Chemical characterization of atmospheric organic aerosol using ultrahigh resolution mass spectrometry and molecular evidence for the association with reactive oxygen species formation

# Dissertation

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"Extension of knowledge lies in the investigation of things"

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# Zusammenfassung

Atmosphärische Aerosolpartikel sind stark mit dem globalen Klima, der Luftqualität und der menschlichen Gesundheit verbunden. Sie beeinflussen die Strahlungsbilanz der Erde direkt, indem sie die solare und terrestrische Strahlung streuen oder absorbieren, oder indirekt, indem sie als Wolkenkondensationskerne und Eiskerne dienen. Darüber hinaus kann die Ablagerung von eingeatmeten Aerosolpartikeln in den menschlichen Atemwegen zur Bildung von reaktiven Sauerstoffspezies (ROS) führen, die möglicherweise oxidativen Stress und Zellschäden verursachen. Insbesondere organisches Aerosol (OA) macht oft einen erheblichen Anteil der Partikelmasse aus und sein Beitrag zur partikelinduzierten Toxizität hat in den letzten Jahren mehr und mehr Aufmerksamkeit erhalten. Aufgrund der komplexen chemischen Zusammensetzung von Feinstaub (PM) ist das derzeitige Wissen jedoch unzureichend um die gesundheitsrelevanten Auswirkungen abschießend zu beurteilen.

Das Ziel dieser Arbeit war i) die chemische Zusammensetzung von OA-Proben, die in verschiedenen Regionen gesammelt wurden, basierend auf ultrahochauflösender Massenspektrometrie (UHRMS) zu charakterisieren und ii) molekulare Hinweise auf den Zusammenhang zwischen der ROS-Bildung und partikelgetragenen organischen Verbindungen zu untersuchen. Insbesondere wurde eine neue Metrik, das "Maximum Carbonyl Ratio (MCR)" vorgeschlagen, um die UHRMS-Daten zu interpretieren.

Der erste Teil dieser Arbeit befasst sich mit in der Entwicklung einer Methode zur Analyse von atmosphärischen Aerosolpartikeln mit Durchmessern  $\leq 2,5 \,\mu$ m (PM<sub>2.5</sub>) und von im Labor erzeugten Proben von sekundären organischen Aerosolen (SOA). Die PM<sub>2.5</sub>-Aerosolproben wurden in vier chinesischen Megastädten (Peking, Shanghai, Guangzhou und Xi'an), einer mitteleuropäischen Stadt (Mainz, Deutschland) und einer abgelegenen Region (Hyytiälä, Finnland) gesammelt, während die SOA-Proben durch Ozonolyse von  $\alpha$ -Pinen,  $\beta$ -Pinen und Limonen in einem Strömungsrohr bzw. durch Photooxidation von Isopren und Naphthalin in einer Smogkammer erzeugt wurden. Ultrahochleistungs-Flüssigkeitschromatographie (UHPLC) gekoppelt an ein Orbitrap-Massenspektrometer mit Elektrospray-Ionisation (ESI) wurde angewendet, um Tausende von organischen Verbindungen auf molekularer Ebene zu charakterisieren. Die Ergebnisse zeigen deutliche Unterschiede in der chemischen Zusammensetzung der organischen Verbindungen in den Proben aus den verschiedenen Regionen sowie in den SOA-Proben, die aus verschiedenen Vorläufern gebildet wurden. Beispielsweise wurden mehr aromatische organische Verbindungen und eine beträchtliche Anzahl von Organosulfaten mit langer Kohlenstoffkette und niedrigem Ungesättigtheitsgrad in Pekinger OA im Vergleich zu OA in Mainz beobachtet.

Der zweite Teil dieser Studie konzentriert sich auf die Anwendung der neuen Metrik MCR, die auf der Grundlage der aus den UHRMS-Daten gewonnenen molekularen Zusammensetzung berechnet und zur Abschätzung der maximalen Anzahl von Carbonylgruppen in einem Molekül verwendet werden kann. Darüber hinaus wurde durch die Kombination des MCR-Wertes mit dem traditionellen VK-Diagramm das MCR-Van Krevelen (MCR-VK)-Diagramm, ein aktualisiertes Visualisierungswerkzeug entwickelt. Entsprechend der Position typischer SOA-Verbindungen im MCR-VK-Diagramm (z. B. Pinonsäure oder 2-Methyl-Tetrole) wurde das Diagramm in fünf spezifische Regionen unterteilt und zwar, sehr stark oxidierte organische Verbindungen, stark oxidierte organische Verbindungen, mittelmäßig oxidierte organische Verbindungen, oxidierte ungesättigte organische Verbindungen und stark ungesättigte organische Verbindungen. Anschließend wurde dieser Ansatz angewandt, um die Aerosolproben aus den verschiedenen Städten und den im Labor erzeugten SOA-Proben zu klassifizieren. Die Verteilung von Hyytiälä-OA im MCR-VK-Diagramm war dabei ähnlich wie die von  $\alpha$ -Pinen-SOA und  $\beta$ -Pinen-SOA, was darauf hindeutet, dass Monoterpene die primäre OA-Quelle an diesem Standort im borealen Wald sind. Darüber hinaus wurden in Hyytiälä OA mehr sehr hoch oxidierte organische Verbindungen und hoch oxidierte organische Verbindungen im Vergleich zu denen in  $\alpha$  und  $\beta$ -Pinen SOA beobachtet, was darauf hindeutet, dass die Partikel in der Umgebungsatmosphäre komplexere Oxidationsprozesse im Vergleich zu im Labor erzeugtem SOA durchlaufen haben. Dies deutet darauf hin, dass die Anwendung der MCR-Metrik und des MCR-VK-Diagramms helfen kann, die Quellen und Entstehungsprozesse der atmosphärischen OA-Komponenten, die mit dem UHRMS erfasst wurden, besser zu verstehen.

Schließlich wurden die vorgeschlagene MCR-Metrik und das MCR-VK-Diagramm verwendet, um gegebenenfalls auch gesundheitsrelevante organische Komponenten zu identifizieren, da die MCR-Werte Informationen über die Häufigkeit von hoch oxidierten Nicht-Carbonyl-Organismen (niedrige MCR-Werte, die oxidativen Stress verursachen können) und hoch elektrophilen organischen Verbindungen (hohe MCR-Werte, die elektrophilen Stress verursachen können) liefern. Die von PM<sub>2,5</sub>-Proben aus der Umgebung und von im Labor erzeugten SOA-Proben in Wasser produzierten ROS wurden als Index zur Bewertung der Toxizität von Aerosolpartikeln quantifiziert. Die Ausbeute an ROS bezog sich auf die Summe der H<sub>2</sub>O<sub>2</sub>-Ausbeute und der Radikalausbeute, die mit einer fluorometrischen Sonde bzw. mit der paramagnetischen Elektronenresonanz gemessen wurden. Die Ergebnisse deuten darauf hin, dass die Gesamtintensität der oxidierten organische Verbindungen (d.h. sehr hoch oxidierte organische Verbindungen, hoch oxidierte organische Verbindungen, intermediär oxidierte organische Verbindungen) in städtischen PM2,5-Proben und im Labor erzeugten SOA signifikant positiv mit der ROS-Ausbeute korreliert, was darauf hindeutet, dass diese oxidierten organischen Verbindungen einen erheblichen Beitrag zur ROS-Bildung leisten.

Zusammenfassend lässt sich festhaten, dass die in dieser Arbeit entwickelte UHPLC-Orbitrap-MS-Methode sich als effektiv erwiesen hat, um die komplexe chemische Zusammensetzung in OA besser zu verstehen. Die vorgeschlagene MCR-Metrik und das Visualisierungstool des MCR-VK-Diagramms können zur Verbesserung der Klassifizierung von OA und zur Identifizierung der gesundheitsrelevanten organischen Komponenten verwendet werden. Dies liefert neue Einblicke, um die chemische Zusammensetzung, die Bildungsprozesse und die gesundheitlichen Auswirkungen von atmosphärischen Aerosolen besser zu verstehen.

# Abstract

Atmospheric aerosol particles are strongly associated with global climate, air quality, and human health. They influence the Earth's radiative balance directly by scattering or absorbing solar and terrestrial radiation, or indirectly by serving as cloud condensation nuclei and ice nuclei. Moreover, the deposition of inhaled aerosol particles in the human respiratory tract can lead to the formation of reactive oxygen species (ROS), potentially causing oxidative stress and cell damage. Particularly, organic aerosol (OA) often accounts for a substantial fraction of particulate mass, and its contribution to particle-induced toxicity has received more attention. However, due to the complex chemical composition of fine particulate matter (PM), current knowledge is insufficient for qualitative characterization of the health-related organic compounds.

The aim of this work was i) to characterize the chemical composition of OA samples collected in ambient regions by using ultrahigh resolution mass spectrometry (UHRMS) and ii) to explore the molecular evidence for the association of ROS formation with organic compounds. In particular, a new metric 'maximum carbonyl ratio (MCR)' was proposed to interpret the UHRMS data by unveiling the information of carbonyl functional groups in the structures of these organic compounds.

The first part of this study was development of an analytical method for analysis of ambient particulate aerosol samples with diameters of PM  $\leq 2.5 \ \mu m$  (PM<sub>2.5</sub>) and laboratory-generated secondary organic aerosol (SOA) samples. The ambient PM<sub>2.5</sub> samples were collected in four Chinese megacities (Beijing, Shanghai, Guangzhou, and Xi'an), a central European city (Mainz, Germany), and a remote region (Hyytiälä, Finland), whereas SOA samples were generated by ozonolysis of  $\alpha$ -pinene,  $\beta$ -pinene, and limonene in a flow tube, respectively and photo-oxidation of isoprene and naphthalene in a smog chamber, respectively. Ultrahigh performance liquid chromatography (UHPLC) coupled to the UHRMS-Orbitrap with electrospray ionization (ESI) was applied to characterize thousands of organic compounds at the molecular level. The results showed clear differences in the chemical composition of organic compounds in ambient samples from different regions as well as in SOA samples derived from different precursors, e.g., more aromatic organic compounds and a substantial number of organosulfates with long-carbon chain and low degree of unsaturation were observed in Beijing OA compared to OA in Mainz. It indicates that sources probably play important roles in the chemical processes of OA formation.

The second part of this study focused on the application of the new metric of MCR, which can be calculated based on the molecular composition obtained from the UHRMS data and be used to estimate the maximum number of carbonyl groups in a molecule. Furthermore, the MCR-Van Krevelen (MCR-VK) diagram, an updated visualization tool, was developed by the combination of the MCR value and the traditional VK diagram. According to the location of typical SOA compounds (e.g., pinonic acid and 2-methyl-tetrols) in the MCR–VK diagram, MCR–VK diagram was divided into five specific regions corresponding to very highly oxidized organic compounds, highly oxidized organic compounds, intermediately oxidized organic compounds, oxidized unsaturated organic compounds, and highly unsaturated organic compounds, respectively. Then, this approach was applied to classify the organic compounds observed in the ambient aerosol samples and laboratory-generated SOA samples and their distributions in the MCR-VK diagram were obtained. The distribution of Hyytiälä OA in the MCR-VK diagram was similar with that of  $\alpha$ -pinene SOA and  $\beta$ -pinene SOA, indicating that monoterpenes may be the primary OA source at this boreal forest site. Furthermore, more very highly oxidized organic compounds and highly oxidized organic compounds were observed in Hyytiälä OA compared to those in  $\alpha/\beta$ -pinene SOA, indicating that the particles in the ambient atmosphere experienced more complex oxidation processes compared to the laboratory-generated SOA. This suggests that the application of MCR metric and MCR-VK diagram can help to better understand the sources and formation processes of atmospheric OA components detected by the UHRMS.

Finally, the proposed MCR metric and MCR-VK diagram were utilized to identify the healthrelevant organics components, since the MCR values give the information about the abundance of highly oxidized non-carbonyl organics (low MCR values, which are able to cause oxidative stress) and highly electrophilic organic compounds (high MCR values, which can induce electrophilic stress). The ROS produced by ambient PM<sub>2.5</sub> samples and laboratory-generated SOA samples in water was quantified as an index of assessing the toxicity of aerosol particles. The yield of ROS referred to the sum of H<sub>2</sub>O<sub>2</sub> yield and radical yield, which were measured using a fluorometric probe and electron paramagnetic resonance, respectively. The results suggest that the total intensity of oxidized organic compounds (i.e., very highly oxidized organic compounds, highly oxidized organic compounds, intermediately oxidized organic compounds) in ambient urban PM<sub>2.5</sub> samples and laboratory-generated SOA both had significantly positive correlations with the ROS yield, indicating that these oxidized organic compounds made considerable contribution to the ROS formation.

In conclusion, the UHPLC-Orbitrap MS method developed in this work has been proved to be effective to identify the complex chemical composition in OA. The proposed metric of MCR and the visualization tool of MCR-VK diagram can be used to improve the classification of OA and to identify the health-related organic components. This provides a new insight to better understand the chemical composition, formation processes, and health effects of atmospheric aerosols.

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# **1.1** Atmospheric aerosol

Atmospheric aerosols, defined as solid or liquid particles suspended in air, are ubiquitous in Earth's atmosphere. They play a key role in many environmental processes and impact the climate (Pöschl, 2005; Seinfeld and Pandis, 2006). Aerosol particles influence the Earth's radiative balance directly by scattering and absorbing solar and terrestrial radiation, or indirectly by acting in the formation of clouds and precipoitaiton as cloud condensation nuclei (CCN) and ice nuclei (IN) (Pöschl, 2005; Hallquist et al., 2009). Participating in heterogeneous chemical reactions and multiphase processes may affect the distribution and abundance of atmospheric trace gases (Pöschl, 2005; George et al., 2015) Moreover, atmospheric aerosol particles can have adverse effects on human health by entering and damaging the respiratory and cardiovascular system or causing infectious and allergic diseases (Pöschl, 2005; Brüggemann, 2015; Pöschl and Shiraiwa, 2015).

According to their origin, atmospheric aerosols can be classified as primary and secondary aerosols. Primary aerosols are directly emitted into the air from natural and anthropogenic sources, including biomass burning, combustion of fossil fuels, volcanic eruptions, wind-driven or traffic-related suspension of soil and dust, sea spray, and biological materials (plant and animal debris, microorganisms, pollen, spore, etc.). Secondary aerosols, on the other hand, are formed in the atmosphere by chemical reactions of gaseous precursors and gas-to-particle conversion (Pöschl, 2005; Seinfeld and Pandis, 2006). Figure 1.1.1 represents the formation, growth, and processing of atmospheric aerosols.



Figure 1.1.1: Schematic representation of the formation, growth and processing of atmospheric aerosols (Zhang et al., 2015).

The size of aerosol particles is mainly determined by their formation mechanisms. Particles larger than 1  $\mu$ m in diameter (coarse mode) are usually primary in nature and contribute largely to the mass of aerosol populations. Due to fast gravitational setting, long-range transport of these particles is rather limited resulting in short atmospheric lifetimes (Seinfeld and Pandis, 2006). Despite of their large size and low number concentration, primary particles in the coarse mode are essentially important for the formation of clouds and precipitation due to the ability to act as IN (Cantrell and Heymsfield, 2005; Seinfeld and Pandis, 2006; Vogel, 2014; Brüggemann, 2015). Particles smaller than 1  $\mu$ m in diameter, generally defined as fine mode, are typically secondary in nature and contribute largely to the number and surface area of particle populations. The fine mode can be further divided into accumulation mode (0.1–1  $\mu$ m), Aitken mode (0.01–0.1  $\mu$ m), and nucleation mode (< 0.01  $\mu$ m) (Seinfeld and Pandis, 2006). Particles in the nucleation and the Aitken mode, formed by the condensation of low volatile compounds onto thermodynamically stable clusters, usually grow rapidly to the accumulation mode with the longest atmospheric lifetimes through condensation of vapors or coagulation with other particle (Kulmala et al., 2016). Fine paticles are mainly removed from the atmosphere by wet deposition. Figure 1.1.2 provides an

overview of the size range and composition of atmospheric particles as well as the major types of multiphase chemical processes in the atmosphere.



Figure 1.1.2: Overview of atmospheric aerosol particles: (a) Size range of aerosols, hydrometeors, cells and organelles. (b) Chemical reactions in the gas phase, at the interface, and in the particle bulk; mass transformation and phase transition in and between the gas phase, clusters, aerosols, cloud, and precipitation particles (Pöschl and Shiraiwa, 2015).

Atmospheric aerosol represents highly dynamic and complex system with a huge temporal and spatial variability in terms of chemical composition and size distribution. Concerning the chemical composition, atmospheric aerosols are complete mixtures consisting of inorganics and organics. The inorganic species have been observed with relatively high concentration in submicrometer aerosols at multiple locations around the world (Jimenez et al., 2009). The commen inorganics include sulfate, nitrate, and ammonium, formed via the oxidation and neutralization of sulfur dioxide (SO<sub>2</sub>), nitrogen oxides (NO<sub>x</sub>) and ammonia (NH<sub>3</sub>) (Koo et al., 2003; Fu et al., 2016). Organic components in atmospheric aerosol include hydrocarbons, alcohols, aldehydes, carboxylic acids, organosulfates, and organic aerosols (OA) is still limited due to a variety and complexity of organic species in atmospheric aerosol. Figure 1.1.3 shows an overview of the inorganic species and organic components in atmospheric aerosols in the Northern Hemisphere, observed using aerosol mass spectrometer (AMS) measurements.



Figure 1.1.3: Total mass concentration (μg m<sup>-3</sup>) and mass fractions of nonrefractory inorganic species and organic components in submicrometer aerosols at muilti surface locations on the Northern Hemisphere.
 Organic aerosols are classified into hydrocarbon-like OA (HOA), semi-volatile oxygenated OA (SV-OOA) and low-volatile oxygenated OA (LV-OOA) (Jimenez et al., 2009).

## 1.2 Secondary organic aerosol

Organic aerosol (OA) constitutes 20–90% of tropospheric aerosol and there is increasing evidence that a major fraction of OA can be attribution to secondary organic aerosol (SOA) (Heald et al., 2005; Kroll and Seinfeld, 2008; Jimenez et al., 2009; Hallquist et al., 2009). SOA is formed by chemical reaction and gas-to-particle conversion of volatile organic compouns (VOCs) in the atmosphere, which may proceed through different pathways, as disscussed in the following sections.

## 1.2.1 Formation mechanisms

The formation of secondary organic aerosol (SOA) starts with the emission of volatile organic compounds (VOCs) into the atmosphere, which are biogenic and anthropogenic in origin. On a global scale, the dominant precursors for SOA generation are biogenic VOCs, such as isoprene ( $C_5H_8$ ), monoterpene ( $C_{10}H_{16}$ :  $\alpha$ - and  $\beta$ -pinene, limonene, etc.), and sesquiterpenes ( $C_{15}H_{24}$ ). Large amounts of biogenic VOCs emitted over forested areas like the Amazon rainforest and the boreal forest contribute to an increasing SOA fraction of local aerosol populations. Compared to the biogenic emissions, emissions of anthropogenic VOCs (e.g., alkanes and aromatics) are almost one order of magnitude smaller, however, they play a key role on local or regional scales (Atkinson & Arey, 2003; Goldstein and Galbally, 2007). VOCs release into the air and then react with atmospheric oxidants, such as hydroxyl radical (•OH), ozone (O<sub>3</sub>) and nitrate radical (NO<sub>3</sub>). The produced condensable organic vapors form SOA by gas-to-particle conversion (i.e., condensation on pre-existing particles or nucleation). Figure 1.2.1 displays the formation mechanisms of atmospheric aerosols (Hoffmann et al., 2011).



Figure 1.2.1 Formation mechanisms of atmospheric aerosols (Hoffmann et al., 2011).

VOCs react with •OH, NO<sub>3</sub>, and O<sub>3</sub> in an initial step and form an alkyl radical which further react with oxygen producing an alkylperoxy radical (RO<sub>2</sub>). Depending on the conecentraion of NOx, HO<sub>2</sub>, and RO<sub>2</sub>, the RO<sub>2</sub> radicals recombine to products such as alcohols, hydroperoxides, peroxynitrates or organic nitrates. Moreover, the RO<sub>2</sub> radicals can react with NO forming alkoxy radical (RO) which can isomerize or dissociate resulting again in an alkyl radical or react with oxygen to produce a carbonyl (Kroll and Seinfeld, 2008). Additionally, recent studies suggested that a class of extremely low-volatile organic compounds (ELVOCs) can be formed via further oxidation of alkylperoxy radicals. Intramolecular hydrogen shifts of an RO<sub>2</sub> radical followed by an autoxidation process involving oxygen addition at the alkyl radical site resultes in forming a more oxidized peroxy radical (R<sub>ELVOC</sub>O<sub>2</sub>) (Brüggemann, 2015; Jokinen et al., 2015; Mentel et al., 2015). Subsequently, ongoing H-shifts and oxygen additions lead to gas-phase formation of ELVOCs in dimer-, monomer-, and organic nitrate (in the presence of NO) channels (Ehn et al., 2014; Jokinen et al., 2014). Figure 1.2.2 shows a simplified schematic initial gas-phase oxidation of VOCs and formation of ELVOCs.

1 Introduction



Figure 1.2.2: Simplified schematic of initial gas-phase oxidation of VOCs and formation of ELVOCs (green frames). The black arrows denote reactions that can lead to a volatility decrease, whereas the gray arrows denote reactions that can lead to a volatility increase (Brüggemann, 2015; Wang, 2018).

## 1.2.2 Gas-particle partitioning

SOA comprises large amounts of organic compounds with higher vapor pressure, considered as semi-volatile organic compounds (SVOCs), typically partition between the gas phase and the particle phase. Theoretical foundation on gas-particle partitioning of organic compounds was developed by Pankow (Pankow, 1994a, 1994b) and extended by Odum to SOA formation (Odum et al., 1996). Partitioning of each SVOCs is described by the equilibrium partitioning coefficient  $K_{p,i}$  (m<sup>3</sup>µg<sup>-1</sup>) or the saturation vapor concentration  $C_i^*$  (µg m<sup>-3</sup>) (Donahue et al., 2006) as described by equation 1.1:

$$\frac{c_i^p}{c_i^g} = K_{p,i} C_{OA} = \frac{c_{OA}}{c_i^*}$$
(1.1)

where  $C_i^g$  and  $C_i^p$  represent the mass concentrations of species *i* per unit volume of air (µg m<sup>-3</sup>) in the gas phase and in the particle phase, respectively, and  $C_{OA}$  is the mass concentration per unit volume of air (µg m<sup>-3</sup>) of the total absorbing particle phase. As long as the absorbing mass is present, some fraction of a given SVOC will partition into the particle phase, even if its gas phase

concentration is below its saturation concentration,  $C_i^*$ . Moreover, the fraction  $F_i$  of a semi-volatile compound in the particle phase can be obtained via equation 1.1 (Hallquist et al., 2009), and depicted in the following equation 1.2:

$$F_{i} = \frac{C_{i}^{p}}{C_{i}^{p} + C_{i}^{g}} = \frac{C_{OA} * K_{p,i}}{1 + C_{OA} * K_{p,i}} = \frac{1}{1 + C_{i}^{*} / C_{OA}}$$
(1.2)

This hypothesis implies that compounds of greater volatility will increasingly partition into the particle phase as the amount of  $C_{OA}$  increases. When  $C_{OA} = C_i^*$ , half of the semivolatile mass of the compounds distribute in the particle phase. Whereas, if  $C_{OA} >> C_i^*$ , the compound will reside essentially in the particle phase.

This partitioning theory is limited due to the wide range of  $C_{OA}$  in the atmosphere and the ongoing oxidation of SVOCs in both the gas and particle phases. Donahue et al. proposed the approach of "volatility basis set" (VBS) (Donahue et al., 2006; Presto and Donahue, 2006; Pathak et al., 2007). Using the VBS, semi-volatile compounds can be mapped into the sets of bins with predefined value of  $C_i^*$ . Moreover, they suggested that oxidation of numerous intermediate volatility vapors may contribute significantly to ambient SOA formation.

## 1.2.3 Condensed phase chemistry

Organic compounds may undergo particle phase reactions in the condensed phase, affecting their chemical properties and volatility. These reactions, which include both heterogeneous and multiphase reactions, can be either non-oxidative or oxidative (Kroll & Seinfeld, 2008). The oligomeric and high-molecular-weight species can be formed via non-oxidative association reactions (also termed " accretion reactions"), in which the oxidation state of the total carbon is unchanged. (Barsanti & Pankow, 2004) Due to the vapor pressure will decrease significantly, such reactions can play an important role in the formation of SOA. Another mechanism of chemical evolution of organic aerosols is the oxidation of particle-phase organics by atmospheric oxidants (OH, NO<sub>3</sub>, O<sub>3</sub>, etc.), which often refers to "aerosol aging" (Rudich et al., 2007). Although the oxidative mechanisms in the particle phase are generally the same as those in the gas phase, the large difference of branching ratios among the various pathways may significantly affect on the vapor pressures of the oxidation products. Furthermore, photolytic processes may also influence the the oxidation state and volatility of particle-phase organics.

## 1.3 Mass spectrometry for the analysis of atmospheric aerosol

To assess the impact of atmospheric aerosols on the environment and human health, detailed information of their chemical composition and physical properties is required. This challenging task drives the development and application of analytical techniques for aerosol measurements. There are different types of analytical techniques used and developed for the analysis of atmospheric organic compounds, as shown in Figure 1.3.1 (Nozière et al., 2015). Therein, mass spectrometry (MS) is a powerful tool in the chemical characterization in aerosol research. Due to its high sensitivity with fast response time, MS offers a great potential for qualitative and quantitative analysis of a broad range of chemical components in OA (Farmer and Jimenez, 2010; Vogel, 2014; Brüggemann, 2015; Laskin, 2018). Until now, many of the significant advances in our understanding of atmospheric aerosols can be attributed to the applications of mass spectrometry (Pratt & Prather, 2012a; Pratt & Prather, 2012b).



Figure 1.3.1: Summary of analytical techniques used to characterize atmospheric organic compounds. A decreasing *I* factor describes the increasing ability of a technique to identify the molecular structure of a compound, whereas the y-axis describes the fraction of the total organic mass of aerosol samples analyzed by a technique (Nozière et al., 2015).

The following will give a brief overview of online and offline MS techniques, and then introduce the applied MS technique as well as parameters and visualization tools used for data analysis in this dissertation. More detailed description of the application and recent development of MS analysis in atmospheric chemistry can be found in published reviews by Pratt and Prather (2012a, 2012b), Nizkorodov (2011) and Laskin (2018).

## 1.3.1 Online and offline mass spectrometry techniques

Generally, the MS techniques can be divided into online and offline techniques. Online MS is performed on introduced particles in or near real time, thereby providing high time resolution for insighting the chemical changes in atmospheric aerosol populations on short timescales, and eliminating potential artifacts associated with offline analysis methods, such as evaporation and chemical reactions during long sample collection and analysis time (Pratt & Prather, 2012b). In contrast, offline MS is performed on collected particles, requiring sample collection over hours to days and sample preparation prior to the analysis by mass spectrometer. However, much more information of chemical composition and structural speciation can be observed by the offline techniques compared to those obtained by online techniques (Pratt and Prather, 2012a).

Online MS techniques can be subdivided into two categories: bulk aerosol measurements which obtain statistical information on the average chemical composition of particle ensembles and single-particle measurements which measure the chemistry of individual particles. The general principle of online mass spectrometry techniques is to introduce airbone particles into the instrument, vaporize and ionize the species, and then analyze the ions using mass spectrometer (Hoffmann, 2011). Commonly, bulk aerosol measurements thermally vaporize particles prior to ionization, whereas single-particle measurements desorb particles one at a time using pulsed lazer techniques (Pratt & Prather, 2012b; Brüggemann, 2015; Zuth, 2018). The Aerodyne aerosol mass spectrometer (AMS) is the main instrument used for bulk measurements, providing real-time MS analysis of size-resolved mass concentration of non-refractory aerosol species (e.g., most organics, ammonium, sulfate, and nitrate), for chemical characterization of bulk aerosol particles (Canagaratna et al., 2007; Pratt & Prather, 2012b). Recent approaches utilized online atmospheric pressure chemical ionization mass spectrometry (APCI-MS) for the analysis of ambient SOA particles (Vogel et al., 2013; Brüggemann et al., 2014; Zuth et al. 2018). Furthermore, the aerosol flowing atmospheric-pressure afterglow mass spectrometry (AeroFAPA-MS) measurements were also applied for the real time analysis of OA particles (Brüggemann et al., 2015; Brüggemann et al., 2017).

Offline MS techniques are preferred in cases when it is impractical to bring the instrument to the measurement location or when time-averaged composition of aerosol particles is needed (Laskin et al., 2018). In such cases, particles are collected traditionally on quartz or polytetrafluoroethylene-coated fiber filters. Alternatively, particles can be sampled by cascade impactors and separated base on size when particles transverse a series of impaction plates. Gases are mostly sampled by suitable sorbents or in gas-tight containers. Prior to the offline analysis, the samples are mostly processed by extraction, sonication, or derivatization in the laboratory (Brüggemann, 2015; Laskin et al., 2018; Zuth, 2018). The aerosol samples are usually analyzed by the separation techniques followed by MS detection.

The characterization of single or multiple individual aerosol constituents at the molecular level in highly complex mixtures generally requires chromatographic separation, of which the two most employed techniques are gas chromatography (GC) and liquid chromatography (LC) (Hallquist et al., 2009; Nozière et al., 2015; Brüggemann, 2015; Zuth, 2018). LC/MS is a commonly analytical method for the chemical characterization and quantification of moderately polar to polar organic analytes (Nozière et al., 2015). Nowadays, LC/MS analysis has been used to investigate the formation and aging of SOA from a series of precursors (e.g., glyoxal and acetic acid) (Surratt et al., 2008; Nozière et al., 2015). The selection of LC or high performance liquid chromatography (HPLC) columns and separation conditions requires knowledge of the properties of OA compounds. In most cases, reversed phase columns (e.g., C18 and C8 columns) are employed for separation of the analytes, whereas hydrophilic interaction liquid chromatography (HILIC) columns provide successful separation of atmospherically relevant monosaccharide anhydrides (e.g., levoglucosan, galactosan, and mannosan) (Hallquist et al., 2009; Laskin et al., 2018).

## 1.3.2 Ionization method

Among the ionization methods, the hard ionization techniques such as electron ionization (EI) or laser deposition ionization (LDI) mostly lead to the high degree of fragmentation, thus the identification power is generally low for individual particle phase organics (Hoffmann et. al., 2011; Nozière et. al., 2015).

By contrast, soft ionization techniques convert the precursor molecules into positive or negative ions without fragmentation, is a key prerequisite for the molecular assignment of organic compounds (Nizkorodov et al., 2011). Atmospheric pressure chemical ionization (APCI), frequently used in atmospheric mass spectrometry, is sensitive to nonpolar compounds such as PAHs, even be used for very labile analytes (e.g., hydroperoxides) (Hoffmann et. al., 2011; Nozière

et. al., 2015; Laskin et al., 2018; Zuth, 2018). Electrospray ionization (ESI) is another widespread used ionization technique for aerosol samples, which performed at atmospheric pressure. In contrast to APCI, ESI is well-suited for the analysis of polar molecules (Müller-Tautges, 2014; Nozière et. al., 2015; Laskin et al., 2018; Zuth, 2018; Wang, 2019). The use of a light source is also a possibility technique to softly ionize organics, for instance, vacuum ultraviolet photoionization or atmospheric pressure photoionization (APPI) (Müller-Tautges, 2014; Nozière et. al., 2015; Zuth, 2018; Wang, 2019). An overview of the application range of different ionization techniques is given in Figure 1.3.2 (Müller-Tautges, 2014; Wang, 2019).



Figure 1.3.2: An overview of application range of different ionization techniques as function of analyte polarity and molecular weight (Müller-Tautges, 2014).

## 1.3.2.1 Electrospray ionization

ESI uses electrical energy to assist the transfer of ions from solution into the gaseous phase prior to mass spectrometric analysis. Neutral compounds can be converted to ionic form in solution or in gaseous phase by protonation or cationization (Ho et al., 2003). The ESI process involves three steps: (1) dispersal of a fine spray of charge droplets, followed by (2) solvent evaporation and (3) the formation of gaseous ions (Ho et al., 2003; Müller-Tautges, 2014; Wang, 2018).

Within an ESI source, a continuous stream of sample solution is pumped through a stainless steel or quartz silica capillary with a very low flow rate (0.1–10  $\mu$ L/min). An either negative or positive high voltage (2–5 kV) is applied on the tip of the capillary, which can provide the electric

field gradient required to produce charge separation on the surface of the liquid droplets. This leads to the generation of a mist of highly charged droplets with the same polarity as the capillary voltage. The liquid protrudes from the capillary tip forming the "Taylor cone". The charged droplets pass down a pressure gradient and potential gradient toward the analyzer region of the mass spectrometer. With the aid of a sheath gas steam (usually nitrogen drying gas) and/or an elevated ESI-source temperature, the solvent of the charged droplets is continuously evaporated, leading to a decrease of droplets size and an increase of surface charge density. When the Coulombic repulsion of the surface charge exceeds the surface tension of the charged droplets, they reach the Rayleigh limit and disintegrate into smaller droplets, which is called droplet jet fission process (Cech and Enke, 2001; Ho et al., 2003; Müller-Tautges, 2014; Wang, 2018).

The generation of gaseous ions can be explained by two proposed mechanisms: (1) The ion evaporation model (IEM) assumes that the increased charge density due to solvent evaporation causes Coulombic repulsion to overcome the surface tension of liquid, resulting in a release of ions from droplet surfaces (Iribarne & Thomson, 1976). This model is suitable for describing the ionization of small molecules. (2) The charge residue model (CRM) assumes that the increased charge density through desolvation causes the large droplets to divide into smaller and smaller droplets and eventually consist only of single ions (Dole et al., 1968). This model is well suited for describing the ionization of large molecules (Cech and Enke, 2001; Müller-Tautges, 2014; Wang, 2018). Figure 1.3.3 illustrates the electrospray ionization process.

The typical ions generated in ESI source are deprotonated ions in the negative mode  $([M-H]^-$  with M = molecule). Positive mode ESI spectra typically contain protonated ions  $([M+H]^+)$  or adducts  $([M+Na]^+, [M+K]^+, and [M+NH_4]^+)$  (Müller-Tautges, 2014; Wang, 2018). The heated electrospray ionization (HESI) source, developed by Thermo Scientific, is applied in this work. HESI transforms ions in solution into ions in the gas phase by using ESI in combination with heated auxiliary gas, providing better desolvation and nebulization performance (Müller-Tautges, 2014).



Figure 1.3.3: Schematic illustration of electrospray ionization process (Müller-Tautges, 2014).

## 1.3.3 High resolution mass spectrometer

High resolution mass spectrometry (HRMS) or ultrahigh resolution mass spectrometry (UHRMS) is a powerful tool for chemical characterization at molecular level with features of high resolution and high mass accuracy (Stock, 2017; Hoffmann et al., 2011; Nizkorodov et al., 2011; Laskin et al., 2018; Wang, 2018). Mass accuracy is defined as the difference between the measured and theoretical mass (equation 1.3), and usually expressed in parts per million (ppm).

$$Mass\ accuracy = \left(\frac{\frac{m}{z}_{experimental} - \frac{m}{z}_{theoretical}}{\frac{m}{z}_{theoretical}}\right) \times 10^{6}$$
(1.3)

For instance, the mass measurement error of 0.001 mass-to-charge (m/z) for a singly charged ion at m/z 500 corresponds to mass accuracy of 2 ppm (Nizkorodov et al., 2011; Nozière et al., 2015). Resolving power (R) is defined as the ratio of the peak position to its full width at half maximum (equation 1.4):

$$R = (m/z) / peak full width at half maximum$$
(1.4)

which determines the ability of the instrument to separate two adjacent peaks on the m/z scale (Nizkorodov et al., 2011; Nozière et al., 2015). High accuracy coupled with high resolution allows one to determine unambiguous elemental formulas for each ion peak, in turn can be used to characterize thousands of organic compounds present in complex atmospheric aerosol samples.

Three major types of HRMS are well-suited for complex samples analysis: (1) high resolution quadrupole time-of-flight (HR-Q-TOF) mass spectrometers which have a resolving power of up to 40,000 across a m/z 100–500 mass range; (2) the Orbitrap mass spectrometers which have higher resolving power in excess of 1,000,000 at m/z < 300-400 within a 3 seconds detection time making it compatible with several types of chromatographic separations; (3) the Fourier transform ion cyclotron (FTICR) mass spectrometers which provide the highest mass resolution and mass accuracy of all existing MS technologies, offering the best resolution power with a record resolution of 40,000,000 at m/z 609 at a magnetic field of 7 T (Nozière et al., 2015; Wang, 2018). Figure 1.3.4 illustrates the advantages of high resolving power for OA analysis, and the comparison of different types of HRMS.



Figure 1.3.4: (a) An ESI mass spectrum of isoprene/ozone SOA. (b) peaks around m/z 251 recorded at the Orbitrap resolving power of R = 100,000. (c) how the same mass range would look like if recorded at a typical resolving power of a reflection-TOF instrument with R = 5,000 (Nizkorodov et al., 2011).

In last years, HRMS coupled with the soft ionization sources (e.g., ESI and APCI) has been successfully used for detailed chemical characterization of atmospheric aerosols (Nizkorodov et al., 2011; Lin et al., 2012a; Lin et al., 2012b; Rincón et al., 2012; Kourtchev et al., 2014; Nozière et al., 2015; Kourtchev et al., 2016; Wang et al., 2016; Wang et al., 2017; Laskin et al., 2018; Wang et al., 2018; Wang et al., 2019). In this study, the Orbitrap MS is applied for the idenfication of chemical composition of OA and described in the following chapter.

## 1.3.3.1 Q-Exactive hybrid quadrupole-orbitrap mass spectrometer

The roots of the Orbitrap analyzer can be traced back to 1923 when the Kingdon trap was developed, later improved by Makarov and finally commercialized by Thermo Fisher Scientific in 2005 (Makarov, 2000; Zubarev and Makarov, 2013). In this study, the Q-Exactive hybrid quadrupole-orbitrap mass spectrometer (built by Thermo Fisher Scientific in 2011) was applied. The instrument has a maximum resolution of 140,000 at m/z 200 and a mass accuracy <3 ppm (external calibration) and <1 ppm (internal calibration). Figure 1.3.7 displays the schematic of the Q-Exactive hybrid quadrupole-orbitrap mass spectrometer.

The ions generated in an ion source (commonly ESI or APCI) are focused by a lens stack and further transmitted by a bent flatapole to a quadrupole for optional precursor ion selection. Subsequently, the ions enter a curved linear trap (C-Trap), where ions are focused by collisional cooling. After that, ions are either transmitted directly to the Orbitrap mass analyzer for detection or led into the higher-energy collisional dissociation (HCD) cell for fragmentation. For MS<sup>2</sup> analysis, the fragmented product ions are again focused in the C-Trap and then transmitted to the Orbitrap for detection (Scigelova and Makarov, 2006; Müller-Tautges, 2014; Zuth, 2018; Wang, 2018).

The Orbitrap consists of a spindle-shaped electrode in the center and an outer barrel-shaped electrode, which is split in the middle by a ceramic ring (see Figure 1.3.5). The ions are injected into the Orbitrap essentially perpendicular to the z-axis and trapped by means of an electrostatic field between the central and out electrodes. A radial electric field bends the ions trajectory toward the central electrode whereas tangential velocity creates an opposing centrifugal force, forcing the ions to a rotational movement around the central electrode, which is like the trajectory of a planet in the solar system. At the same time, the axial electric field caused by the special conical shape of electrodes pushes ions toward the widest part of the trap, initiating a harmonic axial oscillation. The frequency ( $\omega$ axial) of the axial oscillation does not depend on the tangential velocity or the distribution of the circulating ions, but on the m/z ratios of the ions as described by equation 1.5:

$$\omega_{axial} = \sqrt{k\left(\frac{z}{m_i}\right)} \tag{1.5}$$

where k is the force constant of the electrical potential. The frequency of the harmonic axial oscillation induces an image current in the two parts of outer electrode, which is detected and multiplied. Finally, the image current is converted to a mass spectrum by fast Fourier transformation (Scigelova and Makarov, 2006; Zubarev and Makarov, 2013; Müller-Tautges, 2014;

Zuth, 2018; Wang, 2018).



Figure 1.3.5: A schematic of the Q Exactive hybrid quadrupole-orbitrap mass spectrometer, which is composed of the ion source, lens stack, bent flatapole, quadrupole, C-trap, orbitrap mass analyzer and HCD cell. The inset depicts the cross section of Orbitrap consisting of a spindle-shaped central electrode (a), a barrel-shaped outer electrode, composed of two parts (b) and a ceramic ring for segregation (c). The movement of the ions along the z-axis is highlighted with a red orbit (Scigelova and Makarov, 2006; Müller-Tautges, 2014; Zuth, 2018; Wang, 2018).

## 1.3.4 Data analysis and visualization

UHRMS allows the assignment of molecular formulae to the measured hundreds or thousands of compounds. When determining elemental formulas from the accurate mass measurements, there are several constraints applied to eliminate the compounds not likely to occur in nature, which include the restriction for the number of possible elements present in the molecule (e.g., C, H, O, N, and S), reasonable elemental ratios such as oxygen to carbon (O/C) ratios and hydrogen to carbon (H/C) ratios, nitrogen rule, and double bond equivalent (Nozière et al., 2015). Due to the large amounts and complexity of the UHRMS data, a variety of parameters and visualization tools have been developed to facilitate the interpretation of HRMS data, and are described below.

The double bond equivalent (DBE) reflects the number of double bonds and rings in a molecule,

which can be calculated using equation 1.6 (McLafferty and Turecek, 1993):

$$DBE = 1 + c - 0.5x + 0.5y \tag{1.6}$$

where c is the number of carbon atoms, x is the total number of monovalent atoms (e.g., H, Cl, Br), and y is the totoal number of trivalent atoms (e.g., N and P) in the molecule. It should be noted that certain heteroatoms may have multiple valence states, e.g., the valence of N is 3 in amines and 5 in alkyl nitrites, thus the calculated values of DBE need to be considered with caution. Moreover, the sulfuroxygen double bonds of the sulfate groups in the molecule are not taken into account in DBE equation (Nizkorodov, 2011; Nozière et al., 2015).

The aromaticity index (AI), proposed by Koch and Dittmar, is a parameter for the identification of aromatic structures in nature organic matter (Koch and Dittmar, 2006). It reflects the C–C double bonds 'density' in a molecule, including the possibility that heteroatoms can form double bonds which not contribute to aromaticity. AI can be calculated from molecular formulae of the compounds containing C, H, O, N, S, and P, expressed as equation 1.7:

$$AI = \frac{DBE_{AI}}{C_{AI}} = \frac{1 + C - O - S - 0.5H}{C - O - S - N - P}$$
(1.7)

where  $DBE_{AI}$  is the minimum number of C-C double bonds plus rings in a common molecular structure containing heteroatoms and  $C_{AI}$  is the number of carbon reduced by the number of potential double bonds contributed by heteroatoms and if  $DBE_{AI} \le 0$  or  $C_{AI} \le 0$ , then AI = 0. This approach provides two threshold values for the unequivocal identification of aromatics (AI > 0.5) and condensed aromatics ( $AI \ge 0.67$ ). For aromatic molecules with long alkyl chains, their AI value less than 0.5 and they would not be identified as aromatic structures, which results in a lower estimate for aromatic and condensed aromatic compounds in OA by AI approach (Yassine et al., 2014).

The aromaticity equivalent ( $X_C$ ), introduced by Yassine et al. in 2014, complements the AI classification and improves the identification of aromatic and condensed aromatic structures in OA (Yassine et al., 2014). The  $X_C$  of a compound containing C, H, O, N, S, and P can be calculated by equation 1.8:

$$X_{C} = \frac{3[DBE - (m \, 0 + nS)] - 2}{DBE - (m \, 0 + nS)} \tag{1.8}$$

If DBE  $\leq$  mO + nS, then Xc = 0, where m and n are the fraction of oxygen and sulfur atoms involved in the  $\pi$ -bond structure of a compound, respectively. i.e., m = 1 for aldehyde, ketone, nitroso, and

cyanate chemical classes, m = 0.5 for carboxylic acid, ester, and nitro chemical classes, and m = 0 for alcohol, ether, peroxide, sulfoxide, sulfones, sulfonic, and sulfonic acid chemical classes; whereas n = 1 should be used for thial and thione chemical classes, and n = 0 for thiol, sulfide, and disulfide chemical classes. This approach proposed threshold criteria for aromatic compounds (Xc  $\geq 2.5000$ ) and condensed aromatic compounds (Xc  $\geq 2.7143$ ) (Yassine et al., 2014).

The Van Krevelen diagram (VK), constructed by plotting H/C versus O/C elemental ratios, is often utilized to describe the evolution of organic mixtures. VK diagrams can be used to categorize organic aerosols and differentiate their potential sources by the corresponding position. Commonly, the most oxidized compounds lie in the lower right part of the diagram whereas the most reduced/saturated species populate the upper left part of the plot. As illustrated in Figure 1.3.6, aliphatic compounds generally have high H/C ratios ( $\geq 1.5$ ) and low O/C ratios ( $\leq 0.5$ ), while aromatic hydrocarbons typically have low H/C ratios ( $\leq 1.0$ ) and low O/C ratios ( $\leq 0.5$ ) (Kourtchev et al., 2014; Nozière et al., 2015). However, the complexity of atmospheric aerosol is sometimes not well represented by VK diagrams due to it cannot distinguish formulas with different atom numbers but identical atomic ratios. Thus VK diagrams are frequently plotted as heat maps by adding additional dimensionalities or generated as three-dimensional figures using the N/C ratio or the DBE as a third variable.



Figure 1.3.6: Van Krevelen (VK) diagrams for all detected ions in (a) urban aerosol samples and (b) remote aerosol samples. Ions in areas 'A', 'B', and 'C' attributed to aliphatic, aromatic, and SOA species, respectively (Kourtchev et al., 2014).

The average O/C ratio is a convenient but not accurately metric for describing the degree of oxidation in organic aerosols since nonoxidative processes such as hydration and dehydration can also affect atomic ratios in a molecule. The carbon oxidation state ( $OS_C$ ) was suggested by Kroll et al. in 2011 to describe the evolving composition of atmospheric organics undergoing dynamic oxidation processes, which can be calculated from the following equation 1.9:

$$OS_C \approx 2 \ O/C - H/C \tag{1.9}$$

which is generally used for molecules that contain C, H, and O atoms only (Kroll et al., 2011).  $OS_C$ , when coupled with carbon number ( $n_C$ ), provides a framework for describing the chemical characterization of atmospheric organic aerosol, which can be used to constrain the composition of organic aerosol and facilitate understanding the oxidative evolution of atmospheric organics, as shown in Figure 1.3.7. For instance, hydrocarbon-like organic aerosol (HOA) and biomass burning organic aerosol (BBOA) correspond to primary particulate matter directly emitted into the atmosphere, HOA has OSc value less than -1 and more than 18 carbon atoms whereas BBOA has OSc value between -1.5 and 0 with 7–23 carbon atoms. Semivolatile and low-volatility oxidized organic aerosol (SV-OOA and LV-OOA) produced by multistep oxidation reactions have OSc values between -1 and +1 with 18 or less carbon atoms (Kroll et al., 2011; Nozière et al., 2015).



Figure 1.3.7: Carbon oxidation state plot for organic aerosol taken from measurements using three analysis techniques (combustion analysis, HRMS with ESI, and HR–AMS) (Kroll et al., 2011).

Another useful visualization tool is Kendrick Mass (KM) analysis, which is typically used to identify homologous series of compounds differing only by the number of a specific base unit (e.g.

CH<sub>2</sub>, CH<sub>2</sub>O, etc.). (Kendrick, 1963; Hughey et al., 2001). For example, the Kendrick mass of CH<sub>2</sub> unit is calculated by renormalizing the IUPAC mass (14.01565) of CH<sub>2</sub> to exactly 14.00000 using equation 1.10:

$$KM_{CH_2} = Observed \ mass \times \frac{14.00000}{14.01565}$$
 (1.10)

The Kendrick mass defect (KMD) is defined as the exact Kendrick mass subtracted from the nominal Kendrick mass, calculated using equation 1.11:

$$KMD_{CH_2} = Nominal Mass - KM_{CH_2}$$
(1.11)

As a consequence, compounds with identical KMD can be easily grouped into a homologous series. When the KMD is plotted versus nominal Kendrick mass, homologous series will fall on horizontal lines, as illustrated in Figure 1.3.8 (Hughey et al., 2001; Nizkorodov, 2011; Nozière et al., 2015).



Figure 1.3.8: Kendrick mass defect vs nominal Kendrick mass for odd-mass <sup>12</sup>Cc ions. The visual vertical separation of compound classes (e.g., O, O<sub>2</sub> and O<sub>3</sub>S) and types (compounds with different number of rings plus double bonds) based on mass defect and the visual horizontal distribution of number of CH<sub>2</sub> groups for a given compound class and type (Hughey et al., 2001).

## 1.4 Formation of reactive oxygen species by particulate matter

Numerous epidemiological studies show that ambient and indoor air pollution as well as inhalation and deposition of fine particulate matter are correlated with adverse health impacts, including allergic, respiratory, and cardiovascular diseases, lung cancer and increased mortality (Pope et al., 2002; Pöschl, 2005; Pope and Dockery, 2006; Brook et al., 2010; Beelen et al., 2014; Pöschl and Shiraiwa, 2015). One of the most plausible pathophysiological mechanisms to explain the association of PM exposure with adverse health effects is oxidative stress caused by formation of reactive oxygen species (ROS) (Apel and Hirt 2004; Fang et al, 2019). ROS contain hydroxyl radicals (•OH), hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>), and superoxide (•O<sub>2</sub><sup>-</sup>) as well as organic radicals, which can be formed by redox-active components in PM such as transition metals and quinones (Pöschl and Shiraiwa, 2015). Hydroxyl radicals are the most reactive form of ROS, which can cause a variety of oxidative damage to membrane lipids, proteins, and DNA of cells (Valavanidis et al., 2008; Wang et al., 2011).  $H_2O_2$  is relative long lived and generally regarded as having significant indirect biological effects since this small uncharged molecule diffuses across membranes easily (Feierman et al., 1985; LaCagnin et al., 1990). A number of studies have shown that excess ROS can cause oxidative stress leading to cell death and tissue injury in the respiratory tract. Thus, characterizing the formation of ROS is essential to understand how air pollution can cause adverse health effects.

## 1.4.1 Endogenous formation of ROS

Upon inhalation and deposition in the respiratory tract, redox-active components in PM can induce and involve chemical reactions that endogenously produce ROS in the epithelial lining fluid (ELF). ELF covering the airways contains a range of surfactants and antioxidants such as ascorbate (Asc), uric acid (UA), reduced glutathione (GSH), and  $\alpha$ -tocopherol ( $\alpha$ -Toc). As shown in Figure 1.4.1, the redox-active species and ROS undergo a multitude of redox reaction cycles. This process starts with the transfer of electrons from antioxidants (e.g. Acs) to transition metals (iron or copper ions) and/or quinones (see equation 1.12 and 1.13). The formed reduced metal ions and/or semiquinones react with O<sub>2</sub> to regenerate the oxidized metal ions and/or quinones and produce  $\cdot O_2^{-1}$ (see equation 1.14 and 1.15). O<sub>2</sub><sup>-</sup>radicals are further converted into H<sub>2</sub>O<sub>2</sub> (see equation 1.16 and 1.17) and then OH radicals can be formed via Fenton-like reactions of H<sub>2</sub>O<sub>2</sub> with iron or copper ions (see equation 1.18) (Kok et al., 2006; Shen et al, 2011; Wang et al., 2011; Lakey et al., 2016; Fang et al., 2019).
$$TM(ox) + Asc \rightarrow TM(red) + \cdot Asc$$
 (1.12)

$$Quinone + Asc \rightarrow Semiquinone + \cdot Asc$$
(1.13)

$$TM(red) + O_2 \to TM(ox) + \cdot O_2^- \tag{1.14}$$

$$Semiquinone + O_2 \to Quinone + \cdot O_2^- \tag{1.15}$$

$$TM(red) + \cdot O_2^- + 2H^+ \to TM(ox) + H_2O_2$$
 (1.16)

$$Semiquinone + \cdot O_2^- + 2H^+ \to Quinone + H_2O_2$$
(1.17)

$$TM(red) + H_2O_2 \to TM(ox) + OH + OH^-$$
(1.18)

where (ox) and (red) represent oxidized and reduced forms of transition metals (TM), respectively.



Fig. 1.4.1 Interaction of air pollutions and reactive oxygen species in the epithelial lining fluid of the human respiratory tract (Lakey et al., 2016).

## 1.4.2 Components in PM related to ROS formation

ROS can directly derived from PM. Laboratory measurements indicates the majority of  $H_2O_2$  associated with ambient particles is generated by the particles themseleves in aqueous solutions (Hasson and Paulson 2003; Arellanes et al. 2006). Moreover, ROS can also be produced by redox-active species in PM, including transition metals, environmentally persistent free radicals (EPFRs; e.g. semiquinones), humic-like substances (HULIS), and SOA produced from aromatics such as naphthalene (Wang et al., 2012; Pöschl and Shiraiwa, 2015; Lakey et al., 2016; Fang et al., 2017).

Transition metals play an important role in the formation of ROS. Iron (Fe) and copper (Cu), the most abundant transition metals in particles, are capable of chemically producing ROS via redox reactions (see equations 1.7–1.9). Numerous studies have showen significant correlations between  $H_2O_2$  generation with concentrations of soluble Fe and Cu in PM extracts (Shen et al., 2011; Wang et al., 2012). Furthermore, the Fenton reaction (Fe<sup>2+</sup> + H<sub>2</sub>O<sub>2</sub>) is one of the most fundamental and widespread reactions in the multiphase chemistry of ROS, which leads to the generation of hydroxyl radicals (Pöschl and Shiraiwa, 2015). The other transition metals like manganese (Mn), nickel (Ni), cobalt (Co), and vanadium (V) can also produce ROS under some conditions. However, these metals may not produce significant levels of ROS due to their low soluble metal concentrations expected from PM (Pöschl and Shiraiwa, 2015).

Quinones are generally originated from engine exhaust or cigarette smoke or can be generated via oxidation of aromatic precursors (Lakey et al., 2016; Fang et al., 2017). Laboratory studies show that 1,4-naphthoquinone, 1,2-naphthoquinone, and phenanthrenequinone are the most reactive quinones associated with ROS generation. Figure 1.4.2 shows redox reaction cycling of quinone-mediated  $H_2O_2$  generation. In the presence of an electron donor, quinones are converted into semiquinone radical anions accompanied by the generation of superoxide radicals and hydrogen peroxide. Superoxide facilitates the regeneration of quinone as well as additional  $H_2O_2$  formation (Wang et al., 2012; Kuang, 2017).

1 Introduction



Fig. 1.4.2 Scheme of possible quinone cycling reactions (Wang et al., 2011).

Several studies have found that contributions from transition metals and quinones alone cannot account for all of the observed ROS, indicating there are additional compounds in PM responsible for the production of ROS. Water-soluble humic-Like substances (HULIS) are a mixture of compounds containing polycyclic ring structures with aliphatic side chains and multiple polar functional groups, which derived from biomass burning (Hoffer et al., 2006; Mukai and Ambe 1986; Zappoli et al., 1999) or produced by complex secondary reactions (e.g. heterogeneous and photosensitized reactions) (Decesari et al., 2001; Limbeck et al., 2005). They have recently been recognized to be highly redox-active and play a significant role in driving PM-associated ROS formation (Lin and Yu, 2011; Verma et al., 2015; Ma et al., 2018). The reversible redox sites in the HULIS could serve as an electron transfer intermediate leading to the continuous generation of ROS (Lin and Yu, 2011). In addition, due to HULIS contain organics that chelate transition metals, interactions of which could lead to synergistic or antagonistic effects on ROS formation.

The contribution of SOA to the generation of ROS has got increasing attention. A few studies have shown that SOA derived from both biogenic and anthropogenic precursors can generate a considerable amount of  $H_2O_2$  or radicals in the aqueous phase (Hewitt and Kok, 1991; Hasson et al., 2001; Wang et al., 2011; Kramer et al., 2016; Tong et al., 2018; Tong et al., 2019). The formation of  $H_2O_2$  associated with SOA is likely the decomposition or hydrolysis of organic (hydro)peroxides and related species (Pöschl and Shiraiwa, 2015). Wang et al. suggested SOA formed via ozonolysis and photo-oxidation of  $\alpha$ -pinene,  $\beta$ -pinene, and toluene all produced  $H_2O_2$ in the aqueous phase, and  $\alpha$ -pinene and  $\beta$ -pinene SOA have higher  $H_2O_2$  generation ability than toluene SOA (Wang et al., 2011). Moreover, isoprene SOA and naphthalene SOA were observed to release substantial amounts of  $H_2O_2$ , OH radicals, and organic radirals upon interaction with water (Tong et al., 2018). In addition,

## **1.5** Thesis objectives and outline

Atmospheric aerosol contains thousands of chemical compounds due to various biogenic and anthropogenic sources as well as complex multiphase chemical reactions. In particular, OA often constitutes a substantial fraction of aerosol mass and organic compounds in OA cover a wide range of chemical space with respect to molecular mass, polarity, and functional groups. Furthermore, epidemiological studies have indicated associations of adverse respiratory and cardiovascular health effects with organic fractions of ambient PM. Thus, investigating the chemical characterization of OA is an essential and challenging task, which helps to better understand the chemical composition, sources, and atmospheric processes of OA as well as to identify the healthrelated organic compounds.

The aim of this work was to characterize the organic compounds in  $PM_{2.5}$  collected in different cities and remote regions using the UHPLC-Orbitrap technique and further to provide molecular evidence for the association of ROS formation with organic compounds. Based on the identified elemental compositions, a new parameter 'maximum carbonyl ratio (MCR)' was proposed to improve the classification of organic compounds in OA. This work can be described in three parts as follows:

1. The first part focused on the development of analytical method for OA measurement. PM2.5 samples were collected in Beijing (Chinese megacity) and Mainz (a city within the Rhine-Main area, Germany). OA was extracted by a solvent mixture of acetonitrile and water and detected using UHPLC coupled to the UHRMS-Orbitrap with electrospray ionization (ESI). The chemical composition and properties, and related sources of OA in Beijing and Mainz were analyzed and compared.

2. In the second part, we developed a new parameter 'MCR' to interpret the UHRMS data. The MCR expresses the maximum number of carbonyl groups in a molecule and can be calculated based on the elemental composition. By the combination of MCR values and the traditional visualization tool Van Krevelen (VK) diagram, we created the MCR-VK diagram and allocated the typical SOA compounds in the MCR-VK diagram for region division. The approach was tested by using ambient  $PM_{2.5}$  samples, which were collected in Hyytiälä (boreal forest region, Finland) and Beijing, respectively, and SOA samples generated from ozonolysis of  $\alpha$ -pinene and photo-oxidation of isoprene, respectively. The distributions of OA derived from different samples in the MCR-VK diagram were observed and compared.

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3. In the third part, we characterized the chemical composition of organic compounds in ambient  $PM_{2.5}$  samples and laboratory-generated SOA samples using the UHPLC-Orbitrap MS method developed in the first part of this work. The  $PM_{2.5}$  samples were collected in five urban cities (Mainz, Beijing, Shanghai, Guangzhou, and Xi'an) and a remote region (Hyytiälä), while SOA samples were generated from ozonolysis of  $\alpha$ -pinene,  $\beta$ -pinene and limonene, and photo-oxidation of isoprene and naphthalene. Then we proposed the concept 'ratio of relative peak area-weighted fraction of oxidized organic compounds to relative peak area-weighted fraction of unsaturated organic compounds ( $R_{OOC/UOC}$ )' base on the classification of organic compounds by their MCR values. Furthermore, we quantified the ROS yield of the samples in water, which was the sum of  $H_2O_2$  yield using a fluorometric probe and radical yield measured by electron paramagnetic resonance. The correlations of  $R_{OOC/UOC}$  of OA with ROS yield were investigated and organic compounds that contributed to the ROS formation were explored.

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This chapter is a reprint of the article:

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UHPLC- Orbitrap mass spectrometric characterization of organic aerosol from a central European city (Mainz, Germany) and a Chinese megacity (Beijing)

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Abstract. Fine urban aerosol particles with aerodynamic equivalent dimeter  $\leq 2.5 \ \mu m (PM_{2.5})$  were collected in Mainz (a city within the Rhine-Main area, the third largest metropolitan region in Germany) and Beijing (Chinese megacity). A solvent mixture of acetonitrile-water was used to extract the organic aerosol fraction (OA) from the particle samples. The extracts were analyzed by an ultrahigh resolution mass spectrometer (UHRMS) Orbitrap coupled with ultra-high-performance liquid chromatography (UHPLC) both in the negative and positive ion mode. The number of compounds observed in Beijing is a factor of 2–10 higher compared to Mainz. The clear differences on chemical composition of OA in the two cities were observed. The majority of organics in Beijing OA is characterized by lower elemental H/C and O/C ratio but a higher degree of unsaturation and a larger aromaticity equivalent (X<sub>C</sub>) compared to Mainz OA, suggesting that aromatics, which are related to direct combustion compounds (e.g., oxidized polycyclic aromatic hydrocarbon (PAH)), play an important role for OA in Beijing. A significant number of organosulfates (OSs) with long-carbon chain and low degree of unsaturation were observed in Beijing OA, indicating that long-chain alkanes emitted by vehicle might be their precursors.

Keywords: Organic aerosol, Orbitrap MS, UHPLC, Megacity, Molecular characterization

# **2.1 Introduction**

Organic aerosol (OA) constitutes a substantial fraction (20–90%) of submicrometer aerosol mass (Jimenez et al., 2009; Kroll et al., 2011) and influences air quality, climate, and human health (Pöschl, 2005;Hallquist et al., 2009). Previous studies have shown that OA contains a variety of organic species, including hydrocarbons, alcohols, aldehydes, carboxylic acids, organosulfates and organonitrates. However, only about 10–30% of OA has been chemically specified so far (Hoffmann et al., 2011). A better understanding of the chemical composition, properties and reactivity of OA are therefore important for assessing the effects of atmospheric aerosols. Since the thousands of compounds in OA covers a very large chemical space with respect to molecular mass, functional group distribution and polarity at trace level concentrations (Lin et al., 2012a; Nozière et al., 2015), characterization of OA is a challenging analytical task.

With the development of mass spectrometric techniques, considerable advances have been made over the past decade in terms of a better understanding of OA. The Aerodyne aerosol mass spectrometer (AMS) has been widely used to measure OA elemental composition and to study the

sources and atmospheric processes (e.g. oxidation state) of OA (Canagaratna et al., 2015; Dall'Osto et al., 2015; Lee et al., 2015). However, the use of 70 eV electron ionization of the AMS leads to a high degree of fragmentation of OA and therefore difficulties in the identification and quantification of individual organics. Several approaches have been developed recently to introduce soft ionization techniques for OA studies, including atmospheric pressure chemical ionization (APCI) and electrospray ionization (ESI) (Hoffmann et al., 2011; Nozière et al., 2015). Especially ultrahigh resolution mass spectrometry (UHRMS) coupled with ESI allows the characterization of complex organic mixtures at the molecular level (Nizkorodov et al., 2011; Lin et al., 2012a; Rincón et al., 2012; Wang and Schrader, 2015). Fourier transform ion cyclotron (FTICR), Orbitrap and high-resolution quadrupole time-of-flight (HR-Q-TOF) are the three major high-resolution mass analyzers (Nozière et al., 2015). Due to the high mass resolving power ( $\geq$ 40000) and high mass accuracy ( $\leq 5$  ppm), the UHRMS techniques can detect thousands of individual organic aerosol components and provide their accurate chemical composition for each analysis. A recent review by Nizkorodov et al. (Nizkorodov et al., 2011) shows that UHRMS analysis of secondary OA from smog chamber studies and aerosol samples collected from e.g. biomass burning, forest, rural and urban environment can provide improved understanding of the molecular composition and fundamental chemical transformations of OA. However, UHRMS analysis is instrumentally demanding and UHRMS studies of urban OA are still very scarce. Previous studies focused on the characterization of bulk OA or a group of specific compounds. For example, Lin et al. (Lin et al., 2012a) characterized the element composition of humic-like substances in the Pearl River Delta Region, China. Tao et al. (Tao et al., 2014) reported the analysis of organosulfates (OSs) in OA from Shanghai and Los Angeles. Wang et al. (Wang et al., 2016) studied the OSs in three Chinese cities. Wang et al. investigated the month and diurnal variation of the OA chemical composition in Shanghai. Rincon et al. (Rincón et al., 2012) characterized the chemical composition of OA collected in different seasons at Cambridge, UK. Reemtsma et al. (T. et al., 2006) and Roach et al. (Roach et al., 2010) studied the OA from Riverside, CA and Mexico city, respectively.

Over the past decade, particulate air pollution has become a serious environmental problem in China. Severe and persistent haze pollution occurred frequently in China in recent winters, particularly in megacities and urban complexes (Huang et al., 2014). Very recent studies show that outdoor air pollution, mostly by PM<sub>2.5</sub>, leads to 3.3 million premature deaths per year worldwide, predominantly in Asia (Lelieveld et al., 2015). The yearly mass concentrations of PM<sub>2.5</sub> often exceed the WHO guideline concentration of 10  $\mu$ g m<sup>-3</sup>, even in many European urban areas. Given that about 55–75% of population lives in urban areas in China and European countries, a better understanding of the chemical composition, sources and atmospheric processes of aerosol in urban areas is important. This is particularly true for the OA fraction as it is much more complex and uncertain than the inorganic aerosol fraction. In this study, PM<sub>2.5</sub> samples were collected from Beijing (the capital of China with more than 20 million residents) and Mainz (a city within the Rhine-Main area, the third largest metropolitan region in Germany with more than 5.8 million population). However, the two urban regions experience very different natural and anthropogenic influences and it is worthwhile to investigate the similarities and differences in the OA composition in these two citie. Therefore, the organic fraction of the PM<sub>2.5</sub> samples in Beijing and Mainz were analyzed using UHPLC-Orbitrap MS in both negative and positive polarity and the difference in OA chemical composition is discussed.

# 2.2 Methodology

## 2.2.1 Sample collection and preparation

24-h integrated urban  $PM_{2.5}$  samples were collected in Beijing (6 samples) and Mainz (3 samples). For the six Beijing samples, three were collected from 7–12 January 2014, during a relatively clean period with  $PM_{2.5}$  mass concentrations between 32 and 38 µg m<sup>-3</sup> (sample ID: BJL (Beijing Low)). The other three samples were collected from 15–23 January 2014, during a severe haze pollution period with high  $PM_{2.5}$  mass concentrations of 197–319 µg m<sup>-3</sup> (sample ID: BJH (Beijing High)). The three Mainz samples were taken from 15–28 January 2015 with relatively low  $PM_{2.5}$  concentrations of 20–28 µg m<sup>-3</sup> (sample ID: MZL (Mainz Low)). The Beijing samples were collected on prebaked quartz-fiber filters (8×10 inch) using a high-volume sampler at a flow rate of 1.05 m<sup>3</sup> min<sup>-1</sup>, while the Mainz samples were collected on borosilicate glass fiber coated with fluorocarbon filters (Ø 70 mm, Pallflex T60A20, Pall Life Science, USA) using a low-volume sampler at a flow rate of 38.3 L min<sup>-1</sup>. At each sampling site field blank samples were taken. The filter samples were stored at –20 °C until analysis. It should be noted that the  $PM_{2.5}$  samples in Mainz and Beijing were collected in two consecutive years. An influence of year-to-year variability due to changing meteorological conditions cannot be excluded, however, both periods were wintertime periods with a similar regional scenario (Chang et al., 2017).

Portions of the filters  $(1.08-19.23 \text{ cm}^2, \text{ corresponding to around 600 } \mu\text{g}$  particle mass in each extracted filter) were extracted with 1.5 mL acetonitrile-water (8/2, v/v) in an ultrasonic bath for 30 min. The extraction step was repeated twice with 1 mL of the extraction solution. Then the

combined extracts were filtered with a 0.2  $\mu$ m Teflon syringe filter to remove insoluble particulate matter. Afterwards the solvent mixture was evaporated to dryness under a gentle stream of nitrogen. The residual was dissolved in 500  $\mu$ L acetonitrile-water (1/9, v/v) for subsequent analysis.

## 2.2.2 UHRMS analysis

The analysis of the filter extracts was carried out using an ultrahigh resolution mass spectrometer (Q-Exactive mass spectrometer; Thermo Scientific, Germany) coupled to an UHPLC system (Dionex UltiMate 3000, Thermo Scientific, Germany). A Hypersil Gold column (C18, 50 x 2.0 mm, 1.9  $\mu$ m particle size, Thermo Scientific, Germany) was used for separation. Eluent A (ultrapure water with 2% acetonitrile and 0.04% formic acid) and eluent B (acetonitrile with 2% ultrapure water) were used in a gradient mode with a flow rate of 500  $\mu$ L min<sup>-1</sup>. The optimized gradient was as follows: 0–1.5 min 2% B, 1.5–2.5 min from 2% to 20% B, 2.5–5.5 min 20% B, 5.5–6.5 min from 20% to 30% B, 6.5–7.5 min from 30% to 50% B, 7.5–8.5 min from 50% to 98% B, 8.5–11.0 min 98% B, 11.0–11.05 min from 98% to 2% B, 11.05–11.1 min 2% B. Each sample extract was measured in triplicate with an injection volume of 20  $\mu$ L.

The Q Exactive mass spectrometer was equipped with a heated ESI source at 120 °C in the negative ion mode (ESI–) and 150 °C in the positive ion mode (ESI+). It was operated with 40 psi sheath gas, 20 psi auxillary gas, 320 °C capillary temperature and -3.3 kV spray voltage in the ESI– mode and 4.0 kV spray voltage in the ESI+ mode. The mass spectrometer was calibrated with standard solution for ESI– and ESI+, respectively (See supporting information, SI). Mass spectra of all samples were acquired in both ESI– and ESI+ in the mass range between m/z 80 and m/z 500 with a resolving power of 70,000 @ m/z 200. The field blank filters were analyzed to correct for the background spectra. The mass accuracy of the measurements was < 3 ppm.

## 2.2.3 UHRMS data processing

Data were analyzed by a non-target screening approach using a commercially available software (SIEVE<sup>®</sup>, Thermo Scientific, Germany). This software provides the core functionality of MS data processing: peak detection, background subtraction and molecular formula assignment. The processing steps and settings are described in the following. A threshold intensity value of  $1 \times 10^5$  arbitrary units in the two-dimensional space of the retention time window from 0–11.05 min and m/z from 80–500 was applied to all measurements. The software automatically searched the

ions with their peak abundance above the threshold intensity value and only ions with peak abundance in the ambient samples 3 times greater than those in the blank samples were retained. After that, the molecular formulas of observed individual peaks were assigned by SIEVE with following constraints: #12C: 1 to 39, #1H: 1 to 72, #16O: 0 to 20, #14N: 0 to 7, #32S: 0 to 4 and #35Cl: 0 to 2 with mass tolerance of  $\pm 2$  ppm. In ESI+ mode, 0–1 of Na was also included in the formula calculation because of the high tendency of sodium to form adducts with polar organic molecules. In addition, the isotope signals and ion-adducts (e.g. M-H+ACN) were checked and removed. Furthermore, to eliminate the chemically unreasonable formulas, the identified formulas were constrained by setting H/C, O/C, N/C, S/C and Cl/C ratios in the ranges of 0.3–3, 0–3, 0–1.3, 0–0.8 and 0–0.8, respectively (Kind and Fiehn, 2007; Wozniak et al., 2008; Lin et al., 2012a). The resulting neutral formulas with a non-integer or negative double bond equivalent (DBE) or elemental composition which disobey the nitrogen rule for even electron ions were also removed. It should be noted that only molecular formulas observed in all three samples for each sample ID were considered for further calculation and discussion. The peak abundance of a compound in each sample ID corresponded to the average area of its chromatographic peak in the three filter samples and was blank-corrected. The DBE value was calculated by Eq. (2.1) for elemental composition  $C_cH_hO_oN_nS_sCl_x$ :

$$DBE = c - \frac{(h+x)}{2} + \frac{n}{2} + 1$$
(2.1)

Additionally, the aromaticity equivalent ( $X_C$ ) was used to improve the identification and characterization of aromatic and condensed aromatic compounds in OA, which was described in detail by Yassine et al. (Yassine et al., 2014). The  $X_C$  value can be calculated by Eq. (2):

$$X_{C} = \frac{3(DBE - (mN_{0} + nN_{S})) - 2}{DBE - (mN_{0} + nN_{S})}$$
(2.2)

where 'm' and 'n' correspond to a fraction of oxygen and sulfur atoms in  $\pi$ -bond structure of a compound, which varied depending on the compound. If DBE  $\leq mN_0 + nN_s$  or  $X_C \leq 0$ , then  $X_C$  was defined as zero. Due to the extreme complexity of urban OA, we used m=n=1 for the conservative calculation of the  $X_C$ , which means every oxygen and sulfur atom was considered as  $\pi$ -bond structure (e.g., ketone and thioketone).

The assigned elemental formulas were classified into six species, including CHO, CHN, CHON, CHOS, CHONS and "other". CHONS referred to compounds containing carbon, hydrogen, oxygen, nitrogen and sulfur. The other species were defined analogously, while "other" includes CHS, CHNS and chlorine-containing compounds, which represented very low intensity and are not

discussed here.

Since the response of each organic species to the mass spectrometer varies greatly, the average molecular weight (MW), H/C, O/C and DBE values were number-weighted calculated by following equations (2.3–2.6) (Lin et al., 2012a):

$$MW = \sum MW_i / \sum N_i \tag{2.3}$$

$$H/C = \sum H/C_i / \sum N_i \tag{2.4}$$

$$O/C = \sum O/C_i / \sum N_i \tag{2.5}$$

$$DBE = \sum DBE_i / \sum N_i \tag{2.6}$$

where  $N_i$  is the number of individual molecular formula i.

# 2.3 Results and discussion

## 2.3.1 General characteristics

As shown in Table 2.3.1, 1961–28696 mass peaks were detected in this study and the majority (57%–78%) of these detected peaks could be assigned with unambiguous formulas with mass tolerance less than 2 ppm, reflecting the high mass resolution power and high mass accuracy of the UHRMS technique. 1081–1955 molecular formulas of organic compounds with various numbers of isomers for each formula were detected in Mainz samples, while around 2-10 times more molecular formulas (2597–17596) were observed in Beijing samples, indicating the high complex of Beijing OA. The number of molecular formulas in this study is much higher compared to other UHRMS studies used direct infusion (Lin et al., 2012a; Lin et al., 2012b; Rincón et al., 2012; Kourtchev et al., 2016) and a previous UHPLC-Orbitrap MS study (Wang et al., 2017). This can be explained because UHPLC not only separates a large number of isomers, it also reduces ion suppression by coelution. In addition, the use of the mixture of ACN/H<sub>2</sub>O is more efficient for OA extraction, especially for the less polar compounds (e.g. aromatics), compared to pure water or methanol used in previous studies. Moreover, the high organic carbon concentration (around 200  $\mu g \text{ cm}^{-2}$  in BJH) can significantly result in more organic compounds observed in BJH in this study. It should be noted that the number of detected organic compounds is highly depending on the threshold intensity values applied for background subtraction, which always vary in different

studies. 61–92% of molecular formulas in this study contains isomers, indicating that UHPLC technique is very important tool for the characterization of complex ambient OA. And a representative UHPLC chromatogram for the UHPLC performance is shown in Figure S2.3.1 in the Supporting Information (SI).

Table 2.3.1: The number of overall peaks observed in UHRMS, the number of assigned reasonable formulas and the relative abundance of each subgroup depending on their UHPLC chromatographic peaks (%), number-weighted average values of molecular weight, elemental ratios and DBE, and the isomer fraction in each subgroup.

Polarity and subgroup	Number of overall peak <sup>a</sup>	Number of formulas <sup>b</sup>	%	MW (Da)	H/C	O/C	DBE	Isomer fraction (%)
MZL								
total(-)	1961(70%)	1081(100%)	100	243	1.23	0.62	5.38	61
CHO-		347(32%)	23	206	1.05	0.44	6.13	70
CHON-		376(35%)	40	239	1.06	0.56	6.52	57
CHOS-		166(15%)	15	241	1.66	0.78	2.51	51
CHONS-		192(18%)	22	318	1.54	0.91	4.26	61
total(+)	5053(57%)	1955(100%)	100	225	1.34	0.27	5.76	61
CHO+		446(23%)	13	215	1.07	0.33	7.02	64
CHN+		302(15%)	11	177	1.33	0.00	5.93	79
CHON+		1103(56%)	74	236	1.42	0.28	5.34	60
CHONS+		104(6%)	2	292	1.65	0.68	4.29	11
BJL								
total(-)	3950(78%)	2597(100%)	100	241	1.22	0.51	5.85	72
CHO-		937(36%)	24	217	0.98	0.34	7.29	81
CHON-		799(31%)	53	230	0.96	0.50	7.28	68
CHOS-		494(19%)	16	256	1.81	0.63	2.02	70
CHONS-		367(14%)	7	305	1.57	0.81	4.26	57

									-
total(+)	13168(72%)	7473(100%)	100	229	1.26	0.19	6.73	80	
CHO+		1705(23%)	22	238	1.11	0.24	7.33	80	
CHN+		1298(17%)	35	199	1.12	0.00	8.01	92	
CHON+		3848(52%)	40	225	1.24	0.19	6.71	82	
CHONS+		622(8%)	3	292	2.10	0.42	2.52	41	
BJH									
total(-)	6745(72%)	3941(100%)	100	244	1.19	0.45	6.07	78	
CHO-		1718(44%)	35	223	0.93	0.34	7.76	89	
CHON-		842(21%)	48	221	0.92	0.50	7.24	73	
CHOS-		831(21%)	12	280	1.74	0.51	2.26	80	
CHONS-		550(14%)	5	292	1.56	0.59	4.74	48	
total(+)	28696(75%)	17596(100%)	100	235	1.28	0.21	6.75	89	
CHO+		3990(23%)	21	226	1.08	0.22	7.27	91	
CHN+		2831(16%)	39	210	1.14	0.00	8.16	96	
CHON+		8400(48%)	36	229	1.20	0.21	7.15	90	
CHONS+		2375(13%)	4	302	2.04	0.44	2.74	71	

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	mas	s spectrometry				

<sup>a</sup>Values in the parentheses are the percentage of peaks that can be assigned with unambiguous fomulas.

<sup>b</sup>Values in the parentheses are the percentage of different subgroups among the assigned reasonable formulas.

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Figure 2.3.1: Mass spectra of detected organic compounds in ESI- and ESI+. The pie chats are proportional to the peak areas of an organic compound subgroup in each sample.

Mass spectra of observed organic compounds were reconstructed in both ESI– and ESI+ (see Figure 2.3.1). It should be noted that different organic species have different signal response in the mass spectrometer, so uncertainties exist when comparing the peak areas of organics in different subgroups. In this work, all species are assumed to have the same signal response when we compare peak areas of organics among different samples. A significant difference between ESI– and ESI+ is observed in terms of both the number and abundance of the detected compounds (Table 2.3.1 and Figure 2.3.1). Except CHOS compounds, all other subgroups have much more formulas in ESI+ mode compared to ESI– mode, indicating the less ionization suppression for these compounds

in ESI+. However, according to the peak abundance showed in Figure 2.3.1, the abundance fractions of CHO, CHOS and CHONS compounds in ESI– mode are higher than that in ESI+ mode, while CHN compounds have higher abundance fraction in ESI+ and the fractions for CHON compounds vary depending on different samples. This is due to the different mechanisms between negative and positive ionization mode in the electrospray, where ESI– is especially sensitive to deprotonatable compounds (e.g. organic acids) and ESI+ is prone to protonatable compounds (e.g. organic basic compounds). In both Mainz and Beijing samples, CHON compounds show the highest total peak abundance of the detected compounds, which is consistent with other urban OA studies (Lin et al., 2012a; Rincón et al., 2012; Wang et al., 2017), indicating the importance of CHON compounds to the urban atmosphere.

Table 2.3.1 shows that the number-weighted averaged molecular weight of the total detected compounds is similar between Mainz and Beijing samples (241–244 Da in ESI– and 225–229 in ESI+). However, the number-weighted averaged H/C and O/C ratios of total compounds in Beijing samples are significantly lower compared to Mainz samples and the number-weighted averaged DBE in Beijing samples is higher than that in Mainz samples. This observation suggests that organics in Beijing OA are more condensed and unsaturated compared to Mainz OA and aromatics (e.g. oxidized PAH) have an important impact on the Beijing atmosphere.

#### 2.3.2 CHO compounds

In this study, CHO compounds account for 23–35% of the peak abundance among the organic compounds detected in ESI–, while the fraction decreases to 13–22% in ESI+ mode (see Table 2.3.1), indicating CHO compound in this study are more sensitive in ESI- mode. This is consistent with a previous study from Lin et al. (Lin et al., 2012a), which shows that most CHO compounds in OA contain carboxylic groups and are prone to deprotonate in ESI– mode. To further characterize the CHO compounds, Van Krevelen (VK) and carbon oxidation state (OS<sub>c</sub>) diagrams are produced. The VK diagram is often utilized to describe the compositional characteristics of complex organic mixtures. It provides a broad overview on their average composition and can be used to qualitatively classify different composition domains (Hockaday et al., 2009; Lin et al., 2012a; Rincón et al., 2012). The VK diagram for CHO compounds observed in ESI– is shown in Figure 2.3.2, while the VK diagram for CHO compounds observed in ESI+ is showed in Figure S2.3.2. According to the H/C and O/C ratios, organic compounds can be divided into two different classes: aliphatic compounds with high H/C ratio ( $\geq$  1.5) and low O/C ratios ( $\leq$  0.5) (area A in Figure 2.3.2) and low-oxygen-containing aromatic hydrocarbons with low H/C ratio ( $\leq$  1.0) and low O/C ratio

(< 0.5) (area B in Figure 2.3.2) (Kourtchev et al., 2014). As can be seen in Figure 2.3.2 (and Figure S2.3.2), the majority of CHO compounds are located in the region A and B, which agrees well with previous urban OA studies (Rincón et al., 2012; Kourtchev et al., 2014). However, much more CHO compounds detected in Beijing samples were plotted in the region B, indicating that Beijing OA contains more low-oxygen-containing aromatic hydrocarbons. The number weighted averaged H/C and O/C ratios of CHO compounds detected in ESI- are 1.05 and 0.44, respectively, in Mainz samples, while lower H/C and O/C ratios (0.98 and 0.34 in BJL; 0.93 and 0.34 in BJH) are observed in Beijing samples. This result is also consistent with previous studies, for example, the H/C and O/C ratios are lower in the samples from the Pearl River Delta region in Southern China compared to those from Cambridge in the UK (Lin et al., 2012a;Rincón et al., 2012). The low H/C and O/C ratios indicate the unsaturated characteristics of CHO in urban aerosol samples from China. This is further confirmed by the aromaticity equivalent  $(X_{C})$ , which is a parameter determining the presence of aromatics ( $X_C \ge 2.5$ ) and condensed aromatics ( $X_C \ge 2.7$ ) (Yassine et al., 2014). As shown in the pie chart of Figure 2.3.2, the fractions of aromatics and condensed aromatics are about 2 times and 1.7 times higher, respectively, in Beijing than in Mainz. The large difference in chemical characteristics of CHO compounds in Beijing and Mainz is likely associated with the different emission sources and/or atmospheric processes.

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Figure 2.3.2: The Van Krevelen diagram for CHO compounds detected in ESI– mode. Areas 'A' and 'B' refer to aliphatic compounds and low-oxygen-containing aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity equivalent (gray with X<sub>C</sub> < 2.50, purple with 2.50 ≤ X<sub>C</sub> < 2.70 and red with X<sub>C</sub> ≥ 2.70). The pie chat shows the percentage of the number of each color-coded compound in each sample.

The carbon oxidation state  $(OS_C)$ , introduced by Kroll et al. (Kroll et al., 2011) is another parameter used to describe the composition of a complex mixture of organics experiencing dynamic oxidation processes.  $OS_C$  can be calculated for each molecular formula of CHO compounds

identified in the mass spectra following Eq. (2.7).

$$OS_C \approx 2 \, O/C - H/C \tag{2.7}$$

Figure 2.3.3 shows the overlaid  $OS_C$  as a function of carbon number for samples from Beijing and Mainz. Consistent with previous studies (Kourtchev et al., 2015; Kourtchev et al., 2016; Wang et al., 2017), the majority of molecules in the CHO subgroup have  $OS_C$  between -1.5 and +1 with number of carbon atoms up to 30. The molecules with  $OS_C$  between -1 and -2 with 18 or more carbon atoms are suggested to be associated with hydrocarbon-like organic aerosol (HOA). The molecules with  $OS_C$  between -1.25 and -0.25 with 7-23 carbon atoms are associated with biomass burning organic aerosol (BBOA) directly emitted into the atmosphere. The molecules with  $OS_C$ between -0.5 and +0.25 with 5–18 carbon atoms are associated with semi-volatile oxygenated organic aerosol (SV-OOA), while the molecules with  $OS_{C}$  between +0.25 and +1.0 with 4–13 carbon atoms are associated with low-volatility oxygenated organic aerosol (LV-OOA) as defined by Kroll et al. (Kroll et al., 2011). As shown in Figure 2.3.3, a large majority of CHO molecules are attributed to SV-OOA for both Beijing and Mainz samples, indicating the importance of atmospheric oxidation and aging in OA production. Significantly more BBOA associated molecules are obtained in Beijing compared to Mainz, reflecting the enhanced biomass burning activities in Beijing and surrounding areas (Zhang et al., 2008; Cheng et al., 2013; Huang et al., 2014; Elser et al., 2016). It should be noted that coal combustion is also an important OA source (Zhang et al., 2013; Huang et al., 2014; Elser et al., 2016; Zhang et al., 2016), which is not discussed here due to the lack of source characterization with UHRMS study.



Figure 2.3.3: Carbon oxidation state plots for CHO compounds detected in ESI- mode. The black dash ovals area marked as HOA, BBOA, SV-OOA and LV-OOA correspond to hydrocarbon-like organic aerosol, biomass burning organic aerosol, semivolatile and low-volatility organic aerosol.

## 2.3.3 CHON compounds

A large amount of organic nitrogen compounds has been observed in fog water, continental precipitation as well as aerosol samples (Altieri et al., 2009; Mazzoleni et al., 2010; Lin et al., 2012a; Jiang et al., 2016). In this study, 376–842 of CHON– compounds (CHON compounds detected in ESI–) and 1103–8400 of CHON+ compounds (CHON compounds detected in ESI+) were determined. The peak area of CHON– accounts for 40% in Mainz samples and it increases to 74%

for CHON+. On the contrary, the peak area fractions of CHON– in Beijing samples (53% in BJL and 48% in BJH) are higher compared to that for CHON+ (40% in BJL and 36% in BJH). This observation indicates that most CHON compounds in Mainz samples contain amino functional groups, which are prone to be protonated in ESI+ mode, while CHON compounds in Beijing samples contain more nitro groups, which are preferentially to be deprotonated in ESI- mode.

The CHON compounds are further classified into different subgroups based on the O/N ratios. Figure 2.3.4 shows the relative contribution of each subgroup to the sum of CHON peak intensities observed in ESI+ and ESI- mode. Compounds in the subgroups with O/N < 3 are preferentially detected in ESI+ mode, again likely due to the presence of reduced nitrogen containing functional groups (e.g. amines). Interestingly, in ESI+ mode, a large fraction (~40%) of CHON+ compounds have O/N ratio of 2 for samples from Mainz, while compounds with O/N ratio of 1 dominate (~55%) for samples from Beijing regardless of the pollution level. This is an indication that CHON+ compounds in Beijing OA contain more reduced nitrogen atoms, which could be produced from a minor pyrolytic and oxidative processing (e.g. smoldering burning) of N-heterocycle compounds (e.g. imidazole) (Lin et al., 2012a). The number-weighted averaged DBE for CHON+ compounds is 5.34 in Mainz samples, while higher averaged DBEs (6.71 in BJL and 7.15 in BJH) are observed in Beijing samples, indicating CHON+ compounds in Beijing OA are more unsaturated. This is further confirmed by the VK diagram in Figure S2.3.3, which shows that much more CHON+ compounds in Beijing samples are suggested to be low-oxygen-containing aromatic hydrocarbons in area B. And, the pie chat in Figure S2.3.3 shows that the fractions of aromatics and condensed aromatics in Beijing samples are about 1.25 times and 6 times higher, respectively, compared to Mainz samples. It indicates that reduced nitrogen- containing aromatic precursors have more influence on CHON+ compounds in Beijing than in Mainz. Another interesting subgroup of CHON compounds are those compounds with  $O/N \ge 3$ , which are preferentially observed in ESI- mode, likely associated with the nitrooxy (-ONO<sub>2</sub>) or oxygenated nitrooxy group (O/N  $\geq$  4). The majority of CHON- compounds has O/N ratio of 3 or 4, indicating that besides the nitrooxy group most CHON- compounds contain additionally not more than one oxidized group. This observation is confirmed by the modified VK diagram for CHON– compounds in Figure S2.3.4 (in which the VK diagram was constructed by plotting the H/C ratio versus the (O-3N)/C ratio instead of O/C ratio), showing a large number of CHON– compounds are observed with low (O-3N)/C ratio between 0 and 0.2. However, compared to the CHON- compounds in MZL and BJL samples dominating with O/N ratio of 3, the CHON– compounds in BJH samples are dominated with O/N ratio of 4, suggesting CHON- compounds undergo relatively higher oxidized process in polluted air. Consistent with the CHON+ compounds, the number-weighted averaged DBE (see Table 2.3.1)

and the fraction of aromatics of CHON– compounds (see Figure S2.3.4) in Beijing samples are higher than those in Mainz samples, indicating that nitrogen containing aromatics are more important precursors in Beijing OA, which agrees well with Wang et al.'s study (Wang et al., 2017) showing many nitrooxy-aromatic compounds (e.g., nitrophenol) with high abundance observed in the OA of Shanghai. It should be noted that only a small fraction of CHON compounds is observed in both ESI+ and ESI– modes (see overlapped bar in Figure 2.3.4). Actually this fraction of CHNO compounds could consist of amino acids, which contain both acidic (-COOH) and basic (-NH<sub>2</sub>) functional groups and which have been identified in biomass burning and fossil fuel combustion emissions (Mace, 2003;Barbaro et al., 2011).



Figure 2.3.4: Classification of CHON compounds into different subgroups according to O/N ratios in their molecules. The y-axis indicates the relative contribution of each subgroup to the sum of CHON compounds peak intentities observed in the ESI– and ESI+ modes, respectively.

## 2.3.4 CHN compounds

The CHN compounds can be detected only in ESI, which are very likely associated with nitrile and amine species (Lin et al., 2012a). The number-weighted averaged molecular weight of CHN compounds is the smallest in all subgroups. However, the number-weighted averaged DBE (5.93–8.16) of CHN compounds is the highest, indicating that this group of molecules is highly unsaturated. CHN compounds accounts for around 11% of the total peak abundance in Mainz sample, while it is more than three times higher in Beijing samples (35% in BJL and 39% in BJL), suggesting that CHN compounds have more important impact on Beijing OA compared to Mainz OA.

Figure 2.3.5 shows the Kendrick mass defect (KMD) diagram for the CHN compounds observed in Mainz and Beijing samples. The KMD diagram is commonly used to investigate the relationship among a large set of molecular formulas in the UHRMS study (Kendrick, 1963; Hughey et al., 2001; Lin et al., 2012a; Rincón et al., 2012). Here, we set the molar mass of CH<sub>2</sub> to exactly 14 u as the reference mass for calculating the Kendrick mass (KM) following Eq. (2.8) and the KMD is defined as the difference between the nominal mass and the KM as shown in Eq. (2.9).

$$KM(CH_2) = mass \times [mass CH_2]/mass CH_2$$
(2.8)

$$KMD(CH_2) = [mass] - KM(CH_2)$$
(2.9)

where brackets refer to the nominal mass obtained by rounding the mass to the nearest integer. When the KMD of a compound is plotted *vs.* its neutral molecular weight, homologous series of compounds differing only by CH<sub>2</sub> fall on horizontal lines and are clearly distinguishable. As can be seen in Figure 2.3.5, the majority of CHN compounds belong to members of several different homologous series. However, compared to the homologous series of CHN compounds in Mainz samples, the homologous series in Beijing samples often have a higher number of members with larger molecular weights. This could be explained by more primary biological aerosol particles with long chain aromatic amines or N-heterocycle compounds in Beijing atmosphere (Rincón et al., 2012; Jiang et al., 2014). The  $X_C$  values suggest that most CHN compounds are condensed aromatics ( $X_C \ge 2.7$ ) and aromatics ( $X_C \ge 2.5$ ). To facilitate the imagination of possible chemical species within Figure 2.3.5, the elemental composition, the DBE and a potential chemical structure for the first compound of three homologous series are also illustrated in the figure, representing a condensed aromatic species, an aromatic compound and a non-aromatic species. In previous MS/MS studies of CHN compounds (Simoneit et al., 2003; Laskin et al., 2009; Lin et al., 2012a),

these nitrogen containing aromatic compounds are suggested to be alkaloids with one or two nitrogen atoms embedded into five-membered (e.g., pyrazole, imidazole, and their derivatives) or six-membered rings (e.g., pyridazine and their derivatives), which are likely formed during biomass burning from dialkanoic acids and ammonia. It is worth noting that a significant number of CHN compounds with 12–23 DBE and 15–29 carbon atoms (those above the dash line in Figure 2.3.5) are exclusively present in Beijing samples. These compounds are assigned to polycyclic aromatic N-heterocycle hydrocarbons (PANH) with four or more aromatic rings, which are strong mutagens and potential human carcinogens. This result is consistent with a previous study in which several PANH with 4–8 aromatic rings were observed in ambient organic aerosol from Beijing (Jiang et al., 2014).



**Figure 2.3.5:** Kendrick mass defect diagram of CHN compounds detected in ESI+ mode. The colour bar denotes the aromaticity equivalent (gray with  $X_C < 2.50$ , purple with  $2.50 \le X_C < 2.70$  and red with  $X_C \ge 2.70$ ). The element composition, DBE and a potential chemical structure for the first compound (the black asterisk) of three homologous series are illustrated in the figure.

## 2.3.5 Sulfur compounds (CHOS and CHONS subgroups)

A large number of S-containing organic compounds have been observed in urban and rural OA (Tao et al., 2014; Jiang et al., 2016; Wang et al., 2016; Wang et al., 2017). In this study, 166-831 CHOS formulas were determined in ESI- mode. 86-93% of CHOS formulas are assigned to possess a molecular composition with O/S ratio  $\geq 4$ , suggesting they represent organosulfates (OSs), which is consistent with previous studies (Tao et al., 2014; Wang et al., 2016). The numberweighted average molecular weight of CHOS compounds in Beijing samples (250 Da in BJL and 280 Da in BJH) is larger than that (241 Da) in Mainz samples. In contrast, the number-weighted average DBE in Beijing samples (2.02 in BJL and 2.26 in BJH) is lower than that (2.51) in Mainz samples. Moreover, the DBE vs. carbon number diagram in Figure S2.3.5 shows that more CHOS compounds with low DBE and high carbon numbers were observed in Beijing samples, indicating that CHOS compounds with longer carbon chain and lower degree of unsaturation make an important contribution to Beijing OSs. This result is similar to a previous study (Tao et al., 2014), which revealed that the OSs in Shanghai have longer aliphatic carbon chains and lower degree of unsaturation than the OSs in Los Angeles. As observed in smog chamber studies(Riva et al., 2016), the OSs with high molecular weight and low degree of unsaturation can be formed from long-chain alkanes (e.g. dodecane) emitted from combustion sources. Besides the CHOS compounds, the other S-containing organics are assigned to be CHONS compounds, which are also prone to be measured in ESI- mode. The CHONS compounds account for around 22% of the total peak abundance in ESI- mode in the Mainz samples, while the fraction decreases to 5–7% in the samples from Beijing. The compound with the formula  $C_{10}H_{17}O_7NS$ , which has been identified as an  $\alpha$ -pinene-derived nitrooxy-OSs, shows the highest concentration in Mainz (see Figure 2.3.1), while its concentration is much smaller in Beijing, indicating the important role of monoterpene precursor on CHONS compounds in Mainz OA. In Mainz and BJL samples, 61–65% of detected CHONS- formulas have the O/(4S+3N) ratio  $\geq$  1, allowing their assignment to nitrooxy-OSs with both -OSO<sub>3</sub>H and -ONO<sub>2</sub> groups. However, in BJH samples, only 29% of the CHONS- formulas are suggested to be nitrooxy-Oss. To further understand the chemical properties of these CHONS compounds, MS/MS analysis should be performed in the future.

## 2.4 Conclusion and implication

In this study, we applied the UHPLC-Orbitrap MS for the analysis of the organic fraction of PM<sub>2.5</sub> samples from one European city Mainz and one Chinese city Beijing. Roughly 18000 organic

compounds were identified based on unambiguous elemental composition in the urban OA, while the number of organics in Beijing samples are around 2–10 times more than Mainz samples. The information of these organic compounds can enrich the database of the molecular composition of OA in urban regions. 61–92% of the detected organics have more than one isomer, indicating that the UHPLC separation is important for the OA characterization and suggested to be applied prior to the mass spectrometer for the identification or quantification of individual organic substances in the OA in future studies.

The chemical characteristics of OA in Mainz and Beijing shows clear differences. The organic species of CHO, CHON and CHN in Beijing OA have lower elemental H/C and O/C (except CHN) but higher DBE and Xc compared to Mainz OA, demonstrating that organics in Beijing OA are highly unsaturated. The Van Krevelen and KMD diagrams show that much more mono/poly aromatics were observed in Beijing OA, suggesting that they are combustion related compounds. The majority of CHOS compounds are suggested to be OSs, while OSs in the two cities have different molecular characteristics showing that many OS with low DBE and high carbon numbers were only detected in Beijing OA. Most CHONS compounds were observed in low concentrations in PM<sub>2.5</sub> (MZL and BJL). These elemental compositions can be assigned to represent mostly nitrooxy-OS. Only 29% of CHONS compounds collected during high PM<sub>2.5</sub> episodes (BJH) are suggested to be nitrooxy-OSs, point out the large differences in the chemical composition of CHONS compounds in the heavily and in the less polluted atmosphere. In future studies more detailed MS studies (e.g. MS/MS analysis) should be performed for a better understanding the molecular structures, sources or formation pathways of these compounds. As shown in this study, biogenic and anthropogenic precursors have a different influence on the Beijing OA and Mainz OA. Therefore, dedicated smog chamber experiments with mixtures of biogenic (e.g.  $\alpha$ -pinene) and anthropogenic (e.g. naphthalene) precursors might be conducted to better understand their influence on OA formation in urban regions.

#### **Supporting Information**

The description of the calibration standard solution for mass spectrometer, five supporting figures (Figure S2.3.1–S2.3.5).

#### Acknowledgements

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# 2.5 Additional information and results

This following results and information are not part of the actual manuscript, however are supporting the results discussed above.

# 2.5.1 Difference of chemical composition between ACN/H<sub>2</sub>O and H<sub>2</sub>O extraction method

In previous studies, pure water (H<sub>2</sub>O) were always used for the OA sample extraction with the following steps: Portions of OA filter samples were extracted using 2.5 mL pure water in an ultrasonic bath for 30 min two times, respectively. The extracts were filtered with a 0.2  $\mu$ m Teflon syringe filter and acidified to pH = 2 using HCl before performing a solid phase extraction (SPE) step. The filter extracts were then loaded on a SPE cartridge (Oasis HLB, 30  $\mu$ m, 60 mg per cartridge, Waters Corporation, Milford, MA) with the aim to remove inorganic ions, low molecular weight organic molecules and sugars. The loaded cartridge was subsequently rinsed two times with 1 mL pure water and then eluted with 1.5 mL of methanol containing 2% (w/w) ammonia. Immediately after eluting from the SPE column the extract was evaporated to dryness under a gentle stream of nitrogen. The residues were dissolved in 500  $\mu$ L acetonitrile and water (1/9, v/v) for LC-MS analysis.

Previous studies have shown the effect of the solvent on the characterization of OA (Bateman et al., 2008;Heaton et al., 2009;Tao et al., 2014). However, it is still not clear to what extent the extraction solvent affects the characterization of OA from different sources and mass loadings. Therefore, the PM<sub>2.5</sub> samples from Beijing and Mainz, representing high and low mass loading and different pollution sources, were extracted with ACN/H<sub>2</sub>O (A/W) and H<sub>2</sub>O (W), respectively. Figure 2.5.1 shows the number of individually assigned molecular formulas in Mainz and Beijing samples. As can be seen in the figure the number of organic compounds observed in the Beijing samples are 2–10 times higher than in the Mainz samples. However, large solvent-dependent differences are observed for ESI+ and ESI–. While the number of compounds extracted with ACN/H<sub>2</sub>O (A/W–) is similar to those extracted with pure H<sub>2</sub>O (W–) for ESI– analysis, much more organic compounds are observed with ESI+ analysis when ACN/H<sub>2</sub>O (A/W+) is used for extraction

compared to pure  $H_2O$  (W+). A plausible explanation for this observation is that most of organics detected in the ESI- contain carboxylic acid functional groups, which enhance the water solubility of the compounds. A more detailed analysis compares the overlapping percentage of number and intensity of compounds observed in ESI+ and ESI– using the two extraction methods (see Table 2.5.1). For example, in ESI– mode 72% of compounds observed in the H<sub>2</sub>O extracts are also observed in ACN/H<sub>2</sub>O extracts, while only 56% of compounds observed in the ACN/H<sub>2</sub>O extracts are obtained in H<sub>2</sub>O extracts. Meanwhile, 90% of the total peak intensity from the H<sub>2</sub>O extracts matches the peak intensity from the ACN/H<sub>2</sub>O extracts, while only 75% of the total peak intensity from the ACN/H<sub>2</sub>O extracts, in the H<sub>2</sub>O extracts. It is clear that a majority of organics observed in the H<sub>2</sub>O extracts can also be measured in the ACN/H<sub>2</sub>O can extract more organic compounds which are not found in the H<sub>2</sub>O extracts. In summary, the results demonstrate that ACN/H<sub>2</sub>O is superior to H<sub>2</sub>O for the extraction of organics in OA.



Figure 2.5.1: The number of individually assigned molecular formulas observed in ACN/H<sub>2</sub>O and H<sub>2</sub>O methods in Mainz and Beijing samples. Each subgroup is marked by the different colors.

Sample ID	Method	Number of the overlapped molecular formulas (%)		Intensity of the overlapped formulas (%)		
		ESI-	ESI+	ESI-	ESI+	
	ACN-H <sub>2</sub> O	56	20	75	32	
MZL	H <sub>2</sub> O	72	60	90	65	
	ACN-H <sub>2</sub> O	70	46	92	78	
BJL	H <sub>2</sub> O	70	68	95	92	
BJH	ACN-H <sub>2</sub> O	59	43	91	80	
	H <sub>2</sub> O	60	70	95	94	

 Table 2.5.1: The overlapping percentage of number and intensity of compounds extracted in the two

 extraction methods

# **3** The maximum carbonyl ratio as a metric for the structural classification of OA

This chapter is a reprint of the article:

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The maximum carbonyl ratio (MCR) as a new index for the structural classification of secondary organic aerosol components

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Abstract. Organic aerosols (OA) account for a large fraction of atmospheric fine particulate matter and thus are affecting climate and public health. Elucidation of the chemical composition of OA is the key for addressing the role of ambient fine particles at the atmosphere-biosphere interface and mass spectrometry is the main method to achieve this goal. High resolution mass spectrometry (HRMS) is on its way to become one of the most prominent techniques, also for the analysis of atmospheric aerosols. The combination of high mass resolution and accurate mass determination allows the elemental composition of numerous compounds to be easily elucidated. Here a new parameter for the improved classification of OA is introduced - the maximum carbonyl ratio (MCR) - which is directly derived from the molecular composition and is particularly suitable for the identification and characterization of secondary organic aerosols (SOA). The concept is exemplified by the analysis of ambient OA samples from two measurement sites (Hyytiälä, Finland; Beijing, China) and of laboratory-generated SOA based on ultrahigh performance liquid chromatography (UHPLC) coupled to Orbitrap MS. To interpret the results, MCR-Van Krevelen (VK) diagrams are generated for the different OA samples and the individual compounds are categorized into specific areas of the diagrams. The results show that the MCR index is a valuable parameter for representing atmospheric SOA components in composition and structure-dependent visualization tools such as VK diagrams. Therefore, the MCR index is suggested as a tool for a better characterization of the sources and the processing of atmospheric OA components based on HRMS data. Since the MCR contains information on the concentration of highly electrophilic organic compounds in particulate matter (PM) as well as on the concentration of organic (hydro)peroxides, the MCR could be a promising metric for identifying health-related particulate matter parameters by HRMS.

# **3.1 Introduction**

Organic aerosols (OA) account for a large fraction (20–90%) of submicron particulate mass in the atmosphere with consequences for climate and public health (Pöschl, 2005; Jimenez et al., 2009; Hallquist et al., 2009; Kroll et al., 2011; Pöschl and Shiraiwa, 2015). Atmospheric OA, including primary organic aerosol particles emitted directly from sources and secondary organic aerosol (SOA) formed by oxidation of precursors in the atmosphere, originate from a wide variety of biogenic (e.g., terrestrial vegetation) and anthropogenic (e.g., biomass burning and fossil fuel combustion) sources (Seinfeld and Pandis, 2016). Due to their diverse sources, various formation

pathways and complex multiphase aging processes, the OA fraction is composed of thousands of different compounds, which contain various functional groups including hydroxyl, hydroperoxide, carbonyl and carboxyl groups but also sulfur and nitrogen containing functional groups (organic nitrates and sulfates). The vast number of individual compounds not only results in a wide range of physical, chemical and toxicological properties and complicates the OA characterization, this complexity in combination with sophisticated mass spectrometric instrumentation also offers the possibility to decipher OA sources, formation pathways and their fate in the atmosphere (Lin et al., 2012; Kourtchev et al., 2016; Glasius et al., 2016; Wang et al., 2018; Glasius et al., 2018; Daellenbach et al., 2019; Yee et al., 2020). Thus, it is essential to develop highly efficient analytical techniques to gather detailed, compound-specific chemical information.

In the last decade, analytical methods based on high-resolution mass spectrometry (HRMS), such as Fourier transform ion cyclotron (FTICR) and Orbitrap MS, in combination with soft ionization techniques, including atmospheric pressure chemical ionization (APCI) and electrospray ionization (ESI) have been successfully applied to OA research (Lin et al., 2012; Nozière et al., 2015; Kourtchev et al., 2016; Glasius et al., 2016; Song et al., 2018; Laskin, et al., 2018; Wang et al., 2018; Glasius et al., 2018). HRMS benefits from two outstanding features, high mass spectrometric resolution (> 40,000) and high mass accuracy (< 5 ppm). As a consequence, HRMS allows the assignment of unique elemental compositions and enables the calculation of the molecular formulae for the analytes of interest even in highly complex samples, often hundreds or thousands of compounds. However, accompanying the complexity and size of the datasets, new needs and challenges arise concerning the interpretation and visualization of the HRMS results. Consequently, visualization tools like Van Krevelen (VK) diagrams (Kim et al., 2003; Sleighter et al., 2007; Hockaday et al., 2009), Kendrick mass defect (KMD) analysis (Kendrick et al., 1963; Hughey et al., 2001) and carbon oxidation state (OSc) plots (Kroll et al., 2011; Wang et al., 2018) were developed. Most often VK diagrams are applied, which place every assigned unique chemical formula on a 2D scatterplot of H/C ratio versus O/C ratio, to sort and group the organic compounds identified by the HR mass spectra.

One obvious chemical feature which directly results from the elemental composition of the analytes is their degree of unsaturation (DU) or double bond equivalents (DBE). The DBE represents the sum of the number of double bonds and rings in a molecule and is a well established and helpful tool in mass spectrometry (Barrow et al., 2009; Yassine et al., 2014). However, a limitation of this metric is that the DBE cannot distinguish C-C double bonds from C-O/C-S double bonds when divalent atoms (e.g., O and S) are present in the molecules. By definition of the DBE the divalent oxygen does not influence the DBE value, although obviously oxygen can also

contribute to double bonds of organic molecules. Therefore, aiming towards a better structural characterization of complex organic mixtures, the aromaticity index (AI) (Koch and Dittmar, 2016) and aromaticity equivalent (Xc) (Yassine et al., 2014) have been introduced in recent years. The advantage of AI and Xc over the simple use of DBE is that they also consider heteroatoms (O, S, N) as contributors to the degree of unsaturation and that they define threshold values to quantify the aromaticity of the organic molecules. As a consequence, parameters such as AI or Xc are beneficial for the characterization of aromatic/condensed aromatic compounds. However, for the characterization of chemical structures of typical ambient SOA compounds, AI or Xc are less appropriate. First of all, the majority of typical SOA components rarely contain aromatic structures, since the main gaseous SOA precursors are non-aromatic compounds (Hallquist et al., 2009). Moreover, even when aromatic VOCs serve as SOA precursors, which can be expected in mostly anthropogenically influenced areas, their aromaticity is frequently lost during the initial oxidation steps, i.e., due to the dominant OH addition to the aromatic ring followed by rapid further oxidation steps (Ziemann and Atkinson, 2012). Actually, also other structural elements influencing the DBE of SOA precursor molecules, such as C-C multiple bonds or carbon ring structures, are prone to be lost in the process of SOA formation. This is especially true for C-C double bounds, which represent the main chemical feature of biogenic VOCs (e.g., isoprene, monoterpenes, sesquiterpenes), which in turn are the most important SOA precursors on the global scale. The double bonds are preferentially attacked by atmospheric oxidants (OH, ozone, nitrate radicals), hence tend to disappear prior to the gas-to-particle conversion of the products. Less obvious but with the same tendency behave cyclic compounds, for which ring-opening pathways yield especially low-volatile oxidation products that finally make a notable contribution to the particle phase. Therefore, in the process of SOA formation most structural elements (C=C and rings) which usually contribute to a carbon related degree of unsaturation in organic matter disappear and are replaced by unsaturation connected with the introduced oxygen containing functionalities.

In principle, SOA components contain oxygen atoms in the form of hydroxyl (OH), hydroperoxide (OOH) or peroxide (-OO-), carbonyl (C=O), carboxyl (COOH) and epoxide groups (Nozière et al., 2015). Obviously, the carbonyl group, in the form of an aldehyde, ketone or carboxyl group as well as the epoxide group can contribute to the degree of unsaturation. In contrast, in the absence of unsaturation of a specific SOA compound (oxygen is always present in SOA) alcohol or peroxide functionalities must be present. In the context of SOA chemistry especially the latter functionality has created pronounced scientific interest, since highly oxidized multifunctional organic compounds (HOMs) are supposed to be multifunctional hydroperoxides formed via autooxidation (Bianchi et al., 2019). Due to their low vapour pressure, HOMs are able to contribute

to the formation of new particles in the atmosphere and thus, via their function as cloud condensation nuclei, ultimately have a major impact on the atmospheric radiation balance (Carslaw et al., 2017). However, peroxide functionalities may also play an important role in health-related effects of SOA, since organic (hydro)peroxides are thought to contribute to the formation of reactive oxygen species (ROS) by transporting oxidants on/in particles into the respiratory system (Verma et al., 2015; Tong et al., 2018).

It is noteworthy to point out that the degree of unsaturation as discussed above results in distinct chemical properties. For example, both carbonyls and epoxides possess a high electrophilic reactivity. The polarized double bond in carbonyls and even more pronounced the 3-membered ring in epoxides induce a high reactivity towards nucleophilic addition reactions. This reactivity enables the formation of covalent bonds between the electrophile (carbonyl/epoxide carbon) and a nucleophilic partner molecule (alcohols, other carbonyls, amines). On the one hand, this reactivity is directly relevant for atmospheric heterogeneous/multiphase chemistry and the formation of higher molecular weight compounds in SOA. In other words, higher concentrations of carbonyls/epoxides cause a higher potential for condensed phase chemistry and the formation of oligomers by homogeneous aging (Rudich et al., 2007). In contrast, low carbonyl/epoxide content together with the presence of high molecular weight compounds could indicate that condensed phase chemistry already happend (homogeneously aged SOA). On the other hand, and probably diagnostically more valuable, represents the high electrophilic reactivity of the oxygen-related degree of unsaturation a chemical feature that determines the biochemical behavior towards bioactive sites. The majority of biological macromolecules (nucleic acids, proteins) are nucleophilic. For example, in proteins, accessible thiol and primary amino groups constitute strongly nucleophilic centers. Chemical modification of these nucleophilic sites often alters or decreases protein function, resulting in cytotoxicity (Zimniak, 2011). Therefore, a measure of the presence of carbonyls/epoxides in aerosol particles might assist in the prediction of electrophilic stress induced by airborne particle-bound chemicals. Otherwise, oxygen-rich organics in SOA with no or a low contribution of carbonyls/epoxides functionalities suggests that the oxygen is present as peroxides, in this case potentially increasing oxidative stress and causing disruptions in normal mechanisms of cellular signaling leading to many pathophysiological conditions. Since the awareness of health effects of particulate matter is increasing, knowledge about the potential carbonyl/epoxide contribution or its absence could help to understand physiological impacts of atmospheric particulate matter (Schwöbel et al., 2011).

For the above-mentioned reasons, we suggest a new metric – the maximum carbonyl ratio (MCR) –, which describes the maximal contribution of carbonyl/epoxide functionalities in

individual molecules composing organic aerosols, that can be directly derived from HRMS datasets. It should be clearly noted here that the proposed MCR is meant as a metric for the interpretation of mass spectrometry data sets in which hundreds to thousands of compounds are identified. Similar to other metrics that have been successfully used in the interpretation of HRMS data (e.g., DBE, AI), a calculated MCR value of a single molecular formula is not unequivocal evidence of the presence of carbonyl functionalities. Applied to a variety of compounds, however, the presented metric can be useful to visualize and interpret results on the chemical composition of complex, oxygen-rich multifunctional mixtures such as atmospheric SOA. Actually, based on the discussion above the suggested metric should be named 'maximum carbonyl/epoxide ratio'. However, it is generally assumed that the contribution of epoxides to SOA is low (Atkinson et al., 1991; Ji et al., 2017) and therefore most of the degree of unsaturation introduced by oxygen functionalities in connection with SOA formation can be expected to result from carbonyl groups. Consequently, from now on just the expressions 'carbonyls' or 'carbonyl ratio' are used for convenience instead of 'carbonyl/epoxide' when we refer to the degree of unsaturation by oxygen functionalities. Nevertheless, atmospheric chemical interest in epoxy chemistry has recently increased considerably, especially in connection with isoprene chemistry and the formation of organosulfates (Paulot et al., 2009; Shrivastava et al., 2019). But also the very high electrophilicity of epoxides and thus their high toxic potency, means that the contribution of epoxides to the MCR value should not be ignored. The purpose of this paper is to introduce MCR as a new metric for the analysis of HRMS data and to present it in combination with Van Krevelen diagrams as a visualization tool (MCR-VK diagrams) to achieve a better categorization of complex ambient OA samples. The validation and applicability of the MCR-VK diagram are tested by applying the concept to selected samples of ambient organic aerosols and a few samples from laboratory-generated SOA.

# 3.2 Material and methods

#### 3.2.1 Laboratory SOA generation and collection

SOA was formed from the ozonolysis and photooxidation of selected volatile organic compounds (VOC) in a 7 L quartz flow tube (Tong et al., 2016). Ozonolysis was performed by mixing  $\alpha$ -pinene in the flow tube with ozone. The concentrations of the SOA precursor were adjusted in the range between 400 and 700 ppb and the O<sub>3</sub> concentration between 980 and 1100 ppb. Isoprene SOA was generated in a 33 L smog chamber through gas phase photo-oxidation of
the SOA precursor. The isoprene concentration was adjusted in the range between 300 and 500 ppb and the concentration of OH radicals during the experiments was estimated to be  $\sim 5.2 \times 10^{11}$  cm<sup>-3</sup>. A Scanning Mobility Particle Sizer (SMPS, GRIMM Aerosol Technik GmbH & Co. KG) was used to measure the number and size distribution of the formed SOA particles. SOA was collected on 47 mm Omnipore Teflon filters (100 nm pore size, Merck Chemicals GmbH).

#### 3.2.2 Ambient PM sampling

The 24-hour integrated PM samples were collected at the SMEAR II station in Hyytiälä, a boreal forest monitoring station in Finland, and at a central urban site in Beijing (China). A three-stage Dekati PM<sub>10</sub> impactor (Pallflex Tissuquartz 2500QAT-UP) was used for the boreal forest samples collected from 17-19 July 2017. The sampling flow rate through the sampler was set to 35 L min<sup>-1</sup>. The fine particle mode (< 2.5  $\mu$ m) were collected on Teflon filters (PALL, 47 mm diameter). The samples from Beijing were collected from January 7 to 9, 2014 on prebaked quartz fiber filters (8×10 inches) using a large volume sampler (Tisch, Cleveland, OH, USA) at a flow rate of 1050 L min<sup>-1</sup>. All filters were stored in glass vials at - 20 °C or -80 °C until analysis.

### 3.2.3 Sample preparation and UHRMS analysis

The analysis of the filter samples was carried out at the Johannes Gutenberg University in Mainz. Parts of the filters were extracted twice with 1.5 mL methanol in an ultrasonic bath for 30 min. After insoluble particles had been removed by a 0.2  $\mu$ m Teflon filter, the extracts were evaporated to dryness under a gentle nitrogen stream. Finally, the extracts were dissolved with a variable volume of an acetonitrile-water mixture (1/9, v/v) to adjust the particle mass concentration between 150 and 400  $\mu$ g/mL.

The filter extract solution was then analyzed by an ultrahigh performance liquid chromatography (UHPLC) system (Dionex UltiMate 3000, Thermo Scientific, Germany) coupled to a Q Exactive Hybride-Quadrupole-Orbitrap mass spectrometer (Thermo Scientific, Germany) (HPLC-Orbitrap MS). The detailed description of the UHPLC-Orbitrap MS method can be found in a previous study (Wang et al., 2018). In brief, analytes were separated using a Hypersil Gold column (C18, 50 x 2.0 mm, 1.9  $\mu$ m particle size, Thermo Scientific, Germany) with the mobile phase consisting of (A) ultrapure water with 2% acetonitrile and 0.04% formic acid and (B) acetonitrile with 2% ultrapure water. The gradient elution was performed by the A/B mixture at a

total flow rate of 500  $\mu$ L/min as follows: 0–1.5 min 2% B, 1.5–2.5 min from 2% to 20% B, 2.5– 5.5 min 20% B, 5.5–6.5 min from 20% to 30% B, 6.5–7.5 min from 30% to 50% B, 7.5–8.5 min from 50% to 98% B, 8.5–11.0 min 98% B, 11.0–11.05 min from 98% to 2% B, 11.05–11.1 min 2% B. The Q Exactive Orbitrap MS was equipped with a heated ESI source at 120 °C, using a spray voltage of –3.3 Kv for the negative ion mode. The mass resolution power was 70000 at *m*/*z* 200 and the mass scanning range was set to *m*/*z* 80–500.

#### 3.2.4 Data processing

The data obtained from UHPLC-Orbitrap MS were analyzed by an open-source software for mass spectrometry data processing with the main focus on LC-MS data (MZmine 2.37). The detailed processing steps and parameters in the software are shown in the supporting information (Table S3.2.1). The output of MZmine data includes m/z ratios, formulas, retention times and peak areas of detected organic compounds. Molecular formulas were expressed as  $C_CH_HO_0N_NS_5$ , where c, H, o, N, and s correspond to the numbers of carbon, hydrogen, oxygen, nitrogen and sulfur atoms in the molecular formula. To remove chemically unreasonable formulae, identified assignments were constraint by setting H/C, O/C, N/C and S/C ratios in the ranges of 0.3–3, 0–3, 0–1.3 and 0–0.8, respectively (Wang et al., 2018).

## 3.3 Results and discussion

#### 3.3.1 Definition of maximum carbonyl ratio (MCR)

It is recognized that the structral characteristics of organic molecules in aerosols are essential for the evaluation of their behaviour and their environmental interactions, i.e., chemical reactivity, vapour pressure, interaction with water or biological activity. A central metric, which can be directly calculated from the elemental composition, is the number of double bonds in a molecule (double-bond equivalent (DBE) also named degree of unsaturation). The DBE is calculated assuming that all atoms obey the octet rule (except for hydrogen) and that the degree of unsaturation is caused by covalent bonds between carbons. For  $C_CH_HO_ON_NS_S$  compounds the DBE can than be expressed as equation 3.1:

$$DBE = 1 + C - 0.5H + 0.5N \tag{3.1}$$

Based on this definition, the DBE describes the number of C-C multiple bonds plus rings in a molecule and is a well-established metric to assess the degree of unsaturation of molecules obtained by mass spectrometry. By its definition the DBE is thus independent of the number of O and S atoms, which results in a potential overestimation of the number of C-C double/triple bonds in O/S-containing molecules. Therefore, the aromaticity index (AI) (Koch and Dittmar, 2016) and the aromaticity equivalent (Xc) (Yassine et al., 2014) for  $C_CH_HO_ON_NS_S$  compounds were introduced, which also consider the influence of O and S on the degree of unsaturation:

$$AI = \frac{DBE_{AI}}{C_{AI}} = \frac{1 + C - O - S - 0.5H}{C - O - S - N}$$
(3.2)

$$X_{C} = \frac{3[DBE - (m0 + nS)] - 2}{DBE - (m0 + nS)}$$
(3.3)

where *m* and *n* are the fraction of oxygen atoms and sulfur atoms involved in  $\pi$ -bond structure of the compound, respectively.

The AI reflects the C-C double bond density in a molecule including the possibility that heteroatoms can also form double bonds, the Xc further refines this concept by making it independent from the degree of alkylation. In principle, both indices are minimum criteria for the presence of aromatics and condensed aromatics in the sample material by correcting the DBE assuming contributions from heteroatom  $\pi$ -bond structures, such as C=O or S=O containing functionalities. Both parameters are succesfully used for the characterization of natural organic matter (NOM) or mineral oils and have been proved to represent a step towards structural identification of complex organic mixtures. The concept presented here follows a similar approach, but now by estimating a maximum criterion for the presence of carbonyl functionalities. This is done first for pure CHO compounds, often the largest group of organic compounds in atmospheric aerosol particles. A simple distinction of the cases is the basis for the MCR definition. When the number of oxygen atoms *O* in a C<sub>*c*</sub>H<sub>*H*</sub>O<sub>*o*</sub> compound is larger or equals the DBE of this compound ( $O \ge DBE$ ), then the MCR is calculated as:

$$MCR = \frac{DBE}{O}$$
(3.4)

or in other words, it is assumed that in case unsaturation is observed, all oxygen atoms contribute to it (i.e., the molecule's unsaturation is only contributed by oxygen atoms by forming the carbonyl group and all oxygen atoms are part of a C=O functionality). For example, for  $C_2H_2O_2$  (DBE = 2) MCR is 1 (e.g. glyoxal), for  $C_2H_4O_2$  (DBE = 1) MCR is 0.5 (e.g. glycolaldehyde) and for  $C_2H_6O_2$  (DBE = 0) MCR is zero (e.g. glycol). If the number of oxygen atoms in the molecule is smaller than its DBE value (O < DBE), then MCR is considered to equal one (i.e., all oxygen atoms contribute to the DBE), again the maximum criteria for the presence of carbonyl functionalities. In this case all of oxygen atoms are assumed in the form of carbonyl group (e.g., aldehydes or ketones). Thus, MCR is a metric to predict the possible maximum of carbonyl groups in the molecules.

#### 3.3.2 MCR-VK diagram

Motivated by the capabilities of HRMS in combination with soft ionization techniques to observe protonated or deprotonated molecular ions and directly assign thousands of elemental compositions, a useful concept was recently introduced which is named the "compositional space of molecules" (Herkorn et al., 2007). It represents the isomer-filtered complement of the entire space of molecular structures based on a given elemental composition, e.g.  $C_CH_HO_O$ . The compositional space is defined by the laws of chemical binding and is typically restricted to a certain mass range. This concept was also used here to relate the variety of observed organic aerosol components to all possible CHO compounds within the framework of VK diagrams. Consequently, an artificial dataset was constructed which comprise all theoretical  $C_CH_HO_O$  molecular formulae for CHO compounds with up to 15 carbon atoms. To further explore the resulting chemical space the MCR values of all individual compound were calculated as described above.

In Figure 3.3.1, the dots represent the C,H,O-compositional space of molecules within the molecular H/C range between 0–2.5 and O/C range between 0 and 1.2. The different gray scale colours relate to defined MCR ranges based on the theoretically possible functionalities of the underlying chemical components. The white dots represent all compounds in the MCR range between 0 and 0.2 and include compounds without any carbonyl functionality (MCR = 0), i.e., completely saturated compounds, up to compounds in which 20% of the oxygen atoms can be present in a carbonyl functionality. Aiming on a practicable categorization system we introduce three threshold lines (A, B, C; see Figure 3.3.1). Compounds between line A and line B possess MCR values in the range 0.2–0.5, compounds between line B and line C have MCR values in the range 0.5–0.9, and compounds below line C values in the range 0.9–1.0. This means that, for example, compounds located above line A either contain no carbonyl functionalilties or a maximum of 20% of the oxygen atoms can be carbonyl oxygen (C=O), the majority (80–100%) of the oxygens within these compounds has to be single-bounded hydroxyl (R-OH), hydroperoxy (R-OOH), ether (R-O-R) or peroxy oxygen (R-OOR). In contrast, in compounds appearing below line C in the VK diagram, 90 % of the unsaturation can be present in the form of carbonylic oxygen. As in the case

of AI and Xc, one cannot read a certain chemical functionality from the position of a dot (e.g., number of carbonyl O or number of aromatic rings), the MCR parameter is simply a limit value consideration to better structure the VK diagram in a region that is not covered by AI or Xc.



Figure 3.3.1: The MCR-VK diagram of all possible CHO subgroups with up to 15 carbon numbers. The different colors indicate the value of maximum carbonyl ratio (MCR). The dashed lines (A, B and C) represent different boundaries for a practicable categorization of SOA CHO compounds.

To get an idea about potential candidates contributing to the different areas in the MCR-VK diagram, lines A, B and C shown in Figure 3.3.1 are also depicted in Figure 3.3.2, where selected typical SOA precursors and SOA compounds are shown (Ramdahl, 1989; Myoseon, 1997; Matthew and Fraser, 2000; Edney et al., 2005; Kenneth et al., 2005; Henze and Seinfeld, 2006; Jaoui et el., 2007; Sakulyanontvittaya et al., 2008; Fu et al., 2009; Kautzman et al., 2010; Surratt et al., 2010; Ding et al., 2011; Borrás and Tortajada-Genaro, 2012; Ehn et al., 2012; Ehn et al., 2014; Kristensen et al., 2014; Nguyen et al., 2014; Yu et al., 2014; Shen et al., 2015; Zhang et al., 2015; González et al., 2016; Kurten et al., 2016; Utieyin, 2016; Tu et al., 2016; Al-Naiema and Stone, 2017; Martinsson et al., 2017; Pecha, 2017; Yee et al., 2018; Zhu et al., 2018). The molecular formulas, structures, DBE values, MCR values and suggested precursors of the selected marker molecules are listed in Table S3.3.1 in the supporting information. SOA compounds formed from gas phase chemistry are colored in blue, compounds which are known to be formed from condensed

phase chemistry are represented in purple, while a selection of marker compounds related to combustion processes are yellow-colored and a selection of SOA precursors are colored in grey. The biogenic SOA markers generated from gas phase chemistry are further divided based on their origin from isoprene (light blue), monoterpene (MT, blue) or sesquiterpene (SQT, dark blue) oxidation. The shape of the data points indicates whether the specific marker is mainly biogenic (circles), anthropogenic (triangle) or from mixed sources (square).



Figure 3.3.2: MCR-VK diagram of well-known organic marker compounds, which are defined as different colors and shapes according to their source and functionality. MCR-VK diagram was divided into five areas: I for very highly oxidized organic compounds (VHOOCs), II for highly oxidized organic compounds (HOOCs), III for intermediately oxidized organic compounds (IOOCs), IV for oxidized unsaturated organic compounds (OUOCs) and V for highly unsaturated organic compounds (HUOCs).

Although definitely the data points scatter within the MCR-VK diagram, a certain structure is visible. Most of the typical SOA compounds are located in the areas I, II and III, defined by the MCR as explained above. For example, isoprene particle phase oxidation products show up in area I, which generally includes products from the oxidation of smaller VOCs. Several MT and SQT first generation products (e.g. pinic acid) are located in area III, while higher generation oxidation products, such as 3-methyl-1,2,3-butanetricarboxylic acid (MBTCA) or highly oxygenated organic molecules (HOMs), which are formed by multiple oxidation steps, are preferentially located in area II (Yasmeen et al., 2012; Wang et al., 2017; Wang et al., 2018). These observations can be

explained by the well-known gas/particle partitioning behaviour of the products: Smaller VOC precursors, such as the  $C_5$  hydrocarbon isoprene, have to undergo multiple oxidation steps and the introduction of more oxygen-containing functionalities before the vapour pressure of the products enables them to partition into the particle phase. Several of the atmospheric gas phase oxidation mechanisms not only introduce oxygen (shifting the molecules to the right along the x-axis in the VK diagram) and use up unsaturation of C-C double bonds or cyclic structures, but also introduce hydrogen (reaction with HO<sub>2</sub>, hydrolysis), shifting the products up in the VK diagram. However, when the SOA precursors are larger VOCs, exemplified here by MT or SQT derived SOA, the products will partition into the particle phase much earlier, i.e., not necessarily have to undergo multiple oxidation steps before they enter the particle phase. Nevertheless, a certain degree of chemical aging still proceeds, shifting these products from area III into area II. To name the described areas more specifically, we characterize them as very highly oxidized organic compounds (VHOOCs) (area I), highly oxidized organic compounds (HOOCs) (area II) and intermediately oxidized organic compounds (IOOCs) (area III). In addition, according to the degree of unsaturation and oxygen content, the MCR-VK diagram in Figure 3.3.2 is further differentiated into the areas IV and V. Within area IV, named oxidized unsaturated organic compounds (OUOCs), primarily released aromatic OA components and oxidation products from aromatic VOCs are located, compounds which still contain aromatic ring structures. Finally, in area V condensed aromatic structures are showing up, including polycyclic aromatic hydrocarbons (PAHs) or oxygen containing PAHs, defined here as highly unsaturated organic compounds (HUOCs). In this region most of the oxygen atoms are suggested to be present in the form of carbonyl oxygen. These combustion-related compounds are able to explain the observed very low H/C ratios. Another group of compounds which might contribute to area V are products from aqueous phase chemistry for example of phenolic compounds or glyoxal heterogeneous chemistry (Sun et al., 2011; Yu et al., 2014). However, there is no doubt that the MCR value loses meaningfulness in regions IV and V, but here the use of the aromatic indices AI and Xc already introduced above helps to further categorise the CHO compounds localised in these areas (see Figure 3.3.3).

#### 3.3.3 MCR-VK diagram application on aerosol samples

To test the usefulness or limitations of the proposed MCR concept and MCR-VK diagrams in the analysis of complex atmospheric aerosol samples we analysed the chemical composition of SOA samples from both laboratory experiments and field measurements. The chemical composition of the samples was measured by UHPLC combined with ESI Orbitrap MS as described above.

The MCR-VK diagrams from samples of laboratory  $\alpha$ -pinene and isoprene SOA, as well as of field samples from Hyytiälä and Beijng are shown in Figure 3.3.3. It should be noted that in Figure 3.3.3 only compounds consisting of carbon, hydrogen and oxygen atoms (CHO compounds) are presented. The size of the dots in Figure 3.3.3 are logarithmically scaled by the fourth root of peak area of the respective CHO compounds and the colours are selected based on the Xc value (with 0  $\leq$  Xc < 2.5 (grey), 2.5  $\leq$  Xc < 2.7143 (purple) and Xc  $\geq$  2.7143 (red), background colors of areas of I–V are the same as in Figure 3.3.2).



Figure 3.3.3: MCR-VK diagrams of α-pinene ozonolysis SOA (a), isoprene photo-oxidation SOA (b), Hyytiälä OA (c) and Beijing OA (d). The size of the bubbles indicates the fourth root of the intensity of each compound and the colors correspond to the Xc value. The blue dot in (a) shows the results of Claflin et al. 2018, who studied functional group composition of SOA formed from ozonolysis of α-pinene under similar experimental conditions.

Figure 3.3.3a shows particle phase  $\alpha$ -pinene SOA composition depicted in the MCR-VK diagram. The largest fraction (53%) of  $\alpha$ -pinene SOA components is located in area III, while only a few compounds show up in area I. This observation indicates that most SOA products from ozone-oxidation of  $\alpha$ -pinene are carbonyl oxygen-containing compounds with MCR value of 0.5–0.9 and

only a few of them are pure hydroxyl or peroxide oxygen containing compounds with MCR values between 0–0.2. Since these laboratory flow tube experiments allowed only a low level of further oxidation processes, the aerosol consists mainly of first-generation oxidation products of the monoterpene. The blue dot in Figure 3.3.3a is taken from a study by Claflin et al. (2018) in which a combination of derivatization and spectrophotometric methods were used to quantify peroxide, carbonyl, carboxyl, ester, and hydroxyl groups to examine the  $\alpha$ -pinene/ozone SOA composition, actually under similar experimental conditions. Although completely different analytical methods were used and, of course, only one data point is available on the total composition, the results of the Claflin et al. study are not only roughly in the centre of the data shown here (they report average O/C an H/C ratios), but the [carbonyl-O] to [total-O] ratio of 0.56 calculated by Claflin et al. also fits well with the MCR concept as presented here (Claflin et al., 2018). Figure 3.3.3b shows MCR-VK diagram of SOA products from isoprene reacted with OH radicals. As can be seen in the figure, the distribution of products generated from  $\alpha$ -pinene and isoprene to areas of I-V are quite different. Isoprene SOA products span over a considerably larger region of the MCR-VK diagram than the  $\alpha$ -pinene SOA products. Most isoprene SOA products (40%) show up in area I, clearly demonstrating that these compounds are VHOOCs with a very low MCR value (0-0.2) and that the majority of oxygen functionalities are presented in the form of non-carbonyl groups (e.g., OH and OOH). This observation agrees well with the fact that a large amount of diols, tetrols and hydroperoxides were identified in isoprene-derived SOA in previous studies (Carlton et al., 2009). Figure 3.3.3c and 3.3.3d show MCR-VK diagrams for ambient aerosol samples. Figure 3.3.3c, which shows the results of the LC-MS analysis of aerosol field samples from Hyytiälä, indicates a similar aerosol composition as in the case of  $\alpha$ -pinene SOA (Figure 3.3.3a). The largest fraction (40%) of the compounds are located in area III, followed by areas of II (26%), I (21%), IV (11%) and V (2%). The observed similarity can be explained by the fact that at this measurement site monoterpenes are the primary source of SOA and  $\alpha$ -pinene is one of the most important individual monoterpene released at this site. Also previous studies have shown that the photo-oxidation and ozonolysis of biogenic VOCs contribute to the major fraction of aerosol components in Hyytiälä (Cavalli et al., 2006; Lee et al., 2006; Kourchev et al., 2013). However, compared to the laboratory  $\alpha$ -pinene SOA shown in Figure 3.3.3a, significantly more particle phase products in areas of I and II were observed, indicating that the particles in the ambient atmosphere experienced more intensive oxidation processes and oxidative ageing compared to laboratory  $\alpha$ -pinene SOA. Finally, Figure 3.3.3d shows the application of MCR-VK diagram on the Beijing aerosol samples, certainly a location with very different atmospheric conditions compared to the boreal forest station. The majority of Beijing particle phase compounds are located in the highly unsaturated and less

oxidized region of the MCR-VK diagram, i.e., areas of IV (30%) and V (26%). As already discussed above, the indication of the presence of are OUOCs (IV) and HUOCs (V), which mostly contain aromatic structures with low degree of oxidation, are probably related to combustion processes (Wang et al., 2018). The numeric comparison yield, 20%, 9% and 15% of Beijing aerosol products are located in areas of I (VHOOCs), II (HOOCs) and III (IOOCs), respectively, indicating that also in Beijing samples a significant contribution from oxidative processing of SOA components and probably SOA generated by biomass burning (Ding et al., 2016; Ding et al., 2016).

## **3.4 Conclusion and implication**

The maximum carbonyl ratio (MCR) is a metric that can be used to estimate the contribution of carbonyl groups in a molecule. According to the MCR value, the maximum number of carbonyl groups in molecules can be quantified. Furthermore, an updated visualization tool, the MCR-VK diagram, is developed by the combination of the MCR value and a traditional VK diagram. By locating selected typical SOA compounds within the MCR-VK diagram, five areas were defined referring to very highly oxidized organic compounds (area I, VHOOCs), highly oxidized organic compounds (area II, HOOCs), intermediately oxidized organic compounds (area III, IOOCs), oxidized unsaturated organic compounds (area IV, OUOCs) and highly unsaturated organic compounds (area V, HUOCs), to better understand the structural information of SOA compounds in terms of the carbonyl functional group. The MCR-VK diagram approch was tested and validated using laboratory-generated SOA from ozonolysis of  $\alpha$ -pinene, photo-oxidation of isoprene and ambient aerosol samples collected in Hyytiälä (boreal forest) and Beijing (megacity). Distinct distributions in the MCR-VK diagram were observed in the various aerosol samples and the comparison between them can improve the characterization of organic aerosol samples, especially an improved understanding of SOA sources and formation pathways. In summary, the use of the MCR concept or the application of MCR-VK diagrams should help to better understand the sources and the processing of atmospheric OA components based on HRMS data. As discussed above, the MCR might also prove useful for the evaluation of health-related effects of organic aerosols, since the MCR contains information about the presence of eletrophilic particle-bound multifunctional organics (larger MCR values) or the presence of highly oxidized non-carbonly organics (low MCR values), such as (hydro)peroxides, inducing oxidative stress in the respiratory system. Although oxidative and electrophilic stress are linked, the biological pathways causing the adverse health effects of particulate air pollution are poorly understood and there is no conclusive evidence as to which particle properties are causing their toxicity. Chemical components in the particle phase are

likely a key factor, but are difficult to accurately define. The suggested MCR value, easily extracted from HRMS data, might be a valuable tool to identify health-relevant particle parameters, components and sources, information which is crucial for improved and efficient air pollution mitigation strategies. In future work, the combination of MCR or MCR-VK diagrams and other metrics such as AI, Xc and OSc could be further used to better understand the composition, origin, history and effects of complex organic aerosols.

#### **Supporting Information**

The detailed description of the data processing (Table S3.2.1) and the information of selected SOA markers (Table S3.3.1).

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# 4 Molecular evidence for the association of reactive oxygen species yield with oxidized organic compounds

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# Molecular Evidence for the Association of Reactive Oxygen Species Yield with Oxidized Organic Compounds

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**Abstract.** The health effects of atmospheric fine particulate matter with aerodynamic diameter  $\leq$  2.5 µm (PM<sub>2.5</sub>) are closely correlated with redox-active components. However, the health-related organic components and relationship between the redox activities and chemical characteristics of PM<sub>2.5</sub> are largely unknown. In this study, the molecular composition of organic aerosols was analyzed by ultra-high resolution mass spectrometry (UHRMS) Orbitrap coupled with ultra-high performance liquid chromatography (UHPLC) in the negative electrospray ionization mode. After the assignment of molecular formulas for the detected compounds, the compounds were categorized into oxidized organic compounds (OOC) and unsaturated organic compounds (UOC) based on the value of maximum carbonyl ratio (MCR) of individual compound. Afterwards, the parameter defined as the 'ratio of relative peak area-weighted fraction of OOC to relative peak area-weighted fraction of UOC (R<sub>OOC/UOC</sub>)' was proposed. The yield of reactive oxygen species (ROS) generated by ambient  $PM_{2.5}$  and laboratory-generated secondary organic aerosol (SOA) samples were quantified to characterize the redox activities of aerosols, which referred to the sum of  $H_2O_2$  yield and radical yield measured by a fluorometric probe and electron paramagnetic resonance, respectively. We found that the ROOC/UOC of both urban PM2.5 samples and laboratorygenerated SOA samples had significant positive correlations with ROS yield (mainly contributed to  $H_2O_2$  yield). It indicates that organic components, particularly oxidized organic compounds, might make important contribution to the ROS formation. Our study highlights the important contribution of organic aerosols to the formation of reactive species and the relationship between the chemical characteristics of organic aerosols and the ROS formation. The ROOC/UOC can be utilized as a valuable parameter to identify health-related organic components, furthermore, the curve-fitting equations with good performance offer the possibility to predict of the ROS yield of PM<sub>2.5</sub>.

## 4.1 Introduction

Exposure to atmospheric particulate has been associated with adverse health outcomes including respiratory illnesses and cardiovascular diseases (Fuzzi et al., 2015; Pöschl and Shiraiwa, 2015). One proposed mechanism is particulate metter (PM) exposure leading to increased production of reactive oxygen species (ROS) in biological system and target cells, which causes oxidative stress and cell damage (Pöschl and Shiraiwa, 2015; Lakey et al., 2016; Arangio et al., 2016). ROS are a class of reactive oxygen-bearing compounds, including hydrogen peroxide

 $(H_2O_2)$ , hydroxyl radicals (•OH), superoxide radicals (•O<sub>2</sub><sup>-</sup>) and organic radicals (Lakey et al., 2016). Previous studies have shown that ROS can be generated by different redox-active components in PM, such as transition metals, quinones and secondary organic aerosol (SOA) (Chung et al., 2006; Wang et al., 2010; Shen et al., 2011; Wang et al., 2012; Badali et al., 2015; Lakey et al., 2016; Arangio et al., 2016; Tong et al., 2016; Hems et al., 2017; Tong et al., 2018; Bates et al., 2019; Chowdhury et al., 2019; Lin and Yu, 2020). In particular, the impacts of the redox-active organic components on the oxidative potential of PM and the association with ROS formation have been received increasing attention. Tong et al. (2018) reported that the SOA generated by isoprene,  $\beta$ -pinene and naphthalene was able to produce a substantial amount of H<sub>2</sub>O<sub>2</sub> upon interaction with water, furthermore, the organic hydroperoxides in the biogenic SOA were suggested to be the important precursors of ROS formation. Recently, we found that highly oxygenated molecules (HOMs) are closely associated with the radical formation by PM in water (Tong et al., 2018). These studies mainly investigated the ROS yield of the bulk SOA or the correlation of ROS yield with a class of specific compounds (e.g. peroxides). However, it is difficult to target the chemical components related to the adverse health effects in complex aerosol samples due to our limited understanding of detailed chemical composition of organic aerosols (Hoffmann et al., 2011; Wang et al., 2018).

Identification of organic compounds in atmospheric aerosols is always a challenging task due to the high complexity of organic aerosols (Nozière et al., 2015). Recent years, analytical methods based on ultrahigh resolution mass spectrometry (UHRMS), e.g., Orbitrap MS and Fourier transform ion cyclotron (FTICR), coupled with soft ionization techniques including atmospheric pressure chemical ionization (APCI) and electrospray ionization (ESI) have been successfully applied to characterize the chemical composition of organic aerosols at a molecular level (Lin et al., 2012; Vogel et al., 2016; Song et al., 2018; Zuth et al., 2018; Wang et al., 2019). Based on the UHRMS technique, thousands of unambitious molecular formulas have been assigned to the organic compounds in aerosol samples. Moreover, several metrics (e.g., double bond equivalent (DBE) and aromaticity equivalent) have been used to interpret these assigned molecular formulas to further understand the chemical properties of organic aerosols, such as the degrees of unsaturation and aromaticity (Koch and Dittmar, 2006; Yassine et al., 2014). Very recently, we proposed a new metric named maximum carbonyl ratio (MCR), which is used to improve the characterization of organic aerosol samples. Furthermore, in the combination with the composition dependent visualization tool Van Krevelen diagram, the MCR was suggested as a tool for better characterizing the sources and processing the components of atmospheric OA based on UHRMS data. The MCR might also be useful for the identification of health-relevant organic components

in PM, since the MCR containing information on the highly electrophilic organic compounds related to electrophilic stress as well as organic (hydro)peroxides linked to oxidative stress.

In this study, we investigated the relationship between the ROS yield and molecular composition of atmospheric aerosols. Particulate aerosol samples were collected at several cities, a forest site and a laboratory chamber facility. The molecular composition of particulate aerosol samples was characterized by an Ultra High-Performance Liquid Chromatograph coupled to an Electrospray Ionization source of an Orbitrap Mass Spectrometer (UHPLC/ESI-Orbitrap-MS). The identified organic compounds were classified into oxidized organic compounds (OOC) and unsaturated organic compounds (UOC) according to the MCR value of individual compound. We introduced a new index defined as 'the ratio of relative peak area-weighted fraction of OOC to relative peak area-weighted fraction of UOC (ROOC/UOC)' and calculated the values of ROOC/UOC for different samples. Moreover, the  $H_2O_2$  yield and radical yield of particulate aerosol samples were quantified using a fluorometric probe and electron paramagnetic resonance spectrometry in combination with a spin-trapping technique, respectively. Finally, the correlation of ROS yield with the chemical characteristics of aerosols was studied, giving simple equations for fitting the ROS yield based on the molecular composition of aerosols and the abundance of individual moleculea. The results of this study will help to provide a new insight into the link between the chemical composition of PM and ROS formation as well as improve the assessment of the toxicity of PM.

### 4.2 Material and methods

#### 4.2.1 Ambient particle sampling

Ambient fine PM samples were collected at a boreal forest site (Hyytiälä, Finland), an European city (Mainz, Germany) and four Chinese megacities (i.e., Beijing, Xi'an, Shanghai and Guangzhou). The Hyytiälä PM<sub>2.5</sub> samples were collected at Station for Measuring Forest Ecosystem-Atmosphere Relations station (SMEAR II) (61.51°N, 24.17°E) during 5–14 June 2017 using a Dekati impactor with 47 mm diameter Teflon filters (PALL, Teflon) at an air flow rate of 35 L min<sup>-1</sup>. The Mainz PM<sub>1.8</sub> (particulate matter with aerodynamic equivalent dimeter  $\leq 1.8 \mu m$ ) samples were collected on 47 mm diameter Teflon filters (100 nm pore size, Merck Chemicals GmbH) with a micro-orifice uniform deposition impactor (MOUDI, 110-R, MSP Corporation) at the air flow rate of 30 L min<sup>-1</sup> on the roof of Max Planck Institute for Chemistry (49.99°N, 8.23°E) during 22–30 August 2017. The Beijing PM<sub>2.5</sub> samples were collected from 26 February to 10 March 2019 on 47mm diameter Teflon filters (Whatman®) at the campus of Beihang University

(40.15°N, 116.27°E) using a low-volume sampler at a flow rate of 15 L min<sup>-1</sup>. The Xi'an PM<sub>2.5</sub> samples were collected on 90 mm diameter Teflon filters (100 nm pore size, Omnipore JVWP09025, Millipore) during 5–9 November 2018 using a low-pressure cascade impactor at a flow rate of 50 L min<sup>-1</sup> at the campus of Xi'an Jiaotong University (34.25°N, 108.98°E). The PM<sub>2.5</sub> samples of Shanghai (31.30°N, 121.50°E) and Guangzhou (12.12°N, 113.36°E) were collected on prebaked quartz-fiber filters (20.3×25.4 cm, Whatman®) in the period of 5–27 of January 2014 using a high-volume air sampler at a flow rate of 1050 L min<sup>-1</sup>. Information about the detailed location of sampling sites and samples can be found in Table S4.2.1.

#### 4.2.2 Laboratory SOA formation

Laboratory SOA experiments were performed in a 7 L quartz flow tube and a 19 L potential aerosol mass (PAM) chamber, respectively. The particulate SOA were generated from the gas phase ozonolysis of  $\alpha$ -pinene,  $\beta$ -pinene and limonene, respectively, with the O<sub>3</sub> concentration of ~1000 ppb in the flow tube. The isoprene- and naphthalene- SOA were generated from the gas phase photooxidation of isoprene and naphthalene, repectively, with the concentration of OH· radical of ~5.0×10<sup>11</sup> cm<sup>-3</sup> in the PAM chamber. The concentration of precursors was estimated to be 1–2 ppm for  $\alpha$ -pinene,  $\beta$ -pinene and limonene and 0.5–1 ppm for isoprene and naphthalene. SOA samples were collected on 47 mm diameter Teflon filters (JVWP04700, Omnipore membrane filter) and extracted immediately after sampling. More information about the SOA formation and collection processes can be found in our previous study (Tong et al., 2019).

#### 4.2.3 UHRMS measurements and Data processing

The procedure of filter extraction was presented in detail in our previous studies (Wang et al., 2018; Wang et al., 2019; Wang et al., 2019; Tong et al., 2019). In brief, a portion of filter (corresponding to approximate 600  $\mu$ g particle mass in each extracted filter) was extracted twice with 1.5 ml of methanol in an ultrasonic bath for 30 min. The combined extracts were filtered with a 0.2  $\mu$ m polytetrafluoroethylene (PTFE) membrane syringe filter to remove insoluble particulate matter, and then the extracts were evaporated to dryness under a gentle stream of nitrogen. Afterwards, the extracts were dissolved in 1.0 mL of acetonitrile/ultrapure water (ACN/H<sub>2</sub>O) mixture (1/9, v/v) for subsequent analysis.

The chemical measurement of organic compounds was carried out based on ultrahigh

resolution mass spectrometry (UHRMS) using an Orbitrap mass spectrometer (Q-Exactive, Thermo Scientific, Germany) coupled to an UHPLC system (Dionex UltiMate 3000, Thermo Scientific, Germany). A Hypersil Gold column (C18, 50 ×2.0 mm, 1.9 µm particle size, Thermo Scientific, Germany) was used for separation of analytes. The mobile phase was applied on a gradient mode at a flow rate of 0.5 mL min<sup>-1</sup>, consisting of eluent A (ultrapure H<sub>2</sub>O with 2% ACN and 0.04% formic acid) and eluent B (ACN with 2% ultrapure H<sub>2</sub>O). The Orbitrap was equipped with a heated electrospray ionization source (HESI) and operated in the negative ion mode (ESI–) with a -3.3 kV spray voltage. A mass resolving power of 70,000 @ *m*/*z* 200 and a scanning range of 50–500 *m*/*z* were applied. Detailed information of optimized gradient of mobile phase and MS approach can be found in our previous studies (Wang et al., 2018; Wang et al., 2019; Tong et al., 2019).

The obtained chromatograms and mass spectra were proceeded by a non-target screening approach using an open-source software (MZmine 2.37). The detailed processing steps and parameters applied in the software are shown in Table S2. The software automatically searched the ions with absolute peak abundance above  $1 \times 10^5$  and calculated all mathematically possible molecular formulas for ion signals with a mass tolerance of  $\pm 2$  ppm. The molecular formulas were presented as  $C_cH_hO_oN_nS_s$ , where c, h, o, n and s are the number of carbon, hydrogen, oxygen, nitrogen and sulfur atoms, respectively, which were in the range of 1–39, 1–72, 0–20, 0–7 and 0–4. To eliminate chemically unreasonable molecular formulas, ratios of H/C, O/C, N/C and S/C were further constrainted in the range of 0.3–3, 0–3, 0–1.3 and 0–0.8, respectively (Tong et al., 2019).

#### 4.2.4 Quantification of $H_2O_2$ yield

One fourth of each ambient PM filter or a whole SOA-loaded filter was extracted with 1.0 mL of ultra-pure water by stirring with a vortex shaker for 15 minutes. Afterwards, the extracts were centrifuged at 9000 rpm using a centrifuge (Eppendorf Minispin) for 3 minutes. Finally, the concentration of  $H_2O_2$  in the supernatants was quantified using a fluorometric Hydrogen Peroxide Assay Kit (MAK165, Sigma). The detailed procedure of  $H_2O_2$  measurement has been presented in our previous study (Tong et al., 2018). Briefly, 50 µL of supernatant and 50 µL of detection reagent containing horseradish peroxidase and Amplex Red substrate were mixed in a 96-well plate. The fluorescence was detected using a microplate reader (Synergy<sup>TM</sup> NEO, BioTek; excitation at 540 nm and emission at 590 nm) after 30 minutes of incubation. The concentration of  $H_2O_2$  in extracts was determined using a  $H_2O_2$  calibration curve obtained using standard  $H_2O_2$  solutions and was

corrected by blank measurements.

#### 4.2.5 Measurement of radical yield by EPR

The procedure of radical yield measurement was presented in our previous studies (Tong et al., 2018; Tong et al., 2019). In brief, one fourth of each ambient PM filter or a whole SOA-loaded filter was extracted with 10 mM 5-tert-Butoxycarbonyl-5-methyl-1-pyrroline N-oxide (BMPO, high purity, Enzo Life Sciences GmbH), which was used as the spin-trapping agent by vortex shaking (Heidolph Reax 1) for 15 minutes. A continuous-wave electron paramagnetic resonance (CW-EPR) X-band spectrometer (EMXplus-10/12; Bruker Corporation) was applied for identification and quantification of radicals. The operating parameters of EPR is briefly displayed as following: a modulation frequency of 100 KHz, a modulation amplitude of 1 G, a microwave power of 2.1 mW (20 dB), a receiver gain of 40 dB, a scan number of 50 and a sweep width of 100 G. The spin-counting method named Xenon embedded in the Bruker software was used to quantify the radicals.

## 4.3 Results and discussion

#### 4.3.1 MCR-VK diagram

UHRMS technique has been increasingly applied to elucidate the unambiguous the molecular formulas of organic compounds in atmospheric aerosols. However, the interpretation of molecular structures based on the assigned molecular formulas by UHRMS technique is limited. The metrics of double bond equivalent (DBE), aromaticity index (AI) and aromaticity equivalent (Xc) have been successfully introduced to indicate the double bonds and aromatic rings in molecular structures of organic compounds (Koch and Dittmar, 2006; Yassine et al., 2014). We proposed a new metric named maximum carbonyl ratio (MCR), which describes the potentially maximal contribution of carbonyl functionalities in the molecular structures of organic compounds detected by HRMS technique. For a given molecular formula of  $C_cH_hO_oN_nS_s$ , the MCR can be calculated by equation 4.1:

$$MCR = \frac{DBE}{o}, \text{ for } o \ge DBE$$
(4.1)

where o was the number of oxygen atoms in the compound. MCR is considered to equal one if o < v

DBE.

An updated visualization tool, the MCR-VK diagram, is developed by the combination of the MCR value and the traditional VK diagram. In this study, as shown in Figure 4.3.1a, MCR-VK diagram is divided to two regions by the black dash line, which represents the MCR value of 0.9. Compounds located in the blue area in Figure 4.3.1a are classified as oxidized organic compounds (OOC) with the MCR values less than 0.9, while compounds in the gray area are classified as unsaturated organic compounds (UOC) with the value of MCR  $\geq 0.9$ . OOC include several types of compounds, such as very highly oxidized organic compounds (e.g., peroxides and isoprene epoxydiols), highly oxidized organic compounds (e.g. 3-methyl-1, 2, 3-butanetricarboxylic acid (MBTCA)) and intermediately oxidized organic compounds (e.g., pinic acid and pinonic acid) (Yasmeen et al., 2012; Müller et al., 2012; Nguyen et al., 2014; Wang et al., 2018) as shown in Figure S4.3.1a. Highly oxidized multifunctional molecules (HOMs) (Mutzel et al., 2015; Wang et al., 2017), which undergo different oxidation and aging processes, can also be assigned to OOC. UOC mainly include oxidized unsaturated organic compounds (e.g., primary organic compounds and oxidation products from aromatic volatile organic compounds) and highly unsaturated organic compounds (e.g., combustion related compounds and compounds from condensational ageing) (see Figure S4.3.1a).



Figure 4.3.1: (a) MCR-VK diagram applied to classify the organic compounds in particulate organic aerosols. The black dash line represents the boundary (MCR = 0.9) between the oxidized organic compounds (OOC, MCR < 0.9) located in the blue region and the unsaturated organic compounds (UOC, MCR ≥ 0.9) in the gray region. (b) Ratio of relative peak area-weighted fraction of OOC to relative peak area-weighted fraction of UOC (R<sub>OOC/UOC</sub>) of the ambient fine PM samples (blank pattern) and laboratory-generated SOA samples (slash pattern). The error bars represent the standard deviations of R<sub>OOC/UOC</sub> of the samples collected at each location or each laboratory experiment.

# 4.3.2 Contribution of OOC and UOC to ambient and laboratory particulate aerosol samples

Based on the compound classification by MCR-VK diagram, a new parameter was defined as 'ratio of relative peak area-weighted fraction of OOC to relative peak area-weighted fraction of UOC (R<sub>OOC/UOC</sub>)' in this study, which reflected the relative contribution of OOC and UOC to the particulate organic aerosol. Figure 4.3.1b displays the ROOC/UOC of the ambient fine PM and laboratory-generated SOA samples, which were averaged from all samples collected at each location or laboratory experiment. It shows that the R<sub>OOC/UOC</sub> of isoprene SOA is highest with the value of 54, followed by Hyytiälä PM<sub>2.5</sub> (20),  $\alpha/\beta$ -pinene SOA (17), limonene SOA (8), urban fine PM (i.e., Mainz (6), Beijing (1.3), Xi'an (1.2), Guangzhou (1.1) and Shanghai (0.75)) and naphthalene SOA (0.57). The extremely high value (54) of  $R_{OOC/UOC}$  of isoprene SOA indicates the major contribution of OOC to the organic compounds in isoprene SOA. It can be explained by that the oxygen atoms in the molecular structures of typical products generated from photooxidation of isoprene (e.g., 2-methyl-tetrols) (Wang et al., 2018) are in the form of OH functional group, which are assigned to OOC with the low value of MCR. The  $R_{OOC/UOC}$  of  $\alpha/\beta$ -pinene SOA with the valueu of 17 is also very high and OOC in  $\alpha$ -pinene SOA and  $\beta$ -pinene SOA account for 95% and 94%, respectively (See Figure S4.3.1b). It agrees well with our recent study showing that the typical products formed through the ozonolysis of  $\alpha$ -pinene and  $\beta$ -pinene, e.g., pinonic acid, pinic acid and MBTCA from  $\alpha$ -pinene oxidation and nopinone and pinic acid from  $\beta$ -pinene oxidation (Yasmeen et al., 2012; Müller et al., 2012; Zhang et al., 2015), were located in the blue area of MCR-VK diagram. Interestingly, the R<sub>OOC/UOC</sub> (20) of PM<sub>2.5</sub> samples collected at a remote forest site of Hyytiälä is comparable to that of  $\alpha$ -/ $\beta$ -pinene SOA, which can probably be explained by that  $\alpha/\beta$ pinene make important contribution to the formation of SOA at Hyytiälä location (Cavalli et al., 2006; Kourtchev et al., 2013).

On the contrary, the  $R_{OOC/UOC}$  (0.57) of naphthalene SOA is significantly lower compared to the  $R_{OOC/UOC}$  (54) of the SOA generated from biogenic precursors. Such low value of  $R_{OOC/UOC}$  of naphthalene SOA indicates that the products formed through the photooxidation of naphthalene are dominated by UOC with relative fraction value of 64% (see Figure S4.3.1b). Previous studies showed that compounds located at the lower left corner of the VK diagram with H/C ratio  $\leq 1.0$ and O/C ratio  $\leq 0.5$  were suggested to be low-oxygen-containing aromatic hydrocarbons (Kourtchev et al., 2014; Wang et al., 2018). Since the majority of UOC are also located at the lower left corner of the MCR-VK diagram, these UOC are likely to be aromatic compounds. This observation is consistent with a previous study by Kautzman et al. (2010) showing that the SOA generated from the photooxidation of naphthalene under low-NO<sub>x</sub> conditions were dominated by ring-retaining compounds (e.g. 1,4-benzoquinone) and ring-opening species (e.g. phthaldialdehyde). It can be explained by that the photo-oxidation process is not able to break the two benzene rings in the structure of naphthalene, resulting in one benzene ring remaining in the structure of the products.

In urban fine PM, the relative peak area-weighted fractions of UOC span a wide range from ~15% to ~57% (see Figure S4.3.1b), indicating the complex chemical composition of urban organic aerosol due to various kinds of precursors and formation processes in urban regions. The  $R_{OOC/UOC}$  of ambient PM<sub>2.5</sub> samples collected at Beijing, Xi'an, Guangzhou and Shanghai are 1.3, 1.2, 1.1 and 0.75, respectively, which are close to the  $R_{OOC/UOC}$  (0.57) of naphthalene SOA but highly different from the  $R_{OOC/UOC}$  (8–54) of SOA generated from the biogenic precursors. It indicates that a large amount of aromatic compounds were probably generated in these Chinese urban regions. This observation agrees well with our previous studies showing that the majority of compounds in the Chinese cities of Beijing, Shanghai, Guangzhou and Changchun were considered to mono- and poly-aromatics (Wang et al., 2019). However, the  $R_{OOC/UOC}$  (6) of Mainz fine PM samples is much higher than that of the Chinese megacities, indicting the less aromatic compounds in Mainz fine PM samples, which is again consistent with our previous study (Wang et al., 2018).

Interestingly, the  $R_{OOC/UOC}$  (20) of the Hyytiälä PM<sub>2.5</sub> is in the range of the  $R_{OOC/UOC}$  (8–54) of biogenic SOA and much higher than the  $R_{OOC/UOC}$  (0.57) of anthropogenic SOA, while all the  $R_{OOC/UOC}$  (0.75–6) of urban samples are lower than the  $R_{OOC/UOC}$  of biogenic SOA and close to that of anthropogenic SOA. It implies that the SOA in urban areas is affected by a large degree of anthropogenic sources compared to remote forest regions.

#### 4.3.3 Yield and formation potential of ROS by ambient fine PM

Chemical characteristic of organic aerosols is likely a key factor linked to health effect, however, it is difficult to identify a set of chemical reactions or redox-active components responsible for reactive species formation due to the complexity of organic aerosols. Since the MCR might release the health-related information, as introduced in our recent study, the MCR index together with the  $R_{OOC/UOC}$  parameter are promising to identify the health-related organic compound in the complex aerosol samples.

Figure 4.3.2a and 4.3.2b display the volume-normalized (pmol  $m^{-3}$ ) and mass-normalized (pmol  $\mu g^{-1}$ ) ROS yield, i.e., the sum of H<sub>2</sub>O<sub>2</sub> yield and radical yield, by ambient fine PM as a function of the concentration of PM. Beijing PM<sub>2.5</sub> exhibited the highest formation potential of

ROS with 263 pmol m<sup>-3</sup>, whereas the Hyytiälä PM<sub>2.5</sub> samples with concentration of 5  $\mu$ g m<sup>-3</sup> generated only 13 pmol m<sup>-3</sup> ROS. Figure 4.3.2a shows that the volume-normalized ROS yield generated by the ambient fine PM has a positive linear correlation (R<sup>2</sup> = 0.81) with the mass concentration of PM, indicating that the potential of ROS formation by ambient fine PM increases with the increase of pollution levels. This positive correlation is not surprising, since this ROS yield is volume-normalized and higher PM concentration refers to more PM mass in each volume of air, generating more ROS. It is very interesting that the linear coefficient of R<sup>2</sup> between the volume-normalized ROS yield and PM concentration has a high value of 0.8, meaning that we could estimate the volume-normalized ROS yield of ambient fine PM samples simply based on the PM concentration. Moreover, since the ROS yield presented in Figure 4.3.2a and 4.3.2b is the sum of H<sub>2</sub>O<sub>2</sub> yield and radical yield, we also presented the volume-normalized H<sub>2</sub>O<sub>2</sub> yield and radical volume-normalized yield as a function of the concentration of PM in Figure S4.3.4, again showing positive linear correlations with R<sup>2</sup> = 0.79 and R<sup>2</sup> = 0.91, respectively.

In comparison to the volume-normalized ROS yields, the mass-normalized yield of ROS is independent of filter loading, which can better reflect the redox potential associated with redoxactive species (e.g., peroxides and transition metals) in PM. As shown in Figure 4.3.2b, no obvious correlation was observed between the mass-normalized ROS yield and the concentration of PM. Figure S4.3.4c shows that the mass-normalized H<sub>2</sub>O<sub>2</sub> yield had no obvious correlation with the concentration of PM. While the mass-specific radical yield of ambient fine PM exhibits a good negative linear correlation with PM concentration (see Figure S4.3.4d), which agrees well with our previous study (Tong et al., 2019).

The correlation of  $R_{OOC/UOC}$  of ambient fine PM samples with the concentration of PM is displayed in Figure 4.3.2c. It shows that the  $R_{OOC/UOC}$  of organic aerosols is negatively correlated with the PM concentration, indicating that PM in clean areas exhibits higher  $R_{OOC/UOC}$  value, whereas PM is associated with low  $R_{OOC/UOC}$  in polluted regions. Interestingly, the  $R_{OOC/UOC}$  of ambient fine PM decreases with the increasing concentration of PM, showing a similar trend with mass-specific ROS yields by urban fine PM samples (see Figure 4.3.2b), particularly for urban fine PM (i.e., Mainz, Beijing, Xi'an, Guangzhou, and Shanghai). Thus, the relationship between chemical characteristics of organic aerosols based on  $R_{OOC/UOC}$  parameter and ROS generated by ambient fine PM as well as laboratory-generated SOA samples was further explored.



Figure 4.3.2: Correlation of volume-normalized ROS yields (a), mass-specific ROS yields (b) and R<sub>OOC/UOC</sub> (c) with the concentration of ambient fine PM. The error bars represent standard deviations.

#### 4.3.4 Correlation between ROOC/UOC and ROS yield

To get insights into the relationship between chemical characteristics of organic aerosols and ROS generation, the correlations of particle mass normalized  $H_2O_2$  yield, radical yield, and the sum of them, with the  $R_{OOC/UOC}$  of organic compounds in ambient fine PM and laboratory-generated SOA samples were shown in Figure 4.3.3.

As shown in Figure 4.3.3a, a significant positive exponential correlation (y = 3.2 - 7.6exp(-1.5x),  $R^2 = 0.94$ ) was observed between the ROS yield and the  $R_{OOC/UOC}$  of urban fine PM samples (i.e., Mainz, Beijing, Xi'an, Guangzhou, and Shanghai). It indicates that ROS yield is closely associated with organic components, moreover, the ROS generated by organic aerosols in water increase exponentially with  $R_{OOC/UOC}$  value of fine PM. It should be noted that the dot of Hyytiälä PM<sub>2.5</sub> (the gray dot) was not fit the exponential curve, which may be explained by the large different chemical characteristics between the Hyytiälä PM<sub>2.5</sub> samples and urban fine PM samples.

Figure 4.3.3b shows that  $H_2O_2$  yield is positive exponential correlated (y = 3.0 - 8.0exp(-1.6x),  $R^2 = 0.98$ ) with the  $R_{OOC/UOC}$  of ambient samples, which is highly similar to the correlation shown in Figure 4.3.3a, impling that the relatively stable  $H_2O_2$  may make an important contribution to the ROS formation by ambient fine PM. Furthermore, Figure S4.3.5 indicates  $H_2O_2$  yield accounts for the majority fraction (77%–99%) of the total ROS yield by ambient fine PM and laboratory-generated SOA samples.

The good correlations of  $H_2O_2$  yield with the  $R_{OOC/UOC}$  of urban fine PM (see Figure 4.3.3b) as well as relative fraction of OOC in urban fine PM (see Figure S4.3.6b) indicate that the organic components, especially OOC, in urban aerosols make significant contribution to the  $H_2O_2$ generation. This observation agrees well with the previous studies showing that decomposition or hydrolysis of hydroperoxides and organic peroxides (assigned to OOC) is likely an important pathway of  $H_2O_2$  formation in the water (Wang et al., 2011; Badali et al., 2015; Tong et al., 2018).

Another interesting observation is that the data dot of ROS yield of Hyytiälä  $PM_{2.5}$  (the gray dot in Figure 4.3.3a), as well as the ROS yield of Hyytiälä  $PM_{2.5}$  (the gray dot in Figure 4.3.3b) of Hyytiälä  $PM_{2.5}$ , are beyond the exponential curve fitted by the urban fine PM samples. It implies that the curve equations of urban aerosols are not suitable to apply for the forest aerosols samples of Hyytiälä. This observation reflects that the sources and mechanisms of  $H_2O_2$  formation may be different between the urban aerosols and remote forest aerosols due to their large difference in term of chemical composition. For example, some quinones (assigned to UOC) and several transition metals (e.g., Fe, Cu, and Mn) commonly found in urban fine PM samples can also contribute to  $H_2O_2$  yield. On the contrary, remote fine PM samples contain a rare number of metals and quinones

but a large amount of biogenic precusor-generated particles.

Figure 4.3.33c shows that the radical yield of Hyytiälä  $PM_{2.5}$  samples with extremely high  $R_{OOC/UOC}$  value is much higher compared to urban fine PM samples with lower  $R_{OOC/UOC}$  value. It can be explained by our previous study showing that HOMs (assigned to OOC) may play an important role in radical formation in water and a higher relative fraction of HOMs in Hyytiälä  $PM_{2.5}$  was observed compared to that in the urban fine PM.

In contrast to ambient fine PM, laboratory-generated SOA samples exhibited much higher ROS yields as shown in Figure 4.3.3d. Among laboratory-generated SOA, isoprene SOA had the highest ROS yield of 5.9 pmol  $\mu g^{-1}$ , followed by  $\alpha$ -pinene SOA (4.5 pmol  $\mu g^{-1}$ ),  $\beta$ -pinene SOA (3.4 pmol  $\mu g^{-1}$ ) and limonene SOA (3.4 pmol  $\mu g^{-1}$ ), whereas naphthalene SOA had the lowest ROS yield of 1.8 pmol  $\mu g^{-1}$ . The positive linear correlation (y = 47.8 + 5.8x, R<sup>2</sup> = 0.95) of R<sub>OOC/UOC</sub> of laboratory SOA with ROS yield could confirm the significant effect of organic aerosols, especially OOC, on ROS formation. It agrees well with the finding of Tong et al. (2018) showing that a positive correlation was observed between the total peroxide concentration and ROS yield generated by isoprene SOA,  $\beta$ -pinene SOA and naphthalene SOA, indicating that organic (hydro)peroxides (assigned to OOC) may play an important role in ROS formation.

As shown in Figure 4.3.3e, similar with ambient samples, the increasing trend of  $H_2O_2$  yield of SOA generated from different precursors is consistent with that of ROS yield (see Figure 4.3.3d). This observation may mainly be due to that  $H_2O_2$  is the most abundance ROS species accounting for 95%–99% (see Figure S4.3.5b). It clearly shows that higher  $H_2O_2$  yield by biogenic SOA (i.e.,  $\alpha/\beta$ -pinene SOA, limonene SOA, and isoprene SOA) was observed than that by naphthalene SOA. The positive linear correlation (y = 46.1 + 5.7x,  $R^2 = 0.94$ ) between the  $H_2O_2$  yield generated by laboratory-generated SOA samples and the R<sub>OOC/UOC</sub> values implies that SOA samples with high R<sub>OOC/UOC</sub> can generate more  $H_2O_2$ . Furthermore, OOC likely make significant contribution to  $H_2O_2$ generation. Previous studies reported that  $H_2O_2$  generated in water by organic aerosols is likely due to decomposition or hydrolysis of a certain type of organic compounds, e.g., hydroxyhydroperoxides (products from ozonolysis of  $\alpha$ - and  $\beta$ -pinene) and peroxy acids (RC(O)OOH, formed from ozonolysis of  $\alpha$ -pinene) (Hasson et al., 2001; Venkatachari and Hopke, 2008; Wang et al., 2011; Badali et al., 2015).

No obvious correlation is found between the radical yield and the  $R_{OOC/UOC}$  values for these laboratory-generated SOA samples as shown in Figure 4.3.3f. Tong et al. (2018) found that the radical production rates of SOA in water was related with the abundance of total peroxides in SOA, however, naphthalene SOA can generate more  $\cdot O_2^-$ , which is most likely generated by redox reactions of semiquinones contained in naphthalene SOA.



Figure 4.3.3: Correlation of mass-specific ROS yields (a),  $H_2O_2$  yields (b) and radical yields (c) with  $R_{OOC/UOC}$  of ambient fine PM samples and correlation of mass-specific ROS yields (d),  $H_2O_2$  yields (e) and radical yields (f) with  $R_{OOC/UOC}$  of laboratory-generated SOA samples, respectively. The error bars represent standard deviations.

## 4.4 Conclusion and implication

Particulate aerosol samples were collected at six cities (Mainz, Beijing, Shanghai, Guangzhou, and Xi'an), a forest site (Hyytiälä), as well as laboratory flow tube and chamber facilities. The organic compounds identified by UHRMS were classified into oxidized organic compounds (OOC) and unsaturated organic compounds (UOC) according to the MCR value of individual compound. Moreover, the  $H_2O_2$  yield and radical yield of particulate aerosol samples were quantified using a fluorometric probe and electron paramagnetic resonance spectrometry, respectively. A new index defined as 'the ratio of relative peak area-weighted fraction of OOC to relative peak area-weighted fraction of UOC ( $R_{OOC/UOC}$ )' based on the MAC metric was introduced to investigate the relationship between the ROS yield and molecular composition of atmospheric aerosol.

We found that the positive correlations between the ROS yield and the  $R_{OOC/UOC}$  were observed in both ambient urban fine PM and laboratory-generated SOA, indicating that the ROS generation is closely associated with organic components in the particulate aerosol samples, particularly with the oxidized organic compounds. The results of this study will help to provide more evidence for the link between the organic compounds in PM and ROS formation, furthermore, the proposed  $R_{OOC/UOC}$  is suggested to infer the health-related organic species in PM. In the future, by investigating the relationship between the chemical composition and ROS formation of more different locations and generated from different types of precursors, the equations could be improved and be used to predict the ROS yield by the concentration of PM and further better assess the toxicity of PM.

#### **Supporting Information**

The detailed information of ambient PM sampling (Table S4.2.1), molecular formulas of organic compounds detected in ambient PM and laboratory-generated SOA (Table S4.3.1–S4.3.5), and seven figures (Figure S4.2.1, S4.3.1–S4.3.6)

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4 Molecular evidence for the association of reactive oxygen species yield with oxidized organic compounds

## **5** Conclusions and Outlook

The application of ultrahigh resolution mass spectrometry (UHRMS) in the field of atmospheric aerosol research, that was, the chemical composition characterization of organic aerosols (OA) at a molecular level was demonstrated within this thesis. A rapid and simple sample pre-treatment method using a solvent mixture of acetonitrile and water was developed to extract the organic compounds, which was proved to be efficient for both polar compounds like organic acids and non-polar compounds such as polycyclic aromatic hydrocarbons. Ultrahigh performance liquid chromatography (UHPLC) technique was applied prior to UHRMS coupled with electrospray ionization source, which was able to achieve the separation of the isomer compounds and reduction of the ion suppression. Based on the mass spectra data obtained by UHRMS, nontarget screening methods were developed with a commercial software 'SIEVE' and an open-source software 'MZmine', respectively. The identified thousands of organic compounds were classified into CHO, CHON, CHOS, CHONS, and CHN (only in positive mode) according to their elemental composition. Various typical metrics including double bond equivalent, carbon oxidation state, and aromaticity equivalent and several visualization tools, i.e., Van Krevelen diagram and Kendrick mass defect diagram, were applied to interpret the UHRMS data and describe the chemical properties and possible sources of OA.

A new metric – the maximum carbonyl ratio (MCR) – was suggested in this work, which described the maximal contribution of carbonyl/epoxide functionalities in individual compounds in OA, that can be directly derived from the molecular composition. MCR was presented in combination with Van Krevelen diagrams as an updated visualization tool (MCR-VK diagram) aiming to better categorize complex organic compounds in ambient aerosol samples. By locating selected typical SOA compounds, MCR-VK diagram was divided into five regions corresponding to very highly oxidized organic compounds, highly oxidized organic compounds, intermediately oxidized organic compounds, oxidized unsaturated organic compounds, and highly unsaturated organic compounds, respectively. The approach was applied to the ambient OA samples and laboratory-generated SOA samples based on the UHRMS data. By observing and comparing the distributions of organic compounds in the MCR-VK diagram, the understanding of chemical properties, sources, and formation pathways of OA was improved.

Investigating the sources, formation processes, and amount of ROS is an effective pathway to evaluate the redox activity and toxicity of OA. Chemical components in OA are likely a key factor but are difficult to be identified accurately. The suggested metric of MCR, easily extracted from UHRMS data, might be a valuable tool to identify health-relevant particle parameters and components. The ROS yield, which refers to the sum of  $H_2O_2$  yield and radical yield in this thesis, produced by ambient  $PM_{2.5}$  samples and laboratory-generated SOA samples in water was quantified. The yield of  $H_2O_2$  was measured using a fluorometric probe, while the yield of radicals was detected by electron paramagnetic resonance. The total intensity of oxidized organic compounds (i.e., very highly oxidized organic compounds, highly oxidized organic compounds, intermediately oxidized organic compounds) in ambient urban  $PM_{2.5}$  samples and laboratory-generated SOA both showed significant positive correlations with the ROS yield, indicating oxidized organic compounds, e.g. (hydro)peroxides, might make an important contribution to the ROS formation.

The UHRMS technique presented in this thesis is allowed to give the molecular formula information of thousands of organic compounds from complex OA matrix. However, due to such high numbers of organic compounds, it is difficult to elucidate the molecular structures of these organic compounds. In the future, more detailed tandem MS (MS<sup>n</sup>) studies should be performed for a better understanding of the molecular structures. Meanwhile, the interpretation method for UHRMS data should be further developed, like combining the information of molecular formulas and retention times in UHPLC to predict the volatilities of different compounds. Moreover, the proposed MCR metric might be utilized as a valuable parameter to identify health-related organic components, providing new insights into the ROS formation. In future work, the combination between MCR or MCR-VK diagram and other metrics, such as carbon oxidation states, can be further explored to analyze the chemical structures in the complex aerosol components.

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6 References

- **A.** Supplementary material to chapter 2
- **B.** Supplementary material to chapter 3
- C. Supplementary material to chapter 4
- **D.** List of related publications and presentations
- E. Acknowledgements
- **F.** Curriculum vitae

## A. Supplementary material to chapter 2

## "UHPLC-Orbitrap mass spectrometric characterization of organic aerosol from a central European city (Mainz, Germany) and a Chinese megacity (Beijing)"

This supplementary material contains one appendice and five figures (S2.3.1–S2.3.5).

#### The description of calibration standard solution for mass spectrometer

Calibration standard solution were purchased from Sigama-Aldrich, Germany. For positive mode: caffeine (molecular weight 194 Da), MRFA (L-methionyl-arginyl-phenylalanyl-alanine, molecular weight 523 Da), Ultramark 1621 (a mixture of perfluorinated phosphazenes, molecular weight in the range of 1021–1921 Da) and n-butylamine (molecular weight 73 Da). For negative mode: sodium dodecyl sulfate (molecular weight 288 Da), sodium taurocholate hydrate (molecular weight 537 Da) and Ultramark 1621.



Figure S2.3.1: The UHPLC chromatograms of tentatively determined M/Z 161.02394 Da in Maniz and Beijing samples.

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Figure S2.3.2: The Van Krevelen diagram for CHO compounds detected in ESI+ mode. Areas 'A' and 'B' refer to aliphatic compounds and oxidised aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity equivalent (gray ball with  $X_C < 2.50$ , purple ball with  $2.50 \le X_C < 2.70$  and red ball with  $X_C \ge 2.70$ ). The pie chat shows the percentage of the number of each color-coded compound in each sample.



Figure S2.3.3: The Van Krevelen diagram of CHON compounds detected in ESI+ mode. Areas 'A' and 'B' refer to aliphatic compounds and oxidised aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity equivalent (gray ball with  $X_C < 2.50$ , purple ball with  $2.50 \le X_C < 2.70$  and red ball with  $X_C \ge 2.70$ ). The pie chat shows the percentage of the number of each color-coded compound in each sample.



Figure S2.3.4: The Van Krevelen diagram constructed by plotting the H/C ratio agaist the (O–3N)/C ratio for CHON compounds detected in ESI- mode. Areas 'A' and 'B' refer to aliphatic compounds and oxidised aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity equivalent (gray ball with  $X_C < 2.50$ , purple ball with  $2.50 \le X_C < 2.70$  and red ball with  $X_C \ge 2.70$ ). The pie chat shows the percentage of the number of each color-coded compound in each sample.

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Figure S2.3.5: The DBE vs. carbon number diagram of CHOS compounds observed in MZL (circles), BJL (triangles) and BJH (dots). The stars in the figure indicate the averaged DBE and carbon number of CHOS compounds in MZL (red star), BJL (green star) and BJH (blue star).

# **B.** Supplementary material to chapter 3

# "The maximum carbonyl ratio as a metric for the structural classification of OA"

This supplementary material contains two tables (S3.2.1 and S3.3.1).

Table S3.2.1: Parameters and settings for the non-target data analysis workflow in Mzmine 2.37

1) Import data		
Raw data methods	Raw data import	
2) Peak detection		
Raw data methods	Peak dectection	Mass dectection
Parameters	Raw data files	All raw data files
	Scans_set filters	All
	Mass detector	Wavelet transform
		Noise level = 1000
	Mass list name	masses
3) FTMS shoulder peaks	filter	· · · ·
Raw data methods	Peak dectection	FTMS shoulder peak filter
Parameters	Raw data files	All raw data files
	Mass list	masses
	Mass resolution	70000
	Peak model function	Gaussian
	Suffix	filtered
	Remove original peak list	Off
4) ADAP chromatogram	builder	
Raw data methods	Peak dectection	ADAP chromatogram builder
Parameters	Raw data files	All raw data files
	Scans_set filters	
		MS level: 1
		Polarity: Any
		Spectrum type: Any
	Mass list	masses
	Min group size in # of scans	6
	Group intensity threshold	1000
	Min highest intensity	10000
	m/z tolerance	4.0E–4 <i>m/z</i> or 2.0 ppm
	Suffix	chromatograms
5) Smoothing		
Peak list methods	Smoothing	
Parameters	Peak lists	Those created by previous batch step

	Filename suffix	smoothed
	Filter width	5
	Remove original peak list	Off
6) Chromatogram dec	onvolution	
Peak list methods	Chromatogram deconvolution	
	Peak lists	Those created by previous batch step
	Suffix	deconvoluted
	Algorithm	Wavelets (ADAP)
		S/N threshold = 10
		S/N estimator = Intensity window SN
		Min feature height $= 10000$
		coefficient/area threshold = 110
		Peak duration range = $0.03 - 1.00$
		RT wavelet range = $0.01-0.2$
	m/z center calculation	MEDIAN
	m/z range for MS <sup>2</sup> scan pairing	Off
	RT range for MS <sup>2</sup> scan pairing	Off
	Remove original peak list	Off
7) Remove isotope chr	omatograms	
Peak list methods	isotopes	Isotopic peaks grouper
	Peak lists	Those created by previous batch step
	Name suffix	deisotoped
	m/z tolerance	4.0E–4 <i>m/z</i> or 2.0 ppm
	RT tolerance	0.1 absolute (min)
	Monotonic shaoe	Off
	Maximum charge	1
	Representative isotope	Most intense
	Remove original peak list	Off
8) Finds and removes a	adduct signals from peak list	
Peak list methods	Identification	Adduct search
	Peak lists	Those created by previous batch step
	RT tolerance	0.1 absolute (min)
	Adducts	[M+CH <sub>2</sub> O <sub>2</sub> ] 46.0055 <i>m</i> / <i>z</i>
		[M+ACN] 41.0266 <i>m/z</i>
	m/z tolerance	4.0E–4 <i>m</i> / <i>z</i> or 2.0 ppm
	Max relative adduct peak height	50%
9) Finds and removes i	ion complexes from peak list	
Peak list methods	Identification	Complex search
	Peak lists	Those created by previous batch step
	Ionization method	[M–H] <sup>–</sup>
	RT tolerance	0.1 absolute (min)
	m/z tolerance	4.0E–4 <i>m/z</i> or 2.0 ppm
	Max complex peak height	50%

Peak list methods	Alignment	Join aligner
	Peak lists	Those created by previous batch step
	Peak list name	Aligned peak list
	m/z tolerance	4.0E–4 <i>m/z</i> or 2.0 ppm
	Weight for $m/z$	5
	Retention time tolerance	0.2 absolute (min)
	Weight for RT	4
	Require same charge state	Off
	Require same ID	Off
	Compare isotope patter	On
		Isotope $m/z$ tolerance = 0.001 $m/z$ or 5.
		ppm
		Minimum absolute intensity = 1000
		Minimum score = 85%
11) Formula predictio		
Peak list methods	Identification	Formula prediction
	Charge	
	ionization type	
	Peak lists	Those created by previous batch step
	m/z tolerance	4.0E–4 <i>m/z</i> or 2.0 ppm
	max best formulas per peak	1
	Elements	
		C = 1–39
		H = 1 - 72
		O = 0–20
		N = 0 - 7
		S = 0-4
	Element count heuristics	On
		H/C ratio: yes
		NOPS/C ratio: yes
		Multiple element counts: yes
	RDBE restritions	On
		RDBE range=0-30
		RDBE must be an integer: yes
	Isotope pattern filter	On
		Isotope $m/z$ tolerance: 0.001 $m/z$ or 5.0 ppm
		Minimum absolute intensity: 500
		Minimum score = 75%
	MS/MS filter	Off
12) Export data		
Peak list methods	Export	Export to CSV file

Marker	Molecular formula	Structure (or possible structure)	DBE	MCR	Precursor
Isoprene	C <sub>5</sub> H <sub>8</sub>		2	1.00	
MT (monoterpene)	$C_{10}H_{16}$		3	1.00	
SQT (sesquiterprene)	C15H24		4	1.00	
Benzene	$C_6H_6$		4	1.00	
Naphtalene	$C_{10}H_{8}$		7	1.00	
Anthracene	$C_{14}H_{10}$		10	1.00	

#### Table S3.3.1: Molecular formula, possible structure, DBE value, MCR value and suggested precursor of typical marke

IEPOX	$C_5H_{10}O_3$	OH OH	1	0.33	isoprene
2-methyl-tetrols	$C_{5}H_{12}O_{4}$	но	0	0.00	isoprene
2-methylglyceric acid	$C_4H_8O_4$	но	1	0.25	isoprene
Pinic acid	$C_9H_{14}O_4$	о о о о о о о о о о о о о о о о о о о	3	0.75	monoterpenes
MBTCA	$C_8H_{12}O_6$	он он он	3	0.50	monoterpenes
3-OH-4,4-DMG [Jaoui et al., 2008, doi: 10.1029/2007JD009426]	$C_7H_{12}O_5$	но ОН ОН ОН	2	0.40	monoterpenes

Pinonic acid	$C_{10}H_{16}O_3$	ОН СОН	3	1.00	monoterpenes
α-Pinene HOM	$C_{10}H_{16}O_9$	он он он он он	3	0.33	monoterpenes
α-pinene HOM	$C_{10}H_{14}O_7$	ноо	4	0.57	monoterpenes
α-pinene dimer [Beck et al., 2016, doi: 10.1016/j.atmosenv.2015.0 9.012]	$C_{17}H_{26}O_8$	но в страна стра	5	0.63	monoterpenes
sesquiterpene oxidation product [van Eijck et al., 2013, doi: 10.1016/j.atmosenv.2013.0 7.060]	$C_{10}H_{16}O_4$	HOHO	3	0.75	sesquiterpenes

β-caryophyllinic acid [van Eijck et al., 2013, doi: 10.1016/j.atmosenv.2013.0 7.060]	C <sub>14</sub> H <sub>22</sub> O <sub>4</sub>	но	4	1.00	sesquiterpenes
Tolene oxidation tracer [Jaoui et al., 2008, doi0: 10.1029/2007JD009426]	C <sub>5</sub> H <sub>8</sub> O <sub>5</sub>	Но ОН	2	0.40	toluene
Oligomers aqSOA I [Kalberer et al., 2004, doi: 10.1126/science.1092185]	$C_{15}H_{18}O_5$		7	1.00	phenolic
Oligomers aqSOA I [Kalberer et al., 2004, doi: 10.1126/science.1092185]	$C_{12}H_{18}O_9$	он Стон	4	0.44	cellulose
Adipic acid	$C_{6}H_{10}O_{4}$	но он	2	0.50	cyclohexene
Methylphthalic acid	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	HO	6	1.00	benzene

Phthalic acid	$C_8H_6O_4$	HO OH	6	1.00	benzene
C25-dicarboxylic acid	$C_{25}H_{48}O_4$	Но	2	0.50	fatty acids
Phenol	C <sub>6</sub> H <sub>6</sub> O	OH OH	4	1.00	
dimer aqueous phenol [Yu, et al., 2016, doi: 10.5194/acp-16-4511- 2016]	$C_{12}H_{10}O_2$	ОН НО	8	1.00	
Imidazole-carboxaldehyde [Kampf et al., 2016, doi: 10.1039/c6cp03029g]	C <sub>4</sub> H <sub>4</sub> ON <sub>2</sub>	H H	4	1.00	
Benzo(a)pyrene	C <sub>20</sub> H <sub>12</sub>		15	1.00	BB

Benzo(a)pyrene-dione	$C_{20}H_{10}O_2$		16	1.00	BB
combustion soot			1.07	1.00	BB
Abietic acid	$C_{20}H_{30}O_2$	но	6	1.00	BB
Nitro-catechol	C <sub>6</sub> H <sub>5</sub> O <sub>4</sub> N		5	1.00	BB, phenolic
Levoglucosan	$C_6H_{10}O_5$	он	2	0.40	BB, cellulose

# C. Supplementary material to chapter 4

## "Molecular evidence for the association of reactive oxygen species yield with oxidized organic compounds"

This supplementary material contains six figures (Figure S4.2.1, S4.3.1–S4.3.6) and twelve tables (Table S4.2.1, S4.3.1–S4.3.11).



Figure S4.2.1: Schematic outline of the experimental approach: collection of ambient fine particulate matter (PM) samples and sampling of secondary organic aerosols (SOA), samples extraction and application of different experimental techniques to measure organic components, H<sub>2</sub>O<sub>2</sub> yield and radical yield.



Figure S4.3.1: (a) Maximum carbonyl ratio (MCR)-Van Krevelen (VK) diagram. Oxidized organic compounds (OOC) include very highly oxidized organic compounds (dark blue), highly oxidized organic compounds (blue) and intermediately oxidized organic compounds (light blue), while unsaturated organic compounds (UOC) include oxidized unsaturated organic compounds (gray) and highly unsaturated organic compounds (dark gray). (b) Relative peak area-weighted fractions of OOC (blue) and UOC (gray) in the ambient PM<sub>2.5</sub> and laboratory SOA samples. The error bars represent the standard deviations of the relative peak area-weighted fractions of OOC and UOC in the samples collected at each location.

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Figure S4.3.2: Mass spectra (a–f) and MCR-VK diagrams (g–l) of OOC (blue) and UOC (gray) in ambient fine PM samples collected from different locations. The size of symbols in MCR-VK diagrams is proportional to the fourth root of the abundance of each compound.

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Figure S4.3.3: Mass spectra (a–f) and MCR-VK diagrams (g–l) of OOC (blue) and UOC (gray) in ambient fine PM samples collected from different locations. The size of symbols in MCR-VK diagrams is proportional to the fourth root of the abundance of each compound.

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Figure S4.3.4: Correlation of volume-normalized H<sub>2</sub>O<sub>2</sub> yield (a), volume-specific radical yield (b), mass-specific H<sub>2</sub>O<sub>2</sub> yield (c) and mass-specific radical yield (d) with the concentration of ambient fine PM samples. The error bars at x-axis represent the standard deviations of the concentration of fine PM samples collected at each location, and the error bars at y-axis represent the standard deviations of H<sub>2</sub>O<sub>2</sub> yield (a, b) and radical yield (c, d), respectively.



Figure S4.3.5: Relative fraction of  $H_2O_2$  (concentration of  $H_2O_2$  to the sum of  $H_2O_2$  and radicals, orange color) and relative fraction of radical (concentration of radical to the sum of  $H_2O_2$  and radicals, green color) generated by ambient  $PM_{2.5}$  samples from each site (a) or SOA samples from each laboratory experiment

(b). The error bars represent the standard deviations of the relative fraction of  $H_2O_2$  and radical.



Figure S4.3.6: Correlation of mass-specific ROS yield (a, d), H<sub>2</sub>O<sub>2</sub> yield (b, e) radical yield (c, f) with the relative peak area-weighted fraction of OOC of ambient fine PM samples (a, b, c) and laboratory SOA samples (d, e, f), respectively.

Site	Location	Air flow rate L <sup>-1</sup> min <sup>-1</sup>	Volume of air/m <sup>3</sup>	Particle size	Sampler	Sampling time
			293	PM <sub>2.5</sub>		02-05/06/2017
II	61.85°N,	25	252	PM <sub>2.5</sub>	Dekati PM <sub>10</sub> impactor	21-26/06/2017
нуупага	24.29°E	55	100	PM <sub>2.5</sub>	(Dekati Ltd., Tampere, Finland)	26-28/06/2017
			99	PM <sub>2.5</sub>		28-30/06/2017
			80	PM <sub>1.8</sub>		22-24/08/2017
Maina	Mainz 49.99°N,		80	PM <sub>1.8</sub>	MOUDI (122R, MSP	26-28/08/2017
Maniz	8.23°E	29	80	PM <sub>1.8</sub>	corporation, USA)	28-30/08/2017
			80	PM <sub>1.8</sub>		25-27/09/2017
			22	PM <sub>2.5</sub>		26-27/02/2019
			22	PM <sub>2.5</sub>		27-28/02/2019
			22	PM <sub>2.5</sub>		28-29/02/2019
Beijing 116.27°E 40.15°N			22	PM <sub>2.5</sub>		01-02/03/2019
	116.27°E,	15	22	PM <sub>2.5</sub>	Homemade PM <sub>2.5</sub>	02-03/03/2019
	40.15°N	15	21	PM <sub>2.5</sub>	sampler	03-04/03/2019
			22	PM <sub>2.5</sub>		04-05/03/2019
			22	PM <sub>2.5</sub>		08-09/03/2019
			22	PM <sub>2.5</sub>		09-10/03/2019
			22	PM <sub>2.5</sub>		10-11/03/2019
			1612	PM <sub>2.5</sub>		01-02/01/2014
			1585	PM <sub>2.5</sub>	Homemade PM <sub>2.5</sub> sampler	19-20/01/2014
Shanahai	121.43°E, 34.50°N	1050	1620	PM <sub>2.5</sub>		20-21/01/2014
Shanghai		1050	1628	PM <sub>2.5</sub>		24-25/01/2014
			1614	PM <sub>2.5</sub>		26-27/01/2014
			1612	PM <sub>2.5</sub>		27-28/01/2014
			1690	PM <sub>2.5</sub>		05-06/01/2014
			1599	PM <sub>2.5</sub>		06-07/01/2014
Guanazhou	113.27°Е,	1050	1596	PM <sub>2.5</sub>	Homemade PM <sub>2.5</sub>	11-12/01/2014
Gualigzilou	23.13°N	1050	1601	PM <sub>2.5</sub>	sampler	08-09/01/2014
			1616	PM <sub>2.5</sub>		12-13/01/2014
			1646	PM <sub>2.5</sub>		13-14/01/2014
			72	PM <sub>2.5</sub>		05-06/11/2018
	108 95°F		72	PM <sub>2.5</sub>	Tisch TE-20-800	06-07/11/2018
Xi'an	34.27°N	50	72	PM <sub>2.5</sub>	USA	07-08/11/2018
			72	PM <sub>2.5</sub>		08-09/11/2018
			60	PM <sub>2.5</sub>		09-10/11/2018

### Table S4.2.1: Ambient particle sampling information

Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
C4H6O5	134.0215	0.41	0.40	1.50	1.25
C8H12O6	204.0634	2.29	0.50	1.50	0.75
C5H12O7S	216.0304	0.37	0.00	2.40	1.40
C3H4O4	104.0110	0.41	0.50	1.33	1.33
C7H10O5	174.0528	0.77	0.60	1.43	0.71
C8H12O5	188.0685	1.27	0.60	1.50	0.63
C7H10O6	190.0477	0.55	0.50	1.43	0.86
C9H14O5	202.0841	2.76	0.60	1.56	0.56
C10H16O5	216.0998	2.98	0.60	1.60	0.50
C9H12O6	216.0634	2.40	0.67	1.33	0.67
C9H12O6	216.0634	1.53	0.67	1.33	0.67
C8H12O6	204.0634	1.52	0.50	1.50	0.75
C8H12O6	204.0634	0.61	0.50	1.50	0.75
C6H8O5	160.0372	0.47	0.60	1.33	0.83
C13H20O5	256.1311	4.97	0.80	1.54	0.38
C7H10O4	158.0579	1.65	0.75	1.43	0.57
C5H8O4	132.0423	0.47	0.50	1.60	0.80
C7H8O5	172.0372	0.74	0.80	1.14	0.71
C8H10O6	202.0477	0.79	0.67	1.25	0.75
C9H14O5	202.0841	1.49	0.60	1.56	0.56
C5H6O5	146.0215	0.39	0.60	1.20	1.00
C12H18O5	242.1154	3.87	0.80	1.50	0.42
C7H8O6	188.0321	0.48	0.67	1.14	0.86
C5H8O6	164.0321	0.38	0.33	1.60	1.20
C10H14O5	214.0841	2.60	0.80	1.40	0.50
C3H6O5S	153.9936	0.40	0.20	2.00	1.67
C6H8O4	144.0423	0.69	0.75	1.33	0.67
C9H12O7	232.0583	0.82	0.57	1.33	0.78
C7H10O6	190.0477	0.96	0.50	1.43	0.86
C8H14O5	190.0841	1.23	0.40	1.75	0.63
C9H12O5	200.0685	2.35	0.80	1.33	0.56
C9H14O6	218.0790	1.26	0.50	1.56	0.67
C9H12O6	216.0634	0.67	0.67	1.33	0.67
C8H10O7	218.0427	0.48	0.57	1.25	0.88
C7H12O7S	240.0304	0.49	0.29	1.71	1.00
C10H16O4	200.1049	4.23	0.75	1.60	0.40
C6H14O6	182.0790	0.34	0.00	2.33	1.00
C10H18O7S	282.0773	0.75	0.29	1.80	0.70
C2H4O5S	139.9779	0.37	0.20	2.00	2.50
C8H14O6	206.0790	0.57	0.33	1.75	0.75
C2H4O2	60.0211	0.42	0.50	2.00	1.00
C6H10O7S	226.0147	0.49	0.29	1.67	1.17
C3H6O4S	137.9987	0.38	0.25	2.00	1.33
C8H14O4	174.0892	1.36	0.50	1.75	0.50
C7H10O4	158.0579	1.19	0.75	1.43	0.57
C2H4N2O5	136.0120	0.35	0.40	2.00	2.50
C8H12O8S	268.0253	0.55	0.38	1.50	1.00
C3H4N2O4	132.0171	0.37	0.75	1.33	1.33
C4H6O4	118.0266	0.54	0.50	1.50	1.00
C5H8O5	148.0372	0.46	0.40	1.60	1.00
C9H16O4	188.1049	3.71	0.50	1.78	0.44
C6H10O5	162.0528	0.57	0.40	1.67	0.83
C5H8O4	132.0423	0.78	0.50	1.60	0.80
C3H4O3	88.0160	0.38	0.67	1.33	1.00
C5H6O4	130.0266	0.59	0.75	1.20	0.80
C4H4O4	116.0110	0.46	0.75	1.00	1.00
C6H10O4	146.0579	1.66	0.50	1.67	0.67
C6H10O4	146.0579	0.62	0.50	1.67	0.67
C4H8O4	120.0423	0.44	0.25	2.00	1.00
C7H12O4	160.0736	0.86	0.50	1.71	0.57
C5H8O4	132.0423	1.08	0.50	1.60	0.80
C5H10O4	134.0579	0.47	0.25	2.00	0.80
C6H5NO3	139.0269	3.73	1.00	0.83	0.50

Table S4.3.1 Molecular formulas of organic compounds detected in Hyytiälä OA in ESI- mode.
For	mula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
0	C2H4O4	92.0110	0.15	0.25	2.00	2.00
С	2H4O6S	155.9729	0.36	0.17	2.00	3.00
C	8H10O5	186.0528	3.02	0.80	1.25	0.63
C	5H8O7S	211.9991	0.45	0.29	1.60	1.40
C	7H10O5	174.0528	0.76	0.60	1.43	0.71
C	4H8O6S	184.0042	0.44	0.17	2.00	1.50
Ce	oH1007S	226.0147	0.50	0.29	1.67	1.17
CS	0H4N2O3	140.0222	2.36	1.00	0.80	0.60
C.	3H0U05	169.9885	0.40	0.17	2.00	2.00
	оп12075 8H1205	188 0685	0.38	0.00	2.40	0.63
C	9H16O4	188.0085	3.71	0.50	1.50	0.03
CI	0H16O6	232.0947	3.04	0.50	1.60	0.60
0	C5H8O6	164.0321	0.37	0.33	1.60	1.20
C5	5H10O6S	198.0198	0.56	0.17	2.00	1.20
C5H	10N2O11S	306.0005	2.58	0.18	2.00	2.20
C	C5H6O5	146.0215	0.38	0.60	1.20	1.00
C7	7H12O7S	240.0304	0.63	0.29	1.71	1.00
C	C7H8O6	188.0321	0.48	0.67	1.14	0.86
C8	H11NO7	233.0536	3.02	0.57	1.38	0.88
С	4H4O6S	179.9729	0.46	0.50	1.00	1.50
Ce	5H12O7S	228.0304	0.48	0.14	2.00	1.17
C	5H8O6S	196.0042	0.46	0.33	1.60	1.20
C	8H1006	202.0477	0.78	0.67	1.25	0.75
CSH	10N20115	306.0005	2.33	0.18	2.00	2.20
	0H12U05	212.0555	0.94	0.17	2.00	1.00
	0111008 0112078	249.0485	2.00	0.30	1.30	1.00
C,	9H12075	232 0583	0.91	0.57	1.71	0.78
C	7H10O6	190.0477	0.93	0.57	1.33	0.86
0	C5H8O4	132.0423	0.47	0.50	1.60	0.80
C	7H7NO4	169.0375	3.80	1.00	1.00	0.57
С	9H12O6	216.0634	1.52	0.67	1.33	0.67
С	6H10O2	114.0681	2.73	1.00	1.67	0.33
C51	H9NO10S	274.9947	0.58	0.20	1.80	2.00
C101	H17NO10S	343.0573	2.65	0.30	1.70	1.00
C	C6H6O6	174.0164	0.40	0.67	1.00	1.00
C	7H12O5	176.0685	2.35	0.40	1.71	0.71
C	8H1007	218.0427	0.48	0.57	1.25	0.88
	3H12O8S	268.0253	0.60	0.38	1.50	1.00
	H10085	234.0096	0.49	0.58	1.43	1.14
Co	SH1006S	249.0485	2.49	0.30	1.38	1.00
C1	0H14O6	230.0790	2 23	0.55	1.07	0.60
(	27H8O7	204 0270	0.43	0.57	1.14	1.00
C7	7H12O6S	224.0355	0.85	0.33	1.71	0.86
C10	H15NO9S	325.0468	3.00	0.44	1.50	0.90
C5H	10N2O11S	306.0005	3.07	0.18	2.00	2.20
C	4H6O6S	181.9885	0.44	0.33	1.50	1.50
CS	H16O7S	268.0617	2.15	0.29	1.78	0.78
C	C5H8O3	116.0473	0.50	0.67	1.60	0.60
C	3H4O8S	199.9627	0.36	0.25	1.33	2.67
C13	H24N2O4	272.1736	2.30	0.75	1.85	0.31
C	7H10O2	126.0681	1.23	1.00	1.43	0.29
Cl	1H16O6	244.0947	2.68	0.67	1.45	0.55
	оп14U/S	254.0460	1.00	0.29	1.75	0.88
C111	22030U8	422.1941	0.90	1.00	1.30	0.30
	8H1005	202.0909 186.0529	0.22	0.33	1./3	1.09
C C	7H5NO5	183.0520	2.20	1.00	0.71	0.05
C10	H17NO10S	343 0573	2.95	0.30	1 70	1.00
C10	3H20O3	224 1412	8.13	1.00	1.54	0.23
(	C4H4O5	132.0059	0.39	0.60	1.00	1.25

Table S4.3.2 Molecular formulas of organic compounds detected in Mainz OA in ESI- mode.

C5H8O2	100 0524	0.70	1.00	1.60	0.40
C6H10O	08 0732	3.02	1.00	1.67	0.17
CONTOO	98.0732	5.02	1.00	1.07	0.17
C10H18N2011S	374.0631	4.40	0.27	1.80	1.10
C10H16O7S	280.0617	1.06	0.43	1.60	0.70
C10H16O7S	280.0617	2.53	0.43	1.60	0.70
C8H12N2O10	296.0492	3.02	0.40	1.50	1.25
C5H6O3	114 0317	0.46	1.00	1.20	0.60
C(11002	120.0620	0.40	1.00	1.20	0.00
COHIOOS	150.0050	0.73	0.07	1.07	0.50
C/H/NO4	169.0375	4.60	1.00	1.00	0.57
C5H10O5S	182.0249	0.56	0.20	2.00	1.00
C10H7NO3	189.0426	7.73	1.00	0.70	0.30
C9H6O5	194.0215	2.59	1.00	0.67	0.56
C10H17NO8S	311.0675	3 70	0.38	1 70	0.80
C2112NO2	90.0112	0.29	0.58	1.70	1.50
C2H3NO3	89.0115	0.38	0.67	1.50	1.50
C5H10N2O11S	306.0005	1.70	0.18	2.00	2.20
C2H2O3	74.0004	0.37	0.67	1.00	1.50
C8H13NO11S	331.0209	1.05	0.27	1.63	1.38
C8H14O10S	302 0308	0.58	0.20	1 75	1 25
C61607	100.0114	0.30	0.57	1.00	1.25
C0H0O7	190.0114	0.58	0.57	1.00	1.17
C6H8O3	128.0473	0.49	1.00	1.33	0.50
C6H12O9S	260.0202	0.56	0.11	2.00	1.50
C8H6N2O2	162.0429	6.01	1.00	0.75	0.25
C8H10O6	202.0477	1 48	0.67	1.25	0.75
C7H12O2	128 0837	1.74	1.00	1.20	0.29
C/III202	154.0270	1.74	1.00	1.71	0.2)
C6H6N2O3	154.0378	2.84	1.00	1.00	0.50
C10H10O4	194.0579	3.76	1.00	1.00	0.40
C5H7NO5	161.0324	0.37	0.60	1.40	1.00
C5H9NO9S	258,9998	0.71	0.22	1.80	1.80
C5H0NO0S	258 0008	1.07	0.22	1.80	1.80
COLIONOA	238.9998	1.07	0.22	1.00	1.60
C8H9NO4	183.0532	3.34	1.00	1.13	0.50
C6H12O4	148.0736	0.54	0.25	2.00	0.67
C14H10O4	242.0579	5.00	1.00	0.71	0.29
C10H18N2O11S	374.0631	3.88	0.27	1.80	1.10
C7H4N2O7	228 0019	4.13	1.00	0.57	1.00
COLIONO5	100.0491	7.15	1.00	0.57	1.00
CongNO3	199.0481	5.52	1.00	1.15	0.05
C7H9NO7	219.0379	2.78	0.57	1.29	1.00
C7H10O4	158.0579	2.74	0.75	1.43	0.57
C4H6O5S	165.9936	0.40	0.40	1.50	1.25
C8H7NO3	165 0426	5.03	1.00	0.88	0.38
C8H1407S	254 0460	0.74	0.20	1 75	0.88
C3114073	201.0054	0.74	0.29	1.75	0.88
CITHT/NO8	291.0954	2.95	0.50	1.55	0.73
C9H6O5	194.0215	0.84	1.00	0.67	0.56
C10H18N2O11S	374.0631	3.23	0.27	1.80	1.10
C8H14O7S	254,0460	2.29	0.29	1.75	0.88
C2H4O2	76 0160	0.72	0.22	2.00	1.50
C2H4O3	70.0100	0.73	0.55	2.00	1.50
C9H6O6	210.0164	1.15	1.00	0.07	0.07
C8H7NO4	181.0375	3.86	1.00	0.88	0.50
C11H18N2O11	354.0911	8.07	0.36	1.64	1.00
C5H3NO4S	172.9783	0.60	1.00	0.60	0.80
C7H10O2	126 0681	2.88	1.00	1.43	0.29
C10H16089	206 0566	0.76	0.39	1.60	0.20
C10110003	290.0300	0.70	0.30	1.00	0.00
C3H3N3O3	129.0174	0.39	1.00	1.00	1.00
C10H15NO9	293.0747	3.26	0.44	1.50	0.90
C8H14O9S	286.0359	1.23	0.22	1.75	1.13
C9H16O7S	268.0617	0.87	0.29	1.78	0.78
C8H1406S	238 0511	1 55	0.33	1 75	0.75
C7U14049	230.0311	1.55	0.33	2.00	0.75
C/H14005	220.0511	2.1/	0.1/	2.00	0.80
C10H16O6	232.0947	0.87	0.50	1.60	0.60
C8H10O7	218.0427	1.04	0.57	1.25	0.88
C9H6O6	210.0164	1.90	1.00	0.67	0.67
C8H6O5	182 0215	2 80	1.00	0.75	0.63
C9U14O105	202.0213	2.00	0.20	1 75	1.05
	502.0508	2.28	0.20	1.75	1.25
C6H8O2	112.0524	1.14	1.00	1.33	0.33
C6H8O4	144.0423	1.29	0.75	1.33	0.67
C7H7NO3	153.0426	5.16	1.00	1.00	0.43
C11H21NO9	311 1216	2 48	0.22	1 91	0.82
CQHONO2	167 0592	755	1.00	1.71	0.02
	107.0382	1.55	1.00	1.13	0.38
C*/H/N2()38	195,9943	3.15	1.00	0.57	0.43
071141(2035					
C5H3NO5	157.0011	0.75	1.00	0.60	1.00

C7H12O9S	272 0202	0.76	0.22	1 71	1 29
COLIONOS	100.0491	0.70	1.00	1.71	0.62
Conginos	199.0481	2.47	1.00	1.15	0.05
C/H804	156.0423	2.57	1.00	1.14	0.57
C10H10O4	194.0579	3.14	1.00	1.00	0.40
C6H6O4	142.0266	0.46	1.00	1.00	0.67
C4H9NO9S	246,9998	0.53	0.11	2.25	2.25
C4H3NO2S	128 0884	0.55	1.00	0.75	0.50
C4H5NO25	128.9884	0.00	1.00	0.73	0.30
C9H15N08S	297.0518	3.28	0.38	1.6/	0.89
C5H5NO3	127.0269	1.05	1.00	1.00	0.60
C13H20O6	272.1260	3.12	0.67	1.54	0.46
C5H10O5S	182,0249	0.96	0.20	2.00	1.00
C4H608	182.0063	0.70	0.25	1.50	2.00
C411008	182.0005	0.47	0.25	1.00	2.00
Continuos	2/3.0155	2.69	0.22	1.83	1.50
C12H14O5	238.0841	3.40	1.00	1.17	0.42
C5H4O4	128.0110	0.43	1.00	0.80	0.80
C7H5NO6	199.0117	3.47	1.00	0.71	0.86
C8H6O5	182 0215	1.09	1.00	0.75	0.63
C7111002	142.0620	0.77	1.00	1.42	0.03
C/H1003	142.0630	0.77	1.00	1.43	0.43
C6H3N3O7	228.9971	4.12	1.00	0.50	1.17
C7H6O6	186.0164	0.46	0.83	0.86	0.86
C8H7NO5	197.0324	4.71	1.00	0.88	0.63
C7H6N2O6	214.0226	3 52	1.00	0.86	0.86
C111119N2O10	229.00(1	7.72	0.40	1.64	0.00
CITHI8N2010	338.0961	1.47	0.40	1.64	0.91
C8H13N08	251.0641	1.23	0.38	1.63	1.00
C7H8O8S	251.9940	0.58	0.50	1.14	1.14
C12H15NO3	221.1052	7.05	1.00	1.25	0.25
C20H14N2OS	330 0827	673	1.00	0.70	0.05
C12U19O5	254 1154	7.40	1.00	1.20	0.05
C13H1805	254.1154	7.40	1.00	1.58	0.38
C8H6N2O5	210.0277	7.33	1.00	0.75	0.63
C10H12O7	244.0583	0.67	0.71	1.20	0.70
C10H20O5S2	284.0752	3.54	0.20	2.00	0.50
C11H19NO9	309 1060	3 80	0.33	1 73	0.82
Cellie	210,0026	5.07	0.55	1.75	0.62
C8H18045	210.0926	0.47	0.00	2.23	0.50
C14H22O4	254.1518	6.69	1.00	1.57	0.29
C8H10O4	170.0579	1.09	1.00	1.25	0.50
C4H8O4	120.0423	0.95	0.25	2.00	1.00
C9H16O4	188 1049	2.58	0.50	1 78	0.44
C5H7NOOS	256 0842	1 77	0.22	1.40	1.80
C3H/N093	230.9842	1.//	0.33	1.40	1.60
C/HIINOI0S	301.0104	1.08	0.30	1.57	1.43
C7H10O3	142.0630	2.33	1.00	1.43	0.43
C4H8O2	88.0524	0.49	0.50	2.00	0.50
C13H18O7	286,1053	2.78	0.71	1.38	0.54
C74604	154.0266	1.21	1.00	0.86	0.57
C/H004	134.0200	1.51	1.00	0.80	0.57
C12H16O7	272.0896	2.69	0.71	1.33	0.58
C14H24O4	256.1675	3.92	0.75	1.71	0.29
C12H18O5	242.1154	3.87	0.80	1.50	0.42
C8H11NO8	249 0485	0.82	0.50	1 38	1.00
C64602	126.0217	0.02	1.00	1.00	0.50
C011003	120.0317	0.47	1.00	1.00	0.50
C10H14O2	166.0994	7.20	1.00	1.40	0.20
C7H4N2O4	180.0171	3.50	1.00	0.57	0.57
C6H8O3	128.0473	2.33	1.00	1.33	0.50
C14H6N4O5	310.0338	1.22	1.00	0.43	0.36
C10H12N2O6	256.0605	8.02	1.00	1.20	0.50
C10H12N2O0	230.0093	0.03	1.00	1.20	0.00
C9H16O5	204.0998	0.88	0.40	1./8	0.56
C12H9NO3	215.0582	8.10	1.00	0.75	0.25
C8H8O3	152.0473	2.64	1.00	1.00	0.38
C9H13NO8	263 0641	3.10	0.50	1 44	0.89
C74805	172 0272	2 70	0.20	1 1/	0.71
	1/2.03/2	2.19	0.80	1.14	0.71
C9H10O6	214.04/7/	0.71	0.83	1.11	0.67
C8H8O6	200.0321	0.55	0.83	1.00	0.75
C6H4O5	156.0059	0.72	1.00	0.67	0.83
C8H18O3S	194 0977	5 21	0.00	2.25	0.38
C9U12NO4	210.0742	2.02	0.00	1.42	0.30
ContSINUO	219.0/45	5.02	0.50	1.03	0.75
C12H7NO4	229.0375	7.99	1.00	0.58	0.33
C7H13NO9S	287.0311	2.78	0.22	1.86	1.29
C6H6O3S	158,0038	0.76	1.00	1.00	0.50
C5H4O3	112.0160	0.42	1.00	0.80	0.60
651403	00.0270	0.42	1.00	1.00	0.00
	98 11368	04/	1.00	1.20	0.40
C5H6O2	20.0500	0.17			~ ~ ~
C6H10O5S	194.0249	0.54	0.40	1.67	0.83

C8H5NO5	105 0168	3.14	1.00	0.63	0.63
Consider	195.0108	5.14	1.00	0.05	0.03
C9H13NO7	247.0692	3.28	0.57	1.44	0.78
C6H8O2	112.0524	0.56	1.00	1.33	0.33
C1011409	200 0045	2.69	0.62	1.22	0.67
C12H10O8	288.0843	2.08	0.05	1.55	0.07
C14H22O7	302.1366	3.06	0.57	1.57	0.50
C6H12O6S	212 0355	1 57	0.17	2.00	1.00
CTHONOA	171.0533	0.40	1.00	2.00	1.00
C/H9NO4	1/1.0532	0.49	1.00	1.29	0.57
C6H11NO10S	289.0104	0.70	0.20	1.83	1.67
C13H18O6	270 1103	2.88	0.83	1 38	0.46
015111800	270.1103	2.00	0.85	1.56	0.40
C11H19NO9	309.1060	5.63	0.33	1.73	0.82
C5H12O5S	184 0405	0.54	0.00	2.40	1.00
C9U1409S	270.0400	1 20	0.25	1 75	1.00
C6H14O65	270.0409	1.20	0.25	1.75	1.00
C7H5NO6	199.0117	2.68	1.00	0.71	0.86
C11H10O5	222.0528	2.90	1.00	0.91	0.45
COLLIENOC	222.0800	2.22	0.50	1.77	0.67
C9HI5NO6	255.0899	3.23	0.50	1.07	0.67
C8H13NO8	251.0641	0.85	0.38	1.63	1.00
C9H7NO6	225 0273	3 20	1.00	0.78	0.67
C)11/1000	225.0275	3.20	1.00	0.70	0.07
C13H20O5	256.1311	4.64	0.80	1.54	0.38
C6H5NO3	139.0269	0.49	1.00	0.83	0.50
C7H8O3	140.0473	0.52	1.00	1.14	0.43
0/11805	140.0473	0.52	1.00	1.14	0.43
C9H14O8S	282.0409	1.91	0.38	1.56	0.89
C6H10O5	162.0528	2.43	0.40	1.67	0.83
CIOUITNOTS	205.0726	4.71	0.42	1.70	0.70
CIUHI/NO/S	293.0726	4./1	0.45	1.70	0.70
C8H6O2	134.0368	1.80	1.00	0.75	0.25
C8H12N2O11	312 0441	3 49	0.36	1 50	1 38
C511405	144.0050	0.20	0.00	0.90	1.00
C5H4O5	144.0059	0.39	0.80	0.80	1.00
C4H4O2	84.0211	0.39	1.00	1.00	0.50
C5H8O	84 0575	0.75	1.00	1.60	0.20
0.51180	84.0373	0.75	1.00	1.00	0.20
C5H9NO8S	243.0049	2.59	0.25	1.80	1.60
C8H8O6	200.0321	2.60	0.83	1.00	0.75
C9H12NO0	267.0500	1.07	0.22	1.62	1 12
C8H15N09	267.0390	1.07	0.55	1.05	1.15
C7H9NO9	251.0277	0.66	0.44	1.29	1.29
C12H9NO4	231 0532	7 42	1.00	0.75	0.33
0121191101	102.0050	2.02	1.00	0.15	0.55
C9H4O5	192.0059	2.82	1.00	0.44	0.56
C3H2N2O3	114.0065	0.42	1.00	0.67	1.00
C16H12OS	252.0609	2 23	1.00	0.75	0.06
CIALIZINO	202.1016	2.23	1.00	1.75	0.00
CI2H2INO9	323.1216	3.34	0.33	1.75	0.75
C10H17NO7S	295.0726	7.04	0.43	1.70	0.70
COMONICO	228 0382	4.05	1.00	1.00	0.75
Conolv200	228.0382	4.05	1.00	1.00	0.75
C11H19N3O15	433.0816	8.09	0.27	1.73	1.36
C7H5NO5	183 0168	1.27	1.00	0.71	0.71
C201112N2O2S	275 0679	0.02	1.00	0.65	0.15
C20H15N3055	373.0078	0.23	1.00	0.05	0.15
C8H9NO4	183.0532	7.00	1.00	1.13	0.50
C11H6N4OS	242,0262	0.63	1.00	0.55	0.09
CTUENOS	151 0002	2.02	1.00	0.71	0.14
C/H5NOS	151.0092	5.95	1.00	0.71	0.14
C9H15NO8S	297.0518	2.92	0.38	1.67	0.89
C13H22O4	242 1518	674	0.75	1 69	0.31
C10U140(S	2(2.0511	2.01	0.75	1.05	0.01
C10H14005	202.0511	5.01	0.07	1.40	0.00
C15H22O6	298.1416	3.14	0.83	1.47	0.40
C4H6O	70 0419	0.44	1.00	1.50	0.25
COLLEGO	200 0515	1 22	0.11	2.00	1.12
Con10095	200.0515	1.22	0.11	2.00	1.13
C10H12O7	244.0583	2.46	0.71	1.20	0.70
C5H5NO4	143.0219	1.25	1.00	1.00	0.80
C16112607	214 1720	7 01	0 47	1 42	0.20
C16H26O6	314.1729	1.21	0.07	1.05	0.38
C8H15NO9S	301.0468	2.34	0.22	1.88	1.13
C5H5NO3	127 0269	0.38	1.00	1.00	0.60
041123102	112 0112	0.50	1.00	1.00	0.00
C4H3NO3	113.0113	0.54	1.00	0.75	0.75
C8H16N2O5S2	284.0501	1.45	0.40	2.00	0.63
C9H16O4	188 1049	1 46	0.50	1 78	0.44
C/III00+	100.1047	1.70	0.00	1.70	1.50
C6H11NO9S	2/3.0155	0.99	0.22	1.83	1.50
C8H13NO10S	315.0260	2.69	0.30	1.63	1.25
C0H15NO7	240 0840	2 01	0.43	1.67	0.78
CHIJNU/	247.0047	2.91	0.45	1.07	0.70
C6H7NO5	173.0324	0.75	0.80	1.17	0.83
C9H8O5	196.0372	2.76	1.00	0.89	0.56
C7U604	154 0266	2.70	1.00	0.02	0.57
C/H0U4	134.0200	2.39	1.00	0.80	0.57
C7H7NO2	137.0477	2.36	1.00	1.00	0.29
C15H22O9	346 1264	2 92	0.56	1 47	0.60
0(110)005	104 0100	4.40	1.00	1.77	0.00
C6H4N2O5	184.0120	4.48	1.00	0.67	0.83
C10H14O8S	294.0409	0.87	0.50	1.40	0.80
C7H9NO8	235 0328	1.05	0.50	1 20	1.14
0/11/11/00	233.0320	1.05	0.50	1.47	1.17

C8H6O3	150 0317	0.84	1.00	0.75	0.38
C8H14O2	142 0004	2.17	1.00	1.75	0.36
C71111NO2	227.0495	5.17	0.29	1.75	0.23
C/HIINO8	237.0485	1.54	0.38	1.57	1.14
C10H13NO4	211.0845	7.68	1.00	1.30	0.40
C10H18N2O11S	374.0631	5.00	0.27	1.80	1.10
C9H9NO6	227.0430	3.37	1.00	1.00	0.67
C11H9NO3	203.0582	8.07	1.00	0.82	0.27
C7H4N2O3	164 0222	3.08	1.00	0.57	0.43
C0111002	150.0691	2.76	1.00	1.11	0.43
C9H1002	150.0681	3.70	1.00	1.11	0.22
C10H6N2O5	234.0277	7.62	1.00	0.60	0.50
C5H11N3O11	289.0394	2.67	0.18	2.20	2.20
C8H6O3	150.0317	1.16	1.00	0.75	0.38
C10H6O5	206.0215	3.17	1.00	0.60	0.50
C5H10N2O8	226 0437	2 91	0.25	2.00	1.60
C101119N2O9	204 1062	672	0.29	1.00	0.80
C10H18N208	294.1003	0.73	0.38	1.00	0.80
C8HTINO5	201.0637	0.93	0.80	1.38	0.63
C13H8O2	196.0524	7.53	1.00	0.62	0.15
C7H5NO4	167.0219	3.77	1.00	0.71	0.57
C11H15NO2	193.1103	7.18	1.00	1.36	0.18
C12H16O5	240.0998	5 50	1.00	1 33	0.42
C01111NO2	191.0720	7.05	1.00	1.55	0.42
C7U902	101.0/39	1.95	1.00	1.22	0.55
C/H8O3	140.0473	2.53	1.00	1.14	0.43
C5H10O2	102.0681	0.62	0.50	2.00	0.40
C8H9NO5	199.0481	5.36	1.00	1.13	0.63
C10H17N3O11	355,0863	7.47	0.36	1.70	1.10
C3H2N2O4	130 0015	0.59	1.00	0.67	1 33
C12U2009	201 0070	0.57	0.20	1 47	0.67
C12H20085	324.0879	2.75	0.58	1.07	0.07
C8H12O2	140.0837	1.16	1.00	1.50	0.25
C16H19NO3	273.1365	7.39	1.00	1.19	0.19
C8H10O5	186.0528	8.26	0.80	1.25	0.63
C9H12O7S	264 0304	1.74	0.57	1.33	0.78
C11H6N/OS	242 0262	0.91	1.00	0.55	0.09
COLIONADS	242.0202	1.96	1.00	1.00	0.03
C8H8N4055	272.0215	1.80	1.00	1.00	0.65
C8H8O6	200.0321	0.93	0.83	1.00	0.75
C9H16O6S	252.0668	4.10	0.33	1.78	0.67
C12H12O5	236.0685	3.15	1.00	1.00	0.42
C7H6N2O3	166.0378	3.45	1.00	0.86	0.43
C8H7NO3	165 0426	2.13	1.00	0.88	0.38
C5H8O	84.0575	0.54	1.00	1.60	0.30
CJHOU	84.0373	0.34	1.00	1.00	0.20
C/H9NO9S	282.9998	0.99	0.44	1.29	1.29
C13H18O5	254.1154	3.11	1.00	1.38	0.38
C6H11NO8S	257.0205	2.08	0.25	1.83	1.33
C6H10O9S	258.0046	0.96	0.22	1.67	1.50
C10H17NO7S	295.0726	6.32	0.43	1.70	0.70
C10H18068	266 0824	2.61	0.33	1.80	0.60
COLLIZNOS	200.0824	2.01	0.33	1.00	0.00
CONTSINUS	227.0641	0.70	0.15	2.17	1.55
C10H20O4	204.1362	2.84	0.25	2.00	0.40
C16H29NO8	363.1893	8.19	0.38	1.81	0.50
C9H6O5	194.0215	1.25	1.00	0.67	0.56
C8H8O5S	216.0092	1.01	1.00	1.00	0.63
C8H6O5	182.0215	2.51	1.00	0.75	0.63
C10H17N078	295 0726	6.62	0.43	1 70	0.70
	273.0720	1 01	1.00	1.70	0.70
C10H9NU4	207.0552	4.84	1.00	0.90	0.40
C11H8O6	236.0321	2.98	1.00	0.73	0.55
C9H11NO4	197.0688	6.59	1.00	1.22	0.44
C7H14N2O8S	286.0471	1.26	0.25	2.00	1.14
C8H10O3	154.0630	2.68	1.00	1.25	0.38
C5H9N3O13S	350 9856	6.68	0.23	1.80	2.60
C15H20O10	360 1056	2 70	0.23	1.00	0.67
C13H20010	300.1030	2.19	0.00	1.33	0.07
C8H8N4O5S	272.0215	1.28	1.00	1.00	0.63
C4H7NO8S	228.9892	1.09	0.25	1.75	2.00
C6H9NO3	143.0582	0.64	1.00	1.50	0.50
C9H8N4O3S2	284.0038	2.29	1.00	0.89	0.33
C5H9N078	227 0100	3 14	0.29	1.80	1 40
C10H0NO4	207 0522	1 50	1.00	0.00	0.40
C10117INU4	201.0332	4.32	1.00	1.90	1.00
C11H20N2O11	356.1067	3.75	0.27	1.82	1.00
C8H8N2O6	228.0382	3.76	1.00	1.00	0.75
C5H8O2	100.0524	2.37	1.00	1.60	0.40
C15H24O6	300.1573	7.11	0.67	1.60	0.40
C6H12O4	148 0736	1.28	0.25	2.00	0.67
20111201	1.0.0750	1.20	0.20	2.00	0.07

C12H15NO4	227 1001	5.60	1.00	1.25	0.22
C12H15N04	257.1001	5.00	1.00	1.23	0.33
C9H10O3	166.0630	3.07	1.00	1.11	0.33
C8H7NO3	165 0426	3 18	1.00	0.88	0.38
011/1005	105.0420	5.10	1.00	0.00	0.50
C4H5N3O2	127.0382	1.08	1.00	1.25	0.50
C10H11NO6	241 0586	3 52	1.00	1 10	0.60
CIONINGO	211.0500	0.66	1.00	1.10	0.00
C10H18O6	234.1103	0.66	0.33	1.80	0.60
C10H19NO7	265.1162	3.16	0.29	1.90	0.70
CTULINOC	205.0596	2.94	0.50	1 57	0.96
C/HIINO6	205.0580	2.84	0.50	1.57	0.80
C14H26O4	258.1831	4.33	0.50	1.86	0.29
C0H16O2	172 1000	2 75	0.67	1 79	0.22
C9H10O3	172.1099	2.75	0.07	1.70	0.33
C10H17N3O10	339.0914	8.22	0.40	1.70	1.00
C10H16N2O10S	356 0526	7 39	0.40	1.60	1.00
C1011101(20105	350.0520	7.57	0.40	1.00	1.00
C8H16O4	176.1049	2.39	0.25	2.00	0.50
C13H8O2	196 0524	7.16	1.00	0.62	0.15
C71111NO100	201.0104	1.04	0.20	1.57	1.42
C/HIINOI0S	301.0104	1.84	0.30	1.57	1.43
C10H14O7S	278.0460	2.56	0.57	1.40	0.70
COLIZNOS	200 0224	2.06	1.00	0.79	0.56
C9H/NO5	209.0524	5.90	1.00	0.78	0.30
C8H13NO7	235.0692	2.72	0.43	1.63	0.88
C7H11NO7	221.0536	3 13	0.43	1.57	1.00
C/IIIINO/	221.0550	5.15	0.45	1.57	1.00
C17H24O10	388.1369	3.05	0.60	1.41	0.59
C7H9NO5	187 0481	2 79	0.80	1 29	0.71
C1011105	107.0401	2.79	0.00	1.27	0.71
C13H16O6	268.0947	2.98	1.00	1.23	0.46
C5H7NO9S	256,9842	0.76	0.33	1.40	1.80
CELENIOS	122 0220	1 57	1.00	0.02	0.22
CONJNU2	125.0520	1.37	1.00	0.85	0.55
C15H13NO2S	271.0667	4.11	1.00	0.87	0.13
C15H25NO7	331 1631	7 70	0.57	1.67	0.47
C1511251007	551.1051	7.70	0.57	1.07	0.47
C8H9NO4	183.0532	4.14	1.00	1.13	0.50
C10H22O4	31/ 1518	7 71	1.00	1 16	0.21
01/11/22/04	514.1510	7.71	1.00	1.10	0.21
C8H18O4S	210.0926	7.18	0.00	2.25	0.50
C6H5NO5	171 0168	1.05	1.00	0.83	0.83
COLIZINOS	225.0272	2.60	1.00	0.05	0.65
C9H/NO6	225.0273	3.68	1.00	0.78	0.67
C6H12N2O5S	224.0467	7.57	0.40	2.00	0.83
C0H12NO10S	227 0260	2.16	0.40	1.4.4	1 1 1
CONTINUIUS	527.0200	5.10	0.40	1.44	1.11
C3H6O	58.0419	0.54	1.00	2.00	0.33
C13H9NO3	227 0582	8 23	1.00	0.69	0.23
0151151105	227.0502	0.25	1.00	0.07	0.20
C5H8O	84.0575	2.79	1.00	1.60	0.20
C10H17NO7	263 1005	4.19	0.43	1.70	0.70
COULCOAS	220.07(0	2.01	0.50	1 70	0.44
C9H1004S	220.0769	2.01	0.50	1./8	0.44
C16H19NO3	273.1365	7.72	1.00	1.19	0.19
C9H9N2O4	106 0484	2 1 9	1.00	1.00	0.50
ConoN204	190.0484	5.18	1.00	1.00	0.30
C18H14O8	358.0689	7.45	1.00	0.78	0.44
C13H0NO28	243 0354	1.64	1.00	0.60	0.15
C151191(025	243.0334	1.04	1.00	0.09	0.15
C4H4O3	100.0160	2.78	1.00	1.00	0.75
C11H22O7	266 1366	0.76	0.14	2.00	0.64
G10111207	200.1500	2.07	1.00	2.00	0.01
C12H18O4	226.1205	3.07	1.00	1.50	0.33
C9H13NO10S	327.0260	2.78	0.40	1.44	1.11
C7U7NO5	195 0224	2.50	1.00	1.00	0.71
C/H/NO3	185.0524	2.39	1.00	1.00	0.71
C16H20O10	372.1056	2.77	0.70	1.25	0.63
C4H4N2O4	144 0171	0.95	1.00	1.00	1.00
	100.0122	0.75	1.00	1.00	1.00
C9H8O4	180.0423	1.36	1.00	0.89	0.44
C9H15NO7	249.0849	4.78	0.43	1.67	0.78
CAUNIO7	207 0270	2 62	0.42	1 50	1 17
CONSINU/	207.0379	2.03	0.43	1.50	1.1/
C11H14N2O4	238.0954	7.57	1.00	1.27	0.36
C12H16O4	224 1049	3.08	1.00	1 33	0.33
001004	227.1047	5.00	1.00	1.55	0.55
C9H9NO7S	275.0100	3.34	0.86	1.00	0.78
C8H6O5	182 0215	1.90	1.00	0.75	0.63
017110400	256 1471	1.70	1.00	1 41	0.05
C1/H2408	356.14/1	3.13	0.75	1.41	0.47
C3H6O2	74.0368	3.02	0.50	2.00	0.67
C9U14O	126 1045	2.02	1.00	1 75	0.12
C8H14O	120.1045	2.33	1.00	1./5	0.15
C6H7NO	109.0528	0.72	1.00	1.17	0.17
C8H15NO8S	285 0518	3 22	0.25	1 99	1.00
Contightoos	203.0310	5.55	0.23	1.00	1.00
C10H16N2O10	324.0805	7.68	0.40	1.60	1.00
C8H8O4	168 0423	3 12	1.00	1.00	0.50
011004	100.0423	3.14	1.00	1.00	0.50
C9H9NO4	195.0532	6.23	1.00	1.00	0.44
C8H13NO4	187 0845	0.91	0.75	1.63	0.50
001700	1/2 0217	0.71	1.00	1.00	0.22
C9H6O3	162.0317	3.16	1.00	0.67	0.33
C9H6O3	162.0317	2.87	1.00	0.67	0.33
C14U0NO2	220.0592	0.01	1.00	0.64	0.21
C14H9NU3	239.0582	ð.21	1.00	0.64	0.21
C8H15NO10S	317.0417	2.72	0.20	1.88	1.25
C8H16O2	160 1000	1 10	0.33	2.00	0.38
0111003	100.1077	1.10	0.55	2.00	0.50

C16H20O11	388 1006	2 78	0.64	1.25	0.69
C10H22O5	340 2250	2.70	0.04	1.69	0.05
C19H52O5	270.0575	7.65	0.80	1.08	0.20
CI3HI0N40S	270.0575	2.15	1.00	0.77	0.08
C15H10N4O2S2	342.0245	1.22	1.00	0.67	0.13
C10H19NO11S	361.0679	2.82	0.18	1.90	1.10
C9H17NO7	251.1005	3.07	0.29	1.89	0.78
C13H6O10	321,9961	0.83	1.00	0.46	0.77
C14H1004S2	306.0020	0.88	1.00	0.71	0.29
C10117NO05	227.0624	4.24	0.22	0.71	0.29
CIUHI/NO9S	327.0624	4.54	0.55	1.70	0.90
CITH/NO5	233.0324	7.26	1.00	0.64	0.45
C16H10N4O4S2	386.0143	1.23	1.00	0.63	0.25
C7H5NO6	199.0117	0.97	1.00	0.71	0.86
C8H9NO3	167.0582	2.80	1.00	1.13	0.38
C7H6O5	170 0215	1.46	1.00	0.86	0.71
C9119045	200.0142	1.40	1.00	1.00	0.71
C0H0U45	200.0143	1.00	1.00	1.00	0.50
C8H/NO6	213.0273	3.26	1.00	0.88	0.75
C17H29NO9	391.1842	7.50	0.44	1.71	0.53
C8H16O3	160.1099	1.48	0.33	2.00	0.38
C8H9NO4	183.0532	4.70	1.00	1.13	0.50
C5H9NO3	131 0582	0.89	0.67	1.80	0.60
C5H806S	196.0042	1.05	0.33	1.60	1.20
CUINO2	141.0426	1.05	1.00	1.00	1.20
COH/NO3	141.0426	2.47	1.00	1.17	0.50
C9H10O5S	230.0249	2.53	1.00	1.11	0.56
C7H10O6S	222.0198	1.08	0.50	1.43	0.86
C12H20O7S	308.0930	2.82	0.43	1.67	0.58
C10H17NO7	263.1005	5.48	0.43	1.70	0.70
C7H5NO6	100.0117	1 57	1.00	0.71	0.86
C10H0N400	256.0410	1.57	1.00	0.71	0.00
C12H8N4OS	256.0419	1.06	1.00	0.67	0.08
C9H7NO3	177.0426	2.76	1.00	0.78	0.33
C7H6O4	154.0266	1.06	1.00	0.86	0.57
C16H19NO3	273.1365	8.21	1.00	1.19	0.19
C15H24O8S	364 1192	3.06	0.50	1.60	0.53
C14H10O5	258 0528	3.66	1.00	0.71	0.36
CONTINO	191 0275	1.49	1.00	0.71	0.50
C8H/NO4	181.0375	1.48	1.00	0.88	0.50
C11H20O/S	296.0930	2.52	0.29	1.82	0.64
C8H12O5	188.0685	8.07	0.60	1.50	0.63
C18H34O5	330.2406	7.45	0.40	1.89	0.28
C9H17NO8	267.0954	2.70	0.25	1.89	0.89
C12H12O4	220.0736	3 20	1.00	1.00	0.33
C8H6N2O7	242 0175	6.55	1.00	0.75	0.88
C011010207	242.0173	0.55	1.00	0.75	0.00
CITHI/NOI0S	355.0573	3.02	0.40	1.55	0.91
C12H16O10	320.0743	2.59	0.50	1.33	0.83
C16H26O6	314.1729	3.39	0.67	1.63	0.38
C11H19NO7	277.1162	7.00	0.43	1.73	0.64
C20H14N2OS	330.0827	4.28	1.00	0.70	0.05
C14H9NO5	271 0481	7.51	1.00	0.64	0.36
C111114N2O4	222 0054	7.01	1.00	1.27	0.36
C11H14N2O4	238.0934	7.91	1.00	1.27	0.30
C10H14O6	230.0790	8.23	0.67	1.40	0.60
C19H28O7	368.1835	7.18	0.86	1.47	0.37
C10H12O3	180.0786	7.88	1.00	1.20	0.30
C9H9NO3	179.0582	2.96	1.00	1.00	0.33
C13H17NO3	235.1208	7.58	1.00	1.31	0.23
C20H14N2OS	330 0827	5 50	1.00	0.70	0.05
C2U1141205	120 0770	2.50	0.20	2.00	2 50
0121100222	137.7/17	2.00	0.20	2.00	2.30
C13H10O3S2	2/8.00/1	1.64	1.00	0.77	0.23
C16H17NO4	287.1158	3.82	1.00	1.06	0.25
C10H13NO5	227.0794	3.99	1.00	1.30	0.50
C3H6O5S	153.9936	2.59	0.20	2.00	1.67
C6H6N2O2	138.0429	0.94	1.00	1.00	0.33
C10H18N2O10	326 0061	3 80	0.30	1.00	1.00
C17H24O7	242 1670	J.07	0.50	1.00	0.41
	342.10/9	1.91	0./1	1.55	0.41
C16H29NO7	347.1944	7.95	0.43	1.81	0.44
C6H6N2O3	154.0378	2.14	1.00	1.00	0.50
C14H18O5	266.1154	3.30	1.00	1.29	0.36
C14H8O4	240.0423	3.96	1.00	0.57	0.29
C9H8O2	148 0524	2 38	1.00	0.89	0.22
C10U16N200	200 0052	2.30	0.44	1 40	0.22
C10H10N209	508.0850	1.51	0.44	1.00	0.90
C8H8O4S	200.0143	2.70	1.00	1.00	0.50
C5H4O8S2	255.9348	2.05	0.50	0.80	1.60
C15H22O3	250.1569	8.28	1.00	1.47	0.20

C4H7NO3	117.0426	0.88	0.67	1.75	0.75
C7H12O	112.0888	2.69	1.00	1.71	0.14
C11H13NO5	239.0794	8.09	1.00	1.18	0.45
C14H20O5	268.1311	7.66	1.00	1.43	0.36
C7H12O	112.0888	1.33	1.00	1.71	0.14
C27H22O3	394.1569	8.39	1.00	0.81	0.11
C8H12O	124.0888	2.83	1.00	1.50	0.13
C11H19NO7	277.1162	3.89	0.43	1.73	0.64
C9H17NO9S	315.0624	6.32	0.22	1.89	1.00
C8H6N2O5	210.0277	3.41	1.00	0.75	0.63
C11H19N3O12	385.0969	7.68	0.33	1.73	1.09
C7H11NO4	173.0688	1.73	0.75	1.57	0.57
C13H8O3	212.0473	7.50	1.00	0.62	0.23
C11H19NO9S	341.0781	3.51	0.33	1.73	0.82
C13H23NO10S	385.1043	4.78	0.30	1.77	0.77
C13H18O4	238.1205	3.17	1.00	1.38	0.31
C12H21NO7	291.1318	7.49	0.43	1.75	0.58
C12H18O4	226.1205	5.85	1.00	1.50	0.33
C10H16N2O9	308.0856	7.86	0.44	1.60	0.90
C14H30O3S	278.1916	8.39	0.00	2.14	0.21
C5H7NO9S	256.9842	2.22	0.33	1.40	1.80
C9H15NO4	201.1001	1.52	0.75	1.67	0.44
C8H4N2O10S	319.9587	8.61	0.80	0.50	1.25
C10H13NO4	211.0845	6.62	1.00	1.30	0.40
C8H5NO7	227.0066	2.28	1.00	0.63	0.88
C13H20O3	224.1412	7.65	1.00	1.54	0.23
C16H24O2	248.1776	8.55	1.00	1.50	0.13
C20H14N2OS	330.0827	7.31	1.00	0.70	0.05
C6H11NO3	145.0739	1.45	0.67	1.83	0.50
C17H24O7	340.1522	8.11	0.86	1.41	0.41
C16H26N2O10	406.1587	8.39	0.50	1.63	0.63

Table S4.3.3 Molecular formulas of organic compounds detected in Beijing OA in ESI- mode.

Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
C6H5NO3	139.0269	3.72	1.00	0.83	0.50
C2H4O6S	155.9729	0.36	0.17	2.00	3.00
C4H6O5	134.0215	0.38	0.40	1.50	1.25
C3H6O6S	169.9885	0.38	0.17	2.00	2.00
C7H6O2	122.0368	2.70	1.00	0.86	0.29
C5H6O5	146.0215	0.38	0.60	1.20	1.00
C5H6O4	130.0266	0.40	0.75	1.20	0.80
C5H4N2O3	140.0222	2.36	1.00	0.80	0.60
C4H2O11S2	289.9039	0.34	0.36	0.50	2.75
C8H7NO3	165.0426	5.04	1.00	0.88	0.38
C13H8O2	196.0524	7.53	1.00	0.62	0.15
C7H6N2O5	198.0277	7.39	1.00	0.86	0.71
C7H7NO3	153.0426	5.95	1.00	1.00	0.43
C4H8O3	104.0473	0.10	0.33	2.00	0.75
C5H6O3	114.0317	0.40	1.00	1.20	0.60
C7H7NO3	153.0426	5.15	1.00	1.00	0.43
C5H8O3	116.0473	0.09	0.67	1.60	0.60
C6H6N2O3	154.0378	2.83	1.00	1.00	0.50
C5H8O4	132.0423	0.41	0.50	1.60	0.80
C2H4O2	60.0211	0.40	0.50	2.00	1.00
C8H8O3	152.0473	2.64	1.00	1.00	0.38
C9H6O6	210.0164	1.15	1.00	0.67	0.67
C8H6N2O2	162.0429	6.01	1.00	0.75	0.25
C18H14O8	358.0689	7.45	1.00	0.78	0.44
C4H6O6S	181.9885	0.39	0.33	1.50	1.50
C9H8O2	148.0524	3.08	1.00	0.89	0.22
C4H10O5S	170.0249	0.40	0.00	2.50	1.25
C5H4O4	128.0110	0.39	1.00	0.80	0.80
C5H10O3	118.0630	0.14	0.33	2.00	0.60
C15H6OS	234.0139	2.69	1.00	0.40	0.07

C8H0NO4	183 0532	7.00	1.00	1 13	0.50
01191004	185.0552	7.00	1.00	1.15	0.50
C2H3NO3	89.0113	0.39	0.67	1.50	1.50
C13H8O2	196.0524	7.16	1.00	0.62	0.15
C17H14O6	214.0700	7.07	1.00	0.82	0.25
C1/H1400	514.0790	7.97	1.00	0.82	0.55
C2H2O3	74.0004	0.36	0.67	1.00	1.50
C7H6O4	154 0266	1 30	1.00	0.86	0.57
C2114O2	72.0211	0.40	1.00	1.22	0.07
C3H4O2	72.0211	0.40	1.00	1.55	0.07
C7H6O5S	201.9936	0.64	1.00	0.86	0.71
C12H6O4	214 0266	5 48	1.00	0.50	0.33
C1211004	214.0200	3.40	1.00	1.50	0.55
C9H16O5	204.0998	2.77	0.40	1.78	0.56
C4H4O5	132.0059	0.37	0.60	1.00	1.25
C6H12O3	132 0786	0.15	0.33	2.00	0.50
0111203	152.0780	0.15	0.55	2.00	0.50
C/H6O4	154.0266	2.59	1.00	0.86	0.57
C3H3N3O3	129.0174	0.38	1.00	1.00	1.00
C14U8O2	224 0473	7 57	1.00	0.57	0.21
C1411803	224.0473	7.57	1.00	0.57	0.21
C8H6O6	198.0164	3.13	1.00	0.75	0.75
C9H7NO4	193.0375	3.46	1.00	0.78	0.44
C44602	96.0269	0.40	1.00	1.50	0.50
C4H0O2	80.0308	0.40	1.00	1.50	0.50
C7H12O7S	240.0304	0.58	0.29	1.71	1.00
C4H4O3	100.0160	0.41	1.00	1.00	0.75
C2119045	140.0142	0.51	0.00	2.67	1.22
C3H8U4S	140.0143	0.51	0.00	2.07	1.55
C8H9NO7S	263.0100	3.60	0.71	1.13	0.88
C5H5NO3	127.0269	1.03	1.00	1.00	0.60
CTUENCO	125.0200	1.05	1.00	0.71	0.00
C/H5NO2	155.0320	2.66	1.00	0.71	0.29
C6H6O4	142.0266	0.40	1.00	1.00	0.67
C6H3N3O7	228 9971	4 09	1.00	0.50	1 17
Colloco	152.0472	4.07	1.00	0.50	1.17
C8H8O3	152.0473	1.72	1.00	1.00	0.38
C13H7NO4	241.0375	7.83	1.00	0.54	0.31
C5H4O2	112 0160	0.20	1.00	0.80	0.60
0511405	112.0100	0.39	1.00	0.00	0.00
C3H3NO4	117.0062	0.40	0.75	1.00	1.33
C8H6O2	134 0368	1.77	1.00	0.75	0.25
C12U11NO2	220.0720	0.11	1.00	0.95	0.22
CISHIINOS	229.0739	8.11	1.00	0.85	0.25
C7H5NO6	199.0117	3.46	1.00	0.71	0.86
C8H5NO6	211 0117	3.03	1.00	0.63	0.75
011600	162.0217	3.05	1.00	0.05	0.75
C9H6O3	162.0317	3.16	1.00	0.67	0.33
C9H16O5	204.0998	2.57	0.40	1.78	0.56
C7H12O6S	224 0355	0.81	0.33	1 71	0.86
C/1112005	224.0555	0.01	1.00	1.71	0.00
C4H5NO2	99.0320	0.11	1.00	1.25	0.50
C8H8N2O5	212.0433	7.91	1.00	1.00	0.63
C8H9NO5	199 0/81	2 47	1.00	1 13	0.63
Collando	199.0481	2.47	1.00	1.15	0.05
C6H8O2	112.0524	1.00	1.00	1.33	0.33
C6H6N2O2	138.0429	0.40	1.00	1.00	0.33
C6H5NO2	122 0220	0.40	1.00	0.92	0.22
CONSINO2	125.0520	0.40	1.00	0.85	0.55
C10H16O7S	280.0617	1.03	0.43	1.60	0.70
C5H5NO3	127.0269	0.39	1.00	1.00	0.60
C12H8O4	216 0423	4.03	1.00	0.67	0.33
01211804	210.0423	4.03	1.00	0.07	0.35
C10H17NO7S	295.0726	4.68	0.43	1.70	0.70
C8H9NO4	183.0532	6.44	1.00	1.13	0.50
C6H0NO4	150 0532	0.40	0.75	1 50	0.67
01510104	137.0332	0.40	1.00	1.50	0.07
CI5H9NO3S	283.0303	3.79	1.00	0.60	0.20
C9H7NO	145.0528	2.26	1.00	0.78	0.11
C7H5NO6	199 0117	2.68	1.00	0.71	0.86
	177.0117	2.00	1.00	0.71	0.00
C14H10O4S	2/4.0300	7.11	1.00	0.71	0.29
C5H4N2O3	140.0222	0.41	1.00	0.80	0.60
C13H8O3	212 0473	7.03	1.00	0.62	0.23
C1511005	212.0473	7.03	1.00	0.02	0.25
C9H/NO3	177.0426	3.21	1.00	0.78	0.33
C16H10O	218.0732	8.36	1.00	0.63	0.06
C5H5NO4	143 0219	0.30	1.00	1.00	0.80
CJIIJN04	143.0219	0.39	1.00	1.00	0.80
C4H4N2O2	112.0273	0.39	1.00	1.00	0.50
C7H5NO	119.0371	3.12	1.00	0.71	0.14
C9H6O7	226.0114	2 91	1.00	0.67	0.78
0711007	127.0477	2.71	1.00	1.00	0.70
C/H/NO2	137.0477	2.36	1.00	1.00	0.29
C8H18O4S	210.0926	7.17	0.00	2.25	0.50
C13H0O2	212 0472	7 51	1.00	0.62	0.22
C13110U3	212.04/3	7.51	1.00	0.02	0.23
C10H10O2	162.0681	3.39	1.00	1.00	0.20
C5H3N3O2	137.0225	3.17	1.00	0.60	0.40
C6H4N205	18/ 0120	6.20	1.00	0.67	0.83
C011411200	104.0120	0.20	1.00	0.07	0.03
C6H4O4	140.0110	0.39	1.00	0.67	0.67
C5H8O2	100.0524	0.67	1.00	1.60	0.40
C6H7NO	109 0528	0.40	1.00	1 17	0.17
011/110	107.0320	0.47	1.00	1.1/	0.17

C9H7NO4	193 0375	2 35	1.00	0.78	0.44
0911/1004	195.0575	2.35	1.00	0.78	0.44
C10H18N2O11S	374.0631	4.38	0.27	1.80	1.10
C8H6O	118.0419	3.17	1.00	0.75	0.13
C14U905	256 0272	7.07	1.00	0.57	0.26
C14H8O5	256.0372	/.0/	1.00	0.57	0.36
C15H10O2	222.0681	7.22	1.00	0.67	0.13
COHONO3	170.0582	7 /3	1.00	1.00	0.33
C9H9N03	179.0382	7.43	1.00	1.00	0.55
C9H6O7	226.0114	1.07	1.00	0.67	0.78
C6H11NO3	145 0739	0.64	0.67	1.83	0.50
Commos	145.0757	0.04	0.07	1.05	0.50
C4H3N3O4	157.0124	3.21	1.00	0.75	1.00
C9H7NO4	193 0375	1 35	1.00	0.78	0.44
conno c	115.0575	1.55	1.00	0.70	0.11
C3H2O5	117.9902	0.38	0.60	0.67	1.67
C4H8O2	88.0524	0.43	0.50	2.00	0.50
COLIZNO	145.0529	2.47	1.00	0.70	0.11
C9H/NO	145.0528	3.47	1.00	0.78	0.11
C7H6N2O3	166.0378	3.45	1.00	0.86	0.43
C7U9N2O2	169.0525	2 72	1.00	1 1 4	0.42
C/H8N203	168.0555	3.72	1.00	1.14	0.45
C11H8O3	188.0473	7.77	1.00	0.73	0.27
CELISN204	192 0290	4.00	1.00	0.92	0.67
C0H3N304	165.0260	4.90	1.00	0.85	0.07
C11H18O6	246.1103	4.35	0.50	1.64	0.55
C13H8O3	212 0473	6 5 2	1.00	0.62	0.23
C13H805	212.0473	0.52	1.00	0.02	0.23
C12H5NO6	259.0117	3.94	1.00	0.42	0.50
C15H8O4	252 0423	7.61	1.00	0.53	0.27
CUIDIOCT	150.0501	1.01	1.00	1.55	0.27
C6H10N2O3	158.0691	1.06	1.00	1.6/	0.50
C11H8O3	188.0473	7.26	1.00	0.73	0.27
CTHONO	122 0694	0.40	1.00	1.00	0.14
C/H9NU	123.0684	0.69	1.00	1.29	0.14
C9H9NO4	195.0532	6.23	1.00	1.00	0.44
C6H4N2O5	184 0120	4 47	1.00	0.67	0.92
C0H4N2O3	164.0120	4.47	1.00	0.07	0.85
C10H6O6	222.0164	1.35	1.00	0.60	0.60
C14H13NO3	243 0805	8 27	1.00	0.03	0.21
C14H15N05	243.0893	0.27	1.00	0.93	0.21
C8H6N2O6	226.0226	3.01	1.00	0.75	0.75
C15H8O4	252 0423	5 25	1.00	0.53	0.27
01511804	252.0425	5.25	1.00	0.55	0.27
C13H10O4	230.0579	5.35	1.00	0.77	0.31
C8H9NO4	183 0532	4 14	1.00	1 13	0.50
C011/1104	105.0552	4.14	1.00	1.15	0.50
C14H8O3	224.0473	6.88	1.00	0.57	0.21
C14H8O5	256.0372	6.45	1.00	0.57	0.36
C12U9O2	106.0524	4.05	1.00	0.62	0.15
C15H802	190.0324	4.95	1.00	0.02	0.15
C10H17NO4	215.1158	3.62	0.75	1.70	0.40
C18H34O5	330 2406	7.45	0.40	1.80	0.28
C18H34O3	330.2400	7.43	0.40	1.09	0.28
C12H8N2O6	276.0382	7.94	1.00	0.67	0.50
C15H12O2	224 0827	8 10	1.00	0.80	0.12
CIJHI202	224.0837	8.10	1.00	0.80	0.15
C7H12O	112.0888	3.12	1.00	1.71	0.14
C4H4N4O7S	251 9801	0.82	0.71	1.00	1 75
	251.9001	0.82	0.71	1.00	1.75
C8H5NO6	211.0117	2.57	1.00	0.63	0.75
C9H16O4	188 1049	3 72	0.50	1 78	0.44
6211404	104.0110	5.72	0.50	1.70	1.00
C3H4O4	104.0110	0.39	0.50	1.33	1.33
C5H8O5	148.0372	0.40	0.40	1.60	1.00
CALIGOA	119 0266	0.52	0.50	1 50	1.00
04004	110.0200	0.55	0.50	1.50	1.00
C4H4O4	116.0110	0.40	0.75	1.00	1.00
C2H4O5S	139 9779	0.36	0.20	2.00	2 50
02114055	137.7/17	0.50	0.20	2.00	2.50
C6H8O5	160.0372	0.40	0.60	1.33	0.83
C5H8O4	132.0423	0.76	0.50	1.60	0.80
C0111405	202.0041	0.70	0.00	1.00	0.50
C9H14O5	202.0841	2.68	0.60	1.56	0.56
C10H18O4	202.1205	5.19	0.50	1.80	0.40
C2UCO4S	127.0097	0.27	0.25	2.00	1.22
C3H6O4S	137.9987	0.37	0.25	2.00	1.33
C10H16O5	216.0998	2.95	0.60	1.60	0.50
C7111005	174.0529	0.02	0.60	1.42	0.71
C/111005	1/4.0328	0.93	0.00	1.45	0.71
C6H8O4	144.0423	0.67	0.75	1.33	0.67
C8H12O5	188 0685	1.83	0.60	1.50	0.63
C01120J	100.0003	1.05	0.00	1.50	0.05
C10H12N4OS2	268.0453	3.72	1.00	1.20	0.10
C7H12O3	144,0786	1.10	0.67	1.71	0.43
0111205	204.0624	0.07	0.50	1.50	0.75
C8H12U6	204.0634	2.27	0.50	1.50	0.75
C16H22O4	278.1518	8.48	1.00	1.38	0.25
C2U6O2	74 0269	0.42	0.50	2.00	0.47
C3H0U2	/4.0368	0.42	0.50	2.00	0.67
C6H12O4	148.0736	0.54	0.25	2.00	0.67
C8H15NO2	172 1052	2 50	0.67	1 00	0.29
Contisinus	175.1052	2.39	0.07	1.00	0.56
C8H14O	126.1045	3.71	1.00	1.75	0.13
C10H18O4	202 1205	2 80	0.50	1 80	0.40
010111004	202.1203	2.09	0.50	1.00	0.40
C3H5NO3	103.0269	0.39	0.67	1.67	1.00
C13H20O6	272 1260	3 11	0.67	1.54	0.46
CTHENAOSO	275 0092	1 1 4	1.00	0.94	0.14
C/HOIN4US2	223.9983	1.64	1.00	0.86	0.14

Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
C2H4O4	92.0110	0.18	0.25	2.00	2.00
C2H4O4	92 0110	0.41	0.25	2.00	2.00
C6H8O7	192.0270	0.38	0.43	1 33	1.17
C10H7NO3	189.0426	7 73	1.00	0.70	0.30
C7H7NO4	169.0420	3.82	1.00	1.00	0.50
C7H7NO4	109.0375	3.62	1.00	1.00	0.57
C/H/NO4	169.0375	4.66	1.00	1.00	0.57
C/H6O3	138.0317	2.34	1.00	0.86	0.43
C6H5N3O4	183.0280	4.91	1.00	0.83	0.67
C8H5NO2	147.0320	3.26	1.00	0.63	0.25
C13H8O2	196.0524	7.52	1.00	0.62	0.15
C18H14O8	358.0689	7.43	1.00	0.78	0.44
C10H6O5	206.0215	3.14	1.00	0.60	0.50
C8H6O5S	213.9936	1.59	1.00	0.75	0.63
C8H5NO3	163.0269	2.66	1.00	0.63	0.38
C3H8O5S	156 0092	0.36	0.00	2.67	1.67
C4H6O7S	197 9834	0.35	0.29	1.50	1 75
C9H6O5	194 0215	0.83	1.00	0.67	0.56
C10H17N07S	205 0726	0.85	0.42	1.70	0.30
C011902	148.0524	4.00	0.43	1.70	0.70
C9H8O2	148.0524	3.09	1.00	0.89	0.22
C8H/NO5	197.0324	4.69	1.00	0.88	0.63
C7H6O3	138.0317	2.77	1.00	0.86	0.43
C13H8O2	196.0524	7.18	1.00	0.62	0.15
C8H6N2O2	162.0429	6.07	1.00	0.75	0.25
C8H6O5	182.0215	2.46	1.00	0.75	0.63
C8H8O3	152.0473	2.64	1.00	1.00	0.38
C5H4N2O3	140.0222	2.40	1.00	0.80	0.60
C12H9NO3	215.0582	7.86	1.00	0.75	0.25
C4H1005S	170 0249	0.38	0.00	2 50	1.25
C11H9NO3	203 0582	7 97	1.00	0.82	0.27
C14H10O4	242.0570	5.04	1.00	0.82	0.27
C714055	242.0379	0.62	1.00	0.71	0.29
C/H0U35	201.9936	0.05	1.00	0.80	0.71
C9H6O5	194.0215	2.60	1.00	0.67	0.56
C8H12O4	1/2.0/36	2.47	0.75	1.50	0.50
C3H4N2O2S	131.9993	0.33	1.00	1.33	0.67
C8H6O5	182.0215	1.07	1.00	0.75	0.63
C8H9NO7S	263.0100	3.59	0.71	1.13	0.88
C7H6O4	154.0266	2.60	1.00	0.86	0.57
C12H8O4	216.0423	4.04	1.00	0.67	0.33
C9H8O4	180.0423	2.75	1.00	0.89	0.44
C5H5NO4S	174.9939	0.36	1.00	1.00	0.80
C9H5NO4	191.0219	2.64	1.00	0.56	0.44
C9H9NO7S	275.0100	4 20	0.86	1.00	0.78
C5H8O6	164 0321	0.36	0.33	1.60	1 20
C8H9NO4	183 0532	7.04	1.00	1.00	0.50
C104805	208 0272	2.55	1.00	0.80	0.50
C10H8OJ	102 0422	2.55	1.00	0.80	0.30
C10H6O4	192.0425	5.10	1.00	0.80	0.40
C9H0U5	194.0215	2.79	1.00	0.67	0.56
CI3H3IN3OII	405.1959	8.00	0.00	2.38	0.85
C12H7NO4	229.0375	8.00	1.00	0.58	0.33
C9H6O6	210.0164	1.98	1.00	0.67	0.67
C8H6O5	182.0215	1.93	1.00	0.75	0.63
C8H8O2	136.0524	3.04	1.00	1.00	0.25
C6H6N2O3	154.0378	2.84	1.00	1.00	0.50
C8H16O6S	240.0668	2.86	0.17	2.00	0.75
C10H8O5	208.0372	2.81	1.00	0.80	0.50
C8H9NO4	183.0532	5.67	1.00	1.13	0.50
C4H10O4S	154,0300	0.93	0.00	2.50	1.00
C7H4N2O4	180 0171	3 51	1.00	0.57	0.57
C8H6O4	166 0266	1 3/	1.00	0.75	0.50
C10U904	102.0422	1.34	1.00	0.75	0.50
	192.0423	0.98	1.00	0.80	0.40
C6H6O6	1/4.0164	0.37	0.67	1.00	1.00
C8H6O6S	229.9885	2.52	1.00	0.75	0.75
C6H8O4	144.0423	0.70	0.75	1.33	0.67
C8H6O3	150.0317	0.82	1.00	0.75	0.38

Table S4.3.4 Molecular formulas of organic compounds detected in Shanghai OA in ESI- mode.

C14H14N2O5S2	354.0344	2.65	1.00	1.00	0.36
C12H9NO4	231 0532	7 43	1.00	0.75	0.33
CPU5NO2	162 0260	2.00	1.00	0.62	0.29
Consinos	103.0209	2.99	1.00	0.05	0.58
C8H7NO5	197.0324	4.29	1.00	0.88	0.63
C9H8O3	164.0473	2.48	1.00	0.89	0.33
C5H10058	182 0240	0.51	0.20	2.00	1.00
CJHIOOJS	182.0249	0.51	0.20	2.00	1.00
C8H8O3	152.0473	5.33	1.00	1.00	0.38
C10H10O4	194.0579	3.67	1.00	1.00	0.40
C6H14O6S	214 0511	0.38	0.00	2 33	1.00
0114005	214.0011	0.38	0.00	2.55	1.00
C9H5NO4	191.0219	2.05	1.00	0.56	0.44
C5H5NO5S	190.9888	0.38	0.80	1.00	1.00
C3H3NO2	85 0164	0.09	1.00	1.00	0.67
C10111002	170.0620	2.00	1.00	1.00	0.07
C10H10O3	178.0630	3.80	1.00	1.00	0.30
C9H6O3	162.0317	3.14	1.00	0.67	0.33
C10H20O5S	252,1031	7.00	0.20	2.00	0.50
C12H0NO4	231.0532	7.80	1.00	0.75	0.33
61(1100	210.0722	7.00	1.00	0.75	0.55
C16H100	218.0732	8.36	1.00	0.63	0.06
C11H8O3	188.0473	7.77	1.00	0.73	0.27
C6H6O5	158.0215	0.38	0.80	1.00	0.83
C5H6O3	114 0317	0.38	1.00	1 20	0.60
C01115N000	207.0510	0.50	0.20	1.20	0.00
C9HI5N08S	297.0518	3.26	0.38	1.67	0.89
C13H7NO4	241.0375	7.83	1.00	0.54	0.31
C5H7NO6S	208.9994	0.38	0.50	1.40	1.20
C14H10O3	226.0630	7 20	1.00	0.71	0.21
	178.0266	7.20	1.00	0.71	0.21
C9H6O4	178.0266	2.95	1.00	0.67	0.44
C3H7NO5S	169.0045	0.36	0.20	2.33	1.67
C10H17NO7S	295.0726	6.60	0.43	1.70	0.70
C12H11NO3	217 0739	8 21	1.00	0.92	0.25
C1411004	217.0735	0.21	1.00	0.52	0.25
C14H804	240.0423	1.25	1.00	0.57	0.29
C12H14O5	238.0841	3.41	1.00	1.17	0.42
C7H10O6	190.0477	0.39	0.50	1.43	0.86
C0H7NO5S	241.0045	2.11	1.00	0.78	0.56
C9111(035	200.07(0	2.11	1.00	0.70	0.50
C8H1604S	208.0769	4.84	0.25	2.00	0.50
C6H5NO3	139.0269	3.24	1.00	0.83	0.50
C6H12O5S	196.0405	0.84	0.20	2.00	0.83
C8H7NO3	165.0426	5.07	1.00	0.88	0.38
C7U(N)2O2	166 0279	2.45	1.00	0.00	0.30
C/H0N2O5	100.0378	5.45	1.00	0.80	0.45
C4H8O3	104.0473	0.61	0.33	2.00	0.75
C9H11NO4	197.0688	7.36	1.00	1.22	0.44
C10H17N07S	295 0726	6 30	0.43	1 70	0.70
C5U0050	100.0002	0.50	0.40	1.70	1.00
C5H805S	180.0092	0.39	0.40	1.60	1.00
C6H5NO3	139.0269	0.38	1.00	0.83	0.50
C4H9NO7S	215.0100	1.49	0.14	2.25	1.75
C6H8O4	144 0423	1 34	0.75	1 33	0.67
COLLOG	100.0117	1.54	1.00	0.71	0.07
C/H5NO6	199.0117	2.66	1.00	0.71	0.86
C9H16O5S	236.0718	2.65	0.40	1.78	0.56
C8H9NO4	183.0532	3.50	1.00	1.13	0.50
C8H9NO5	199 0/181	1 24	1.00	1 13	0.63
CONTROL	224 0719	7.24	0.20	2.00	0.03
C8H10035	224.0718	2.70	0.20	2.00	0.05
C14H10O4	242.0579	6.91	1.00	0.71	0.29
C11H12N2O3S2	284.0289	3.85	1.00	1.09	0.27
C6H5NO5	171.0168	2.31	1.00	0.83	0.83
C9119O2	152 0472	6.00	1.00	1.00	0.29
C8H8U3	132.0475	0.22	1.00	1.00	0.58
C13H8O4	228.0423	7.87	1.00	0.62	0.31
C9H9NO6S	259.0151	0.59	1.00	1.00	0.67
C9H9NO3	179.0582	3 33	1.00	1.00	0.33
C6H10O4	146.0579	2.48	0.50	1.67	0.67
C011004	152.0472	2.40	0.50	1.07	0.07
C8H8O3	152.0473	4.37	1.00	1.00	0.38
C11H8O3	188.0473	7.28	1.00	0.73	0.27
C7H8O6	188.0321	0.38	0.67	1.14	0.86
C6H14O4S	182,0613	3 50	0.00	2.33	0.67
00100	120.0575	2.00	1.00	1.00	0.12
Consu	120.0575	3.06	1.00	1.00	0.13
C2H6O3S	110.0038	0.35	0.00	3.00	1.50
C10H18O5S	250.0875	3.08	0.40	1.80	0.50
C15H10O2	222.0681	7.23	1.00	0.67	0.13
Cereose	158 0029	0.74	1.00	1.00	0.50
C0110035	130.0030	0.74	1.00	1.00	0.50
C/H6N2O6	214.0226	3.53	1.00	0.86	0.86
C4H6O6S	181.9885	0.38	0.33	1.50	1.50
C12H8O4	216.0423	4.44	1.00	0.67	0.33
C7H1004	158 0579	2 75	0.75	1 43	0.57
0/11/004	100.0077	2.15	0.15	1.10	0.07

C7H4N2O3         164.0222         4.00         1.00           C8H14N2O6S         266.0573         7.38         0.50           C7H6O4         154.0266         1.30         1.00           C3H803         212.0473         7.01         1.00           C9H8O4         180.0423         4.12         1.00           C6H10O4         146.0579         0.59         0.50           C8H9NO4         183.0532         6.49         1.00           C7H4N2O7         228.0019         4.06         1.00           C7H4N2O7         226.0114         2.87         1.00           C7H16O4S         196.0769         5.12         0.00           C7H16O4S         196.0769         5.12         0.00           C4H3NO3S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C8H6O2         134.0368         1.83         1.00           C3H4O3         82.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         30.1315         3.07         0.63	0.57 1.75 0.86 0.62 0.89 1.67 1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.43 0.75 0.57 0.23 0.44 0.67 0.50 1.00 0.36 0.78 0.57
C8H14N2O6S         160.022         1.00         1.00           C3H402065         154.0266         1.30         1.00           C13H803         212.0473         7.01         1.00           C9H804         180.0423         4.12         1.00           C6H1004         146.0579         0.59         0.50           C8H9N04         183.0532         6.49         1.00           C7H4N207         228.0019         4.06         1.00           C14H805         256.0372         7.07         1.00           C9H607         226.0114         2.87         1.00           C7H1604S         196.0769         5.12         0.00           C2H3N03S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C8H602         134.0368         1.83         1.00           C3H403         212.0473         7.49         1.00           C3H403         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C3H403         30.0118         3.84         0.20 <td>1.75 0.86 0.62 0.89 1.67 1.13 0.57 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75</td> <td>0.75 0.75 0.23 0.44 0.67 0.50 1.00 0.36 0.78 0.57</td>	1.75 0.86 0.62 0.89 1.67 1.13 0.57 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.75 0.75 0.23 0.44 0.67 0.50 1.00 0.36 0.78 0.57
CSH14N2DOS         200.0373         7.38         0.30           C7H604         154.0266         1.30         1.00           C13H8O3         212.0473         7.01         1.00           C9HR04         180.0423         4.12         1.00           C6H1004         146.0579         0.59         0.50           C8H9N04         183.0532         6.49         1.00           C7H4N2O7         228.0019         4.06         1.00           C14H805         256.0372         7.07         1.00           C7H40207         226.0114         2.87         1.00           C7H1604S         196.0769         5.12         0.00           C2H3NO3S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C8H602         134.0368         1.83         1.00           C13H803         212.0473         7.49         1.00           C8H602         134.0368         1.83         1.00           C3H403         88.0160         0.06         0.67           C9H17N08         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00 <td>1.75 0.86 0.62 0.89 1.67 1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75</td> <td>0.73 0.23 0.44 0.67 0.50 1.00 0.36 0.78 0.57</td>	1.75 0.86 0.62 0.89 1.67 1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.73 0.23 0.44 0.67 0.50 1.00 0.36 0.78 0.57
C7/H604         154.0266         1.30         1.00           C13H803         212.0473         7.01         1.00           C9H804         180.0423         4.12         1.00           C6H1004         146.0579         0.59         0.50           C8H9N04         183.0532         6.49         1.00           C7H4N207         228.0019         4.06         1.00           C14H805         256.0372         7.07         1.00           C9H607         226.0114         2.87         1.00           C9H607         226.0114         2.87         1.00           C2H3N03S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C8H602         134.0368         1.83         1.00           C8H602         134.0368         1.83         1.00           C8H5N04         179.0219         5.38         1.00           C3H403         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63	0.86 0.62 0.89 1.67 1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.57 0.23 0.44 0.67 0.50 1.00 0.36 0.78 0.57
C13H8O3         212.0473         7.01         1.00           C9H8O4         180.0423         4.12         1.00           C6H10O4         146.0579         0.59         0.50           C8H9NO4         183.0532         6.49         1.00           C7H4N2O7         228.0019         4.06         1.00           C14H8O5         256.0372         7.07         1.00           C9H6O7         226.0114         2.87         1.00           C7H16O4S         196.0769         5.12         0.00           C2H3NO3S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C8H6O2         134.0368         1.83         1.00           C13H8O3         212.0473         7.49         1.00           C8H5NO4         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C4H603         102.0317         0.38         0.67           C10H2005S2         284.0752         7.78         0.20 <td>0.62 0.89 1.67 1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75</td> <td>0.23 0.44 0.67 0.50 1.00 0.36 0.78 0.57</td>	0.62 0.89 1.67 1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.23 0.44 0.67 0.50 1.00 0.36 0.78 0.57
C9H804         180.0423         4.12         1.00           C6H1004         146.0579         0.59         0.50           C8H9N04         183.0532         6.49         1.00           C7H4N207         228.0019         4.06         1.00           C14H805         256.0372         7.07         1.00           C9H607         226.0114         2.87         1.00           C7H1604S         196.0769         5.12         0.00           C2H3N03S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C8H5N03         139.0269         2.94         1.00           C8H602         134.0368         1.83         1.00           C3H403         212.0473         7.49         1.00           C3H403         28.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         30.1315         3.07         0.63           C7H5NO6         199.0117         3.42         1.00           C9H7NO4         193.0375         7.16         1.00	0.89 1.67 1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.44 0.67 0.50 1.00 0.36 0.78 0.57
C6H1004         146.0579         0.59         0.50           C8H9N04         183.0532         6.49         1.00           C7H4N207         228.0019         4.06         1.00           C14H805         256.0372         7.07         1.00           C9H607         226.0114         2.87         1.00           C9H607         226.0114         2.87         1.00           C116025         242.0249         2.98         1.00           C6H5N03         139.0269         2.94         1.00           C8H602         134.0368         1.83         1.00           C8H5N04         179.0219         5.38         1.00           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5NO6         199.0117         3.42         1.00	1.67 1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.67 0.50 1.00 0.36 0.78 0.57
Control         140.0379         0.39         0.30           C8H9N04         183.0532         6.49         1.00           C7H4N2O7         228.0019         4.06         1.00           C14H8O5         256.0372         7.07         1.00           C9H6O7         226.0114         2.87         1.00           C7H16O4S         196.0769         5.12         0.00           C2H3N03S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C6H5N03         139.0269         2.94         1.00           C8H6O2         134.0368         1.83         1.00           C3H4O3         212.0473         7.49         1.00           C8H5NO4         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17NO8S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5NO6         199.0117         3.42         1.00           C4H10N4010S         306.0118         3.84         0.20	1.03 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.50 1.00 0.36 0.78 0.57
C8H9N04         183.0552         6.49         1.00           C7H4N2O7         228.0019         4.06         1.00           C14H8O5         256.0372         7.07         1.00           C9H6O7         226.0114         2.87         1.00           C7H16O4S         196.0769         5.12         0.00           C2H3N03S         120.9834         0.35         0.67           C10H10O5S         242.0249         2.98         1.00           C8H5N03         139.0269         2.94         1.00           C8H6O2         134.0368         1.83         1.00           C13H8O3         212.0473         7.49         1.00           C8H5NO4         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78	1.13 0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.50 1.00 0.36 0.78 0.57
C7H4N207         228.0019         4.06         1.00           C14H805         256.0372         7.07         1.00           C9H607         226.0114         2.87         1.00           C7H1604S         196.0769         5.12         0.00           C2H3NO3S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C6H5NO3         139.0269         2.94         1.00           C8H602         134.0368         1.83         1.00           C13H803         212.0473         7.49         1.00           C3H403         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5NO6         199.0117         3.42         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1	0.57 0.57 0.67 2.29 1.50 1.00 0.83 0.75	1.00 0.36 0.78 0.57
C14H805         256.0372         7.07         1.00           C9H607         226.0114         2.87         1.00           C7H1604S         196.0769         5.12         0.00           C2H3N03S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C6H5N03         139.0269         2.94         1.00           C8H602         134.0368         1.83         1.00           C3H403         212.0473         7.49         1.00           C8H5N04         179.0219         5.38         1.00           C3H403         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.0	0.57 0.67 2.29 1.50 1.00 0.83 0.75	0.36 0.78 0.57
C9H607         226.0114         2.87         1.00           C7H1604S         196.0769         5.12         0.00           C2H3N03S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C6H5N03         139.0269         2.94         1.00           C8H602         134.0368         1.83         1.00           C13H803         212.0473         7.49         1.00           C8H5N04         179.0219         5.38         1.00           C3H403         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C4H603         102.0317         0.38         0.67           C10H200S52         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00 <td>0.67 2.29 1.50 1.00 0.83 0.75</td> <td>0.78 0.57</td>	0.67 2.29 1.50 1.00 0.83 0.75	0.78 0.57
C91007         220.0114         2.87         1.00           C7H16O4S         196.0769         5.12         0.00           C2H3NO3S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C6H5NO3         139.0269         2.94         1.00           C8H602         134.0368         1.83         1.00           C13H8O3         212.0473         7.49         1.00           C8H5NO4         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C4H10N40108         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C9H7NO3         166.0630         7.30         1.	2.29 1.50 1.00 0.83 0.75	0.78
C7H1604S         196.0769         5.12         0.00           C2H3N03S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C6H5N03         139.0269         2.94         1.00           C8H602         134.0368         1.83         1.00           C13H803         212.0473         7.49         1.00           C8H5N04         179.0219         5.38         1.00           C3H403         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C4H10N4010S         306.0118         3.84         0.20           C4H603         102.0317         0.38         0.67           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.	2.29 1.50 1.00 0.83 0.75	0.57
C2H3NO3S         120.9834         0.35         0.67           C10H1005S         242.0249         2.98         1.00           C6H5NO3         139.0269         2.94         1.00           C8H602         134.0368         1.83         1.00           C13H803         212.0473         7.49         1.00           C8H5NO4         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17NO8S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5NO6         199.0117         3.42         1.00           C9H7NO4         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C9H7NO2         135.0320         2.68         1.00           C9H7NO3         166.0630         7.30         1.	1.50 1.00 0.83 0.75	1 50
C10H1005S         242.0249         2.98         1.00           C6H5NO3         139.0269         2.94         1.00           C8H6O2         134.0368         1.83         1.00           C13H8O3         212.0473         7.49         1.00           C8H5NO4         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17NO8S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5NO6         199.0117         3.42         1.00           C9H7NO4         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H8O4         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.00           C6H14O4S         182.0613         3.03         0.00           C9H7NO3         177.0426         3.27         1.	1.00 0.83 0.75	1.50
C6H5N03         139.0269         2.94         1.00           C8H6O2         134.0368         1.83         1.00           C13H8O3         212.0473         7.49         1.00           C8H5NO4         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5NO6         199.0117         3.42         1.00           C9H7NO4         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C4H6O3         166.0630         7.30         1.00           C9H1003         166.0630         7.30         1.00           C9H9N06         227.0430         3.36         1.00 </td <td>0.83 0.75</td> <td>0.50</td>	0.83 0.75	0.50
C0111/CO3         139.0209         2.94         1.00           C8H6O2         134.0368         1.83         1.00           C13H8O3         212.0473         7.49         1.00           C8H5NO4         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17NO8S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5NO6         199.0117         3.42         1.00           C9H7NO4         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.00           C6H14O4S         182.0613         3.03         0.00           C9H7NO3         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.	0.75	0.50
C8H602         134.0568         1.85         1.00           C13H803         212.0473         7.49         1.00           C8H5N04         179.0219         5.38         1.00           C3H403         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C4H603         102.0317         0.38         0.67           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C9H1003         166.0630         7.30         1.00           C9H9N06         227.0430         3.36         1.00           C10H806         224.0321         2.46         1.00 </td <td>0.75</td> <td>0.50</td>	0.75	0.50
C13H803         212.0473         7.49         1.00           C8H5N04         179.0219         5.38         1.00           C3H403         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H603         102.0317         0.38         0.67           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H7NO3         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C13H8N03         227.0582         8.23         1.00           C13H9N03         227.0582         8.23         1.00 </td <td></td> <td>0.25</td>		0.25
C8H5N04         179.0219         5.38         1.00           C3H4O3         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C4H10N3         166.0630         7.30         1.00           C9H1003         166.0630         7.30         1.00           C9H1N03         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C16H16N205S2         380.0501         7.43         1.00           C16H806         224.0321         2.46 <td< td=""><td>0.62</td><td>0.23</td></td<>	0.62	0.23
C3H4O3         88.0160         0.06         0.67           C9H17N08S         299.0675         3.37         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H9N06         227.0430         3.36         1.00           C10H804         240.0321         2.46         1.00           C16H16N205S2         380.0501         7.43         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         <	0.63	0.50
C9H17N03S         299.0675         3.37         0.25           C1H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H7NO3         166.0630         7.30         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C10H804         224.0321         2.46         1.00           C16H16N205S2         380.0501         7.43         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46	1 33	1.00
C9H17N08S         299.0675         3.57         0.25           C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H7N03         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H806         224.0321         2.46         1.00           C10H803         176.0473         3.23	1.00	1.00
C11H1005         222.0528         2.90         1.00           C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H10N40108         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H7N03         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C16H16N205S2         380.0501         7.43         1.00           C10H806         224.0321         2.46         1.00           C10H806         224.0321         2.46         1.00           C10H806         259.0117         3.86         1.00           C10H806         259.0117         3.86 <t< td=""><td>1.89</td><td>0.89</td></t<>	1.89	0.89
C15H2208         330.1315         3.07         0.63           C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H7N03         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H806         259.0117         3.86         1.00           C10H803         176.0473         3.23         1.00           C7H622         122.0368         0.83         1.00           C12H5N06         259.0117         3.86         1.0	0.91	0.45
C7H5N06         199.0117         3.42         1.00           C9H7N04         193.0375         7.16         1.00           C4H10N4O10S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H603         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H1003         166.0630         7.30         1.00           C9H1003         166.0630         7.33         1.00           C9H9N06         227.0430         3.36         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H806         259.0117         3.86         1.00           C1H5N06         259.0117         3.86         1.00           C1H5N06         259.0117         3.86         1.00           C1H5N06         259.0117         3.86         1.00	1.47	0.53
CHIAROO         193.0375         7.16         1.00           C9H7NO4         193.0375         7.16         1.00           C4H10N4O10S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C13H9NO3         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H806         224.0321         2.46         1.00           C10H803         176.0473         3.23         1.00           C7H12N2O3         172.0848         2.49         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.	0.71	0.86
C9H7N04         193.0575         7.16         1.00           C4H10N4010S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H7N03         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H806         224.0321         2.46         1.00           C10H806         259.0117         3.86         1.00           C1H2N203         172.0848         2.49         1.00           C1H5N06         259.0117         3.86         1.00           C1H805         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.	0.71	0.00
C4H10N4O10S         306.0118         3.84         0.20           C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H8O4         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.00           C6H14O4S         182.0613         3.03         0.00           C9H10O3         166.0630         7.30         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9NO6         227.0430         3.36         1.00           C13H9NO3         227.0582         8.23         1.00           C10H8O6         224.0321         2.46         1.00           C10H8O3         176.0473         3.23         1.00           C10H8O3         176.0473         3.23         1.00           C10H8O6         259.0117         3.86         1.00           C1H12N2O3         172.0848         2.49         1.00           C12H5NO6         259.0117         3.86         1.00           C1H6O2         122.0368         0.83         1.00           C7H6O2         122.0368         0.45         0.6	0.78	0.44
C10H2005S2         284.0752         7.78         0.20           C4H6O3         102.0317         0.38         0.67           C10H8O4         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.00           C6H14O4S         182.0613         3.03         0.00           C9H10O3         166.0630         7.30         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9NO6         227.0430         3.36         1.00           C16H16N205S2         380.0501         7.43         1.00           C13H9NO3         227.0582         8.23         1.00           C10H8O6         224.0321         2.46         1.00           C10H8O6         259.0117         3.86         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	2.50	2.50
C4H6O3         102.0317         0.38         0.67           C10H8O4         192.0423         3.28         1.00           C7H5NO2         135.0320         2.68         1.00           C6H14O4S         182.0613         3.03         0.00           C9H10O3         166.0630         7.30         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9NO6         227.0430         3.36         1.00           C16H16N205S2         380.0501         7.43         1.00           C13H9NO3         227.0582         8.23         1.00           C10H8O6         224.0321         2.46         1.00           C10H8O6         224.0321         2.46         1.00           C10H8O6         259.0117         3.86         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H10O5S         266.0249         3.33         1.00	2.00	0.50
C1000         102.017         0.36         0.07           C10H804         192.0423         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H7N03         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H803         176.0473         3.23         1.00           C10H803         176.0473         3.23         1.00           C7H12N203         172.0848         2.49         1.00           C12H5N06         259.0117         3.86         1.00           C7H602         122.0368         0.83         1.00           C5H605S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	1.50	0.75
C10H804         192.0425         3.28         1.00           C7H5N02         135.0320         2.68         1.00           C6H1404S         182.0613         3.03         0.00           C9H1003         166.0630         7.30         1.00           C9H7N03         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C16H16N205S2         380.0501         7.43         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H803         176.0473         3.23         1.00           C10H803         172.0848         2.49         1.00           C12H5N06         259.0117         3.86         1.00           C7H602         122.0368         0.83         1.00           C5H605S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.80	0.10
C7H5NO2         135.0320         2.68         1.00           C6H14O4S         182.0613         3.03         0.00           C9H10O3         166.0630         7.30         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9NO6         227.0430         3.36         1.00           C16H16N205S2         380.0501         7.43         1.00           C13H9NO3         227.0582         8.23         1.00           C10H8O6         224.0321         2.46         1.00           C10H8O3         176.0473         3.23         1.00           C10H8O3         176.0473         3.23         1.00           C10H8O6         259.0117         3.86         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.80	0.40
C6H14O4S         182.0613         3.03         0.00           C9H10O3         166.0630         7.30         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9NO6         227.0430         3.36         1.00           C16H16N205S2         380.0501         7.43         1.00           C13H9NO3         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H803         176.0473         3.23         1.00           C7H12N2O3         172.0848         2.49         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.71	0.29
C9H10O3         166.0630         7.30         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9NO6         227.0430         3.36         1.00           C16H16N2O5S2         380.0501         7.43         1.00           C13H9NO3         227.0582         8.23         1.00           C10H8O6         224.0321         2.46         1.00           C10H8O3         176.0473         3.23         1.00           C7H12N2O3         172.0848         2.49         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	2.33	0.67
C9H1005         100.0050         1.00         1.00           C9H7NO3         177.0426         3.27         1.00           C9H9NO6         227.0430         3.36         1.00           C16H16N2O5S2         380.0501         7.43         1.00           C13H9NO3         227.0582         8.23         1.00           C10H8O6         224.0321         2.46         1.00           C10H8O3         176.0473         3.23         1.00           C10H8O3         172.0848         2.49         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	1.11	0.33
C9H7N05         177.0426         3.27         1.00           C9H9N06         227.0430         3.36         1.00           C16H16N205S2         380.0501         7.43         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H803         176.0473         3.23         1.00           C7H12N2O3         172.0848         2.49         1.00           C12H5N06         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.79	0.33
C9H9N06         227.0430         3.36         1.00           C16H16N2O5S2         380.0501         7.43         1.00           C13H9N03         227.0582         8.23         1.00           C10H806         224.0321         2.46         1.00           C10H803         176.0473         3.23         1.00           C7H12N2O3         172.0848         2.49         1.00           C12H5N06         259.0117         3.86         1.00           C7H602         122.0368         0.83         1.00           C5H605S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.78	0.33
C16H16N2O5S2         380.0501         7.43         1.00           C13H9NO3         227.0582         8.23         1.00           C10H8O6         224.0321         2.46         1.00           C10H8O3         176.0473         3.23         1.00           C7H12N2O3         172.0848         2.49         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	1.00	0.67
C13H9NO3227.05828.231.00C10H8O6224.03212.461.00C10H8O3176.04733.231.00C7H12N2O3172.08482.491.00C12H5NO6259.01173.861.00C7H6O2122.03680.831.00C5H6O5S177.99360.450.60C12H1005S266.02493.331.00	1.00	0.31
C10101005         221.0302         0.25         1.00           C101806         224.0321         2.46         1.00           C10H803         176.0473         3.23         1.00           C7H12N2O3         172.0848         2.49         1.00           C12H5N06         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.69	0.23
C10H806         224.0521         2.40         1.00           C10H803         176.0473         3.23         1.00           C7H12N203         172.0848         2.49         1.00           C12H5N06         259.0117         3.86         1.00           C7H602         122.0368         0.83         1.00           C5H605S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.02	0.23
C10H803         176.0473         3.23         1.00           C7H12N2O3         172.0848         2.49         1.00           C12H5NO6         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.80	0.00
C7H12N2O3         172.0848         2.49         1.00           C12H5N06         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.80	0.30
C12H5N06         259.0117         3.86         1.00           C7H6O2         122.0368         0.83         1.00           C5H6O5S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	1.71	0.43
C7H602         122.0368         0.83         1.00           C5H605S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.42	0.50
C7H002         122.0508         0.85         1.00           C5H605S         177.9936         0.45         0.60           C12H1005S         266.0249         3.33         1.00	0.96	0.20
C5H6O5S 177.9936 0.45 0.60 C12H1005S 266.0249 3.33 1.00	0.80	0.29
C12H1005S 266.0249 3.33 1.00	1.20	1.00
	0.83	0.42
C8H8O5S 216 0092 1.81 1.00	1.00	0.63
	0.67	0.05
C9R005 102.0517 2.90 1.00	0.07	0.55
C9H9NO3 179.0582 7.45 1.00	1.00	0.33
C14H8O4 240.0423 7.45 1.00	0.57	0.29
C9H7NO 145 0528 2 25 1 00	0.78	0.11
	2.00	1.00
212.0353 1.00 0.17	2.00	1.00
C5H5NO3 127.0269 1.03 1.00	1.00	0.60
C9H5NO5 207.0168 3.93 1.00	0.56	0.56
C13H9NO4 243.0532 7.74 1.00	0.69	0.31
C9H6O7 226 0114 1 07 1 00	0.67	0.78
C511007 220.0117 1.07 1.00 C511902 116.0472 0.40 0.47	1.60	0.70
0.000 110.0475 0.40 0.67	1.00	0.00
C11H4O6 232.0008 3.17 1.00	0.36	0.55
C7H5NO4 167.0219 0.35 1.00	0.71	0.57
C8H7NO5 197.0324 3.26 1.00	0.88	0.63
C10H806 $2240321$ $200$ $100$	0.80	0.60
C1011000 224.0321 3.07 1.00 C10110NO4 207.0520 2.02 1.00	0.00	0.00
C10H9NO4 207.0532 2.82 1.00	0.90	0.40
C11H6O5 218.0215 3.04 1.00	0.55	0.45
C7H14O5S 210.0562 1.94 0.20	2.00	0.71
C9H5NO5 207 0168 2 50 1 00	0.56	0.56
COLLIZOGE 252 0449 2.50 1.00	1 70	0.50
C71110005 252.0006 2.01 0.55	1./0	0.07
C/H12O4 160.0736 0.91 0.50	1.71	0.57
C8H6O 118.0419 3.14 1.00	0.75	0.13
C15H8O4 252 0423 5 28 1 00	0.53	0.27
C11H12O6S 272.0255 2.40 1.00	1.00	0.55
C11112005 272.0555 2.49 1.00	1.09	0.55
C10H/NO/S 284.9943 1.03 1.00	0.70	0.70
C13H10O3 214.0630 8.03 1.00		0.23
C2H4O4S 123.9830 0.70 0.25	0.77	2.00
C15H10O4 254.0579 7.89 1.00	0.77 2.00	2.00
CIGINIOUT 2J7.0377 7.07 1.00 CIGINIOCC 250.0100 1.75 1.00	0.77 2.00 0.67	2.00
C10H10O6S 258.0198 1.75 1.00	0.77 2.00 0.67	0.27

C8H15NO8S	285.0518	2.98	0.25	1 88	1.00
CollishOos	285.0518	2.98	0.25	1.00	1.00
C8H9NO4	183.0532	5.95	1.00	1.13	0.50
C10H6O3S2	237.9758	0.52	1.00	0.60	0.30
C8H9NO6S	247.0151	1.43	0.83	1.13	0.75
C10H10O3	178 0630	2 99	1.00	1.00	0.30
C2U2NO2	101 0112	0.05	1.00	1.00	1.00
CSH5NO5	101.0113	0.05	1.00	1.00	1.00
C3H4O6S	167.9729	0.37	0.33	1.33	2.00
C12H10O2	186.0681	7.16	1.00	0.83	0.17
C9H8O	132 0575	3 10	1.00	0.89	0.11
C11U1905	220.1154	2.20	0.00	1.64	0.11
CITH1805	230.1154	5.20	0.00	1.04	0.45
C5H10O4S	166.0300	0.39	0.25	2.00	0.80
C15H10O3	238.0630	7.99	1.00	0.67	0.20
C5H12O4S	168 0456	2 22	0.00	240	0.80
C15H10O2	222.0681	2.22	1.00	0.67	0.00
C13H1002	222.0081	0.00	1.00	0.07	0.13
C5H12O5S	184.0405	0.53	0.00	2.40	1.00
C14H8O4	240.0423	4.25	1.00	0.57	0.29
C5H4N2O3	140 0222	1.16	1.00	0.80	0.60
C6H5NO2	122 0220	0.29	1.00	0.82	0.22
CONSINCE	125.0520	0.38	1.00	0.85	0.33
C6H5NO6S	218.9838	2.92	0.83	0.83	1.00
C4H10O4S	154.0300	1.30	0.00	2.50	1.00
C8H6O4	166.0266	1 89	1.00	0.75	0.50
C8H5NO4	179 0219	/ 01	1.00	0.63	0.50
COLLOPAG	172.0007	7.71	1.00	1.00	0.50
C6H6O4S	1/3.998/	0.98	1.00	1.00	0.67
C7H14O5S	210.0562	2.50	0.20	2.00	0.71
C5H7NO8	209.0172	0.35	0.38	1.40	1.60
C18H10O4	290 0579	7 68	1.00	0.56	0.22
C1/11004	270.0377	2 20	1.00	0.50	0.22
C14H8U4	240.0423	0.38	1.00	0.57	0.29
C10H10O2	162.0681	3.61	1.00	1.00	0.20
C6H5NO4	155.0219	0.39	1.00	0.83	0.67
C6H5NO3	139 0269	0.59	1.00	0.83	0.50
C0H10O2	166 0620	2 20	1.00	1 1 1	0.22
C9H1003	100.0050	3.30	1.00	1.11	0.33
C/H1406S	226.0511	2.22	0.17	2.00	0.86
C7H6N2O4	182.0328	3.45	1.00	0.86	0.57
C13H8O3	212.0473	7.98	1.00	0.62	0.23
C16H8O3	248 0473	7.40	1.00	0.50	0.19
	128.0473	7.40	1.00	1.00	0.17
C4H4N2O3	128.0222	0.55	1.00	1.00	0.75
C15H25NO7S	363.1352	8.03	0.57	1.67	0.47
C9H18O6S	254.0824	3.52	0.17	2.00	0.67
C7H8O5	172 0372	0.38	0.80	1.14	0.71
COLLOCE	244.0042	2.94	1.00	0.90	0.71
0918005	244.0042	2.64	1.00	0.89	0.07
C13H8O4	228.0423	8.21	1.00	0.62	0.31
C7H7NO4	169.0375	6.30	1.00	1.00	0.57
C13H8O3	212 0473	6 52	1.00	0.62	0.23
CI2UONO4S	212.0475	2.04	1.00	0.02	0.23
C12H9N045	203.0232	2.94	1.00	0.75	0.33
C5H10O5S	182.0249	0.90	0.20	2.00	1.00
C10H10O3	178.0630	3.38	1.00	1.00	0.30
C11H7NO5	233.0324	7.21	1.00	0.64	0.45
C11H8O6	236 0321	2.86	1.00	0.73	0.55
C6U12N079	242 0412	2.00	0.14	0.75	1 17
CONTRINU/S	245.0415	5.55	0.14	2.17	1.1/
C/H14O6S	226.0511	2.48	0.17	2.00	0.86
C9H8O6S	244.0042	0.81	1.00	0.89	0.67
C6H6O4	142.0266	0.39	1.00	1.00	0.67
C9H5NO4	191 0219	0.18	1.00	0.56	0.44
C1/II100F	750 0520	2 44	1.00	0.50	0.77
01401005	236.0528	5.00	1.00	0./1	0.30
C11H8N2O5	248.0433	8.16	1.00	0.73	0.45
C9H7NO6	225.0273	3.16	1.00	0.78	0.67
C7H7NO3	153.0426	0.38	1.00	1.00	0.43
C10H2005S	252 1031	3.86	0.20	2.00	0.50
051120033	252.1051	3.00	0.20	2.00	0.50
C5H3N3O2	137.0225	3.19	1.00	0.60	0.40
C9H19NO8S	301.0831	3.36	0.13	2.11	0.89
C8H7NO3	165.0426	6.74	1.00	0.88	0.38
C9H15NO8S	297 0518	2 91	0.38	1.67	0.89
C10111404	227.0510	2.71	1.00	1.07	0.07
C12H14O4	222.0892	8.03	1.00	1.1/	0.33
C9H9NO5	211.0481	6.99	1.00	1.00	0.56
C7H6O2	122.0368	1.34	1.00	0.86	0.29
C8H12O5	188 0685	1 29	0.60	1.50	0.63
C1/H11NO2	241 0720	2 10	1.00	0.70	0.00
CI4HIINUS	241.0739	5.48	1.00	0.79	0.21
C10H16O7S	280.0617	2.48	0.43	1.60	0.70
C8H18O5S	226.0875	2.94	0.00	2.25	0.63
C7H7NO5	185 0324	2.62	1.00	1.00	0.71
0,11,1100	100.0027	2.02	1.00	1.00	0.71

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C5H12O3S	152 0507	1.88	0.00	2 40	0.60
C(112035	132.0307	2.50	0.00	2.40	0.50
C0H12O5	152.0780	2.39	0.55	2.00	0.50
C8H7NO3	165.0426	2.41	1.00	0.88	0.38
C6H12O4S	180.0456	2.55	0.25	2.00	0.67
C9H11NO4	197.0688	7.77	1.00	1.22	0.44
C14H9O5	256 0272	6 50	1.00	0.57	0.26
C14H8O3	250.0372	0.50	1.00	0.57	0.30
C16H8O4	264.0423	7.59	1.00	0.50	0.25
C17H10O2	246.0681	8.30	1.00	0.59	0.12
C2H4O4S	123 9830	3 52	0.25	2.00	2.00
C15H12O2	240.0786	7 70	1.00	0.80	0.20
C13H12O3	240.0780	7.70	1.00	0.80	0.20
C3H5NO3	103.0269	0.37	0.67	1.67	1.00
C9H7NO4	193.0375	2.36	1.00	0.78	0.44
C4H8O6S	184 0042	0.72	0.17	2.00	1.50
C0H16O4	188 10/0	2.04	0.50	1 78	0.44
C7117NO2	100.1047	2.24	1.00	1.70	0.44
C/H/NO2	137.0477	2.39	1.00	1.00	0.29
C7H14O7S	242.0460	0.57	0.14	2.00	1.00
C7H6N2O6	214.0226	7.08	1.00	0.86	0.86
C10H7NO3	189 0426	3 21	1.00	0.70	0.30
C121124055	280 1244	7.14	0.20	2.00	0.42
C12H24O5S	280.1344	/.14	0.20	2.00	0.42
C8H4N2O	144.0324	3.70	1.00	0.50	0.13
C20H16O8	384.0845	8.25	1.00	0.80	0.40
C14H8O4	240.0423	7.96	1.00	0.57	0.29
C1/H8O/	240.0423	3.06	1.00	0.57	0.20
01/01/100/	240.0423	5.90	1.00	0.57	0.29
C16H10O4	266.0579	6.98	1.00	0.63	0.25
C14H28O5S	308.1657	7.92	0.20	2.00	0.36
C8H7NO4	181.0375	2.14	1.00	0.88	0.50
C13H0NO4	243 0532	8 26	1.00	0.60	0.31
C131191104	243.0332	0.20	1.00	0.09	0.51
C9H16O6S	252.0668	2.65	0.33	1.78	0.67
C11H6O7	250.0114	2.83	1.00	0.55	0.64
C9H7NO	145 0528	3 47	1.00	0.78	0.11
COH8N2O2	176.0586	7.46	1.00	0.80	0.22
Collonad	170.0580	7.40	1.00	0.89	0.22
C9H9NO4	195.0532	6.32	1.00	1.00	0.44
C9H7NO5	209.0324	0.57	1.00	0.78	0.56
C4H11NO3S	153.0460	0.64	0.00	2.75	0.75
C13H6O5	242 0215	3 77	1.00	0.46	0.38
C7117NO2	152.0426	2.50	1.00	1.00	0.42
C/H/NO3	153.0426	2.59	1.00	1.00	0.43
C13H8O5	244.0372	8.17	1.00	0.62	0.38
C8H7NO3	165.0426	2.65	1.00	0.88	0.38
C7H13N07S	255 0413	3 41	0.29	1.86	1.00
COLITIONS	287.0675	2.09	0.12	2.12	1.00
C8H1/NO85	287.0075	2.98	0.15	2.15	1.00
C10H9NO5S	255.0201	2.84	1.00	0.90	0.50
C15H12O4	256.0736	6.95	1.00	0.80	0.27
C9H8O6S	244 0042	3.12	1.00	0.89	0.67
C7H7NO	121.0528	2 10	1.00	1.00	0.14
C/II/NO	121.0528	5.19	1.00	1.00	0.14
C5H6N2O	110.0480	0.14	1.00	1.20	0.20
C9H6O4	178.0266	2.43	1.00	0.67	0.44
C8H8O3	152.0473	1.75	1.00	1.00	0.38
C5H6N2O4S	190 0048	0.82	1.00	1 20	0.80
COLUMNO	144.0224	2.42	1.00	0.50	0.12
Con4IN2U	144.0324	5.45	1.00	0.50	0.15
C9H6N2O3	190.0378	2.75	1.00	0.67	0.33
C9H9NO7S	275.0100	3.70	0.86	1.00	0.78
C7H6O3	138.0317	0.16	1.00	0.86	0.43
C13H10O2	198 0681	7 07	1.00	0.77	0.15
011002	120.0575	2.20	1.00	1.00	0.12
ConoU	120.0575	5.28	1.00	1.00	0.15
C9H7NO3	177.0426	2.75	1.00	0.78	0.33
C9H9NO3	179.0582	6.99	1.00	1.00	0.33
C13H6O5	242.0215	2.84	1.00	0.46	0.38
C5H5NO5	150 0168	0.30	0.80	1.00	1.00
CHINOS	137.0108	0.59	0.00	1.00	1.00
COH/NO4S	189.0096	0.39	1.00	1.17	0.67
C8H5NO6	211.0117	3.00	1.00	0.63	0.75
C9H17NO7S	283.0726	7.24	0.29	1.89	0.78
C8H16O6S	240 0668	3.78	0.17	2.00	0.75
CALISNO2	2-10.0000	0.46	1.00	2.00	0.75
C4H5INU2	99.0320	0.46	1.00	1.25	0.50
C6H12N4O10S	332.0274	5.04	0.30	2.00	1.67
C6H14O5S	198.0562	0.83	0.00	2.33	0.83
C6H4N2O5	184 0120	6 29	1.00	0.67	0.83
C15U005	268 0272	1 20	1.00	0.52	0.22
	208.0572	4.28	1.00	0.55	0.55
C5H5N3O4	171.0280	3.94	1.00	1.00	0.80
C5H4O3	112.0160	0.38	1.00	0.80	0.60
C7H5NO4	167.0219	3 80	1.00	0.71	0.57
	-0//021/	0.00	1.00	0.7.2	5.07

C5H8O3	116.0473	0.07	0.67	1.60	0.60
C8H8O3	152.0473	2.26	1.00	1.00	0.38
C8H8O6S	232 0042	3.09	0.83	1.00	0.75
C6H4N2O6	200,0069	1.82	1.00	0.67	1.00
C10140200	200.0009	4.02	1.00	0.07	1.00
C10H0O0	222.0104	1.55	1.00	0.00	0.00
C13H10O3	214.0630	/.61	1.00	0.77	0.23
C/H12O5	176.0685	1.15	0.40	1.71	0.71
C4H3NO2	97.0164	0.38	1.00	0.75	0.50
C8H6N2O5	210.0277	7.60	1.00	0.75	0.63
C8H6O3	150.0317	3.05	1.00	0.75	0.38
C6H12O6S	212.0355	2.55	0.17	2.00	1.00
C9H8O6S	244 0042	2.36	1.00	0.89	0.67
C4H6O3	102 0317	0.09	0.67	1 50	0.75
C4H3N3O4	157.0124	3.24	1.00	0.75	1.00
C4H3N3O4	212.0255	5.24	1.00	0.73	1.00
C0H12005	212.0555	1.62	0.17	2.00	1.00
C9H12O5S	232.0405	2.74	0.80	1.33	0.56
C9H9NO4	195.0532	6.61	1.00	1.00	0.44
C8H9NO4	183.0532	4.18	1.00	1.13	0.50
C12H10O6	250.0477	2.97	1.00	0.83	0.50
C7H7NO4	169.0375	6.68	1.00	1.00	0.57
C13H26O5S	294.1501	7.61	0.20	2.00	0.38
C5H4N2O3	140 0222	0.39	1.00	0.80	0.60
C5H10O3	118.0630	1 00	0.33	2 00	0.60
C8H7NO	133 0578	2 22	1.00	0.88	0.13
	155.0528	2.33	1.00	0.00	0.15
Constant	108.0423	5.19	1.00	1.00	0.50
CI0H5NO2S	203.0041	0.52	1.00	0.50	0.20
C12H6O5	230.0215	6.72	1.00	0.50	0.42
C9H10O5S	230.0249	2.77	1.00	1.11	0.56
C9H10O5S	230.0249	2.69	1.00	1.11	0.56
C14H10O5	258.0528	3.36	1.00	0.71	0.36
C9H7NO4S	225.0096	1.84	1.00	0.78	0.44
C3H4N2O3S	147 9943	0.41	1.00	1 33	1.00
C9U14O4	174 0902	0.41	0.50	1.55	0.50
Con1404	174.0692	2.52	0.50	1.75	0.50
C8H5NO4	179.0219	3.13	1.00	0.63	0.50
C8H14O4	174.0892	2.69	0.50	1.75	0.50
C7H8O4S	188.0143	2.57	1.00	1.14	0.57
C15H30O5S	322.1814	8.12	0.20	2.00	0.33
C6H8O3	128.0473	0.59	1.00	1.33	0.50
C6H5NO3	139.0269	0.08	1.00	0.83	0.50
C4H8O4S	152.0143	2.84	0.25	2.00	1.00
C8H8N2O4	196 0484	4.06	1.00	1.00	0.50
C12H24O6S	206 1204	6.06	0.17	2.00	0.50
C711124005	230.1234	0.50	0.17	2.00	0.50
C/H10005	228.0008	0.57	0.00	2.29	0.80
C16H10O6	298.0477	3.46	1.00	0.63	0.38
C7H8N2O3	168.0535	3.75	1.00	1.14	0.43
C10H14O5	214.0841	2.67	0.80	1.40	0.50
C10H10O7S	274.0147	1.02	0.86	1.00	0.70
C5H6O6S	193.9885	0.65	0.50	1.20	1.20
C10H18O6S	266.0824	3.00	0.33	1.80	0.60
C7H14O4	162.0892	0.87	0.25	2.00	0.57
C10H10O5S	242.0249	2.76	1.00	1.00	0.50
C8H8O4	168 0/23	1 11	1.00	1.00	0.50
C12U804	200.0423	1.11	1.00	0.62	0.30
C13H6U4	220.0425	1.25	1.00	0.02	0.51
C6H12O6S	212.0355	2.82	0.17	2.00	1.00
C11H6O3	186.0317	6.60	1.00	0.55	0.27
C8H8O4S	200.0143	1.22	1.00	1.00	0.50
C7H6O2	122.0368	6.99	1.00	0.86	0.29
C12H8O4	216.0423	3.33	1.00	0.67	0.33
C15H10O4	254.0579	7.19	1.00	0.67	0.27
C8H7NO4S	213 0096	1 11	1.00	0.88	0.50
C8H18O3S	194 0077	5 17	0.00	2 25	0.38
CALISNO2	00.0220	0.04	1.00	1.25	0.50
C4H5NO2	99.0520	0.04	1.00	1.25	0.50
C6H10N2O3	158.0691	1.11	1.00	1.6/	0.50
C15H8O5	268.0372	5.09	1.00	0.53	0.33
C6H3N3O7	228.9971	4.08	1.00	0.50	1.17
C9H16O8S	284.0566	2.48	0.25	1.78	0.89
C6H4O4S	171.9830	1.56	1.00	0.67	0.67
C13H12O2	200.0837	7.71	1.00	0.92	0.15
C17H12O3	264.0786	7.70	1.00	0.71	0.18
C6H6O3	126 0317	0.38	1.00	1.00	0.50
011005	120.0317	0.50	1.00	1.00	0.50

C11H7NO3	201 0426	3 23	1.00	0.64	0.27
C14U20055	210 1014	7.02	0.00	0.04	0.27
C14H30O5S	310.1814	7.83	0.00	2.14	0.36
C8H5NO7	227.0066	2.78	1.00	0.63	0.88
C11H5NO3	199.0269	3.02	1.00	0.45	0.27
C10H18O4	202 1205	2.88	0.50	1.80	0.40
C15U20065	202.1205	2.00	0.17	2.00	0.40
C15H3006S	558.1705	/.0/	0.17	2.00	0.40
C9H10O2	150.0681	3.74	1.00	1.11	0.22
C12H8O3	200.0473	4.40	1.00	0.67	0.25
C7H12O7S	240 0304	0.91	0.29	1 71	1.00
C2117NO75	200.0042	0.91	0.14	1.71	1.00
C3H/NO/S	200.9943	0.85	0.14	2.33	2.33
C9H18O4	190.1205	2.81	0.25	2.00	0.44
C9H7NO6	225.0273	3.60	1.00	0.78	0.67
C6H7NO4	157 0375	0.69	1.00	1 17	0.67
C11H2007S	206.0020	2.01	0.20	1.92	0.64
C11H2007S	296.0930	2.91	0.29	1.62	0.04
C10H17NO8S	311.0675	3.77	0.38	1.70	0.80
C10H9NO	159.0684	2.63	1.00	0.90	0.10
C8H8O5S	216 0092	2 58	1.00	1.00	0.63
COLLIZNOOS	215.0624	2.50	0.22	1.00	1.00
C9H1/NO95	313.0624	2.34	0.22	1.69	1.00
C9H5NO5	207.0168	3.18	1.00	0.56	0.56
C7H14O6S	226.0511	0.60	0.17	2.00	0.86
C16H22O8S	374 1035	7 37	0.75	1.38	0.50
C12H2005	244 1211	3.01	0.75	1.50	0.42
01202003	244.1511	5.01	0.00	1.0/	0.42
C4H9NO7S	215.0100	1.94	0.14	2.25	1.75
C6H5NO4	155.0219	1.84	1.00	0.83	0.67
C9H4N2O2	172.0273	2.95	1.00	0.44	0.22
C10H11NO3	193 0730	7.91	1.00	1 10	0.30
CTUTTINUS	193.0739	1.01	1.00	1.10	0.50
C/H16O5S	212.0718	3.01	0.00	2.29	0.71
C20H26O4	330.1831	7.61	1.00	1.30	0.20
C15H12O4S	288.0456	7.51	1.00	0.80	0.27
C919055	216 0002	1.09	1.00	1.00	0.62
C6H6U35	218.0092	1.08	1.00	1.00	0.05
C10H17NO10S	343.0573	2.68	0.30	1.70	1.00
C11H8O7	252.0270	2.65	1.00	0.73	0.64
C10H12O3	180 0786	7.82	1.00	1.20	0.30
C111120N2O10	240 1119	6.70	0.20	1.20	0.01
	340.1118	0.79	0.30	1.62	0.91
C/H8N2O3	168.0535	3.35	1.00	1.14	0.43
C8H5NO5	195.0168	3.14	1.00	0.63	0.63
C10H6O4S	221,9987	3.88	1.00	0.60	0.40
C12H10O3	202.0630	8 13	1.00	0.83	0.25
C12H1003	202.0030	0.15	1.00	0.83	0.23
CI2H9NO3	215.0582	3.34	1.00	0.75	0.25
C11H7NO	169.0528	7.37	1.00	0.64	0.09
C16H9NO2	247.0633	7.08	1.00	0.56	0.13
C13H10O3	214.0630	3.47	1.00	0.77	0.23
	214.0030	5.47	1.00	0.77	0.23
C4H4N2O4S	175.9892	0.43	1.00	1.00	1.00
C15H12O3	240.0786	6.87	1.00	0.80	0.20
C9H6O8	242.0063	3.11	0.88	0.67	0.89
C7H6O2	122 0368	7.64	1.00	0.86	0.29
C15U7NO22	220.0000	0.00	1.00	0.30	0.27
CI5H/NUS2	280.9969	0.60	1.00	0.47	0.07
C8H10O3S	186.0351	2.78	1.00	1.25	0.38
C6H6O	94.0419	3.55	1.00	1.00	0.17
C9H10O	134 0732	3.80	1.00	1.11	0.11
C114907	252 0270	1 17	1.00	0.72	0.64
	232.0270	1.17	1.00	0.75	0.04
C/H6O2	122.0368	1.91	1.00	0.86	0.29
C12H8O4	216.0423	2.84	1.00	0.67	0.33
C13H28O5S	296.1657	8.19	0.00	2.15	0.38
C0H10O4	182 0570	2 21	1.00	1 11	0.44
0411004	102.03/9	2.31	1.00	1.11	0.44
C4H6N2O2	114.0429	0.04	1.00	1.50	0.50
C15H8O3	236.0473	7.83	1.00	0.53	0.20
C8H14O7S	254.0460	1.07	0.29	1.75	0.88
C11H2405S	268 1344	7.66	0.00	2.18	0.45
C10H2007C	200.1344	2.00	0.00	2.10	0.40
C10H2006S	268.0981	5.79	0.17	2.00	0.60
C19H22O4	314.1518	7.70	1.00	1.16	0.21
C5H8O2	100.0524	0.68	1.00	1.60	0.40
C8H7NO4	181 0375	2.89	1.00	0.88	0.50
CALLON	102.00/2	2.07	0.05	1 50	2.00
C4H6U8	182.0063	0.39	0.25	1.50	2.00
C8H6O6	198.0164	1.25	1.00	0.75	0.75
C8H10O5	186.0528	0.65	0.80	1.25	0.63
C7H8O4	156 0423	1.07	1.00	1 14	0.57
COLLING	204.0624	1.07	0.50	1.17	0.37
C8H12U6	204.0634	0.65	0.50	1.50	0.75
C15H10O5	270.0528	4.14	1.00	0.67	0.33
C10H7NO2	173.0477	3.45	1.00	0.70	0.20

C6H4O5	156 0059	0.68	1.00	0.67	0.83
C011+05	150.0057	0.00	1.00	0.07	0.05
C11H1804	214.1205	6.74	0.75	1.64	0.36
C6H13NO8S	259.0362	1.45	0.13	2.17	1.33
C13H28O5S	296.1657	7.55	0.00	2.15	0.38
C11H2006S	280,0081	3 1 5	0.33	1.82	0.55
C111120005	200.0701	5.15	0.55	1.02	0.55
C6H9NO2	127.0633	0.20	1.00	1.50	0.33
C6H5NO7S	234.9787	2.81	0.71	0.83	1.17
C8H16O3	160 1099	3 14	0.33	2.00	0.38
C1011100/5	259.0109	0.77	1.00	2.00	0.50
C10H1006S	258.0198	0.77	1.00	1.00	0.60
C10H9NO4	207.0532	2.44	1.00	0.90	0.40
C9H9NO4	195 0532	3 94	1.00	1.00	0.44
C9111002	154.0620	1 50	1.00	1.00	0.29
C8H1005	134.0650	1.38	1.00	1.23	0.58
C10H16O4	200.1049	4.58	0.75	1.60	0.40
C4H10O3S	138.0351	0.70	0.00	2.50	0.75
C6H8O2	112 0524	1.03	1.00	1 33	0.33
C1011002	200.0272	1.05	1.00	1.55	0.55
C10H805	208.0372	3.63	1.00	0.80	0.50
C11H13NO3	207.0895	8.17	1.00	1.18	0.27
C15H8O2	220 0524	7.85	1.00	0.53	0.13
CTUTNO	121.0529	1.07	1.00	1.00	0.13
C/H/NO	121.0528	1.07	1.00	1.00	0.14
C15H31NO8S	385.1770	7.99	0.13	2.07	0.53
C5H10N2O11S	306.0005	2.60	0.18	2.00	2.20
C6H5N3O2	151 0382	3 88	1.00	0.83	0.33
001510502	131.0302	3.00	1.00	0.05	0.33
C8H5NO7	227.0066	4.07	1.00	0.63	0.88
C13H9NO	195.0684	4.46	1.00	0.69	0.08
C5H14N2O6S	230 0573	6 64	0.00	2.80	1.20
COLIDNO2	151 0622	0.04	1.00	1.12	0.25
Congino2	151.0633	2./1	1.00	1.13	0.25
C6H7NO3	141.0426	2.47	1.00	1.17	0.50
C10H10O6S	258 0198	1.07	1.00	1.00	0.60
COLLAGE	102.0050	1.07	1.00	0.44	0.00
C9H4O5	192.0059	1.95	1.00	0.44	0.50
C6H11NO4S	193.0409	0.56	0.50	1.83	0.67
C23H10OS	334.0452	7.23	1.00	0.43	0.04
C1/1905	256 0272	7.57	1.00	0.57	0.26
C14H805	230.0372	7.57	1.00	0.57	0.50
C17H12O4	280.0736	7.73	1.00	0.71	0.24
C8H8O4S	200.0143	1.69	1.00	1.00	0.50
C10H18O6S	266 0824	2.66	0.33	1.80	0.60
COLIONOSS	200.0824	2.00	1.00	1.00	0.00
C8H9NO5S	231.0201	2.73	1.00	1.13	0.63
C9H18O6S	254.0824	4.28	0.17	2.00	0.67
C12H25NO7S	327 1352	8 10	0.14	2.08	0.58
C0111406	218.0700	0.10	0.14	1.50	0.50
C9H14O6	218.0790	0.89	0.50	1.56	0.67
C7H16O3S	180.0820	3.56	0.00	2.29	0.43
C10H6O4	190.0266	3.33	1.00	0.60	0.40
C0H16085	284.0566	2.65	0.25	1 79	0.90
0,01100003	254.0500	2.03	0.25	1.78	0.89
C12H14N2O4	250.0954	5.27	1.00	1.17	0.33
C16H10O5	282.0528	7.47	1.00	0.63	0.31
C10H17NO8	279.0954	2 97	0.38	1 70	0.80
C1011(05	200.0015	2.97	1.00	1.70	0.00
CIUHOUS	200.0215	2.48	1.00	0.00	0.50
C8H5NO4	179.0219	2.56	1.00	0.63	0.50
C8H18O5S	226.0875	2.62	0.00	2.25	0.63
C15H3205S	324 1970	8 07	0.00	2.13	0.33
C01102000	324.17/0	0.07	1.00	2.13	0.55
C9H10O4S	214.0300	2.59	1.00	1.11	0.44
C12H20N2O2	224.1525	2.88	1.00	1.67	0.17
C4H4O5	132.0059	0.35	0.60	1.00	1.25
C9U16049	208 0760	6 00	0.25	2.00	0.50
Con10045	208.0769	0.80	0.25	2.00	0.50
C12H24O6S	296.1294	7.49	0.17	2.00	0.50
C8H11NO5S	233.0358	0.63	0.80	1.38	0.63
C10H6O6	222.0164	3 60	1.00	0.60	0.60
C1011000	214.0742	5.09	1.00	0.00	0.00
C12H10N2O2	214.0742	8.26	1.00	0.83	0.1/
C12H14O4	222.0892	3.18	1.00	1.17	0.33
C12H8O3	200.0473	7.12	1.00	0.67	0.25
C9U16059	200.0175	274	0.20	2.00	0.62
Con10033	224.0718	5.74	0.20	2.00	0.05
C14H9NO5	271.0481	7.50	1.00	0.64	0.36
C17H24O3	276.1725	7.56	1.00	1.41	0.18
C5H5NO2	111 0320	0.38	1.00	1.00	0.40
CONDICO 22	100.0025	1.25	1.00	1.00	0.00
C6H6O5S	189.9936	1.35	0.80	1.00	0.83
C7H7NO7S	248.9943	2.88	0.71	1.00	1.00
C7H16N2O5S	240 0780	8.00	0.20	2 29	0.71
C(11404	140.0110	0.00	1.00	0.67	0.71
C0H4U4	140.0110	0.58	1.00	0.67	0.0/
C11H18O4	214.1205	4.41	0.75	1.64	0.36
C11H8O3	188.0473	5.16	1.00	0.73	0.27
C0U10050	228 0075	2.10	0.20	2.00	0.56
C9U19032	230.08/3	2.12	0.20	2.00	0.30

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C8H16O3	160 1000	5.84	0.33	2.00	0.38
0011005	100.1099	5.64	0.33	2.00	0.58
C7H5N3O6	227.0178	3.31	1.00	0.71	0.86
C7H5N3O7	243.0127	5.68	1.00	0.71	1.00
CITITINO	221.0699	2.05	1.00	1.00	0.26
CITHIIN04	221.0088	5.05	1.00	1.00	0.50
C8H16O4	176.1049	2.41	0.25	2.00	0.50
C5H12N2O8S	260.0314	7 59	0.13	2.40	1.60
C(112056	106.0405	0.01	0.15	2.40	1.00
C6H1205S	196.0405	2.31	0.20	2.00	0.83
C10H8O3	176.0473	4.14	1.00	0.80	0.30
C221112NO65	421 0464	4.70	1.00	0.57	0.26
C25H15N005	451.0404	4.70	1.00	0.57	0.20
C7H7NO3	153.0426	3.35	1.00	1.00	0.43
C8H1406S	238.0511	1.52	0.33	1 75	0.75
C0114005	230.0511	1.52	0.55	1.75	0.75
C4H9NO8S	231.0049	0.71	0.13	2.25	2.00
C6H7NO	109.0528	0.53	1.00	1.17	0.17
COH8O2	148 0524	2.40	1.00	0.80	0.22
0911802	148.0524	2.40	1.00	0.89	0.22
C10H9NO3	191.0582	4.43	1.00	0.90	0.30
C9H11NO4	197 0688	5.79	1.00	1.22	0.44
CELIZNO2	112.0477	0.44	1.00	1.40	0.40
C5H/NO2	113.0477	0.44	1.00	1.40	0.40
C15H8O6	284.0321	3.45	1.00	0.53	0.40
C20H28O2	216 2028	8 12	1.00	1.40	0.15
C20H28O3	310.2038	0.42	1.00	1.40	0.15
C13H10O2	198.0681	7.20	1.00	0.77	0.15
C6H6O5S	189,9936	0.54	0.80	1.00	0.83
COLLENDOC	206.0006	2.00	1.00	0.75	0.75
Corroin200	220.0226	3.00	1.00	0.75	0.75
C9H7NO5	209.0324	4.00	1.00	0.78	0.56
C8H16O6S	240 0668	1 22	0.17	2 00	0.75
01110005	240.0000	1.44	0.17	2.00	0.75
C13H8O3	212.0473	5.77	1.00	0.62	0.23
C11H20O4	216.1362	3.17	0.50	1.82	0.36
61112001	124.01.60	2.00	1.00	0.67	0.50
C6H4O3	124.0160	5.08	1.00	0.67	0.50
C10H17NO8S	311.0675	3.45	0.38	1.70	0.80
C9H0NO2	167.0592	0.76	1.00	1 1 2	0.28
C8H9N03	107.0382	0.70	1.00	1.15	0.56
C12H7NO3	213.0426	3.46	1.00	0.58	0.25
C10H14O6	230.0790	2.81	0.67	1 40	0.60
01111400	230.0790	2.01	0.07	1.40	0.00
C11H8O6	236.0321	2.48	1.00	0.73	0.55
C5H14N2O6S	230.0573	6.27	0.00	2.80	1.20
C11H22058	266 1199	5 16	0.20	2.00	0.45
C11H22033	200.1188	5.40	0.20	2.00	0.45
C13H13NO3	231.0895	8.33	1.00	1.00	0.23
C7H5NO5	183 0168	1.28	1.00	0.71	0.71
C101102049	229,1220	1.20	1.00	0.71	0.71
C10H22O4S	238.1239	/.64	0.00	2.20	0.40
C10H17NO3	199.1208	6.95	1.00	1.70	0.30
C10H2006S	268 0081	2 71	0.17	2.00	0.60
C10H20005	208.0981	2.71	0.17	2.00	0.00
C14H9NO2	223.0633	7.59	1.00	0.64	0.14
C10H20N2O8S	328 0940	8 16	0.25	2.00	0.80
C101120112000D	110.0620	0.14	0.25	2.00	0.00
C5H10O3	118.0630	0.14	0.33	2.00	0.60
C9H6N2O3	190.0378	3.04	1.00	0.67	0.33
C7H9N4O9S2	220.0784	2.79	0.75	1 1 4	1.14
C/HolN40052	339.9764	2.70	0.75	1.14	1.14
C11H18O6	246.1103	4.37	0.50	1.64	0.55
C10H6O6	222.0164	2.44	1.00	0.60	0.60
0110050	222.0104	1.0	1.00	0.00	0.50
C9H805S	228.0092	1.69	1.00	0.89	0.56
C14H6O3S2	285.9758	2.62	1.00	0.43	0.21
C6H10O2	114 0681	1 23	1.00	1.67	0.33
0011002	117.0001	1.23	1.00	1.07	0.55
C3H6O4S	137.9987	1.64	0.25	2.00	1.33
C7H4N2O6	212.0069	2.81	1.00	0.57	0.86
C12H10O2	202.0620	7 91	1.00	0.83	0.25
01201003	202.0030	1.01	1.00	0.03	0.23
C7H10O6	190.0477	0.99	0.50	1.43	0.86
C10H6O5	206 0215	2.89	1.00	0.60	0.50
C111122055	200.0210	2.07	0.00	2.00	0.45
CT1H2205S	200.1188	0.43	0.20	2.00	0.45
C11H8O8S	299.9940	3.85	1.00	0.73	0.73
C13H10O2	198 0681	7 18	1.00	0.77	0.15
C13111002	170.0001	7.40	1.00	0.77	0.15
C9H18O6S	254.0824	2.49	0.17	2.00	0.67
C6H6O	94.0419	2.34	1.00	1.00	0.17
C9U14O4	174 0902	2.04	0.50	1 75	0.50
Con1404	1/4.0892	5.90	0.50	1./5	0.50
C7H7NO3	153.0426	4.70	1.00	1.00	0.43
C8H6N2O	146 0480	3.00	1.00	0.75	0.13
C111111204	221 0200	0.00	1.00	1.00	0.15
CITHTINO4	221.0688	8.03	1.00	1.00	0.36
C10H18O5	218.1154	2.84	0.40	1.80	0.50
C8H18049	242 0824	1.50	0.00	2.00	0.75
00110005	242.0024	1.32	0.00	2.23	0.75
C4H4N2O4	144.0171	0.92	1.00	1.00	1.00
C7H12O2	128 0837	2 47	1.00	1 71	0.29
C0111012002	220.0722	2.7/	1.00	1./1	1.00
C9H18N2O9S	330.0733	1.35	0.22	2.00	1.00
C12H12O6	252.0634	4.82	1.00	1.00	0.50
C13H904	228 0422	671	1.00	0.62	0.31
01511004	220.0423	0.71	1.00	0.02	0.31

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C8H7NO5	197.0324	5.56	1.00	0.88	0.63
Connicos	177.0521	5.50	1.00	0.00	0.05
CI3H2/NO/S	341.1508	8.34	0.14	2.08	0.54
C18H12O3	276.0786	8.06	1.00	0.67	0.17
C20112004	224.0144	0.10	1.00	1.50	0.20
C20H30O4	334.2144	8.12	1.00	1.50	0.20
C12H20O4	228 1362	6.61	0.75	1.67	0.33
CILLIONO	211.0(22	7.05	1.00	0.00	0.15
CI3H9NO2	211.0633	7.95	1.00	0.69	0.15
C14H22O4	254 1518	6 66	1.00	1 57	0.29
Gruppion	100.0400	0.00	0.00	1.00	0.02
C6H8N2O5	188.0433	2.17	0.80	1.33	0.83
C3H6O9S	217,9733	4.06	0.11	2.00	3.00
65110075	217.9755	1.00	0.11	2.00	5.00
C5H8N2O3	144.0535	0.57	1.00	1.60	0.60
C7H6O4	154 0266	2 11	1.00	0.86	0.57
C/11004	154.0200	2.11	1.00	0.00	0.57
C16H14O4	270.0892	7.54	1.00	0.88	0.25
C11H18N2O4	242 1267	2.87	1.00	1 64	0.36
6111101(204	272.1207	2.07	1.00	1.04	0.50
C9HIINO/S	277.0256	2.21	0.71	1.22	0.78
C8H8N2O6	228 0382	4 68	1.00	1.00	0.75
CININZO	105.0502	4.00	1.00	1.00	0.75
CI3H9NO	195.0684	7.65	1.00	0.69	0.08
C10H7NO2	173 0477	2.96	1.00	0.70	0.20
6711005	173.0177	1.04	1.00	1.1.4	0.20
C/H805	172.0372	1.04	0.80	1.14	0.71
C7H9NO5S	219 0201	1.26	0.80	1 29	0.71
Children	217.0201	1.20	0.00	1.29	0.71
C12H10O2	186.0681	5.66	1.00	0.83	0.17
C7H12N2O7S	268 0365	5.07	0.43	1 71	1.00
C511100.40	200.0305	0.70	0.15	2.00	1.00
C5H10O4S	166.0300	0.72	0.25	2.00	0.80
C10H13NO4	211 0845	7 84	1.00	1 30	0.40
C(H14050	100.0550	7.04	1.00	1.50	0.40
C6H14O5S	198.0562	2.20	0.00	2.33	0.83
C15H6O4S2	313 9707	0.82	1.00	0.40	0.27
011100452	515.9707	0.02	1.00	0.40	0.27
C8H/NO3	165.0426	7.38	1.00	0.88	0.38
C3H4N2O3	116 0222	0.64	1.00	1 33	1.00
031141(20)3	110.0222	0.04	1.00	1.55	1.00
C11H23NO7S	313.1195	7.96	0.14	2.09	0.64
C8H8O5S	216 0092	1 55	1.00	1.00	0.63
0010055	210.0092	1.55	1.00	1.00	0.05
C12H8O2	184.0524	5.15	1.00	0.67	0.17
C10H17N3O13S	419 0482	7.61	0.31	1 70	1 30
610111/1050155	419.0402	7.01	0.51	1.70	1.50
C10H6O7	238.0114	1.10	1.00	0.60	0.70
C16H32O5S	336 1970	8 27	0.20	2.00	0.31
0101152055	550.1770	0.27	0.20	2.00	0.51
C12H8O3	200.0473	8.05	1.00	0.67	0.25
C11H8O2	172 0524	6.82	1.00	0.73	0.18
01111002	172.0524	0.02	1.00	0.75	0.10
C9H11NO4	197.0688	6.64	1.00	1.22	0.44
C9H12O5	200.0685	2 49	0.80	1 33	0.56
0/11/2005	200.0085	2.47	0.00	1.55	0.50
C13H26O6S	310.1450	7.39	0.17	2.00	0.46
C11H7NO6	240 0273	2 75	1.00	0.64	0.55
CIIII/NO0	249.0273	2.15	1.00	0.04	0.55
C11H10O2	174.0681	3.34	1.00	0.91	0.18
C16H1004S	208 0200	7 19	1.00	0.62	0.25
C101110045	298.0300	7.40	1.00	0.05	0.25
C11H22O6S	282.1137	6.97	0.17	2.00	0.55
C16H0NO2	247 0622	9.16	1.00	0.56	0.12
C101191002	247.0033	8.10	1.00	0.50	0.15
C12H8O2	184.0524	8.05	1.00	0.67	0.17
C15H16O2S2	202 0502	2 70	1.00	1.07	0.13
C1511100252	292.0392	2.19	1.00	1.07	0.15
C7H8N4O7S2	323.9834	2.94	0.86	1.14	1.00
C10H19NO7S	297 0882	7.46	0.29	1.90	0.70
C1011171(075	277.0002	7.40	0.2)	1.90	0.70
C11H6O7S2	313.9555	2.59	1.00	0.55	0.64
C6H5N3O2	151 0382	4 22	1.00	0.83	0.33
001101002	101.0002	7.22	1.00	0.05	1.17
C6H16N2O/S2	292.0399	3.58	0.00	2.67	1.1/
C10H14N2O7S	306.0522	7 83	0.71	1.40	0.70
C01114075	266.0460	1.24	0.42	1.50	0.79
C9H14U/S	∠00.0400	1.34	0.43	1.30	0.78
C12H20O6	260,1260	3.43	0.50	1.67	0.50
C1111(O4	202.0266	2.10	1.00	0.55	0.20
C11H604	202.0266	2.79	1.00	0.55	0.30
C6H4N2O	120.0324	2.26	1.00	0.67	0.17
CIOLICOS	292.0120	7.00	1.00	0.22	0.05
C19H0US	282.0139	7.09	1.00	0.32	0.05
C10H7NO5	221.0324	4.17	1.00	0.70	0.50
CITITEOE	224 0164	1.00	1.00	0.55	0.55
01111000	234.0104	1.00	1.00	0.55	0.55
C10H18O6	234.1103	2.74	0.33	1.80	0.60
C5112N2O2	127 0225	202	1.00	0.60	0.40
CJH5N502	137.0223	2.02	1.00	0.00	0.40
C12H7NO2	197.0477	3.84	1.00	0.58	0.17
COHENDOD	162 0420	3 1 2	1.00	0.75	0.25
CORUNZUZ	102.0429	5.15	1.00	0.75	0.23
C15H22O2	234.1620	0.13	1.00	1.47	0.13
C4H4N2O	96 0324	0.55	1.00	1.00	0.25
	10.0324	0.55	1.00	1.00	0.25
C5H4O2S	127.9932	1.57	1.00	0.80	0.40
C10H7NO5	221 0324	3 15	1.00	0.70	0.50
	221.0324	5.45	1.00	0.70	0.50
C9H6O6	210.0164	3.06	1.00	0.67	0.67
C4H5N3O2	127 0382	1.09	1.00	1 25	0.50
	127.0302	1.00	1.00	1.43	0.50
C8H8O6S	232.0042	3.49	0.83	1.00	0.75
C15H5NOS2	278 9813	1 76	1.00	0 33	0.07
0101101002	2,0.7015	1.70	1.00	0.00	0.07

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C8H18O5S	226 0875	3 71	0.00	2 25	0.63
CALINNOOSO	199.0079	2.50	1.00	1.22	0.05
COH8N2OS2	188.0078	2.59	1.00	1.55	0.17
C9H19NO/S	285.0882	7.41	0.14	2.11	0.78
C8H6N2O3	178.0378	6.49	1.00	0.75	0.38
C10H18O4	202.1205	7 45	0.50	1.80	0.40
C6H7NO5	173 0324	0.77	0.80	1 17	0.83
COH/NO3	173.0324	0.77	0.80	1.17	0.83
C11H8O3	188.0473	3.82	1.00	0.73	0.27
C7H8O9S	267.9889	3.55	0.44	1.14	1.29
C23H28N4OS2	440,1705	7.16	1.00	1.22	0.04
COULINOS	212.0627	2 50	1.00	1.22	0.56
CHIINOJ	213.0037	5.59	1.00	1.22	0.50
C10H7NO5	221.0324	3.05	1.00	0.70	0.50
C5H4N2O4	156.0171	1.24	1.00	0.80	0.80
C9H10O6S	246 0198	2.88	0.83	1.11	0.67
C14H0NO5	271.0481	7.80	1.00	0.64	0.36
C14119N0J	271.0481	7.09	1.00	0.04	0.30
C16H14O3	254.0943	8.03	1.00	0.88	0.19
C7H7NO7S	248.9943	2.50	0.71	1.00	1.00
C9H6N2O3	190.0378	4.44	1.00	0.67	0.33
C8H10O5	186 0528	3.04	0.80	1.25	0.63
C1111(2)202	214.0279	2.59	1.00	1.25	0.03
C11H6N2O3	214.0378	3.52	1.00	0.55	0.27
C7H7NO2	137.0477	2.92	1.00	1.00	0.29
C13H8O5	244.0372	3.68	1.00	0.62	0.38
C9H8O4S	212 0143	1 59	1.00	0.89	0.44
COUDOO29	200 1122	7 10	0.00	2.02	0.22
C9H20U35	200.1155	1.12	0.00	2.22	0.55
C15H5NOS2	278.9813	1.11	1.00	0.33	0.07
C8H12N2OS2	216.0391	3.63	1.00	1.50	0.13
C8H18O6S	242 0824	1.08	0.00	2.25	0.75
C7H13N009	287 0211	2.00	0.00	1.25	1 20
C/HISNU95	207.0311	2.09	0.22	1.80	1.29
C14H8O3	224.0473	7.86	1.00	0.57	0.21
C9H8O6	212.0321	3.70	1.00	0.89	0.67
C6H15N3O5S	241.0732	7.67	0.20	2.50	0.83
C10H2006S	268 0081	4.01	0.17	2.00	0.60
C10H20005	208.0981	4.91	0.17	2.00	0.00
C/H9NO5S	219.0201	2.47	0.80	1.29	0.71
C15H10O7	302.0427	3.03	1.00	0.67	0.47
C9H10O3	166.0630	4.30	1.00	1.11	0.33
C11H9NO5	235 0481	7.48	1.00	0.82	0.45
CI119NOJ	235.0481	7.40	1.00	0.82	0.45
CI3H1604	236.1049	7.80	1.00	1.23	0.31
C16H24O8	344.1471	3.49	0.63	1.50	0.50
C10H14O4	198.0892	2.64	1.00	1.40	0.40
C0H7NO	145 0528	4.14	1.00	0.78	0.11
COLIONOC	227.0420	7.14	1.00	1.00	0.11
C9H9INO0	227.0450	2.99	1.00	1.00	0.07
C7H12N2O7S	268.0365	4.44	0.43	1.71	1.00
C13H26O6S	310.1450	7.79	0.17	2.00	0.46
C14H10O	194 0732	7.08	1.00	0.71	0.07
C10117N076	284 0042	6.69	1.00	0.70	0.07
CIOH/NO/S	204.9943	0.08	1.00	0.70	0.70
C18H13NO3	291.0895	7.35	1.00	0.72	0.17
C18H14O3	278.0943	8.02	1.00	0.78	0.17
C9H18O3	174.1256	3.80	0.33	2.00	0.33
C14H20NO8S	371 1614	7 8/	0.13	2.07	0.57
C011(2)1000	170.0270	2.50	1.00	0.75	0.20
C8H0N2U3	1/8.03/8	2.50	1.00	0.75	0.58
C5H7NO2	113.0477	0.10	1.00	1.40	0.40
C7H10N2O5	202.0590	3.13	0.80	1.43	0.71
C8H11NO4S	217 0409	0.91	1.00	1.38	0.50
COMENTO	202 0001	2.00	0.75	1.00	1.00
071112005	292.0001	2.70	0.75	1.00	1.00
C/H16O5S	212.0/18	1.52	0.00	2.29	0.71
C11H22O6S	282.1137	7.89	0.17	2.00	0.55
C12H8O5	232.0372	3.87	1.00	0.67	0.42
C14H11NO3	241 0739	8 34	1.00	0.79	0.21
C121005	244.0272	6.54	1.00	0.72	0.21
C13H8U5	244.0372	0.70	1.00	0.62	0.58
C9H6O2	146.0368	3.07	1.00	0.67	0.22
C4H4O3	100.0160	0.11	1.00	1.00	0.75
C6H6N2O4	170.0328	0.39	1.00	1.00	0.67
071171100	127 0477	2 10	1.00	1.00	0.20
C/H/NU2	137.0477	5.10	1.00	1.00	0.29
C/H16015	340.0489	7.15	0.00	2.29	2.14
C9H6O2S	178.0088	3.89	1.00	0.67	0.22
C8H7NO4	181.0375	4.76	1.00	0.88	0.50
C10H12O4	106.0726	267	1.00	1 20	0.40
C10H12U4	190.0750	2.07	1.00	1.20	0.40
C5H10N2O11S	306.0005	2.37	0.18	2.00	2.20
C10H11NO5	225.0637	3.49	1.00	1.10	0.50
C12H7NO4	229.0375	7.41	1.00	0.58	0.33
C7H0NO3S	187 0303	0.02	1.00	1 20	0.43
0/11/1000	107.0303	0.72	1.00	1.27	0.75

C5H2N2O3	138 0065	0.47	1.00	0.40	0.60
C511211203	156.0005	0.47	1.00	0.40	0.00
C5H4N2O4	156.01/1	0.39	1.00	0.80	0.80
CITH5NO4	215.0219	3.15	1.00	0.45	0.36
C6H8O4	144.0423	2.43	0.75	1.33	0.67
C14H24O5	272.1624	7.35	0.60	1.71	0.36
C16H14O2	254 0042	7.50	1.00	0.99	0.10
C10H14O3	234.0943	7.59	1.00	0.00	0.19
C9H8O5	196.0372	5.42	1.00	0.89	0.56
C8H8O6S	232.0042	1.34	0.83	1.00	0.75
C14H9NO4	255.0532	8.07	1.00	0.64	0.29
C12U904	228.0422	4.20	1.00	0.62	0.21
013H804	228.0425	4.29	1.00	0.62	0.51
C6H9NO3	143.0582	0.63	1.00	1.50	0.50
C8H14N2O10S	330.0369	3.13	0.30	1.75	1.25
C8H14O7S	254,0460	2.32	0.29	1.75	0.88
C18H32O6S	376 1020	7.54	0.50	1 78	0.33
0181132003	370.1920	7.54	0.50	1.78	0.55
C/H4O/	199.9957	2.22	0.86	0.57	1.00
C7H6N4O6S	274.0008	3.85	1.00	0.86	0.86
C9H11NO5	213.0637	3.24	1.00	1.22	0.56
C9H6O4	178 0266	0.80	1.00	0.67	0.44
C12U240552	224.1065	0.00	1.00	1.07	0.30
CI3H24O5S2	324.1065	6.57	0.40	1.85	0.38
C9H7NO4	193.0375	2.10	1.00	0.78	0.44
C8H9NO2	151.0633	1.80	1.00	1.13	0.25
C13H4N4OS2	205 0827	3 85	1.00	0.31	0.08
C13114104032	275.7627	5.05	1.00	0.51	0.00
C8H10O4S	202.0300	3.17	1.00	1.25	0.50
C9H8O5	196.0372	4.11	1.00	0.89	0.56
C11H22O6S	282.1137	7.39	0.17	2.00	0.55
C7H8058	204 0092	2 77	0.80	1 14	0.71
0100100	207.0072	2.11	1.00	1.17	0.71
C12H12O6	252.0634	3.37	1.00	1.00	0.50
C12H10O7	266.0427	2.90	1.00	0.83	0.58
C6H7NO3S	173.0147	0.60	1.00	1.17	0.50
C10H5NO2	171 0320	2 92	1.00	0.50	0.20
C(I)(O	04.0410	2.72	1.00	1.00	0.20
C6H6O	94.0419	2.78	1.00	1.00	0.17
C8H8O4	168.0423	1.60	1.00	1.00	0.50
C10H22N2O11S2	410.0665	7.96	0.09	2.20	1.10
C10H20O4	204 1362	3 15	0.25	2.00	0.40
C111112NO9	207.0641	2.15	0.25	2.00	0.70
CITHISNO8	287.0641	2.65	0.75	1.18	0.75
C8H4N2O2	160.0273	3.15	1.00	0.50	0.25
C9H14O8S	282.0409	0.90	0.38	1.56	0.89
C14H8O4S	272 01/13	7 17	1.00	0.57	0.29
C74110045	201.0006	0.55	1.00	1.00	0.27
C/H/N045	201.0096	0.55	1.00	1.00	0.57
C9H11NO7S	277.0256	4.93	0.71	1.22	0.78
C6H4N2O	120.0324	0.39	1.00	0.67	0.17
C7H12N2O9S	300 0264	3 44	0.33	1 71	1 29
C0119075	250,0001	1 15	0.96	0.90	0.79
0918075	239.9991	1.15	0.80	0.89	0.78
C4H8O4S	152.0143	7.83	0.25	2.00	1.00
C12H22O4	230.1518	3.72	0.50	1.83	0.33
C5H4O3	112,0160	0.67	1.00	0.80	0.60
C16H12O2	226 0927	<u>8</u> 10	1.00	0.75	0.12
C10H12O2	250.0857	0.19	1.00	0.75	0.15
C11H22O5S	266.1188	6.81	0.20	2.00	0.45
C7H8O3S	172.0194	1.33	1.00	1.14	0.43
C9H16O6S	252.0668	0.79	0.33	1.78	0.67
C10H19NO9S	329 0781	2 60	0.22	1.90	0.90
C15U1000	222.0701	5 66	1.00	0.47	0.12
01311002	222.0081	3.00	1.00	0.07	0.15
C9H10N4O4S	270.0423	3.72	1.00	1.11	0.44
C10H9NO	159.0684	2.87	1.00	0.90	0.10
C11H7NO5	233,0324	4 53	1.00	0.64	0.45
C10H1004	104 0570	1.10	1.00	1.00	0.40
	174.03/9	1.12	1.00	1.00	0.40
C/H9NO9S	282.9998	3.21	0.44	1.29	1.29
C16H32O7S	368.1869	7.08	0.14	2.00	0.44
C4H3NO2	97.0164	0.08	1.00	0.75	0.50
C7H16O5S	212 0718	1 97	0.00	2 20	0.71
CALIONOA	150.0522	1.77	0.00	1.27	0.71
C0H9INU4	139.0532	0.88	0.75	1.50	0.07
C13H9NO5	259.0481	7.63	1.00	0.69	0.38
C8H6N2O5	210.0277	6.96	1.00	0.75	0.63
C7H9NO	123 0684	0.72	1.00	1 20	0.14
C71110055	206 0240	0.72	0.00	1.42	0.14
C/H10055	200.0249	0.50	0.00	1.43	0./1
C15H9NO	219.0684	8.19	1.00	0.60	0.07
C8H6O5	182.0215	3.70	1.00	0.75	0.63
C7H4N2O5	196 0120	3 38	1.00	0.57	0.71
COHIOS	208 0000	1.06	1.00	0.44	0.67
C7H4U0	200.0000	1.00	1.00	0.44	0.07
COLLONG	210 0277	0.00	1 00	0.55	0.62

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C12H26O3S	250,1603	8.13	0.00	2.17	0.25
C15H14O4	258,1805	7.71	1.00	0.02	0.25
C10U21NO95	215 0092	2.76	0.12	0.95	0.27
CIUHZINO85	315.0988	3.76	0.13	2.10	0.80
C3H5NO2	87.0320	0.04	1.00	1.67	0.67
C18H18O4S	330.0926	8.07	1.00	1.00	0.22
C9H16N2O5S	264.0780	7.92	0.60	1.78	0.56
C11H10O3	190.0630	2.67	1.00	0.91	0.27
C13H8O3	212 0473	4.23	1.00	0.62	0.23
CIJIBOS	212.0473	4.23	1.00	1.20	1.20
C5H6IN4O6S	250.0008	3.09	0.83	1.20	1.20
C12H18O6	258.1103	2.95	0.67	1.50	0.50
C9H8N2O3	192.0535	2.49	1.00	0.89	0.33
C20H28O4	332.1988	7.58	1.00	1.40	0.20
C13H10O2	198 0681	5.03	1.00	0.77	0.15
C7H5NO6	199.0117	1 49	1.00	0.71	0.86
671151(00	100.0410	0.92	1.00	0.71	0.00
	100.0419	0.82	1.00	0.80	0.14
C6H7NO	109.0528	2.48	1.00	1.17	0.17
C4H4N2O3	128.0222	0.11	1.00	1.00	0.75
C5H11NO8S	245.0205	0.81	0.13	2.20	1.60
C19H24O3	300.1725	8.19	1.00	1.26	0.16
C13H6O5	242 0215	4.65	1.00	0.46	0.38
	242.0213	4.05	1.00	0.40	0.38
C16H8O6	296.0321	4.24	1.00	0.50	0.38
C10H10O6S	258.0198	2.78	1.00	1.00	0.60
C10H10O5	210.0528	6.63	1.00	1.00	0.50
C10H7NO4	205.0375	3.62	1.00	0.70	0.40
C7H5NO6	199.0117	0.66	1.00	0.71	0.86
C5H6049	161 0087	0.66	0.75	1 20	0.80
CJ00045	101.770/	0.00	0.75	1.20	0.00
CI0H/NO/S	284.9943	1.99	1.00	0.70	0.70
C14H11NO4	257.0688	8.08	1.00	0.79	0.29
C5H3NO3	125.0113	0.42	1.00	0.60	0.60
C10H11NO3	193.0739	4.08	1.00	1.10	0.30
C8H6N2O6	226.0226	2 43	1.00	0.75	0.75
C0H6078	257.0824	0.71	1.00	0.75	0.79
C9H0U/S	237.9834	0.71	1.00	0.07	0.78
C8H/NO2	149.0477	1.43	1.00	0.88	0.25
C5H6N2O5	174.0277	2.54	0.80	1.20	1.00
C6H8O6S	208.0042	1.38	0.50	1.33	1.00
C6H6O4	142.0266	0.88	1.00	1.00	0.67
C6H6O2	110.0368	0.39	1.00	1.00	0.33
C13H22O5	258 1467	6.47	0.60	1.60	0.38
CT31122O3	155.0592	0.47	0.00	1.09	0.38
C/H9NO3	155.0582	0.54	1.00	1.29	0.43
C4H5N3O2	127.0382	0.81	1.00	1.25	0.50
C8H6O2	134.0368	2.98	1.00	0.75	0.25
C7H12O5	176.0685	2.41	0.40	1.71	0.71
C9H12O3	168 0786	2.80	1.00	1 33	0.33
C12H2007S	308.0930	2.00	0.43	1.55	0.55
C12H2007S	308.0930	2.03	0.43	1.07	0.38
CITH/NO5	233.0324	2.89	1.00	0.64	0.45
C5H8O	84.0575	0.56	1.00	1.60	0.20
C13H7NO2	209.0477	8.00	1.00	0.54	0.15
C10H6O6	222.0164	2.86	1.00	0.60	0.60
C10H11NO7S	289.0256	2.54	0.86	1.10	0.70
C12H11NO5	249 0637	2.68	1.00	0.92	0.42
C12HP029	279.0037	2.00	1.00	0.52	0.15
C15H8U25	220.0245	0.10	1.00	0.62	0.15
C10H6N2O	1/0.0480	2.15	1.00	0.60	0.10
C7H15NO7S	257.0569	4.10	0.14	2.14	1.00
C9H10O6S	246.0198	0.96	0.83	1.11	0.67
C8H8O6S	232.0042	0.59	0.83	1.00	0.75
C8H16O6S	240.0668	4.06	0.17	2.00	0.75
C18H100S	274 0452	3.67	1.00	0.56	0.06
COLLONDOLOG	214.0432	3.07	1.00	0.50	1 1 1
C9H18N2O105	340.0682	7.40	0.20	2.00	1.11
C9H5NO6	223.0117	2.62	1.00	0.56	0.67
C8H6N2O3	178.0378	5.58	1.00	0.75	0.38
C24H34O2	354.2559	9.06	1.00	1.42	0.08
C10H17NO9S	327.0624	3.17	0.33	1.70	0.90
C11H8O2	172 0524	4 46	1.00	0.73	0.18
C9U1405	100 00/1	0.47	0.40	1 75	0.62
0011405	190.0641	0.07	0.40	1.73	0.05
C15H26O5	286.1780	1.35	0.60	1./3	0.33
C10H19NO10S	345.0730	1.05	0.20	1.90	1.00
C10H11NO5	225.0637	6.78	1.00	1.10	0.50
C4H4O6S	179,9729	0.41	0.50	1.00	1.50
C9H11NO4	197 0688	4 41	1.00	1 22	0 44
C12H1004	250 0477	2.45	1.00	0.92	0.50
01201000	230.0477	5.45	1.00	0.85	0.30

C18H13NO3	291.0895	7.79	1.00	0.72	0.17
CIONISI (OS	2)1.00)5	7.72	1.00	0.72	0.17
CITH2INO/S	311.1039	7.71	0.29	1.91	0.64
C10H8N2O6	252 0382	7 80	1.00	0.80	0.60
6101101(200	100.0525	2.52	1.00	1.00	0.00
C8H8N2O3	180.0535	2.53	1.00	1.00	0.38
C11H8O2	172.0524	7.42	1.00	0.73	0.18
C12U90282	262.0015	0.00	1.00	0.77	0.05
C12H8O3S2	263.9915	0.69	1.00	0.67	0.25
C8H8O6S	232 0042	2 85	0.83	1.00	0.75
GIOLOGIA	20210012	2.00	0.02	2.00	0.70
C12H24O6S	296.1294	8.14	0.17	2.00	0.50
C13H27N08S	357 1457	7.55	0.13	2.08	0.62
619112/110005	337.1157	1.55	0.15	2.00	0.02
C13H8O3	212.0473	4.93	1.00	0.62	0.23
C10H6N2O2	186 0429	3 48	1.00	0.60	0.20
01011011202	100.0429	3.40	1.00	0.00	0.20
C8H/NO2	149.0477	2.94	1.00	0.88	0.25
C11H14N2O7S	318 0522	7.64	0.86	1 27	0.64
C111141(2075	510.0522	7.04	0.00	1.27	0.04
C14H10O	194.0732	8.15	1.00	0.71	0.07
C18H12O4S	324 0456	7 78	1.00	0.67	0.22
C101112010	250,0225	2.20	1.00	0.07	0.22
C5H10N2O10	258.0335	2.39	0.20	2.00	2.00
C6H8N2O	124 0637	0.46	1.00	1 33	0.17
601101(20	121.0037	0.10	1.00	1.55	0.17
C9H6O/S	257.9834	2.28	1.00	0.67	0.78
C14H27NO8S	369 1457	7 79	0.25	1 93	0.57
G10111 (070	200.0617	1.05	0.40	1.55	0.57
C10H16O/S	280.0617	1.06	0.43	1.60	0.70
C6H7NO10S	284 9791	3.08	0.40	1 17	1 67
GLUUIAGA	212 0027	0.00	1.00	1.17	0.14
C14H12O2	212.0837	8.20	1.00	0.86	0.14
C7H7NO7S	248 9943	3 37	0.71	1.00	1.00
GIUNNO2	121.0592	0.00	0.71	1.00	1.00
C5H9NO3	131.0582	0.89	0.67	1.80	0.60
C11H14O3	194 0943	8 28	1.00	1 27	0.27
C01101202	102.0525	0.20	1.00	1.27	0.27
C9H8N2O3	192.0535	4.81	1.00	0.89	0.33
C9H11NO7S	277 0256	4 4 2	0.71	1 22	0.78
CENTRA COMP	277.0250	1.12	0.71	1.22	0.70
C/H8N4O8S2	339.9784	1.07	0.75	1.14	1.14
C11H8O2	172 0524	5 13	1.00	0.73	0.18
cillioo2	101.0021	5.15	1.00	0.75	0.10
C8H7NO4	181.0375	6.13	1.00	0.88	0.50
C6H7NO4S	189 0096	0.78	1.00	1 17	0.67
CONTROL D	101.0000	0.76	1.00	1.17	0.07
C10H9NO3	191.0582	2.85	1.00	0.90	0.30
C13H12OS2	248 0330	2 21	1.00	0.92	0.08
679102002	152.05350	1.50	1.00	1.1.4	0.00
C/H8N2O2	152.0586	1.73	1.00	1.14	0.29
C10H6O7	238 0114	2 78	1.00	0.60	0.70
CIALIONOA	2022 0 (222	7.17	1.00	0.64	0.1.4
CI4H9NO2	223.0633	/.1/	1.00	0.64	0.14
C12H18N2O6S	318 0886	7 97	0.83	1 50	0.50
GIANNAGA	220.0726	7.57	1.00	1.00	0.20
C12H12O4	220.0736	1.12	1.00	1.00	0.33
C8H6N2O7	242 0175	646	1.00	0.75	0.88
C10101207	242.0175	0.40	1.00	0.75	0.00
C13H22O/S	322.1086	3.07	0.43	1.69	0.54
C11H11N3O4	249 0750	2 98	1.00	1.00	0.36
CONTRACT	249.0750	2.90	1.00	1.00	0.50
C9H7NO3	177.0426	6.98	1.00	0.78	0.33
C5H5NO4	143 0219	1 21	1.00	1.00	0.80
00111(020	102.0219	2.00	0.00	2.00	0.00
C8H16O3S	192.0820	3.98	0.33	2.00	0.38
C14H9NO3	239.0582	2 69	1.00	0.64	0.21
051110000	220,0006	1.70	0.12	2.00	1.00
C5H1008S	230.0096	1.70	0.13	2.00	1.60
C12H7NO6	261.0273	2.92	1.00	0.58	0.50
COLLOCAC	200.0142	2.65	1.00	1.00	0.50
C8H8045	200.0145	2.65	1.00	1.00	0.50
C12H16O7	272.0896	2.66	0.71	1.33	0.58
C10U1204	106.0726	2.24	1.00	1.20	0.40
01011204	190.0730	5.54	1.00	1.20	0.40
C7H8N2O2	152.0586	0.55	1.00	1.14	0.29
C10H6N4O5S	294 0059	3.07	1.00	0.60	0.50
01011014035	277.0037	3.07	1.00	0.00	0.50
C12H8O6	248.0321	3.27	1.00	0.67	0.50
C14H10O3	226.0630	4.17	1.00	0.71	0.21
014111003	220.0030	4.17	1.00	0.71	0.21
C7H12N2O7S	268.0365	7.09	0.43	1.71	1.00
C5H5N3O3	155 0331	1 60	1.00	1.00	0.60
010111000	155.0551	1.07	1.00	1.00	0.00
C10H16O7S	280.0617	1.55	0.43	1.60	0.70
C14H11NO4	257 0688	8 36	1.00	0.79	0.29
	207.0000	0.00	1.00	0.17	0.27
CT/H8O3S	292.0194	2.87	1.00	0.47	0.18
C14H10O3	226.0630	5 28	1.00	0.71	0.21
00111003	142.00050	2.20	1.00	1.75	0.21
C8H14O2	142.0994	2.95	1.00	1.75	0.25
C10H11NO7S	289 0256	6.11	0.86	1.10	0.70
0(1110/15	100.0455	0.11	0.00	2.00	0.70
C6H12O4S	180.0456	0.55	0.25	2.00	0.67
C12H10O3	202.0630	7.18	1.00	0.83	0.25
C11U22N20100	274 0005	7.07	0.00	2.00	0.01
C11H22N2O10S	374.0995	1.95	0.20	2.00	0.91
C7H18N2O7S	274.0835	3.89	0.00	2.57	1.00
C011004	169.0402	4 40	1.00	1.00	0.50
C8H8U4	108.0423	4.40	1.00	1.00	0.50
C7H13NO8S	271.0362	2.77	0.25	1.86	1.14
C16H31NO0S	413 1720	8.07	0.22	1.04	0.56
C10H31N095	415.1/20	0.07	0.22	1.94	0.50
C10H7NO5	221.0324	6.27	1.00	0.70	0.50

C22H33NO5S2	455 1800	7 59	1.00	1 50	0.23
61711210562	155.1000	0.00	1.00	1.50	0.20
CI/H34055	350.2127	8.38	0.20	2.00	0.29
C7H8O	108.0575	2.73	1.00	1.14	0.14
C7H6N2O4	182 0328	4 70	1.00	0.86	0.57
C01151107	227.0066	4.70	1.00	0.00	0.07
C8H5NO/	227.0066	2.21	1.00	0.65	0.88
C11H13NO5	239.0794	7.35	1.00	1.18	0.45
C8H605S	213 0036	2 74	1.00	0.75	0.63
000000	215.7750	2.74	1.00	0.75	0.05
C8H7NO8S	276.9892	3.26	0.75	0.88	1.00
C17H14O7	330.0740	8.06	1.00	0.82	0.41
C7H14O7S	242 0460	2.60	0.14	2.00	1.00
C/III40/3	242.0400	2.00	0.14	2.00	1.00
C8H12N2O8S	296.0314	3.48	0.50	1.50	1.00
C9H6O5	194.0215	3.17	1.00	0.67	0.56
C7H5NO2	151 0260	2.80	1.00	0.71	0.42
C/HSNO5	131.0209	2.09	1.00	0.71	0.45
C4H4N4O7S	251.9801	0.83	0.71	1.00	1.75
C6H12N2O18S	431 9806	6.48	0.11	2.00	3.00
C7HONO4	171.0522	1.29	1.00	1 20	0.57
C/H9N04	171.0332	1.38	1.00	1.29	0.57
C12H20O8S	324.0879	2.84	0.38	1.67	0.67
C10H15N3O7S	321.0631	8.07	0.71	1.50	0.70
C12U1004	218.0570	2 21	1.00	0.02	0.22
C12H1004	218.0579	3.21	1.00	0.85	0.55
C7H9NO2	139.0633	1.02	1.00	1.29	0.29
C4H5NO5	147 0168	0.34	0.60	1 25	1 25
COLLINO2	1(0.0720	2.70	1.00	1.20	0.20
Continuos	169.0739	2.70	1.00	1.38	0.38
C15H14O5	274.0841	6.76	1.00	0.93	0.33
C7H14O4	162 0892	2 45	0.25	2.00	0.57
C/III404	102.0072	2.43	0.25	2.00	0.37
C9H6O2S2	209.9809	0.63	1.00	0.67	0.22
C3H5NO4S	150.9939	0.50	0.50	1.67	1.33
C0H16O6S	252 0668	4.08	0.22	1 79	0.67
09110003	232.0008	4.06	0.55	1.70	0.07
C18H35NO8S	425.2083	8.26	0.25	1.94	0.44
C10H5NO3	187.0269	2.95	1.00	0.50	0.30
CINIZNOA	220.0275	2 40	1.00	0.59	0.22
C12H/N04	229.0373	5.42	1.00	0.58	0.55
C7H5NO5	183.0168	0.66	1.00	0.71	0.71
C14H13NO4	259 0845	8 13	1.00	0.93	0.29
C14U2605	239.0013	7.40	0.40	1.96	0.25
C14H20O3	274.1780	7.40	0.40	1.60	0.50
C8H6N2O3	178.0378	5.40	1.00	0.75	0.38
C15H14O3	242,0943	8.22	1.00	0.93	0.20
COLLONDO2	179.0279	6.24	1.00	0.75	0.20
C8H6N2O3	1/8.03/8	0.24	1.00	0.75	0.38
C12H16N2O7S	332.0678	8.00	0.86	1.33	0.58
C13H4N4O6	312 0131	2 72	1.00	0.31	0.46
C011100/0	254.0924	2.72	1.00	0.51	0.40
C9H1806S	254.0824	6.92	0.17	2.00	0.67
C8H7N3O2	177.0538	3.38	1.00	0.88	0.25
C7H10O	110.0732	2 49	1.00	1 /3	0.14
C/11100	110.0732	2.49	1.00	1.45	0.14
C8H6O10S	293.9682	1.95	0.60	0.75	1.25
C9H11NO4	197.0688	4.76	1.00	1.22	0.44
C8H16O6S	240.0668	4.65	0.17	2.00	0.75
00110005	240.0008	4.05	0.17	2.00	0.75
C6H5N3O5	199.0229	7.41	1.00	0.83	0.83
C11H5NO4	215.0219	3.59	1.00	0.45	0.36
C8H16O3S2	224 0541	286	0.33	2.00	0.38
C811100332	224.0341	2.80	0.55	2.00	0.38
C8H10O6S	234.0198	0.63	0.67	1.25	0.75
C8H6N2O6	226.0226	4.75	1.00	0.75	0.75
C10H0NO2	175 0633	3.18	1.00	0.00	0.20
0000002	171.0000	5.10	1.00	0.90	0.20
C6H5N3O2	151.0382	3.37	1.00	0.83	0.33
C6H12O5S	196.0405	2.79	0.20	2.00	0.83
C9H7NO5	209 0324	3 / 1	1.00	0.78	0.56
CHINOS	207:0324	5.41	1.00	0.70	0.50
C3H6O4S	137.9987	2.76	0.25	2.00	1.33
C12H18O4	226.1205	5.86	1.00	1.50	0.33
C14H25NO78	351 1352	8 1 1	0.43	1 70	0.50
	211.0775	0.11	0.75	1.79	0.50
CIUHI/NO8S	311.0675	3.10	0.38	1.70	0.80
C14H14O2	214.0994	8.12	1.00	1.00	0.14
C10H7NO2	173 0477	5.02	1.00	0.70	0.20
01011/102	1,3.04/7	2.02	1.00	1.00	0.20
C12H12O3	204.0786	3.37	1.00	1.00	0.25
C7H12N2O8S2	316.0035	5.35	0.38	1.71	1.14
C15H0NO5	283 0481	3 24	1.00	0.60	0.33
010112025	203.0401	0.44	1.00	1.00	0.55
C10H12O5	212.0685	2.62	1.00	1.20	0.50
C9H5NO5	207.0168	1.85	1.00	0.56	0.56
C8H6N2O6	226 0226	4 96	1.00	0.75	0.75
	210.0220	7.70	1.00	0.75	0.75
C14H16O4	248.1049	7.71	1.00	1.14	0.29
C8H12N2O6S	264.0416	6.99	0.67	1.50	0.75
C4H8O4S	152 01/13	5 11	0.25	2 00	1.00
	176.1040	J.11 1.40	0.25	2.00	1.00
C8H16O4	1/6.1049	1.48	0.25	2.00	0.50
C10H11NO6	241.0586	4.16	1.00	1.10	0.60

C13H6N4OS2	297 9983	1 72	1.00	0.46	0.08
01511014052	271.7705	1.72	1.00	0.40	0.00
C12H11NO6	265.0586	2.64	1.00	0.92	0.50
CINICNIO	200.0790	0.11	1.00	1 22	0.42
C12H10N2055	300.0780	8.11	1.00	1.55	0.42
C8H12O2	140.0837	2 77	1.00	1 50	0.25
00111202	140.0037	2.11	1.00	1.50	0.25
C7H6N2O6	214.0226	6.75	1.00	0.86	0.86
COLLIANACOOR	206.0214	7.20	0.50	1 50	1.00
C8H12N2O8S	296.0314	7.38	0.50	1.50	1.00
COHONO2	151 0622	0.75	1.00	1 1 2	0.25
CongNO2	131.0055	0.73	1.00	1.15	0.25
C8H8N2O4	196 0484	2 94	1.00	1.00	0.50
011011204	170.0404	2.74	1.00	1.00	0.50
C6H13NO8S	259.0362	2.60	0.13	2.17	1.33
G101000	200.0452	2.00	1.00	0.47	0.05
C12H8O3	200.0473	3.09	1.00	0.67	0.25
071160	106.0410	264	1.00	0.96	0.14
C/H0U	100.0419	2.04	1.00	0.80	0.14
C6H7NO9S	268 9842	3 75	0.44	1 17	1 50
connicobb	200.9012	5.75	0.11	1.17	1.50
C18H18O4	298.1205	7.67	1.00	1.00	0.22
C011402	140.01/0	1.0.4	1.00	0.50	0.20
C8H4O3	148.0160	1.94	1.00	0.50	0.38
C10H18N2068	20/ 0886	8.00	0.50	1.80	0.60
C101110102005	294.0000	8.00	0.50	1.00	0.00
C8H12N2O10S	328.0213	3.16	0.40	1.50	1.25
G101110000	2260000		1.00	0.55	0.50
C13H1008S	326.0096	5.04	1.00	0.77	0.62
C101126055	261 2202	0 76	0.20	2.00	0.28
C18H50055	304.2283	0.20	0.20	2.00	0.28
C17H14O12S	442 0206	7 43	0.92	0.82	0.71
01711140125	442.0200	7.45	0.72	0.02	0.71
C6H4N2O5	184.0120	3.99	1.00	0.67	0.83
CLOUIDONIDOOG	220,00,40	7.05	0.05	2.00	0.00
C10H20N2O8S	328.0940	1.25	0.25	2.00	0.80
C10H1006S	258 0108	3 65	1.00	1.00	0.60
C101110005	238.0198	5.05	1.00	1.00	0.00
C10H8O2	160.0524	3.55	1.00	0.80	0.20
01011002	100.0521	5.55	1.00	0.00	0.20
C8H6O6S	229.9885	1.34	1.00	0.75	0.75
CELIONO70	007 0100	2.10	0.00	1.00	1 40
C5H9N0/S	227.0100	3.10	0.29	1.80	1.40
C6H13N07S	243 0413	3.07	0.14	2 17	1 17
Comprovis	243.0413	3.91	0.14	2.17	1.17
C20H30O5	350,2093	7.89	1.00	1.50	0.25
0201100000	22012092		1.00	1.00	0.20
C9H8O5S	228.0092	1.50	1.00	0.89	0.56
CTUISNOOD	272.0519	2.04	0.12	2.14	1 1 4
C/HISNO8S	2/3.0518	2.04	0.13	2.14	1.14
C5H0NO8S	243 0040	1.68	0.25	1.80	1.60
0511910005	243.0049	1.00	0.25	1.00	1.00
C12H9NO5	247 0481	7.70	1.00	0.75	0.42
	21/10/01		1.00	0.10	0.12
C14H14O6	278.0790	3.30	1.00	1.00	0.43
CINTNO	107.0477	6.94	1.00	0.50	0.17
CI2H/NO2	197.0477	0.84	1.00	0.58	0.17
C4H8O2	88 0524	1.09	0.50	2.00	0.50
0411002	00.0524	1.07	0.50	2.00	0.50
C8H8O6S	232.0042	2.31	0.83	1.00	0.75
01211(07	074 0114	C 1 C	1.00	0.46	0.54
C13H607	2/4.0114	5.15	1.00	0.46	0.54
C0H18N2O0S	330 0733	6.92	0.22	2.00	1.00
C/11101020/J	550.0755	0.92	0.22	2.00	1.00
C8H15NO9S	301.0468	3.11	0.22	1.88	1.13
G10110070	200.01.15		1.00	0.00	0.50
C12H1007S	298.0147	2.36	1.00	0.83	0.58
COLIONO75	262 0100	1 0 1	0.71	1 1 2	0.88
Con91075	203.0100	4.04	0.71	1.15	0.88
C7H9NO3	155 0582	1 38	1.00	1 29	0.43
0/11/11/05	155.0502	1.50	1.00	1.27	0.45
C7H12N2O8S2	316.0035	5.63	0.38	1.71	1.14
CTUIANACCO	252.0416	6.60	0.50	1 71	0.00
C/H12N2O6S	252.0416	6.62	0.50	1./1	0.86
C12H8O4	216 0423	672	1.00	0.67	0.33
C1211004	210.0425	0.72	1.00	0.07	0.55
C7H14O3S2	210.0384	2.59	0.33	2.00	0.43
General	210,0020	0.00	0.02	0.00	1.00
C6H5NO6S	218.9838	0.38	0.83	0.83	1.00
C17U16O2	268 1000	8 22	1.00	0.04	0.19
C1/H1003	208.1099	0.22	1.00	0.94	0.18
C14H10O5	258.0528	7.61	1.00	0.71	0.36
COLIDNIC 10	007.0050	1 //	1.00	1.00	0.44
C9H9NO4S	227.0252	1.66	1.00	1.00	0.44
C10H14N2O5S	274 0623	6 00	1.00	1.40	0.50
0101114102035	277.0023	0.77	1.00	1.40	0.50
C8H5NO8	243.0015	4.16	0.88	0.63	1.00
CTHONICOC	102.0614	0.10	1.00	1.00	0.40
C/H9N3O3	183.0644	3.10	1.00	1.29	0.43
C10H17NO5	231 1107	262	0.60	1 70	0.50
CIUTI/NU3	231.1107	2.02	0.00	1.70	0.50
C15H8O7S2	363,9711	2.94	1.00	0.53	0.47
010100752	202.2711		2.00		0.17
C17H28O5	312.1937	7.80	0.80	1.65	0.29
COLIZONIZOES	260 1002	700	0.20	2.22	0.56
C9H20N2O55	208.1093	/.80	0.20	2.22	0.56
C11H1006S	270 0198	2 57	1.00	0.91	0.55
011110005	270.0170	2.37	1.00	0.71	0.55
C9H8O2	148.0524	3.78	1.00	0.89	0.22
COLIONO 40	227.0252	0.01	1.00	1.00	0.44
C9H9NO4S	227.0252	2.21	1.00	1.00	0.44
C12H2205	246 1467	2.02	0.40	1 92	0.42
C12H22O5	240.140/	5.02	0.40	1.83	0.42
C13H24O5	260 1624	6 77	0.40	1.85	0.38
015112405	200.1024	0.77	0.70	1.05	0.50
C4H4N4O8S	267.9750	1.94	0.63	1.00	2.00
CLINANCO	211 101 4	0.51	0.00	1.01	0.00
CTTH21NO9	311.1216	2.51	0.22	1.91	0.82
CELEON	110 0369	2 60	1.00	1.00	0.32
011002	110.0500	2.00	1.00	1.00	0.55
C11H18O7S	294,0773	2.62	0.43	1.64	0.64
	22		0.00	1.50	0.01
C10H17NO9S	327.0624	3.50	0.33	1.70	0.90
COULINOS	201 0627	0.70	0.00	1 20	0 42
COLLINOS	201.0037	0.79	0.80	1.38	0.05
C9H10O2	150 0681	5.00	1.00	1 1 1	0.22
0111002	150.0001	5.00	1.00	1.11	0.22
C10H8N2O4	220.0484	1.22	1.00	0.80	0.40
C14UZNO5	200 0224	7.02	1.00	0.50	0.24
C14H/N05	209.0324	1.85	1.00	0.50	0.30

C16H14O2	238 0994	8 26	1.00	0.88	0.13
010111402	250.0774	0.20	1.00	0.00	0.15
C9H9NO4	195.0532	7.34	1.00	1.00	0.44
C4H12N2O7S	232 0365	3 49	0.00	3.00	1 75
C41112112075	252.0505	5.42	0.00	5.00	1.75
C15H18O4	262.1205	8.01	1.00	1.20	0.27
C11H7NO6	249 0273	2 46	1.00	0.64	0.55
CITIL/100	219.0275	2.10	1.00	0.01	0.55
C11H20O5S	264.1031	3.90	0.40	1.82	0.45
C8H9NO4	183 0532	0.55	1.00	1 13	0.50
01101104	105.0552	0.55	1.00	1.15	0.50
C15H25NO8S	379.1301	7.56	0.50	1.67	0.53
C7H7N05S	217 0045	2 29	1.00	1.00	0.71
C/11/1055	217.0045	2.2)	1.00	1.00	0.71
C13H10O	182.0732	7.10	1.00	0.77	0.08
C1046N405S	204 0050	2 28	1.00	0.60	0.50
C10H0N4035	294.0039	3.20	1.00	0.00	0.50
C9H7NO	145.0528	0.91	1.00	0.78	0.11
C12H12NO4	225 0845	8 22	1.00	1.09	0.22
C12H15N04	235.0645	0.23	1.00	1.06	0.55
C13H22O5	258.1467	3.16	0.60	1.69	0.38
COLIZNOS	200 0224	1 10	1.00	0.79	0.56
C9H/NO3	209.0524	1.10	1.00	0.78	0.50
C7H5NO4	167.0219	2.93	1.00	0.71	0.57
C91114O105	202 0208	2.49	0.20	1 75	1.25
C8H140105	502.0508	2.40	0.20	1.75	1.23
C8H16O4S	208.0769	6.31	0.25	2.00	0.50
CTUCNOO	124.0490	2.95	1.00	0.96	0.14
C/HoN2O	134.0480	2.85	1.00	0.80	0.14
C10H20O3	188.1412	5.47	0.33	2.00	0.30
C51110N2O10	259 0225	2.00	0.20	2.00	2.00
C5H10N2O10	258.0335	2.96	0.20	2.00	2.00
C7H8O2	124.0524	0.63	1.00	1.14	0.29
C121125N000	271 1250	7.04	0.00	1.00	0.00
C13H25N09S	3/1.1250	7.24	0.22	1.92	0.69
C9H7NO	145.0528	3.01	1.00	0.78	0.11
CCU1202	116,0027	0.71	0.50	2.00	0.22
C6H12O2	116.0837	2.71	0.50	2.00	0.33
C12H13NO4	235 0845	2.91	1.00	1.08	0.33
CILINGIA	200.0015	2.91	1.00	1.00	0.55
C8H11NO8S	281.0205	3.04	0.50	1.38	1.00
C3H6O9S	217 9733	7 58	0.11	2.00	3.00
05110075	217.9733	7.50	0.11	2.00	5.00
C6H5NO5	171.0168	0.41	1.00	0.83	0.83
C9H13NO5S	247.0514	1.02	0.80	1.44	0.56
011151(055	247.0314	1.02	0.00	1.77	0.50
C16H12O5	284.0685	4.32	1.00	0.75	0.31
C4H11N3O8S	261 0267	4.27	0.13	2 75	2.00
C4IIIIN3085	201.0207	4.27	0.15	2.15	2.00
C17H14O3	266.0943	8.08	1.00	0.82	0.18
C6H7N058	205 0045	1.07	0.80	1 17	0.83
011/1035	205.0045	1.07	0.80	1.17	0.85
C10H20O4	204.1362	6.68	0.25	2.00	0.40
C11H22O4	218 1518	3 70	0.25	2.00	0.36
CI1112204	210.1310	3.19	0.25	2.00	0.50
C10H9NO5	223.0481	5.90	1.00	0.90	0.50
C4H3NO2S	128 0884	0.55	1.00	0.75	0.50
C41151NO25	120.9004	0.55	1.00	0.75	0.50
C8H7N3O7	257.0284	6.95	1.00	0.88	0.88
C14U1002	210.0691	6 00	1.00	0.71	0.14
C14H1002	210.0081	0.00	1.00	0.71	0.14
C9H6O2	146.0368	2.51	1.00	0.67	0.22
C5U(O)	09.0269	0.20	1.00	1.20	0.40
C5H6O2	98.0308	0.39	1.00	1.20	0.40
C20H10O5S2	393,9970	5.04	1.00	0.50	0.25
C7111404	1(2,0902	2.74	0.25	2.00	0.57
C/H1404	162.0892	2.74	0.25	2.00	0.57
C17H24O4	292,1675	6.83	1.00	1.41	0.24
CIDINNOCECO	200.0975	1.40	1.00	0.00	0.50
C10H8N20552	299.9875	1.49	1.00	0.80	0.50
C10H10O6S	258.0198	3 44	1.00	1.00	0.60
CITICOS	265,0960	0.01	1.00	0.40	0.07
C15H6052	205.9800	0.81	1.00	0.40	0.07
C11H10N2O8S	330.0158	3.71	1.00	0.91	0.73
C14U26079	220 1200	2 1 1	0.20	1 04	0.50
C14H20U/3	330.1399	5.11	0.29	1.00	0.30
C15H10O4S	286.0300	7.18	1.00	0.67	0.27
COMENIOOD	162 0420	1 16	1.00	0.75	0.25
COHUNZUZ	102.0429	1.10	1.00	0.75	0.23
C4H8O7	168.0270	1.12	0.14	2.00	1.75
C121127NO55	200 1610	2 60	0.20	2.09	0.29
C13H2/NU33	309.1010	5.08	0.20	2.08	0.56
C9H18O8S	286.0722	5.22	0.13	2.00	0.89
CISUISNO2	257 1052	0 10	1.00	1.00	0.20
CISHISNO3	257.1052	8.40	1.00	1.00	0.20
C26H50O4	426.3709	10.38	0.50	1.92	0.15
CTUTNO	121 0529	2 65	1.00	1.00	0.14
C/H/NU	121.0528	2.00	1.00	1.00	0.14
C12H20O6S	292.0981	2.98	0.50	1.67	0.50
CTUCNOO2	166 0270	1 1 1	1.00	0.97	0.42
C/HoN2O3	100.03/8	1.11	1.00	0.86	0.43
C11H19NO5	245.1263	3.04	0.60	1.73	0.45
C11111407	250 0740	2.50	0.71	1 07	0 64
CHHI4U/	258.0740	2.59	0.71	1.27	0.04
C8H6N2O	146.0480	2.40	1.00	0.75	0.13
COLLIANIAOCO	264.0416	0.27	0.7	1.50	0.75
C0112N2005	204.0410	0.37	0.07	1.50	0.75
C12H10O2	186.0681	7.55	1.00	0.83	0.17
CTHENAOSO	225 0002	1 71	1.00	0.94	0.14
C/H0N4US2	223.9983	1./1	1.00	0.80	0.14
C10H9NO6S	271.0151	2.36	1.00	0.90	0.60
C201160292	257 0759	< 00	1.00	0.20	0.15
020000000000000000000000000000000000000	551.9138	0.99	1.00	0.30	0.15
C10H14O3	182.0943	3.07	1.00	1.40	0.30
CAUTNO2S	140.0147	0.62	0.67	1 75	0.75
C4H/NU35	147.0147	0.02	0.07	1./3	0.75

C16H22O5	294 1467	<b>8</b> /11	1.00	1 38	0.31
C10H22O3	294.1407	0.41	1.00	1.30	0.51
C/H6O5	170.0215	1.42	1.00	0.86	0.71
C10H12O6	228.0634	2.65	0.83	1.20	0.60
C29H9NO3S	451.0303	3.57	1.00	0.31	0.10
C13H25N07S	330 1352	8 22	0.20	1.02	0.54
C1311251NO73	339.1352	0.22	0.29	1.92	0.54
C13H12O4	232.0736	3.90	1.00	0.92	0.31
C7H9NO2	139.0633	2.52	1.00	1.29	0.29
C15H5NO3S	278,9990	0.85	1.00	0.33	0.20
C12H24058	280 1344	8 10	0.20	2.00	0.42
C121124055	280.1344	0.19	0.20	2.00	0.42
C12H12O2	188.0837	4.24	1.00	1.00	0.17
C16H30O5	302.2093	7.51	0.40	1.88	0.31
C16H9NO2S	279.0354	6.38	1.00	0.56	0.13
C16H1007	314 0427	3 52	1.00	0.63	0.44
C(H12N2O(S	255 0525	5.52	0.22	0.05	1.00
Contonouos	255.0525	0.91	0.55	2.17	1.00
C10H16N2O10S	356.0526	7.71	0.40	1.60	1.00
C8H14N2O10S	330.0369	3.73	0.30	1.75	1.25
C11H13NO5	239.0794	4 58	1.00	1 18	0.45
C7119055	201 0002	4.50	1.00	1.10	0.45
C/H8055	204.0092	0.99	0.80	1.14	0.71
C18H28O3	292.2038	8.29	1.00	1.56	0.17
C8H7NO2	149.0477	0.66	1.00	0.88	0.25
C10H16O3	184 1099	7 80	1.00	1.60	0.30
C10111005	210 1099	7.09	1.00	1.00	0.50
C12H22O/S	510.1086	3.94	0.29	1.85	0.58
C9H19NO4S	237.1035	6.86	0.25	2.11	0.44
C11H8O3	188.0473	6.44	1.00	0.73	0.27
C8H13NO4	187 0845	2 70	0.75	1.63	0.50
0111007	252 0220	2.70	1.00	1.05	0.50
CITH8U/	252.0270	5.54	1.00	0.73	0.64
C10H9NO6	239.0430	4.25	1.00	0.90	0.60
C8H10O6	202.0477	1.59	0.67	1.25	0.75
C11H13NO4	223 0845	7.85	1.00	1 18	0.36
	223.0845	1.05	1.00	1.10	0.50
C/H8O	108.0575	4.37	1.00	1.14	0.14
C6H8N2O7	220.0332	0.68	0.57	1.33	1.17
C10H19NO13S2	425.0298	4.68	0.15	1.90	1.30
C15H27NO7S	365 1508	8 24	0.43	1.80	0.47
C15112/110/15	105.0007	0.24	1.00	1.00	0.47
C/H6O4S	185.9987	1.42	1.00	0.86	0.57
C18H10O4S	322.0300	7.72	1.00	0.56	0.22
C9H16O4S	220.0769	2.06	0.50	1.78	0.44
C8H15NO9S	301 0468	2 37	0.22	1.88	1 13
COLLIZNO2	155 0046	2.37	1.00	1.00	0.25
C8H15NO2	133.0946	5.54	1.00	1.05	0.23
C4H8O2	88.0524	0.39	0.50	2.00	0.50
C9H13NO3	183.0895	2.73	1.00	1.44	0.33
C8H9NO7S	263 0100	3 13	0.71	1 13	0.88
C14U2207	202 1266	2.09	0.57	1.15	0.50
C14H22O7	502.1500	5.08	0.57	1.57	0.50
C8H16O5S	224.0718	1.81	0.20	2.00	0.63
C8H10N2O2	166.0742	2.79	1.00	1.25	0.25
C9H5NO6	223.0117	2.33	1.00	0.56	0.67
C16H1007	314 0427	3 3 2	1.00	0.63	0.44
Citilitio0/	314.0427	5.52	1.00	0.05	0.44
C9H20O5S	240.1031	5.60	0.00	2.22	0.56
C11H22O6S	282.1137	6.17	0.17	2.00	0.55
C13H7NO4	241.0375	3.41	1.00	0.54	0.31
C14H8O4	240 0423	3 54	1.00	0.57	0.29
CISUONOS	292 0491	2 57	1.00	0.60	0.22
CISHSNUS	205.0481	5.57	1.00	0.00	0.55
C14H16O4	248.1049	7.80	1.00	1.14	0.29
C9H11NO5	213.0637	4.33	1.00	1.22	0.56
C15H28O6	304.1886	7.30	0.33	1.87	0.40
COHIINOA	107.0699	3 60	1.00	1 22	0.44
	197.0000	5.00	1.00	1.22	1.40
C5H14N2O7S	246.0522	3.43	0.00	2.80	1.40
C13H22O5	258.1467	7.26	0.60	1.69	0.38
C7H4O3	136.0160	3.12	1.00	0.57	0.43
C9H11NO6	229.0586	2.62	0.83	1 22	0.67
015110004	227.0300	2.02	1.00	1.22	0.07
C15H20O4	204.1302	8.19	1.00	1.33	0.27
C9H8N2O3	192.0535	6.89	1.00	0.89	0.33
C8H8N4OS2	240.0140	2.72	1.00	1.00	0.13
C9H11NO2	165 0790	3 26	1.00	1 22	0.22
COLIDNOS	100.0491	5.40	1.00	1.12	0.62
Compileo	199.0481	5.42	1.00	1.15	0.03
C5H7NO8S	240.9892	1.10	0.38	1.40	1.60
C10H18O6S	266.0824	5.42	0.33	1.80	0.60
C17H30O4	298 2144	8.18	0.75	1.76	0.24
C14H12NO7S	330 0/12	7 17	1.00	0.02	0.50
	225 0045	1.41	1.00	1.00	0.50
C12H13NO4	235.0845	1.54	1.00	1.08	0.33
<u>C16H8O</u> S	<u>248.0296</u>	3.92	1.00	0.50	0.06

C7H7N3O2	165 0538	3 72	1.00	1.00	0.29
C/11/10502	105.0550	5.72	1.00	1.00	0.27
C11H1205S	256.0405	2.73	1.00	1.09	0.45
C6H10O7	194.0427	2.90	0.29	1.67	1.17
C9H7NO5S	241 0045	2 / 8	1.00	0.78	0.56
	241.0045	2.40	1.00	0.78	0.50
CI5H5NOS2	2/8.9813	2.69	1.00	0.33	0.07
C4H12N2O7S	232.0365	4.93	0.00	3.00	1.75
C11U9O2S2	251 0015	1.00	1.00	0.72	0.27
C11H80352	231.9913	1.09	1.00	0.75	0.27
C11H20O6S	280.0981	7.03	0.33	1.82	0.55
C7H10O5S	206 0249	0.96	0.60	1 43	0.71
COULINO2	101.0720	0.57	1.00	1.10	0.22
C9HTINO3	181.0739	2.57	1.00	1.22	0.33
C5H14N2O9S	278.0420	2.77	0.00	2.80	1.80
C11H10NO7S	309 0882	7.60	0.43	1 73	0.64
	505.0002	7.00	0.45	1.75	0.04
C/H5NO6	199.0117	0.97	1.00	0.71	0.86
C11H11NO5	237.0637	7.46	1.00	1.00	0.45
C2H7N088	216 0802	1.52	0.12	2 22	2.67
C3H/N085	210.9892	4.55	0.15	2.33	2.07
C4H8O4S	152.0143	1.20	0.25	2.00	1.00
C13H24O5	260 1624	7.21	0.40	1.85	0.38
Cellianaoes	206.0214	5.27	0.10	1.00	1.00
C8H12N2O8S	296.0314	5.27	0.50	1.50	1.00
C8H12N2O8S	296.0314	3.96	0.50	1.50	1.00
C12H16O4	224 1049	3.03	1.00	1 33	0.33
012111004	224.1047	5.05	1.00	1.55	0.55
C/H/NO/S	248.9943	3.80	0.71	1.00	1.00
C7H6O5	170.0215	2.13	1.00	0.86	0.71
C8H14N2068	266 0572	2 51	0.50	1 75	0.75
01511112005	200.0575	5.54	0.50	1.75	0.75
CI5HIINO5	285.0637	7.79	1.00	0.73	0.33
C16H14O6	302.0790	5.12	1.00	0.88	0.38
C8H14O9	238 0680	3 10	0.25	1 75	1.00
Con1408	238.0089	5.10	0.25	1./5	1.00
C14H9NO2	223.0633	6.82	1.00	0.64	0.14
C14H26N4O12	442 1547	3 71	0.33	1.86	0.86
G1014002	442.1347	5.71	0.55	1.00	0.00
C10H609S	301.9733	0.48	0.89	0.60	0.90
C9H12O7	232.0583	2.52	0.57	1.33	0.78
C23H13NO6S	431 0464	6 33	1.00	0.57	0.26
023111310003	451.0404	0.55	1.00	0.57	0.20
C8H6N2O3	178.0378	4.26	1.00	0.75	0.38
C11H22O4	218 1518	3.29	0.25	2.00	0.36
C121122NO05	257 1004	2 50	0.22	1.02	0.75
C12H25IN095	557.1094	3.30	0.22	1.92	0.75
C7H9NO	123.0684	0.95	1.00	1.29	0.14
C5H2N4OS2	197 9670	0.53	1.00	0.40	0.20
CELIONOOS	259,0009	0.55	0.00	1.00	1.20
C5H9NO9S	258.9998	0.74	0.22	1.80	1.80
C10H12O7	244.0583	0.63	0.71	1.20	0.70
C0H11NO4	107.0688	4.12	1.00	1 22	0.44
CHIIINO4	197.0088	4.12	1.00	1.22	0.44
C13H1805	254.1154	3.13	1.00	1.38	0.38
C9H8N2O3	192.0535	7.32	1.00	0.89	0.33
C12H8O282	247 0066	0.52	1.00	0.67	0.17
0121180232	247.9900	0.52	1.00	0.07	0.17
C13H23NO2	225.1729	8.19	1.00	1.77	0.15
C4H8O5S	168.0092	0.85	0.20	2.00	1.25
C12U19O4	226 1205	2.17	1.00	1.50	0.22
C12H1804	220.1205	5.17	1.00	1.50	0.55
C16H16O5	288.0998	7.49	1.00	1.00	0.31
C10H15NO4	213 1001	3.82	1.00	1 50	0.40
C7111200	213.1001	2.02	0.25	1.50	1.14
C/H12U8	224.0552	2.98	0.25	1./1	1.14
C15H15NO4	273.1001	8.27	1.00	1.00	0.27
C7H6N2O6	214.0226	4 34	1.00	0.86	0.86
C7H12N2O49	225 0627	7 57	0.75	1.04	0.57
C/HISNS048	233.002/	1.57	0.75	1.80	0.57
C11H20O8S	312.0879	3.79	0.25	1.82	0.73
C14H12O3	228 0786	4 41	1.00	0.86	0.21
C7114N205	106 0120	2.71	1.00	0.00	0.21
C/H4N205	196.0120	3.37	1.00	0.57	0.71
C6H7NO3S	173.0147	1.30	1.00	1.17	0.50
C14H28O4	260 1988	7 50	0.25	2.00	0.20
C011112004	200.1700	1.54	1.00	2.00	0.27
C9H11N3OS2	241.0344	0.58	1.00	1.22	0.11
C11H8O3	188.0473	3.15	1.00	0.73	0.27
C5H8O	84 0575	1 71	1.00	1.60	0.20
C31100	07.0075	1./1	1.00	1.00	0.20
C9H6O7S	257.9834	1.71	1.00	0.67	0.78
C11H12O4	208.0736	7.58	1.00	1.09	0.36
01111201		671	1.00	1 77	0.22
C13H23N2O2	260 1720		1.00	1.//	0.25
C13H23N3O3	269.1739	0.71	1.00		
C13H23N3O3 C5H14N2O9S	269.1739 278.0420	3.01	0.00	2.80	1.80
C13H23N3O3 C5H14N2O9S C12H12O3	269.1739 278.0420 204.0786	3.01 4.07	0.00	2.80 1.00	1.80 0.25
C13H23N3O3 C5H14N2O9S C12H12O3 C10H2NO5	269.1739 278.0420 204.0786	3.01 4.07	0.00	2.80 1.00	1.80 0.25
C13H23N3O3 C5H14N2O9S C12H12O3 C10H9NO5	269.1739 278.0420 204.0786 223.0481	3.01 4.07 5.01	0.00 1.00 1.00	2.80 1.00 0.90	1.80 0.25 0.50
C13H23N3O3 C5H14N2O9S C12H12O3 C10H9NO5 C16H30O5	269.1739 278.0420 204.0786 223.0481 302.2093	3.01 4.07 5.01 7.96	0.00 1.00 1.00 0.40	2.80 1.00 0.90 1.88	1.80 0.25 0.50 0.31
C13H23N3O3 C5H14N2O9S C12H12O3 C10H9NO5 C16H30O5 C8H6O6S	269.1739 278.0420 204.0786 223.0481 302.2093 229.9885	3.01 4.07 5.01 7.96 0.92	0.00 1.00 1.00 0.40	2.80 1.00 0.90 1.88 0.75	1.80 0.25 0.50 0.31 0.75
C13H23N3O3 C5H14N2O9S C12H12O3 C10H9NO5 C16H30O5 C8H606S	269.1739 278.0420 204.0786 223.0481 302.2093 229.9885	3.01 4.07 5.01 7.96 0.92	0.00 1.00 1.00 0.40 1.00	2.80 1.00 0.90 1.88 0.75	1.80 0.25 0.50 0.31 0.75
C13H23N3O3 C5H14N2O9S C12H12O3 C10H9NO5 C16H30O5 C8H6O6S C9H6O3	269.1739 278.0420 204.0786 223.0481 302.2093 229.9885 162.0317	3.01 4.07 5.01 7.96 0.92 1.07	0.00 1.00 1.00 0.40 1.00 1.00	2.80 1.00 0.90 1.88 0.75 0.67	1.80 0.25 0.50 0.31 0.75 0.33
C13H23N3O3 C5H14N2O9S C12H12O3 C10H9NO5 C16H30O5 C8H6O6S C9H6O3 C11H9NO6	269.1739 278.0420 204.0786 223.0481 302.2093 229.9885 162.0317 251.0430	0.71 3.01 4.07 5.01 7.96 0.92 1.07 2.73	0.00 1.00 1.00 0.40 1.00 1.00 1.00	2.80 1.00 0.90 1.88 0.75 0.67 0.82	1.80 0.25 0.50 0.31 0.75 0.33 0.55
C13H23N3O3 C5H14N2O9S C12H12O3 C10H9NO5 C16H30O5 C8H6O6S C9H6O3 C11H9NO6 C6H2NO49	269.1739 278.0420 204.0786 223.0481 302.2093 229.9885 162.0317 251.0430	0.71 3.01 4.07 5.01 7.96 0.92 1.07 2.73	$\begin{array}{c} 0.00\\ 1.00\\ 1.00\\ 0.40\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ \end{array}$	2.80 1.00 0.90 1.88 0.75 0.67 0.82	1.80 0.25 0.50 0.31 0.75 0.33 0.55

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C8H15NO6	221 0899	3 73	0.33	1.88	0.75
CIFULCOA	260.1040	7.02	1.00	1.00	0.75
C15H1604	260.1049	7.85	1.00	1.07	0.27
C/H14N2O8S	286.0471	4.94	0.25	2.00	1.14
C12H4O13	355.9652	0.18	0.85	0.33	1.08
C20H20N4O3	364 1535	7.50	1.00	1.00	0.15
C14H10O2	226.0620	2 55	1.00	0.71	0.21
C14H1003	220.0030	5.55	1.00	0.71	0.21
C5H13N3O/S	259.0474	6.98	0.14	2.60	1.40
C16H10N4O6	354.0600	5.21	1.00	0.63	0.38
C11H6O6	234 0164	1.59	1.00	0.55	0.55
COHOMOOSO	226 1017	6.75	1.00	2 22	0.11
C9H20N2OS2	230.1017	0.73	1.00	2.22	0.11
C9H8N2O3	192.0535	7.63	1.00	0.89	0.33
C11H12N2O10	332.0492	6.18	0.70	1.09	0.91
C8H6N2O7	242.0175	2.26	1.00	0.75	0.88
C10H808S	287 9940	1.51	0.88	0.80	0.80
C10118085	207.9940	1.51	0.88	0.80	0.80
C13H12O3	216.0786	7.80	1.00	0.92	0.23
C11H10O2	174.0681	3.55	1.00	0.91	0.18
C6H5NO5	171.0168	1.06	1.00	0.83	0.83
C8H801152	3/3 0508	1 50	0.45	1.00	1 38
C811801132	343.9508	1.39	0.45	1.00	1.56
C6H13NO9S	275.0311	0.71	0.11	2.17	1.50
C20H26OS2	346.1425	7.49	1.00	1.30	0.05
C8H8O5	184.0372	1.82	1.00	1.00	0.63
C9H13NO5S	247 0514	1 20	0.80	1 44	0.56
CONTROLS	247.0314	1.27	0.00	1.44	0.50
C8H/NO2	149.0477	2.44	1.00	0.88	0.25
C9H8O6	212.0321	4.14	1.00	0.89	0.67
C5H8O10S2	291.9559	8.87	0.20	1.60	2.00
C4H7NO8S	228 9892	0.86	0.25	1 75	2 00
CIDIONOCC	220.7072	0.00	1.00	1.73	2.00
CIUH9NU6S	2/1.0151	0.89	1.00	0.90	0.60
C16H30O6	318.2042	7.62	0.33	1.88	0.38
C4H4N4O8S	267.9750	1.09	0.63	1.00	2.00
C16H20O4	276 1362	8 30	1.00	1.25	0.25
C10112004	270.1302	0.50	1.00	1.25	0.23
C8H6N2O3	1/8.03/8	3.88	1.00	0.75	0.38
C8H15N3O5S	265.0732	8.44	0.60	1.88	0.63
C18H10OS	274.0452	4.15	1.00	0.56	0.06
C14H16O3	232 1000	7.40	1.00	1.14	0.21
	232.1099	7.40	1.00	1.14	0.21
C6H12N2O10	272.0492	3.33	0.20	2.00	1.6/
C7H7NO5S	217.0045	1.09	1.00	1.00	0.71
C5H3NO4S	172.9783	0.56	1.00	0.60	0.80
C15H26O3	254 1882	8 37	1.00	1 73	0.20
C101/C04	100.0000	0.57	1.00	1.75	0.20
C10H6O4	190.0266	4.24	1.00	0.60	0.40
C10H22N2O2S2	266.1123	3.80	0.50	2.20	0.20
C14H16O4	248.1049	6.78	1.00	1.14	0.29
C11H12O6S	272 0355	1.07	1.00	1.09	0.55
C211122005	272.0555	7.01	1.00	1.05	0.55
C21H22N4O3	378.1092	7.81	1.00	1.05	0.14
C9H9NO4	195.0532	7.56	1.00	1.00	0.44
C10H6O12S2	381.9301	0.13	0.67	0.60	1.20
C9H16O4	188.1049	3.72	0.50	1.78	0.44
C6H5NO3	130.0260	275	1.00	0.82	0.50
CONJINUS	139.0209	5.75	1.00	0.85	0.50
C4H6O4	118.0266	0.52	0.50	1.50	1.00
C7H12O4	160.0736	2.72	0.50	1.71	0.57
C6H10O4	146.0579	1.70	0.50	1.67	0.67
C4H8O4	120 0423	0.38	0.25	2 00	1.00
C10U1004	202 1205	5.00	0.25	1.00	0.40
C10H1804	202.1205	5.21	0.50	1.80	0.40
C4H4O4	116.0110	0.38	0.75	1.00	1.00
C5H8O4	132.0423	0.76	0.50	1.60	0.80
C7H7NO3	153 0426	6.04	1.00	1.00	0.43
C5H1004	134 0570	0.04	0.25	2.00	0.10
C3H10O4	134.0379	0.38	0.25	2.00	0.80
C8H7NO5	197.0324	3.66	1.00	0.88	0.63
C8H12O6	204.0634	2.33	0.50	1.50	0.75
C7H7NO3	153.0426	5.21	1.00	1.00	0.43
COLLOG	180.0422	2 15	1.00	0.00	0.44
07111462	100.0423	5.15	1.00	0.09	0.44
C/H14O3	146.0943	3.23	0.33	2.00	0.43
C3H6O5S	153.9936	0.36	0.20	2.00	1.67
C2H3NO4S	136,9783	0.38	0.50	1.50	2.00
C5U005	140 0272	0.20	0.20	1.50	1.00
05H805	148.0372	0.38	0.40	1.60	1.00
C8H9NO3	167.0582	7.56	1.00	1.13	0.38
C12H14O4	222.0892	7.43	1.00	1.17	0.33
C8H9NO3	167 0582	7.26	1.00	1 13	0.38
	107.0502	7.20	1.00	1.13	0.30
C16H6N4O6S2	413.9729	7.95	1.00	0.38	0.38
C6H5NO4	155.0219	3.08	1.00	0.83	0.67

C4H8O4S	152 0143	0.38	0.25	2 00	1.00
C III CO IB	192.0119	0.50	0.25	2.00	1.00
C9H14O5	202.0841	2.69	0.60	1.56	0.56
C15H16O5S2	340 0439	3.72	1.00	1.07	0.33
012112(02	220 1002	7.00	0.22	2.00	0.02
C13H26O3	230.1882	7.99	0.33	2.00	0.23
C7H5NO5	183.0168	3.26	1.00	0.71	0.71
C10U1(O)5	016 0000	2.04	0.00	1.00	0.50
C10H16O5	216.0998	2.94	0.60	1.60	0.50
C6H12O5	164 0685	0.36	0.20	2.00	0.83
CTUSNOS	102.01.00	0.00	1.00	0.71	0.02
C/H5NO5	183.0168	2.94	1.00	0.71	0.71
C10H12N4OS2	268 0453	3.71	1.00	1.20	0.10
GGUIAGA	140.0726	0.50	0.05	2.00	0.10
C6H12O4	148.0/36	0.58	0.25	2.00	0.67
C6H10O5	162 0528	0.49	0.40	1.67	0.83
G11112005	102.0520	0.12	0.10	1.07	0.05
C11H20O5	232.1311	3.53	0.40	1.82	0.45
C14H28O4S	292 1708	8 27	0.25	2.00	0.29
C1 411200 15	2/2.1700	0.21	1.00	2.00	0.21
C14H13N03	243.0895	8.31	1.00	0.93	0.21
C2H6O4S	125,9987	0.38	0.00	3.00	2.00
COLUNIAO2S	409.0217	2 71	1.00	0.20	0.14
C22H8N4O3S	408.0317	5.71	1.00	0.30	0.14
C5H8O6S	196 0042	0.36	0.33	1.60	1.20
C2H2N2O2	120.0174	0.26	1.00	1.00	1.00
C3H3N3O3	129.0174	0.36	1.00	1.00	1.00
C8H14O	126 1045	3.71	1.00	1.75	0.13
CTUCNDOC	214.0226	4.92	1.00	0.96	0.96
C/H6N2O6	214.0226	4.82	1.00	0.86	0.86
C5H6O5	146 0215	0.37	0.60	1.20	1.00
C7111005	174.0529	0.05	0.00	1.42	0.71
C/H1005	1/4.0528	0.95	0.60	1.45	0.71
C13H16O3	220.1099	8.07	1.00	1.23	0.23
0211404	104.0110	0.27	0.50	1.22	1.22
C3H4O4	104.0110	0.37	0.50	1.55	1.55
C2H4O5S	139,9779	0.34	0.20	2.00	2.50
0711(02)	120 0217	2.55	1.00	0.00	0.42
C/H6O3	138.0317	3.55	1.00	0.86	0.43
C7H6O2	122.0368	2.67	1.00	0.86	0.29
COLICOA	166.0266	2.67	1.00	0.75	0.50
C8H6O4	166.0266	2.64	1.00	0.75	0.50
C4H8O6S	184 0042	0.38	0.17	2.00	1.50
COLLIAGA	10 ( 0002	0.00	0.75	1.50	0.44
C9H14O4	186.0892	2.96	0.75	1.56	0.44
C5H10O5	150 0528	0.34	0.20	2.00	1.00
COLICOLO	127.0007	0.25	0.25	2.00	1.00
C3H6O4S	137.9987	0.35	0.25	2.00	1.33
C2H4O6S	155,9729	0.35	0.17	2.00	3.00
0511001	122.0422	0.20	0.50	1.00	0.00
C5H8O4	132.0423	0.39	0.50	1.60	0.80
C5H8O4	132.0423	1.10	0.50	1.60	0.80
COLLCO2	150.0217	2.62	1.00	0.75	0.20
C8H6O3	150.0317	2.63	1.00	0.75	0.38
C7H7NO4	169.0375	4.11	1.00	1.00	0.57
07111004	159.0570	1.60	0.75	1.42	0.57
C/H1004	158.0579	1.69	0.75	1.43	0.57
C7H7NO4	169 0375	2 94	1.00	1.00	0.57
610112005	105.0575	2.91	1.00	1.00	0.07
C18H30O5	326.2093	8.01	0.80	1.67	0.28
C8H6O3	150 0317	1 14	1.00	0.75	0.38
6011005	164.0472	2.04	1.00	0.75	0.50
C9H8O3	164.04/3	3.06	1.00	0.89	0.33
C4H8O5S	168 0092	0.39	0.20	2.00	1.25
CONTINOS	165.0496	1.07	1.00	2.00	0.20
C8H/NO3	165.0426	1.07	1.00	0.88	0.38
C4H6O5S	165 9936	0.36	0.40	1.50	1.25
C12HONO2	215 0592	8.00	1.00	0.75	0.25
CI2H9NO3	215.0582	8.09	1.00	0.75	0.25
C13H28O4S	280.1708	8.59	0.00	2.15	0.31
C12U2204	242 1519	7 49	0.75	1.60	0.21
C13H22O4	242.1318	7.40	0.75	1.09	0.51
C7H5NO	119.0371	3.13	1.00	0.71	0.14
C64805	160 0372	0.30	0.60	1 22	0.83
011005	100.0572	0.39	0.00	1.33	0.05
C9H10N2O5	226.0590	8.15	1.00	1.11	0.56
C0H0NO3	179 0582	2.88	1.00	1.00	0.33
	102.0202	2.00	1.00	1.00	0.35
C/H6N2O4	182.0328	3.12	1.00	0.86	0.57
C8H7NO3	165 0426	3 19	1.00	0.88	0.38
Collinios	105.0120	5.17	1.00	0.00	0.50
C8H7NO4	181.0375	3.91	1.00	0.88	0.50
C7H12O6	192 0634	0.37	0 33	1 71	0.86
0/11/200	120.0034	0.57	0.55	1./1	0.00
C6H6N2O2	138.0429	0.92	1.00	1.00	0.33
C9H16O5	204 0998	2 58	0.40	1.78	0.56
05111003	100.0155	2.50	0.70	2.10	0.00
C5H12O4S	168.0456	2.81	0.00	2.40	0.80
C10H18O4	202.1205	6.80	0.50	1.80	0.40
01011007	202.1203	5.00	0.50	1.00	0.70
C12H20O4	228.1362	/.36	0.75	1.67	0.33
C8H12O5	188 0685	1.91	0.60	1.50	0.63
CELI2NO 4	141.0000	0.27	1.00	0.00	0.00
C5H3NO4	141.0062	0.37	1.00	0.60	0.80
C3H3NO4	117,0062	0.39	0.75	1.00	1.33
CELIONOA	150.0522	0.20	0.75	1.00	0.07
COH9INU4	139.0332	0.38	0.75	1.50	0.07
C16H32O6S	352,1920	7.86	0.17	2.00	0.38
COLLINGA	100 1205	2 47	0.25	2.00	0.44
C9H18O4	190.1205	5.47	0.25	2.00	0.44
C12H8N2O5	260.0433	8.31	1.00	0.67	0.42
CELENICA	155 0010	2 01	1.00	0.02	0.67
CONSINU4	155.0219	5.81	1.00	0.85	0.07
C3H8O4S	140.0143	0.50	0.00	2.67	1.33

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C10H11NO5	225.0637	4.15	1.00	1.10	0.50
C10H10O4	194.0579	6.38	1.00	1.00	0.40
C8H8N2O6	228.0382	7.67	1.00	1.00	0.75
C12H12N2O3	232.0848	7.63	1.00	1.00	0.25
C5H4O4	128.0110	0.37	1.00	0.80	0.80
C14H26O3	242.1882	8.40	0.67	1.86	0.21
C11H8O2	172.0524	3.84	1.00	0.73	0.18
C16H32O4	288.2301	7.56	0.25	2.00	0.25
C12H20O5	244.1311	4.34	0.60	1.67	0.42
C8H14O5	190.0841	2.24	0.40	1.75	0.63
C13H5NOS	223.0092	3.55	1.00	0.38	0.08
C8H6O5	182.0215	2.78	1.00	0.75	0.63
C7H12O	112.0888	3.12	1.00	1.71	0.14
C9H15NO2	169.1103	4.41	1.00	1.67	0.22

Table S4.3.5 Molecular formulas of organic compounds detected in Guangzhou OA in ESI- mode.

Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	0/0
C7H5NO5	183.0168	3.23	1.00	0.71	0.71
C7H7NO4	169.0375	2.93	1.00	1.00	0.57
C10H7NO3	189.0426	7.73	1.00	0.70	0.30
C7H5NO5	183.0168	2.93	1.00	0.71	0.71
C8H9NO5	199.0481	2.49	1.00	1.13	0.63
C8H9NO4	183.0532	7.04	1.00	1.13	0.50
C10H10O5	210.0528	3.01	1.00	1.00	0.50
C8H12O4	172.0736	2.46	0.75	1.50	0.50
C5H4N2O3	140.0222	2.38	1.00	0.80	0.60
C7H7NO5	185.0324	3.28	1.00	1.00	0.71
C13H25NO3	243.1834	7.36	0.67	1.92	0.23
C8H10O5S	218.0249	1.40	0.80	1.25	0.63
C6H12O7S	228.0304	0.38	0.14	2.00	1.17
C7H6O3	138.0317	2.23	1.00	0.86	0.43
C18H14O8	358.0689	7.43	1.00	0.78	0.44
C8H9NO4	183.0532	5.66	1.00	1.13	0.50
C5H6O7S	209.9834	0.37	0.43	1.20	1.40
C9H6O6	210.0164	1.08	1.00	0.67	0.6
C8H8O3	152.0473	2.63	1.00	1.00	0.38
C6H6O6	174.0164	0.37	0.67	1.00	1.00
C9H6O6	210.0164	1.90	1.00	0.67	0.6
C6H6O5	158.0215	0.38	0.80	1.00	0.8
C17H14O6	314.0790	7.96	1.00	0.82	0.3
C14H10O4S	274.0300	7.08	1.00	0.71	0.29
C4H10O5S	170.0249	0.38	0.00	2.50	1.2
C9H14O4	186.0892	2.92	0.75	1.56	0.4
C8H7NO5	197.0324	4.69	1.00	0.88	0.6
C10H17NO10S	343.0573	2.71	0.30	1.70	1.0
C5H1007S	214.0147	0.37	0.14	2.00	1.4
C6H5N3O4	183.0280	4.90	1.00	0.83	0.6
C7H6O3	138.0317	2.76	1.00	0.86	0.4
C6H5NO5	171.0168	2 29	1.00	0.83	0.8
C9H11NO4	197.0688	7.36	1.00	1.22	0.44
C11H9NO3	203 0582	7.98	1.00	0.82	0.2
C10H17N07S	295.0726	6.58	0.43	1.70	0.7
C13H8O2	196.0524	7 54	1.00	0.62	0.14
C9H16O5S	236.0718	2.64	0.40	1.78	0.5
C6H8O4	144 0423	0.69	0.75	1 33	0.6
C7H6N2O6	214 0226	3 53	1.00	0.86	0.8
C3H4O3	88 0160	0.36	0.67	1 33	1.00
C9H15N08S	297.0518	3.26	0.38	1.55	0.89
C9H8O2	148 0524	3.08	1.00	0.89	0.0
C9H9N07S	275 0100	4.19	0.86	1.00	0.7
C7H8O6	188 0321	0.39	0.67	1.14	0.70
C5H8O4	132.0423	0.39	0.50	1.60	0.80
C9H7NO4	193 0375	3.46	1.00	0.78	0.4
C/H606S	181 9885	0.38	0.33	1 50	1.50

C8H5NO3	163 0269	2.66	1.00	0.63	0.38
661151105	160.0209	2.00	1.00	0.05	0.50
C5H4N4O3	168.0283	0.37	1.00	0.80	0.60
C12H10O5S	266.0249	3.32	1.00	0.83	0.42
COLLICOCO	252.0669	2.00	0.22	1.70	0.02
C9H1606S	252.0668	2.60	0.33	1./8	0.67
C7H4N2O3	164 0222	3.99	1.00	0.57	0.43
0711(04	154.0266	1.00	1.00	0.07	0.57
C/H6O4	154.0266	1.28	1.00	0.86	0.57
C9H18O6S	254 0824	3.20	0.17	2.00	0.67
CONTRACT	107.0221	2.20	1.00	2.00	0.07
C8H/NO5	197.0324	3.25	1.00	0.88	0.63
C10H18O5S	250.0875	3.08	0.40	1.80	0.50
GOLISION	147.0000	2.00	1.00	0.00	0.05
C8H5NO2	147.0320	3.25	1.00	0.63	0.25
C10H17N3O13S	419 0482	7.61	0.31	1 70	1 30
GOLONOA	102.0522	7.01	1.00	1.10	0.50
C8H9NO4	183.0532	6.51	1.00	1.13	0.50
C8H8O2	136 0524	3 10	1.00	1.00	0.25
C101002	106.0521	5.10	1.00	1.00	0.15
C13H8O2	196.0524	7.18	1.00	0.62	0.15
C22H10O3S	354 0351	2 62	1.00	0.45	0.14
C51110055	100.0100	0.44	0.17	0.15	1.00
C5H1006S	198.0198	0.44	0.17	2.00	1.20
C11H18O5	230,1154	3.20	0.60	1.64	0.45
CTUANOOA	100.0171	2.51	1.00	0.57	0.77
C/H4N2O4	180.01/1	3.51	1.00	0.57	0.57
C10H16O5S	248 0718	2.98	0.60	1.60	0.50
C11110035	172.0524	2.20	1.00	0.72	0.50
CTTH802	172.0524	3.84	1.00	0.73	0.18
C3H5NO5	135.0168	0.38	0.40	1.67	1.67
COLLIAOS	100.0605	0.24	0.00	1.50	0.62
C8H12O5	188.0685	2.34	0.60	1.50	0.63
C6H10O4	146 0579	0.58	0.50	1 67	0.67
COLLIDOS	106.0520	2.02	0.00	1.07	0.07
C8H1005	186.0528	3.03	0.80	1.25	0.63
C10H10O4	194 0579	3 66	1.00	1.00	0.40
GOLIONIOO	191.0379	5.00	1.00	1.00	0.10
C8H8N2O6	228.0382	7.58	1.00	1.00	0.75
C4H8O5S	168 0092	0.42	0.20	2.00	1 25
6110055	100.0092	0.12	0.20	2.00	1.20
C5H3N3O2	137.0225	3.18	1.00	0.60	0.40
C7H12O7S	240 0304	0.57	0.29	1 71	1.00
C/III20/B	210.0301	0.57	0.27	1.71	1.00
C10H8O4	192.0423	3.08	1.00	0.80	0.40
C8H9NO4	183 0532	5 95	1.00	1 1 3	0.50
GIOUOOF	105.0552	0.55	1.00	0.00	0.50
C10H8O5	208.0372	2.54	1.00	0.80	0.50
C7H6O5S	201 9936	0.62	1.00	0.86	0.71
G100110	201.5550	1.02	1.00	1.00	1.10
C10H18N2O11S	374.0631	4.36	0.27	1.80	1.10
C9H8O3	164 0473	2 47	1.00	0.89	0.33
CINNOC	201.0221	2.07	1.00	0.00	0.00
C10H8O6	224.0321	2.86	1.00	0.80	0.60
C9H5NO4	191.0219	2.64	1.00	0.56	0.44
651131101	100.0110	2.01	1.00	0.00	0.11
C5H4O4	128.0110	0.37	1.00	0.80	0.80
C9H8O3	164 0473	3.06	1.00	0.89	0.33
C)11005	104.0475	5.00	1.00	0.07	0.55
C8H6O5	182.0215	1.89	1.00	0.75	0.63
C10H19NO8S	313 0831	3 38	0.25	1.90	0.80
	100.0117	2.11	1.00	1.90	0.00
C/H5NO6	199.0117	3.41	1.00	0.71	0.86
C9H9NO6	227 0430	3 36	1.00	1.00	0.67
C1411004	227.0450	5.50	1.00	1.00	0.07
C14H10O4	242.0579	5.03	1.00	0.71	0.29
C7H5NO6	199.0117	2.65	1.00	0.71	0.86
CHISTOD	100.0017	2.05	1.00	1.50	0.00
C4H6O3	102.0317	0.39	0.67	1.50	0.75
C4H10O4S	154 0300	0.92	0.00	2 50	1.00
C14U002	224.0472	7.54	1.00	0.57	0.01
C14H8O3	224.04/3	1.56	1.00	0.57	0.21
C6H5NO3	139.0269	0.39	1.00	0.83	0.50
COLLISNOOS	295 0519	2.07	0.25	1 00	1.00
COLIDINO92	283.0318	2.91	0.23	1.00	1.00
C5H10O5S	182.0249	0.52	0.20	2.00	1.00
C10H605	206 0215	3 1 2	1.00	0.60	0.50
0101003	200.0213	5.15	1.00	0.00	0.50
C8H6O3	150.0317	0.81	1.00	0.75	0.38
C0H16O5	204 0008	276	0.40	1 79	0.56
0111005	207.0770	2.70	0.40	1./0	0.50
C12H6O4	214.0266	5.46	1.00	0.50	0.33
C10H6O382	237 9758	0.52	1.00	0.60	0.30
010100352	231.3130	0.52	1.00	0.00	0.50
C9H6O3	162.0317	3.14	1.00	0.67	0.33
C0H8O4	180 0423	2 75	1.00	0.80	0.44
	05.0123	2.13	1.00	1.00	0.77
C3H3NO2	85.0164	0.05	1.00	1.00	0.67
C6H4N2O5	184 0120	6.28	1.00	0.67	0.83
001110203	100.0727	0.20	1.00	1.00	0.05
C3H4O8S	199.9627	0.31	0.25	1.33	2.67
C9H11NO4	197 0688	7 76	1.00	1 22	0.44
0/11/10/4	10/.0000	1.10	1.00	1.22	0.44
C6H12O5S	196.0405	0.97	0.20	2.00	0.83
C7H10O4	158 0579	1.67	0.75	1 43	0.57
051151204	171 0200	1.07	1.00	1.70	0.07
C5H5N3O4	171.0280	3.93	1.00	1.00	0.80
C8H9NO4	183 0532	4 16	1.00	1 1 3	0.50
	105.0552	7.10	1.00	1.15	0.50
C/H6N2O6	214.0226	7.13	1.00	0.86	0.86
C9H15NO8S	297.0518	2 90	0.38	1.67	0.89
0011731000	165.0406	2.10	1.00	0.00	0.02
C8H/NU3	165.0426	5.18	1.00	0.88	0.38
C3H5NO5S	166.9888	0.36	0.40	1.67	1.67
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C9H7N04         193.0375         7.16         1.00         0.78         0.444           C8H5N04         179.0219         5.38         1.00         0.67         1.00           C4H43N304         157.0124         3.23         1.00         0.67         0.33           C6H8075         223.9991         0.38         0.43         1.33         1.17           C7H1406S         226.0511         2.18         0.17         2.00         0.86           C10H1604         200.1049         3.39         0.75         1.60         0.40           C10H17078         295.0726         6.29         0.43         1.70         0.70           C10H11N04         209.0688         7.17         1.00         1.10         0.40           CSH13N016         391.0224         3.08         0.25         1.44         1.78           C6H1002         114.0681         2.74         1.00         1.67         0.33           C7H1406         218.0790         2.72         0.50         1.56         0.67           C8H5N05         195.0168         3.13         1.00         0.63         0.63           C1H1405         224.075         1.83         0.06         0.67	C5H4N2O3	140.0222	1.14	1.00	0.80	0.60
CRH5N04         179.0219         5.38         1.00         0.63         0.53           CH4N2O7         228.0019         4.05         1.00         0.75         1.00           C9H603         162.0317         2.96         1.00         0.67         0.33           C6H807S         223.9991         0.38         0.43         1.33         1.17           C7H1406S         226.0511         2.18         0.17         2.00         0.86           C10H11604         220.0499         3.39         0.75         1.60         0.40           C10H11NO4         229.0628         7.17         1.00         1.10         0.40           C10H11NO4         299.0688         7.17         1.00         1.00         0.38           C10H11NO4         299.0688         7.17         1.00         1.60         0.33           C10H1405         214.0841         2.66         0.80         1.40         0.50           C9H1406         218.0790         2.72         0.50         1.56         0.67           C9H1406         218.0790         2.72         0.50         1.56         0.67           C9H1405         224.0375         8.19         0.00         2.18         0	C9H7NO4	193.0375	7.16	1.00	0.78	0.44
CH43X204         157.0124         3.23         1.00         0.57         1.00           CH4N3Q04         157.0124         3.23         1.00         0.675         0.23           CHBOTS         223.9991         0.38         0.43         1.33         1.17           CHH1406X         226.0511         2.18         0.17         2.00         0.86           C10H1604         200.1049         3.39         0.75         1.60         0.40           C10H1707S         295.0726         6.29         0.43         1.70         0.70           C10H11NO4         209.0688         7.17         1.00         1.10         0.40           CSH13ND16         391.0234         3.08         0.25         1.44         1.78           CH11405         214.0841         2.66         0.80         1.40         0.57           CH13ND16         391.0234         3.08         0.25         1.44         1.78           CH11405         214.0841         2.66         0.80         1.40         0.57           CH143ND16         218.0790         2.72         0.50         1.56         0.67           CH14204S         22.1395         8.19         0.00         0.30         <	C8H5NO4	179.0219	5.38	1.00	0.63	0.50
C9H603         1620317         256         1.00         0.67         0.03           C6H807S         223.9991         0.38         0.43         1.33         1.17           C7H14065         226.0511         218         0.17         2.00         0.86           C10H1604         200.1049         3.39         0.75         1.60         0.40           C10H17N07S         295.0726         6.29         0.43         1.70         0.70           C10H117N07S         295.0726         6.29         0.43         1.70         0.70           C10H11004         209.0688         7.17         1.00         1.00         0.38           C10H11005         214.0841         2.66         0.80         1.44         1.78           C6H1002         114.0681         2.74         1.00         1.67         0.33           C7H18N04         167.0219         3.79         1.00         0.63         0.63           C1H42045         252.1395         8.19         0.00         2.18         0.30         1.50           C1H420445         252.1395         8.19         0.00         2.18         0.36         C10H4N204         2.60.075         1.43         0.50	C/H4N2O/ C4H2N2O4	228.0019	4.05	1.00	0.57	1.00
Coffworfs         223.9991         0.38         0.43         1.33         0.17           CTH1406S         226.0511         2.18         0.17         2.00         0.86           C10H1604         200.1049         3.39         0.75         1.60         0.40           C1H1707S         224.0355         0.82         0.33         1.71         0.80           C1H17N07S         295.0726         6.29         0.43         1.70         0.70           C1H11N04         209.0688         7.17         1.00         1.10         0.40           C8H803         152.0473         3.22         1.00         1.67         0.33           C1H1405         214.0681         2.74         1.00         1.67         0.33           C7H15N04         167.0219         3.79         1.00         0.61         0.63           CH1405         252.1395         8.19         0.00         2.18         0.66           C1H4404S         252.1395         8.19         0.00         2.18         0.36           C1H4404S         252.1395         8.19         0.00         2.18         0.36           C1H4404S         252.1395         8.19         0.00         0.40	C9H6O3	162 0317	2.25	1.00	0.73	0.33
CTH4005         226.0511         2.18         0.17         2.00         0.88           C10H1604         200.1049         3.39         0.75         1.60         0.40           C10H110707S         226.0726         6.29         0.43         1.70         0.70           C10H11NO4         209.0688         7.17         1.00         1.00         0.43           C10H1405         214.0841         2.66         0.80         1.44         1.75           C6H1002         114.0681         2.74         1.00         0.71         0.57           C9H1405         214.0841         2.66         0.80         1.66         0.67           C9H1406         218.0790         2.72         0.50         1.56         0.67           C9H1406         218.0790         2.72         0.50         1.56         0.67           C10H48204115         374.0651         3.23         0.27         1.80         0.36           C10H48204115         374.0651         3.23         0.27         1.80         0.36           C10H48204115         374.0651         3.23         0.27         1.80         0.36           C10H48204         216.0171         0.12         1.00         0.40 <td>C6H8O7S</td> <td>223 9991</td> <td>0.38</td> <td>0.43</td> <td>1.33</td> <td>1.17</td>	C6H8O7S	223 9991	0.38	0.43	1.33	1.17
C10H16O4         200.1049         3.39         0.75         1.60         0.40           C7H12O6S         224.0355         0.82         0.33         1.71         0.86           C10H17NO7S         295.0726         6.29         0.43         1.70         0.70           C10H11NO4         209.0888         7.17         1.00         1.10         0.40           CSH30016         391.0234         3.08         0.25         1.44         1.78           C9H13NO16         391.0234         3.08         0.25         1.44         1.78           C6H1002         114.0681         2.74         1.00         0.71         0.57           C9H1406         218.0790         2.72         0.50         1.56         0.67           C8H5NO5         195.0168         3.13         1.00         0.63         0.63           C1H42O4S         252.1395         8.19         0.00         2.18         0.36           C1H42O4S         252.1395         8.19         0.00         2.18         0.36           C1H42O4S         25.1390         0.67         1.60         0.60           C1H418N2011S         374.0631         3.23         0.27         1.80         0.63     <	C7H14O6S	226.0511	2.18	0.13	2.00	0.86
C7H1206S         2240355         0.82         0.33         1.71         0.86           C10H11NO4         295.0726         6.29         0.43         1.70         0.70           C10H11NO4         295.0726         6.29         0.43         1.70         0.70           C10H14O5         214.0841         2.66         0.80         1.40         0.53           C10H14O5         214.0841         2.66         0.80         1.40         0.53           C6H10O2         114.0681         2.74         1.00         0.71         0.57           C9H14O6         218.0790         2.72         0.50         1.56         0.67           C9H14O6         218.0790         2.72         0.50         1.56         0.67           C2H60XS         110.0038         0.35         0.00         3.00         1.60           C1H24O4S         252.1395         8.19         0.00         2.18         0.36           C10H18N2011S         374.0631         3.23         0.27         1.80         1.10           C10H4RO4         126.0379         1.22         0.75         1.43         0.57           C8H803         116.0473         0.39         0.67         1.40 <t< td=""><td>C10H16O4</td><td>200.1049</td><td>3.39</td><td>0.75</td><td>1.60</td><td>0.40</td></t<>	C10H16O4	200.1049	3.39	0.75	1.60	0.40
C10H117N07S         295.0726         6.29         0.43         1.70         0.70           C10H11N04         209.0688         7.17         1.00         1.10         0.40           C10H11A05         214.0841         2.66         0.80         1.40         0.53           C10H1A05         214.0841         2.66         0.80         1.40         0.53           C10H1A05         214.0841         2.74         1.00         1.67         0.33           C7H5NO4         167.0219         3.79         1.00         0.71         0.57           C9H14O6         218.0790         2.72         0.50         1.56         0.67           C2H5NO5         195.0168         3.13         1.00         0.63         0.63         0.63           C10H18N2011S         374.0631         3.23         0.07         1.80         0.10         0.40         0.40           C10H18N204         126.0473         0.39         0.67         1.60         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.40         0.50	C7H12O6S	224.0355	0.82	0.33	1.71	0.86
C10H1NO4         209.0688         7.17         1.00         1.10         0.40           CSH803         152.0473         3.22         1.00         1.00         0.38           C10H1405         214.0841         2.66         0.80         1.40         0.50           C9H13N016         391.0234         3.08         0.25         1.44         1.78           C6H1002         114.0681         2.74         1.00         1.67         0.33           C7H5N04         167.0219         3.79         1.00         0.63         0.63           C2H603S         119.0038         0.35         0.00         3.00         1.50           C1H14X04S         252.1395         8.19         0.00         2.18         0.36           C10H18X04         216.0171         0.12         1.00         0.40         0.40           C10H18X04         120.423         6.98         1.00         0.80         0.40           C1H18X04         192.0423         6.98         1.00         1.03         0.57           C8H80X05         295.9838         2.65         0.50         1.00         1.25           C8H80X05         295.9971         4.07         1.00         0.063 <t< td=""><td>C10H17NO7S</td><td>295.0726</td><td>6.29</td><td>0.43</td><td>1.70</td><td>0.70</td></t<>	C10H17NO7S	295.0726	6.29	0.43	1.70	0.70
CSHR03         152.0473         3.22         1.00         1.00         0.38           C10H1405         214.0841         2.66         0.80         1.40         0.55           C6H1002         114.0681         2.74         1.00         1.67         0.33           C7H5N04         167.0219         3.79         1.00         0.71         0.57           C9H1406         218.0790         2.72         0.50         1.56         0.63           C11H2A04S         252.1395         8.19         0.00         2.18         0.36           C10H18N2O11S         374.0631         3.23         0.27         1.80         1.10           C10H8N2O4         216.0171         0.12         1.00         0.40         0.40           C70H7N2O4         216.0171         0.12         1.00         0.40         0.40           C10H4N2O4         126.023         6.98         1.00         0.40         0.40           C10H4N2O4         126.023         6.98         1.00         0.40         0.40           C10H4N2O4         126.023         6.98         1.00         1.13         0.50           C10H4N2O4         126.031         1.60         0.50         1.00	C10H11NO4	209.0688	7.17	1.00	1.10	0.40
C1011405         214.0841         2.66         0.80         1.40         0.78           C9H13N016         391.0234         3.08         0.25         1.44         1.78           C6H1002         114.0681         2.74         1.00         0.71         0.57           C9H1406         218.0790         2.72         0.50         1.56         0.67           C8H5NO5         195.0168         3.13         1.00         0.63         0.63           C2H603S         110.0038         0.35         0.00         3.00         1.50           C1H12404S         252.1395         8.19         0.00         2.18         0.36           C10H18N2011S         374.0631         3.23         0.27         1.80         0.10           C10H18N204         216.0171         0.12         0.75         1.43         0.57           C8H3005         199.0481         4.23         1.00         1.00         0.80         0.40           C7H19N05         185.0324         2.61         1.00         1.00         0.71         C8H8010S         259.9838         2.65         0.50         1.12         C8H503         0.50         C7H17N05         183.0324         2.61         1.00         1.00 <td>C8H8O3</td> <td>152.0473</td> <td>3.22</td> <td>1.00</td> <td>1.00</td> <td>0.38</td>	C8H8O3	152.0473	3.22	1.00	1.00	0.38
CH13N016         3910234         3.08         0.25         1.44         1.78           C6H1002         114.0681         2.74         1.00         0.71         0.37           C9H1406         218.0790         2.72         0.50         1.56         0.67           C8H5N05         195.0168         3.13         1.00         0.63         0.63           C2H603S         110.0038         0.35         0.00         3.00         1.50           C1H14204S         252.1395         8.19         0.00         2.18         0.36           C10H4N204         216.0171         0.12         1.00         0.40         0.40           C5H803         116.0473         0.39         0.67         1.60         0.60           C10H4N204         128.0579         1.22         0.75         1.43         0.63           C10H180A         192.0423         6.69         1.00         1.03         0.63           C1H1004         158.0324         2.61         1.00         1.00         1.25           C8H8N05         199.0481         4.23         1.00         1.25         C8H8         2.5         1.90         0.80           C10H18N06         255.9838         2.6	C10H14O5	214.0841	2.66	0.80	1.40	0.50
C7HSNO4         167,0219         3.79         1.00         0.71         0.57           C7HSNO5         195,0168         3.13         1.00         0.63         0.63           C8HSNO5         195,0168         3.13         1.00         0.63         0.63           C1H2AO4S         252,1395         8.19         0.00         2.18         0.36           C1H4AO4S         252,1395         8.19         0.00         2.18         0.36           C1H4N2O4         216,0171         0.12         1.00         0.40         0.40           CSH803         116,0473         0.39         0.67         1.60         0.60           C10H1804         192,0423         6.98         1.00         0.80         0.40           C7H1004         158,057         1.22         0.75         1.43         0.63           C10H19NO8S         313,0831         3.08         0.25         1.90         0.80           C7H1N05         185,0324         2.61         1.00         1.00         0.71           C8HSN04         179,0219         4.90         1.00         0.63         0.50           C7H1N05         185,0324         2.61         1.00         0.00         0.30<	C9H13N016	391.0234	3.08	0.25	1.44	1./8
C9H1466         12180790         2.72         0.50         0.51         6.07           C9H1466         12180790         2.72         0.50         1.56         0.63           C2H603S         110.0038         0.35         0.00         3.00         1.50           C1H24O4S         252.1395         8.19         0.00         2.18         0.36           C10H18V204         216.0171         0.12         1.00         0.40         0.40           C10H18V204         216.0171         0.12         1.00         0.40         0.40           C10H18V204         192.0423         6.98         1.00         0.80         0.40           C10H8V05         199.0481         4.23         1.00         1.13         0.63           C1H19N0S8         313.0831         3.08         0.25         1.90         0.80           C7H7N05         185.0324         2.61         1.00         1.00         0.71           C8H8N03         295.9838         2.65         0.50         1.00         1.25           C8H8N03         294.0304         0.89         0.29         1.11         1.00           C4H19O5         132.0059         0.35         0.60         1.00         <	C7H5NO4	167 0219	2.74	1.00	0.71	0.55
C8H5NO5         195.0168         3.13         1.00         0.63         0.63           C2H6O35         110.0038         0.35         0.00         3.00         1.50           C11H24O4S         252.1395         8.19         0.00         2.18         0.36           C10H18N2O11S         374.0631         3.23         0.27         1.80         1.10           C10HAN2O4         216.0171         0.12         1.00         0.40         0.40           C10H3N2O4         126.0171         0.12         1.00         0.40         0.40           C7H10O4         158.0579         1.22         0.75         1.43         0.57           C10H19NOSS         130.081         3.08         0.25         1.90         0.80           C10H19NOSS         130.081         3.08         0.25         1.90         0.80           C7H7NO5         185.0324         2.61         1.00         1.00         1.63         0.55           C8H8NO4         179.0219         4.90         1.00         0.63         0.55         1.17           C8H8037         122.8971         4.07         1.00         0.50         1.17           C8H8030         1.62         0.299 <t< td=""><td>C9H14O6</td><td>218 0790</td><td>2 72</td><td>0.50</td><td>1.56</td><td>0.57</td></t<>	C9H14O6	218 0790	2 72	0.50	1.56	0.57
C2HG03S         1100038         0.35         0.00         3.00         1.50           C1H24O4S         252.1395         8.19         0.00         2.18         0.10           C10H18X2011S         374.0651         3.23         0.27         1.80         1.10           C10H4N2O4         216.0171         0.12         1.00         0.40         0.40           C5H803         116.0473         0.39         0.67         1.60         0.60           C10H804         192.0423         6.98         1.00         0.80         0.40           CTH7N05         199.04481         4.23         1.00         1.13         0.63           C10H19N08S         313.0831         3.08         0.25         1.90         0.80           C7H7N05         185.0324         2.61         1.00         1.00         1.25           C8H8N04         179.0219         4.90         1.00         0.63         0.50           C7H12O7S         240.0304         0.89         0.29         1.71         1.00           C6H3N307         228.9971         4.07         1.00         0.75         0.63           C19H1003         178.0630         2.98         1.00         1.00         <	C8H5NO5	195.0168	3.13	1.00	0.63	0.63
C11H2404S         252,1395         8,19         0.00         2.18         0.36           C10H18N2011S         374,0631         3.23         0.27         1.80         1.10           C10H4N204         216,0171         0.12         1.00         0.40         0.40           C10H4N204         126,0473         0.39         0.67         1.60         0.60           C10H4N204         158,0579         1.22         0.75         1.43         0.67           C8H9N05         199,0481         4.23         1.00         1.13         0.63           C10H19N08S         313,0831         3.08         0.25         1.90         0.80           C7H7NO5         185,0324         2.61         1.00         1.01         1.25           C8H5N04         179,0219         4.90         1.00         0.63         0.50           C7H1207S         240,0304         0.89         0.29         1.71         1.00           C6H3N307         228,9971         4.07         1.00         0.75         0.63           C10H1003         178,0630         2.98         1.00         1.00         0.60           CH41405         132,0059         0.35         0.66         1.00	C2H6O3S	110.0038	0.35	0.00	3.00	1.50
C10H18N2011S         374 0631         3.23         0.27         1.80         1.10           C10H4N204         216.0171         0.12         1.00         0.40         0.40           CSH803         116.0473         0.39         0.67         1.60         0.60           C10HR04         192.0423         6.98         1.00         0.80         0.40           C7H1004         158.0579         1.22         0.75         1.43         0.63           C10H19N08S         313.0831         3.08         0.25         1.90         0.80           C7H7N05         185.0324         2.61         1.00         1.01         1.25           C8H8N04         179.0219         4.90         1.00         0.63         0.50           C7H12075         240.0304         0.89         0.29         1.71         1.00           C8H8N03         194.0977         5.17         0.00         0.53         0.60         1.00         1.25           C10H1003         178.0630         2.98         1.00         1.00         0.30         C4H405         132.0059         0.35         0.60         1.00         1.25           C10H406         230.0790         2.79         0.67         <	C11H24O4S	252.1395	8.19	0.00	2.18	0.36
C10H4N2O4         2160171         0.12         1.00         0.40         0.40           CSH8O3         116.0473         0.39         0.67         1.60         0.60           C10H8O4         192.0423         6.98         1.00         0.80         0.40           CTH10O4         158.0579         1.22         0.75         1.43         0.63           C10H19NO8S         313.0831         3.08         0.25         1.90         0.80           C7H7NO5         185.0324         2.61         1.00         1.00         0.71           C8H8N04         179.0219         4.90         1.00         0.63         0.50           C7H12OTS         240.0304         0.89         0.29         1.71         1.00           C6H3N3O7         228.9971         4.07         1.00         0.50         1.17           C8H6N2O5         210.0277         7.59         1.00         0.75         0.63           C10H14O6         1230.059         0.35         0.60         1.00         0.60           C1H4O5         127.0269         1.01         1.00         0.00         0.30           C1HH004         128.0320         2.67         1.00         0.71         0.29	C10H18N2O11S	374.0631	3.23	0.27	1.80	1.10
C5H803         116.0473         0.39         0.67         1.60         0.60           C10H804         192.0423         6.98         1.00         0.80         0.40           C7H1004         158.0579         1.22         0.75         1.43         0.57           C8H9N05         199.0481         4.23         1.00         1.13         0.63           C10H19N08S         313.0831         3.08         0.25         1.90         0.80           C7H7N05         185.0324         2.61         1.00         1.00         0.71           C8H8010S         295.9838         2.65         0.50         1.00         1.75           C8H5N04         179.0219         4.90         1.00         0.53         0.50           C7H12O7S         240.0304         0.89         0.29         1.71         1.00           C6H3N307         228.971         4.07         1.00         0.50         C3         0.63         0.63         0.50           C10H1405         132.0059         0.35         0.60         1.00         1.25         C10H1406         230.0790         2.79         0.67         1.40         0.60           C10H405         132.0059         1.31         1.0	C10H4N2O4	216.0171	0.12	1.00	0.40	0.40
C10H8O4         192.0423         6.98         1.00         0.80         0.43           C7H10O4         158.0579         1.22         0.75         1.43         0.63           C10H19N08S         313.0831         3.08         0.25         1.90         0.80           C1H7N05         185.0324         2.61         1.00         1.00         1.71           C8H8010S         295.9838         2.65         0.50         1.00         1.65           C7H7N05         1240.0304         0.89         0.29         1.71         1.00           C6H3N307         228.9971         4.07         1.00         0.50         1.17           C8H16N205         210.0277         7.59         1.00         0.75         0.63           C10H1003         178.0630         2.98         1.00         1.00         0.30           C4H405         132.0059         0.35         0.60         1.00         1.25           C10H1406         230.0790         2.79         0.67         1.40         0.60           C7H5N02         135.0320         2.67         1.00         0.71         0.29           C5H604         166.0266         1.33         1.00         0.75         0.	C5H8O3	116.0473	0.39	0.67	1.60	0.60
C RH9N05         199.0481         4.23         1.00         1.13         0.63           C10H19N08S         313.0831         3.08         0.25         1.90         0.80           C7H7N05         185.0324         2.61         1.00         1.00         0.71           C8H8N010S         295.9838         2.65         0.50         1.00         1.25           C8H5N04         179.0219         4.90         1.00         0.63         0.50           C7H12O7S         240.0304         0.89         0.29         1.71         1.00           C6H3N3O7         228.9971         4.07         1.00         0.50         1.17           C8H6N2O5         210.0277         7.59         1.00         0.75         0.63           C10H1003         178.0630         2.98         1.00         1.00         1.25           C10H1406         230.0790         2.79         0.67         1.40         0.60           C7H5N02         135.0320         2.67         1.00         0.75         0.50           C1H4006         248.1260         3.03         0.33         1.82         0.55           C9H18068         254.0824         3.51         0.17         2.00 <t< td=""><td>C10H8O4</td><td>192.0423</td><td>6.98</td><td>1.00</td><td>0.80</td><td>0.40</td></t<>	C10H8O4	192.0423	6.98	1.00	0.80	0.40
C10H19NOSS         133.0831         3.08         0.25         1.90         0.80           C1H7NOS         185.0324         2.61         1.00         1.00         0.71           C8H8010S         295.9838         2.65         0.50         1.00         0.71           C8H5NO4         179.0219         4.90         1.00         0.63         0.50           C7H12O7S         240.0304         0.89         0.29         1.71         1.00           C6H5N3O7         228.9971         4.07         1.00         0.55         1.17           C8H6N2OS         210.0277         7.59         1.00         0.75         0.63           C10H10O3         178.0630         2.98         1.00         1.00         0.30           C4H405         132.0059         0.35         0.60         1.00         1.25           C10H1003         177.0269         1.01         1.00         0.77         0.29           C5H5N03         127.0269         1.01         1.00         0.75         0.50           C1H12O6         248.1260         3.03         3.33         1.82         0.55           C9H18O6S         252.0668         4.01         0.33         1.78         0	C/HI004	158.0579	1.22	0.75	1.43	0.57
C1017005         15.0631         3.06         0.22         1.50         0.60           CTH7N05         185.0324         2.61         1.00         1.00         0.71           C8H8010S         295.9838         2.65         0.50         1.00         0.50           C7H12O7S         240.0304         0.89         0.29         1.71         1.00           C6H3N307         228.9971         4.07         1.00         0.55         1.17           C8H6N2O5         210.0277         7.59         1.00         0.75         0.63           C10H10O3         178.0630         2.98         1.00         1.00         0.30           C4H405         132.0059         0.35         0.60         1.00         1.25           C300790         2.79         0.67         1.40         0.60           C7H5N02         135.0320         2.67         1.00         0.75         0.50           C11H2006         248.1260         3.03         0.33         1.82         0.55           C9H18065         254.0824         3.51         0.17         2.00         0.67           C1H2006         248.1260         3.03         0.33         1.78         0.67	C10H10NO8S	313 0831	4.25	0.25	1.15	0.05
C8H8010S         295338         2.65         0.50         1.00         0.12           C8H5N04         179.0219         4.90         1.00         0.63         0.50           C7H1207S         240.0304         0.89         0.29         1.71         1.00           C6H3N307         228.9971         4.07         1.00         0.53         0.63           C6H5035         210.0277         7.59         1.00         0.75         0.63           C10H1003         178.0630         2.98         1.00         1.00         0.50           C10H1406         230.0790         2.79         0.67         1.40         0.60           C7H5N02         135.0320         2.67         1.00         0.71         0.29           C5H5N03         127.0269         1.01         1.00         1.00         0.60           C8H604         166.0266         1.33         1.00         0.75         0.50           C1H2006         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C1H2006         248.1260         3.03         0.33         1.78         0.67 <td>C7H7NO5</td> <td>185 0324</td> <td>2 61</td> <td>1.00</td> <td>1.90</td> <td>0.80</td>	C7H7NO5	185 0324	2 61	1.00	1.90	0.80
C8H5NO4         179.0219         4.90         1.00         0.63         0.50           C7H12O7S         240.0304         0.89         0.29         1.71         1.00           C6H5N3O7         228.9971         4.07         1.00         0.50         1.17           C8H1803S         194.0977         5.17         0.00         2.25         0.38           C10H1003         178.0630         2.98         1.00         1.00         0.50           C10H1003         178.0630         2.98         1.00         0.75         0.63           C10H1003         178.0630         2.97         0.67         1.40         0.60           C7H5NO2         135.0320         2.67         1.00         0.71         0.29           C5H5NO3         127.0269         1.01         1.00         1.00         0.60           C8H6O4         166.0266         1.33         1.00         0.75         0.50           C11H2006         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C1H1H2003         126.0630         7.14         1.00         0.11         0	C8H8O10S	295.9838	2.65	0.50	1.00	1.25
C7H1207S         240.0304         0.89         0.29         1.71         1.00           C6H3N3O7         228.9971         4.07         1.00         0.50         1.17           C8H1803S         194.0977         7.59         1.00         0.75         0.63           C10H10O3         178.0630         2.98         1.00         1.00         0.30           C4H405         132.0059         0.35         0.60         1.00         1.25           C10H1406         230.0790         2.79         0.67         1.40         0.60           C7H5NO2         135.0320         2.67         1.00         1.00         0.60           C8H604         166.0266         1.33         1.00         0.75         0.50           C11H2006         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C1H2003         154.0630         1.56         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C14H1003         226.0630         7.14         1.00         0.71         0.2	C8H5NO4	179.0219	4.90	1.00	0.63	0.50
C6H3N3O7         228.9971         4.07         1.00         0.50         1.17           C8H1803S         194.0977         5.17         0.00         2.25         0.38           C8H6N2O5         210.0277         7.59         1.00         1.00         0.30           C4H4O5         132.0059         0.35         0.60         1.00         1.25           C10H14O6         230.0790         2.79         0.67         1.40         0.60           C7H5NO2         135.0320         2.67         1.00         0.71         0.29           CSH6NO3         127.0269         1.01         1.00         1.00         0.60           C8H6O4         166.0266         1.33         1.00         0.75         0.50           C1H2O6         248.1260         3.03         0.33         1.82         0.55           C9H18O6S         254.0824         3.51         0.17         2.00         0.67           C1H2O6         48.86         1.00         1.25         0.38           C9H18O3         154.0630         1.54         1.00         1.25         0.38           C9H1003         154.0630         7.14         1.00         0.67         0.78	C7H12O7S	240.0304	0.89	0.29	1.71	1.00
C8H1803S         194.0977         5.17         0.00         2.25         0.38           C8H6N205         210.0277         7.59         1.00         0.75         0.63           C10H1003         178.0630         2.98         1.00         1.00         0.30           C4H405         132.0059         0.35         0.60         1.00         1.25           C10H1406         230.0790         2.79         0.67         1.40         0.60           C7H5N02         135.0320         2.67         1.00         0.71         0.29           C5H5N03         127.0269         1.01         1.00         1.00         0.60           C8H604         166.0266         1.33         1.01         2.00         0.67           C1H2006         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C1H2006         248.1260         3.03         0.33         1.78         0.67           C1H2006         154.0630         1.56         1.00         1.25         0.38           C9H1607S         252.0668         4.01         0.33         1.78         0.67 </td <td>C6H3N3O7</td> <td>228.9971</td> <td>4.07</td> <td>1.00</td> <td>0.50</td> <td>1.17</td>	C6H3N3O7	228.9971	4.07	1.00	0.50	1.17
C8H6N205         210.0277         7.59         1.00         0.75         0.63           C10H1003         178.0630         2.98         1.00         1.00         0.30           C4H405         132.0059         0.35         0.60         1.00         1.25           C10H1406         230.0790         2.79         0.67         1.40         0.60           C7H5N02         135.0320         2.67         1.00         0.71         0.29           C5H5N03         127.0269         1.01         1.00         1.00         0.66           C8H604         166.0266         1.33         1.00         0.75         0.50           C11H2006         248.1260         3.03         0.33         1.82         0.65           C8H604         166.0264         1.56         1.00         0.62         0.15           C8H1003         154.0630         1.56         1.00         1.25         0.38           C9H16068         252.0668         4.01         0.33         1.78         0.67           C4H1003         226.0630         7.14         1.00         0.71         0.21           C6H1204         148.0736         0.53         0.25         2.00         0.67 <td>C8H18O3S</td> <td>194.0977</td> <td>5.17</td> <td>0.00</td> <td>2.25</td> <td>0.38</td>	C8H18O3S	194.0977	5.17	0.00	2.25	0.38
C10H1003         178.0630         2.98         1.00         1.00         0.30           C4H405         132.0059         0.35         0.60         1.00         1.25           C10H1406         230.0790         2.79         0.67         1.40         0.60           C7H5N02         135.0320         2.67         1.00         0.71         0.29           C5H5N03         127.0269         1.01         1.00         0.60         0.66           C8H604         166.0266         1.33         1.00         0.75         0.50           C11H2006         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C13H802         196.0524         4.86         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C14H1003         226.0630         7.14         1.00         0.71         0.21           C6H1204         148.0736         0.53         0.25         2.00         0.67           C8H607         226.0114         1.05         1.00         0.67         0.78 <td>C8H6N2O5</td> <td>210.0277</td> <td>7.59</td> <td>1.00</td> <td>0.75</td> <td>0.63</td>	C8H6N2O5	210.0277	7.59	1.00	0.75	0.63
C10H1405         152.0059         0.35         0.00         1.00         1.25           C10H1406         230.0790         2.79         0.67         1.40         0.60           C7H5NO2         135.0320         2.67         1.00         0.71         0.29           C5H5NO3         127.0269         1.01         1.00         0.00         0.66           C8H604         166.0266         1.33         1.00         0.75         0.50           C11H2006         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C13H802         196.0524         4.86         1.00         0.62         0.15           C8H1003         154.0630         1.56         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C1H11003         226.0630         7.14         1.00         0.71         0.21           C6H1204         148.0736         0.53         0.25         2.00         0.67           C8H17N08S         287.0675         2.99         0.13         2.13         1.0	C10H10O3	1/8.0630	2.98	1.00	1.00	0.30
C7H5NO2         L35.030         L75         0.00         1.76         0.03           CSH5NO3         127.0269         1.01         1.00         0.00         0.60           CSH604         166.0266         1.33         1.00         0.75         0.50           C11H2006         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C13H802         196.0524         4.86         1.00         0.62         0.15           C8H1003         154.0630         1.56         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C4H1003         226.0630         7.14         1.00         0.71         0.21           C6H1204         148.0736         0.53         0.25         2.00         0.67           C8H17N08S         287.0675         2.99         0.13         2.13         1.00           C5H403         112.0160         0.38         1.00         0.67         0.78           C4H803         104.0473         0.60         0.33         2.00         0.75	C10H14O6	230.0790	0.33	0.00	1.00	0.60
C5H5NO3         127.0269         1.01         1.00         1.00         0.60           C8H6O4         166.0266         1.33         1.00         0.75         0.50           C11H20O6         248.1260         3.03         0.33         1.82         0.55           C9H18O6S         254.0824         3.51         0.17         2.00         0.67           C13H8O2         196.0524         4.86         1.00         0.62         0.15           C8H10O3         154.0630         1.56         1.00         1.25         0.38           C9H16O6S         252.0668         4.01         0.33         1.78         0.67           C14H10O3         226.0630         7.14         1.00         0.71         0.21           C6H12O4         148.0736         0.53         0.25         2.00         0.67           C8H4O3         112.0160         0.38         1.00         0.80         0.60           C9H6O7         226.0114         1.05         1.00         0.67         0.78           C4H8O3         104.0473         0.60         0.33         2.00         0.75           C9H18O75         270.0773         3.03         0.14         2.00         0.78	C7H5NO2	135.0320	2.67	1.00	0.71	0.29
C8H6O4         166.0266         1.33         1.00         0.75         0.50           C11H20O6         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C13H802         196.0524         4.86         1.00         0.62         0.15           C8H1003         154.0630         1.56         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C14H1003         226.0630         7.14         1.00         0.71         0.21           C6H12O4         148.0736         0.53         0.25         2.00         0.67           C8H17N08S         287.0675         2.99         0.13         2.13         1.00           C5H4O3         112.0160         0.38         1.00         0.80         0.60           C7H12O4         160.0736         0.91         0.50         1.71         0.57           C9H6O7         226.0114         1.05         1.00         0.67         0.33           C9H18O7S         270.0773         3.03         0.14         2.00         0.78 </td <td>C5H5NO3</td> <td>127.0269</td> <td>1.01</td> <td>1.00</td> <td>1.00</td> <td>0.60</td>	C5H5NO3	127.0269	1.01	1.00	1.00	0.60
C11H2006         248.1260         3.03         0.33         1.82         0.55           C9H1806S         254.0824         3.51         0.17         2.00         0.67           C13H802         196.0524         4.86         1.00         0.62         0.15           C8H1003         154.0630         1.56         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C14H1003         226.0630         7.14         1.00         0.71         0.21           C6H1204         148.0736         0.53         0.25         2.00         0.67           C8H17N08S         287.0675         2.99         0.13         2.13         1.00           C5H403         112.0160         0.38         1.00         0.80         0.60           C7H1204         160.0736         0.91         0.50         1.71         0.57           C9H607         226.0114         1.05         1.00         0.67         0.78           C12H804         216.0423         4.04         1.00         0.67         0.33           C9H1807S         270.0773         3.03         0.14         2.00         0.75<	C8H6O4	166.0266	1.33	1.00	0.75	0.50
C9H1806S         254.0824         3.51         0.17         2.00         0.67           C13H802         196.0524         4.86         1.00         0.62         0.15           C8H1003         154.0630         1.56         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C14H1003         226.0630         7.14         1.00         0.71         0.21           C6H1204         148.0736         0.53         0.25         2.00         0.67           C8H17N08S         287.0675         2.99         0.13         2.13         1.00           C5H403         112.0160         0.38         1.00         0.80         0.60           C7H1204         160.0736         0.91         0.50         1.71         0.57           C9H607         226.0114         1.05         1.00         0.67         0.78           C4H803         104.0473         0.60         0.33         2.00         0.75           C9H1807S         270.0773         3.03         0.14         2.00         0.78           C12H804         216.0423         4.04         1.00         0.67         0.33 <td>C11H20O6</td> <td>248.1260</td> <td>3.03</td> <td>0.33</td> <td>1.82</td> <td>0.55</td>	C11H20O6	248.1260	3.03	0.33	1.82	0.55
C13H802         196.0524         4.86         1.00         0.62         0.15           C8H1003         154.0630         1.56         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C14H1003         226.0630         7.14         1.00         0.71         0.21           C6H12O4         148.0736         0.53         0.25         2.00         0.67           C8H17N08S         287.0675         2.99         0.13         2.13         1.00           C5H403         112.0160         0.38         1.00         0.80         0.60           C7H12O4         160.0736         0.91         0.50         1.71         0.57           C9H607         226.0114         1.05         1.00         0.67         0.33           C4H803         104.0473         0.60         0.33         2.00         0.75           C9H1807S         270.0773         3.03         0.14         2.00         0.78           C12H804         216.0423         4.04         1.00         0.67         0.33           C9H1003         166.0630         3.23         1.00         1.11         0.33 <td>C9H18O6S</td> <td>254.0824</td> <td>3.51</td> <td>0.17</td> <td>2.00</td> <td>0.67</td>	C9H18O6S	254.0824	3.51	0.17	2.00	0.67
CSH1003         154.0630         1.56         1.00         1.25         0.38           C9H1606S         252.0668         4.01         0.33         1.78         0.67           C14H1003         226.0630         7.14         1.00         0.71         0.21           C6H12O4         148.0736         0.53         0.25         2.00         0.67           C8H17N08S         287.0675         2.99         0.13         2.13         1.00           C5H4O3         112.0160         0.38         1.00         0.80         0.60           C7H12O4         160.0736         0.91         0.50         1.71         0.57           C9H6O7         226.0114         1.05         1.00         0.67         0.78           C4H803         104.0473         0.60         0.33         2.00         0.75           C9H1807S         270.0773         3.03         0.14         2.00         0.78           C12H804         216.0423         4.04         1.00         0.67         0.33           C9H1003         166.0630         3.23         1.00         1.11         0.33           C8H602         134.0368         1.79         1.00         0.63         0.38	C13H8O2	196.0524	4.86	1.00	0.62	0.15
C9H10003226.00084.010.531.780.07C14H1003226.06307.141.000.710.21C6H1204148.07360.530.252.000.67C8H17N08S287.06752.990.132.131.00C5H403112.01600.381.000.800.60C7H1204160.07360.910.501.710.57C9H607226.01141.051.000.670.78C4H803104.04730.600.332.000.75C9H1807S270.07733.030.142.000.78C12H804216.04234.041.000.670.33C9H1003166.06303.231.001.110.33C8H602134.03681.791.000.750.25C13H11NO3229.07398.121.000.630.38C5H802100.05240.671.001.600.40C5H4N203140.02220.391.000.600.60C8H1005186.05280.650.801.250.63C8H604166.02661.861.000.750.50C6H607190.01140.350.571.001.17C6H1404S182.06133.490.002.330.67C5H4N204156.01711.221.000.800.80C9H1607S268.06172.350.291.780.78C9H7N04139.02692.961.00 </td <td>C8H10O3</td> <td>154.0630</td> <td>1.56</td> <td>1.00</td> <td>1.25</td> <td>0.38</td>	C8H10O3	154.0630	1.56	1.00	1.25	0.38
C6H11005         2200050         1.14         1.00         0.11         0.21           C6H1204         148.0736         0.53         0.25         2.00         0.67           C8H17N08S         287.0675         2.99         0.13         2.13         1.00           C5H403         112.0160         0.38         1.00         0.80         0.60           C7H1204         160.0736         0.91         0.50         1.71         0.57           C9H607         226.0114         1.05         1.00         0.67         0.78           C4H803         104.0473         0.60         0.33         2.00         0.75           C9H1807S         270.0773         3.03         0.14         2.00         0.78           C12H804         216.0423         4.04         1.00         0.67         0.33           C9H1003         166.0630         3.23         1.00         1.11         0.33           C8H602         134.0368         1.79         1.00         0.75         0.25           C13H11N03         229.0739         8.12         1.00         0.85         0.23           C8H5N03         163.0269         2.99         1.00         0.63         0.38	C14H10O3	232.0008	4.01	1.00	0.71	0.07
C8H17NO8S         287.0675         2.99         0.13         2.13         1.00           C5H4O3         112.0160         0.38         1.00         0.80         0.60           C7H12O4         160.0736         0.91         0.50         1.71         0.57           C9H6O7         226.0114         1.05         1.00         0.67         0.78           C4H8O3         104.0473         0.60         0.33         2.00         0.75           C9H18O7S         270.0773         3.03         0.14         2.00         0.78           C12H8O4         216.0423         4.04         1.00         0.67         0.33           C9H10O3         166.0630         3.23         1.00         1.11         0.33           C8H6O2         134.0368         1.79         1.00         0.75         0.25           C13H11NO3         229.0739         8.12         1.00         0.85         0.23           C8H5NO3         163.0269         2.99         1.00         0.63         0.38           C5H8O2         100.0524         0.67         1.00         1.60         0.40           C5H4N2O3         140.0222         0.39         1.00         0.80         0.63	C6H12O4	148 0736	0.53	0.25	2.00	0.21
C5H4O3112.01600.381.000.800.60C7H12O4160.07360.910.501.710.57C9H6O7226.01141.051.000.670.78C4H8O3104.04730.600.332.000.75C9H18O7S270.07733.030.142.000.78C12H8O4216.04234.041.000.670.33C9H10O3166.06303.231.001.110.33C8H6O2134.03681.791.000.750.25C13H11NO3229.07398.121.000.850.23C8H5NO3163.02692.991.000.630.38C5H8O2100.05240.671.001.600.40C5H4N2O3140.02220.391.000.800.60C8H10O5186.05280.650.801.250.63C8H6O4166.02661.861.000.750.50C6H6O7190.01140.350.571.001.17C6H14O4S182.06133.490.002.330.67C5H4N2O4156.01711.221.000.800.80C9H7NO4193.03756.771.000.780.74C6H5NO3139.02692.961.000.830.50C6H6O4142.02660.391.001.000.67	C8H17NO8S	287.0675	2.99	0.13	2.13	1.00
C7H12O4160.07360.910.501.710.57C9H6O7226.01141.051.000.670.78C4H8O3104.04730.600.332.000.75C9H18O7S270.07733.030.142.000.78C12H8O4216.04234.041.000.670.33C9H10O3166.06303.231.001.110.33C8H6O2134.03681.791.000.750.25C13H11NO3229.07398.121.000.850.23C8H5NO3163.02692.991.000.630.38C5H8O2100.05240.671.001.600.40C5H4N2O3140.02220.391.000.800.60C8H10O5186.05280.650.801.250.63C8H6O4166.02661.861.000.750.50C6H6O7190.01140.350.571.001.17C6H14O4S182.06133.490.002.330.67C5H4N2O4156.01711.221.000.800.80C9H7NO4193.03756.771.000.780.78C9H7NO4193.03756.771.000.780.44C6H5NO3139.02692.961.000.830.50C6H6O4142.02660.391.001.000.67	C5H4O3	112.0160	0.38	1.00	0.80	0.60
C9H6O7226.01141.051.000.670.78C4H8O3104.04730.600.332.000.75C9H18O7S270.07733.030.142.000.78C12H8O4216.04234.041.000.670.33C9H10O3166.06303.231.001.110.33C8H6O2134.03681.791.000.750.25C13H11NO3229.07398.121.000.850.23C8H5NO3163.02692.991.000.630.38C5H8O2100.05240.671.001.600.40C5H4N2O3140.02220.391.000.800.60C8H10O5186.05280.650.801.250.63C8H6O4166.02661.861.000.750.50C6H6O7190.01140.350.571.001.17C6H14O4S182.06133.490.002.330.67C5H4N2O4156.01711.221.000.800.80C9H7NO4193.03756.771.000.780.44C6H5NO3139.02692.961.000.830.50C6H6O4142.02660.391.001.000.67	C7H12O4	160.0736	0.91	0.50	1.71	0.57
C4H803         104.0473         0.60         0.33         2.00         0.75           C9H1807S         270.0773         3.03         0.14         2.00         0.78           C12H804         216.0423         4.04         1.00         0.67         0.33           C9H1003         166.0630         3.23         1.00         1.11         0.33           C8H602         134.0368         1.79         1.00         0.75         0.25           C13H11N03         229.0739         8.12         1.00         0.85         0.23           C8H5N03         163.0269         2.99         1.00         0.63         0.38           C5H802         100.0524         0.67         1.00         1.60         0.40           C5H4N203         140.0222         0.39         1.00         0.80         0.60           C8H604         166.0266         1.86         1.00         0.75         0.50           C6H607         190.0114         0.35         0.57         1.00         1.17           C6H1404S         182.0613         3.49         0.00         2.33         0.67           C5H4N204         156.0171         1.22         1.00         0.80         0.80	C9H6O7	226.0114	1.05	1.00	0.67	0.78
C9H18O/S         270.07/3         3.03         0.14         2.00         0.78           C12H8O4         216.0423         4.04         1.00         0.67         0.33           C9H10O3         166.0630         3.23         1.00         1.11         0.33           C9H10O3         166.0630         3.23         1.00         0.75         0.25           C13H11NO3         229.0739         8.12         1.00         0.85         0.23           C8H5NO3         163.0269         2.99         1.00         0.63         0.38           C5H8O2         100.0524         0.67         1.00         1.60         0.40           C5H4N2O3         140.0222         0.39         1.00         0.80         0.60           C8H10O5         186.0528         0.65         0.80         1.25         0.63           C8H6O4         166.0266         1.86         1.00         0.75         0.50           C6H6O7         190.0114         0.35         0.57         1.00         1.17           C6H14O4S         182.0613         3.49         0.00         2.33         0.67           C5H4N2O4         156.0171         1.22         1.00         0.80         0.80 <td>C4H8O3</td> <td>104.0473</td> <td>0.60</td> <td>0.33</td> <td>2.00</td> <td>0.75</td>	C4H8O3	104.0473	0.60	0.33	2.00	0.75
C12H804         216.0425         4.04         1.00         0.67         0.33           C9H10O3         166.0630         3.23         1.00         1.11         0.33           C8H6O2         134.0368         1.79         1.00         0.75         0.25           C13H11NO3         229.0739         8.12         1.00         0.85         0.23           C8H5NO3         163.0269         2.99         1.00         0.63         0.38           C5H8O2         100.0524         0.67         1.00         1.60         0.40           C5H4N2O3         140.0222         0.39         1.00         0.80         0.60           C8H6O4         166.0266         1.86         1.00         0.75         0.50           C6H6O7         190.0114         0.35         0.57         1.00         1.17           C6H14O4S         182.0613         3.49         0.00         2.33         0.67           C5H4N2O4         156.0171         1.22         1.00         0.80         0.80           C9H16O7S         268.0617         2.35         0.29         1.78         0.78           C9H16O7S         268.0617         2.35         0.29         1.78         0.78 <td>C9H1807S</td> <td>270.0773</td> <td>3.03</td> <td>0.14</td> <td>2.00</td> <td>0.78</td>	C9H1807S	270.0773	3.03	0.14	2.00	0.78
CSH1003         100.0630         3.23         1.00         1.11         0.53           C8H6O2         134.0368         1.79         1.00         0.75         0.25           C13H11NO3         229.0739         8.12         1.00         0.85         0.23           C8H5NO3         163.0269         2.99         1.00         0.63         0.38           C5H802         100.0524         0.67         1.00         1.60         0.40           C5H4N2O3         140.0222         0.39         1.00         0.80         0.60           C8H6O4         166.0266         1.86         1.00         0.75         0.50           C6H6O7         190.0114         0.35         0.57         1.00         1.17           C6H14O4S         182.0613         3.49         0.00         2.33         0.67           C5H4N2O4         156.0171         1.22         1.00         0.80         0.80           C9H16O7S         268.0617         2.35         0.29         1.78         0.78           C9H7NO4         193.0375         6.77         1.00         0.78         0.44           C6H5NO3         139.0269         2.96         1.00         0.83         0.50 <td>C12H8O4 C01110O2</td> <td>216.0423</td> <td>4.04</td> <td>1.00</td> <td>0.67</td> <td>0.33</td>	C12H8O4 C01110O2	216.0423	4.04	1.00	0.67	0.33
Consol         177         180         0.15         0.125           C13H11NO3         229.0739         8.12         1.00         0.85         0.23           C8H5NO3         163.0269         2.99         1.00         0.63         0.38           C5H8O2         100.0524         0.67         1.00         1.60         0.40           C5H4N2O3         140.0222         0.39         1.00         0.80         0.60           C8H10O5         186.0528         0.65         0.80         1.25         0.63           C8H6O4         166.0266         1.86         1.00         0.75         0.50           C6H6O7         190.0114         0.35         0.57         1.00         1.17           C6H14O4S         182.0613         3.49         0.00         2.33         0.67           C5H4N2O4         156.0171         1.22         1.00         0.80         0.80           C9H16O7S         268.0617         2.35         0.29         1.78         0.78           C9H7NO4         193.0375         6.77         1.00         0.78         0.44           C6H5NO3         139.0269         2.96         1.00         0.83         0.50	C8H6O2	134 0368	3.23	1.00	0.75	0.33
C8H5N03         163.0269         2.99         1.00         0.63         0.38           C5H8O2         100.0524         0.67         1.00         1.60         0.40           C5H4N2O3         140.0222         0.39         1.00         0.80         0.60           C8H10O5         186.0528         0.65         0.80         1.25         0.63           C8H6O4         166.0266         1.86         1.00         0.75         0.50           C6H6O7         190.0114         0.35         0.57         1.00         1.17           C6H14O4S         182.0613         3.49         0.00         2.33         0.67           C5H4N2O4         156.0171         1.22         1.00         0.80         0.80           C9H16O7S         268.0617         2.35         0.29         1.78         0.78           C9H7NO4         193.0375         6.77         1.00         0.78         0.44           C6H5NO3         139.0269         2.96         1.00         0.83         0.50           C6H6O4         142.0266         0.39         1.00         1.00         0.67	C13H11NO3	229.0739	8.12	1.00	0.85	0.23
C5H802100.05240.671.001.600.40C5H4N2O3140.02220.391.000.800.60C8H10O5186.05280.650.801.250.63C8H6O4166.02661.861.000.750.50C6H6O7190.01140.350.571.001.17C6H14O4S182.06133.490.002.330.67C5H4N2O4156.01711.221.000.800.80C9H16O7S268.06172.350.291.780.78C9H7NO4193.03756.771.000.780.44C6H5NO3139.02692.961.000.830.50C6H6O4142.02660.391.001.000.67	C8H5NO3	163.0269	2.99	1.00	0.63	0.38
C5H4N2O3140.02220.391.000.800.60C8H10O5186.05280.650.801.250.63C8H6O4166.02661.861.000.750.50C6H6O7190.01140.350.571.001.17C6H14O4S182.06133.490.002.330.67C5H4N2O4156.01711.221.000.800.80C9H16O7S268.06172.350.291.780.78C9H7NO4193.03756.771.000.780.44C6H5NO3139.02692.961.000.830.50C6H6O4142.02660.391.001.000.67	C5H8O2	100.0524	0.67	1.00	1.60	0.40
C8H1005         186.0528         0.65         0.80         1.25         0.63           C8H604         166.0266         1.86         1.00         0.75         0.50           C6H607         190.0114         0.35         0.57         1.00         1.17           C6H1404S         182.0613         3.49         0.00         2.33         0.67           C5H4N204         156.0171         1.22         1.00         0.80         0.80           C9H1607S         268.0617         2.35         0.29         1.78         0.78           C9H7N04         193.0375         6.77         1.00         0.78         0.44           C6H5N03         139.0269         2.96         1.00         0.83         0.50           C6H604         142.0266         0.39         1.00         1.00         0.67	C5H4N2O3	140.0222	0.39	1.00	0.80	0.60
C8H6O4166.02661.861.000.750.50C6H6O7190.01140.350.571.001.17C6H14O4S182.06133.490.002.330.67C5H4N2O4156.01711.221.000.800.80C9H16O7S268.06172.350.291.780.78C9H7NO4193.03756.771.000.780.44C6H5NO3139.02692.961.000.830.50C6H6O4142.02660.391.001.000.67	C8H10O5	186.0528	0.65	0.80	1.25	0.63
C6H6O7         190.0114         0.35         0.57         1.00         1.17           C6H14O4S         182.0613         3.49         0.00         2.33         0.67           C5H4N2O4         156.0171         1.22         1.00         0.80         0.80           C9H16O7S         268.0617         2.35         0.29         1.78         0.78           C9H7NO4         193.0375         6.77         1.00         0.78         0.44           C6H5NO3         139.0269         2.96         1.00         0.83         0.50           C6H6O4         142.0266         0.39         1.00         1.00         0.67	C8H6O4	166.0266	1.86	1.00	0.75	0.50
Con14045182.00153.490.002.330.67C5H4N2O4156.01711.221.000.800.80C9H16O7S268.06172.350.291.780.78C9H7NO4193.03756.771.000.780.44C6H5NO3139.02692.961.000.830.50C6H6O4142.02660.391.001.000.67	C6H6O7	190.0114	0.35	0.57	1.00	1.17
C5H4N204         150.0171         1.22         1.00         0.80         0.80           C9H16O7S         268.0617         2.35         0.29         1.78         0.78           C9H7N04         193.0375         6.77         1.00         0.78         0.44           C6H5N03         139.0269         2.96         1.00         0.83         0.50           C6H604         142.0266         0.39         1.00         1.00         0.67	C5H4N2O4	182.0613	5.49	0.00	2.33	0.67
C9H10075         2000017         2.35         0.29         1.76         0.78           C9H7NO4         193.0375         6.77         1.00         0.78         0.44           C6H5NO3         139.0269         2.96         1.00         0.83         0.50           C6H6O4         142.0266         0.39         1.00         1.00         0.67	C3H4N2O4 C9H16O7S	130.01/1 268.0617	1.22	0.29	0.80	0.80
C6H5NO3         139.0269         2.96         1.00         0.73         0.74           C6H6O4         142.0266         0.39         1.00         0.67	C9H7NO4	193 0375	677	1.00	0.78	0.78
C6H6O4 142.0266 0.39 1.00 1.00 0.67	C6H5NO3	139.0269	2.96	1.00	0.83	0.50
	C6H6O4	142.0266	0.39	1.00	1.00	0.67

C7H6O2	122.0368	0.81	1.00	0.86	0.29
COLIZNOC	225 0272	2 10	1.00	0.79	0.07
C9H/NO6	225.0273	5.19	1.00	0.78	0.67
C10H8O3	176.0473	3.23	1.00	0.80	0.30
C10H9NO4	207 0532	4.54	1.00	0.90	0.40
	207.0332	4.54	1.00	0.90	0.40
C6H4O5	156.0059	0.67	1.00	0.67	0.83
C5H11NO7S	229.0256	2.73	0.14	2.20	1.40
C12U0NO2	227.0592	0.02	1.00	0.60	0.22
CISH9NOS	227.0382	0.23	1.00	0.09	0.23
C9H17NO9S	315.0624	2.52	0.22	1.89	1.00
C10H10N2O6	254 0539	7 79	1.00	1.00	0.60
C1011101(200	234.0337	1.17	1.00	1.00	0.00
C10H14O4	198.0892	3.73	1.00	1.40	0.40
C9H9NO6	227.0430	2.98	1.00	1.00	0.67
07111205	176.0695	1.00	0.40	1.71	0.71
С/п1203	1/0.0085	1.00	0.40	1./1	0.71
C9H7NO5	209.0324	4.07	1.00	0.78	0.56
C7H14O4	162 0892	0.84	0.25	2.00	0.57
0/111404	102.0092	0.04	0.25	2.00	0.57
C9H7NO3	177.0426	3.24	1.00	0.78	0.33
C10H9NO4	207.0532	7.65	1.00	0.90	0.40
C711604	154 0266	2.50	1.00	0.96	0.57
C/H004	134.0200	2.39	1.00	0.80	0.57
C9H16O4	188.1049	2.60	0.50	1.78	0.44
C3H4O3	88.0160	0.07	0.67	1 33	1.00
C511405	176.0605	0.07	0.07	1.55	1.00
C/H1205	1/6.0685	1.65	0.40	1./1	0.71
C9H9NO7S	275.0100	3.69	0.86	1.00	0.78
0711602	129 0217	1.05	1.00	0.96	0.42
C/H005	158.0517	1.05	1.00	0.80	0.45
C9H8O	132.0575	3.09	1.00	0.89	0.11
COH10NO8S	301 0831	3 20	0.13	2.11	0.80
0111/10005	501.0051	5.20	0.15	2.11	0.07
C10H8O6	224.0321	2.44	1.00	0.80	0.60
C8H5NO6	211.0117	2.57	1.00	0.63	0.75
C7111004	159.0570	2.27	0.75	1.42	0.57
C/H1004	158.0579	2.75	0.75	1.43	0.57
C6H8O3	128.0473	0.52	1.00	1.33	0.50
C3H6O3S	122 0038	0.38	0.33	2.00	1.00
05110055	122.0038	0.38	0.55	2.00	1.00
C12H20O5	244.1311	3.80	0.60	1.67	0.42
C6H5NO4	155 0219	0.40	1.00	0.83	0.67
COLIDITOT	00.0112	0.10	0.67	1.50	1.50
C2H3NO3	89.0113	0.02	0.67	1.50	1.50
C8H14O7S	254.0460	2.30	0.29	1.75	0.88
C6U6O2	126 0217	0.27	1.00	1.00	0.50
011003	120.0317	0.37	1.00	1.00	0.50
C8H14O7S	254.0460	1.04	0.29	1.75	0.88
C9H8N2O2	176.0586	7 46	1.00	0.89	0.22
C111110N2O2	210.1269	2.70	1.00	1.64	0.10
CITHI8N202	210.1368	2.70	1.00	1.04	0.18
C7H7NO3	153.0426	0.38	1.00	1.00	0.43
C64904	144 0422	1 22	0.75	1 22	0.67
C0H804	144.0423	1.32	0.75	1.55	0.07
C9H16O4	188.1049	2.94	0.50	1.78	0.44
C8H5NO6	211 0117	3.00	1.00	0.63	0.75
CINUOS	211.0117	5.00	1.00	0.05	0.75
C10H805	208.0372	2.14	1.00	0.80	0.50
C8H8N2O6	228.0382	4.68	1.00	1.00	0.75
C12H0NO4	242.0522	774	1.00	0.60	0.21
C13H9N04	243.0332	1.14	1.00	0.09	0.51
C8H14O4	174.0892	2.69	0.50	1.75	0.50
C9H6N2O3	190.0378	2 76	1.00	0.67	0.33
C14115N029	251.0041	2.70	1.00	0.07	0.55
CI4H5NO2S	251.0041	2.62	1.00	0.36	0.14
C13H22O4	242.1518	7.48	0.75	1.69	0.31
Ceheose	158 0038	0.74	1.00	1.00	0.50
0110055	150.0050	0.74	1.00	1.00	0.50
C/H8N2O3	168.0535	3.74	1.00	1.14	0.43
C5H9NO7S	227.0100	3.08	0.29	1.80	1.40
C8H7NO2	165.0426	675	1.00	0.00	0.29
Continuos	105.0420	0.75	1.00	0.00	0.38
C10H7NO5	221.0324	3.45	1.00	0.70	0.50
C7H16O4S	196 0769	5 1 2	0.00	2.29	0.57
GIOUSDIOOG	190.0709	0.12	1.00	0.50	0.07
CI0H5NO2S	203.0041	0.52	1.00	0.50	0.20
C10H9NO4	207.0532	4.85	1.00	0.90	0.40
C0H16099	284 0566	2 40	0.25	1 79	0.80
031110005	204.0300	2.49	0.25	1./0	0.09
C13H26O5S	294.1501	7.59	0.20	2.00	0.38
C9H18O7S	270 0773	2.52	0.14	2.00	0.78
C10U19070	2/0.0775	2.02	0.22	1.00	0.70
C10H1806S	200.0824	2.96	0.33	1.80	0.60
C9H17NO8S	299.0675	3.34	0.25	1.89	0.89
C16H16O4	272 1049	8 1 5	1.00	1.00	0.25
C10H10O4	2/2.1049	0.13	1.00	1.00	0.23
C14H10O4	242.0579	6.91	1.00	0.71	0.29
C10H7NO5	221 0324	5 83	1.00	0.70	0.50
010110005	221.0324	4.24	0.00	1 77	0.30
C12H20O5	244.1311	4.34	0.60	1.6/	0.42
C8H6O6	198.0164	0.89	1.00	0.75	0.75
C8H8O4	168 0422	3.00	1.00	1.00	0.50
00004	100.0425	5.08	1.00	1.00	0.50
C11H16O5	228.0998	2.85	0.80	1.45	0.45
C10H8N2O6	252.0382	7.80	1.00	0.80	0.60
001011200	101 0112	7.00	1.00	1.00	1.00
C3H3NU3	101.0113	0.07	1.00	1.00	1.00

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C4H4N2O3	128.0222	0.55	1.00	1.00	0.75
C6H5NO2	123.0320	0.38	1.00	0.83	0.33
C9H10O6S	246.0198	2.87	0.83	1.11	0.67
C10H13NO4	211.0845	7.85	1.00	1.30	0.40
C6H10O5	162.0528	0.91	0.40	1.67	0.83
C/H6N2O4	182.0328	3.45	1.00	0.86	0.57
C9H10O4	182.0579	2.79	1.00	1.11	0.44
C14H0NO2	100.0730	1.52	0.50	1./1	0.57
C8H14O6S	239.0382	0.21	0.33	1.75	0.21
C5H11NO9S	258.0511	0.53	0.33	2 20	1.80
C11H8N2O5	201.0133	8.16	1.00	0.73	0.45
C6H7NO5	173 0324	0.37	0.80	1.17	0.83
C9H6O6	210.0164	2.20	1.00	0.67	0.67
C10H11NO4	209.0688	7.55	1.00	1.10	0.40
C9H7NO	145.0528	2.22	1.00	0.78	0.11
C10H16O4	200.1049	4.58	0.75	1.60	0.40
C8H6O6	198.0164	3.08	1.00	0.75	0.75
C5H3N3O2	137.0225	2.79	1.00	0.60	0.40
C10H7NO4	205.0375	3.04	1.00	0.70	0.40
C9H10O7S	262.0147	2.65	0.71	1.11	0.78
C10H10O2	162.0681	3.61	1.00	1.00	0.20
C10H18O6S	266.0824	2.65	0.33	1.80	0.60
C9H6N2O6	238.0226	7.25	1.00	0.67	0.67
C10H11NO3	193.0739	7.79	1.00	1.10	0.30
C7H7NO5	108.0430	2.19	1.00	2.40	0.80
C8H5NO8	243 0015	2.42	0.88	0.63	1.00
C7H6N2O3	166 0378	2.88	1.00	0.05	0.43
C8H6O6	198.0164	1 22	1.00	0.00	0.45
C14H10O2	210.0681	7.79	1.00	0.71	0.14
C9H11NO5	213.0637	3.58	1.00	1.22	0.56
C15H5NOS2	278.9813	1.09	1.00	0.33	0.07
C12H14O4	222.0892	8.04	1.00	1.17	0.33
C15H10O6	286.0477	3.49	1.00	0.67	0.40
C8H4N2O6	224.0069	4.13	1.00	0.50	0.75
C5H3NO4	141.0062	0.37	1.00	0.60	0.80
C12H5NO6	259.0117	3.85	1.00	0.42	0.50
C6H8O2	112.0524	1.02	1.00	1.33	0.33
CI5H5NOS2	278.9813	1.73	1.00	0.33	0.07
C12H8O4	216.0423	4.44	1.00	0.67	0.33
C15U2009	180.0425	4.11	1.00	0.89	0.44
C31H2203	442 1569	7.50	1.00	0.71	0.55
C7H7NO4	169.0375	6.29	1.00	1.00	0.10
C11H20O5	232.1311	3.52	0.40	1.82	0.45
C8H6N2O5	210.0277	6.96	1.00	0.75	0.63
C7H12O2	128.0837	2.45	1.00	1.71	0.29
C4H4O3	100.0160	0.46	1.00	1.00	0.75
C10H18O4	202.1205	2.88	0.50	1.80	0.40
C9H7NO	145.0528	3.46	1.00	0.78	0.11
C20H18O9	402.0951	7.43	1.00	0.90	0.45
C13H8O3	212.0473	7.08	1.00	0.62	0.23
C9H12O5S	232.0405	2.74	0.80	1.33	0.56
C6H5N3O2	151.0382	3.87	1.00	0.83	0.33
C8H6O3	150.0317	1.13	1.00	0.75	0.38
C0H4N4O12	275 0775	1.20	1.00	0.44	0.55
C4H4N2O4	1/4 0171	0.91	1.00	1.00	1.44
C13H8O3	212 0473	6.53	1.00	0.62	0.23
C12H8N2O6	276.0382	7.94	1.00	0.67	0.50
C13H8O3	212.0473	7.51	1.00	0.62	0.23
C5H10O3	118.0630	0.80	0.33	2.00	0.60
C13H20O6	272.1260	3.11	0.67	1.54	0.46
C15H16OS2	276.0643	3.20	1.00	1.07	0.07
C8H8N2O4	196.0484	4.03	1.00	1.00	0.50
C8H16O3	160.1099	3.13	0.33	2.00	0.38
C8H8O3	152.0473	1.72	1.00	1.00	0.38
C13H9NO4	243.0532	8.26	1.00	0.69	0.31
C21H36O9	432.2359	7.62	0.44	1.71	0.43
C6H12N2O6S	240 0416	7 24	0.33	2 00	1.00
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000020000	240.0410	1.24	0.55	2.00	1.00
C5H5NO4	143.0219	1.19	1.00	1.00	0.80
C101124000	410 1074	0.10	0.25	1.90	0.44
C18H34085	410.1974	0.10	0.25	1.69	0.44
C12H20N2O10S	384 0839	8 25	0.40	1 67	0.83
61201020105	226.0605	0.14	1.00	1.00	0.00
C12H12O5	236.0685	3.14	1.00	1.00	0.42
C11H6O3	186 0317	6.60	1.00	0.55	0.27
C1111005	180.0517	0.00	1.00	0.55	0.27
C16H10O4	266.0579	7.39	1.00	0.63	0.25
C15U1002	222.0691	7 22	1.00	0.77	0.12
C15H1002	222.0681	1.23	1.00	0.07	0.15
C9H10O4S	214 0300	2.58	1.00	1.11	0.44
071110010	17.0000	2.00	2.00		0.11
C7H12O5	176.0685	2.39	0.40	1.71	0.71
COLIANO	144 0224	2 60	1.00	0.50	0.12
Con4N2O	144.0324	3.09	1.00	0.50	0.15
C16H10O4S	298.0300	7.48	1.00	0.63	0.25
G10H200 CG	2 <0.0001	0.40	0.17	2.00	0.00
C10H20O6S	268.0981	3.43	0.17	2.00	0.60
C12H8O3	200 0473	4.40	1.00	0.67	0.25
01211005	200.0475	4.40	1.00	0.07	0.25
C15H8O4	252.0423	5.27	1.00	0.53	0.27
CGU4N2OG	200,0060	1 79	1.00	0.67	1.00
C0H4N2O0	200.0009	4.70	1.00	0.07	1.00
C8H5NO7	227.0066	4.07	1.00	0.63	0.88
CTLCC/	120.0266	0.07	0.75	1.00	0.00
C5H6O4	130.0266	0.96	0.75	1.20	0.80
C5H6O2	98 0368	0.39	1.00	1.20	0.40
0511002	90.0500	0.57	1.00	1.20	0.40
C7H8O4	156.0423	1.04	1.00	1.14	0.57
COLICNI2O2	170 0270	C 19	1.00	0.75	0.20
C8H0N2O5	1/8.05/8	0.48	1.00	0.75	0.56
C11H8O3	188 0473	7.77	1.00	0.73	0.27
California	151.0202	1.00	1.00	0.02	0.00
C6H5N3O2	151.0382	4.22	1.00	0.83	0.33
C6H6N2O2	138 0/29	0.91	1.00	1.00	0.33
001014202	130.0427	0.91	1.00	1.00	0.55
C6H4O4	140.0110	0.38	1.00	0.67	0.67
C7U12NO0S	297 0211	2 69	0.22	1 06	1 20
C/HI3N093	287.0511	2.08	0.22	1.80	1.29
C5H6O6S	193,9885	0.63	0.50	1.20	1.20
COLLCOC	210.0164	0.52	1.00	0.67	0.67
C9H6O6	210.0164	2.55	1.00	0.07	0.07
C12H18O6	258,1103	2.93	0.67	1.50	0.50
GAUTINOS	1 <5 0272	0.00	0.00	1.77	1.50
C4H/NO6	165.0273	0.38	0.33	1.75	1.50
C9H4O5	192.0059	1.89	1.00	0.44	0.56
6911100	192100009	2.50	1.00	0.70	0.20
C9H/N06	225.0273	3.59	1.00	0.78	0.67
C6H13NO8S	259 0362	2 62	0.13	2 17	1 33
011151(005	259.0502	2.02	0.15	2.17	1.55
C10H10O7S	274.0147	2.78	0.86	1.00	0.70
C7H7NO4	160 0375	6 67	1.00	1.00	0.57
C/II/N04	109.0375	0.07	1.00	1.00	0.57
C9H15NO9S	313.0468	3.20	0.33	1.67	1.00
C10U1(07	256 0906	7 70	1.00	0.04	0.27
C19H1007	550.0890	1.18	1.00	0.84	0.57
C6H12O3	132.0786	2.58	0.33	2.00	0.50
GUISNOS	147.01.00	2.00	0.00	1.05	1.05
C4H5NO5	147.0168	0.34	0.60	1.25	1.25
C15H12N2O14S	476 0009	3.08	0.79	0.80	0.03
01011121(20145	470.0009	5.00	0.75	0.00	0.75
C6H7NO4	157.0375	0.71	1.00	1.17	0.67
COHONO3	170.0582	3 3 2	1.00	1.00	0.33
C31191003	179.0382	5.52	1.00	1.00	0.55
C9H16O7S	268.0617	0.71	0.29	1.78	0.78
COLLOOA	169 0422	1.00	1.00	1.00	0.50
C6H6U4	108.0425	1.09	1.00	1.00	0.50
C11H10O2	174.0681	3.33	1.00	0.91	0.18
CIQUIDANOC	220 0742	7.95	1.00	0.70	0.22
C18H13N06	339.0743	7.85	1.00	0.72	0.33
C7H7N3O4	197 0437	6 94	1.00	1.00	0.57
C/11/1004	177.0457	0.54	1.00	1.00	0.57
C14H10O5	258.0528	3.66	1.00	0.71	0.36
C7H7NO2	137 0477	2 36	1.00	1.00	0.29
6/11/1(02	101.0111	2.50	1.00	1.00	0.27
C8H10O5	186.0528	2.31	0.80	1.25	0.63
C10H16O7S	280.0617	2.05	0.43	1.60	0.70
Cionico/b	200.0017	2:05	0.45	1.00	0.70
CTTH9NO5	235.0481	7.48	1.00	0.82	0.45
C16H20O5	292 1311	7 51	1.00	1 25	0.31
0101120005	272.1311	7.51	1.00	1.23	0.51
C5H10O3	118.0630	2.91	0.33	2.00	0.60
C8H0NO2	151 0633	1 76	1.00	1 1 3	0.25
001191102	151.0055	1.70	1.00	1.15	0.25
C10H15NO10S	341.0417	2.98	0.40	1.50	1.00
CORRNOOD	176 0586	672	1.00	0.80	0.22
C7110IN2U2	170.0300	0.72	1.00	0.09	0.22
C13H11NO4	245.0688	7.89	1.00	0.85	0.31
CEUTNO2	141.0426	0.47	1.00	1 17	0.50
COLINOS	141.0420	0.4/	1.00	1.1/	0.50
C8H15NO9S	301.0468	3.09	0.22	1.88	1.13
COLISNI2O2	197 0292	2.00	1.00	0.50	0.22
C9H5N3O2	187.0382	3.99	1.00	0.56	0.22
C6H9NO3	143.0582	0.58	1.00	1.50	0.50
C111111NO4	221.0702	6.00	1.00	1.00	0.26
CITHTINO4	221.0688	6.97	1.00	1.00	0.36
C9H18O6S	254 0824	4.27	0.17	2.00	0.67
012120005	25 10021	7.01	0.00	1.00	0.20
C13H20O5	256.1311	7.91	0.80	1.54	0.38
C8H12O9S	284 0202	1.08	0.33	1 50	1 1 3
01101000	100.0250	1.00	1.00	1.50	1.15
C9H6N2O3	190.0378	4.44	1.00	0.67	0.33
C9H10O2	150.0681	3 71	1.00	1 1 1	0.22
C011103207	226.0500	0.17	1.00	1 1 1	0.22
C9H10N2O5	226.0590	8.17	1.00	1.11	0.56
C8H7NO6	213 0273	4 60	1.00	0.88	0.75
00111100	210.0210		1.00	0.00	0.10

C5H8O3	116.0473	0.05	0.67	1.60	0.60
CITUSNOSO	070 0012	2.60	1.00	0.22	0.07
CI5H5NOS2	278.9813	2.69	1.00	0.33	0.07
C11H7NO4	217.0375	6.97	1.00	0.64	0.36
C20112004	224 2144	0.12	1.00	1.50	0.20
C20H30O4	554.2144	0.15	1.00	1.50	0.20
C6H5NO4	155.0219	1.79	1.00	0.83	0.67
C91112005	284 0202	0.60	0.22	1.50	1 1 2
C8H12095	284.0202	0.09	0.55	1.50	1.15
C9H7NO3	177.0426	6.97	1.00	0.78	0.33
C11119O6	226 0221	2.57	1.00	0.72	0.55
C11H8O0	250.0521	2.37	1.00	0.75	0.55
C12H8O3S2	263.9915	0.67	1.00	0.67	0.25
COLIONIQOC	228 0282	2 (9	1.00	1.00	0.75
C8H8N2O6	228.0382	3.08	1.00	1.00	0.75
C7H6O2	122.0368	1.87	1.00	0.86	0.29
CELIZNOS	172 0224	0.76	0.80	1 17	0.92
COH/NO5	1/5.0524	0.76	0.80	1.1/	0.85
C8H4N2O	144.0324	3.42	1.00	0.50	0.13
C71116058	212 0719	1 49	0.00	2.20	0.71
C/H10055	212.0718	1.48	0.00	2.29	0.71
C15H8O4	252.0423	7.60	1.00	0.53	0.27
C14U10028	259 0251	0.52	1.00	0.71	0.21
C14H10035	238.0331	0.55	1.00	0.71	0.21
C10H9NO4	207.0532	2.82	1.00	0.90	0.40
Cellente	172 0097	0.07	1.00	1.00	0.67
C0H0043	1/3.9987	0.97	1.00	1.00	0.07
C10H9NO5	223.0481	5.89	1.00	0.90	0.50
C11H12NO4	222 0845	7 97	1.00	1 1 9	0.26
CITHI3N04	223.0843	1.07	1.00	1.10	0.50
C11H8O3	188.0473	7.28	1.00	0.73	0.27
C12H11NO7	202 0526	7 66	1.00	0.85	0.54
CI3HINO/	293.0330	7.00	1.00	0.85	0.54
C4H8O2	88.0524	0.39	0.50	2.00	0.50
COH7NO4	102 0275	2 24	1.00	0.78	0.44
C9H/NO4	195.0575	2.34	1.00	0.78	0.44
C4H8O3	104.0473	0.09	0.33	2.00	0.75
C9H16O4	176 1040	2.40	0.25	2.00	0.50
Con1004	170.1049	2.40	0.23	2.00	0.50
C13H22O5	258.1467	6.47	0.60	1.69	0.38
COLLOCAS	200.0142	1.20	1.00	1.00	0.50
C8H8045	200.0143	1.20	1.00	1.00	0.50
C6H4O3	124.0160	3.07	1.00	0.67	0.50
COLICNI2OC	228 0226	6.00	1.00	0.77	0.7
C9H6N2O6	238.0226	0.99	1.00	0.67	0.67
C7H16O4S	196.0769	3.67	0.00	2.29	0.57
C14U9O2	224 0472	4.40	1.00	0.57	0.21
C14H8O3	224.0475	4.49	1.00	0.57	0.21
C9H10O5S	230.0249	2.53	1.00	1.11	0.56
C011002	152 0472	1 26	1.00	1.00	0.20
Cono03	132.0475	4.30	1.00	1.00	0.58
C8H16O4	176.1049	1.44	0.25	2.00	0.50
C6H7NO2	141 0426	2.46	1.00	1 17	0.50
COHINOS	141.0420	2.40	1.00	1.17	0.50
C14H8O4	240.0423	6.38	1.00	0.57	0.29
COLO	118 0/10	2 1 2	1.00	0.75	0.12
Сопоо	116.0419	5.15	1.00	0.75	0.15
C8H15NO9S	301.0468	2.36	0.22	1.88	1.13
C17U2204	200 1519	7.24	1.00	1.20	0.24
C1/H2204	290.1518	1.24	1.00	1.29	0.24
C8H8O3	152.0473	5.32	1.00	1.00	0.38
COLISNOA	170.0210	2 1 2	1.00	0.62	0.50
Consino4	179.0219	5.12	1.00	0.05	0.50
C8H8O	120.0575	3.06	1.00	1.00	0.13
C4H5NO2	00.0220	0.00	1.00	1.25	0.50
C4HJNO2	99.0320	0.09	1.00	1.25	0.50
C5H5N3O3	155.0331	1.67	1.00	1.00	0.60
C10H16N2O10S	356 0526	7 72	0.40	1.60	1.00
C10H10N20105	330.0320	1.12	0.40	1.00	1.00
C9H8N2O6	240.0382	7.70	1.00	0.89	0.67
C10H0NO3	101 0582	1 13	1.00	0.00	0.30
C101191003	191.0382	4.45	1.00	0.90	0.50
C4H4O4S	147.9830	0.40	0.75	1.00	1.00
C6H6N2O4	170 0328	2 35	1.00	1.00	0.67
CALCOR	114.0420	0.05	1.00	1.00	0.57
C4H6N2O2	114.0429	0.05	1.00	1.50	0.50
C8H9NO4	183.0532	2.34	1.00	1.13	0.50
012111002	100.0001	7.07	1.00	0.77	0.15
C13H1002	198.0681	1.97	1.00	0.77	0.15
C12H11NO7S	313.0256	7.11	1.00	0.92	0.58
C71114075	226.0511	0.94	0.17	2.00	0.94
C/H1406S	220.0511	0.84	0.17	2.00	0.86
C13H8O4	228.0423	7.86	1.00	0.62	0.31
C7117N2O4	107.0427	571	1.00	1.00	0.57
C/H/N304	197.0437	5.74	1.00	1.00	0.57
C7H6O2	122.0368	6.99	1.00	0.86	0.29
COLICOA	179.0200	2.42	1.00	0.07	0.44
09004	1/6.0200	2.42	1.00	0.07	0.44
C9H7NO6	225.0273	4.06	1.00	0.78	0.67
C1111002	172.0524	2 77	1.00	0.72	0.10
C11H802	172.0524	0.//	1.00	0.73	0.18
C15H8O4	252.0423	7.25	1.00	0.53	0.27
C10111000	106 0601	7.05	1.00	0.02	0.17
C12H10O2	180.0081	1.25	1.00	0.85	0.17
C14H9NO5	271.0481	7.51	1.00	0.64	0.36
C10HONO2	101 0592	2 50	1.00	0.00	0.20
CIUMPINOS	191.0362	5.52	1.00	0.90	0.30
C4H8O4S	152.0143	2.83	0.25	2.00	1.00
COLISNIDOS	102 0525	1 80	1.00	0.80	0.32
C7H0IN2U3	192.0333	4.00	1.00	0.09	0.35
C6H5NO6S	218.9838	2.92	0.83	0.83	1.00
C8H5NO4	179 0219	2 55	1.00	0.63	0.50
01151104	1/2.0217	2.55	1.00	0.05	0.50
C5H5NO4	143.0219	0.38	1.00	1.00	0.80

C9H8O6	212 0321	2 92	1.00	0.89	0.67
0,11000	212.0521	2.72	1.00	0.07	0.07
C8H8O	120.0575	3.27	1.00	1.00	0.13
C14H6O3S2	285 9758	2.61	1.00	0.43	0.21
611100352	200.0750	2.01	1.00	0.15	0.21
C9H16O4S	220.0769	2.02	0.50	1.78	0.44
C7H14O3	146 0943	3 22	0.33	2.00	0.43
C/111105	1 10.09 15	3.22	0.55	2.00	0.15
C9H14O2	154.0994	3.13	1.00	1.56	0.22
C10H15NO8S	309.0518	3 22	0.50	1.50	0.80
0101115110005	505.0510	5.22	0.50	1.50	0.00
C8H10O5S	218.0249	1.81	0.80	1.25	0.63
C16H24O8	344 1471	3 /7	0.63	1 50	0.50
010112400	544.1471	5.47	0.05	1.50	0.50
C13H6O6	258.0164	3.26	1.00	0.46	0.46
C64804	144 0422	2.40	0.75	1 22	0.67
C0H804	144.0423	2.40	0.75	1.55	0.07
C10H19NO7S	297.0882	7.48	0.29	1.90	0.70
C6H10N2O2	158 0601	1.00	1.00	1.67	0.50
COHION205	138.0091	1.09	1.00	1.07	0.50
C18H16O6	328.0947	8.16	1.00	0.89	0.33
C10H14O2	182 0042	2.07	1.00	1.40	0.20
C10H14O3	182.0945	3.07	1.00	1.40	0.50
C12H8O3	200.0473	5.95	1.00	0.67	0.25
C9U5NO2S	104 0000	7 41	1.00	0.62	0.28
Conjinoss	194.9990	7.41	1.00	0.05	0.56
C10H19NO10S	345.0730	1.04	0.20	1.90	1.00
C9U16O68	240.0668	1 17	0.17	2.00	0.75
C8H10005	240.0008	1.17	0.17	2.00	0.75
C11H7NO7	265.0223	6.71	1.00	0.64	0.64
CALIONO2	127 0622	0.12	1.00	1.50	0.22
Conginoz	127.0055	0.12	1.00	1.50	0.55
C8H14O10S	302.0308	2.46	0.20	1.75	1.25
C12U10O2	109 0691	7 20	1.00	0.77	0.15
C15H1002	198.0081	7.20	1.00	0.77	0.15
C10H12O6	228.0634	2.64	0.83	1.20	0.60
C0119O2	149.0524	2.29	1.00	0.00	0.22
C9H8O2	148.0524	2.38	1.00	0.89	0.22
C4H5N3O2	127.0382	1.06	1.00	1.25	0.50
C41110026	120.0251	0.60	0.00	2.50	0.75
C4H10O3S	138.0351	0.69	0.00	2.50	0.75
C13H18O6	270.1103	3.05	0.83	1.38	0.46
CIQUONOZ	270.0270	3.05	1.00	0.75	0.10
CI2H9NO/	2/9.03/9	7.47	1.00	0.75	0.58
C12H22O5	246 1467	4 69	0.40	1.83	0.42
C10111204	106.0726	2.21	1.00	1.00	0.12
C10H12O4	196.0736	3.31	1.00	1.20	0.40
C13H9NO5	259 0481	7 63	1.00	0.69	0.38
CISII/105	257.0401	7.05	1.00	1.02	1.00
C6H11NO8S	257.0205	2.11	0.25	1.83	1.33
C14H26O6	290 1729	6 5 2	0.33	1.86	0.43
C14112000	200.1720	0.52	0.55	1.00	0.45
C12H22O4	230.1518	3.72	0.50	1.83	0.33
C5H10O8S	230.0096	1.68	0.13	2.00	1.60
6511100005	230.0070	1.00	0.15	2.00	1.00
C6H8O5S	192.0092	0.89	0.60	1.33	0.83
C13H12O2	200.0837	7 73	1.00	0.92	0.15
015111202	200.0057	1.15	1.00	0.72	0.15
C6H7NO	109.0528	0.45	1.00	1.17	0.17
C12H14N2O4	250.0954	5.26	1.00	1 17	0.33
012111411204	250.0754	5.20	1.00	1.17	0.55
C10H16O5S	248.0718	2.61	0.60	1.60	0.50
C7H10O6	100 0477	1 / 8	0.50	1 / 3	0.86
C/111000	190.0477	1.48	0.50	1.45	0.80
C12H12O3	204.0786	3.31	1.00	1.00	0.25
C11H17NO7S	307 0726	6 70	0.57	1 55	0.64
CIIII/NO/S	307.0720	0.70	0.57	1.55	0.04
C7H7NO7S	248.9943	2.87	0.71	1.00	1.00
C7H16O3S	180.0820	3 55	0.00	2 20	0.43
C/1110055	180.0820	5.55	0.00	2.29	0.45
C12H25NO3S2	295.1276	3.04	0.33	2.08	0.25
C12H15N3O4S	207 0783	1.67	1.00	1 25	0.33
0121115115045	277.0785	4.07	1.00	1.23	0.55
C11H11NO4	221.0688	6.46	1.00	1.00	0.36
C12H13N3O4	263,0906	7 94	1.00	1.08	0 33
COLIDITOOT	203.0300	7.27	1.00	1.00	0.55
C9H8N2O5	224.0433	1./1	1.00	0.89	0.56
C15H8O5	268.0372	5.08	1.00	0.53	0.33
CELENOS	150.01/0	0.42	0.00	1.00	1.00
COHONOS	159.0168	0.43	0.80	1.00	1.00
C6H7NO3	141.0426	0.94	1.00	1.17	0.50
Gelleoka	211.00120	0.07	1.00	0.00	0.67
C9H8O6S	244.0042	2.37	1.00	0.89	0.67
C10H9NO5	223 0481	5.02	1.00	0.90	0.50
0011100	100.0570	1.17	1.00	1.11	0.50
C9H10O4	182.0579	4.17	1.00	1.11	0.44
C6H6O2	110.0368	0.38	1.00	1.00	0 33
001002	102.0505	0.50	1.00	1.00	0.33
C9H8N2O3	192.0535	2.48	1.00	0.89	0.33
C6H8N2O5	188 0433	2 77	0.80	1 33	0.83
00111002	100.0733	2.77	0.00	1.55	0.00
C9H18O3	174.1256	3.80	0.33	2.00	0.33
C18H10O3	274 0630	7 98	1.00	0.56	0.17
0111005	277.0050	7.50	1.00	0.50	0.17
C9H12O7	232.0583	2.51	0.57	1.33	0.78
C8H8O4S	200 01/13	1.67	1.00	1.00	0.50
	200.01+3	1.07	1.00	1.00	0.50
C14H8O3	224.0473	6.88	1.00	0.57	0.21
C8H14O4	174 0892	3 95	0.50	1 75	0.50
	1/7.00/2	5.75	0.50	1.75	0.50
C10H17NO4	215.1158	3.61	0.75	1.70	0.40
C11H12O3	192 0786	3 60	1.00	1.00	0.27
015111203	172.0700	5.07	1.00	1.07	0.27
C15H10O3	238.0630	7.98	1.00	0.67	0.20
C10H6O5	206 0215	2 42	1.00	0.60	0.50
01011005	200.0213	2.72	1.00	0.00	0.50

C7H10O2	126 0681	1 25	1.00	1 43	0.29
G10124075	201.0001	1.20	0.00	1.00	0.20
C18H34O/S	394.2025	7.66	0.29	1.89	0.39
C7H6O4	154 0266	2.07	1.00	0.86	0.57
CINTRO I	151.0200	2.07	1.00	0.00	0.57
C10H/N3O4	233.0437	7.61	1.00	0.70	0.40
C7H5NO6	199.0117	0.96	1.00	0.71	0.86
6/1151(60	177.0117	0.90	1.00	0.71	0.00
C10H16N2O10S	356.0526	7.36	0.40	1.60	1.00
C10H11NO7S	289 0256	6.10	0.86	1 10	0.70
CI0IIIII075	207.0250	0.10	0.00	1.10	0.70
C6H5NO7S	234.9787	1.08	0.71	0.83	1.17
C14U8O2	224 0472	5 87	1.00	0.57	0.21
C14H6O3	224.0473	5.62	1.00	0.57	0.21
C13H9NO5	259.0481	8.07	1.00	0.69	0.38
CELLOO	94 0575	0.55	1.00	1.0	0.20
CSH8O	84.0373	0.55	1.00	1.00	0.20
C13H24O6	276.1573	4.37	0.33	1.85	0.46
C211122007	206 21 49	7.07	0.96	1.50	0.22
C21H32O/	390.2148	1.87	0.80	1.52	0.55
C15H12O4	256.0736	6.95	1.00	0.80	0.27
015111405	074 0041	676	1.00	0.02	0.22
C15H14O5	274.0841	0.70	1.00	0.93	0.55
C17H24O4	292.1675	8.59	1.00	1.41	0.24
C101114N204	226 0054	1.02	1.00	1.40	0.40
C10H14N204	226.0954	1.03	1.00	1.40	0.40
C13H6O6	258.0164	4.37	1.00	0.46	0.46
015110402	252 1725	8.04	1.00	1.0	0.00
C15H24O3	252.1725	8.04	1.00	1.60	0.20
C13H8O4	228 0423	7.26	1.00	0.62	0.31
01211(05	0.40.0015	2 77	1.00	0.46	0.20
C13H6O5	242.0215	3.77	1.00	0.46	0.38
C8H6N2O4	194 0328	5.21	1.00	0.75	0.50
Capital Abaon	220,0027	6.20	1.00	0.70	0.05
C20H14N2OS	330.0827	6.79	1.00	0.70	0.05
C10H11NO7S	289 0256	4 98	0.86	1 10	0.70
	207.0250	1.50	0.00	1.10	0.70
C15H32O5S	324.1970	8.07	0.00	2.13	0.33
C15H23NO8S	377 1144	7 34	0.63	1 53	0.53
015112510065	577.1144	7.54	0.05	1.55	0.55
C10H12O5	212.0685	2.58	1.00	1.20	0.50
C10H2005S	252 1031	3 60	0.20	2.00	0.50
0101120055	252.1051	5.00	0.20	2.00	0.50
C7H8O5S	204.0092	2.77	0.80	1.14	0.71
C15H10O2	222.0681	8.08	1.00	0.67	0.13
C15H1002	222.0081	0.00	1.00	0.07	0.15
C8H9NO2	151.0633	0.74	1.00	1.13	0.25
C11H20N2O11	256 1067	1 91	0.27	1.92	1.00
C11H20N2011	550.1007	4.01	0.27	1.62	1.00
C5H10O4S	166.0300	0.72	0.25	2.00	0.80
COLIANDOD	172 0272	0.10	1.00	0.44	0.22
C9H4N2O2	172.0273	0.10	1.00	0.44	0.22
C7H5NO4	167.0219	2.93	1.00	0.71	0.57
C9H12N2O4	200.0707	2 27	1.00	1 50	0.50
C6H12N2O4	200.0797	2.57	1.00	1.50	0.50
C15H24O9	348.1420	3.25	0.44	1.60	0.60
CTHONOAS	202 0252	0.52	1.00	1.20	0.57
C/H9NO4S	203.0252	0.55	1.00	1.29	0.57
C11H10O6	238.0477	4 09	1.00	0.91	0.55
CIFILIENCOR	072 0902	2.71	1.00	1.00	0.12
CI5HI5NO25	275.0825	3.71	1.00	1.00	0.15
C10H12O7	244 0583	0.69	0.71	1.20	0.70
CIQUADOCC	2(0.0001	1.00	0.17	2.00	0.70
C10H2006S	268.0981	4.90	0.17	2.00	0.60
C7H7N3O2	165 0538	3 72	1.00	1.00	0.29
C12U24N20109	100.0000	7.00	0.20	1.00	0.27
CI3H24N2O10S	400.1152	7.99	0.30	1.85	0.77
C5H10O3	118 0630	0.11	0.33	2.00	0.60
Collabora	200.1122	5.12	0.00	2.00	0.00
C9H20O3S	208.1133	7.12	0.00	2.22	0.33
C10H21NO8S	315 0988	3 79	0.13	2 10	0.80
C1011211(005	313.0700	5.77	1.00	2.10	0.00
C13H8O3	212.04/3	5.77	1.00	0.62	0.23
C9H15NO18	425.0289	4.67	0.17	1.67	2.00
CTUTNOTS	248 0042	2.24	0.71	1.00	1.00
C/H/NU/S	240.9943	5.54	0.71	1.00	1.00
C7H8O3S	172.0194	1.32	1.00	1.14	0.43
COLIMNOSS	221 0201	0.70	1.00	1 1 2	0.62
COURINO22	251.0201	2.12	1.00	1.13	0.03
C12H21NO9S	355.0937	6.47	0.33	1.75	0.75
C11U12NO2	207 0905	0 10	1.00	1 10	0.27
CHHISNOS	207.0895	0.10	1.00	1.10	0.27
C15H8O3	236.0473	7.80	1.00	0.53	0.20
CIOLCOS	206 0215	2.00	1.00	0.00	0.50
C10H6O5	200.0215	2.89	1.00	0.60	0.50
C13H8O3	212.0473	7.98	1.00	0.62	0.23
C14U12NO4	250 0045	0 1 2	1.00	0.02	0.20
C14H15INU4	239.0843	8.13	1.00	0.93	0.29
C10H13NO5	227.0794	4.01	1.00	1.30	0.50
C0111(02	160 1000	5 05	0.22	2.00	0.20
C8H16U3	100.1099	5.85	0.55	2.00	0.38
C6H9NO4	159.0532	0.87	0.75	1.50	0.67
COLLINGIAGO	202.0772	2 50	0.21	1 20	1.00
Continui352	392.96/2	3.39	0.51	1.58	1.63
C13H7NO5	257.0324	7.25	1.00	0.54	0.38
07115206	100 0117	0.55	1.00	0.71	0.00
C/H5NO6	199.0117	0.65	1.00	0.71	0.86
C17H24O4	292,1675	6.82	1.00	1.41	0.24
01011011010	207.0002	0.02	1.00	0.70	1.00
C12H6N4O12	397.9982	2.57	1.00	0.50	1.00
C9H18O4S	222,0926	8 11	0.25	2.00	0.44
COLLECTO	1.00.1102	0.11	1.00	2.00	0.77
C9H15NO2	169.1103	4.41	1.00	1.67	0.22
C13H24O5	260 1624	6.77	0.40	1.85	0.38
011110300	200.1024	0.77	1.00	1.05	0.50
C11H9NO5	235.0481	7.13	1.00	0.82	0.45

C10H20O6S	268.0981	7.36	0.17	2.00	0.60
C15U10O4	254.0570	7 15	1.00	0.67	0.27
C13H1004	234.0379	7.15	1.00	0.07	0.27
C11H8O5S2	283.9813	0.76	1.00	0.73	0.45
COLENIOS	102 0220	150	1.00	0.02	0.22
COHSINO2	125.0520	1.30	1.00	0.85	0.55
C15H10O6	286.0477	4.01	1.00	0.67	0.40
C101110N202	206.0601	2.02	1.00	1.00	0.20
C10H10N2O3	206.0691	2.85	1.00	1.00	0.50
C4H6N4O6S	238.0008	3.15	0.67	1.50	1.50
CTHONOLOG	200.0017	2.01	0.40	1.00	1.40
C/H9NO10S	298.9947	3.81	0.40	1.29	1.43
C12H13NO4	235 0845	7.60	1.00	1.08	0.33
01211101101	255.0015	7.00	1.00	1.00	0.55
C8H8N4O6S	288.0165	2.31	1.00	1.00	0.75
C5H4N2O4	156 0171	2 50	1.00	0.80	0.80
0311411204	150.0171	2.5)	1.00	0.00	0.00
C12H7NO2S	229.0197	0.68	1.00	0.58	0.17
C0H4O6	208 0008	1.06	1.00	0.44	0.67
C9H4O0	208.0008	1.00	1.00	0.44	0.07
C11H18N2O10	338.0961	7.49	0.40	1.64	0.91
C17U1002	246.0691	7.65	1.00	0.50	0.12
C1/H1002	240.0081	7.05	1.00	0.59	0.12
C10H7NO5	221.0324	2.74	1.00	0.70	0.50
C15U21NO9C	295 1770	7.00	0.12	2.07	0.52
CISH3INO8S	385.1770	7.99	0.13	2.07	0.53
C7H10N2O4	186 0641	0.97	1.00	1 4 3	0.57
6/1101(201	100.0011	0.57	1.00	1.15	0.57
C9H8O5	196.0372	1.77	1.00	0.89	0.56
C9H7NO4	193 0375	0.64	1.00	0.78	0.44
Chintof	175.0575	0.04	1.00	0.70	0.44
C6H5N3O2	151.0382	3.36	1.00	0.83	0.33
C16U12058	216 0405	6 1 6	1.00	0.75	0.21
C10H12035	510.0405	0.40	1.00	0.75	0.51
C16H31NO9S	413,1720	8.13	0.22	1.94	0.56
C10U17N2O2	227 1270	2.11	1.00	1.70	0.20
C10H1/N505	227.1270	3.11	1.00	1.70	0.50
C3H5NO3	103 0269	0.03	0.67	1 67	1.00
031131103	105.0209	0.05	0.07	1.07	1.00
C16H30O5	302.2093	7.50	0.40	1.88	0.31
C12H0NO	105 0694	1 16	1.00	0.60	0.08
CISHINO	195.0064	4.40	1.00	0.09	0.08
C7H12O8	224.0532	2.85	0.25	1.71	1.14
COLLCOR	242.00/2	2 10	0.00	0.67	0.90
C9H6O8	242.0065	5.10	0.88	0.07	0.89
C3H7NO8S	216,9892	0.48	0.13	2.33	2.67
CONTINUES	210.0002	4.00	1.00	2.55	2.07
C20H13NOS2	347.0439	4.32	1.00	0.65	0.05
C6H6O2	110.0368	1.28	1.00	1.00	0.33
011002	110.0508	1.20	1.00	1.00	0.55
C9H10N4OS2	254.0296	3.11	1.00	1.11	0.11
C749N40982	220 0784	1.05	0.75	1.14	1.14
C/1101040052	339.9704	1.05	0.75	1.14	1.14
C7H9NO8S	267.0049	2.50	0.50	1.29	1.14
CIDUISNOOS	225 0469	2.01	0.44	1.50	0.00
C10H15N095	525.0408	5.01	0.44	1.50	0.90
C13H25NO8S	355,1301	7.63	0.25	1.92	0.62
CTUONO	100.0604	0.00	1.00	1.00	0.1.4
C/H9NO	123.0684	0.69	1.00	1.29	0.14
C12H9NO5	247 0481	7 70	1.00	0.75	0.42
	247.0401	1.10	1.00	0.75	0.42
C14H11NO3	241.0739	8.34	1.00	0.79	0.21
C12H7NO2	107 0477	3 83	1.00	0.58	0.17
C1211/102	197.0477	5.65	1.00	0.56	0.17
C8H9NO2	151.0633	2.70	1.00	1.13	0.25
Cell11NO08	272 0155	2 10	0.22	1.02	1.50
CONTINU93	275.0155	2.19	0.22	1.05	1.50
C4H8O2	88.0524	1.08	0.50	2.00	0.50
C1 4112 402	240 1725	7.00	1.00	1 7 1	0.01
C14H24O3	240.1725	/.90	1.00	1./1	0.21
C10H20O6S	268 0981	7.60	0.17	2 00	0.60
GIOLIZO COD	200.0701	7.00	1.00	2.00	0.00
C19H24O4	316.16/5	7.61	1.00	1.26	0.21
C13H24N2O4	272 1736	1 46	0.75	1.85	0.31
	2,2.1,30	1.10	1.00	1.05	0.51
C/H6N4OS2	225.9983	1.68	1.00	0.86	0.14
C14H8O4	240 0423	4 24	1.00	0.57	0.29
	100.0123		1.00	0.57	0.27
C11H8O3	188.0473	6.44	1.00	0.73	0.27
C14H14O4	246 0892	7 41	1.00	1.00	0.29
	210.0072	7.71	1.00	1.00	0.27
C16H30O8S	382.1661	7.76	0.25	1.88	0.50
C14H16O4	248 1049	8 25	1.00	1 1/	0.20
014111004	240.1047	0.20	1.00	1.14	0.29
C8H8O4	168.0423	4.40	1.00	1.00	0.50
CEULINO2	145 0720	1 47	0.67	1 02	0.50
CONTINUS	143.0739	1.4/	0.07	1.83	0.50
C10H8O7	240.0270	2.87	1.00	0.80	0.70
CIDIDENOOS	242 1201	6 00	0.12	2.00	0.77
C12H25N085	343.1301	0.88	0.13	2.08	0.67
C9H8N2O3	192.0535	6.89	1.00	0.89	0.33
001001200	102.0535	7.00	1.00	0.02	0.00
C9H8N2O3	192.0535	1.32	1.00	0.89	0.33
C15H6O7S2	361 9555	1 89	1.00	0.40	0.47
011100/02	301.2333	1.07	1.00	0.40	017
C9H19NO7S	285.0882	7.41	0.14	2.11	0.78
C11H8O3	188 0/73	5 1 5	1.00	0.73	0.27
0111003	100.0473	5.15	1.00	0.75	0.27
C9H7NO	145.0528	4.13	1.00	0.78	0.11
C6H6O	94 0410	2 22	1.00	1.00	0.17
COHOO	74.0417	2.32	1.00	1.00	0.17
C14H13NO3S	275.0616	3.11	1.00	0.93	0.21
CGUANDO	120.0224	2.24	1.00	0.47	0.17
COH4N2O	120.0324	2.24	1.00	0.07	0.17
C12H14O3	206.0943	7.26	1.00	1.17	0.25
012111/04	20010210	2.04	1.00	1 22	0.22
C12H16O4	224.1049	3.04	1.00	1.55	0.33
C8H5NO8	243 0015	3 31	0.88	0.63	1.00
20110100	2.0.0010	0.01	0.00	0.05	1.00

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C19H18O6	342.1103	8.30	1.00	0.95	0.32
C15H8O6	284.0321	3.43	1.00	0.53	0.40
C15H12O3	240.0786	6.87	1.00	0.80	0.20
C7H3NO5S	212.9732	6.63	1.00	0.43	0.71
C7H7NO	121.0528	3.18	1.00	1.00	0.14
C11H8O2	172.0524	5.13	1.00	0.73	0.18
C15H24O3	252.1725	7.88	1.00	1.60	0.20
C20H36O8	404.2410	7.43	0.38	1.80	0.40
CI0H2INO/S	299.1039	1.13	0.14	2.10	0.70
C6H4N4OS2	211.9827	0.76	1.00	0.67	0.17
C9H14O	138.1045	2.76	1.00	1.56	0.11
CIUH9NU3	191.0582	0.77	1.00	0.90	0.30
COHIZOSS	196.0405	2.29	0.20	2.00	0.85
COLLINGOS	281.0203	5.01	0.30	1.50	1.00
C9H10U05	280.0722	5.20	0.15	2.00	0.89
C7H0NO2	130.0633	1.41	1.00	1.20	0.30
C12H7NO2	197.0033	3.63	1.00	0.58	0.29
C13H7NO2	257 0324	7.66	1.00	0.50	0.17
C16H34O5S	338 2127	8 25	0.00	2.13	0.30
C8H11NO4S	217 0/09	0.90	1.00	1 38	0.51
C8H4O3	148 0160	1.91	1.00	0.50	0.30
C12H12O2	188 0837	1.21	1.00	1.00	0.30
C11H13NO5	239.0794	4.59	1.00	1.00	0.17
C5H7NO2	113 0477	0.12	1.00	1.10	0.40
C10H10N2O3	206.0691	6.55	1.00	1.40	0.40
C7H14O4	162 0892	2 43	0.25	2.00	0.50
C4H4N407S	251 9801	0.81	0.25	2.00	1.75
C9H16O10S	316 0464	8.07	0.71	1.00	1.75
C12H18O8	290 1002	2.63	0.20	1.70	0.67
C9H8N2O3	192 0535	2.03	1.00	0.89	0.07
C11H14O4	210.0892	3.01	1.00	1.27	0.35
C9H17NO9S	315.0624	6.29	0.22	1.27	1.00
C0H7NO5	209.0324	6.22	1.00	0.78	0.56
C4H7NO5	149 0324	0.52	0.40	1 75	1.25
C13H10O2	198.0681	7 48	1.00	0.77	0.15
C13H8O4	228 0423	8 21	1.00	0.62	0.15
C23H10OS	334.0452	7.23	1.00	0.43	0.04
C4H8O4S	152 0143	5.12	0.25	2.00	1.00
C13H8O4	228 0423	673	1.00	0.62	0.31
C10H2006S	268 0981	6.61	0.17	2.00	0.60
C9H7NO5	209.0324	0.57	1.00	0.78	0.56
C15H16O3S2	308 0541	3.71	1.00	1.07	0.20
C19H18O7	358 1053	7.83	1.00	0.95	0.37
C5H3NO3	125.0113	0.42	1.00	0.60	0.60
C10H11NO7S	289.0256	4.44	0.86	1.10	0.70
C8H10O6S	234.0198	0.70	0.67	1.25	0.75
C8H9NO5	199.0481	5.41	1.00	1.13	0.63
C7H6O	106.0419	0.82	1.00	0.86	0.14
C11H23NO7S	313.1195	7.93	0.14	2.09	0.64
C11H8O3S2	251.9915	1.09	1.00	0.73	0.27
C9H20O4S	224.1082	7.19	0.00	2.22	0.44
C7H5NO3	151.0269	2.89	1.00	0.71	0.43
C12H8N2O6	276.0382	7.60	1.00	0.67	0.50
C14H11NO3	241.0739	3.47	1.00	0.79	0.21
C17H16O5	300.0998	7.78	1.00	0.94	0.29
C9H6O2	146.0368	3.06	1.00	0.67	0.22
C7H4N2O5	196.0120	3.37	1.00	0.57	0.71
C8H6N2O2	162.0429	3.11	1.00	0.75	0.25
C12H9NO5	247.0481	4.12	1.00	0.75	0.42
C16H18OS2	290.0799	3.43	1.00	1.13	0.06
C8H13NO5	203.0794	2.51	0.60	1.63	0.63
C9H10O	134.0732	3.80	1.00	1.11	0.11
C11H12N2O4	236.0797	4.25	1.00	1.09	0.36
C6H7NO2	125.0477	2.92	1.00	1.17	0.33
C8H6O2	134.0368	2.95	1.00	0.75	0.25
C16H30O5S	334.1814	8.04	0.40	1.88	0.31
C6H10O8	210.0376	2.54	0.25	1.67	1.33
C9H8N2O5	224.0433	3.68	1.00	0.89	0.56
C8H10O4S	202.0300	3.14	1.00	1.25	0.50

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C5H8O	84 0575	1 67	1.00	1.60	0.20
651100	01.0575	1.07	1.00	1.00	0.20
C6H6O	94.0419	2.77	1.00	1.00	0.17
C11H18N2O10	338 0961	7 1 5	0.40	1 64	0.91
6111101(2010	1 54 0222	1.10	0.10	1.01	0.71
C/H4N2O3	164.0222	1.10	1.00	0.57	0.43
C18H28O3	292 2038	8 29	1.00	1 56	0.17
010112005	292.2030	1.00	1.00	1.50	0.17
C11H8O5S2	283.9813	1.09	1.00	0.73	0.45
C10H20N2O10S	360.0830	7.64	0.20	2.00	1.00
C1011201020105	500.0859	7.04	0.20	2.00	1.00
C8H16O6S	240.0668	4.03	0.17	2.00	0.75
COLLOC	212 0221	2 (0	1.00	0.90	0.7
C9H8O0	212.0321	5.09	1.00	0.89	0.07
C7H6O6S	217,9885	1.17	0.83	0.86	0.86
6/110005	211.0000		0.00	0.00	0.00
CITH2INO/S	311.1039	7.71	0.29	1.91	0.64
C19H32O9	404 2046	7.09	0.44	1 68	0.47
01)11320)	404.2040	7.05	0.44	1.00	0.47
C9H7NO	145.0528	0.90	1.00	0.78	0.11
C13H20O11	352 1006	0.60	0.36	1.54	0.85
0151120011	552.1000	0.00	0.50	1.54	0.05
C12H8O4	216.0423	5.80	1.00	0.67	0.33
C11U100155	412 0740	7.05	0.47	0.01	1.26
C111100155	413.9740	1.95	0.47	0.91	1.50
C6H6O2	110.0368	1.84	1.00	1.00	0.33
CIDUSNO7S	207 1250	8.00	0.14	2.00	0.59
C12H25N0/S	327.1352	8.09	0.14	2.08	0.58
C10H19NO9S	329 0781	1.43	0.22	1.90	0.90
GUIDOUG	152.01.02	1.15	0.22	1.90	1.00
C4H8O4S	152.0143	1.18	0.25	2.00	1.00
C11H6O3	186 0317	5 69	1.00	0.55	0.27
0111005	100.0517	5.09	1.00	0.55	0.27
C9H7NO7	241.0223	3.62	1.00	0.78	0.78
C6H7NO	100 0528	2 47	1.00	1 17	0.17
COILING	109.0528	2.47	1.00	1.1/	0.17
C8H4N2O10S	319.9587	0.10	0.80	0.50	1.25
C7111404	162 0802	2.74	0.25	2.00	0.57
C/H1404	162.0892	2.74	0.25	2.00	0.57
C13H20O3	224,1412	7.36	1.00	1.54	0.23
G11111002	174.0601	2.55	1.00	0.01	0.10
C11H1002	1/4.0681	3.55	1.00	0.91	0.18
C19H14O4	306 0892	7 73	1.00	0.74	0.21
017111404	500.0072	1.15	1.00	0.74	0.21
C7H10N2O5	202.0590	3.15	0.80	1.43	0.71
C9U16O2	144 1150	1.06	0.50	2.00	0.25
00111002	144.1150	4.00	0.50	2.00	0.25
C15H6O6S2	345.9606	0.81	1.00	0.40	0.40
C10117NO2	212 0426	2 16	1.00	0.59	0.25
CI2H/NO3	213.0420	3.40	1.00	0.58	0.25
C11H20N2O10	340.1118	8.15	0.30	1.82	0.91
61111201(2010	2101110	0.10	0.00	1.02	0.01
C15H24O13	412.1217	0.55	0.31	1.60	0.87
C12H21NO9S	355 0937	5 17	0.33	1 75	0.75
01211211(0)5	555.6757	5.17	0.55	1.75	0.75
C6H10O	98.0732	0.91	1.00	1.67	0.17
C7H6N2O5	198 0277	2.68	1.00	0.86	0.71
C/1101v205	190.0277	2.08	1.00	0.80	0.71
C12H20O6	260.1260	6.52	0.50	1.67	0.50
C10U11NO76	280.0256	5 (7	0.96	1 10	0.70
CI0HIINO/S	289.0256	5.67	0.86	1.10	0.70
C12H8O5	232 0372	3 4 9	1.00	0.67	0.42
61211005	232.0372	1.07	1.00	0.07	0.12
C9H8O5S	228.0092	1.97	1.00	0.89	0.56
C10H17NO8	279 0954	5 40	0.38	1 70	0.80
C1011171000	279.0934	5.40	0.50	1.70	0.00
C8H6N2O8	258.0124	7.55	0.88	0.75	1.00
C10U19N2O115	274 0621	7 67	0.27	1.80	1 10
C10H16N20115	574.0051	7.07	0.27	1.60	1.10
C9H8N2O4	208.0484	3.60	1.00	0.89	0.44
COLIONOC	227.0420	1.24	1.00	1.00	0.67
COHONOO	227.0430	4.34	1.00	1.00	0.07
C13H26O4	246,1831	7.07	0.25	2.00	0.31
C17U22O2	274 15 (0	7.00	1.00	1.20	0.10
CI/H22O3	2/4.1309	/.00	1.00	1.29	0.18
C14H8O3	224.0473	3.30	1.00	0.57	0.21
C1011907	240.0270	2 01	1.00	0.00	0.70
CIUH8U/	240.0270	3.81	1.00	0.80	0.70
C9H8O5S	228.0092	2.57	1.00	0.89	0.56
COLLIZNOOS	215.0024	4 70	0.00	1.00	1.00
C9H1/INU98	313.0624	4.79	0.22	1.89	1.00
C14H14O2	214,0994	8.11	1.00	1.00	0.14
011005	106.0072	- 40	1.00	0.00	0.57
C9H8O5	196.0372	5.40	1.00	0.89	0.56
C8H5NO8	243 0015	4 14	0.88	0.63	1.00
	2-13.0013	T.1T	0.00	0.05	1.00
C6H8N2O7	220.0332	0.68	0.57	1.33	1.17
C10H17NO7S	295 0726	3 20	0.43	1 70	0.70
	275.0720	3.47	0.+5	1.70	0.70
C13H20O7	288.1209	6.22	0.57	1.54	0.54
C15H220482	220 0050	2 70	1.00	1 47	0.27
C13H22O452	330.0939	2.70	1.00	1.4/	0.27
C7H12O	112,0888	2.64	1.00	1.71	0.14
01011120	112.0000	2.07	1.00	0.77	0.17
C18H12O4	292.0736	7.86	1.00	0.67	0.22
C5H4O2S	127 9932	1 53	1.00	0.80	0.40
0114025	121.7732	1.55	1.00	0.00	0.40
C11H17NO9	307.0903	3.19	0.44	1.55	0.82
C14H20O3	236 1412	7 0/	1.00	1 / 2	0.21
014112003	230.1412	1.74	1.00	1.45	0.21
C16H8O4	264.0423	7.87	1.00	0.50	0.25
CIGUZINOOS	207 1770	0 11	0.25	1.0.4	0.50
C10H31N085	397.1770	0.21	0.23	1.94	0.50
C8H9NO6	215.0430	1.50	0.83	1.13	0.75
CTUIINCOS	205 0155	1.00	0.22	1 57	1.00
C/HIINO9S	285.0155	1.69	0.33	1.57	1.29
C14H7NO2	221.0477	7.65	1.00	0.50	0.14
01012407	274 2205	0.00	0.40	1.70	0.27
<u>C19H34</u> O7	374.2305	8.26	0.43	1.79	0.37

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C15H15NO4	273.1001	8.28	1.00	1.00	0.27
C11H6O4	202.0266	2.79	1.00	0.55	0.36
C11H11NO6	253.0586	6.95	1.00	1.00	0.55
C8H7NO6	213.0273	5.35	1.00	0.88	0.75
C6H6N2O7	218.0175	0.69	0.71	1.00	1.17
C12H21N3O3	255.1583	4.43	1.00	1.75	0.25
C8H18O4S	210.0926	6.37	0.00	2.25	0.50
C12H8O8	280.0219	1.27	1.00	0.67	0.67
C/H9NO2	139.0633	2.50	1.00	1.29	0.29
C12H14O3	258.0841	2.00	1.00	1.17	0.42
C12H12NO5	240.1407	4.19	1.00	1.05	0.42
C6H3NO7	200 9910	1.03	0.86	0.50	1.17
C8H6N2O	146 0480	2 99	1.00	0.50	0.13
C8H8N2O3	180.0535	2.52	1.00	1.00	0.38
C7H7NO	121.0528	2.64	1.00	1.00	0.14
C8H7NO2	149.0477	3.79	1.00	0.88	0.25
C15H6O5S2	329.9657	1.07	1.00	0.40	0.33
C6H12O4	148.0736	0.93	0.25	2.00	0.67
C18H30O9	390.1890	6.56	0.44	1.67	0.50
C9H14N2O5S	262.0623	7.84	0.80	1.56	0.56
C7H7N3O2	165.0538	6.52	1.00	1.00	0.29
C8H16O5	192.0998	0.61	0.20	2.00	0.63
C10H7NO4	205.0375	5.86	1.00	0.70	0.40
C13H27NO7S	341.1508	8.25	0.14	2.08	0.54
C9H14N2O5S	262.0623	8.12	0.80	1.56	0.56
C10H8N2O3	204.0535	5.57	1.00	0.80	0.30
C13H15N04	249.1001	7.94	1.00	1.15	0.31
C21H300/S	426.1712	/.61	1.00	1.43	0.33
C10H12NO0S	149.0477	0.01	1.00	0.88	0.25
C15H26O3	254 1882	2.30	1.00	1.30	0.90
C10H12003	244 0583	2.60	0.71	1.73	0.20
C15H10O4	254 0579	2.00 4.46	1.00	0.67	0.70
C16H16N2O5S2	380.0501	4 68	1.00	1.00	0.31
C9H6O8S	273.9783	2.50	0.88	0.67	0.89
C9H16N2O6S	280.0729	7.74	0.50	1.78	0.67
C10H8O8S	287.9940	1.45	0.88	0.80	0.80
C13H6O5	242.0215	4.65	1.00	0.46	0.38
C9H13NO4	199.0845	2.57	1.00	1.44	0.44
C17H32O5	316.2250	8.14	0.40	1.88	0.29
C15H6O5S2	329.9657	1.90	1.00	0.40	0.33
C14H16O5	264.0998	7.42	1.00	1.14	0.36
C10H7NO2	173.0477	3.48	1.00	0.70	0.20
C15H15N03	257.1052	8.38	1.00	1.00	0.20
CI3H25NU/S	339.1352	8.18	0.29	1.92	0.54
C5H1002	102.0681	1.68	0.50	2.00	0.40
C11H12N2O2	204.0800	7.59	1.00	1.75	0.75
C18H16O7	344 0896	7 32	1.00	0.89	0.18
C6H11NO8S	257 0205	2.80	0.25	1.83	1.33
C12H22O7	278.1366	2.75	0.29	1.83	0.58
C17H8O5	292.0372	3.98	1.00	0.47	0.29
C14H11NO3S	273.0460	1.25	1.00	0.79	0.21
C18H8N4O6S2	439.9885	1.68	1.00	0.44	0.33
C12H10O2	186.0681	5.65	1.00	0.83	0.17
C6H11NO8S	257.0205	1.74	0.25	1.83	1.33
C13H10O2	198.0681	5.02	1.00	0.77	0.15
C11H20O6	248.1260	1.67	0.33	1.82	0.55
C9H11NO2	165.0790	3.21	1.00	1.22	0.22
C13H24O6	276.1573	3.10	0.33	1.85	0.46
C10H13NO4	211.0845	5.35	1.00	1.30	0.40
C13H26N2O10	370.1587	8.18	0.20	2.00	0.77
C8H15NO7S	269.0569	4.13	0.29	1.88	0.88
C9H6U3	162.0317	1.05	1.00	0.6/	0.33
C01100N4US	242.0202	0.89	1.00	0.33	0.09
C4H8048	152.0575	5.55 7 8/	0.25	2 00	1.00
C13H23N08S	353 1144	7.39	0.38	1.77	0.62
C9H8N4O6S	300.0165	5.04	1.00	0.89	0.67
		- /			

C3H5N04S         150.9939         0.51         0.50         1.67         1.83           CTHNNO         123.0684         0.95         1.00         0.80         0.27           C1SH12O4         268.1675         4.08         1.00         0.60         0.77           C13H2NOTS         337.1195         7.99         0.43         1.77         0.43           C1H1INO9S         226.0630         5.27         1.00         0.71         0.22           C1H1INO2         155.0790         2.87         1.03         0.86         0.86           C1H1INO2         155.0790         2.87         1.00         0.71         0.21           CTHIDN2O4         188.0797         0.99         0.75         1.71         0.57           CTHSINO3         130.0457         7.98         1.00         0.89         0.56           CTH60         196.0372         4.10         1.00         0.71         0.43           CHH1005         2.88.0528         5.01         1.00         0.87         1.00           C1H12N204         122.0028         5.01         1.00         0.71         0.43           C1H1005         2.88.0528         7.21         1.00         0.71 <t< th=""><th></th><th></th><th></th><th></th><th></th><th></th></t<>						
C7H9NO         123,0084         0.95         1.00         1.29         0.14           C15H1204         256,0736         4.35         1.00         0.75         0.47           C15H12404         268,1757         4.08         1.00         0.75         0.42           C13H12NO7S         337,1195         7.99         0.43         1.77         1.02           C1H11NO2S         2826,0530         5.27         1.00         0.71         1.021           C1H1003         226,0630         5.27         1.00         0.71         0.21           C1H1003         126,0750         2.87         1.00         1.16         0.72           C1H1003         126,0700         2.87         1.00         0.71         0.32           C1H12N204         188,0797         0.99         0.75         1.71         0.57           C1H12N204         186,0172         4.10         1.00         0.71         0.33           C1H14N05         258,0528         5.01         1.00         0.71         0.36           C1H11N2012S         360,0524         4.40         2.55         1.60         0.71         0.36           C1H14N05         258,0528         7.21         1.00	C3H5NO4S	150 9939	0.51	0.50	1.67	1.33
C. HYNO         12.308-4         0.35         1.00         1.29         0.12           C. ISH12O4         226.0736         4.33         1.00         1.60         0.27           C. ISH12NOTS         337.1195         7.99         0.43         1.77         0.42           C. HHINOS         237.0185         0.87         0.33         1.57         1.29           C. HHINOS         226.0155         2.78         0.33         1.66         0.57           C. HHINOS         226.0157         0.87         0.33         0.86         0.86           C. HHINOS         158.0790         2.87         1.00         1.22         0.22           C. CHINOS         138.0797         0.99         0.75         1.71         0.43           C. CHINOS         136.0772         4.10         1.00         0.89         0.56           C. CHINOS         136.0772         4.10         1.00         0.89         0.56           C. CHINOS         258.0528         5.01         1.00         0.71         0.36           C. CHHINOS         258.0528         5.01         1.00         0.86         0.71         0.36           C. CHHINOS         258.0528         5.01         1.	CTUONO	102.0694	0.05	1.00	1.20	0.14
C15H12O4         268,1675         4.08         1.00         0.80         0.27           C15H2O4         268,1675         4.08         1.00         0.75         0.42           C13H2NOTS         337,1195         7.99         0.43         1.77         0.54           C1H1INO9S         285,0155         2.78         0.33         1.57         1.02           C1H1INO2         165,0790         2.87         1.00         0.71         0.21           C1H1INO2         155,0790         2.87         1.00         1.71         0.52           C1H1INO2         156,0790         2.87         1.00         0.71         0.43           C1H1INO2         156,0790         2.87         1.00         0.71         0.43           C1H11NO2         156,0790         0.97         1.00         0.71         0.43           C1H11NO2         28,0528         5.01         1.00         0.71         0.36           C1H11NO15         28,0528         7.21         1.00         0.71         0.36           C1H11NO2         28,0528         7.21         1.00         0.86         0.14           C1H11NO3         24,0934         1.67         1.00         0.86 <td< td=""><td>C/H9NO</td><td>123.0684</td><td>0.95</td><td>1.00</td><td>1.29</td><td>0.14</td></td<>	C/H9NO	123.0684	0.95	1.00	1.29	0.14
C15H24O4         268.1675         4.08         1.00         1.60         0.27           C13H23NOTS         337.1195         7.99         0.43         1.77         0.43           CTH11NOS         225.0155         2.78         0.33         1.57         1.29           CHH10O3         226.0630         5.27         1.00         0.71         0.21           CH606S         217.988         0.87         0.83         0.86         0.86           CH11NO2         165.0790         2.87         1.00         1.10         0.75           C1912205         330.1467         7.98         1.00         0.71         0.43           CH805         196.0372         4.10         1.00         0.71         0.43           CH41005         238.0528         5.01         1.00         0.71         0.32           C14H1005         238.0528         7.21         1.00         0.67         0.21	C15H12O4	256.0736	4.35	1.00	0.80	0.27
C 12H5NO5         247,0481         7.44         1.00         1.07         0.42           C 13H2NO75         337,1195         7.99         0.43         1.77         0.13           C THIINO9S         226,0650         5.27         1.00         0.71         0.22           C H4000S         217,9885         0.87         0.83         0.86         0.86           C PHIINO2         165,0790         2.87         1.00         1.22         0.22           C THISNO3         188,0797         0.99         0.75         1.71         0.43           C CPHISNO3         182,9990         0.97         1.00         0.71         0.43           C CHHOOS         196,0372         4.10         1.00         0.89         0.55           C THINO5         258,0528         5.01         1.00         0.71         0.36           C CHHINO5         258,0528         7.21         1.00         0.71 </td <td>C15H24O4</td> <td>268 1675</td> <td>4.08</td> <td>1.00</td> <td>1.60</td> <td>0.27</td>	C15H24O4	268 1675	4.08	1.00	1.60	0.27
C12H9R05         24/.0481         7.41         1.00         0.75         0.42           C1H1IN098         285.0155         2.78         0.33         1.57         1.29           C14H1003         226.0630         5.27         1.00         0.71         0.21           CTH606S         217.9885         0.87         0.83         0.86         0.86           CH11N02         165.0790         2.87         1.00         1.12         0.22           CTH12N204         188.0797         0.99         0.75         1.71         0.57           C19H2D35         330.1467         7.98         1.00         1.16         0.26           CTHSN03S         182.9990         0.97         1.00         0.71         0.43           CH4H005         126.01         1.60.01         0.86         0.11         0.05           C14H1005         258.0528         7.21         1.00         0.71         0.36           C14H1005         258.0528         7.21         1.00         0.73         0.20           C14H1005         258.0528         7.21         1.00         0.71         0.36           C14H1005         258.0528         7.21         1.00         0.71         <	612404	200.1075	4.00	1.00	1.00	0.27
C13H23NO7S         337.1195         7.99         0.43         1.77         0.54           C7H11NO9S         228.0650         5.27         1.00         0.71         0.21           CH1606S         217.9885         0.87         0.83         0.86         0.86           C9H11NO2         165.0790         2.87         1.00         1.22         0.22           C7H12N2O4         188.0777         0.99         0.75         1.71         0.57           C19H22O5         330.1467         7.98         1.00         0.16         0.43           C7HRO         106.0419         2.63         1.00         0.86         0.85           C7H6O         106.0419         2.63         1.00         0.86         0.14           C14410O5         258.0528         5.01         1.00         0.71         0.36           C1411NO25         258.0528         7.21         1.00         0.86         0.14           C1411NO25         258.0528         7.21         1.00         0.86         0.14           C1411NO25         258.0528         7.21         1.00         0.86         0.14           C1411NO25         258.0528         7.21         1.00         0.80	C12H9N05	247.0481	7.41	1.00	0.75	0.42
C7H11N095         285(0155         2.78         0.33         1.57         1.29           C1H61003         226(053)         5.27         1.00         0.71         0.21           C7H61068         217,9885         0.87         1.03         0.86         0.86           C7H12N204         188.0797         0.99         0.75         1.71         0.57           C19H12N05         330.1467         7.98         1.00         1.16         0.26           C7H5N03S         182.9990         0.97         1.00         0.71         0.43           C9H80C5         196.0372         4.10         1.00         0.88         0.44           C6H406         172.0008         0.68         0.83         0.67         1.00           C14H1005         258.0528         7.21         1.00         0.71         0.33           C14H1005         258.0528         4.69         1.00         0.86         0.57           C15H1403         242.0943         8.21         1.00         0.71         0.33           C15H14005         258.0528         7.21         1.00         0.73         0.20           C15H14005         258.0528         4.69         1.00         0.66	C13H23NO7S	337.1195	7.99	0.43	1.77	0.54
C (1111003) 226,0630 5.27 1.00 0.71 0.21 C7H606S 217.9885 0.87 0.83 0.86 0.86 C9H11N02 165,0790 0.87 0.89 0.75 1.71 0.57 C19H2205 330.1467 7.98 1.00 1.16 0.25 C7H10N3S 182,9990 0.97 1.00 0.71 0.43 C9H805 196,0372 4.10 1.00 0.89 0.55 C7H60 106,0419 2.63 1.00 0.86 0.44 C6H406 172,0008 0.68 0.83 0.67 1.00 C14H1005 258,0528 5.01 1.00 0.71 0.36 C10H18N20125 390,0580 4.44 0.25 1.80 1.20 C14H1005 258,0528 7.21 1.00 0.86 0.57 C19H220 1.34,0480 2.85 1.00 0.86 0.57 C19H220 1.34,0480 2.85 1.00 0.86 0.57 C19H8N20125 243,0354 1.67 1.00 0.69 0.15 C19H18N22 243,0354 1.67 1.00 0.69 0.15 C19H18N25 243,0354 1.67 1.00 0.63 0.20 C13H19025 243,0354 1.67 1.00 0.63 0.20 C13H19025 243,0354 1.67 1.00 0.63 0.20 C13H19025 243,0354 1.67 1.00 0.63 0.20 C13H1804 2242,0735 6.85 1.00 1.03 0.31 0.19 C18H180552 367,9813 3.83 1.00 0.44 0.22 C19H1805 210,056 2.74 0.66 1.53 0.67 C19H1805 210,056 2.74 0.66 1.53 0.67 C19H1805 210,056 2.74 0.66 1.53 0.67 C19H1805 210,0528 6.62 1.00 1.00 0.50 C29H3N06 227,0430 6.85 1.00 1.00 0.50 C29H3N06 227,0430 6.85 1.00 1.00 0.57 0.43 C13H1902 102,0681 0.81 0.50 2.00 0.44 C3H1002 102,0681 0.81 0.50 2.00 0.44 C3H1002 210,0528 6.62 1.00 1.00 0.57 0.43 C13H1204 326,2301 8.31 1.00 1.68 0.22 C13H1004 326,2301 8.31 1.00 1.61 0.22 C13H1004 288,1362 7.38 1.00 0.17 0.22 C13H1008 326,0096 5.04 1.00 0.57 0.43 C13H2004 288,1362 8.14 1.00 1.54 0.22 C13H1008 326,0096 5.04 1.00 0.57 0.43 C13H2004 288,1362 8.14 1.00 1.54 0.23 C17H2004 288,1362 8.14 1.00 0.57 0.43 C3H40A0 116,010 0.36 0.50 1.33 1.33 C4H40A 116,0110 0.36 0.50 1.33 1.33 C4H40A 116,0110 0.36 0.50 1.50 1.30 C4H40A 116,0110 0.36 0.50 1.50 1.50 C1H120A 189,0375 4.11 1.00 1.08 0.57 C1H120A 189,0375 4.11 1.00 1.46 0.50	C7H11NO0S	285 0155	2 78	0.22	1 57	1 20
C14H10O3         226.0630         5.27         1.00         0.71         0.21           C7H1DO2         165.0790         2.87         1.00         1.22         0.22           C7H12N2O4         188.0797         0.99         0.75         1.71         0.57           C19H22O5         330.1467         7.98         1.00         0.71         0.43           CHISNOS         196.0372         4.10         1.00         0.89         0.56           C7H6O         106.0419         2.63         1.00         0.87         1.03           C14H10O5         258.0528         5.01         1.00         0.71         0.36           C14H1NO2         258.0528         7.21         1.00         0.76         0.36           C14H1NO2         134.0480         2.85         1.00         0.86         0.14           C1HINNO2         134.0480         2.85         1.00         0.86         0.14           C1HINNO2         134.0480         2.85         1.00         0.86         0.15           C1HINNO2         134.0480         2.85         1.00         0.86         0.15           C1HINNO2         134.0480         2.85         1.00         0.67         0	C/HINO95	285.0155	2.78	0.55	1.57	1.29
C7H606S         217.9885         0.87         0.83         0.86         0.085           C7H12N204         188.0797         0.99         0.75         1.71         0.57           C19H2205         330.1467         7.98         1.00         0.16         0.22           C7H1SN03S         182.9990         0.97         1.00         0.71         0.43           C7H60         106.0419         2.63         1.00         0.86         0.14           C6H406         172.0008         0.68         0.83         0.67         1.00           C14H1005         258.0528         5.01         1.00         0.71         0.35           C1H18X2012S         390.0580         4.44         0.25         1.80         1.20           C1H11005         258.0528         7.21         1.00         0.71         0.35           C1H1403         242.0943         8.21         1.00         0.86         0.57           C15H1403         242.0943         8.21         1.00         0.63         0.20           C15H1803         290.990         3.98         1.00         0.61         0.33         0.67           C15H1804         262.1205         8.05         1.00 <td< td=""><td>C14H10O3</td><td>226.0630</td><td>5.27</td><td>1.00</td><td>0.71</td><td>0.21</td></td<>	C14H10O3	226.0630	5.27	1.00	0.71	0.21
C9H11NO2         165.0790         2.87         1.00         1.22         0.22           C7H12N2O4         188.0797         0.99         0.75         1.71         0.57           C19H2ZO5         330.1467         7.98         1.00         0.71         0.43           C7HRO3S         182.9990         0.97         1.00         0.71         0.43           C7HRO         106.0419         2.63         1.00         0.86         0.44           C6H406         172.0008         0.68         0.83         0.67         1.00           C14H1005         258.0528         7.21         1.00         0.71         0.36           C1H1N2O122         390.0550         4.44         0.25         1.80         1.20           C14H1005         258.0528         7.21         1.00         0.71         0.36           C1H1N2O12         124.0334         1.67         1.00         0.69         0.15           C15H1A03         242.0943         8.21         1.00         0.48         0.22           C15H1A024         262.1205         6.85         1.00         1.06         0.67         0.22           C15H1A03         240.043         6.81         1.00 <td< td=""><td>C7H6O6S</td><td>217 9885</td><td>0.87</td><td>0.83</td><td>0.86</td><td>0.86</td></td<>	C7H6O6S	217 9885	0.87	0.83	0.86	0.86
CFH INO2         10.0         1.22         0.23           CTH INO2         188.077         0.99         0.75         1.71         0.57           C19H22O5         330.1467         7.98         1.00         1.16         0.26           CHISOS         196.0372         4.10         1.00         0.89         0.55           CTH6O         106.0419         2.63         1.00         0.86         0.14           C6H4O6         172.0008         0.68         0.83         0.67         1.00           C14H10O5         258.0528         5.01         1.00         0.71         0.35           C10H18N2012S         390.0580         4.44         0.25         1.80         1.20           C14H10O5         258.0528         7.21         1.00         0.86         0.14           CTH6N20         13.40480         2.85         1.00         0.86         0.14           C14H10O5         258.0528         7.21         1.00         0.93         0.20           C15H14O3         242.0943         8.21         1.00         0.86         0.15           C16H5N03S         290.990         3.98         1.00         0.67         0.22           C15H1003<	COLLINO2	165.0700	0.07	1.00	1.00	0.00
C7H12N204         188.0797         0.99         0.75         1.71         0.57           C19H205         330.1467         7.98         1.00         0.71         0.43           C9H805         196.0372         4.10         1.00         0.89         0.55           C7H60         106.0419         2.63         1.00         0.71         0.56           C14406         172.0008         0.68         0.83         0.67         1.00           C1441005         258.0528         7.21         1.00         0.71         0.35           C14H1005         258.0528         7.21         1.00         0.71         0.36           C14H1005         258.0528         7.21         1.00         0.71         0.36           C15H1403         242.0943         8.21         1.00         0.86         0.57           C15H1403         242.0943         8.21         1.00         0.86         0.77           C15H1403         242.0943         8.21         1.00         0.44         0.22           C15H1403         242.0943         8.21         1.00         0.67         0.22           C15H1403         242.0943         8.21         1.00         0.67         0.22	C9HIINO2	165.0790	2.87	1.00	1.22	0.22
C19H2205         330.1467         7.98         1.00         1.16         0.25           C7HSN035         182.9990         0.97         1.00         0.71         0.43           C9HR05         196.0372         4.10         1.00         0.89         0.36           C7HGO         106.0419         2.63         1.00         0.86         0.14           C6H406         172.0008         0.68         0.83         0.67         1.00           C10H1RN20125         390.0580         4.44         0.25         1.80         1.20           C14H1005         258.0528         7.21         1.00         0.71         0.36           C7H6N204         182.0328         4.69         1.00         0.86         0.14           C1SH1403         242.043         8.21         1.00         0.93         0.20           C1SH1403         242.043         8.21         1.00         0.44         0.28           C1SH1403         242.043         8.21         1.00         0.44         0.28           C1SH180552         367.9813         3.83         1.00         0.47         0.22           C1SH180652         21.055         8.05         1.00         1.20         0	C7H12N2O4	188.0797	0.99	0.75	1.71	0.57
CH1220         J301400         1.93         1.00         0.71         0.43           CH8003S         196,0372         4.10         1.00         0.86         0.41           CH4006         172,0008         0.68         0.83         0.67         1.00           C14H1005         258,0528         5.01         1.00         0.71         0.36           C10H18N2012S         390,0580         4.44         0.25         1.80         1.20           C14H1005         258,0528         7.21         1.00         0.71         0.36           CTH6N204         182,0328         4.69         1.00         0.86         0.14           CTH6N204         182,0328         4.69         1.00         0.86         0.14           C18H1403         242,0943         8.21         1.00         0.69         0.57           C16H15N03S         290,9990         3.98         1.00         0.67         0.22           C18H1803S2         367,9813         3.83         1.00         0.44         0.28           C18H1803S2         367,9813         3.83         1.00         1.20         0.27           C18H1804         262,1205         8.05         1.00         1.60	C10H22O5	330 1467	7.08	1.00	1 16	0.26
C/HSNOSIS         182.9990         0.97         1.00         0.11         0.43           C9H8OS         196.0372         4.10         1.00         0.89         0.56           C7H6O         106.0419         2.63         1.00         0.86         0.44           C6H4D6         172.0008         0.68         0.83         0.67         1.00           C14H10O5         258.0528         7.21         1.00         0.71         0.36           C1HN2O4         184.0480         2.85         1.00         0.86         0.57           C15H1403         242.0943         8.21         1.00         0.93         0.20           C13H18024         182.0328         4.69         1.00         0.69         0.15           C15H1403         242.0943         8.21         1.00         0.43         0.29           C15H18022         367.9813         3.83         1.00         0.44         0.28         0.77           C15H1804         262.1205         8.05         1.00         1.00         0.67         0.22           C15H1804         262.1205         8.05         1.00         1.20         0.47           C15H1804         262.1205         8.05         1.	01/11/2203	330.1407	7.90	1.00	1.10	0.20
C9H805         196.0372         4.10         1.00         0.86         0.45           C1H60         106.0419         2.63         1.00         0.86         0.14           C6H406         172.0008         0.68         0.83         0.67         1.00           C10H11N2012S         390.0580         4.44         0.25         1.80         1.20           C1H41005         258.0528         7.21         1.00         0.71         0.36           CTH6N20         134.0480         2.85         1.00         0.86         0.14           CTH6N204         182.0328         4.69         1.00         0.86         0.14           C13H9N02S         243.0354         1.67         1.00         0.93         0.20           C13H9N02S         243.0354         1.67         1.00         0.44         0.28           C18H1204         292.0736         6.85         1.00         0.44         0.28           C18H12041         262.1205         8.05         1.00         1.20         0.27           C18H12041         262.1205         8.05         1.00         1.00         0.50           C18H12041         262.1205         8.05         1.00         1.20	C/H5NO3S	182.9990	0.97	1.00	0.71	0.43
CTH60         106.0419         2.63         1.00         0.66         0.14           C6H406         172.0008         0.68         0.83         0.67         1.00           C14H1005         258.0528         5.01         1.00         0.71         0.36           C14H1005         258.0528         7.21         1.00         0.71         0.35           C7H6N20         134.0480         2.85         1.00         0.86         0.57           C15H1403         242.0943         8.21         1.00         0.93         0.20           C15H1403         242.0943         8.21         1.00         0.66         0.57           C15H18035         290.9990         3.98         1.00         0.47         0.22           C18H80352         367.9813         3.83         1.00         0.44         0.22         0.27           C18H804         262.1205         8.05         1.00         1.00         0.67         0.22           C18H80552         267.0430         6.85         1.00         1.20         0.27           C18H80552         366.01056         2.74         0.60         1.33         0.67         0.22           C19H9N06         227.0430 <td< td=""><td>C9H8O5</td><td>196.0372</td><td>4.10</td><td>1.00</td><td>0.89</td><td>0.56</td></td<>	C9H8O5	196.0372	4.10	1.00	0.89	0.56
C) H00         100,01 j         2.03         1.00         0.38         0.14           C6H406         172.0008         0.68         0.83         0.67         1.00           C10H1RN2012S         390.0580         4.44         0.25         1.80         1.20           C14H1005         258.0528         7.21         1.00         0.71         0.36           CTH6N20         134.0480         2.85         1.00         0.86         0.14           C15H1403         242.0943         8.21         1.00         0.93         0.20           C13H19N2S         243.0354         1.67         1.00         0.69         0.15           C16H5N03S         290.9990         3.98         1.00         0.31         0.44         0.28           C18H1204         292.0736         6.85         1.00         0.67         0.22           C15H12010         360.1056         2.74         0.60         1.33         0.67           C15H1407         262.1205         8.05         1.00         0.67         0.27           C15H1407         366.740         3.73         1.00         1.60         0.20           C15H1407         366.740         3.73         1.00         <	071160	106.0410	2.62	1.00	0.96	0.14
C6H406         172,0008         0.68         0.83         0.67         1.00           C14H1005         258,0528         5.01         1.00         0.71         0.53           C10H18N2012S         390,0580         4.44         0.25         1.80         1.20           C14H1005         258,0528         7.21         1.00         0.71         0.53           CTH6N204         182,0328         4.69         1.00         0.86         0.14           CTH6N204         182,0328         4.69         1.00         0.86         0.57           C15H1403         242,0943         8.21         1.00         0.93         0.20           C13H9N025         243,0354         1.67         1.00         0.69         0.55           C16H1503S         290,9990         3.98         1.00         0.67         0.22           C18H12041         292,0736         6.85         1.00         1.20         0.27           C18H1804         262,1205         8.05         1.00         1.20         0.27           C15H1804         262,1205         8.05         1.00         1.00         0.55           C27H2010         366,0740         3.73         1.00         0.67	C/H00	100.0419	2.03	1.00	0.80	0.14
C14H1005         258.0528         5.01         1.00         0.71         0.56           C10H18N2012S         390.0580         4.44         0.25         1.80         1.20           C14H1005         258.0528         7.21         1.00         0.71         0.36           C7H6N2O         134.0480         2.85         1.00         0.86         0.17           C1SH1403         242.0943         8.21         1.00         0.93         0.20           C13H9N02S         243.0354         1.67         1.00         0.69         0.15           C16H5N03S         290.9990         3.98         1.00         0.67         0.22           C18H8OSS2         367.9813         3.83         1.00         0.67         0.22           C15H20010         360.1056         2.74         0.60         1.33         0.67           C15H1804         262.1205         8.05         1.00         1.20         0.27           C15H1804         262.1205         8.05         1.00         1.60         0.20           C19H9N06         27.0430         8.31         1.00         1.60         0.20           C15H1804         262.1205         8.05         1.00         0.67	C6H4O6	172.0008	0.68	0.83	0.67	1.00
C10H18N2012S         390.0580         4.44         0.25         1.80         1.20           C14H1005         258.0528         7.21         1.00         0.71         0.36           C7H6N2O         134.0480         2.85         1.00         0.86         0.14           C7H6N2O4         182.0328         4.69         1.00         0.86         0.57           C15H1403         242.0943         8.21         1.00         0.93         0.20           C13H9NO2S         243.0354         1.67         1.00         0.69         0.15           C16H1204         292.0736         6.85         1.00         0.44         0.28           C18H1204         292.0736         6.85         1.00         1.00         0.67           C18H1804         262.105         8.05         1.00         1.00         0.67           C15H1804         262.105         8.05         1.00         1.00         0.50           C15H1407         306.0740         3.73         1.00         1.60         0.20           C15H1407         306.0740         3.73         1.00         1.67         0.17           C15H1407         306.0740         3.73         1.00         1.67	C14H10O5	258.0528	5.01	1.00	0.71	0.36
C10116/C20125         390.080         4.44         0.23         1.80         1.62           CTH6N201         134.0480         2.85         1.00         0.86         0.17           CTI6N201         134.0480         2.85         1.00         0.86         0.17           C1SH1403         242.0943         8.21         1.00         0.93         0.20           C13H9N02S         243.0354         1.67         1.00         0.69         0.15           C16H5N03S         290.9990         3.98         1.00         0.44         0.22           C18H8OSS2         367.9813         3.83         1.00         0.67         0.22           C15H20010         360.1056         2.74         0.60         1.33         0.67           C15H1804         262.1205         8.05         1.00         1.20         0.27           C15H1407         306.0740         3.73         1.00         0.67         0.17           C1H1407         306.0740         3.73         1.00         1.60         0.20           C1H1407         306.0740         3.73         1.00         1.60         0.20           C1H14024         236.2301         8.31         1.00         0.67	CIOLINNOCIO	200.0590	4.44	0.25	1.90	1.20
C14H1005         258.0528         7.21         1.00         0.71         0.36           C7H6N2O         134.0480         2.85         1.00         0.86         0.57           C15H14O3         242.0943         8.21         1.00         0.93         0.20           C13H9NO2S         243.0354         1.67         1.00         0.69         0.15           C16H5NO3S         290.9990         3.98         1.00         0.41         0.22           C18H0SS2         367.9813         3.83         1.00         0.44         0.22           C18H0SS2         367.9813         3.83         1.00         0.67         0.22           C15H20010         360.1056         2.74         0.60         1.33         0.67           C19H9N06         227.0430         6.85         1.00         1.00         0.67           C15H1804         262.1205         8.05         1.00         1.60         0.20           C15H1407         366.0740         3.73         1.00         0.67         0.77           C15H1407         266.42         1.00         1.60         0.20         C17H2004         288.1362         7.38         1.00         1.67         0.43         C1H4N0S2	C10H18N20125	390.0380	4.44	0.25	1.60	1.20
C7H6N2O         134.0480         2.85         1.00         0.86         0.57           C15H14O3         242.0943         8.21         1.00         0.93         0.20           C13H9NO2S         243.0354         1.67         1.00         0.69         0.15           C16H5NO3S         290.990         3.98         1.00         0.44         0.28           C18H12O4         292.0736         6.85         1.00         0.67         0.22           C15H2O010         360.1056         2.74         0.60         1.33         0.67           C15H18O4         262.105         8.05         1.00         1.00         0.67           C15H14O7         306.0740         3.73         1.00         0.93         0.47           C5H1002         102.0681         0.81         0.50         2.00         0.40           C16H1005         210.0528         6.62         1.00         1.60         0.20           C17H2O04         288.1362         7.38         1.00         1.60         0.20           C17H2O04         288.1362         7.38         1.00         0.67         0.22           C13H10N438         326.096         5.04         1.00         0.77         <	C14H10O5	258.0528	7.21	1.00	0.71	0.36
CTH6N204         182.0328         4.69         1.00         0.86         0.57           C15H1403         242.0943         8.21         1.00         0.93         0.20           C13H9N02S         243.0354         1.67         1.00         0.69         0.15           C16H5N03S         290.9990         3.98         1.00         0.31         0.19           C18H805S2         367.9813         3.83         1.00         0.44         0.28           C18H1204         292.0736         6.85         1.00         1.00         0.67           C15H120010         360.1056         2.74         0.60         1.33         0.67           C15H1804         262.1205         8.05         1.00         1.00         0.67           C15H1804         262.1205         8.05         1.00         1.00         0.50           C1H1407         306.0740         3.73         1.00         1.60         0.20           C1H1407         306.0740         3.73         1.00         1.60         0.20           C1H1407         306.0740         3.73         1.00         1.60         0.20           C1H14003         241.052         1.03         1.00         0.67	C7H6N2O	134 0480	2.85	1.00	0.86	0.14
C (FB) 8204         182,0323         4,09         1,00         0,88         0,20           C (13H9NO2S         243,0354         1,67         1,00         0,69         0,15           C (16HSNO3S         290,9990         3.98         1,00         0,31         0,19           C (18HSO5S2         367,9813         3.83         1,00         0,44         0,28           C (18H12O4         292,0736         6,85         1,00         0,67         0,22           C (15H20010         360,1056         2.74         0,60         1,33         0,67           C (15H18O4         262,1205         8,05         1,00         1,20         0,27           C (15H14O7         306,0740         3,73         1,00         0,93         0,47           C (1H10O5         210,0528         6,62         1,00         1,00         0,50           C (20H3204         366,2301         8,31         1,00         1,66         0,22           C (1H2O04         288,1362         7,38         1,00         1,18         0,24           C (14HXO52         211,9827         1,09         1,00         0,67         0,22           C (13H100K8         326,0096         5,04         1,00	CTUCNDOA	192.0229	4.00	1.00	0.00	0.57
C13H1403         242.0943         8.21         1.00         0.93         0.23           C13H19N02S         243.0354         1.67         1.00         0.69         0.15           C16H5N03S         290.9990         3.98         1.00         0.31         0.19           C18H18O5S2         367.9813         3.83         1.00         0.67         0.22           C15H2O010         360.1056         2.74         0.60         1.33         0.67           C15H18O4         262.1205         8.05         1.00         1.20         0.27           C15H18O4         262.1205         8.05         1.00         1.20         0.27           C15H18O4         262.1205         8.05         1.00         1.20         0.27           C15H14O7         306.0740         3.73         1.00         0.93         0.47           C1H10O5         210.0528         6.62         1.00         1.60         0.20           C1H12O04         288.1362         7.38         1.00         1.68         0.24           CH41N4OS2         211.9827         1.09         1.00         0.67         0.43           C13H2O03         242.1412         4.74         1.00         1.54	C/H6N2O4	182.0328	4.69	1.00	0.86	0.57
C13H9NO2S         243.0354         1.67         1.00         0.69         0.15           C16H5NO3S         290.9990         3.98         1.00         0.31         0.19           C18H8O5S2         367.9813         3.83         1.00         0.44         0.28           C18H2O4         292.0736         6.85         1.00         0.67         0.22           C15H2O10         360.1056         2.74         0.60         1.33         0.67           C15H1407         306.0740         3.73         1.00         0.93         0.47           C1H1407         306.0740         3.73         1.00         0.93         0.47           C5H1002         102.0681         0.81         0.50         2.00         0.40           C10H1005         210.0528         6.62         1.00         1.60         0.20           C20H3204         386.321         8.31         1.00         1.67         0.22           C5H4N0S2         211.9827         1.09         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         0.57         0.43           C13H2003         224.1412         4.74         1.00         1.54 <t< td=""><td>C15H14O3</td><td>242.0943</td><td>8.21</td><td>1.00</td><td>0.93</td><td>0.20</td></t<>	C15H14O3	242.0943	8.21	1.00	0.93	0.20
C1611NO35         240.0990         3.98         1.00         0.31         0.19           C18H8O5S2         367.9813         3.83         1.00         0.44         0.22           C18H1204         292.0736         6.85         1.00         1.67         0.22           C15H20010         360.1056         2.74         0.60         1.33         0.67           C19H3N06         227.0430         6.85         1.00         1.20         0.27           C15H1407         306.0740         3.73         1.00         0.93         0.47           CSH1002         102.0681         0.81         0.50         2.00         0.40           C10H1005         210.0528         6.62         1.00         1.60         0.20           C17H2004         288.1362         7.38         1.00         1.66         0.22           C14HX052         211.9827         1.09         1.00         0.67         0.43           C13H2003         224.1412         4.74         1.00         1.54         0.33           C13H2003         224.1412         4.74         1.00         0.67         0.22           C13H10088         326.0096         5.044         1.00         0.77	C13H9NO2S	243 0354	1.67	1.00	0.69	0.15
C16H5NO3S         290.9990         3.98         1.00         0.31         0.12           C18H1204         292.0736         6.85         1.00         0.44         0.22           C15H20010         360.1056         2.74         0.60         1.33         0.67           C19H9N06         227.0430         6.85         1.00         1.20         0.27           C15H1407         306.0740         3.73         1.00         0.93         0.47           C19H1005         210.0528         6.62         1.00         1.00         0.50           C20H3204         286.2301         8.31         1.00         1.60         0.20           C2H4N022         211.9827         1.09         1.00         0.67         0.17           C7H4N03         164.0222         1.36         1.00         0.57         0.43           C13H2003         224.1412         4.74         1.00         0.57         0.43           C13H1008S         326.0096         5.04         1.00         0.67         0.22           C13H1003S         422.0474         5.20         1.00         0.77         0.62           C13H100A3S         42.0474         5.20         1.00         0.75	CI (HENO2S	243.0334	1.07	1.00	0.07	0.15
C18H805S2         367.9813         3.83         1.00         0.44         0.28           C18H12O4         292.0736         6.85         1.00         0.67         0.22           C15H2O010         360.056         2.74         0.60         1.33         0.67           C15H18O4         262.1205         8.05         1.00         1.20         0.27           C15H14O7         306.0740         3.73         1.00         0.93         0.47           C19H10O5         210.0528         6.62         1.00         1.00         0.50           C10H10O5         210.0528         6.62         1.00         1.00         0.50           C20H32O4         336.2301         8.31         1.00         1.60         0.20           C1H4N4OS2         211.9827         1.09         1.00         0.67         0.17           C7HAN2O3         164.0222         1.36         1.00         0.67         0.22           C13H10O35         326.0096         5.04         1.00         0.67         0.22           C13H10A35         422.0474         5.20         1.00         0.43         0.13           C17H20O5         304.1311         7.50         1.00         0.75	CI6H5NO3S	290.9990	3.98	1.00	0.31	0.19
C18H12O4         292.0736         6.85         1.00         0.67         0.22           C1SH2O010         360.1056         2.74         0.60         1.33         0.67           C9H9N06         227.0430         6.85         1.00         1.00         0.67           C1SH1407         306.0740         3.73         1.00         0.93         0.47           CSH1002         102.0681         0.81         0.50         2.00         0.44           C10H1005         210.0528         6.62         1.00         1.00         0.50           C20H3204         336.2301         8.31         1.00         1.18         0.24           C6H4N40S2         211.9827         1.09         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         0.57         0.43           C13H12003         224.1412         4.74         1.00         1.54         0.23           C13H1008S         326.0096         5.04         1.00         0.77         0.62           C13H1008S         326.0096         5.04         1.00         0.75         0.50           C17H2005         304.1311         7.50         1.00         0.43	C18H8O5S2	367.9813	3.83	1.00	0.44	0.28
C18H1204         292.0730         0.63         1.00         0.01         0.22           C19H12041         360.1056         2.74         0.66         1.33         0.67           C19H1804         262.1205         8.05         1.00         1.20         0.27           C15H1804         262.1205         8.05         1.00         0.93         0.47           C19H1005         210.0528         6.62         1.00         1.60         0.20           C17H2004         288.1362         7.38         1.00         1.60         0.20           C1H42004         288.1362         7.38         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         0.57         0.43           C13H12003         224.1412         4.74         1.00         1.54         0.23           C13H1008S         326.0096         5.04         1.00         0.77         0.62           C13H1008S         326.0096         5.04         1.00         0.77         0.62           C13H1008S         326.0096         5.04         1.00         0.77         0.50           C17H2004         288.1362         8.14         1.00         1.18	C18U12O4	202.0726	6.95	1.00	0.67	0.22
C15H20010         360.1056         2.74         0.60         1.33         0.67           C9H9N06         227.0430         6.85         1.00         1.00         0.67           C15H1804         262.1205         8.05         1.00         1.20         0.27           C15H1407         306.0740         3.73         1.00         0.93         0.47           C9H1005         210.0528         6.62         1.00         1.00         0.50           C20H3204         336.2301         8.31         1.00         1.18         0.24           C6H4N40S2         211.9827         1.09         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         1.54         0.23           C13H1008S         326.096         5.04         1.00         0.67         0.22           C13H1008S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3N02S         128.9884         0.53         1.00         0.83	C18H1204	292.0730	0.85	1.00	0.07	0.22
C9H9NO6         227,0430         6.85         1.00         1.00         0.67           C15H18O4         262,1205         8.05         1.00         0.23         0.27           C15H14O7         306,0740         3.73         1.00         0.93         0.47           CSH10O2         102,0681         0.81         0.50         2.00         0.40           C10H10O5         210,0528         6.62         1.00         1.60         0.20           C17H20O4         288,1362         7.38         1.00         1.60         0.20           C7H4N2O3         164,0222         1.36         1.00         0.57         0.43           C13H2003         224,1412         4.74         1.00         1.54         0.23           C9H6O2         146,0368         2.51         1.00         0.67         0.22           C13H10O8S         326,0096         5.04         1.00         0.77         0.62           C23H10N403S         422,0474         5.20         1.00         0.43         0.13           C17H20O4         288,1362         8.14         1.00         1.76         0.50           C17H20O4         288,1362         8.14         1.00         0.75         <	C15H20O10	360.1056	2.74	0.60	1.33	0.67
C15H1804         262.1205         8.05         1.00         1.20         0.27           C15H1407         306.0740         3.73         1.00         0.93         0.47           CSH1002         102.0681         0.81         0.50         2.00         0.40           C10H1005         210.0528         6.62         1.00         1.00         0.50           C20H3204         336.2301         8.31         1.00         1.60         0.20           C17H2004         288.1362         7.38         1.00         1.18         0.24           C6H4N4OS2         211.9827         1.09         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         0.57         0.43           C13H1008S         326.0096         5.04         1.00         0.67         0.22           C13H1008S         326.0096         5.04         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           CH3N02S         128.984         0.53         1.00         1.83	C9H9NO6	227 0430	6.85	1.00	1.00	0.67
C15H1804         202.1205         8.05         1.00         1.20         0.24           C15H1407         306.0740         3.73         1.00         0.93         0.47           C5H1002         102.0681         0.81         0.50         2.00         0.40           C10H1005         210.0528         6.62         1.00         1.60         0.50           C20H3204         336.2301         8.31         1.00         1.60         0.20           C17H2004         288.1362         7.38         1.00         1.67         0.43           C13H2003         224.1412         4.74         1.00         0.57         0.43           C13H1008S         326.0096         5.04         1.00         0.67         0.22           C13H1008S         326.0096         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         418.0737         7.43         0.33         1.67         1.00           C4H3NO2S         128.9884         0.53         1.00         0.83	C15U1904	262 1205	0.05	1.00	1.00	0.07
C15H1407         306.0740         3.73         1.00         0.93         0.47           C5H1002         102.0681         0.81         0.50         2.00         0.40           C10H1005         210.0528         6.62         1.00         1.00         0.50           C20H3204         336.2301         8.31         1.00         1.16         0.20           C17H2004         288.1362         7.38         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         0.67         0.43           C13H2003         224.1412         4.74         1.00         1.54         0.23           C9H602         146.0368         2.51         1.00         0.67         0.22           C13H10088         326.0096         5.04         1.00         0.18         0.29           C13H10088         326.0096         5.04         1.00         1.18         0.29           C13H10081         422.0474         5.20         1.00         0.18         0.29           C13H10082         128.984         0.53         1.00         1.18         0.24           CH3NO2S         128.984         0.53         1.00         1.83 <td< td=""><td>C15H1804</td><td>262.1205</td><td>8.05</td><td>1.00</td><td>1.20</td><td>0.27</td></td<>	C15H1804	262.1205	8.05	1.00	1.20	0.27
C5H1002         102.0681         0.81         0.50         2.00         0.40           C10H1005         210.0528         6.62         1.00         1.00         0.50           C20H3204         336.2301         8.31         1.00         1.60         0.20           C17H2004         288.1362         7.38         1.00         1.18         0.24           C6H4N40S2         211.9827         1.09         1.00         0.67         0.17           C7H4N2O3         124.1412         4.74         1.00         1.54         0.23           C13H2003         224.1412         4.74         1.00         0.67         0.22           C13H1008S         326.0096         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         0.43         0.13           C12H20N2012S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         1.8         0.24           C6H5N03         139.0269         3.74         1.00         0.83	C15H14O7	306.0740	3.73	1.00	0.93	0.47
Clintion         102.001         0.03         0.03         0.03         0.03         0.03           C20H3204         336.2301         8.31         1.00         1.60         0.20           C17H2004         288.1362         7.38         1.00         1.18         0.24           C6H4N40S2         211.9827         1.09         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         0.57         0.43           C13H2003         224.1412         4.74         1.00         1.54         0.23           C9H602         146.0368         2.51         1.00         0.67         0.22           C13H1008S         326.096         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3N02S         128.9884         0.53         1.00         0.83         0.50           C17H2004         288.1362         8.14         1.00	C5H10O2	102 0681	0.81	0.50	2.00	0.40
C10H1005         210.0528         6.62         1.00         1.00         0.03           C20H3204         336.2301         8.31         1.00         1.60         0.20           C17H2004         288.1362         7.38         1.00         1.18         0.24           C6H4N40S2         211.9827         1.09         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         0.57         0.43           C13H2003         224.1412         4.74         1.00         0.67         0.22           C13H10088         326.0996         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3N02S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         1.88         0.56           C17H2004         288.1362         8.14         1.00         1.830	0.0111002	102.0001	0.01	0.50	2.00	0.40
C20H3204         336,2301         8.31         1.00         1.60         0.20           C17H2004         288,1362         7.38         1.00         1.18         0.24           C6H4N40S2         211.9827         1.09         1.00         0.67         0.17           C7H4N203         164.0222         1.36         1.00         0.57         0.43           C13H2003         224.1412         4.74         1.00         1.54         0.23           C9H602         146.0368         2.51         1.00         0.67         0.22           C13H1008S         326.0996         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H5NO4         288.1362         8.14         1.00         1.18         0.24           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C4H405         134.0215         0.36         0.40         1.50	C10H10O5	210.0528	6.62	1.00	1.00	0.50
C17H2004         288.1362         7.38         1.00         1.18         0.24           C6H4N40S2         211.9827         1.09         1.00         0.67         0.17           C7H4N2O3         164.0222         1.36         1.00         0.57         0.43           C13H2O03         224.1412         4.74         1.00         0.57         0.43           C9H6O2         146.0368         2.51         1.00         0.67         0.22           C13H100S3         322.0474         5.20         1.00         0.43         0.13           C17H20O5         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           CH4H3NO2S         128.9884         0.53         1.00         0.75         0.50           C17H2O04         288.1362         8.14         1.00         1.88         0.24           C6H5NO4         155.0219         3.07         1.00         0.83         0.67           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         <	C20H32O4	336.2301	8.31	1.00	1.60	0.20
C1/H2004         286.1362         7.58         1.00         1.16         0.24           C6H4N4OS2         211.9827         1.09         1.00         0.67         0.17           C7H4N2O3         164.0222         1.36         1.00         0.57         0.43           C13H2O03         224.1412         4.74         1.00         1.54         0.23           C9H6O2         146.0368         2.51         1.00         0.67         0.22           C13H10O8S         326.0096         5.04         1.00         0.77         0.62           C23H10N4O3S         422.0474         5.20         1.00         0.43         0.13           C17H20O5         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3NO2S         128.9884         0.53         1.00         0.83         0.50           C17H2004         288.1362         8.14         1.00         1.18         0.24           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C3H4O4         104.0110         0.36         0.50         1.33	C17U2004	200 1262	7 20	1.00	1 10	0.24
C6H4N40S2         211.9827         1.09         1.00         0.67         0.17           C7H4N2O3         164.0222         1.36         1.00         0.57         0.43           C13H2O03         224.1412         4.74         1.00         1.54         0.23           C9H6O2         146.0368         2.51         1.00         0.67         0.22           C13H1008S         326.0096         5.04         1.00         0.77         0.62           C23H10N4O3S         422.0474         5.20         1.00         0.43         0.13           C17H2O05         304.1311         7.50         1.00         1.18         0.29           C12H20N2O12S         416.0737         7.43         0.33         1.67         1.00           C4H3NO2S         128.9884         0.53         1.00         0.75         0.50           C17H2O04         288.1362         8.14         1.00         1.88         0.50           C4H6N04         155.0219         3.07         1.00         0.83         0.50           C4H6O5         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.38         0.75         1.00	01/H2004	200.1302	1.30	1.00	1.10	0.24
C7H4N2O3         164.0222         1.36         1.00         0.57         0.43           C13H2OO3         224.1412         4.74         1.00         1.54         0.23           C9H6O2         146.0368         2.51         1.00         0.67         0.22           C13H10O8S         326.0096         5.04         1.00         0.77         0.62           C23H10N4O3S         422.0474         5.20         1.00         0.43         0.13           C17H20O5         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3NO2S         128.9884         0.53         1.00         0.18         0.24           C6H5NO4         155.0219         3.07         1.00         0.83         0.67           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H6O4         104.0110         0.36         0.50         1.33         1.33           C4H6O5         134.0215         0.36         0.40         1.60 <t< td=""><td>C6H4N4OS2</td><td>211.9827</td><td>1.09</td><td>1.00</td><td>0.67</td><td>0.17</td></t<>	C6H4N4OS2	211.9827	1.09	1.00	0.67	0.17
C13H2003         224.1412         4.74         1.00         1.54         0.23           C9H602         146.0368         2.51         1.00         0.67         0.22           C13H10088S         326.0096         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3NO2S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         1.18         0.24           C6H5N03         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.38         0.75         1.00         0.00           C4H605         148.0372         0.38         0.40         1.60 <t< td=""><td>C7H4N2O3</td><td>164 0222</td><td>1.36</td><td>1.00</td><td>0.57</td><td>0.43</td></t<>	C7H4N2O3	164 0222	1.36	1.00	0.57	0.43
C15H2005         224.1412         4.74         1.00         1.54         0.25           C9H602         146.0368         2.51         1.00         0.67         0.22           C13H1008S         326.0096         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3N02S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         1.18         0.24           C6H5N03         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H604         118.0266         0.53         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         104.0110         0.38         0.75         1.00 <td< td=""><td>C12U2002</td><td>224.1412</td><td>4.74</td><td>1.00</td><td>1 5 4</td><td>0.13</td></td<>	C12U2002	224.1412	4.74	1.00	1 5 4	0.13
C9H602         146.0368         2.51         1.00         0.677         0.22           C13H1008S         326.0096         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3N02S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         1.18         0.24           C6H5N03         139.0269         3.74         1.00         0.83         0.67           C3H405         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H605         148.0372         0.38         0.40         1.60         1.00           C4H404         116.0110         0.38         0.75         1.00         1	C13H20O3	224.1412	4./4	1.00	1.54	0.23
C13H1008S         326.0096         5.04         1.00         0.77         0.62           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3NO2S         128.984         0.53         1.00         0.75         0.50           C17H20O4         288.1362         8.14         1.00         1.18         0.24           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         104.0110         0.38         0.75         1.00         1.00           C4H404         116.0110         0.38         0.75         1.00         1.	C9H6O2	146.0368	2.51	1.00	0.67	0.22
C13110083         320030         3.04         1.00         0.71         0.02           C23H10N403S         422.0474         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3N02S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         1.18         0.24           C6H5N04         155.0219         3.07         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H605         148.0372         0.38         0.40         1.60         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C4H604         116.0110         0.38         0.75         1.00         1.0	C13H1008S	326 0006	5.04	1.00	0.77	0.62
C23H10N403S         422.04/4         5.20         1.00         0.43         0.13           C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3NO2S         128.9884         0.53         1.00         0.75         0.50           C17H20O4         288.1362         8.14         1.00         1.18         0.24           C6H5NO4         155.0219         3.07         1.00         0.83         0.67           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C2H4O6S         155.9729         0.33         0.17         2.00         3.00           C4H6O5         134.0215         0.36         0.40         1.50         1.25           C3H4O4         104.0110         0.36         0.50         1.33         1.33           C4H6O4         118.0266         0.53         0.50         1.50         1.00           C5H8O5         148.0372         0.38         0.40         1.60         1.00           C5H8O5         148.0372         7.41         1.00         0.86         0.2	0151110085	320.0090	5.04	1.00	0.77	0.02
C17H2005         304.1311         7.50         1.00         1.18         0.29           C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3N02S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         1.18         0.24           C6H5N03         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         116.0110         0.38         0.75         1.00         1.00           C4H404         116.0110         0.38         0.40         1.60         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C4H404         176.012         2.25         0.50         0.50         1.50	C23H10N4O3S	422.0474	5.20	1.00	0.43	0.13
C12H20N2012S         416.0737         7.43         0.33         1.67         1.00           C4H3N02S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         1.18         0.24           C6H5N04         155.0219         3.07         1.00         0.83         0.67           C6H5N03         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N205         198.0277         7.41         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.86         0.29           C3H1404         174.0892         3.11         0.50         1.75         0.50 <td>C17H20O5</td> <td>304.1311</td> <td>7.50</td> <td>1.00</td> <td>1.18</td> <td>0.29</td>	C17H20O5	304.1311	7.50	1.00	1.18	0.29
C12H20120123         1410.0137         1.43         0.33         1.107         1.00           C4H3NO2S         128.9884         0.53         1.00         0.75         0.50           C17H2004         288.1362         8.14         1.00         0.18         0.24           C6H5NO3         139.0269         3.74         1.00         0.83         0.67           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.20           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         116.0110         0.38         0.75         1.00         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N205         198.0277         7.41         1.00         0.86         0.71           C9H804         174.0892         3.11         0.50         1.75         0.50 </td <td>C12H20N2O12S</td> <td>416.0727</td> <td>7.42</td> <td>0.22</td> <td>1.67</td> <td>1.00</td>	C12H20N2O12S	416.0727	7.42	0.22	1.67	1.00
C4H3N02S         128,9884         0.53         1.00         0.75         0.50           C17H2004         288,1362         8.14         1.00         1.18         0.24           C6H5N03         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         116.0110         0.38         0.75         1.00         1.00           C4H805         148.0372         0.38         0.40         1.60         1.00           C4H804         180.0423         3.14         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.86         0.29           C3H1044         174.0892         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29 </td <td>C12H20N2O125</td> <td>410.0737</td> <td>7.43</td> <td>0.55</td> <td>1.07</td> <td>1.00</td>	C12H20N2O125	410.0737	7.43	0.55	1.07	1.00
C17H2004         288.1362         8.14         1.00         1.18         0.24           C6H5NO4         155.0219         3.07         1.00         0.83         0.67           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         116.0110         0.38         0.75         1.00         1.00           C4H404         116.0110         0.38         0.40         1.60         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N205         198.0277         7.41         1.00         0.86         0.71           C9H804         180.0423         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29 </td <td>C4H3NO2S</td> <td>128.9884</td> <td>0.53</td> <td>1.00</td> <td>0.75</td> <td>0.50</td>	C4H3NO2S	128.9884	0.53	1.00	0.75	0.50
Control         Dote         Ont         Dote         Dote           C6H5NO4         155.0219         3.07         1.00         0.83         0.67           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H6O5         134.0215         0.36         0.40         1.50         1.25           C3H4O4         104.0110         0.36         0.50         1.33         1.33           C4H6O5         148.0266         0.53         0.50         1.50         1.00           C4H4O4         116.0110         0.38         0.75         1.00         1.00           C4H8O5         148.0372         0.38         0.40         1.60         1.00           C7H0N2O5         198.0277         7.41         1.00         0.86         0.71           C9H8O4         180.0423         3.14         1.00         0.86         0.29           C3H6O5         143.03936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70 <t< td=""><td>C17H20O4</td><td>288 1362</td><td>8 14</td><td>1.00</td><td>1 18</td><td>0.24</td></t<>	C17H20O4	288 1362	8 14	1.00	1 18	0.24
C6H5NO4         155.0219         3.07         1.00         0.83         0.67           C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C2H4O6S         155.9729         0.33         0.17         2.00         3.00           C4H6O5         134.0215         0.36         0.40         1.50         1.25           C3H4O4         104.0110         0.36         0.50         1.33         1.33           C4H6O4         118.0266         0.53         0.50         1.50         1.00           C4H4O4         116.0110         0.38         0.75         1.00         1.00           C5H8O5         148.0372         0.38         0.40         1.60         1.00           C7H6N2O5         198.0277         7.41         1.00         0.86         0.71           C9H8O4         180.0423         3.14         1.00         0.86         0.71           C9H8O4         174.0892         3.11         0.50         1.75         0.50           C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67 <td>C(USNO4</td> <td>155.0010</td> <td>2.07</td> <td>1.00</td> <td>0.02</td> <td>0.21</td>	C(USNO4	155.0010	2.07	1.00	0.02	0.21
C6H5NO3         139.0269         3.74         1.00         0.83         0.50           C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         116.0110         0.38         0.40         1.60         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N205         198.0277         7.41         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.86         0.71           C9H804         180.0423         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29           C3H605S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70	C6H5NO4	155.0219	3.07	1.00	0.83	0.67
C2H406S         155.9729         0.33         0.17         2.00         3.00           C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         116.0110         0.38         0.75         1.00         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N205         198.0277         7.41         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.86         0.71           C9H804         174.0892         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29           C3H605S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H204         89.9953         0.36         0.50         1.00         2.00 </td <td>C6H5NO3</td> <td>139.0269</td> <td>3.74</td> <td>1.00</td> <td>0.83</td> <td>0.50</td>	C6H5NO3	139.0269	3.74	1.00	0.83	0.50
C2H4005         133.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         116.0110         0.38         0.75         1.00         1.00           C4H404         116.0110         0.38         0.75         1.00         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N205         198.0277         7.41         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.86         0.71           C9H804         174.0892         3.11         0.50         1.75         0.50           C8H1404         174.0892         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29           C3H605S         153.9936         0.36         0.20         2.00         1.67           C10H17N07S         295.0726         4.67         0.43         1.70         0.70	C2H4O6S	155 9729	0.33	0.17	2.00	3.00
C4H605         134.0215         0.36         0.40         1.50         1.25           C3H404         104.0110         0.36         0.50         1.33         1.33           C4H604         118.0266         0.53         0.50         1.50         1.00           C4H404         116.0110         0.38         0.75         1.00         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N205         198.0277         7.41         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.86         0.71           C9H804         174.0892         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29           C3H605S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H204         89.9953         0.36         0.50         1.00         2.00 <td>C2114005</td> <td>133.9729</td> <td>0.35</td> <td>0.17</td> <td>2.00</td> <td>5.00</td>	C2114005	133.9729	0.35	0.17	2.00	5.00
C3H4O4         104.0110         0.36         0.50         1.33         1.33           C4H6O4         118.0266         0.53         0.50         1.50         1.00           C4H4O4         116.0110         0.38         0.75         1.00         1.00           C5H8O5         148.0372         0.38         0.40         1.60         1.00           C7H6N2O5         198.0277         7.41         1.00         0.86         0.71           C9H8O4         180.0423         3.14         1.00         0.89         0.44           C8H18O4S         210.0926         7.15         0.00         2.25         0.50           C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80	C4H6O5	134.0215	0.36	0.40	1.50	1.25
C4H6O4         118.0266         0.53         0.50         1.50         1.00           C4H4O4         116.0110         0.38         0.75         1.00         1.00           C5H8O5         148.0372         0.38         0.40         1.60         1.00           C7H6N2O5         198.0277         7.41         1.00         0.86         0.71           C9H8O4         180.0423         3.14         1.00         0.86         0.71           C9H8O4         180.0423         3.14         1.00         0.89         0.44           C8H18O4S         210.0926         7.15         0.00         2.25         0.50           C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80	C3H4O4	104.0110	0.36	0.50	1.33	1.33
CHIOO         116.0200         0.33         0.30         1.30         1.60           C4H404         116.0110         0.38         0.75         1.00         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N2O5         198.0277         7.41         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.89         0.44           C8H1804S         210.0926         7.15         0.00         2.25         0.50           C8H1404         174.0892         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29           C3H605S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H204         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33	C4H6O4	118 0266	0.53	0.50	1.50	1.00
C4H404         116.0110         0.38         0.75         1.00         1.00           C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N205         198.0277         7.41         1.00         0.86         0.71           C9H804         180.0423         3.14         1.00         0.89         0.44           C8H1804S         210.0926         7.15         0.00         2.25         0.50           C8H1404         174.0892         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29           C3H605S         153.9936         0.36         0.20         2.00         1.67           C10H17N07S         295.0726         4.67         0.43         1.70         0.70           C2H204         89.9953         0.36         0.50         1.00         2.00           C9H17N03         187.1208         2.98         0.67         1.89         0.33           C5H804         132.0423         0.77         0.50         1.60         0.80           C7H7N04         169.0375         4.11         1.00         1.00         0.57		116.0200	0.33	0.50	1.00	1.00
C5H805         148.0372         0.38         0.40         1.60         1.00           C7H6N2O5         198.0277         7.41         1.00         0.86         0.71           C9H8O4         180.0423         3.14         1.00         0.89         0.44           C8H18O4S         210.0926         7.15         0.00         2.25         0.50           C8H14O4         174.0892         3.11         0.50         1.75         0.50           C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00	C4H4O4	116.0110	0.38	0.75	1.00	1.00
C7H6N2O5         198.0277         7.41         1.00         0.86         0.71           C9H8O4         180.0423         3.14         1.00         0.89         0.44           C8H18O4S         210.0926         7.15         0.00         2.25         0.50           C8H14O4         174.0892         3.11         0.50         1.75         0.50           C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60	C5H8O5	148.0372	0.38	0.40	1.60	1.00
CHINEOD         150.0277         7.41         1.00         0.80         0.71           C9H804         180.0423         3.14         1.00         0.89         0.44           C8H1804S         210.0926         7.15         0.00         2.25         0.50           C8H1404         174.0892         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29           C3H605S         153.9936         0.36         0.20         2.00         1.67           C10H17N07S         295.0726         4.67         0.43         1.70         0.70           C2H204         89.9953         0.36         0.50         1.00         2.00           C9H17N03         187.1208         2.98         0.67         1.89         0.33           C5H804         132.0423         0.77         0.50         1.60         0.80           C7H7N04         169.0375         4.11         1.00         1.00         0.57           C5H605         146.0215         0.37         0.60         1.20         1.00           C5H7N03         129.0426         0.38         1.00         1.40         0.60	C7H6N2O5	198 0277	7 / 1	1.00	0.86	0.71
C9H804         180.0423         3.14         1.00         0.89         0.44           C8H1804S         210.0926         7.15         0.00         2.25         0.50           C8H1404         174.0892         3.11         0.50         1.75         0.50           C7H602         122.0368         2.63         1.00         0.86         0.29           C3H605S         153.9936         0.36         0.20         2.00         1.67           C10H17N07S         295.0726         4.67         0.43         1.70         0.70           C2H204         89.9953         0.36         0.50         1.00         2.00           C9H17N03         187.1208         2.98         0.67         1.89         0.33           C5H804         132.0423         0.77         0.50         1.60         0.80           C7H7N04         169.0375         4.11         1.00         1.00         0.57           C5H605         146.0215         0.37         0.60         1.20         1.00           C5H7N03         129.0426         0.38         1.00         1.40         0.60           C8H605         182.0215         2.77         1.00         0.75         0.63	C/1101N2OJ	190.0277	1.41	1.00	0.00	0.71
C8H1804S         210.0926         7.15         0.00         2.25         0.50           C8H14O4         174.0892         3.11         0.50         1.75         0.50           C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50	C9H8O4	180.0423	3.14	1.00	0.89	0.44
C8H14O4         174.0892         3.11         0.50         1.75         0.50           C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H4O5S         139.979         0.33         0.20         2.00         2.50           C6HU004         146         0579         1.69         0.50         1.67	C8H18O4S	210.0926	7.15	0.00	2.25	0.50
Control         174.0892         5.11         0.30         1.75         0.50           C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17N07S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6HU004         146.0579         1.69         0.50         1.67         0.67	C8H14O4	174 0802	2 11	0.50	1 75	0.50
C7H6O2         122.0368         2.63         1.00         0.86         0.29           C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H8O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6HU004         146.0579         1.69         0.50         1.67         0.67	Соп1404	1/4.0692	5.11	0.50	1./3	0.50
C3H6O5S         153.9936         0.36         0.20         2.00         1.67           C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6HU004         146.0579         1.69         0.50         1.67         0.67	C7H6O2	122.0368	2.63	1.00	0.86	0.29
C10H17NO7S         295.0726         4.67         0.43         1.70         0.70           C2H2O4         89.9953         0.36         0.50         1.00         2.00	C3H6O5S	153,9936	0.36	0.20	2.00	1.67
C10m1/NO/5         293.0/20         4.0/         0.43         1./0         0./0           C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6H1004         146.0579         1.69         0.50         1.67         0.67	C10U17NO79	205.0726	1 27	0.42	1.70	0.70
C2H2O4         89.9953         0.36         0.50         1.00         2.00           C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H4O5S         139.9779         0.33         0.20         2.00         2.50           C6HU004         146.0579         1.69         0.50         1.67         0.67	CIUHI/NU/S	293.0726	4.0/	0.43	1.70	0.70
C9H17NO3         187.1208         2.98         0.67         1.89         0.33           C5H8O4         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6H1004         146.0579         1.69         0.50         1.67         0.67	C2H2O4	89.9953	0.36	0.50	1.00	2.00
C5H804         132.0423         0.77         0.50         1.60         0.80           C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H605         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H605         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6H1004         146.0579         1.69         0.50         1.67         0.67	C9H17NO3	187,1208	2 98	0.67	1.89	0 33
C5H804         132.0423         0.77         0.50         1.60         0.80           C7H7N04         169.0375         4.11         1.00         1.00         0.57           C5H605         146.0215         0.37         0.60         1.20         1.00           C5H7N03         129.0426         0.38         1.00         1.40         0.60           C8H605         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6H1004         146.0579         1.69         0.50         1.67         0.67	0511004	122.0402	0.77	0.57	1.07	0.00
C7H7NO4         169.0375         4.11         1.00         1.00         0.57           C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6H1004         146.0579         1.69         0.50         1.67         0.67	С5Н8О4	132.0423	0.77	0.50	1.60	0.80
C5H6O5         146.0215         0.37         0.60         1.20         1.00           C5H7NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H4O5S         139.9779         0.33         0.20         2.00         2.50           C6H1004         146.0579         1.69         0.50         1.67         0.63	C7H7NO4	169.0375	4.11	1.00	1.00	0.57
C5H7005         140.0215         0.37         0.00         1.20         1.00           C5H7N03         129.0426         0.38         1.00         1.40         0.60           C8H605         182.0215         2.77         1.00         0.75         0.63           C2H405S         139.9779         0.33         0.20         2.00         2.50           C6H1004         146.0579         1.69         0.50         1.67         0.67	C54605	146 0215	0.37	0.60	1.20	1.00
C5H/NO3         129.0426         0.38         1.00         1.40         0.60           C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H4O5S         139.9779         0.33         0.20         2.00         2.50           C6H1004         146.0579         1.69         0.50         1.67         0.67		170.0213	0.57	0.00	1.40	1.00
C8H6O5         182.0215         2.77         1.00         0.75         0.63           C2H4O5S         139.9779         0.33         0.20         2.00         2.50           C6H10O4         146.0579         1.69         0.50         1.67         0.67	C5H7NO3	129.0426	0.38	1.00	1.40	0.60
C2H4O5S 139.9779 0.33 0.20 2.00 2.50 C6H10O4 146.0579 1.69 0.50 1.67 0.67	C8H6O5	182.0215	2.77	1.00	0.75	0.63
C6H10O4 146 0579 1 69 0 50 1 67 0 67	C2H405S	130 0770	0.22	0.20	2.00	2 50
C6H10O4 146 0579 1 69 0 50 1 67 0 67	0204035	139.9/19	0.55	0.20	2.00	2.30
140.0577 1.07 0.07	C6H10O4	146.0579	1.69	0.50	1.67	0.67
C6H8O5 160.0372 0.38 0.60 1.33 0.83	C6H8O5	160 0372	0.38	0.60	1.33	0.83
	C211005	150.0072	0.00	0.00	1.55	1.67
<u>C3R6035</u> 130.0092 0.30 0.00 2.6/ 1.6/	C3H8032	156.0092	0.36	0.00	2.67	1.67

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C5H8O6	164.0321	0.36	0.33	1.60	1.20
C2H6O4S	125.9987	0.38	0.00	3.00	2.00
C5H6O3	114.0317	0.38	1.00	1.20	0.60
C8H6N2O2	162.0429	6.07	1.00	0.75	0.25
C5H8O4	153.0426	5.20	1.00	1.00	0.43
C10H6N2O5	234 0277	7.60	1.00	1.60	0.80
C3H6O4S	137 9987	0.35	0.25	2.00	1 33
C9H14O5	202.0841	2.68	0.60	1.56	0.56
C8H9NO4	183.0532	3.49	1.00	1.13	0.50
C7H6N2O4	182.0328	3.12	1.00	0.86	0.57
C8H6O3	150.0317	2.62	1.00	0.75	0.38
C12H22O6	262.1416	3.42	0.33	1.83	0.50
C7H12O7	208.0583	0.37	0.29	1.71	1.00
C5H10O5	150.0528	0.34	0.20	2.00	1.00
C6H10O6	1/8.04//	0.38	0.33	1.67	1.00
C7H6O3	190.0477	0.38	0.50	1.45	0.80
C10H16O5	216.0998	2.93	0.60	1.60	0.43
C5H12O4S	168.0456	2.95	0.00	2.40	0.80
C6H10O5	162.0528	0.49	0.40	1.67	0.83
C8H9NO3	167.0582	7.25	1.00	1.13	0.38
C16H22O4	278.1518	8.48	1.00	1.38	0.25
C15H22O8	330.1315	3.07	0.63	1.47	0.53
C3H8O4S	140.0143	0.50	0.00	2.67	1.33
C12H22O4	230.1518	7.58	0.50	1.83	0.33
C6H5NO4	120.0422	3.80	1.00	0.83	0.67
C5H10O4	120.0425	0.38	0.23	2.00	0.80
C8H7NO5	197.0324	3.61	1.00	0.88	0.60
C12H14O4	222.0892	7.46	1.00	1.17	0.33
C4H6O5S	165.9936	0.37	0.40	1.50	1.25
C3H6O4	106.0266	0.35	0.25	2.00	1.33
C9H20O4S	224.1082	7.64	0.00	2.22	0.44
C4H8O4S	152.0143	0.38	0.25	2.00	1.00
C3H3NO4	117.0062	0.38	0.75	1.00	1.33
C10H32U0S	552.1920 181.0730	7.80	0.17	2.00	0.38
C2H3NO3	89.0113	0.32	0.67	1.22	1.50
C8H16O8S	272.0566	3.71	0.13	2.00	1.00
C7H5NO3S2	214.9711	2.79	1.00	0.71	0.43
C6H10O4	146.0579	2.48	0.50	1.67	0.67
C10H22O4S	238.1239	7.95	0.00	2.20	0.40
C15H8N4O6	340.0444	3.71	1.00	0.53	0.40
C2H3NO4S	136.9783	0.37	0.50	1.50	2.00
C5H/NO5	161.0324	0.36	0.60	1.40	1.00
C16H30O4	214.0220	4.81	0.50	0.80	0.80
C8H14O	126 1045	3 71	1.00	1.00	0.23
C6H6N2O2	138.0429	0.38	1.00	1.00	0.33
C6H9NO4	159.0532	0.38	0.75	1.50	0.67
C4H4N2O2	112.0273	0.38	1.00	1.00	0.50
C10H10O4	194.0579	6.37	1.00	1.00	0.40
C10H18O6	234.1103	2.73	0.33	1.80	0.60
C14H21NO6	299.1369	4.59	0.83	1.50	0.43
CTH5NO	246.1103	4.30	0.50	1.64	0.55
C18H30O5	326 2093	3.13 8.01	0.80	0.71	0.14
C18H34O5	330,2406	7 44	0.80	1.89	0.28
C5H4N2O4	156.0171	0.39	1.00	0.80	0.80
C15H28O4	272.1988	8.28	0.50	1.87	0.27
C14H28O3	244.2038	8.21	0.33	2.00	0.21
C12H14O4	222.0892	3.95	1.00	1.17	0.33
C7H8O3S	172.0194	1.74	1.00	1.14	0.43
CIUHIINO3	193.0739	5.04	1.00	1.10	0.30
C7H13NO3	100.1099 150 0805	4.45	0.33	2.00	0.38
C18H32O4	312 2301	8.29	0.75	1.78	0.43
C7H12O	112.0888	3.11	1.00	1.71	0.14
C11H15NO3	209.1052	8.37	1.00	1.36	0.27

C15H30O3	258.2195	8.38	0.33	2.00	0.20
C15H28O3	256.2038	8.27	0.67	1.87	0.20
C18H26O4	306.1831	8.71	1.00	1.44	0.22

Neutral mass (Da) RT (min) MCR H/C O/C Formula [M] C2H4O6S 155.9729 0.39 0.17 2.00 3.00 C7H7NO4 169.0375 2.92 1.00 1.00 0.57 C10H7NO3 189.0426 7.72 1.00 0.70 0.30 C9H12O4 184.0736 1.07 1.00 1.33 0.44 C5H12O4S 2.80 0.00 0.80 168.0456 2.40 C10H17NO7S 295.0726 4.70 0.43 1.70 0.70 C8H7NO3 5.03 0.38 165.0426 1.00 0.88 C7H7NO4 169.0375 3.79 1.00 1.00 0.57 C3H6O6S 169.9885 0.39 0.17 2.00 2.00 C9H15NO8S 297.0518 3.27 0.38 1.67 0.89 C10H17NO7S 295.0726 6.31 0.43 1.70 0.70 C3H8O5S 156.0092 0.38 0.00 2.67 1.67 C4H8O6S 184.0042 0.40 0.17 2.00 1.50 C8H9NO3 167.0582 7.24 1.00 1.13 0.38 C8H12O5 188.0685 1.21 0.60 1.50 0.63 314.0790 C17H14O6 7.96 1.00 0.82 0.35 C8H5NO2 147.0320 3.25 0.25 1.00 0.63 C7H7NO4 0.57 169.0375 4.60 1.00 1.00 C8H18O5S 2.95 2.25 0.63 226.0875 0.00 C8H9NO3 167.0582 7.55 1.00 1.13 0.38 C10H20N2O4 232.1423 3.00 0.50 2.00 0.40 0.70 C10H17NO7S 295.0726 6.63 0.43 1.70 C9H15NO8S 297.0518 2.91 0.38 1.67 0.89 C4H4O6S 1.50 179.9729 0.41 0.50 1.00 C6H10O8S 242.0096 0.39 0.25 1.67 1.33 C9H16O6S 252.0668 2.60 0.33 1.78 0.67 C8H9NO5 199.0481 2.81 1.00 1.13 0.63 C4H10O5S 170.0249 0.40 0.00 2.50 1.25 C10H17NO10S 343.0573 2.67 0.30 1.70 1.00 228.0304 0.40 C6H12O7S 0.14 2.001.17 C10H15NO9S 325.0468 2.99 0.44 1.50 0.90 C7H12O7S 240.0304 0.59 0.29 1.71 1.00 C8H16O4S 208.0769 4.86 0.25 2.00 0.50 C6H5N3O4 183.0280 4.85 1.00 0.83 0.67 C10H8O4 192.0423 6.96 1.00 0.80 0.40 C5H4N2O3 140.0222 2.34 0.80 0.60 1.00 C6H8O6 176.0321 0.38 0.50 1.33 1.00 280.0617 C10H16O7S 2.48 0.43 0.70 1.60 C10H14O6S 262.0511 3.00 0.67 1.40 0.60 C8H7NO5 197.0324 4.71 1.00 0.88 0.63 C10H18N2O11S 374.0631 4.40 0.27 1.80 1.10 C6H6O5 158.0215 0.39 0.80 1.00 0.83 C10H17NO8S 311.0675 3.78 0.38 1.70 0.80 C8H7NO4 181.0375 3.87 1.00 0.88 0.50 C8H9NO4 183.0532 5.59 1.00 1.13 0.50 4.22 0.78 C9H9NO7S 275.0100 0.86 1.00 C8H8O3 152.0473 2.63 1.00 1.00 0.38 C11H9NO3 203.0582 8.05 0.82 0.27 1.00 C5H11NO7S 229.0256 2.73 0.14 2.20 1.40 0.63 C8H16O5S 224.0718 2.55 0.20 2.00 C10H19NO8S 3.40 0.25 1.90 0.80 313.0831 0.29 0.70 C10H18O7S 282.0773 2.79 1.80 0.40 0.20 2.00 1.25 C4H8O5S 168.0092 C10H18O4 202.1205 7.12 0.50 1.80 0.40 0.63 C8H12O5 188.0685 2.41 0.60 1.50 C8H5NO3 163.0269 2.66 1.00 0.63 0.38 C9H18O6S 254.0824 2.67 2.00 0.67 0.17 C4H6O6S 181.9885 0.40 0.33 1.50 1.50

Table S4.3.6 Molecular formulas of organic compounds detected in Xi'an OA in ESI- mode.

C3H5NO5	135.0168	0.40	0.40	1.67	1.67
0511006	164.0201	0.27	0.22	1.00	1.00
C5H8O6	164.0321	0.37	0.33	1.60	1.20
C10H18N2O11S	374.0631	3.27	0.27	1.80	1.10
GIOLICORG	227 0750	0.54	1.00	0.00	0.00
C10H6O3S2	237.9758	0.54	1.00	0.60	0.30
C5H10O6S	198 0198	0.44	0.17	2.00	1.20
051112059	104.0405	0.44	0.00	0.40	1.00
C5H12055	184.0405	0.44	0.00	2.40	1.00
C4H6O5S	165 9936	0.38	0.40	1 50	1 25
C III0055	105.5550	0.50	0.10	1.00	1.20
C6H11NO8	225.0485	0.37	0.25	1.83	1.33
C6H8O6S	208 0042	0.40	0.50	1 33	1.00
00100005	200.0042	0.40	0.50	1.55	1.00
C8H12O7	220.0583	0.40	0.43	1.50	0.88
COLIONO76	262 0100	2 61	0.71	1 1 2	0.00
Consino/3	203.0100	5.01	0.71	1.15	0.00
C9H19NO8S	301.0831	3.41	0.13	2.11	0.89
CELLEDE	174.0164	0.40	0.67	1.00	1.00
Сопосо	174.0104	0.40	0.07	1.00	1.00
C6H5NO4	155.0219	3.78	1.00	0.83	0.67
C10111(076	200.0617	1.02	0.42	1.00	0.70
C10H100/S	280.0017	1.02	0.45	1.00	0.70
C9H18O6S	254.0824	3.22	0.17	2.00	0.67
COLLIZNIOSC	220 0827	2.24	0.20	0.12	0.62
C8H1/NO5S	239.0827	2.24	0.20	2.13	0.63
C10H18O6S	266.0824	1.19	0.33	1.80	0.60
GIOHIOOGG	200.0021	0.62	0.00	1.00	0.00
C10H1806S	266.0824	0.63	0.33	1.80	0.60
C7H6O5S	201 9936	0.66	1.00	0.86	0.71
67110055	201.9950	0.00	1.00	0.00	0.71
C7H8O6	188.0321	0.40	0.67	1.14	0.86
C9H14O5	202 0841	1.61	0.60	1 56	0.56
0/111405	202.0041	1.01	0.00	1.50	0.50
C14H14N2O5S2	354.0344	2.68	1.00	1.00	0.36
C10H10O4	104.0570	6 22	1.00	1.00	0.40
C10H1004	194.0379	0.33	1.00	1.00	0.40
C3H8O3S	124.0194	0.40	0.00	2.67	1.00
CTUCNOOA	192 0229	2 11	1.00	0.00	0.57
C/HolN204	182.0328	3.11	1.00	0.80	0.57
C5H6O6S	193,9885	0.59	0.50	1.20	1.20
CIOLIONOOG	220.0701	0.00	0.00	1.00	0.00
C10H19N09S	329.0781	2.70	0.22	1.90	0.90
C7H8O5	172 0372	0.40	0.80	1 14	0.71
C711005	172.0372	0.40	0.00	1.14	0.71
C/H12O5	176.0685	0.77	0.40	1.71	0.71
C5H8O5S	180.0092	0.40	0.40	1.60	1.00
05110055	100.0072	0.40	0.40	1.00	1.00
C7H12O6S	224.0355	0.80	0.33	1.71	0.86
C12H9NO3	215.0582	7 85	1.00	0.75	0.25
C121191003	215.0582	7.85	1.00	0.75	0.25
C12H11NO3	217.0739	8.21	1.00	0.92	0.25
C10H20O5S	252 1031	7.03	0.20	2.00	0.50
01011200005	252.1051	7.05	0.20	2.00	0.50
C10H18N2O11S	374.0631	3.88	0.27	1.80	1.10
C2112O2	74.0004	0.29	0.67	1.00	1.50
C2H2O3	74.0004	0.38	0.07	1.00	1.50
C14H10O4S	274.0300	7.12	1.00	0.71	0.29
COLIZINO	102 0275	2.45	1.00	0.70	0.44
C9H/NO4	193.0375	3.45	1.00	0.78	0.44
C9H18O6S	254 0824	3 54	0.17	2 00	0.67
CTUTNOS	105.0001	2.27	1.00	1.00	0.01
C/H/NO5	185.0324	3.27	1.00	1.00	0.71
C6H6N2O3	154 0378	2.82	1.00	1.00	0.50
011011205	154.0570	2.02	1.00	1.00	0.50
C7H4N2O7	228.0019	4.12	1.00	0.57	1.00
C9H16O3	172 1009	4 17	0.67	1 78	0.33
0/11/005	172.1077	4.17	0.07	1.70	0.55
C7H14O7S	242.0460	0.54	0.14	2.00	1.00
C6H4O5	156 0059	0.68	1.00	0.67	0.83
011405	150.0059	0.08	1.00	0.07	0.85
C3H3NO4	117.0062	0.40	0.75	1.00	1.33
C12H10N2O6	278 0520	3 77	1.00	0.92	0.50
C1211101N2O0	210.0339	5.12	1.00	0.05	0.50
C9H16O3	172.1099	2.67	0.67	1.78	0.33
COLICOS	162 0317	2.06	1.00	0.67	0.33
0,711003	102.0517	2.90	1.00	0.07	0.55
C12H7NO4	229.0375	7.98	1.00	0.58	0.33
C10H16N2O10S	356 0526	7.40	0.40	1.60	1.00
0101101/20105	550.0520	7.40	0.40	1.00	1.00
C14H8O3	224.0473	7.56	1.00	0.57	0.21
C10H16058	248 0718	2 00	0.60	1.60	0.50
0101110035	240.0710	2.99	0.00	1.00	0.50
C17H26O5	310.1780	8.07	1.00	1.53	0.29
CGUIINOOS	257 0205	2.05	0.25	1 02	1 22
COLLINOSS	237.0205	2.05	0.25	1.83	1.33
C8H7NO5	197.0324	4.32	1.00	0.88	0.63
CIOLIONOOS	220.0791	2.04	0.22	1.00	0.00
CIUHI9N09S	329.0781	3.04	0.22	1.90	0.90
C7H14O6S	226.0511	2.09	0.17	2.00	0.86
0010070	222,0001		0.42	1.00	1 17
COH8U/S	223.9991	0.40	0.43	1.33	1.17
C6H11NO9S	273 0155	2.15	0.22	1.83	1 50
001112020	102 0020	2.13	0.22	1.05	1.50
C8H16O3S	192.0820	3.61	0.33	2.00	0.38
C0H8O4	180 0423	4 11	1.00	0.80	0.44
011004	100.0423	7.11	1.00	0.07	0.77
C11H23NO5S	281.1297	2.91	0.20	2.09	0.45
CSHOORS	229 9885	2 51	1.00	0.75	0.75
0110005	227.7005	2.31	1.00	0.15	0.75
C10H14O6	230.0790	2.16	0.67	1.40	0.60
C8H12088	268 0253	0.63	0.38	1 50	1.00
00112005	200.0233	0.05	0.50	1.50	1.00
C7H16O4S	196.0769	5.15	0.00	2.29	0.57
C5H4N4O3	168 0283	0.38	1.00	0.80	0.60
0311411403	100.0205	0.50	1.00	0.00	0.00
C8H16O3S	192.0820	4.01	0.33	2.00	0.38

C8H12O5	188 0685	1.81	0.60	1.50	0.63
COLLING	107.0000	7.24	1.00	1.00	0.44
C9HTINO4	197.0688	7.34	1.00	1.22	0.44
C9H8O4	180.0423	2.77	1.00	0.89	0.44
C8H7NO5	197 0324	3 33	1.00	0.88	0.63
00171003	197.0324	5.55	1.00	0.88	0.05
C10H18N2O11S	374.0631	4.99	0.27	1.80	1.10
C4H10O4S	154 0300	0.91	0.00	2.50	1.00
CALLENIO2	115 0200	0.20	1.00	1.05	0.75
C4H5NO3	115.0269	0.39	1.00	1.25	0.75
C9H17NO9S	315.0624	2.50	0.22	1.89	1.00
C0H16078	268 0617	0.60	0.20	1 79	0.78
C9H100/3	208.0017	0.00	0.29	1.70	0.78
C7H5NO4	167.0219	3.77	1.00	0.71	0.57
C6H14O5S	198 0562	0.81	0.00	2 33	0.83
C0114035	198.0502	0.01	0.00	2.55	0.85
C8H17NO8S	287.0675	2.99	0.13	2.13	1.00
C9H7NO4	193 0375	7 14	1.00	0.78	0.44
COLICIDO2	100.0279	2.75	1.00	0.77	0.22
C9H6N2O3	190.0378	2.75	1.00	0.67	0.55
C6H5NO4	155.0219	0.41	1.00	0.83	0.67
C10H15NO10S	341 0417	2 99	0.40	1 50	1.00
	541.0417	2.))	0.40	1.50	1.00
C3H7NO7S	200.9943	0.85	0.14	2.33	2.33
C11H18O5	230 1154	3 20	0.60	1 64	0.45
CTHENO(	100.0117	3.20	1.00	0.71	0.15
C/H5NO6	199.0117	3.46	1.00	0.71	0.86
C8H16O4S	208.0769	6.33	0.25	2.00	0.50
CSUGOSS	177.0026	0.42	0.60	1 20	1.00
C5H6055	177.9930	0.42	0.60	1.20	1.00
C5H6O4S	161.9987	0.64	0.75	1.20	0.80
C10H16088	206.0566	0.50	0.38	1.60	0.80
C10H10085	290.0300	0.39	0.38	1.00	0.80
C6H13NO8S	259.0362	1.38	0.13	2.17	1.33
C5H12O3S	152 0507	1.80	0.00	2.40	0.60
031112035	152.0507	1.00	0.00	2.40	0.00
C6H3N3O7	228.9971	4.12	1.00	0.50	1.17
C24H24O3S	392,1446	8.14	1.00	1.00	0.13
6211121055	106.0270	0.11	1.00	0.00	0.15
C9H8O5	196.0372	2.76	1.00	0.89	0.56
C8H9NO4	183.0532	6.43	1.00	1.13	0.50
COLLINOZ	222.0526	2.01	0.57	1 20	0.00
Contino/	255.0550	5.01	0.57	1.56	0.88
C6H13NO7S	243.0413	3.25	0.14	2.17	1.17
C11H18N2O2	210 1368	2 60	1.00	1.64	0.18
C1111181N2O2	210.1308	2.09	1.00	1.04	0.18
C6H10O3	130.0630	0.66	0.67	1.67	0.50
C15H28O8S	368 1505	7.60	0.25	1.87	0.53
C71115N000	372.0519	7.00	0.23	1.07	1.1.4
C/HI5NO8S	273.0518	2.68	0.13	2.14	1.14
C10H22O4S	238,1239	8.01	0.00	2.20	0.40
COLISNOA	170.0210	1 97	1.00	0.62	0.50
Consinu4	179.0219	4.07	1.00	0.05	0.50
C9H8N2O2	176.0586	7.45	1.00	0.89	0.22
C10H1807S	282 0773	0.68	0.20	1.80	0.70
C10H18073	282.0773	0.08	0.29	1.60	0.70
C11H20O6S	280.0981	3.85	0.33	1.82	0.55
C11H21NO8	295 1267	3.01	0.25	1 91	0.73
CI IIIZINO0	295.1207	5.01	0.23	1.71	0.15
C13H19N06	285.1212	1.37	0.83	1.46	0.46
C7H6N2O6	214 0226	3.51	1.00	0.86	0.86
C711140(S	226.0511	2.46	0.17	2.00	0.00
C/H14065	226.0511	2.40	0.17	2.00	0.80
C8H14O10S	302.0308	2.25	0.20	1.75	1.25
C0H18N2O4	218 1267	2.67	0.50	2.00	0.44
C9H18N2O4	218.1207	2.07	0.50	2.00	0.44
C16H10O	218.0732	8.36	1.00	0.63	0.06
C7H14O5S	210.0562	1.83	0.20	2.00	0.71
C12111004	210.0502	1.05	0.20	2.00	0.71
C13H10O4	230.0579	5.34	1.00	0.77	0.31
C13H9NO3	227.0582	8.23	1.00	0.69	0.23
C19U2602	284 2715	0.52	0.50	2.00	0.11
C16H30U2	204.2/13	9.55	0.50	2.00	0.11
C9H6O6	210.0164	1.15	1.00	0.67	0.67
C9H8O5	196 0372	3 30	1.00	0.80	0.56
0014003	150.0372	2.01	1.00	0.07	0.50
C8H6O3	150.0317	3.01	1.00	0.75	0.38
C5H5NO4	143.0219	1.22	1.00	1.00	0.80
011111005	113.0217	1.22	1.00	1.00	0.00
CHHI0O5	222.0528	2.92	1.00	0.91	0.45
C9H16O6S	252.0668	0.83	0.33	1.78	0.67
C10H20049	260 0001	2 02	0.17	2.00	0.60
010020005	208.0981	3.63	0.17	2.00	0.00
C9H9NO6	227.0430	3.36	1.00	1.00	0.67
C7H13NO7S	255 0/12	3 17	0.20	1 86	1.00
	233.0413	J.+2	0.27	1.00	1.00
C7H14O4	162.0892	0.81	0.25	2.00	0.57
C7H7NO3	153 0426	2 57	1.00	1.00	0.43
0014050	133.0420	1.51	1.00	1.00	0.43
C8H6O5S	213.9936	1.54	1.00	0.75	0.63
C6H8O2	112.0524	1.01	1.00	1.33	0.33
C011002	126.0524	2 50	1.00	1.00	0.25
С8н802	130.0524	5.50	1.00	1.00	0.25
C11H20O7S	296.0930	2.90	0.29	1.82	0.64
C6H13NOVS	250 0262	2.61	0.12	2 17	1 22
CONTSINUAS	239.0302	2.01	0.15	2.17	1.33
C12H14O5	238.0841	3.39	1.00	1.17	0.42
C7H12O2	128 0837	1 71	1.00	1 71	0.29
0711202	110.0051	1./1	1.00	1./1	0.27
C/H5NO	119.0371	3.12	1.00	0.71	0.14

C7H4N2O4	180.0171	3.49	1.00	0.57	0.57
C10U19075	282 0772	1 /2	0.20	1.90	0.70
C10H18075	282.0773	1.45	0.29	1.60	0.70
C10H19NO9S	329.0781	2.30	0.22	1.90	0.90
C8H10O5	186 0528	0.62	0.80	1 25	0.63
C0111 (070	269.0617	0.02	0.00	1.20	0.05
C9H1607S	208.0017	2.39	0.29	1./8	0.78
C13H11NO3	229.0739	8.12	1.00	0.85	0.23
C13H8O10	324 0117	2.26	1.00	0.62	0.77
015118010	524.0117	2.20	1.00	0.02	0.77
C14H22O4	254.1518	6.61	1.00	1.57	0.29
C9H16O6S	252,0668	3.71	0.33	1.78	0.67
CTIKOA	154.0266	2.59	1.00	0.96	0.57
C/H604	154.0266	2.58	1.00	0.80	0.57
C8H8N2O4	196.0484	3.18	1.00	1.00	0.50
C10H6O4	190.0266	3 34	1.00	0.60	0.40
C1011004	190.0200	5.54	1.00	0.00	0.40
C20H1809	402.0951	7.44	1.00	0.90	0.45
C8H6O3	150.0317	0.83	1.00	0.75	0.38
C9H5NO4	170.0210	5 22	1.00	0.62	0.50
Collon04	179.0219	5.55	1.00	0.05	0.50
C5H5N3O4	171.0280	3.93	1.00	1.00	0.80
C8H6O2	134.0368	1.77	1.00	0.75	0.25
CIOULINOA	200.0688	7.16	1.00	1 10	0.40
CIUHIIN04	209.0088	/.10	1.00	1.10	0.40
C9H14O5S	234.0562	2.53	0.60	1.56	0.56
C8H9NO5	199 0481	4 22	1.00	1 13	0.63
Collonoo	1/0.0401	1.12	1.00	1.15	0.05
C5H4N2O3	140.0222	1.13	1.00	0.80	0.60
C9H7NO	145.0528	3.46	1.00	0.78	0.11
C12H11NO2S	261.0460	2.65	1.00	0.85	0.22
CISHINOSS	201.0400	2.05	1.00	0.85	0.23
C9H17NO8S	299.0675	3.36	0.25	1.89	0.89
C6H12O6S	212 0355	1.52	0.17	2.00	1.00
C01112005	212.0355	1.52	0.17	2.00	0.70
C9H10O/S	262.0147	2.68	0.71	1.11	0.78
C8H14O7S	254.0460	2.27	0.29	1.75	0.88
C12H0NO4	221 0522	7 42	1.00	0.75	0.22
C12H9N04	231.0332	1.42	1.00	0.75	0.33
C5H6O3	114.0317	0.85	1.00	1.20	0.60
C10H8O5	208 0372	240	1.00	0.80	0.50
COLLOS	192.0215	2.10	1.00	0.75	0.50
C8H0U5	182.0215	2.48	1.00	0.75	0.65
C6H6O4	142.0266	0.40	1.00	1.00	0.67
C14H10O2	210.0681	7.86	1.00	0.71	0.14
C14111002	210.0081	7.00	1.00	0.71	0.14
C12H21NO9S	355.0937	6.51	0.33	1.75	0.75
C9H16O6S	252.0668	4.10	0.33	1.78	0.67
C11U17NO8	201.0054	2.04	0.50	1.55	0.72
CITHI/NO8	291.0934	2.94	0.50	1.55	0.75
C9H5NO5	207.0168	3.90	1.00	0.56	0.56
C7H13NO9S	287 0311	2 70	0.22	1.86	1 29
C12U002	210.0311	2.70	1.00	0.60	0.02
C13H8O3	212.0473	7.04	1.00	0.62	0.23
C8H16O7S	256.0617	0.76	0.14	2.00	0.88
C18H13NO6	330 0743	7.86	1.00	0.72	0.33
C18H15N00	339.0743	7.80	1.00	0.72	0.33
C15H25NO7S	363.1352	8.09	0.57	1.67	0.47
C9H8O5S	228 0092	2 45	1.00	0.89	0.56
COLIZNO2	177.0426	2.15	1.00	0.79	0.20
C9H/NO3	177.0426	3.32	1.00	0.78	0.33
C9H7NO	145.0528	2.22	1.00	0.78	0.11
C8H6O3	150 0317	1 11	1.00	0.75	0.38
6011005	150.0517	1.11	1.00	0.75	0.50
C5H11NO8S	245.0205	0.85	0.13	2.20	1.60
C5H9NO7S	227.0100	3.12	0.29	1.80	1.40
C12U7NO4	241 0275	7.94	1.00	0.54	0.21
	271.0373	7.04	1.00	1.00	1.22
C6H11NO8S	257.0205	2.77	0.25	1.83	1.33
C13H8O4	228.0423	7.86	1.00	0.62	0.31
C5H5NO2	127.0260	1.02	1.00	1.00	0.60
CJHJNOJ	127.0209	1.05	1.00	1.00	0.00
C10H11NO3	193.0739	7.88	1.00	1.10	0.30
C7H7NO2	137 0477	2.34	1.00	1.00	0.29
C101111102	241.0506	5.00	1.00	1.00	0.29
CIUHIINO6	241.0586	5.33	1.00	1.10	0.60
C9H20O3S	208.1133	7.15	0.00	2.22	0.33
C7H13NO8S	271 0362	282	0.25	1 86	1.14
0/111510005	2/1.0302	2.02	0.23	1.00	1.14
C11H18O4	214.1205	6.72	0.75	1.64	0.36
C14H13NO3S	275.0616	3.09	1.00	0.93	0.21
CIOLIONOA	207.0522	7 40	1.00	0.00	0.40
CIUH9INO4	207.0532	1.09	1.00	0.90	0.40
C13H8O3	212.0473	7.51	1.00	0.62	0.23
C8H7NO3	165 0426	1 28	1.00	0.88	0.38
	270.1201	1.20	1.00	0.00	0.50
C15H25NO8S	379.1301	7.65	0.50	1.67	0.53
C7H11NO9S	285.0155	1.58	0.33	1.57	1.29
C7H/N2O2	164 0222	3.07	1.00	0.57	0.42
C/H4IN2U3	104.0222	3.91	1.00	0.57	0.45
C10H12O5S	244.0405	4.97	1.00	1.20	0.50
C9H10O5S	230 0249	2 54	1.00	1 11	0.56
C111110035	200.0279	2.0 1	1.00	0.01	0.26
CITH1004	206.0579	5.17	1.00	0.91	0.36
C9H20O4S	224.1082	6.18	0.00	2.22	0.44
C10H0NO4	207 0532	1 82	1.00	0 00	0.40
0101171104	201.0332	7.02	1.00	0.70	0.40

C8H15NO9S	301.0468	2.33	0.22	1.88	1.13
C20H14N2OS	330 0827	672	1.00	0.70	0.05
C101104068	350.0027	0.72	0.17	0.70	0.05
C12H24O6S	296.1294	7.01	0.17	2.00	0.50
C9H6O6	210.0164	1.84	1.00	0.67	0.67
C11H17NO8	201 0054	3 23	0.50	1 55	0.73
	271.0754	5.25	0.50	1.55	0.75
C11H8O2	172.0524	3.83	1.00	0.73	0.18
C14H11NO2S	257.0510	2.43	1.00	0.79	0.14
C14U0NO2	220.0592	0.00	1.00	0.64	0.21
CI4H9NO5	239.0582	8.22	1.00	0.64	0.21
C9H7NO4	193.0375	6.74	1.00	0.78	0.44
C9H7NO4	193 0375	1 33	1.00	0.78	0.44
011/104	175.0575	1.55	1.00	0.70	0.44
C9H14O/S	266.0460	1.28	0.43	1.56	0.78
C11H18N2O4S	274.0987	2.36	1.00	1.64	0.36
C15H8O4	252 0422	5 24	1.00	0.52	0.27
015H804	232.0423	5.24	1.00	0.55	0.27
C10H10O4	194.0579	2.79	1.00	1.00	0.40
C9H9NO6	227 0430	2 97	1.00	1.00	0.67
C9112N4011	240.0502	7 10	0.45	1.60	1 20
C6H12N4O11	540.0505	/.10	0.45	1.50	1.56
C7H9NO8S	267.0049	2.45	0.50	1.29	1.14
C4H4N2O2	112 0273	2.06	1.00	1.00	0.50
C1011102	112.0275	2.00	1.00	1.00	0.50
C18H16O6	328.0947	8.16	1.00	0.89	0.33
C8H11NO5S	233.0358	0.59	0.80	1.38	0.63
C12H10O2	108 0681	7.07	1.00	0.77	0.15
015111002	198.0081	1.91	1.00	0.77	0.15
C/H6O2	122.0368	0.83	1.00	0.86	0.29
C8H9NO5S	231.0201	2.72	1.00	1.13	0.63
CIOUIONOOS	220.0791	1 20	0.22	1.00	0.00
C10H19N095	529.0781	1.30	0.22	1.90	0.90
C19H12O4	304.0736	8.03	1.00	0.63	0.21
C8H13NO9S	299.0311	3.00	0.33	1.63	1 1 3
C1 (111002	2222000	5.00	1.00	1.05	1.15
C14H10O3	226.0630	7.88	1.00	0.71	0.21
C13H26O5S	294.1501	7.63	0.20	2.00	0.38
C6U12068	212 0255	2.52	0.17	2.00	1.00
C0H12005	212.0555	2.32	0.17	2.00	1.00
C11H8N2O5	248.0433	8.17	1.00	0.73	0.45
C11H16O5	228 0998	3 27	0.80	1 45	0.45
C(1111NOOS	272.0155	0.00	0.00	1.10	1.50
C6H11NO9S	273.0155	0.96	0.22	1.83	1.50
C7H6O4S	185.9987	1.37	1.00	0.86	0.57
C10H9NO4	207 0532	4.52	1.00	0.00	0.40
C1011/1004	207.0552	4.52	1.00	0.90	0.40
C6H10O5S	194.0249	0.59	0.40	1.67	0.83
C9H6O4	178.0266	2.95	1.00	0.67	0.44
COUTNO	122.0528	2.20	1.00	0.88	0.12
Contino	133.0328	2.29	1.00	0.88	0.15
C7H9NO9S	282.9998	3.20	0.44	1.29	1.29
C7H16O5S	212 0718	1.89	0.00	2 29	0.71
C01115N00	212:0710	2.10	0.00	1.27	0.71
C9HI5NO8	265.0798	3.10	0.38	1.67	0.89
C3H2N2O4	130.0015	0.55	1.00	0.67	1.33
C10H16088	206.0566	2 72	0.38	1.60	0.80
0101110083	290.0500	2.12	0.58	1.00	0.80
C23H28N4OS2	440.1705	7.19	1.00	1.22	0.04
C14H9NO2	223 0633	7.60	1.00	0.64	0.14
C0119O	122.0575	2.00	1.00	0.00	0.11
C9H8O	132.0575	3.09	1.00	0.89	0.11
C8H11NO8S	281.0205	2.98	0.50	1.38	1.00
C10H21NO8S	315 0988	3 79	0.13	2 10	0.80
COLIONOZO	275.0100	2.70	0.15	2.10	0.00
C9H9NO/S	275.0100	3.72	0.80	1.00	0.78
C5H11NO8S	245.0205	1.09	0.13	2.20	1.60
C4H10O3S	138 0351	0.62	0.00	2 50	0.75
01111030010	220.0051	7.02	0.00	2.50	0.75
C11H18N2O10	338.0961	/.88	0.40	1.64	0.91
C8H5NO5	195.0168	3.14	1.00	0.63	0.63
C0H17NO7S	283 0726	7 26	0.20	1 80	0.78
	203.0720	1.20	1.00	1.07	0.70
C14H10O4	242.0579	6.66	1.00	0.71	0.29
C10H10O6S	258.0198	1.63	1.00	1.00	0.60
C13H600	306 0012	2 57	1.00	0.46	0.60
015/1009	300.0012	2.37	1.00	0.40	0.09
C5H12O4S	168.0456	2.12	0.00	2.40	0.80
C8H5NO6	211.0117	2.56	1.00	0.63	0.75
COLINO	148 0524	2 27	1.00	0.00	0.22
0911802	146.0524	5.57	1.00	0.89	0.22
C9H8O5S	228.0092	2.76	1.00	0.89	0.56
C7H10O2	126 0681	2.77	1.00	1.43	0.29
07111002	140.0001	0.01	1.00	1.40	0.42
C/H10O3	142.0630	0.81	1.00	1.43	0.43
C9H7NO6	225.0273	3.17	1.00	0.78	0.67
C7H8O5	172 0372	1.07	0.80	1.14	0.71
	172.0372	1.07	0.00	1.14	0.71
C4H/NO9S	244.9842	0.59	0.22	1.75	2.25
C7H12N2O3	172.0848	2.45	1.00	1.71	0.43
C7H7NO4	169 0375	6 22	1.00	1.00	0.57
	107.0373	0.22	1.00	1.00	0.57
C10H17NO4	215.1158	3.60	0.75	1.70	0.40
C8H7NO3	165.0426	6.71	1.00	0.88	0.38
CSULLOCS	100 0100	1.00	0.17	2.00	1 20
C3H1000S	190.0198	1.00	0.17	2.00	1.20

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C5H11NO9S	261.0155	0.54	0.11	2.20	1.80
GTHING	201.0155	0.51	0.11	2.20	1.00
C/H10O2	126.0681	1.21	1.00	1.43	0.29
C11H12N2O4S	268 0518	7.18	1.00	1.09	0.36
0511211200	127,0225	2.17	1.00	0.00	0.40
C5H3N3O2	137.0225	3.17	1.00	0.60	0.40
C9H11N3OS2	241 0344	0.58	1.00	1.22	0.11
07111000	100.0001	2.06	1.00	1.42	0.00
C/H10O2	126.0681	2.06	1.00	1.43	0.29
C14H28O5S	308.1657	7.90	0.20	2.00	0.36
C0111002	166.0620	2.24	1.00	1 1 1	0.22
C9H10O3	166.0630	3.34	1.00	1.11	0.33
C15H9NO3S	283.0303	2.92	1.00	0.60	0.20
C1411120462	200.0177	1.01	1.00	0.00	0.20
C14H12O4S2	308.0177	1.21	1.00	0.86	0.29
C10H11NO3	193 0739	2 99	1.00	1 10	0.30
071171204	107.0427	5.67	1.00	1.00	0.57
C/H/N304	197.0437	5.67	1.00	1.00	0.57
C8H16O5S	224.0718	1.70	0.20	2.00	0.63
C10U10NO7S	207 0992	7 16	0.20	1.00	0.70
C10H19N075	297.0882	7.40	0.29	1.90	0.70
C9H18O6S	254.0824	4.30	0.17	2.00	0.67
C0H8O4	180.0422	1 22	1.00	0.80	0.44
0911804	180.0423	1.55	1.00	0.89	0.44
C8H7NO7S	260.9943	2.81	0.86	0.88	0.88
C13H8O3	212 0473	6 5 2	1.00	0.62	0.23
C1511805	212.0475	0.52	1.00	0.02	0.25
C6H12O6S	212.0355	2.83	0.17	2.00	1.00
C7H12O3	144 0786	1.08	0.67	1 71	0.43
0/111203	144.0780	1.00	0.07	1./1	0.45
C8H14O6S	238.0511	2.57	0.33	1.75	0.75
C10H17N08S	311.0675	6 59	0.38	1 70	0.80
010111/10005	511.0075	0.57	0.50	1.70	0.00
C6H5N3O2	151.0382	4.18	1.00	0.83	0.33
C8H8N2O6	228 0382	7 57	1.00	1.00	0.75
C011011200	220.0302	1.51	1.00	1.00	0.75
C9H5NO5	207.0168	3.18	1.00	0.56	0.56
C12H8O3	200.0473	4 38	1.00	0.67	0.25
01211005	200.0475	<b>-</b>	1.00	0.07	0.25
C11H18N2O10	338.0961	7.48	0.40	1.64	0.91
C8H8O3	152 0473	6.12	1.00	1.00	0.38
001005	152.0475	0.12	1.00	1.00	0.50
C7H5NO6	199.0117	2.68	1.00	0.71	0.86
C15H8O4	252 0423	7.61	1.00	0.53	0.27
C1311004	252.0425	1.01	1.00	0.00	0.27
C12H10O3S2	266.00/1	1.62	1.00	0.83	0.25
C8H16O6S	240.0668	3 28	0.17	2.00	0.75
CTHENOD	210.0000	5.20	1.00	2.00	0.75
C/H5NO2	135.0320	2.65	1.00	0.71	0.29
C13H16O3	220 1099	8.10	1.00	1.23	0.23
015111000	224.0027	0.10	1.00	0.00	0.12
C15H12O2	224.0837	8.10	1.00	0.80	0.13
C11H13NO3	207.0895	8.17	1.00	1.18	0.27
COLLICOTE	256.0617	1.01	0.14	2.00	0.00
C8H160/S	250.0017	1.01	0.14	2.00	0.88
C11H20O4	216.1362	3.18	0.50	1.82	0.36
0(1114059	100.0560	0.11	0.00	0.00	0.02
C6H14O5S	198.0562	2.11	0.00	2.33	0.83
C7H7N3O4	197.0437	6 90	1.00	1.00	0.57
COLIZINOS	200.0224	2.07	1.00	0.70	0.50
C9H/NO5	209.0324	3.97	1.00	0.78	0.56
C5H10N2O10	258.0335	2.33	0.20	2.00	2.00
CELIONOOG	259,0009	1.04	0.22	1.00	1.00
C5H9NO95	258.9998	1.04	0.22	1.80	1.80
C7H8O4S	188.0143	2.55	1.00	1.14	0.57
C10U7NO4	205 0275	2.00	1.00	0.70	0.40
C10H/N04	203.0373	5.09	1.00	0.70	0.40
C8H14O9S	286.0359	1.21	0.22	1.75	1.13
C8H7NO2	165 0426	7 26	1.00	0 80	0.30
0311/1005	105.0420	7.50	1.00	0.88	0.58
C7H7NO4	169.0375	6.61	1.00	1.00	0.57
C11H21NO9	311 1216	2 47	0.22	1 91	0.82
01111107	222.0522	2.77	1.00	1.71	0.02
CTIHI005	222.0528	3.57	1.00	0.91	0.45
C10H10O7S	274 0147	2.79	0.86	1.00	0.70
CCHPOA	144.0402	2.72	0.00	1 22	0.77
C0H8U4	144.0423	2.52	0.75	1.55	0.67
C10H8N2O3	204.0535	2.96	1.00	0.80	0.30
C10H22O4	31/ 1510	7 71	1.00	1 16	0.21
C19H22U4	514.1518	/./1	1.00	1.10	0.21
C13H13NO3	231.0895	8.36	1.00	1.00	0.23
C0H14099	282 0400	1 97	0.38	1 56	0.80
03114003	202.0409	1.0/	0.30	1.50	0.09
C11H20O8S	312.0879	2.42	0.25	1.82	0.73
C9H10O3	166 0630	7 77	1.00	1 1 1	0 33
0111005	100.0050	1.41	1.00	1.11	0.55
C6H10O	98.0732	3.01	1.00	1.67	0.17
C7H15NO8S	273 0518	1 95	0.13	2 14	1.14
01110005	273.0310	1.75	1.00	2.17	0.17
CITH/NO5	233.0324	7.26	1.00	0.64	0.45
C9H10N2O5	226.0590	3.01	1.00	1.11	0.56
0015203	151 0000	2.01	1.00	0.02	0.20
C6H5N3O2	151.0382	3.84	1.00	0.83	0.33
C10H10O6S	258.0198	0.76	1.00	1.00	0.60
C12U1(O)	256.0047	2.00	0.02	1 22	0.50
C12H10O6	230.0947	2.90	0.83	1.35	0.50
C6H6N2O3	154.0378	2.14	1.00	1.00	0.50
C15U1002	228.0620	7.00	1.00	0.67	0.20
CISHI005	238.0030	7.99	1.00	0.07	0.20
C10H7NO5	221.0324	5.77	1.00	0.70	0.50
C11H602	186 0217	6.57	1.00	0.55	0.27
0111005	100.0317	0.57	1.00	0.55	0.27
C18H10O3	274.0630	7.99	1.00	0.56	0.17

C11H11NO4	221.0688	8.04	1.00	1.00	0.36
CLINICOL	221.0000	0.01	1.00	1.00	0.50
CITHI808S	310.0722	2.68	0.38	1.64	0.73
C11H12O3	192.0786	3.47	1.00	1.09	0.27
C0H11N2OS2	241 0244	0.88	1.00	1 22	0.11
C9H11N3O52	241.0344	0.88	1.00	1.22	0.11
C7H11NO8S	269.0205	4.53	0.38	1.57	1.14
C13H24OS2	260 1269	3 41	1.00	1.85	0.08
COLIENIO2C	104,0000	7.40	1.00	0.62	0.00
COHSINUSS	194.9990	7.40	1.00	0.65	0.38
C11H22N2O8S	342.1097	8.31	0.25	2.00	0.73
C1/H1005	258 0528	3 66	1.00	0.71	0.36
014111005	258.0528	5.00	1.00	0.71	0.50
C10H17NO9S	327.0624	6.29	0.33	1.70	0.90
C9H8N2O2	176 0586	6 69	1.00	0.89	0.22
C14U2002	214 2020	0.02	0.00	0.00	0.21
C14H28O3	244.2038	8.23	0.55	2.00	0.21
C10H20O5S	252.1031	3.82	0.20	2.00	0.50
C8H5NO6	211 0117	3.02	1.00	0.63	0.75
Constructo	211.0117	5.02	1.00	0.03	0.75
C9H/NO4	193.0375	2.34	1.00	0.78	0.44
C7H16O5S	212.0718	1.44	0.00	2.29	0.71
C16U1004	266.0570	7.40	1.00	0.62	0.25
C10H1004	200.0379	7.40	1.00	0.05	0.23
C10H10N2O2	190.0742	7.93	1.00	1.00	0.20
C12H25NO8S	3/13 1301	6.90	0.13	2.08	0.67
C1211251(005	1 70 0 60 1	0.50	0.15	2.00	0.07
CI0H9NO	159.0684	2.64	1.00	0.90	0.10
C10H9NO4	207.0532	2.81	1.00	0.90	0.40
COLIZNI2O5	225 0296	6.01	1.00	0.00	0.62
C8H/N3O3	223.0380	0.01	1.00	0.88	0.05
C6H8O6S	208.0042	1.15	0.50	1.33	1.00
C15H23NO88	377 1144	7 38	0.63	1 53	0.53
C1511251(085	377.1144	7.50	0.05	1.55	0.55
C8H6N2O5	210.0277	7.33	1.00	0.75	0.63
C11H11NO4	221.0688	6.95	1.00	1.00	0.36
COLICNIDOS	210.0277	6.50	1.00	0.75	0.00
C8H0N2O5	210.0277	0.93	1.00	0.75	0.65
C12H20O3	212.1412	8.41	1.00	1.67	0.25
C15H30O5S	322 1814	8 18	0.20	2.00	0.33
0151150055	522.1814	0.10	0.20	2.00	0.55
C12H21NO9S	355.0937	5.20	0.33	1.75	0.75
C12H18O5	242.1154	5.03	0.80	1.50	0.42
C(U7NO2	141.0426	2.60	1.00	1.17	0.50
COH/NO3	141.0420	2.40	1.00	1.1/	0.50
C14H20O6	284.1260	3.10	0.83	1.43	0.43
C10H0NO3	101 0582	4.40	1.00	0.00	0.30
	171.0502	4.40	1.00	0.90	0.50
C14H12O4	244.0736	7.21	1.00	0.86	0.29
C7H13NO6	207.0743	3.10	0.33	1.86	0.86
C10U12NO4	211.0945	7 00	1.00	1.20	0.40
C10H15N04	211.0843	7.00	1.00	1.50	0.40
C9H7NO6	225.0273	3.67	1.00	0.78	0.67
C14H28O6S	324 1607	7 70	0.17	2.00	0.43
C14I128003	324.1007	1.10	0.17	2.00	0.43
C10H11NO6	241.0586	4.15	1.00	1.10	0.60
C14H22O6	286,1416	3.15	0.67	1.57	0.43
COLLINOS	212.0627	4 21	1.00	1.00	0.56
C9HTINO5	213.0637	4.51	1.00	1.22	0.56
C9H6N2O3	190.0378	4.42	1.00	0.67	0.33
C16H10O4S	298.0300	7 53	1.00	0.63	0.25
0101110045	298.0300	1.55	1.00	0.05	0.25
C9H5NO5	207.0168	2.54	1.00	0.56	0.56
C13H26O6S	310.1450	7.40	0.17	2.00	0.46
CITITINO	221.0699	6.40	1.00	1.00	0.26
CITHIIN04	221.0088	0.42	1.00	1.00	0.50
C8H12O9S	284.0202	1.07	0.33	1.50	1.13
C8H13NO8	251 0641	2.42	0.38	1.63	1.00
Cellenace	120 0 420	0.02	1.00	1.00	1.00
COHON2O2	138.0429	0.92	1.00	1.00	0.55
C7H6N2O4	182.0328	3.45	1.00	0.86	0.57
C7H14O4	162 0892	2.40	0.25	2.00	0.57
	102.0072	2.70	0.20	2.00	0.57
C9H11NO5	213.0637	3.29	1.00	1.22	0.56
C8H6N2O5	210.0277	3.40	1.00	0.75	0.63
C11U12NO5	220.0704	1 52	1.00	1 10	0.45
CIIIIISNOS	239.0794	4.33	1.00	1.18	0.45
C20H30O4	334.2144	8.13	1.00	1.50	0.20
C10H1006S	258 0198	1.03	1.00	1.00	0.60
C101110005	230.0170	1.05	1.00	1.00	0.00
C10H12O11S	340.0100	3.01	0.45	1.20	1.10
C9H18O5S	238,0875	2.74	0.20	2.00	0.56
C12H12NO4	225 0945	754	1.00	1.00	0.22
C12n13IN04	255.0845	1.50	1.00	1.08	0.33
C6H6N2O6	202.0226	3.72	0.83	1.00	1.00
C8H8O	120.0575	3 28	1.00	1.00	0.13
	120.0373	5.20	1.00	1.00	0.15
C9H19NO7	253.1162	6.77	0.14	2.11	0.78
C10H17N3O3	227,1270	3.11	1.00	1.70	0.30
C8H12NO9	251.0641	0.02	0.29	1.62	1.00
CONTOINOO	231.0041	0.82	0.58	1.05	1.00
C13H23NO10S	385.1043	4.77	0.30	1.77	0.77
C5H9NO9S	258 9998	0.74	0.22	1.80	1.80
	200.000	0.74	1.00	1.00	1.00
C12H15NO3	221.1052	8.35	1.00	1.25	0.25
C4H5N3O2	127.0382	1.06	1.00	1.25	0.50
C14U2005	269 1211	2 72	1.00	1 42	0.24
01402003	200.1311	3.23	1.00	1.43	0.30

C11H8O2	172.0524	5.12	1.00	0.73	0.18
CGH12049	100.0456	5.12	1.00	0.75	0.10
C6H12O4S	180.0456	7.34	0.25	2.00	0.67
C16H14O4	270 0892	7.51	1.00	0.88	0.25
CIONOS	222.0491	5.00	1.00	0.00	0.50
CIUH9NO5	223.0481	5.82	1.00	0.90	0.50
C17H10O2	246 0681	7.61	1.00	0.59	0.12
C1 (111 4020	070 0714	1.24	1.00	0.00	0.12
C16H14O2S	2/0.0/14	1.34	1.00	0.88	0.13
C10H12O3	180.0786	7.89	1.00	1.20	0.30
015112(04	070 1021	0.14	0.75	1.70	0.07
C15H26O4	270.1831	8.14	0.75	1./3	0.27
C9H11NO4	197.0688	6.58	1.00	1.22	0.44
0101110070	074.0147	0.05	0.00	1.00	0.70
C10H10O/S	2/4.014/	0.95	0.86	1.00	0.70
C12H12O4	220.0736	7.71	1.00	1.00	0.33
CTUTNO	121.0529	2.10	1.00	1.00	0.14
C/H/NO	121.0528	3.18	1.00	1.00	0.14
C11H8O2	172.0524	6.74	1.00	0.73	0.18
C12U902	194.0524	5.15	1.00	0.77	0.17
C12H8O2	184.0524	5.15	1.00	0.67	0.17
C13H18O6	270 1103	2.99	0.83	1.38	0.46
C12U24N4OC62	206 1127	9.40	0.7	1.05	0.46
CI3H24IN40052	590.1157	8.49	0.07	1.65	0.40
C13H9NO	195.0684	4.52	1.00	0.69	0.08
C101120065	269 0091	4.04	0.17	2.00	0.60
C10H20005	208.0981	4.94	0.17	2.00	0.00
C20H13N3O3S	375.0678	8.24	1.00	0.65	0.15
CTUTNO	121 0529	1.02	1.00	1.00	0.14
C/H/NO	121.0328	1.02	1.00	1.00	0.14
C15H30O10	370.1839	8.47	0.10	2.00	0.67
C44902	88.0524	1.05	0.50	2.00	0.50
C4H8O2	88.0324	1.05	0.50	2.00	0.50
C14H8O3	224.0473	6.88	1.00	0.57	0.21
C11U1406	242.0700	2.00	0.92	1.07	0.55
CI1H1400	242.0790	2.99	0.85	1.27	0.55
C12H10O4	218.0579	3.16	1.00	0.83	0.33
0711605	170.0215	1.42	1.00	0.96	0.71
C/H003	170.0215	1.45	1.00	0.80	0.71
C8H9NO4	183.0532	7.60	1.00	1.13	0.50
C10111407	242.0740	7.74	1.00	0.70	0.20
C18H14O/	342.0740	1.14	1.00	0.78	0.39
C9H17NO9S	315.0624	4.83	0.22	1.89	1.00
012111002	014.0620	2.00	1.00	0.77	0.00
C13H10O3	214.0630	3.90	1.00	0.77	0.23
C10H12O4	196.0736	3.30	1.00	1.20	0.40
COLLINOA	107.0699	5 71	1.00	1.00	0.44
C9HTINO4	197.0688	5./1	1.00	1.22	0.44
C14H8O4	240.0423	6.44	1.00	0.57	0.29
0711100	110.0722	0.45	1.00	1.42	0.14
C/H100	110.0732	2.45	1.00	1.45	0.14
C18H32O9S	424.1767	7.44	0.33	1.78	0.50
C1911004	200.0570	7.60	1.00	050	0.22
C18H1004	290.0379	7.00	1.00	0.30	0.22
C13H11NO4	245.0688	7.97	1.00	0.85	0.31
CINIONIO	224 1525	2.00	1.00	1.77	0.17
C12H20N2O2	224.1323	2.00	1.00	1.07	0.17
C14H12O2	212.0837	8.21	1.00	0.86	0.14
C12U10O2	100 0601	7 19	1.00	0.77	0.15
C13H1002	198.0681	7.18	1.00	0.77	0.15
C11H9NO5	235.0481	7.46	1.00	0.82	0.45
C14U12NO4	250 0845	9.12	1.00	0.02	0.20
C14H15N04	239.0843	0.12	1.00	0.95	0.29
C14H8O4	240.0423	7.96	1.00	0.57	0.29
C0116O2	162 0217	2.02	1.00	0.67	0.22
C9H0O3	102.0317	3.95	1.00	0.07	0.55
C14H8O3	224.0473	5.86	1.00	0.57	0.21
C11U9O2	199 0472	5 1 2	1.00	0.72	0.27
C11H803	100.0475	5.12	1.00	0.75	0.27
C11H13NO6	255.0743	3.61	1.00	1.18	0.55
C6H10N2O3	158 0601	1.06	1.00	1.67	0.50
C01101203	130.00/1	1.00	1.00	1.07	0.50
C9H17NO9S	315.0624	6.32	0.22	1.89	1.00
C11H18N2O4	242, 1267	2.86	1.00	1.64	0.36
	272.0460	1.01	1.00	0.70	0.00
C14H11NO3S	2/3.0460	1.21	1.00	0.79	0.21
C13H18O3	222,1256	7.68	1.00	1.38	0.23
C10U12NO5	227.0704	4.00	1.00	1 20	0.50
CIUHISINUS	227.0794	4.00	1.00	1.50	0.50
C18H34O7S	394.2025	8.51	0.29	1.89	0.39
C12U24N2O4	272 1726	1 44	0.75	1 05	0.21
C13H24N2O4	212.1/30	1.40	0.75	1.80	0.51
C12H10O3	202.0630	7.17	1.00	0.83	0.25
C12H10O2	186 0691	7 14	1.00	0.92	0.17
012111002	100.0001	/.14	1.00	0.05	0.17
C8H7NO6	213.0273	4.71	1.00	0.88	0.75
C13H27N099	357 1457	7 62	0.12	2.00	0.62
013112/11/003	557.1457	7.05	0.15	2.00	0.02
C10H8N2O6	252.0382	7.81	1.00	0.80	0.60
C10H10N2O2	190 0742	7 58	1.00	1.00	0.20
	190.0742	1.50	1.00	1.00	0.20
C11H20O8S	312.0879	3.81	0.25	1.82	0.73
C12H25NO78	327 1352	8 23	0.14	2.08	0.58
012112311073	521.1552	0.23	0.14	2.00	0.50
C12H10O2	186.0681	7.54	1.00	0.83	0.17
C11H8O3	188 0473	4 83	1.00	0.73	0.27
C111005	100.0475	1.00	1.00	0.75	0.27
C14H8O3	224.0473	4.49	1.00	0.57	0.21
C13H8O3	212 0473	5 75	1.00	0.62	0.23
C10151055	212.0775	0.10	1.00	0.02	0.23
C10H/N05	221.0324	3.46	1.00	0.70	0.50
C14H12O2	212.0837	7.76	1.00	0.86	0.14
00111002	212.0057	0.50	0.00	1.54	0.17
C9H14O8S	282.0409	2.58	0.38	1.56	0.89

C9H10O2	150.0681	4.96	1.00	1.11	0.22
C12H10O3	202 0630	7.85	1.00	0.83	0.25
C(14N2O5	184.0120	( 20	1.00	0.05	0.23
C6H4N2O5	184.0120	0.20	1.00	0.67	0.85
C12H9NO4	231.0532	7.78	1.00	0.75	0.33
C13H10O2	198.0681	7.47	1.00	0.77	0.15
C10H7NO5	221 0324	4 14	1.00	0.70	0.50
C11U2004	216 1262	2.02	0.50	1.00	0.26
C11H20O4	210.1302	5.85	0.50	1.82	0.30
C10H6N2O2	186.0429	3.49	1.00	0.60	0.20
C15H25NO7	331.1631	7.70	0.57	1.67	0.47
C12H13NO4	235 0845	8 25	1.00	1.08	0.33
C14U905	255:0045	0.25	1.00	1.00	0.55
C14H805	256.0372	6.46	1.00	0.57	0.36
C14H11NO4	257.0688	8.35	1.00	0.79	0.29
C16H22O5	294.1467	8.42	1.00	1.38	0.31
C15H15NO4	273 1001	8 28	1.00	1.00	0.27
CI III O I	275.1001	0.20	1.00	1.00	0.27
C14H8O4	240.0423	3.96	1.00	0.57	0.29
C12H8O2	184.0524	5.39	1.00	0.67	0.17
C12H26O4S	266.1552	8.49	0.00	2.17	0.33
C9H16O4	188 10/9	3 71	0.50	1 78	0.44
C)111004	100.104)	3.71	0.50	1.70	0.44
C11H23N305	2/7.1638	2.56	0.40	2.09	0.45
C7H6O2	122.0368	2.72	1.00	0.86	0.29
C4H4O4	116 0110	0.40	0.75	1.00	1.00
C8H6O4	166.0266	2.68	1.00	0.75	0.50
001004	100.0200	2.08	1.00	0.75	0.50
C11H20O4	216.1362	7.06	0.50	1.82	0.36
C6H5NO3	139.0269	3.72	1.00	0.83	0.50
C5H8O4	132 0423	1.06	0.50	1.60	0.80
C9111005	196.0529	2.00	0.00	1.00	0.60
C8H1003	180.0328	2.99	0.80	1.23	0.05
C15H22O2	234.1620	8.55	1.00	1.47	0.13
C5H6O4	130.0266	0.62	0.75	1.20	0.80
C9H14O4	186 0892	2.84	0.75	1.56	0.44
C511905	149.0272	2.04	0.75	1.50	1.00
C5H805	148.0372	0.40	0.40	1.00	1.00
C8H12O4	172.0736	2.43	0.75	1.50	0.50
C3H4O4	104.0110	0.40	0.50	1.33	1.33
C10H10O5	210.0528	3.02	1.00	1.00	0.50
C10111005	210:0520	3.02	1.00	1.00	0.30
C16H24O5	296.1624	7.88	1.00	1.50	0.31
C3H6O5S	153.9936	0.39	0.20	2.00	1.67
C8H10O5	186.0528	2.27	0.80	1.25	0.63
C9H8O2	148 0524	3.05	1.00	0.89	0.22
C011002	140.0324	3.05	1.00	0.07	0.22
C9H8O3	164.0473	3.28	1.00	0.89	0.33
C9H14O5	202.0841	2.65	0.60	1.56	0.56
C7H6O3	138.0317	2.31	1.00	0.86	0.43
C4H6O5	134 0215	0.30	0.40	1 50	1.25
C411005	154.0215	0.39	0.40	1.50	1.23
C6H10O5	162.0528	0.48	0.40	1.67	0.83
C9H8O4	180.0423	3.14	1.00	0.89	0.44
C2H4O5S	139.9779	0.39	0.20	2.00	2.50
C6H8O4	144 0423	0.65	0.75	1 33	0.67
C011804	144.0423	0.05	0.75	1.55	0.07
C10H804	192.0423	3.09	1.00	0.80	0.40
C18H14O8	358.0689	7.44	1.00	0.78	0.44
C5H10O5	150.0528	0.37	0.20	2.00	1.00
C13H2005	256 1311	3 78	0.80	1.54	0.38
C13112003	72.0211	5.20	1.00	1.24	0.50
C3H4O2	72.0211	0.40	1.00	1.55	0.67
C10H16O5	216.0998	2.90	0.60	1.60	0.50
C7H7NO3	153.0426	5.95	1.00	1.00	0.43
C10H10O4	194 0579	3 60	1.00	1.00	0.40
C0111(05	204.0009	3.00	0.40	1.00	0.40
C9H1605	204.0998	2.57	0.40	1./8	0.56
C8H12O3	156.0786	2.85	1.00	1.50	0.38
C7H13NO3	159.0895	2.83	0.67	1.86	0.43
C5H6O5	146.0215	0.39	0.60	1.20	1.00
0211003	127 0007	0.57	0.00	2.00	1.00
03H6048	137.9987	0.37	0.25	2.00	1.55
C7H7NO3	153.0426	5.14	1.00	1.00	0.43
C7H10O5	174.0528	0.73	0.60	1.43	0.71
C5H6O3	114 0317	0.40	1.00	1 20	0.60
001003	114.0402	1.20	0.75	1.20	0.00
C6H8O4	144.0423	1.29	0.75	1.33	0.67
C9H18O4	190.1205	4.18	0.25	2.00	0.44
C12H8N2O5	260.0433	8.31	1.00	0.67	0.42
C7H7NO4	169 0375	4 07	1.00	1.00	0.57
	220 1215	2.07	0.62	1.00	0.57
C15H22O8	330.1315	3.06	0.63	1.4/	0.53
C8H6O3	150.0317	2.61	1.00	0.75	0.38
C8H14O5	190.0841	2.52	0.40	1.75	0.63
C6H8O3	128 0473	0.65	1.00	1 33	0.50
0011003	210.0026	7.10	1.00	2.55	0.50
C8H18045	210.0926	/.18	0.00	2.23	0.50

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G11111001	214 1205	2.10	0.75	1.74	0.04
CITH1804	214.1205	3.19	0.75	1.64	0.36
C10H14O6	230.0790	2.76	0.67	1.40	0.60
CITH1804	214.1205	3.79	0.75	1.64	0.36
C15H20N2O4S	324.1144	8.49	1.00	1.33	0.27
C11H20O3	200.1412	7.61	0.67	1.82	0.27
C12H9NO3	215.0582	8.09	1.00	0.75	0.25
C18H30O5	326.2093	8.02	0.80	1.67	0.28
C10H13NO4	211.0845	8.16	1.00	1.30	0.40
C7H5NO5	183.0168	3.26	1.00	0.71	0.71
C8H14O	126.1045	3.70	1.00	1.75	0.13
C10H18O4	202.1205	2.93	0.50	1.80	0.40
C18H34O5	330.2406	7.45	0.40	1.89	0.28
C13H24O2S2	276.1218	2.75	1.00	1.85	0.15
C2H4O2	60.0211	2.72	0.50	2.00	1.00
C2H4O2	60.0211	0.41	0.50	2.00	1.00
C7H6N2O3	166.0378	3.44	1.00	0.86	0.43
C3H8O4S	140.0143	0.50	0.00	2.67	1.33
C12H25NO5S	295.1453	4.62	0.20	2.08	0.42
C9H20O4S	224.1082	7.68	0.00	2.22	0.44
C11H24O4S	252.1395	8.26	0.00	2.18	0.36
C6H10O2	114.0681	2.71	1.00	1.67	0.33
C8H16O6S	240.0668	2.88	0.17	2.00	0.75
C11H18O6	246.1103	4.34	0.50	1.64	0.55
C9H16O3	172.1099	3.01	0.67	1.78	0.33
C8H18O3S	194.0977	5.22	0.00	2.25	0.38
C4H6O2	86.0368	0.53	1.00	1.50	0.50
C6H10O2	114.0681	1.23	1.00	1.67	0.33
C7H8O4	156.0423	1.01	1.00	1.14	0.57
C9H11NO3	181.0739	7.87	1.00	1.22	0.33
C6H5NO4	155.0219	3.06	1.00	0.83	0.67
C12H22O4	230.1518	3.74	0.50	1.83	0.33
C12H18O5	242.1154	3.06	0.80	1.50	0.42
C8H16O4	176.1049	1.43	0.25	2.00	0.50
C14H13NO3	243 0895	8.30	1.00	0.93	0.21
C8H7NO3	165.0426	3.19	1.00	0.88	0.38
C7H6O3	138 0317	2 77	1.00	0.86	0.43
C7H1006	190.0477	0.40	0.50	1 43	0.15
C10H12O3	180.0786	3 13	1.00	1 20	0.30
C11H22O4	218 1518	7 55	0.25	2.00	0.36
C9H12O4	184 0736	2 77	1.00	1.33	0.30
C9H12O4	168.0786	2.77	1.00	1.33	0.33
C6H8O3	128 0473	2.75	1.00	1.33	0.55
C15H15NO2S	273 0823	3 70	1.00	1.00	0.13
C6H12O4	1/8 0736	1.22	0.25	2.00	0.13
C10H11NO5	225.0637	3 53	1.00	2.00	0.07
C13H2006	223.0037	3.06	0.67	1.10	0.30
C14H5NO29	272.1200	2.00	1.00	0.36	0.40
C14H27NO4	231.0041	2.00 7.78	0.50	1.03	0.14
C7U5NO5	273.1940 192.0169	2.05	1.00	1.95	0.29
C2H7NO6	103.0100	2.93	1.00	0.71	0.71
COL/NO0	213.0273	5.55	1.00	0.88	0.75

Table S4.3.7 Molecular formulas of organic compounds detected in  $\alpha$ -pinene SOA in ESI- mode.

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Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
C9H14O4	186.0892	2.96	0.75	1.56	0.44
C9H14O4	186.0892	0.37	0.75	1.56	0.44
C8H12O4	172.0736	0.36	0.75	1.50	0.50
C10H16O5	216.0998	3.39	0.60	1.60	0.50
C10H16O4	200.1049	0.37	0.75	1.60	0.40
C10H16O3	184.1099	3.48	1.00	1.60	0.30
C8H12O4	172.0736	2.53	0.75	1.50	0.50
C8H14O4	174.0892	0.36	0.50	1.75	0.50
C10H14O5	214.0841	0.36	0.80	1.40	0.50
C10H16O4	200.1049	2.72	0.75	1.60	0.40
C19H28O7	368.1835	7.21	0.86	1.47	0.37

C10H14O4	198 0892	0.36	1.00	1 40	0.40
010111404	170.0072	0.50	1.00	1.40	0.40
C8H14O3	158.0943	2.92	0.67	1.75	0.38
C0111205	100.0005	2.29	0.00	1.50	0.02
C8H12O5	188.0685	3.28	0.60	1.50	0.05
C11H18O6	246 1103	2 71	0.50	1.64	0.55
CIIII000	240.1105	2.71	0.50	1.04	0.55
C7H10O4	158.0579	3.37	0.75	1.43	0.57
00111402	170.0042	0.20	1.00	1.50	0.22
C9H14O3	170.0943	0.38	1.00	1.56	0.33
C4H4O2	100.0160	0.26	1.00	1.00	0.75
C4H4O5	100.0100	0.50	1.00	1.00	0.75
C9H14O3	170 0943	3.09	1.00	1 56	0.33
6,111,105	170.0915	5.07	1.00	1.00	0.55
C4H8O2	88.0524	0.35	0.50	2.00	0.50
C0111202	150 0790	0.29	1.00	1.50	0.20
C8H12O3	156.0786	0.38	1.00	1.50	0.38
C0H14O3	170.0043	7 71	1.00	1 56	0.33
0311403	170.0945	/./1	1.00	1.50	0.55
C11H18O7	262.1053	3.06	0.43	1.64	0.64
00111405	100.0041	2.44	0.40	1.77	0.60
C8H14O5	190.0841	2.44	0.40	1.75	0.63
C9U12O2	156 0786	2 97	1.00	1.50	0.29
C6H12O3	130.0780	2.07	1.00	1.50	0.58
C18H26O6	338 1729	7 51	1.00	1 44	0.33
0101120000	000000		1.00	4 50	0.00
C4H6O2	86.0368	0.36	1.00	1.50	0.50
C711904	156 0422	0.26	1.00	1 1 4	0.57
C/H804	130.0425	0.50	1.00	1.14	0.57
C10H14O4	198 0892	7 14	1.00	1 40	0.40
	190.0092		1.00	1110	0.110
C20H32O7	384.2148	6.76	0.71	1.60	0.35
C17U2(00	259 1 (29	4.00	0.62	1 5 2	0.47
C1/H2608	338.1028	4.90	0.65	1.55	0.47
C20H32O7	384 2148	6.07	0.71	1.60	0.35
C20115207	304.2140	0.97	0.71	1.00	0.55
C9H14O5	202.0841	1.68	0.60	1.56	0.56
C10111.00 F	21 6 0 0 0 0		0.00	4 60	0.50
C10H16O5	216.0998	1.76	0.60	1.60	0.50
C20H2000	209 10/1	7 05	0.75	1.50	0.40
C20H30O8	396.1941	1.00	0.75	1.50	0.40
C20H32O7	384 2148	8 08	0.71	1.60	0.35
C20115207	504.2140	0.00	0.71	1.00	0.55
C5H8O2	100.0524	0.36	1.00	1.60	0.40
CCURON	110.0504	0.26	1.00	1.22	0.22
C6H8O2	112.0524	0.36	1.00	1.33	0.33
C9U1205	199 0695	2 97	0.60	1.50	0.62
C6H12O3	100.0005	2.07	0.00	1.50	0.05
C9H12O4	184.0736	0.36	1.00	1.33	0.44
	10110720	0.20	1.00	1.00	0
C7H10O3	142.0630	0.37	1.00	1.43	0.43
C7U1404	162 0802	2.04	0.25	2.00	0.57
C/H1404	102.0892	2.94	0.23	2.00	0.57
C7H8O3	140.0473	0.37	1.00	1.14	0.43
C/11005	140.0475	0.57	1.00	1.14	0.45
C19H28O5	336.1937	8.02	1.00	1.47	0.26
07111202	120,0007	0.04	1.00	1 7 1	0.00
C/H12O2	128.0837	0.36	1.00	1./1	0.29
C20H30O8	308 10/1	7 52	0.75	1 50	0.40
C201150008	390.1941	1.52	0.75	1.50	0.40
C19H30O5	338,2093	8.09	1.00	1.58	0.26
010115005	550.2095	0.09	1.00	1.50	0.20
C6H10O2	114.0681	0.36	1.00	1.67	0.33
C10U2(O0	270 1 (29	7 70	0.75	1 4 4	0.44
C18H2008	370.1628	1.12	0.75	1.44	0.44
C10H14O3	182 09/3	3.81	1.00	1.40	0.30
C10111403	182.0945	5.61	1.00	1.40	0.50
C8H14O2	142.0994	0.37	1.00	1.75	0.25
CALLIALOO	100.0000	5.10	0.54	1.00	0.40
C21H34O9	430.2203	7.13	0.56	1.62	0.43
C20H22O0	416 2046	7.40	0.56	1.60	0.45
C20H32O9	410.2040	7.49	0.50	1.00	0.45
C19H30O5	338 2093	6 99	1.00	1 58	0.26
0101150055	550.2075	0.77	1.00	1.50	0.20
C7H8O3	140.0473	2.99	1.00	1.14	0.43
0211(0	50.0410	0.27	1.00	2.00	0.22
CSHOU	58.0419	0.37	1.00	2.00	0.55
C8H14O6	206.0790	2 34	0.33	1 75	0.75
0011400	200.0770	2.54	0.55	1.75	0.75
C21H34O9	430.2203	7.66	0.56	1.62	0.43
COLLIDOA	170.0570	2.07	1.00	1.05	0.50
C8H1004	170.0579	3.27	1.00	1.25	0.50
C19H32O8	388 2097	7 39	0.50	1 68	0.42
017115200	11500.2077		0.50	1.00	0.12
C7H14O3	146.0943	2.59	0.33	2.00	0.43
C7111002	126 0601	0.20	1.00	1 42	0.20
C/H1002	120.0081	0.30	1.00	1.45	0.29
C19H30O6	354 2042	7 41	0.83	1.58	0.32
010110000	000.100.2		1.00	1.00	0.02
C19H28O6	352.1886	7.81	1.00	1.47	0.32
C17U2600	250 1600	6.20	0.62	1 5 2	0.47
C1/H20U8	536.1028	0.30	0.05	1.33	0.47
C8H10O4	170 0579	0.37	1.00	1 25	0.50
0111004	170.0077	0.57	1.00	1.20	0.50
C19H32O8	388.2097	7.22	0.50	1.68	0.42
0711000	104.0504	0.27	1.00	1 1 /	0.00
C/H802	124.0524	0.37	1.00	1.14	0.29
C0H12O2	168 0786	0.36	1.00	1 32	0 33
071112003	100.0700	0.50	1.00	1.55	0.55
C11H16O6	244.0947	3.31	0.67	1.45	0.55
0001122011	440.1045	7.50	0.45	1 (0	0.55
C20H32O11	448.1945	7.53	0.45	1.60	0.55
C21U3600	122 2250	Q 15	0.44	1 71	0.42
C21H3009	+32.2339	0.13	0.44	1./1	0.43
C9H12O4	184 0736	2.92	1.00	1.33	0.44
CIOLICO -	101.0750	2.72	1.00	1.55	0.00
C19H28O6	352.1886	7.53	1.00	1.47	0.32
C16U2607	220 1670	1 12	0.57	1 42	0.44
C10H20U/	550.1079	4.15	0.57	1.03	0.44
C20H32O6	368 2199	8 31	0.83	1.60	0.30
020115200	500.2177	0.51	0.00	1.00	0.50
C10H16O7	248.0896	3.00	0.43	1.60	0.70
CIOUZOOC	256 2100	7 (2)	0.77	1 (0	0.22
C19H32O6	330.2199	1.62	0.67	1.68	0.32
C8H12O2	140 0837	0.36	1.00	1 50	0.25
0111202	140.0007	0.50	1.00	1.50	0.25
C11H20O8	280.1158	2.47	0.25	1.82	0.73
C10112C07	254 1 (70)	(75	0.07	1 4 4	0.20
C18H26U/	354.16/9	0.75	0.86	1.44	0.39
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C7H12O5	176.0685	0.89	0.40	1.71	0.71
C18H28O9	388.1733	5.60	0.56	1.56	0.50
C14H20O8	316.1158	3.15	0.63	1.43	0.57
C17H28O5	312.1937	7.47	0.80	1.65	0.29
C19H28O4	320.1988	8.47	1.00	1.47	0.21
C18H28O5	324.1937	7.90	1.00	1.56	0.28
C16H24O8	344.1471	4.73	0.63	1.50	0.50
C16H24O6	312.1573	6.33	0.83	1.50	0.38
C11H18O8	278.1002	3.43	0.38	1.64	0.73
C20H32O6	368.2199	7.78	0.83	1.60	0.30
C16H26O6	314.1729	8.60	0.67	1.63	0.38
C16H28O6	316.1886	8.38	0.50	1.75	0.38
C9H14O5	202.0841	0.36	0.60	1.56	0.56
C10H16O5	216.0998	0.36	0.60	1.60	0.50
C7H10O4	158.0579	0.36	0.75	1.43	0.57
C5H8O3	116.0473	0.36	0.67	1.60	0.60
C5H8O4	132.0423	0.35	0.50	1.60	0.80
C3H4O4	104.0110	0.35	0.50	1.33	1.33
C8H12O5	188.0685	0.36	0.60	1.50	0.63
C8H14O3	158.0943	0.37	0.67	1.75	0.38
C9H16O5	204.0998	0.35	0.40	1.78	0.56
C4H4O4	116.0110	0.36	0.75	1.00	1.00
C4H6O4	118.0266	0.35	0.50	1.50	1.00
C7H12O4	160.0736	0.36	0.50	1.71	0.57
C6H8O4	144.0423	0.36	0.75	1.33	0.67
C4H6O3	102.0317	0.37	0.67	1.50	0.75
C7H10O5	174.0528	0.36	0.60	1.43	0.71
C5H6O4	130.0266	0.36	0.75	1.20	0.80
C6H8O3	128.0473	0.37	1.00	1.33	0.50
C10H18O5	218.1154	0.36	0.40	1.80	0.50
C9H16O4	188.1049	2.99	0.50	1.78	0.44
C7H12O3	144.0786	0.36	0.67	1.71	0.43

Table S4.3.8 Molecular formulas of organic compounds detected in  $\beta$ -pinene SOA in ESI- mode.

Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
C9H14O4	186.0892	2.96	0.75	1.56	0.44
C9H14O4	186.0892	0.37	0.75	1.56	0.44
C8H12O4	172.0736	0.36	0.75	1.50	0.50
C10H16O4	200.1049	0.37	0.75	1.60	0.40
C10H16O3	184.1099	3.48	1.00	1.60	0.30
C8H12O4	172.0736	2.53	0.75	1.50	0.50
C8H14O4	174.0892	0.36	0.50	1.75	0.50
C10H14O5	214.0841	0.36	0.80	1.40	0.50
C10H16O4	200.1049	2.72	0.75	1.60	0.40
C19H28O7	368.1835	7.21	0.86	1.47	0.37
C10H14O4	198.0892	0.36	1.00	1.40	0.40
C8H14O3	158.0943	2.92	0.67	1.75	0.38
C8H12O5	188.0685	3.28	0.60	1.50	0.63
C11H18O6	246.1103	2.71	0.50	1.64	0.55
C4H4O3	100.0160	0.36	1.00	1.00	0.75
C4H8O2	88.0524	0.35	0.50	2.00	0.50
C8H12O3	156.0786	0.38	1.00	1.50	0.38
C8H14O5	190.0841	2.44	0.40	1.75	0.63
C8H12O3	156.0786	2.87	1.00	1.50	0.38
C18H26O6	338.1729	7.51	1.00	1.44	0.33
C4H6O2	86.0368	0.36	1.00	1.50	0.50
C7H8O4	156.0423	0.36	1.00	1.14	0.57
C17H26O8	358.1628	4.90	0.63	1.53	0.47
C20H30O8	398.1941	7.85	0.75	1.50	0.40
C20H32O7	384.2148	8.08	0.71	1.60	0.35
C5H8O2	100.0524	0.36	1.00	1.60	0.40
C6H8O2	112.0524	0.36	1.00	1.33	0.33
C9H12O4	184.0736	0.36	1.00	1.33	0.44
C7H10O3	142.0630	0.37	1.00	1.43	0.43

C7H14O4	162.0892	2.94	0.25	2.00	0.57
C7H8O3	140.0473	0.37	1.00	1.14	0.43
C19H28O5	336.1937	8.02	1.00	1.47	0.26
C7H12O2	128.0837	0.36	1.00	1.71	0.29
C19H30O5	338.2093	8.09	1.00	1.58	0.26
C6H10O2	114.0681	0.36	1.00	1.67	0.33
C18H26O8	370.1628	7.72	0.75	1.44	0.44
C8H14O2	142.0994	0.37	1.00	1.75	0.25
C19H30O5	338.2093	6.99	1.00	1.58	0.26
C/H8O3	140.0473	2.99	1.00	1.14	0.43
C3H6O	58.0419	0.37	1.00	2.00	0.33
C10U2208	200.0790	2.34	0.55	1.75	0.75
C19H32O8	388.2097	7.39	0.50	1.08	0.42
C7H10O2	140.0945	2.39	1.00	2.00	0.43
C19H30O6	354 2042	7.41	0.83	1.43	0.29
C19H28O6	352 1886	7.41	1.00	1.38	0.32
C17H26O8	358 1628	6.30	0.63	1.47	0.32
C8H10O4	170.0579	0.37	1.00	1.25	0.50
C9H12O3	168.0786	0.36	1.00	1.33	0.33
C11H16O6	244.0947	3.31	0.67	1.45	0.55
C9H12O4	184.0736	2.92	1.00	1.33	0.44
C16H26O7	330.1679	4.13	0.57	1.63	0.44
C8H12O2	140.0837	0.36	1.00	1.50	0.25
C7H12O5	176.0685	0.89	0.40	1.71	0.71
C14H20O8	316.1158	3.15	0.63	1.43	0.57
C17H28O5	312.1937	7.47	0.80	1.65	0.29
C18H28O5	324.1937	7.90	1.00	1.56	0.28
C16H24O8	344.1471	4.73	0.63	1.50	0.50
C16H24O6	312.1573	6.33	0.83	1.50	0.38
C11H18O8	278.1002	3.43	0.38	1.64	0.73
C16H26O6	314.1729	8.60	0.67	1.63	0.38
C16H28O6	316.1886	8.38	0.50	1.75	0.38
C8H12O4	172.0736	2.76	0.75	1.50	0.50
C20H32O9	416.2046	7.67	0.56	1.60	0.45
C8H12O5	188.0685	8.28	0.60	1.50	0.63
C8H12O4	1/2.0/30	8.54	0.75	1.50	0.50
C14H2007	200 1200	0.24 7.62	0.73	1.30	0.44
C14H2007	300.1209	7.02	0.71	1.43	0.50
C18H28O6	340 1886	7.50	0.83	1.07	0.33
C7H10O5	174 0528	8.25	0.60	1.50	0.33
C19H30O6	354.2042	7.22	0.83	1.58	0.32
C18H28O5	324.1937	7.37	1.00	1.56	0.28
C9H14O3	170.0943	7.94	1.00	1.56	0.33
C10H18O6	234.1103	6.07	0.33	1.80	0.60
C6H10O3	130.0630	8.23	0.67	1.67	0.50
C4H6O4	118.0266	8.20	0.50	1.50	1.00
C5H8O3	116.0473	8.22	0.67	1.60	0.60
C19H32O6	356.2199	8.17	0.67	1.68	0.32
C17H26O7	342.1679	7.49	0.71	1.53	0.41
C9H14O3	170.0943	3.11	1.00	1.56	0.33
C20H32O10	432.1995	8.24	0.50	1.60	0.50
C8H14O6	206.0790	8.27	0.33	1.75	0.75
C7H10O4	158.0579	1.88	0.75	1.43	0.57
C6H8O4	144.0423	3.42	0.75	1.33	0.67
C9H14O3	170.0943	0.39	1.00	1.56	0.33
C/H12O3	144.0786	8.33	0.67	1./1	0.43
C0H10O2	114.0081	8.43	1.00	1.07	0.55
C6H8O3	174.0692	3.40 8.30	1.00	1.75	0.50
C5H8O2	120.0475	3 12	1.00	1.55	0.50
C9H14O5	202 0841	2 51	0.60	1.00	0.40
C7H12O3	144.0786	3.27	0.67	1.71	0.30
C8H14O6	206.0790	3.15	0.33	1.75	0.75
C19H32O8	388.2097	7.61	0.50	1.68	0.42
C10H16O5	216.0998	3.04	0.60	1.60	0.50
C10H14O6	230.0790	0.35	0.67	1.40	0.60
C10H18O6	234.1103	7.98	0.33	1.80	0.60
C19H32O7	372.2148	8.31	0.57	1.68	0.37

C8H14O4	174.0892	8.63	0.50	1.75	0.50
C17H26O8	358.1628	3.15	0.63	1.53	0.47
C17H26O8	358.1628	8.22	0.63	1.53	0.47
C7H12O5	176.0685	7.96	0.40	1.71	0.71
C6H10O5	162.0528	0.62	0.40	1.67	0.83
C6H10O5	162.0528	8.73	0.40	1.67	0.83
C13H22O6	274.1416	7.78	0.50	1.69	0.46
C19H32O6	356.2199	7.93	0.67	1.68	0.32
C15H24O7	316.1522	6.71	0.57	1.60	0.47
C20H30O9	414.1890	7.27	0.67	1.50	0.45
C19H32O8	388.2097	7.87	0.50	1.68	0.42
C7H10O3	142.0630	8.23	1.00	1.43	0.43
C20H30O7	382.1992	8.21	0.86	1.50	0.35
C16H26O10	378.1526	4.35	0.40	1.63	0.63
C19H32O7	372.2148	7.98	0.57	1.68	0.37
C8H14O5	190.0841	1.50	0.40	1.75	0.63
C19H30O5	338.2093	8.43	1.00	1.58	0.26
C18H30O6	342.2042	8.32	0.67	1.67	0.33
C20H32O9	416.2046	3.90	0.56	1.60	0.45
C13H20O7	288.1209	8.11	0.57	1.54	0.54
C10H14O4	198.0892	8.17	1.00	1.40	0.40
C11H20O6	248.1260	3.09	0.33	1.82	0.55
C11H20O7	264.1209	2.61	0.29	1.82	0.64
C9H14O5	202.0841	0.36	0.60	1.56	0.56
C10H16O5	216.0998	0.36	0.60	1.60	0.50
C7H10O4	158.0579	0.36	0.75	1.43	0.57
C5H8O3	116.0473	0.36	0.67	1.60	0.60
C5H8O4	132.0423	0.35	0.50	1.60	0.80
C3H4O4	104.0110	0.35	0.50	1.33	1.33
C8H12O5	188.0685	0.36	0.60	1.50	0.63
C8H14O3	158.0943	0.37	0.67	1.75	0.38
C9H16O5	204.0998	0.35	0.40	1.78	0.56
C4H4O4	116.0110	0.36	0.75	1.00	1.00
C3H6O3	90.0317	0.36	0.33	2.00	1.00
C4H6O4	118.0266	0.35	0.50	1.50	1.00
C7H12O4	160.0736	0.36	0.50	1.71	0.57
C6H8O4	144.0423	0.36	0.75	1.33	0.67
C4H6O3	102.0317	0.37	0.67	1.50	0.75
C2H4O3	76.0160	0.34	0.33	2.00	1.50
C7H10O5	174.0528	0.36	0.60	1.43	0.71
C5H6O4	130.0266	0.36	0.75	1.20	0.80
C6H10O4	146.0579	0.36	0.50	1.67	0.67
C6H8O3	128.0473	0.37	1.00	1.33	0.50
C10H18O5	218.1154	0.36	0.40	1.80	0.50
C7H12O3	144.0786	0.36	0.67	1.71	0.43
C8H14O4	174.0892	3.21	0.50	1.75	0.50

Table S4.3.9 Molecular formulas of organic compounds detected in limonene SOA in ESI- mode.

Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
C9H14O4	186.0892	0.37	0.75	1.56	0.44
C8H12O4	172.0736	0.36	0.75	1.50	0.50
C10H16O4	200.1049	0.37	0.75	1.60	0.40
C8H14O4	174.0892	0.36	0.50	1.75	0.50
C10H14O5	214.0841	0.36	0.80	1.40	0.50
C10H14O4	198.0892	0.36	1.00	1.40	0.40
C8H14O3	158.0943	2.92	0.67	1.75	0.38
C8H12O5	188.0685	3.28	0.60	1.50	0.63
C11H18O6	246.1103	2.71	0.50	1.64	0.55
C7H10O4	158.0579	3.37	0.75	1.43	0.57
C4H4O3	100.0160	0.36	1.00	1.00	0.75
C4H8O2	88.0524	0.35	0.50	2.00	0.50
C8H12O3	156.0786	0.38	1.00	1.50	0.38
C9H14O3	170.0943	7.71	1.00	1.56	0.33
C18H26O6	338.1729	7.51	1.00	1.44	0.33

CHH602         86.0368         0.36         1.00         1.50         0.53           C2DH3008         398.1941         7.85         0.75         1.50         0.40           C2DH3207         384.2148         8.08         0.71         1.60         0.35           CSH802         100.0524         0.36         1.00         1.33         0.33           CSH1204         184.0736         0.36         1.00         1.43         0.43           CTH1003         142.0630         0.37         1.00         1.14         0.43           CTH1205         336.1937         8.02         1.00         1.58         0.26           CTH1205         128.0837         0.36         1.00         1.57         0.35           CSH1402         120.094         0.37         1.00         1.57         0.35           CSH1402         126.0681         0.36         1.00         1.43         0.39           CSH1402         126.0681         0.36         1.00         1.43         0.39           CSH1604         170.0579         0.37         1.00         1.25         0.57           CSH1604         170.0579         0.37         1.00         1.44         0.30						
C71180A         156.0423         0.36         1.00         1.14         0.57           C20113207         384.144         8.08         0.71         1.60         0.40           C20113207         100.0524         0.36         1.00         1.33         0.40           C311802         100.0524         0.36         1.00         1.33         0.44           C7H1003         148.0736         0.37         1.00         1.43         0.44           C7H1003         140.0473         0.36         1.00         1.47         0.43           C19H2805         336.1937         8.02         1.00         1.47         0.29           C19H3005         338.2093         8.09         1.00         1.58         0.23           C19H2805         336.1937         1.00         1.58         0.23         C184         0.34         0.29         C1943005         338.2093         8.09         1.00         1.58         0.23         C184         0.35         1.00         1.43         0.32         C184         0.35         C144         0.34         0.32         C184         0.35         C144         0.35         C144         0.35         C144         0.35         C144         0.35	C4H6O2	86.0368	0.36	1.00	1 50	0.50
CH804         156.0423         0.36         1.00         1.14         0.57           C2H43207         334.2148         8.08         0.71         1.60         0.35           CSH802         112.0524         0.36         1.00         1.33         0.33           CSH102         112.0524         0.36         1.00         1.43         0.44           CTH1003         142.0630         0.37         1.00         1.44         0.43           CTH102         128.0837         8.02         1.00         1.47         0.26           CTH102         128.0837         8.02         1.00         1.67         0.29           CTH1002         128.0837         8.03         1.00         1.58         0.26           CH1002         114.0681         0.36         1.00         1.57         0.25           C3H1002         126.0681         0.36         1.00         1.47         0.32           C19H2806         352.1886         7.81         1.00         1.47         0.32           C19H2080         358.1628         6.30         0.63         1.53         0.47           C19H2080         358.1628         6.36         1.00         1.33         0.33	C411002	80.0508	0.50	1.00	1.50	0.50
C20H3008         398,1941         7.85         0.75         1.50         0.035           C20H3207         344,2148         8.08         0.71         1.60         0.35           CSH802         112,0524         0.36         1.00         1.33         0.34           CFH1003         142,0630         0.37         1.00         1.43         0.43           CTH1003         142,0630         0.37         1.00         1.44         0.43           C19H2805         336,1937         8.02         1.00         1.47         0.26           C1H1202         128,0857         0.35         1.00         1.67         0.33           C19H2805         336,1937         8.02         1.00         1.47         0.26           C1H1202         128,0857         7.12         0.75         1.44         0.44           C19H2806         370,1628         7.72         0.75         1.44         0.44           C19H2806         352,1886         7.81         1.00         1.47         0.32           C1H1002         126,0681         0.35         1.00         1.33         0.33           C1H1208         358,1628         6.30         0.35         1.63         0.47	C7H8O4	156.0423	0.36	1.00	1.14	0.57
C 20H4008 398.1941 7.85 0.75 1.50 0.40 C 20H4207 384.2148 8.08 0.71 1.60 0.35 C 5H802 100.0524 0.36 1.00 1.33 0.33 C 5H802 112.0524 0.36 1.00 1.33 0.43 C 7H1003 142.0630 0.37 1.00 1.14 0.43 C 7H1003 142.0630 0.37 1.00 1.14 0.43 C 7H1003 142.0630 0.37 1.00 1.71 0.29 C 19H3005 338.2093 8.09 1.00 1.58 0.26 C 6H1002 114.0681 0.36 1.00 1.57 0.35 C 6H1002 114.0681 0.36 1.00 1.57 0.35 C 18H2008 370.1628 7.72 0.75 1.44 0.44 C 28H1402 142.0994 0.37 1.00 1.75 0.25 C 3H60 58.0419 0.37 1.00 1.75 0.25 C 3H60 58.0419 0.37 1.00 1.75 0.25 C 3H60 58.0419 0.37 1.00 1.43 0.29 C 19H306 335.1628 6.30 0.63 1.53 0.47 C 7H1002 126.0681 0.36 1.00 1.47 0.32 C 17H2068 358.1628 6.30 0.63 1.53 0.47 C 7H1002 126.0681 0.36 1.00 1.44 0.32 C 17H206 352.1886 7.81 1.00 1.44 0.32 C 17H206 352.1886 7.81 1.00 1.44 0.32 C 17H206 352.1886 7.81 0.00 1.43 0.39 C 7H1002 124.0524 0.37 1.00 1.14 0.32 C 17H206 356.2199 8.31 0.33 1.60 0.30 C 20H3206 368.2199 7.62 0.67 1.68 0.32 C 3H1202 124.0524 0.37 1.00 1.50 0.35 C 11H208 280.158 2.477 0.25 1.50 0.35 C 11H208 280.158 2.477 0.26 0.67 1.68 0.32 C 20H3206 368.2199 7.62 0.67 1.68 0.32 C 20H3206 368.2199 7.62 0.67 1.68 0.32 C 20H3206 368.2199 7.61 0.05 1.50 0.35 C 11H208 280.1158 2.47 0.25 1.50 0.33 C 20H3206 368.2199 7.61 0.50 1.60 0.45 C 21H2205 344.1937 7.90 1.00 1.56 0.33 C 21H1205 334.1937 7.90 1.00 1.56 0.33 C 21H1206 330.82097 7.61 0.50 1.68 0.42 C 20H3206 340.1886 7.52 0.83 1.56 0.33 C 21H1205 334.1937 7.90 1.00 1.56 0.33 C 21H1206 348.2042 7.22 0.83 1.56 0.33 C 21H1206 340.1860 7.52 0.83 1.50 0.35 C 21H1207 2.64.1209 2.61 0.40 0.40 C 21H1208 2.88.2097 7.61 0.50 1.68 0.42 C 21H1207 3.41.03 3.402 7.51 0.50 1.68 0.42 C 21H1207 3.42.192 8.21 0.86 1.50 0.35 C 21H1207 3.44.102 3.58.075 1.56 0.44 C 20H1404 1.98.0892 8.55 1.00 1.40 0.40 C 20H1404 1.98.0892 8.55 1.00 1.40 0.40 C 20H1404 1.98.0892 8.55 1.00 1.40 0.40 C	C20110001	200.1011	7.05	0.75	1.50	0.40
C2H3207         384,2148         8.08         0.71         1.60         0.33           C5H802         112,0524         0.36         1.00         1.33         0.34           C7H1003         142,0630         0.37         1.00         1.43         0.43           C7H1003         142,0630         0.37         1.00         1.43         0.43           C7H1003         142,0630         0.37         1.00         1.47         0.26           C7H1022         128,0837         8.02         1.00         1.47         0.26           C19H3005         338,2093         8.09         1.00         1.58         0.26           C4H1002         144,0681         0.36         1.00         1.67         0.33           C1H2008         370,1628         7.72         0.75         1.44         0.44           C3H1402         142,0944         0.37         1.00         1.47         0.32           C3H605         86,0749         0.37         1.00         1.43         0.29           C1H1202         126,0681         0.36         1.00         1.43         0.32           C1H1202         124,0524         0.37         1.00         1.14         0.32	C20H30O8	398.1941	7.85	0.75	1.50	0.40
C2H12207         364,2143         8365         0.71         1.60         0.30           C4H802         112 00524         0.36         1.00         1.33         0.34           C7H1003         142 06530         0.37         1.00         1.43         0.44           C7H1003         142 06530         0.37         1.00         1.44         0.43           C1H202         128 0837         8.02         1.00         1.47         0.29           C1H1202         128 0837         8.02         1.00         1.58         0.26           CH14002         142 0.094         0.37         1.00         1.58         0.25           C1H1202         128 0.037         1.00         1.67         0.33         C11         0.29           C1H1202         126 0.0681         0.36         1.00         1.47         0.32         C3         0.37         1.00         1.43         0.29           C1H1202         126 0.0681         0.36         1.00         1.43         0.29         C1H1208         358 1628         6.30         0.63         1.53         0.33         C3         0.07         0.33         C3         0.07         1.55         0.33         C3         0.60	C20H22O7	284 2148	8 <u>0</u> 8	0.71	1.60	0.25
CSH802         100.0524         0.36         1.00         1.60         0.43           CSH1204         184.0736         0.36         1.00         1.33         0.44           CTH1003         142.0630         0.37         1.00         1.14         0.43           CTH1205         336.1937         8.02         1.00         1.47         0.36           CCH1205         338.2093         8.09         1.00         1.67         0.35           CCH11005         338.2093         8.09         1.00         1.67         0.33           CSH1002         114.0681         0.36         1.00         1.67         0.33           CSH1002         126.0681         0.36         1.00         1.47         0.32           CSH1002         126.0681         0.36         1.00         1.43         0.29           C1H208         358.1628         6.30         0.63         1.53         0.47           CSH1004         170.0579         0.37         1.00         1.25         0.50           CH1208         358.1628         6.30         0.63         1.00         1.33         0.33           CSH1004         170.0579         0.37         1.00         1.44	C20H3207	364.2146	0.00	0.71	1.00	0.55
C6H802         112.0524         0.36         1.00         1.33         0.33           C7H1003         144.0736         0.37         1.00         1.43         0.43           C7H1023         140.0473         0.37         1.00         1.44         0.43           C19H2805         336.1937         8.02         1.00         1.47         0.26           C19H3005         338.2093         8.09         1.00         1.67         0.33           C1H1202         128.06837         0.36         1.00         1.67         0.33           C1H1202         142.0994         0.37         1.00         1.75         0.25           C3H60         58.0419         0.37         1.00         1.43         0.29           C1H12005         328.1286         7.81         1.00         1.43         0.29           C1H12006         325.1886         7.81         1.00         1.44         0.32           C1H12005         328.1628         6.30         0.63         1.53         0.47           C2H12006         352.1886         7.81         1.00         1.14         0.29           C1H12005         124.0524         0.37         1.00         1.14         0.29 </td <td>C5H8O2</td> <td>100.0524</td> <td>0.36</td> <td>1.00</td> <td>1.60</td> <td>0.40</td>	C5H8O2	100.0524	0.36	1.00	1.60	0.40
CHH02         112(b)24         0.36         1.00         1.33         0.34           C7H1003         142(b)30         0.37         1.00         1.43         0.44           C7H1003         142(b)30         0.37         1.00         1.44         0.43           C19H2805         336(b)37         8.02         1.00         1.47         0.26           C19H1202         128(b)37         8.02         1.00         1.58         0.26           C19H1202         128(b)37         8.02         1.00         1.58         0.26           C19H1202         128(b)37         8.02         1.00         1.57         0.25           C3H1002         124(b)294         0.37         1.00         1.67         0.25           C3H402         142(b)294         0.37         1.00         1.47         0.32           C19H2806         352(b)37         0.37         1.00         1.43         0.39           C19H203         168(b)786         0.36         1.00         1.33         0.30           C19H203         168(b)786         0.36         1.00         1.34         0.29           C1H1202         140(b)37         0.36         1.00         1.36         0.33	C (TROOP		0.04	1.00	4.00	0.00
COH1204         184 0736         0.36         1.00         1.43         0.43           CTHR03         140.0473         0.37         1.00         1.14         0.43           CTHR03         36,1937         8.02         1.00         1.71         0.26           CTH1205         336,1937         8.02         1.00         1.58         0.26           CGH1002         1144 0681         0.35         1.00         1.58         0.26           CGH1002         1144 0681         0.35         1.00         1.58         0.22           C3H60         58.0419         0.37         1.00         2.00         0.33           C1H1202         122.06081         0.36         1.00         1.47         0.32           C1H1208         358.1628         6.30         0.63         1.53         0.47           CH1402         124.0524         0.37         1.00         1.43         0.29           CH1402         124.0524         0.37         1.00         1.25         0.50           CH1402         124.0524         0.37         1.00         1.25         0.50           CH1402         124.0524         0.37         1.00         1.43         0.30 <td>C6H8O2</td> <td>112.0524</td> <td>0.36</td> <td>1.00</td> <td>1.33</td> <td>0.33</td>	C6H8O2	112.0524	0.36	1.00	1.33	0.33
C3H1204         194.073         0.30         1.00         1.43         0.43           CTHR03         142.0630         0.37         1.00         1.14         0.43           CTHR2S         336.1937         8.02         1.00         1.71         0.26           CTH1202         128.0837         0.36         1.00         1.71         0.29           C19H3005         338.2093         8.09         1.00         1.67         0.33           C18H2008         370.1628         7.72         0.75         1.44         0.44           C8H1402         142.0994         0.37         1.00         1.75         0.25           C3H160         58.0419         0.37         1.00         1.43         0.39           C19H206         352.1886         7.81         1.00         1.43         0.39           C19H206         352.1886         7.81         1.00         1.34         0.32           C1H202         124.0524         0.37         1.00         1.34         0.32           C1H2008         356.1299         7.62         0.67         1.68         0.32           C1H2020         1368.2798         0.36         1.00         1.33         0.33	C0111204	184 0726	0.26	1.00	1 22	0.44
C7H1003         140.0473         0.37         1.00         1.43         0.43           C19H28O5         336.1937         8.02         1.00         1.47         0.29           C19H13O05         338.2093         8.09         1.00         1.58         0.26           C19H13O05         338.2093         8.09         1.00         1.58         0.26           C19H13O02         114.0681         0.36         1.00         1.57         0.23           C18H26O8         370.1628         7.72         0.75         1.44         0.44           C8H1402         126.0681         0.36         1.00         1.43         0.22           C19H28O6         358.1628         6.30         0.63         1.53         0.47           C3H1004         170.0579         0.37         1.00         1.14         0.29           C7H1802         126.0524         0.37         1.00         1.14         0.29           C7H1802         126.0524         0.37         1.00         1.43         0.29           C7H1802         126.0532         0.63         1.00         1.33         0.33           C20H3206         356.2199         7.62         0.67         1.68	C9H12O4	184.0730	0.50	1.00	1.55	0.44
CHR03         140.0473         0.37         1.00         1.47         0.43           C1912805         336.1937         8.02         1.00         1.47         0.26           C191202         128.0837         0.36         1.00         1.47         0.26           C19113005         338.2093         8.09         1.00         1.58         0.23           C18112608         370.1628         7.72         0.75         1.44         0.44           C1811402         142.0994         0.37         1.00         1.75         0.25           C31H02         126.0681         0.36         1.00         1.47         0.32           C19112608         358.1628         6.30         0.63         1.53         0.47           C31H02         124.0524         0.37         1.00         1.25         0.50           C7H1203         168.0786         0.36         1.00         1.33         0.33         0.33           C20H3206         362.199         7.62         0.67         1.68         0.32         0.71         1.60         1.50         0.25         1.82         0.73         0.83         1.60         0.30         C20H320         240.1158         2.47         0.25 <td>C7H10O3</td> <td>142 0630</td> <td>0.37</td> <td>1.00</td> <td>1 / 3</td> <td>0.43</td>	C7H10O3	142 0630	0.37	1.00	1 / 3	0.43
C7H803         140.0473         0.37         1.00         1.14         0.43           C7H1202         128.0837         0.36         1.00         1.71         0.29           CFM13005         338.2093         8.09         1.00         1.58         0.26           CFM13005         338.2093         8.09         1.00         1.67         0.33           CI8H2608         370.1628         7.72         0.75         1.44         0.44           CSH1402         142.0994         0.37         1.00         1.03         0.23           C3H400         58.0419         0.37         1.00         1.43         0.22           C17H2608         352.1886         7.81         1.00         1.47         0.32           C3H1004         170.0579         0.37         1.00         1.14         0.29           C4H1203         168.0786         0.36         1.00         1.33         0.33           C20H3206         368.2199         8.31         0.08         1.33         0.33           C20H3206         368.2199         7.78         0.83         1.60         0.30           C20H3206         368.199         7.78         0.83         1.60         0.33 <td>C/111005</td> <td>142.0050</td> <td>0.57</td> <td>1.00</td> <td>1.+5</td> <td>0.45</td>	C/111005	142.0050	0.57	1.00	1.+5	0.45
C19H28O5         336,1937         8.02         1.00         1.47         0.26           CTH13O2         128,0837         0.36         1.00         1.58         0.26           CH110O2         114,0681         0.36         1.00         1.67         0.33           C18H2608         370.1628         7.72         0.75         1.44         0.44           C8H1402         142,0994         0.37         1.00         1.75         0.22           C19H2806         358.1628         6.30         0.63         1.53         0.47           CSH1004         170.0579         0.37         1.00         1.47         0.32           C17H2806         358.1628         6.30         0.63         1.53         0.47           CSH1004         170.0579         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C17H206         368.2199         7.62         0.67         1.68         0.32           C9H1203         168.0787         0.36         1.00         1.50         0.25           C11H2008         280.1158         2.47         0.25         1.82         0.73<	C7H8O3	140.0473	0.37	1.00	1.14	0.43
C1912305         33.6         1.00         1.47         0.29           C1913005         338.2093         8.09         1.00         1.58         0.26           C1913005         338.2093         8.09         1.00         1.58         0.29           C1913005         338.2093         8.09         1.00         1.58         0.22           C1812608         370.1628         7.72         0.75         1.44         0.44           C1811200         126.0681         0.36         1.00         1.47         0.32           C19112806         352.1866         7.81         1.00         1.47         0.32           C19112608         358.1628         6.30         0.63         1.53         0.47           C19112306         136.0759         0.37         1.00         1.44         0.29           C19112306         362.199         7.62         0.67         1.68         0.32           C1811202         140.0837         0.36         1.00         1.50         0.25           C1811202         140.0837         0.36         1.00         1.56         0.28           C20013206         368.2199         7.78         0.83         1.66         0.32	010110005	226 1027	0.00	1.00	1 47	0.00
C7H1202         128.0837         0.36         1.00         1.71         0.26           C6H1002         114.0681         0.36         1.00         1.67         0.33           C1BH2608         370.1628         7.72         0.75         1.44         0.44           C8H1402         142.0994         0.37         1.00         1.75         0.25           C3H60         58.0149         0.36         1.00         1.43         0.29           C19H2806         352.1886         7.81         1.00         1.47         0.32           C19H2806         358.1628         6.30         0.63         1.53         0.47           C3H1004         170.0579         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C20H1202         140.0837         0.36         1.00         1.50         0.25           C1H1202         140.0837         0.36         1.00         1.56         0.28           C20H3206         368.2199         7.78         0.83         1.66         0.30           C20H3206         368.2199         7.78         0.83         1.66         0.33 <td>C19H28O5</td> <td>336.1937</td> <td>8.02</td> <td>1.00</td> <td>1.4/</td> <td>0.26</td>	C19H28O5	336.1937	8.02	1.00	1.4/	0.26
C1913005         138.2003         8.09         1.00         1.78         0.26           CH11002         114.0681         0.36         1.00         1.67         0.33           C1814208         370.1628         7.72         0.75         1.44         0.44           C8H1402         142.0994         0.37         1.00         1.75         0.25           C3H400         \$8.0419         0.37         1.00         1.43         0.29           C19H2806         358.1628         6.30         0.63         1.53         0.47           C8H1004         170.0579         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C20H3206         368.2199         8.31         0.83         1.60         0.30           C19H3206         356.1199         7.62         0.67         1.66         0.25           C1H2028         280.1158         2.47         0.25         1.82         0.73           C1H20208         324.1937         7.90         1.00         1.56         0.30           C20H3206         368.2199         7.78         0.83         1.60         0.30<	C7H12O2	128 0837	0.36	1.00	1 71	0.29
C19H3005         338.2093         8.09         1.00         1.58         0.23           C18H2608         370.1628         7.72         0.75         1.44         0.44           C8H1402         142.0994         0.37         1.00         1.75         0.25           C3H60         58.0419         0.37         1.00         1.43         0.22           C19H2806         358.1628         6.30         0.63         1.53         0.47           C1H12004         170.0579         0.37         1.00         1.14         0.32           C1H12004         170.0579         0.37         1.00         1.14         0.29           CH1203         168.0786         0.36         1.00         1.33         0.33           C20H3206         356.2199         7.62         0.67         1.68         0.32           C1H2008         280.1158         2.47         0.25         1.82         0.73           C1H2008         280.1158         2.477         0.25         1.82         0.73           C20H3206         340.1886         7.52         0.83         1.60         0.30           C20H3206         340.1886         7.52         0.83         1.66         0.32<	C/III202	120.0057	0.50	1.00	1./1	0.27
C6H1002         114,0681         0.36         1.00         1.67         0.33           C18H2608         370,1628         7.72         0.75         1.44         0.44           C8H1402         142,0994         0.37         1.00         1.75         0.25           C3H60         58,0149         0.37         1.00         1.43         0.29           C17H2608         352,1886         7.81         1.00         1.47         0.32           C17H2068         352,1886         6.30         0.63         1.53         0.47           C3H1004         170,0579         0.37         1.00         1.14         0.29           C9H1203         168,0786         0.36         1.00         1.33         0.33           C20H3206         362,199         7.62         0.67         1.68         0.32           C1H12008         280,1158         2.47         0.25         1.82         0.73           C1812805         324,1937         7.90         1.00         1.56         0.28           C20H3206         368,2199         7.72         0.83         1.66         0.33           C19H3206         354,2042         7.22         0.83         1.56         0.33 </td <td>C19H30O5</td> <td>338.2093</td> <td>8.09</td> <td>1.00</td> <td>1.58</td> <td>0.26</td>	C19H30O5	338.2093	8.09	1.00	1.58	0.26
CCH1002         114,0681         0.36         1.00         1.67         0.434           CSH1402         142,0994         0.37         1.00         1.75         0.25           CSH160         58,0419         0.37         1.00         1.75         0.22           CJH1202         126,0681         0.36         1.00         1.43         0.22           CJH12806         358,1628         6.30         0.63         1.53         0.47           CSH1004         170,0579         0.37         1.00         1.14         0.29           CH1203         168,0786         0.36         1.00         1.33         0.33           C20H3206         368,2199         8.31         0.83         1.60         0.30           C1H202         140,0837         0.36         1.00         1.56         0.25           C1H2008         280,1158         2.47         0.25         1.82         0.73           C1H2020         46,2046         7.67         0.56         1.60         0.45           C1H20208         324,1937         7.90         1.00         1.56         0.33           C1H2008         324,1937         7.90         1.00         1.46         0.43	0(111000	114.0601	0.26	1.00	1 (7	0.22
C18H2608         370.1628         7.72         0.75         1.44         0.44           C3H60         58.0419         0.37         1.00         1.75         0.25           C3H60         350.419         0.37         1.00         1.43         0.29           C19H2806         352.1886         7.81         1.00         1.47         0.32           C17H2608         358.1628         6.30         0.63         1.53         0.47           C8H1004         170.0579         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C19H3206         368.2199         7.62         0.67         1.68         0.32           C1H12008         280.1158         2.47         0.25         1.82         0.73           C1H2008         281.1597         7.90         1.00         1.56         0.28           C20H3206         368.199         7.78         0.83         1.60         0.45           C18H2805         324.1937         7.90         1.00         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71	C6H10O2	114.0681	0.36	1.00	1.67	0.33
C8H1402         142.094         0.37         1.00         1.75         0.25           C3H60         58.0419         0.37         1.00         2.00         0.33           C7H1002         126.0681         0.36         1.00         1.43         0.29           C17H2806         352.1886         7.81         1.00         1.47         0.32           C7H12068         358.1628         6.30         0.63         1.53         0.47           C8H1004         170.0579         0.37         1.00         1.14         0.29           C9H1203         128.0786         0.36         1.00         1.33         0.33           C19H3206         356.2199         7.62         0.67         1.68         0.32           C18H2005         324.1937         7.90         1.00         1.56         0.28           C18H2805         324.1937         7.90         1.00         1.56         0.28           C18H2806         340.1886         7.52         0.83         1.66         0.45           C18H2806         340.1886         7.52         0.83         1.56         0.33           C18H2806         340.1886         7.52         0.83         1.56         0.33 </td <td>C18H26O8</td> <td>370 1628</td> <td>7 72</td> <td>0.75</td> <td>1 44</td> <td>0.44</td>	C18H26O8	370 1628	7 72	0.75	1 44	0.44
C8H1402         142.0994         0.37         1.00         1.75         0.25           C7H1002         126.0681         0.36         1.00         1.43         0.29           C19H2806         352.1886         7.81         1.00         1.47         0.32           C17H2608         358.1628         6.30         0.63         1.53         0.47           C8H1004         170.0579         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C20H1206         356.2199         7.62         0.67         1.68         0.32           C1H12005         230.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.32           C18H2805         324.1937         7.90         1.00         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.44         0.6	010112000	570.1020	1.12	0.75	1.77	0.77
C3H60         S8.0419         0.37         1.00         2.00         0.33           C7H1002         126.0681         0.36         1.00         1.43         0.29           C19H2806         352.1886         7.81         1.00         1.47         0.32           C17H2608         358.1628         6.30         0.63         1.53         0.47           C8H1004         170.0579         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C20H3206         368.2199         8.31         0.83         1.60         0.30           C19H3206         368.2199         7.62         0.67         1.88         0.32           C1H2008         280.1158         2.47         0.25         1.82         0.73           C1H2005         324.1937         7.90         1.00         1.56         0.28           C20H3209         41.6246         7.67         0.56         1.60         0.45           C1H206         340.186         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71	C8H14O2	142.0994	0.37	1.00	1.75	0.25
C3HBO         35.0419         0.37         1.00         2.00         0.33           C7HHO2         126.0681         0.36         1.00         1.43         0.29           C19H2806         352.1886         7.81         1.00         1.43         0.29           C7HB02         124.0524         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C19H2806         368.2199         8.31         0.83         1.60         0.30           C19H206         368.2199         7.62         0.67         1.68         0.32           C1H1203         140.0837         0.36         1.00         1.50         0.25           C1H12008         280.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.33           C20H3209         416.2046         7.67         0.56         1.60         0.45           C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71	COLLO	59.0410	0.27	1.00	2.00	0.22
C7H1002         1260681         0.36         1.00         1.43         0.29           C19H2806         352.1886         7.81         1.00         1.47         0.32           C17H2608         353.1628         6.30         0.63         1.53         0.47           C8H1004         170.0579         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C20H3206         356.2199         7.62         0.67         1.68         0.32           C1H1202         140.0837         0.36         1.00         1.50         0.25           C1H206         324.1937         7.90         1.00         1.56         0.32           C20H3205         324.1937         7.90         1.00         1.56         0.33           C1BH2805         324.1937         7.90         1.00         1.56         0.33           C1H205         174.0528         8.25         0.60         1.43         0.71           C19H3206         354.2042         7.22         0.83         1.56         0.33           C19H1403         170.0943         0.39         1.00         1.56         0.33 </td <td>C3H0U</td> <td>38.0419</td> <td>0.57</td> <td>1.00</td> <td>2.00</td> <td>0.55</td>	C3H0U	38.0419	0.57	1.00	2.00	0.55
C1912806         152.1886         7.81         1.00         1.47         0.32           C17112608         352.1886         7.81         1.00         1.47         0.32           C17112608         358.1628         6.30         0.63         1.53         0.47           C811004         170.0579         0.37         1.00         1.14         0.29           C911203         168.0786         0.36         1.00         1.33         0.33           C1913206         368.2199         8.31         0.83         1.60         0.32           C111202         140.0837         0.36         1.00         1.56         0.28           C111202         140.0837         0.36         1.00         1.56         0.28           C111202         140.0837         0.36         1.00         1.56         0.28           C20113206         368.199         7.78         0.83         1.60         0.45           C1181205         314.1937         7.90         1.00         1.56         0.33           C1911206         340.186         7.52         0.83         1.56         0.33           C181205         146.0746         7.61         0.50         1.48         0.	C7H10O2	126 0681	0.36	1.00	1 4 3	0.29
C19H2806         352,1886         7,81         1,00         1,47         0.32           C17H2608         358,1628         6,30         0,63         1,53         0,47           C8H1004         170,0579         0,37         1,00         1,14         0,29           C9H1203         168,0786         0,36         1,00         1,33         0,33           C20H3206         368,2199         8,31         0,83         1,60         0,30           C1H12008         280,1158         2,47         0,25         1,82         0,73           C1H12008         280,1158         2,47         0,25         1,82         0,73           C1H12008         280,1158         2,47         0,25         1,82         0,73           C1H12008         368,2199         7,78         0,83         1,60         0,45           C18H2806         340,1886         7,52         0,83         1,56         0,33           C19H3005         174,0528         8,25         0,60         1,43         0,71           C19H3006         354,2042         7,22         0,83         1,58         0,32           C9H1403         170,0943         0,39         1,00         1,66	0/111002	120.0001	0.50	1.00	1.45	0.29
C17H2608         358.1628         6.30         0.63         1.53         0.47           C8H1004         170.0579         0.37         1.00         1.25         0.50           C7H802         124.0524         0.36         1.00         1.33         0.33           C20H1203         168.0786         0.36         1.00         1.33         0.33           C20H3206         356.2199         7.62         0.67         1.68         0.32           C8H1202         140.0837         0.36         1.00         1.50         0.25           C1H2008         280.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.33           C20H3209         416.2046         7.67         0.56         1.60         0.43           C18H2806         340.1886         7.52         0.83         1.58         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.33           C19H3005         152.0528         0.67         1.40         0.60      <	C19H28O6	352.1886	7.81	1.00	1.47	0.32
C8H1004         170.0579         0.37         1.00         1.25         0.50           C7H802         124.0524         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C20H3206         368.2199         8.31         0.83         1.60         0.30           C19H3206         365.2199         7.62         0.67         1.68         0.32           C8H1202         140.0837         0.36         1.00         1.50         0.25           C1H2008         280.1158         2.47         0.25         1.82         0.73           C1H2008         280.1158         2.47         0.25         1.82         0.73           C1H2005         364.1937         7.90         1.00         1.56         0.28           C20H3209         416.2046         7.67         0.56         1.60         0.33           C1H2005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C19H3006         354.1028         3.15         0.63         1.53         0.47 </td <td>C17U2(O9</td> <td>259 1 (29</td> <td>6.20</td> <td>0.02</td> <td>1 5 2</td> <td>0.47</td>	C17U2(O9	259 1 (29	6.20	0.02	1 5 2	0.47
C8H1004         170.0579         0.37         1.00         1.25         0.50           C7H802         124.0554         0.36         1.00         1.33         0.33           C20H32O6         368.2199         8.31         0.83         1.60         0.30           C1H12O2         140.0837         0.36         1.00         1.50         0.25           C1H2O08         280.1158         2.47         0.25         1.82         0.73           C18H2R05         324.1937         7.90         1.00         1.56         0.28           C20H32O6         368.2199         7.78         0.83         1.60         0.45           C18H2R05         324.1937         7.90         1.00         1.56         0.30           C20H32O9         416.2046         7.67         0.56         1.60         0.45           C18H2R06         340.1886         7.52         0.83         1.56         0.33           C79H1403         170.0943         0.39         1.00         1.56         0.33           C19H3006         354.2042         7.22         0.83         1.53         0.47           C19H3005         162.0528         0.62         0.40         1.67         0.	C1/H2008	338.1028	0.30	0.05	1.55	0.47
C7H802         124.0524         0.37         1.00         1.14         0.29           C9H1203         168.0786         0.36         1.00         1.33         0.33           C0H13206         356.2199         7.62         0.67         1.68         0.30           C19H3206         356.2199         7.62         0.67         1.68         0.32           C8H1202         140.0837         0.36         1.00         1.50         0.25           C11H2008         280.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.30           C20H3209         416.2046         7.67         0.56         1.60         0.30           C2H3209         416.2046         7.67         0.56         1.60         0.33           C19H3006         342.042         7.22         0.83         1.58         0.33           C19H3006         354.2042         7.22         0.83         1.58         0.33           C19H3006         354.2042         7.22         0.83         1.58         0.33           C19H3006         358.1628         3.15         0.63         1.53         0.4	C8H10O4	170.0579	0.37	1.00	1 25	0.50
C7H802         1240524         0.37         1.00         1.14         0.29           C9H1203         166.0786         0.36         1.00         1.33         0.33           C20H3206         356.2199         7.62         0.67         1.68         0.32           C8H1202         140.0837         0.36         1.00         1.50         0.25           C1H2008         280.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.28           C20H3206         382.199         7.78         0.83         1.60         0.45           C18H2805         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C19H3005         174.0528         0.62         0.40         1.67         0.83           C19H3006         354.1028         3.15         0.63         1.53         0.47           C1H406         230.0790         0.35         1.60         0.40         0.64 <td>0011004</td> <td>170.0577</td> <td>0.57</td> <td>1.00</td> <td>1.25</td> <td>0.50</td>	0011004	170.0577	0.57	1.00	1.25	0.50
C9H1203         168.0786         0.36         1.00         1.33         0.33           C20H3206         368.2199         8.31         0.63         1.60         0.30           C1H1202         140.0837         0.36         1.00         1.50         0.25           C1H12008         280.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.28           C20H3206         368.2199         7.78         0.83         1.60         0.45           C18H2805         324.1937         7.90         1.00         1.56         0.28           C20H3206         340.1886         7.52         0.83         1.56         0.33           C18H2806         340.1886         7.52         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C10H1404         198.0892         8.17         1.00         1.40	C7H8O2	124.0524	0.37	1.00	1.14	0.29
C9H1205         168.0780         0.30         1.00         1.33         0.33           C20H3206         356.2199         7.62         0.67         1.68         0.32           C8H1202         140.0837         0.36         1.00         1.50         0.25           C1H4208         280.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.28           C20H3209         416.2046         7.67         0.56         1.60         0.30           C2H3209         416.2046         7.67         0.56         1.60         0.43           C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C1H1403         170.0943         0.39         1.00         1.56         0.33           C19H3006         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83	C0111202	169.0796	0.26	1.00	1.22	0.22
C20H3206         368.2199         7.62         0.67         1.68         0.32           C8H1202         140.0837         0.36         1.00         1.50         0.25           C1H12008         280.1158         2.47         0.25         1.82         0.73           C18H205         324.1937         7.90         1.00         1.56         0.28           C20H3206         368.2199         7.78         0.83         1.60         0.30           C20H3206         368.2192         7.78         0.83         1.56         0.33           C1H12005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         358.1628         3.15         0.63         1.53         0.47           C16H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0	C9H12O3	168.0786	0.36	1.00	1.33	0.33
C20112500         256-2199         7.62         0.67         1.68         0.32           C811202         140.0837         0.36         1.00         1.50         0.25           C11142008         280.1158         2.47         0.25         1.82         0.73           C1812805         324.1937         7.90         1.00         1.56         0.28           C20H3209         416.2046         7.67         0.56         1.60         0.35           C71H005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.55           C10H1404         198.0892         2.61         0.29         1.82 <td< td=""><td>C20H32O6</td><td>368 2100</td><td>8 31</td><td>0.83</td><td>1.60</td><td>0.30</td></td<>	C20H32O6	368 2100	8 31	0.83	1.60	0.30
C19H3206         356.2199         7.62         0.67         1.68         0.32           C8H1202         140.0837         0.36         1.00         1.50         0.25           C11H2008         280.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.28           C20H3209         416.2046         7.67         0.56         1.60         0.45           C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C1H1403         170.0943         0.39         1.00         1.66         0.42           C19H3208         388.2097         7.61         0.50         1.68         0.42           C1H1406         230.0790         0.35         0.67         1.40         0.60           C1H4208         388.1628         3.15         0.63         1.50         0.33           C1H1404         198.0892         8.17         1.00         1.40         0.4	020113200	500.2177	0.51	0.05	1.00	0.50
C8H1202         140.0837         0.36         1.00         1.50         0.25           C11H2008         280.1158         2.47         0.25         1.82         0.73           C18H2R05         324.1937         7.90         1.00         1.56         0.28           C20H3206         368.2199         7.78         0.83         1.60         0.30           C20H3209         416.2046         7.67         0.56         1.60         0.45           C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.56         0.33           C19H1403         170.0943         0.39         1.00         1.56         0.33           C19H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C1H12006         248.1260         3.09         0.33         1.82         0.55           C1H1404         198.0892         3.25         0.75         1.56	C19H32O6	356.2199	7.62	0.67	1.68	0.32
C8H1202         140.0837         0.36         1.00         1.53         0.25           C1H2008         280.1158         2.47         0.25         1.82         0.73           C18H2805         332.1937         7.90         1.00         1.56         0.28           C20H3209         416.2046         7.67         0.56         1.60         0.35           C1H12806         340.1886         7.52         0.83         1.56         0.33           C1H13005         174.0528         8.25         0.60         1.43         0.71           C1H3208         388.2097         7.61         0.50         1.58         0.32           C1H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.17         1.00         1.40         0.40           C1H2006         248.1260         3.09         0.33         1.82         0.55           C1H404         198.0892         3.25         0.75         1.56         0.44<	COLLIAGO	140.0007	0.04	1.00	1.50	0.05
C11H2008         280.1158         2.47         0.25         1.82         0.73           C18H2805         324.1937         7.90         1.00         1.56         0.28           C20H3209         416.2046         7.67         0.56         1.60         0.30           C20H3209         416.2046         7.67         0.56         1.60         0.45           C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.66         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C1H42608         388.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C10H1404         198.0892         8.17         1.00         1.40	C8H12O2	140.0837	0.36	1.00	1.50	0.25
C11112005         230.1136         2.47         0.23         1.62         0.73           C11112005         324.1937         7.90         1.00         1.56         0.28           C20H3206         368.2199         7.78         0.83         1.60         0.30           C20H3206         340.1886         7.52         0.83         1.56         0.33           C1H12005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C1H12007         264.1260         3.09         0.33         8.2         0.63         1.50         0.35           C1H2007         264.1209         2.61         0.29         1.82         0.64           C1H2007         264.1209         2.61         0.29         1.82         0.64           C1H2006         248.1260         3.04 <td< td=""><td>C11H20O8</td><td>280 1158</td><td>2 47</td><td>0.25</td><td>1.82</td><td>0.73</td></td<>	C11H20O8	280 1158	2 47	0.25	1.82	0.73
C18H2805         324.1937         7.90         1.00         1.56         0.28           C20H3206         368.2199         7.78         0.83         1.60         0.45           C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.65           C1H404         198.0892         3.25         0.75         1.56         0.44           C1H2007         264.1209         2.61         0.29         1.82         0.	0111120008	200.1150	2.47	0.25	1.02	0.75
C20H3206         368.2199         7.78         0.83         1.60         0.30           C20H3209         416.2046         7.67         0.56         1.60         0.45           C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3206         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C1H2006         248.1260         3.09         0.33         1.82         0.55           C1H2007         264.1209         2.61         0.29         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.56         0.4	C18H28O5	324,1937	7.90	1.00	1.56	0.28
C20H3206         368.2199         7.78         0.83         1.60         0.30           C20H3209         416.2046         7.67         0.55         1.60         0.45           C19H3206         340.1886         7.52         0.83         1.56         0.33           C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.33           C10H1404         198.0892         8.17         1.00         1.40         0.40           C1H2006         248.1260         3.09         0.33         1.82         0.55           C1H2007         264.1209         2.51         0.56         0.44           C10H1604         200.1049         3.04         0.75         1.56         0.44	G0011000	2 40 2100		0.00	4 40	0.00
C20H3209         416.2046         7.67         0.56         1.60         0.45           C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C1H42006         248.1260         3.09         0.33         1.82         0.55           C1H42007         264.1209         2.61         0.29         1.82         0.64           C19H1404         186.0892         3.25         0.75         1.60	C20H32O6	368.2199	7.78	0.83	1.60	0.30
C20H3209         410.2040         7.00         0.30         1.00         0.43           C18H3206         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         388.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C10H1404         198.0892         8.17         1.00         1.40         0.40           C1H2006         248.1260         3.09         0.33         1.82         0.64           C1H2007         264.1209         2.61         0.29         1.82         0.64           C10H1604         200.1049         3.04         0.75         1.60         0.40           C10H1604         188.092         2.62         1.00         1.40         0.	C20H22O0	416 2046	7 67	0.56	1.60	0.45
C18H2806         340.1886         7.52         0.83         1.56         0.33           C7H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C1H12006         248.1260         3.09         0.33         1.82         0.64           C1H12007         264.1209         2.61         0.29         1.82         0.64           C10H1604         120.0149         3.04         0.75         1.60         0.40           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.58 <td< td=""><td>C20H32O9</td><td>410.2040</td><td>7.07</td><td>0.50</td><td>1.00</td><td>0.45</td></td<>	C20H32O9	410.2040	7.07	0.50	1.00	0.45
CHH005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C1H2007         264.1209         2.61         0.29         1.82         0.64           C10H1604         200.1049         3.04         0.75         1.60         0.44           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.40         0.	C18H28O6	340 1886	7 52	0.83	1 56	0.33
C/H1005         174.0528         8.25         0.60         1.43         0.71           C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C10H1404         198.0892         8.17         1.00         1.40         0.40           C1H2006         248.1260         3.09         0.33         1.82         0.55           C1H2007         264.1209         2.61         0.29         1.82         0.64           C10H1604         200.1049         3.04         0.75         1.56         0.44           C10H1604         200.1049         3.89         1.00         1.60         0.30           C19H3005         382.093         7.48         1.00         1.40         0.4	610112000	510.1000	1.52	0.00	1.50	0.55
C19H3006         354.2042         7.22         0.83         1.58         0.32           C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.55           C1H404         186.0892         3.25         0.75         1.56         0.44           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0	C7H10O5	174.0528	8.25	0.60	1.43	0.71
C1911403         17.22         0.83         1.38         0.32           C1911403         170.0943         0.39         1.00         1.56         0.33           C1911406         230.0790         0.35         0.67         1.40         0.60           C1712608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C1H2006         248.1260         3.09         0.33         1.82         0.55           C1H2007         264.1209         2.61         0.29         1.82         0.64           C19H1404         186.0892         3.25         0.75         1.60         0.44           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.50         0.38           C10H1603         184.1099         3.85         1.00         1.40         0.40      <	C10U2006	254 2042	7 22	0.02	1 50	0.22
C9H1403         170.0943         0.39         1.00         1.56         0.33           C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.56         0.44           C10H1604         200.1049         3.04         0.75         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.50         0.38           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40	C19H3006	354.2042	1.22	0.85	1.58	0.32
C19H32O8         188.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.55           C11H2007         264.1209         2.61         0.29         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.66         0.44           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.40         0.40           C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40 <td< td=""><td>C9H14O3</td><td>170 0943</td><td>0.39</td><td>1.00</td><td>1 56</td><td>0.33</td></td<>	C9H14O3	170 0943	0.39	1.00	1 56	0.33
C19H3208         388.2097         7.61         0.50         1.68         0.42           C10H1406         230.0790         0.35         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.55           C11H2007         264.1209         2.61         0.29         1.82         0.64           C10H1604         200.1049         3.04         0.75         1.60         0.40           C10H1603         184.1099         3.89         1.00         1.50         0.38           C10H1404         198.0892         2.92         1.00         1.40         0.40           C19H3005         338.2093         7.44         1.00         1.40         0.40           C10H1404         198.0892         7.57         0.60         1.60 <t< td=""><td>05111405</td><td>170.0745</td><td>0.57</td><td>1.00</td><td>1.50</td><td>0.55</td></t<>	05111405	170.0745	0.57	1.00	1.50	0.55
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C19H32O8	388.2097	7.61	0.50	1.68	0.42
C1011406         230.0790         0.33         0.67         1.40         0.60           C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.55           C11H2007         264.1209         2.61         0.29         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.56         0.44           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.75	C1011140C	220.0700	0.25	0.7	1.40	0.00
C17H2608         358.1628         3.15         0.63         1.53         0.47           C6H1005         162.0528         0.62         0.40         1.67         0.83           C20H3007         382.1992         8.21         0.86         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.55           C11H2007         264.1209         2.61         0.29         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.60         0.40           C10H1604         200.1049         3.04         0.75         1.60         0.40           C10H1603         184.1099         3.89         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.78         0.44           C8H1402         142.0994         3.21         0.60         1.50         0	C10H14O6	230.0790	0.35	0.67	1.40	0.60
Cirinioos         J.1.5         J.1.5 <thj.15< th="">         J.1.5         J.1.5         &lt;</thj.15<>	C17H26O8	358 1628	3 1 5	0.63	1 53	0.47
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	01/112000	550.1020	5.15	0.05	1.55	0.47
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C6H10O5	162.0528	0.62	0.40	1.67	0.83
C20H3007         382.1992         8.21         0.86         1.50         0.35           C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.56         0.44           C10H1604         200.1049         3.04         0.75         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.50         0.38           C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C9H1604         188.1049         3.31         0.50         1.75         0.25           C10H1806         234.1103         3.54         0.33         1.80	000110007	202 1002	0.01	0.07	1 50	0.05
C10H1404         198.0892         8.17         1.00         1.40         0.40           C11H2006         248.1260         3.09         0.33         1.82         0.55           C11H2007         264.1209         2.61         0.29         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.60         0.40           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         230.0790         3.15         0.67         1.40         0	C20H30O/	382.1992	8.21	0.86	1.50	0.35
C1011404         198.0892         8.17         1.100         1.40         0.40           C11142006         248.1260         3.09         0.33         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.56         0.44           C10H1604         200.1049         3.04         0.75         1.60         0.40           C10H1603         184.1099         3.89         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.50         0.38           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.75         0.25           C10H1404         198.0892         8.55         1.00         1.76         0.25           C10H1404         198.0892         8.55         1.00         1.75         0.25           C10H1404         198.0892         8.55         1.00         1.75         <	C10U14O4	108 0802	9 17	1.00	1.40	0.40
C11H2006         248.1260         3.09         0.33         1.82         0.55           C11H2007         264.1209         2.61         0.29         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.56         0.44           C10H1604         200.1049         3.04         0.75         1.60         0.40           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.40         0.40           C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         2.57         0.60         1.60         0.50           C10H1404         198.0892         8.55         1.00         1.40         0.40           C9H1604         188.1049         3.31         0.50         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         234.1103         3.54         0.33         1.80         0	C10H1404	196.0692	0.17	1.00	1.40	0.40
C11H2007         264,1209         2.61         0.29         1.82         0.64           C9H14O4         186,0892         3.25         0.75         1.56         0.44           C10H16O4         200,1049         3.04         0.75         1.60         0.40           C10H16O3         184,1099         3.89         1.00         1.60         0.30           C19H30O5         338,2093         7.48         1.00         1.58         0.26           C8H12O3         156,0786         2.62         1.00         1.40         0.40           C10H14O4         198,0892         2.92         1.00         1.40         0.40           C10H14O4         198,0892         7.64         1.00         1.40         0.40           C10H16O5         216,0998         2.57         0.60         1.60         0.50           C10H16O4         198,0892         8.55         1.00         1.75         0.25           C10H16O4         188,1049         3.31         0.50         1.78         0.44           C8H14O2         142,0994         3.25         1.00         1.75         0.25           C10H18O6         234,1103         3.54         0.33         1.80	C11H20O6	248 1260	3.09	0.33	1.82	0.55
C11H2007         264.1209         2.61         0.29         1.82         0.64           C9H1404         186.0892         3.25         0.75         1.56         0.44           C10H1604         200.1049         3.04         0.75         1.60         0.40           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.40         0.40           C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         234.1103         3.54         0.33         1.80         0.60           C8H1402         142.0994         3.25         0.60         1.50         0.63           C10H1806         230.0790         3.15         0.67         1.40         0	0111120000	2.0.1200	2.05	0.00	1.02	0.00
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C11H20O7	264.1209	2.61	0.29	1.82	0.64
C911404         180.092         3.23         0.73         1.50         0.44           C10H1604         200.1049         3.04         0.75         1.60         0.40           C10H1603         184.1099         3.89         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.40         0.40           C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C9H1604         188.1049         3.31         0.50         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         230.0790         3.15         0.67         1.40         0.60           C8H1205         188.0685         1.39         0.60         1.56         0.5	C0H14O4	186 0802	2 25	0.75	1 56	0.44
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0911404	180.0892	5.25	0.75	1.50	0.44
C1011603         184.1099         3.81         1.00         1.60         0.30           C19H3005         338.2093         7.48         1.00         1.58         0.26           C8H1203         156.0786         2.62         1.00         1.50         0.38           C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         234.1103         3.54         0.33         1.80         0.60           C8H1205         188.0685         1.39         0.60         1.50         0.63           C10H1406         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0	C10H16O4	200 1049	3.04	0.75	1.60	0.40
C10H16O3         184.1099         3.89         1.00         1.60         0.30           C19H30O5         338.2093         7.48         1.00         1.58         0.26           C8H12O3         156.0786         2.62         1.00         1.50         0.38           C10H14O4         198.0892         2.92         1.00         1.40         0.40           C10H14O4         198.0892         7.64         1.00         1.40         0.40           C10H14O4         198.0892         8.55         1.00         1.40         0.40           C10H16O5         216.0998         2.57         0.60         1.60         0.50           C10H14O4         198.0892         8.55         1.00         1.40         0.40           C9H16O4         188.1049         3.31         0.50         1.78         0.44           C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H14O2         188.0685         1.39         0.60         1.50         0.63           C10H14O6         230.0790         3.15         0.67         1.40         0	CIONICO I	200.1019	3.01	0.75	1.00	0.10
C19H30O5         338.2093         7.48         1.00         1.58         0.26           C8H12O3         156.0786         2.62         1.00         1.50         0.38           C10H14O4         198.0892         2.92         1.00         1.40         0.40           C10H14O4         198.0892         7.64         1.00         1.40         0.40           C10H14O4         198.0892         8.55         1.00         1.40         0.40           C10H14O4         198.0892         8.55         1.00         1.40         0.40           C9H16O4         188.1049         3.31         0.50         1.78         0.44           C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H12O5         188.0685         1.39         0.60         1.50         0.63           C10H14O6         230.0790         3.15         0.67         1.40         0.60           C9H14O5         202.0841         0.36         0.60         1.56         0.56           C10H14O6         230.0790         3.15         0.67         1.43         0.	C10H16O3	184.1099	3.89	1.00	1.60	0.30
C19H3003         138.2093         1.48         1.00         1.38         0.20           C8H1203         156.0786         2.62         1.00         1.50         0.38           C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C10H1404         198.0892         8.55         1.00         1.40         0.40           C9H1604         188.1049         3.31         0.50         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         234.1103         3.54         0.33         1.80         0.60           C8H1205         188.0685         1.39         0.60         1.50         0.63           C10H1806         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.	C10U2005	228 2002	7 49	1.00	1 50	0.26
C8H12O3         156.0786         2.62         1.00         1.50         0.38           C10H14O4         198.0892         2.92         1.00         1.40         0.40           C10H14O4         198.0892         7.64         1.00         1.40         0.40           C10H16O5         216.0998         2.57         0.60         1.60         0.50           C10H14O4         198.0892         8.55         1.00         1.40         0.40           C9H16O4         188.1049         3.31         0.50         1.78         0.44           C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H12O5         188.0685         1.39         0.60         1.50         0.63           C10H14O6         230.0790         3.15         0.67         1.40         0.60           C9H14O5         202.0841         0.36         0.60         1.56         0.56           C10H14O6         230.0790         3.15         0.67         1.43         0.57           C5H803         116.0473         0.36         0.60         1.50         0.50	C19H50O5	558.2095	7.40	1.00	1.38	0.20
C10H14O4         198.0892         2.92         1.00         1.40         0.40           C10H14O4         198.0892         7.64         1.00         1.40         0.40           C10H14O4         198.0892         7.64         1.00         1.40         0.40           C10H14O4         198.0892         8.55         1.00         1.40         0.40           C10H14O4         198.0892         8.55         1.00         1.40         0.40           C9H16O4         188.1049         3.31         0.50         1.78         0.44           C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H12O5         188.0685         1.39         0.60         1.50         0.63           C10H14O6         230.0790         3.15         0.67         1.40         0.60           C9H14O5         202.0841         0.36         0.60         1.56         0.56           C10H16O5         216.0998         0.36         0.67         1.60         0.80           C7H10O4         158.0579         0.36         0.67         1.60         0.	C8H12O3	156.0786	2.62	1.00	1.50	0.38
C10H1404         198.0892         2.92         1.00         1.40         0.40           C10H1404         198.0892         7.64         1.00         1.40         0.40           C10H1605         216.0998         2.57         0.60         1.60         0.50           C10H1404         198.0892         8.55         1.00         1.40         0.40           C9H1604         188.1049         3.31         0.50         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         234.1103         3.54         0.33         1.80         0.60           C8H1205         188.0685         1.39         0.60         1.50         0.63           C11H2005         232.1311         3.88         0.40         1.82         0.45           C10H1406         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.56           C10H1605         216.0998         0.36         0.67         1.60         0.60           C5H803         116.0473         0.36         0.67         1.60         0.8	60111200	100.0700	2.02	1.00	1.00	0.00
C10H14O4         198.0892         7.64         1.00         1.40         0.40           C10H16O5         216.0998         2.57         0.60         1.60         0.50           C10H14O4         198.0892         8.55         1.00         1.40         0.40           C9H16O4         188.1049         3.31         0.50         1.78         0.44           C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H12O5         188.0685         1.39         0.60         1.50         0.63           C11H2OO5         232.1311         3.88         0.40         1.82         0.45           C10H14O6         230.0790         3.15         0.67         1.40         0.60           C9H14O5         202.0841         0.36         0.60         1.56         0.56           C10H16O5         216.0998         0.36         0.67         1.60         0.60           C5H8O3         116.0473         0.36         0.67         1.60         0.60           C5H8O4         132.0423         0.35         0.50         1.33         1.33<	C10H14O4	198.0892	2.92	1.00	1.40	0.40
C1011404         190.0692         7.04         1.00         1.40         0.40           C10H16O5         216.0998         2.57         0.60         1.60         0.50           C10H1404         198.0892         8.55         1.00         1.40         0.40           C9H16O4         188.1049         3.31         0.50         1.78         0.44           C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H12O5         188.0685         1.39         0.60         1.50         0.63           C10H14O6         230.0790         3.15         0.67         1.40         0.60           C9H14O5         202.0841         0.36         0.60         1.56         0.56           C10H16O5         216.0998         0.36         0.67         1.43         0.57           C5H8O3         116.0473         0.36         0.67         1.60         0.60           C5H8O3         116.0473         0.36         0.67         1.60         0.80           C3H4O4         104.0110         0.35         0.50         1.33         1.33 <td>C10U14O4</td> <td>108 0802</td> <td>7.64</td> <td>1.00</td> <td>1.40</td> <td>0.40</td>	C10U14O4	108 0802	7.64	1.00	1.40	0.40
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	010111404	190.0092	/.04	1.00	1.40	0.40
C10H1404         198.0892         8.55         1.00         1.40         0.40           C9H1604         188.1049         3.31         0.50         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         234.1103         3.54         0.33         1.80         0.60           C8H1205         188.0685         1.39         0.60         1.50         0.63           C10H1406         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.56           C10H1406         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.56           C10H1605         216.0998         0.36         0.67         1.43         0.57           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.66         1.50         0.63 <td>C10H16O5</td> <td>216.0998</td> <td>2.57</td> <td>0.60</td> <td>1.60</td> <td>0.50</td>	C10H16O5	216.0998	2.57	0.60	1.60	0.50
C1011404         198.0892         8.55         1.00         1.40         0.40           C9H1604         188.1049         3.31         0.50         1.78         0.44           C8H1402         142.0994         3.25         1.00         1.75         0.25           C10H1806         234.1103         3.54         0.33         1.80         0.60           C8H1205         188.0685         1.39         0.60         1.50         0.63           C10H1406         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.56           C10H1605         216.0998         0.36         0.60         1.60         0.50           C7H1004         158.0579         0.36         0.75         1.43         0.57           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38 <td>C10111404</td> <td>100 0000</td> <td>0 55</td> <td>1.00</td> <td>1 40</td> <td>0.40</td>	C10111404	100 0000	0 55	1.00	1 40	0.40
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C10H14O4	198.0892	8.33	1.00	1.40	0.40
C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H12O5         188.0685         1.39         0.60         1.50         0.63           C11H2O05         232.1311         3.88         0.40         1.82         0.45           C10H14O6         230.0790         3.15         0.67         1.40         0.60           C9H14O5         202.0841         0.36         0.60         1.56         0.56           C10H16O5         216.0998         0.36         0.60         1.60         0.50           C7H10O4         158.0579         0.36         0.75         1.43         0.57           C5H8O3         116.0473         0.36         0.67         1.60         0.60           C5H8O4         132.0423         0.35         0.50         1.33         1.33           C8H14O3         158.0943         0.37         0.67         1.75         0.38 <td>C9H16O4</td> <td>188 1049</td> <td>3 31</td> <td>0.50</td> <td>1 78</td> <td>0.44</td>	C9H16O4	188 1049	3 31	0.50	1 78	0.44
C8H14O2         142.0994         3.25         1.00         1.75         0.25           C10H18O6         234.1103         3.54         0.33         1.80         0.60           C8H12O5         188.0685         1.39         0.60         1.50         0.63           C11H2OO5         232.1311         3.88         0.40         1.82         0.45           C10H14O6         230.0790         3.15         0.67         1.40         0.60           C9H14O5         202.0841         0.36         0.60         1.56         0.56           C10H16O5         216.0998         0.36         0.67         1.43         0.57           C5H8O3         116.0473         0.36         0.67         1.60         0.60           C5H8O4         132.0423         0.35         0.50         1.33         1.33           C8H12O5         188.0685         0.36         0.67         1.60         0.60           C5H8O4         132.0423         0.35         0.50         1.33         1.33           C8H12O5         188.0685         0.36         0.60         1.50         0.63           C8H14O3         158.0943         0.37         0.67         1.75         0.38 <td>00111004</td> <td>1 10 000</td> <td>0.01</td> <td>1.00</td> <td>1.70</td> <td>0.77</td>	00111004	1 10 000	0.01	1.00	1.70	0.77
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C8H14O2	142.0994	3.25	1.00	1.75	0.25
Contractor         2.34,1105         3.34         0.55         1.80         0.60           C8H1205         188.0685         1.39         0.60         1.50         0.63           C11H2005         232.1311         3.88         0.40         1.82         0.45           C10H1406         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.56           C10H1605         216.0998         0.36         0.60         1.60         0.50           C7H1004         158.0579         0.36         0.67         1.60         0.60           C5H803         116.0473         0.36         0.67         1.60         0.80           C3H404         104.0110         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.71         0.57 </td <td>C10H1906</td> <td>234 1102</td> <td>3 5 1</td> <td>0.22</td> <td>1 20</td> <td>0.60</td>	C10H1906	234 1102	3 5 1	0.22	1 20	0.60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C10111800	234.1105	5.54	0.55	1.60	0.00
C11H2005         232.1311         3.88         0.40         1.82         0.45           C10H1406         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.56           C10H1605         216.0998         0.36         0.60         1.60         0.50           C7H1004         158.0579         0.36         0.75         1.43         0.57           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.60         0.80           C3H404         104.0110         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.71         0.57           C6H804         144.0423         0.36         0.75         1.33         0.67	C8H12O5	188.0685	1.39	0.60	1.50	0.63
C11H2005         232.1311         3.88         0.40         1.82         0.45           C10H1406         230.0790         3.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.56           C10H1605         216.0998         0.36         0.60         1.60         0.50           C7H1004         158.0579         0.36         0.75         1.43         0.57           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.67         1.60         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.50         1.71         0.57           C4H603         102.0317         0.37         0.67         1.50         0.75	0111200	200.0000	2.00	0.00	1.00	0.05
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C11H20O5	232.1311	3.88	0.40	1.82	0.45
C1011400         250.0750         5.15         0.67         1.40         0.60           C9H1405         202.0841         0.36         0.60         1.56         0.56           C10H1605         216.0998         0.36         0.60         1.60         0.50           C7H1004         158.0579         0.36         0.75         1.43         0.57           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.67         1.60         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.50         1.71         0.57           C4H603         102.0317         0.37         0.67         1.50         0.75           C4H603         102.0317         0.36         0.60         1.43         0.71	C10U1404	220 0700	2 1 5	0 47	1.40	0 60
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C10/11400	230.0790	5.15	0.07	1.40	0.00
C10H1605         216.0998         0.36         0.60         1.60         0.50           C7H1004         158.0579         0.36         0.67         1.60         0.60           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.60         0.80           C3H404         104.0110         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.50         1.71         0.57           C6H804         144.0423         0.36         0.75         1.33         0.67           C4H603         102.0317         0.37         0.67         1.50         0.75           C4H603         102.0317         0.36         0.60         1.43         0.71	C9H14O5	202.0841	0.36	0.60	1.56	0.56
C10111005         216.0998         0.36         0.60         1.60         0.50           C7H1004         158.0579         0.36         0.75         1.43         0.57           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.60         0.80           C3H404         104.0110         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.50         1.71         0.57           C6H804         144.0423         0.36         0.75         1.33         0.67           C4H603         102.0317         0.37         0.67         1.50         0.75           C7H1005         174.0528         0.36         0.60         1.43         0.71	010111 (05	016 0000	0.25	0.00	1 (0	0.50
C7H1004         158.0579         0.36         0.75         1.43         0.57           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.60         0.80           C3H404         104.0110         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.75         1.33         0.67           C4H603         102.0317         0.37         0.67         1.50         0.75           C4H603         102.0317         0.37         0.67         1.50         0.75           C7H1005         174.0528         0.36         0.60         1.43         0.71	C10H16O5	216.0998	0.36	0.60	1.60	0.50
C5H803         150.077         0.30         0.75         1.43         0.57           C5H803         116.0473         0.36         0.67         1.60         0.60           C5H804         132.0423         0.35         0.50         1.60         0.80           C3H404         104.0110         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.50         1.71         0.57           C6H804         144.0423         0.36         0.75         1.33         0.67           C4H603         102.0317         0.37         0.67         1.50         0.75           C7H1005         174.0528         0.36         0.60         1.43         0.71	C7H10O4	158 0570	0.36	0.75	1 / 2	0.57
C5H8O3         116.0473         0.36         0.67         1.60         0.60           C5H8O4         132.0423         0.35         0.50         1.60         0.80           C3H4O4         104.0110         0.35         0.50         1.33         1.33           C8H12O5         188.0685         0.36         0.60         1.50         0.63           C8H14O3         158.0943         0.37         0.67         1.75         0.38           C9H16O5         204.0998         0.35         0.40         1.78         0.56           C4H6O4         118.0266         0.35         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C4H6O3         102.0317         0.36         0.60         1.43         0.71	0/111004	130.0379	0.50	0.75	1.43	0.57
C5H804         132.0423         0.35         0.50         1.60         0.80           C3H404         104.0110         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.50         1.71         0.57           C6H804         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H1005         174.0528         0.36         0.60         1.43         0.71	C5H8O3	116.0473	0.36	0.67	1.60	0.60
C5H804         132.0423         0.35         0.50         1.60         0.80           C3H404         104.0110         0.35         0.50         1.33         1.33           C8H1205         188.0685         0.36         0.60         1.50         0.63           C8H1403         158.0943         0.37         0.67         1.75         0.38           C9H1605         204.0998         0.35         0.40         1.78         0.56           C4H604         118.0266         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.75         1.33         0.67           C4H603         102.0317         0.37         0.67         1.50         0.75           C7H1005         174.0528         0.36         0.60         1.43         0.71	0511000	122.0.122	0.00	0.50	1.00	0.00
C3H4O4         104.0110         0.35         0.50         1.33         1.33           C8H12O5         188.0685         0.36         0.60         1.50         0.63           C8H14O3         158.0943         0.37         0.67         1.75         0.38           C9H16O5         204.0998         0.35         0.40         1.78         0.56           C4H6O4         118.0266         0.35         0.50         1.50         1.00           C7H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	C5H8O4	132.0423	0.35	0.50	1.60	0.80
C3H4O4         104.0110         0.35         0.30         1.35         1.35           C8H12O5         188.0685         0.36         0.60         1.50         0.63           C8H14O3         158.0943         0.37         0.67         1.75         0.38           C9H16O5         204.0998         0.35         0.40         1.78         0.56           C4H6O4         118.0266         0.35         0.50         1.50         1.00           C7H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	C3H4O4	104 01 10	0.25	0.50	1 22	1 22
C8H12O5         188.0685         0.36         0.60         1.50         0.63           C8H14O3         158.0943         0.37         0.67         1.75         0.38           C9H16O5         204.0998         0.35         0.40         1.78         0.56           C4H6O4         118.0266         0.35         0.50         1.50         1.00           C7H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	C311404	104.0110	0.55	0.50	1.33	1.33
C8H14O3         158.0943         0.37         0.67         1.75         0.38           C9H16O5         204.0998         0.35         0.40         1.78         0.56           C4H6O4         118.0266         0.35         0.50         1.50         1.00           C7H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	C8H12O5	188.0685	0.36	0.60	1.50	0.63
C8H14O3         158.0943         0.37         0.67         1.75         0.38           C9H16O5         204.0998         0.35         0.40         1.78         0.56           C4H6O4         118.0266         0.35         0.50         1.50         1.00           C7H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	0011100	150.0010	0.00	0.00	1.00	0.00
C9H16O5         204.0998         0.35         0.40         1.78         0.56           C4H6O4         118.0266         0.35         0.50         1.50         1.00           C7H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	C8H14O3	158.0943	0.37	0.67	1.75	0.38
C4H603         118.0266         0.35         0.40         1.78         0.30           C4H604         118.0266         0.35         0.50         1.50         1.00           C7H1204         160.0736         0.36         0.50         1.71         0.57           C6H804         144.0423         0.36         0.75         1.33         0.67           C4H603         102.0317         0.37         0.67         1.50         0.75           C7H1005         174.0528         0.36         0.60         1.43         0.71	C9H16O5	204 0998	0.35	0.40	1 78	0.56
C4H6O4         118.0266         0.35         0.50         1.50         1.00           C7H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	0,111003	204.0770	0.55	0.40	1.70	0.50
C7H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	C4H6O4	118.0266	0.35	0.50	1.50	1.00
C/H12O4         160.0736         0.36         0.50         1.71         0.57           C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H1005         174.0528         0.36         0.60         1.43         0.71	CTUIDOA	160.0726	0.26	0.50	1 71	0.57
C6H8O4         144.0423         0.36         0.75         1.33         0.67           C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	C/H12O4	160.0736	0.36	0.50	1./1	0.57
C4H6O3         102.0317         0.36         0.75         1.55         0.67           C7H1005         174.0528         0.36         0.60         1.43         0.71	C6H8O4	144 0423	0.36	0.75	1 22	0.67
C4H6O3         102.0317         0.37         0.67         1.50         0.75           C7H10O5         174.0528         0.36         0.60         1.43         0.71	011004	144.0423	0.50	0.75	1.55	0.07
<u>C7H1005</u> 174.0528 0.36 0.60 1.43 0.71	C4H6O3	102.0317	0.37	0.67	1.50	0.75
<u> </u>	CTUIDOS	174.0500	0.26	0.00	1.40	0.71
	C/H1005	1/4.0528	0.30	0.00	1.45	0.71

C5H6O4	130.0266	0.36	0.75	1.20	0.80
C6H10O4	146.0579	0.36	0.50	1.67	0.67
C6H8O3	128.0473	0.37	1.00	1.33	0.50
C10H18O5	218.1154	0.36	0.40	1.80	0.50
C7H12O3	144.0786	0.36	0.67	1.71	0.43
C8H14O4	174.0892	3.21	0.50	1.75	0.50

Table S4.3.10 Molecular formulas of organic compounds detected in isoprene SOA in ESI- mode.

Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
C6H14O7	198.0740	0.39	0.00	2.33	1.17
C6H14O6	182.0790	0.37	0.00	2.33	1.00
C5H6O3	114.0317	0.66	1.00	1.20	0.60
C6H14O8	214.0689	0.39	0.00	2.33	1.33
C3H6O2	74.0368	0.40	0.50	2.00	0.67
C5H6O4	130.0266	0.38	0.75	1.20	0.80
C5H8O4	132.0423	0.40	0.50	1.60	0.80
C4H6O3	102.0317	0.43	0.67	1.50	0.75
C2H2O4	89.9953	2.07	0.50	1.00	2.00
C4H6O5	134.0215	0.38	0.40	1.50	1.25
C6H10O5	162.0528	0.48	0.40	1.67	0.83
C3H4O3	88.0160	0.37	0.67	1.33	1.00
C3H4O2	72.0211	0.38	1.00	1.33	0.67
C5H6O5	146 0215	0.38	0.60	1.20	1.00
C4H6O2	86.0368	0.86	1.00	1.50	0.50
C5H8O4	132 0423	1.18	0.50	1.60	0.80
C4H8O2	88.0524	0.48	0.50	2.00	0.50
C6H10O5	162 0528	0.40	0.50	1.67	0.83
C4H6O2	86.0368	0.02	1.00	1.50	0.05
C14H6O2	206.0368	0.32	1.00	0.43	0.50
C5H12O4	136.0736	0.36	0.00	2.40	0.14
C5H12O4	152.0685	0.30	0.00	2.40	1.00
C17U2604	204 1921	0.37	0.00	2.40	0.24
C7H16O7	212 0806	0.05	1.00	1.33	1.00
C/HI60/	212.0890	0.50	0.00	2.29	1.00
CT1H2208	282.1315	2.74	0.13	2.00	0.73
C5H12O6	108.0034	0.39	0.00	2.40	1.20
C11H22O8	282.1315	0.95	0.13	2.00	0.73
C4H8O3	104.0473	0.58	0.33	2.00	0.75
C14H60	190.0419	0.40	1.00	0.43	0.07
C8H12O3	156.0786	2.61	1.00	1.50	0.38
C5H12O7	184.0583	0.46	0.00	2.40	1.40
C5H8O3	116.04/3	0.81	0.67	1.60	0.60
C9H14O4	186.0892	2.51	0.75	1.56	0.44
C2H4O2	60.0211	0.39	0.50	2.00	1.00
C5H8O3	116.04/3	0.38	0.67	1.60	0.60
C6H8O5	160.0372	0.63	0.60	1.33	0.83
C2H2O3	74.0004	0.37	0.67	1.00	1.50
C7H12O5	176.0685	1.48	0.40	1.71	0.71
C5H4O4	128.0110	0.39	1.00	0.80	0.80
C11H22O8	282.1315	2.38	0.13	2.00	0.73
C5H12O4	136.0736	2.73	0.00	2.40	0.80
C4H6O3	102.0317	2.76	0.67	1.50	0.75
C7H12O5	176.0685	2.47	0.40	1.71	0.71
C14H22O4	254.1518	7.79	1.00	1.57	0.29
C4H6O	70.0419	0.73	1.00	1.50	0.25
C7H12O4	160.0736	3.00	0.50	1.71	0.57
C6H8O4	144.0423	0.96	0.75	1.33	0.67
C13H4O	176.0262	0.35	1.00	0.31	0.08
C5H10O3	118.0630	0.82	0.33	2.00	0.60
C5H12O4	136.0736	2.52	0.00	2.40	0.80
C8H12O4	172.0736	1.47	0.75	1.50	0.50
C10H14O5	214.0841	2.73	0.80	1.40	0.50
C8H16O8	240.0845	0.74	0.13	2.00	1.00
C2H4O2	60.0211	0.63	0.50	2.00	1.00
C11H20O8	280.1158	1.23	0.25	1.82	0.73

C'H1005         174.0528         0.82         0.60         1.43         0.71           CTH805         172.0372         0.38         0.80         1.14         0.71           CH1205         164.0685         0.97         0.20         2.00         0.83           C1011204         196.0736         2.80         1.00         1.20         0.40           C511403         112.0160         3.22         1.00         0.80         0.60           C1011809         282.0951         1.14         0.22         1.80         0.90           C1011605         21.60998         3.74         0.60         1.60         0.50           C1011605         21.60998         3.74         0.60         1.60         0.50           C11122010         310.1264         3.02         0.22         1.83         0.75           C6118007         74.0368         2.88         0.50         1.33         1.00           C1112209         298.1224         1.09         0.51         1.33         1.00           C31600         54.0419         0.45         1.00         2.00         0.33           C411802         80.0524         3.00         0.55         2.00         0.55 <th></th> <th></th> <th></th> <th></th> <th></th> <th></th>						
CT805         172.0372         0.38         0.80         1.14         0.71           C1812002         20.1463         7.99         1.00         1.54         0.15           C011205         164.0685         0.97         0.20         2.00         0.83           C1011300         312.2         1.00         0.80         0.60           C1011800         282.0951         1.14         0.22         1.80         0.90           C1011800         22.010         0.78         0.25         1.80         0.80           C1011605         21.60998         3.74         0.60         1.60         0.50           C1112209         310.1264         3.02         0.22         1.83         0.75           C1112209         298.1264         0.63         0.11         2.00         0.33           C1112209         298.1264         0.63         0.11         2.00         0.35           C11112209         298.1264         0.63         0.11         2.00         0.35           C11112209         298.1264         0.63         0.11         0.14         0.44           C4H603         100.0137         6.20         0.67         1.50         0.50	C7H10O5	174.0528	0.82	0.60	1.43	0.71
C1312002 208.1463 7.99 1.00 1.54 0.15 C6H1205 164.0685 0.97 0.20 2.00 0.83 C10H1804 196.0736 2.80 1.00 1.20 0.40 C5H403 112.0160 3.22 1.00 0.80 0.60 C10H1808 266.1002 0.78 0.25 1.80 0.90 C10H1805 216.0998 3.74 0.60 1.60 0.50 C10H1605 216.0998 3.74 0.60 1.60 0.50 C10H1605 216.0998 3.74 0.60 1.60 0.50 C10H1605 216.0998 3.74 0.60 1.60 0.50 C1H20010 312.1056 0.87 0.20 1.83 0.75 C6H802 74.0368 2.53 0.50 2.00 0.67 C12H209 310.1264 3.02 0.22 1.83 0.75 C6H806 1.76.0321 1.09 0.50 1.33 1.00 C1H12209 298.1264 0.63 0.11 2.00 0.82 C4H802 88.0524 3.00 0.50 2.00 0.50 C3H60 2.80.017 6.20 0.45 1.00 2.00 0.50 C3H60 2.80.017 6.20 0.45 1.00 2.00 0.50 C3H60 2.80.017 6.20 0.67 1.15 0.075 C4H803 102.0317 6.20 0.67 1.15 0.075 C4H803 100.0160 0.43 1.00 1.00 0.75 C4H803 100.0160 0.43 1.00 1.00 0.75 C4H803 100.0160 0.43 1.00 1.00 0.75 C4H803 2.02.0841 2.98 0.63 1.55 0.38 C9H1004 182.03947 0.69 0.33 1.78 0.67 C4H803 2.02.0841 2.98 0.60 1.55 0.56 C4H805 2.20.0947 0.69 0.33 1.78 0.67 C4H805 2.30.790 3.05 0.67 1.40 0.00 C9H1606 2.20.0947 0.69 0.33 1.78 0.67 C4H105 188.0685 2.53 0.16 1.50 0.63 C4H105 188.0685 2.53 0.14 2.00 0.64 C4H205 188.0685 2.53 0.11 2.00 0.64 C4H205 188.0685 2.53 0.17 2.00 0.60 C7H1003 142.0630 1.44 1.00 1.43 0.43 C4H205 188.0685 2.53 0.11 2.00 0.82 C7H1007 206.0427 0.93 0.43 1.43 1.00 C10H206 230.1790 3.05 0.67 1.40 0.60 C9H1808 254.1002 0.81 0.13 2.00 0.89 C7H1003 120.0681 2.83 0.50 2.00 0.40 C3H1205 188.0685 0.83 0.60 1.50 0.63 C4H105 192.0988 2.43 0.50 2.00 0.40 C3H1205 188.0685 0.83 0.60 1.50 0.63 C4H105 192.0988 2.43 0.50 2.00 0.40 C3H1205 188.0685 0.83 0.60 1.50 0.63 C1H1209 2.98.1264 2.55 0.11 2.00 0.82 C7H1003 174.1256 7.51 0.33 2.00 0.33 C3H40 5.0026 2.79 0.13 2.00 0.83 C3H40 5.0026 2.79 0.13 2.00 0.83 C3H40 5.0026 2.79 0.13 2.00 0.33 C3H40 5.00841 0.48 0.60 1.50 0.55 C3H1205 198.0845 0.83 0.40 1.57 C3H1205 196.0	C7H8O5	172.0372	0.38	0.80	1.14	0.71
C6H1205         164.0685         0.97         0.20         2.00         0.83           C10H1204         196.0736         2.80         1.00         1.20         0.40           C10H1809         282.0951         1.14         0.22         1.80         0.90           C10H1805         246.1002         0.78         0.25         1.80         0.80           C10H205         24.0368         2.88         0.50         2.00         0.67           C10H2010         312.1056         0.87         0.20         1.82         0.91           C3H602         74.0368         2.53         0.50         2.00         0.67           C1H2209         310.1264         3.02         0.22         1.83         0.75           C4H802         88.0524         3.00         0.50         2.00         0.33           C4H603         102.0317         6.20         0.67         1.50         0.75           C4H603         102.0317         6.20         0.67         1.50         0.75           C4H403         1.00         1.00         1.00         1.04         4.20         0.00         0.33           C4H603         1.00.0160         0.43         1.00	C13H20O2	208.1463	7.99	1.00	1.54	0.15
C10H1204         196.0736         2.80         1.00         1.20         0.40           C5H403         112.0160         3.22         1.00         0.80         0.60           C10H1809         282.0951         1.14         0.22         1.80         0.90           C10H1605         216.0998         2.88         0.50         2.00         0.67           C10H1605         216.0998         3.74         0.60         1.83         0.75           C3H602         74.0568         2.53         0.50         2.20         0.67           C12H2209         310.1264         3.02         0.22         1.83         0.75           C4H802         88.0524         3.00         0.50         1.33         1.00           C3H60         58.0419         0.43         1.00         2.00         0.33           C4H803         10.2017         6.20         0.67         1.50         0.75           C10H1607         248.0896         3.02         0.43         1.60         0.70           C4H403         100.0160         0.43         1.00         1.75         0.75           C10H1806         234.1103         2.74         0.33         1.78         0.67	C6H12O5	164.0685	0.97	0.20	2.00	0.83
CSH403         112.0160         3.22         1.00         0.80         0.60           C10H1809         282.0951         1.14         0.22         1.80         0.90           C10H1805         266.1002         0.78         0.25         1.80         0.80           C10H1605         216.0998         3.74         0.60         1.60         0.50           C1H20010         312.1056         0.87         0.20         1.82         0.91           C3H602         74.0368         2.53         0.50         2.33         1.00           CH806         176.0321         1.09         0.50         1.33         1.00         0.82           CH806         156.0321         1.09         0.50         2.00         0.67         1.50         0.75           CH806         156.0321         6.20         0.67         1.50         0.75         0.75           CH4103         100.0160         4.33         1.00         1.00         0.33         1.78         0.67           CH4103         100.0160         0.43         1.00         1.00         0.75         CH4103         1.00         1.60         0.75           CH4105         20.0843         1.65 <td< td=""><td>C10H12O4</td><td>196.0736</td><td>2.80</td><td>1.00</td><td>1.20</td><td>0.40</td></td<>	C10H12O4	196.0736	2.80	1.00	1.20	0.40
C101H1809         282.0951         1.14         0.22         1.80         0.90           C101H1808         266.1002         0.78         0.25         1.80         0.80           C101H1605         216.0998         3.74         0.60         1.60         0.50           C11H20010         312.1056         0.87         0.20         1.82         0.91           C3H602         74.0368         2.83         0.50         2.00         0.67           C1H2209         310.1264         3.02         0.22         1.83         0.75           C4H802         88.0524         3.00         0.50         2.00         0.50           C3H60         58.0419         0.43         1.00         2.00         0.51           C4H603         102.0577         2.69         1.00         1.11         0.44           C4H603         102.017         6.20         0.67         1.50         0.75           C10H1607         248.0896         3.02         0.43         1.60         0.70           C4H403         100.0160         0.43         1.00         1.78         0.67           C1H1405         202.0841         2.98         0.60         1.56         0.56	C5H4O3	112.0160	3.22	1.00	0.80	0.60
C10H1808         266.1002         0.78         0.25         1.80         0.80           C3H602         74.0368         2.88         0.50         2.00         0.67           C1H20010         312.1056         0.87         0.20         1.82         0.91           C3H602         74.0368         2.53         0.50         2.00         0.67           C1H2209         310.1264         3.02         0.22         1.83         0.75           C6H806         176.0521         1.09         0.50         1.33         1.00           C1H2209         298.1264         0.63         0.11         2.00         0.82           C4H802         88.0524         3.00         0.50         2.00         0.33           C5H1004         182.0579         2.69         1.00         1.11         0.44           C4H603         100.0160         0.43         1.00         1.00         0.75           C1H1806         220.0947         2.89         0.33         1.78         0.67           C1H1207         220.6833         1.65         0.43         1.50         0.88           C9H1405         220.0947         0.69         0.33         1.76         0.67 </td <td>C10H18O9</td> <td>282.0951</td> <td>1.14</td> <td>0.22</td> <td>1.80</td> <td>0.90</td>	C10H18O9	282.0951	1.14	0.22	1.80	0.90
C3H602         74.0368         2.88         0.50         2.00         0.67           C10H1605         216.0998         3.74         0.60         1.82         0.91           C3H602         74.0368         2.53         0.50         2.00         0.67           C12H2209         310.1264         3.02         0.22         1.83         0.75           C4H802         88.0524         3.00         0.50         2.00         0.50           C3H60         58.0419         0.45         1.00         1.11         0.44           C4H802         88.0524         3.00         0.50         2.00         0.57           C3H1004         182.0579         2.69         1.00         1.11         0.44           C4H603         102.017         2.20.0947         2.89         0.33         1.78         0.67           C4H403         100.0160         0.43         1.00         1.00         0.75         C8H1207         220.09843         2.98         0.63         1.56         0.56           C10H1806         234.1103         2.74         0.33         1.80         0.66         C9H1405         220.0947         0.69         0.33         1.78         0.66	C10H18O8	266.1002	0.78	0.25	1.80	0.80
C1011605         216.098         3.74         0.60         1.60         0.50           C111620010         312.1056         0.87         0.20         1.82         0.91           C31602         74.0368         2.53         0.50         2.00         0.67           C1212209         310.1264         3.02         0.22         1.83         0.75           C618006         176.0321         1.09         0.50         1.33         1.00           C1112209         298.1264         3.00         0.50         2.00         0.33           C41802         88.0524         3.00         0.50         2.00         0.33           C911004         182.0579         2.69         1.00         1.01         0.44           C414603         100.0160         0.43         1.00         0.75         C           C1011607         248.0896         3.02         0.43         1.50         0.75           C1114207         220.0881         1.68         0.43         1.50         0.68           C10111806         234.1103         2.74         0.33         1.80         0.60           C1114207         266.1366         2.54         0.14         2.00         0.64 <td>C3H6O2</td> <td>74.0368</td> <td>2.88</td> <td>0.50</td> <td>2.00</td> <td>0.67</td>	C3H6O2	74.0368	2.88	0.50	2.00	0.67
C1H220010         312,1056         0.87         0.20         1.82         0.91           C3H602         74,0368         2.53         0.50         2.00         0.67           C12H2209         310,1264         3.02         0.22         1.83         0.75           C6H806         176,0321         1.09         0.50         1.33         1.00           C1H2209         288,1264         0.63         0.11         2.00         0.82           C4H802         88,0524         3.00         0.50         2.00         0.33           C9H1004         182,0579         2.69         1.00         1.11         0.44           C4H403         102,017         2.20         0.43         1.60         0.75           C10H1606         220,0947         2.89         0.33         1.78         0.67           C4H403         100,0160         0.43         1.50         0.88         0.78           C10H1806         224,1103         2.74         0.33         1.78         0.67           C1H2207         266,1366         2.54         0.14         2.00         0.64           C8H1405         188,0685         2.53         0.60         1.50         0.25	C10H16O5	216.0998	3.74	0.60	1.60	0.50
C3H602         74.0368         2.53         0.50         2.00         0.67           C12H2209         310.1264         3.02         0.22         1.83         0.075           C6H806         176.0321         1.09         0.50         1.33         1.00           C1H2209         298.1264         0.63         0.11         2.00         0.53           C3H60         58.0419         0.45         1.00         2.10         0.33           C3H1004         182.0579         2.69         1.00         1.11         0.44           C4H403         102.0317         6.20         0.67         1.50         0.75           C10H1607         248.0896         3.02         0.43         1.50         0.75           C4H403         1000.160         0.43         1.50         0.87         0.66           C4H403         1000.160         0.43         1.50         0.88         0.66         0.56         0.56           C10H1806         234.1103         2.74         0.33         1.80         0.60         0.61         5.5         0.56           C10H1806         230.0790         3.05         0.67         1.40         0.60         0.61         0.61         <	C11H20O10	312.1056	0.87	0.20	1.82	0.91
C12H2209         310.1264         3.02         0.22         1.83         0.75           C6H806         176.0321         1.09         0.50         1.33         1.00           C1HB209         288.0524         3.00         0.50         2.00         0.82           C4H802         88.0524         3.00         0.50         2.00         0.33           C9H1004         182.0579         2.69         1.00         1.11         0.44           C4H603         102.0317         6.20         0.67         1.50         0.75           C10H1607         248.0896         3.02         0.43         1.60         0.77           C9H1606         220.0947         2.89         0.33         1.80         0.66           C1H1405         202.0841         2.98         0.60         1.56         0.56           C1H1806         234.1103         2.74         0.33         1.80         0.66           C1H18207         266.1366         2.53         0.60         1.50         0.25           C7H1003         142.0630         1.44         1.00         1.53         0.25           C7H1007         266.1260         2.78         0.17         2.00         0.60	C3H6O2	74.0368	2.53	0.50	2.00	0.67
CoH806         1760321         1.09         0.30         1.33         1.00           C1HH209         298.1264         0.63         0.11         2.00         0.82           C4H802         88.0524         3.00         0.50         2.00         0.53           C3H60         58.0419         0.45         1.00         1.11         0.44           C4H603         102.0317         6.20         0.67         1.50         0.75           C10H1607         248.0896         3.02         0.43         1.60         0.70           C9H1606         220.0947         2.89         0.60         1.56         0.56           C1H1205         220.0841         2.98         0.60         1.56         0.56           C1H1205         220.0841         2.98         0.60         1.56         0.56           C1H1207         22661366         2.54         0.14         2.00         0.64           CH1405         220.0947         0.69         0.33         1.78         0.67           C1H2207         2661366         2.54         0.14         2.00         0.64           C1H2207         2661366         2.54         0.17         2.00         0.60	C12H22O9	310.1264	3.02	0.22	1.83	0.75
C11H2209         298.1264         0.63         0.11         2.00         0.82           C4H802         88.0524         3.00         0.50         2.00         0.33           C9H1004         182.0579         2.69         1.00         2.11         0.44           C4H603         102.0317         6.20         0.67         1.50         0.75           C10H1607         248.0896         3.02         0.43         1.60         0.70           C9H1606         220.0947         2.89         0.33         1.78         0.67           C4H403         1000160         0.43         1.00         1.00         0.75           C10H1806         223.1103         2.74         0.33         1.80         0.66           C10H1806         234.1103         2.74         0.33         1.80         0.66           C1H1207         266.1366         2.54         0.14         2.00         0.64           C8H1205         188.0685         2.53         0.60         1.50         0.63           C7H1007         206.0427         0.93         0.43         1.43         1.00           C10H1206         230.0790         3.05         0.67         1.40         0.60	C6H8O6	176.0321	1.09	0.50	1.33	1.00
C3H802         88.049         0.45         1.00         2.00         0.30           CSH60         38.0419         0.45         1.00         1.11         0.44           C4H603         102.0317         6.20         0.67         1.50         0.75           C10H1607         248.0896         3.02         0.43         1.60         0.70           C9H1606         220.0947         2.89         0.33         1.78         0.67           C4H403         100.0160         0.43         1.00         1.00         0.75           C8H1207         220.0883         1.65         0.43         1.50         0.88           C9H1405         220.0947         0.69         0.33         1.78         0.67           C1H2207         266.1366         2.54         0.14         2.00         0.64           C8H1205         188.0685         2.53         0.60         1.50         0.25           C7H1003         142.0630         1.44         1.00         1.43         0.43           C10H1206         236.1260         2.78         0.17         2.00         0.60           C9H1808         254.1002         0.81         0.13         2.00         0.43 </td <td>C11H22O9</td> <td>298.1264</td> <td>0.63</td> <td>0.11</td> <td>2.00</td> <td>0.82</td>	C11H22O9	298.1264	0.63	0.11	2.00	0.82
C9H1004         138.0519         2.69         1.00         2.10         0.33           C9H1004         182.0579         2.69         1.00         1.11         0.43           C10H1607         248.0896         3.02         0.43         1.60         0.75           C9H1066         220.0947         2.89         0.33         1.78         0.67           C4H403         100.0160         0.43         1.00         1.00         0.75           C8H1207         220.0583         1.65         0.43         1.50         0.88           C10H1806         234.1103         2.74         0.33         1.80         0.60           C1H12207         266.1366         2.54         0.14         2.00         0.64           C4H60         70.0419         0.40         1.00         1.50         0.63           C4H60         70.0419         0.40         1.00         1.43         0.43           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.67         1.40         0.60           C9H1006         236.1260         2.78         0.17         2.00         0.89	C4H8O2	88.0524	5.00	0.50	2.00	0.50
C3H603         102.0317         6.20         0.67         1.50         0.73           C10H1607         248.0896         3.02         0.43         1.60         0.70           C9H1606         220.0947         2.89         0.33         1.78         0.67           C4H403         100.0160         0.43         1.00         1.00         0.75           C8H1207         220.0583         1.65         0.43         1.50         0.88           C9H1405         202.0841         2.98         0.60         1.56         0.56           C10H1806         234.1103         2.74         0.33         1.78         0.67           C1H2207         266.1366         2.54         0.14         2.00         0.64           C8H1205         188.0685         2.53         0.60         1.50         0.25           C7H1003         142.0630         1.44         1.00         1.43         1.00           C10H2006         236.1260         2.78         0.17         2.00         0.60           C9H1808         254.1002         0.81         0.13         2.00         0.43           C1H14206         190.0477         2.11         0.50         2.03         0.55 <td>C0H10O4</td> <td>182 0570</td> <td>2.60</td> <td>1.00</td> <td>2.00</td> <td>0.55</td>	C0H10O4	182 0570	2.60	1.00	2.00	0.55
C1011607         248.0896         3.02         0.43         1.60         0.70           C911606         220.0947         2.89         0.33         1.78         0.67           C41403         100.0160         0.43         1.00         1.00         0.75           C811207         220.0583         1.65         0.43         1.50         0.88           C911405         202.0841         2.98         0.60         1.56         0.56           C1011806         234.1103         2.74         0.33         1.80         0.60           C911606         220.0947         0.69         0.33         1.78         0.67           C11112207         266.1366         2.54         0.14         2.00         0.64           C811205         188.0685         2.53         0.60         1.50         0.63           C7H1007         206.0427         0.93         0.43         1.43         1.00           C1011406         230.0790         3.05         0.67         1.40         0.60           C1014106         230.0790         3.05         0.67         1.40         0.60           C1014106         230.0790         3.05         0.67         1.40         0.60	C/H6O3	102.0379	2.09	1.00	1.11	0.44
C9111606         220.0947         2.89         0.33         1.78         0.67           C4H403         100.0160         0.43         1.00         1.00         0.75           C8H1207         220.0583         1.65         0.43         1.50         0.88           C9H1405         202.0581         1.65         0.43         1.50         0.66           C19H1606         234.1103         2.74         0.33         1.80         0.67           C1H12207         266.1366         2.54         0.14         2.00         0.63           C4H60         70.0419         0.40         1.00         1.43         1.00           C10H1205         188.0685         2.53         0.60         1.50         0.63           C7H1007         206.0427         0.93         0.43         1.43         1.00           C10H1406         230.0790         3.05         0.67         1.40         0.60           C9H1808         254.1002         0.81         0.13         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.60           C9H1803         174.1256         7.51         0.33         2.00         0.33	C10H16O7	2/18 0896	3.02	0.07	1.50	0.75
C3H403         100.0160         0.43         1.00         1.00         0.75           C8H1207         220.0883         1.65         0.43         1.50         0.88           C9H1405         202.0841         2.98         0.60         1.56         0.56           C10H1806         234.1103         2.74         0.33         1.78         0.67           C11H2207         266.1366         2.54         0.14         2.00         0.64           C4H60         70.0419         0.40         1.00         1.50         0.25           C7H1003         142.0630         1.44         1.00         1.43         0.43           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.67         1.43         0.86           C5H1002         102.0681         2.83         0.50         2.00         0.43           C3H2808         432.1784         8.02         1.00         1.22         0.35           C1H020         234.0740         2.70         0.43         1.56         0.78	C9H16O6	240.0070	2.89	0.45	1.00	0.70
C8H1207         220.0833         1.65         0.43         1.50         0.88           C9H1405         220.0841         2.98         0.60         1.56         0.56           C10H1806         224.1103         2.74         0.33         1.78         0.67           C11H2207         266.1366         2.54         0.14         2.00         0.64           C8H1205         188.0685         2.53         0.60         1.50         0.63           C7H1003         142.0630         1.44         1.00         1.43         0.43           C7H1007         206.0427         0.93         0.43         1.43         1.00           C10H1406         230.0790         3.05         0.67         1.44         0.60           C9H1808         254.1002         0.81         0.13         2.00         0.86           C5H1002         102.0681         2.83         0.50         2.00         0.40           C3H18208         432.1784         8.02         1.00         1.22         0.33           C1H1407         234.0740         2.70         0.43         1.56         0.78           C1H14209         298.1264         2.55         0.11         2.00         0.33<	C4H4O3	100.0160	0.43	1.00	1.70	0.75
C9H1405         202.0841         2.98         0.60         1.56         0.55           C10H1806         234.1103         2.74         0.33         1.80         0.60           C9H1606         220.0947         0.69         0.33         1.78         0.67           C1H2207         266.1366         2.54         0.14         2.00         0.64           C4H60         70.0419         0.40         1.00         1.50         0.25           C7H1003         142.0630         1.44         1.00         1.43         0.43           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.67         1.40         0.60           C9H1808         254.1002         0.81         0.13         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.86           C3H1808         432.178         8.02         1.00         1.22         0.35           C1H2209         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.43         1.56         0.78	C8H12O7	220.0583	1.65	0.43	1.50	0.88
C10H1806         234.1103         2.74         0.33         1.80         0.60           C9H1606         220.0947         0.69         0.33         1.78         0.67           C11H2207         266.1366         2.54         0.14         2.00         0.64           C8H1205         188.0685         2.53         0.60         1.50         0.63           C4H60         70.0419         0.40         1.00         1.43         0.43           C7H1007         206.0427         0.93         0.43         1.43         1.00           C10H1406         230.0790         3.05         0.67         1.40         0.60           C1H12006         236.1260         2.78         0.17         2.00         0.60           C9H1808         254.1002         0.81         0.13         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.86           C3H18208         432.1784         8.02         1.00         1.82         0.55           C11H2209         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.43         1.56         0.78 <td>C9H14O5</td> <td>202.0841</td> <td>2.98</td> <td>0.60</td> <td>1.56</td> <td>0.56</td>	C9H14O5	202.0841	2.98	0.60	1.56	0.56
C9H1606         220.0947         0.69         0.33         1.78         0.67           C11H2207         266.1366         2.54         0.14         2.00         0.63           C4H60         70.0419         0.40         1.00         1.50         0.63           C7H1003         142.0630         1.44         1.00         1.43         0.43           C7H1007         206.0427         0.93         0.43         1.43         1.00           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H2006         236.1260         2.78         0.17         2.00         0.89           C7H1002         102.0681         2.83         0.50         2.00         0.40           C23H2808         432.1784         8.02         1.00         1.22         0.35           C1H209         298.1264         2.55         0.11         2.00         0.82           C9H1407         174.0277         0.39         0.00         2.50         1.75           C7H803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75	C10H18O6	234.1103	2.74	0.33	1.80	0.60
C11H2207         266.1366         2.54         0.14         2.00         0.64           C8H1205         188.0685         2.53         0.60         1.50         0.25           C7H1003         142.0630         1.44         1.00         1.43         0.43           C10H106         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.07         1.43         0.86           C7H1007         100.0477         2.11         0.50         1.43         0.86           C3H1002         102.0681         2.83         0.50         2.00         0.40           C23H2808         432.1784         8.02         1.00         1.82         0.35         C11           C11H2209         298.1264         2.55         0.11         2.00         0.82         C9H1407         1.75         C7H805         1.72.0372         1.23         0.80         1.14         0.71           CH1803         174.0473         0.05	C9H16O6	220.0947	0.69	0.33	1.78	0.67
C8H1205         188.0685         2.53         0.60         1.50         0.63           C7H1003         142.0630         1.44         1.00         1.43         0.43           C7H1007         206.0427         0.93         0.43         1.43         1.00           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H2006         236.1260         2.78         0.17         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.86           CSH1002         102.0681         2.83         0.50         2.00         0.40           C23H2808         432.1784         8.02         1.00         1.22         0.35           C1H12209         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75	C11H22O7	266.1366	2.54	0.14	2.00	0.64
C4H60         70.0419         0.40         1.00         1.50         0.25           C7H10O3         142.0630         1.44         1.00         1.43         0.43           C7H10O7         206.0427         0.93         0.43         1.43         1.00           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H206         236.1260         2.78         0.17         2.00         0.60           C9H1808         254.1002         0.81         0.13         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.86           C3H12808         432.1784         8.02         1.00         1.22         0.35           C1H2209         298.1264         2.55         0.11         2.00         0.82           C9H1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H805         172.0372         1.23         0.80         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63	C8H12O5	188.0685	2.53	0.60	1.50	0.63
C7H1003         142.0630         1.44         1.00         1.43         0.43           C7H1007         206.0427         0.93         0.43         1.43         1.00           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H2006         236.1260         2.78         0.17         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.86           CSH1002         102.0681         2.83         0.50         2.00         0.40           C23H2808         432.1784         8.02         1.00         1.22         0.35           C1H1H2209         298.1264         2.55         0.11         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H803         140.0473         0.05         1.00         1.14         0.43           CH11205         188.0685         0.83         0.60         1.50         0.63           C1H1808         278.1002         2.51         0.38         1.64         0.73           C1H1808         278.1002         2.51         0.38         1.64         0.73 </td <td>C4H6O</td> <td>70.0419</td> <td>0.40</td> <td>1.00</td> <td>1.50</td> <td>0.25</td>	C4H6O	70.0419	0.40	1.00	1.50	0.25
CTH1007         206.0427         0.93         0.43         1.43         1.00           C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H2006         236.1260         2.78         0.17         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.86           CSH1002         102.0681         2.83         0.50         2.00         0.40           C23H2808         432.1784         8.02         1.00         1.22         0.35           C1H209         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.43         1.56         0.78           CH1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H803         140.0473         0.05         1.00         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C1H1808         278.1002         2.51         0.38         1.64         0.73	C7H10O3	142.0630	1.44	1.00	1.43	0.43
C10H1406         230.0790         3.05         0.67         1.40         0.60           C10H2006         236.1260         2.78         0.17         2.00         0.60           C9H1808         234.1002         0.81         0.13         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.86           C3H1808         432.1784         8.02         1.00         1.22         0.35           C1H2209         298.1264         2.55         0.11         2.00         0.82           C9H1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H803         140.0473         0.05         1.00         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C1H1808         278.1002         2.51         0.38         1.64         0.73           C7H1203         144.0786         0.07         0.67         1.71         0.43           C3H402         72.0211         2.90         1.00         1.33         0.67	C7H10O7	206.0427	0.93	0.43	1.43	1.00
C10H2006         256.1260         2.78         0.17         2.00         0.60           C9H1808         254.1002         0.81         0.13         2.00         0.89           C7H1006         190.0477         2.11         0.50         1.43         0.86           C3H1802         432.1784         8.02         1.00         1.22         0.35           C1H2209         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.43         1.56         0.78           CH1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H803         140.0473         0.05         1.00         1.14         0.71           C7H803         140.0473         0.05         1.00         1.14         0.43           C3H1205         188.0685         0.83         0.60         1.50         0.63           C1H1808         278.1002         2.51         0.38         1.64         0.73           C7H1203         144.0786         0.07         0.67         1.71         0.43	C10H14O6	230.0790	3.05	0.67	1.40	0.60
CM1808         254,1002         0.81         0.13         2.00         0.89           CM1006         190.0477         2.11         0.50         1.43         0.86           CSH1002         102.0681         2.83         0.50         2.00         0.40           C23H2808         432.1784         8.02         1.00         1.22         0.35           C1H209         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.43         1.56         0.78           C9H1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H805         172.0372         1.23         0.80         1.14         0.71           C7H803         140.0473         0.05         1.00         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C1H1108         278.1002         2.51         0.38         1.64         0.73           C7H1203         144.0786         0.07         0.67         1.71         0.43	C10H20O6	236.1260	2.78	0.17	2.00	0.60
CYH1000         190.0477         2.11         0.30         1.43         0.30           CSH1002         102.0681         2.83         0.50         2.00         0.40           C23H2808         432.1784         8.02         1.00         1.22         0.35           C11H22O9         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.43         1.56         0.78           C9H1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H805         172.0372         1.23         0.80         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C11H1808         278.1002         2.51         0.38         1.64         0.73           C7H203         144.0786         0.07         0.67         1.71         0.43           C3H402         72.0211         2.90         1.00         1.33         0.63           CH1805         158.0215         0.38         0.00         1.33         0.33	C9H18O8	254.1002	0.81	0.13	2.00	0.89
C23H2808         432.1784         8.02         1.00         1.22         0.35           C11H2209         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.43         1.56         0.78           C9H1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H805         172.0372         1.23         0.80         1.14         0.71           C7H803         140.0473         0.05         1.00         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C11H1808         278.1002         2.51         0.38         1.64         0.73           C7H1203         144.0786         0.07         0.67         1.71         0.43           C3H402         72.0211         2.90         1.00         1.33         0.67           C16H28011         396.1632         2.89         0.27         1.75         0.69           C9H1607         236.0896         0.91         0.29         1.78         0.78	C5H10O2	190.0477	2.11	0.50	1.45	0.80
C11H2209         298.1264         2.55         0.11         2.00         0.82           C9H1407         234.0740         2.70         0.43         1.56         0.78           C9H1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H805         172.0372         1.23         0.80         1.14         0.71           C7H805         172.0372         1.23         0.80         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C1H1808         278.1002         2.51         0.38         1.64         0.73           C7H1203         144.0786         0.07         0.67         1.71         0.43           C3H402         72.0211         2.90         1.00         1.33         0.67           C1H28011         396.1632         2.89         0.27         1.75         0.69           C9H1607         236.0896         0.91         0.29         1.78         0.78           C6H605         158.0215         0.38         0.80         1.00         0.83	C23H28O8	432 1784	2.83	1.00	1.22	0.40
C9H1407         234.0740         2.70         0.43         1.56         0.78           C9H1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H805         172.0372         1.23         0.80         1.14         0.71           C7H803         140.0473         0.05         1.00         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C1H1808         278.1002         2.51         0.38         1.64         0.73           C7H1203         144.0786         0.07         0.67         1.71         0.43           C3H402         72.0211         2.90         1.00         1.33         0.67           C16H28011         396.1632         2.89         0.27         1.75         0.69           C9H1607         236.0896         0.91         0.29         1.78         0.78           C6H605         158.0215         0.38         0.80         1.00         0.83           C9H1808         254.1002         2.79         0.13         2.00         0.63	C11H22O9	298 1264	2.55	0.11	2.00	0.82
C9H1803         174.1256         7.51         0.33         2.00         0.33           C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H805         172.0372         1.23         0.80         1.14         0.71           C7H803         140.0473         0.05         1.00         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C1H1808         278.1002         2.51         0.38         1.64         0.73           C7H1203         144.0786         0.07         0.67         1.71         0.43           C3H402         72.0211         2.90         1.00         1.33         0.67           C16H28011         396.1632         2.89         0.27         1.75         0.69           C9H1607         236.0896         0.91         0.29         1.78         0.78           C6H605         158.0215         0.38         0.80         1.00         0.83           C3H40         56.0262         0.38         1.00         1.33         0.33           C9H1808         254.1002         2.79         0.13         2.00         0.82 </td <td>C9H14O7</td> <td>234.0740</td> <td>2.70</td> <td>0.43</td> <td>1.56</td> <td>0.78</td>	C9H14O7	234.0740	2.70	0.43	1.56	0.78
C4H1007         170.0427         0.39         0.00         2.50         1.75           C7H805         172.0372         1.23         0.80         1.14         0.71           C7H803         140.0473         0.05         1.00         1.14         0.43           C8H1205         188.0685         0.83         0.60         1.50         0.63           C11H1808         278.1002         2.51         0.38         1.64         0.73           C7H1203         144.0786         0.07         0.67         1.71         0.43           C3H402         72.0211         2.90         1.00         1.33         0.67           C1H1808         278.1002         2.89         0.27         1.75         0.69           C9H1607         236.0896         0.91         0.29         1.78         0.78           C6H605         158.0215         0.38         0.80         1.00         0.83           C3H40         56.0262         0.38         1.00         1.33         0.33           C9H1805         192.0998         0.90         0.20         2.00         0.63           C1H2209         298.1264         2.82         0.11         2.00         0.82 <td>C9H18O3</td> <td>174.1256</td> <td>7.51</td> <td>0.33</td> <td>2.00</td> <td>0.33</td>	C9H18O3	174.1256	7.51	0.33	2.00	0.33
C7H805172.03721.230.801.140.71C7H803140.04730.051.001.140.43C8H1205188.06850.830.601.500.63C11H1808278.10022.510.381.640.73C7H1203144.07860.070.671.710.43C3H40272.02112.901.001.330.67C16H28011396.16322.890.271.750.69C9H1607236.08960.910.291.780.78C6H605158.02150.381.001.330.33C9H1808254.10022.790.132.000.89C8H1605192.09980.900.202.000.63C11H2209298.12642.820.112.000.82C6H1204148.07360.560.252.000.67C10H1605216.09982.850.601.600.50C8H1206204.06342.680.501.500.75C6H1405166.08410.400.002.330.83C4H40284.02110.381.001.000.50C7H1205176.06851.840.401.710.71C11H1809294.09511.090.331.640.82C8H1405190.08410.890.401.750.63C8H1405190.08410.890.401.750.63C8H1405190.08410.391.00 <t< td=""><td>C4H10O7</td><td>170.0427</td><td>0.39</td><td>0.00</td><td>2.50</td><td>1.75</td></t<>	C4H10O7	170.0427	0.39	0.00	2.50	1.75
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7H8O5	172.0372	1.23	0.80	1.14	0.71
C8H12O5         188.0685         0.83         0.60         1.50         0.63           C11H1808         278.1002         2.51         0.38         1.64         0.73           C7H12O3         144.0786         0.07         0.67         1.71         0.43           C3H4O2         72.0211         2.90         1.00         1.33         0.67           C16H28011         396.1632         2.89         0.27         1.75         0.69           C9H1607         236.0896         0.91         0.29         1.78         0.78           C6H605         158.0215         0.38         0.80         1.00         0.83           C3H40         56.0262         0.38         1.00         1.33         0.33           C9H1808         254.1002         2.79         0.13         2.00         0.63           C1H2O9         298.1264         2.82         0.11         2.00         0.82           C6H12O4         148.0736         0.56         0.25         2.00         0.67           C10H1605         216.0998         2.85         0.60         1.60         0.50           C8H12O6         204.0634         2.68         0.50         1.50         0.75	C7H8O3	140.0473	0.05	1.00	1.14	0.43
C11H1808         278.1002         2.51         0.38         1.64         0.73           C7H12O3         144.0786         0.07         0.67         1.71         0.43           C3H4O2         72.0211         2.90         1.00         1.33         0.67           C16H28011         396.1632         2.89         0.27         1.75         0.69           C9H1607         236.0896         0.91         0.29         1.78         0.78           C6H605         158.0215         0.38         0.80         1.00         0.83           C3H4O         56.0262         0.38         1.00         1.33         0.33           C9H1808         254.1002         2.79         0.13         2.00         0.63           C1H2209         298.1264         2.82         0.11         2.00         0.82           C6H1204         148.0736         0.56         0.25         2.00         0.67           C10H1605         216.0998         2.85         0.60         1.60         0.50           C8H1206         204.0634         2.68         0.50         1.50         0.75           C6H1405         166.0841         0.40         0.00         2.33         0.83	C8H12O5	188.0685	0.83	0.60	1.50	0.63
C7H12O3144.07860.070.671.710.43C3H4O272.02112.901.001.330.67C16H28011396.16322.890.271.750.69C9H16O7236.08960.910.291.780.78C6H6O5158.02150.380.801.000.83C3H4O56.02620.381.001.330.33C9H18O8254.10022.790.132.000.89C8H16O5192.09980.900.202.000.63C1H22O9298.12642.820.112.000.82C6H12O4148.07360.560.252.000.67C10H1605216.09982.850.601.600.50C8H12O6204.06342.680.501.500.75C6H14O5166.08410.400.002.330.83C4H4O284.02110.381.001.000.50C7H12O5176.06851.840.401.710.71C11H18O9294.09511.090.331.640.82C8H14O5190.08410.830.401.750.63C5H4O3112.01600.391.000.800.60C9H14O5202.08411.090.601.560.56C1H26010354.15262.880.201.860.71C1H26010354.15262.890.181.880.69C5H10O2102.06810.680.50	C11H18O8	278.1002	2.51	0.38	1.64	0.73
C3H40272.02112.901.001.330.67C16H28011396.16322.890.271.750.69C9H1607236.08960.910.291.780.78C6H605158.02150.380.801.000.83C3H4056.02620.381.001.330.33C9H1808254.10022.790.132.000.89C8H1605192.09980.900.202.000.63C1H2209298.12642.820.112.000.82C6H1204148.07360.560.252.000.67C10H1605216.09982.850.601.600.50C8H1206204.06342.680.501.500.75C6H1405166.08410.400.002.330.83C4H40284.02110.381.001.000.50C7H1205176.06851.840.401.710.71C11H1809294.09511.090.331.640.82C8H1405190.08410.830.401.750.63C5H403112.01600.391.000.800.60C9H1405202.08411.090.601.560.56C1H26010354.15262.880.201.860.71C1H26010354.15262.890.181.880.69C5H1002102.06810.680.502.000.40C1H203202.15697.000.332	C7H12O3	144.0786	0.07	0.67	1.71	0.43
C16H28011396.16322.890.271.750.69C9H1607236.08960.910.291.780.78C6H605158.02150.380.801.000.83C3H4056.02620.381.001.330.33C9H1808254.10022.790.132.000.89C8H1605192.09980.900.202.000.63C11H2209298.12642.820.112.000.82C6H1204148.07360.560.252.000.67C10H1605216.09982.850.601.600.50C8H1206204.06342.680.501.500.75C6H1405166.08410.400.002.330.83C4H40284.02110.381.001.000.50C7H1205176.06851.840.401.710.71C11H1809294.09511.090.331.640.82C8H1405190.08410.830.401.750.63C8H1405190.08410.830.401.750.63C5H403112.01600.391.000.800.60C9H1405202.08411.090.601.560.56C14H26010354.15262.880.201.860.71C16H30011398.17882.890.181.880.69C5H1002102.06810.680.502.000.40C1H2203202.15697.000.33 <td>C3H4O2</td> <td>72.0211</td> <td>2.90</td> <td>1.00</td> <td>1.33</td> <td>0.67</td>	C3H4O2	72.0211	2.90	1.00	1.33	0.67
C9H1607         236.0896         0.91         0.29         1.78         0.78           C6H605         158.0215         0.38         0.80         1.00         0.83           C3H40         56.0262         0.38         1.00         1.33         0.33           C9H1808         254.1002         2.79         0.13         2.00         0.89           C8H1605         192.0998         0.90         0.20         2.00         0.63           C1H2209         298.1264         2.82         0.11         2.00         0.82           C6H1204         148.0736         0.56         0.25         2.00         0.67           C10H1605         216.0998         2.85         0.60         1.60         0.50           C8H1206         204.0634         2.68         0.50         1.50         0.75           C6H1405         166.0841         0.40         0.00         2.33         0.83           C4H402         84.0211         0.38         1.00         1.00         0.50           C7H1205         176.0685         1.84         0.40         1.71         0.71           C1H1809         294.0951         1.09         0.33         1.64         0.82     <	C16H28O11	396.1632	2.89	0.27	1.75	0.69
C6H005138.02130.380.381.001.300.33C3H4O56.02620.381.001.330.33C9H18O8254.10022.790.132.000.89C8H16O5192.09980.900.202.000.63C11H22O9298.12642.820.112.000.82C6H12O4148.07360.560.252.000.67C10H16O5216.09982.850.601.600.50C8H12O6204.06342.680.501.500.75C6H14O5166.08410.400.002.330.83C4H4O284.02110.381.001.000.50C7H12O5176.06851.840.401.710.71C1H18O9294.09511.090.331.640.82C8H14O5190.08410.830.401.750.63C8H14O5190.08410.830.401.750.63C5H4O3112.01600.391.000.800.60C9H14O5202.08411.090.601.560.56C14H26010354.15262.880.201.860.71C16H30011398.17882.890.181.880.69C5H10O2102.06810.680.502.000.40C1H22O3202.15697.000.332.000.27C6H14O7198.07402.420.002.331.17	C9H10U/	230.0890	0.91	0.29	1.78	0.78
C9H1808         254.1002         2.79         0.13         2.00         0.89           C8H1605         192.0998         0.90         0.20         2.00         0.63           C1H2209         298.1264         2.82         0.11         2.00         0.82           C6H1204         148.0736         0.56         0.25         2.00         0.67           C10H1605         216.0998         2.85         0.60         1.60         0.50           C8H1206         204.0634         2.68         0.50         1.50         0.75           C6H1405         166.0841         0.40         0.00         2.33         0.83           C4H402         84.0211         0.38         1.00         1.00         0.50           C7H1205         176.0685         1.84         0.40         1.71         0.71           C1H1809         294.0951         1.09         0.33         1.64         0.82           C8H1405         190.0841         0.83         0.40         1.75         0.63           C8H1405         190.0841         0.83         0.40         1.75         0.63           C8H1405         190.0841         0.83         0.40         1.75         0.63	C3H4O	56 0262	0.38	1.00	1.00	0.33
C8H1605         192.0998         0.90         0.20         2.00         0.63           C8H1605         192.0998         0.90         0.20         2.00         0.63           C1H2209         298.1264         2.82         0.11         2.00         0.82           C6H1204         148.0736         0.56         0.25         2.00         0.67           C10H1605         216.0998         2.85         0.60         1.60         0.50           C8H1206         204.0634         2.68         0.50         1.50         0.75           C6H1405         166.0841         0.40         0.00         2.33         0.83           C4H402         84.0211         0.38         1.00         1.00         0.50           C7H1205         176.0685         1.84         0.40         1.71         0.71           C1H1809         294.0951         1.09         0.33         1.64         0.82           C8H1405         190.0841         0.89         0.40         1.75         0.63           C5H403         112.0160         0.39         1.00         0.80         0.60           C9H1405         202.0841         1.09         0.60         1.56         0.56	C9H18O8	254 1002	2.79	0.13	2.00	0.89
C11H2209         298,1264         2.82         0.11         2.00         0.82           C6H1204         148.0736         0.56         0.25         2.00         0.67           C10H1605         216.0998         2.85         0.60         1.60         0.50           C8H1206         204.0634         2.68         0.50         1.50         0.75           C6H1405         166.0841         0.40         0.00         2.33         0.83           C4H402         84.0211         0.38         1.00         1.00         0.50           C7H1205         176.0685         1.84         0.40         1.71         0.71           C1H1809         294.0951         1.09         0.33         1.64         0.82           C8H1405         190.0841         0.89         0.40         1.75         0.63           C8H1405         190.0841         0.83         0.40         1.75         0.63           C5H403         112.0160         0.39         1.00         0.80         0.60           C9H1405         202.0841         1.09         0.60         1.56         0.56           C14H26010         354.1526         2.88         0.20         1.86         0.71	C8H16O5	192,0998	0.90	0.20	2.00	0.63
C6H12O4148.07360.560.252.000.67C10H16O5216.09982.850.601.600.50C8H12O6204.06342.680.501.500.75C6H14O5166.08410.400.002.330.83C4H4O284.02110.381.001.000.50C7H12O5176.06851.840.401.710.71C1H18O9294.09511.090.331.640.82C8H14O5190.08410.890.401.750.63C8H14O5190.08410.830.401.750.63C5H4O3112.01600.391.000.800.60C9H14O5202.08411.090.601.560.56C14H26010354.15262.880.201.860.71C16H30011398.17882.890.181.880.69C5H10O2102.06810.680.502.000.40C1H22O3202.15697.000.332.000.27C6H14O7198.07402.420.002.331.17	C11H22O9	298.1264	2.82	0.11	2.00	0.82
C10H16O5216.09982.850.601.600.50C8H12O6204.06342.680.501.500.75C6H14O5166.08410.400.002.330.83C4H4O284.02110.381.001.000.50C7H12O5176.06851.840.401.710.71C11H18O9294.09511.090.331.640.82C8H14O5190.08410.890.401.750.63C8H14O5190.08410.830.401.750.63C5H4O3112.01600.391.000.800.60C9H14O5202.08411.090.601.560.56C14H26010354.15262.880.201.860.71C16H30011398.17882.890.181.880.69C5H10O2102.06810.680.502.000.40C11H22O3202.15697.000.332.000.27C6H14O7198.07402.420.002.331.17	C6H12O4	148.0736	0.56	0.25	2.00	0.67
C8H12O6         204.0634         2.68         0.50         1.50         0.75           C6H14O5         166.0841         0.40         0.00         2.33         0.83           C4H4O2         84.0211         0.38         1.00         1.00         0.50           C7H12O5         176.0685         1.84         0.40         1.71         0.71           C1H18O9         294.0951         1.09         0.33         1.64         0.82           C8H14O5         190.0841         0.89         0.40         1.75         0.63           C8H14O5         190.0841         0.83         0.40         1.75         0.63           C5H4O3         112.0160         0.39         1.00         0.80         0.60           C9H14O5         202.0841         1.09         0.60         1.56         0.56           C1H26010         354.1526         2.88         0.20         1.86         0.71           C16H30011         398.1788         2.89         0.18         1.88         0.69           C5H10O2         102.0681         0.68         0.50         2.00         0.40           C1H22O3         202.1569         7.00         0.33         2.00         0.27	C10H16O5	216.0998	2.85	0.60	1.60	0.50
C6H14O5166.08410.400.002.330.83C4H4O284.02110.381.001.000.50C7H12O5176.06851.840.401.710.71C11H18O9294.09511.090.331.640.82C8H14O5190.08410.890.401.750.63C8H14O5190.08410.830.401.750.63C5H4O3112.01600.391.000.800.60C9H14O5202.08411.090.601.560.56C14H26010354.15262.880.201.860.71C16H30011398.17882.890.181.880.69C5H10O2102.06810.680.502.000.40C11H22O3202.15697.000.332.000.27C6H14O7198.07402.420.002.331.17	C8H12O6	204.0634	2.68	0.50	1.50	0.75
C4H4O284.02110.381.001.000.50C7H12O5176.06851.840.401.710.71C11H18O9294.09511.090.331.640.82C8H14O5190.08410.890.401.750.63C8H14O5190.08410.830.401.750.63C5H4O3112.01600.391.000.800.60C9H14O5202.08411.090.601.560.56C14H26010354.15262.880.201.860.71C16H30011398.17882.890.181.880.69C5H10O2102.06810.680.502.000.40C11H22O3202.15697.000.332.000.27C6H14O7198.07402.420.002.331.17	C6H14O5	166.0841	0.40	0.00	2.33	0.83
C7H12O5176.06851.840.401.710.71C11H18O9294.09511.090.331.640.82C8H14O5190.08410.890.401.750.63C8H14O5190.08410.830.401.750.63C5H4O3112.01600.391.000.800.60C9H14O5202.08411.090.601.560.56C14H26010354.15262.880.201.860.71C16H30011398.17882.890.181.880.69C5H10O2102.06810.680.502.000.40C11H22O3202.15697.000.332.000.27C6H14O7198.07402.420.002.331.17	C4H4O2	84.0211	0.38	1.00	1.00	0.50
C11H1809294.09511.090.331.640.82C8H1405190.08410.890.401.750.63C8H1405190.08410.830.401.750.63C5H403112.01600.391.000.800.60C9H1405202.08411.090.601.560.56C14H26010354.15262.880.201.860.71C16H30011398.17882.890.181.880.69C5H1002102.06810.680.502.000.40C11H22O3202.15697.000.332.000.27C6H1407198.07402.420.002.331.17	C7H12O5	176.0685	1.84	0.40	1.71	0.71
C8H14O5         190.0841         0.89         0.40         1.75         0.63           C8H14O5         190.0841         0.83         0.40         1.75         0.63           C5H4O3         112.0160         0.39         1.00         0.80         0.60           C9H14O5         202.0841         1.09         0.60         1.56         0.56           C14H26010         354.1526         2.88         0.20         1.86         0.71           C16H30011         398.1788         2.89         0.18         1.88         0.69           C5H10O2         102.0681         0.68         0.50         2.00         0.40           C11H22O3         202.1569         7.00         0.33         2.00         0.27           C6H14O7         198.0740         2.42         0.00         2.33         1.17	C11H18O9	294.0951	1.09	0.33	1.64	0.82
Contracts         190.0641         0.85         0.40         1.75         0.63           C5H4O3         112.0160         0.39         1.00         0.80         0.60           C9H14O5         202.0841         1.09         0.60         1.56         0.56           C14H26O10         354.1526         2.88         0.20         1.86         0.71           C16H30O11         398.1788         2.89         0.18         1.88         0.69           C5H10O2         102.0681         0.68         0.50         2.00         0.40           C1H2O3         202.1569         7.00         0.33         2.00         0.27           C6H14O7         198.0740         2.42         0.00         2.33         1.17	C8H14O5	190.0841	0.89	0.40	1.75	0.63
C9H1405         202.0841         1.09         0.60         1.56         0.56           C9H1405         202.0841         1.09         0.60         1.56         0.56           C14H26010         354.1526         2.88         0.20         1.86         0.71           C16H30011         398.1788         2.89         0.18         1.88         0.69           C5H1002         102.0681         0.68         0.50         2.00         0.40           C1H22O3         202.1569         7.00         0.33         2.00         0.27           C6H1407         198.0740         2.42         0.00         2.33         1.17	C5H4O2	190.0841	0.85	0.40	1.75	0.03
C14H26O10         354.1526         2.88         0.20         1.86         0.71           C16H30O11         398.1788         2.89         0.18         1.88         0.69           C5H10O2         102.0681         0.68         0.50         2.00         0.40           C11H22O3         202.1569         7.00         0.33         2.00         0.27           C6H14O7         198.0740         2.42         0.00         2.33         1.17	C9H14O5	202 08/1	1 00	0.60	1.56	0.00
C16H30011         398.1788         2.89         0.18         1.88         0.69           C5H1002         102.0681         0.68         0.50         2.00         0.40           C1H22O3         202.1569         7.00         0.33         2.00         0.27           C6H1407         198.0740         2.42         0.00         2.33         1.17	C14H26O10	354 1526	2.88	0.20	1.86	0.71
C5H10O2         102.0681         0.68         0.50         2.00         0.40           C11H22O3         202.1569         7.00         0.33         2.00         0.27           C6H14O7         198.0740         2.42         0.00         2.33         1.17	C16H30O11	398.1788	2.89	0.18	1.88	0.69
C11H22O3         202.1569         7.00         0.33         2.00         0.27           C6H14O7         198.0740         2.42         0.00         2.33         1.17	C5H10O2	102.0681	0.68	0.50	2.00	0.40
C6H14O7 198.0740 2.42 0.00 2.33 1.17	C11H22O3	202.1569	7.00	0.33	2.00	0.27
	C6H14O7	198.0740	2.42	0.00	2.33	1.17

C9H12O5	200.0685	2 79	0.80	1 33	0.56
C0111/04	199 1040	2.79	0.50	1.55	0.30
C9H16O4	188.1049	2.60	0.50	1./8	0.44
C8H12O3	156.0786	2.90	1.00	1.50	0.38
C6H12O5	164.0685	2.99	0.20	2.00	0.83
C11H18O8	278 1002	0.69	0.38	1.64	0.73
6711000	278.1002	0.09	0.38	1.04	0.73
C/H804	156.0423	1.04	1.00	1.14	0.57
C8H10O4	170.0579	1.95	1.00	1.25	0.50
C16H28O11	396 1632	2.68	0.27	1 75	0.69
C011120011	174 1256	5.00	0.22	2.00	0.22
C9H1803	174.1256	5.25	0.55	2.00	0.55
C6H6O4	142.0266	0.40	1.00	1.00	0.67
C5H6O2	98.0368	0.39	1.00	1.20	0.40
C11H22O10	31/ 1213	0.94	0.10	2.00	0.91
C101122010	250,1052	0.74	0.10	2.00	0.71
C10H1807	250.1053	2.55	0.29	1.80	0.70
C5H8O2	100.0524	0.41	1.00	1.60	0.40
C7H16O8	228 0845	0.78	0.00	2.29	1.14
C12H22O9	310 1264	2.45	0.22	1.83	0.75
C12H22O9	310.1204	2.45	0.22	1.65	0.73
C8H6O3	150.0317	3.86	1.00	0.75	0.38
C10H16O6	232.0947	0.69	0.50	1.60	0.60
C9H10O3	166 0630	4 15	1.00	1 1 1	0.33
C12112000	208 1107	4.15	0.22	1.11	0.55
C12H2009	308.1107	2.74	0.33	1.67	0.75
C4H10O5	138.0528	0.47	0.00	2.50	1.25
C10H20O7	252.1209	0.98	0.14	2.00	0.70
C16H28O10	380 1682	2.05	0.30	1 75	0.63
C(111400	214.0200	2.75	0.50	1.75	1.22
C6H14O8	214.0689	0.94	0.00	2.33	1.55
C16H30O11	398.1788	2.64	0.18	1.88	0.69
C8H10O4	170 0579	1.23	1.00	1.25	0.50
C14U29O2	244 2028	0.62	0.22	2.00	0.21
C14H28U3	244.2038	8.05	0.55	2.00	0.21
C7H12O8	224.0532	0.73	0.25	1.71	1.14
C9H8O4	180.0423	0.14	1.00	0.89	0.44
C11H24O9	300 1420	2 4 3	0.00	2.18	0.82
C(111240)	106.0592	2.43	0.00	2.10	1.17
C6H12O7	196.0583	0.98	0.14	2.00	1.1/
C10H22O9	286.1264	0.73	0.00	2.20	0.90
C13H24O10	340.1369	2.75	0.20	1.85	0.77
C4460	70.0410	2.05	1.00	1.50	0.25
C41100	70.0419	2.95	1.00	1.50	0.23
C19H16O3	292.1099	0.41	1.00	0.84	0.16
C9H16O4	188.1049	3.30	0.50	1.78	0.44
C6H6O4	142.0266	1.38	1.00	1.00	0.67
Cell1004	170.0570	2.62	1.00	1.00	0.50
004	170.0379	2.05	1.00	1.23	0.50
C11H18O7	262.1053	1.12	0.43	1.64	0.64
C11H24O9	300.1420	1.35	0.00	2.18	0.82
C6H10O5	162 0528	2 74	0.40	1.67	0.83
C10U2002	102.0520	2.74	0.40	2.00	0.05
C10H20O3	188.1412	7.98	0.33	2.00	0.30
C14H24O10	352.1369	2.69	0.30	1.71	0.71
C4H4O5	132.0059	0.37	0.60	1.00	1.25
C10H20O0	284 1107	0.99	0.11	2.00	0.00
C10112009	204.0051	0.88	0.11	2.00	0.90
C11H1809	294.0951	2.46	0.33	1.64	0.82
C14H26O10	354.1526	2.58	0.20	1.86	0.71
C3H6O	58 0419	2.56	1.00	2.00	0.33
C/14205	126 0272	6.59	0.20	2.00	1.25
C4110UJ	150.0372	0.50	0.20	2.00	1.23
C/H804	156.0423	0.66	1.00	1.14	0.57
C2H2O2	58.0055	0.37	1.00	1.00	1.00
C5H6O5	146.0215	0.94	0.60	1.20	1.00
C10H18O8	266 1002	1.56	0.25	1.80	0.80
C1411000	200.1002	1.50	0.23	1.00	0.00
C14H28O12	588.1581	0.61	0.08	2.00	0.86
C4H10O6	154.0477	0.35	0.00	2.50	1.50
C11H22O7	266,1366	0.64	0.14	2.00	0.64
C10H1806	23/ 1102	1 32	0.33	1.80	0.60
C101118000	234.1103	1.52	0.55	1.60	0.00
C/H10O6	190.0477	2.37	0.50	1.43	0.86
C4H8O	72.0575	0.41	1.00	2.00	0.25
C10H14O8	262,0689	1.63	0.50	1.40	0.80
C8H14O6	205.0000	2.00	0.32	1 75	0.75
	200.0790	2.31	0.33	1.75	0.75
С9Н14О8	250.0689	1.20	0.38	1.56	0.89
C11H18O9	294.0951	2.62	0.33	1.64	0.82
C2H4O2	60.0211	3 63	0.50	2.00	1.00
C8H1005	196 0570	0.72	0.00	1.05	0.62
	100.0328	0.72	0.80	1.23	0.05
C9H12O5	200.0685	0.83	0.80	1.33	0.56
C9H12O4	184.0736	2.19	1.00	1.33	0.44
C7H12O6	192.0634	1 20	0.33	1.71	0.86
074206	100 0201	0.74	0.55	1 1 /	0.00
C/H8U0	100.0321	0.74	0.07	1.14	0.80
C12H22O9	310.1264	0.91	0.22	1.83	0.75

C11H24O8	284.1471	0.85	0.00	2.18	0.73
C4H4O	68.0262	0.39	1.00	1.00	0.25
C10H18O6	234.1103	0.62	0.33	1.80	0.60
C14H24O9	336.1420	2.56	0.33	1.71	0.64
C8H10O3	154.0630	0.03	1.00	1.25	0.38
C8H12O8	236.0532	0.97	0.38	1.50	1.00
C12H22O10	326.1213	2.28	0.20	1.83	0.83
C6H8O2	112.0524	1.09	1.00	1.33	0.33
C10H14O6	230.0790	0.75	0.67	1.40	0.60
C10H16O5	216.0998	1.05	0.60	1.60	0.50
C12H20O9	308.1107	0.84	0.33	1.67	0.75
C6H12O8	212.0532	2.36	0.13	2.00	1.33
C9H12O5	200.0685	1.23	0.80	1.33	0.56
C11H22O7	266.1366	2.13	0.14	2.00	0.64
C6H14O8	214.0689	2.35	0.00	2.33	1.33
C3H6O	58.0419	1.40	1.00	2.00	0.33
C4H4O	68.0262	0.73	1.00	1.00	0.25
C16H32O2	256.2402	9.24	0.50	2.00	0.13
C2H4O3	76.0160	0.38	0.33	2.00	1.50
C4H6O4	118.0266	0.56	0.50	1.50	1.00
C5H8O5	148.0372	0.43	0.40	1.60	1.00
C3H6O4	106.0266	0.37	0.25	2.00	1.33
C3H4O4	104.0110	0.38	0.50	1.33	1.33
C5H6O4	130.0266	0.63	0.75	1.20	0.80
C6H8O4	144.0423	0.66	0.75	1.33	0.67
C4H4O4	116.0110	0.41	0.75	1.00	1.00
C7H12O4	160.0736	0.93	0.50	1.71	0.57
C8H12O4	172.0736	2.54	0.75	1.50	0.50

Table S4.3.11 Molecular formulas of organic compounds detected in naphthalene SOA in ESI- mode.

Formula [M]	Neutral mass (Da)	RT (min)	MCR	H/C	O/C
C5H6O3	114.0317	0.66	1.00	1.20	0.60
C3H6O2	74.0368	0.40	0.50	2.00	0.67
C5H6O4	130.0266	0.38	0.75	1.20	0.80
C5H8O4	132.0423	0.40	0.50	1.60	0.80
C4H6O3	102.0317	0.43	0.67	1.50	0.75
C4H6O5	134.0215	0.38	0.40	1.50	1.25
C6H10O5	162.0528	0.48	0.40	1.67	0.83
C3H4O3	88.0160	0.37	0.67	1.33	1.00
C3H4O2	72.0211	0.38	1.00	1.33	0.67
C5H6O5	146.0215	0.38	0.60	1.20	1.00
C4H6O2	86.0368	0.39	1.00	1.50	0.50
C17H26O4	294.1831	8.05	1.00	1.53	0.24
C2H4O2	60.0211	0.39	0.50	2.00	1.00
C5H8O3	116.0473	0.38	0.67	1.60	0.60
C2H2O3	74.0004	0.37	0.67	1.00	1.50
C5H4O4	128.0110	0.39	1.00	0.80	0.80
C7H12O4	160.0736	3.00	0.50	1.71	0.57
C7H10O5	174.0528	0.82	0.60	1.43	0.71
C7H8O5	172.0372	0.38	0.80	1.14	0.71
C13H20O2	208.1463	7.99	1.00	1.54	0.15
C3H6O	58.0419	0.45	1.00	2.00	0.33
C9H10O4	182.0579	2.69	1.00	1.11	0.44
C4H4O3	100.0160	0.43	1.00	1.00	0.75
C4H6O	70.0419	0.40	1.00	1.50	0.25
C23H28O8	432.1784	8.02	1.00	1.22	0.35
C7H8O5	172.0372	1.23	0.80	1.14	0.71
C3H4O2	72.0211	2.90	1.00	1.33	0.67
C6H6O5	158.0215	0.38	0.80	1.00	0.83
C3H4O	56.0262	0.38	1.00	1.33	0.33
C4H4O2	84.0211	0.38	1.00	1.00	0.50
C5H4O3	112.0160	0.39	1.00	0.80	0.60
C11H22O3	202.1569	7.00	0.33	2.00	0.27
C6H6O4	142.0266	0.40	1.00	1.00	0.67

C5H6O2	98.0368	0 39	1.00	1.20	0.40
C5H8O2	100.0524	0.41	1.00	1.60	0.40
C10H20O2	198 1412	7.08	0.22	2.00	0.40
C10H20O5	122,0050	7.90	0.33	2.00	0.30
C4H4O5	132.0059	0.37	0.60	1.00	1.25
C2H2O2	58.0055	0.37	1.00	1.00	1.00
C8H10O5	186.0528	0.72	0.80	1.25	0.63
C4H4O	68.0262	0.39	1.00	1.00	0.25
C4H4O	68.0262	0.73	1.00	1.00	0.25
C8H6O4	166 0266	2.62	1.00	0.75	0.50
C8H6O3	150.0200	2.62	1.00	0.75	0.38
C311003	129.0217	2.08	1.00	0.75	0.38
C/H6O3	138.0317	3.39	1.00	0.80	0.43
C9H8O4	180.0423	3.33	1.00	0.89	0.44
C10H8O4	192.0423	3.13	1.00	0.80	0.40
C9H8O3	164.0473	3.10	1.00	0.89	0.33
C10H8O5	208.0372	3.30	1.00	0.80	0.50
C9H6O4	178.0266	2.92	1.00	0.67	0.44
C9H8O5	196 0372	2.81	1.00	0.89	0.56
C0H8O3	164 0473	2.51	1.00	0.89	0.33
C71603	154.0266	2.54	1.00	0.85	0.55
C/H0U4	134.0200	2.00	1.00	0.80	0.37
C10H8O4	192.0423	3.83	1.00	0.80	0.40
C7H6O3	138.0317	2.83	1.00	0.86	0.43
C9H6O3	162.0317	2.49	1.00	0.67	0.33
C9H8O2	148.0524	3.13	1.00	0.89	0.22
C9H6O5	194.0215	2.70	1.00	0.67	0.56
C9H18O3	174 1256	6 95	0.33	2.00	0.33
C6H10O4	146.0579	1 78	0.50	1.67	0.67
C10U1004	226 0477	2.40	1.00	1.07	0.60
C10H1000	220.0477	2.49	1.00	1.00	0.00
C9H8O4	180.0423	1.45	1.00	0.89	0.44
C9H6O5	194.0215	0.87	1.00	0.67	0.56
C10H8O5	208.0372	2.42	1.00	0.80	0.50
C8H6O5	182.0215	1.16	1.00	0.75	0.63
C6H8O5	160.0372	1.03	0.60	1.33	0.83
C8H6O2	134 0368	1.94	1.00	0.75	0.25
C3H4O5	120,0059	0.42	0.40	1 33	1.67
C7H6O	106.0419	2.68	1.00	0.86	0.14
C/1100	100.0419	2.08	1.00	1.00	0.14
C0H0O5	120.0317	0.58	1.00	1.00	0.30
C/H6O4	154.0266	2.20	1.00	0.86	0.57
C10H8O3	176.0473	3.50	1.00	0.80	0.30
C5H4O3	112.0160	2.93	1.00	0.80	0.60
C8H8O	120.0575	3.10	1.00	1.00	0.13
C9H8O5	196.0372	0.83	1.00	0.89	0.56
C6H4O5	156.0059	0.75	1.00	0.67	0.83
C9H6O4	178 0266	0.83	1.00	0.67	0.44
C8H6O5	182 0215	2.01	1.00	0.75	0.44
C101807	240.0270	2.01	1.00	0.75	0.05
	240.0270	0.02	1.00	0.60	0.70
C9H6O3	162.0317	3.06	1.00	0.67	0.33
C9H6O3	162.0317	3.31	1.00	0.67	0.33
C5H6O	82.0419	0.38	1.00	1.20	0.20
C9H10O2	150.0681	0.10	1.00	1.11	0.22
C8H6O6	198.0164	0.99	1.00	0.75	0.75
C11H12O7	256.0583	2.25	0.86	1.09	0.64
C12H24O3	216.1725	8.32	0.33	2.00	0.25
C9H8O5	196 0372	1.83	1.00	0.89	0.56
C5H6O2	98 0368	0.60	1.00	1 20	0.20
CJH002	98.0308	0.09	1.00	1.20	0.40
CIOHIOOS	210.0528	1.00	1.00	1.00	0.50
C8H8O	120.0575	2.53	1.00	1.00	0.13
C8H8O4	168.0423	1.14	1.00	1.00	0.50
C11H14O6	242.0790	0.63	0.83	1.27	0.55
C10H10O4	194.0579	1.24	1.00	1.00	0.40
C2H2O4	89.9953	0.37	0.50	1.00	2.00
C3H2O5	117,9902	0.36	0.60	0.67	1.67
C10H6O4	190.0266	3 25	1.00	0.60	0.40
C3H204	101 0053	0.34	0.75	0.67	1 33
C611204	101.7733	0.54	0.75	1.00	1.33
	200.0003	0.30	0.50	1.00	1.55
C5H4O5	144.0059	0.36	0.80	0.80	1.00
C10H6O5	206.0215	2.88	1.00	0.60	0.50
C6H6O7	190.0114	0.36	0.57	1.00	1.17
C7H6O2	122.0368	2.71	1.00	0.86	0.29
C4H6O4	118.0266	0.36	0.50	1.50	1.00
C8H8O8	232.0219	0.36	0.63	1.00	1.00

C7H8O7	204.0270	0.36	0.57	1.14	1.00
C8H6O5	182.0215	0.96	1.00	0.75	0.63
C6H4O6	172.0008	0.38	0.83	0.67	1.00
C8H6O4	166.0266	2.13	1.00	0.75	0.50
C7H6O7	202.0114	0.37	0.71	0.86	1.00
C8H6O7	214 0114	0.69	0.86	0.75	0.88
C10H6O5	206.0215	3 45	1.00	0.60	0.50
C5H6O5	146 0215	0.63	0.60	1.20	1.00
C4H2O4	113 9953	0.05	1.00	0.50	1.00
C7H6O6	186 0164	0.50	0.83	0.50	0.86
C5H4O6	160.0008	0.01	0.67	0.80	1.20
C8H6O8	230,0063	1 14	0.75	0.30	1.20
C7H6O5	170.0215	0.00	1.00	0.75	0.71
C8H8O7	216 0270	0.39	0.71	1.00	0.88
C5H4O4	128 0110	0.50	1.00	0.80	0.80
C6H4O7	123.0110	0.09	0.71	0.80	1 17
C10H8O5	208 0372	2.04	1.00	0.07	0.50
C10H805	108.0372	2.04	1.00	0.80	0.30
C101406	222.0164	0.08	1.00	0.75	0.75
C0H6O4	178.0266	2.81	1.00	0.60	0.00
C9H0O4	242.0062	2.07	1.00	0.67	0.44
C9H0O8	242.0003	2.01	0.88	0.07	0.89
C9H6O4	180.0423	2.72	1.00	0.89	0.44
C10H8O5	208.0372	1.18	1.00	0.80	0.50
C/H6U3	158.0517	3.09	1.00	0.86	0.43
C10H6O/	238.0114	2.57	1.00	0.60	0.70
C5H6O3	114.0317	0.39	1.00	1.20	0.60
C6H4O5	156.0059	0.37	1.00	0.67	0.83
C6H8O5	160.0372	0.38	0.60	1.33	0.83
C8H6O4	166.0266	1.34	1.00	0.75	0.50
C6H6O5	158.0215	0.59	0.80	1.00	0.83
C8H6O6	198.0164	2.58	1.00	0.75	0.75
C5H4O4	128.0110	1.48	1.00	0.80	0.80
C8H6O5	182.0215	2.82	1.00	0.75	0.63
C9H6O7	226.0114	2.73	1.00	0.67	0.78
C9H8O6	212.0321	2.41	1.00	0.89	0.67
C7H6O5	170.0215	1.31	1.00	0.86	0.71
C11H12O5	224.0685	2.49	1.00	1.09	0.45
C9H6O7	226.0114	0.40	1.00	0.67	0.78
C8H6O3	150.0317	0.85	1.00	0.75	0.38
C10H8O5	208.0372	0.73	1.00	0.80	0.50
C10H6O6	222.0164	2.59	1.00	0.60	0.60
C9H8O5	196.0372	4.16	1.00	0.89	0.56
C6H4O4	140.0110	0.37	1.00	0.67	0.67
C6H6O	94.0419	3.59	1.00	1.00	0.17
C8H8O3	152.0473	2.93	1.00	1.00	0.38
C10H10O4	194.0579	3.68	1.00	1.00	0.40
C10H8O6	224.0321	2.49	1.00	0.80	0.60
C8H8O6	200.0321	0.38	0.83	1.00	0.75
C9H6O3	162.0317	3.92	1.00	0.67	0.33
C9H6O5	194.0215	3.23	1.00	0.67	0.56
C10H6O6	222.0164	3.64	1.00	0.60	0.60
C4H2O5	129.9902	0.35	0.80	0.50	1.25
C11H8O6	236.0321	2.76	1.00	0.73	0.55
C7H6O2	122.0368	0.85	1.00	0.86	0.29
C9H8O6	212.0321	0.57	1.00	0.89	0.67
C9H8O2	148.0524	3.83	1.00	0.89	0.22
C6H8O4	144.0423	0.38	0.75	1.33	0.67
C6H4O6	172.0008	0.75	0.83	0.67	1.00
C10H8O6	224 0321	1.70	1.00	0.80	0.60
C9H8O6	212.0321	1.57	1.00	0.89	0.67
C7H4O6	184 0008	0.38	1.00	0.57	0.86
C9H4O5	192 0059	2.97	1.00	0.44	0.56
C10H1005	210 0528	0.58	1.00	1.00	0.50
C10H8O2	160 0524	5 48	1.00	0.80	0.20
C6H4O5	156 0059	1 08	1.00	0.67	0.83
C19H12O5	320.0685	7 47	1.00	0.63	0.05
C10H807	240.0005	7. <del>4</del> 7 2.55	1.00	0.05	0.20
C11H8O6	270.0270	2.55	1.00	0.30	0.55
C8H4O7	230.0321	1 3/	1.00	0.75	0.35
C6H6O4	117 0766	0.60	1.00	1.00	0.00
C011004	142.0200	0.09	1.00	1.00	0.07

C8H6O8	230.0063	0.58	0.75	0.75	1.00
C11H12O7	256.0583	1.96	0.86	1.09	0.64
C8H8O5	184.0372	0.40	1.00	1.00	0.63
C10H6O8	254.0065	2.08	1.00	0.60	0.80
C10H6O7	220.0114	2.94	1.00	0.60	0.70
C6H6O3	126.0317	0.78	1.00	1.00	0.50
C9H8O	132.0575	3.12	1.00	0.89	0.11
C3H2O2	70.0055	0.36	1.00	0.67	0.67
C8H8O4	168.0423	2.32	1.00	1.00	0.50
C5H2O5	141.9902	0.39	1.00	0.40	1.00
C9H10O4	182.0579	1.16	1.00	1.11	0.44
C10H8O3	140.0110	0.75 4.08	1.00	0.07	0.87
C8H6O2	134.0368	2.96	1.00	0.75	0.25
C11H10O7	254.0427	2.79	1.00	0.91	0.64
C10H6O6	222.0164	3.14	1.00	0.60	0.60
C11H12O6	240.0634	0.95	1.00	1.09	0.55
C11H14O6	242.0790	1.19	0.83	1.27	0.55
C5H2O4	125.9953	0.36	1.00	0.40	0.80
C10H6O5	226.0114	0.89	1.00	0.67	0.78
C7H6O	106 0419	0.85	1.00	0.86	0.14
C10H8O7	240.0270	1.82	1.00	0.80	0.70
C11H10O7	254.0427	1.09	1.00	0.91	0.64
C10H10O4	194.0579	2.94	1.00	1.00	0.40
C9H6O3	162.0317	1.15	1.00	0.67	0.33
C10H10O7	242.0427	2.45	0.86	1.00	0.70
C11H10O6	238.0477	2.72	1.00	0.91	0.55
C10H807	240.0270	2.92	1.00	0.80	0.70
C11H8O3	188.0473	5.57	1.00	0.73	0.27
C7H4O5	168.0059	1.23	1.00	0.57	0.71
C7H8O4	156.0423	0.38	1.00	1.14	0.57
C9H8O	132.0575	3.51	1.00	0.89	0.11
C11H10O5	222.0528	2.97	1.00	0.91	0.45
C13H806	260.0321	4.66	1.00	0.62	0.46
C9H8O2	230.0383	1.04	1.00	0.89	0.04
C7H4O5	168.0059	0.37	1.00	0.57	0.22
C6H4O3	124.0160	0.36	1.00	0.67	0.50
C9H10O4	182.0579	1.60	1.00	1.11	0.44
C9H10O5	198.0528	0.76	1.00	1.11	0.56
C5H4O2	96.0211	0.38	1.00	0.80	0.40
C9H6O3	162.0317	1.49	1.00	0.67	0.33
C5H4O3	112 0160	0.78	1.00	0.91	0.55
C6H6O2	110.0368	1.87	1.00	1.00	0.33
C6H6O2	110.0368	0.38	1.00	1.00	0.33
C11H8O4	204.0423	3.20	1.00	0.73	0.36
C10H10O3	178.0630	3.26	1.00	1.00	0.30
C14H10O8	306.0376	2.82	1.00	0.71	0.57
C11H1005	222.0528	2.40	1.00	0.91	0.45
C7H8O	108.0575	3 33	1.00	1.00	0.33
C9H6O2	146.0368	1.18	1.00	0.67	0.22
C9H10O2	150.0681	2.82	1.00	1.11	0.22
C10H6O4	190.0266	1.65	1.00	0.60	0.40
C8H4O6	196.0008	2.35	1.00	0.50	0.75
C10H6O9	270.0012	2.79	0.89	0.60	0.90
C12H8U0 C4H2O3	248.0521	2.90	1.00	0.07	0.50
C16H10O4	266.0579	3.26	1.00	0.63	0.25
C7H4O5	168.0059	0.57	1.00	0.57	0.71
C9H18O3	174.1256	7.50	0.33	2.00	0.33
C7H6O5	170.0215	2.66	1.00	0.86	0.71
C7H4O6	184.0008	1.19	1.00	0.57	0.86
C7H4O6	184.0008	0.80	1.00	0.57	0.86
C10H10O4	194.0579	0.96	1.00	1.00	0.40
C0H4O4	104.0110	0.01	1.00	0.30	0.30

C6H2O5	153.9902	0.32	1.00	0.33	0.83
C9H4O7	223.9957	2.54	1.00	0.44	0.78
C15H10O4	254.0579	7.58	1.00	0.67	0.27
C15H10O8	318.0376	3.07	1.00	0.67	0.53
C9H6O2	146.0368	3.17	1.00	0.67	0.22
C10H6O5	206.0215	4 57	1.00	0.60	0.50
C7H4O6	184 0008	2 38	1.00	0.57	0.86
C6H6O2	110 0368	3.05	1.00	1.00	0.33
C6H6O	04 0410	1.15	1.00	1.00	0.33
C16U1005	282.0528	5.51	1.00	1.00	0.17
COLLO	202.0320	2.51	1.00	0.03	0.31
CICIDAOR	118.0419	2.47	1.00	0.75	0.13
C16H24O8	344.1471	3.53	0.63	1.50	0.50
C3H2O3	86.0004	0.36	1.00	0.67	1.00
C18H12O9	372.0481	3.10	1.00	0.67	0.50
C8H4O5	180.0059	1.97	1.00	0.50	0.63
C12H10O6	250.0477	2.90	1.00	0.83	0.50
C10H8O2	160.0524	5.14	1.00	0.80	0.20
C3H2O	54.0106	0.37	1.00	0.67	0.33
C17H12O7	328.0583	3.26	1.00	0.71	0.41
C7H4O3	136.0160	1.28	1.00	0.57	0.43
C11H8O5	220.0372	3.14	1.00	0.73	0.45
C17H14O10	378.0587	3.01	1.00	0.82	0.59
C13H10O6	262.0477	2.99	1.00	0.77	0.46
C12H10O7	266.0427	2.57	1.00	0.83	0.58
C13H1007	278.0427	2.80	1.00	0.77	0.54
C4H4O4	116 0110	3.04	0.75	1.00	1.00
C12H1007	266 0427	2 79	1.00	0.83	0.58
C14H1009	322 0325	2.75	1.00	0.03	0.64
C14H10O6	274 0477	2.70	1.00	0.71	0.04
C7116O	2/4.0477	3.12	1.00	0.71	0.43
C7U4O4	152 0110	2.00	1.00	0.80	0.14
C/H404	132.0110	0.58	1.00	0.37	0.37
C5H4O	80.0262	0.38	1.00	0.80	0.20
C15H1009	334.0325	2.93	1.00	0.67	0.60
C8H10O3	154.0630	1.62	1.00	1.25	0.38
C6H6O	94.0419	2.37	1.00	1.00	0.17
C15H12O7	304.0583	3.03	1.00	0.80	0.47
C15H10O6	286.0477	3.39	1.00	0.67	0.40
C10H12O5	212.0685	0.96	1.00	1.20	0.50
C11H6O7	250.0114	2.79	1.00	0.55	0.64
C14H12O8	308.0532	2.98	1.00	0.86	0.57
C4H2O	66.0106	0.37	1.00	0.50	0.25
C5H6O6	162.0164	2.74	0.50	1.20	1.20
C12H12O6	252.0634	2.92	1.00	1.00	0.50
C8H4O5	180.0059	0.42	1.00	0.50	0.63
C8H6O8	230,0063	2.83	0.75	0.75	1.00
C8H4O9	243 9855	0.54	0.78	0.50	1 13
C14H1008	306.0376	2.58	1.00	0.71	0.57
C18H36O5	332 2563	8.00	0.20	2 00	0.28
C9H18O3	174 1256	5 21	0.20	2.00	0.33
C7H4O4	152 0110	1 32	1.00	0.57	0.57
CINHON	254 0063	0.74	1.00	0.57	0.57
C11H8O4	204.0003	1 02	1.00	0.00	0.00
C2H4O2	60.0211	7.05	0.50	2.00	1.00
C/H2O	66.0106	2.90	1.00	2.00	0.25
C1111607	250.0114	2.08	1.00	0.50	0.25
	250.0114	2.85	1.00	0.55	0.04
C11H12O4	208.0736	5.82	1.00	1.09	0.36
CI0HI0O8	258.0376	2.67	0.75	1.00	0.80
C10H12O5	212.0685	1.30	1.00	1.20	0.50
C12H10O7	266.0427	0.96	1.00	0.83	0.58
C9H6O9	258.0012	0.84	0.78	0.67	1.00
C8H10O6	202.0477	1.00	0.67	1.25	0.75
C4H4O	68.0262	2.43	1.00	1.00	0.25
C12H12O7	268.0583	0.67	1.00	1.00	0.58
C7H8O	108.0575	2.11	1.00	1.14	0.14
C8H10O4	170.0579	0.75	1.00	1.25	0.50
C20H18O10	418.0900	2.27	1.00	0.90	0.50
C9H10O7	230.0427	2.63	0.71	1.11	0.78
C8H8O	120.0575	1.16	1.00	1.00	0.13
C9H4O7	223.9957	1.03	1.00	0.44	0.78
C7H8O5	172.0372	1.82	0.80	1 14	0.71
0,11000	1,2.00/2	1.02	0.00		0.71

C3H4O C9H8O4					
C9H8O4	56.0262	1.47	1.00	1.33	0.33
0/11001	180.0423	3.24	1.00	0.89	0.44
C6H6O6	174.0164	0.36	0.67	1.00	1.00
C10H8O5	208.0372	3.32	1.00	0.80	0.50
C10H6O3	174.0317	3.76	1.00	0.60	0.30
C8H6O6	198.0164	1.25	1.00	0.75	0.75
C8H8O7	216.0270	0.37	0.71	1.00	0.88
C10H10O5	210.0528	2.98	1.00	1.00	0.50
C8H4O4	164.0110	2.79	1.00	0.50	0.50
C7H6O3	138.0317	4.17	1.00	0.86	0.43
C8H6O7	214 0114	1.37	0.86	0.75	0.88
C10H6O4	190.0266	3.61	1.00	0.60	0.40
C2H4O3	76.0160	2.88	0.33	2.00	1.50
C7H6O2	122.0368	2.96	1.00	0.86	0.29
C10H8O6	224.0321	0.92	1.00	0.80	0.60
C9H6O4	178.0266	3.51	1.00	0.67	0.44
C7H6O2	122.0368	2.37	1.00	0.86	0.29
C10H10O4	194.0579	3.28	1.00	1.00	0.40
C9H6O6	210.0164	1.33	1.00	0.67	0.67
C10H6O4	190.0266	4.32	1.00	0.60	0.40
C10H6O3	174 0317	2.76	1.00	0.60	0.30
C11H12O5	224 0685	2.76	1.00	1.09	0.45
C11H1007	254.0005	2.70	1.00	0.91	0.43
C6H4O6	172 0008	2.78	0.83	0.91	1.00
C5H2O5	1/1 0002	0.37	1.00	0.07	1.00
C3H2O3	141.9902	0.37	1.00	1.00	0.25
C0H6O6	210.0164	2.11	1.00	1.00	0.23
C10U1405	210.0104	2.03	1.00	0.07	0.07
C12H14O5	238.0841	2.07	1.00	1.17	0.42
C10U10O4	104.0570	3.07	1.00	1.00	0.73
C10H1004	194.0379	4.30	1.00	1.00	0.40
C8H8U2	150.0524	2.78	1.00	1.00	0.25
C16H10O4	266.0579	3.44	1.00	0.63	0.25
C18H1008	354.0376	3.48	1.00	0.56	0.44
C11H6O6	234.0164	3.23	1.00	0.55	0.55
C18H12O4	292.0736	7.66	1.00	0.67	0.22
C10H8O8	256.0219	2.85	0.88	0.80	0.80
C12H10O5	234.0528	2.81	1.00	0.83	0.42
C13H1005	246.0528	3.06	1.00	0.77	0.38
C12H8O5	232.0372	3.82	1.00	0.67	0.42
C16H10O9	346.0325	3.04	1.00	0.63	0.56
C13H10O3	214.0630	6.83	1.00	0.77	0.23
C/H8O3	140.0473	0.37	1.00	1.14	0.43
C10H8O2	160.0524	7.62	1.00	0.80	0.20
(34/05	180.0059	<b>A A F</b>	1 00	11 511	0.70
001405	100.0059	2.95	1.00	0.30	0.63
C11H8O3	188.0473	2.95 7.80	1.00 1.00	0.30	0.63 0.27
C11H8O3 C7H6O	188.0473 106.0419	2.95 7.80 3.05	1.00 1.00 1.00	0.30 0.73 0.86	0.63 0.27 0.14
C11H8O3 C11H8O3 C7H6O C8H8O5	188.0473 106.0419 184.0372	2.95 7.80 3.05 1.50	1.00 1.00 1.00 1.00	0.30 0.73 0.86 1.00	0.63 0.27 0.14 0.63
C11H8O3 C7H6O C8H8O5 C14H10O6	188.0473 106.0419 184.0372 274.0477	2.95 7.80 3.05 1.50 3.43	1.00 1.00 1.00 1.00 1.00	0.30 0.73 0.86 1.00 0.71	0.63 0.27 0.14 0.63 0.43
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4	188.0473 106.0419 184.0372 274.0477 292.0736	2.95 7.80 3.05 1.50 3.43 7.22	$ \begin{array}{c} 1.00 \\ 1.00 \\ 1.00 \\ 1.00 \\ 1.00 \\ 1.00 \\ 0.06 \\ \end{array} $	0.30 0.73 0.86 1.00 0.71 0.67	0.63 0.27 0.14 0.63 0.43 0.22
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427	2.95 7.80 3.05 1.50 3.43 7.22 3.19	1.00 1.00 1.00 1.00 1.00 1.00 0.86	0.30 0.73 0.86 1.00 0.71 0.67 1.00	0.63 0.27 0.14 0.63 0.43 0.22 0.70
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215	2.95 7.80 3.05 1.50 3.43 7.22 3.19 2.81	1.00 1.00 1.00 1.00 1.00 1.00 0.86 1.00	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.55\\ 0.55\\ \end{array}$	$\begin{array}{c} 0.63 \\ 0.27 \\ 0.14 \\ 0.63 \\ 0.43 \\ 0.22 \\ 0.70 \\ 0.45 \\ \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215 230.0063	2.95 7.80 3.05 1.50 3.43 7.22 3.19 2.81 2.32	$ \begin{array}{c} 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 0.86\\ 1.00\\ 0.75\\ \end{array} $	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.75\\ \end{array}$	$\begin{array}{c} 0.63 \\ 0.27 \\ 0.14 \\ 0.63 \\ 0.43 \\ 0.22 \\ 0.70 \\ 0.45 \\ 1.00 \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215 230.0063 232.0372	2.95 7.80 3.05 1.50 3.43 7.22 3.19 2.81 2.32 3.03	$ \begin{array}{c} 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 0.86\\ 1.00\\ 0.75\\ 1.00\\ 1.00\\ 0.75\\ 1.00\\ 1.00\\ 0.75\\ 1.00\\ 1.00\\ 0.75\\ 1.00\\ 0.75\\ 0.02$	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.67\\ \end{array}$	$\begin{array}{c} 0.63 \\ 0.27 \\ 0.14 \\ 0.63 \\ 0.43 \\ 0.22 \\ 0.70 \\ 0.45 \\ 1.00 \\ 0.42 \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215 230.0063 232.0372 300.0634	2.95 7.80 3.05 1.50 3.43 7.22 3.19 2.81 2.32 3.03 3.16	$ \begin{array}{c} 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 0.86\\ 1.00\\ 0.75\\ 1.00\\ 1.00\\ 1.00\\ 1.00 \end{array} $	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.67\\ 0.75\\ 0.75\\ 0.67\\ 0.75\\ 0.67\\ 0.75\\ 0.67\\ 0.75\\ 0.75\\ 0.67\\ 0.75\\ 0.75\\ 0.67\\ 0.75\\ 0.75\\ 0.67\\ 0.75\\ 0.75\\ 0.67\\ 0.75\\ 0.75\\ 0.67\\ 0.75\\ 0.75\\ 0.67\\ 0.75\\ 0.75\\ 0.67\\ 0.75\\$	$\begin{array}{c} 0.63 \\ 0.27 \\ 0.14 \\ 0.63 \\ 0.43 \\ 0.22 \\ 0.70 \\ 0.45 \\ 1.00 \\ 0.42 \\ 0.38 \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215 230.0063 232.0372 300.0634 304.0883	$2.95 \\ 7.80 \\ 3.05 \\ 1.50 \\ 3.43 \\ 7.22 \\ 3.19 \\ 2.81 \\ 2.32 \\ 3.03 \\ 3.16 \\ 3.17 \\ $	$ \begin{array}{c} 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 0.86\\ 1.00\\ 0.75\\ 1.00$	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.67\\ 0.75\\ 0.67\\ 0.75\\ 0.86\\$	$\begin{array}{c} 0.63 \\ 0.27 \\ 0.14 \\ 0.63 \\ 0.43 \\ 0.22 \\ 0.70 \\ 0.45 \\ 1.00 \\ 0.45 \\ 1.00 \\ 0.42 \\ 0.38 \\ 0.47 \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215 230.0063 232.0372 300.0634 304.0583 192.0059	$2.95 \\ 7.80 \\ 3.05 \\ 1.50 \\ 3.43 \\ 7.22 \\ 3.19 \\ 2.81 \\ 2.32 \\ 3.03 \\ 3.16 \\ 3.17 \\ 2.76 \\ 5.75 \\ 0.17 \\ 0.17 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.17 \\ 0.16 \\ 0.16 \\ 0.17 \\ 0.16 \\ $	$ \begin{array}{c} 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 0.86\\ 1.00\\ 0.75\\ 1.00$	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.67\\ 0.75\\ 0.80\\ 0.44\\ 0.41\end{array}$	$\begin{array}{c} 0.63 \\ 0.27 \\ 0.14 \\ 0.63 \\ 0.43 \\ 0.22 \\ 0.70 \\ 0.45 \\ 1.00 \\ 0.45 \\ 1.00 \\ 0.42 \\ 0.38 \\ 0.47 \\ 0.56 \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C14H1007	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215 230.0063 232.0372 300.0634 304.0583 192.0059 290.0427	$\begin{array}{c} 2.95 \\ 7.80 \\ 3.05 \\ 1.50 \\ 3.43 \\ 7.22 \\ 3.19 \\ 2.81 \\ 2.32 \\ 3.03 \\ 3.16 \\ 3.17 \\ 2.76 \\ 3.28 \end{array}$	$ \begin{array}{c} 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 0.86\\ 1.00\\ 0.75\\ 1.00$	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.67\\ 0.75\\ 0.80\\ 0.44\\ 0.71\\ 0.75\\ \end{array}$	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.50\\ 0.55\\$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C14H10O7 C18H12O5	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215 230.0063 232.0372 300.0634 304.0583 192.0059 290.0427 308.0685	$2.95 \\ 7.80 \\ 3.05 \\ 1.50 \\ 3.43 \\ 7.22 \\ 3.19 \\ 2.81 \\ 2.32 \\ 3.03 \\ 3.16 \\ 3.17 \\ 2.76 \\ 3.28 \\ 7.88 \\ $	$ \begin{array}{c} 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 0.86\\ 1.00\\ 0.75\\ 1.00$	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.67\\ 0.75\\ 0.80\\ 0.44\\ 0.71\\ 0.67\\$	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C14H1007 C18H12O5 C9H6O2	188.0473 106.0419 184.0372 274.0477 292.0736 242.0427 218.0215 230.0063 232.0372 300.0634 304.0583 192.0059 290.0427 308.0685 146.0368	$2.95 \\ 7.80 \\ 3.05 \\ 1.50 \\ 3.43 \\ 7.22 \\ 3.19 \\ 2.81 \\ 2.32 \\ 3.03 \\ 3.16 \\ 3.17 \\ 2.76 \\ 3.28 \\ 7.88 \\ 4.32 \\ 5.6 \\ $	$ \begin{array}{c} 1.00\\ 1.00\\ 1.00\\ 1.00\\ 1.00\\ 0.86\\ 1.00\\ 0.75\\ 1.00$	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.22\\ 0.21\\ 0.55\\ 0.21\\ 0.25\\ 0.22\\ 0.22\\ 0.25\\$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C14H10O7 C18H12O5 C9H6O2 C18H16O7	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\$	1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.89 0.85	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.45\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.22\\ 0.39\\ 0.55\\$
C1114803 C71460 C81805 C14H1006 C18H1204 C10H1007 C1114605 C8H608 C12H805 C16H1206 C15H1207 C9H405 C14H1007 C18H1205 C9H602 C18H1607 C11H606	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\end{array}$	1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.67	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ \end{array}$
C1114803 C71460 C818805 C14H1006 C18H1204 C10H1007 C1114605 C8H608 C12H805 C16H1206 C15H1207 C9H405 C14H1007 C18H1205 C9H602 C18H1607 C11H606 C14H1207	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$ $292.0583$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\\ 2.86\\ 2.86\end{array}$	1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.67\\ 0.75\\ 0.80\\ 0.44\\ 0.71\\ 0.67\\ 0.67\\ 0.67\\ 0.89\\ 0.55\\ 0.86\end{array}$	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ 0.50\\ \end{array}$
C111H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C19H4O5 C14H10O7 C18H12O5 C9H6O2 C18H16O7 C11H6O6 C14H12O7 C11H6O6 C14H12O7 C17H12O6	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$ $292.0583$ $312.0634$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\\ 2.86\\ 2.86\\ 6.41\\ \end{array}$	1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	$\begin{array}{c} 0.30\\ 0.73\\ 0.86\\ 1.00\\ 0.71\\ 0.67\\ 1.00\\ 0.55\\ 0.75\\ 0.67\\ 0.75\\ 0.80\\ 0.44\\ 0.71\\ 0.67\\ 0.67\\ 0.67\\ 0.89\\ 0.55\\ 0.86\\ 0.71\\ \end{array}$	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ 0.50\\ 0.35\\ \end{array}$
C1114803 C71460 C818805 C14H1006 C18H1204 C10H1007 C1114605 C8H608 C12H805 C16H1206 C15H1207 C9H405 C14H1007 C18H1205 C9H602 C18H1607 C11H606 C14H1207 C11H606 C14H1207 C17H1206 C6H605	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$ $292.0583$ $312.0634$ $158.0215$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\\ 2.86\\ 2.86\\ 6.41\\ 0.95\\ \end{array}$	1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00 $1.001$	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.55 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.75 0.80 0.67 0.67 0.67 0.67 0.75 0.80 0.71 0.67 0.67 0.67 0.75 0.67 0.75 0.80 0.71 0.67 0.67 0.67 0.67 0.67 0.75 0.67 0.75 0.80 0.67 0.89 0.55 0.86 0.71 1.00	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ 0.50\\ 0.35\\ 0.83\\ \end{array}$
C111H8O3 C71H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C16H12O5 C9H4O5 C14H1007 C18H12O5 C9H6O2 C18H16O7 C11H6O6 C14H12O7 C11H6O6 C14H12O7 C17H12O6 C6H6O5 C16H14O9	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$ $292.0583$ $312.0634$ $158.0215$ $350.0638$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\\ 2.86\\ 6.41\\ 0.95\\ 2.97\\ \end{array}$	1.00 1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00 $1.001$	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.55 0.80 0.44 0.71 0.67 0.89 0.55 0.86 0.71 1.00 0.88	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ 0.50\\ 0.35\\ 0.83\\ 0.56\\ \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H10O7 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C16H12O5 C9H4O5 C14H1007 C18H12O5 C9H6O2 C18H16O7 C11H6O6 C14H12O7 C17H12O6 C6H6O5 C16H14O9 C11H8O6	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$ $292.0583$ $312.0634$ $158.0215$ $350.0638$ $236.0321$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\\ 2.86\\ 6.41\\ 0.95\\ 2.97\\ 3.15\\ \end{array}$	1.00 1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.55 0.80 0.44 0.71 0.67 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.55 0.80 0.44 0.71 0.67 0.89 0.55 0.86 0.71 0.07 0.89 0.55 0.86 0.71 0.07 0.89 0.75 0.80 0.71 0.07 0.80 0.71 0.07 0.80 0.71 0.07 0.80 0.71 0.07 0.80 0.71 0.00 0.73 0.80 0.71 0.00 0.88 0.73	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ 0.50\\ 0.35\\ 0.83\\ 0.56\\ 0.55\\ \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H1007 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C14H1007 C18H12O5 C9H6O2 C18H16O7 C11H6O6 C14H12O7 C17H12O6 C6H6O5 C16H14O9 C11H8O6 C18H12O7	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$ $292.0583$ $312.0634$ $158.0215$ $350.0638$ $236.0321$ $340.0583$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\\ 2.86\\ 6.41\\ 0.95\\ 2.97\\ 3.15\\ 3.73\\ \end{array}$	1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.55 0.80 0.44 0.71 0.67 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.80 0.44 0.71 0.67 0.89 0.55 0.86 0.71 0.67 0.89 0.55 0.86 0.71 0.00 0.88 0.71 1.00 0.88 0.73 0.67	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ 0.50\\ 0.35\\ 0.83\\ 0.56\\ 0.55\\ 0.39\\ \end{array}$
C11H8O3 C7H6O C8H8O5 C14H10O6 C18H12O4 C10H1007 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C14H1007 C18H12O5 C9H6O2 C18H16O7 C11H6O6 C14H12O7 C17H12O6 C6H6O5 C16H14O9 C11H8O6 C18H12O7 C13H1007	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$ $292.0583$ $312.0634$ $158.0215$ $350.0638$ $236.0321$ $340.0583$ $278.0427$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\\ 2.86\\ 6.41\\ 0.95\\ 2.97\\ 3.15\\ 3.73\\ 2.49\\ \end{array}$	1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.67 0.55 0.80 0.44 0.71 0.67 0.67 0.88 0.71 1.00 0.88 0.71 1.00 0.88 0.71 1.00 0.88 0.73 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.67 0.75 0.80 0.71 0.67 0.71 0.67 0.71 0.67 0.75 0.80 0.71 0.67 0.71 0.67 0.73 0.67 0.73 0.67 0.73 0.67 0.73 0.73 0.67 0.73 0.67 0.73 0.73 0.67 0.73 0.77 0.77	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ 0.50\\ 0.35\\ 0.83\\ 0.56\\ 0.55\\ 0.39\\ 0.54\\ \end{array}$
C111H8O3 C71H6O C8H8O5 C14H10O6 C18H12O4 C10H1007 C11H6O5 C8H6O8 C12H8O5 C16H12O6 C15H12O7 C9H4O5 C14H1007 C18H12O5 C9H6O2 C18H16O7 C11H6O6 C14H12O7 C17H12O6 C6H6O5 C16H14O9 C11H8O6 C18H12O7 C13H1007 C13H1007 C9H1005	188.0473 $106.0419$ $184.0372$ $274.0477$ $292.0736$ $242.0427$ $218.0215$ $230.0063$ $232.0372$ $300.0634$ $304.0583$ $192.0059$ $290.0427$ $308.0685$ $146.0368$ $344.0896$ $234.0164$ $292.0583$ $312.0634$ $158.0215$ $350.0638$ $236.0321$ $340.0583$ $278.0427$ $198.0528$	$\begin{array}{c} 2.95\\ 7.80\\ 3.05\\ 1.50\\ 3.43\\ 7.22\\ 3.19\\ 2.81\\ 2.32\\ 3.03\\ 3.16\\ 3.17\\ 2.76\\ 3.28\\ 7.88\\ 4.32\\ 3.84\\ 2.86\\ 2.86\\ 6.41\\ 0.95\\ 2.97\\ 3.15\\ 3.73\\ 2.49\\ 3.31\end{array}$	1.00 1.00 1.00 1.00 1.00 0.86 1.00 0.75 1.00	0.30 0.73 0.86 1.00 0.71 0.67 1.00 0.55 0.75 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.67 0.75 0.80 0.44 0.71 0.67 0.67 0.67 0.67 0.67 0.67 0.75 0.80 0.44 0.71 0.67 0.71 1.00 0.88 0.73 0.67 0.71 1.00 0.88	$\begin{array}{c} 0.63\\ 0.27\\ 0.14\\ 0.63\\ 0.43\\ 0.22\\ 0.70\\ 0.45\\ 1.00\\ 0.45\\ 1.00\\ 0.42\\ 0.38\\ 0.47\\ 0.56\\ 0.50\\ 0.28\\ 0.22\\ 0.39\\ 0.55\\ 0.50\\ 0.35\\ 0.83\\ 0.56\\ 0.55\\ 0.39\\ 0.54\\ 0.56\end{array}$

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C6H6O2	110.0368	0.93	1.00	1.00	0.33
C11H8O5	220.0372	3.56	1.00	0.73	0.45
C19H16O9	388.0794	3.09	1.00	0.84	0.47
C14H10O5	258.0528	3.34	1.00	0.71	0.36
C18H12O10	388.0430	3.02	1.00	0.67	0.56
C17H14O8	346.0689	3.00	1.00	0.82	0.47
C15H1007	302.0427	3.26	1.00	0.67	0.47
CI/H1006	310.0477	6.67	1.00	0.59	0.35
C18H12O4	292.0736	8.17	1.00	0.67	0.22
C11H803	188.0473	/.34	1.00	0.73	0.27
C19H12O4	304.0736	0.99	1.00	0.05	0.21
C0H10O2	150.0681	4.21	1.00	1 11	0.37
C17H12O5	296.0685	5 44	1.00	0.71	0.22
C16H10O4	256.0003	7.40	1.00	0.71	0.25
C15H12O6	288.0634	3.06	1.00	0.80	0.25
C17H12O10	376.0430	2.98	1.00	0.71	0.59
C16H12O7	316.0583	3.16	1.00	0.75	0.44
C13H8O7	276.0270	3.13	1.00	0.62	0.54
C17H10O6	310.0477	7.29	1.00	0.59	0.35
C19H10O6	334.0477	7.33	1.00	0.53	0.32
C12H8O6	248.0321	3.19	1.00	0.67	0.50
C16H10O5	282.0528	3.07	1.00	0.63	0.31
C18H12O3	276.0786	7.93	1.00	0.67	0.17
C14H12O7	292.0583	2.78	1.00	0.86	0.50
C18H16O8	360.0845	2.12	1.00	0.89	0.44
C15H10O9	334.0325	2.78	1.00	0.67	0.60
C6H14O6	182.0790	0.03	0.00	2.33	1.00
C9H18O3	174.1256	6.59	0.33	2.00	0.33
C16H10O7	314.0427	3.48	1.00	0.63	0.44
C8H4O6	196.0008	2.62	1.00	0.50	0.75
C11H14O6	242.0790	1.69	0.83	1.27	0.55
C7H8O	108.0575	2.97	1.00	1.14	0.14
C11H10O4	206.0579	6.28	1.00	0.91	0.36
C18H12O9	372.0481	3.40	1.00	0.67	0.50
C19H12O4	304.0736	7.74	1.00	0.63	0.21
C1/H12O6	312.0634	0.83	1.00	0.71	0.35
C11H1004	206.0579	2.90	1.00	0.91	0.30
C16H12O6	324.0034	7.15	1.00	0.67	0.33
C12H12O7	280.0582	3.13	1.00	0.03	0.44
C13H12O7	260.0583	2.03	1.00	1.00	0.54
C18H1009	370.0325	3.09	1.00	0.56	0.58
C9H6O2	146 0368	6.99	1.00	0.50	0.30
C18H12O11	404 0380	3.02	1.00	0.67	0.22
C13H8O8	292 0219	3.20	1.00	0.62	0.62
C18H14O7	342.0740	5.31	1.00	0.78	0.39
C9H4O6	208.0008	2.33	1.00	0.44	0.67
C19H14O11	418.0536	3.02	1.00	0.74	0.58
C19H12O5	320.0685	6.93	1.00	0.63	0.26
C10H6O3	174.0317	1.01	1.00	0.60	0.30
C12H12O6	252.0634	2.79	1.00	1.00	0.50
C10H8O2	160.0524	6.91	1.00	0.80	0.20
C4H6O3	102.0317	1.23	0.67	1.50	0.75
C12H8O6	248.0321	7.27	1.00	0.67	0.50
C16H12O6	300.0634	3.51	1.00	0.75	0.38
C14H12O8	308.0532	2.38	1.00	0.86	0.57
C20H12O6	348.0634	7.33	1.00	0.60	0.30
C11H8O2	172.0524	6.87	1.00	0.73	0.18
C15H12O5	272.0685	7.19	1.00	0.80	0.33
C6H6O7	190.0114	0.71	0.57	1.00	1.17
C10H6O6	222.0164	0.57	1.00	0.60	0.60
C14H12O6	276.0634	2.99	1.00	0.86	0.43
C19H18O9	390.0951	2.14	1.00	0.95	0.47
C6H4O7	187.9957	0.60	0.71	0.67	1.17
C10H10O10	302.02/4	3.04	1.00	0.03	0.63
C13H12U6	204.0034	3.00	1.00	0.92	0.40
C16H14O7	210.0270	2.03 2.07	1.00	0.02	0.34
C14H807	288 0270	2.27	1.00	0.00	0.44
01411007	200.0270	5.00	1.00	0.57	0.50

C18H10O7	338.0427	3.75	1.00	0.56	0.39
C17H16O10	380.0743	2.71	1.00	0.94	0.59
C20H14O5	334.0841	7.51	1.00	0.70	0.25
C12H8O8	280.0219	2.93	1.00	0.67	0.67
C16H10O4	266.0579	7.94	1.00	0.63	0.25
C12H8O5	232.0372	1.35	1.00	0.67	0.42
C12U8O2	340.0089	5.55 5.50	1.00	0.82	0.47
C12H8O4	200.0475	5.52	1.00	0.67	0.23
C15H804	220.0423	3.40 4 77	1.00	0.02	0.31
C10H8O2	160.0524	4.77	1.00	0.03	0.31
C15H10O3	238.0630	7 36	1.00	0.67	0.20
C8H16O3	160 1099	3.03	0.33	2.00	0.38
C8H4O5	180.0059	2.46	1.00	0.50	0.63
C6H4O5	156.0059	2.78	1.00	0.67	0.83
C19H18O8	374.1002	3.83	1.00	0.95	0.42
C5H4O4	128.0110	3.10	1.00	0.80	0.80
C18H12O11	404.0380	2.72	1.00	0.67	0.61
C14H10O9	322.0325	1.21	1.00	0.71	0.64
C12H8O3	200.0473	2.95	1.00	0.67	0.25
C14H12O9	324.0481	2.44	1.00	0.86	0.64
C12H14O7	270.0740	2.17	0.86	1.17	0.58
C18H14O5	310.0841	6.84	1.00	0.78	0.28
C15H14O7	306.0740	3.04	1.00	0.93	0.47
C17H10O6	310.0477	4.26	1.00	0.59	0.35
C8H4O5	180.0059	2.45	1.00	0.50	0.63
C4H8O5	136.0372	6.84	0.20	2.00	1.25
C4H2O6	145.9851	0.38	0.67	0.50	1.50
C18H12O7	340.0583	4.65	1.00	0.67	0.39
C9H16O3	172.1099	3.62	0.67	1.78	0.33
C3H2O	54.0106	2.67	1.00	0.67	0.33
CITHI207	256.0583	3.23	0.86	1.09	0.64
CoHoOS	158.0215	2.01	0.80	1.00	0.85
C0H0O0 C14H8O7	288 0270	2.00	1.00	0.57	0.50
C9H6O2	146.0368	2.68	1.00	0.57	0.22
C6H6O5	158 0215	2.08	0.80	1.00	0.22
C17H10O8	342 0376	3.23	1.00	0.59	0.47
C16H8O8	328.0219	6.47	1.00	0.50	0.50
C7H8O5	172.0372	2.45	0.80	1.14	0.71
C6H12O6	180.0634	7.47	0.17	2.00	1.00
C12H14O8	286.0689	2.74	0.75	1.17	0.67
C19H16O9	388.0794	1.89	1.00	0.84	0.47
C14H14O8	310.0689	2.94	1.00	1.00	0.57
C14H14O8	310.0689	2.94	1.00	1.00	0.57
C14H10O7	290.0427	2.54	1.00	0.71	0.50
C5H6O5	146.0215	2.62	0.60	1.20	1.00
C12H12O7	268.0583	2.57	1.00	1.00	0.58
C13H10O5	246.0528	3.35	1.00	0.77	0.38
C10H10O8	258.0376	2.69	0.75	1.00	0.80
C9H8O6	212.0321	3.63	1.00	0.89	0.67
C15H1006	286.0477	7.62	1.00	0.67	0.40
C4H4U2 C12U1000	84.0211	0.74	1.00	1.00	0.50
C11H8O2	510.0525 188.0472	2.30	1.00	0.77	0.09
C10H12O6	100.0475	0.00	0.82	1.20	0.27
C7H12O4	160.0736	0.04	0.85	1.20	0.00
C18H12O8	356 0532	1.86	1.00	0.67	0.44
C13H14O8	298.0689	0.90	0.88	1.08	0.62
C10H6O7	238.0114	0.77	1.00	0.60	0.70
C9H10O9	262.0325	0.84	0.56	1.11	1.00
C8H10O4	170.0579	0.49	1.00	1.25	0.50
C9H10O8	246.0376	0.99	0.63	1.11	0.89
C9H10O8	246.0376	0.99	0.63	1.11	0.89
C10H8O2	160.0524	4.37	1.00	0.80	0.20
C7H8O	108.0575	1.41	1.00	1.14	0.14
C12H6O4	214.0266	4.70	1.00	0.50	0.33
C12H8O8	280.0219	2.50	1.00	0.67	0.67
C15H14O7	306.0740	2.80	1.00	0.93	0.47
C17H16O9	364.0794	2.16	1.00	0.94	0.53
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C7H6O9	234.0012	0.84	0.56	0.86	1.29	Ī
C7H14O3	146.0943	0.73	0.33	2.00	0.43	
C17H12O5	296.0685	3.48	1.00	0.71	0.29	
C7H6O6	186.0164	2.74	0.83	0.86	0.86	
C13H12O9	312.0481	0.74	0.89	0.92	0.69	
C17H14O10	378.0587	0.96	1.00	0.82	0.59	
C6H6O7	190.0114	1.03	0.57	1.00	1.17	
C3H2O2	70.0055	2.83	1.00	0.67	0.67	
C9H8O10	276.0117	0.79	0.60	0.89	1.11	
C10H10O8	258.0376	2.29	0.75	1.00	0.80	
C10H4O5	204.0059	1.34	1.00	0.40	0.50	
C12H12O8	284.0532	2.59	0.88	1.00	0.67	
C7H6O8	218.0063	0.88	0.63	0.86	1.14	
C7H8O10	252.0117	0.91	0.40	1.14	1.43	
C14H12O9	324.0481	0.58	1.00	0.86	0.64	
C3H4O2	72.0211	4.22	1.00	1.33	0.67	
C8H4O8	227.9906	1.11	0.88	0.50	1.00	
C9H10O3	166.0630	1.55	1.00	1.11	0.33	
C16H14O10	366.0587	0.82	1.00	0.88	0.63	
C7H14O3	146.0943	8.72	0.33	2.00	0.43	
C5H4O	80.0262	0.76	1.00	0.80	0.20	
C8H4O6	196.0008	1.96	1.00	0.50	0.75	
C7H4O6	184.0008	1.79	1.00	0.57	0.86	
C8H6O6	198.0164	8.82	1.00	0.75	0.75	
C7H8O2	124.0524	0.02	1.00	1.14	0.29	
C7H12O4	160.0736	8.82	0.50	1.71	0.57	
C5H8O5	148.0372	0.43	0.40	1.60	1.00	
C3H6O4	106.0266	0.37	0.25	2.00	1.33	
C3H4O4	104.0110	0.38	0.50	1.33	1.33	
C4H4O4	116.0110	0.41	0.75	1.00	1.00	
C8H8O2	136.0524	3.14	1.00	1.00	0.25	

# **D.** List of related publications and presentations

#### **Peer-reviewed publications:**

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<u>Zhang Y.</u>, Wang K., Tong H. J., and Hoffmann, T.:  $H_2O_2$  formation by PM<sub>2.5</sub> associated with highly oxygenated molecules. *European Aerosol Conference*, online, September 2020, post presentation.

Zhang. Y., Wang K., Lelieveld S., Ren H., Li L. J., Yue S. Y., Fu P. Q., Pöschl U., and Tong H. J., and Hoffmann T.: Organic chemical composition by Orbitrap MS and oxidative potential of particulate aerosols. *Asian Aerosol Conference*, Hong Kong, China, May 2019, oral presentation.

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# F. Curriculum vitae

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