# Chemical characterization of organic aerosol from Chinese cities using high resolution mass spectrometry

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by

Kai Wang

born in Xiaobai, Shengzhou, China

JG|U
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UNIVERSITÄT MAINZ

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1st supervisor:

2nd supervisor:

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Mainz, June 2018

“路漫漫其修远兮 吾将上下而求索”

“The way ahead is long, I shall search high and low”

屈原《离骚》

Qu Yuan, 《Li Sao》

# Zusammenfassung

Atmosphärische Aerosole üben einen großen Einfluss auf die Luftqualität, das Klima und die Gesundheit des Menschen aus. Dabei können sie die Sonnenstrahlung direkt streuen oder absorbieren, oder indirekt als Nukleationskeime für Wolkentröpfchen zu einem erhöhten Reflektionsverhalten von Wolken beitragen. Darüber hinaus können sie negative Auswirkungen auf das menschliche Atmungs- und Herz-Kreislauf-System haben. In den letzten Jahrzehnten kam es in China zu schweren und andauernden Luftverschmutzungsperioden, wobei die Feinstaubpartikel (PM) in vielen Städten ein beispiellos hohes Niveau erreichten und damit die regionale Luftqualität und die Gesundheit von Millionen von Menschen beeinflusste. Daraus ergibt sich die Notwendigkeit die chemische Zusammensetzung und die Quellen der Aerosolpartikel während der Verschmutzungsperioden besser zu verstehen.

Das Ziel dieser Arbeit lag daher in einer Charakterisierung der chemischen Zusammensetzung von organischen Aerosolpartikeln (OA), und zwar konkret für Luftproben, die während Verschmutzungsperioden im Januar 2014 in verschiedenen chinesischen Städten gesammelt wurden. Dazu wurde die ultrahochauflösende Massenspektrometrie (UHRMS) eingesetzt. Der erste Teil dieser Studie beschäftigte sich mit der Entwicklung einer analytischen Methode zur Analyse von Aerosolproben mit Partikeldurchmessern kleiner als 2,5 μm ($PM_{2,5}$) und der Gegenüberstellung der Resultate aus Proben, die in einer chinesischen Stadt (Peking) und einer mitteleuropäischen Stadt (Mainz, Deutschland), gesammelt wurden. In Kombination mit der Ultrahochleistungs-Flüssigkeitschromatographie (UHPLC) und der Elektrospray-Ionisierung (ESI) ist die UHRMS (Orbitrap-MS) in der Lage Tausende organische Verbindungen auf molekularer Ebene zu identifizieren. Vergleicht man die chemische Zusammensetzung von OA in Peking und Mainz, wurde im Rahmen dieser Arbeit beobachtet, dass OA in Peking ungesättigter ist und deutlich mehr aromatische Verbindungen enthält als OA in Mainz, ein deutlicher Hinweis auf höhere Beiträge aus Verbrennungsprozessen (z. B. Autoabgasemissionen) in der chinesischen Megacity. Ein weiterer Schwerpunkt der vorgelegten Studie bestand in der Identifizierung und dem Vergleich von OA, die in drei repräsentativen chinesischen Städten beprobt wurden. Dabei kam die im ersten Teil der Arbeit entwickelte UHPLC-Orbitrap-MS-Methode zum Einsatz. Die drei chinesischen Städte Changchun (CC), Shanghai (SH) und Guangzhou (GZ) befinden sich jeweils in den nordöstlichen, zentralen und südöstlichen Regionen Chinas. Die Ergebnisse zeigen, dass die wichtigsten organischen Verbindungen mit hohen Konzentrationen in allen Städten eine ähnliche chemische Charakteristik zeigen und aromatische Verbindungen dominieren, während OA in SH und GZ generell eine recht hohe Ähnlichkeit aufweisen. Im Vergleich zu OA in SH und GZ, zeigt sich OA in CC weniger hoch oxidiert und höher konzentriert bzgl. polyzyklischen aromatischen Verbindungen, wahrscheinlich hervorgerufen durch höhere Beiträge aus der Kohleverbrennung im Winter in Nordost-China. Schließlich wurde eine wichtige atmosphärische Substanzgruppe (Organosulfate (OSs)) in OA-Proben aus Peking und Mainz mit der UHPLC-Orbitrap MS-Methode analysiert und charakterisiert. Gemäß den Ergebnissen zur chemischen Zusammensetzung aus existierenden Simulationskammerexperimenten wurde ein Diagramm zur Vorhersage der OSs-Vorläufer erstellt. Basierend auf diesem Vorläuferdiagramm wird im Rahmen dieser Arbeit vorgeschlagen, dass OSs in Mainz hauptsächlich aus Isopren oder anderen kleinen Moleküken mit

einer Kohlenstoffatomzahl von weniger als fünf gebildet werden, während OSs in Beijing sowohl aus Isopren als auch aus anthropogenen Vorläufern (z. B. langkettige Alkane sowie Aromaten) erzeugt werden.

Zusammenfassend konnte gezeigt werden, dass die in dieser Arbeit entwickelte UHPLC-Orbitrap-MS-Methode zur Analyse der komplexen chemischen Zusammensetzung von OA geeignet ist. Die vorgelegte Arbeit bietet einen umfassenden Überblick über OAs in verschiedenen chinesischen Städten und ermöglicht ein besseres Verständnis ihrer chemischen Eigenschaften und der zugrundeliegenden Quellen.

# Abstract

Atmospheric aerosols are strongly related to air quality, global climate and human health. They influence the Earth's radiative balance directly by scatting and absorbing solar radiation and indirectly by nucleating cloud droplets. Aerosol particles can also have adverse effects to the human respiratory and cardiovascular systems. Within the last decades, China has experienced severe and persistent haze pollution with the fine particulate matter (PM) reaching unprecedentedly high levels across many cities, which is influencing the regional air quality and million people's health. Hence, understanding the chemical composition and sources of the PM during the haze events is essential for assessing the effects of polluted aerosols.

The aim of this work is to characterize the chemical composition of organic aerosol (OA) samples collected from different Chinese cities during the haze events in January 2014 based on ultrahigh resolution mass spectrometry (UHRMS) and to present a comprehensive overview of OA in Chinese urban regions. The first part of this study was the development of an analytical method to analyze the aerosol samples with diameters of PM ≤ 2.5 μm ($PM_{2.5}$) collected in a Chinese city (Beijing) and a central European city (Mainz, Germany). In combination with ultrahigh performance liquid chromatography (UHPLC), the UHRMS-Orbitrap technique coupled with electrospray ionization (ESI) was able to identify thousands of organic compounds at the molecular level. The comparison of the chemical composition of OA in Beijing and Mainz showed that OA in Beijing was more unsaturated and contained more aromatics than OA in Mainz, indicating that combustion emission (e.g., automotive exhaust emission) played a more important role in Beijing OA. The second part of this study focused on the identification and comparison of chemical components in OA collected from three representative Chinese cities using again the UHPLC-Orbitrap MS method. The three Chinese cities Changchun (CC), Shanghai (SH) and Guangzhou (GZ) locate, respectively, in the northeast, central east and southeast regions of China. The results showed that the major organic compounds with high concentrations in all cities had similar chemical composition and were dominant by aromatics, while OA in SH and GZ showed a higher similarity. Compared to the OA in SH and GZ, OA in CC obviously experienced less oxidation processes and contained more polycyclic aromatics, which were probably generated from the coal burning for the residential heating in winter in northeast China. Finally, an important organic species named organosulfates (OSs) in OA samples from Beijing and Mainz were characterized using the UHPLC-Orbitrap MS method. By summarizing the elemental composition information of OSs generated in previous OSs chamber simulation experiments, a diagram for the prediction of OSs precursors was created. Based on this OSs precursor diagram, OSs in Mainz OA is suggested to be mainly derived from isoprene or other small molecules with carbon atom number less than five, while OSs in Beijing OA was generated from both isoprene and anthropogenic precursors (e.g., long chain alkanes and aromatics).

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. This thesis offers a comprehensive overview about the molecular composition of OA in different Chinese cities, which helps to better understand their chemical characteristics and sources as well as provide the chemical database for haze control strategies in China.

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# 1 Introduction

## 1.1 Atmospheric aerosol

Atmospheric aerosols are defined as a suspension system of solid or liquid particles in air, with particle diameters in the range of $10^{-9}$-$10^{-4}$ m (Pöschl, 2005;Seinfeld and Pandis, 2006). They are ubiquitous throughout the atmosphere and play an important role in many environmental processes. Aerosol particles scatter and absorb solar and terrestrial radiation as well as serve as cloud condensation nuclei (CCN) and ice nuclei (IN) for could and precipitation formation, thereby directly or indirectly affecting the Earth’s radiative balance (Pöschl, 2005;Hallquist et al., 2009a). As a result, atmospheric aerosols play a central role in Earth’s climate and their contribution to the Earth’s radiative budget is progressively taken into account in the model calculations of the Intergovernmental Panel for Climate Change (IPCC) (Noziere et al., 2015). In addition, ambient aerosol particles have adverse effects on human health through damaging the respiratory and cardiovascular system or causing infectious and allergic diseases (Pöschl, 2005;Brüggemann, 2015;Pöschl and Shiraiwa, 2015).

The size of particles in the aerosols mainly depend on their formation mechanisms. Particles with diameters larger than 1 μm (coarse mode) are typically primarily generated in nature, which contribute largely to the mass of aerosol populations. Due to fast gravitational setting, their transport in the atmosphere is limited, resulting in short atmospheric lifetimes (Seinfeld and Pandis, 2006). However, these coarse particles 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 with diameters smaller than 1 μm (fine mode) are usually secondary in nature and contribute largely to the number and surface area of particle populations. The fine mode can be further classified into three different submicron size modes: accumulation mode (0.1-1 μm), Aitken mode (0.01-0.1 μm) and nucleation mode (< 0.01 μm) (Seinfeld and Pandis, 2006). It is noted that the nucleation and Aitken mode particles can grow fast through condensation or coagulation to the accumulation mode, which has the longest atmospheric lifetimes (Kulmala et al., 2016). Figure 1.1.1 shows an overview of the size range and composition of atmospheric particles and their corresponding source as well as the major types of multiphase chemical processes.

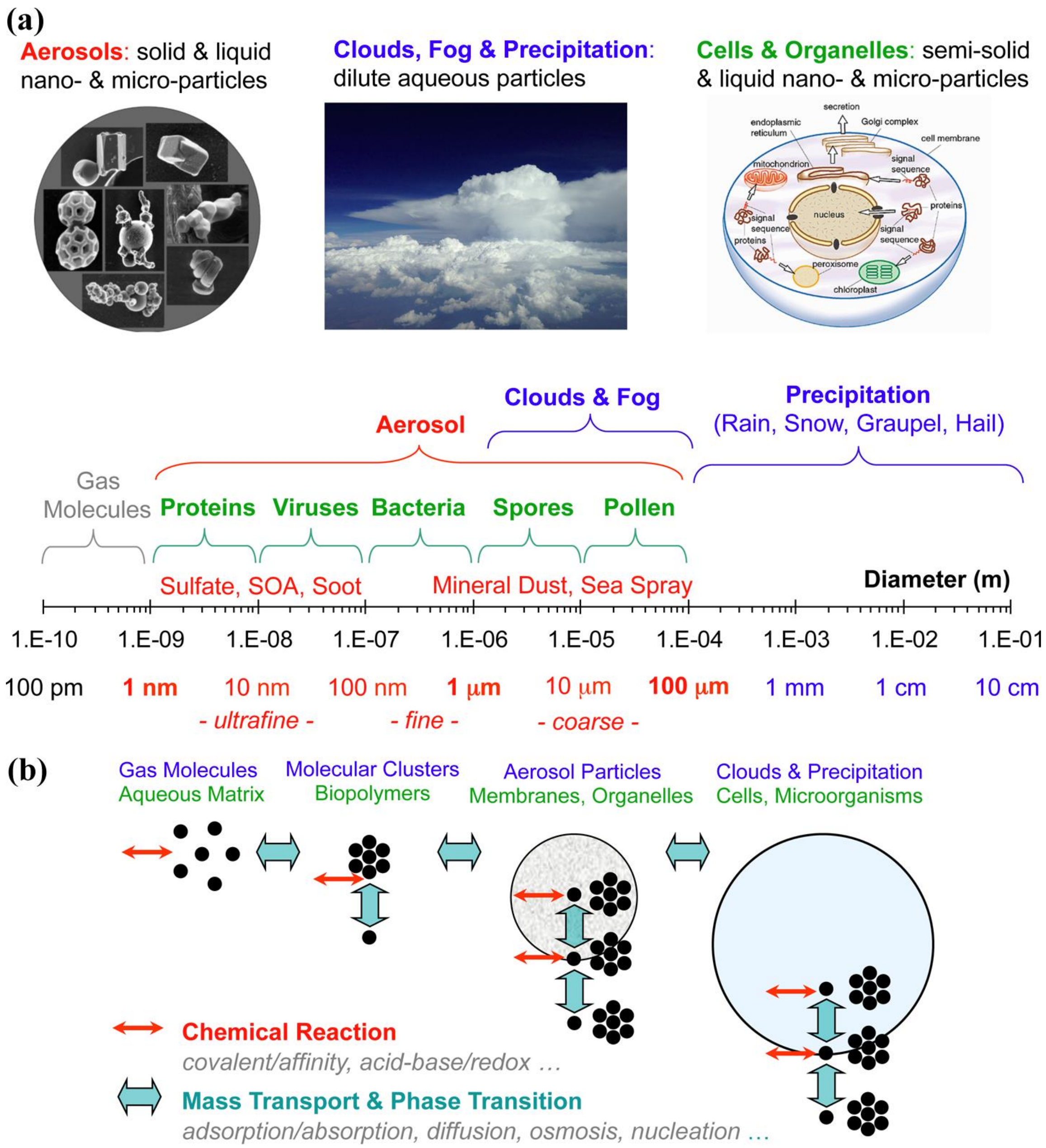

Figure 1.1.1: Overview of atmospheric particles: (a) Size range of aerosols, hydrometeors, cells and organelles. (b) Chemical reactions and mass transformation in the course of aerosol-cloud-precipitation interactions in the atmosphere (Pöschl and Shiraiwa, 2015).

According to the formation processes, atmospheric aerosols can be divided into two categories: primary aerosols are directly emitted into the atmosphere from natural or anthropogenic sources (e.g., sea spray, dust, biomass burning, volcanic eruption and fossil fuels combustion), whereas secondary aerosols are formed from precursor gases in the atmosphere through gas-to-particle conversion processes (e.g., nucleation, condensation and multiphase chemical reactions) (Seinfeld and Pandis, 2006). Figure 1.1.2 represents the formation, growth, and processing of atmospheric aerosols. Due to a wide variety of natural and anthropogenic sources as well as the complex multiphase chemical reactions, atmospheric aerosols represent a huge temporal and spatial variability in terms of chemical composition and size distribution. Atmospheric aerosols consist of complex mixtures of inorganics and organics. The inorganic components include sulfate, nitrate and ammonium, generated mainly through the oxidation and neutralization of sulfur dioxide ($SO_2$), nitrogen oxides ($NO_x$) and ammonia ($NH_3$) (Koo et al., 2003;Fu et al., 2016). Inorganic compounds in atmospheric aerosols have been fairly well understood and applied in different aerosol models, such as atmospheric chemistry global model (EMAC) (Aquila et al., 2011). However, the knowledge on the organic components is still very limited due to a variety of organic species in atmospheric aerosol, including hydrocarbons, alcohols, aldehydes, carboxylic acids, organosulfates and organonitrates (Jimenez et al., 2009;Rincón et al., 2012;Wang et al., 2018). The complexity of organic aerosol (OA) is compounded further by the fact that precursor gases or particles experience a series of atmospheric oxidation. Figure 1.1.3 shows an overview of the inorganic components and organic species in atmospheric aerosols in the Northern Hemisphere, observed using aerosol mass spectrometer (AMS) measurements.

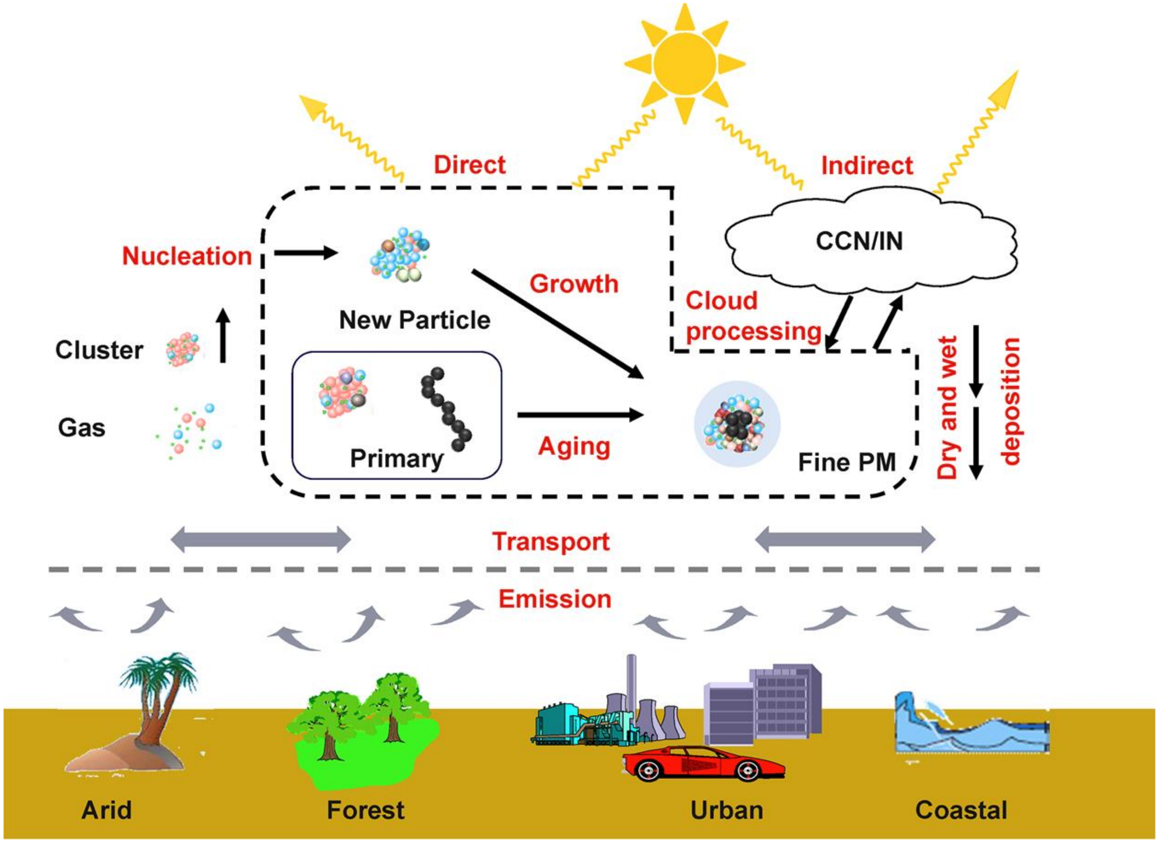

Figure 1.1.2: Schematic representation of the formation, growth and processing of atmospheric aerosols (Zhang et al., 2015).

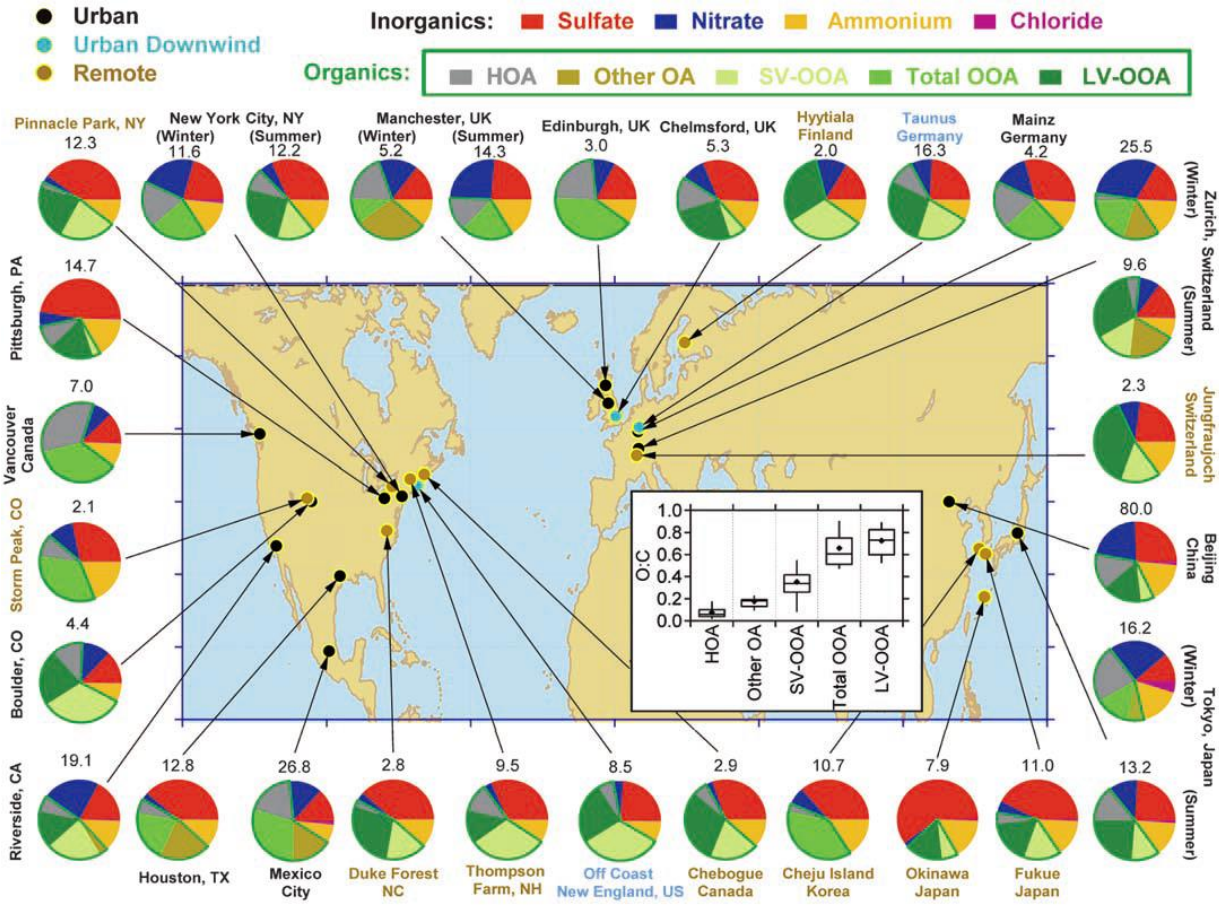

Figure 1.1.3: Total mass concentration (μg/m$^3$) and mass fractions of nonrefractory inorganic species and organic components in submicrometer aerosols at different surface locations on the Northern Hemisphere. Organic species are classified into hydrocarbon-like OA (HOA), semi-volatile oxygenated OA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

## 1.2 Secondary organic aerosol

OA constitutes 20-90% of the total submicron aerosols and is typically dominated by secondary organic aerosol (SOA) (Kroll and Seinfeld, 2008;Hallquist et al., 2009b). SOA is formed from a variety of biogenic and anthropogenic precursors through a series of complex photochemical gas and aqueous reactions. Depending on different global aerosol models, the SOA annual production rates vary from 13-119 teragrams per year (Tg/yr) and its lifetime is in the range of 5-15 days (Hodzic et al., 2016). Despite the importance of SOA effect on climate and public health, our knowledge about the chemical composition and formation mechanisms of SOA is still insufficient.

### *1.2.1 SOA formation*

The emission of volatile organic compounds (VOCs) into the atmosphere is a precondition for the formation of SOA. VOCs are organic chemicals that have a high vapor pressure at ordinary room temperature, including saturated, unsaturated and other substituted hydrocarbons. VOCs in atmosphere arise from both biogenic and anthropogenic emissions. On a global scale, the estimated budget of VOCs from biogenic emissions is 1150 teragrams of carbon per year (Tg C/yr), while anthropogenic VOCs budget (142 Tg C/yr ) is almost one order of magnitude smaller, however, they play a crucial role in urban atmospheric chemistry (Goldstein and Galbally, 2007). Among the biogenic VOCs, isoprene ($C_5H_8$), monoterpene ($C_{10}H_{16}$) and sesquiterpenes ($C_{15}H_{24}$) have the largest amount, which are naturally emitted from vegetation (Vogel, 2014;Brüggemann, 2015). The anthropogenic VOCs, such as alkanes and aromatic compounds, are mainly from fossil fuels combustion and biomass burning (IPCC report).

In general, SOA is formed when the VOCs in gas phase transforms to low-volatile organic compounds (LVOCs) in liquid or particle phase by the reaction with atmospheric oxidants, such as hydroxyl radical (OH), ozone ($O_3$) and nitrate radical ($NO_3$). Initially, an alkyl radical can be generated by the reaction of a VOC with $OH/NO_3/O_3$, which will be further oxidized with oxygen to produce an alkylperoxy radical After that, the alkylperoxy radical either reacts with organic peroxy and hydroperoxyl to produce alcohols and hydroperoxides, or with the presence of $NO_x$ it reacts with NO forming organic nitrates or alkoxy radical. The alkoxy radical can either result again in alky radical by isomerization and dissociation or form carbonyl with oxygen (Kroll and Seinfeld, 2008). Additionally, recent studies show that extremely low-volatile organic compounds (ELVOCs) can be formed through the further oxidation of alkylperoxy radicals by intramolecular hydrogen shifts followed by a rapid reaction with oxygen (Brüggemann, 2015;Jokinen et al., 2015;Mentel et al., 2015). Figure 1.2.1 shows a simplified mechanism for the atmospheric oxidation of VOCs and ELVOCs.

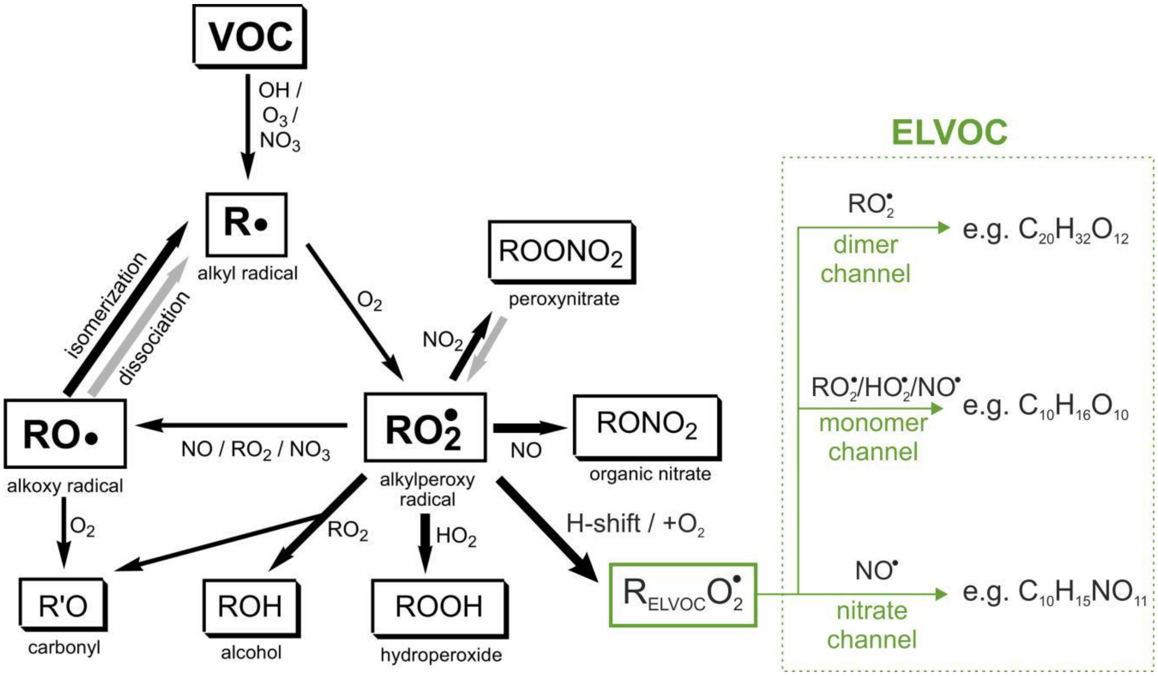

Figure 1.2.1: Simplified atmospheric oxidation mechanisms of VOCs and LVOCs. The black arrows denote reactions that can lead to a volatility decrease, whereas the gray arrows denote reactions that can lead to volatility increase ((Brüggemann, 2015).

## 1.3 Air pollution in China

### *1.3.1 Persistent haze events in China*

In recent years, China has experienced severe and persistent particulate air pollution accompanying with rapid industrialization and urbanization (Huang et al., 2014;Song et al., 2017). For example, the haze events happened in the first quarter of 2013 affecting around 1.3 million km$^2$ territories and 800 million people in China (Huang et al., 2014). The measurements of $PM_{2.5}$ (particulate matter with an aerodynamic diameter less than 2.5 μm) concentrations at 74 major Chinese cities in January 2013 showed that the daily average concentrations of $PM_{2.5}$ exceeded the Chinese air quality standards of 75 μg/m$^3$ (around twice higher compared to the US EPA standards of 35 μg/m$^3$), with a record-breaking daily concentration of 772 μg/m$^3$) (Huang et al., 2014). Figure 1.3.1 shows the annual average $PM_{2.5}$ concentrations in eastern China in 2014. Such extremely acute air pollution is not only influencing the regional air quality and human health in China, but also leading to a global environment problem in some case by long-time and long-distance transport of pollutants from China. In response to these severe air pollution events, several significant efforts have been implemented by the Chinese government to tackle the air pollution and protect the public health, such as upgrading the quality of gasoline and diesel for vehicles, reducing the production of steel and of coal-fired electricity, and encouraging the investments on environmentally-friendly energy (e.g., wind and solar power). On 10th September of 2013, the Chinese government promulgated the "Air Pollution Prevention and Control Action Plan" baked by US $277 billion investments from the central government aiming to reduce the $PM_{2.5}$ concentrations in the three key regions, namely, the Beijing-Tianjian-Hebei (BTH) region with around 110 million population, the Yangtze River Delta (YRD) region with 150 million population, and the Pearl River Delta (PRD) region with about 50 million residents, by 25%, 20% and 15% as compared to the 2012 level (Huang et al., 2014;Zheng et al., 2017).

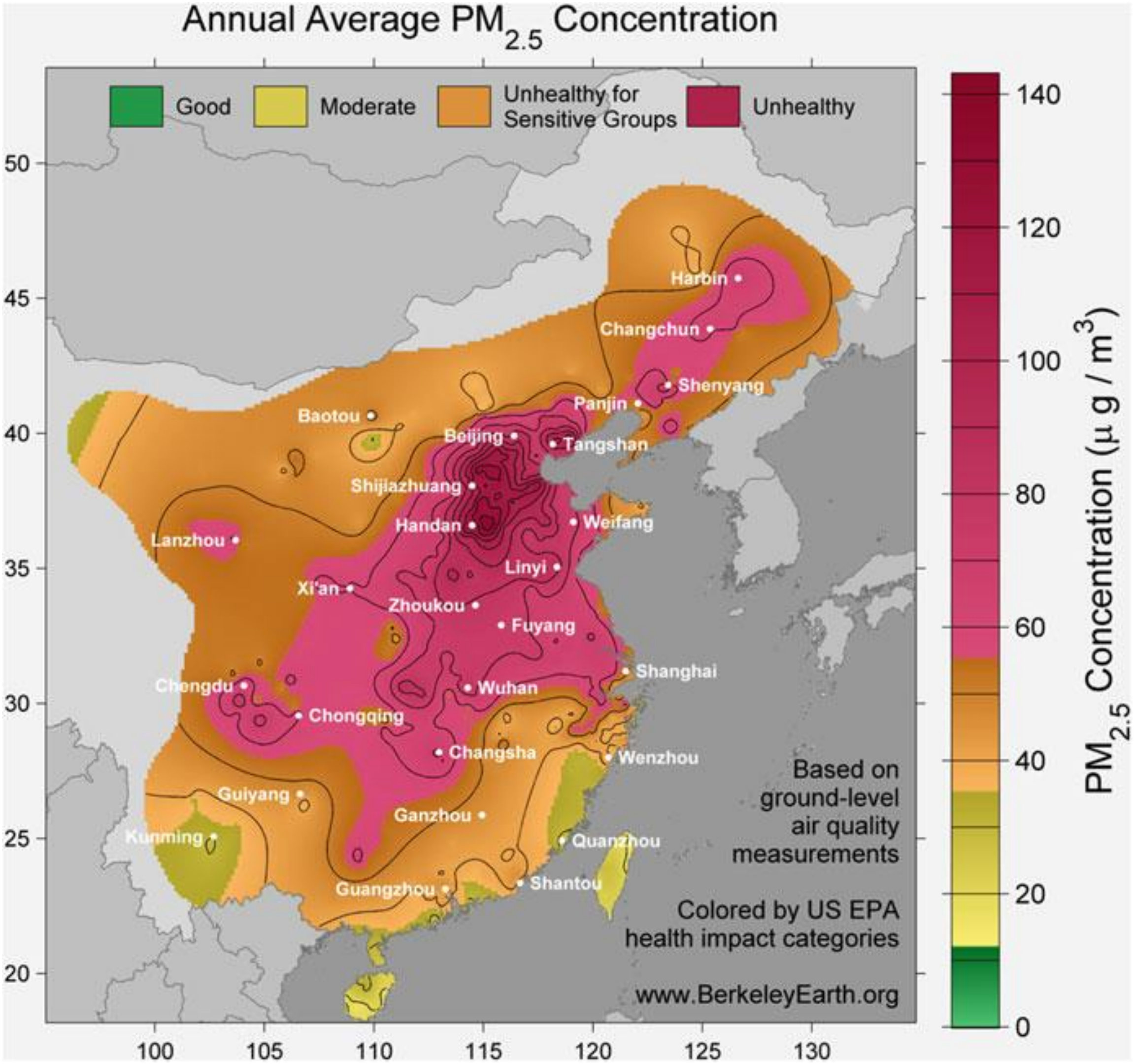

Figure 1.3.1: Annual average $PM_{2.5}$ concentrations in eastern China in 2014 measured by the Berkeley Earth based on ground-level measurements made at 27 monitoring stations in China (Bouarar et al., 2017).

### 1.3.2 Chemical composition of particulate matter during haze pollution in China

The chemical composition and sources of particulate matter (PM) in atmospheric aerosols in China are extremely complex and vary according to different locations resulting from the diverse human activities and inter-regional air pollutant transport. PM consists of a highly complex mixture of organic and inorganic components produced from both biogenic and anthropogenic sources, which has been outlined in section 1.1. Despite the relatively higher PM concentrations in China, numerous aerosol studies show that the PM compositions in Chinese cities are similar with those in urban areas of USA and European cities, which mainly consist of organic matter (OM) followed by secondary sulfate ($SO_4^{2-}$), nitrate ($NO_3^-$), ammonium ($NH_4^+$), and elemental carbon (EC) (Zhang et al., 2015;Bouarar et al., 2017). Measurements of $PM_{2.5}$ samples collected at 14 Chinese cities in January and June 2003 by Cao et al. show the following profile of chemical compositions (see Figure 1.3.2): OM (25-45%), $SO_4^{2-}$ (12-24%), $NO_3^-$ (2-14%), $NH_4^+$ (6-11%) in wintertime; and OM (26-41%), $SO_4^{2-}$ (14-22%), $NO_3^-$ (3-8%), $NH_4^+$ (1-7%) in summertime. These results also present the regional and seasonal variation in terms of PM concentration and relative contribution of individual species. Recently, Huang et al. investigated the chemical nature and sources of $PM_{2.5}$ collected at urban regions in four Chinese cities during the severe haze pollution events of January 2013 (Huang et al., 2014). It shows that OM constitutes the major fraction (30-50%) of the total $PM_{2.5}$ in the four cities, followed by $SO_4^{2-}$ (8-18%), $NO_3^-$ (7-14%), $NH_4^+$ (5-10%), EC (2-5%) and chloride (2-4%) (see Figure 1.3.3). This study also showed that the severe haze pollution events were driven to a large extent by secondary aerosol formation, contributing 30-77% and 44-71% of $PM_{2.5}$ and organic aerosol, respectively. Compared to relatively comprehensive identification of inorganic compounds in atmospheric aerosols, OM is much more complex and only around 10-30% of particulate OM has been chemically specified so far (Hoffmann et al., 2011). Studies on OM in China mainly focus on the quantification of organic acids, carbonyls, anhydrosugars, polycyclic aromatic hydrocarbons (PAHs) and their derivatives (Bouarar et al., 2017). However, due to the important effect of OM on Earth climate and human health, more efforts need to be made to further identify the OM and clarify the OM profile of chemical composition.

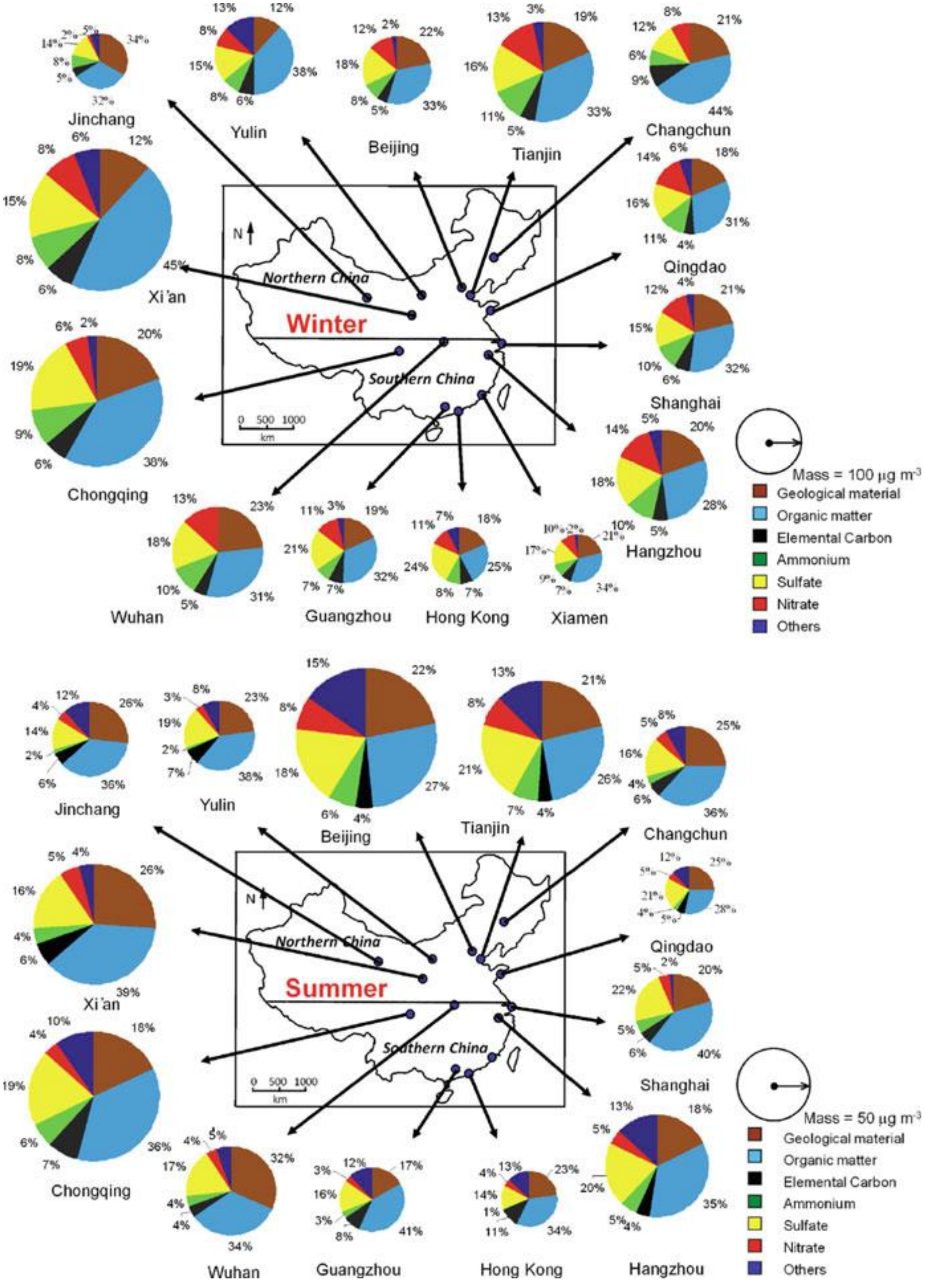

Figure 1.3.2: Chemical composition of $PM_{2.5}$ in wintertime and summertime in 14 Chinese cities (Cao et al., 2012).

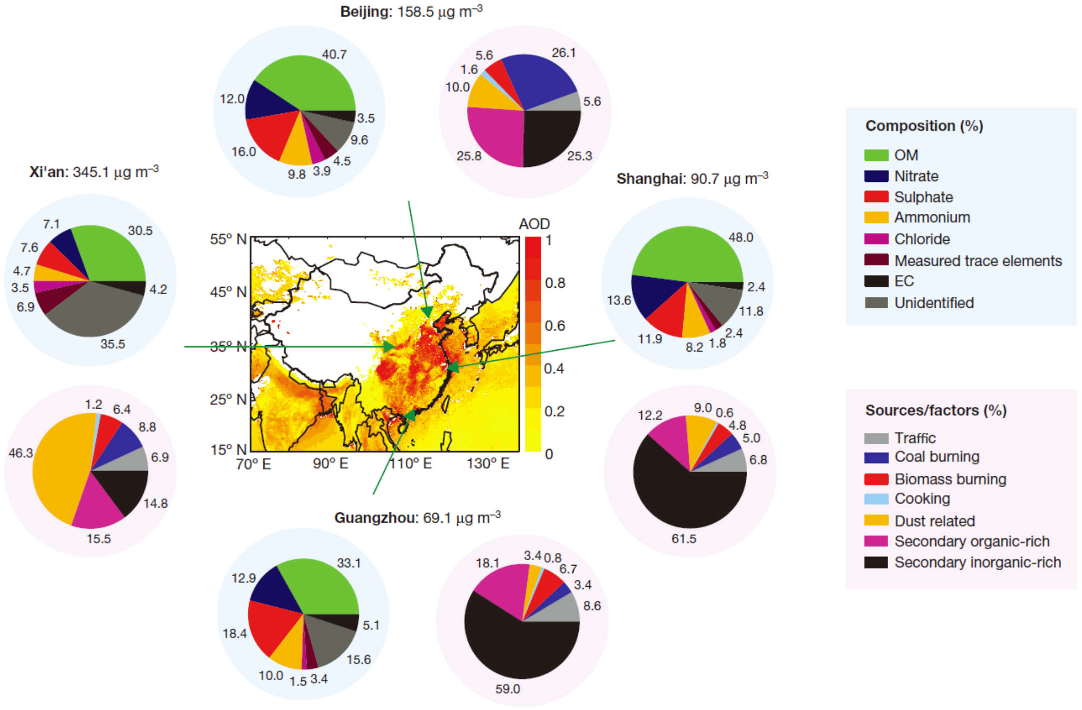

Figure 1.3.3: Chemical compostition and source apportionment of $PM_{2.5}$ collected druring the high pollution events in January 2013 at the urban regions of four Chinese cities: Beijing, Shanghai, Guangzhou and Xi'an (Huang et al., 2014).

## 1.4 Mass spectrometry in aerosol research

Mass spectrometry (MS) is the most commonly applied technique for the chemical analysis of PM in atmospheric aerosols, providing high sensitivity and selectivity to individual chemical compounds (Farmer and Jimenez, 2010;Vogel, 2014;Brüggemann, 2015). Generally, the MS techniques can be classified into online and offline techniques: online techniques commonly operate in or near real time with a time resolution of 0.1 s to 1 h (Brüggemann, 2015), providing the ability to examine chemical changes during the process of aerosol formation on short timescales as well as avoid potential artifacts associated with offline analysis methods (Pratt and Prather, 2012). However, the information of chemical compositions observed by the online techniques is normally less specific compared to those obtained by offline techniques, which require sample collection but provide detailed molecular speciation (Pratt and Prather, 2012). In particular, offline mass spectrometry utilizing high resolution mass analyzers is recently used for aerosol research, which allows the characterization of complex organic mixtures at the molecular level (Nizkorodov et al., 2011). In the following a brief introduction of the applied MS technique in this thesis is displayed. A more detailed description of the current status of MS techniques used for the chemical analysis of atmospheric aerosol can be found in the recently published reviews by Pratt and Prather (2012a, 2012b), Nizkorodov (2011) and Laskin (2018).

### *1.4.1 Electrospray ionization*

Atmospheric pressure ionization (API) methods have become indispensable tools in analytical chemistry as well as in aerosol research (Müller-Tautges, 2014;Laskin et al., 2018). Compared to the "hard" techniques such as electron ionization (EI) and chemical ionization (CI), the API techniques are much softer and suitable for the analysis of non-volatile, medium to highly polar and thermally unstable compounds (Rosenberg, 2003). Based on the formation of ionization spray, API techniques can be classified into electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), and atmospheric pressure photoionization (APPI). Among the three API techniques, ESI is the most widely used for targeting both biomolecules and small molecules (see Figure 1.4.1). In last twenty decades, various MS techniques have been developed for aerosol measurements based on the ESI technique (Noziere et al., 2015;Laskin et al., 2018).

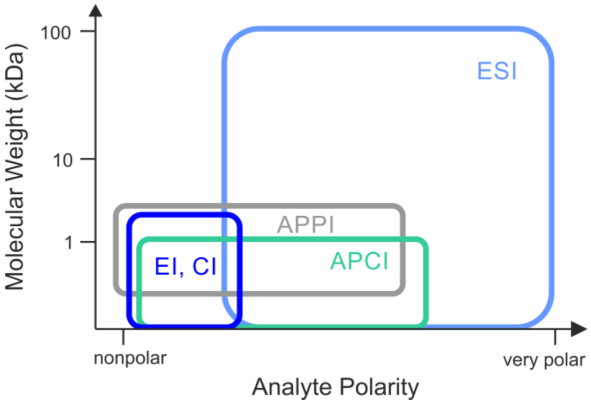

Figure 1.4.1: Application range of different ionization techniques as function of analyte polarity and molecular weight (Müller-Tautges, 2014).

ESI technique is based on the formation of gaseous ions from a mist of electrically charged droplets in an electric field (Müller-Tautges, 2014). In general, the ESI process involves the following three steps: (1) dispersal of a fine spray of electrically charged droplets, followed by (2) the evaporation of solvent and (3) the formation of gaseous ions (see Figure 1.4.2) (Ho et al., 2003). Within an ESI source, the analyte solution is pumped through a metal spray capillary (around 10 µm in diameter) with a low flow rate of 0.1-10 µL/min. A high voltage (2-5 kV) in negative or positive mode is applied on the tip of the spray capillary, which can provide the electric field gradient to produce charge separation on the surface of the liquid droplets. As a result, the liquid protrudes from the tip of the capillary forming the “Taylor cone”. Then, the charged droplets that comprise the Taylor cone can be accelerated towards or away from the counter electrode, according to their charge in the electric field. With the aid of a sheath gas stream (usually nitrogen gas) and an elevated ESI source temperature, the solvent in the charged droplets is continuously evaporated resulting in the decrease of the droplet size and increase of the 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 eject smaller droplets, which is called droplet jet fission process. Accompanying with the successive droplet jet fission process, the charged droplets are getting more and more smaller and finally converted to gaseous ions by two different models: (1) the ion emission model (IEM) assumes that the emission of ions from the highly charged droplet, which is commonly used for describing the ionization of small molecules. (2) the charge residue model (CRM) assumes that the increased charge density through desolvation causes the successive decrease of the droplet size and eventually a single ionized molecule is produced. This model is suited for describing the ionization of large molecules (Cech and Enke, 2001;Müller-Tautges, 2014). The typical ions generated in ESI source are deprotonated ions ($[M-H]^-$ with M = parent molecule) in negative mode and protonated ions ($[M+H]^+$ or adducts ($[M+Na]^+$ and $[M+NH_4]^+$) in positive mode.

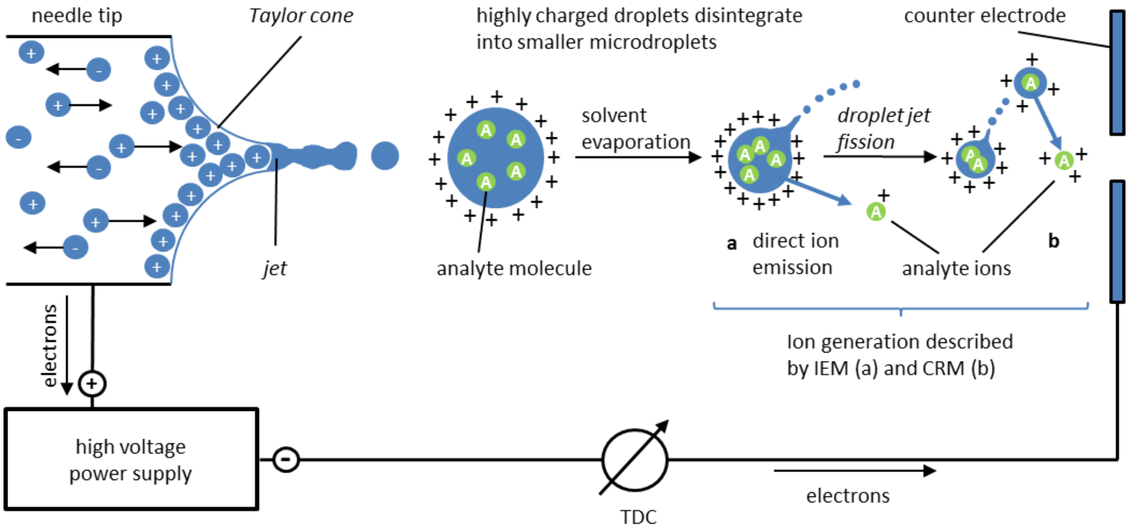

Figure 1.4.2: Schematic illustration of electrospray ionization process with ion emission model (IEM) and charge residue model (CRM) (Müller-Tautges, 2014).

### 1.4.2 High resolution mass spectrometer

High resolution mass spectrometry (HRMS) or ultrahigh resolution mass spectrometry (UHRMS) is a powerful tool for molecular-level chemical analysis with two outstanding features of high resolution and high mass accuracy (Stock, 2017;Laskin et al., 2018). There are three major types high resolution analyzers: the high resolution quadrupole time-of-flight (HR-qTOF), the Orbitrap and the Fourier transform ion cyclotron (FTICR). HR-qTOF instruments have a relatively low resolving power of up to 40,000 at mass range of m/z 100-500. Orbitrap instruments have shown the resolving power in excess of 1,000,000 at m/z < 300-400 within a 3s detection time which makes it compatible with several types of chromatographic separations. FTICR represents the best resolution power with a record resolution of 40,000,000 at m/z 609 at a magnetic field of 7 T (Noziere et al., 2015). In last decade, UHRMS coupled with the soft ionization sources (e.g., ESI and APCI) has been applied for the identification of chemical composition in atmospheric aerosol (Nizkorodov et al., 2011;Lin et al., 2012a;Lin et al., 2012b;Rincón et al., 2012;Kourtchev et al., 2014;Noziere et al., 2015;Kourtchev et al., 2016;Wang et al., 2016;Wang et al., 2017;Laskin et al., 2018;Wang et al., 2018), which allows the unambiguous characterization of thousands of organic compounds by determination of the corresponding elemental compositions, as can be seen in Figure 1.4.3.. In this study, the Orbitrap instrument is used for the chemical analysis of OA and described in the following chapter.

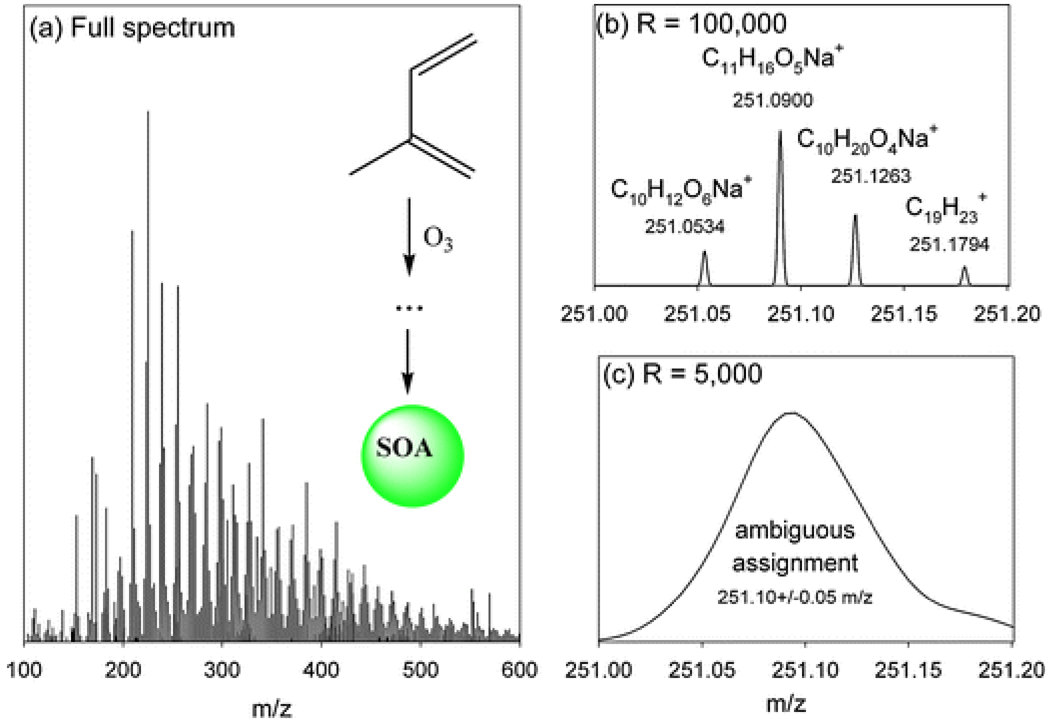

Figure 1.4.3: (a) positive mode ion mode ESI-MS spectra for isoprene/ozone SOA. (b) zooms in on peaks near m/z 251 recorded at the Orbitrap resolving power of R = 100,000. (c) shows how the same mass range would loo like if recorded at a typical resolution power of reflection-TOF instrument with R = 5000 (Nizkorodov et al., 2011).

### *1.4.2.1 Q-Exactive hybrid quadrupole-orbitrap mass spectrometer*

The Orbitrap MS is a modification of the Kingdon trap which was already developed in the early 1920s and debuted in mainstream MS as an accurate and compact mass detector in 2005 (Zubarev and Makarov, 2013). In this study, the Orbitrap instrument called Q-Exactive hybrid quadrupole-orbitrap mass spectrometer (built by Thermo Fisher Scientific in 2011) was applied, which has a maximum resolution of 140,000 at m/z 200 and a mass accuracy lower than 3 ppm (external calibration) or 1 ppm (internal calibration). Figure 1.4.4 shows the schematic of the Q-Exactive hybrid quadrupole-orbitrap mass spectrometer. The ions generated in the ionization source (1, ESI or APCI) are focused by a lens stack (2) and further transmitted by a bent flatapole (3) to a quadrupole (4) for optional parent ion selection. Subsequently, the ions enter a covered linear trap (C-trap, 5), where they are accumulated and loose their kinetic energy in collisions with nitrogen bath gas. After that, the ions either are directly injected into the Orbitrap analyzer (6) for detection or into the high energy collisional dissociation cell (HCD, 7) for fragmentation as MS$^2$

analysis. The fragmented product ions are again collected in the C-trap and then injected into the Orbitrap analyzer (Scigelova and Makarov, 2006;Müller-Tautges, 2014).

The Orbitrap consists of a spindle-like central electrode and an outer barrel-shaped electrode, which is isolated into two halves by a ceramic ring (see Figure 1.4.4). The ions from the C-trap are injected into the Orbitrap essentially perpendicular to the z-axis and trapped the electrostatic field between the central and outer electrodes. The ions are forced to a rotational movement toward the central electrode while the tangential velocity creates an opposing centrifugal force, which is like the trajectory of a planet in the solar system. At the same time, the ions have an axial oscillation along the axis of the central electrode caused by the axial electrostatic field gradient due to the special shape of electrodes. The frequency ($\omega_{axial}$) of the axial oscillation only depends on the m/z ratios of the ions and the instrumental constant k regardless of the tangential velocity as described by equation 1.4.1:

$$\boldsymbol{\omega_{axial} = \sqrt{k\left(\frac{z}{m_i}\right)}} \tag{1.4.1}$$

The image current produced by the oscillating ions is detected and multiplied and finally converted to a mass spectrum by fast Fourier transformation (Scigelova and Makarov, 2006;Zubarev and Makarov, 2013).

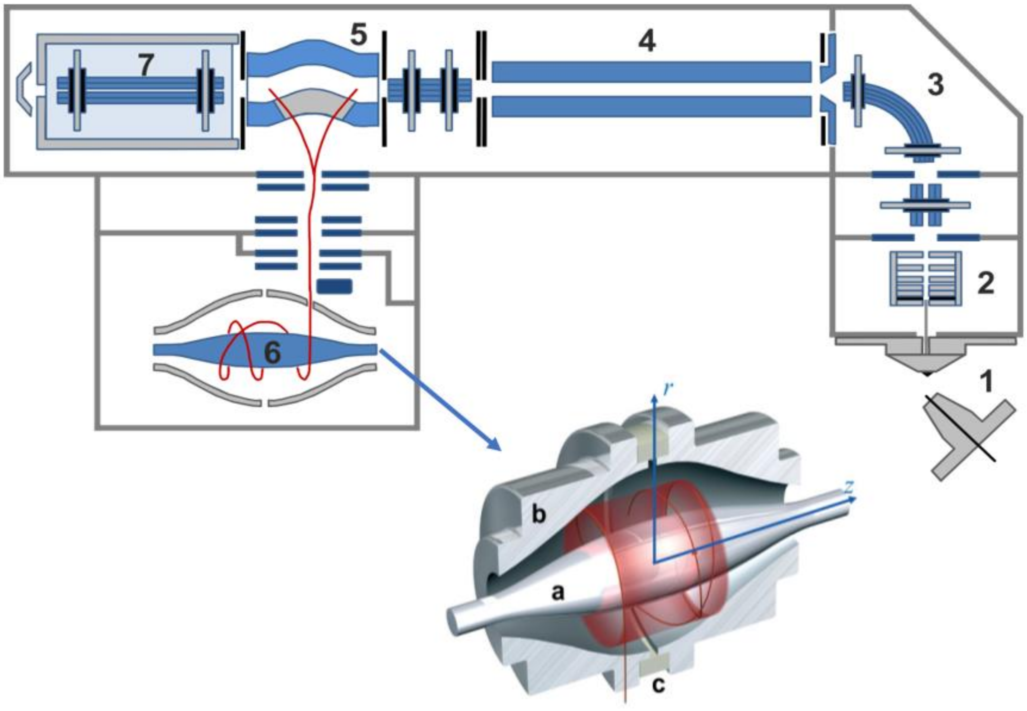

Figure 1.4.4: Schematic view of the Q Exactive hybrid quadrupole-orbitrap mass spectrometer including the following components: (1) the ion source region (2) lens stack (3) bent flatapole, (4) quadrupole (5) C-trap (6) orbitrap and (7) HCD cell. The inset depicts the cross section of Orbitrap consisting 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).

## 1.5 Thesis objectives and outline

Ambient aerosols represent a highly complexity with thousands of different compounds due to various biogenic and anthropogenic sources as well as complex multiphase chemical reactions. In particular, organic compounds in OA cover a very large chemical space with respect to molecular mass, functional group distribution and polarity at a trace level concentration. Therefor, a comprehensive characterization of OA is a challenging analytical task. Over the past decade, China, the world’s second largest economy with ~1/6 of the total world population, has experienced sever air pollution particularly in megacities and urban complexes. Since the OA has the profound impacts on human health and ecosystems, a better understanding of the chemical composition, sources and atmospheric processes of OA in Chinese urban regions is getting more and more important.

The aim of this work is to identify the elemental compositions of organic compounds in $PM_{2.5}$ collected in Chinese cities using the UHPLC-Orbitrap technique. Based on the identified elemental compositions, the chemical properties (e.g., oxidation state, unsaturation degree and aromaticity index) and possible sources of $PM_{2.5}$ in different cities have been compared and discussed. This work can be described in three parts as follows:

1. The first part focuses on the analytical method development for OA measurement and the comparison of chemical composition of OA in a European city (Mainz, Germany) and a Chinese city (Beijing). A solvent mixture of acetonitrile and water was used for the OA extraction and Orbitrap coupled with ultra-high-performance liquid chromatography (UHPLC) was applied for detection, where UHPLC technique is efficient for isomer separation and reducing the ion suppression. Since the natural sources and human activities strongly influence the OA properties, $PM_{2.5}$ samples collected from Mainz (a city within the Rhine-Main area, the third largest metropolitan region in Germany with more than 5.8 million population) and Beijing (the capital of China with more than 20 million residents) were analyzed and their chemical properties and related sources were compared.
2. In the second part, we characterized the chemical composition of organic compounds in $PM_{2.5}$ samples from three Chinese cities using UHPLC-Orbitrap MS method developed in first part of the work. The three Chinse cities are Changchun (CC), Shanghai (SH) and Guangzhou (GZ), which are located, respectively, in the northeast, central east and southeast regions of China with around 50 million population in total. Characteristics of OA in these three Chinese megacities including the molecular weight, number of isomers, degrees of oxidation and unsaturation were analyzed and compared.
3. In the third part, we created a 'OSs precursor map' by summarizing the elemental composition of OSs generated in several smog chamber experiments. Then, according to this 'OSs precursor map', we estimated the possible sources and molecular structures of OSs in the ambient $PM_{2.5}$ samples, which were collected in Beijing and Mainz and analyzed by UHPLC-Orbitrap MS.

# 2 Analytical method development and chemical characterization of urban OA using ultrahigh resolution mass spectrometry

This chapter is a reprint of the article:

Kai Wang, Yun Zhang, Rujin Huang, Junji Cao, and Thorsten Hoffmann

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

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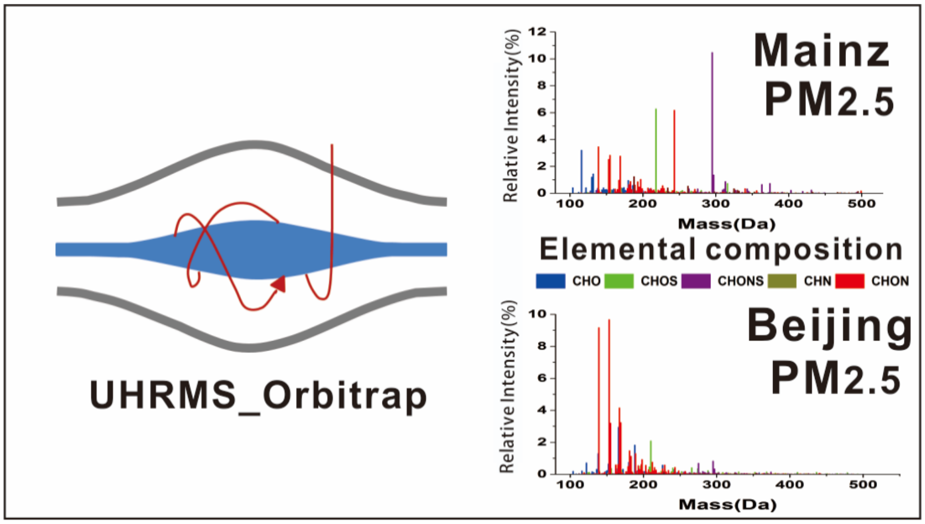

**Abstract.** Fine urban aerosol particles with aerodynamic equivalent dimeter ≤ 2.5 μm ($PM_{2.5}$) were collected in Mainz (a city within the Rhine-Main area, the third largest metropolitan region in Germany) and Beijing (Chinese megacity). A solvent mixture of acetonitrile-water was used to extract 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 ($X_C$) 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., 2009a). 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;Noziere 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;Noziere 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 (Noziere et al., 2015). Due to the high mass resolving power (≥40000) and high mass accuracy (≤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 $PM_{2.5}$, leads to 3.3 million premature deaths per year worldwide, predominantly in Asia (Lelieveld et al., 2015). The yearly mass concentrations of $PM_{2.5}$ often exceed the WHO guideline concentration of 10 $\mu g\ m^{-3}$, 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, $PM_{2.5}$ 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 $PM_{2.5}$ 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 $m^{-3}$ (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 $m^{-3}$ (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 $m^{-3}$ (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 $m^3$ $min^{-1}$, 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 $min^{-1}$. 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 $cm^2$, corresponding to around 600 µg 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 μm 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 μL 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 µm 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 µL min$^{-1}$. 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 μL.

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®, 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 $1\times10^5$ 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 ±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. (1) for elemental composition $C_cH_hO_oN_nS_sCl_x$:

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

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):

$$X_C = \frac{3(\mathrm{DBE} - (\mathrm{m}N_O + nN_S)) - 2}{\mathrm{DBE} - (\mathrm{m}N_O + nN_S)} \tag{2}$$

where ‘m’ and ‘n’ correspond to a fraction of oxygen and sulfur atoms in π-bond structure of a compound, which varied depending on the compound. If $\mathrm{DBE} \le mN_O + nN_S$ or $X_C \le 0$, 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 π-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 (3-6) (Lin et al., 2012a):

$$MW = \sum MW_i / \sum N_i \tag{3}$$

$$H / C = \sum H / C_i / \sum N_i \tag{4}$$

$$\mathrm{O}/ C = \sum \mathrm{O}/ C_i / \sum N_i \tag{5}$$

$$DBE = \sum DBE_i / \sum N_i \tag{6}$$

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

## 2.3 Result 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/$H_2O$ 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 μg/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[a] | Number of formulas[b] | % | 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 |

[a] Values in the parentheses are the percentage of peaks that can be assigned with unambiguous fomulas.

[b] Values in the parentheses are the percentage of different subgroups among the assigned reasonable formulas.

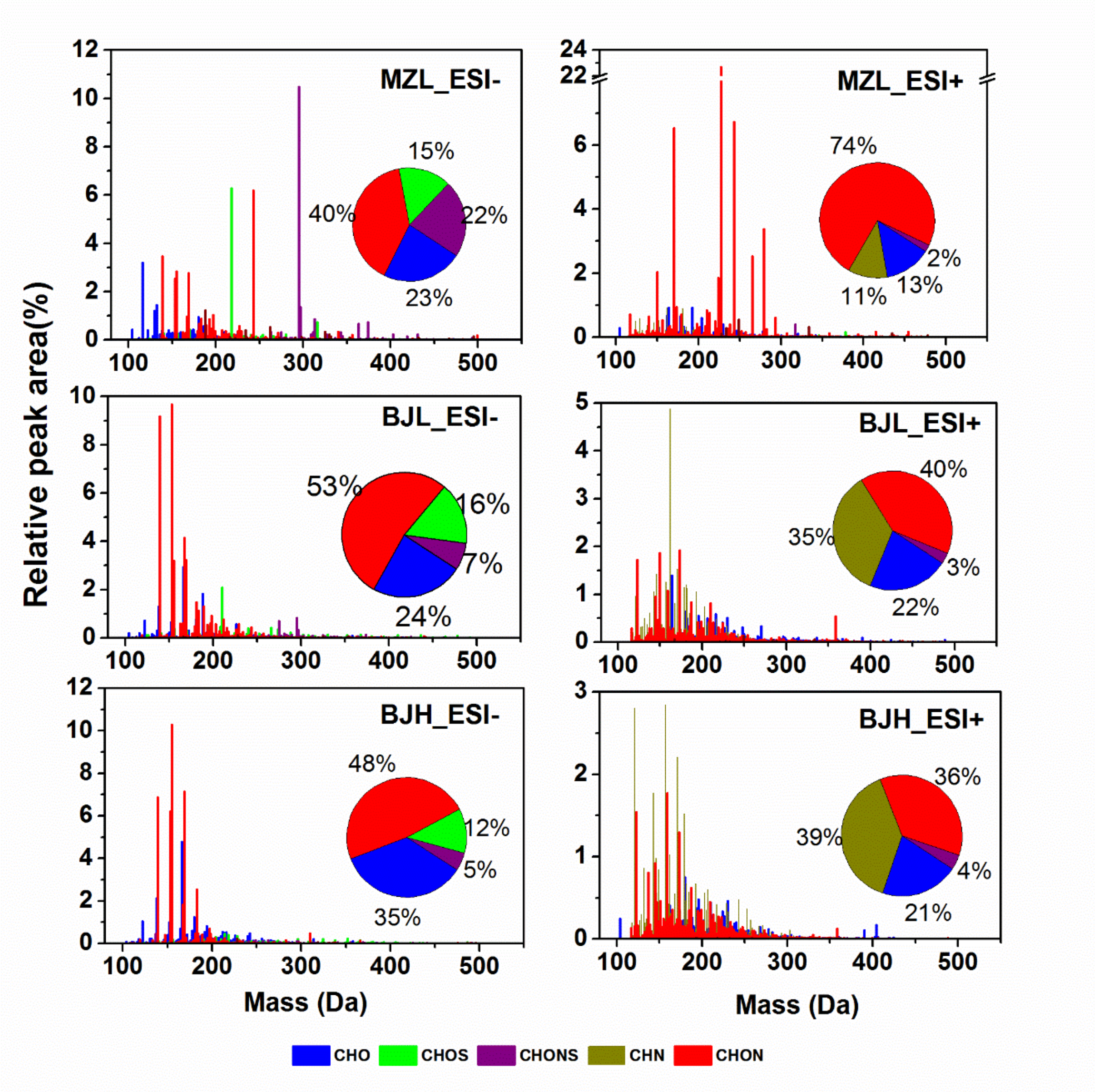

Figure 2.3.1: Mass spectra of detected organic compounds in ESI- and ESI+. The pie chats are proportional to the peak areas of an organic compound subgroup in each sample.

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 ($OS_c$) 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 (≥ 1.5) and low O/C ratios (≤ 0.5) (area A in Figure 2.3.2) and low-oxygen-containing aromatic hydrocarbons with low H/C ratio (≤ 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 ($X_C \geq 2.5$) and condensed aromatics ($X_C \geq 2.7$) (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.

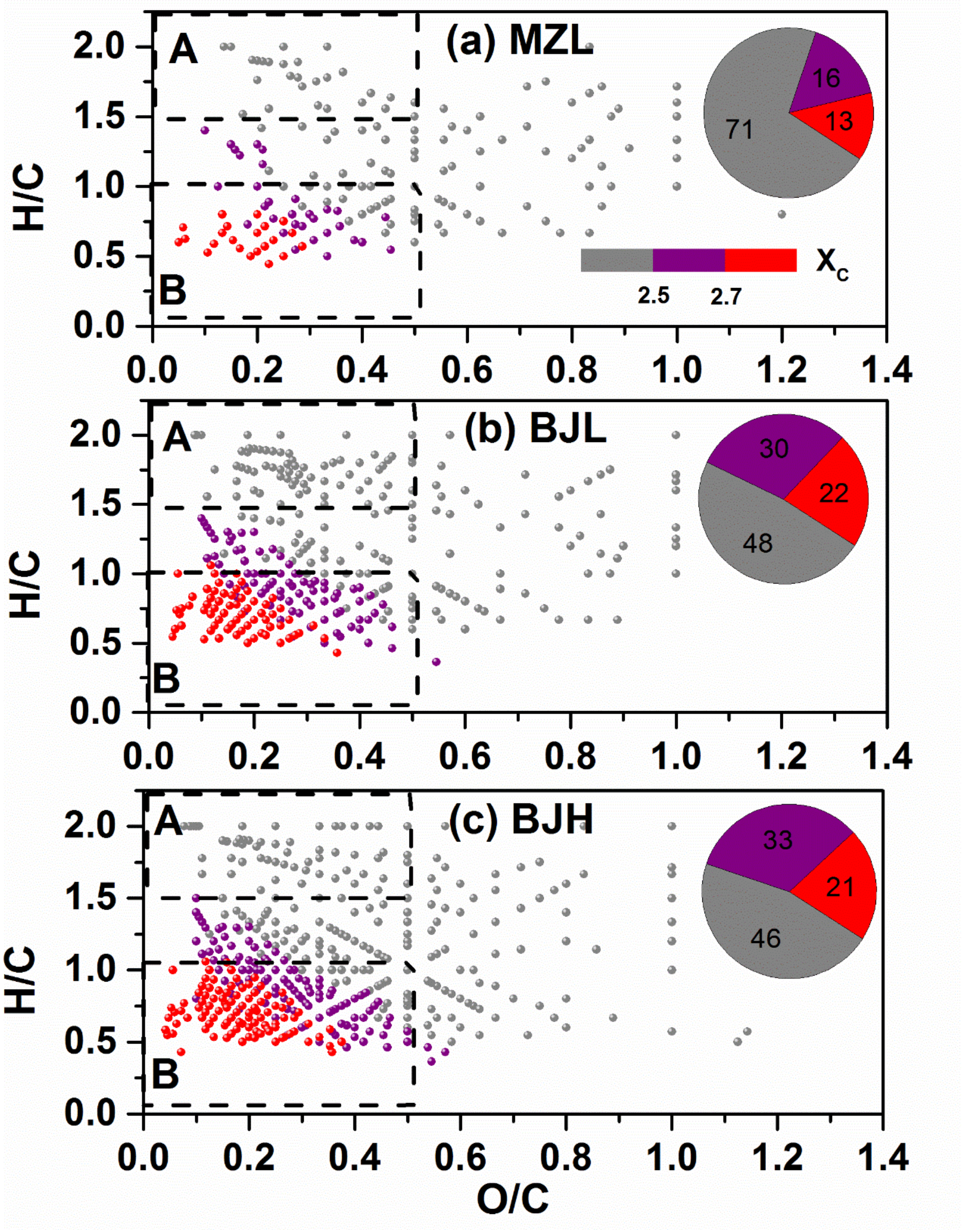

**Figure 2.3.2:** The van Krevelen diagram for CHO compounds detected in ESI- mode. Areas 'A' and 'B' refer to aliphatic compounds and low-oxygen-containing aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity equivalent (gray with $X_C < 2.50$, purple with $2.50 \leq X_C < 2.70$ and red with $X_C \geq 2.70$). 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. (7).

$$OS_C \approx 2\,O/C - H/C \tag{7}$$

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.

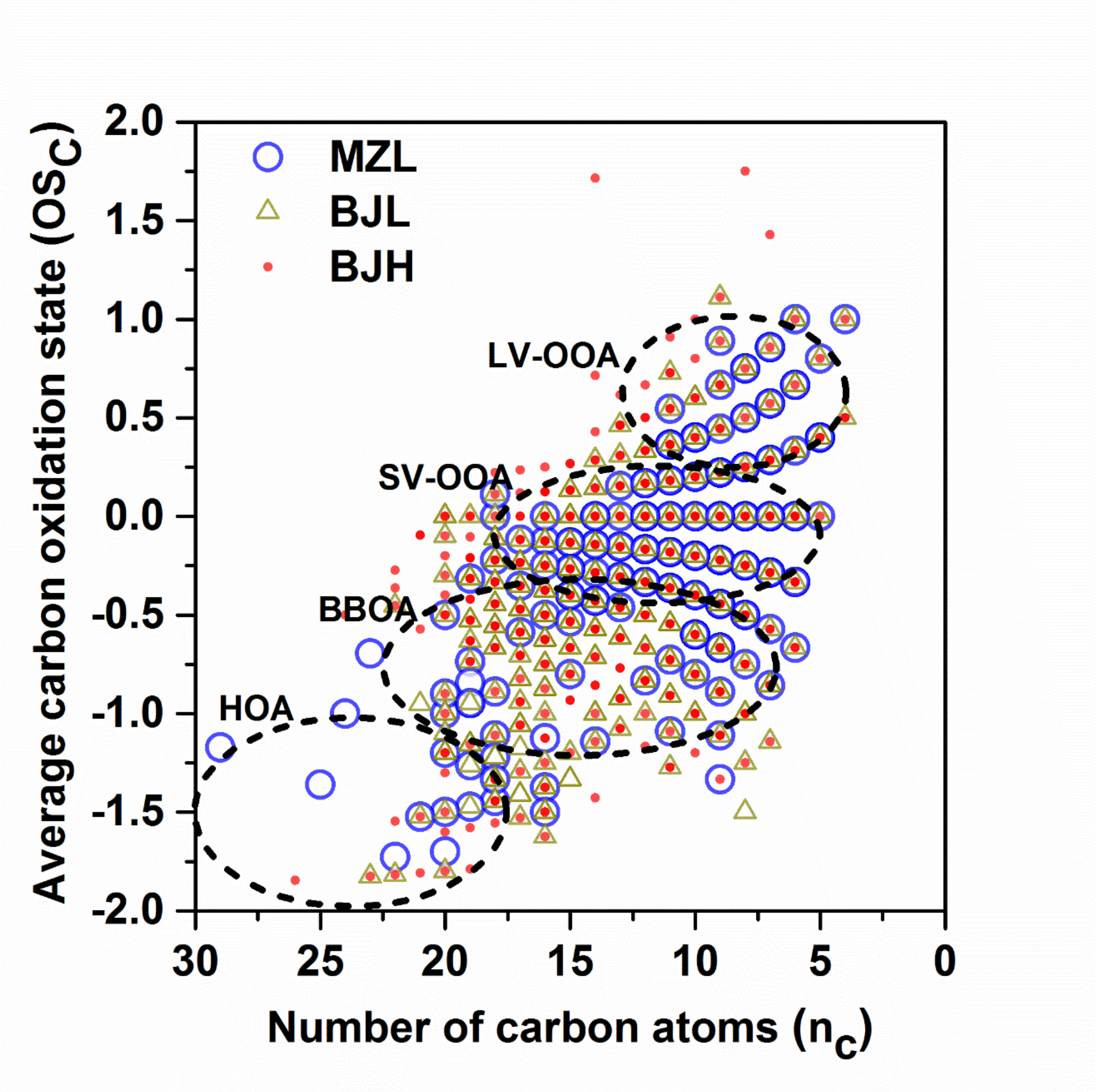

**Figure 2.3.3:** Carbon oxidation state plots for CHO compounds detected in ESI- mode. The black dash ovals area marked as HOA, BBOA, SV-OOA and LV-OOA correspond to hydrocarbon-like organic aerosol, biomass burning organic aerosol, semivolatile and low-volatility organic aerosol.

### *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., 2010b;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 ≥ 3, which are preferentially observed in ESI- mode, likely associated with the nitrooxy ($-ONO_2$) or oxygenated nitrooxy group (O/N ≥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 (-$NH_2$) functional groups and which have been identified in biomass burning and fossil fuel combustion emissions (Mace, 2003;Barbaro et al., 2011).

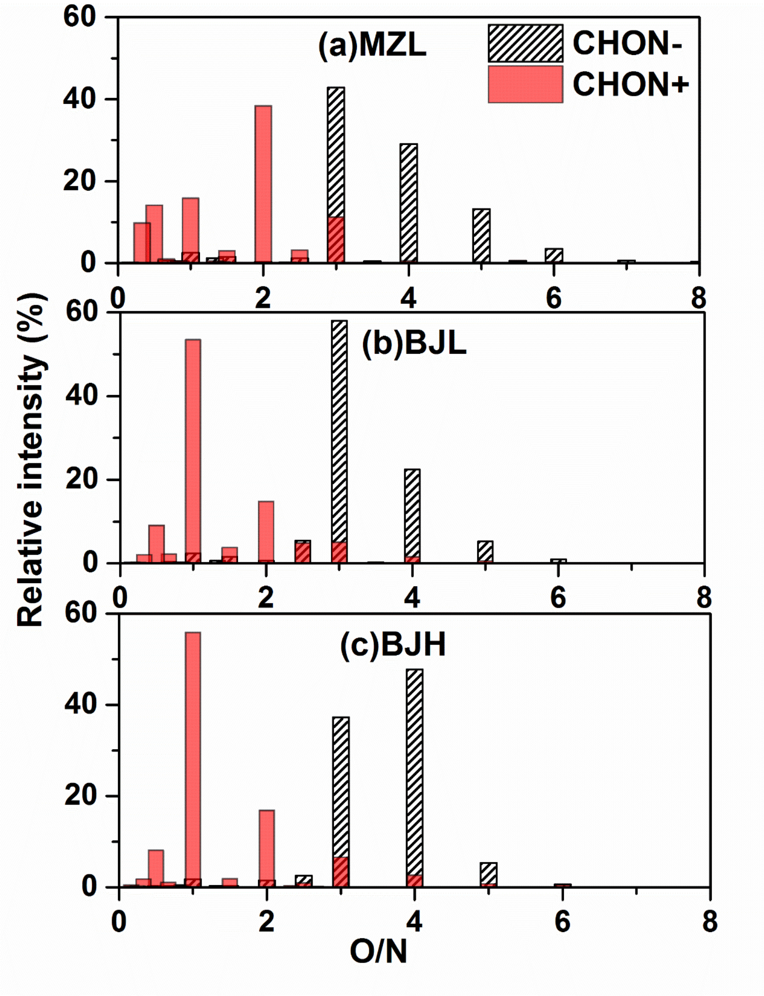

**Figure 2.3.4:** Classification of CHON compounds into different subgroups according to O/N ratios in their molecules. The y-axis indicates the relative contribution of each subgroup to the sum of CHON compounds peak intentities observed in the ESI- and ESI+ modes, respectively.

### 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 $CH_2$ to exactly 14 u as the reference mass for calculating the Kendrick mass (KM) following Eq. (8) and the KMD is defined as the difference between the nominal mass and the KM as shown in Eq. (9).

$$KM\left(CH_2\right) = mass \times \left[mass\ CH_2\right] / mass\ CH_2 \tag{8}$$

$$KMD\left(CH_2\right) = \left[mass\right] - KM\left(CH_2\right) \tag{9}$$

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 $CH_2$ 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 ($X_C \geq 2.7$) and aromatics ($X_C \geq 2.5$). 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).

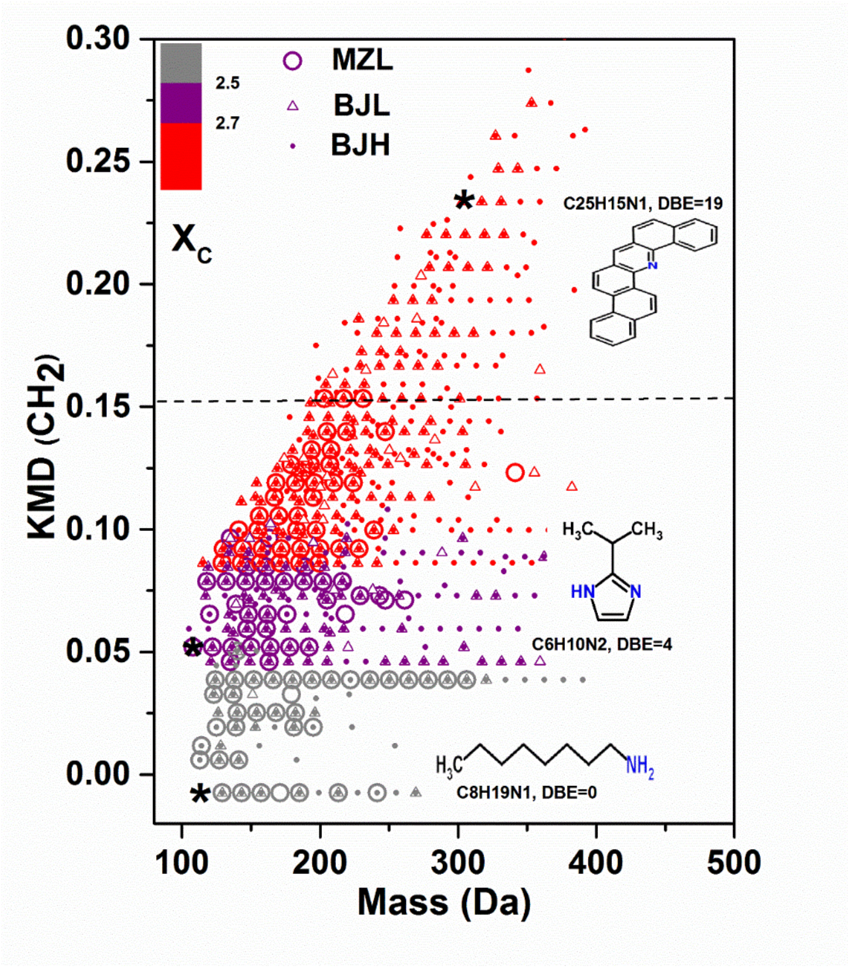

**Figure 2.3.5:** Kendrick mass defect diagram of CHN compounds detected in ESI+ mode. The colour bar denotes the aromaticity equivalent (gray with $X_C < 2.50$, purple with $2.50 \leq X_C < 2.70$ and red with $X_C \geq 2.70$). The element composition, DBE and a potential chemical structure for the first 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 ≥ 4, suggesting they represent organosulfates (OSs), which is consistent with previous studies (Tao et al., 2014;Wang et al., 2016). The number-weighted 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 α-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 ≥1, allowing their assignment to nitrooxy-OSs with both –$OSO_3H$ and –$ONO_2$ 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 $PM_{2.5}$ samples from one European city Mainz and one Chinese city Beijing. Roughly 18000organic 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 $PM_{2,5}$ (MZL and BJL). These elemental compositions can be assigned to represent mostly nitrooxy-OS. Only 29% of CHONS compounds collected during high $PM_{2.5}$ 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., α-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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Atmospheric Physics, Johannes Gutenberg University of Mainz) for his assistance in sample collection in Mainz.

## 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/H2O and H2O extraction method*

In previous studies, pure water ($H_2O$) 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 µm 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 µm, 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 µL 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 PM2.5 samples from Beijing and Mainz, representing high and low mass loading and different pollution sources, were extracted with ACN/H2O (A/W) and H2O (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/H2O (A/W-) is similar to those extracted with pure H2O (W-) for ESI- analysis, much more organic compounds are observed with ESI+ analysis when ACN/H2O (A/W+) is used for extraction compared to pure H2O (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 obertained in the H2O extracts are also observed in ACN/H2O extracts, while only 56% of compounds observed in the ACN/H2O extracts are obtained in H2O extracts. Meanwhile, 90% of the total peak intensity from the H2O extracts matches the peak intensity from the ACN/H2O extracts, while only 75% of the total peak intensity from the ACN/H2O extracts matched assigned peaks in the H2O extracts. It is clear that a majority of organics observed in the H2O extracts can also be measured in the ACN/H2O extracts, in particular for those organics of high concentrations. More important, ACN/H2O can extract more organic compounds which are not found in the H2O extracts. In summary, the results demonstrate that ACN/H2O is superior to H2O for the extraction of organics in OA.

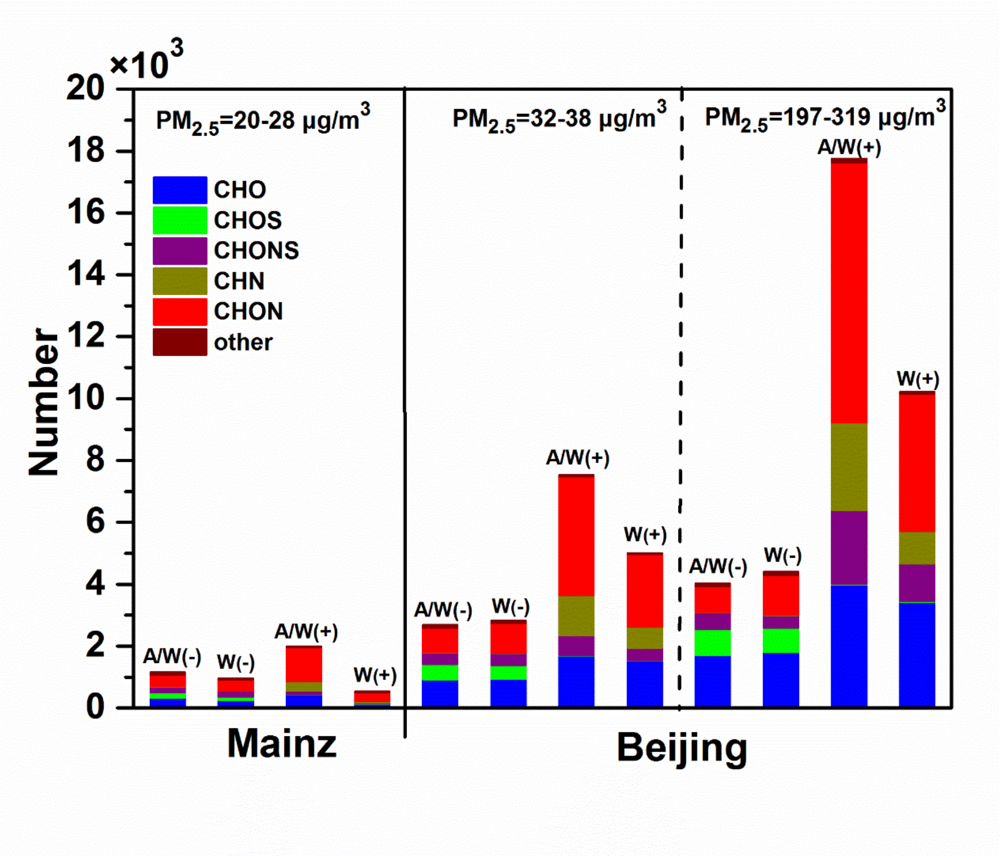

Figure 2.5.1: The number of individually assigned molecular formulas observed in ACN/$H_2O$ and $H_2O$ methods in Mainz and Beijing samples. Each subgroup is marked by the different colors.

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

| Sample ID | Method | Number of the overlapped molecular formulas (%) | | Intensity of the overlapped formulas (%) | |
|---|---|---|---|---|---|
| | | ESI- | ESI+ | ESI- | ESI+ |
| MZL | ACN-$H_2O$ | 56 | 20 | 75 | 32 |
| | H2O | 72 | 60 | 90 | 65 |
| BJL | ACN-$H_2O$ | 70 | 46 | 92 | 78 |
| | H2O | 70 | 68 | 95 | 92 |
| BJH | ACN-$H_2O$ | 59 | 43 | 91 | 80 |
| | H2O | 60 | 70 | 95 | 94 |

# 3 Comparison of OA chemical composition from different Chinese cities

This chapter is a reprint of the manuscript:

Kai Wang, Yun Zhang, Rujin Huang, Junji Cao, Christopher Kampf, Yafang Cheng, Ulrich Pöschl and Thorsten Hoffmann

## Molecular characterization of organic aerosols in three cities at the northeast, central east and southeast of China using UHPLC-Orbitrap mass spectrometry

*In preparation for Atmospheric Chemistry and physics*

**Abstract.** Aerosol samples with the diameter of particulate matter ≤ 2.5 μm ($PM_{2.5}$) were collected in January 2014 in three Chinese cities located in northeast, centraleast and southeast of China: Changchun (CC), Shanghai (SH) and Guangzhou (GZ). The organic fraction of the $PM_{2.5}$ samples were analyzed by ultrahigh performance liquid chromatography (UHPLC) coupled with Orbirtrap mass spectrometry (MS). The formulas of the identified compounds were classified into five main subgroups: CHO, CHON, CHN, CHOS and CHONS. In total, 416-769 organic compounds in the negative electrospray ionization (ESI-) and 687-2943 in the positive electrospray ionization (ESI+), respectively, were determined. CHO, CHON and CHN compounds with high concentrations in the the three urban samples share large similarity of chemical composition and the majority of them are assigned as mono or poly aromatics, suggesting that anthropogenic emission is an especially important source for the Chinese urban OA. Additionally, significantly more polyaromatics were observed in CC samples, which were probably generated from the coal burning for the residential heating in winter in northeast China. Moreover, higher H/C and O/C ratios of organic compounds in ESI- were observed in SH and GZ than those in CC, indicating that OA in low latitude regions of China experienced more intense photochemical oxidation processes. The majority of CHOS and CHONS compounds in all samples were identified as aliphatic compounds with low unsaturation and aromaticity, while CHOS and CHONS compounds between SH and GZ share higher similarity.

## 3.1 Introduction

In last decade, China has experienced severe and persistent particulate air pollution accompanying with rapid industrialization and urbanization (Huang et al., 2014;Song et al., 2017). Especially, in January 2013, the large-scare and severe particulate pollution affected around 1.3 million km$^2$ territories and 800 million inhabitants in China. Measurements of $PM_{2.5}$ (particulate matter with an aerodynamic diameter less than 2.5 μm) concentrations in 74 major Chinese cities in January 2013 showed that the daily average concentrations of $PM_{2.5}$ exceeded the Chinese air quality standards of 75 μg/m$^3$, which were around twice higher compared to the US EPA standards of 35 μg/m$^3$ (Huang et al., 2014). Such extremely acute air pollution could not only influence the regional air quality and human health in China, but also lead to a global environment problem in some case by long-time and long-distance transport of pollutants from China. However, despite the important influence of particular aerosols on air quality, climate and human health (Pöschl, 2005;Pöschl and Shiraiwa, 2015), the chemical composition of particulate aerosol is still poorly understood due to a wide variety of natural and anthropogenic sources as well as the complex multiphase chemical reactions (Lin et al., 2012a;Noziere et al., 2015;Wang et al., 2017;Wang et al., 2018). In particular, compared to the fairly well understanding of inorganic fraction in particulate aerosol, the organic fraction, also named organic aerosol (OA), is considerably unclear in terms of chemical composition and precursors (Hallquist et al., 2009b).

OA accounts for a substantial fraction (20-90%) of submicrometer aerosol mass (Jimenez et al., 2009;Kroll et al., 2011;Wang et al., 2017) and contains thousands of organic compounds including alcohols, aldehydes, organic acids, organosulfates, organonitrates and polycyclic aromatic hydrocarbons (PAHs) (Lin et al., 2012a;Rincón et al., 2012;Kourtchev et al., 2014;Wang et al., 2018). However, only around 10-30% of OA has been identified as specific compounds (Hoffmann et al., 2011). Since compounds in OA cover a large chemical space with respect to molecular weight, functional groups and polarity (Rincón et al., 2012), chemical characterization of OA is vital but challenging analytical task(Wang et al., 2017;Laskin et al., 2018).

With the development of mass spectrometric techniques, recently, ultrahigh resolution mass spectrometry (UHRMS), such as Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) and Orbitrap-MS, coupled with soft ionization sources (e.g., electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI)) have been introduced to elucidate the organic components in OA (Noziere et al., 2015;Laskin et al., 2018). Due to the two outstanding features of high resolution and high mass accuracy, UHRMS can give the information of precise elemental compositions of individual organic compounds. Previous UHRMS studies mainly focused on the chemical characterization of OA samples collected from laboratory simulations, forest, rain water, biomass burning and rural regions (Nizkorodov et al., 2011;Kourtchev et al., 2016;Tu et al., 2016). For example, Tu et al. (2016) identified the highly oxidized multifunctional molecules (HOMs) in fresh and aged secondary organic aerosol (SOA) generated from a flow tube reactor using Orbitrap-MS. Kourtchev et al. (2016) applied the Orbitrap-MS technique to analyze the organic fraction of $PM_{2.5}$ aerosol samples collected during dry and wet seasons in central Amazonia and showed that OA in central Amazonia was influenced not only by biogenic emission but also anthropogenic emissions from near urban environment. However, less studies on urban OA have been conducted by UHRMS techniques. Rincon et al. (2012) compared the chemical composition of OA collected in summer and winter times at Cambridge, UK and showed that more organic compounds, especially the PAHs, were observed in summer OA samples probably due to more intense photo-chemical aging processes during summer time. Lin et al. (Lin et al., 2012b), Tao et al. (Tao et al., 2014) and Wang at al. (Wang et al., 2016) identified the organosulfates in OA collected from seven rural and urban locations in East Asia, Shanghai and Los Angeles, and Shanghai, respectively. Very recently, Wang et al. (Wang et al., 2017) characterized the OA in Shanghai and showed the variations of chemical composition of OA among different months and between daytime and nighttime. Our recent study (Wang et al., 2018) analyzed the OA in a Chinese city (Beijing) and a German city (Mainz) and showed that the chemical composition of OA in Beijing and Mainz had a big difference. Since the severe particulate pollution in China happened in a large-scale with inter-regional air pollutant transport, more UHRMS studies need to be conducted to elucidate the chemical composition of OA from different Chinese cities.

In this study, $PM_{2.5}$ aerosol samples were collected from three Chinese cities: Changchun (CC), Shanghai (SH) and Guangzhou (GZ) and their organic fraction were detected using ultra-high-performance liquid chromatography (UHPLC) coupled with Orbitrap MS. The Chinese cities of CC, SH and GZ are located, respectively, in the northeast, central east and southeast regions of China with around 50 million population in total. The geographic positions of these three cities cover a large latitude span from $23.12^0$N to $43.53^0$N resulting in different meteorological conditions including insolation duration, average daily temperature and monsoon climate. In addition, the industrial structure, energy consumption and energy in these three cities are different, which can cause various anthropogenic emission influencing the chemical composition of OA. For example, OA in CC are strongly affected by the coal burning used for residential heating in winter in northeast China. Therefor, this study presents a comprehensive overview of chemical composition of OA in three representative Chinese cities, which can promote our understanding of OA effect on climate and public health as well as provide chemical database for the haze control strategies in China.

## 3.2 Material and methods

### *3.2.1 Collection of $PM_{2.5}$ samples*

Three 24-h integrated urban $PM_{2.5}$ samples were collected during the severe haze pollution events in each of the three Chinese cities: CC, ($43.53^0$N, $125.19^0$E), SH ($31.30^0$N, $121.50^0$E) and GZ ($23.12^0$N, $113.36^0$E), which are located respectively in the northeast, central east and southeast regions of China (see Figure 3.2.1). Samples in CC were collected in 4, 24 and 29 of January 2014 with $PM_{2.5}$ mass concentrations of 185-222 μg $m^{-3}$, samples in SH were collected in 1, 19 and 20 of January 2014 with $PM_{2.5}$ mass concentrations of 159-172 μg $m^{-3}$ and samples in GZ were collected in 5, 6 and 11 of January 2014 with $PM_{2.5}$ mass concentrations of 138-152 μg $m^{-3}$. All $PM_{2.5}$ samples were collected on the prebaked quartz-fiber filters (8×10 inch) using a high-volume sampler at a flow rate of 1.05 $m^3$ $min^{-1}$ and at each sampling site field blank samples were taken. After sample collection, filters were stored at -20 °C until analysis.

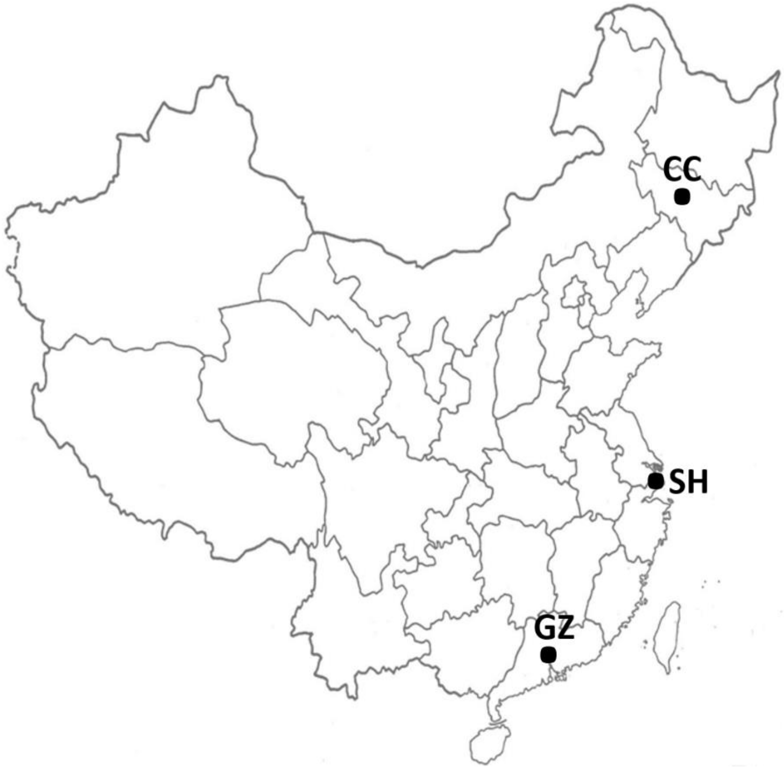

Figure 3.2.1: Locations of Changchun (CC), Shanghai (SH) and Guangzhou (GZ) in China.

### 3.2.2 Sample analysis

Detailed description on the filter sample extraction and UHPLC-Orbitrap MS analysis can be found in our previous study (Wang et al., 2018). Briefly, a part of the filters (around 1.13 $cm^2$, corresponding to about 600 μg particle mass in each extracted filter) was extracted three times with 1.5 mL of acetonitrile-water (8/2, v/v) in an ultrasonic bath. The extracts were combined, filtered through a 0.2 μm Teflon syringe filter and evaporated to almost dryness under a gentle nitrogen stream. Finally, the residual was redissovled in 1000 μL acetonitrile-water (1/9, v/v) for subsequent analysis.

The analytes were separated using Hypersil Gold column (C18, 50 x 2.0 mm, 1.9 µm particle size) with mobile phases consisting of (A) 0.04% formic acid and 2% acetonitrile in water and (B) 2% water in acetonitrile. Gradient elution was applied with the A and B mixture at a flow rate of

500 µL $min^{-1}$ as follows: 0-1.5 min 2% B, 1.5-2.5 min from 2% to 20% B (linear), 2.5-5.5 min 20% B, 5.5-6.5 min from 20% to 30% B (linear), 6.5-7.5 min from 30% to 50% B (linear), 7.5-8.5 min from 50% to 98% B (linear), 8.5-11.0 min 98% B, 11.0-11.05 min from 98% to 2% B (linear), 11.05-11.1 min 2% B. The Q Exactive Hybrid Quadrupole-Orbitrap MS was equipped with a heated ESI source at 120 °C, applying a spray voltage of -3.3 kV and 4.0 kV for negative ESI (ESI-) and positive ESI (ESI+), respectively. The mass scanning range was set between m/z 50 and m/z 500 with a resolving power of 70,000 @ m/z 200. The Orbitrap MS was externally calibrated before each measurement sequence using an Ultramark 1621 solution (Sigama-Aldrich, Germany) providing the mass accuracy of the instrument lower than 3 ppm. Each sample was measured in triplicate with an injection volume of 10 µL.

### *3.2.3 Data Processing*

Custom software (SIEVE®, Thermo Fisher Scientific, Germany) was used to calculate all mathematically possible formulas for all detected ions with a sample-to-blank abundance ratio ≥ 10 with a mass tolerance of ±2 ppm. The permitted maximum elemental numbers of atoms were set as follows: $^{12}C$ (39), $^{1}H$ (72), $^{16}O$ (20), $^{14}N$ (7), $^{32}S$ (4), $^{35}Cl$ (2) and $^{23}Na$ (1). The assigned formulas containing isotopes (e.g., $^{13}C$, $^{18}O$ and $^{34}S$) were not discussed in this study due to much less abundance of these formulas. To remove the chemically unreasonable formulas, further constraint was applied 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. For chemical formula $C_cH_hO_oN_nS_sCl_x$, the double bond equivalent (DBE) was calculated by the equation: $DBE = (2c + 2 – h – x + n) / 2$, and the aromaticity equivalent ($X_C$) as a modified index for aromatic compounds was obtained using the equation: $Xc = [3(DBE – (p \times o + q \times n)) – 2] / [DBE – (p \times o + q \times n)]$, where p and q, respectively, refer to the fraction of oxygen and sulfur atoms involved in π-bond structure of a compound. $Xc \geq 2.50$ and $Xc \geq 2.71$ are suggested to unambiguous minimum criteria for the presence of monoaromatics and polyaromatics, respectively (Yassine et al., 2014). Detailed data processing is presented in the Supporting Information (SI) and the molecular formulas assigned in each sample is also shown in Table S3.2.1-S3.2.6 in SI.

## 3.3 Results and discussion

### *3.3.1 General Characteristics*

The main purpose of this study is to tentatively identify and compare the chemical composition of organic compounds in the $PM_{2.5}$ samples collected from the three Chinese cities of CC, SH and GZ. The number of organic compounds detected in each city and the abundance-weighted average values of molecular weight (MW), elemental ratios, DBE and Xc for each subgroup are listed in Table 3.3.1. Overall, 416-769 and 687-2943 organic compounds were determined in ESI- and ESI+, respectively. The greatest number of organic compounds was observed in CC samples in both ESI- and ESI+, indicating that OA collected in winter season in the northeast region of China were more complex compared to that in central east and southeast regions of China. It could be explained by the extensive use of coal burning for the residential heating in winter in northeast China, which can produce various numbers of organics. In addition, the temperatures (-10 ℃ to -6℃) during the sample collection dates in CC were lowest, which inhibited the diffusion of formed organics enhancing the air pollution. It should be noted that in this study we focused on the organic compounds with relatively high concentrations, so the compounds with low concentration were excluded through reducing the injection volume from 20 μL in our previous study to 10 μL and increasing the sample-to-blank ratio from 3 in our previous study to 10 in data process, which leaded to many fewer numbers of organic compounds detected in this study compared to our previous study (Wang et al., 2018).

As shown in Table 3.3.1, the abundance-weighted average values of MW, H/C and O/C ratio of the total assigned formulas in CC- are 169, 1.03 and 0.58, respectively, which are significantly lower compared to those in SH- (MW=176, H/C=1.05 and O/C=0.69) and in GZ- (MW=183, H/C=1.14 and O/C=0.74). On the contrary, the Xc (2.13) of the organics detected in CC- is relatively higher than that in SH- (Xc = 1.92) and GZ- (Xc = 1.65). These observations indicate that OA in northeast China features lower degree of oxidation but higher degree of aromaticity compared to those in central east and southeast China. It could be caused by that the low temperature and hydroxy radical concentration in winter time in northeast China suppressed the photooxidation process of OA, meanwhile, a large number of PAHs were emitted from coal burning (Huang et al., 2014). Figure 3.3.2 shows the reconstructed mass spectra of organic compounds detected in ESI- and ESI+. It should be noted that uncertainties always exist when comparing the peak abundance of organic compounds in different subgroups due to their different signal response in the mass spectrometer. In this study, we assume that all organic compounds have the same mass spectrum response and the peak abundance of organic compounds were compared among different samples. The major organic species detected in ESI- are attributed to CHO- and CHON-, accounting for 30-42% and 39-55% in terms of peak abundance, respectively, which is consistent with other OA studies by Lin et al. and Wang et al. (Lin et al., 2012a;Wang et al., 2017). Comparing the organics detected in ESI- among the three samples, we find that 139 formulas were observed in all samples as common formulas (see Figure 3.3.3), which account for 35-51% and 78-87% of all assigned formulas in terms of peak numbers and peak abundance, respectively. It demonstrates that despite the different sampling locations a large number of common organic compounds exist in Chinese urban OAs, in particular for those organics with high abundances. Furthermore, the pie chat in Figure 3.3.3b shows that these common formulas are also dominated by CHON- and CHO-, respectively accounting for 59% and 33% of the total common formulas in terms of peak abundance.

As we know that ESI source has a different mechanism between negative and positive ionization mode, where ESI- is especially sensitive to deprotonatable compounds (e.g., organic acids) and ESI+ is prone to protonatable compounds (e.g., organic amines). Due to the different mechanism between ESI- and ESI, a remarkable difference of mass spectra (see Figure 3.3.2) and chemical characteristics (see Table 3.3.1) between ESI- and ESI+ was represented. For example, in this study, CHO compounds were preferentially detected in ESI- with relatively higher fraction (30-42%) compared to 4-13% in ESI+, while CHN compounds could only be observed in ESI+ with great peak abundance fraction of 40-71%. This observation indicates that most CHO compounds with high concentrations are probably organic acids and the major CHN compounds in this study are likely organic amines, which agrees well with previous studies (Lin et al., 2012a;Wang et al., 2017;Wang et al., 2018). Organic compounds in ESI+ are dominated by CHN+ and CHON+ compounds and these compounds are characterized with higher H/C ratio and lower O/C ratios (see Table 3.3.1), showing that they are less oxidized. The venn diagram in Figure 3.3.3a shows that 168 formulas were found in all samples as common formulas, which account for 25-44% and 65-90% of all assigned formulas in terms of peak numbers and peak abundance, respectively. Among these common formulas, CHN+ and CHON+ have the highest abundance fractions of 65% and 35% (see Figure 3.3.3b), respectively. In the following chapters, the chemical properties including oxidation, unsaturation and aromaticity degrees of each organic species (CHO, CHON, CHN, CHOS and CHONS) observed in the three samples were compared and discussed.

Table 3.3.1 Number of organic compounds in each subgroup and the abundance-weighted average values of molecular weight (MW), elemental ratios, double bond equivalent (DBE) and aromaticity equivalent (Xc) for detected organic compounds in ESI- and ESI+ in the three Chinese cities.

| Sample ID | Subgroup | Number of compounds | Abundance (%) | MW | H/C | O/C | DBE | Xc | Isomer fraction (%) |
|---|---|---|---|---|---|---|---|---|---|
| CC- | total | 769 | 100 | 169 | 1.03 | 0.58 | 5.02 | 2.13 | 64 |
| | CHO | 346 | 30 | 162 | 0.96 | 0.41 | 5.65 | 2.28 | 81 |
| | CHON | 180 | 55 | 163 | 0.94 | 0.51 | 5.24 | 2.44 | 66 |
| | CHOS | 155 | 10 | 198 | 1.56 | 1.17 | 2.55 | 0.50 | 51 |
| | CHONS | 88 | 5 | 214 | 1.35 | 1.07 | 3.75 | 1.06 | 18 |
| SH- | total | 416 | 100 | 176 | 1.05 | 0.69 | 4.99 | 1.92 | 55 |
| | CHO | 164 | 40 | 171 | 0.97 | 0.59 | 5.37 | 1.94 | 68 |
| | CHON | 135 | 44 | 169 | 0.86 | 0.56 | 5.67 | 2.47 | 59 |
| | CHOS | 75 | 12 | 190 | 1.85 | 1.41 | 1.79 | 0.34 | 29 |
| | CHONS | 42 | 4 | 266 | 1.56 | 1.00 | 3.30 | 0.44 | 36 |
| GZ- | total | 488 | 100 | 183 | 1.14 | 0.74 | 4.55 | 1.65 | 59 |
| | CHO | 196 | 42 | 172 | 1.10 | 0.65 | 4.68 | 1.57 | 68 |
| | CHON | 161 | 39 | 173 | 0.89 | 0.58 | 5.56 | 2.41 | 60 |
| | CHOS | 86 | 14 | 201 | 1.85 | 1.48 | 1.71 | 0.21 | 38 |
| | CHONS | 45 | 5 | 293 | 1.56 | 0.82 | 3.45 | 0.43 | 53 |
| CC+ | total | 2943 | 100 | 160 | 1.21 | 0.13 | 5.58 | 2.36 | 90 |
| | CHO | 609 | 13 | 174 | 0.94 | 0.28 | 6.55 | 2.22 | 87 |
| | CHN | 696 | 40 | 154 | 1.22 | 0.00 | 5.84 | 2.60 | 96 |
| | CHON | 1594 | 46.5 | 161 | 1.27 | 0.19 | 5.11 | 2.22 | 90 |
| | CHONS | 44 | 5 | 196 | 1.91 | 0.70 | 2.64 | 0.09 | 23 |
| SH+ | total | 704 | 100 | 162 | 1.37 | 0.09 | 4.91 | 2.32 | 63 |
| | CHO | 87 | 4 | 184 | 1.13 | 0.43 | 5.46 | 1.46 | 38 |
| | CHN | 253 | 71 | 159 | 1.38 | 0.00 | 5.08 | 2.55 | 85 |
| | CHON | 350 | 24.7 | 167 | 1.40 | 0.27 | 4.34 | 1.81 | 57 |
| | CHONS | 14 | 0.3 | 241 | 1.17 | 0.61 | 5.32 | 0.91 | 0 |
| GZ+ | total | 687 | 100 | 161 | 1.41 | 0.17 | 4.58 | 2.07 | 58 |
| | CHO | 125 | 8 | 185 | 1.12 | 0.42 | 5.19 | 1.20 | 49 |
| | CHN | 205 | 62 | 156 | 1.42 | 0.00 | 4.80 | 2.47 | 82 |
| | CHON | 336 | 29 | 165 | 1.47 | 0.45 | 4.00 | 1.51 | 50 |
| | CHONS | 21 | 1 | 209 | 1.84 | 0.71 | 3.05 | 0.31 | 10 |

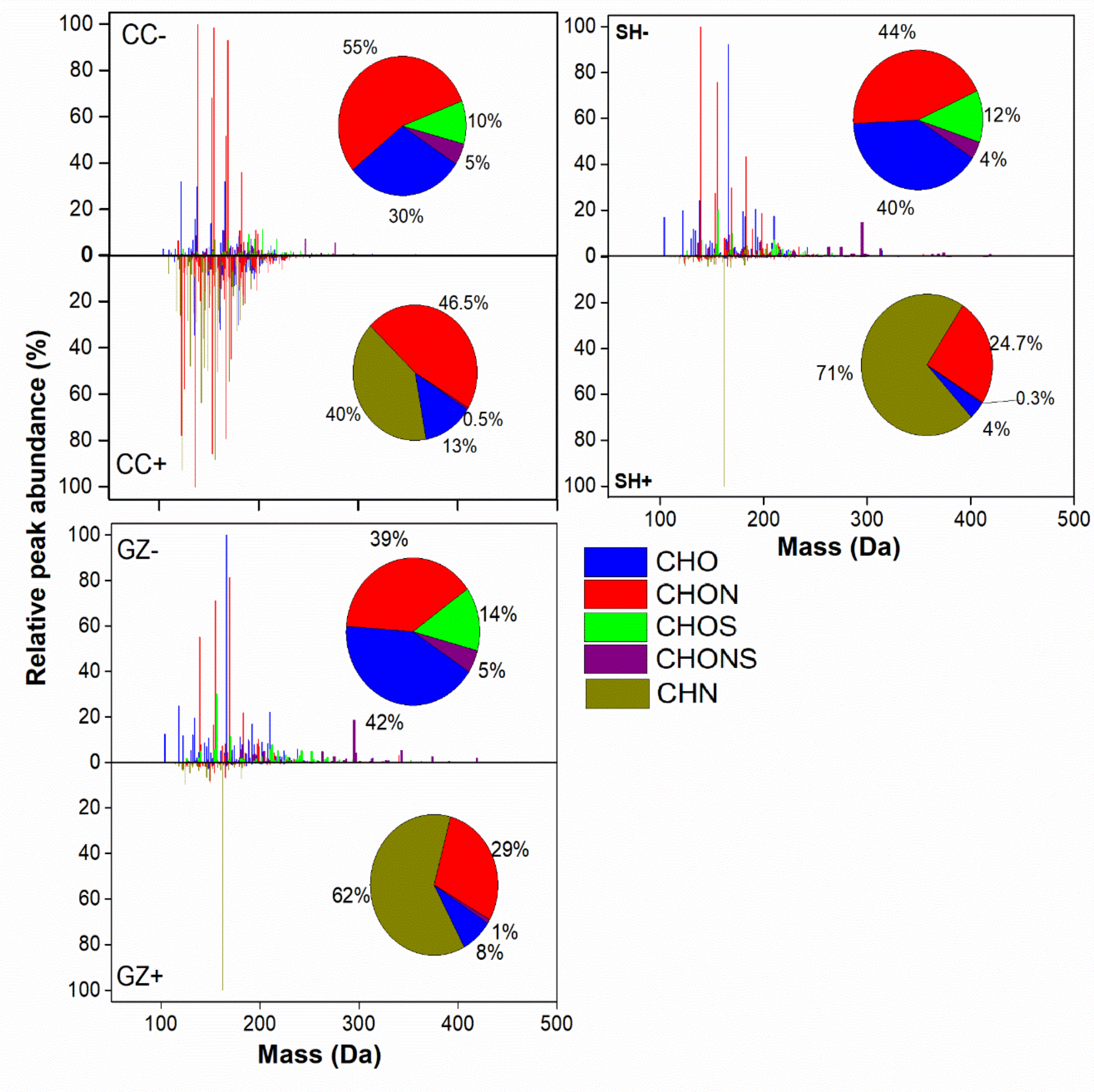

Figure 3.3.2: Mass spectra of detected organic compounds reconstructed from extracted ion chromatograms in ESI- and ESI+. X axis refers to the molecular mass (Da) of the identified species. Y axis refers to the relative peak abundance of each individual compound to the compound with the greatest peak abundance. The sizes of pie chats are proportional to the abundances of a subgroup in all detected organics.

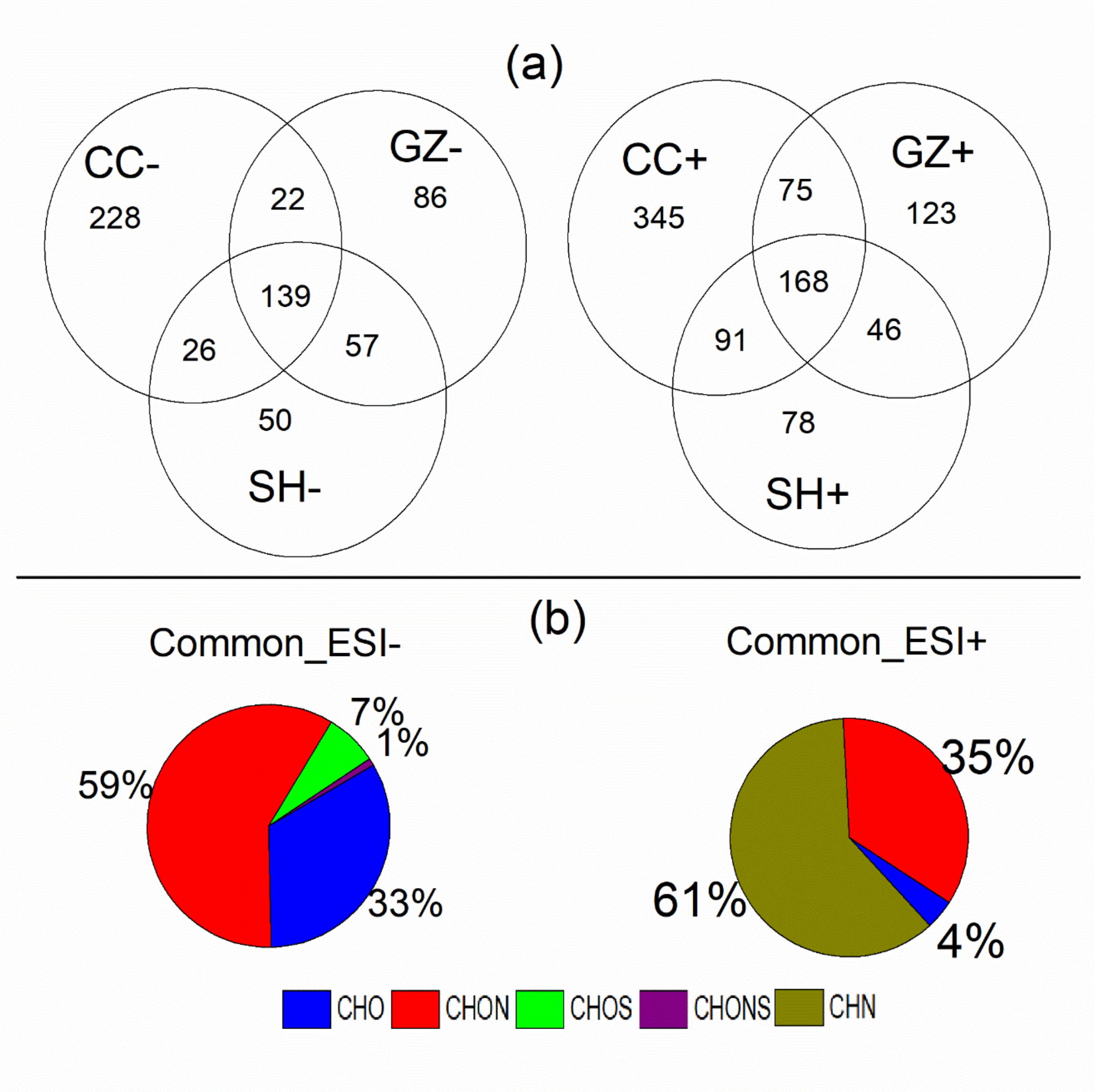

Figure 3.3.3: (a)Venn diagrams shows the number distribution of all molecular formulas detected in ESI- and ESI+ in all samples. (b) Peak abundance contribution of each elemental formula category to the total common formulas.

### 3.3.2 CHO

CHO compounds have been widely observed in urban OA with a substantial fraction (13-41%) of OA (Mazzoleni et al., 2010a;Lin et al., 2012a;Rincón et al., 2012;Wang et al., 2017;Wang et al., 2018). Previous studies showed that the majority of CHO compounds in urban OA were identified as organic acids containing carboxyl functional groups, which are prone to be detected in the negative mode in mass spectrometer. As shown in Table 3.3.1, a total of 346, 164, and 196 CHO- compounds were detected in ESI- in CC-, SH- and GZ- samples, which account for 30%, 40% and 42% of the overall peak abundance of compounds in each sample. The average H/C values (0.96-1.10) are similar among the three samples, while the average O/C values in SH- (O/C = 0.59) and GZ- (O/C = 0.65) are relatively higher than that (0.41) in CC-. Furthermore, the van Krevelen diagram in Figure S3.3.1 also shows that more CHO- compounds with high O/C ratio were found in SH- and GZ- compared to CC-. These results together indicate that CHO- compounds in the OA collected from central east and southeast China were generated after a more intensive oxidation process. 52 common CHO- formulas were obtained in all samples, accounting for 13-17% and 74-88% of all identified CHO- formulas in terms of numbers and abundance, respectively. It indicates that the chemical composition of CHO- compounds with high concentration among these three Chinese cities are similar.

Figure 3.3.4 shows the DBE against C number of CHO- compounds in the three samples. As shown in Figure 3.3.4, the abundance-weighted average molecular formulas for CHO- compounds in CC-, SH- and GZ- are $C_{8.58}H_{7.86}O_{3.22}$ (MW = 162), $C_8H_{7.27}O_{4.22}$ (MW = 171) and $C_{7.7}H_{8.04}O_{4.48}$ (MW = 172), respectively. It shows that CHO- compounds in SH- and GZ- have relatively higher abundance-weighted MW with greater content of O, whereas the CHO- compounds in CC- have lower abundance-weighted MW with less C content. In Figure 3.3.4, a wide range of DBE values (0-15) was obtained in the CHO- compounds, increasing with the increase of carbon content. The CHO- compounds with high peak abundance were mainly assigned as monoaromatics with $2.5 \leq Xc < 2.7$ (purple circles in Figure 3.3.4) in the region of 7-12 C numbers and 5-7 DBE values, which have the highest fraction (49-67%) of the total CHO- compounds. In addition, 4-14% of CHO- compounds are identified as polyaromatics with $Xc \geq 2.7$ (red circles in Figure 3.3.4), which are suggested to be emitted from coal combustion (Song et al., 2018). These results are consistent with a previous study by Wang et al. (Wang et al., 2017) showing that aromatics account for 51% of total CHO- compounds in Shanghai OA. It indicates that aromatic compounds are an important fraction in Chinese urban OA, which are probably generated from combustion emission (e.g., biomass burning and fossil fuel fuel combustion) (Huang et al., 2014;Kourtchev et al., 2016;Fleming et al., 2018). Beside the monoaromatics and polyaromatics, the rest CHO- compounds are assigned as aliphatic compounds with Xc lower than 2.5 (grey circles in Figure 3.3.4), which are likely derived from biogenic precursors (Lin et al., 2012a;Rincón et al., 2012). Comparing with the high fraction (47%) of CHO aliphatic compounds in GZ-, they account for much lower fraction in CC- (19%) and SH- (28%), indicating that biogenic sources have more impact on GZ- OA than that in CC- and SH-.

In CC-, formulas of $C_8H_6O_4$, $C_7H_6O_2$, $C_7H_6O_3$, $C_8H_8O_2$, and $C_8H_8O_3$ with DBE values of 6, 5, 5, 5, and 5 are dominant. According to previous studies, $C_8H_6O_4$, $C_7H_6O_2$ and $C_7H_6O_3$ are suggested to phthalic acid, benzoic acid and monohydroxybenzoic acid, respectively, which are derived from naphthalene (Kautzman et al., 2010;Riva et al., 2015;Wang et al., 2017). $C_8H_8O_2$ and $C_8H_8O_3$ are likely hydroxyphenylacetaldehyde and 4-methoxybenzoic acid derived from estragole (Lee et al., 2006;Pereira et al., 2014). In SH-, besides $C_8H_6O_4$, $C_7H_6O_3$ and $C_7H_6O_2$, formulas of $C_6H_8O_7$ and $C_9H_8O_4$ with DBE values of 3 and 6 were observed with high peak abundance. $C_6H_8O_7$ was identified as citric acid in the pollen sample in previous study(Jung and Kawamura, 2011) and $C_9H_8O_4$ are probably homophthalic acid derived from estragole (Pereira et al., 2014). In GZ-, besides the formulas of $C_8H_6O_4$ and $C_6H_8O_7$ discussed above, $C_4H_6O_4$ and $C_4H_6O_5$ with low DBE values of 2 were also detected with high abundance and they are suggested to succinic acid and malic acid, respectively (Claeys et al., 2004;Wang et al., 2017).

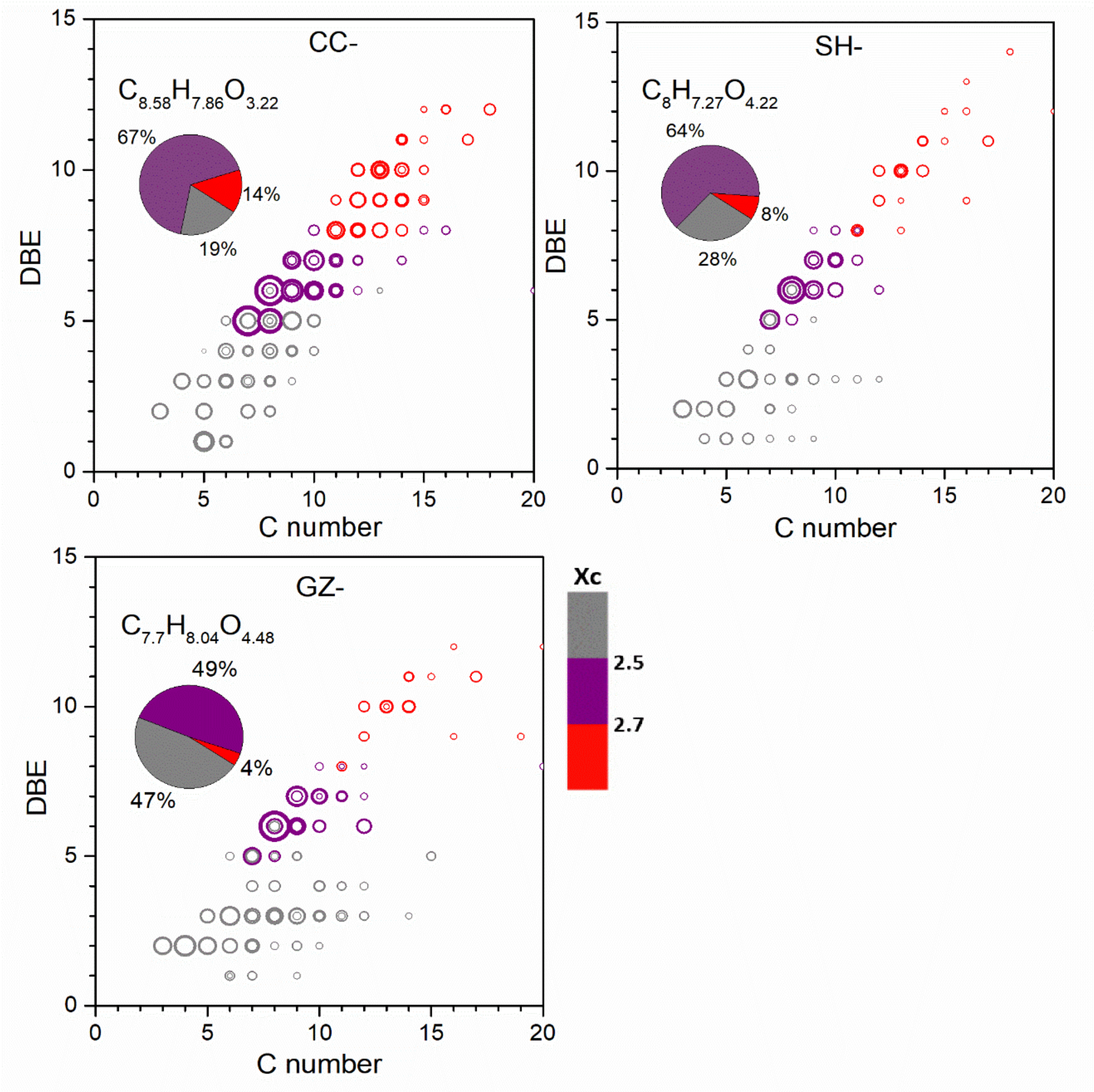

Figure 3.3.4: Double bond equivalent (DBE) vs C number for all CHO- compounds of all samples. The molecular formula represents the abundance-weighted average CHO- formula and the size of circles is proportional to the fourth root of the peak abundance of a individual compound. The color bar denotes the aromaticity equivalent (gray with XC < 2.50, purple with 2.50 ≤ XC < 2.70 and red with XC ≥ 2.70). The size of pie chats is proportional to the peak abundances of each color-coded compounds in each sample.

### 3.3.3 CHON

A large amount of organic nitrogen compounds was detected in CC, SH and GZ samples, accounting for 39-55% and 24.7-46.5% of total peak abundance detected in ESI- and ES+, respectively. 51 common CHON- and 89 common CHON+ formulas were observed in all samples, taking up 90-96% and 61-75% fraction of all CHON compounds detected in ESI- and ESI+, respectively, in terms of peak abundance. It indicates that the chemical composition of CHON compounds with high concentrations are quite similar in the OA of these three Chinese cities.

According to the O/N ratios in CHON formulas, the CHON compounds were further classified into different subgroups in Figure 3.3.5 for CHON- and Figure S2 for CHON+. As shown in Figure 3.3.5, the majority (84-96%) of CHON- compounds have O/N ratios ≥ 3, allowing the assignment of one nitro (-$NO_2$) or nitrooxy (-$ONO_2$) group in these formulas, which are preferentially ionized in ESI- (Lin et al., 2012b;Wang et al., 2017;Song et al., 2018;Wang et al., 2018). In addition, the excess of O atoms to the -$ONO_2$ functional group in the CHON- subgroups with O/N ratios ≥ 4 suggests these compounds also contain other oxygenated functional groups, such as hydroxy group (-OH). 59% of CHON- compounds were found with O/N ratios ≥ 4 in GZ-, which is significantly higher than 51% in CC- and 45% in SH-, indicating that CHON- compounds in southeast China present a higher degree of oxidation compared to those in northeast and central east of China. Not surprisingly, CHON+ compounds come with lower O/N ratios (see Figure S3.3.2), which probably contain reduced nitrogen functional group (e.g., amines) and are prone to be detected in ESI+. As shown in Figure S3.3.2, CHON+ compounds with O/N ratio of 1 are dominant in CC+, whereas CHON+ compounds in SH+ and GZ+ have a relatively wider ranges of O/N ratios from 1 to 3. Moreover, the average O/C ratios (0.27-0.45) in SH+ and GZ+ (see Table 3.3.1) are much greater than that (0.19) in CC+. These results together indicate that CHON+ compounds in the OA of central east and southeast China experienced more intensive oxidation process.

Figure 3.3.6 shows the DBE versus C number of CHON- compounds in the three samples. The majority of CHON- compounds are in the region with 5-15 C and 3-10 DBE values. 67% of CHON- compounds were assigned as mono or poly aromatics in SH-, which is significant higher than 52% in GZ- and 54.7% in CC-. Additionally, the average DBE value (5.67) in SH- is relatively greater compared to 5.24 in CC- and 5.56 in GZ-. It indicates that CHON- compounds are dominated with aromatic compounds in all samples, while they have higher degree of aromaticity and unsaturation in SH- compared with those in CC- and GZ-. The abundance-weighted average molecular formulas for CHON- compounds in CC-, SH- and GZ- are $C_{7.1}H_{6.76}O_{3.56}N_{1.03}$, $C_{7.07}H_{6.03}O_{3.8}N_{1.24}$ and $C_{7.12}H_{6.36}O_{3.99}N_{1.24}$, respectively showing that CHON- formulas in SH- and GZ- contain more O and N atoms than that in CC-. Formulas of $C_6H_5O_3N_1$, $C_6H_5O_4N_1$, $C_7H_7O_3N_1$, $C_7H_7O_4N_1$, $C_8H_9O_3N_1$, and $C_8H_9O_4N_1$ were detected in all samples with the highest abundance. These compounds are probably nitrophenol or nitrocatechol analogs, which have been identified in previous urban OA study (Wang et al., 2017). Furthermore, these nitrooxy-aromatic compounds are proved to be responsible for the light absorption in OA (Laskin et al., 2015;Lin et al., 2015). In addition, it should be noted that the Xc values for $C_6H_5O_4N_1$, $C_7H_7O_4N_1$ and $C_8H_9O_4N_1$ were calculated lower than 2.5, suggesting that the fraction of aromatics in CHON- compounds has been underestimated.

In Figure S3.3.3, the DBE versus C diagram shows that the major CHON+ compounds have the similar C number range from 5 to 15 with CHON- compounds in Figure 3.3.6, whereas more CHON+ compounds with DBE values lower than 5 were observed. The average molecular formulas for CHON+ compounds in CC+, SH+ and GZ+ are $C_{8.73}H_{10.74}O_{1.52}N_{1.5,}$ $C_{8.35}H_{11.56}O_{2.08}N_{1.54}$ and $C_{7.6}H_{10.75}O_{2.6}N_{1.56}$, respectively, showing that they contain lower O contents but higher H contents than in CHON- compounds due to the different mechanism between ESI+ and ESI-. As shown in Figure S3.3.3, the majority (61-85.8%) of CHON+ compounds in the three samples are assigned as aliphatic compounds, while aromatics accounts for 39%, 18% and 14.2% in CC+, SH+ and GZ+, respectively. In addition, Table 3.3.1 shows that the DBE and Xc values in CC+ are significantly greater than those in SH+ and GZ+, while the O/C ratio (0.19) in CC+ is relatively lower than that in SH+ (O/C = 0.27) and GZ+ (O/C = 0.45). These results together demonstrate that CHON+ compounds in CC+ contain more aromatics with low degree of oxidation, while most CHON+ compounds in SH+ and GZ+ are identified as aliphatic compounds with relatively higher degree of oxidation.

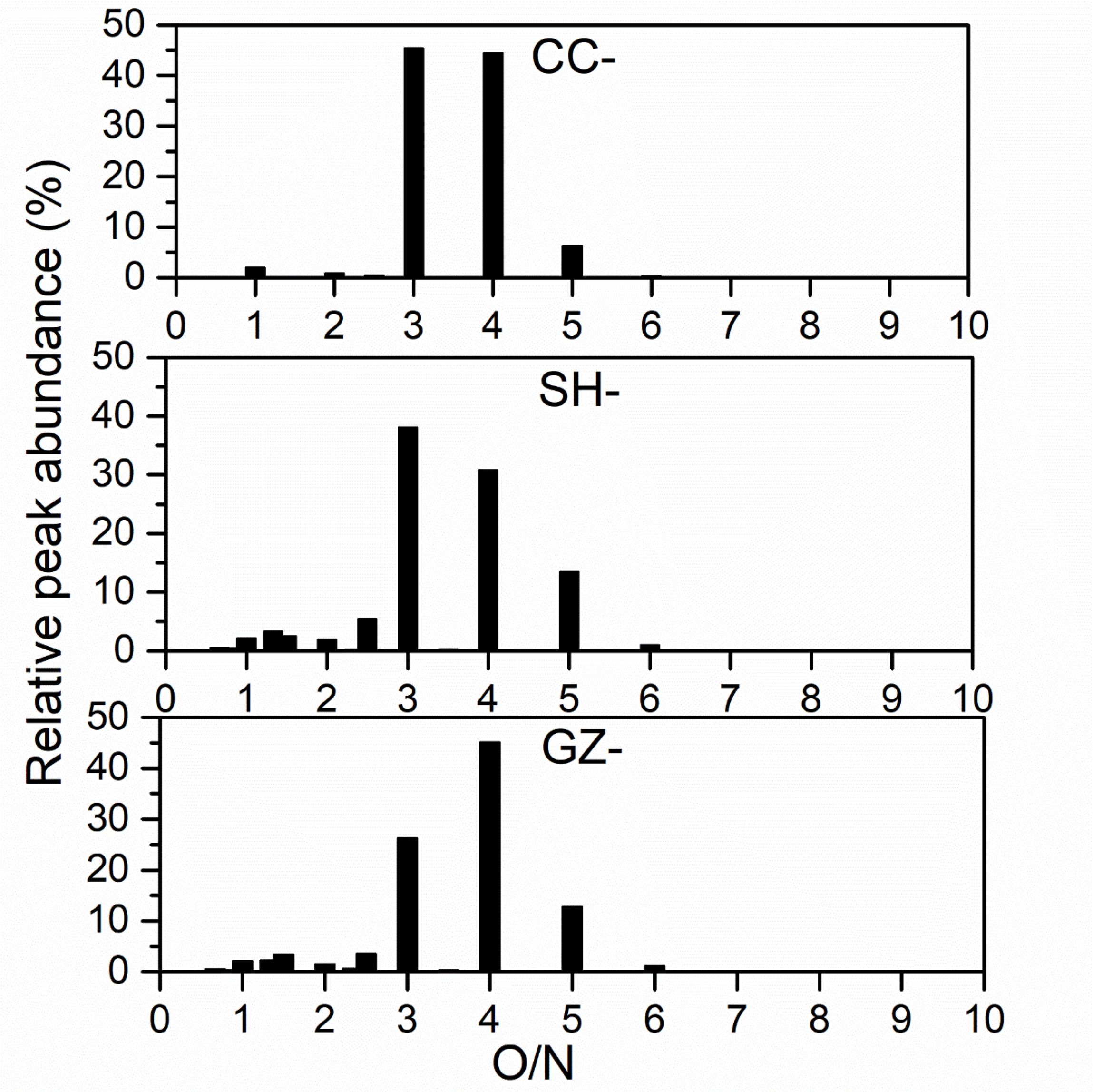

Figure 3.3.5: Classification of CHON- compounds into different subgroups according to O/N ratios in their formulas. The y-axis indicates the relative contribution of each subgroup to the sum of peak abundance of CHON- compounds.

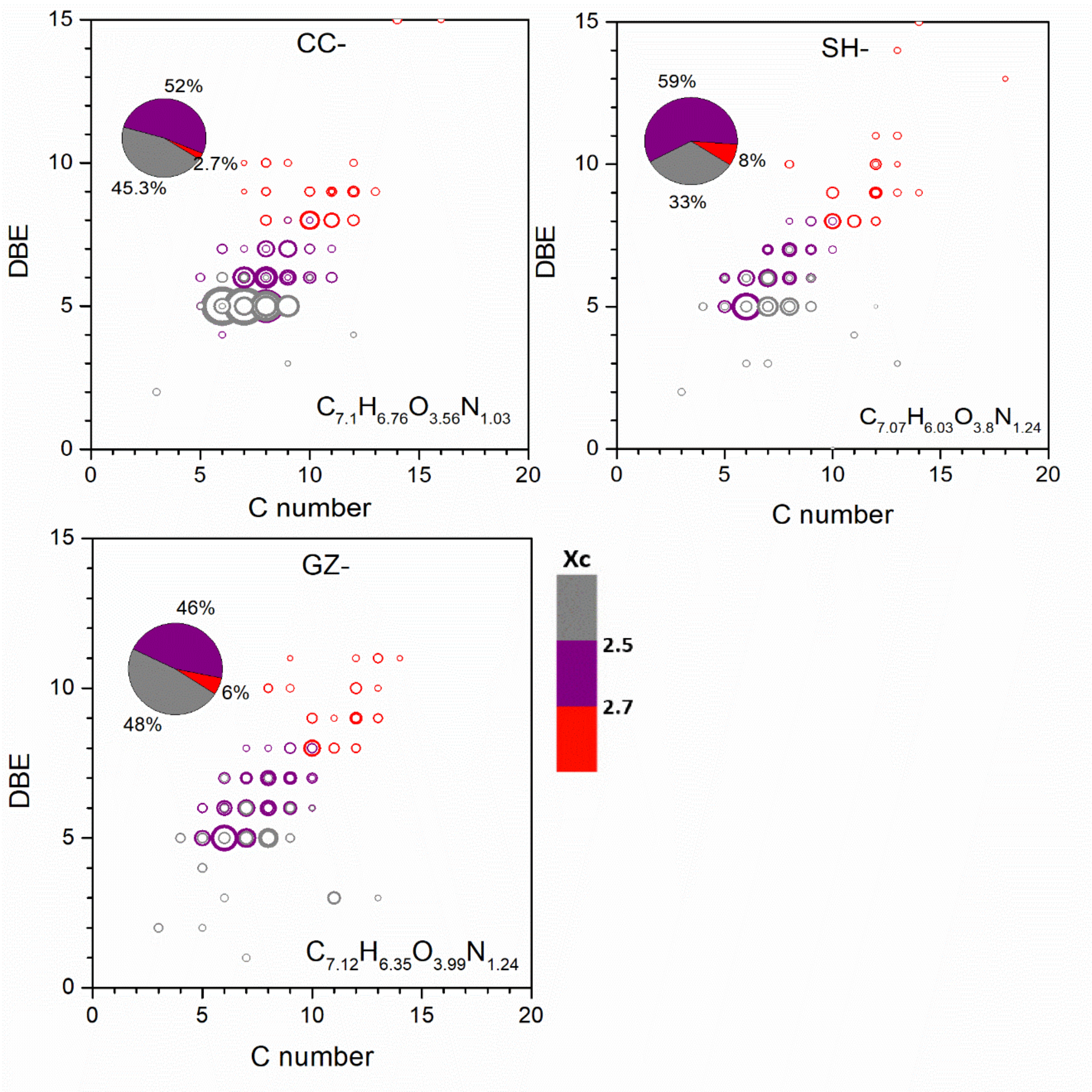

Figure 3.3.6: Double bond equivalent (DBE) vs C number for all CHON- compounds of all samples. The molecular formula represents the abundance-weighted average CHON- formula and the size of circles is proportional to the fourth root of the peak abundance of a individual compound. The color bar denotes the aromaticity equivalent (gray with XC < 2.50, purple with 2.50 ≤ XC < 2.70 and red with XC ≥ 2.70). The size of pie chats is proportional to the peak abundances of each color-coded compounds in each sample.

### *3.3.4 CHN+*

205-696 CHN+ compounds were detected in ESI+, which are likely amines according to previous studies (Rincón et al., 2012;Wang et al., 2017;Wang et al., 2018). The number of CHN+ compounds accounts for 24%, 36% and 30% of the total organic compounds in CC+, SH+ and

GZ+, respectively, whereas the peak abundance of these compounds accounts for 40%, 71% and 62%, correspondingly. Comparing the CHN+ compounds in these three samples, we find that 58 common CHN+ formulas were observed in all samples, which contributes 83-98% fraction to the total abundance of CHN+ formulas. It indicates that CHN+ compounds with high concentrations in CC+, SH+ and GZ+ are characterized with similar chemical compositions.

A van Krevelen diagram of CHN+ compounds detected in the three samples is shown in Figure 3.3.7, where H/C ratio is plotted versus the N/C ratio. The major CHN+ compounds are found in the region with H/C ratios between 0.5 and 2 with N/C ratios lower than 0.5. The pie chats in Figure 3.3.7 show that the major (83-87%) CHN+ compounds are assigned as mono or poly-aromatics with $Xc \geq 2.5$. In addition, Table 3.3.1 shows that the average DBE and Xc values of CHN+ compounds are the highest among all organic species. These observations imply that CHN+ compounds are the most aromatic organics in the urban OAs, which is consistent with previous studies (Lin et al., 2012b;Rincón et al., 2012). Polyaromatics with $Xc \geq 2.7$ are obtained at the lower left corner of the van Krevelen diagram accounting for 41% of CHN+ compounds detected in CC+, while they have less fraction (9-10%) in SH+ and GZ+. Moreover, the average DBE and Xc values of CHN+ compounds in CC+ are significantly higher than those in SH+ and GZ+ indicating that CHN+ compounds in CC+ have higher degree of aromaticity, which can be caused by heavy coal burning emission in the winter time in CC (Huang et al., 2014). An interesting observation in Figure 3.3.7 is that the abundance of CHN+ compounds in CC+ distributes evenly among different individual CHN+ compounds, while in SH+ and GZ+ they are absolutely dominated by the formula of $C_{10}H_{14}N_2$ (the biggest purple circle in Figure 3.3.7) with DBE value of 5, which is suggested to nicotine generated from tobacco smoke (Wang et al., 2017). Formulas of $C_7H_{12}N_2$, $C_{11}H_{11}N_1$, $C_{10}H_9N_1$, and $C_{12}H_{13}N_1$ were detected with high abundance in CC+. $C_7H_{12}N_2$ is likely imidazoles, while the others are related to polyaromatics with a naphthalene core structure, such as 1-naphthalenemethylamine ($C_{11}H_{11}N_1$), 1-naphthalenelamine ($C_{10}H_9N_1$), and N-ethyl-1-naphthylamine ($C_{12}H_{13}N_1$) (Laskin et al., 2009;Wang et al., 2017). According to previous smog chamber studies (Laskin et al., 2010), most CHN+ aromatics are probably generated from biomass burning through the addition of reduced nitrogen (e.g., $NH_3$) to the organic molecules via imine formation reaction.

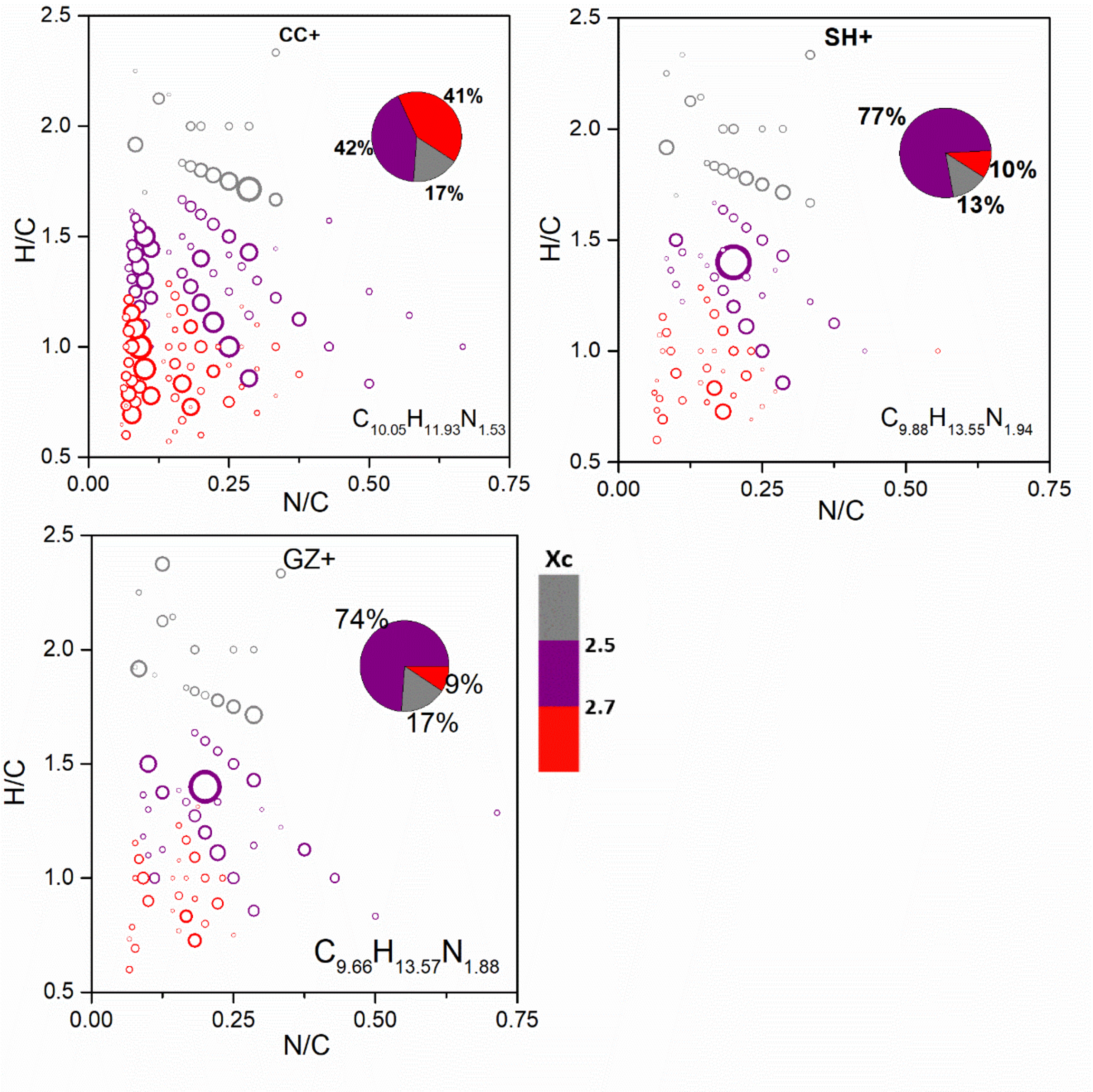

Figure 3.3.7: The van Krevelen diagram for CHN+ compounds in CC, SH and GZ samples. The size of circles is proportional to the fourth root of the peak abundance of a individual compound and the color bar denotes the aromaticity equivalent (gray with XC < 2.50, purple with 2.50 ≤ XC < 2.70 and red with XC ≥ 2.70).

### *3.3.5 CHOS-*

In this study, 75-155 CHOS- compounds were observed, accounting for 10%, 12% and 14% of the total peak abundance of all organics in CC-, SH- and GZ-, respectively. Around 89-96% of these CHOS- compounds were assigned to contain enough oxygen atoms to allow the assignment of -$OSO_3H$ functional group, which are suggested to organosulfates (OSs) according to previous studies (Lin et al., 2012a;Lin et al., 2012b;Tao et al., 2014;Wang et al., 2016;Wang et al., 2017). The OSs could affect the surface activity and hygroscopic properties of the aerosol particles, leading to potential impacts on climate (Hansen et al., 2015;Huang et al., 2018). 28 common CHOS- formulas were detected in the three samples, accounting for 39%, 68% and 65% of the CHOS- peak abundance in CC-, SH- and GZ-, respectively. It indicates that the chemical composition of the major CHOS- compounds in SH- and GZ- are similar, while they have a big chemical difference with the CHOS- compounds in CC-.

Figure 3.3.8 shows the DBE vs. C number for all CHOS- compounds detected in the three samples. The CHOS- compounds exhibit a DBE range from 0 to 10 and carbon number range from 2-15. However, the majority of CHOS- compounds with high abundance concentrate on the region with low DBE values of 0-5. The average H/C (1.56-1.85) and O/C (1.17-1.48) ratios of CHOS- compounds are relatively higher than other organic species, while the average DBE values (1.71-2.55) of CHOS- compounds are the lowest. This result indicates that CHOS- compounds in the OA of the three Chinses cities are characterized with low degree of unsaturation and high degree of oxidation. Moreover, the pie chats in Figure 3.3.8 show that aliphatic compounds with Xc $\leq$ 2.5 are dominant in CHOS- compounds with a fraction of 96-99%, which is significantly higher than that in CHO, CHON and CHN species. The most CHOS- compounds were assigned with carbon number less than 10, which are probably formed from biogenic precursors (e.g., isoprene) or other small molecules (Lim et al., 2010;McNeill et al., 2012;Hansen et al., 2014). However, more CHOS- compounds with C > 10 and with DBE lower than 1 are observed in CC-, such as $C_{14}H_{28}O_5S_1$, $C_{13}H_{26}O_5S_1$, $C_{12}H_{24}O_5S_1$, $C_{11}H_{22}O_5S_1$ and $C_{11}H_{20}O_6S_1$. These high-carbon-number-containing CHOS- compounds are likely formed from long-alkyl-chain compounds with less oxygenated functional groups and traffic emissions are suggested to the source of these long-chain alkanes (Tao et al., 2014). It indicates that anthropogenic emissions (e.g., fossil fuel burning) make more influence on the CHOS- formation in CC-. Comparing the average values of H/C, O/C and DBE of CHOS- in the three samples (see Table 3.3.1), we find that the H/C ratios (1.85) and O/C ratios (1.41-1.48) in SH- and GZ- are relatively higher than those (H/C = 1.56 and O/C = 1.17) in CC-, whereas the DBE values (1.71-1.79) in SH- and GZ- are relatively lower than that (2.55) in CC-. These observations indicate that CHOS- compounds in the OA from northeast China are less oxidized but more unsaturated compared to those in central east and southeast China.

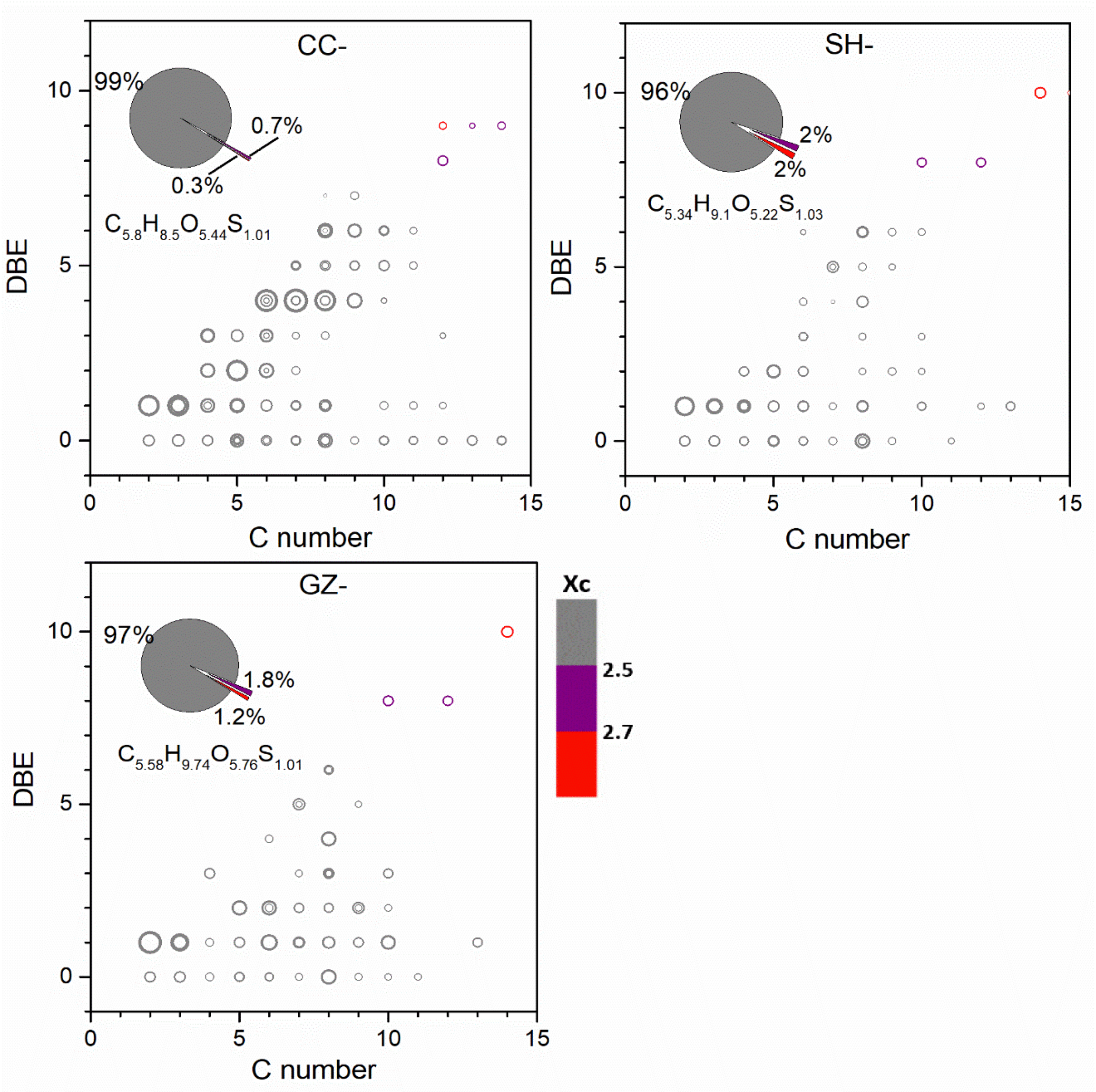

Figure 3.3.8: Double bond equivalent (DBE) vs C number for all CHOS- compounds of all samples. The molecular formula represents the abundance-weighted average CHOS- formula and the size of circles is proportional to the fourth root of the peak abundance of a individual compound. The color bar denotes the aromaticity equivalent (gray with $XC < 2.50$, purple with $2.50 \leq XC < 2.70$ and red with $XC \geq 2.70$). The size of pie chats is proportional to the peak abundances of each color-coded compounds in each sample.

### *3.3.6 CHONS*

4-5% of the total organics detected in ESI- were identified as CHONS- compounds, while it decreases to 0.3-1% in ESI+. The average MW of the CHONS- compounds are 214-293, showing greater masse than other organic species likely due to the presence of nitrate and sulfate functional groups. Only 8 common CHOS- formulas were detected in all three samples, accounting for 8%, 58% and 56% of the CHONS- peak abundance in CC-, SH- anf GZ-, respectively. It implies that the CHONS- compounds in SH- and GZ are characterized with similar chemical composition, while they are significantly different with those in CC-.

In the OA samples of SH- and GZ-, 78-87% of CHONS- formulas have 7 or more O atoms, allowing the assignment of one $-OSO_3H$ and one $-NO_3$ functional groups in the molecular structures and regarded as nitrooxy-OSs. However, in CC-, only 26% of CHONS- compounds were assigned as nitroooxy-OSs with more than 7 oxygen numbers, indicating that the most N atoms in the CHONS- compounds of CC- are presented in reduction state N, such as amine. The average DBE and Xc values of CHONS- compounds in SH- and GZ- are 3.3-3.45 and 0.43-0.44, respectively, while they are relatively higher in CC- with DBE of 3.75 and Xc of 1.06, indicating that CHONS- compounds in CC- have higher degree of unsaturation and aromaticity compared to SH- and GZ-. Interestingly, the compound with formula $C_{10}H_{17}O_7NS$ has the highest relatively abundance (32%) in SH- and GZ-, whereas in CC- the compound with formula $C_2H_3O_4NS$ is dominant. $C_{10}H_{17}O_7NS$ has been identified as pinanediol mononitrate generated from α-pinene (Surratt et al., 2008;Lin et al., 2012b;Wang et al., 2017), while $C_2H_3O_4NS$ are probably cyanomethyl hydrogen sulfate. It further illuminates that the precursors for CHONS- compounds in SH- and GZ- are different with those in CC-.

## 3.4 Conclusion

The molecular composition of the organic fraction of $PM_{2.5}$ samples collected in three Chinese megacities (CC, SH and GZ) was investigated using a UHPLC-Orbitrap MS. In total, 416-769 (ESI-) and 687-2943 (ESI+) organic compounds were observed, including five subgroups: CHO, CHN, CHON, CHOS and CHONS. 139 common formulas in ESI- and 168 common formulas in ESI+ were detected in all samples, accounting for 78-87% and 65-90% in terms of peak abundance. It indicates that the major organic compounds with high concentrations in CC, SH and GZ are characterized with similar chemical composition.

The most organic species including CHO, CHN and CHON compounds are dominated with mono or poly-aromatics in all three OA samples, indicating that anthropogenic emissions are the leading sources for Chinese urban OA. In addition, more polyaromatics were observed in CC samples, suggesting that coal burning plays an important role in the OA formation in CC. Moreover, the abundance-weighted average DBE and Xc values of the total organic compounds in CC are relatively higher than those in SH and GZ, showing that organic compounds in CC have higher degree of unsaturation and aromaticity. The average H/C and O/C ratios of compounds detected in ESI- in GZ is highest, followed by SH and GZ, indicating that OA collected in lower latitude regions of China experience more intense photochemical oxidation processes. The major CHOS- compounds are suggested to OSs, while OSs in SH and GZ share more similarity. The major CHONS- compounds in SH and GZ are assigned as nitrooxy-OSs and generated from biogenic precursor (e.g., α-pinene), whereas only 26% of CHONS- compounds are assigned to be nitrooxy-OSs, indicating that CHONS- compounds in SH and GZ are similar in terms of chemical composition, while they have big chemical difference with CHONS- in CC. This study gives a comprehensive overview of the chemical composition and possible sources of OA in three representative Chinese cities and in the future OA samples from more other Chinese cities could be analyzed by UHPLC-Orbitrap MS technique to better understand the formation mechanism of haze events in China.

**Supporting Information**

The detailed description of the data processing, six tables (Table S3.2.1-S3.2.6) and three supporting figures (Figure S3.3.1-S3.3.3).

**Acknowledgements**

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# 4 Molecular identification and source prediction of sulfur-containing compounds in urban OA

This chapter is a reprint of the manuscript:

Kai Wang, Yun Zhang, Rujin Huang, Junji Cao, Christopher Kampf, Yafang Cheng, Ulrich Pöschl, Marianne Glasius and Thorsten Hoffmann

## Molecular characterization and source prediction of atmospheric particulate organosulfates using ultrahigh resolution mass spectrometry

*In preparation for Atmospheric Chemistry and physics*

**Abstract.** Organosulfates (OSs) have been observed as substantial constituents of atmospheric organic aerosol (OA) in a wide range of environment, however, the chemical composition, sources and formation mechanism of OSs are still not yet well understood. In this study, we first created a 'OSs precursor map' based on the elemental composition information of previous OSs chamber experiments. Then according to this 'OSs precursor map', we estimated the possible sources and molecular structures of OSs in the ambient $PM_{2.5}$ (aerosol particles with aerodynamic equivalent diameter ≤ 2.5) samples, which were collected in the urban areas of Beijing (a Chinese city) and Mainz (a German city) and analyzed by an ultrahigh performance liquid chromatography (UHPLC) coupled with Orbitrap mass spectrometry (MS). As many as about 10 times more OSs species were observed in Beijing samples compared to Mainz samples. Based on the 'OSs precursor map', OSs in Mainz samples are suggested to be mainly derived from isoprene or other small polar organic compounds, while OSs in Beijing samples were generated from both isoprene and anthropogenic sources (e.g., long alkanes and aromatics). The nitrooxy-OSs in the aerosol samples collected in cleaner air in Mainz were mainly derived from monoterpenes, while much fewer monoterpene-derived nitrooxy-OSs were obtained in the polluted aerosol samples, showing that nitrooxy-OS formation is affected by different precursors in clean air condition and polluted air condition.

## 4.1 Introduction

Organic aerosol (OA) accounts for an important fraction (20-90%) of submicron atmospheric particulate mass (Jimenez et al., 2009;Kroll et al., 2011) and influences global climate, air quality and human health (Pöschl, 2005;Hallquist et al., 2009a;Pöschl and Shiraiwa, 2015). Atmospheric OA can be divided into two categories, as primary organic aerosol (POA) is directly emitted into the atmosphere from biogenic or anthropogenic source, whereas secondary organic aerosol (SOA) is formed from the condensation of primary gas precursors (Seinfeld and Pankow, 2003). Due to a wide variety of natural and anthropogenic sources as well as the complex multiphase chemical reactions, organic compounds in OA present a large space of physicochemical properties, including hydrocarbons, alcohols, carboxylic acids, organosulfates (OSs) and organonitrates. Hence, characterizing the chemical composition of the organics in OA is a challenging but vital task (Glasius and Goldstein, 2016;Wang et al., 2016;Wang et al., 2017;Wang et al., 2018).

Recently, OSs have been observed as an important fraction in the ambient OA (Iiuma et al., 2007;Kristensen and Glasius, 2011;Lin et al., 2012b;Lin et al., 2014;Nguyen et al., 2014;Tao et al., 2014;Wang et al., 2017;Huang et al., 2018;Wang et al., 2018). Due to the presence of a deprotonated functional group R-O-$SO_3^-$, OSs are acidic and highly water soluble and therefore may affect the surface activity and hygroscopic properties of the atmospheric particles, leading to potential impacts on climate (Hansen et al., 2015). To understand the sources, formation process and chemical composition of OSs, a few laboratory smog chamber studies have been conducted. In the presence of acidified sulfate aerosol seed, OSs have been produced in the chamber studies from $O_3$, OH or $NO_3$ oxidation of (Surratt et al., 2008) biogenic volatile organic compounds, such as isoprene, monoterpenes, sesquiterpene and unsaturated aldehydes (Surratt et al., 2007;Ng et al., 2008;Surratt et al., 2008;Iinuma et al., 2009) Recently, OSs derived from aromatics and long-chain alkanes have been reported by Riva et al. (Riva et al., 2015;Riva et al., 2016) to understand the effect of anthropogenic sources on OSs formation. However, due to a lack of authentic standards, identification and quantification of OSs is still a challenging task (Huang et al., 2018).

Previous studies on OSs were conducted mainly in Europe and USA (Iiuma et al., 2007;Surratt et al., 2007;Surratt et al., 2008;Kristensen and Glasius, 2011;Worton et al., 2011;Nguyen et al., 2012;Nguyen et al., 2014;Shalamzari et al., 2016;Martinsson et al., 2017), and only a few in China (Lin et al., 2012b;He et al., 2014;Ma et al., 2014;Tao et al., 2014;Wang et al., 2016;Huang et al., 2018). Over the past decade, severe air pollution has occurred frequently in China, seriously affecting the human health (Huang et al., 2014;Jiang et al., 2016;Wang et al., 2017). Therefore, a better understanding of the chemical composition and reactivity of OA including the OSs in China is important. Since OSs in urban areas are highly related to the anthropogenic emission and human activities, OSs formed in different cities present different characteristics (Tao et al., 2014). In this study, we have created a ‘OSs precursor map’ based on the elemental composition information of previous chamber experiments and compared the chemical composition and possible sources of OSs in atmospheric $PM_{2.5}$ samples (aerosol particles with aerodynamic equivalent diameter ≤ 2.5 μm) collected in two metropolises, Mainz (Germany) and Beijing (China), where the biogenic/anthropogenic emission and human activities present a large difference. Ultrahigh performance liquid chromatography (UHPLC) coupled to Orbitrap mass spectrometry was used for the detailed characterization of OS at a molecular level. Several synthesized/commercial OSs standards including isoprene/β-pinene/benzene-derived OSs, octyl hydrogen sulfate and laurilsulfate were used as markers to better identify the OSs detected in the ambient samples.

## 4.2 Material and methods

### *4.2.1 Collection of PM2.5 samples*

The 24-h integrated Chinese unban $PM_{2.5}$ samples were collected onto prebaked quartz-fiber filters (8×10 inch, Whatman, QM-A, USA) using a high-volume sampler at a flow rate of 1.05 $m^3$ $min^{-1}$ from 7-23 January 2014. Similarly, the 24-h integrated German urban $PM_{2.5}$ 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 $min^{-1}$ from 15-28 January 2015. The sampling site for Chinese samples was located at the urban site of Beijing (39.99 $^oN$, 116.39 $^oE$) surrounded by residential areas, while the German sampling site was in the campus of Johannes Gutenberg University of Mainz (50 $^oN$, 98 $^oE$). According to the $PM_{2.5}$ mass concentration in the atmosphere during the sample collection, the $PM_{2.5}$ samples in Beijing were divided into two categories for further analysis: Beijing low air pollution level samples with $PM_{2.5}$ mass concentrations lower than 35 μg $m^{-3}$ (sample ID: BJL); Beijing high air pollution samples with $PM_{2.5}$ mass concentrations higher than 150 μg $m^{-3}$ (sample ID: BJH). Since the $PM_{2.5}$ mass concentrations in Mainz were all lower than 35 μg $m^{-3}$ during sample collection, we regarded these samples as Mainz low level samples (sample ID: MZL). The field blank samples were collected at each site and all the filter samples were stored at -20 °C until analysis.

### *4.2.2 Sample analysis*

A portion of the filters (1.05-19.23 $cm^2$, corresponding to about 600 μg particle mass in each extracted filter) were ultrasonicated for 30 min with 1.5 mL acetonitrile/ultrapure water ($ACN/H_2O$) mixture (8/2, v/v). The extraction step was repeated twice with 1 mL of the $ACN/H_2O$ solution. After that, the extracts were combined and filtered through a 0.2 μm polytetrafluoroethylene (PTFE) membrane syringe filter to remove insoluble particulate matter. Then, the extracted solution was evaporated to dryness with a gentle stream of nitrogen at 20 °C. Afterwards, 1.0 mL $ACN/H_2O$ (1/9, v/v) was used to redissolve the residue for subsequent analysis.

The chemical identification of OSs was conducted using an UHPLC system (Dionex UltiMate 3000, Thermo Scientific, Germany) coupled to an ultrahigh resolution mass spectrometer (UHRMS) _Orbitrap (Q-Exactive mass spectrometer, Thermo Scientific, Germany). Analytes were separated by a Hypersil Gold column (C18, 50 x 2.0 mm, 1.9 µm particle size, Thermo Scientific, Germany). The mobile phase consisted of eluent A (ACN with 2% ultrapure $H_2O$) and eluent B (ultrapure $H_2O$ with 2% ACN and 0.04% formic acid). Gradient elution was optimized at flow rate of 0.5 mL $min^{-1}$ as follows: 2% A for 1.5 min, a linear increase to 20% A in the next 1 min, 20% A for 3 min, another linear increase to 30% A in 1 min, 30% A for another 1 min, a linear gradient to 50% A in 1 min and immediate increase to 98% A in the next 1 min, 98% A for 2.5 min, back to 2% A in

0.05 min and then 2% A for 0.05 min. The Orbitrap MS was equipped with a heated electrospray ionization source (HESI). It was operated in both negative ion mode (ESI-) and positive mode (ESI+) with a -3.3 kV and + 4.0 kV spray voltage, respectively. A mass resolving power of 70,000 @ m/z 200 and a scanning range of 50-500 m/z were applied. The mass spectrometer was externally mass calibrated using commercial standard calibration solution Ultramark 1621 (Thermo Scientific, Germany) with mass range of 73-1921 m/z. Each sample extracted was analyzed in triplicate with an injection volume of 10.0 μL.

### *4.2.3 Data processing*

The obtained chromatograms and mass spectra were analyzed by a non-target screening approach using a commercially available software (SIEVE®, Thermo Scientific, Germany). A threshold intensity value of $1\times10^5$ arbitrary units in the two-dimensional space of the retention time window from 0.0-11.05 min and m/z from 50-500 was applied to all measurements. The software automatically searched peaks above the threshold value which were significantly different from the background and assigned the molecular formulas with mass tolerance of ±2 ppm. The molecular formulas were presented as $C_cH_hO_oN_nS_s$, where c was the number of carbon atoms in the range of 1-39, h was the number of hydrogen atoms in the range of 1-72, o was the number of oxygen atoms in the range of 0-20, n was the number of nitrogen atoms in the range of 0-7, and s was the number of sulfur atoms in the range of 0-4. To remove the chemically non-meaningful molecular formulas, formulas were further constrained 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. Meanwhile, the resulting neutral formulas with a non-integer or negative double bond equivalent (DBE) or elemental composition which disobeyed the nitrogen rule for even electron ions were removed.

All molar ratios, DBE factors and molecular formulas presented in this paper refer to neutral molecules and only molecular formulas found in all $PM_{2.5}$ samples for BJL, BJH and MZL samples, respectively, were considered. The abundance of a compound refers to its average chromatographic peak area and only compounds with a sample-to-blank abundance ratio ≥ 10 were retained. Subsequently, the abundance of the retained compounds in the samples was blank-subtracted.

The DBE value (number of rings plus double bonds) of a molecule reflects the degree of its unsaturation and was calculated by Eq. (1) for the elemental composition $C_cH_hO_oN_nS_s$:

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

It should be noted that the main purpose of this study is to compare the difference of chemical composition and sources of OSs in Mainz and Beijing, so we excluded the OSs with low concentrations through reducing the injection volume from 20.0 µL in our previous study to 10 µL in this study and increasing the sample-to-blank ratio from 3 in our previous study to 10 in this study for data processing, which lead to much fewer organic compounds obtained in this study compared to our previous UHRMS study (Wang et al., 2018).

## 4.3 Results and discussion

### *4.3.1 Isomers*

The UHPLC system enables separation of potential isomers which could otherwise be hidden behind a given m/z value, as well as it provides additional information (e.g., retention time), which is helpful for elucidation of the molecular structures of organic compounds. In addition, hundreds of organic compounds can be separated using UHPLC before the ionization process, which can reduce the ion suppression in the ESI source, improving the sensitivity of detection.

Figure 4.3.1 shows the extracted ion chromatograms for the formula $C_{10}H_{17}O_7NS$, which has been identified as a nitrooxy-OSs derived from monoterpenes and presents relatively higher abundance compared to other S-containing compounds (Surratt et al., 2008; Lin et al., 2012; Wang et al., 2016; Brüggemann et al., 2016). As most of previous UHRMS studies on OSs mainly used direct infusion (Lin et al., 2012b;Tao et al., 2014;Kourtchev et al., 2016), no isomers with the formula $C_{10}H_{17}O_7NS$ were reported. Compared to three isomers of $C_{10}H_{17}O_7NS$ identified in α/β-pinene-derived chamber experiment by Surratt et al. (Surratt et al., 2008), in our study, 6 isomers of $C_{10}H_{17}O_7NS$ were obtained in all samples with varying abundances of each isomer in different sample IDs (See Fig. 4.3.1), indicating that nitrooxy-OSs are more complex in ambient atmosphere than those in the smog chamber simulations. The abundance of each isomer varies from sample to sample, reflecting the concentrations of corresponding precursors in different samples.

Figure 4.3.2 shows the reconstructed mass spectra of CHOS and CHONS compounds observed in Mainz and Beijing samples, where the x-axis corresponds to the neutral molecular weight of detected organic compounds, the y axis represents their relative abundances, and the number of isomers per detected mass is color-coded. Fig. 4.3.2 clearly shows that many more molecular formulas related to CHOS and CHONS compounds were detected in Beijing samples than in Mainz samples, indicating the relatively high abundance of S-containing compounds in Beijing OA, which are suggested to be formed from the burning of coal and oil (Huang et al., 2014). In Beijing samples, 34-57% of CHOS and CHONS compounds contain more than one isomer, while significantly fewer isomers were observed in Mainz samples. This result indicates that organic isomers widely exist in aerosol samples, especially in the polluted OA samples, and S-containing compounds are more complex in Beijing than those in Mainz samples.

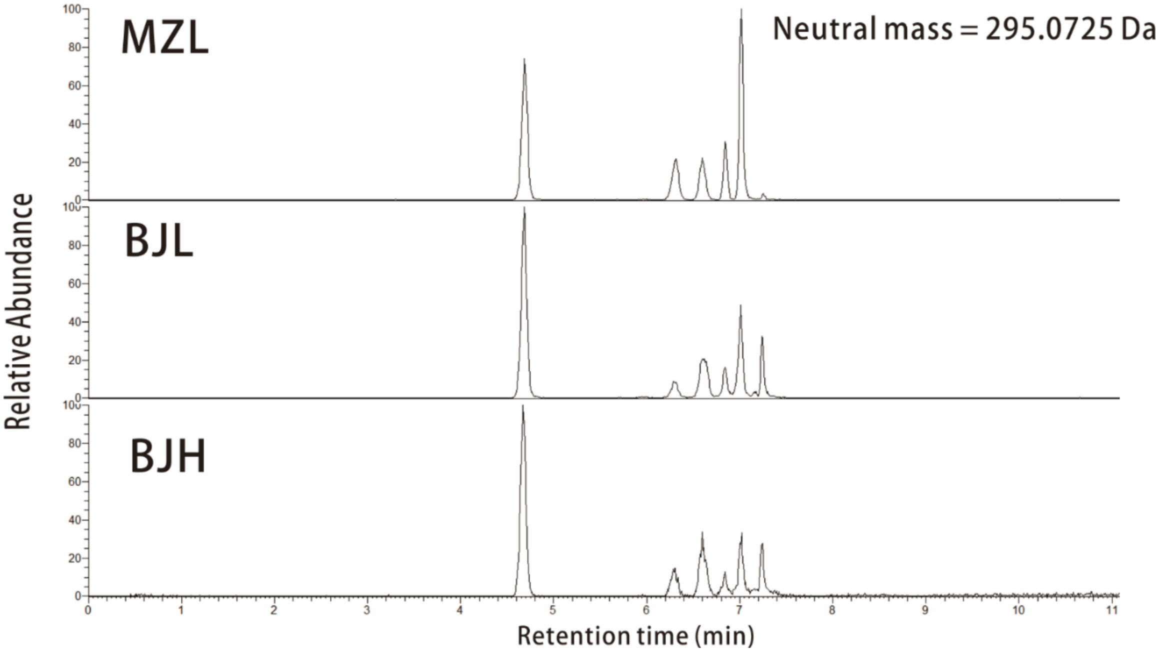

Figure 4.3.1: UHPLC chromatograms of tentatively determined $C_{10}H_{17}O_7NS$ (potentially derived from monoterpenes) in Mainz and Beijing samples.

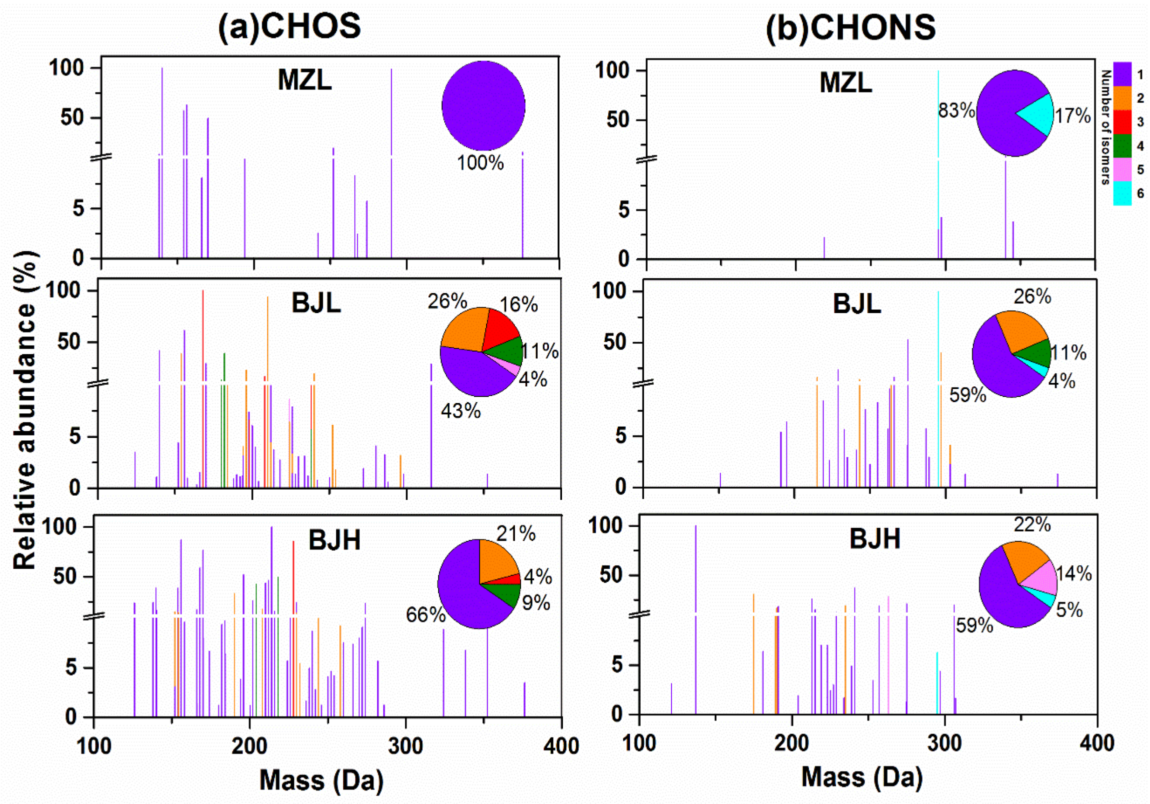

Figure 4.3.2: ESI- orbitrap mass spectra of detected CHOS (a) and CHONS (b) reconstructed from extracted ion chromatograms. The x-axis corresponds to the molecular weight (Da) of the identified species. The number of isomers for an assigned formula is marked by colors.

### 4.3.2 OSs precursor map

In previous studies, several smog chamber experiments have been conducted to understand the formation and chemical composition of OSs and nitrooxy-OSs generated from different precursors (Surratt et al., 2007;Surratt et al., 2008;Chan et al., 2011;Riva et al., 2015;Riva et al., 2016). In this study, we summarized the information (e.g., elemental composition, molecular weight, elemental ratios and DBE) of the identified OSs and nitrooxy-OSs (see Table S4.3.1) and then created a 'OSs precursor map' (see Figure 4.3.3a-b), which can be used to estimate the precursors of OSs and nitrooxy-OSs from the complex ambient aerosols.

Figure 4.3.3a-b show the 'OSs precursor map' for the OSs and nitrooxy-OSs generated from oxidation of biogenic precursors including isoprene, monoterpene and sesquiterpene as well as anthropogenic sources, like long alkane, benzene and naphthalene. The color bar in Figure 4.3.3 indicates the oxidation state of OSs and nitrooxy-OSs by (o-3s)/c and (o-3s-2n)/c ratios, respectively. Since the sulfate group and nitrate group respectively contains three and two more oxygen atoms compared to common oxygen-containing groups (e.g., hydroxyl and carbonyl), the use of (o-3s)/c and (o-3s-2n)/c ratios instead of traditional o/c ratio could better illustrate the number of additional oxidized groups per carbon atom. As shown in Figure 4.3.3a, the majority of OSs, except the benzene-derived OSs (solid star marks in Figure 4.3.3a), fall into a molecular corridor with upper and lower boundaries represented by linear alkane-derived OSs ($C_nH_{2n+1}SO_4$, red dashed line) and sugar alcohol-derived OSs ($C_nH_{2n+1}O_nSO_4$, black dashed line), respectively. Similarly, most nitroxy-OSs are plotted into a molecular corridor with upper and lower boundaries represented by linear alkane-derived nitrooxy-OSs ($C_nH_{2n}NO_3SO_4$, red dashed line) and sugar alcohol nitrooxy-OSs ($C_nH_{2n}O_nNO_3SO_4$, black dashed line). It indicates that this 2-D space of molecular weight and carbon number can constrain most of the OSs and nitrooxy-OSs generated from different precursors. Most isoprene-derived OSs (asterisk marks in Figure 4.3.3a) are situated close to the sugar alcohol-derived OSs line in the range of 2-5 carbon numbers (region I in Figure 4.3.3a) with high (o-3s)/c ratios (0.67≤ (0-3s)/c≤1.5), indicating that they are highly oxidized. And several OSs from isoprene dimers are also reported with carbon numbers exceeding 5 (region II in Figure 4.3.3a). The majority of OSs derived from monoterpenes (circle marks in Figure 4.3.3a), long alkanes (square marks in Figure 4.3.3a) and naphthalene (hollow star marks in Figure 4.3.3a) have a carbon number of 7-11 (region III in Figure 4.3.3a) with (0-3s)/c ratio between 0.12 and 0.57, while the sesquiterpene-derived OSs (triangle marks in Figure 4.3.3a) are in the range of 14-16 carbon atoms (region IV in Figure 4.3.3a) with (0-3s)/c ratio between 0.2 and 0.36. The OSs derived from benzene are located outside of the molecular corridor but close to the linear alkane-derived OSs line in the range of 6-9 carbon numbers (region V in Figure 4.3.3a) with low (0-3s)/c ratio. Meanwhile, according to the precursors, three different source regions for nitrooxy-OSs were defined as follows: region A with carbon number of 5 is dominant with isoprene-derived nitrooxy-OSs; region B with carbon number of 9 and 10 is occupied by the nitrooxy-OSs derived from monoterpene and naphthalene; region C with carbon number of 14 and 15 represents the sesquiterpene-derived nitrooxy-OSs.

As the UHPLC technique was applied in this study, the retention time of the organic compounds could be used as an additional information to approach the chemical structure properties, such as the polarity. Figure 4.3.3c shows the retention time of two synthesized isoprene-derived OSs (IEPOX OSs with formula $C_5H_{12}O_7S$ and hydroxyacetone OSs with formula $C_3H_6O_5S$), one β-pinene-derived OSs with formula $C_{10}H_{18}O_5S$, five benzene-derived OSs with formulas $C_6H_6O_4S$, $C_7H_8O_4S$, $C_8H_{10}O_4S$ (two isomers), and $C_9H_{12}O_4S$, and two commercial OSs standards (laurilsulfate with formula $C_{12}H_{26}O_4S$ and octyl hydrogen sulfate with formula $C_8H_{18}O_4S$). The synthetic procedures for these OSs standards have been previously described (Zhang et al., 2012;Huang et al., 2018). The retention time of the two synthesized isoprene-derived OSs is less than 1 minute. Such short retention time is caused by the polar functional groups of hydroxyl and carbonyl existing in the structures of isoprene-derived OSs, which are easily rinsed in the hydrophobic C18 column. The synthesized β-pinene-derived OSs and five benzene-derived OSs have the retention time between 1 and 4 minutes, indicating that less-polar functional groups exist in the chemical structures of OSs from monoterpene and aromatic precursors compared to isoprene-derived OSs. The two commercially available long alkane-derived OSs present the longest retention time (>4 minutes) compared to the other OSs, which is due to the strong bonding between the long alkane groups in OSs and the hydrophobic C18 column. Though the OSs and nitrooxy-OSs observed in the chamber simulations can not cover all the OSs and nitrooxy-OSs in the ambient organic aerosol, the ‘OSs precursor map’ and the retention time of OSs standards in Figure 4.3.3 can be used to estimate the precursors of OSs and nitrooxy-OSs generated in the ambient OA as well as better understand their molecular structures.

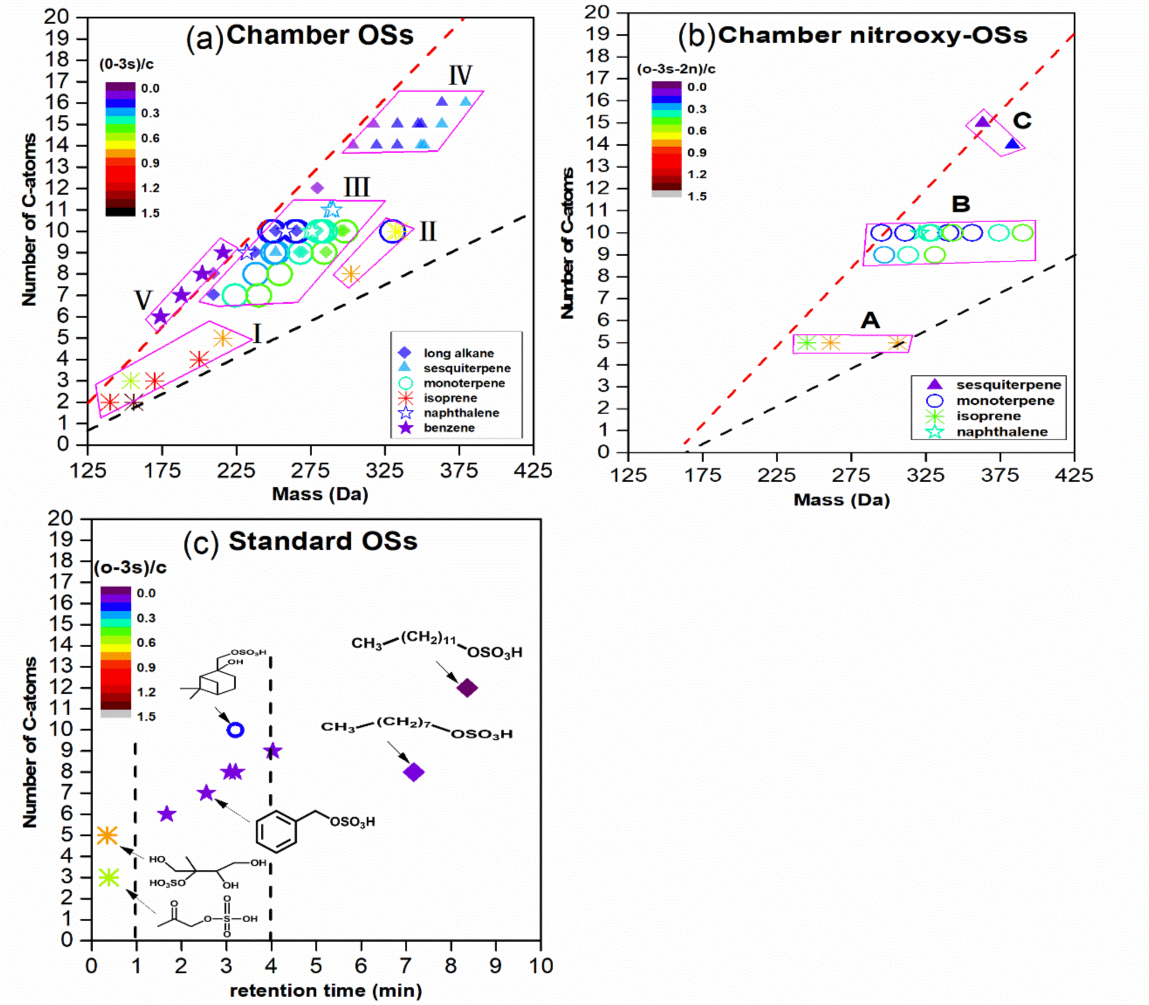

Figure 4.3.3: The OSs precursor map for OSs (a) and nitrooxy-OSs (b) represented by the molar mass and carbon number in the formulas. The dashed lines represent the molecular corridor by linear alkane OSs $C_nH_{2n+1}SO_4$ or nitrooxy-OSs $C_nH_{2n}NO_3SO_4$ (red dashed line) and sugar alcohol OSs $C_nH_{2n+1}O_nSO_4$ or nitrooxy-OSs $C_nH_{2n}O_nNO_3SO_4$ (black dashed line). The regions marked in roman numbers (I-V) in Fig. a represent OS derived from isoprene (I), isoprene dimers (II), monoterpenes/long alkene/naphthalene (III), sesquiterpene (IV) and benzene (V). The regions of A, B and C in Fig. b represent nitrooxy-OSs derived from isoprene, monoterpenes/naphthalene and sesquiterpenes, respectively. The chromatographic retention time of several standards of OSs together with their structures is shown in Fig. c. It should be noted that only one molecular structure of benzene-derived Os is shown in Fig. c due to the similar moleculare structures of these five benzene-derived OSs. The color bar indicates the (o-3s)/c or (o-3s-2n)/c ratio

### *4.3.3 Comparison of CHOS in Mainz and Beijing samples*

Table 4.3.1 summarizes the averaged characteristics (MW, elemental ratios, retention time and

DBE) of assigned CHOS and CHONS compounds. Compounds with a number of oxygen atoms greater that or equal to four were tentatively regarded as OSs (Lin et al., 2012b;Wang et al., 2016). However, tandem MS experiments were not conducted on the S-containing ions detected in these samples, and therefore, other S-containing compounds, such as sulfonates, may also assigned to this group. As many as 15-22% of organic compounds in Beijing samples were identified as CHOS compounds, while the fraction decreases to 11% in Mainz samples (Table 4.3.1). The majority (92-94%) of CHOS formulae were assigned with o/4s ≥ 1, suggesting that these compounds are OSs, which is consistent with previous studies (Lin et al., 2012b;Tao et al., 2014;Wang et al., 2016). The averaged O/C of CHOS compounds in Mainz samples is 1.44, which is significantly higher than that in Beijing samples (0.84 in BJL and 0.88 in BJH), indicating the higher oxidation state of OSs in Mainz OA. To estimate the precursors of OSs observed in Mainz and Beijing samples, the 'OSs precursor map' was applied in Figure 4.3.4a-c. The majority of OSs in both Mainz and Beijing samples fall into the molecular corridor represented by linear alkane OSs and sugar alcohol OSs, indicating that the the 2-D space of molar mass and carbon number can constrain not only the chamber OSs, but also the complex ambient aerosol OSs. As shown in Figure 4.3.4a, the most OSs in Mainz samples are plotted in the region I in a range of carbon number 2-5 with high (o-3s)/c ratio, indicating that OSs in Mainz were mainly derived from isoprene or other low carbon atom containing precursors. However, the OSs observed in Beijing samples covere almost all regions of I-V with the carbon number of 2-16, while OSs in region I (represented by isoprene-derived OSs) and region III (represented by monoterpene, long alkane and naphthalene derived OSs) are dominant. These observations together demonstrate that OSs in Mainz samples were mainly formed from biogenic source isoprene or other small molecules with carbon number ≤ 5 from anthropogenic emissions (Hansen et al., 2014), while OSs in Beijing samples are more complex and were generated from both biogenic and anthropogenic sources. Figure 4.3.4d-f show the retention time of OSs in the UHPLC system. The majority of OSs from Mainz samples have retention time below 1 minute with high (o-3s)/c ratio and 2-7 carbon numbers (see Figure 4.3.4d), further indicating that they are isoprene-derived. However, the OSs in Beijing samples showe a broad range of retention times between 0 and 9 minutes (see Figure 4.3.4e-f). As discussed above, OSs with a retention time of 0-1 minute are probably derived from isoprene or other small, polar molecules (Hansen et al., 2014), OSs with a retention time of 1-4 minutes are likely derived from monoterpenes, benzene and naphthalene, while OSs with a retention time of 4-9 minutes are probably derived from long alkane and sesquiterpenes, the broad rang of retention time additionally illuminates that OSs in Beijing aerosol were generated from both biogenic and anthropogenic precursors. Based on the carbon number, Figure 4.3.4g-i present the relative abundance of OSs detected in Mainz and Beijing samples. It shows that $C_3$-OSs are dominant in Mainz samples, which is suggested to be hydroxyacetone sulfate originated from photochemical oxidation of isoprene or anthropogenic emissions (e.g., biomass burning and fossil fuel combustion) (Hansen et al., 2014;Huang et al., 2018). However, $C_5$-OSs (probably related to isoprene-derived OSs) and $C_8$-OSs (likely related to aromatic OSs) showe the maximum intensities in BJL and BJH samples, respectively. Moreover, OSs with high carbon number ($C \geq 10$) in BJH samples have significantly higher abundance compared to those in MZL and BJL samples. This indicates that more OSs in polluted air are generated from long carbon-chain alkanes, which is consistent with Tao et al.'s study showing that the molecular structures of OSs collected in Shanghai contain longer carbon chain than those collected in Los Angeles (Tao et al., 2014).

Table 4.3.1 Summary of formula number, molecular weight (MW), elemental ratios, double bond equivalents (DBE) and retention time (RT) of assigned CHOS and CHONS detected in ESI- and ESI+ mode.

| Sample ID | Subgroup | Number of formulae[a] | Number of formulae with O/4S (or O/(4S+3N)) ≥ 1[b] | MW | H/C | O/C | DBE | RT (min) |
|---|---|---|---|---|---|---|---|---|
| MZL | CHOS- | 16 (11%) | 15 (94%) | 212 | 1.57 | 1.44 | 2.81 | 1.29 |
| | CHONS- | 9 (6%) | 6 (67%) | 297 | 1.55 | 0.61 | 4.33 | 4.54 |
| | CHONS+ | 11 (5%) | 0 (0%) | 247 | 1.27 | 0.44 | 5.55 | 3.48 |
| BJL | CHOS- | 114 (22%) | 105 (92%) | 212 | 1.89 | 0.84 | 1.46 | 2.73 |
| | CHONS- | 38 (7%) | 22 (58%) | 265 | 1.44 | 0.84 | 4.55 | 3.81 |
| | CHONS+ | 12 (1.4%) | 0 (0%) | 240 | 1.28 | 0.95 | 4.17 | 1.57 |
| BJH | CHOS- | 86 (15%) | 81 (94%) | 216 | 1.57 | 0.88 | 2.79 | 2.40 |
| | CHONS- | 36 (6.4%) | 14 (39%) | 229 | 1.28 | 0.95 | 4.17 | 1.78 |
| | CHONS+ | 18 (1.6%) | 0 (0%) | 235 | 1.62 | 0.82 | 3.50 | 1.84 |

[a]Values in the parentheses are the percentages of CHOS formulae among the total number of assigned formulae. [b]Values in the parentheses are the percentages of CHOS formulae with o/4s ≥1 and CHONS formulae with o/(4s+3n) ≥1 among the total number of CHOS formulae and CHONS formulae, respectively.

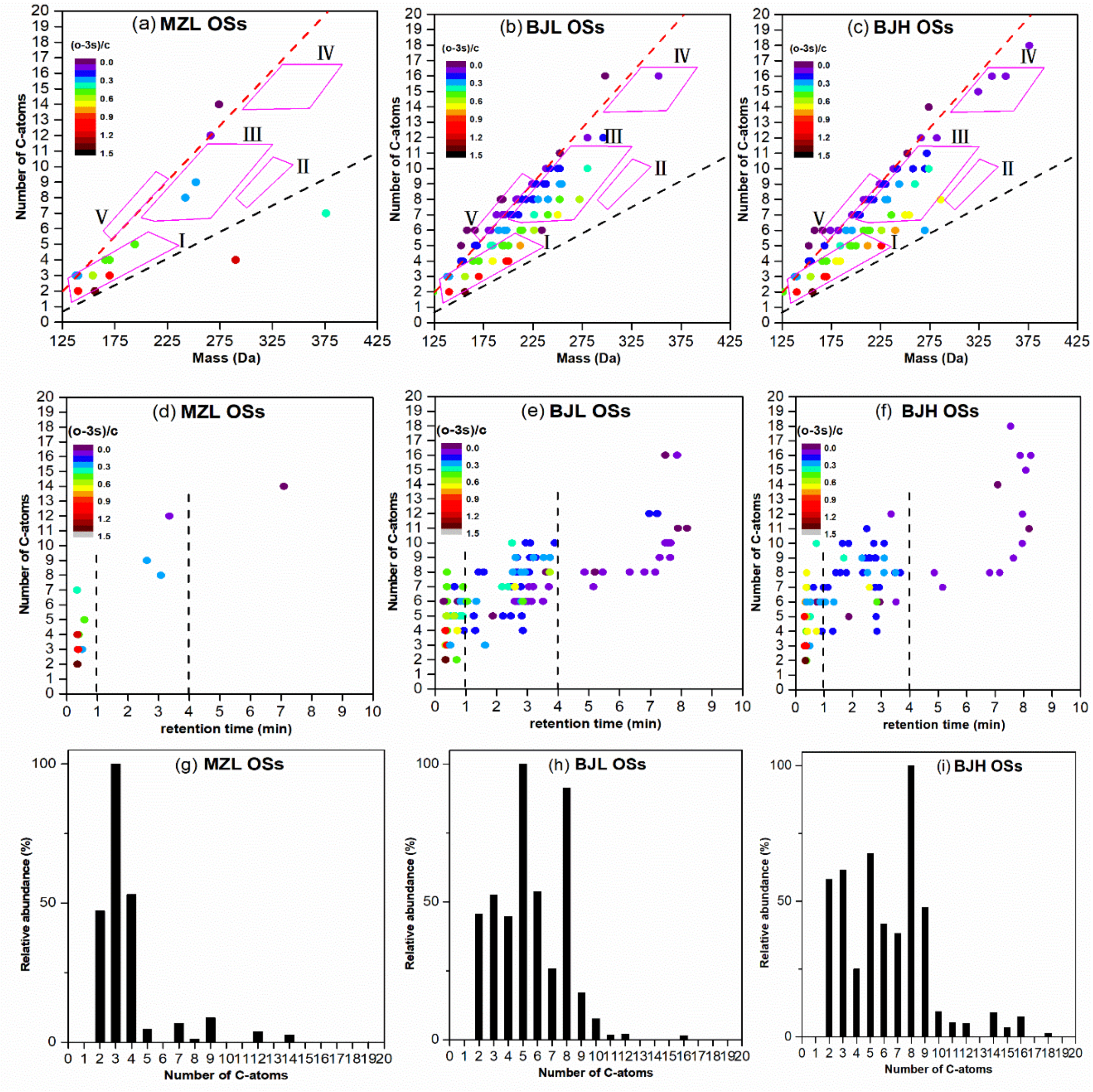

Figure 4.3.4: (a-c) the 'OSs precursor map' applied on the OSs detected in Mainz and Beijing samples. (d-f) the retention time of OSs in Mainz and Beijing samples. (g-i) the relative abundance distribution of OSs in Mainz and Beijing samples.

### 4.3.4 Comparison of CHONS in Mainz and Beijing samples

As shown in Table 4.3.1, 9-38 CHONS compounds were observed in Mainz and Beijing samples, which have higher averaged MW (235-297 Da) compared to CHOS compounds. In ESI-mode, 58-57% of CHONS- in Mainz and BJL samples containe enough oxygen atoms to allow assignment of -$OSO_3H$ and -$ONO_2$ groups ($o/(4s+3n) \geq 1$) in their formulas, indicating that they are nitrooxy-OSs (Lin et al., 2012b;Wang et al., 2016). However, only 39% of CHONS- compounds were assigned as nitrooxy-OSs in BJH samples, showing the large difference in chemical composition of CHONS- compounds in clean and polluted atmosphere.

Figure 4.3.5 shows the application of ‘OSs precursor map’ on the CHONS- compounds observed in Mainz and Beijing samples. As shown in Figure 4.3.5a-c, no nitrooxy-OSs plots (circles in Figure 4.3.5) are observed in region A and C, indicating that no isoprene or sesquiterpene-derived nitrooxy OSs were detected in Mainz and Beijing samples. A few nitrooxy-OSs plots are located in the region B, suggesting that they were probably generated from monoterpene or naphthalene precursors. In Beijing samples, many nitrooxy-OSs compounds are found outside of the molecular corridor but close to the linear alkane-derived nitrooxy-OSs line (see Figure 4.3.5b-c), indicating that the precursors of these nitrooxy-OSs are similar with linear alkane but more unsaturated. Meanwhile, several non-nitrooxy-OSs CHONS- compounds (triangle plots in Figure 4.3.5) were also obtained in Mainz and Beijing samples.

The diagrams of retention time plotted by carbon number in Figure 4.3.5d-f show that CHONS- compounds in both Mainz and Beijing samples have a broad retention time between 0 and 9 minutes. However, more CHONS- compounds with retention time less than four minutes were detected in Beijing samples, showing that more polar functional groups (e.g., hydroxy group) were formed in the Beijing CHONS- compounds. This observation is consistent with the results in Table 4.3.1 showing that higher O/C ratio of CHONS- are observed in Beijing samples compared to Mainz samples. The relative abundance of each subgroup of CHONS- compounds based on the carbon number is shown in Figure 4.3.5g-i. The CHONS compounds with carbon number of 10 (e.g., $C_{10}H_{17}O_7NS$) are dominant in Mainz and BJL samples, indicating that monoterpenes are the most important nitrooxy-OSs precursors in clean OA. However, in BJH samples, the CHONS compound with molecular formulae of $C_2H_2O_4NS$ shows the maximum abundance, which could be assigned as cyanogroup-containing OSs, indicating the different precursors for CHONS compounds between clean and polluted OA.

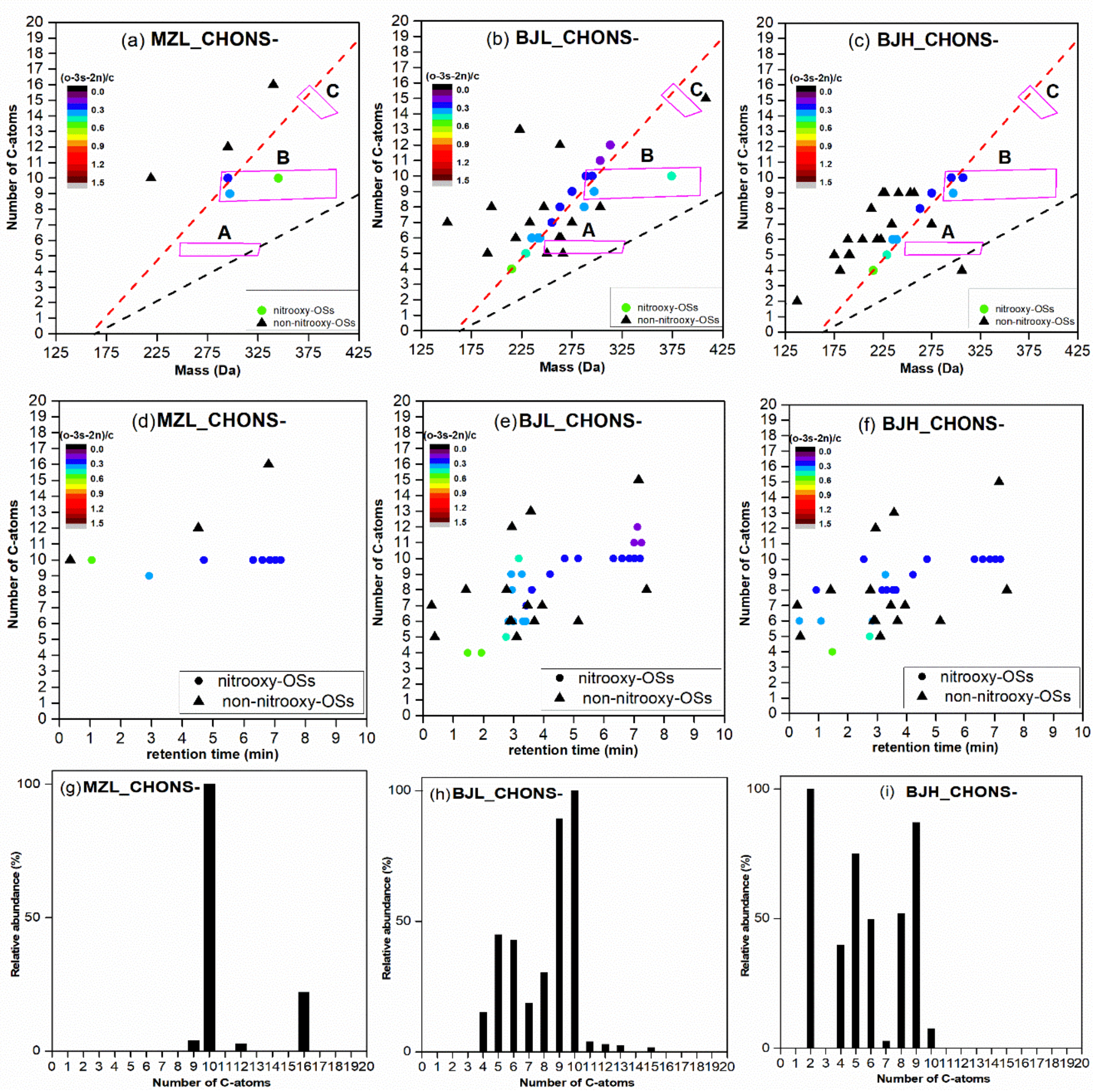

Figure 4.3.5: (a-c) the 'OSs precursor map' applied on the CHONS in Mainz and Beijing samples. (d-f) the retention time of CHONS in Mainz and Beijing samples. (g-i) the relative abundance distribution of CHONS in Mainz and Beijing samples.

## 4.4 Conclusion

In this study, $PM_{2.5}$ samples in Mainz and Beijing were analyzed using a UHPLC-Orbitrap MS technique. Only 16 molecular formulas of CHOS and 9-11 formulas of CHONS were detected in Mainz samples, while a large number of molecular formulas of CHOS and CHONS (86-114 formulas of CHOS and 12-38 formulas of CHONS) with various numbers of isomers were determined in Beijing samples. The majority (92-94%) of CHOS compounds were assigned as OSs, while 39-67% of CHONS compounds were identified as nitrooxy-OSs.

By summarizing the elemental composition information of OSs and nitrooxy-OSs observed in previous smog chamber studies, a ‘OSs precursor map’ with carbon number and molecular mass was established to constrain and estimate the precursors of OSs and nitrooxy-OSs obtained in ambient atmospheric OA. The majority of OSs in Mainz and Beijing samples can be constrained by the OSs molecular corridor from chamber studies in the ‘OSs precursor map’, while the molecular corridor of nitrooxy-OSs cannot constrain the ambient nitrooxy-OSs well due to the insufficient nitrooxy-OSs information from the chamber simulations. OSs derived from isoprene or other small molecules with less than five carbon atoms were dominant in Mainz samples, while in Beijing samples, OSs generated from anthropogenic sources (e.g., long alkane and aromatics) also showe a significant fraction. Nitrooxy-OSs generated from monoterpenes have the highest abundance in Mainz and BJL samples, while much fewer monoterpene-derived nitrooxy-OSs were observed in BJH samples, indicating that nitrooxy-OSs in clean OA have different chemical composition with those in polluted OA. The ‘OSs precursor map’ developed in this study for OSs and nitrooxy-OSs has been shown to provide important information on possible precursors and chemical properties of these compounds and will be useful in future studies of their formation and occurrence. Meanwhile, more information of elemental composition of OSs and nitrooxy-OSs identified in future chamber simulations can be used to perfect this ‘OSs precursor map’.

**Supporting Information**

Table S4.3.1 the information of elemental composition of identified OSs and nitrooxy-OSs in smog chamber experiments.

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# 5 Conclusions and Outlook

The application of ultrahigh resolution mass spectrometry (UHRMS) to characterize the chemical composition of the urban organic aerosol (OA) at a molecular level was demonstrated within this thesis. Based on the solvent mixture of acetonitrile and water, a simple OA extraction method was developed and proved to be efficient for both polar compounds (e.g., organic acids) and non-polar compounds (e.g., PAHs). UHPLC technique was applied prior to UHRMS coupled with ESI source, which was able to separate the isomer compounds and reduce the ion suppression. Since a large number of isomer compounds were detected in this thesis, UHPLC technique is highly suggested to be applied prior to the UHRMS in the future atmospheric analytical chemistry research. According to the mass spectra data observed in UHRMS, a non-target screening method was developed based a commercial software and more than 17000 organic compounds were identified in this thesis, which were classified in to CHO, CHON, CHN, CHOS, and CHONS compounds. Based on the molecular formulas of there organic compounds, various indexes (e.g., DBE, carbon oxidation state, and aromaticity equivalent) and diagrams, i.e. van Krevelen and Kendrick mass defect, were applied to interpret the UHRMS data and describe the chemical properties and possible sources of OA.

Comparing the UHRMS data between Mainz OA samples and Beijing OA samples, we found that 2-10 times more organic compounds were observed in Beijing than Mainz, indicating the highly complexity of Beijing OA. The majority organic compounds in Beijing shows a higher degree of unsaturation and aromaticity and lower degree of oxidation sate compared to that in Mainz, indicating the important influence of combustion emission (e.g., fossil fuel burning) on Beijing OA. Furthermore, the OA chemical composition from three Chinese cities: Changchun (CC, northeast of China), Shanghai (SH, central east of China) and Guangzhou (GZ, northeast of China) were identified and compared. The majority of organic compounds in these three cities have similar chemical composition and were dominant by aromatic compounds, indicating that anthropogenic sources are the most important precursors for the Chinses urban OA. More polycyclic aromatics were detected in CC, which were related to coal burning for the residential heating in winter in northeast China. The oxidation state of organic compounds in GZ was highest, followed by SH and CC, indicating that OA collected in lower latitude regions of China experienced more intense photochemical oxidation processes. In addition, by summarizing the chemical composition data of previous organosulfates (OSs) chamber experiments, a 'OSs precursor map' was created to estimate the possible sources for OSs in ambient OA. According to the 'OSs precursor map', OSs in Mainz is suggested to be mainly derived from biogenic sources (e.g., isoprene and monoterpene) or other small molecules, while OSs in Beijing were effected by both biogenic sources and anthropogenic sources (e.g., long alkane and aromatics).

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 ($MS^n$) 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, since the UHPLC-Orbitrap MS technique is unefficient for analyzing the high volatile compounds in aerosols as well as time limited, it is better to combine the UHPLC-Orbitrap MS technique with other MS techniques, such as gas chromatography (GC)-MS and online Aerosol Mass Spectrometer (AMS).

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# 7 Appendix

**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.

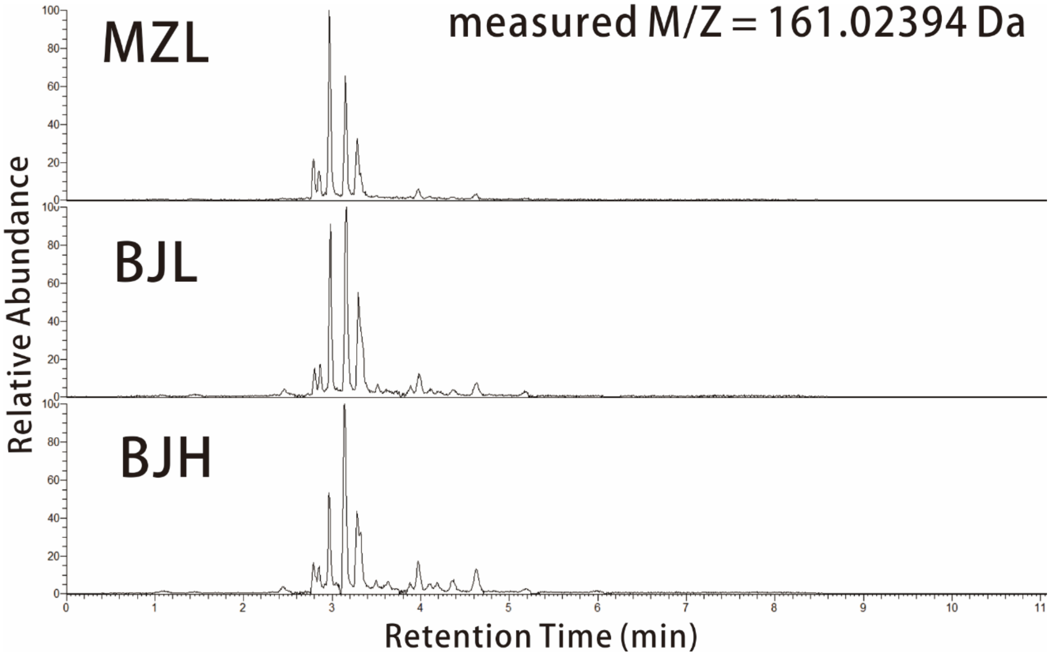

Figure S2.3.1: The UHPLC chromatograms of tentatively determined M/Z 161.02394 Da in Maniz and Beijing samples.

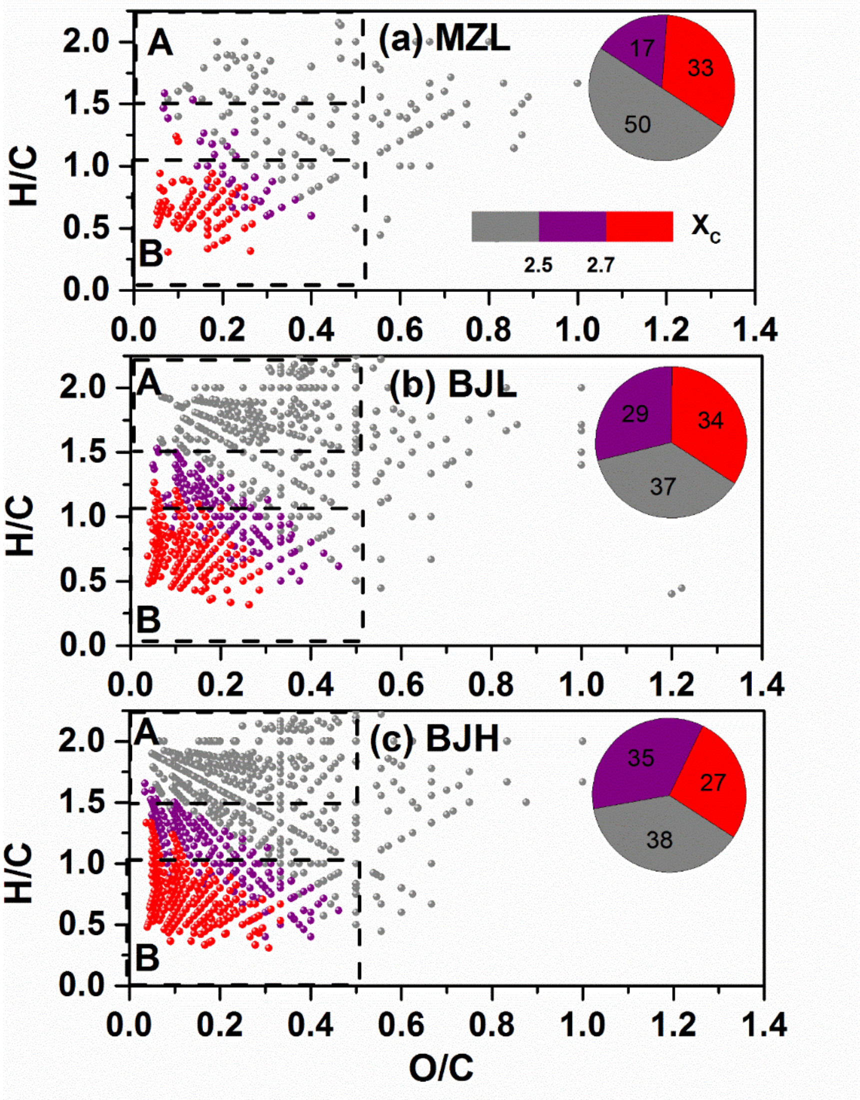

Figure S2.3.2: The van Krevelen diagram for CHO compounds detected in ESI+ mode. Areas ‘A’ and ‘B’ refer to aliphatic compounds and oxidised aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity equivalent (gray ball with $X_C < 2.50$, purple ball with $2.50 \leq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

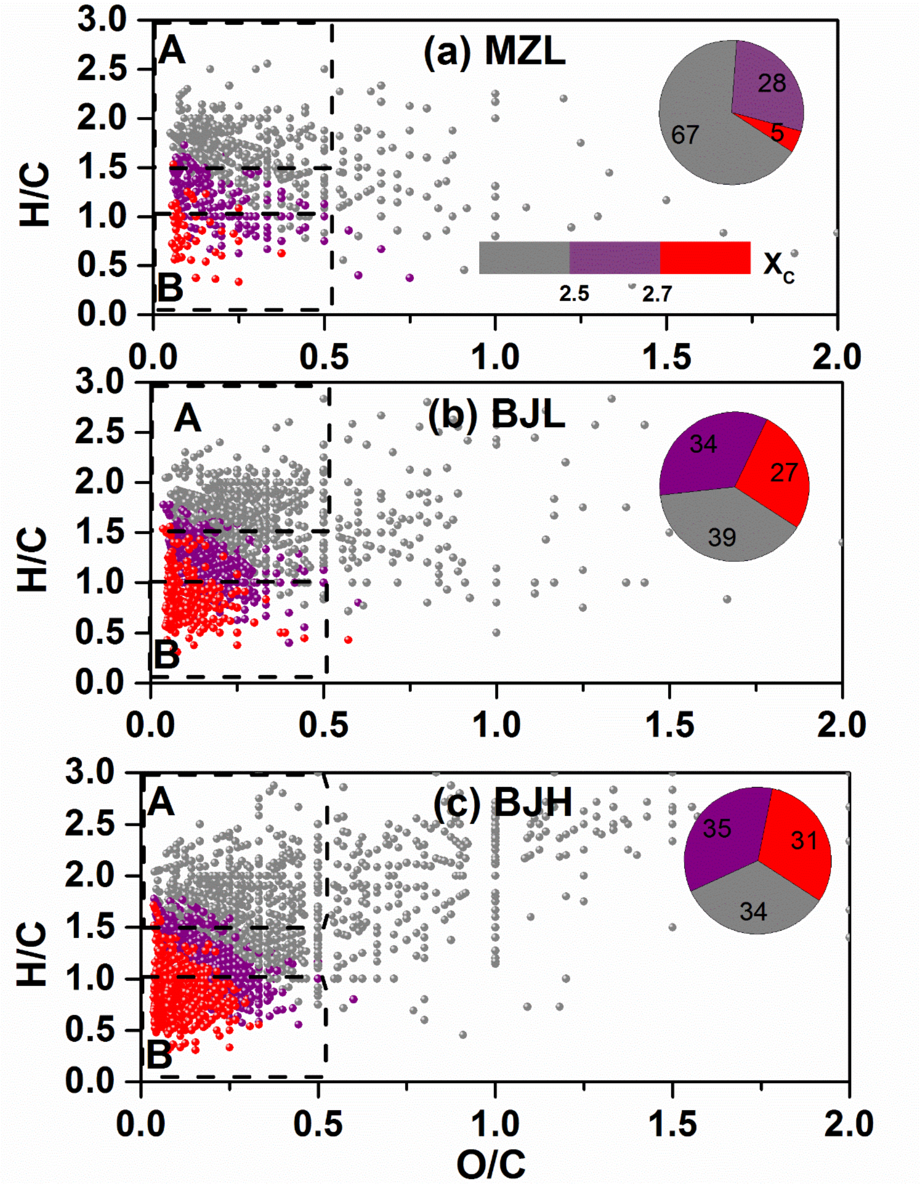

Figure S2.3.3: The van Krevelen diagram of CHON compounds detected in ESI+ mode. Areas 'A' and 'B' refer to aliphatic compounds and oxidised aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity equivalent (gray ball with $X_C < 2.50$, purple ball with $2.50 \leq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

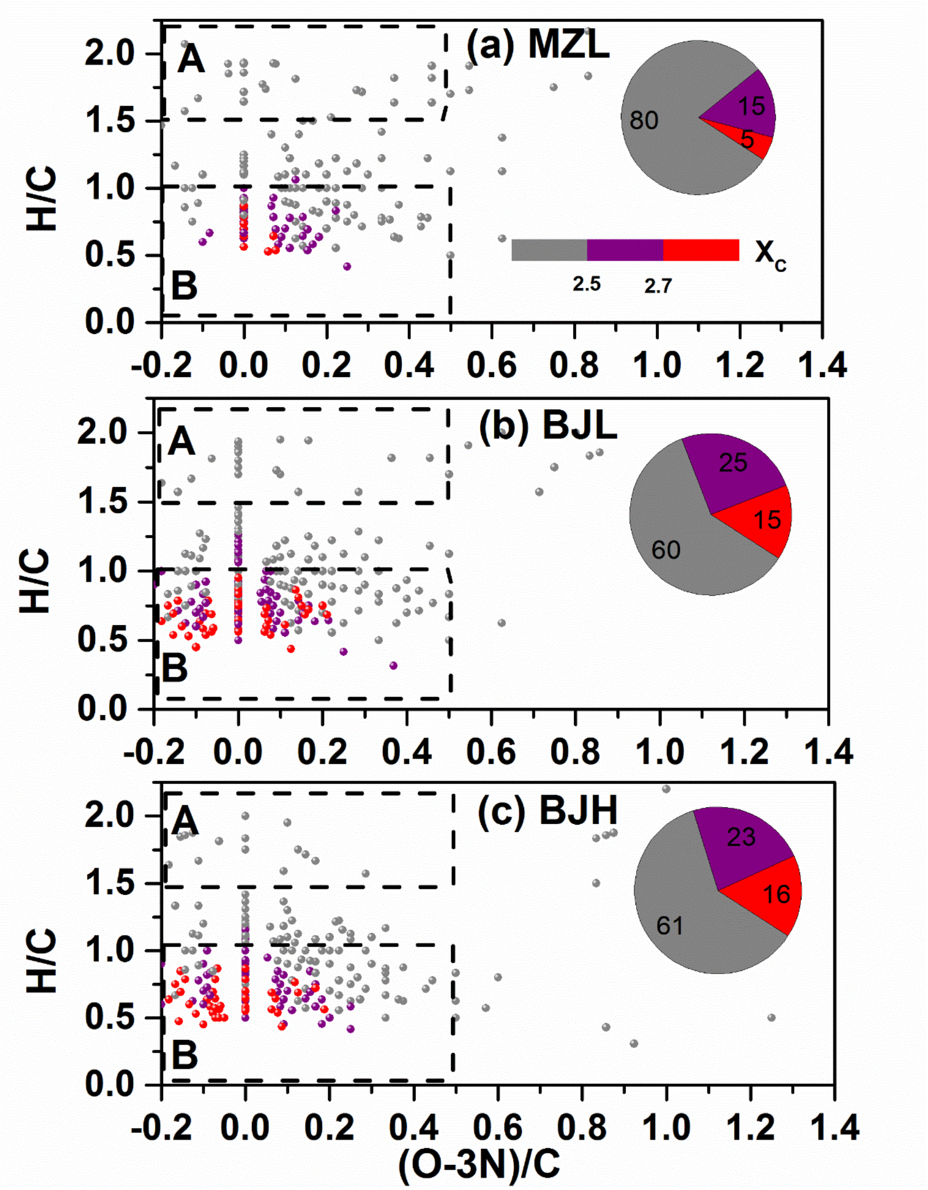

Figure S2.3.4: The van Krevelen diagram constructed by plotting the H/C ratio agaist the (O-3N)/C ratio for CHON compounds detected in ESI- mode. Areas ‘A’ and ‘B’ refer to aliphatic compounds and oxidised aromatic hydrocarbons in organic aerosol, respectively. The colour bar denotes the aromaticity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

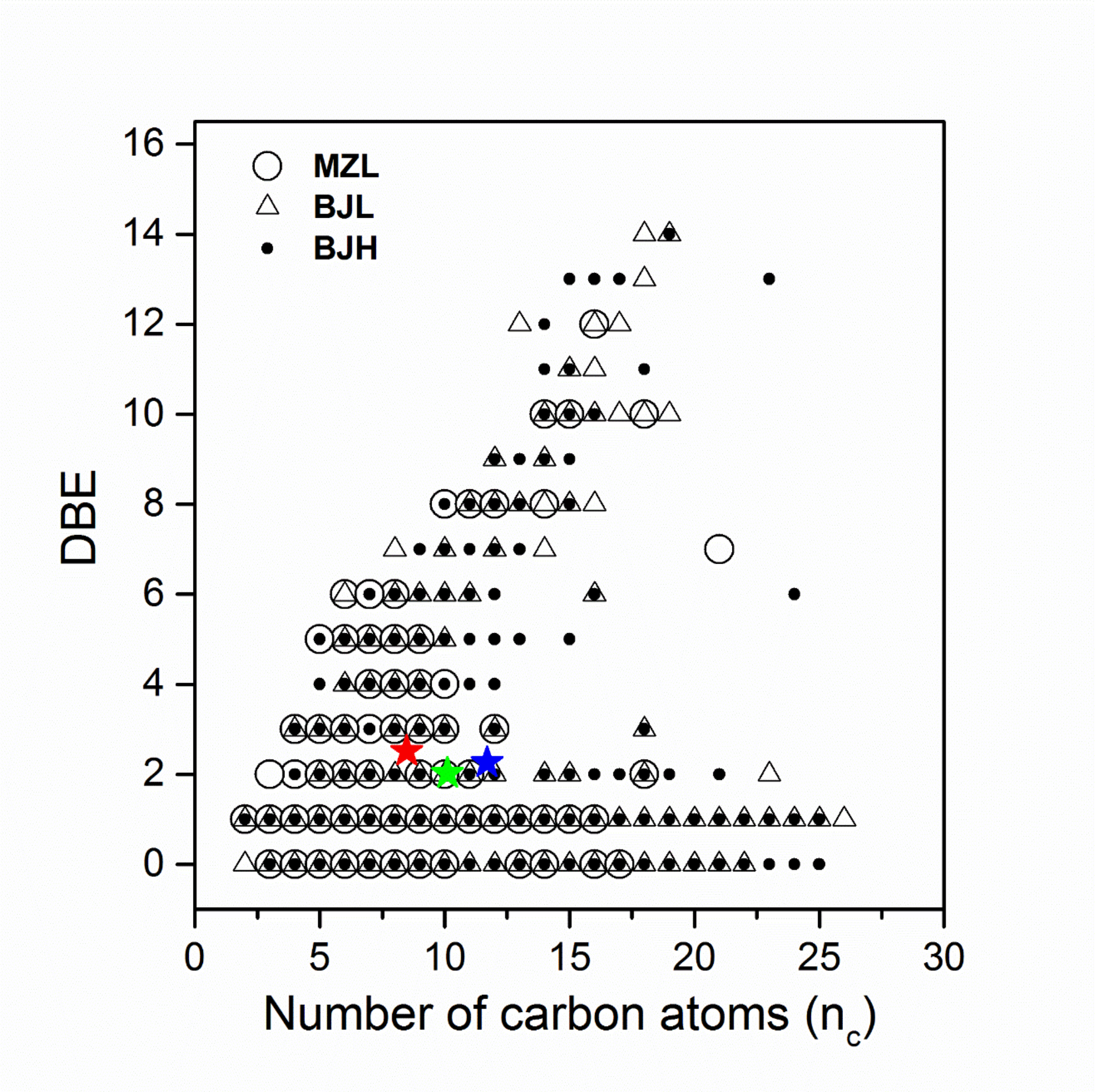

Figure S2.3.5: The DBE vs. carbon number diagram of CHOS compounds observed in MZL (circles), BJL (triangles) and BJH (dots). The stars in the figure indicate the averaged DBE and carbon number of CHOS compounds in MZL (red star), BJL (green star) and BJH (blue star).

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

## “Molecular characterization of organic aerosols in three cities at the northeast, central east and southeast of China using ultrahigh performance liquid chromatography coupled with Orbitrap mass spectrometry”

This supplementary material contains one appendice, six tables (S3.2.1-S3.2.6) and three figures (S3.3.1-S3.3.3).

Data processing for UHRMS:

The mass spectra were processed using a custom software named SIEVE, which was developed by Thermo Scientific in Germany. The detailed processing steps and settings in the software are showed as follows: A threshold peak abundance of $1\times10^5$ arbitrary units in the the two-dimensional space of the retention time window from 0-11.05 min and m/z window from 50-500 was applied to to all ions. The software automatically searched the ions with their peak abundance above the threshold and only ions with peak abundance in the ambient samples 10 times higher than those in the blank samples were retained. Subsequently, all mathematically possible formulas for these ions were calculated with a mass tolerance of ±2 ppm with the elemental number ranges of 1-39 ($^{12}C$), 1-72 ($^{1}H$), 0-20 ($^{16}O$), 0-7 ($^{14}N$), 0-4 ($^{32}S$) and 0-2 ($^{35}Cl$). In the positive mode (ESI+), 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. To remove the chemically unreasonable formulas, the identified formulas were further constraint 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. Meanwhile, 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 formulas detected in the three repetitions and observed in all three filter samples for each city were discussed in this study. The peak abundance of a compound in each city sample refers to the average area of its chromatographic peak in the three filter samples and was blank-corrected. After that, the arbitrary abundances of all isomers for a given formula were added up.

To reflect the degree of unsaturation of a compound, the double-boud equivalence (DBE) was calculated for chemical formula $C_cH_hO_oN_nS_sCl_x$:

$$DBE = (2c + 2 - h - x + n) / 2$$

Where c, h, x and n represent the numbers of atoms of carbon, hydrogen, chlorine and nitrogen, respectively.

Additionally, the aromaticity equivalent (Xc) was suggested to improve the identification and characterization of monoaromatic and polyaromatic compounds (Yassine et al., 2014;Kourtchev et al., 2016;Wang et al., 2017). Xc of the formula $C_cH_hO_oN_nS_sCl_x$ was calculated as follows:

$Xc = [3(DBE – (p × o + q × n)) – 2] / [DBE – (p × o + q × n)]$

where p and q, respectively, refer to the fraction of oxygen and sulfur atoms involved in in π-bond structure of a compound that varies based on the category of the compound. For example, carboxylic acids and esters are characterized using p = q = 0.5, while p = q = 1 and p = q = 0 are used for carbonyl and hydroxyl, respectively. Since it is impossible to identify the structurers of the hundreds of formulas observed in this study, we can not know the exact values of p and q in an individual compound. Therefor, in this study, p = q = 0.5 was applied for compounds detected in ESI- due to carboxylic compounds are prone to be ionized in negative mode. However, because of the high complexity of compounds detected in ESI+, p = q = 1 was used in ESI+ to avoid an overestimation of the amount of aromatics. Moreover, if $DBE \leq (p \times o + q \times n)$ or $X_C \leq 0$, then $X_C$ was defined as zero. When using p = q = 0.5 and (p × o + q × n) gave an odd number, the value of (p × o + q × n) was rounded down to the lower integer (Yassine et al., 2014). $Xc \geq 2.50$ and $Xc \geq 2.71$ are suggested to unambiguous minimum criteria for the presence of monoaromatics and polyaromatics, respectively (Yassine et al., 2014).

It is noted that different organic compounds have different signal response in the mass spectrometer, so uncertainties exist when comparing the peak areas of different. In this work, we assume that all organic compounds observed in this study have the same abundance response in the mass spectrometer when they are compared. And the abundance-weighted molecular weight, elemental ratios, DBE and Xc for formula $C_cH_hO_oN_nS_sCl_x$ were calculated using following equations:

$MW_w = \sum (MW_i \times A_i) / \sum A_i$

$O/C_w = \sum (O/C_i \times A_i) / \sum A_i$

$H/C_w = \sum (O/C_i \times A_i) / \sum A_i$

$DBE_w = \sum (O/C_i \times A_i) / \sum A_i$

$Xc_w = \sum (O/C_i \times A_i) / \sum A_i$

where $A_i$ was the peak abundance for each individual formula i.

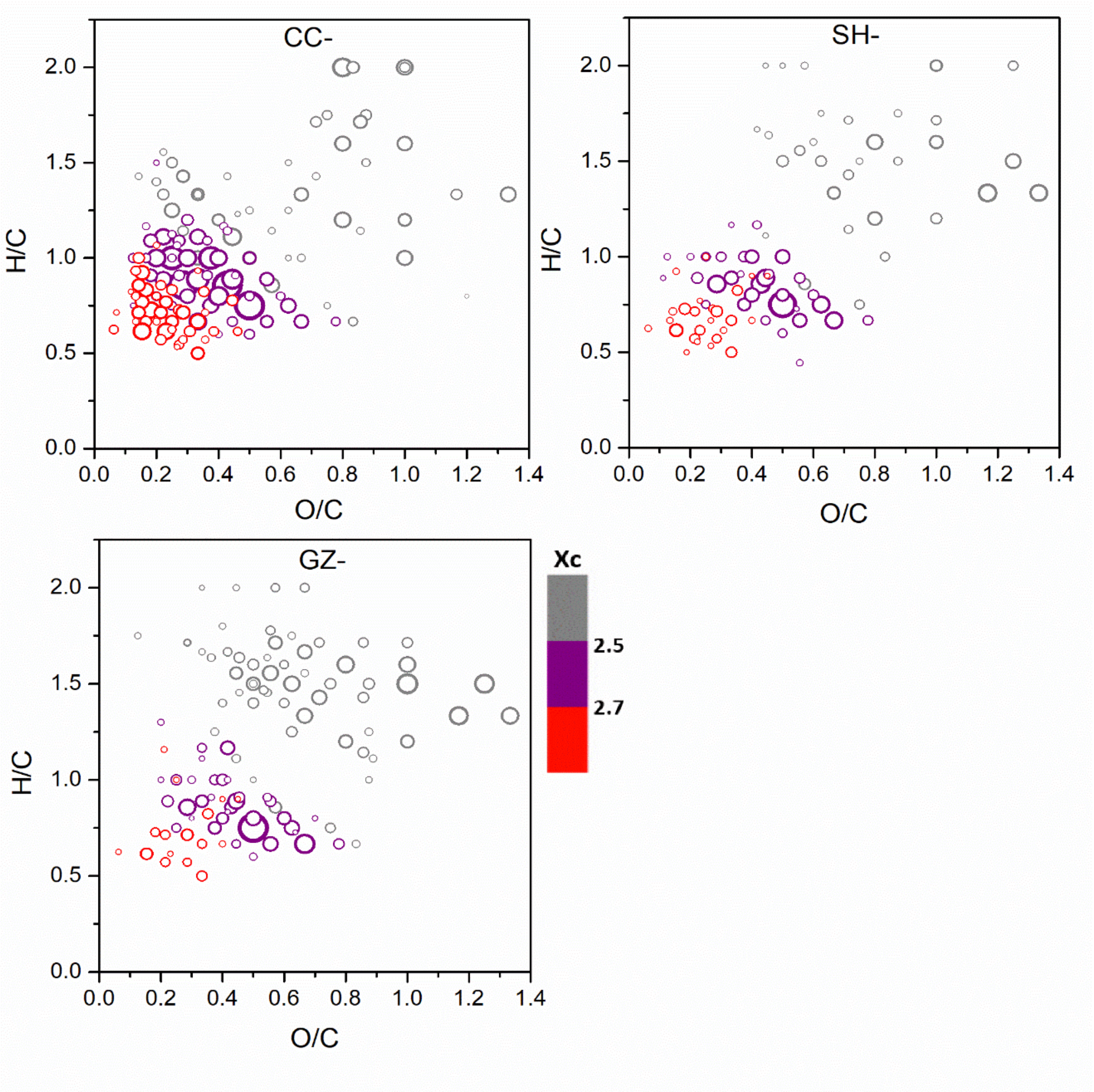

Figure S3.3.1. The van Krevelen diagram for CHO- compounds in CC, SH and GZ samples. The size of circles is proportional to the fourth root of the peak abundance of a individual compound and the color bar denotes the aromaticity equivalent (gray with XC < 2.50, purple with 2.50 ≤ XC < 2.70 and red with XC ≥ 2.70).

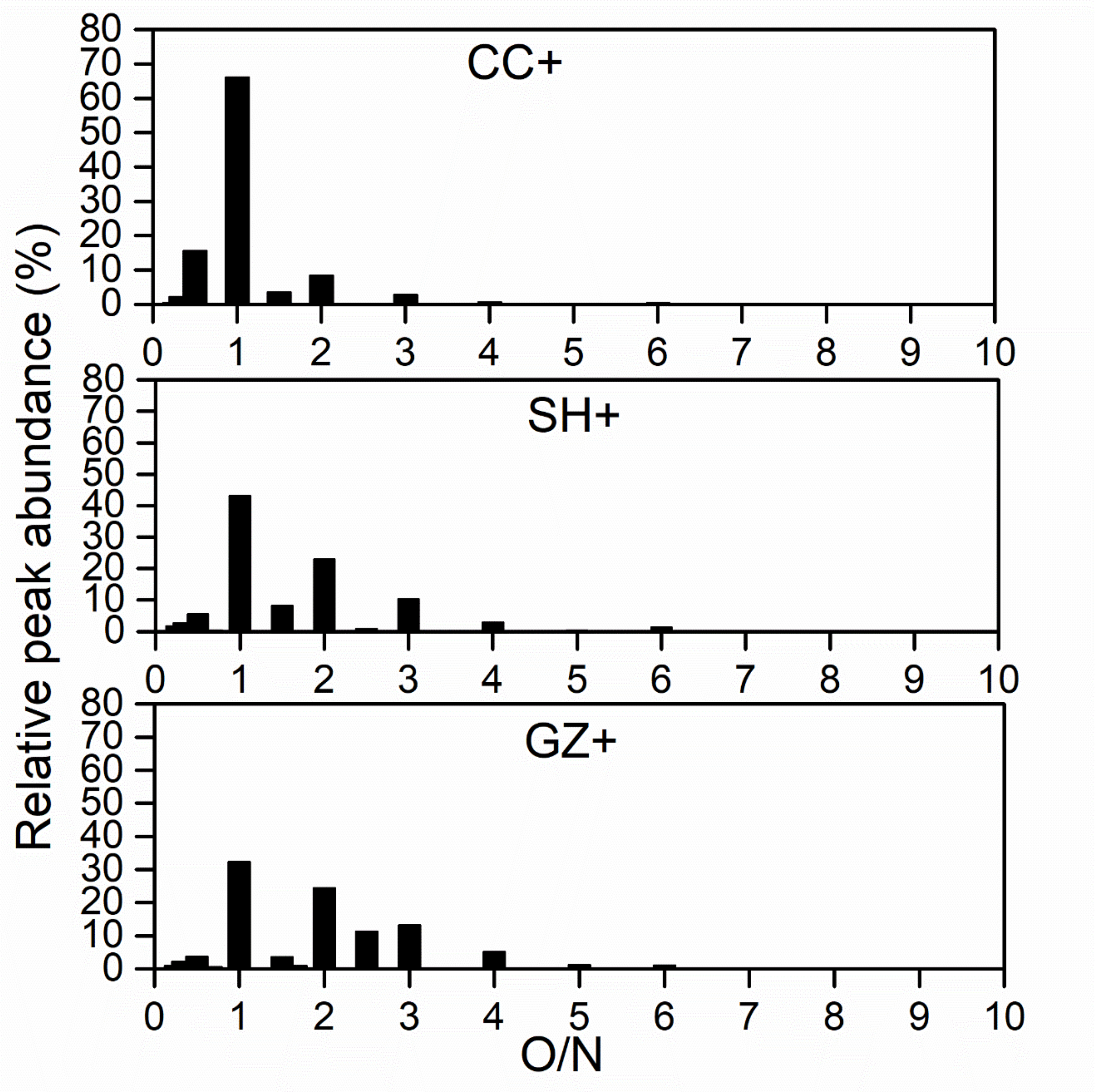

Figure S3.3.2: Classification of CHON+ compounds into different subgroups according to O/N ratios in their formulas. The y-axis indicates the relative contribution of each subgroup to the sum of peak abundance of CHON+ compounds.

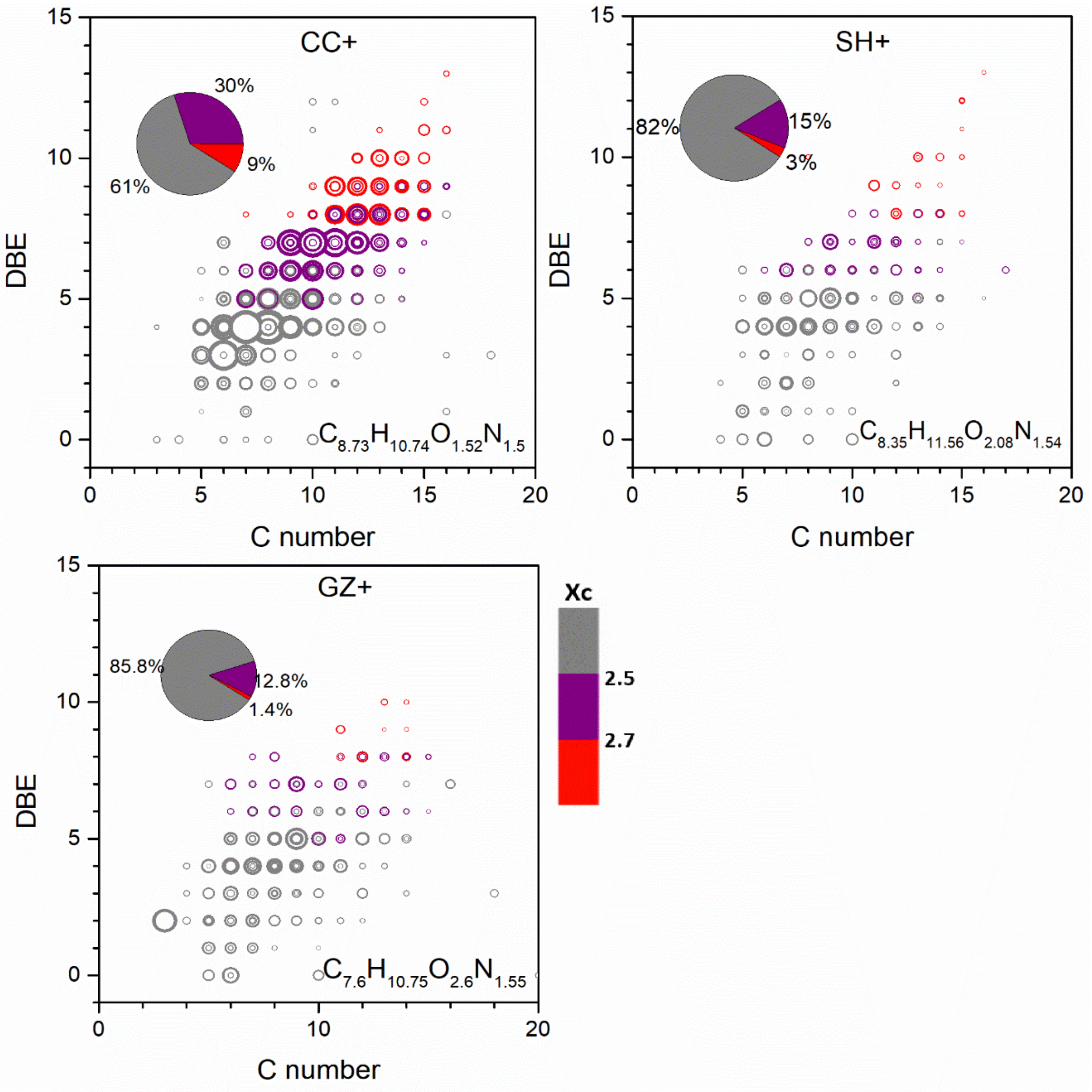

Figure S3.3.3: Double bond equivalent (DBE) vs C number for all CHON+ compounds of all samples. The molecular formula represents the abundance-weighted average CHON+ formula and the size of circles is proportional to the fourth root of the peak abundance of a individual compound. The color bar denotes the aromaticity equivalent (gray with XC < 2.50, purple with 2.50 ≤ XC < 2.0 and red with XC ≥ 2.70). The size of pie chats is proportional to the peak abundances of each color-coded compounds in each sample.

Table S3.2.1 Molecular formulas of organic compounds detected in CC in ESI- mode.

| Formula [M-H] | Neutral mass (Da) | RT (min) | DBE | H/C | O/C |
|---|---|---|---|---|---|
| C3H5O6S1 | 169.9885 | 0.39 | 1 | 2.00 | 2.00 |
| C3H3O4 | 104.0110 | 0.37 | 2 | 1.33 | 1.33 |
| C6H6O1N1 | 109.0528 | 0.47 | 4 | 1.17 | 0.17 |
| C6H5O2 | 110.0368 | 1.87 | 4 | 1.00 | 0.33 |
| C7H9O1 | 110.0732 | 2.53 | 3 | 1.43 | 0.14 |
| C5H7O5 | 148.0372 | 0.38 | 2 | 1.60 | 1.00 |
| C6H7O2 | 112.0524 | 1.02 | 3 | 1.33 | 0.33 |
| C6H7O2 | 112.0524 | 3.25 | 3 | 1.33 | 0.33 |
| C4H3O4 | 116.0110 | 0.39 | 3 | 1.00 | 1.00 |
| C3H4O5N1 | 135.0168 | 0.39 | 2 | 1.67 | 1.67 |
| C8H5O1 | 118.0419 | 3.17 | 6 | 0.75 | 0.13 |
| C7H4O1N1 | 119.0371 | 3.16 | 6 | 0.71 | 0.14 |
| C7H4O1N1 | 119.0371 | 3.36 | 6 | 0.71 | 0.14 |
| C8H7O1 | 120.0575 | 3.09 | 5 | 1.00 | 0.13 |
| C8H7O1 | 120.0575 | 3.37 | 5 | 1.00 | 0.13 |
| C7H6O1N1 | 121.0528 | 3.20 | 5 | 1.00 | 0.14 |
| C5H9O7S1 | 214.0147 | 0.38 | 1 | 2.00 | 1.40 |
| C7H5O2 | 122.0368 | 2.77 | 5 | 0.86 | 0.29 |
| C2H4O3N1S1 | 122.9990 | 0.29 | 1 | 2.50 | 1.50 |
| C2H3O4S1 | 123.9830 | 0.71 | 1 | 2.00 | 2.00 |
| C2H3O4S1 | 123.9830 | 1.66 | 1 | 2.00 | 2.00 |
| C7H7O2 | 124.0524 | 3.07 | 4 | 1.14 | 0.29 |
| C2H5O4S1 | 125.9987 | 0.38 | 0 | 3.00 | 2.00 |
| C6H7O7S1 | 223.9991 | 0.38 | 3 | 1.33 | 1.17 |
| C7H9O2 | 126.0681 | 2.05 | 3 | 1.43 | 0.29 |
| C7H9O2 | 126.0681 | 2.54 | 3 | 1.43 | 0.29 |
| C5H5O5 | 146.0215 | 0.38 | 3 | 1.20 | 1.00 |
| C5H8O7N1S2 | 258.9820 | 0.29 | 2 | 1.80 | 1.40 |
| C5H5O4 | 130.0266 | 0.60 | 3 | 1.20 | 0.80 |
| C5H7O4 | 132.0423 | 0.77 | 2 | 1.60 | 0.80 |
| C5H7O4 | 132.0423 | 1.11 | 2 | 1.60 | 0.80 |
| C8H9O4N2S1 | 230.0361 | 3.12 | 5 | 1.25 | 0.50 |
| C8H8O7N1S1 | 263.0100 | 3.61 | 5 | 1.13 | 0.88 |
| C8H6O1N1 | 133.0528 | 4.04 | 6 | 0.88 | 0.13 |
| C8H6O1N1 | 133.0528 | 4.50 | 6 | 0.88 | 0.13 |
| C8H6O1N1 | 133.0528 | 4.83 | 6 | 0.88 | 0.13 |
| C8H5O2 | 134.0368 | 1.80 | 6 | 0.75 | 0.25 |
| C5H9O4 | 134.0579 | 0.39 | 1 | 2.00 | 0.80 |
| C7H4O2N1 | 135.0320 | 2.71 | 6 | 0.71 | 0.29 |
| C7H4O2N1 | 135.0320 | 2.92 | 6 | 0.71 | 0.29 |
| C8H7O2 | 136.0524 | 3.02 | 5 | 1.00 | 0.25 |
| C8H7O2 | 136.0524 | 3.19 | 5 | 1.00 | 0.25 |
| C8H7O2 | 136.0524 | 3.36 | 5 | 1.00 | 0.25 |
| C8H7O2 | 136.0524 | 3.55 | 5 | 1.00 | 0.25 |
| C8H7O2 | 136.0524 | 3.75 | 5 | 1.00 | 0.25 |
| C2H2O4N1S1 | 136.9783 | 0.38 | 2 | 1.50 | 2.00 |
| C3H5O4S1 | 137.9987 | 0.35 | 1 | 2.00 | 1.33 |
| C3H5O4S1 | 137.9987 | 1.60 | 1 | 2.00 | 1.33 |
| C7H5O3 | 138.0317 | 2.14 | 5 | 0.86 | 0.43 |
| C7H5O3 | 138.0317 | 2.29 | 5 | 0.86 | 0.43 |

| | | | | | |
|---|---|---|---|---|---|
| C7H5O3 | 138.0317 | 2.80 | 5 | 0.86 | 0.43 |
| C7H5O3 | 138.0317 | 3.59 | 5 | 0.86 | 0.43 |
| C8H9O2 | 138.0681 | 2.94 | 4 | 1.25 | 0.25 |
| C8H9O2 | 138.0681 | 4.12 | 4 | 1.25 | 0.25 |
| C8H9O2 | 138.0681 | 4.22 | 4 | 1.25 | 0.25 |
| C6H4O3N1 | 139.0269 | 3.79 | 5 | 0.83 | 0.50 |
| C6H3O4 | 140.0110 | 0.39 | 5 | 0.67 | 0.67 |
| C3H7O4S1 | 140.0143 | 0.50 | 0 | 2.67 | 1.33 |
| C5H3O3N2 | 140.0222 | 2.42 | 5 | 0.80 | 0.60 |
| C7H7O3 | 140.0473 | 0.79 | 4 | 1.14 | 0.43 |
| C6H9O6N2S1 | 238.0260 | 0.37 | 3 | 1.67 | 1.00 |
| C8H11O2 | 140.0837 | 2.79 | 3 | 1.50 | 0.25 |
| C8H11O2 | 140.0837 | 2.93 | 3 | 1.50 | 0.25 |
| C6H5O4 | 142.0266 | 0.40 | 4 | 1.00 | 0.67 |
| C6H5O4 | 142.0266 | 0.86 | 4 | 1.00 | 0.67 |
| C7H9O3 | 142.0630 | 2.85 | 3 | 1.43 | 0.43 |
| C8H4O12N1 | 306.9812 | 0.36 | 7 | 0.63 | 1.50 |
| C8H3O1N2 | 144.0324 | 3.47 | 8 | 0.50 | 0.13 |
| C8H3O1N2 | 144.0324 | 3.73 | 8 | 0.50 | 0.13 |
| C6H7O4 | 144.0423 | 0.70 | 3 | 1.33 | 0.67 |
| C9H6O1N1 | 145.0528 | 2.28 | 7 | 0.78 | 0.11 |
| C9H6O1N1 | 145.0528 | 3.51 | 7 | 0.78 | 0.11 |
| C9H6O1N1 | 145.0528 | 4.19 | 7 | 0.78 | 0.11 |
| C8H4O2N1 | 147.0320 | 3.29 | 7 | 0.63 | 0.25 |
| C9H7O2 | 148.0524 | 2.98 | 6 | 0.89 | 0.22 |
| C9H9O3 | 166.0630 | 3.12 | 5 | 1.11 | 0.33 |
| C9H7O2 | 148.0524 | 3.25 | 6 | 0.89 | 0.22 |
| C8H2O8N5 | 296.9982 | 0.39 | 10 | 0.38 | 1.00 |
| C8H6O2N1 | 149.0477 | 3.39 | 6 | 0.88 | 0.25 |
| C8H5O3 | 150.0317 | 2.66 | 6 | 0.75 | 0.38 |
| C8H5O3 | 150.0317 | 2.90 | 6 | 0.75 | 0.38 |
| C5H9O5 | 150.0528 | 0.35 | 1 | 2.00 | 1.00 |
| C9H9O2 | 150.0681 | 3.71 | 5 | 1.11 | 0.22 |
| C9H9O2 | 150.0681 | 3.90 | 5 | 1.11 | 0.22 |
| C9H9O2 | 150.0681 | 4.34 | 5 | 1.11 | 0.22 |
| C9H9O2 | 150.0681 | 5.08 | 5 | 1.11 | 0.22 |
| C9H9O2 | 150.0681 | 5.23 | 5 | 1.11 | 0.22 |
| C8H8O2N1 | 151.0633 | 1.78 | 5 | 1.13 | 0.25 |
| C5H9O6S1 | 198.0198 | 0.38 | 1 | 2.00 | 1.20 |
| C8H7O3 | 152.0473 | 1.78 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 2.67 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 3.08 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 3.26 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 3.40 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 3.55 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 3.67 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 3.82 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 4.40 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 5.42 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 5.58 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 6.30 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 3.77 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 4.65 | 5 | 1.00 | 0.38 |

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| C9H11O2 | 152.0837 | 6.11 | 4 | 1.33 | 0.22 |
| C9H11O2 | 152.0837 | 6.63 | 4 | 1.33 | 0.22 |
| C9H11O2 | 152.0837 | 7.16 | 4 | 1.33 | 0.22 |
| C7H6O3N1 | 153.0426 | 5.28 | 5 | 1.00 | 0.43 |
| C7H6O3N1 | 153.0426 | 6.13 | 5 | 1.00 | 0.43 |
| C3H5O5S1 | 153.9936 | 0.37 | 1 | 2.00 | 1.67 |
| C7H5O4 | 154.0266 | 1.32 | 5 | 0.86 | 0.57 |
| C7H5O4 | 154.0266 | 2.27 | 5 | 0.86 | 0.57 |
| C7H5O4 | 154.0266 | 2.71 | 5 | 0.86 | 0.57 |
| C7H5O4 | 154.0266 | 2.96 | 5 | 0.86 | 0.57 |
| C7H5O4 | 154.0266 | 3.34 | 5 | 0.86 | 0.57 |
| C4H9O4S1 | 154.0300 | 0.94 | 0 | 2.50 | 1.00 |
| C9H13O2 | 154.0994 | 3.27 | 3 | 1.56 | 0.22 |
| C2H4O5N1S1 | 154.9888 | 0.32 | 1 | 2.50 | 2.50 |
| C6H4O4N1 | 155.0219 | 0.48 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 3.11 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 3.83 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 4.21 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 4.28 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 3.55 | 5 | 0.83 | 0.67 |
| C2H3O6S1 | 155.9729 | 0.33 | 1 | 2.00 | 3.00 |
| C6H3O5 | 156.0059 | 0.68 | 5 | 0.67 | 0.83 |
| C5H3O4N2 | 156.0171 | 1.27 | 5 | 0.80 | 0.80 |
| C7H7O4 | 156.0423 | 1.08 | 4 | 1.14 | 0.57 |
| C6H5O3S1 | 158.0038 | 0.74 | 4 | 1.00 | 0.50 |
| C10H8O1N1 | 159.0684 | 2.66 | 7 | 0.90 | 0.10 |
| C5H7O6S1 | 196.0042 | 0.37 | 2 | 1.60 | 1.20 |
| C5H3O6 | 160.0008 | 0.36 | 4 | 0.80 | 1.20 |
| C10H7O2 | 160.0524 | 4.03 | 7 | 0.80 | 0.20 |
| C10H7O2 | 160.0524 | 4.41 | 7 | 0.80 | 0.20 |
| C9H6O2N1 | 161.0477 | 2.83 | 7 | 0.78 | 0.22 |
| C9H6O2N1 | 161.0477 | 2.89 | 7 | 0.78 | 0.22 |
| C9H8O3N1 | 179.0582 | 3.40 | 6 | 1.00 | 0.33 |
| C9H6O2N1 | 161.0477 | 3.04 | 7 | 0.78 | 0.22 |
| C9H5O3 | 162.0317 | 2.81 | 7 | 0.67 | 0.33 |
| C9H5O3 | 162.0317 | 2.99 | 7 | 0.67 | 0.33 |
| C9H5O3 | 162.0317 | 3.17 | 7 | 0.67 | 0.33 |
| C9H5O3 | 162.0317 | 3.31 | 7 | 0.67 | 0.33 |
| C9H5O3 | 162.0317 | 4.00 | 7 | 0.67 | 0.33 |
| C9H5O3 | 162.0317 | 4.12 | 7 | 0.67 | 0.33 |
| C9H5O3 | 162.0317 | 4.65 | 7 | 0.67 | 0.33 |
| C8H5O2N2 | 162.0429 | 6.18 | 7 | 0.75 | 0.25 |
| C10H9O2 | 162.0681 | 3.40 | 6 | 1.00 | 0.20 |
| C10H9O2 | 162.0681 | 3.54 | 6 | 1.00 | 0.20 |
| C10H9O2 | 162.0681 | 3.65 | 6 | 1.00 | 0.20 |
| C10H9O2 | 162.0681 | 3.83 | 6 | 1.00 | 0.20 |
| C8H4O3N1 | 163.0269 | 2.69 | 7 | 0.63 | 0.38 |
| C4H3O5S1 | 163.9779 | 0.38 | 3 | 1.00 | 1.25 |
| C7H3O3N2 | 164.0222 | 4.27 | 7 | 0.57 | 0.43 |
| C9H7O3 | 164.0473 | 2.51 | 6 | 0.89 | 0.33 |
| C9H7O3 | 164.0473 | 2.77 | 6 | 0.89 | 0.33 |
| C9H7O3 | 164.0473 | 3.09 | 6 | 0.89 | 0.33 |
| C9H7O3 | 164.0473 | 3.33 | 6 | 0.89 | 0.33 |

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| C9H7O3 | 164.0473 | 3.39 | 6 | 0.89 | 0.33 |
| C6H11O5 | 164.0685 | 0.36 | 1 | 2.00 | 0.83 |
| C8H6O3N1 | 165.0426 | 1.50 | 6 | 0.88 | 0.38 |
| C8H6O3N1 | 165.0426 | 3.22 | 6 | 0.88 | 0.38 |
| C8H6O3N1 | 165.0426 | 5.14 | 6 | 0.88 | 0.38 |
| C8H6O3N1 | 165.0426 | 6.80 | 6 | 0.88 | 0.38 |
| C8H6O3N1 | 165.0426 | 7.40 | 6 | 0.88 | 0.38 |
| C4H5O5S1 | 165.9936 | 0.37 | 2 | 1.50 | 1.25 |
| C8H5O4 | 166.0266 | 1.35 | 6 | 0.75 | 0.50 |
| C8H5O4 | 166.0266 | 2.69 | 6 | 0.75 | 0.50 |
| C8H5O4 | 166.0266 | 2.85 | 6 | 0.75 | 0.50 |
| C8H5O4 | 166.0266 | 2.96 | 6 | 0.75 | 0.50 |
| C5H9O4S1 | 166.0300 | 3.40 | 1 | 2.00 | 0.80 |
| C9H9O3 | 166.0630 | 2.90 | 5 | 1.11 | 0.33 |
| C9H9O3 | 166.0630 | 3.26 | 5 | 1.11 | 0.33 |
| C9H9O3 | 166.0630 | 3.59 | 5 | 1.11 | 0.33 |
| C9H9O3 | 166.0630 | 3.81 | 5 | 1.11 | 0.33 |
| C9H9O3 | 166.0630 | 4.36 | 5 | 1.11 | 0.33 |
| C9H9O3 | 166.0630 | 5.29 | 5 | 1.11 | 0.33 |
| C9H9O3 | 166.0630 | 7.22 | 5 | 1.11 | 0.33 |
| C9H9O3 | 166.0630 | 4.00 | 5 | 1.11 | 0.33 |
| C6H13O3S1 | 166.0664 | 2.96 | 0 | 2.33 | 0.50 |
| C10H13O2 | 166.0994 | 7.67 | 4 | 1.40 | 0.20 |
| C3H4O5N1S1 | 166.9888 | 0.36 | 2 | 1.67 | 1.67 |
| C7H4O4N1 | 167.0219 | 3.80 | 6 | 0.71 | 0.57 |
| C8H8O3N1 | 167.0582 | 7.17 | 5 | 1.13 | 0.38 |
| C8H8O3N1 | 167.0582 | 7.29 | 5 | 1.13 | 0.38 |
| C8H8O3N1 | 167.0582 | 7.59 | 5 | 1.13 | 0.38 |
| C5H3O3N4 | 168.0283 | 0.38 | 6 | 0.80 | 0.60 |
| C8H7O4 | 168.0423 | 1.12 | 5 | 1.00 | 0.50 |
| C8H7O4 | 168.0423 | 2.92 | 5 | 1.00 | 0.50 |
| C8H7O4 | 168.0423 | 3.09 | 5 | 1.00 | 0.50 |
| C8H7O4 | 168.0423 | 3.29 | 5 | 1.00 | 0.50 |
| C8H7O4 | 168.0423 | 3.34 | 5 | 1.00 | 0.50 |
| C5H11O4S1 | 168.0456 | 2.23 | 0 | 2.40 | 0.80 |
| C5H11O4S1 | 168.0456 | 2.84 | 0 | 2.40 | 0.80 |
| C9H11O3 | 168.0786 | 2.56 | 4 | 1.33 | 0.33 |
| C9H11O3 | 168.0786 | 2.78 | 4 | 1.33 | 0.33 |
| C3H6O5N1S1 | 169.0045 | 0.34 | 1 | 2.33 | 1.67 |
| C7H6O4N1 | 169.0375 | 3.06 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 3.70 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 3.86 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 4.20 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 4.72 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 6.38 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 6.74 | 5 | 1.00 | 0.57 |
| C11H6O1N1 | 169.0528 | 7.44 | 9 | 0.64 | 0.09 |
| C9H14O2N1 | 169.1103 | 4.47 | 3 | 1.67 | 0.22 |
| C8H9O4 | 170.0579 | 2.54 | 4 | 1.25 | 0.50 |
| C6H4O5N1 | 171.0168 | 2.33 | 5 | 0.83 | 0.83 |
| C6H4O5N1 | 171.0168 | 3.01 | 5 | 0.83 | 0.83 |
| C7H7O3S1 | 172.0194 | 1.34 | 4 | 1.14 | 0.43 |
| C11H7O2 | 172.0524 | 3.89 | 8 | 0.73 | 0.18 |

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| C11H7O2 | 172.0524 | 4.10 | 8 | 0.73 | 0.18 |
| C11H7O2 | 172.0524 | 5.21 | 8 | 0.73 | 0.18 |
| C11H7O2 | 172.0524 | 6.82 | 8 | 0.73 | 0.18 |
| C11H7O2 | 172.0524 | 7.10 | 8 | 0.73 | 0.18 |
| C11H7O2 | 172.0524 | 7.44 | 8 | 0.73 | 0.18 |
| C5H5O3N2S1 | 174.0099 | 0.39 | 4 | 1.20 | 0.60 |
| C7H9O5 | 174.0528 | 0.83 | 3 | 1.43 | 0.71 |
| C11H9O2 | 174.0681 | 3.38 | 7 | 0.91 | 0.18 |
| C11H9O2 | 174.0681 | 3.55 | 7 | 0.91 | 0.18 |
| C11H9O2 | 174.0681 | 4.48 | 7 | 0.91 | 0.18 |
| C11H9O2 | 174.0681 | 6.95 | 7 | 0.91 | 0.18 |
| C11H9O2 | 174.0681 | 7.11 | 7 | 0.91 | 0.18 |
| C11H9O2 | 174.0681 | 7.35 | 7 | 0.91 | 0.18 |
| C10H8O2N1 | 175.0633 | 3.37 | 7 | 0.90 | 0.20 |
| C6H7O4S1 | 176.0143 | 1.38 | 3 | 1.33 | 0.67 |
| C6H7O4S1 | 176.0143 | 1.80 | 3 | 1.33 | 0.67 |
| C10H7O3 | 176.0473 | 3.01 | 7 | 0.80 | 0.30 |
| C10H7O3 | 176.0473 | 3.21 | 7 | 0.80 | 0.30 |
| C10H7O3 | 176.0473 | 3.29 | 7 | 0.80 | 0.30 |
| C10H7O3 | 176.0473 | 3.51 | 7 | 0.80 | 0.30 |
| C10H7O3 | 176.0473 | 3.84 | 7 | 0.80 | 0.30 |
| C10H7O3 | 176.0473 | 4.12 | 7 | 0.80 | 0.30 |
| C10H7O3 | 176.0473 | 4.47 | 7 | 0.80 | 0.30 |
| C8H13O7 | 222.0740 | 0.41 | 2 | 1.75 | 0.88 |
| C7H11O5 | 176.0685 | 0.56 | 2 | 1.71 | 0.71 |
| C7H11O5 | 176.0685 | 0.97 | 2 | 1.71 | 0.71 |
| C7H11O5 | 176.0685 | 1.18 | 2 | 1.71 | 0.71 |
| C11H11O2 | 176.0837 | 4.06 | 6 | 1.09 | 0.18 |
| C11H11O2 | 176.0837 | 4.15 | 6 | 1.09 | 0.18 |
| C11H11O2 | 176.0837 | 4.28 | 6 | 1.09 | 0.18 |
| C11H11O2 | 176.0837 | 4.47 | 6 | 1.09 | 0.18 |
| C11H11O2 | 176.0837 | 4.78 | 6 | 1.09 | 0.18 |
| C11H11O2 | 176.0837 | 5.19 | 6 | 1.09 | 0.18 |
| C9H6O3N1 | 177.0426 | 3.10 | 7 | 0.78 | 0.33 |
| C9H6O3N1 | 177.0426 | 3.34 | 7 | 0.78 | 0.33 |
| C9H6O3N1 | 177.0426 | 7.05 | 7 | 0.78 | 0.33 |
| C9H5O4 | 178.0266 | 0.81 | 7 | 0.67 | 0.44 |
| C9H5O4 | 178.0266 | 2.71 | 7 | 0.67 | 0.44 |
| C10H7O6 | 224.0321 | 2.85 | 7 | 0.80 | 0.60 |
| C9H5O4 | 178.0266 | 3.43 | 7 | 0.67 | 0.44 |
| C9H5O4 | 178.0266 | 3.02 | 7 | 0.67 | 0.44 |
| C10H9O3 | 178.0630 | 2.74 | 6 | 1.00 | 0.30 |
| C10H9O3 | 178.0630 | 3.01 | 6 | 1.00 | 0.30 |
| C10H9O3 | 178.0630 | 3.21 | 6 | 1.00 | 0.30 |
| C10H9O3 | 178.0630 | 3.79 | 6 | 1.00 | 0.30 |
| C10H9O3 | 178.0630 | 4.32 | 6 | 1.00 | 0.30 |
| C10H9O3 | 178.0630 | 4.54 | 6 | 1.00 | 0.30 |
| C10H9O3 | 178.0630 | 4.65 | 6 | 1.00 | 0.30 |
| C10H9O3 | 178.0630 | 5.42 | 6 | 1.00 | 0.30 |
| C5H6O7N1S1 | 224.9943 | 0.35 | 3 | 1.40 | 1.40 |
| C8H4O4N1 | 179.0219 | 4.98 | 7 | 0.63 | 0.50 |
| C8H4O4N1 | 179.0219 | 5.46 | 7 | 0.63 | 0.50 |
| C9H8O3N1 | 179.0582 | 3.36 | 6 | 1.00 | 0.33 |

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| C9H8O3N1 | 179.0582 | 7.04 | 6 | 1.00 | 0.33 |
| C9H8O3N1 | 179.0582 | 7.30 | 6 | 1.00 | 0.33 |
| C9H8O3N1 | 179.0582 | 7.47 | 6 | 1.00 | 0.33 |
| C9H8O3N1 | 179.0582 | 7.66 | 6 | 1.00 | 0.33 |
| C4H3O6S1 | 179.9729 | 0.40 | 3 | 1.00 | 1.50 |
| C9H7O4 | 180.0423 | 2.65 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 2.79 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 2.93 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 3.06 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 3.18 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 4.16 | 6 | 0.89 | 0.44 |
| C6H11O4S1 | 180.0456 | 2.57 | 1 | 2.00 | 0.67 |
| C6H11O6 | 180.0634 | 0.34 | 1 | 2.00 | 1.00 |
| C10H11O3 | 180.0786 | 3.19 | 5 | 1.20 | 0.30 |
| C10H11O3 | 180.0786 | 3.83 | 5 | 1.20 | 0.30 |
| C10H11O3 | 180.0786 | 3.93 | 5 | 1.20 | 0.30 |
| C10H11O3 | 180.0786 | 4.53 | 5 | 1.20 | 0.30 |
| C10H11O3 | 180.0786 | 3.25 | 5 | 1.20 | 0.30 |
| C8H6O4N1 | 181.0375 | 2.64 | 6 | 0.88 | 0.50 |
| C8H6O4N1 | 181.0375 | 3.83 | 6 | 0.88 | 0.50 |
| C8H6O4N1 | 181.0375 | 3.95 | 6 | 0.88 | 0.50 |
| C8H6O4N1 | 181.0375 | 4.34 | 6 | 0.88 | 0.50 |
| C9H10O3N1 | 181.0739 | 2.18 | 5 | 1.22 | 0.33 |
| C9H10O3N1 | 181.0739 | 7.78 | 5 | 1.22 | 0.33 |
| C9H10O3N1 | 181.0739 | 7.89 | 5 | 1.22 | 0.33 |
| C9H10O3N1 | 181.0739 | 8.05 | 5 | 1.22 | 0.33 |
| C8H5O5 | 182.0215 | 1.08 | 6 | 0.75 | 0.63 |
| C8H5O5 | 182.0215 | 1.95 | 6 | 0.75 | 0.63 |
| C8H5O5 | 182.0215 | 2.48 | 6 | 0.75 | 0.63 |
| C5H9O5S1 | 182.0249 | 0.41 | 1 | 2.00 | 1.00 |
| C5H9O5S1 | 182.0249 | 0.50 | 1 | 2.00 | 1.00 |
| C7H5O4N2 | 182.0328 | 3.14 | 6 | 0.86 | 0.57 |
| C9H9O4 | 182.0579 | 2.67 | 5 | 1.11 | 0.44 |
| C9H9O4 | 182.0579 | 2.94 | 5 | 1.11 | 0.44 |
| C9H9O4 | 182.0579 | 3.13 | 5 | 1.11 | 0.44 |
| C6H13O4S1 | 182.0613 | 3.03 | 0 | 2.33 | 0.67 |
| C5H7O8N6 | 280.0404 | 3.14 | 5 | 1.60 | 1.60 |
| C6H13O4S1 | 182.0613 | 3.54 | 0 | 2.33 | 0.67 |
| C8H9O3N2 | 182.0691 | 0.72 | 5 | 1.25 | 0.38 |
| C7H4O5N1 | 183.0168 | 2.96 | 6 | 0.71 | 0.71 |
| C7H4O5N1 | 183.0168 | 3.28 | 6 | 0.71 | 0.71 |
| C7H4O5N1 | 183.0168 | 3.40 | 6 | 0.71 | 0.71 |
| C7H4O5N1 | 183.0168 | 3.63 | 6 | 0.71 | 0.71 |
| C8H8O4N1 | 183.0532 | 3.39 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 3.54 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 4.22 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 5.76 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 6.03 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 6.58 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 7.09 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 7.64 | 5 | 1.13 | 0.50 |
| C4H7O6S1 | 184.0042 | 0.73 | 1 | 2.00 | 1.50 |
| C8H7O5 | 184.0372 | 2.79 | 5 | 1.00 | 0.63 |

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| C5H11O5S1 | 184.0405 | 0.81 | 0 | 2.40 | 1.00 |
| C12H7O2 | 184.0524 | 5.25 | 9 | 0.67 | 0.17 |
| C12H7O2 | 184.0524 | 8.09 | 9 | 0.67 | 0.17 |
| C7H6O5N1 | 185.0324 | 2.63 | 5 | 1.00 | 0.71 |
| C7H6O5N1 | 185.0324 | 3.32 | 5 | 1.00 | 0.71 |
| C11H5O3 | 186.0317 | 6.67 | 9 | 0.55 | 0.27 |
| C8H9O5 | 186.0528 | 1.26 | 4 | 1.25 | 0.63 |
| C12H9O2 | 186.0681 | 7.18 | 8 | 0.83 | 0.17 |
| C12H9O2 | 186.0681 | 7.30 | 8 | 0.83 | 0.17 |
| C7H11O6S1 | 224.0355 | 1.02 | 2 | 1.71 | 0.86 |
| C7H7O4S1 | 188.0143 | 2.60 | 4 | 1.14 | 0.57 |
| C7H7O6 | 188.0321 | 0.53 | 4 | 1.14 | 0.86 |
| C11H7O3 | 188.0473 | 3.44 | 8 | 0.73 | 0.27 |
| C11H7O3 | 188.0473 | 7.31 | 8 | 0.73 | 0.27 |
| C11H7O3 | 188.0473 | 7.51 | 8 | 0.73 | 0.27 |
| C11H7O3 | 188.0473 | 7.79 | 8 | 0.73 | 0.27 |
| C8H11O5 | 188.0685 | 1.29 | 3 | 1.50 | 0.63 |
| C12H11O2 | 188.0837 | 4.15 | 7 | 1.00 | 0.17 |
| C12H11O2 | 188.0837 | 4.36 | 7 | 1.00 | 0.17 |
| C6H6O4N1S1 | 189.0096 | 0.72 | 4 | 1.17 | 0.67 |
| C6H6O4N1S1 | 189.0096 | 0.86 | 4 | 1.17 | 0.67 |
| C6H6O4N1S1 | 189.0096 | 1.32 | 4 | 1.17 | 0.67 |
| C10H6O3N1 | 189.0426 | 7.75 | 8 | 0.70 | 0.30 |
| C6H5O5S1 | 189.9936 | 0.29 | 4 | 1.00 | 0.83 |
| C6H5O5S1 | 189.9936 | 0.36 | 4 | 1.00 | 0.83 |
| C6H9O7S1 | 226.0147 | 0.52 | 2 | 1.67 | 1.17 |
| C6H5O5S1 | 189.9936 | 1.33 | 4 | 1.00 | 0.83 |
| C5H5O4N2S1 | 190.0048 | 0.36 | 4 | 1.20 | 0.80 |
| C5H5O4N2S1 | 190.0048 | 0.82 | 4 | 1.20 | 0.80 |
| C10H5O4 | 190.0266 | 3.24 | 8 | 0.60 | 0.40 |
| C9H5O3N2 | 190.0378 | 2.77 | 8 | 0.67 | 0.33 |
| C6H9O3N2S1 | 190.0412 | 0.38 | 3 | 1.67 | 0.50 |
| C11H9O3 | 190.0630 | 3.04 | 7 | 0.91 | 0.27 |
| C11H9O3 | 190.0630 | 3.40 | 7 | 0.91 | 0.27 |
| C11H9O3 | 190.0630 | 3.64 | 7 | 0.91 | 0.27 |
| C11H9O3 | 190.0630 | 4.50 | 7 | 0.91 | 0.27 |
| C11H9O3 | 190.0630 | 4.62 | 7 | 0.91 | 0.27 |
| C12H13O2 | 190.0994 | 6.92 | 6 | 1.17 | 0.17 |
| C5H4O5N1S1 | 190.9888 | 0.39 | 4 | 1.00 | 1.00 |
| C10H8O3N1 | 191.0582 | 4.49 | 7 | 0.90 | 0.30 |
| C6H7O5S1 | 192.0092 | 0.40 | 3 | 1.33 | 0.83 |
| C6H7O5S1 | 192.0092 | 0.83 | 3 | 1.33 | 0.83 |
| C6H7O7 | 192.0270 | 0.38 | 3 | 1.33 | 1.17 |
| C10H7O4 | 192.0423 | 2.91 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.00 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.12 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.32 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.52 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 4.10 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 7.03 | 7 | 0.80 | 0.40 |
| C7H11O6 | 192.0634 | 0.55 | 2 | 1.71 | 0.86 |
| C11H11O3 | 192.0786 | 3.50 | 6 | 1.09 | 0.27 |
| C11H11O3 | 192.0786 | 3.74 | 6 | 1.09 | 0.27 |

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|---|---|---|---|---|---|
| C11H11O3 | 192.0786 | 4.65 | 6 | 1.09 | 0.27 |
| C9H6O4N1 | 193.0375 | 6.83 | 7 | 0.78 | 0.44 |
| C9H6O4N1 | 193.0375 | 7.05 | 7 | 0.78 | 0.44 |
| C9H6O4N1 | 193.0375 | 7.19 | 7 | 0.78 | 0.44 |
| C10H10O3N1 | 193.0739 | 7.98 | 6 | 1.10 | 0.30 |
| C5H5O6S1 | 193.9885 | 0.61 | 3 | 1.20 | 1.20 |
| C5H5O6S1 | 193.9885 | 0.70 | 3 | 1.20 | 1.20 |
| C9H5O5 | 194.0215 | 0.83 | 7 | 0.67 | 0.56 |
| C9H5O5 | 194.0215 | 2.76 | 7 | 0.67 | 0.56 |
| C9H5O5 | 194.0215 | 2.92 | 7 | 0.67 | 0.56 |
| C10H9O4 | 194.0579 | 2.90 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.01 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.08 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.29 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.57 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.67 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.82 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 6.46 | 6 | 1.00 | 0.40 |
| C14H9O1 | 194.0732 | 8.20 | 10 | 0.71 | 0.07 |
| C8H17O3S1 | 194.0977 | 5.27 | 0 | 2.25 | 0.38 |
| C8H4O3N1S1 | 194.9990 | 7.44 | 7 | 0.63 | 0.38 |
| C8H4O5N1 | 195.0168 | 3.66 | 7 | 0.63 | 0.63 |
| C9H8O4N1 | 195.0532 | 3.99 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 4.80 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 5.07 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 5.67 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 6.39 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 6.56 | 6 | 1.00 | 0.44 |
| C9H7O5 | 196.0372 | 1.83 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 2.49 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.04 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.20 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.33 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.76 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.43 | 6 | 0.89 | 0.56 |
| C6H11O5S1 | 196.0405 | 1.08 | 1 | 2.00 | 0.83 |
| C13H7O2 | 196.0524 | 4.62 | 10 | 0.62 | 0.15 |
| C13H7O2 | 196.0524 | 4.67 | 10 | 0.62 | 0.15 |
| C13H7O2 | 196.0524 | 7.20 | 10 | 0.62 | 0.15 |
| C13H7O2 | 196.0524 | 7.55 | 10 | 0.62 | 0.15 |
| C10H11O4 | 196.0736 | 2.75 | 5 | 1.20 | 0.40 |
| C10H11O4 | 196.0736 | 3.22 | 5 | 1.20 | 0.40 |
| C10H11O4 | 196.0736 | 3.34 | 5 | 1.20 | 0.40 |
| C7H15O4S1 | 196.0769 | 3.72 | 0 | 2.29 | 0.57 |
| C7H15O4S1 | 196.0769 | 5.22 | 0 | 2.29 | 0.57 |
| C8H6O5N1 | 197.0324 | 2.81 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 3.28 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 3.47 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 3.70 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 4.06 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 4.41 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 4.76 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 3.73 | 6 | 0.88 | 0.63 |

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|---|---|---|---|---|---|
| C9H10O4N1 | 197.0688 | 7.29 | 5 | 1.22 | 0.44 |
| C9H10O4N1 | 197.0688 | 7.39 | 5 | 1.22 | 0.44 |
| C9H10O4N1 | 197.0688 | 7.59 | 5 | 1.22 | 0.44 |
| C9H10O4N1 | 197.0688 | 7.78 | 5 | 1.22 | 0.44 |
| C13H10O1N1 | 197.0841 | 8.08 | 9 | 0.85 | 0.08 |
| C8H5O6 | 198.0164 | 3.10 | 6 | 0.75 | 0.75 |
| C5H9O6S1 | 198.0198 | 1.60 | 1 | 2.00 | 1.20 |
| C5H9O6S1 | 198.0198 | 1.74 | 1 | 2.00 | 1.20 |
| C5H9O6S1 | 198.0198 | 1.89 | 1 | 2.00 | 1.20 |
| C7H5O5N2 | 198.0277 | 7.44 | 6 | 0.86 | 0.71 |
| C6H13O5S1 | 198.0562 | 2.82 | 0 | 2.33 | 0.83 |
| C13H9O2 | 198.0681 | 7.23 | 9 | 0.77 | 0.15 |
| C13H9O2 | 198.0681 | 7.50 | 9 | 0.77 | 0.15 |
| C13H9O2 | 198.0681 | 7.99 | 9 | 0.77 | 0.15 |
| C13H9O2 | 198.0681 | 7.28 | 9 | 0.77 | 0.15 |
| C7H4O6N1 | 199.0117 | 2.69 | 6 | 0.71 | 0.86 |
| C7H4O6N1 | 199.0117 | 3.44 | 6 | 0.71 | 0.86 |
| C8H8O5N1 | 199.0481 | 2.51 | 5 | 1.13 | 0.63 |
| C8H8O5N1 | 199.0481 | 4.29 | 5 | 1.13 | 0.63 |
| C6H3O6N2 | 200.0069 | 4.85 | 6 | 0.67 | 1.00 |
| C12H7O1S1 | 200.0296 | 0.78 | 9 | 0.67 | 0.08 |
| C12H7O3 | 200.0473 | 4.47 | 9 | 0.67 | 0.25 |
| C12H7O3 | 200.0473 | 6.05 | 9 | 0.67 | 0.25 |
| C12H7O3 | 200.0473 | 7.16 | 9 | 0.67 | 0.25 |
| C12H7O3 | 200.0473 | 8.07 | 9 | 0.67 | 0.25 |
| C13H11O2 | 200.0837 | 7.80 | 8 | 0.92 | 0.15 |
| C13H11O2 | 200.0837 | 7.90 | 8 | 0.92 | 0.15 |
| C13H11O2 | 200.0837 | 7.59 | 8 | 0.92 | 0.15 |
| C7H5O5S1 | 201.9936 | 0.63 | 5 | 0.86 | 0.71 |
| C6H5O4N2S1 | 202.0048 | 0.57 | 5 | 1.00 | 0.67 |
| C7H9O3N2S1 | 202.0412 | 1.10 | 4 | 1.43 | 0.43 |
| C12H9O3 | 202.0630 | 3.46 | 8 | 0.83 | 0.25 |
| C12H9O3 | 202.0630 | 4.54 | 8 | 0.83 | 0.25 |
| C12H9O3 | 202.0630 | 7.74 | 8 | 0.83 | 0.25 |
| C12H9O3 | 202.0630 | 7.82 | 8 | 0.83 | 0.25 |
| C7H8O4N1S1 | 203.0252 | 0.49 | 4 | 1.29 | 0.57 |
| C11H8O3N1 | 203.0582 | 7.98 | 8 | 0.82 | 0.27 |
| C11H8O3N1 | 203.0582 | 8.08 | 8 | 0.82 | 0.27 |
| C5H3O1N2S3 | 203.9486 | 0.31 | 5 | 0.80 | 0.20 |
| C7H7O5S1 | 204.0092 | 0.40 | 4 | 1.14 | 0.71 |
| C7H7O5S1 | 204.0092 | 0.99 | 4 | 1.14 | 0.71 |
| C7H7O5S1 | 204.0092 | 1.15 | 4 | 1.14 | 0.71 |
| C7H7O5S1 | 204.0092 | 1.40 | 4 | 1.14 | 0.71 |
| C7H7O5S1 | 204.0092 | 1.71 | 4 | 1.14 | 0.71 |
| C7H7O5S1 | 204.0092 | 2.80 | 4 | 1.14 | 0.71 |
| C7H7O5S1 | 204.0092 | 2.95 | 4 | 1.14 | 0.71 |
| C12H11O3 | 204.0786 | 3.35 | 7 | 1.00 | 0.25 |
| C12H11O3 | 204.0786 | 7.65 | 7 | 1.00 | 0.25 |
| C6H6O5N1S1 | 205.0045 | 0.60 | 4 | 1.17 | 0.83 |
| C6H6O5N1S1 | 205.0045 | 1.03 | 4 | 1.17 | 0.83 |
| C10H6O4N1 | 205.0375 | 3.13 | 8 | 0.70 | 0.40 |
| C11H10O3N1 | 205.0739 | 7.71 | 7 | 1.00 | 0.27 |
| C6H5O6S1 | 205.9885 | 0.44 | 4 | 1.00 | 1.00 |

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|---|---|---|---|---|---|
| C10H5O5 | 206.0215 | 3.17 | 8 | 0.60 | 0.50 |
| C11H9O4 | 206.0579 | 3.21 | 7 | 0.91 | 0.36 |
| C11H9O4 | 206.0579 | 3.46 | 7 | 0.91 | 0.36 |
| C11H9O4 | 206.0579 | 4.03 | 7 | 0.91 | 0.36 |
| C11H9O4 | 206.0579 | 6.01 | 7 | 0.91 | 0.36 |
| C8H13O6 | 206.0790 | 0.76 | 2 | 1.75 | 0.75 |
| C9H4O5N1 | 207.0168 | 3.97 | 8 | 0.56 | 0.56 |
| C10H8O4N1 | 207.0532 | 4.57 | 7 | 0.90 | 0.40 |
| C10H8O4N1 | 207.0532 | 7.82 | 7 | 0.90 | 0.40 |
| C11H12O3N1 | 207.0895 | 8.18 | 6 | 1.18 | 0.27 |
| C10H7O5 | 208.0372 | 2.44 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.57 | 7 | 0.80 | 0.50 |
| C11H11O4 | 208.0736 | 2.91 | 6 | 1.09 | 0.36 |
| C11H11O4 | 208.0736 | 3.98 | 6 | 1.09 | 0.36 |
| C11H11O4 | 208.0736 | 5.07 | 6 | 1.09 | 0.36 |
| C8H15O4S1 | 208.0769 | 4.92 | 1 | 2.00 | 0.50 |
| C9H8O4N1S1 | 227.0252 | 2.24 | 6 | 1.00 | 0.44 |
| C9H6O3N1S1 | 209.0147 | 7.92 | 7 | 0.78 | 0.33 |
| C6H10O5N1S1 | 209.0358 | 0.39 | 2 | 1.83 | 0.83 |
| C10H10O4N1 | 209.0688 | 7.21 | 6 | 1.10 | 0.40 |
| C10H10O4N1 | 209.0688 | 7.52 | 6 | 1.10 | 0.40 |
| C10H10O4N1 | 209.0688 | 7.64 | 6 | 1.10 | 0.40 |
| C9H5O6 | 210.0164 | 1.11 | 7 | 0.67 | 0.67 |
| C9H5O6 | 210.0164 | 1.91 | 7 | 0.67 | 0.67 |
| C6H9O6S1 | 210.0198 | 0.48 | 2 | 1.67 | 1.00 |
| C10H9O5 | 210.0528 | 3.03 | 6 | 1.00 | 0.50 |
| C14H9O2 | 210.0681 | 7.52 | 10 | 0.71 | 0.14 |
| C14H9O2 | 210.0681 | 7.69 | 10 | 0.71 | 0.14 |
| C14H9O2 | 210.0681 | 7.77 | 10 | 0.71 | 0.14 |
| C14H9O2 | 210.0681 | 7.90 | 10 | 0.71 | 0.14 |
| C14H9O2 | 210.0681 | 8.08 | 10 | 0.71 | 0.14 |
| C8H17O4S1 | 210.0926 | 7.18 | 0 | 2.25 | 0.50 |
| C9H8O5N1 | 211.0481 | 4.30 | 6 | 1.00 | 0.56 |
| C9H8O5N1 | 211.0481 | 4.57 | 6 | 1.00 | 0.56 |
| C9H8O5N1 | 211.0481 | 4.97 | 6 | 1.00 | 0.56 |
| C9H8O5N1 | 211.0481 | 7.08 | 6 | 1.00 | 0.56 |
| C6H11O6S1 | 212.0355 | 2.57 | 1 | 2.00 | 1.00 |
| C6H11O6S1 | 212.0355 | 2.76 | 1 | 2.00 | 1.00 |
| C6H11O6S1 | 212.0355 | 2.84 | 1 | 2.00 | 1.00 |
| C8H7O5N2 | 212.0433 | 7.70 | 6 | 1.00 | 0.63 |
| C8H7O5N2 | 212.0433 | 7.83 | 6 | 1.00 | 0.63 |
| C13H7O3 | 212.0473 | 4.30 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 6.45 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 6.60 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 7.03 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 7.22 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 7.39 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 7.51 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 7.78 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 8.00 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 7.55 | 10 | 0.62 | 0.23 |
| C7H15O5S1 | 212.0718 | 3.09 | 0 | 2.29 | 0.71 |
| C14H11O2 | 212.0837 | 7.68 | 9 | 0.86 | 0.14 |

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| C14H11O2 | 212.0837 | 7.91 | 9 | 0.86 | 0.14 |
| C14H11O2 | 212.0837 | 8.21 | 9 | 0.86 | 0.14 |
| C4H6O7N1S1 | 212.9943 | 0.31 | 2 | 1.75 | 1.75 |
| C8H6O4N1S1 | 213.0096 | 1.10 | 6 | 0.88 | 0.50 |
| C8H6O6N1 | 213.0273 | 3.45 | 6 | 0.88 | 0.75 |
| C8H5O5S1 | 213.9936 | 1.61 | 6 | 0.75 | 0.63 |
| C7H5O6N2 | 214.0226 | 7.15 | 6 | 0.86 | 0.86 |
| C12H5O4 | 214.0266 | 5.56 | 10 | 0.50 | 0.33 |
| C13H9O3 | 214.0630 | 7.67 | 9 | 0.77 | 0.23 |
| C13H9O3 | 214.0630 | 7.86 | 9 | 0.77 | 0.23 |
| C13H9O3 | 214.0630 | 7.96 | 9 | 0.77 | 0.23 |
| C13H9O3 | 214.0630 | 8.04 | 9 | 0.77 | 0.23 |
| C13H9O3 | 214.0630 | 8.27 | 9 | 0.77 | 0.23 |
| C14H13O2 | 214.0994 | 8.14 | 8 | 1.00 | 0.14 |
| C4H8O7N1S1 | 215.0100 | 1.50 | 1 | 2.25 | 1.75 |
| C12H8O3N1 | 215.0582 | 7.87 | 9 | 0.75 | 0.25 |
| C12H8O3N1 | 215.0582 | 8.11 | 9 | 0.75 | 0.25 |
| C8H7O5S1 | 216.0092 | 0.81 | 5 | 1.00 | 0.63 |
| C5H11O7S1 | 216.0304 | 0.35 | 0 | 2.40 | 1.40 |
| C12H7O4 | 216.0423 | 3.14 | 9 | 0.67 | 0.33 |
| C12H7O4 | 216.0423 | 3.40 | 9 | 0.67 | 0.33 |
| C12H7O4 | 216.0423 | 3.89 | 9 | 0.67 | 0.33 |
| C12H7O4 | 216.0423 | 4.10 | 9 | 0.67 | 0.33 |
| C8H11O3N2S1 | 216.0569 | 2.43 | 4 | 1.50 | 0.38 |
| C11H6O4N1 | 217.0375 | 7.03 | 9 | 0.64 | 0.36 |
| C12H10O3N1 | 217.0739 | 8.22 | 8 | 0.92 | 0.25 |
| C7H5O6S1 | 217.9885 | 1.20 | 5 | 0.86 | 0.86 |
| C8H9O5S1 | 218.0249 | 0.53 | 4 | 1.25 | 0.63 |
| C8H9O5S1 | 218.0249 | 1.44 | 4 | 1.25 | 0.63 |
| C8H9O5S1 | 218.0249 | 2.52 | 4 | 1.25 | 0.63 |
| C8H9O5S1 | 218.0249 | 2.69 | 4 | 1.25 | 0.63 |
| C8H9O5S1 | 218.0249 | 2.78 | 4 | 1.25 | 0.63 |
| C8H9O5S1 | 218.0249 | 3.67 | 4 | 1.25 | 0.63 |
| C7H9O4N2S1 | 218.0361 | 0.39 | 4 | 1.43 | 0.57 |
| C16H9O1 | 218.0732 | 8.36 | 12 | 0.63 | 0.06 |
| C6H4O6N1S1 | 218.9838 | 2.95 | 5 | 0.83 | 1.00 |
| C7H7O6S1 | 220.0042 | 0.42 | 4 | 1.14 | 0.86 |
| C7H3O3N6 | 220.0345 | 3.69 | 9 | 0.57 | 0.43 |
| C8H11O7 | 220.0583 | 0.39 | 3 | 1.50 | 0.88 |
| C11H10O4N1 | 221.0688 | 8.10 | 7 | 1.00 | 0.36 |
| C7H9O6S1 | 222.0198 | 0.78 | 3 | 1.43 | 0.86 |
| C11H9O5 | 222.0528 | 2.72 | 7 | 0.91 | 0.45 |
| C11H9O5 | 222.0528 | 2.89 | 7 | 0.91 | 0.45 |
| C15H9O2 | 222.0681 | 8.09 | 11 | 0.67 | 0.13 |
| C8H13O7 | 222.0740 | 0.49 | 2 | 1.75 | 0.88 |
| C15H15O3 | 244.1099 | 7.59 | 8 | 1.07 | 0.20 |
| C6H9O8S1 | 242.0096 | 0.38 | 2 | 1.67 | 1.33 |
| C10H7O6 | 224.0321 | 3.16 | 7 | 0.80 | 0.60 |
| C7H11O6S1 | 224.0355 | 0.66 | 2 | 1.71 | 0.86 |
| C14H7O3 | 224.0473 | 7.58 | 11 | 0.57 | 0.21 |
| C8H15O5S1 | 224.0718 | 2.69 | 1 | 2.00 | 0.63 |
| C8H15O5S1 | 224.0718 | 2.70 | 1 | 2.00 | 0.63 |
| C8H15O5S1 | 224.0718 | 2.71 | 1 | 2.00 | 0.63 |

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|---|---|---|---|---|---|
| C15H11O2 | 224.0837 | 7.94 | 10 | 0.80 | 0.13 |
| C9H19O4S1 | 224.1082 | 7.65 | 0 | 2.22 | 0.44 |
| C12H19O2N2 | 224.1525 | 2.90 | 4 | 1.67 | 0.17 |
| C9H6O4N1S1 | 225.0096 | 3.05 | 7 | 0.78 | 0.44 |
| C10H10O5N1 | 225.0637 | 5.23 | 6 | 1.10 | 0.50 |
| C5H5O8S1 | 225.9783 | 0.30 | 3 | 1.20 | 1.60 |
| C9H5O7 | 226.0114 | 0.82 | 7 | 0.67 | 0.78 |
| C9H5O7 | 226.0114 | 1.08 | 7 | 0.67 | 0.78 |
| C7H13O6S1 | 226.0511 | 2.56 | 1 | 2.00 | 0.86 |
| C7H13O6S1 | 226.0511 | 3.28 | 1 | 2.00 | 0.86 |
| C7H13O6S1 | 226.0511 | 3.40 | 1 | 2.00 | 0.86 |
| C9H9O5N2 | 226.0590 | 3.05 | 6 | 1.11 | 0.56 |
| C14H9O3 | 226.0630 | 7.28 | 10 | 0.71 | 0.21 |
| C14H9O3 | 226.0630 | 7.68 | 10 | 0.71 | 0.21 |
| C14H9O3 | 226.0630 | 7.89 | 10 | 0.71 | 0.21 |
| C8H17O5S1 | 226.0875 | 2.97 | 0 | 2.25 | 0.63 |
| C8H17O5S1 | 226.0875 | 3.76 | 0 | 2.25 | 0.63 |
| C15H13O2 | 226.0994 | 8.37 | 9 | 0.93 | 0.13 |
| C8H8O3N3S1 | 227.0365 | 0.39 | 6 | 1.13 | 0.38 |
| C9H8O6N1 | 227.0430 | 3.40 | 6 | 1.00 | 0.67 |
| C9H9O6S1 | 246.0198 | 2.37 | 5 | 1.11 | 0.67 |
| C9H7O5S1 | 228.0092 | 2.47 | 6 | 0.89 | 0.56 |
| C9H7O5S1 | 228.0092 | 2.60 | 6 | 0.89 | 0.56 |
| C9H7O5S1 | 228.0092 | 2.76 | 6 | 0.89 | 0.56 |
| C9H7O5S1 | 228.0092 | 2.83 | 6 | 0.89 | 0.56 |
| C8H7O6N2 | 228.0382 | 3.67 | 6 | 1.00 | 0.75 |
| C13H7O4 | 228.0423 | 7.88 | 10 | 0.62 | 0.31 |
| C13H7O4 | 228.0423 | 8.22 | 10 | 0.62 | 0.31 |
| C7H15O6S1 | 228.0668 | 0.61 | 0 | 2.29 | 0.86 |
| C14H11O3 | 228.0786 | 7.98 | 9 | 0.86 | 0.21 |
| C4H6O6N1S2 | 228.9715 | 0.29 | 2 | 1.75 | 1.50 |
| C4H6O8N1S1 | 228.9892 | 0.31 | 2 | 1.75 | 2.00 |
| C5H10O7N1S1 | 229.0256 | 0.38 | 1 | 2.20 | 1.40 |
| C12H6O4N1 | 229.0375 | 8.00 | 10 | 0.58 | 0.33 |
| C12H6O4N1 | 229.0375 | 8.07 | 10 | 0.58 | 0.33 |
| C13H10O3N1 | 229.0739 | 8.13 | 9 | 0.85 | 0.23 |
| C13H10O3N1 | 229.0739 | 8.29 | 9 | 0.85 | 0.23 |
| C8H5O6S1 | 229.9885 | 2.54 | 6 | 0.75 | 0.75 |
| C8H9O2N2S2 | 230.0184 | 0.34 | 5 | 1.25 | 0.25 |
| C9H9O5S1 | 230.0249 | 2.47 | 5 | 1.11 | 0.56 |
| C7H4O2N1S3 | 230.9482 | 0.33 | 6 | 0.71 | 0.29 |
| C8H8O5N1S1 | 231.0201 | 2.83 | 5 | 1.13 | 0.63 |
| C12H8O4N1 | 231.0532 | 7.82 | 9 | 0.75 | 0.33 |
| C8H7O6S1 | 232.0042 | 1.36 | 5 | 1.00 | 0.75 |
| C8H7O6S1 | 232.0042 | 3.11 | 5 | 1.00 | 0.75 |
| C8H7O6S1 | 232.0042 | 3.53 | 5 | 1.00 | 0.75 |
| C9H11O5S1 | 232.0405 | 3.01 | 4 | 1.33 | 0.56 |
| C9H11O5S1 | 232.0405 | 3.22 | 4 | 1.33 | 0.56 |
| C9H11O5S1 | 232.0405 | 3.34 | 4 | 1.33 | 0.56 |
| C9H11O5S1 | 232.0405 | 2.76 | 4 | 1.33 | 0.56 |
| C7H2O3N7 | 233.0297 | 3.22 | 10 | 0.43 | 0.43 |
| C11H6O5N1 | 233.0324 | 7.24 | 9 | 0.64 | 0.45 |
| C8H10O5N1S1 | 233.0358 | 0.63 | 4 | 1.38 | 0.63 |

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|---|---|---|---|---|---|
| C8H9O6S1 | 234.0198 | 0.48 | 4 | 1.25 | 0.75 |
| C10H5O5N2 | 234.0277 | 7.62 | 9 | 0.60 | 0.50 |
| C7H9O5N2S1 | 234.0310 | 0.37 | 4 | 1.43 | 0.71 |
| C6H4O7N1S1 | 234.9787 | 0.36 | 5 | 0.83 | 1.17 |
| C6H4O7N1S1 | 234.9787 | 1.10 | 5 | 0.83 | 1.17 |
| C6H4O7N1S1 | 234.9787 | 2.78 | 5 | 0.83 | 1.17 |
| C6H4O7N1S1 | 234.9787 | 2.86 | 5 | 0.83 | 1.17 |
| C7H7O7S1 | 235.9991 | 0.39 | 4 | 1.14 | 1.00 |
| C15H9O3 | 238.0630 | 7.99 | 11 | 0.67 | 0.20 |
| C12H13O5 | 238.0841 | 3.05 | 6 | 1.17 | 0.42 |
| C10H21O4S1 | 238.1239 | 7.53 | 0 | 2.20 | 0.40 |
| C10H21O4S1 | 238.1239 | 7.66 | 0 | 2.20 | 0.40 |
| C10H21O4S1 | 238.1239 | 7.94 | 0 | 2.20 | 0.40 |
| C10H8O4N1S1 | 239.0252 | 3.18 | 7 | 0.90 | 0.40 |
| C8H16O5N1S1 | 239.0827 | 2.29 | 1 | 2.13 | 0.63 |
| C14H7O4 | 240.0423 | 7.31 | 11 | 0.57 | 0.29 |
| C14H7O4 | 240.0423 | 7.52 | 11 | 0.57 | 0.29 |
| C8H15O6S1 | 240.0668 | 2.90 | 1 | 2.00 | 0.75 |
| C15H11O3 | 240.0786 | 7.72 | 10 | 0.80 | 0.20 |
| C15H11O3 | 240.0786 | 8.15 | 10 | 0.80 | 0.20 |
| C8H8O7N1S1 | 263.0100 | 3.11 | 5 | 1.13 | 0.88 |
| C10H10O6N1 | 241.0586 | 4.08 | 6 | 1.10 | 0.60 |
| C10H9O5S1 | 242.0249 | 3.28 | 6 | 1.00 | 0.50 |
| C7H13O7S1 | 242.0460 | 0.68 | 1 | 2.00 | 1.00 |
| C14H9O4 | 242.0579 | 5.13 | 10 | 0.71 | 0.29 |
| C14H9O4 | 242.0579 | 7.50 | 10 | 0.71 | 0.29 |
| C14H9O4 | 242.0579 | 7.90 | 10 | 0.71 | 0.29 |
| C14H9O4 | 242.0579 | 8.19 | 10 | 0.71 | 0.29 |
| C6H12O7N1S1 | 243.0413 | 3.29 | 1 | 2.17 | 1.17 |
| C13H7O5 | 244.0372 | 6.75 | 10 | 0.62 | 0.38 |
| C13H7O5 | 244.0372 | 7.00 | 10 | 0.62 | 0.38 |
| C13H7O5 | 244.0372 | 8.18 | 10 | 0.62 | 0.38 |
| C10H11O5S1 | 244.0405 | 3.14 | 5 | 1.20 | 0.50 |
| C15H15O3 | 244.1099 | 7.84 | 8 | 1.07 | 0.20 |
| C9H10O5N1S1 | 245.0358 | 1.06 | 5 | 1.22 | 0.56 |
| C9H9O6S1 | 246.0198 | 2.89 | 5 | 1.11 | 0.67 |
| C10H13O5S1 | 246.0562 | 3.68 | 4 | 1.40 | 0.50 |
| C8H8O6N1S1 | 247.0151 | 1.44 | 5 | 1.13 | 0.75 |
| C12H8O5N1 | 247.0481 | 4.18 | 9 | 0.75 | 0.42 |
| C8H7O7S1 | 247.9991 | 2.83 | 5 | 1.00 | 0.88 |
| C5H11O9S1 | 248.0202 | 0.35 | 0 | 2.40 | 1.80 |
| C8H3O4N6 | 248.0294 | 3.15 | 10 | 0.50 | 0.50 |
| C8H3O4N6 | 248.0294 | 4.17 | 10 | 0.50 | 0.50 |
| C7H6O7N1S1 | 248.9943 | 2.50 | 5 | 1.00 | 1.00 |
| C8H5O4N6 | 250.0451 | 2.94 | 9 | 0.75 | 0.50 |
| C17H13O2 | 250.0994 | 8.14 | 11 | 0.82 | 0.12 |
| C3H8O8N1S2 | 250.9770 | 0.35 | 0 | 3.00 | 2.67 |
| C8H11O7S1 | 252.0304 | 0.64 | 3 | 1.50 | 0.88 |
| C7H11O6N2S1 | 252.0416 | 5.37 | 3 | 1.71 | 0.86 |
| C15H7O4 | 252.0423 | 7.62 | 12 | 0.53 | 0.27 |
| C11H23O4S1 | 252.1395 | 8.20 | 0 | 2.18 | 0.36 |
| C9H18O5N1S1 | 253.0984 | 1.33 | 1 | 2.11 | 0.56 |
| C10H21O5S1 | 254.1188 | 7.26 | 0 | 2.20 | 0.50 |

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|---|---|---|---|---|---|
| C10H21O5S1 | 254.1188 | 7.36 | 0 | 2.20 | 0.50 |
| C14H7O5 | 256.0372 | 7.11 | 11 | 0.57 | 0.36 |
| C9H6O6N1S1 | 256.9994 | 1.50 | 7 | 0.78 | 0.67 |
| C9H5O7S1 | 257.9834 | 0.73 | 7 | 0.67 | 0.78 |
| C10H9O6S1 | 258.0198 | 1.81 | 6 | 1.00 | 0.60 |
| C10H9O6S1 | 258.0198 | 2.52 | 6 | 1.00 | 0.60 |
| C14H9O5 | 258.0528 | 7.60 | 10 | 0.71 | 0.36 |
| C11H13O5S1 | 258.0562 | 3.68 | 5 | 1.27 | 0.45 |
| C11H13O5S1 | 258.0562 | 4.10 | 5 | 1.27 | 0.45 |
| C13H7O6 | 260.0321 | 7.60 | 10 | 0.62 | 0.46 |
| C6H15O7N2S1 | 260.0678 | 7.67 | 0 | 2.67 | 1.17 |
| C15H15O4 | 260.1049 | 7.85 | 8 | 1.07 | 0.27 |
| C9H10O6N1S1 | 261.0307 | 2.64 | 5 | 1.22 | 0.67 |
| C8H9O6N2S1 | 262.0260 | 0.38 | 5 | 1.25 | 0.75 |
| C10H13O6S1 | 262.0511 | 2.98 | 4 | 1.40 | 0.60 |
| C4H8O8N1S2 | 262.9770 | 0.30 | 1 | 2.25 | 2.00 |
| C8H8O7N1S1 | 263.0100 | 0.91 | 5 | 1.13 | 0.88 |
| C4H7O9S2 | 263.9610 | 0.34 | 1 | 2.00 | 2.25 |
| C7H6O8N1S1 | 264.9892 | 3.04 | 5 | 1.00 | 1.14 |
| C12H9O5S1 | 266.0249 | 3.35 | 8 | 0.83 | 0.42 |
| C16H9O4 | 266.0579 | 7.40 | 12 | 0.63 | 0.25 |
| C10H19O6S1 | 268.0981 | 3.00 | 1 | 2.00 | 0.60 |
| C13H15O6 | 268.0947 | 3.13 | 6 | 1.23 | 0.46 |
| C10H19O6S1 | 268.0981 | 7.57 | 1 | 2.00 | 0.60 |
| C11H23O5S1 | 268.1344 | 7.67 | 0 | 2.18 | 0.45 |
| C6H5O8S2 | 269.9504 | 0.39 | 4 | 1.00 | 1.33 |
| C6H7O8S2 | 271.9661 | 0.30 | 3 | 1.33 | 1.33 |
| C5H7O7N2S2 | 271.9773 | 0.35 | 3 | 1.60 | 1.40 |
| C11H11O6S1 | 272.0355 | 2.74 | 6 | 1.09 | 0.55 |
| C9H6O7N1S1 | 272.9943 | 2.31 | 7 | 0.78 | 0.78 |
| C10H10O6N1S1 | 273.0307 | 3.41 | 6 | 1.10 | 0.60 |
| C10H10O6N1S1 | 273.0307 | 2.86 | 6 | 1.10 | 0.60 |
| C5H9O7N2S2 | 273.9929 | 0.36 | 2 | 2.00 | 1.40 |
| C10H9O7S1 | 274.0147 | 1.02 | 6 | 1.00 | 0.70 |
| C6H5O7N6 | 274.0298 | 7.12 | 7 | 1.00 | 1.17 |
| C11H13O6S1 | 274.0511 | 3.30 | 5 | 1.27 | 0.55 |
| C11H13O6S1 | 274.0511 | 3.63 | 5 | 1.27 | 0.55 |
| C15H13O5 | 274.0841 | 6.82 | 9 | 0.93 | 0.33 |
| C16H17O4 | 274.1205 | 7.94 | 8 | 1.13 | 0.25 |
| C9H8O7N1S1 | 275.0100 | 4.26 | 6 | 1.00 | 0.78 |
| C14H11O4S1 | 276.0456 | 3.51 | 9 | 0.86 | 0.29 |
| C6H12O10N1S2 | 322.9981 | 0.38 | 1 | 2.17 | 1.67 |
| C9H10O7N1S1 | 277.0256 | 2.17 | 5 | 1.22 | 0.78 |
| C13H9O5S1 | 278.0249 | 3.13 | 9 | 0.77 | 0.38 |
| C9H5O5N6 | 278.0400 | 3.03 | 10 | 0.67 | 0.56 |
| C14H15O6 | 280.0947 | 4.10 | 7 | 1.14 | 0.43 |
| C8H10O8N1S1 | 281.0205 | 3.07 | 4 | 1.38 | 1.00 |
| C10H18O6N1S1 | 281.0933 | 2.79 | 2 | 1.90 | 0.60 |
| C11H22O5N1S1 | 281.1297 | 2.91 | 1 | 2.09 | 0.45 |
| C11H21O6S1 | 282.1137 | 7.90 | 1 | 2.00 | 0.55 |
| C12H25O5S1 | 282.1501 | 7.97 | 0 | 2.17 | 0.42 |
| C7H8O7N1S2 | 282.9820 | 0.36 | 4 | 1.29 | 1.00 |
| C7H8O9N1S1 | 282.9998 | 3.23 | 4 | 1.29 | 1.29 |

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|---|---|---|---|---|---|
| C9H16O7N1S1 | 283.0726 | 6.64 | 2 | 1.89 | 0.78 |
| C8H14O8N1S1 | 285.0518 | 3.01 | 2 | 1.88 | 1.00 |
| C10H10O7N1S1 | 289.0256 | 2.57 | 6 | 1.10 | 0.70 |
| C6H9O11S1 | 289.9944 | 0.39 | 2 | 1.67 | 1.83 |
| C13H8O5N1S1 | 291.0201 | 3.58 | 10 | 0.69 | 0.38 |
| C14H11O5S1 | 292.0405 | 3.61 | 9 | 0.86 | 0.36 |
| C10H16O7N1S1 | 295.0726 | 7.26 | 3 | 1.70 | 0.70 |
| C12H23O6S1 | 296.1294 | 8.15 | 1 | 2.00 | 0.50 |
| C13H27O5S1 | 296.1657 | 7.56 | 0 | 2.15 | 0.38 |
| C13H27O5S1 | 296.1657 | 8.20 | 0 | 2.15 | 0.38 |
| C9H14O8N1S1 | 297.0518 | 3.30 | 3 | 1.67 | 0.89 |
| C6H4O13N1 | 298.9761 | 0.32 | 5 | 0.83 | 2.17 |
| C7H7O9S2 | 299.9610 | 0.38 | 4 | 1.14 | 1.29 |
| C10H13O7N2S1 | 306.0522 | 0.39 | 5 | 1.40 | 0.70 |
| C10H12O8N1S1 | 307.0362 | 2.56 | 5 | 1.30 | 0.80 |
| C12H19O7S1 | 308.0930 | 3.45 | 3 | 1.67 | 0.58 |
| C13H26O5N1S1 | 309.1610 | 3.73 | 1 | 2.08 | 0.38 |
| C14H29O5S1 | 310.1814 | 7.84 | 0 | 2.14 | 0.36 |
| C17H13O6 | 314.0790 | 7.97 | 11 | 0.82 | 0.35 |
| C6H9O10N6 | 326.0458 | 2.84 | 5 | 1.67 | 1.67 |
| C20H29O4 | 334.2144 | 8.14 | 6 | 1.50 | 0.20 |
| C8H5O13S1 | 341.9529 | 0.28 | 6 | 0.75 | 1.63 |
| C8H4O7N7S1 | 342.9971 | 4.26 | 10 | 0.63 | 0.88 |
| C6H5O11S3 | 349.9072 | 0.30 | 4 | 1.00 | 1.83 |
| C14H5O6N6 | 354.0349 | 2.68 | 15 | 0.43 | 0.43 |
| C18H13O8 | 358.0689 | 7.45 | 12 | 0.78 | 0.44 |
| C16H9O6N6 | 382.0662 | 7.97 | 15 | 0.63 | 0.38 |
| C8H3O12S3 | 387.8865 | 0.28 | 7 | 0.50 | 1.50 |
| C18H6O6N5 | 389.0396 | 2.89 | 18 | 0.39 | 0.33 |
| C7H8O15N5 | 403.0095 | 4.29 | 6 | 1.29 | 2.14 |

Table S3.2.2 Molecular formulas of organic compounds detected in CC in ESI+ mode.

| Formula [M+H]/[M+Na] | Neutral mass (Da) | RT (min) | DBE | H/C | O/C |
|---|---|---|---|---|---|
| C6H6N3 | 119.0483 | 0.39 | 6 | 0.83 | 0.00 |
| C7H10O1N1 | 123.0684 | 0.92 | 4 | 1.29 | 0.14 |
| C6H11O2N2 | 142.0742 | 0.36 | 3 | 1.67 | 0.33 |
| C5H7O2N2 | 126.0429 | 0.37 | 4 | 1.20 | 0.40 |
| C7H7O1 | 106.0419 | 1.03 | 5 | 0.86 | 0.14 |
| C7H10O1N1 | 123.0684 | 1.27 | 4 | 1.29 | 0.14 |
| C7H11O1N2 | 138.0793 | 0.38 | 4 | 1.43 | 0.14 |
| C6H11O1N2 | 126.0793 | 0.39 | 3 | 1.67 | 0.17 |
| C12H15O2N2 | 218.1055 | 2.64 | 7 | 1.17 | 0.17 |
| C6H11N2 | 110.0844 | 0.99 | 3 | 1.67 | 0.00 |
| C5H9O2N2 | 128.0586 | 0.39 | 3 | 1.60 | 0.40 |
| C5H10N3 | 111.0796 | 0.75 | 3 | 1.80 | 0.00 |
| C7H12O1N3 | 153.0902 | 0.36 | 4 | 1.57 | 0.14 |
| C5H9O1N2 | 112.0637 | 4.76 | 3 | 1.60 | 0.20 |
| C7H13O5 | 176.0685 | 0.36 | 2 | 1.71 | 0.71 |
| C7H16N1 | 113.1204 | 0.71 | 1 | 2.14 | 0.00 |
| C6H15N2 | 114.1157 | 1.27 | 1 | 2.33 | 0.00 |
| C5H9O3 | 116.0473 | 0.48 | 2 | 1.60 | 0.60 |
| C5H5O1N1Na1 | 95.0371 | 0.60 | 4 | 1.00 | 0.20 |
| C7H7N2 | 118.0531 | 0.39 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 0.46 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 0.56 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 0.77 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 1.03 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 1.08 | 6 | 0.86 | 0.00 |
| C6H6N3 | 119.0483 | 0.39 | 6 | 0.83 | 0.00 |
| C6H5O1N2 | 120.0324 | 0.74 | 6 | 0.67 | 0.17 |
| C6H5O1N2 | 120.0324 | 1.95 | 6 | 0.67 | 0.17 |
| C6H5O1N2 | 120.0324 | 2.35 | 6 | 0.67 | 0.17 |
| C5H5N4 | 120.0436 | 0.52 | 6 | 0.80 | 0.00 |
| C8H9O1 | 120.0575 | 2.52 | 5 | 1.00 | 0.13 |
| C8H9O1 | 120.0575 | 2.56 | 5 | 1.00 | 0.13 |
| C7H9N2 | 120.0687 | 0.39 | 5 | 1.14 | 0.00 |
| C7H9N2 | 120.0687 | 0.46 | 5 | 1.14 | 0.00 |
| C7H9N2 | 120.0687 | 0.53 | 5 | 1.14 | 0.00 |
| C7H9N2 | 120.0687 | 0.81 | 5 | 1.14 | 0.00 |
| C7H8O1N1 | 121.0528 | 0.39 | 5 | 1.00 | 0.14 |
| C7H8O1N1 | 121.0528 | 0.61 | 5 | 1.00 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.11 | 4 | 1.43 | 0.14 |
| C7H8O1N1 | 121.0528 | 2.31 | 5 | 1.00 | 0.14 |
| C7H8O1N1 | 121.0528 | 2.38 | 5 | 1.00 | 0.14 |
| C8H12O2N1 | 153.0790 | 2.63 | 4 | 1.38 | 0.25 |

| | | | | | |
|---|---|---|---|---|---|
| C8H15N2 | 138.1157 | 1.57 | 3 | 1.75 | 0.00 |
| C7H7O2 | 122.0368 | 2.80 | 5 | 0.86 | 0.29 |
| C7H11N2 | 122.0844 | 0.39 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.47 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.60 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.68 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.91 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.97 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.08 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.26 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.32 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.41 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.66 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.81 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 2.02 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 2.19 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 2.54 | 4 | 1.43 | 0.00 |
| C6H6O2N1 | 123.0320 | 0.38 | 5 | 0.83 | 0.33 |
| C7H10O1N1 | 123.0684 | 0.39 | 4 | 1.29 | 0.14 |
| C7H10O1N1 | 123.0684 | 0.85 | 4 | 1.29 | 0.14 |
| C7H10O1N1 | 123.0684 | 1.34 | 4 | 1.29 | 0.14 |
| C3H9O5 | 124.0372 | 0.28 | 0 | 2.67 | 1.67 |
| C7H9O2 | 124.0524 | 2.48 | 4 | 1.14 | 0.29 |
| C6H9O1N2 | 124.0637 | 0.48 | 4 | 1.33 | 0.17 |
| C7H13N2 | 124.1000 | 0.61 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 0.71 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 0.94 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.08 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.20 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.30 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.87 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.00 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.11 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.25 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.40 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.64 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.47 | 3 | 1.71 | 0.00 |
| C8H11O2N2 | 166.0742 | 0.37 | 5 | 1.25 | 0.25 |
| C6H8O2N1 | 125.0477 | 0.50 | 4 | 1.17 | 0.33 |
| C6H8O2N1 | 125.0477 | 1.18 | 4 | 1.17 | 0.33 |
| C6H8O2N1 | 125.0477 | 1.27 | 4 | 1.17 | 0.33 |
| C6H8O2N1 | 125.0477 | 1.37 | 4 | 1.17 | 0.33 |
| C5H8O1N3 | 125.0589 | 0.39 | 4 | 1.40 | 0.20 |
| C7H12O1N1 | 125.0841 | 2.88 | 3 | 1.57 | 0.14 |
| C10H13O3N2 | 208.0848 | 0.98 | 6 | 1.20 | 0.30 |
| C5H7O2N2 | 126.0429 | 0.60 | 4 | 1.20 | 0.40 |
| C6H11O1N2 | 126.0793 | 0.51 | 3 | 1.67 | 0.17 |
| C7H15N2 | 126.1157 | 0.70 | 2 | 2.00 | 0.00 |
| C7H15N2 | 126.1157 | 0.93 | 2 | 2.00 | 0.00 |
| C7H15N2 | 126.1157 | 1.74 | 2 | 2.00 | 0.00 |

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|---|---|---|---|---|---|
| C7H15N2 | 126.1157 | 1.89 | 2 | 2.00 | 0.00 |
| C8H18N1 | 127.1361 | 1.16 | 1 | 2.13 | 0.00 |
| C9H5O1 | 128.0262 | 0.61 | 8 | 0.44 | 0.11 |
| C6H13O1N2 | 128.0950 | 0.33 | 2 | 2.00 | 0.17 |
| C3H9O3N2S1 | 152.0256 | 0.28 | 1 | 2.67 | 1.00 |
| C9H8N1 | 129.0578 | 0.96 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 1.22 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 1.29 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 1.33 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 1.38 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 1.40 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 1.61 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 1.75 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 2.00 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 2.20 | 7 | 0.78 | 0.00 |
| C9H8N1 | 129.0578 | 2.30 | 7 | 0.78 | 0.00 |
| C7H16O1N1 | 129.1154 | 0.39 | 1 | 2.14 | 0.14 |
| C7H16O1N1 | 129.1154 | 2.47 | 1 | 2.14 | 0.14 |
| C9H13O4N2 | 212.0797 | 0.63 | 5 | 1.33 | 0.44 |
| C9H7O1 | 130.0419 | 3.10 | 7 | 0.67 | 0.11 |
| C9H7O1 | 130.0419 | 3.52 | 7 | 0.67 | 0.11 |
| C8H7N2 | 130.0531 | 0.63 | 7 | 0.75 | 0.00 |
| C8H7N2 | 130.0531 | 0.78 | 7 | 0.75 | 0.00 |
| C8H7N2 | 130.0531 | 0.97 | 7 | 0.75 | 0.00 |
| C8H7N2 | 130.0531 | 1.04 | 7 | 0.75 | 0.00 |
| C8H7N2 | 130.0531 | 1.12 | 7 | 0.75 | 0.00 |
| C8H7N2 | 130.0531 | 1.14 | 7 | 0.75 | 0.00 |
| C8H7N2 | 130.0531 | 1.20 | 7 | 0.75 | 0.00 |
| C5H10O3N1 | 131.0582 | 0.33 | 2 | 1.80 | 0.60 |
| C5H10O3N1 | 131.0582 | 0.39 | 2 | 1.80 | 0.60 |
| C9H10N1 | 131.0735 | 0.41 | 6 | 1.00 | 0.00 |
| C8H5O2 | 132.0211 | 2.66 | 7 | 0.50 | 0.25 |
| C9H9O1 | 132.0575 | 2.76 | 6 | 0.89 | 0.11 |
| C8H9N2 | 132.0687 | 0.64 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 0.77 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 0.86 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 0.94 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.11 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.34 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.49 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.63 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.76 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.97 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 2.14 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 2.32 | 6 | 1.00 | 0.00 |
| C8H8O1N1 | 133.0528 | 0.56 | 6 | 0.88 | 0.13 |
| C8H8O1N1 | 133.0528 | 2.56 | 6 | 0.88 | 0.13 |
| C7H8N3 | 133.0640 | 0.59 | 6 | 1.00 | 0.00 |
| C7H8N3 | 133.0640 | 0.78 | 6 | 1.00 | 0.00 |
| C7H8N3 | 133.0640 | 1.36 | 6 | 1.00 | 0.00 |

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|---|---|---|---|---|---|
| C7H8N3 | 133.0640 | 1.60 | 6 | 1.00 | 0.00 |
| C7H8N3 | 133.0640 | 2.49 | 6 | 1.00 | 0.00 |
| C7H8N3 | 133.0640 | 1.68 | 6 | 1.00 | 0.00 |
| C9H12N1 | 133.0891 | 0.95 | 5 | 1.22 | 0.00 |
| C9H12N1 | 133.0891 | 1.13 | 5 | 1.22 | 0.00 |
| C9H12N1 | 133.0891 | 1.41 | 5 | 1.22 | 0.00 |
| C9H12N1 | 133.0891 | 1.68 | 5 | 1.22 | 0.00 |
| C9H12N1 | 133.0891 | 2.48 | 5 | 1.22 | 0.00 |
| C7H7O1N2 | 134.0480 | 1.04 | 6 | 0.86 | 0.14 |
| C7H7O1N2 | 134.0480 | 1.87 | 6 | 0.86 | 0.14 |
| C7H7O1N2 | 134.0480 | 2.30 | 6 | 0.86 | 0.14 |
| C7H7O1N2 | 134.0480 | 2.71 | 6 | 0.86 | 0.14 |
| C7H7O1N2 | 134.0480 | 2.89 | 6 | 0.86 | 0.14 |
| C6H7N4 | 134.0592 | 0.58 | 6 | 1.00 | 0.00 |
| C6H7N4 | 134.0592 | 0.84 | 6 | 1.00 | 0.00 |
| C11H14O1N1 | 175.0997 | 3.01 | 6 | 1.18 | 0.09 |
| C8H11N2 | 134.0844 | 0.36 | 5 | 1.25 | 0.00 |
| C8H11N2 | 134.0844 | 0.68 | 5 | 1.25 | 0.00 |
| C8H11N2 | 134.0844 | 1.19 | 5 | 1.25 | 0.00 |
| C7H6O2N1 | 135.0320 | 1.72 | 6 | 0.71 | 0.29 |
| C7H6O2N1 | 135.0320 | 2.29 | 6 | 0.71 | 0.29 |
| C6H6O1N3 | 135.0433 | 1.05 | 6 | 0.83 | 0.17 |
| C8H10O1N1 | 135.0684 | 0.39 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 0.62 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 0.76 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 0.82 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 1.26 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 1.38 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 2.27 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 2.36 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 2.51 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 2.68 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 2.78 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 3.01 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 3.12 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 3.35 | 5 | 1.13 | 0.13 |
| C8H10O1N1 | 135.0684 | 3.61 | 5 | 1.13 | 0.13 |
| C9H14N1 | 135.1048 | 1.49 | 4 | 1.44 | 0.00 |
| C9H14N1 | 135.1048 | 1.62 | 4 | 1.44 | 0.00 |
| C9H14N1 | 135.1048 | 1.83 | 4 | 1.44 | 0.00 |
| C9H14N1 | 135.1048 | 1.74 | 4 | 1.44 | 0.00 |
| C7H5O3 | 136.0160 | 1.43 | 6 | 0.57 | 0.43 |
| C5H5O1N4 | 136.0385 | 0.39 | 6 | 0.80 | 0.20 |
| C8H9O2 | 136.0524 | 0.49 | 5 | 1.00 | 0.25 |
| C8H9O2 | 136.0524 | 0.57 | 5 | 1.00 | 0.25 |
| C8H9O2 | 136.0524 | 2.95 | 5 | 1.00 | 0.25 |
| C8H9O2 | 136.0524 | 3.02 | 5 | 1.00 | 0.25 |
| C8H9O2 | 136.0524 | 3.10 | 5 | 1.00 | 0.25 |
| C8H9O2 | 136.0524 | 3.19 | 5 | 1.00 | 0.25 |
| C8H9O2 | 136.0524 | 3.36 | 5 | 1.00 | 0.25 |

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|---|---|---|---|---|---|
| C8H9O2 | 136.0524 | 3.53 | 5 | 1.00 | 0.25 |
| C8H9O2 | 136.0524 | 3.57 | 5 | 1.00 | 0.25 |
| C7H9O1N2 | 136.0637 | 0.39 | 5 | 1.14 | 0.14 |
| C7H9O1N2 | 136.0637 | 0.43 | 5 | 1.14 | 0.14 |
| C7H9O1N2 | 136.0637 | 0.47 | 5 | 1.14 | 0.14 |
| C7H9O1N2 | 136.0637 | 0.49 | 5 | 1.14 | 0.14 |
| C7H9O1N2 | 136.0637 | 0.55 | 5 | 1.14 | 0.14 |
| C7H9O1N2 | 136.0637 | 1.52 | 5 | 1.14 | 0.14 |
| C7H9O1N2 | 136.0637 | 2.38 | 5 | 1.14 | 0.14 |
| C7H9O1N2 | 136.0637 | 2.63 | 5 | 1.14 | 0.14 |
| C8H13N2 | 136.1000 | 0.77 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 0.92 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.12 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.25 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.36 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.55 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.69 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.78 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.90 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.95 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.12 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.32 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.40 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.51 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.68 | 4 | 1.50 | 0.00 |
| C7H8O2N1 | 137.0477 | 0.39 | 5 | 1.00 | 0.29 |
| C8H12O1N1 | 137.0841 | 0.39 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.44 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.50 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.56 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.79 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.89 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.97 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.12 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.22 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.36 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.44 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.60 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.67 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.78 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.88 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.97 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.09 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.20 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.30 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.33 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.54 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.62 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.65 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.87 | 4 | 1.38 | 0.13 |

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|---|---|---|---|---|---|
| C8H12O1N1 | 137.0841 | 3.00 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 3.10 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 3.25 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 3.38 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 3.56 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 3.68 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 3.79 | 4 | 1.38 | 0.13 |
| C7H12N3 | 137.0953 | 0.56 | 4 | 1.57 | 0.00 |
| C7H12N3 | 137.0953 | 1.05 | 4 | 1.57 | 0.00 |
| C7H7O3 | 138.0317 | 2.13 | 5 | 0.86 | 0.43 |
| C7H7O3 | 138.0317 | 2.28 | 5 | 0.86 | 0.43 |
| C7H7O3 | 138.0317 | 2.38 | 5 | 0.86 | 0.43 |
| C6H7O2N2 | 138.0429 | 0.95 | 5 | 1.00 | 0.33 |
| C7H11O1N2 | 138.0793 | 0.48 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 0.64 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 0.72 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.03 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.22 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.32 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.50 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.67 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.77 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.85 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 1.97 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 2.01 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 2.03 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 2.33 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 2.41 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 2.44 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 2.71 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 2.89 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 3.13 | 4 | 1.43 | 0.14 |
| C8H15N2 | 138.1157 | 0.87 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 0.90 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 0.96 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.26 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.40 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.48 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.59 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.65 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.83 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.89 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.07 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.21 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.27 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.40 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.54 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.68 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.80 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.88 | 3 | 1.75 | 0.00 |

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|---|---|---|---|---|---|
| C8H15N2 | 138.1157 | 2.95 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 3.03 | 3 | 1.75 | 0.00 |
| C6H6O3N1 | 139.0269 | 0.38 | 5 | 0.83 | 0.50 |
| C6H6O3N1 | 139.0269 | 0.43 | 5 | 0.83 | 0.50 |
| C7H13O2N2 | 156.0899 | 0.39 | 3 | 1.71 | 0.29 |
| C7H10O2N1 | 139.0633 | 0.51 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 0.73 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 0.95 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 1.30 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 2.49 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 2.62 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 2.80 | 4 | 1.29 | 0.29 |
| C6H10O1N3 | 139.0746 | 0.64 | 4 | 1.50 | 0.17 |
| C5H5O3N2 | 140.0222 | 2.65 | 5 | 0.80 | 0.60 |
| C7H9O3 | 140.0473 | 1.39 | 4 | 1.14 | 0.43 |
| C6H9O2N2 | 140.0586 | 0.68 | 4 | 1.33 | 0.33 |
| C6H9O2N2 | 140.0586 | 1.07 | 4 | 1.33 | 0.33 |
| C7H13O1N2 | 140.0950 | 0.50 | 3 | 1.71 | 0.14 |
| C8H17N2 | 140.1313 | 1.35 | 2 | 2.00 | 0.00 |
| C8H17N2 | 140.1313 | 2.43 | 2 | 2.00 | 0.00 |
| C11H9O4 | 204.0423 | 3.64 | 8 | 0.73 | 0.36 |
| C6H8O3N1 | 141.0426 | 0.35 | 4 | 1.17 | 0.50 |
| C6H8O3N1 | 141.0426 | 0.39 | 4 | 1.17 | 0.50 |
| C6H8O3N1 | 141.0426 | 0.41 | 4 | 1.17 | 0.50 |
| C8H11O3N2 | 182.0691 | 0.65 | 5 | 1.25 | 0.38 |
| C7H12O2N1 | 141.0790 | 0.37 | 3 | 1.57 | 0.29 |
| C6H11O2N2 | 142.0742 | 0.53 | 3 | 1.67 | 0.33 |
| C6H10O1N1S1 | 143.0405 | 0.89 | 3 | 1.50 | 0.17 |
| C9H11O3 | 166.0630 | 3.25 | 5 | 1.11 | 0.33 |
| C7H14O4N1 | 175.0845 | 0.39 | 2 | 1.86 | 0.57 |
| C7H14O4N1 | 175.0845 | 0.39 | 2 | 1.86 | 0.57 |
| C10H10N1 | 143.0735 | 0.67 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.32 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.50 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.56 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.60 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.67 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.77 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.89 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.01 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.19 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.34 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.60 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.65 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.66 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.68 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.68 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.71 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.73 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.89 | 7 | 0.90 | 0.00 |

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|---|---|---|---|---|---|
| C10H10N1 | 143.0735 | 2.90 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.96 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 3.08 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 3.17 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 3.51 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 3.61 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 3.86 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 4.01 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 4.52 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 5.09 | 7 | 0.90 | 0.00 |
| C9H9N2 | 144.0687 | 0.78 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 0.90 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 1.09 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 1.19 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 1.30 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 1.46 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 1.74 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 2.41 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 2.49 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 2.56 | 7 | 0.89 | 0.00 |
| C7H9O1N1Na1 | 123.0684 | 2.63 | 4 | 1.29 | 0.14 |
| C9H8O1N1 | 145.0528 | 0.84 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 0.92 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 1.07 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 1.19 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 1.96 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 2.33 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 2.42 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 2.83 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 3.26 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 3.50 | 7 | 0.78 | 0.11 |
| C8H8N3 | 145.0640 | 0.39 | 7 | 0.88 | 0.00 |
| C8H8N3 | 145.0640 | 0.71 | 7 | 0.88 | 0.00 |
| C6H12O3N1 | 145.0739 | 0.38 | 2 | 1.83 | 0.50 |
| C6H12O3N1 | 145.0739 | 0.60 | 2 | 1.83 | 0.50 |
| C10H12N1 | 145.0891 | 1.70 | 6 | 1.10 | 0.00 |
| C10H12N1 | 145.0891 | 1.95 | 6 | 1.10 | 0.00 |
| C10H12N1 | 145.0891 | 2.21 | 6 | 1.10 | 0.00 |
| C10H12N1 | 145.0891 | 2.37 | 6 | 1.10 | 0.00 |
| C10H12N1 | 145.0891 | 2.51 | 6 | 1.10 | 0.00 |
| C10H12N1 | 145.0891 | 2.20 | 6 | 1.10 | 0.00 |
| C7H16O2N1 | 145.1103 | 0.41 | 1 | 2.14 | 0.29 |
| C7H16O2N1 | 145.1103 | 0.49 | 1 | 2.14 | 0.29 |
| C9H7O2 | 146.0368 | 2.74 | 7 | 0.67 | 0.22 |
| C10H11O3 | 178.0630 | 3.09 | 6 | 1.00 | 0.30 |
| C9H7O2 | 146.0368 | 3.26 | 7 | 0.67 | 0.22 |
| C9H7O2 | 146.0368 | 3.35 | 7 | 0.67 | 0.22 |
| C9H7O2 | 146.0368 | 3.64 | 7 | 0.67 | 0.22 |
| C8H7O1N2 | 146.0480 | 0.39 | 7 | 0.75 | 0.13 |
| C8H7O1N2 | 146.0480 | 0.95 | 7 | 0.75 | 0.13 |

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|---|---|---|---|---|---|
| C8H7O1N2 | 146.0480 | 1.69 | 7 | 0.75 | 0.13 |
| C8H7O1N2 | 146.0480 | 2.31 | 7 | 0.75 | 0.13 |
| C8H7O1N2 | 146.0480 | 2.62 | 7 | 0.75 | 0.13 |
| C8H7O1N2 | 146.0480 | 2.65 | 7 | 0.75 | 0.13 |
| C8H7O1N2 | 146.0480 | 2.77 | 7 | 0.75 | 0.13 |
| C6H11O4 | 146.0579 | 0.37 | 2 | 1.67 | 0.67 |
| C6H11O4 | 146.0579 | 0.45 | 2 | 1.67 | 0.67 |
| C5H11O3N2 | 146.0691 | 0.33 | 2 | 2.00 | 0.60 |
| C10H11O1 | 146.0732 | 3.11 | 6 | 1.00 | 0.10 |
| C9H11N2 | 146.0844 | 0.39 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 0.50 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 0.91 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.02 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.15 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.22 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.31 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.44 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.51 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.63 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.76 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.91 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.98 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.09 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.18 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.27 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.39 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.51 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.61 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.71 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.85 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.88 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 3.19 | 6 | 1.11 | 0.00 |
| C9H10O1N1 | 147.0684 | 0.93 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 1.07 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 1.17 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 1.30 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 1.48 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 1.63 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 1.73 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 1.96 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 1.99 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 2.16 | 6 | 1.00 | 0.11 |
| C10H14O2N1 | 179.0946 | 2.63 | 5 | 1.30 | 0.20 |
| C9H10O1N1 | 147.0684 | 2.77 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 3.01 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 3.08 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 3.22 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 3.34 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 3.45 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 3.56 | 6 | 1.00 | 0.11 |

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|---|---|---|---|---|---|
| C9H10O1N1 | 147.0684 | 3.79 | 6 | 1.00 | 0.11 |
| C9H10O1N1 | 147.0684 | 3.89 | 6 | 1.00 | 0.11 |
| C8H10N3 | 147.0796 | 0.48 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 0.57 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 0.73 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 0.87 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 0.94 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 1.04 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 1.27 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 1.37 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 1.42 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 1.66 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 2.27 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 2.36 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 2.78 | 6 | 1.13 | 0.00 |
| C10H14N1 | 147.1048 | 2.24 | 5 | 1.30 | 0.00 |
| C10H14N1 | 147.1048 | 2.39 | 5 | 1.30 | 0.00 |
| C10H14N1 | 147.1048 | 2.58 | 5 | 1.30 | 0.00 |
| C10H14N1 | 147.1048 | 2.75 | 5 | 1.30 | 0.00 |
| C10H14N1 | 147.1048 | 2.84 | 5 | 1.30 | 0.00 |
| C10H14N1 | 147.1048 | 2.94 | 5 | 1.30 | 0.00 |
| C10H14N1 | 147.1048 | 2.98 | 5 | 1.30 | 0.00 |
| C10H14N1 | 147.1048 | 2.55 | 5 | 1.30 | 0.00 |
| C9H9O2 | 148.0524 | 3.02 | 6 | 0.89 | 0.22 |
| C9H9O2 | 148.0524 | 3.46 | 6 | 0.89 | 0.22 |
| C9H9O2 | 148.0524 | 3.53 | 6 | 0.89 | 0.22 |
| C9H9O2 | 148.0524 | 3.61 | 6 | 0.89 | 0.22 |
| C8H9O1N2 | 148.0637 | 0.45 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 0.48 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 0.73 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 1.05 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 1.17 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 1.27 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 2.39 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 2.52 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 2.72 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 2.93 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 3.01 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 3.04 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 3.12 | 6 | 1.00 | 0.13 |
| C7H9N4 | 148.0749 | 0.91 | 6 | 1.14 | 0.00 |
| C9H13N2 | 148.1000 | 1.26 | 5 | 1.33 | 0.00 |
| C9H13N2 | 148.1000 | 1.43 | 5 | 1.33 | 0.00 |
| C9H13N2 | 148.1000 | 2.47 | 5 | 1.33 | 0.00 |
| C9H13N2 | 148.1000 | 2.78 | 5 | 1.33 | 0.00 |
| C6H11O3N2S1 | 190.0412 | 0.37 | 3 | 1.67 | 0.50 |
| C8H8O2N1 | 149.0477 | 0.38 | 6 | 0.88 | 0.25 |
| C8H8O2N1 | 149.0477 | 0.70 | 6 | 0.88 | 0.25 |
| C8H8O2N1 | 149.0477 | 0.71 | 6 | 0.88 | 0.25 |
| C8H8O2N1 | 149.0477 | 0.96 | 6 | 0.88 | 0.25 |

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|---|---|---|---|---|---|
| C8H8O2N1 | 149.0477 | 1.17 | 6 | 0.88 | 0.25 |
| C8H8O2N1 | 149.0477 | 2.39 | 6 | 0.88 | 0.25 |
| C8H8O2N1 | 149.0477 | 2.75 | 6 | 0.88 | 0.25 |
| C8H8O2N1 | 149.0477 | 2.85 | 6 | 0.88 | 0.25 |
| C8H8O2N1 | 149.0477 | 3.10 | 6 | 0.88 | 0.25 |
| C7H8O1N3 | 149.0589 | 0.40 | 6 | 1.00 | 0.14 |
| C7H8O1N3 | 149.0589 | 2.37 | 6 | 1.00 | 0.14 |
| C7H8O1N3 | 149.0589 | 2.46 | 6 | 1.00 | 0.14 |
| C6H8N5 | 149.0701 | 0.42 | 6 | 1.17 | 0.00 |
| C9H12O1N1 | 149.0841 | 0.51 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 0.89 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 1.11 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 1.26 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 1.45 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 1.58 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 1.88 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 2.40 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 2.47 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 2.82 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 2.85 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 2.93 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 3.18 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 3.45 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 3.56 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 3.63 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 3.76 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 3.87 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 4.31 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 0.66 | 5 | 1.22 | 0.11 |
| C9H12O1N1 | 149.0841 | 3.96 | 5 | 1.22 | 0.11 |
| C6H16O3N1 | 149.1052 | 0.62 | 0 | 2.50 | 0.50 |
| C6H16O3N1 | 149.1052 | 0.64 | 0 | 2.50 | 0.50 |
| C6H16O3N1 | 149.1052 | 0.84 | 0 | 2.50 | 0.50 |
| C10H16N1 | 149.1204 | 2.20 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 2.53 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 2.60 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 2.64 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 2.71 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 2.81 | 4 | 1.50 | 0.00 |
| C10H19N2 | 166.1470 | 2.95 | 3 | 1.80 | 0.00 |
| C10H16N1 | 149.1204 | 2.98 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 3.07 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 3.18 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 3.39 | 4 | 1.50 | 0.00 |
| C5H10O5N3 | 191.0542 | 0.28 | 3 | 1.80 | 1.00 |
| C8H7O3 | 150.0317 | 2.64 | 6 | 0.75 | 0.38 |
| C8H7O3 | 150.0317 | 2.73 | 6 | 0.75 | 0.38 |
| C8H7O3 | 150.0317 | 2.77 | 6 | 0.75 | 0.38 |
| C8H5O2 | 132.0211 | 2.79 | 7 | 0.50 | 0.25 |
| C5H8O2N2Na1 | 128.0586 | 0.37 | 3 | 1.60 | 0.40 |

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|---|---|---|---|---|---|
| C6H7O1N4 | 150.0542 | 0.59 | 6 | 1.00 | 0.17 |
| C6H7O1N4 | 150.0542 | 0.82 | 6 | 1.00 | 0.17 |
| C9H11O2 | 150.0681 | 0.97 | 5 | 1.11 | 0.22 |
| C11H12O1N1 | 173.0841 | 2.84 | 7 | 1.00 | 0.09 |
| C9H11O2 | 150.0681 | 3.60 | 5 | 1.11 | 0.22 |
| C9H11O2 | 150.0681 | 3.70 | 5 | 1.11 | 0.22 |
| C9H11O2 | 150.0681 | 3.93 | 5 | 1.11 | 0.22 |
| C9H11O2 | 150.0681 | 4.12 | 5 | 1.11 | 0.22 |
| C9H11O2 | 150.0681 | 4.29 | 5 | 1.11 | 0.22 |
| C9H11O2 | 150.0681 | 4.44 | 5 | 1.11 | 0.22 |
| C9H11O2 | 150.0681 | 4.64 | 5 | 1.11 | 0.22 |
| C9H11O2 | 150.0681 | 5.07 | 5 | 1.11 | 0.22 |
| C8H11O1N2 | 150.0793 | 0.53 | 5 | 1.25 | 0.13 |
| C8H11O1N2 | 150.0793 | 0.90 | 5 | 1.25 | 0.13 |
| C8H11O1N2 | 150.0793 | 0.98 | 5 | 1.25 | 0.13 |
| C8H11O1N2 | 150.0793 | 1.33 | 5 | 1.25 | 0.13 |
| C8H11O1N2 | 150.0793 | 2.45 | 5 | 1.25 | 0.13 |
| C8H11O1N2 | 150.0793 | 2.75 | 5 | 1.25 | 0.13 |
| C8H11O1N2 | 150.0793 | 2.90 | 5 | 1.25 | 0.13 |
| C8H11O1N2 | 150.0793 | 3.11 | 5 | 1.25 | 0.13 |
| C8H11O1N2 | 150.0793 | 3.27 | 5 | 1.25 | 0.13 |
| C9H15N2 | 150.1157 | 1.25 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 1.49 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 1.66 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 1.97 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.22 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.39 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.59 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.73 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.83 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.92 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 1.69 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 3.03 | 4 | 1.56 | 0.00 |
| C12H10O1Na1 | 170.0732 | 0.28 | 8 | 0.83 | 0.08 |
| C8H10O2N1 | 151.0633 | 0.38 | 5 | 1.13 | 0.25 |
| C10H13O2N2 | 192.0899 | 0.59 | 6 | 1.20 | 0.20 |
| C8H10O2N1 | 151.0633 | 1.08 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 1.36 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 1.37 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 1.74 | 5 | 1.13 | 0.25 |
| C8H13O2N2 | 168.0899 | 2.11 | 4 | 1.50 | 0.25 |
| C8H10O2N1 | 151.0633 | 2.39 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 2.44 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 2.61 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 2.77 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 2.82 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 3.05 | 5 | 1.13 | 0.25 |
| C7H10O1N3 | 151.0746 | 0.53 | 5 | 1.29 | 0.14 |
| C9H14O1N1 | 151.0997 | 0.59 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 0.73 | 4 | 1.44 | 0.11 |

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|---|---|---|---|---|---|
| C9H14O1N1 | 151.0997 | 1.00 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 1.12 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 1.32 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 1.46 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 1.63 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 1.93 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.10 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.25 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.39 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.54 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.64 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 3.37 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 3.53 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 3.61 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 3.74 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 3.83 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 4.06 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.00 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 3.00 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.71 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.46 | 4 | 1.44 | 0.11 |
| C10H18N1 | 151.1361 | 2.85 | 3 | 1.70 | 0.00 |
| C8H9O3 | 152.0473 | 2.67 | 5 | 1.00 | 0.38 |
| C8H9O3 | 152.0473 | 2.94 | 5 | 1.00 | 0.38 |
| C8H9O3 | 152.0473 | 3.00 | 5 | 1.00 | 0.38 |
| C8H9O3 | 152.0473 | 3.25 | 5 | 1.00 | 0.38 |
| C8H9O3 | 152.0473 | 3.56 | 5 | 1.00 | 0.38 |
| C8H9O3 | 152.0473 | 3.64 | 5 | 1.00 | 0.38 |
| C8H9O3 | 152.0473 | 3.72 | 5 | 1.00 | 0.38 |
| C7H9O2N2 | 152.0586 | 0.53 | 5 | 1.14 | 0.29 |
| C7H9O2N2 | 152.0586 | 0.76 | 5 | 1.14 | 0.29 |
| C7H9O2N2 | 152.0586 | 0.94 | 5 | 1.14 | 0.29 |
| C7H9O2N2 | 152.0586 | 1.36 | 5 | 1.14 | 0.29 |
| C7H9O2N2 | 152.0586 | 1.80 | 5 | 1.14 | 0.29 |
| C7H9O2N2 | 152.0586 | 2.67 | 5 | 1.14 | 0.29 |
| C8H13O1N2 | 152.0950 | 0.85 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 0.89 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 0.97 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 1.14 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 1.19 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 1.36 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 1.71 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 2.21 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 2.30 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 2.73 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 2.83 | 4 | 1.50 | 0.13 |
| C8H13O1N2 | 152.0950 | 3.56 | 4 | 1.50 | 0.13 |
| C9H17N2 | 152.1313 | 2.34 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.55 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.70 | 3 | 1.78 | 0.00 |

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|---|---|---|---|---|---|
| C9H17N2 | 152.1313 | 2.79 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.83 | 3 | 1.78 | 0.00 |
| C7H11O3N2 | 170.0691 | 0.89 | 4 | 1.43 | 0.43 |
| C7H8O3N1 | 153.0426 | 2.62 | 5 | 1.00 | 0.43 |
| C8H12O2N1 | 153.0790 | 0.52 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 0.60 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 0.96 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 1.05 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 1.43 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 1.63 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 2.07 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 2.28 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 2.56 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 2.82 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 2.89 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 3.13 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 3.30 | 4 | 1.38 | 0.25 |
| C7H12O1N3 | 153.0902 | 0.86 | 4 | 1.57 | 0.14 |
| C6H7O3N2 | 154.0378 | 0.37 | 5 | 1.00 | 0.50 |
| C10H7N2 | 154.0531 | 3.04 | 9 | 0.60 | 0.00 |
| C10H7N2 | 154.0531 | 3.39 | 9 | 0.60 | 0.00 |
| C7H11O2N2 | 154.0742 | 0.39 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 0.50 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 0.84 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 0.89 | 4 | 1.43 | 0.29 |
| C7H8O2N1 | 137.0477 | 0.98 | 5 | 1.00 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.03 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.07 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.17 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.28 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.41 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.47 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.55 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.68 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.72 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.81 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.86 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 1.94 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 2.06 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 2.14 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 2.26 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 2.36 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 2.40 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 3.08 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 3.25 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 3.75 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 3.86 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 3.89 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 4.50 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 4.57 | 4 | 1.43 | 0.29 |

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|---|---|---|---|---|---|
| C5H11N6 | 154.0967 | 0.71 | 4 | 2.00 | 0.00 |
| C7H10O3N1 | 155.0582 | 0.98 | 4 | 1.29 | 0.43 |
| C7H10O3N1 | 155.0582 | 1.42 | 4 | 1.29 | 0.43 |
| C7H10O3N1 | 155.0582 | 2.61 | 4 | 1.29 | 0.43 |
| C11H10N1 | 155.0735 | 2.14 | 8 | 0.82 | 0.00 |
| C11H10N1 | 155.0735 | 2.29 | 8 | 0.82 | 0.00 |
| C11H10N1 | 155.0735 | 2.39 | 8 | 0.82 | 0.00 |
| C11H10N1 | 155.0735 | 2.52 | 8 | 0.82 | 0.00 |
| C11H10N1 | 155.0735 | 2.78 | 8 | 0.82 | 0.00 |
| C11H10N1 | 155.0735 | 2.86 | 8 | 0.82 | 0.00 |
| C11H10N1 | 155.0735 | 3.03 | 8 | 0.82 | 0.00 |
| C8H14O2N1 | 155.0946 | 0.39 | 3 | 1.63 | 0.25 |
| C7H14O1N3 | 155.1059 | 0.32 | 3 | 1.86 | 0.14 |
| C7H9O4 | 156.0423 | 1.21 | 4 | 1.14 | 0.57 |
| C6H9O3N2 | 156.0535 | 0.39 | 4 | 1.33 | 0.50 |
| C13H12O1N1 | 197.0841 | 2.62 | 9 | 0.85 | 0.08 |
| C13H10N1 | 179.0735 | 2.92 | 10 | 0.69 | 0.00 |
| C10H9N2 | 156.0687 | 1.35 | 8 | 0.80 | 0.00 |
| C10H9N2 | 156.0687 | 1.56 | 8 | 0.80 | 0.00 |
| C10H9N2 | 156.0687 | 1.87 | 8 | 0.80 | 0.00 |
| C10H9N2 | 156.0687 | 2.10 | 8 | 0.80 | 0.00 |
| C7H13O2N2 | 156.0899 | 0.38 | 3 | 1.71 | 0.29 |
| C7H13O2N2 | 156.0899 | 0.64 | 3 | 1.71 | 0.29 |
| C7H13O2N2 | 156.0899 | 0.89 | 3 | 1.71 | 0.29 |
| C10H8O1N1 | 157.0528 | 1.13 | 8 | 0.70 | 0.10 |
| C9H8N3 | 157.0640 | 2.49 | 8 | 0.78 | 0.00 |
| C9H8N3 | 157.0640 | 3.09 | 8 | 0.78 | 0.00 |
| C7H12O3N1 | 157.0739 | 0.58 | 3 | 1.57 | 0.43 |
| C11H12N1 | 157.0891 | 2.54 | 7 | 1.00 | 0.00 |
| C11H12N1 | 157.0891 | 2.61 | 7 | 1.00 | 0.00 |
| C11H12N1 | 157.0891 | 2.67 | 7 | 1.00 | 0.00 |
| C11H12N1 | 157.0891 | 2.79 | 7 | 1.00 | 0.00 |
| C11H12N1 | 157.0891 | 2.95 | 7 | 1.00 | 0.00 |
| C11H12N1 | 157.0891 | 3.02 | 7 | 1.00 | 0.00 |
| C13H15N2 | 198.1157 | 3.06 | 8 | 1.08 | 0.00 |
| C10H7O2 | 158.0368 | 2.76 | 8 | 0.60 | 0.20 |
| C10H7O2 | 158.0368 | 3.36 | 8 | 0.60 | 0.20 |
| C11H11O1 | 158.0732 | 5.62 | 7 | 0.91 | 0.09 |
| C10H11N2 | 158.0844 | 1.14 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 1.30 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 1.47 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 1.63 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 1.73 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 1.97 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.42 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.52 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.71 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.84 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 3.00 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 3.08 | 7 | 1.00 | 0.00 |

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|---|---|---|---|---|---|
| C6H10O4N1 | 159.0532 | 0.63 | 3 | 1.50 | 0.67 |
| C10H10O1N1 | 159.0684 | 1.49 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 1.66 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 1.82 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 1.92 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 2.06 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 2.20 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 2.36 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 2.46 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 2.65 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 2.86 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 3.65 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 3.77 | 7 | 0.90 | 0.10 |
| C10H10O1N1 | 159.0684 | 2.90 | 7 | 0.90 | 0.10 |
| C9H10N3 | 159.0796 | 0.55 | 7 | 1.00 | 0.00 |
| C9H10N3 | 159.0796 | 0.67 | 7 | 1.00 | 0.00 |
| C9H10N3 | 159.0796 | 0.87 | 7 | 1.00 | 0.00 |
| C9H10N3 | 159.0796 | 1.31 | 7 | 1.00 | 0.00 |
| C9H10N3 | 159.0796 | 1.52 | 7 | 1.00 | 0.00 |
| C9H10N3 | 159.0796 | 1.77 | 7 | 1.00 | 0.00 |
| C7H14O3N1 | 159.0895 | 0.39 | 2 | 1.86 | 0.43 |
| C11H14N1 | 159.1048 | 2.52 | 6 | 1.18 | 0.00 |
| C11H14N1 | 159.1048 | 2.64 | 6 | 1.18 | 0.00 |
| C11H14N1 | 159.1048 | 2.70 | 6 | 1.18 | 0.00 |
| C11H14N1 | 159.1048 | 2.76 | 6 | 1.18 | 0.00 |
| C11H14N1 | 159.1048 | 2.91 | 6 | 1.18 | 0.00 |
| C11H14N1 | 159.1048 | 3.00 | 6 | 1.18 | 0.00 |
| C10H9O2 | 160.0524 | 3.61 | 7 | 0.80 | 0.20 |
| C10H9O2 | 160.0524 | 3.64 | 7 | 0.80 | 0.20 |
| C10H9O2 | 160.0524 | 3.81 | 7 | 0.80 | 0.20 |
| C10H9O2 | 160.0524 | 3.98 | 7 | 0.80 | 0.20 |
| C10H9O2 | 160.0524 | 4.09 | 7 | 0.80 | 0.20 |
| C10H9O2 | 160.0524 | 4.53 | 7 | 0.80 | 0.20 |
| C12H10O1N1 | 183.0684 | 3.41 | 9 | 0.75 | 0.08 |
| C10H9O2 | 160.0524 | 4.35 | 7 | 0.80 | 0.20 |
| C10H9O2 | 160.0524 | 4.58 | 7 | 0.80 | 0.20 |
| C9H9O1N2 | 160.0637 | 0.50 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 0.59 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 0.67 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 0.77 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 0.87 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 0.99 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 1.18 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 1.21 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 1.36 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 1.54 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 1.62 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 1.72 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 1.88 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 2.04 | 7 | 0.89 | 0.11 |

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| C9H9O1N2 | 160.0637 | 2.27 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 2.56 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 2.68 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 2.88 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 2.93 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 3.01 | 7 | 0.89 | 0.11 |
| C9H9O1N2 | 160.0637 | 3.24 | 7 | 0.89 | 0.11 |
| C6H13O3N2 | 160.0848 | 0.33 | 2 | 2.00 | 0.50 |
| C10H13N2 | 160.1000 | 0.48 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.05 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.60 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.76 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.98 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 3.17 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 3.25 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 3.37 | 6 | 1.20 | 0.00 |
| C9H8O2N1 | 161.0477 | 1.31 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 1.53 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 1.72 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 2.20 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 2.51 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 2.67 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 2.83 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 2.92 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 3.12 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 3.27 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 3.51 | 7 | 0.78 | 0.22 |
| C9H8O2N1 | 161.0477 | 4.19 | 7 | 0.78 | 0.22 |
| C6H12O4N1 | 161.0688 | 0.37 | 2 | 1.83 | 0.67 |
| C6H12O4N1 | 161.0688 | 0.68 | 2 | 1.83 | 0.67 |
| C10H12O1N1 | 161.0841 | 0.59 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 0.62 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 0.84 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 1.11 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 1.19 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 1.77 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.23 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.31 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.46 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.57 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.65 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.74 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.82 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.88 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.91 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 2.96 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 3.07 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 3.31 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 3.47 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 3.51 | 6 | 1.10 | 0.10 |

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| C10H12O1N1 | 161.0841 | 3.68 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 3.93 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 4.16 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 4.30 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 4.34 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 4.77 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 5.02 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 5.07 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 5.34 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 5.52 | 6 | 1.10 | 0.10 |
| C9H12N3 | 161.0953 | 0.77 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 0.95 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 1.06 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 1.19 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 1.31 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 1.57 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 1.81 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 1.90 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 2.40 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 2.48 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 2.56 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 2.61 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 2.91 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 3.13 | 6 | 1.22 | 0.00 |
| C11H16N1 | 161.1204 | 2.64 | 5 | 1.36 | 0.00 |
| C11H16N1 | 161.1204 | 2.67 | 5 | 1.36 | 0.00 |
| C11H16N1 | 161.1204 | 2.77 | 5 | 1.36 | 0.00 |
| C11H16N1 | 161.1204 | 2.89 | 5 | 1.36 | 0.00 |
| C11H16N1 | 161.1204 | 2.94 | 5 | 1.36 | 0.00 |
| C11H16N1 | 161.1204 | 3.19 | 5 | 1.36 | 0.00 |
| C11H16N1 | 161.1204 | 3.25 | 5 | 1.36 | 0.00 |
| C11H16N1 | 161.1204 | 3.38 | 5 | 1.36 | 0.00 |
| C9H7O3 | 162.0317 | 0.54 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 0.63 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 0.64 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 2.62 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 2.78 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 2.90 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 2.90 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 2.91 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 3.16 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 3.34 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 3.35 | 7 | 0.67 | 0.33 |
| C8H7O2N2 | 162.0429 | 2.29 | 7 | 0.75 | 0.25 |
| C8H7O2N2 | 162.0429 | 2.55 | 7 | 0.75 | 0.25 |
| C6H10O5Na1 | 162.0528 | 0.38 | 2 | 1.67 | 0.83 |
| C5H11O4N2 | 162.0641 | 0.33 | 2 | 2.00 | 0.80 |
| C10H11O2 | 162.0681 | 2.77 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 2.91 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 3.04 | 6 | 1.00 | 0.20 |

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| C10H11O2 | 162.0681 | 3.12 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 3.22 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 3.38 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 3.51 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 3.62 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 3.75 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 4.06 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 4.43 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 4.54 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 4.64 | 6 | 1.00 | 0.20 |
| C10H11O2 | 162.0681 | 4.76 | 6 | 1.00 | 0.20 |
| C9H11O1N2 | 162.0793 | 0.88 | 6 | 1.11 | 0.11 |
| C9H11O1N2 | 162.0793 | 0.97 | 6 | 1.11 | 0.11 |
| C9H11O1N2 | 162.0793 | 1.08 | 6 | 1.11 | 0.11 |
| C9H11O1N2 | 162.0793 | 2.37 | 6 | 1.11 | 0.11 |
| C9H11O1N2 | 162.0793 | 2.46 | 6 | 1.11 | 0.11 |
| C9H11O1N2 | 162.0793 | 2.65 | 6 | 1.11 | 0.11 |
| C9H11O1N2 | 162.0793 | 3.37 | 6 | 1.11 | 0.11 |
| C9H11O1N2 | 162.0793 | 3.53 | 6 | 1.11 | 0.11 |
| C8H11N4 | 162.0905 | 0.76 | 6 | 1.25 | 0.00 |
| C10H15N2 | 162.1157 | 0.39 | 5 | 1.40 | 0.00 |
| C10H15N2 | 162.1157 | 0.49 | 5 | 1.40 | 0.00 |
| C5H10O5N1 | 163.0481 | 0.34 | 2 | 1.80 | 1.00 |
| C9H10O2N1 | 163.0633 | 2.55 | 6 | 1.00 | 0.22 |
| C9H10O2N1 | 163.0633 | 2.62 | 6 | 1.00 | 0.22 |
| C9H10O2N1 | 163.0633 | 2.74 | 6 | 1.00 | 0.22 |
| C9H10O2N1 | 163.0633 | 2.89 | 6 | 1.00 | 0.22 |
| C9H10O2N1 | 163.0633 | 3.00 | 6 | 1.00 | 0.22 |
| C9H10O2N1 | 163.0633 | 3.07 | 6 | 1.00 | 0.22 |
| C9H10O2N1 | 163.0633 | 3.31 | 6 | 1.00 | 0.22 |
| C9H10O2N1 | 163.0633 | 3.63 | 6 | 1.00 | 0.22 |
| C9H10O2N1 | 163.0633 | 3.83 | 6 | 1.00 | 0.22 |
| C8H10O1N3 | 163.0746 | 0.45 | 6 | 1.13 | 0.13 |
| C8H10O1N3 | 163.0746 | 0.86 | 6 | 1.13 | 0.13 |
| C8H10O1N3 | 163.0746 | 1.29 | 6 | 1.13 | 0.13 |
| C8H10O1N3 | 163.0746 | 2.49 | 6 | 1.13 | 0.13 |
| C8H10O1N3 | 163.0746 | 2.61 | 6 | 1.13 | 0.13 |
| C8H10O1N3 | 163.0746 | 2.89 | 6 | 1.13 | 0.13 |
| C8H10O1N3 | 163.0746 | 2.93 | 6 | 1.13 | 0.13 |
| C10H14O1N1 | 163.0997 | 0.59 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 0.66 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 0.78 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 0.85 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 1.12 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 1.49 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 2.37 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 2.53 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 2.72 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 2.79 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 2.79 | 5 | 1.30 | 0.10 |

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|---|---|---|---|---|---|
| C10H14O1N1 | 163.0997 | 2.88 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 2.96 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.06 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.09 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.17 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.36 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.44 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.51 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.58 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.64 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.78 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.83 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.94 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 4.11 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 4.18 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 4.24 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 4.35 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 4.46 | 5 | 1.30 | 0.10 |
| C9H14N3 | 163.1109 | 0.81 | 5 | 1.44 | 0.00 |
| C11H18N1 | 163.1361 | 2.90 | 4 | 1.55 | 0.00 |
| C11H18N1 | 163.1361 | 3.00 | 4 | 1.55 | 0.00 |
| C11H18N1 | 163.1361 | 3.12 | 4 | 1.55 | 0.00 |
| C11H18N1 | 163.1361 | 3.31 | 4 | 1.55 | 0.00 |
| C11H18N1 | 163.1361 | 3.31 | 4 | 1.55 | 0.00 |
| C11H18N1 | 163.1361 | 3.61 | 4 | 1.55 | 0.00 |
| C11H18N1 | 163.1361 | 3.22 | 4 | 1.55 | 0.00 |
| C9H9O3 | 164.0473 | 2.48 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 2.62 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 2.70 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 2.86 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 2.96 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 3.02 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 3.30 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 3.30 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 3.31 | 6 | 0.89 | 0.33 |
| C8H9O2N2 | 164.0586 | 0.29 | 6 | 1.00 | 0.25 |
| C8H9O2N2 | 164.0586 | 0.48 | 6 | 1.00 | 0.25 |
| C8H9O2N2 | 164.0586 | 0.61 | 6 | 1.00 | 0.25 |
| C7H9O1N4 | 164.0698 | 0.88 | 6 | 1.14 | 0.14 |
| C7H9O1N4 | 164.0698 | 1.06 | 6 | 1.14 | 0.14 |
| C7H9O1N4 | 164.0698 | 1.34 | 6 | 1.14 | 0.14 |
| C10H13O2 | 164.0837 | 3.12 | 5 | 1.20 | 0.20 |
| C10H13O2 | 164.0837 | 4.50 | 5 | 1.20 | 0.20 |
| C10H13O2 | 164.0837 | 4.74 | 5 | 1.20 | 0.20 |
| C10H13O2 | 164.0837 | 5.29 | 5 | 1.20 | 0.20 |
| C10H13O2 | 164.0837 | 5.59 | 5 | 1.20 | 0.20 |
| C10H13O2 | 164.0837 | 6.04 | 5 | 1.20 | 0.20 |
| C9H13O1N2 | 164.0950 | 0.44 | 5 | 1.33 | 0.11 |
| C9H13O1N2 | 164.0950 | 0.57 | 5 | 1.33 | 0.11 |
| C9H13O1N2 | 164.0950 | 1.07 | 5 | 1.33 | 0.11 |

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|---|---|---|---|---|---|
| C9H13O1N2 | 164.0950 | 2.62 | 5 | 1.33 | 0.11 |
| C9H13O1N2 | 164.0950 | 2.70 | 5 | 1.33 | 0.11 |
| C9H13O1N2 | 164.0950 | 2.79 | 5 | 1.33 | 0.11 |
| C9H13O1N2 | 164.0950 | 3.09 | 5 | 1.33 | 0.11 |
| C10H17N2 | 164.1313 | 2.49 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.89 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.98 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 3.12 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 3.22 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.62 | 4 | 1.60 | 0.00 |
| C8H8O3N1 | 165.0426 | 3.21 | 6 | 0.88 | 0.38 |
| C9H12O2N1 | 165.0790 | 0.38 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 0.45 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 0.53 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 0.56 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 0.65 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 1.11 | 5 | 1.22 | 0.22 |
| C9H15O2N2 | 182.1055 | 1.42 | 4 | 1.56 | 0.22 |
| C9H12O2N1 | 165.0790 | 1.98 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 2.88 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 2.97 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 3.01 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 3.11 | 5 | 1.22 | 0.22 |
| C8H12O1N3 | 165.0902 | 0.39 | 5 | 1.38 | 0.13 |
| C10H16O1N1 | 165.1154 | 0.52 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 0.95 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 2.66 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 2.76 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 2.91 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 3.03 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 3.15 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 3.19 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 3.36 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 2.83 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 5.15 | 4 | 1.50 | 0.10 |
| C8H7O4 | 166.0266 | 2.58 | 6 | 0.75 | 0.50 |
| C9H11O3 | 166.0630 | 3.12 | 5 | 1.11 | 0.33 |
| C9H11O3 | 166.0630 | 3.19 | 5 | 1.11 | 0.33 |
| C8H11O2N2 | 166.0742 | 0.48 | 5 | 1.25 | 0.25 |
| C8H11O2N2 | 166.0742 | 0.67 | 5 | 1.25 | 0.25 |
| C8H11O2N2 | 166.0742 | 0.77 | 5 | 1.25 | 0.25 |
| C8H11O2N2 | 166.0742 | 0.98 | 5 | 1.25 | 0.25 |
| C8H11O2N2 | 166.0742 | 2.53 | 5 | 1.25 | 0.25 |
| C9H15O1N2 | 166.1106 | 0.72 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 0.96 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 1.07 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 1.17 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 1.29 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 2.70 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 2.84 | 4 | 1.56 | 0.11 |

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|---|---|---|---|---|---|
| C9H15O1N2 | 166.1106 | 2.96 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 3.13 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 3.31 | 4 | 1.56 | 0.11 |
| C9H15O1N2 | 166.1106 | 3.08 | 4 | 1.56 | 0.11 |
| C10H19N2 | 166.1470 | 2.78 | 3 | 1.80 | 0.00 |
| C10H19N2 | 166.1470 | 2.85 | 3 | 1.80 | 0.00 |
| C10H19N2 | 166.1470 | 2.95 | 3 | 1.80 | 0.00 |
| C10H19N2 | 166.1470 | 3.07 | 3 | 1.80 | 0.00 |
| C7H6O4N1 | 167.0219 | 0.37 | 6 | 0.71 | 0.57 |
| C8H10O3N1 | 167.0582 | 0.38 | 5 | 1.13 | 0.38 |
| C10H13O3N2 | 208.0848 | 0.51 | 6 | 1.20 | 0.30 |
| C8H10O3N1 | 167.0582 | 0.67 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 0.77 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 0.94 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 1.12 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 1.36 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 1.48 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 1.60 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 2.45 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 2.55 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 2.80 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 2.96 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 3.07 | 5 | 1.13 | 0.38 |
| C12H10N1 | 167.0735 | 2.79 | 9 | 0.75 | 0.00 |
| C12H10N1 | 167.0735 | 2.96 | 9 | 0.75 | 0.00 |
| C12H10N1 | 167.0735 | 3.33 | 9 | 0.75 | 0.00 |
| C9H14O2N1 | 167.0946 | 2.45 | 4 | 1.44 | 0.22 |
| C9H14O2N1 | 167.0946 | 2.53 | 4 | 1.44 | 0.22 |
| C9H14O2N1 | 167.0946 | 2.64 | 4 | 1.44 | 0.22 |
| C9H14O2N1 | 167.0946 | 2.71 | 4 | 1.44 | 0.22 |
| C8H14O1N3 | 167.1059 | 0.44 | 4 | 1.63 | 0.13 |
| C8H14O1N3 | 167.1059 | 0.59 | 4 | 1.63 | 0.13 |
| C11H5O2 | 168.0211 | 3.86 | 10 | 0.36 | 0.18 |
| C5H5O3N4 | 168.0283 | 0.38 | 6 | 0.80 | 0.60 |
| C4H9O7 | 168.0270 | 2.65 | 1 | 2.00 | 1.75 |
| C8H9O4 | 168.0423 | 2.36 | 5 | 1.00 | 0.50 |
| C8H9O4 | 168.0423 | 2.45 | 5 | 1.00 | 0.50 |
| C8H9O4 | 168.0423 | 2.60 | 5 | 1.00 | 0.50 |
| C8H9O4 | 168.0423 | 2.68 | 5 | 1.00 | 0.50 |
| C8H9O4 | 168.0423 | 3.06 | 5 | 1.00 | 0.50 |
| C12H12O1N1 | 185.0841 | 3.92 | 8 | 0.92 | 0.08 |
| C11H9N2 | 168.0687 | 2.14 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.41 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.55 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.59 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.70 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.78 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.93 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 3.04 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 3.14 | 9 | 0.73 | 0.00 |

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| C11H9N2 | 168.0687 | 3.35 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 3.97 | 9 | 0.73 | 0.00 |
| C8H13O2N2 | 168.0899 | 0.39 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.50 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.59 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.67 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.83 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.93 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 1.04 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 1.17 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 1.33 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 1.47 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 1.56 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 1.77 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 1.89 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 2.13 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 2.51 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 2.69 | 4 | 1.50 | 0.25 |
| C10H21N2 | 168.1626 | 2.74 | 2 | 2.00 | 0.00 |
| C10H21N2 | 168.1626 | 2.86 | 2 | 2.00 | 0.00 |
| C6H8O3N3 | 169.0487 | 0.33 | 5 | 1.17 | 0.50 |
| C11H8O1N1 | 169.0528 | 2.63 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 2.76 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 2.84 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 2.91 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 3.04 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 3.12 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 3.29 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 5.00 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 5.71 | 9 | 0.64 | 0.09 |
| C10H8N3 | 169.0640 | 1.42 | 9 | 0.70 | 0.00 |
| C8H12O3N1 | 169.0739 | 0.75 | 4 | 1.38 | 0.38 |
| C10H7O1N2 | 170.0480 | 2.56 | 9 | 0.60 | 0.10 |
| C10H7O1N2 | 170.0480 | 3.35 | 9 | 0.60 | 0.10 |
| C8H11O4 | 170.0579 | 1.13 | 4 | 1.25 | 0.50 |
| C8H11O4 | 170.0579 | 1.86 | 4 | 1.25 | 0.50 |
| C8H11O4 | 170.0579 | 2.31 | 4 | 1.25 | 0.50 |
| C7H11O3N2 | 170.0691 | 0.37 | 4 | 1.43 | 0.43 |
| C7H11O3N2 | 170.0691 | 0.62 | 4 | 1.43 | 0.43 |
| C12H11O1 | 170.0732 | 3.25 | 8 | 0.83 | 0.08 |
| C12H11O1 | 170.0732 | 3.28 | 8 | 0.83 | 0.08 |
| C11H11N2 | 170.0844 | 2.28 | 8 | 0.91 | 0.00 |
| C11H11N2 | 170.0844 | 2.54 | 8 | 0.91 | 0.00 |
| C11H11N2 | 170.0844 | 2.68 | 8 | 0.91 | 0.00 |
| C8H15O2N2 | 170.1055 | 0.36 | 3 | 1.75 | 0.25 |
| C8H15O2N2 | 170.1055 | 0.39 | 3 | 1.75 | 0.25 |
| C8H15O2N2 | 170.1055 | 0.78 | 3 | 1.75 | 0.25 |
| C8H15O2N2 | 170.1055 | 0.84 | 3 | 1.75 | 0.25 |
| C8H15O2N2 | 170.1055 | 1.13 | 3 | 1.75 | 0.25 |
| C8H15O2N2 | 170.1055 | 1.83 | 3 | 1.75 | 0.25 |

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| C11H10O1N1 | 171.0684 | 1.72 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 1.93 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.05 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.17 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.45 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.53 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.64 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.77 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.88 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 3.03 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 3.64 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 3.89 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 4.02 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 4.50 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 5.11 | 8 | 0.82 | 0.09 |
| C10H10N3 | 171.0796 | 2.50 | 8 | 0.90 | 0.00 |
| C10H10N3 | 171.0796 | 2.78 | 8 | 0.90 | 0.00 |
| C12H14N1 | 171.1048 | 2.77 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 2.83 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 2.96 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.01 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.08 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.23 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.29 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.42 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.50 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.58 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.65 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.69 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.76 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 4.12 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 5.03 | 7 | 1.08 | 0.00 |
| C5H10O5Na1 | 150.0528 | 0.34 | 1 | 2.00 | 1.00 |
| C11H9O2 | 172.0524 | 3.62 | 8 | 0.73 | 0.18 |
| C13H10O1N1 | 195.0684 | 4.26 | 10 | 0.69 | 0.08 |
| C11H9O2 | 172.0524 | 6.81 | 8 | 0.73 | 0.18 |
| C10H9O1N2 | 172.0637 | 2.62 | 8 | 0.80 | 0.10 |
| C10H9O1N2 | 172.0637 | 3.06 | 8 | 0.80 | 0.10 |
| C10H9O1N2 | 172.0637 | 3.17 | 8 | 0.80 | 0.10 |
| C10H9O1N2 | 172.0637 | 3.30 | 8 | 0.80 | 0.10 |
| C8H13O4 | 172.0736 | 2.31 | 3 | 1.50 | 0.50 |
| C7H13O3N2 | 172.0848 | 0.34 | 3 | 1.71 | 0.43 |
| C12H13O1 | 172.0888 | 7.41 | 7 | 1.00 | 0.08 |
| C11H13N2 | 172.1000 | 2.57 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.68 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.74 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.78 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.87 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 3.02 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 3.08 | 7 | 1.09 | 0.00 |

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| C11H13N2 | 172.1000 | 3.17 | 7 | 1.09 | 0.00 |
| C10H11O2N2 | 190.0742 | 2.49 | 7 | 1.00 | 0.20 |
| C10H8O2N1 | 173.0477 | 3.01 | 8 | 0.70 | 0.20 |
| C7H12O4N1 | 173.0688 | 1.15 | 3 | 1.57 | 0.57 |
| C11H12O1N1 | 173.0841 | 0.66 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 1.68 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 1.87 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.43 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.52 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.60 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.67 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.96 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 3.22 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 3.60 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 4.14 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 4.20 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 4.61 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 4.74 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 4.88 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 4.98 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 5.12 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 5.29 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 5.40 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 5.53 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 5.64 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 5.72 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 5.82 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 5.89 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 6.01 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 6.13 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 6.37 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 6.55 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 6.84 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 4.35 | 7 | 1.00 | 0.09 |
| C10H12N3 | 173.0953 | 1.02 | 7 | 1.10 | 0.00 |
| C10H12N3 | 173.0953 | 2.47 | 7 | 1.10 | 0.00 |
| C12H16N1 | 173.1204 | 2.89 | 6 | 1.25 | 0.00 |
| C12H16N1 | 173.1204 | 2.97 | 6 | 1.25 | 0.00 |
| C12H16N1 | 173.1204 | 3.05 | 6 | 1.25 | 0.00 |
| C10H24O1N1 | 173.1780 | 2.75 | 0 | 2.30 | 0.10 |
| C7H11O5 | 174.0528 | 0.66 | 3 | 1.43 | 0.71 |
| C11H11O2 | 174.0681 | 3.09 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 3.37 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 3.59 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 4.14 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 4.26 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 4.42 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 4.53 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 4.67 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 4.76 | 7 | 0.91 | 0.18 |

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| C11H11O2 | 174.0681 | 5.10 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 5.17 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 5.32 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 5.56 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 6.21 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 6.40 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 6.76 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 6.91 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 7.40 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 6.87 | 7 | 0.91 | 0.18 |
| C11H11O2 | 174.0681 | 7.25 | 7 | 0.91 | 0.18 |
| C10H11O1N2 | 174.0793 | 0.55 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 0.98 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 1.25 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 1.36 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 1.62 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 1.93 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 1.98 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 2.19 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 2.42 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 2.59 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 2.77 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 2.99 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 3.19 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 3.30 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 3.33 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 3.41 | 7 | 1.00 | 0.10 |
| C10H11O1N2 | 174.0793 | 3.71 | 7 | 1.00 | 0.10 |
| C11H15N2 | 174.1157 | 2.70 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 2.80 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 2.92 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 3.04 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 3.28 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 3.38 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 3.01 | 6 | 1.27 | 0.00 |
| C5H6O4N1S1 | 174.9939 | 0.43 | 4 | 1.00 | 0.80 |
| C4H10O1N5S1 | 175.0528 | 2.98 | 3 | 2.25 | 0.25 |
| C10H10O2N1 | 175.0633 | 1.50 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 1.72 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.00 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.30 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.36 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.48 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.59 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.79 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.88 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.98 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 3.07 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 3.16 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 3.27 | 7 | 0.90 | 0.20 |

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| C10H10O2N1 | 175.0633 | 3.41 | 7 | 0.90 | 0.20 |
| C9H10O1N3 | 175.0746 | 2.67 | 7 | 1.00 | 0.11 |
| C7H14O4N1 | 175.0845 | 0.37 | 2 | 1.86 | 0.57 |
| C7H14O4N1 | 175.0845 | 1.16 | 2 | 1.86 | 0.57 |
| C11H14O1N1 | 175.0997 | 1.02 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 1.20 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 1.39 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 1.71 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 1.92 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 2.30 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 2.72 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 2.89 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 3.14 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 3.34 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 4.09 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 4.20 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 4.31 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 4.44 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 4.55 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 4.65 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 5.01 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 5.41 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 5.54 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 6.03 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 6.38 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 6.65 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 6.90 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 7.00 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 5.11 | 6 | 1.18 | 0.09 |
| C11H14O1N1 | 175.0997 | 5.68 | 6 | 1.18 | 0.09 |
| C10H14N3 | 175.1109 | 1.01 | 6 | 1.30 | 0.00 |
| C10H14N3 | 175.1109 | 1.16 | 6 | 1.30 | 0.00 |
| C10H14N3 | 175.1109 | 1.35 | 6 | 1.30 | 0.00 |
| C10H14N3 | 175.1109 | 2.12 | 6 | 1.30 | 0.00 |
| C10H14N3 | 175.1109 | 2.30 | 6 | 1.30 | 0.00 |
| C10H14N3 | 175.1109 | 2.52 | 6 | 1.30 | 0.00 |
| C10H14N3 | 175.1109 | 2.69 | 6 | 1.30 | 0.00 |
| C10H14N3 | 175.1109 | 2.78 | 6 | 1.30 | 0.00 |
| C10H14N3 | 175.1109 | 2.93 | 6 | 1.30 | 0.00 |
| C12H18N1 | 175.1361 | 2.89 | 5 | 1.42 | 0.00 |
| C12H18N1 | 175.1361 | 3.01 | 5 | 1.42 | 0.00 |
| C12H18N1 | 175.1361 | 3.11 | 5 | 1.42 | 0.00 |
| C12H18N1 | 175.1361 | 3.41 | 5 | 1.42 | 0.00 |
| C12H18N1 | 175.1361 | 3.44 | 5 | 1.42 | 0.00 |
| C5H9O3N2S1 | 176.0256 | 0.36 | 3 | 1.60 | 0.60 |
| C10H9O3 | 176.0473 | 3.11 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.19 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.27 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.51 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.77 | 7 | 0.80 | 0.30 |

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| C10H9O3 | 176.0473 | 4.03 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 4.38 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 4.44 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 4.49 | 7 | 0.80 | 0.30 |
| C9H9O2N2 | 176.0586 | 0.78 | 7 | 0.89 | 0.22 |
| C9H9O2N2 | 176.0586 | 1.01 | 7 | 0.89 | 0.22 |
| C9H9O2N2 | 176.0586 | 2.43 | 7 | 0.89 | 0.22 |
| C9H9O2N2 | 176.0586 | 3.01 | 7 | 0.89 | 0.22 |
| C7H13O5 | 176.0685 | 0.40 | 2 | 1.71 | 0.71 |
| C7H13O5 | 176.0685 | 0.84 | 2 | 1.71 | 0.71 |
| C7H13O5 | 176.0685 | 0.87 | 2 | 1.71 | 0.71 |
| C7H9N6 | 176.0810 | 2.92 | 7 | 1.14 | 0.00 |
| C13H14O1N1 | 199.0997 | 2.89 | 8 | 1.00 | 0.08 |
| C11H13O2 | 176.0837 | 2.91 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 3.19 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 3.43 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 3.47 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 3.55 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 3.60 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 3.67 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 3.76 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 3.83 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.14 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.19 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.47 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.56 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.63 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.71 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.78 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.88 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 4.92 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.07 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.12 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.16 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.19 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.23 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.28 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.43 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.49 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 5.66 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 6.03 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 6.09 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 6.20 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 6.44 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 6.49 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 6.74 | 6 | 1.09 | 0.18 |
| C11H13O2 | 176.0837 | 6.86 | 6 | 1.09 | 0.18 |
| C10H13O1N2 | 176.0950 | 1.03 | 6 | 1.20 | 0.10 |
| C10H13O1N2 | 176.0950 | 2.49 | 6 | 1.20 | 0.10 |
| C10H13O1N2 | 176.0950 | 2.65 | 6 | 1.20 | 0.10 |

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| C10H13O1N2 | 176.0950 | 2.74 | 6 | 1.20 | 0.10 |
| C10H13O1N2 | 176.0950 | 2.93 | 6 | 1.20 | 0.10 |
| C10H13O1N2 | 176.0950 | 3.01 | 6 | 1.20 | 0.10 |
| C10H13O1N2 | 176.0950 | 5.77 | 6 | 1.20 | 0.10 |
| C10H13O1N2 | 176.0950 | 1.14 | 6 | 1.20 | 0.10 |
| C10H13O1N2 | 176.0950 | 3.08 | 6 | 1.20 | 0.10 |
| C11H17N2 | 176.1313 | 2.85 | 5 | 1.45 | 0.00 |
| C9H8O3N1 | 177.0426 | 2.34 | 7 | 0.78 | 0.33 |
| C9H8O3N1 | 177.0426 | 2.78 | 7 | 0.78 | 0.33 |
| C9H8O3N1 | 177.0426 | 3.10 | 7 | 0.78 | 0.33 |
| C10H12O2N1 | 177.0790 | 2.39 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 2.53 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 2.72 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 2.80 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 2.88 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 2.89 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 3.02 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 3.04 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 3.38 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 3.46 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 3.53 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 3.67 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 3.72 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 4.00 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 4.38 | 6 | 1.10 | 0.20 |
| C10H12O2N1 | 177.0790 | 5.11 | 6 | 1.10 | 0.20 |
| C9H12O1N3 | 177.0902 | 0.67 | 6 | 1.22 | 0.11 |
| C9H12O1N3 | 177.0902 | 0.89 | 6 | 1.22 | 0.11 |
| C9H12O1N3 | 177.0902 | 1.10 | 6 | 1.22 | 0.11 |
| C9H12O1N3 | 177.0902 | 2.51 | 6 | 1.22 | 0.11 |
| C9H12O1N3 | 177.0902 | 3.13 | 6 | 1.22 | 0.11 |
| C9H12O1N3 | 177.0902 | 3.18 | 6 | 1.22 | 0.11 |
| C9H12O1N3 | 177.0902 | 1.21 | 6 | 1.22 | 0.11 |
| C12H20N1 | 177.1517 | 3.19 | 4 | 1.58 | 0.00 |
| C12H20N1 | 177.1517 | 3.32 | 4 | 1.58 | 0.00 |
| C12H20N1 | 177.1517 | 3.48 | 4 | 1.58 | 0.00 |
| C12H20N1 | 177.1517 | 3.58 | 4 | 1.58 | 0.00 |
| C12H20N1 | 177.1517 | 3.69 | 4 | 1.58 | 0.00 |
| C3H3O7N2 | 177.9862 | 0.29 | 4 | 0.67 | 2.33 |
| C9H7O4 | 178.0266 | 1.87 | 7 | 0.67 | 0.44 |
| C9H7O4 | 178.0266 | 2.25 | 7 | 0.67 | 0.44 |
| C9H7O4 | 178.0266 | 3.43 | 7 | 0.67 | 0.44 |
| C10H11O3 | 178.0630 | 2.49 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.08 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.15 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.38 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.61 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.65 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.71 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.84 | 6 | 1.00 | 0.30 |

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| C10H11O3 | 178.0630 | 3.95 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.99 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 4.17 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 4.41 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 4.62 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 4.74 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 5.41 | 6 | 1.00 | 0.30 |
| C9H11O2N2 | 178.0742 | 1.14 | 6 | 1.11 | 0.22 |
| C9H11O2N2 | 178.0742 | 2.46 | 6 | 1.11 | 0.22 |
| C9H11O2N2 | 178.0742 | 2.76 | 6 | 1.11 | 0.22 |
| C8H11O1N4 | 178.0855 | 0.96 | 6 | 1.25 | 0.13 |
| C8H11O1N4 | 178.0855 | 1.29 | 6 | 1.25 | 0.13 |
| C10H15O1N2 | 178.1106 | 0.38 | 5 | 1.40 | 0.10 |
| C10H15O1N2 | 178.1106 | 0.87 | 5 | 1.40 | 0.10 |
| C10H15O1N2 | 178.1106 | 1.09 | 5 | 1.40 | 0.10 |
| C10H15O1N2 | 178.1106 | 2.76 | 5 | 1.40 | 0.10 |
| C10H15O1N2 | 178.1106 | 3.10 | 5 | 1.40 | 0.10 |
| C11H19N2 | 178.1470 | 2.96 | 4 | 1.64 | 0.00 |
| C11H19N2 | 178.1470 | 3.16 | 4 | 1.64 | 0.00 |
| C11H19N2 | 178.1470 | 3.29 | 4 | 1.64 | 0.00 |
| C11H19N2 | 178.1470 | 3.39 | 4 | 1.64 | 0.00 |
| C11H19N2 | 178.1470 | 3.46 | 4 | 1.64 | 0.00 |
| C9H10O3N1 | 179.0582 | 2.44 | 6 | 1.00 | 0.33 |
| C9H10O3N1 | 179.0582 | 2.59 | 6 | 1.00 | 0.33 |
| C13H10N1 | 179.0735 | 3.13 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.19 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.22 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.22 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.29 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.31 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.48 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.56 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 6.83 | 10 | 0.69 | 0.00 |
| C10H14O2N1 | 179.0946 | 0.39 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.80 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.86 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.93 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 1.07 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 1.38 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 1.56 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 1.97 | 5 | 1.30 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.05 | 4 | 1.60 | 0.20 |
| C10H14O2N1 | 179.0946 | 2.48 | 5 | 1.30 | 0.20 |
| C12H12O2N1 | 201.0790 | 2.61 | 8 | 0.92 | 0.17 |
| C10H14O2N1 | 179.0946 | 2.75 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 2.81 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 2.97 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 3.19 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 3.80 | 5 | 1.30 | 0.20 |
| C11H18O1N1 | 179.1310 | 2.58 | 4 | 1.55 | 0.09 |

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| C11H18O1N1 | 179.1310 | 2.76 | 4 | 1.55 | 0.09 |
| C11H18O1N1 | 179.1310 | 2.96 | 4 | 1.55 | 0.09 |
| C11H18O1N1 | 179.1310 | 3.08 | 4 | 1.55 | 0.09 |
| C11H18O1N1 | 179.1310 | 3.12 | 4 | 1.55 | 0.09 |
| C11H18O1N1 | 179.1310 | 3.35 | 4 | 1.55 | 0.09 |
| C9H9O4 | 180.0423 | 2.74 | 6 | 0.89 | 0.44 |
| C9H9O4 | 180.0423 | 3.10 | 6 | 0.89 | 0.44 |
| C9H9O4 | 180.0423 | 3.18 | 6 | 0.89 | 0.44 |
| C8H9O3N2 | 180.0535 | 0.38 | 6 | 1.00 | 0.38 |
| C13H9O1 | 180.0575 | 7.21 | 10 | 0.62 | 0.08 |
| C13H9O1 | 180.0575 | 7.68 | 10 | 0.62 | 0.08 |
| C13H9O1 | 180.0575 | 8.22 | 10 | 0.62 | 0.08 |
| C12H9N2 | 180.0687 | 3.10 | 10 | 0.67 | 0.00 |
| C12H9N2 | 180.0687 | 4.15 | 10 | 0.67 | 0.00 |
| C12H9N2 | 180.0687 | 4.41 | 10 | 0.67 | 0.00 |
| C12H9N2 | 180.0687 | 3.35 | 10 | 0.67 | 0.00 |
| C10H13O3 | 180.0786 | 0.96 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 1.48 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 2.49 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 2.55 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 2.82 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 2.91 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 3.05 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 3.23 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 3.34 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 3.70 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 4.22 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 4.45 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 1.60 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 3.20 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 4.51 | 5 | 1.20 | 0.30 |
| C9H13O2N2 | 180.0899 | 0.45 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 0.58 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 0.84 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 0.88 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 1.29 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 1.75 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 1.98 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 2.43 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 2.56 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 2.63 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 2.74 | 5 | 1.33 | 0.22 |
| C9H13O2N2 | 180.0899 | 2.87 | 5 | 1.33 | 0.22 |
| C10H17O1N2 | 180.1263 | 0.90 | 4 | 1.60 | 0.10 |
| C10H17O1N2 | 180.1263 | 1.49 | 4 | 1.60 | 0.10 |
| C10H17O1N2 | 180.1263 | 1.68 | 4 | 1.60 | 0.10 |
| C10H17O1N2 | 180.1263 | 2.48 | 4 | 1.60 | 0.10 |
| C10H17O1N2 | 180.1263 | 2.74 | 4 | 1.60 | 0.10 |
| C10H17O1N2 | 180.1263 | 2.90 | 4 | 1.60 | 0.10 |
| C10H17O1N2 | 180.1263 | 3.11 | 4 | 1.60 | 0.10 |

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| C10H17O1N2 | 180.1263 | 3.20 | 4 | 1.60 | 0.10 |
| C10H17O1N2 | 180.1263 | 3.29 | 4 | 1.60 | 0.10 |
| C10H17O1N2 | 180.1263 | 3.78 | 4 | 1.60 | 0.10 |
| C11H21N2 | 180.1626 | 3.10 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 3.23 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 3.33 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 3.40 | 3 | 1.82 | 0.00 |
| C5H9O1N3Na1S1 | 159.0466 | 5.13 | 3 | 1.80 | 0.20 |
| C12H8O1N1 | 181.0528 | 4.72 | 10 | 0.58 | 0.08 |
| C12H8O1N1 | 181.0528 | 4.88 | 10 | 0.58 | 0.08 |
| C5H12O6N1 | 181.0586 | 0.37 | 1 | 2.20 | 1.20 |
| C9H12O3N1 | 181.0739 | 0.47 | 5 | 1.22 | 0.33 |
| C9H12O3N1 | 181.0739 | 0.72 | 5 | 1.22 | 0.33 |
| C9H12O3N1 | 181.0739 | 0.92 | 5 | 1.22 | 0.33 |
| C9H12O3N1 | 181.0739 | 1.18 | 5 | 1.22 | 0.33 |
| C9H12O3N1 | 181.0739 | 2.07 | 5 | 1.22 | 0.33 |
| C9H12O3N1 | 181.0739 | 2.47 | 5 | 1.22 | 0.33 |
| C11H13O2N2 | 204.0899 | 2.52 | 7 | 1.09 | 0.18 |
| C9H12O3N1 | 181.0739 | 2.64 | 5 | 1.22 | 0.33 |
| C13H12N1 | 181.0891 | 2.97 | 9 | 0.85 | 0.00 |
| C13H12N1 | 181.0891 | 3.06 | 9 | 0.85 | 0.00 |
| C13H12N1 | 181.0891 | 3.08 | 9 | 0.85 | 0.00 |
| C13H12N1 | 181.0891 | 3.20 | 9 | 0.85 | 0.00 |
| C13H12N1 | 181.0891 | 3.33 | 9 | 0.85 | 0.00 |
| C13H12N1 | 181.0891 | 3.33 | 9 | 0.85 | 0.00 |
| C13H12N1 | 181.0891 | 3.49 | 9 | 0.85 | 0.00 |
| C13H12N1 | 181.0891 | 3.63 | 9 | 0.85 | 0.00 |
| C10H16O2N1 | 181.1103 | 2.96 | 4 | 1.50 | 0.20 |
| C11H20O1N1 | 181.1467 | 7.18 | 3 | 1.73 | 0.09 |
| C12H24N1 | 181.1830 | 3.29 | 2 | 1.92 | 0.00 |
| C8H7O5 | 182.0215 | 1.09 | 6 | 0.75 | 0.63 |
| C12H7O2 | 182.0368 | 4.47 | 10 | 0.50 | 0.17 |
| C9H11O4 | 182.0579 | 3.12 | 5 | 1.11 | 0.44 |
| C8H11O3N2 | 182.0691 | 0.38 | 5 | 1.25 | 0.38 |
| C8H11O3N2 | 182.0691 | 0.65 | 5 | 1.25 | 0.38 |
| C8H11O3N2 | 182.0691 | 1.23 | 5 | 1.25 | 0.38 |
| C8H11O3N2 | 182.0691 | 2.46 | 5 | 1.25 | 0.38 |
| C13H11O1 | 182.0732 | 7.68 | 9 | 0.77 | 0.08 |
| C12H11N2 | 182.0844 | 2.68 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 2.75 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 2.86 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 2.91 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.10 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.13 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.15 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.32 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.46 | 9 | 0.83 | 0.00 |
| C9H15O2N2 | 182.1055 | 0.58 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 0.82 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 0.97 | 4 | 1.56 | 0.22 |

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| C9H15O2N2 | 182.1055 | 1.13 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 1.38 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 1.69 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 1.92 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 2.22 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 2.39 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 2.53 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 2.70 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 2.82 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 2.87 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 1.13 | 4 | 1.56 | 0.22 |
| C11H23N2 | 182.1783 | 3.16 | 2 | 2.00 | 0.00 |
| C11H23N2 | 182.1783 | 3.28 | 2 | 2.00 | 0.00 |
| C11H23N2 | 182.1783 | 3.37 | 2 | 2.00 | 0.00 |
| C9H7O2N1Na1 | 161.0477 | 2.54 | 7 | 0.78 | 0.22 |
| C7H10O3N3 | 183.0644 | 0.38 | 5 | 1.29 | 0.43 |
| C7H10O3N3 | 183.0644 | 0.46 | 5 | 1.29 | 0.43 |
| C12H10O1N1 | 183.0684 | 2.54 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 2.59 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 2.75 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 2.80 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 2.90 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 3.00 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 3.09 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 3.21 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 3.30 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 3.39 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 3.87 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 3.99 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 4.26 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 4.74 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 5.63 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 6.87 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 7.40 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 7.55 | 9 | 0.75 | 0.08 |
| C12H10O1N1 | 183.0684 | 4.04 | 9 | 0.75 | 0.08 |
| C11H10N3 | 183.0796 | 2.55 | 9 | 0.82 | 0.00 |
| C13H14N1 | 183.1048 | 2.89 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 2.98 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 3.11 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 3.27 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 3.27 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 3.47 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 3.58 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 3.74 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 3.82 | 8 | 1.00 | 0.00 |
| C13H14N1 | 183.1048 | 4.12 | 8 | 1.00 | 0.00 |
| C11H22O1N1 | 183.1623 | 2.91 | 2 | 1.91 | 0.09 |
| C12H9O2 | 184.0524 | 2.80 | 9 | 0.67 | 0.17 |
| C12H9O2 | 184.0524 | 3.47 | 9 | 0.67 | 0.17 |

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| C12H9O2 | 184.0524 | 4.72 | 9 | 0.67 | 0.17 |
| C12H9O2 | 184.0524 | 5.52 | 9 | 0.67 | 0.17 |
| C11H9O1N2 | 184.0637 | 0.85 | 9 | 0.73 | 0.09 |
| C11H9O1N2 | 184.0637 | 2.43 | 9 | 0.73 | 0.09 |
| C11H9O1N2 | 184.0637 | 2.59 | 9 | 0.73 | 0.09 |
| C11H9O1N2 | 184.0637 | 2.77 | 9 | 0.73 | 0.09 |
| C11H9O1N2 | 184.0637 | 3.12 | 9 | 0.73 | 0.09 |
| C11H9O1N2 | 184.0637 | 4.67 | 9 | 0.73 | 0.09 |
| C8H13O3N2 | 184.0848 | 0.50 | 4 | 1.50 | 0.38 |
| C8H13O3N2 | 184.0848 | 1.16 | 4 | 1.50 | 0.38 |
| C12H13N2 | 184.1000 | 2.60 | 8 | 1.00 | 0.00 |
| C12H13N2 | 184.1000 | 2.73 | 8 | 1.00 | 0.00 |
| C12H13N2 | 184.1000 | 2.76 | 8 | 1.00 | 0.00 |
| C12H13N2 | 184.1000 | 3.02 | 8 | 1.00 | 0.00 |
| C12H13N2 | 184.1000 | 3.12 | 8 | 1.00 | 0.00 |
| C12H13N2 | 184.1000 | 3.16 | 8 | 1.00 | 0.00 |
| C9H17O2N2 | 184.1212 | 0.60 | 3 | 1.78 | 0.22 |
| C9H17O2N2 | 184.1212 | 0.94 | 3 | 1.78 | 0.22 |
| C9H17O2N2 | 184.1212 | 2.65 | 3 | 1.78 | 0.22 |
| C9H17O2N2 | 184.1212 | 0.68 | 3 | 1.78 | 0.22 |
| C9H17O2N2 | 184.1212 | 2.80 | 3 | 1.78 | 0.22 |
| C5H9O5N1Na1 | 163.0481 | 3.01 | 2 | 1.80 | 1.00 |
| C11H8O2N1 | 185.0477 | 2.28 | 9 | 0.64 | 0.18 |
| C11H8O2N1 | 185.0477 | 3.29 | 9 | 0.64 | 0.18 |
| C11H8O2N1 | 185.0477 | 3.40 | 9 | 0.64 | 0.18 |
| C11H8O2N1 | 185.0477 | 4.18 | 9 | 0.64 | 0.18 |
| C10H8O1N3 | 185.0589 | 3.46 | 9 | 0.70 | 0.10 |
| C12H12O1N1 | 185.0841 | 1.33 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 1.95 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.19 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.32 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.42 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.51 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.63 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.72 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.80 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.90 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.92 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 3.00 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 3.11 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 3.22 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 3.41 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 3.60 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 3.93 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 4.39 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 4.72 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 4.89 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 4.98 | 8 | 0.92 | 0.08 |
| C11H12N3 | 185.0953 | 2.81 | 8 | 1.00 | 0.00 |
| C13H16N1 | 185.1204 | 3.15 | 7 | 1.15 | 0.00 |

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|---|---|---|---|---|---|
| C13H16N1 | 185.1204 | 3.23 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.30 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.37 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.42 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.46 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.52 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.62 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.66 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.72 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.81 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.87 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.93 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 4.01 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 4.34 | 7 | 1.15 | 0.00 |
| C12H28N1 | 185.2143 | 4.15 | 0 | 2.25 | 0.00 |
| C10H7O2N2 | 186.0429 | 3.51 | 9 | 0.60 | 0.20 |
| C6H12O5Na1 | 164.0685 | 0.36 | 1 | 2.00 | 0.83 |
| C12H11O2 | 186.0681 | 3.60 | 8 | 0.83 | 0.17 |
| C12H11O2 | 186.0681 | 7.15 | 8 | 0.83 | 0.17 |
| C12H11O2 | 186.0681 | 7.25 | 8 | 0.83 | 0.17 |
| C12H11O2 | 186.0681 | 7.43 | 8 | 0.83 | 0.17 |
| C11H11O1N2 | 186.0793 | 2.43 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 2.55 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 2.73 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 2.80 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 2.96 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 3.06 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 3.15 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 3.26 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 3.38 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 3.66 | 8 | 0.91 | 0.09 |
| C11H11O1N2 | 186.0793 | 3.96 | 8 | 0.91 | 0.09 |
| C12H15N2 | 186.1157 | 2.78 | 7 | 1.17 | 0.00 |
| C12H15N2 | 186.1157 | 2.89 | 7 | 1.17 | 0.00 |
| C12H15N2 | 186.1157 | 2.99 | 7 | 1.17 | 0.00 |
| C12H15N2 | 186.1157 | 3.31 | 7 | 1.17 | 0.00 |
| C12H15N2 | 186.1157 | 3.37 | 7 | 1.17 | 0.00 |
| C10H19O3 | 186.1256 | 5.05 | 2 | 1.80 | 0.30 |
| C9H19O2N2 | 186.1368 | 2.51 | 2 | 2.00 | 0.22 |
| C7H10O3N1S1 | 187.0303 | 0.37 | 4 | 1.29 | 0.43 |
| C11H10O2N1 | 187.0633 | 0.61 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 1.11 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 2.44 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 2.45 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 2.61 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 2.62 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 2.83 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 3.05 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 3.05 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 3.12 | 8 | 0.82 | 0.18 |

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| C11H10O2N1 | 187.0633 | 3.34 | 8 | 0.82 | 0.18 |
| C11H10O2N1 | 187.0633 | 3.34 | 8 | 0.82 | 0.18 |
| C8H11O4 | 170.0579 | 0.91 | 4 | 1.25 | 0.50 |
| C12H14O1N1 | 187.0997 | 2.71 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 2.82 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 2.87 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 2.95 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 3.03 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 3.07 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 3.16 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 3.33 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 3.32 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 3.43 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 3.49 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 6.75 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 7.09 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 7.11 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 7.25 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 7.31 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 7.49 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 7.52 | 7 | 1.08 | 0.08 |
| C11H14N3 | 187.1109 | 2.61 | 7 | 1.18 | 0.00 |
| C13H18N1 | 187.1361 | 3.22 | 6 | 1.31 | 0.00 |
| C13H18N1 | 187.1361 | 3.41 | 6 | 1.31 | 0.00 |
| C13H18N1 | 187.1361 | 3.46 | 6 | 1.31 | 0.00 |
| C13H18N1 | 187.1361 | 3.65 | 6 | 1.31 | 0.00 |
| C13H18N1 | 187.1361 | 3.63 | 6 | 1.31 | 0.00 |
| C5H10O6Na1 | 166.0477 | 3.57 | 1 | 2.00 | 1.20 |
| C12H13O4 | 220.0736 | 3.46 | 7 | 1.00 | 0.33 |
| C11H9O3 | 188.0473 | 4.30 | 8 | 0.73 | 0.27 |
| C11H9O3 | 188.0473 | 6.54 | 8 | 0.73 | 0.27 |
| C10H9O2N2 | 188.0586 | 0.49 | 8 | 0.80 | 0.20 |
| C8H13O5 | 188.0685 | 0.64 | 3 | 1.50 | 0.63 |
| C8H13O5 | 188.0685 | 0.78 | 3 | 1.50 | 0.63 |
| C8H13O5 | 188.0685 | 2.57 | 3 | 1.50 | 0.63 |
| C12H13O2 | 188.0837 | 3.82 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 4.00 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 4.15 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 4.28 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 4.60 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 4.69 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 4.74 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 4.96 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 5.06 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 5.13 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 5.24 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 5.38 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 5.84 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 6.46 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 6.69 | 7 | 1.00 | 0.17 |

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| C12H13O2 | 188.0837 | 6.84 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 7.09 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 7.33 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 7.49 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 7.62 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 7.79 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 7.88 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 8.03 | 7 | 1.00 | 0.17 |
| C12H13O2 | 188.0837 | 8.11 | 7 | 1.00 | 0.17 |
| C11H13O1N2 | 188.0950 | 0.88 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 1.15 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 1.25 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 1.37 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 1.54 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 1.59 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 1.68 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 2.39 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 2.45 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 2.77 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 2.80 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 3.10 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 3.37 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 3.88 | 7 | 1.09 | 0.09 |
| C8H17O3N2 | 188.1161 | 0.33 | 2 | 2.00 | 0.38 |
| C12H17N2 | 188.1313 | 3.05 | 6 | 1.33 | 0.00 |
| C12H17N2 | 188.1313 | 3.31 | 6 | 1.33 | 0.00 |
| C12H17N2 | 188.1313 | 3.39 | 6 | 1.33 | 0.00 |
| C12H17N2 | 188.1313 | 3.46 | 6 | 1.33 | 0.00 |
| C12H17N2 | 188.1313 | 3.63 | 6 | 1.33 | 0.00 |
| C6H8O4N1S1 | 189.0096 | 0.74 | 4 | 1.17 | 0.67 |
| C11H12O2N1 | 189.0790 | 0.56 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 2.52 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 2.56 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 2.59 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 2.83 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 2.91 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 3.24 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 3.35 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 3.38 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 3.43 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 3.61 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 3.72 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 3.81 | 7 | 1.00 | 0.18 |
| C11H12O2N1 | 189.0790 | 7.32 | 7 | 1.00 | 0.18 |
| C8H16O4N1 | 189.1001 | 0.38 | 2 | 1.88 | 0.50 |
| C12H16O1N1 | 189.1154 | 2.67 | 6 | 1.25 | 0.08 |
| C12H16O1N1 | 189.1154 | 3.17 | 6 | 1.25 | 0.08 |
| C12H16O1N1 | 189.1154 | 3.38 | 6 | 1.25 | 0.08 |
| C12H16O1N1 | 189.1154 | 3.55 | 6 | 1.25 | 0.08 |
| C12H16O1N1 | 189.1154 | 6.56 | 6 | 1.25 | 0.08 |

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| C12H16O1N1 | 189.1154 | 7.33 | 6 | 1.25 | 0.08 |
| C12H16O1N1 | 189.1154 | 7.44 | 6 | 1.25 | 0.08 |
| C12H16O1N1 | 189.1154 | 7.51 | 6 | 1.25 | 0.08 |
| C11H16N3 | 189.1266 | 2.50 | 6 | 1.36 | 0.00 |
| C11H16N3 | 189.1266 | 2.57 | 6 | 1.36 | 0.00 |
| C11H16N3 | 189.1266 | 2.66 | 6 | 1.36 | 0.00 |
| C11H16N3 | 189.1266 | 2.74 | 6 | 1.36 | 0.00 |
| C11H16N3 | 189.1266 | 2.83 | 6 | 1.36 | 0.00 |
| C11H16N3 | 189.1266 | 2.95 | 6 | 1.36 | 0.00 |
| C13H20N1 | 189.1517 | 3.38 | 5 | 1.46 | 0.00 |
| C13H20N1 | 189.1517 | 3.50 | 5 | 1.46 | 0.00 |
| C13H20N1 | 189.1517 | 3.64 | 5 | 1.46 | 0.00 |
| C13H20N1 | 189.1517 | 3.82 | 5 | 1.46 | 0.00 |
| C13H20N1 | 189.1517 | 4.09 | 5 | 1.46 | 0.00 |
| C9H7O3N2 | 190.0378 | 2.77 | 8 | 0.67 | 0.33 |
| C6H11O3N2S1 | 190.0412 | 0.39 | 3 | 1.67 | 0.50 |
| C11H8N2Na1 | 168.0687 | 0.49 | 9 | 0.73 | 0.00 |
| C7H7O1N6 | 190.0603 | 2.84 | 8 | 0.86 | 0.14 |
| C11H11O3 | 190.0630 | 3.64 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 3.94 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 4.03 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 4.10 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 4.26 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 4.35 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 4.48 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 4.90 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 5.07 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 5.24 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 5.37 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 5.46 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 5.63 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 5.71 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 6.15 | 7 | 0.91 | 0.27 |
| C11H11O3 | 190.0630 | 6.64 | 7 | 0.91 | 0.27 |
| C11H15O3N2 | 222.1004 | 0.57 | 6 | 1.27 | 0.27 |
| C10H11O2N2 | 190.0742 | 1.59 | 7 | 1.00 | 0.20 |
| C10H11O2N2 | 190.0742 | 1.81 | 7 | 1.00 | 0.20 |
| C10H11O2N2 | 190.0742 | 2.26 | 7 | 1.00 | 0.20 |
| C10H11O2N2 | 190.0742 | 2.44 | 7 | 1.00 | 0.20 |
| C10H11O2N2 | 190.0742 | 2.55 | 7 | 1.00 | 0.20 |
| C10H11O2N2 | 190.0742 | 2.87 | 7 | 1.00 | 0.20 |
| C10H11O2N2 | 190.0742 | 3.02 | 7 | 1.00 | 0.20 |
| C10H11O2N2 | 190.0742 | 3.11 | 7 | 1.00 | 0.20 |
| C12H15O2 | 190.0994 | 3.14 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 3.42 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 5.82 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 6.04 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 6.63 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 6.76 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 6.86 | 6 | 1.17 | 0.17 |

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| C12H15O2 | 190.0994 | 6.94 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 7.08 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 7.17 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 7.29 | 6 | 1.17 | 0.17 |
| C12H15O2 | 190.0994 | 7.36 | 6 | 1.17 | 0.17 |
| C11H15O1N2 | 190.1106 | 1.13 | 6 | 1.27 | 0.09 |
| C11H13N2 | 172.1000 | 2.47 | 7 | 1.09 | 0.00 |
| C11H15O1N2 | 190.1106 | 2.59 | 6 | 1.27 | 0.09 |
| C11H15O1N2 | 190.1106 | 2.77 | 6 | 1.27 | 0.09 |
| C11H15O1N2 | 190.1106 | 2.89 | 6 | 1.27 | 0.09 |
| C11H15O1N2 | 190.1106 | 3.02 | 6 | 1.27 | 0.09 |
| C11H15O1N2 | 190.1106 | 3.23 | 6 | 1.27 | 0.09 |
| C12H19N2 | 190.1470 | 3.16 | 5 | 1.50 | 0.00 |
| C12H19N2 | 190.1470 | 3.21 | 5 | 1.50 | 0.00 |
| C10H10O3N1 | 191.0582 | 2.95 | 7 | 0.90 | 0.30 |
| C11H14O2N1 | 191.0946 | 2.61 | 6 | 1.18 | 0.18 |
| C11H14O2N1 | 191.0946 | 2.76 | 6 | 1.18 | 0.18 |
| C11H14O2N1 | 191.0946 | 2.91 | 6 | 1.18 | 0.18 |
| C11H14O2N1 | 191.0946 | 3.03 | 6 | 1.18 | 0.18 |
| C11H12O1N1 | 173.0841 | 3.19 | 7 | 1.00 | 0.09 |
| C11H14O2N1 | 191.0946 | 3.32 | 6 | 1.18 | 0.18 |
| C11H14O2N1 | 191.0946 | 3.53 | 6 | 1.18 | 0.18 |
| C10H14O1N3 | 191.1059 | 0.86 | 6 | 1.30 | 0.10 |
| C10H14O1N3 | 191.1059 | 0.98 | 6 | 1.30 | 0.10 |
| C10H14O1N3 | 191.1059 | 1.16 | 6 | 1.30 | 0.10 |
| C10H14O1N3 | 191.1059 | 1.33 | 6 | 1.30 | 0.10 |
| C10H14O1N3 | 191.1059 | 2.48 | 6 | 1.30 | 0.10 |
| C12H18O1N1 | 191.1310 | 2.46 | 5 | 1.42 | 0.08 |
| C12H18O1N1 | 191.1310 | 2.60 | 5 | 1.42 | 0.08 |
| C12H18O1N1 | 191.1310 | 2.75 | 5 | 1.42 | 0.08 |
| C12H18O1N1 | 191.1310 | 3.07 | 5 | 1.42 | 0.08 |
| C12H18O1N1 | 191.1310 | 3.11 | 5 | 1.42 | 0.08 |
| C12H18O1N1 | 191.1310 | 7.49 | 5 | 1.42 | 0.08 |
| C12H18O1N1 | 191.1310 | 7.52 | 5 | 1.42 | 0.08 |
| C13H22N1 | 191.1674 | 4.05 | 4 | 1.62 | 0.00 |
| C13H22N1 | 191.1674 | 4.30 | 4 | 1.62 | 0.00 |
| C10H9O4 | 192.0423 | 2.79 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 2.83 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.00 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.08 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.12 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.26 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.63 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.77 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 4.08 | 7 | 0.80 | 0.40 |
| C13H9N2 | 192.0687 | 2.71 | 11 | 0.62 | 0.00 |
| C13H9N2 | 192.0687 | 2.78 | 11 | 0.62 | 0.00 |
| C13H9N2 | 192.0687 | 2.78 | 11 | 0.62 | 0.00 |
| C11H13O3 | 192.0786 | 2.14 | 6 | 1.09 | 0.27 |
| C13H14O2N1 | 215.0946 | 2.48 | 8 | 1.00 | 0.15 |

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| C11H13O3 | 192.0786 | 3.34 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 3.47 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 3.53 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 3.65 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 3.71 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 3.79 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 4.24 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 4.29 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 4.41 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 4.63 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 4.79 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 4.85 | 6 | 1.09 | 0.27 |
| C11H13O3 | 192.0786 | 5.89 | 6 | 1.09 | 0.27 |
| C10H13O2N2 | 192.0899 | 0.60 | 6 | 1.20 | 0.20 |
| C10H13O2N2 | 192.0899 | 0.75 | 6 | 1.20 | 0.20 |
| C10H13O2N2 | 192.0899 | 1.04 | 6 | 1.20 | 0.20 |
| C10H13O2N2 | 192.0899 | 2.52 | 6 | 1.20 | 0.20 |
| C10H13O2N2 | 192.0899 | 2.61 | 6 | 1.20 | 0.20 |
| C10H13O2N2 | 192.0899 | 2.79 | 6 | 1.20 | 0.20 |
| C12H21N2 | 192.1626 | 3.25 | 4 | 1.67 | 0.00 |
| C12H21N2 | 192.1626 | 3.33 | 4 | 1.67 | 0.00 |
| C12H21N2 | 192.1626 | 3.58 | 4 | 1.67 | 0.00 |
| C12H21N2 | 192.1626 | 3.73 | 4 | 1.67 | 0.00 |
| C12H21N2 | 192.1626 | 3.85 | 4 | 1.67 | 0.00 |
| C12H21N2 | 192.1626 | 3.99 | 4 | 1.67 | 0.00 |
| C10H12O3N1 | 193.0739 | 0.39 | 6 | 1.10 | 0.30 |
| C10H12O3N1 | 193.0739 | 2.78 | 6 | 1.10 | 0.30 |
| C10H12O3N1 | 193.0739 | 2.87 | 6 | 1.10 | 0.30 |
| C14H12N1 | 193.0891 | 3.03 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 3.12 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 3.25 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 3.32 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 3.53 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 3.67 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 3.80 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 3.90 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 4.03 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 4.21 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 4.37 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 5.02 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 5.05 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 6.08 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 6.13 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 6.51 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 7.71 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 7.81 | 10 | 0.79 | 0.00 |
| C9H17O2N1Na1 | 171.1259 | 1.35 | 2 | 1.89 | 0.22 |
| C12H20O1N1 | 193.1467 | 3.35 | 4 | 1.58 | 0.08 |
| C10H11O4 | 194.0579 | 2.76 | 6 | 1.00 | 0.40 |
| C10H11O4 | 194.0579 | 2.82 | 6 | 1.00 | 0.40 |

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|---|---|---|---|---|---|
| $C_{10}H_{11}O_4$ | 194.0579 | 2.88 | 6 | 1.00 | 0.40 |
| $C_{10}H_{11}O_4$ | 194.0579 | 2.98 | 6 | 1.00 | 0.40 |
| $C_{10}H_9O_3$ | 176.0473 | 3.08 | 7 | 0.80 | 0.30 |
| $C_9H_{11}O_3N_2$ | 194.0691 | 0.43 | 6 | 1.11 | 0.33 |
| $C_9H_{11}O_3N_2$ | 194.0691 | 1.21 | 6 | 1.11 | 0.33 |
| $C_{14}H_{11}O_1$ | 194.0732 | 7.68 | 10 | 0.71 | 0.07 |
| $C_{14}H_{11}O_1$ | 194.0732 | 7.74 | 10 | 0.71 | 0.07 |
| $C_{14}H_{11}O_1$ | 194.0732 | 7.80 | 10 | 0.71 | 0.07 |
| $C_{14}H_{11}O_1$ | 194.0732 | 8.03 | 10 | 0.71 | 0.07 |
| $C_{14}H_{11}O_1$ | 194.0732 | 8.20 | 10 | 0.71 | 0.07 |
| $C_{14}H_{11}O_1$ | 194.0732 | 8.29 | 10 | 0.71 | 0.07 |
| $C_{13}H_{11}N_2$ | 194.0844 | 2.90 | 10 | 0.77 | 0.00 |
| $C_{13}H_{11}N_2$ | 194.0844 | 2.98 | 10 | 0.77 | 0.00 |
| $C_{13}H_{11}N_2$ | 194.0844 | 3.01 | 10 | 0.77 | 0.00 |
| $C_{13}H_{11}N_2$ | 194.0844 | 3.22 | 10 | 0.77 | 0.00 |
| $C_{13}H_{11}N_2$ | 194.0844 | 3.33 | 10 | 0.77 | 0.00 |
| $C_{13}H_{11}N_2$ | 194.0844 | 3.53 | 10 | 0.77 | 0.00 |
| $C_{11}H_{15}O_3$ | 194.0943 | 2.56 | 5 | 1.27 | 0.27 |
| $C_{11}H_{15}O_3$ | 194.0943 | 2.88 | 5 | 1.27 | 0.27 |
| $C_{10}H_{15}O_2N_2$ | 194.1055 | 0.62 | 5 | 1.40 | 0.20 |
| $C_{10}H_{15}O_2N_2$ | 194.1055 | 0.90 | 5 | 1.40 | 0.20 |
| $C_{10}H_{15}O_2N_2$ | 194.1055 | 1.11 | 5 | 1.40 | 0.20 |
| $C_{10}H_{15}O_2N_2$ | 194.1055 | 1.55 | 5 | 1.40 | 0.20 |
| $C_{10}H_{15}O_2N_2$ | 194.1055 | 2.72 | 5 | 1.40 | 0.20 |
| $C_{10}H_{15}O_2N_2$ | 194.1055 | 2.86 | 5 | 1.40 | 0.20 |
| $C_{11}H_{19}O_1N_2$ | 194.1419 | 2.60 | 4 | 1.64 | 0.09 |
| $C_{11}H_{19}O_1N_2$ | 194.1419 | 2.90 | 4 | 1.64 | 0.09 |
| $C_{11}H_{19}O_1N_2$ | 194.1419 | 3.19 | 4 | 1.64 | 0.09 |
| $C_{12}H_{23}N_2$ | 194.1783 | 3.47 | 3 | 1.83 | 0.00 |
| $C_{12}H_{23}N_2$ | 194.1783 | 3.54 | 3 | 1.83 | 0.00 |
| $C_{12}H_{23}N_2$ | 194.1783 | 3.65 | 3 | 1.83 | 0.00 |
| $C_{12}H_{23}N_2$ | 194.1783 | 6.87 | 3 | 1.83 | 0.00 |
| $C_9H_{10}O_4N_1$ | 195.0532 | 0.37 | 6 | 1.00 | 0.44 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 2.75 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 2.83 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 2.95 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 3.03 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 3.10 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 3.19 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 3.24 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 3.42 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 3.47 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 4.49 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 6.22 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 6.71 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 6.96 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 7.13 | 10 | 0.69 | 0.08 |
| $C_{13}H_{10}O_1N_1$ | 195.0684 | 7.29 | 10 | 0.69 | 0.08 |
| $C_{10}H_{14}O_3N_1$ | 195.0895 | 0.86 | 5 | 1.30 | 0.30 |
| $C_{10}H_{14}O_3N_1$ | 195.0895 | 1.03 | 5 | 1.30 | 0.30 |

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|---|---|---|---|---|---|
| C10H14O3N1 | 195.0895 | 2.42 | 5 | 1.30 | 0.30 |
| C10H14O3N1 | 195.0895 | 2.53 | 5 | 1.30 | 0.30 |
| C10H14O3N1 | 195.0895 | 2.68 | 5 | 1.30 | 0.30 |
| C10H14O3N1 | 195.0895 | 2.81 | 5 | 1.30 | 0.30 |
| C10H14O3N1 | 195.0895 | 3.56 | 5 | 1.30 | 0.30 |
| C9H14O2N3 | 195.1008 | 0.50 | 5 | 1.44 | 0.22 |
| C14H14N1 | 195.1048 | 3.20 | 9 | 0.93 | 0.00 |
| C14H14N1 | 195.1048 | 3.41 | 9 | 0.93 | 0.00 |
| C14H14N1 | 195.1048 | 3.46 | 9 | 0.93 | 0.00 |
| C14H14N1 | 195.1048 | 3.54 | 9 | 0.93 | 0.00 |
| C14H14N1 | 195.1048 | 3.71 | 9 | 0.93 | 0.00 |
| C14H14N1 | 195.1048 | 3.83 | 9 | 0.93 | 0.00 |
| C14H14N1 | 195.1048 | 3.96 | 9 | 0.93 | 0.00 |
| C12H22O1N1 | 195.1623 | 2.78 | 3 | 1.75 | 0.08 |
| C13H9O2 | 196.0524 | 4.62 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 4.71 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 4.90 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 5.79 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 6.76 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 7.19 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 7.55 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 7.60 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 7.68 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 7.77 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 7.96 | 10 | 0.62 | 0.15 |
| C13H9O2 | 196.0524 | 8.02 | 10 | 0.62 | 0.15 |
| C12H9O1N2 | 196.0637 | 2.78 | 10 | 0.67 | 0.08 |
| C12H9O1N2 | 196.0637 | 3.90 | 10 | 0.67 | 0.08 |
| C12H9O1N2 | 196.0637 | 4.18 | 10 | 0.67 | 0.08 |
| C10H13O4 | 196.0736 | 0.58 | 5 | 1.20 | 0.40 |
| C10H13O4 | 196.0736 | 2.80 | 5 | 1.20 | 0.40 |
| C10H13O4 | 196.0736 | 3.04 | 5 | 1.20 | 0.40 |
| C10H13O4 | 196.0736 | 3.24 | 5 | 1.20 | 0.40 |
| C10H13O4 | 196.0736 | 3.35 | 5 | 1.20 | 0.40 |
| C10H13O4 | 196.0736 | 3.52 | 5 | 1.20 | 0.40 |
| C9H13O3N2 | 196.0848 | 0.93 | 5 | 1.33 | 0.33 |
| C9H13O3N2 | 196.0848 | 1.36 | 5 | 1.33 | 0.33 |
| C14H13O1 | 196.0888 | 8.17 | 9 | 0.86 | 0.07 |
| C13H13N2 | 196.1000 | 3.04 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.14 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.22 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.31 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.39 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.55 | 9 | 0.92 | 0.00 |
| C11H17O3 | 196.1099 | 2.99 | 4 | 1.45 | 0.27 |
| C11H17O3 | 196.1099 | 3.21 | 4 | 1.45 | 0.27 |
| C10H17O2N2 | 196.1212 | 0.74 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 1.28 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.27 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.40 | 4 | 1.60 | 0.20 |

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|---|---|---|---|---|---|
| C10H13N2 | 160.1000 | 2.49 | 6 | 1.20 | 0.00 |
| C10H17O2N2 | 196.1212 | 2.56 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.64 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.70 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.77 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.91 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 3.02 | 4 | 1.60 | 0.20 |
| C4H8O6N1S1 | 196.9994 | 0.56 | 2 | 1.75 | 1.50 |
| C12H8O2N1 | 197.0477 | 3.44 | 10 | 0.58 | 0.17 |
| C12H8O2N1 | 197.0477 | 3.87 | 10 | 0.58 | 0.17 |
| C12H8O2N1 | 197.0477 | 4.20 | 10 | 0.58 | 0.17 |
| C12H8O2N1 | 197.0477 | 4.57 | 10 | 0.58 | 0.17 |
| C13H12O1N1 | 197.0841 | 2.71 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 2.83 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 2.94 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.02 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.14 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.27 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.37 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.51 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.58 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.75 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.84 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.94 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 4.11 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 4.25 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 6.82 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 7.10 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 7.18 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 7.32 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 7.51 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 7.60 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 7.79 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 7.84 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 7.99 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 8.20 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 4.35 | 9 | 0.85 | 0.08 |
| C13H12O1N1 | 197.0841 | 3.94 | 9 | 0.85 | 0.08 |
| C6H16O6N1 | 197.0899 | 0.33 | 0 | 2.50 | 1.00 |
| C12H12N3 | 197.0953 | 2.79 | 9 | 0.92 | 0.00 |
| C14H16N1 | 197.1204 | 3.15 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 3.32 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 3.42 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 3.53 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 3.74 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 3.79 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 3.95 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 4.04 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 4.15 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 4.16 | 8 | 1.07 | 0.00 |

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|---|---|---|---|---|---|
| C14H16N1 | 197.1204 | 4.28 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 4.38 | 8 | 1.07 | 0.00 |
| C14H16N1 | 197.1204 | 4.54 | 8 | 1.07 | 0.00 |
| C12H7O3 | 198.0317 | 3.88 | 10 | 0.50 | 0.25 |
| C12H7O3 | 198.0317 | 6.54 | 10 | 0.50 | 0.25 |
| C5H7O3N6 | 198.0501 | 0.51 | 6 | 1.20 | 0.60 |
| C9H11O5 | 198.0528 | 2.80 | 5 | 1.11 | 0.56 |
| C13H11O2 | 198.0681 | 4.81 | 9 | 0.77 | 0.15 |
| C13H11O2 | 198.0681 | 5.22 | 9 | 0.77 | 0.15 |
| C13H11O2 | 198.0681 | 6.53 | 9 | 0.77 | 0.15 |
| C13H11O2 | 198.0681 | 6.80 | 9 | 0.77 | 0.15 |
| C13H11O2 | 198.0681 | 7.13 | 9 | 0.77 | 0.15 |
| C13H11O2 | 198.0681 | 7.23 | 9 | 0.77 | 0.15 |
| C13H11O2 | 198.0681 | 7.45 | 9 | 0.77 | 0.15 |
| C13H11O2 | 198.0681 | 7.59 | 9 | 0.77 | 0.15 |
| C13H11O2 | 198.0681 | 7.76 | 9 | 0.77 | 0.15 |
| C12H11O1N2 | 198.0793 | 2.60 | 9 | 0.83 | 0.08 |
| C12H11O1N2 | 198.0793 | 2.75 | 9 | 0.83 | 0.08 |
| C12H11O1N2 | 198.0793 | 2.85 | 9 | 0.83 | 0.08 |
| C12H11O1N2 | 198.0793 | 2.93 | 9 | 0.83 | 0.08 |
| C12H11O1N2 | 198.0793 | 3.05 | 9 | 0.83 | 0.08 |
| C12H11O1N2 | 198.0793 | 3.24 | 9 | 0.83 | 0.08 |
| C10H15O4 | 198.0892 | 2.89 | 4 | 1.40 | 0.40 |
| C9H15O3N2 | 198.1004 | 0.45 | 4 | 1.56 | 0.33 |
| C9H15O3N2 | 198.1004 | 0.59 | 4 | 1.56 | 0.33 |
| C9H15O3N2 | 198.1004 | 0.83 | 4 | 1.56 | 0.33 |
| C9H15O3N2 | 198.1004 | 0.89 | 4 | 1.56 | 0.33 |
| C9H15O3N2 | 198.1004 | 1.02 | 4 | 1.56 | 0.33 |
| C9H15O3N2 | 198.1004 | 1.19 | 4 | 1.56 | 0.33 |
| C9H15O3N2 | 198.1004 | 2.46 | 4 | 1.56 | 0.33 |
| C13H15N2 | 198.1157 | 3.07 | 8 | 1.08 | 0.00 |
| C12H10O2N1 | 199.0633 | 2.69 | 9 | 0.75 | 0.17 |
| C12H10O2N1 | 199.0633 | 2.83 | 9 | 0.75 | 0.17 |
| C12H10O2N1 | 199.0633 | 3.14 | 9 | 0.75 | 0.17 |
| C12H10O2N1 | 199.0633 | 3.24 | 9 | 0.75 | 0.17 |
| C12H10O2N1 | 199.0633 | 3.38 | 9 | 0.75 | 0.17 |
| C12H10O2N1 | 199.0633 | 3.53 | 9 | 0.75 | 0.17 |
| C8H14O3N3 | 199.0957 | 0.36 | 4 | 1.63 | 0.38 |
| C13H14O1N1 | 199.0997 | 2.45 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 2.49 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 2.63 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 2.74 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 2.83 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 2.91 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 2.97 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 3.01 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 3.12 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 3.16 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 3.29 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 3.44 | 8 | 1.00 | 0.08 |

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|---|---|---|---|---|---|
| C13H14O1N1 | 199.0997 | 3.50 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 6.89 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 6.94 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 6.99 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 7.30 | 8 | 1.00 | 0.08 |
| C14H18N1 | 199.1361 | 3.46 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 3.54 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 3.61 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 3.78 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 3.86 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 3.92 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 3.98 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 4.05 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 4.22 | 7 | 1.21 | 0.00 |
| C14H18N1 | 199.1361 | 4.41 | 7 | 1.21 | 0.00 |
| C11H22O2N1 | 199.1572 | 2.90 | 2 | 1.91 | 0.18 |
| C12H9O3 | 200.0473 | 7.27 | 9 | 0.67 | 0.25 |
| C12H9O3 | 200.0473 | 7.59 | 9 | 0.67 | 0.25 |
| C9H13O5 | 200.0685 | 3.14 | 4 | 1.33 | 0.56 |
| C13H13O2 | 200.0837 | 4.90 | 8 | 0.92 | 0.15 |
| C13H13O2 | 200.0837 | 5.15 | 8 | 0.92 | 0.15 |
| C13H13O2 | 200.0837 | 7.45 | 8 | 0.92 | 0.15 |
| C13H13O2 | 200.0837 | 7.58 | 8 | 0.92 | 0.15 |
| C13H13O2 | 200.0837 | 8.04 | 8 | 0.92 | 0.15 |
| C13H13O2 | 200.0837 | 8.10 | 8 | 0.92 | 0.15 |
| C12H13O1N2 | 200.0950 | 2.66 | 8 | 1.00 | 0.08 |
| C12H13O1N2 | 200.0950 | 2.84 | 8 | 1.00 | 0.08 |
| C12H13O1N2 | 200.0950 | 3.00 | 8 | 1.00 | 0.08 |
| C12H13O1N2 | 200.0950 | 3.09 | 8 | 1.00 | 0.08 |
| C12H13O1N2 | 200.0950 | 3.17 | 8 | 1.00 | 0.08 |
| C12H13O1N2 | 200.0950 | 3.47 | 8 | 1.00 | 0.08 |
| C12H13O1N2 | 200.0950 | 3.70 | 8 | 1.00 | 0.08 |
| C12H13O1N2 | 200.0950 | 3.81 | 8 | 1.00 | 0.08 |
| C13H17N2 | 200.1313 | 3.11 | 7 | 1.23 | 0.00 |
| C13H17N2 | 200.1313 | 3.19 | 7 | 1.23 | 0.00 |
| C13H17N2 | 200.1313 | 3.44 | 7 | 1.23 | 0.00 |
| C13H17N2 | 200.1313 | 3.63 | 7 | 1.23 | 0.00 |
| C11H21O3 | 200.1412 | 7.11 | 2 | 1.82 | 0.27 |
| C8H12O5N1 | 201.0637 | 0.37 | 4 | 1.38 | 0.63 |
| C12H12O2N1 | 201.0790 | 1.04 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 1.73 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 1.95 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 2.32 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 2.47 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 2.55 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 2.80 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 2.92 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 3.04 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 3.20 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 3.35 | 8 | 0.92 | 0.17 |

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| C12H12O2N1 | 201.0790 | 3.54 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 3.68 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 3.79 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 4.14 | 8 | 0.92 | 0.17 |
| C13H16O1N1 | 201.1154 | 2.62 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 2.79 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.04 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.08 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.16 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.29 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.32 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.40 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.49 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.80 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 3.84 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 7.60 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 7.68 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 7.81 | 7 | 1.15 | 0.08 |
| C13H16O1N1 | 201.1154 | 7.89 | 7 | 1.15 | 0.08 |
| C14H20N1 | 201.1517 | 3.68 | 6 | 1.36 | 0.00 |
| C14H20N1 | 201.1517 | 3.74 | 6 | 1.36 | 0.00 |
| C14H20N1 | 201.1517 | 3.76 | 6 | 1.36 | 0.00 |
| C14H20N1 | 201.1517 | 3.82 | 6 | 1.36 | 0.00 |
| C14H20N1 | 201.1517 | 3.88 | 6 | 1.36 | 0.00 |
| C14H20N1 | 201.1517 | 3.94 | 6 | 1.36 | 0.00 |
| C14H20N1 | 201.1517 | 4.20 | 6 | 1.36 | 0.00 |
| C14H20N1 | 201.1517 | 4.28 | 6 | 1.36 | 0.00 |
| C7H11O3N2S1 | 202.0412 | 0.37 | 4 | 1.43 | 0.43 |
| C12H11O3 | 202.0630 | 3.43 | 8 | 0.83 | 0.25 |
| C12H11O3 | 202.0630 | 3.55 | 8 | 0.83 | 0.25 |
| C12H11O3 | 202.0630 | 4.13 | 8 | 0.83 | 0.25 |
| C12H11O3 | 202.0630 | 5.37 | 8 | 0.83 | 0.25 |
| C12H11O3 | 202.0630 | 6.52 | 8 | 0.83 | 0.25 |
| C12H11O3 | 202.0630 | 7.48 | 8 | 0.83 | 0.25 |
| C11H11O2N2 | 202.0742 | 1.07 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 2.42 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 2.47 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 2.57 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 2.70 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 2.89 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 3.20 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 3.23 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 2.97 | 8 | 0.91 | 0.18 |
| C13H15O2 | 202.0994 | 4.34 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 4.57 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 4.73 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 4.88 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 4.98 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 5.06 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 5.17 | 7 | 1.08 | 0.15 |

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| C13H15O2 | 202.0994 | 5.47 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 5.82 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 5.96 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 6.10 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 6.26 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 6.46 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 6.63 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 6.74 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 6.85 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 7.02 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 7.10 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 7.19 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 7.27 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 7.33 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 7.48 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 5.59 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 6.34 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 7.82 | 7 | 1.08 | 0.15 |
| C13H15O2 | 202.0994 | 5.58 | 7 | 1.08 | 0.15 |
| C12H15O1N2 | 202.1106 | 2.12 | 7 | 1.17 | 0.08 |
| C12H15O1N2 | 202.1106 | 2.26 | 7 | 1.17 | 0.08 |
| C12H15O1N2 | 202.1106 | 2.45 | 7 | 1.17 | 0.08 |
| C12H15O1N2 | 202.1106 | 2.49 | 7 | 1.17 | 0.08 |
| C12H15O1N2 | 202.1106 | 2.67 | 7 | 1.17 | 0.08 |
| C12H15O1N2 | 202.1106 | 2.81 | 7 | 1.17 | 0.08 |
| C12H15O1N2 | 202.1106 | 2.84 | 7 | 1.17 | 0.08 |
| C12H15O1N2 | 202.1106 | 2.93 | 7 | 1.17 | 0.08 |
| C13H16N1 | 185.1204 | 3.34 | 7 | 1.15 | 0.00 |
| C7H10O4N1S1 | 203.0252 | 0.56 | 4 | 1.29 | 0.57 |
| C7H10O4N1S1 | 203.0252 | 0.57 | 4 | 1.29 | 0.57 |
| C11H10O3N1 | 203.0582 | 2.52 | 8 | 0.82 | 0.27 |
| C15H10N1 | 203.0735 | 5.87 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.09 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.60 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.84 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.84 | 12 | 0.60 | 0.00 |
| C9H10O1N5 | 203.0807 | 2.53 | 8 | 1.00 | 0.11 |
| C12H14O2N1 | 203.0946 | 2.92 | 7 | 1.08 | 0.17 |
| C12H14O2N1 | 203.0946 | 3.05 | 7 | 1.08 | 0.17 |
| C12H14O2N1 | 203.0946 | 3.31 | 7 | 1.08 | 0.17 |
| C12H14O2N1 | 203.0946 | 3.65 | 7 | 1.08 | 0.17 |
| C12H14O2N1 | 203.0946 | 3.83 | 7 | 1.08 | 0.17 |
| C12H14O2N1 | 203.0946 | 5.26 | 7 | 1.08 | 0.17 |
| C12H14O2N1 | 203.0946 | 3.46 | 7 | 1.08 | 0.17 |
| C12H14O2N1 | 203.0946 | 3.91 | 7 | 1.08 | 0.17 |
| C11H14O1N3 | 203.1059 | 2.62 | 7 | 1.18 | 0.09 |
| C13H18O1N1 | 203.1310 | 2.79 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 2.84 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 2.91 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 3.07 | 6 | 1.31 | 0.08 |

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| C13H18O1N1 | 203.1310 | 3.20 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 3.26 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 3.36 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 7.34 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 7.61 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 7.77 | 6 | 1.31 | 0.08 |
| C13H18O1N1 | 203.1310 | 7.89 | 6 | 1.31 | 0.08 |
| C12H18N3 | 203.1422 | 2.83 | 6 | 1.42 | 0.00 |
| C12H18N3 | 203.1422 | 2.90 | 6 | 1.42 | 0.00 |
| C12H18N3 | 203.1422 | 3.02 | 6 | 1.42 | 0.00 |
| C12H18N3 | 203.1422 | 3.15 | 6 | 1.42 | 0.00 |
| C12H18N3 | 203.1422 | 3.20 | 6 | 1.42 | 0.00 |
| C11H9O4 | 204.0423 | 3.33 | 8 | 0.73 | 0.36 |
| C8H13O6 | 204.0634 | 0.39 | 3 | 1.50 | 0.75 |
| C8H13O6 | 204.0634 | 0.46 | 3 | 1.50 | 0.75 |
| C8H13O6 | 204.0634 | 0.59 | 3 | 1.50 | 0.75 |
| C8H13O6 | 204.0634 | 0.77 | 3 | 1.50 | 0.75 |
| C14H9N2 | 204.0687 | 7.53 | 12 | 0.57 | 0.00 |
| C14H9N2 | 204.0687 | 8.14 | 12 | 0.57 | 0.00 |
| C11H13O2N2 | 204.0899 | 0.85 | 7 | 1.09 | 0.18 |
| C11H13O2N2 | 204.0899 | 1.05 | 7 | 1.09 | 0.18 |
| C11H13O2N2 | 204.0899 | 1.40 | 7 | 1.09 | 0.18 |
| C11H13O2N2 | 204.0899 | 1.89 | 7 | 1.09 | 0.18 |
| C11H13O2N2 | 204.0899 | 2.34 | 7 | 1.09 | 0.18 |
| C11H13O2N2 | 204.0899 | 2.49 | 7 | 1.09 | 0.18 |
| C11H13O2N2 | 204.0899 | 2.72 | 7 | 1.09 | 0.18 |
| C11H13O2N2 | 204.0899 | 2.83 | 7 | 1.09 | 0.18 |
| C11H13O2N2 | 204.0899 | 2.96 | 7 | 1.09 | 0.18 |
| C13H17O2 | 204.1150 | 7.23 | 6 | 1.23 | 0.15 |
| C13H17O2 | 204.1150 | 7.52 | 6 | 1.23 | 0.15 |
| C12H17O1N2 | 204.1263 | 2.58 | 6 | 1.33 | 0.08 |
| C12H17O1N2 | 204.1263 | 2.70 | 6 | 1.33 | 0.08 |
| C12H17O1N2 | 204.1263 | 2.70 | 6 | 1.33 | 0.08 |
| C12H17O1N2 | 204.1263 | 3.00 | 6 | 1.33 | 0.08 |
| C11H12O3N1 | 205.0739 | 2.37 | 7 | 1.00 | 0.27 |
| C15H12N1 | 205.0891 | 2.79 | 11 | 0.73 | 0.00 |
| C15H12N1 | 205.0891 | 3.65 | 11 | 0.73 | 0.00 |
| C15H12N1 | 205.0891 | 3.96 | 11 | 0.73 | 0.00 |
| C15H12N1 | 205.0891 | 4.75 | 11 | 0.73 | 0.00 |
| C15H12N1 | 205.0891 | 5.39 | 11 | 0.73 | 0.00 |
| C15H12N1 | 205.0891 | 6.39 | 11 | 0.73 | 0.00 |
| C15H12N1 | 205.0891 | 6.89 | 11 | 0.73 | 0.00 |
| C15H12N1 | 205.0891 | 7.33 | 11 | 0.73 | 0.00 |
| C8H16O5N1 | 205.0950 | 2.38 | 2 | 1.88 | 0.63 |
| C12H16O2N1 | 205.1103 | 2.74 | 6 | 1.25 | 0.17 |
| C12H16O2N1 | 205.1103 | 2.91 | 6 | 1.25 | 0.17 |
| C11H16O1N3 | 205.1215 | 2.43 | 6 | 1.36 | 0.09 |
| C13H20O1N1 | 205.1467 | 2.75 | 5 | 1.46 | 0.08 |
| C13H20O1N1 | 205.1467 | 2.88 | 5 | 1.46 | 0.08 |
| C10H7O5 | 206.0215 | 3.16 | 8 | 0.60 | 0.50 |

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| C11H11O4 | 206.0579 | 3.06 | 7 | 0.91 | 0.36 |
| C11H11O4 | 206.0579 | 3.11 | 7 | 0.91 | 0.36 |
| C11H11O4 | 206.0579 | 3.29 | 7 | 0.91 | 0.36 |
| C11H11O4 | 206.0579 | 3.46 | 7 | 0.91 | 0.36 |
| C11H11O4 | 206.0579 | 3.60 | 7 | 0.91 | 0.36 |
| C11H11O4 | 206.0579 | 4.16 | 7 | 0.91 | 0.36 |
| C11H11O4 | 206.0579 | 6.01 | 7 | 0.91 | 0.36 |
| C11H11O4 | 206.0579 | 6.40 | 7 | 0.91 | 0.36 |
| C11H11O4 | 206.0579 | 6.49 | 7 | 0.91 | 0.36 |
| C15H11O1 | 206.0732 | 7.62 | 11 | 0.67 | 0.07 |
| C8H15O6 | 206.0790 | 0.77 | 2 | 1.75 | 0.75 |
| C12H15O3 | 206.0943 | 2.69 | 6 | 1.17 | 0.25 |
| C5H15O1N6S1 | 206.0950 | 2.77 | 2 | 2.80 | 0.20 |
| C5H15O1N6S1 | 206.0950 | 3.27 | 2 | 2.80 | 0.20 |
| C12H15O3 | 206.0943 | 3.44 | 6 | 1.17 | 0.25 |
| C12H15O3 | 206.0943 | 3.56 | 6 | 1.17 | 0.25 |
| C12H15O3 | 206.0943 | 3.62 | 6 | 1.17 | 0.25 |
| C12H15O3 | 206.0943 | 3.76 | 6 | 1.17 | 0.25 |
| C12H15O3 | 206.0943 | 4.26 | 6 | 1.17 | 0.25 |
| C12H15O3 | 206.0943 | 4.57 | 6 | 1.17 | 0.25 |
| C12H15O3 | 206.0943 | 4.74 | 6 | 1.17 | 0.25 |
| C12H15O3 | 206.0943 | 5.04 | 6 | 1.17 | 0.25 |
| C11H15O2N2 | 206.1055 | 0.66 | 6 | 1.27 | 0.18 |
| C11H15O2N2 | 206.1055 | 0.86 | 6 | 1.27 | 0.18 |
| C11H15O2N2 | 206.1055 | 1.31 | 6 | 1.27 | 0.18 |
| C12H19O3N2 | 238.1317 | 2.58 | 5 | 1.50 | 0.25 |
| C11H15O2N2 | 206.1055 | 3.04 | 6 | 1.27 | 0.18 |
| C11H15O2N2 | 206.1055 | 3.20 | 6 | 1.27 | 0.18 |
| C11H15O2N2 | 206.1055 | 3.25 | 6 | 1.27 | 0.18 |
| C12H19O1N2 | 206.1419 | 2.73 | 5 | 1.50 | 0.08 |
| C11H14O3N1 | 207.0895 | 2.94 | 6 | 1.18 | 0.27 |
| C11H14O3N1 | 207.0895 | 3.16 | 6 | 1.18 | 0.27 |
| C15H14N1 | 207.1048 | 3.63 | 10 | 0.87 | 0.00 |
| C15H14N1 | 207.1048 | 3.80 | 10 | 0.87 | 0.00 |
| C15H14N1 | 207.1048 | 3.97 | 10 | 0.87 | 0.00 |
| C15H14N1 | 207.1048 | 4.03 | 10 | 0.87 | 0.00 |
| C15H14N1 | 207.1048 | 4.43 | 10 | 0.87 | 0.00 |
| C15H14N1 | 207.1048 | 4.50 | 10 | 0.87 | 0.00 |
| C15H14N1 | 207.1048 | 4.62 | 10 | 0.87 | 0.00 |
| C15H14N1 | 207.1048 | 4.16 | 10 | 0.87 | 0.00 |
| C12H18O2N1 | 207.1259 | 2.43 | 5 | 1.42 | 0.17 |
| C12H16O1N1 | 189.1154 | 2.50 | 6 | 1.25 | 0.08 |
| C12H18O2N1 | 207.1259 | 2.74 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.80 | 5 | 1.42 | 0.17 |
| C14H19O1N2 | 230.1419 | 2.93 | 7 | 1.29 | 0.07 |
| C11H18O1N3 | 207.1372 | 2.44 | 5 | 1.55 | 0.09 |
| C8H22O3N3 | 207.1583 | 0.35 | 0 | 2.63 | 0.38 |
| C6H13O6N2 | 208.0695 | 0.28 | 2 | 2.00 | 1.00 |
| C9H14O4Na1 | 186.0892 | 2.16 | 3 | 1.56 | 0.44 |
| C11H13O4 | 208.0736 | 3.17 | 6 | 1.09 | 0.36 |

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| C11H13O4 | 208.0736 | 3.54 | 6 | 1.09 | 0.36 |
| C11H13O4 | 208.0736 | 3.96 | 6 | 1.09 | 0.36 |
| C11H13O4 | 208.0736 | 5.78 | 6 | 1.09 | 0.36 |
| C10H13O3N2 | 208.0848 | 0.51 | 6 | 1.20 | 0.30 |
| C10H13O3N2 | 208.0848 | 0.95 | 6 | 1.20 | 0.30 |
| C15H13O1 | 208.0888 | 8.07 | 10 | 0.80 | 0.07 |
| C14H13N2 | 208.1000 | 3.17 | 10 | 0.86 | 0.00 |
| C14H13N2 | 208.1000 | 3.32 | 10 | 0.86 | 0.00 |
| C6H17O2N4S1 | 208.0994 | 3.49 | 1 | 2.67 | 0.33 |
| C11H17O2N2 | 208.1212 | 1.16 | 5 | 1.45 | 0.18 |
| C11H17O2N2 | 208.1212 | 1.24 | 5 | 1.45 | 0.18 |
| C11H17O2N2 | 208.1212 | 1.46 | 5 | 1.45 | 0.18 |
| C11H17O2N2 | 208.1212 | 1.88 | 5 | 1.45 | 0.18 |
| C11H17O2N2 | 208.1212 | 2.46 | 5 | 1.45 | 0.18 |
| C11H17O2N2 | 208.1212 | 2.56 | 5 | 1.45 | 0.18 |
| C11H17O2N2 | 208.1212 | 2.74 | 5 | 1.45 | 0.18 |
| C11H17O2N2 | 208.1212 | 3.02 | 5 | 1.45 | 0.18 |
| C12H21O1N2 | 208.1576 | 2.83 | 4 | 1.67 | 0.08 |
| C12H21O1N2 | 208.1576 | 2.90 | 4 | 1.67 | 0.08 |
| C13H8O2N1 | 209.0477 | 4.43 | 11 | 0.54 | 0.15 |
| C6H12O7N1 | 209.0536 | 0.39 | 2 | 1.83 | 1.17 |
| C10H12O4N1 | 209.0688 | 0.38 | 6 | 1.10 | 0.40 |
| C10H12O4N1 | 209.0688 | 0.48 | 6 | 1.10 | 0.40 |
| C14H12O1N1 | 209.0841 | 3.20 | 10 | 0.79 | 0.07 |
| C14H12O1N1 | 209.0841 | 3.47 | 10 | 0.79 | 0.07 |
| C14H12O1N1 | 209.0841 | 3.56 | 10 | 0.79 | 0.07 |
| C14H12O1N1 | 209.0841 | 3.63 | 10 | 0.79 | 0.07 |
| C14H12O1N1 | 209.0841 | 3.64 | 10 | 0.79 | 0.07 |
| C14H12O1N1 | 209.0841 | 7.27 | 10 | 0.79 | 0.07 |
| C14H12O1N1 | 209.0841 | 7.42 | 10 | 0.79 | 0.07 |
| C14H12O1N1 | 209.0841 | 7.80 | 10 | 0.79 | 0.07 |
| C14H12O1N1 | 209.0841 | 7.88 | 10 | 0.79 | 0.07 |
| C7H16O6N1 | 209.0899 | 0.39 | 1 | 2.14 | 0.86 |
| C15H16N1 | 209.1204 | 3.70 | 9 | 1.00 | 0.00 |
| C15H16N1 | 209.1204 | 3.86 | 9 | 1.00 | 0.00 |
| C15H16N1 | 209.1204 | 4.20 | 9 | 1.00 | 0.00 |
| C12H20O2N1 | 209.1416 | 2.25 | 4 | 1.58 | 0.17 |
| C9H7O6 | 210.0164 | 1.14 | 7 | 0.67 | 0.67 |
| C8H12O5Na1 | 188.0685 | 2.38 | 3 | 1.50 | 0.63 |
| C14H11O2 | 210.0681 | 6.46 | 10 | 0.71 | 0.14 |
| C14H11O2 | 210.0681 | 6.96 | 10 | 0.71 | 0.14 |
| C14H11O2 | 210.0681 | 7.50 | 10 | 0.71 | 0.14 |
| C14H11O2 | 210.0681 | 7.72 | 10 | 0.71 | 0.14 |
| C14H11O2 | 210.0681 | 8.28 | 10 | 0.71 | 0.14 |
| C13H11O1N2 | 210.0793 | 2.83 | 10 | 0.77 | 0.08 |
| C13H11O1N2 | 210.0793 | 7.43 | 10 | 0.77 | 0.08 |
| C11H15O4 | 210.0892 | 1.34 | 5 | 1.27 | 0.36 |
| C11H15O4 | 210.0892 | 2.37 | 5 | 1.27 | 0.36 |
| C11H15O4 | 210.0892 | 3.09 | 5 | 1.27 | 0.36 |
| C11H15O4 | 210.0892 | 3.15 | 5 | 1.27 | 0.36 |

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| C11H15O4 | 210.0892 | 3.31 | 5 | 1.27 | 0.36 |
| C11H15O4 | 210.0892 | 2.45 | 5 | 1.27 | 0.36 |
| C10H15O3N2 | 210.1004 | 0.47 | 5 | 1.40 | 0.30 |
| C10H15O3N2 | 210.1004 | 0.58 | 5 | 1.40 | 0.30 |
| C10H15O3N2 | 210.1004 | 0.67 | 5 | 1.40 | 0.30 |
| C10H15O3N2 | 210.1004 | 0.95 | 5 | 1.40 | 0.30 |
| C10H15O3N2 | 210.1004 | 1.10 | 5 | 1.40 | 0.30 |
| C10H15O3N2 | 210.1004 | 1.20 | 5 | 1.40 | 0.30 |
| C10H15O3N2 | 210.1004 | 1.40 | 5 | 1.40 | 0.30 |
| C10H15O3N2 | 210.1004 | 2.27 | 5 | 1.40 | 0.30 |
| C10H15O3N2 | 210.1004 | 2.55 | 5 | 1.40 | 0.30 |
| C14H15N2 | 210.1157 | 3.27 | 9 | 1.00 | 0.00 |
| C14H15N2 | 210.1157 | 3.29 | 9 | 1.00 | 0.00 |
| C14H15N2 | 210.1157 | 3.36 | 9 | 1.00 | 0.00 |
| C11H19O2N2 | 210.1368 | 2.49 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 2.63 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 2.72 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 2.79 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 2.91 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 2.99 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 3.18 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 3.39 | 4 | 1.64 | 0.18 |
| C10H17O4N2 | 228.1110 | 0.60 | 4 | 1.60 | 0.40 |
| C14H14O1N1 | 211.0997 | 2.89 | 9 | 0.93 | 0.07 |
| C14H14O1N1 | 211.0997 | 2.99 | 9 | 0.93 | 0.07 |
| C14H14O1N1 | 211.0997 | 3.05 | 9 | 0.93 | 0.07 |
| C14H14O1N1 | 211.0997 | 3.14 | 9 | 0.93 | 0.07 |
| C14H14O1N1 | 211.0997 | 3.37 | 9 | 0.93 | 0.07 |
| C14H14O1N1 | 211.0997 | 3.66 | 9 | 0.93 | 0.07 |
| C14H14O1N1 | 211.0997 | 3.88 | 9 | 0.93 | 0.07 |
| C14H14O1N1 | 211.0997 | 7.45 | 9 | 0.93 | 0.07 |
| C14H14O1N1 | 211.0997 | 7.88 | 9 | 0.93 | 0.07 |
| C7H18O6N1 | 211.1056 | 0.38 | 0 | 2.43 | 0.86 |
| C13H14N3 | 211.1109 | 3.03 | 9 | 1.00 | 0.00 |
| C15H18N1 | 211.1361 | 3.65 | 8 | 1.13 | 0.00 |
| C15H18N1 | 211.1361 | 3.73 | 8 | 1.13 | 0.00 |
| C15H18N1 | 211.1361 | 4.13 | 8 | 1.13 | 0.00 |
| C15H18N1 | 211.1361 | 4.21 | 8 | 1.13 | 0.00 |
| C15H18N1 | 211.1361 | 4.26 | 8 | 1.13 | 0.00 |
| C15H18N1 | 211.1361 | 4.66 | 8 | 1.13 | 0.00 |
| C13H9O3 | 212.0473 | 6.20 | 10 | 0.62 | 0.23 |
| C13H9O3 | 212.0473 | 7.03 | 10 | 0.62 | 0.23 |
| C13H9O3 | 212.0473 | 7.31 | 10 | 0.62 | 0.23 |
| C13H9O3 | 212.0473 | 7.56 | 10 | 0.62 | 0.23 |
| C10H13O5 | 212.0685 | 2.87 | 5 | 1.20 | 0.50 |
| C10H13O5 | 212.0685 | 3.90 | 5 | 1.20 | 0.50 |
| C9H13O4N2 | 212.0797 | 0.48 | 5 | 1.33 | 0.44 |
| C9H13O4N2 | 212.0797 | 1.00 | 5 | 1.33 | 0.44 |
| C14H13O2 | 212.0837 | 7.02 | 9 | 0.86 | 0.14 |
| C14H13O2 | 212.0837 | 7.12 | 9 | 0.86 | 0.14 |

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| C14H13O2 | 212.0837 | 7.28 | 9 | 0.86 | 0.14 |
| C14H13O2 | 212.0837 | 7.41 | 9 | 0.86 | 0.14 |
| C14H13O2 | 212.0837 | 7.55 | 9 | 0.86 | 0.14 |
| C14H13O2 | 212.0837 | 7.78 | 9 | 0.86 | 0.14 |
| C14H13O2 | 212.0837 | 8.18 | 9 | 0.86 | 0.14 |
| C13H13O1N2 | 212.0950 | 2.65 | 9 | 0.92 | 0.08 |
| C13H13O1N2 | 212.0950 | 2.87 | 9 | 0.92 | 0.08 |
| C13H13O1N2 | 212.0950 | 3.28 | 9 | 0.92 | 0.08 |
| C11H17O4 | 212.1049 | 3.05 | 4 | 1.45 | 0.36 |
| C10H17O3N2 | 212.1161 | 0.60 | 4 | 1.60 | 0.30 |
| C10H17O3N2 | 212.1161 | 0.68 | 4 | 1.60 | 0.30 |
| C10H17O3N2 | 212.1161 | 0.90 | 4 | 1.60 | 0.30 |
| C10H17O3N2 | 212.1161 | 0.98 | 4 | 1.60 | 0.30 |
| C10H17O3N2 | 212.1161 | 1.11 | 4 | 1.60 | 0.30 |
| C10H17O3N2 | 212.1161 | 1.19 | 4 | 1.60 | 0.30 |
| C14H17N2 | 212.1313 | 3.39 | 8 | 1.14 | 0.00 |
| C5H16O4N3S1 | 213.0783 | 2.79 | 0 | 3.00 | 0.80 |
| C13H12O2N1 | 213.0790 | 2.87 | 9 | 0.85 | 0.15 |
| C13H12O2N1 | 213.0790 | 3.10 | 9 | 0.85 | 0.15 |
| C13H12O2N1 | 213.0790 | 3.27 | 9 | 0.85 | 0.15 |
| C13H12O2N1 | 213.0790 | 3.39 | 9 | 0.85 | 0.15 |
| C5H16O4N3S1 | 213.0783 | 3.46 | 0 | 3.00 | 0.80 |
| C14H16O1N1 | 213.1154 | 2.69 | 8 | 1.07 | 0.07 |
| C14H16O1N1 | 213.1154 | 2.88 | 8 | 1.07 | 0.07 |
| C14H16O1N1 | 213.1154 | 3.22 | 8 | 1.07 | 0.07 |
| C14H16O1N1 | 213.1154 | 3.37 | 8 | 1.07 | 0.07 |
| C14H16O1N1 | 213.1154 | 7.82 | 8 | 1.07 | 0.07 |
| C14H16O1N1 | 213.1154 | 7.93 | 8 | 1.07 | 0.07 |
| C7H12O6Na1 | 192.0634 | 0.54 | 2 | 1.71 | 0.86 |
| C11H12O3Na1 | 192.0786 | 3.01 | 6 | 1.09 | 0.27 |
| C13H11O3 | 214.0630 | 6.37 | 9 | 0.77 | 0.23 |
| C13H11O3 | 214.0630 | 6.52 | 9 | 0.77 | 0.23 |
| C13H11O3 | 214.0630 | 6.77 | 9 | 0.77 | 0.23 |
| C13H11O3 | 214.0630 | 8.04 | 9 | 0.77 | 0.23 |
| C12H11O2N2 | 214.0742 | 1.46 | 9 | 0.83 | 0.17 |
| C10H15O5 | 214.0841 | 3.87 | 4 | 1.40 | 0.50 |
| C14H15O2 | 214.0994 | 6.81 | 8 | 1.00 | 0.14 |
| C14H15O2 | 214.0994 | 6.98 | 8 | 1.00 | 0.14 |
| C14H15O2 | 214.0994 | 7.27 | 8 | 1.00 | 0.14 |
| C14H15O2 | 214.0994 | 7.28 | 8 | 1.00 | 0.14 |
| C14H15O2 | 214.0994 | 7.33 | 8 | 1.00 | 0.14 |
| C14H15O2 | 214.0994 | 8.06 | 8 | 1.00 | 0.14 |
| C14H15O2 | 214.0994 | 8.33 | 8 | 1.00 | 0.14 |
| C13H15O1N2 | 214.1106 | 2.64 | 8 | 1.08 | 0.08 |
| C13H15O1N2 | 214.1106 | 2.87 | 8 | 1.08 | 0.08 |
| C14H19N2 | 214.1470 | 3.43 | 7 | 1.29 | 0.00 |
| C14H19N2 | 214.1470 | 3.63 | 7 | 1.29 | 0.00 |
| C12H10O3N1 | 215.0582 | 2.48 | 9 | 0.75 | 0.25 |
| C12H10O3N1 | 215.0582 | 3.82 | 9 | 0.75 | 0.25 |
| C13H14O2N1 | 215.0946 | 1.83 | 8 | 1.00 | 0.15 |

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| C13H14O2N1 | 215.0946 | 2.24 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 2.52 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 2.92 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 3.12 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 3.30 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 3.46 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 2.88 | 8 | 1.00 | 0.15 |
| C14H18O1N1 | 215.1310 | 3.29 | 7 | 1.21 | 0.07 |
| C14H18O1N1 | 215.1310 | 3.56 | 7 | 1.21 | 0.07 |
| C14H18O1N1 | 215.1310 | 8.05 | 7 | 1.21 | 0.07 |
| C14H18O1N1 | 215.1310 | 8.14 | 7 | 1.21 | 0.07 |
| C9H13O6 | 216.0634 | 1.54 | 4 | 1.33 | 0.67 |
| C9H13O6 | 216.0634 | 2.74 | 4 | 1.33 | 0.67 |
| C13H13O3 | 216.0786 | 7.25 | 8 | 0.92 | 0.23 |
| C12H13O2N2 | 216.0899 | 2.92 | 8 | 1.00 | 0.17 |
| C12H13O2N2 | 216.0899 | 3.05 | 8 | 1.00 | 0.17 |
| C12H13O2N2 | 216.0899 | 3.20 | 8 | 1.00 | 0.17 |
| C12H13O2N2 | 216.0899 | 3.36 | 8 | 1.00 | 0.17 |
| C10H20O5N1 | 233.1263 | 3.17 | 2 | 1.90 | 0.50 |
| C14H17O2 | 216.1150 | 6.75 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 6.87 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 6.94 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.03 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.20 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.25 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.37 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.44 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.53 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.70 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.78 | 7 | 1.14 | 0.14 |
| C14H17O2 | 216.1150 | 7.85 | 7 | 1.14 | 0.14 |
| C13H17O1N2 | 216.1263 | 2.60 | 7 | 1.23 | 0.08 |
| C13H17O1N2 | 216.1263 | 2.74 | 7 | 1.23 | 0.08 |
| C13H17O1N2 | 216.1263 | 2.96 | 7 | 1.23 | 0.08 |
| C13H17O1N2 | 216.1263 | 3.32 | 7 | 1.23 | 0.08 |
| C14H21N2 | 216.1626 | 3.65 | 6 | 1.43 | 0.00 |
| C12H12O3N1 | 217.0739 | 0.71 | 8 | 0.92 | 0.25 |
| C12H12O3N1 | 217.0739 | 1.22 | 8 | 0.92 | 0.25 |
| C12H12O3N1 | 217.0739 | 1.37 | 8 | 0.92 | 0.25 |
| C12H12O3N1 | 217.0739 | 2.95 | 8 | 0.92 | 0.25 |
| C11H14O5N1 | 239.0794 | 0.39 | 6 | 1.18 | 0.45 |
| C13H16O2N1 | 217.1103 | 2.71 | 7 | 1.15 | 0.15 |
| C13H16O2N1 | 217.1103 | 2.85 | 7 | 1.15 | 0.15 |
| C13H16O2N1 | 217.1103 | 2.97 | 7 | 1.15 | 0.15 |
| C12H16O1N3 | 217.1215 | 2.69 | 7 | 1.25 | 0.08 |
| C14H20O1N1 | 217.1467 | 7.80 | 6 | 1.36 | 0.07 |
| C7H11O4N2S1 | 218.0361 | 0.38 | 4 | 1.43 | 0.57 |
| C11H11O3N2 | 218.0691 | 2.52 | 8 | 0.91 | 0.27 |
| C13H15O3 | 218.0943 | 3.25 | 7 | 1.08 | 0.23 |
| C13H15O3 | 218.0943 | 3.75 | 7 | 1.08 | 0.23 |

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| C13H15O3 | 218.0943 | 4.11 | 7 | 1.08 | 0.23 |
| C13H15O3 | 218.0943 | 4.26 | 7 | 1.08 | 0.23 |
| C13H15O3 | 218.0943 | 4.36 | 7 | 1.08 | 0.23 |
| C13H15O3 | 218.0943 | 4.56 | 7 | 1.08 | 0.23 |
| C13H13O2 | 200.0837 | 4.74 | 8 | 0.92 | 0.15 |
| C13H15O3 | 218.0943 | 5.32 | 7 | 1.08 | 0.23 |
| C13H15O3 | 218.0943 | 5.86 | 7 | 1.08 | 0.23 |
| C12H15O2N2 | 218.1055 | 1.66 | 7 | 1.17 | 0.17 |
| C12H15O2N2 | 218.1055 | 2.33 | 7 | 1.17 | 0.17 |
| C12H15O2N2 | 218.1055 | 2.49 | 7 | 1.17 | 0.17 |
| C12H15O2N2 | 218.1055 | 2.81 | 7 | 1.17 | 0.17 |
| C12H15O2N2 | 218.1055 | 2.95 | 7 | 1.17 | 0.17 |
| C13H19O1N2 | 218.1419 | 2.77 | 6 | 1.38 | 0.08 |
| C6H10O4N3S1 | 219.0314 | 0.38 | 4 | 1.50 | 0.67 |
| C15H10O1N1 | 219.0684 | 7.65 | 12 | 0.60 | 0.07 |
| C12H14O3N1 | 219.0895 | 2.66 | 7 | 1.08 | 0.25 |
| C12H14O3N1 | 219.0895 | 3.08 | 7 | 1.08 | 0.25 |
| C16H14N1 | 219.1048 | 3.08 | 11 | 0.81 | 0.00 |
| C16H14N1 | 219.1048 | 3.85 | 11 | 0.81 | 0.00 |
| C16H14N1 | 219.1048 | 3.19 | 11 | 0.81 | 0.00 |
| C13H18O2N1 | 219.1259 | 2.76 | 6 | 1.31 | 0.15 |
| C14H22O1N1 | 219.1623 | 3.07 | 5 | 1.50 | 0.07 |
| C7H13O4N2S1 | 220.0518 | 0.39 | 3 | 1.71 | 0.57 |
| C10H14O4Na1 | 198.0892 | 2.51 | 4 | 1.40 | 0.40 |
| C12H13O4 | 220.0736 | 2.90 | 7 | 1.00 | 0.33 |
| C12H13O4 | 220.0736 | 3.05 | 7 | 1.00 | 0.33 |
| C12H13O4 | 220.0736 | 3.29 | 7 | 1.00 | 0.33 |
| C12H13O4 | 220.0736 | 3.67 | 7 | 1.00 | 0.33 |
| C12H13O4 | 220.0736 | 3.85 | 7 | 1.00 | 0.33 |
| C13H21O1N2 | 220.1576 | 2.88 | 5 | 1.54 | 0.08 |
| C15H25O1 | 220.1827 | 7.77 | 4 | 1.60 | 0.07 |
| C15H12O1N1 | 221.0841 | 2.76 | 11 | 0.73 | 0.07 |
| C15H12O1N1 | 221.0841 | 2.88 | 11 | 0.73 | 0.07 |
| C15H12O1N1 | 221.0841 | 3.00 | 11 | 0.73 | 0.07 |
| C15H12O1N1 | 221.0841 | 3.16 | 11 | 0.73 | 0.07 |
| C15H12O1N1 | 221.0841 | 3.37 | 11 | 0.73 | 0.07 |
| C15H12O1N1 | 221.0841 | 4.64 | 11 | 0.73 | 0.07 |
| C15H12O1N1 | 221.0841 | 3.50 | 11 | 0.73 | 0.07 |
| C8H16O6N1 | 221.0899 | 0.66 | 2 | 1.88 | 0.75 |
| C13H20O2N1 | 221.1416 | 3.03 | 5 | 1.46 | 0.15 |
| C13H20O2N1 | 221.1416 | 3.65 | 5 | 1.46 | 0.15 |
| C15H11O2 | 222.0681 | 6.71 | 11 | 0.67 | 0.13 |
| C15H15N2 | 222.1157 | 3.42 | 10 | 0.93 | 0.00 |
| C10H22O5Na1 | 222.1467 | 2.73 | 0 | 2.20 | 0.50 |
| C4H11O8N1Na1 | 201.0485 | 0.64 | 0 | 2.75 | 2.00 |
| C11H14O4N1 | 223.0845 | 0.50 | 6 | 1.18 | 0.36 |
| C11H14O4N1 | 223.0845 | 0.64 | 6 | 1.18 | 0.36 |
| C10H14O3N3 | 223.0957 | 0.39 | 6 | 1.30 | 0.30 |
| C15H14O1N1 | 223.0997 | 3.05 | 10 | 0.87 | 0.07 |
| C15H14O1N1 | 223.0997 | 3.20 | 10 | 0.87 | 0.07 |

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| C7H18O3N3S1 | 223.0991 | 3.32 | 1 | 2.43 | 0.43 |
| C15H14O1N1 | 223.0997 | 7.30 | 10 | 0.87 | 0.07 |
| C15H14O1N1 | 223.0997 | 7.35 | 10 | 0.87 | 0.07 |
| C15H14O1N1 | 223.0997 | 7.79 | 10 | 0.87 | 0.07 |
| C15H14O1N1 | 223.0997 | 3.36 | 10 | 0.87 | 0.07 |
| C12H22O1N3 | 223.1685 | 2.55 | 4 | 1.75 | 0.08 |
| C14H9O3 | 224.0473 | 7.32 | 11 | 0.57 | 0.21 |
| C10H13O4N2 | 224.0797 | 0.41 | 6 | 1.20 | 0.40 |
| C15H13O2 | 224.0837 | 7.22 | 10 | 0.80 | 0.13 |
| C15H13O2 | 224.0837 | 7.32 | 10 | 0.80 | 0.13 |
| C15H13O2 | 224.0837 | 7.43 | 10 | 0.80 | 0.13 |
| C15H13O2 | 224.0837 | 7.60 | 10 | 0.80 | 0.13 |
| C15H13O2 | 224.0837 | 8.51 | 10 | 0.80 | 0.13 |
| C14H13O1N2 | 224.0950 | 2.58 | 10 | 0.86 | 0.07 |
| C12H17O4 | 224.1049 | 4.10 | 5 | 1.33 | 0.33 |
| C11H17O3N2 | 224.1161 | 0.73 | 5 | 1.45 | 0.27 |
| C11H17O3N2 | 224.1161 | 0.87 | 5 | 1.45 | 0.27 |
| C11H14O3N1 | 207.0895 | 2.61 | 6 | 1.18 | 0.27 |
| C11H17O3N2 | 224.1161 | 2.79 | 5 | 1.45 | 0.27 |
| C12H21O2N2 | 224.1525 | 2.92 | 4 | 1.67 | 0.17 |
| C12H21O2N2 | 224.1525 | 3.00 | 4 | 1.67 | 0.17 |
| C3H9O9N1Na1 | 203.0277 | 3.04 | 0 | 3.00 | 3.00 |
| C6H16O4N3S1 | 225.0783 | 7.81 | 1 | 2.50 | 0.67 |
| C15H16O1N1 | 225.1154 | 3.09 | 9 | 1.00 | 0.07 |
| C15H16O1N1 | 225.1154 | 3.19 | 9 | 1.00 | 0.07 |
| C15H16O1N1 | 225.1154 | 3.34 | 9 | 1.00 | 0.07 |
| C15H16O1N1 | 225.1154 | 3.48 | 9 | 1.00 | 0.07 |
| C15H16O1N1 | 225.1154 | 7.60 | 9 | 1.00 | 0.07 |
| C15H16O1N1 | 225.1154 | 7.94 | 9 | 1.00 | 0.07 |
| C6H7O4N6 | 226.0451 | 0.60 | 7 | 1.00 | 0.67 |
| C8H12O6Na1 | 204.0634 | 0.74 | 3 | 1.50 | 0.75 |
| C14H11O3 | 226.0630 | 7.29 | 10 | 0.71 | 0.21 |
| C14H11O3 | 226.0630 | 7.32 | 10 | 0.71 | 0.21 |
| C14H11O3 | 226.0630 | 7.59 | 10 | 0.71 | 0.21 |
| C14H11O3 | 226.0630 | 7.67 | 10 | 0.71 | 0.21 |
| C14H11O3 | 226.0630 | 7.79 | 10 | 0.71 | 0.21 |
| C14H11O3 | 226.0630 | 7.88 | 10 | 0.71 | 0.21 |
| C14H11O3 | 226.0630 | 7.89 | 10 | 0.71 | 0.21 |
| C10H15O4N2 | 226.0954 | 1.07 | 5 | 1.40 | 0.40 |
| C15H15O2 | 226.0994 | 7.45 | 9 | 0.93 | 0.13 |
| C15H15O2 | 226.0994 | 7.52 | 9 | 0.93 | 0.13 |
| C15H15O2 | 226.0994 | 7.69 | 9 | 0.93 | 0.13 |
| C15H15O2 | 226.0994 | 7.79 | 9 | 0.93 | 0.13 |
| C15H15O2 | 226.0994 | 7.94 | 9 | 0.93 | 0.13 |
| C15H15O2 | 226.0994 | 8.08 | 9 | 0.93 | 0.13 |
| C11H19O3N2 | 226.1317 | 2.96 | 4 | 1.64 | 0.27 |
| C12H23O2N2 | 226.1681 | 1.54 | 3 | 1.83 | 0.17 |
| C15H11N1Na1 | 205.0891 | 7.15 | 11 | 0.73 | 0.00 |
| C14H14O2N1 | 227.0946 | 2.81 | 9 | 0.93 | 0.14 |
| C14H14O2N1 | 227.0946 | 3.00 | 9 | 0.93 | 0.14 |

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| C14H14O2N1 | 227.0946 | 3.09 | 9 | 0.93 | 0.14 |
| C14H14O2N1 | 227.0946 | 3.21 | 9 | 0.93 | 0.14 |
| C11H18O4N1 | 227.1158 | 3.16 | 4 | 1.55 | 0.36 |
| C15H18O1N1 | 227.1310 | 2.92 | 8 | 1.13 | 0.07 |
| C15H18O1N1 | 227.1310 | 3.00 | 8 | 1.13 | 0.07 |
| C15H18O1N1 | 227.1310 | 3.11 | 8 | 1.13 | 0.07 |
| C15H18O1N1 | 227.1310 | 3.21 | 8 | 1.13 | 0.07 |
| C15H18O1N1 | 227.1310 | 3.34 | 8 | 1.13 | 0.07 |
| C15H18O1N1 | 227.1310 | 3.43 | 8 | 1.13 | 0.07 |
| C15H18O1N1 | 227.1310 | 3.57 | 8 | 1.13 | 0.07 |
| C15H18O1N1 | 227.1310 | 3.82 | 8 | 1.13 | 0.07 |
| C15H18O1N1 | 227.1310 | 8.09 | 8 | 1.13 | 0.07 |
| C13H9O4 | 228.0423 | 7.88 | 10 | 0.62 | 0.31 |
| C6H9O4N6 | 228.0607 | 0.56 | 6 | 1.33 | 0.67 |
| C14H13O3 | 228.0786 | 7.72 | 9 | 0.86 | 0.21 |
| C13H13O2N2 | 228.0899 | 2.64 | 9 | 0.92 | 0.15 |
| C13H13O2N2 | 228.0899 | 2.79 | 9 | 0.92 | 0.15 |
| C13H13O2N2 | 228.0899 | 2.96 | 9 | 0.92 | 0.15 |
| C13H13O2N2 | 228.0899 | 3.06 | 9 | 0.92 | 0.15 |
| C10H17O4N2 | 228.1110 | 0.74 | 4 | 1.60 | 0.40 |
| C15H17O2 | 228.1150 | 7.42 | 8 | 1.07 | 0.13 |
| C15H17O2 | 228.1150 | 7.67 | 8 | 1.07 | 0.13 |
| C14H17O1N2 | 228.1263 | 2.84 | 8 | 1.14 | 0.07 |
| C14H17O1N2 | 228.1263 | 3.02 | 8 | 1.14 | 0.07 |
| C14H17O1N2 | 228.1263 | 7.95 | 8 | 1.14 | 0.07 |
| C14H17O1N2 | 228.1263 | 3.15 | 8 | 1.14 | 0.07 |
| C13H12O3N1 | 229.0739 | 2.88 | 9 | 0.85 | 0.23 |
| C17H12N1 | 229.0891 | 8.64 | 13 | 0.65 | 0.00 |
| C14H16O2N1 | 229.1103 | 2.63 | 8 | 1.07 | 0.14 |
| C14H16O2N1 | 229.1103 | 2.84 | 8 | 1.07 | 0.14 |
| C14H16O2N1 | 229.1103 | 3.09 | 8 | 1.07 | 0.14 |
| C14H16O2N1 | 229.1103 | 3.34 | 8 | 1.07 | 0.14 |
| C6H9O3N2S3 | 251.9697 | 0.31 | 4 | 1.33 | 0.50 |
| C10H12O3N2Na1 | 208.0848 | 0.96 | 6 | 1.20 | 0.30 |
| C17H11O1 | 230.0732 | 8.31 | 13 | 0.59 | 0.06 |
| C17H11O1 | 230.0732 | 8.42 | 13 | 0.59 | 0.06 |
| C13H15O2N2 | 230.1055 | 2.79 | 8 | 1.08 | 0.15 |
| C13H15O2N2 | 230.1055 | 3.02 | 8 | 1.08 | 0.15 |
| C13H15O2N2 | 230.1055 | 3.17 | 8 | 1.08 | 0.15 |
| C15H19O2 | 230.1307 | 7.71 | 7 | 1.20 | 0.13 |
| C15H19O2 | 230.1307 | 7.87 | 7 | 1.20 | 0.13 |
| C14H19O1N2 | 230.1419 | 3.12 | 7 | 1.29 | 0.07 |
| C16H10O1N1 | 231.0684 | 8.06 | 13 | 0.56 | 0.06 |
| C13H14O3N1 | 231.0895 | 0.91 | 8 | 1.00 | 0.23 |
| C13H14O3N1 | 231.0895 | 2.32 | 8 | 1.00 | 0.23 |
| C13H14O3N1 | 231.0895 | 2.60 | 8 | 1.00 | 0.23 |
| C13H14O3N1 | 231.0895 | 2.71 | 8 | 1.00 | 0.23 |
| C13H14O3N1 | 231.0895 | 2.87 | 8 | 1.00 | 0.23 |
| C13H14O3N1 | 231.0895 | 3.01 | 8 | 1.00 | 0.23 |
| C16H9O2 | 232.0524 | 7.65 | 13 | 0.50 | 0.13 |

| | | | | | |
|---|---|---|---|---|---|
| C12H13O3N2 | 232.0848 | 2.62 | 8 | 1.00 | 0.25 |
| C12H13O3N2 | 232.0848 | 2.68 | 8 | 1.00 | 0.25 |
| C12H13O3N2 | 232.0848 | 3.04 | 8 | 1.00 | 0.25 |
| C12H13O3N2 | 232.0848 | 3.22 | 8 | 1.00 | 0.25 |
| C14H17O3 | 232.1099 | 4.79 | 7 | 1.14 | 0.21 |
| C14H17O3 | 232.1099 | 5.03 | 7 | 1.14 | 0.21 |
| C14H17O3 | 232.1099 | 6.57 | 7 | 1.14 | 0.21 |
| C13H17O2N2 | 232.1212 | 1.68 | 7 | 1.23 | 0.15 |
| C13H17O2N2 | 232.1212 | 2.51 | 7 | 1.23 | 0.15 |
| C13H17O2N2 | 232.1212 | 2.69 | 7 | 1.23 | 0.15 |
| C13H17O2N2 | 232.1212 | 2.80 | 7 | 1.23 | 0.15 |
| C13H17O2N2 | 232.1212 | 2.88 | 7 | 1.23 | 0.15 |
| C14H21O1N2 | 232.1576 | 2.91 | 6 | 1.43 | 0.07 |
| C12H12O4N1 | 233.0688 | 3.89 | 8 | 0.92 | 0.33 |
| C13H16O3N1 | 233.1052 | 2.78 | 7 | 1.15 | 0.23 |
| C16H11O2 | 234.0681 | 6.97 | 12 | 0.63 | 0.13 |
| C13H15O4 | 234.0892 | 3.27 | 7 | 1.08 | 0.31 |
| C13H15O4 | 234.0892 | 3.34 | 7 | 1.08 | 0.31 |
| C13H15O4 | 234.0892 | 3.45 | 7 | 1.08 | 0.31 |
| C13H15O4 | 234.0892 | 3.86 | 7 | 1.08 | 0.31 |
| C13H15O4 | 234.0892 | 4.77 | 7 | 1.08 | 0.31 |
| C12H15O3N2 | 234.1004 | 2.68 | 7 | 1.17 | 0.25 |
| C16H14O1N1 | 235.0997 | 2.64 | 11 | 0.81 | 0.06 |
| C8H18O3N3S1 | 235.0991 | 3.24 | 2 | 2.13 | 0.38 |
| C16H14O1N1 | 235.0997 | 3.49 | 11 | 0.81 | 0.06 |
| C16H14O1N1 | 235.0997 | 3.57 | 11 | 0.81 | 0.06 |
| C14H22O2N1 | 235.1572 | 3.19 | 5 | 1.50 | 0.14 |
| C9H13O2N6 | 236.1022 | 3.21 | 7 | 1.33 | 0.22 |
| C12H17O3N2 | 236.1161 | 2.44 | 6 | 1.33 | 0.25 |
| C13H21O2N2 | 236.1525 | 2.57 | 5 | 1.54 | 0.15 |
| C13H21O2N2 | 236.1525 | 2.69 | 5 | 1.54 | 0.15 |
| C7H16O4N3S1 | 237.0783 | 2.89 | 2 | 2.14 | 0.57 |
| C8H16O7N1 | 237.0849 | 0.39 | 2 | 1.88 | 0.88 |
| C12H8O4Na1 | 216.0423 | 3.88 | 9 | 0.67 | 0.33 |
| C15H11O3 | 238.0630 | 7.93 | 11 | 0.67 | 0.20 |
| C16H15O2 | 238.0994 | 7.80 | 10 | 0.88 | 0.13 |
| C7H19O3N4S1 | 238.1100 | 3.12 | 1 | 2.57 | 0.43 |
| C12H19O3N2 | 238.1317 | 2.59 | 5 | 1.50 | 0.25 |
| C13H23O2N2 | 238.1681 | 3.09 | 4 | 1.69 | 0.15 |
| C13H23O2N2 | 238.1681 | 3.13 | 4 | 1.69 | 0.15 |
| C8H18O5N1S1 | 239.0827 | 2.32 | 1 | 2.13 | 0.63 |
| C8H22O3N3S1 | 239.1304 | 3.28 | 0 | 2.63 | 0.38 |
| C16H18O1N1 | 239.1310 | 3.54 | 9 | 1.06 | 0.06 |
| C15H13O3 | 240.0786 | 7.80 | 10 | 0.80 | 0.20 |
| C11H17O4N2 | 240.1110 | 0.52 | 5 | 1.45 | 0.36 |
| C16H17O2 | 240.1150 | 7.96 | 9 | 1.00 | 0.13 |
| C16H17O2 | 240.1150 | 8.01 | 9 | 1.00 | 0.13 |
| C16H17O2 | 240.1150 | 8.06 | 9 | 1.00 | 0.13 |
| C16H17O2 | 240.1150 | 8.21 | 9 | 1.00 | 0.13 |
| C12H21O3N2 | 240.1474 | 2.65 | 4 | 1.67 | 0.25 |

| | | | | | |
|---|---|---|---|---|---|
| C12H21O3N2 | 240.1474 | 3.14 | 4 | 1.67 | 0.25 |
| C7H20O4N3S1 | 241.1096 | 3.11 | 0 | 2.71 | 0.57 |
| C16H20O1N1 | 241.1467 | 3.15 | 8 | 1.19 | 0.06 |
| C16H20O1N1 | 241.1467 | 3.19 | 8 | 1.19 | 0.06 |
| C11H19O3N3Na1 | 241.1426 | 3.41 | 4 | 1.73 | 0.27 |
| C16H20O1N1 | 241.1467 | 3.46 | 8 | 1.19 | 0.06 |
| C6H7O5N6 | 242.0400 | 0.39 | 7 | 1.00 | 0.83 |
| C14H11O4 | 242.0579 | 5.11 | 10 | 0.71 | 0.29 |
| C10H15O5N2 | 242.0903 | 0.40 | 5 | 1.40 | 0.50 |
| C15H15O3 | 242.0943 | 7.57 | 9 | 0.93 | 0.20 |
| C14H15O2N2 | 242.1055 | 3.26 | 9 | 1.00 | 0.14 |
| C16H19O2 | 242.1307 | 7.86 | 8 | 1.13 | 0.13 |
| C15H19O1N2 | 242.1419 | 8.28 | 8 | 1.20 | 0.07 |
| C14H14O3N1 | 243.0895 | 2.49 | 9 | 0.93 | 0.21 |
| C14H14O3N1 | 243.0895 | 2.66 | 9 | 0.93 | 0.21 |
| C15H18O2N1 | 243.1259 | 3.05 | 8 | 1.13 | 0.13 |
| C15H18O2N1 | 243.1259 | 3.27 | 8 | 1.13 | 0.13 |
| C9H13O6N2 | 244.0695 | 0.38 | 5 | 1.33 | 0.67 |
| C13H13O3N2 | 244.0848 | 2.61 | 9 | 0.92 | 0.23 |
| C15H17O3 | 244.1099 | 7.84 | 8 | 1.07 | 0.20 |
| C14H17O2N2 | 244.1212 | 3.19 | 8 | 1.14 | 0.14 |
| C10H22O5Na1 | 222.1467 | 2.69 | 0 | 2.20 | 0.50 |
| C16H21O2 | 244.1463 | 8.18 | 7 | 1.25 | 0.13 |
| C15H21O1N2 | 244.1576 | 3.25 | 7 | 1.33 | 0.07 |
| C14H16O3N1 | 245.1052 | 2.43 | 8 | 1.07 | 0.21 |
| C14H16O3N1 | 245.1052 | 2.56 | 8 | 1.07 | 0.21 |
| C14H16O3N1 | 245.1052 | 2.68 | 8 | 1.07 | 0.21 |
| C14H16O3N1 | 245.1052 | 2.83 | 8 | 1.07 | 0.21 |
| C14H16O3N1 | 245.1052 | 3.04 | 8 | 1.07 | 0.21 |
| C6H11O5N6 | 246.0713 | 0.36 | 5 | 1.67 | 0.83 |
| C13H15O3N2 | 246.1004 | 3.15 | 8 | 1.08 | 0.23 |
| C13H15O3N2 | 246.1004 | 3.33 | 8 | 1.08 | 0.23 |
| C15H19O3 | 246.1256 | 7.41 | 7 | 1.20 | 0.20 |
| C15H19O3 | 246.1256 | 7.61 | 7 | 1.20 | 0.20 |
| C14H19O2N2 | 246.1368 | 2.65 | 7 | 1.29 | 0.14 |
| C13H14O4N1 | 247.0845 | 2.76 | 8 | 1.00 | 0.31 |
| C11H22O1N1S2 | 247.1065 | 3.00 | 2 | 1.91 | 0.09 |
| C14H17O4 | 248.1049 | 3.95 | 7 | 1.14 | 0.29 |
| C14H17O4 | 248.1049 | 4.26 | 7 | 1.14 | 0.29 |
| C10H20O6N1 | 249.1212 | 0.57 | 2 | 1.90 | 0.60 |
| C16H11O3 | 250.0630 | 7.65 | 12 | 0.63 | 0.19 |
| C3H3O7N1Na1S2 | 228.9351 | 0.31 | 3 | 1.00 | 2.33 |
| C16H14O2N1 | 251.0946 | 3.09 | 11 | 0.81 | 0.13 |
| C11H18O5Na1 | 230.1154 | 3.22 | 3 | 1.64 | 0.45 |
| C17H17O2 | 252.1150 | 8.18 | 10 | 0.94 | 0.12 |
| C9H19O5N1Na1S1 | 253.0984 | 1.42 | 1 | 2.11 | 0.56 |
| C13H19O5 | 254.1154 | 6.09 | 5 | 1.38 | 0.38 |
| C14H9O5 | 256.0372 | 7.09 | 11 | 0.57 | 0.36 |
| C10H18O6Na1 | 234.1103 | 2.82 | 2 | 1.80 | 0.60 |
| C15H16O3N1 | 257.1052 | 2.51 | 9 | 1.00 | 0.20 |

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|---|---|---|---|---|---|
| C15H16O3N1 | 257.1052 | 2.75 | 9 | 1.00 | 0.20 |
| C15H16O3N1 | 257.1052 | 2.83 | 9 | 1.00 | 0.20 |
| C17H7O3 | 258.0317 | 2.37 | 15 | 0.35 | 0.18 |
| C15H18O3N1 | 259.1208 | 2.68 | 8 | 1.13 | 0.20 |
| C15H18O3N1 | 259.1208 | 2.76 | 8 | 1.13 | 0.20 |
| C15H18O3N1 | 259.1208 | 2.89 | 8 | 1.13 | 0.20 |
| C15H18O3N1 | 259.1208 | 2.92 | 8 | 1.13 | 0.20 |
| C13H13O4N2 | 260.0797 | 2.59 | 9 | 0.92 | 0.31 |
| C15H17O4 | 260.1049 | 7.88 | 8 | 1.07 | 0.27 |
| C14H17O3N2 | 260.1161 | 2.75 | 8 | 1.14 | 0.21 |
| C14H16O4N1 | 261.1001 | 1.25 | 8 | 1.07 | 0.29 |
| C13H15O4N2 | 262.0954 | 2.69 | 8 | 1.08 | 0.31 |
| C14H19O3N2 | 262.1317 | 2.56 | 7 | 1.29 | 0.21 |
| C12H20O3N2Na1 | 240.1474 | 3.97 | 4 | 1.67 | 0.25 |
| C9H20O4N3S1 | 265.1096 | 2.71 | 2 | 2.11 | 0.44 |
| C10H23O4N2S1 | 266.1300 | 8.25 | 1 | 2.20 | 0.40 |
| C3H3O7N1Na1S2 | 228.9351 | 0.31 | 3 | 1.00 | 2.33 |
| C10H14O7Na1 | 246.0740 | 2.02 | 4 | 1.40 | 0.70 |
| C6H3O4N7Na1S1 | 268.9967 | 1.47 | 9 | 0.50 | 0.67 |
| C12H16O6N1 | 269.0899 | 0.38 | 6 | 1.25 | 0.50 |
| C16H18O3N1 | 271.1208 | 2.68 | 9 | 1.06 | 0.19 |
| C16H18O3N1 | 271.1208 | 3.06 | 9 | 1.06 | 0.19 |
| C15H16O4N1 | 273.1001 | 2.61 | 9 | 1.00 | 0.27 |
| C11H24O6Na1 | 252.1573 | 2.67 | 0 | 2.18 | 0.55 |
| C15H18O4N1 | 275.1158 | 2.28 | 8 | 1.13 | 0.27 |
| C15H18O4N1 | 275.1158 | 2.60 | 8 | 1.13 | 0.27 |
| C15H21O3N2 | 276.1474 | 2.75 | 7 | 1.33 | 0.20 |
| C17H25O3 | 276.1725 | 7.58 | 6 | 1.41 | 0.18 |
| C6H4O6N1S3 | 280.9122 | 0.30 | 6 | 0.50 | 1.00 |
| C14H24O3N3 | 281.1739 | 2.49 | 5 | 1.64 | 0.21 |
| C16H18O4N1 | 287.1158 | 2.70 | 9 | 1.06 | 0.25 |
| C6H6O7N1S3 | 298.9228 | 0.29 | 5 | 0.83 | 1.17 |
| C12H22O7Na1 | 278.1366 | 2.90 | 2 | 1.83 | 0.58 |
| C12H4O1N6Na1S1 | 280.0167 | 2.63 | 14 | 0.33 | 0.08 |
| C16H18O5N1 | 303.1107 | 2.69 | 9 | 1.06 | 0.31 |
| C16H20O5N1 | 305.1263 | 2.44 | 8 | 1.19 | 0.31 |
| C13H17O5N2S1 | 312.0780 | 1.10 | 7 | 1.23 | 0.38 |
| C16H30O5N1 | 315.2046 | 2.57 | 3 | 1.81 | 0.31 |
| C16H35O4N2 | 318.2519 | 0.39 | 1 | 2.13 | 0.25 |
| C10H21O4N6S1 | 320.1267 | 6.30 | 4 | 2.00 | 0.40 |
| C20H31O4 | 334.2144 | 8.14 | 6 | 1.50 | 0.20 |
| C10H7O8N6 | 338.0247 | 2.41 | 11 | 0.60 | 0.80 |
| C18H34O5N1 | 343.2359 | 3.26 | 3 | 1.83 | 0.28 |
| C20H25O5 | 344.1624 | 7.35 | 9 | 1.20 | 0.25 |
| C9H22O6N6Na1S1 | 342.1322 | 3.35 | 2 | 2.44 | 0.67 |
| C10H6O9N7 | 367.0149 | 1.45 | 12 | 0.50 | 0.90 |
| C19H24O6Na1 | 348.1573 | 7.62 | 8 | 1.26 | 0.32 |
| C18H38O7Na1 | 366.2618 | 4.96 | 0 | 2.11 | 0.39 |
| C11H8O10N7 | 397.0254 | 2.23 | 12 | 0.64 | 0.91 |
| C21H44O8Na1 | 424.3036 | 6.82 | 0 | 2.10 | 0.38 |

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|---|---|---|---|---|---|
| C26H49O6N2 | 484.3512 | 2.55 | 4 | 1.85 | 0.23 |

Table S3.2.3 Molecular formulas of organic compounds detected in SH in ESI- mode.

| Formula [M-H] | Neutral mass (Da) | RT (min) | DBE | H/C | O/C |
|---|---|---|---|---|---|
| C3H5O6S1 | 169.9885 | 0.38 | 1 | 2.00 | 2.00 |
| C4H7O6S1 | 184.0042 | 0.43 | 1 | 2.00 | 1.50 |
| C3H3O4 | 104.0110 | 0.37 | 2 | 1.33 | 1.33 |
| C5H7O7S1 | 211.9991 | 0.38 | 2 | 1.60 | 1.40 |
| C4H5O5 | 134.0215 | 0.39 | 2 | 1.50 | 1.25 |
| C3H4O5N1 | 135.0168 | 0.39 | 2 | 1.67 | 1.67 |
| C8H7O1 | 120.0575 | 3.07 | 5 | 1.00 | 0.13 |
| C3H4O5N1S1 | 166.9888 | 0.35 | 2 | 1.67 | 1.67 |
| C7H5O2 | 122.0368 | 2.60 | 5 | 0.86 | 0.29 |
| C7H5O2 | 122.0368 | 2.66 | 5 | 0.86 | 0.29 |
| C2H5O4S1 | 125.9987 | 0.38 | 0 | 3.00 | 2.00 |
| C5H5O5 | 146.0215 | 0.38 | 3 | 1.20 | 1.00 |
| C5H7O5 | 148.0372 | 0.39 | 2 | 1.60 | 1.00 |
| C5H5O4 | 130.0266 | 0.59 | 3 | 1.20 | 0.80 |
| C5H3O3N4 | 168.0283 | 0.36 | 6 | 0.80 | 0.60 |
| C5H7O4 | 132.0423 | 0.77 | 2 | 1.60 | 0.80 |
| C5H7O4 | 132.0423 | 1.10 | 2 | 1.60 | 0.80 |
| C9H7O1 | 132.0575 | 3.11 | 6 | 0.89 | 0.11 |
| C8H5O2 | 134.0368 | 1.83 | 6 | 0.75 | 0.25 |
| C7H4O2N1 | 135.0320 | 2.69 | 6 | 0.71 | 0.29 |
| C4H7O5 | 136.0372 | 0.33 | 1 | 2.00 | 1.25 |
| C8H7O2 | 136.0524 | 3.10 | 5 | 1.00 | 0.25 |
| C2H2O4N1S1 | 136.9783 | 0.37 | 2 | 1.50 | 2.00 |
| C5H2O2N3 | 137.0225 | 2.80 | 6 | 0.60 | 0.40 |
| C5H2O2N3 | 137.0225 | 3.20 | 6 | 0.60 | 0.40 |
| C7H6O2N1 | 137.0477 | 2.39 | 5 | 1.00 | 0.29 |
| C3H5O4S1 | 137.9987 | 0.36 | 1 | 2.00 | 1.33 |
| C7H5O3 | 138.0317 | 2.17 | 5 | 0.86 | 0.43 |
| C7H5O3 | 138.0317 | 2.34 | 5 | 0.86 | 0.43 |
| C7H5O3 | 138.0317 | 3.57 | 5 | 0.86 | 0.43 |
| C6H4O3N1 | 139.0269 | 3.76 | 5 | 0.83 | 0.50 |
| C2H3O5S1 | 139.9779 | 0.34 | 1 | 2.00 | 2.50 |
| C3H7O4S1 | 140.0143 | 0.50 | 0 | 2.67 | 1.33 |
| C5H3O3N2 | 140.0222 | 2.40 | 5 | 0.80 | 0.60 |
| C6H7O8S1 | 239.9940 | 0.39 | 3 | 1.33 | 1.33 |
| C8H3O1N2 | 144.0324 | 3.70 | 8 | 0.50 | 0.13 |
| C6H7O4 | 144.0423 | 0.69 | 3 | 1.33 | 0.67 |
| C6H7O4 | 144.0423 | 1.34 | 3 | 1.33 | 0.67 |
| C9H6O1N1 | 145.0528 | 2.26 | 7 | 0.78 | 0.11 |
| C8H4O2N1 | 147.0320 | 3.27 | 7 | 0.63 | 0.25 |
| C9H7O2 | 148.0524 | 2.96 | 6 | 0.89 | 0.22 |
| C9H7O2 | 148.0524 | 3.10 | 6 | 0.89 | 0.22 |

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|---|---|---|---|---|---|
| C8H5O3 | 150.0317 | 0.82 | 6 | 0.75 | 0.38 |
| C8H5O3 | 150.0317 | 2.64 | 6 | 0.75 | 0.38 |
| C5H9O5 | 150.0528 | 0.34 | 1 | 2.00 | 1.00 |
| C4H7O4S1 | 152.0143 | 0.38 | 1 | 2.00 | 1.00 |
| C4H7O4S1 | 152.0143 | 2.85 | 1 | 2.00 | 1.00 |
| C8H7O3 | 152.0473 | 2.65 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 2.99 | 5 | 1.00 | 0.38 |
| C5H11O3S1 | 152.0507 | 1.88 | 0 | 2.40 | 0.60 |
| C7H6O3N1 | 153.0426 | 5.22 | 5 | 1.00 | 0.43 |
| C7H6O3N1 | 153.0426 | 6.06 | 5 | 1.00 | 0.43 |
| C3H5O5S1 | 153.9936 | 0.37 | 1 | 2.00 | 1.67 |
| C7H5O4 | 154.0266 | 1.30 | 5 | 0.86 | 0.57 |
| C7H5O4 | 154.0266 | 2.10 | 5 | 0.86 | 0.57 |
| C7H5O4 | 154.0266 | 2.62 | 5 | 0.86 | 0.57 |
| C4H9O4S1 | 154.0300 | 0.93 | 0 | 2.50 | 1.00 |
| C6H5O3N2 | 154.0378 | 2.85 | 5 | 1.00 | 0.50 |
| C6H5O3N2 | 154.0378 | 3.33 | 5 | 1.00 | 0.50 |
| C6H4O4N1 | 155.0219 | 0.42 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 3.09 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 3.82 | 5 | 0.83 | 0.67 |
| C2H3O6S1 | 155.9729 | 0.34 | 1 | 2.00 | 3.00 |
| C4H2O4N3 | 157.0124 | 3.25 | 5 | 0.75 | 1.00 |
| C6H5O3S1 | 158.0038 | 0.74 | 4 | 1.00 | 0.50 |
| C6H5O5 | 158.0215 | 0.38 | 4 | 1.00 | 0.83 |
| C6H8O4N1 | 159.0532 | 0.38 | 3 | 1.50 | 0.67 |
| C4H3O3N2S1 | 159.9943 | 0.37 | 4 | 1.00 | 0.75 |
| C9H5O3 | 162.0317 | 3.08 | 7 | 0.67 | 0.33 |
| C9H5O3 | 162.0317 | 3.26 | 7 | 0.67 | 0.33 |
| C9H5O3 | 162.0317 | 3.31 | 7 | 0.67 | 0.33 |
| C8H5O2N2 | 162.0429 | 6.09 | 7 | 0.75 | 0.25 |
| C10H9O2 | 162.0681 | 3.63 | 6 | 1.00 | 0.20 |
| C7H13O4 | 162.0892 | 0.85 | 1 | 2.00 | 0.57 |
| C7H3O3N2 | 164.0222 | 4.01 | 7 | 0.57 | 0.43 |
| C7H3O3N2 | 164.0222 | 4.23 | 7 | 0.57 | 0.43 |
| C9H7O3 | 164.0473 | 2.49 | 6 | 0.89 | 0.33 |
| C9H7O3 | 164.0473 | 3.07 | 6 | 0.89 | 0.33 |
| C9H7O3 | 164.0473 | 3.29 | 6 | 0.89 | 0.33 |
| C8H6O3N1 | 165.0426 | 3.20 | 6 | 0.88 | 0.38 |
| C8H6O3N1 | 165.0426 | 5.09 | 6 | 0.88 | 0.38 |
| C8H6O3N1 | 165.0426 | 6.75 | 6 | 0.88 | 0.38 |
| C4H5O5S1 | 165.9936 | 0.36 | 2 | 1.50 | 1.25 |
| C8H5O4 | 166.0266 | 1.09 | 6 | 0.75 | 0.50 |
| C8H5O4 | 166.0266 | 1.34 | 6 | 0.75 | 0.50 |
| C8H5O4 | 166.0266 | 2.67 | 6 | 0.75 | 0.50 |
| C8H5O4 | 166.0266 | 2.94 | 6 | 0.75 | 0.50 |
| C6H11O6S1 | 212.0355 | 0.39 | 1 | 2.00 | 1.00 |
| C7H5O3N2 | 166.0378 | 3.47 | 6 | 0.86 | 0.43 |
| C8H8O3N1 | 167.0582 | 7.26 | 5 | 1.13 | 0.38 |
| C8H8O3N1 | 167.0582 | 7.57 | 5 | 1.13 | 0.38 |
| C5H11O4S1 | 168.0456 | 2.22 | 0 | 2.40 | 0.80 |

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|---|---|---|---|---|---|
| C5H11O4S1 | 168.0456 | 2.82 | 0 | 2.40 | 0.80 |
| C7H6O4N1 | 169.0375 | 2.95 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 2.99 | 5 | 1.00 | 0.57 |
| C6H4O5N1 | 171.0168 | 2.31 | 5 | 0.83 | 0.83 |
| C5H4O4N3 | 171.0280 | 3.94 | 5 | 1.00 | 0.80 |
| C7H11O7 | 208.0583 | 0.39 | 2 | 1.71 | 1.00 |
| C7H7O5 | 172.0372 | 0.54 | 4 | 1.14 | 0.71 |
| C11H7O2 | 172.0524 | 3.86 | 8 | 0.73 | 0.18 |
| C8H11O4 | 172.0736 | 2.48 | 3 | 1.50 | 0.50 |
| C7H11O3N2 | 172.0848 | 2.49 | 3 | 1.71 | 0.43 |
| C7H9O5 | 174.0528 | 0.75 | 3 | 1.43 | 0.71 |
| C7H9O5 | 174.0528 | 0.96 | 3 | 1.43 | 0.71 |
| C5H4O4N1S1 | 174.9939 | 0.38 | 4 | 1.00 | 0.80 |
| C6H8O5N1 | 175.0481 | 0.38 | 3 | 1.50 | 0.83 |
| C10H9O4 | 194.0579 | 3.20 | 6 | 1.00 | 0.40 |
| C9H7O2N2 | 176.0586 | 7.47 | 7 | 0.89 | 0.22 |
| C7H11O5 | 176.0685 | 0.95 | 2 | 1.71 | 0.71 |
| C7H11O5 | 176.0685 | 1.15 | 2 | 1.71 | 0.71 |
| C8H15O4 | 176.1049 | 1.47 | 1 | 2.00 | 0.50 |
| C9H6O3N1 | 177.0426 | 2.77 | 7 | 0.78 | 0.33 |
| C9H6O3N1 | 177.0426 | 3.32 | 7 | 0.78 | 0.33 |
| C9H5O4 | 178.0266 | 2.82 | 7 | 0.67 | 0.44 |
| C9H5O4 | 178.0266 | 2.99 | 7 | 0.67 | 0.44 |
| C10H9O3 | 178.0630 | 3.00 | 6 | 1.00 | 0.30 |
| C10H9O3 | 178.0630 | 3.81 | 6 | 1.00 | 0.30 |
| C8H4O4N1 | 179.0219 | 4.92 | 7 | 0.63 | 0.50 |
| C8H4O4N1 | 179.0219 | 5.40 | 7 | 0.63 | 0.50 |
| C9H8O3N1 | 179.0582 | 3.34 | 6 | 1.00 | 0.33 |
| C9H8O3N1 | 179.0582 | 7.30 | 6 | 1.00 | 0.33 |
| C9H8O3N1 | 179.0582 | 7.45 | 6 | 1.00 | 0.33 |
| C6H9O7S1 | 226.0147 | 0.39 | 2 | 1.67 | 1.17 |
| C7H3O4N2 | 180.0171 | 3.53 | 7 | 0.57 | 0.57 |
| C9H7O4 | 180.0423 | 2.77 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 2.86 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 3.04 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 3.16 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 3.58 | 6 | 0.89 | 0.44 |
| C9H7O4 | 180.0423 | 4.13 | 6 | 0.89 | 0.44 |
| C8H7O3N2 | 180.0535 | 3.83 | 6 | 1.00 | 0.38 |
| C6H11O6 | 180.0634 | 0.34 | 1 | 2.00 | 1.00 |
| C7H2O1N1S2 | 180.9656 | 0.33 | 7 | 0.43 | 0.14 |
| C8H6O4N1 | 181.0375 | 3.91 | 6 | 0.88 | 0.50 |
| C9H10O3N1 | 181.0739 | 7.96 | 5 | 1.22 | 0.33 |
| C8H5O5 | 182.0215 | 1.07 | 6 | 0.75 | 0.63 |
| C8H5O5 | 182.0215 | 1.92 | 6 | 0.75 | 0.63 |
| C8H5O5 | 182.0215 | 2.46 | 6 | 0.75 | 0.63 |
| C8H5O5 | 182.0215 | 2.82 | 6 | 0.75 | 0.63 |
| C5H9O5S1 | 182.0249 | 0.48 | 1 | 2.00 | 1.00 |
| C5H9O5S1 | 182.0249 | 0.68 | 1 | 2.00 | 1.00 |
| C5H9O5S1 | 182.0249 | 0.90 | 1 | 2.00 | 1.00 |

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|---|---|---|---|---|---|
| C7H5O4N2 | 182.0328 | 3.13 | 6 | 0.86 | 0.57 |
| C7H5O4N2 | 182.0328 | 3.47 | 6 | 0.86 | 0.57 |
| C9H9O4 | 182.0579 | 2.30 | 5 | 1.11 | 0.44 |
| C6H13O4S1 | 182.0613 | 3.02 | 0 | 2.33 | 0.67 |
| C6H13O4S1 | 182.0613 | 3.14 | 0 | 2.33 | 0.67 |
| C6H13O4S1 | 182.0613 | 3.51 | 0 | 2.33 | 0.67 |
| C7H4O5N1 | 183.0168 | 2.95 | 6 | 0.71 | 0.71 |
| C7H4O5N1 | 183.0168 | 3.27 | 6 | 0.71 | 0.71 |
| C7H4O5N1 | 183.0168 | 3.34 | 6 | 0.71 | 0.71 |
| C6H4O4N3 | 183.0280 | 4.93 | 6 | 0.83 | 0.67 |
| C6H4O4N3 | 183.0280 | 5.05 | 6 | 0.83 | 0.67 |
| C8H8O4N1 | 183.0532 | 3.37 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 3.45 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 3.52 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 4.18 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 5.69 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 5.97 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 6.52 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 7.05 | 5 | 1.13 | 0.50 |
| C5H11O5S1 | 184.0405 | 0.51 | 0 | 2.40 | 1.00 |
| C7H6O5N1 | 185.0324 | 3.30 | 5 | 1.00 | 0.71 |
| C11H7O3 | 188.0473 | 7.28 | 8 | 0.73 | 0.27 |
| C11H7O3 | 188.0473 | 7.78 | 8 | 0.73 | 0.27 |
| C8H11O5 | 188.0685 | 1.29 | 3 | 1.50 | 0.63 |
| C8H11O5 | 188.0685 | 1.92 | 3 | 1.50 | 0.63 |
| C8H11O5 | 188.0685 | 2.37 | 3 | 1.50 | 0.63 |
| C10H6O3N1 | 189.0426 | 7.74 | 8 | 0.70 | 0.30 |
| C9H5O3N2 | 190.0378 | 2.76 | 8 | 0.67 | 0.33 |
| C8H13O5 | 190.0841 | 2.27 | 2 | 1.75 | 0.63 |
| C9H17O4 | 190.1205 | 2.80 | 1 | 2.00 | 0.44 |
| C9H3O5 | 192.0059 | 1.95 | 8 | 0.44 | 0.56 |
| C6H7O7 | 192.0270 | 0.38 | 3 | 1.33 | 1.17 |
| C10H7O4 | 192.0423 | 2.40 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 2.91 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.00 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.12 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.28 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 6.99 | 7 | 0.80 | 0.40 |
| C8H15O3S1 | 192.0820 | 3.99 | 1 | 2.00 | 0.38 |
| C9H6O4N1 | 193.0375 | 3.48 | 7 | 0.78 | 0.44 |
| C9H6O4N1 | 193.0375 | 3.64 | 7 | 0.78 | 0.44 |
| C9H6O4N1 | 193.0375 | 7.16 | 7 | 0.78 | 0.44 |
| C9H5O5 | 194.0215 | 0.82 | 7 | 0.67 | 0.56 |
| C9H5O5 | 194.0215 | 2.61 | 7 | 0.67 | 0.56 |
| C9H5O5 | 194.0215 | 2.77 | 7 | 0.67 | 0.56 |
| C9H5O5 | 194.0215 | 2.90 | 7 | 0.67 | 0.56 |
| C10H9O4 | 194.0579 | 2.86 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.61 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.74 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 6.39 | 6 | 1.00 | 0.40 |

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|---|---|---|---|---|---|
| C10H9O4 | 194.0579 | 3.96 | 6 | 1.00 | 0.40 |
| C8H17O3S1 | 194.0977 | 5.18 | 0 | 2.25 | 0.38 |
| C8H4O5N1 | 195.0168 | 3.15 | 7 | 0.63 | 0.63 |
| C9H7O5 | 196.0372 | 2.74 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.18 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.41 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.72 | 6 | 0.89 | 0.56 |
| C6H11O5S1 | 196.0405 | 0.83 | 1 | 2.00 | 0.83 |
| C6H11O5S1 | 196.0405 | 1.05 | 1 | 2.00 | 0.83 |
| C8H7O4N2 | 196.0484 | 3.19 | 6 | 1.00 | 0.50 |
| C13H7O2 | 196.0524 | 4.89 | 10 | 0.62 | 0.15 |
| C13H7O2 | 196.0524 | 7.17 | 10 | 0.62 | 0.15 |
| C13H7O2 | 196.0524 | 7.53 | 10 | 0.62 | 0.15 |
| C7H15O4S1 | 196.0769 | 5.15 | 0 | 2.29 | 0.57 |
| C8H6O5N1 | 197.0324 | 4.31 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 4.70 | 6 | 0.88 | 0.63 |
| C7H6O4N3 | 197.0437 | 6.96 | 6 | 1.00 | 0.57 |
| C9H10O4N1 | 197.0688 | 7.36 | 5 | 1.22 | 0.44 |
| C9H10O4N1 | 197.0688 | 7.57 | 5 | 1.22 | 0.44 |
| C8H5O6 | 198.0164 | 0.90 | 6 | 0.75 | 0.75 |
| C8H5O6 | 198.0164 | 1.22 | 6 | 0.75 | 0.75 |
| C8H5O6 | 198.0164 | 3.09 | 6 | 0.75 | 0.75 |
| C7H5O5N2 | 198.0277 | 7.41 | 6 | 0.86 | 0.71 |
| C7H4O6N1 | 199.0117 | 2.67 | 6 | 0.71 | 0.86 |
| C7H4O6N1 | 199.0117 | 3.43 | 6 | 0.71 | 0.86 |
| C8H8O5N1 | 199.0481 | 2.51 | 5 | 1.13 | 0.63 |
| C8H8O5N1 | 199.0481 | 2.81 | 5 | 1.13 | 0.63 |
| C8H8O5N1 | 199.0481 | 4.25 | 5 | 1.13 | 0.63 |
| C6H3O6N2 | 200.0069 | 4.24 | 6 | 0.67 | 1.00 |
| C6H3O6N2 | 200.0069 | 4.80 | 6 | 0.67 | 1.00 |
| C13H11O2 | 200.0837 | 7.72 | 8 | 0.92 | 0.15 |
| C7H5O5S1 | 201.9936 | 0.63 | 5 | 0.86 | 0.71 |
| C9H13O5 | 202.0841 | 2.70 | 3 | 1.56 | 0.56 |
| C11H8O3N1 | 203.0582 | 7.97 | 8 | 0.82 | 0.27 |
| C11H8O3N1 | 203.0582 | 8.07 | 8 | 0.82 | 0.27 |
| C8H13O7 | 222.0740 | 0.39 | 2 | 1.75 | 0.88 |
| C8H11O6 | 204.0634 | 0.55 | 3 | 1.50 | 0.75 |
| C10H6O4N1 | 205.0375 | 3.03 | 8 | 0.70 | 0.40 |
| C10H6O4N1 | 205.0375 | 3.13 | 8 | 0.70 | 0.40 |
| C10H5O5 | 206.0215 | 3.15 | 8 | 0.60 | 0.50 |
| C11H9O4 | 206.0579 | 3.19 | 7 | 0.91 | 0.36 |
| C9H4O5N1 | 207.0168 | 2.52 | 8 | 0.56 | 0.56 |
| C9H4O5N1 | 207.0168 | 3.19 | 8 | 0.56 | 0.56 |
| C9H4O5N1 | 207.0168 | 3.93 | 8 | 0.56 | 0.56 |
| C10H8O4N1 | 207.0532 | 2.83 | 7 | 0.90 | 0.40 |
| C10H8O4N1 | 207.0532 | 7.70 | 7 | 0.90 | 0.40 |
| C6H7O6S1 | 208.0042 | 0.39 | 3 | 1.33 | 1.00 |
| C10H7O5 | 208.0372 | 2.54 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.77 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.87 | 7 | 0.80 | 0.50 |

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| C10H7O5 | 208.0372 | 3.00 | 7 | 0.80 | 0.50 |
| C8H15O4S1 | 208.0769 | 4.86 | 1 | 2.00 | 0.50 |
| C9H5O6 | 210.0164 | 1.10 | 7 | 0.67 | 0.67 |
| C9H5O6 | 210.0164 | 1.95 | 7 | 0.67 | 0.67 |
| C9H5O6 | 210.0164 | 2.24 | 7 | 0.67 | 0.67 |
| C9H5O6 | 210.0164 | 2.55 | 7 | 0.67 | 0.67 |
| C10H9O5 | 210.0528 | 2.85 | 6 | 1.00 | 0.50 |
| C10H9O5 | 210.0528 | 3.02 | 6 | 1.00 | 0.50 |
| C14H9O2 | 210.0681 | 7.75 | 10 | 0.71 | 0.14 |
| C14H9O2 | 210.0681 | 7.88 | 10 | 0.71 | 0.14 |
| C8H17O4S1 | 210.0926 | 7.16 | 0 | 2.25 | 0.50 |
| C11H17O2N2 | 210.1368 | 2.72 | 4 | 1.64 | 0.18 |
| C8H4O6N1 | 211.0117 | 3.01 | 7 | 0.63 | 0.75 |
| C9H8O5N1 | 211.0481 | 7.06 | 6 | 1.00 | 0.56 |
| C6H11O6S1 | 212.0355 | 1.02 | 1 | 2.00 | 1.00 |
| C6H11O6S1 | 212.0355 | 2.85 | 1 | 2.00 | 1.00 |
| C8H7O5N2 | 212.0433 | 7.92 | 6 | 1.00 | 0.63 |
| C13H7O3 | 212.0473 | 6.54 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 7.08 | 10 | 0.62 | 0.23 |
| C13H7O3 | 212.0473 | 7.48 | 10 | 0.62 | 0.23 |
| C8H6O6N1 | 213.0273 | 3.42 | 6 | 0.88 | 0.75 |
| C8H5O5S1 | 213.9936 | 1.58 | 6 | 0.75 | 0.63 |
| C7H5O6N2 | 214.0226 | 3.55 | 6 | 0.86 | 0.86 |
| C7H5O6N2 | 214.0226 | 4.84 | 6 | 0.86 | 0.86 |
| C12H5O4 | 214.0266 | 5.49 | 10 | 0.50 | 0.33 |
| C13H9O3 | 214.0630 | 8.03 | 9 | 0.77 | 0.23 |
| C4H8O7N1S1 | 215.0100 | 1.48 | 1 | 2.25 | 1.75 |
| C12H8O3N1 | 215.0582 | 7.86 | 9 | 0.75 | 0.25 |
| C12H8O3N1 | 215.0582 | 8.10 | 9 | 0.75 | 0.25 |
| C8H7O5S1 | 216.0092 | 1.80 | 5 | 1.00 | 0.63 |
| C12H7O4 | 216.0423 | 3.86 | 9 | 0.67 | 0.33 |
| C12H7O4 | 216.0423 | 4.05 | 9 | 0.67 | 0.33 |
| C12H7O4 | 216.0423 | 4.46 | 9 | 0.67 | 0.33 |
| C12H10O3N1 | 217.0739 | 8.21 | 8 | 0.92 | 0.25 |
| C6H1O3S3 | 217.9166 | 0.54 | 6 | 0.33 | 0.50 |
| C8H9O5S1 | 218.0249 | 1.42 | 4 | 1.25 | 0.63 |
| C16H9O1 | 218.0732 | 8.36 | 12 | 0.63 | 0.06 |
| C6H4O6N1S1 | 218.9838 | 2.93 | 5 | 0.83 | 1.00 |
| C8H11O7 | 220.0583 | 0.38 | 3 | 1.50 | 0.88 |
| C11H9O5 | 222.0528 | 2.91 | 7 | 0.91 | 0.45 |
| C11H9O5 | 222.0528 | 3.04 | 7 | 0.91 | 0.45 |
| C11H9O5 | 222.0528 | 3.16 | 7 | 0.91 | 0.45 |
| C11H9O5 | 222.0528 | 3.30 | 7 | 0.91 | 0.45 |
| C15H9O2 | 222.0681 | 7.23 | 11 | 0.67 | 0.13 |
| C12H13O4 | 222.0892 | 8.04 | 6 | 1.17 | 0.33 |
| C8H3O6N2 | 224.0069 | 4.15 | 8 | 0.50 | 0.75 |
| C10H7O6 | 224.0321 | 2.73 | 7 | 0.80 | 0.60 |
| C10H7O6 | 224.0321 | 2.88 | 7 | 0.80 | 0.60 |
| C10H7O6 | 224.0321 | 3.06 | 7 | 0.80 | 0.60 |
| C10H7O6 | 224.0321 | 3.13 | 7 | 0.80 | 0.60 |

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| C8H13O8S1 | 270.0409 | 0.38 | 2 | 1.75 | 1.00 |
| C14H7O3 | 224.0473 | 7.57 | 11 | 0.57 | 0.21 |
| C8H15O5S1 | 224.0718 | 2.57 | 1 | 2.00 | 0.63 |
| C8H15O5S1 | 224.0718 | 2.67 | 1 | 2.00 | 0.63 |
| C8H15O5S1 | 224.0718 | 2.83 | 1 | 2.00 | 0.63 |
| C9H19O4S1 | 224.1082 | 7.64 | 0 | 2.22 | 0.44 |
| C9H6O6N1 | 225.0273 | 3.13 | 7 | 0.78 | 0.67 |
| C9H6O6N1 | 225.0273 | 3.23 | 7 | 0.78 | 0.67 |
| C9H10O4N3 | 225.0750 | 7.68 | 6 | 1.22 | 0.44 |
| C9H5O7 | 226.0114 | 1.07 | 7 | 0.67 | 0.78 |
| C9H5O7 | 226.0114 | 2.88 | 7 | 0.67 | 0.78 |
| C7H13O6S1 | 226.0511 | 2.49 | 1 | 2.00 | 0.86 |
| C7H13O6S1 | 226.0511 | 2.81 | 1 | 2.00 | 0.86 |
| C14H9O3 | 226.0630 | 7.12 | 10 | 0.71 | 0.21 |
| C14H9O3 | 226.0630 | 7.26 | 10 | 0.71 | 0.21 |
| C8H17O5S1 | 226.0875 | 2.95 | 0 | 2.25 | 0.63 |
| C8H4O7N1 | 227.0066 | 4.08 | 7 | 0.63 | 0.88 |
| C9H8O6N1 | 227.0430 | 2.99 | 6 | 1.00 | 0.67 |
| C9H8O6N1 | 227.0430 | 3.38 | 6 | 1.00 | 0.67 |
| C13H8O3N1 | 227.0582 | 8.23 | 10 | 0.69 | 0.23 |
| C7H3O7N2 | 228.0019 | 4.07 | 7 | 0.57 | 1.00 |
| C8H7O6N2 | 228.0382 | 4.69 | 6 | 1.00 | 0.75 |
| C13H7O4 | 228.0423 | 7.87 | 10 | 0.62 | 0.31 |
| C5H10O7N1S1 | 229.0256 | 2.76 | 1 | 2.20 | 1.40 |
| C5H10O7N1S1 | 229.0256 | 2.84 | 1 | 2.20 | 1.40 |
| C12H6O4N1 | 229.0375 | 7.98 | 10 | 0.58 | 0.33 |
| C12H6O4N1 | 229.0375 | 8.05 | 10 | 0.58 | 0.33 |
| C13H10O3N1 | 229.0739 | 8.12 | 9 | 0.85 | 0.23 |
| C13H10O3N1 | 229.0739 | 8.28 | 9 | 0.85 | 0.23 |
| C8H5O6S1 | 229.9885 | 2.53 | 6 | 0.75 | 0.75 |
| C9H9O5S1 | 230.0249 | 2.57 | 5 | 1.11 | 0.56 |
| C11H17O5 | 230.1154 | 3.22 | 3 | 1.64 | 0.45 |
| C4H8O8N1S1 | 231.0049 | 0.70 | 1 | 2.25 | 2.00 |
| C5H4O6N5 | 231.0240 | 0.37 | 6 | 1.00 | 1.20 |
| C12H8O4N1 | 231.0532 | 7.43 | 9 | 0.75 | 0.33 |
| C12H8O4N1 | 231.0532 | 7.81 | 9 | 0.75 | 0.33 |
| C10H15O6 | 232.0947 | 3.05 | 3 | 1.60 | 0.60 |
| C10H5O5N2 | 234.0277 | 7.61 | 9 | 0.60 | 0.50 |
| C11H7O6 | 236.0321 | 2.59 | 8 | 0.73 | 0.55 |
| C15H9O4 | 254.0579 | 7.87 | 11 | 0.67 | 0.27 |
| C9H15O5S1 | 236.0718 | 2.66 | 2 | 1.78 | 0.56 |
| C7H10O6N1S1 | 237.0307 | 0.38 | 3 | 1.57 | 0.86 |
| C10H5O3S2 | 237.9758 | 0.52 | 8 | 0.60 | 0.30 |
| C8H11O9S1 | 284.0202 | 0.38 | 3 | 1.50 | 1.13 |
| C12H13O5 | 238.0841 | 3.42 | 6 | 1.17 | 0.42 |
| C14H7O4 | 240.0423 | 7.12 | 11 | 0.57 | 0.29 |
| C14H7O4 | 240.0423 | 7.28 | 11 | 0.57 | 0.29 |
| C8H15O6S1 | 240.0668 | 2.88 | 1 | 2.00 | 0.75 |
| C8H15O6S1 | 240.0668 | 2.99 | 1 | 2.00 | 0.75 |
| C13H6O4N1 | 241.0375 | 7.83 | 11 | 0.54 | 0.31 |

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|---|---|---|---|---|---|
| C8H17O2S3 | 242.0469 | 0.47 | 0 | 2.25 | 0.25 |
| C9H9O6N2 | 242.0539 | 6.82 | 6 | 1.11 | 0.67 |
| C14H9O4 | 242.0579 | 5.06 | 10 | 0.71 | 0.29 |
| C14H9O4 | 242.0579 | 7.48 | 10 | 0.71 | 0.29 |
| C8H4O8N1 | 243.0015 | 2.90 | 7 | 0.63 | 1.00 |
| C7H4O7N3 | 243.0127 | 5.69 | 7 | 0.71 | 1.00 |
| C6H12O7N1S1 | 243.0413 | 3.45 | 1 | 2.17 | 1.17 |
| C14H12O3N1 | 243.0895 | 8.31 | 9 | 0.93 | 0.21 |
| C9H7O6S1 | 244.0042 | 2.34 | 6 | 0.89 | 0.67 |
| C12H19O5 | 244.1311 | 4.35 | 3 | 1.67 | 0.42 |
| C8H8O6N1S1 | 247.0151 | 1.43 | 5 | 1.13 | 0.75 |
| C8H3O4N6 | 248.0294 | 3.09 | 10 | 0.50 | 0.50 |
| C8H3O4N6 | 248.0294 | 3.16 | 10 | 0.50 | 0.50 |
| C16H7O3 | 248.0473 | 7.41 | 13 | 0.50 | 0.19 |
| C10H15O5S1 | 248.0718 | 2.99 | 3 | 1.60 | 0.50 |
| C7H5O8S1 | 249.9783 | 2.60 | 5 | 0.86 | 1.14 |
| C10H17O5S1 | 250.0875 | 3.09 | 2 | 1.80 | 0.50 |
| C14H4O2N1S1 | 251.0041 | 2.66 | 13 | 0.36 | 0.14 |
| C8H11O7S1 | 252.0304 | 0.38 | 3 | 1.50 | 0.88 |
| C15H7O4 | 252.0423 | 7.60 | 12 | 0.53 | 0.27 |
| C9H15O6S1 | 252.0668 | 2.62 | 2 | 1.78 | 0.67 |
| C10H19O5S1 | 252.1031 | 7.01 | 1 | 2.00 | 0.50 |
| C11H23O4S1 | 252.1395 | 8.19 | 0 | 2.18 | 0.36 |
| C7H10O7N1S1 | 253.0256 | 0.38 | 3 | 1.57 | 1.00 |
| C8H13O7S1 | 254.0460 | 1.05 | 2 | 1.75 | 0.88 |
| C12H17O4N2 | 254.1267 | 2.67 | 5 | 1.50 | 0.33 |
| C10H9O6S1 | 258.0198 | 1.79 | 6 | 1.00 | 0.60 |
| C12H4O6N1 | 259.0117 | 3.87 | 11 | 0.42 | 0.50 |
| C9H7O7S1 | 259.9991 | 1.71 | 6 | 0.89 | 0.78 |
| C12H7O5N2 | 260.0433 | 8.31 | 10 | 0.67 | 0.42 |
| C8H8O7N1S1 | 263.0100 | 3.61 | 5 | 1.13 | 0.88 |
| C12H9O5S1 | 266.0249 | 3.34 | 8 | 0.83 | 0.42 |
| C16H15O4 | 272.1049 | 8.15 | 9 | 1.00 | 0.25 |
| C13H23O4N2 | 272.1736 | 2.33 | 3 | 1.85 | 0.31 |
| C14H9O4S1 | 274.0300 | 7.09 | 10 | 0.71 | 0.29 |
| C7H4O5N3S2 | 274.9671 | 0.28 | 7 | 0.71 | 0.71 |
| C9H8O7N1S1 | 275.0100 | 4.21 | 6 | 1.00 | 0.78 |
| C12H23O5S1 | 280.1344 | 7.14 | 1 | 2.00 | 0.42 |
| C8H14O8N1S1 | 285.0518 | 2.99 | 2 | 1.88 | 1.00 |
| C15H9O6 | 286.0477 | 3.51 | 11 | 0.67 | 0.40 |
| C8H16O8N1S1 | 287.0675 | 3.07 | 1 | 2.13 | 1.00 |
| C15H11O4S1 | 288.0456 | 7.42 | 10 | 0.80 | 0.27 |
| C18H9O4 | 290.0579 | 7.71 | 14 | 0.56 | 0.22 |
| C13H25O5S1 | 294.1501 | 7.59 | 1 | 2.00 | 0.38 |
| C10H16O7N1S1 | 295.0726 | 4.70 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 6.32 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 6.62 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 6.84 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 7.01 | 3 | 1.70 | 0.70 |
| C9H14O8N1S1 | 297.0518 | 3.27 | 3 | 1.67 | 0.89 |

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|---|---|---|---|---|---|
| C9H16O8N1S1 | 299.0675 | 3.37 | 2 | 1.89 | 0.89 |
| C15H10O4N1S1 | 301.0409 | 3.04 | 11 | 0.73 | 0.27 |
| C9H18O8N1S1 | 301.0831 | 3.22 | 1 | 2.11 | 0.89 |
| C13H5O4N6 | 310.0451 | 5.06 | 14 | 0.46 | 0.31 |
| C10H16O8N1S1 | 311.0675 | 3.50 | 3 | 1.70 | 0.80 |
| C10H18O8N1S1 | 313.0831 | 2.81 | 2 | 1.90 | 0.80 |
| C10H18O8N1S1 | 313.0831 | 2.94 | 2 | 1.90 | 0.80 |
| C10H18O8N1S1 | 313.0831 | 3.09 | 2 | 1.90 | 0.80 |
| C10H18O8N1S1 | 313.0831 | 3.40 | 2 | 1.90 | 0.80 |
| C10H18O8N1S1 | 313.0831 | 3.53 | 2 | 1.90 | 0.80 |
| C17H13O6 | 314.0790 | 7.96 | 11 | 0.82 | 0.35 |
| C9H16O9N1S1 | 315.0624 | 2.54 | 2 | 1.89 | 1.00 |
| C18H12O6N1 | 339.0743 | 7.85 | 13 | 0.72 | 0.33 |
| C7H7O8S4 | 347.9102 | 0.28 | 4 | 1.14 | 1.14 |
| C14H5O6N6 | 354.0349 | 2.59 | 15 | 0.43 | 0.43 |
| C15H24O7N1S1 | 363.1352 | 8.04 | 4 | 1.67 | 0.47 |
| C8H2O8N1S4 | 368.8741 | 0.33 | 8 | 0.38 | 1.00 |
| C10H17O11N2S1 | 374.0631 | 3.18 | 3 | 1.80 | 1.10 |
| C10H17O11N2S1 | 374.0631 | 3.33 | 3 | 1.80 | 1.10 |
| C10H17O11N2S1 | 374.0631 | 4.37 | 3 | 1.80 | 1.10 |
| C20H17O8 | 386.1002 | 8.21 | 12 | 0.90 | 0.40 |
| C20H17O9 | 402.0951 | 7.43 | 12 | 0.90 | 0.45 |
| C10H27O11N6 | 408.1816 | 8.05 | 0 | 2.80 | 1.10 |
| C10H16O13N3S1 | 419.0482 | 7.61 | 4 | 1.70 | 1.30 |

Table S3.2.4 Molecular formulas of organic compounds detected in SH in ESI+ mode.

| Formula [M+H]/[M+Na] | Neutral mass (Da) | RT (min) | DBE | H/C | O/C |
|---|---|---|---|---|---|
| C6H9O3N2 | 156.0535 | 0.32 | 4 | 1.33 | 0.50 |
| C4H12O4N2Na1S3 | 247.9959 | 0.28 | 0 | 3.00 | 1.00 |
| C6H4O5N1S4 | 296.8894 | 0.28 | 6 | 0.50 | 0.83 |
| C12H17O2N2 | 220.1212 | 0.34 | 6 | 1.33 | 0.17 |
| C6H11N2 | 110.0844 | 0.89 | 3 | 1.67 | 0.00 |
| C7H11O2N2 | 154.0742 | 0.43 | 4 | 1.43 | 0.29 |
| C7H16N1 | 113.1204 | 1.00 | 1 | 2.14 | 0.00 |
| C6H15N2 | 114.1157 | 1.24 | 1 | 2.33 | 0.00 |
| C6H15N2 | 114.1157 | 1.50 | 1 | 2.33 | 0.00 |
| C6H9O2N2 | 140.0586 | 0.38 | 4 | 1.33 | 0.33 |
| C7H7N2 | 118.0531 | 0.39 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 0.43 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 0.47 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 0.66 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 0.77 | 6 | 0.86 | 0.00 |
| C5H14O2N1 | 119.0946 | 0.32 | 0 | 2.60 | 0.40 |
| C7H11O1N2 | 138.0793 | 0.39 | 4 | 1.43 | 0.14 |
| C4H12O1N1S1 | 121.0561 | 0.33 | 0 | 2.75 | 0.25 |
| C10H15N2 | 162.1157 | 0.39 | 5 | 1.40 | 0.00 |
| C7H7O2 | 122.0368 | 2.77 | 5 | 0.86 | 0.29 |
| C7H11N2 | 122.0844 | 0.43 | 4 | 1.43 | 0.00 |

| | | | | | |
|---|---|---|---|---|---|
| C7H11N2 | 122.0844 | 0.49 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.97 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.02 | 4 | 1.43 | 0.00 |
| C7H10O1N1 | 123.0684 | 0.50 | 4 | 1.29 | 0.14 |
| C7H10O1N1 | 123.0684 | 2.59 | 4 | 1.29 | 0.14 |
| C3H9O5 | 124.0372 | 0.28 | 0 | 2.67 | 1.67 |
| C7H13N2 | 124.1000 | 0.39 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 0.70 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 0.89 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.30 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.29 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.89 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.96 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.07 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.32 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.42 | 3 | 1.71 | 0.00 |
| C6H8O2N1 | 125.0477 | 0.39 | 4 | 1.17 | 0.33 |
| C6H8O2N1 | 125.0477 | 0.44 | 4 | 1.17 | 0.33 |
| C6H8O2N1 | 125.0477 | 1.22 | 4 | 1.17 | 0.33 |
| C5H7O2N2 | 126.0429 | 0.42 | 4 | 1.20 | 0.40 |
| C5H7O2N2 | 126.0429 | 0.74 | 4 | 1.20 | 0.40 |
| C7H15N2 | 126.1157 | 0.75 | 2 | 2.00 | 0.00 |
| C7H15N2 | 126.1157 | 0.90 | 2 | 2.00 | 0.00 |
| C7H15N2 | 126.1157 | 1.77 | 2 | 2.00 | 0.00 |
| C8H18N1 | 127.1361 | 1.14 | 1 | 2.13 | 0.00 |
| C6H13O1N2 | 128.0950 | 0.33 | 2 | 2.00 | 0.17 |
| C7H16O1N1 | 129.1154 | 0.38 | 1 | 2.14 | 0.14 |
| C8H7N2 | 130.0531 | 1.00 | 7 | 0.75 | 0.00 |
| C8H5O2 | 132.0211 | 2.66 | 7 | 0.50 | 0.25 |
| C8H14O6N1 | 219.0743 | 0.38 | 3 | 1.63 | 0.75 |
| C8H9N2 | 132.0687 | 0.77 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 0.83 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.05 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.31 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 2.14 | 6 | 1.00 | 0.00 |
| C8H8O1N1 | 133.0528 | 2.79 | 6 | 0.88 | 0.13 |
| C7H8N3 | 133.0640 | 1.58 | 6 | 1.00 | 0.00 |
| C9H12N1 | 133.0891 | 1.24 | 5 | 1.22 | 0.00 |
| C7H7O1N2 | 134.0480 | 0.58 | 6 | 0.86 | 0.14 |
| C7H7O1N2 | 134.0480 | 2.71 | 6 | 0.86 | 0.14 |
| C8H11N2 | 134.0844 | 0.36 | 5 | 1.25 | 0.00 |
| C8H11N2 | 134.0844 | 0.65 | 5 | 1.25 | 0.00 |
| C8H11N2 | 134.0844 | 1.18 | 5 | 1.25 | 0.00 |
| C6H6O1N3 | 135.0433 | 1.02 | 6 | 0.83 | 0.17 |
| C9H14N1 | 135.1048 | 1.15 | 4 | 1.44 | 0.00 |
| C5H5O1N4 | 136.0385 | 0.39 | 6 | 0.80 | 0.20 |
| C8H9O2 | 136.0524 | 3.01 | 5 | 1.00 | 0.25 |
| C7H9O1N2 | 136.0637 | 0.41 | 5 | 1.14 | 0.14 |
| C8H13N2 | 136.1000 | 0.71 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 0.83 | 4 | 1.50 | 0.00 |

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|---|---|---|---|---|---|
| C8H13N2 | 136.1000 | 1.05 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.36 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.35 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.48 | 4 | 1.50 | 0.00 |
| C7H8O2N1 | 137.0477 | 0.38 | 5 | 1.00 | 0.29 |
| C8H12O1N1 | 137.0841 | 0.50 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.55 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.91 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.10 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.15 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.22 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 2.31 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 3.10 | 4 | 1.38 | 0.13 |
| C8H15O2N2 | 170.1055 | 0.38 | 3 | 1.75 | 0.25 |
| C7H8O1N1 | 121.0528 | 0.39 | 5 | 1.00 | 0.14 |
| C7H11O1N2 | 138.0793 | 0.44 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 0.68 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 0.73 | 4 | 1.43 | 0.14 |
| C8H15N2 | 138.1157 | 0.93 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.13 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.32 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.50 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.77 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.11 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.29 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.51 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.61 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.77 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 3.03 | 3 | 1.75 | 0.00 |
| C6H6O3N1 | 139.0269 | 0.58 | 5 | 0.83 | 0.50 |
| C7H10O2N1 | 139.0633 | 0.66 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 0.87 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 2.61 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 2.79 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 1.00 | 4 | 1.29 | 0.29 |
| C5H10N5 | 139.0858 | 0.38 | 4 | 1.80 | 0.00 |
| C8H14O1N1 | 139.0997 | 0.38 | 3 | 1.63 | 0.13 |
| C5H5O3N2 | 140.0222 | 2.41 | 5 | 0.80 | 0.60 |
| C8H17N2 | 140.1313 | 2.30 | 2 | 2.00 | 0.00 |
| C8H17N2 | 140.1313 | 2.44 | 2 | 2.00 | 0.00 |
| C6H7O4 | 142.0266 | 0.53 | 4 | 1.00 | 0.67 |
| C5H7O3N2 | 142.0378 | 0.34 | 4 | 1.20 | 0.60 |
| C6H10O3N1 | 143.0582 | 0.89 | 3 | 1.50 | 0.50 |
| C10H10N1 | 143.0735 | 0.70 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.47 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.79 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.26 | 7 | 0.90 | 0.00 |
| C7H14O2N1 | 143.0946 | 0.34 | 2 | 1.86 | 0.29 |
| C9H22N1 | 143.1674 | 6.73 | 0 | 2.33 | 0.00 |
| C9H9N2 | 144.0687 | 1.26 | 7 | 0.89 | 0.00 |

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| C9H9N2 | 144.0687 | 2.35 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 2.40 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 2.46 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 2.46 | 7 | 0.89 | 0.00 |
| C9H8O1N1 | 145.0528 | 2.33 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 2.31 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 3.14 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 3.24 | 7 | 0.78 | 0.11 |
| C9H12O1N3 | 177.0902 | 0.65 | 6 | 1.22 | 0.11 |
| C6H12O3N1 | 145.0739 | 0.33 | 2 | 1.83 | 0.50 |
| C6H12O3N1 | 145.0739 | 0.63 | 2 | 1.83 | 0.50 |
| C7H16O2N1 | 145.1103 | 0.37 | 1 | 2.14 | 0.29 |
| C9H7O2 | 146.0368 | 3.13 | 7 | 0.67 | 0.22 |
| C8H7O1N2 | 146.0480 | 2.63 | 7 | 0.75 | 0.13 |
| C9H11N2 | 146.0844 | 0.52 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 0.93 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.05 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.15 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.28 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.41 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.54 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.64 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.79 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.40 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.52 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.63 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.85 | 6 | 1.11 | 0.00 |
| C9H8N1 | 129.0578 | 0.44 | 7 | 0.78 | 0.00 |
| C8H10N3 | 147.0796 | 0.39 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 0.46 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 0.68 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 2.25 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 2.79 | 6 | 1.13 | 0.00 |
| C10H14N1 | 147.1048 | 2.43 | 5 | 1.30 | 0.00 |
| C10H14N1 | 147.1048 | 2.53 | 5 | 1.30 | 0.00 |
| C4H9O4N2 | 148.0484 | 0.33 | 2 | 2.00 | 1.00 |
| C9H9O2 | 148.0524 | 2.97 | 6 | 0.89 | 0.22 |
| C8H9O1N2 | 148.0637 | 0.77 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 3.23 | 6 | 1.00 | 0.13 |
| C9H13N2 | 148.1000 | 0.38 | 5 | 1.33 | 0.00 |
| C9H13N2 | 148.1000 | 1.25 | 5 | 1.33 | 0.00 |
| C9H13N2 | 148.1000 | 1.53 | 5 | 1.33 | 0.00 |
| C9H13N2 | 148.1000 | 2.36 | 5 | 1.33 | 0.00 |
| C9H13N2 | 148.1000 | 2.56 | 5 | 1.33 | 0.00 |
| C9H13N2 | 148.1000 | 2.69 | 5 | 1.33 | 0.00 |
| C8H8O2N1 | 149.0477 | 2.14 | 6 | 0.88 | 0.25 |
| C7H8O1N3 | 149.0589 | 0.38 | 6 | 1.00 | 0.14 |
| C7H8O1N3 | 149.0589 | 2.40 | 6 | 1.00 | 0.14 |
| C5H12O4N1 | 149.0688 | 0.32 | 1 | 2.20 | 0.80 |
| C9H12O1N1 | 149.0841 | 3.21 | 5 | 1.22 | 0.11 |

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|---|---|---|---|---|---|
| C6H16O3N1 | 149.1052 | 0.32 | 0 | 2.50 | 0.50 |
| C10H16N1 | 149.1204 | 2.67 | 4 | 1.50 | 0.00 |
| C6H7O1N4 | 150.0542 | 0.55 | 6 | 1.00 | 0.17 |
| C9H15N2 | 150.1157 | 1.22 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.14 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.42 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.57 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.63 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.78 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 1.60 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 3.02 | 4 | 1.56 | 0.00 |
| C8H10O2N1 | 151.0633 | 0.51 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 1.74 | 5 | 1.13 | 0.25 |
| C9H14O1N1 | 151.0997 | 0.54 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 0.70 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 1.05 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 1.87 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.09 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.27 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.43 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.56 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.65 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.76 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 3.77 | 4 | 1.44 | 0.11 |
| C10H18N1 | 151.1361 | 2.84 | 3 | 1.70 | 0.00 |
| C8H9O3 | 152.0473 | 2.66 | 5 | 1.00 | 0.38 |
| C7H9O2N2 | 152.0586 | 0.45 | 5 | 1.14 | 0.29 |
| C7H9O2N2 | 152.0586 | 0.73 | 5 | 1.14 | 0.29 |
| C9H17N2 | 152.1313 | 2.32 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.38 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.46 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.55 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.64 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.69 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.80 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.86 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.94 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 3.08 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 3.19 | 3 | 1.78 | 0.00 |
| C7H8O3N1 | 153.0426 | 0.56 | 5 | 1.00 | 0.43 |
| C7H8O3N1 | 153.0426 | 2.59 | 5 | 1.00 | 0.43 |
| C6H8O2N3 | 153.0538 | 0.39 | 5 | 1.17 | 0.33 |
| C8H12O2N1 | 153.0790 | 1.31 | 4 | 1.38 | 0.25 |
| C7H11O2N2 | 154.0742 | 0.49 | 4 | 1.43 | 0.29 |
| C7H10O3N1 | 155.0582 | 1.37 | 4 | 1.29 | 0.43 |
| C10H9N2 | 156.0687 | 1.63 | 8 | 0.80 | 0.00 |
| C7H13O2N2 | 156.0899 | 2.90 | 3 | 1.71 | 0.29 |
| C6H6O3N1 | 139.0269 | 0.39 | 5 | 0.83 | 0.50 |
| C11H12N1 | 157.0891 | 2.72 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 1.82 | 7 | 1.00 | 0.00 |

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|---|---|---|---|---|---|
| C10H11N2 | 158.0844 | 2.37 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.46 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.71 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.83 | 7 | 1.00 | 0.00 |
| C6H10O4N1 | 159.0532 | 0.37 | 3 | 1.50 | 0.67 |
| C7H14O5N1 | 191.0794 | 0.38 | 2 | 1.86 | 0.71 |
| C7H14O3N1 | 159.0895 | 0.33 | 2 | 1.86 | 0.43 |
| C9H9O1N2 | 160.0637 | 1.00 | 7 | 0.89 | 0.11 |
| C10H13N2 | 160.1000 | 0.39 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.41 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.49 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.60 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.69 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.76 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.85 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.99 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 3.10 | 6 | 1.20 | 0.00 |
| C8H17O3 | 160.1099 | 3.16 | 1 | 2.00 | 0.38 |
| C8H13O3N2 | 184.0848 | 0.35 | 4 | 1.50 | 0.38 |
| C10H12O1N1 | 161.0841 | 0.58 | 6 | 1.10 | 0.10 |
| C10H12O1N1 | 161.0841 | 4.02 | 6 | 1.10 | 0.10 |
| C9H12N3 | 161.0953 | 0.85 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 0.95 | 6 | 1.22 | 0.00 |
| C9H12N3 | 161.0953 | 1.21 | 6 | 1.22 | 0.00 |
| C11H16N1 | 161.1204 | 2.86 | 5 | 1.36 | 0.00 |
| C8H20O2N1 | 161.1416 | 0.54 | 0 | 2.38 | 0.25 |
| C9H7O3 | 162.0317 | 2.61 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 3.04 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 3.18 | 7 | 0.67 | 0.33 |
| C6H10O5Na1 | 162.0528 | 0.35 | 2 | 1.67 | 0.83 |
| C10H11O2 | 162.0681 | 3.63 | 6 | 1.00 | 0.20 |
| C10H15N2 | 162.1157 | 0.49 | 5 | 1.40 | 0.00 |
| C9H10O2N1 | 163.0633 | 0.57 | 6 | 1.00 | 0.22 |
| C8H10O1N3 | 163.0746 | 0.49 | 6 | 1.13 | 0.13 |
| C6H14O4N1 | 163.0845 | 0.33 | 1 | 2.17 | 0.67 |
| C10H14O1N1 | 163.0997 | 0.61 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 0.79 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 0.93 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 2.76 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 3.45 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 4.09 | 5 | 1.30 | 0.10 |
| C8H5O4 | 164.0110 | 1.08 | 7 | 0.50 | 0.50 |
| C8H5O4 | 164.0110 | 2.74 | 7 | 0.50 | 0.50 |
| C8H9O2N2 | 164.0586 | 0.34 | 6 | 1.00 | 0.25 |
| C7H9O1N4 | 164.0698 | 0.82 | 6 | 1.14 | 0.14 |
| C7H9O1N4 | 164.0698 | 0.88 | 6 | 1.14 | 0.14 |
| C7H9O1N4 | 164.0698 | 0.90 | 6 | 1.14 | 0.14 |
| C7H9O1N4 | 164.0698 | 0.92 | 6 | 1.14 | 0.14 |
| C7H9O1N4 | 164.0698 | 0.93 | 6 | 1.14 | 0.14 |
| C7H9O1N4 | 164.0698 | 0.93 | 6 | 1.14 | 0.14 |

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|---|---|---|---|---|---|
| C6H13O5 | 164.0685 | 3.08 | 1 | 2.00 | 0.83 |
| C9H16O1N3 | 181.1215 | 0.38 | 4 | 1.67 | 0.11 |
| C9H11N2 | 146.0844 | 0.44 | 6 | 1.11 | 0.00 |
| C9H13O1N2 | 164.0950 | 0.68 | 5 | 1.33 | 0.11 |
| C5H11O2N6 | 186.0865 | 1.45 | 4 | 2.00 | 0.40 |
| C10H17N2 | 164.1313 | 2.41 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.55 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.65 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.86 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 3.03 | 4 | 1.60 | 0.00 |
| C8H8O3N1 | 165.0426 | 1.08 | 6 | 0.88 | 0.38 |
| C8H8O3N1 | 165.0426 | 3.21 | 6 | 0.88 | 0.38 |
| C9H12O2N1 | 165.0790 | 0.47 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 0.66 | 5 | 1.22 | 0.22 |
| C10H16O1N1 | 165.1154 | 0.69 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 0.80 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 0.86 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 1.00 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 2.76 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 3.12 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 3.17 | 4 | 1.50 | 0.10 |
| C10H19N2 | 166.1470 | 2.63 | 3 | 1.80 | 0.00 |
| C10H19N2 | 166.1470 | 2.84 | 3 | 1.80 | 0.00 |
| C10H19N2 | 166.1470 | 2.97 | 3 | 1.80 | 0.00 |
| C10H19N2 | 166.1470 | 3.15 | 3 | 1.80 | 0.00 |
| C8H10O3N1 | 167.0582 | 0.36 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 0.43 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 0.46 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 0.48 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 0.58 | 5 | 1.13 | 0.38 |
| C7H10O2N3 | 167.0695 | 0.39 | 5 | 1.29 | 0.29 |
| C10H18O1N1 | 167.1310 | 2.80 | 3 | 1.70 | 0.10 |
| C11H22N1 | 167.1674 | 2.47 | 2 | 1.91 | 0.00 |
| C9H6O2Na1 | 146.0368 | 0.33 | 7 | 0.67 | 0.22 |
| C11H5O2 | 168.0211 | 3.87 | 10 | 0.36 | 0.18 |
| C5H5O3N4 | 168.0283 | 0.38 | 6 | 0.80 | 0.60 |
| C4H9O7 | 168.0270 | 2.66 | 1 | 2.00 | 1.75 |
| C11H9N2 | 168.0687 | 2.56 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.70 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.85 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.98 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 3.08 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 3.97 | 9 | 0.73 | 0.00 |
| C8H13O2N2 | 168.0899 | 0.38 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.72 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.80 | 4 | 1.50 | 0.25 |
| C10H21N2 | 168.1626 | 2.74 | 2 | 2.00 | 0.00 |
| C10H21N2 | 168.1626 | 2.81 | 2 | 2.00 | 0.00 |
| C10H21N2 | 168.1626 | 2.84 | 2 | 2.00 | 0.00 |
| C10H21N2 | 168.1626 | 2.94 | 2 | 2.00 | 0.00 |

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| C8H4N5 | 169.0388 | 0.30 | 10 | 0.38 | 0.00 |
| C6H8O3N3 | 169.0487 | 0.34 | 5 | 1.17 | 0.50 |
| C11H8O1N1 | 169.0528 | 2.87 | 9 | 0.64 | 0.09 |
| C11H8O1N1 | 169.0528 | 2.91 | 9 | 0.64 | 0.09 |
| C8H15O3N2 | 186.1004 | 0.38 | 3 | 1.75 | 0.38 |
| C8H11O4 | 170.0579 | 0.83 | 4 | 1.25 | 0.50 |
| C8H11O4 | 170.0579 | 0.92 | 4 | 1.25 | 0.50 |
| C7H11O3N2 | 170.0691 | 0.34 | 4 | 1.43 | 0.43 |
| C7H11O3N2 | 170.0691 | 0.55 | 4 | 1.43 | 0.43 |
| C11H11N2 | 170.0844 | 3.06 | 8 | 0.91 | 0.00 |
| C8H15O2N2 | 170.1055 | 0.40 | 3 | 1.75 | 0.25 |
| C6H10O3N3 | 171.0644 | 0.33 | 4 | 1.50 | 0.50 |
| C11H10O1N1 | 171.0684 | 1.77 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.57 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.77 | 8 | 0.82 | 0.09 |
| C13H11N2 | 194.0844 | 3.02 | 10 | 0.77 | 0.00 |
| C12H14N1 | 171.1048 | 2.84 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.22 | 7 | 1.08 | 0.00 |
| C12H14N1 | 171.1048 | 3.25 | 7 | 1.08 | 0.00 |
| C10H22O1N1 | 171.1623 | 3.03 | 1 | 2.10 | 0.10 |
| C11H13N2 | 172.1000 | 2.51 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.64 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.74 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.86 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 3.01 | 7 | 1.09 | 0.00 |
| C4H4O3N2Na1S2 | 191.9663 | 0.28 | 4 | 1.00 | 0.75 |
| C11H12O1N1 | 173.0841 | 2.51 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.62 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.72 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.83 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 3.04 | 7 | 1.00 | 0.09 |
| C9H20O2N1 | 173.1416 | 2.75 | 1 | 2.11 | 0.22 |
| C10H24O1N1 | 173.1780 | 2.74 | 0 | 2.30 | 0.10 |
| C7H11O5 | 174.0528 | 0.54 | 3 | 1.43 | 0.71 |
| C6H11O4N2 | 174.0641 | 0.33 | 3 | 1.67 | 0.67 |
| C10H11O1N2 | 174.0793 | 2.86 | 7 | 1.00 | 0.10 |
| C11H15N2 | 174.1157 | 0.50 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 2.88 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 3.03 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 3.15 | 6 | 1.27 | 0.00 |
| C5H6O4N1S1 | 174.9939 | 0.36 | 4 | 1.00 | 0.80 |
| C6H10O5N1 | 175.0481 | 0.38 | 3 | 1.50 | 0.83 |
| C10H10O2N1 | 175.0633 | 2.55 | 7 | 0.90 | 0.20 |
| C10H10O2N1 | 175.0633 | 2.81 | 7 | 0.90 | 0.20 |
| C7H14O4N1 | 175.0845 | 0.35 | 2 | 1.86 | 0.57 |
| C7H14O4N1 | 175.0845 | 1.32 | 2 | 1.86 | 0.57 |
| C7H18O2N3 | 175.1321 | 0.34 | 1 | 2.43 | 0.29 |
| C12H18N1 | 175.1361 | 2.70 | 5 | 1.42 | 0.00 |
| C5H9O5N2 | 176.0433 | 0.33 | 3 | 1.60 | 1.00 |
| C10H9O3 | 176.0473 | 2.99 | 7 | 0.80 | 0.30 |

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| C10H9O3 | 176.0473 | 3.11 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.20 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.30 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.67 | 7 | 0.80 | 0.30 |
| C6H13O4N2 | 176.0797 | 0.33 | 2 | 2.00 | 0.67 |
| C8H17O4 | 176.1049 | 1.47 | 1 | 2.00 | 0.50 |
| C11H17N2 | 176.1313 | 2.84 | 5 | 1.45 | 0.00 |
| C11H17N2 | 176.1313 | 2.93 | 5 | 1.45 | 0.00 |
| C9H8O3N1 | 177.0426 | 2.34 | 7 | 0.78 | 0.33 |
| C9H8O3N1 | 177.0426 | 2.64 | 7 | 0.78 | 0.33 |
| C9H7O4 | 178.0266 | 2.23 | 7 | 0.67 | 0.44 |
| C10H11O3 | 178.0630 | 3.05 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.75 | 6 | 1.00 | 0.30 |
| C10H11O3 | 178.0630 | 3.82 | 6 | 1.00 | 0.30 |
| C11H19N2 | 178.1470 | 2.84 | 4 | 1.64 | 0.00 |
| C11H19N2 | 178.1470 | 2.96 | 4 | 1.64 | 0.00 |
| C11H19N2 | 178.1470 | 3.07 | 4 | 1.64 | 0.00 |
| C11H19N2 | 178.1470 | 3.15 | 4 | 1.64 | 0.00 |
| C11H19N2 | 178.1470 | 3.27 | 4 | 1.64 | 0.00 |
| C13H10N1 | 179.0735 | 2.90 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.15 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.39 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 4.02 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 3.48 | 10 | 0.69 | 0.00 |
| C10H14O2N1 | 179.0946 | 0.56 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.65 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.90 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 2.64 | 5 | 1.30 | 0.20 |
| C9H14O1N3 | 179.1059 | 0.39 | 5 | 1.44 | 0.11 |
| C11H18O1N1 | 179.1310 | 3.03 | 4 | 1.55 | 0.09 |
| C9H9O4 | 180.0423 | 3.16 | 6 | 0.89 | 0.44 |
| C10H13O3 | 180.0786 | 2.82 | 5 | 1.20 | 0.30 |
| C10H13O3 | 180.0786 | 3.00 | 5 | 1.20 | 0.30 |
| C9H13O2N2 | 180.0899 | 2.24 | 5 | 1.33 | 0.22 |
| C10H17O1N2 | 180.1263 | 2.76 | 4 | 1.60 | 0.10 |
| C11H21N2 | 180.1626 | 3.11 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 3.14 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 3.30 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 3.36 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 3.40 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 4.46 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 5.86 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 5.92 | 3 | 1.82 | 0.00 |
| C8H8O4N1 | 181.0375 | 0.38 | 6 | 0.88 | 0.50 |
| C5H12O6N1 | 181.0586 | 0.37 | 1 | 2.20 | 1.20 |
| C9H12O3N1 | 181.0739 | 0.39 | 5 | 1.22 | 0.33 |
| C14H16O1N1 | 213.1154 | 3.04 | 8 | 1.07 | 0.07 |
| C10H16O2N1 | 181.1103 | 0.49 | 4 | 1.50 | 0.20 |
| C12H24N1 | 181.1830 | 3.28 | 2 | 1.92 | 0.00 |
| C12H7O2 | 182.0368 | 4.45 | 10 | 0.50 | 0.17 |

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|---|---|---|---|---|---|
| C12H11N2 | 182.0844 | 2.72 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 2.85 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 2.91 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.06 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.15 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.23 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 3.38 | 9 | 0.83 | 0.00 |
| C11H23N2 | 182.1783 | 3.13 | 2 | 2.00 | 0.00 |
| C11H23N2 | 182.1783 | 3.24 | 2 | 2.00 | 0.00 |
| C11H23N2 | 182.1783 | 3.32 | 2 | 2.00 | 0.00 |
| C11H23N2 | 182.1783 | 3.37 | 2 | 2.00 | 0.00 |
| C5H14O4N1S1 | 183.0565 | 0.33 | 0 | 2.60 | 0.80 |
| C12H10O1N1 | 183.0684 | 3.15 | 9 | 0.75 | 0.08 |
| C11H10N3 | 183.0796 | 2.66 | 9 | 0.82 | 0.00 |
| C9H12O2N1 | 165.0790 | 0.38 | 5 | 1.22 | 0.22 |
| C13H14N1 | 183.1048 | 3.13 | 8 | 1.00 | 0.00 |
| C12H9O2 | 184.0524 | 3.48 | 9 | 0.67 | 0.17 |
| C8H13O3N2 | 184.0848 | 0.43 | 4 | 1.50 | 0.38 |
| C12H13N2 | 184.1000 | 3.02 | 8 | 1.00 | 0.00 |
| C10H17O3 | 184.1099 | 3.38 | 3 | 1.60 | 0.30 |
| C10H17O3 | 184.1099 | 3.89 | 3 | 1.60 | 0.30 |
| C10H17O3 | 184.1099 | 3.48 | 3 | 1.60 | 0.30 |
| C9H17O2N2 | 184.1212 | 0.40 | 3 | 1.78 | 0.22 |
| C8H12O4N1 | 185.0688 | 0.60 | 4 | 1.38 | 0.50 |
| C12H12O1N1 | 185.0841 | 2.56 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.69 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.86 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 3.02 | 8 | 0.92 | 0.08 |
| C13H16N1 | 185.1204 | 3.29 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.30 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.33 | 7 | 1.15 | 0.00 |
| C12H28N1 | 185.2143 | 4.12 | 0 | 2.25 | 0.00 |
| C11H11O1N2 | 186.0793 | 2.50 | 8 | 0.91 | 0.09 |
| C7H16O4Na1 | 164.1049 | 1.41 | 0 | 2.29 | 0.57 |
| C9H15O4 | 186.0892 | 2.83 | 3 | 1.56 | 0.44 |
| C9H15O4 | 186.0892 | 2.89 | 3 | 1.56 | 0.44 |
| C9H15O4 | 186.0892 | 2.97 | 3 | 1.56 | 0.44 |
| C8H15O3N2 | 186.1004 | 0.34 | 3 | 1.75 | 0.38 |
| C12H15N2 | 186.1157 | 2.89 | 7 | 1.17 | 0.00 |
| C12H15N2 | 186.1157 | 2.97 | 7 | 1.17 | 0.00 |
| C12H15N2 | 186.1157 | 3.16 | 7 | 1.17 | 0.00 |
| C8H19O1N4 | 186.1481 | 1.63 | 2 | 2.25 | 0.13 |
| C11H10O2N1 | 187.0633 | 2.55 | 8 | 0.82 | 0.18 |
| C9H10N5 | 187.0858 | 2.57 | 8 | 1.00 | 0.00 |
| C12H14O1N1 | 187.0997 | 2.80 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 2.92 | 7 | 1.08 | 0.08 |
| C12H14O1N1 | 187.0997 | 3.06 | 7 | 1.08 | 0.08 |
| C10H9O2N2 | 188.0586 | 0.63 | 8 | 0.80 | 0.20 |
| C11H13O1N2 | 188.0950 | 0.89 | 7 | 1.09 | 0.09 |
| C11H13O1N2 | 188.0950 | 2.64 | 7 | 1.09 | 0.09 |

| | | | | | |
|---|---|---|---|---|---|
| C12H17N2 | 188.1313 | 2.98 | 6 | 1.33 | 0.00 |
| C12H17N2 | 188.1313 | 3.16 | 6 | 1.33 | 0.00 |
| C12H17N2 | 188.1313 | 3.32 | 6 | 1.33 | 0.00 |
| C11H12O2N1 | 189.0790 | 3.08 | 7 | 1.00 | 0.18 |
| C8H16O4N1 | 189.1001 | 0.40 | 2 | 1.88 | 0.50 |
| C11H16N3 | 189.1266 | 2.47 | 6 | 1.36 | 0.00 |
| C11H16N3 | 189.1266 | 2.77 | 6 | 1.36 | 0.00 |
| C11H15O1N2 | 190.1106 | 0.64 | 6 | 1.27 | 0.09 |
| C11H15O1N2 | 190.1106 | 0.96 | 6 | 1.27 | 0.09 |
| C11H15O1N2 | 190.1106 | 2.79 | 6 | 1.27 | 0.09 |
| C11H15O1N2 | 190.1106 | 3.02 | 6 | 1.27 | 0.09 |
| C9H10O2N3 | 191.0695 | 2.43 | 7 | 1.00 | 0.22 |
| C7H14O5N1 | 191.0794 | 0.94 | 2 | 1.86 | 0.71 |
| C6H8O7Na1 | 192.0270 | 0.38 | 3 | 1.33 | 1.17 |
| C10H9O4 | 192.0423 | 3.13 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.18 | 7 | 0.80 | 0.40 |
| C10H13O2N2 | 192.0899 | 0.39 | 6 | 1.20 | 0.20 |
| C12H21N2 | 192.1626 | 4.04 | 4 | 1.67 | 0.00 |
| C11H16O4N1 | 225.1001 | 0.38 | 5 | 1.36 | 0.36 |
| C10H12O3N1 | 193.0739 | 2.83 | 6 | 1.10 | 0.30 |
| C14H12N1 | 193.0891 | 3.36 | 10 | 0.79 | 0.00 |
| C14H12N1 | 193.0891 | 3.45 | 10 | 0.79 | 0.00 |
| C14H11O1 | 194.0732 | 7.70 | 10 | 0.71 | 0.07 |
| C11H19O1N2 | 194.1419 | 2.45 | 4 | 1.64 | 0.09 |
| C12H23N2 | 194.1783 | 3.94 | 3 | 1.83 | 0.00 |
| C12H23N2 | 194.1783 | 4.09 | 3 | 1.83 | 0.00 |
| C12H23N2 | 194.1783 | 6.83 | 3 | 1.83 | 0.00 |
| C13H10O1N1 | 195.0684 | 6.93 | 10 | 0.69 | 0.08 |
| C10H14O3N1 | 195.0895 | 0.50 | 5 | 1.30 | 0.30 |
| C10H14O3N1 | 195.0895 | 0.85 | 5 | 1.30 | 0.30 |
| C10H14O3N1 | 195.0895 | 3.32 | 5 | 1.30 | 0.30 |
| C12H22O1N1 | 195.1623 | 2.63 | 3 | 1.75 | 0.08 |
| C12H22O1N1 | 195.1623 | 2.76 | 3 | 1.75 | 0.08 |
| C13H9O2 | 196.0524 | 4.92 | 10 | 0.62 | 0.15 |
| C13H13N2 | 196.1000 | 3.10 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.21 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.44 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.57 | 9 | 0.92 | 0.00 |
| C10H17O2N2 | 196.1212 | 2.23 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.56 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.65 | 4 | 1.60 | 0.20 |
| C13H12O1N1 | 197.0841 | 3.83 | 9 | 0.85 | 0.08 |
| C12H12N3 | 197.0953 | 2.90 | 9 | 0.92 | 0.00 |
| C10H16O3N1 | 197.1052 | 0.39 | 4 | 1.50 | 0.30 |
| C14H16N1 | 197.1204 | 3.27 | 8 | 1.07 | 0.00 |
| C12H7O3 | 198.0317 | 3.87 | 10 | 0.50 | 0.25 |
| C9H15O3N2 | 198.1004 | 0.77 | 4 | 1.56 | 0.33 |
| C9H15O3N2 | 198.1004 | 2.56 | 4 | 1.56 | 0.33 |
| C13H14O1N1 | 199.0997 | 2.84 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 2.97 | 8 | 1.00 | 0.08 |

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|---|---|---|---|---|---|
| C10H18O3N1 | 199.1208 | 0.66 | 3 | 1.70 | 0.30 |
| C12H9O3 | 200.0473 | 4.41 | 9 | 0.67 | 0.25 |
| C8H13O4N2 | 200.0797 | 0.34 | 4 | 1.50 | 0.50 |
| C12H13O1N2 | 200.0950 | 2.79 | 8 | 1.00 | 0.08 |
| C13H17N2 | 200.1313 | 3.17 | 7 | 1.23 | 0.00 |
| C12H12O2N1 | 201.0790 | 0.81 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 2.47 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 2.55 | 8 | 0.92 | 0.17 |
| C7H11O5N2 | 202.0590 | 0.33 | 4 | 1.43 | 0.71 |
| C11H11O2N2 | 202.0742 | 2.64 | 8 | 0.91 | 0.18 |
| C11H11O2N2 | 202.0742 | 2.96 | 8 | 0.91 | 0.18 |
| C12H15O1N2 | 202.1106 | 2.65 | 7 | 1.17 | 0.08 |
| C12H15O1N2 | 202.1106 | 2.99 | 7 | 1.17 | 0.08 |
| C13H19N2 | 202.1470 | 3.44 | 6 | 1.38 | 0.00 |
| C15H10N1 | 203.0735 | 3.30 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.10 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.61 | 12 | 0.60 | 0.00 |
| C13H18O1N1 | 203.1310 | 2.78 | 6 | 1.31 | 0.08 |
| C9H17O5 | 204.0998 | 2.71 | 2 | 1.78 | 0.56 |
| C15H12N1 | 205.0891 | 2.78 | 11 | 0.73 | 0.00 |
| C13H20O1N1 | 205.1467 | 2.78 | 5 | 1.46 | 0.08 |
| C13H20O1N1 | 205.1467 | 2.89 | 5 | 1.46 | 0.08 |
| C10H7O5 | 206.0215 | 2.45 | 8 | 0.60 | 0.50 |
| C10H7O5 | 206.0215 | 2.88 | 8 | 0.60 | 0.50 |
| C11H11O4 | 206.0579 | 3.80 | 7 | 0.91 | 0.36 |
| C8H11O1N6 | 206.0916 | 3.19 | 7 | 1.25 | 0.13 |
| C11H15O2N2 | 206.1055 | 0.39 | 6 | 1.27 | 0.18 |
| C11H15O2N2 | 206.1055 | 3.18 | 6 | 1.27 | 0.18 |
| C12H19O1N2 | 206.1419 | 2.76 | 5 | 1.50 | 0.08 |
| C13H10N3 | 207.0796 | 7.39 | 11 | 0.69 | 0.00 |
| C11H14O3N1 | 207.0895 | 3.15 | 6 | 1.18 | 0.27 |
| C15H14N1 | 207.1048 | 3.63 | 10 | 0.87 | 0.00 |
| C12H18O2N1 | 207.1259 | 2.28 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.40 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.43 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.44 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.44 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.59 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.62 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.71 | 5 | 1.42 | 0.17 |
| C11H18O1N3 | 207.1372 | 2.39 | 5 | 1.55 | 0.09 |
| C13H22O1N1 | 207.1623 | 2.88 | 4 | 1.62 | 0.08 |
| C14H8O2Na1 | 208.0524 | 7.48 | 11 | 0.57 | 0.14 |
| C14H13N2 | 208.1000 | 3.09 | 10 | 0.86 | 0.00 |
| C14H13N2 | 208.1000 | 3.32 | 10 | 0.86 | 0.00 |
| C11H17O2N2 | 208.1212 | 3.02 | 5 | 1.45 | 0.18 |
| C9H20O5Na1 | 208.1311 | 2.47 | 0 | 2.22 | 0.56 |
| C13H25N2 | 208.1939 | 7.33 | 3 | 1.85 | 0.00 |
| C14H12O1N1 | 209.0841 | 7.60 | 10 | 0.79 | 0.07 |
| C11H20O1N3 | 209.1528 | 1.80 | 4 | 1.73 | 0.09 |

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|---|---|---|---|---|---|
| C9H7O6 | 210.0164 | 1.09 | 7 | 0.67 | 0.67 |
| C8H12O5Na1 | 188.0685 | 1.95 | 3 | 1.50 | 0.63 |
| C10H15O3N2 | 210.1004 | 0.43 | 5 | 1.40 | 0.30 |
| C14H15N2 | 210.1157 | 3.38 | 9 | 1.00 | 0.00 |
| C11H19O2N2 | 210.1368 | 2.63 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 2.96 | 4 | 1.64 | 0.18 |
| C6H14O7N1 | 211.0692 | 0.36 | 1 | 2.17 | 1.17 |
| C11H18O5N1 | 243.1107 | 0.38 | 4 | 1.55 | 0.45 |
| C13H14N3 | 211.1109 | 3.04 | 9 | 1.00 | 0.00 |
| C9H13O4N2 | 212.0797 | 0.93 | 5 | 1.33 | 0.44 |
| C13H13O1N2 | 212.0950 | 2.48 | 9 | 0.92 | 0.08 |
| C10H17O3N2 | 212.1161 | 0.58 | 4 | 1.60 | 0.30 |
| C10H17O3N2 | 212.1161 | 3.13 | 4 | 1.60 | 0.30 |
| C10H16O4N1 | 213.1001 | 0.38 | 4 | 1.50 | 0.40 |
| C14H16O1N1 | 213.1154 | 2.77 | 8 | 1.07 | 0.07 |
| C14H16O1N1 | 213.1154 | 3.07 | 8 | 1.07 | 0.07 |
| C10H15O5 | 214.0841 | 2.69 | 4 | 1.40 | 0.50 |
| C11H19O4 | 214.1205 | 4.45 | 3 | 1.64 | 0.36 |
| C14H19N2 | 214.1470 | 3.70 | 7 | 1.29 | 0.00 |
| C13H14O2N1 | 215.0946 | 2.42 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 2.67 | 8 | 1.00 | 0.15 |
| C10H18O4N1 | 215.1158 | 0.38 | 3 | 1.70 | 0.40 |
| C10H17O5 | 216.0998 | 3.16 | 3 | 1.60 | 0.50 |
| C13H17O1N2 | 216.1263 | 2.72 | 7 | 1.23 | 0.08 |
| C11H21O4 | 216.1362 | 3.06 | 2 | 1.82 | 0.36 |
| C11H21O4 | 216.1362 | 7.08 | 2 | 1.82 | 0.36 |
| C14H21N2 | 216.1626 | 3.63 | 6 | 1.43 | 0.00 |
| C8H12O6N1 | 217.0586 | 0.38 | 4 | 1.38 | 0.75 |
| C6H12O7Na1 | 196.0583 | 0.33 | 1 | 2.00 | 1.17 |
| C12H15O2N2 | 218.1055 | 2.88 | 7 | 1.17 | 0.17 |
| C15H10O1N1 | 219.0684 | 7.63 | 12 | 0.60 | 0.07 |
| C8H14O6N1 | 219.0743 | 0.38 | 3 | 1.63 | 0.75 |
| C16H14N1 | 219.1048 | 3.07 | 11 | 0.81 | 0.00 |
| C16H14N1 | 219.1048 | 3.17 | 11 | 0.81 | 0.00 |
| C13H18O2N1 | 219.1259 | 2.81 | 6 | 1.31 | 0.15 |
| C14H22O1N1 | 219.1623 | 3.04 | 5 | 1.50 | 0.07 |
| C10H14O4Na1 | 198.0892 | 2.73 | 4 | 1.40 | 0.40 |
| C12H13O4 | 220.0736 | 3.40 | 7 | 1.00 | 0.33 |
| C11H13O3N2 | 220.0848 | 0.38 | 7 | 1.09 | 0.27 |
| C13H21O1N2 | 220.1576 | 2.77 | 5 | 1.54 | 0.08 |
| C13H21O1N2 | 220.1576 | 2.85 | 5 | 1.54 | 0.08 |
| C13H21O1N2 | 220.1576 | 2.95 | 5 | 1.54 | 0.08 |
| C15H12O1N1 | 221.0841 | 2.76 | 11 | 0.73 | 0.07 |
| C8H16O6N1 | 221.0899 | 0.42 | 2 | 1.88 | 0.75 |
| C8H16O6N1 | 221.0899 | 0.54 | 2 | 1.88 | 0.75 |
| C13H20O2N1 | 221.1416 | 2.76 | 5 | 1.46 | 0.15 |
| C13H20O2N1 | 221.1416 | 2.95 | 5 | 1.46 | 0.15 |
| C12H19O2N2 | 222.1368 | 2.48 | 5 | 1.50 | 0.17 |
| C12H22O1N3 | 223.1685 | 2.54 | 4 | 1.75 | 0.08 |
| C9H14O5Na1 | 202.0841 | 2.65 | 3 | 1.56 | 0.56 |

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|---|---|---|---|---|---|
| C9H14O5Na1 | 202.0841 | 2.70 | 3 | 1.56 | 0.56 |
| C12H21O2N2 | 224.1525 | 2.89 | 4 | 1.67 | 0.17 |
| C12H21O2N2 | 224.1525 | 2.98 | 4 | 1.67 | 0.17 |
| C12H21O2N2 | 224.1525 | 3.13 | 4 | 1.67 | 0.17 |
| C13H12O1N3 | 225.0902 | 3.18 | 10 | 0.85 | 0.08 |
| C8H12O6Na1 | 204.0634 | 0.56 | 3 | 1.50 | 0.75 |
| C7H11O3N6 | 226.0814 | 2.69 | 6 | 1.43 | 0.43 |
| C11H19O3N2 | 226.1317 | 2.47 | 4 | 1.64 | 0.27 |
| C12H23O2N2 | 226.1681 | 2.34 | 3 | 1.83 | 0.17 |
| C7H3O1N5Na1S1 | 205.0058 | 0.78 | 9 | 0.43 | 0.14 |
| C9H14O4N3 | 227.0906 | 0.37 | 5 | 1.44 | 0.44 |
| C14H14O2N1 | 227.0946 | 2.69 | 9 | 0.93 | 0.14 |
| C14H17O1N2 | 228.1263 | 2.72 | 8 | 1.14 | 0.07 |
| C12H21O4 | 228.1362 | 6.64 | 3 | 1.67 | 0.33 |
| C14H16O2N1 | 229.1103 | 2.77 | 8 | 1.07 | 0.14 |
| C14H16O2N1 | 229.1103 | 2.80 | 8 | 1.07 | 0.14 |
| C14H16O2N1 | 229.1103 | 3.16 | 8 | 1.07 | 0.14 |
| C12H24O3N1 | 229.1678 | 2.93 | 2 | 1.92 | 0.25 |
| C17H11O1 | 230.0732 | 8.31 | 13 | 0.59 | 0.06 |
| C17H11O1 | 230.0732 | 8.46 | 13 | 0.59 | 0.06 |
| C9H15O5N2 | 230.0903 | 0.33 | 4 | 1.56 | 0.56 |
| C7H15O3N6 | 230.1127 | 2.33 | 4 | 2.00 | 0.43 |
| C11H19O5 | 230.1154 | 3.25 | 3 | 1.64 | 0.45 |
| C14H19O1N2 | 230.1419 | 2.99 | 7 | 1.29 | 0.07 |
| C16H10O1N1 | 231.0684 | 8.26 | 13 | 0.56 | 0.06 |
| C14H21O1N2 | 232.1576 | 2.92 | 6 | 1.43 | 0.07 |
| C15H11O1N2 | 234.0793 | 7.44 | 12 | 0.67 | 0.07 |
| C10H16O3N2Na1 | 212.1161 | 3.09 | 4 | 1.60 | 0.30 |
| C7H7O5N3Na1 | 213.0386 | 0.59 | 6 | 1.00 | 0.71 |
| C8H18O3N3S1 | 235.0991 | 2.76 | 2 | 2.13 | 0.38 |
| C14H22O2N1 | 235.1572 | 2.95 | 5 | 1.50 | 0.14 |
| C14H22O2N1 | 235.1572 | 3.25 | 5 | 1.50 | 0.14 |
| C8H16O7N1 | 237.0849 | 0.39 | 2 | 1.88 | 0.88 |
| C15H15O1N2 | 238.1106 | 3.12 | 10 | 0.93 | 0.07 |
| C12H19O3N2 | 238.1317 | 2.76 | 5 | 1.50 | 0.25 |
| C13H23O2N2 | 238.1681 | 3.08 | 4 | 1.69 | 0.15 |
| C13H23O2N2 | 238.1681 | 3.14 | 4 | 1.69 | 0.15 |
| C13H23O2N2 | 238.1681 | 3.36 | 4 | 1.69 | 0.15 |
| C14H9O4 | 240.0423 | 5.27 | 11 | 0.57 | 0.29 |
| C12H21O3N2 | 240.1474 | 2.68 | 4 | 1.67 | 0.25 |
| C8H12O7Na1 | 220.0583 | 0.38 | 3 | 1.50 | 0.88 |
| C10H15O5N2 | 242.0903 | 0.39 | 5 | 1.40 | 0.50 |
| C12H19O5 | 242.1154 | 3.01 | 4 | 1.50 | 0.42 |
| C15H19O1N2 | 242.1419 | 8.27 | 8 | 1.20 | 0.07 |
| C13H23O4 | 242.1518 | 7.49 | 3 | 1.69 | 0.31 |
| C7H3O2N5Na1S1 | 221.0007 | 0.41 | 9 | 0.43 | 0.29 |
| C15H18O2N1 | 243.1259 | 3.02 | 8 | 1.13 | 0.13 |
| C14H17O2N2 | 244.1212 | 3.13 | 8 | 1.14 | 0.14 |
| C14H17O2N2 | 244.1212 | 3.24 | 8 | 1.14 | 0.14 |
| C15H21O1N2 | 244.1576 | 3.21 | 7 | 1.33 | 0.07 |

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|---|---|---|---|---|---|
| C8H17O6N1Na1 | 223.1056 | 3.69 | 1 | 2.13 | 0.75 |
| C12H24O4N1 | 245.1627 | 2.86 | 2 | 1.92 | 0.33 |
| C12H24O4N1 | 245.1627 | 3.02 | 2 | 1.92 | 0.33 |
| C14H21O2N2 | 248.1525 | 0.33 | 6 | 1.43 | 0.14 |
| C16H11O3 | 250.0630 | 7.63 | 12 | 0.63 | 0.19 |
| C12H20O4Na1 | 228.1362 | 2.82 | 3 | 1.67 | 0.33 |
| C13H21O3N2 | 252.1474 | 2.82 | 5 | 1.54 | 0.23 |
| C11H24O6Na1 | 252.1573 | 2.70 | 0 | 2.18 | 0.55 |
| C14H25O2N2 | 252.1838 | 3.62 | 4 | 1.71 | 0.14 |
| C12H19O4N2 | 254.1267 | 2.69 | 5 | 1.50 | 0.33 |
| C13H23O3N2 | 254.1630 | 2.76 | 4 | 1.69 | 0.23 |
| C14H25O4 | 256.1675 | 7.86 | 3 | 1.71 | 0.29 |
| C12H14O5Na1 | 238.0841 | 3.42 | 6 | 1.17 | 0.42 |
| C16H26O2N1 | 263.1885 | 3.68 | 5 | 1.56 | 0.13 |
| C12H20O5Na1 | 244.1311 | 4.38 | 3 | 1.67 | 0.42 |
| C13H21O4N2 | 268.1423 | 2.88 | 5 | 1.54 | 0.31 |
| C16H29O3 | 268.2038 | 7.89 | 3 | 1.75 | 0.19 |
| C8H5O3N7Na1 | 247.0454 | 7.42 | 10 | 0.63 | 0.38 |
| C5H5O5N1Na1S3 | 254.9330 | 0.33 | 4 | 1.00 | 1.00 |
| C8H15O7N4 | 278.0862 | 7.71 | 4 | 1.75 | 0.88 |
| C14H19O4N2 | 278.1267 | 0.32 | 7 | 1.29 | 0.29 |
| C12H15O6N2 | 282.0852 | 0.39 | 7 | 1.17 | 0.50 |
| C14H23O4N2 | 282.1580 | 2.87 | 5 | 1.57 | 0.29 |
| C14H25O4N2 | 284.1736 | 2.71 | 4 | 1.71 | 0.29 |
| C4H12O11N2Na1 | 264.0441 | 2.62 | 0 | 3.00 | 2.75 |
| C11H15O7N2 | 286.0801 | 0.39 | 6 | 1.27 | 0.64 |
| C17H27O2N2 | 290.1994 | 2.98 | 6 | 1.53 | 0.12 |
| C15H22O3N1S1 | 295.1242 | 2.52 | 6 | 1.40 | 0.20 |
| C14H23O5N2 | 298.1529 | 2.73 | 5 | 1.57 | 0.36 |
| C12H4O1N6Na1S1 | 280.0167 | 2.62 | 14 | 0.33 | 0.08 |
| C20H27O4 | 330.1831 | 7.60 | 8 | 1.30 | 0.20 |
| C6H5O10N1Na1S4 | 378.8796 | 0.29 | 5 | 0.83 | 1.67 |
| C16H26O5N6Na1S1 | 414.1685 | 8.30 | 7 | 1.63 | 0.31 |

Table S3.2.5 Molecular formulas of organic compounds detected in GZ in ESI- mode.

| Formula [M-H] | Neutral mass (Da) | RT (min) | DBE | H/C | O/C |
|---|---|---|---|---|---|
| C3H5O6S1 | 169.9885 | 0.38 | 1 | 2.00 | 2.00 |
| C6H11O4 | 148.0736 | 0.48 | 1 | 2.00 | 0.67 |
| C3H3O4 | 104.0110 | 0.37 | 2 | 1.33 | 1.33 |
| C5H7O5 | 148.0372 | 0.38 | 2 | 1.60 | 1.00 |
| C5H7O7S1 | 211.9991 | 0.38 | 2 | 1.60 | 1.40 |
| C4H5O5 | 134.0215 | 0.38 | 2 | 1.50 | 1.25 |
| C6H11O2 | 116.0837 | 2.94 | 1 | 2.00 | 0.33 |
| C3H4O5N1 | 135.0168 | 0.39 | 2 | 1.67 | 1.67 |
| C4H5O4 | 118.0266 | 0.53 | 2 | 1.50 | 1.00 |
| C7H5O2 | 122.0368 | 2.66 | 5 | 0.86 | 0.29 |
| C7H5O2 | 122.0368 | 2.76 | 5 | 0.86 | 0.29 |
| C2H5O4S1 | 125.9987 | 0.38 | 0 | 3.00 | 2.00 |

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|---|---|---|---|---|---|
| C8H9O7 | 218.0427 | 0.38 | 4 | 1.25 | 0.88 |
| C8H13O1 | 126.1045 | 3.72 | 2 | 1.75 | 0.13 |
| C5H4O3N1 | 127.0269 | 1.02 | 4 | 1.00 | 0.60 |
| C5H5O5 | 146.0215 | 0.38 | 3 | 1.20 | 1.00 |
| C7H11O2 | 128.0837 | 2.47 | 2 | 1.71 | 0.29 |
| C7H11O2 | 128.0837 | 2.68 | 2 | 1.71 | 0.29 |
| C5H5O4 | 130.0266 | 0.60 | 3 | 1.20 | 0.80 |
| C5H8O3N1 | 131.0582 | 0.44 | 2 | 1.80 | 0.60 |
| C5H3O3N4 | 168.0283 | 0.35 | 6 | 0.80 | 0.60 |
| C5H7O4 | 132.0423 | 0.77 | 2 | 1.60 | 0.80 |
| C5H7O4 | 132.0423 | 1.10 | 2 | 1.60 | 0.80 |
| C8H5O2 | 134.0368 | 1.83 | 6 | 0.75 | 0.25 |
| C7H4O2N1 | 135.0320 | 2.69 | 6 | 0.71 | 0.29 |
| C8H7O2 | 136.0524 | 3.10 | 5 | 1.00 | 0.25 |
| C5H2O2N3 | 137.0225 | 2.79 | 6 | 0.60 | 0.40 |
| C5H2O2N3 | 137.0225 | 3.20 | 6 | 0.60 | 0.40 |
| C3H5O4S1 | 137.9987 | 0.36 | 1 | 2.00 | 1.33 |
| C7H5O3 | 138.0317 | 2.34 | 5 | 0.86 | 0.43 |
| C6H4O3N1 | 139.0269 | 3.76 | 5 | 0.83 | 0.50 |
| C2H3O5S1 | 139.9779 | 0.33 | 1 | 2.00 | 2.50 |
| C3H7O4S1 | 140.0143 | 0.51 | 0 | 2.67 | 1.33 |
| C5H3O3N2 | 140.0222 | 1.16 | 5 | 0.80 | 0.60 |
| C5H3O3N2 | 140.0222 | 2.40 | 5 | 0.80 | 0.60 |
| C6H7O4 | 144.0423 | 0.56 | 3 | 1.33 | 0.67 |
| C6H7O4 | 144.0423 | 0.68 | 3 | 1.33 | 0.67 |
| C9H6O1N1 | 145.0528 | 2.26 | 7 | 0.78 | 0.11 |
| C6H9O4 | 146.0579 | 1.71 | 2 | 1.67 | 0.67 |
| C8H4O2N1 | 147.0320 | 3.26 | 7 | 0.63 | 0.25 |
| C9H7O2 | 148.0524 | 2.95 | 6 | 0.89 | 0.22 |
| C9H7O2 | 148.0524 | 3.10 | 6 | 0.89 | 0.22 |
| C8H5O3 | 150.0317 | 0.82 | 6 | 0.75 | 0.38 |
| C8H5O3 | 150.0317 | 2.64 | 6 | 0.75 | 0.38 |
| C8H8O2N1 | 151.0633 | 1.80 | 5 | 1.13 | 0.25 |
| C8H7O3 | 152.0473 | 2.65 | 5 | 1.00 | 0.38 |
| C8H7O3 | 152.0473 | 3.04 | 5 | 1.00 | 0.38 |
| C7H6O3N1 | 153.0426 | 5.23 | 5 | 1.00 | 0.43 |
| C7H6O3N1 | 153.0426 | 6.07 | 5 | 1.00 | 0.43 |
| C3H5O5S1 | 153.9936 | 0.37 | 1 | 2.00 | 1.67 |
| C7H5O4 | 154.0266 | 1.30 | 5 | 0.86 | 0.57 |
| C7H5O4 | 154.0266 | 2.61 | 5 | 0.86 | 0.57 |
| C4H9O4S1 | 154.0300 | 0.93 | 0 | 2.50 | 1.00 |
| C6H5O3N2 | 154.0378 | 2.83 | 5 | 1.00 | 0.50 |
| C6H5O3N2 | 154.0378 | 3.34 | 5 | 1.00 | 0.50 |
| C8H9O3 | 154.0630 | 1.59 | 4 | 1.25 | 0.38 |
| C6H4O4N1 | 155.0219 | 0.46 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 3.09 | 5 | 0.83 | 0.67 |
| C6H4O4N1 | 155.0219 | 3.83 | 5 | 0.83 | 0.67 |
| C2H3O6S1 | 155.9729 | 0.33 | 1 | 2.00 | 3.00 |
| C6H3O5 | 156.0059 | 0.69 | 5 | 0.67 | 0.83 |
| C5H3O4N2 | 156.0171 | 1.24 | 5 | 0.80 | 0.80 |

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|---|---|---|---|---|---|
| C4H2O4N3 | 157.0124 | 3.25 | 5 | 0.75 | 1.00 |
| C6H5O3S1 | 158.0038 | 0.74 | 4 | 1.00 | 0.50 |
| C7H11O4 | 160.0736 | 2.73 | 2 | 1.71 | 0.57 |
| C9H7O4 | 180.0423 | 3.13 | 6 | 0.89 | 0.44 |
| C9H5O3 | 162.0317 | 3.29 | 7 | 0.67 | 0.33 |
| C8H5O2N2 | 162.0429 | 6.11 | 7 | 0.75 | 0.25 |
| C10H9O2 | 162.0681 | 3.38 | 6 | 1.00 | 0.20 |
| C7H13O4 | 162.0892 | 0.86 | 1 | 2.00 | 0.57 |
| C7H3O3N2 | 164.0222 | 4.02 | 7 | 0.57 | 0.43 |
| C7H3O3N2 | 164.0222 | 4.23 | 7 | 0.57 | 0.43 |
| C9H7O3 | 164.0473 | 2.48 | 6 | 0.89 | 0.33 |
| C9H7O3 | 164.0473 | 3.07 | 6 | 0.89 | 0.33 |
| C9H7O3 | 164.0473 | 3.29 | 6 | 0.89 | 0.33 |
| C8H6O3N1 | 165.0426 | 3.20 | 6 | 0.88 | 0.38 |
| C8H6O3N1 | 165.0426 | 5.09 | 6 | 0.88 | 0.38 |
| C8H6O3N1 | 165.0426 | 6.78 | 6 | 0.88 | 0.38 |
| C6H9O9S1 | 258.0046 | 0.37 | 2 | 1.67 | 1.50 |
| C8H5O4 | 166.0266 | 1.34 | 6 | 0.75 | 0.50 |
| C8H5O4 | 166.0266 | 2.66 | 6 | 0.75 | 0.50 |
| C8H5O4 | 166.0266 | 2.94 | 6 | 0.75 | 0.50 |
| C7H5O3N2 | 166.0378 | 3.46 | 6 | 0.86 | 0.43 |
| C9H9O3 | 166.0630 | 3.25 | 5 | 1.11 | 0.33 |
| C6H13O3S1 | 166.0664 | 2.95 | 0 | 2.33 | 0.50 |
| C3H4O5N1S1 | 166.9888 | 0.36 | 2 | 1.67 | 1.67 |
| C7H4O4N1 | 167.0219 | 3.81 | 6 | 0.71 | 0.57 |
| C8H8O3N1 | 167.0582 | 7.26 | 5 | 1.13 | 0.38 |
| C8H8O3N1 | 167.0582 | 7.57 | 5 | 1.13 | 0.38 |
| C8H7O4 | 168.0423 | 3.15 | 5 | 1.00 | 0.50 |
| C5H11O4S1 | 168.0456 | 2.46 | 0 | 2.40 | 0.80 |
| C5H11O4S1 | 168.0456 | 2.82 | 0 | 2.40 | 0.80 |
| C7H7O3N2 | 168.0535 | 3.76 | 5 | 1.14 | 0.43 |
| C7H6O4N1 | 169.0375 | 2.94 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 2.99 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 3.67 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 3.83 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 4.15 | 5 | 1.00 | 0.57 |
| C7H6O4N1 | 169.0375 | 4.68 | 5 | 1.00 | 0.57 |
| C6H4O5N1 | 171.0168 | 2.31 | 5 | 0.83 | 0.83 |
| C5H4O4N3 | 171.0280 | 3.92 | 5 | 1.00 | 0.80 |
| C11H7O2 | 172.0524 | 3.86 | 8 | 0.73 | 0.18 |
| C8H11O4 | 172.0736 | 2.48 | 3 | 1.50 | 0.50 |
| C7H9O5 | 174.0528 | 0.56 | 3 | 1.43 | 0.71 |
| C7H9O5 | 174.0528 | 0.75 | 3 | 1.43 | 0.71 |
| C7H9O5 | 174.0528 | 0.96 | 3 | 1.43 | 0.71 |
| C6H8O5N1 | 175.0481 | 0.38 | 3 | 1.50 | 0.83 |
| C10H7O3 | 176.0473 | 3.29 | 7 | 0.80 | 0.30 |
| C9H7O2N2 | 176.0586 | 7.47 | 7 | 0.89 | 0.22 |
| C7H11O5 | 176.0685 | 0.95 | 2 | 1.71 | 0.71 |
| C7H11O5 | 176.0685 | 1.15 | 2 | 1.71 | 0.71 |
| C9H6O3N1 | 177.0426 | 3.28 | 7 | 0.78 | 0.33 |

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| C9H5O4 | 178.0266 | 2.44 | 7 | 0.67 | 0.44 |
| C9H5O4 | 178.0266 | 2.82 | 7 | 0.67 | 0.44 |
| C9H7O5 | 196.0372 | 2.99 | 6 | 0.89 | 0.56 |
| C10H9O3 | 178.0630 | 3.81 | 6 | 1.00 | 0.30 |
| C8H4O4N1 | 179.0219 | 2.90 | 7 | 0.63 | 0.50 |
| C8H4O4N1 | 179.0219 | 4.92 | 7 | 0.63 | 0.50 |
| C8H4O4N1 | 179.0219 | 5.41 | 7 | 0.63 | 0.50 |
| C9H8O3N1 | 179.0582 | 7.01 | 6 | 1.00 | 0.33 |
| C9H8O3N1 | 179.0582 | 7.45 | 6 | 1.00 | 0.33 |
| C4H3O6S1 | 179.9729 | 0.40 | 3 | 1.00 | 1.50 |
| C6H9O7S1 | 226.0147 | 0.39 | 2 | 1.67 | 1.17 |
| C7H3O4N2 | 180.0171 | 3.52 | 7 | 0.57 | 0.57 |
| C9H7O4 | 180.0423 | 2.76 | 6 | 0.89 | 0.44 |
| C8H6O4N1 | 181.0375 | 2.15 | 6 | 0.88 | 0.50 |
| C8H6O4N1 | 181.0375 | 2.62 | 6 | 0.88 | 0.50 |
| C8H6O4N1 | 181.0375 | 3.90 | 6 | 0.88 | 0.50 |
| C9H10O3N1 | 181.0739 | 7.99 | 5 | 1.22 | 0.33 |
| C8H5O5 | 182.0215 | 1.07 | 6 | 0.75 | 0.63 |
| C8H5O5 | 182.0215 | 1.92 | 6 | 0.75 | 0.63 |
| C8H5O5 | 182.0215 | 2.46 | 6 | 0.75 | 0.63 |
| C6H11O7S1 | 228.0304 | 0.40 | 1 | 2.00 | 1.17 |
| C5H9O5S1 | 182.0249 | 0.52 | 1 | 2.00 | 1.00 |
| C7H5O4N2 | 182.0328 | 3.13 | 6 | 0.86 | 0.57 |
| C7H5O4N2 | 182.0328 | 3.46 | 6 | 0.86 | 0.57 |
| C9H9O4 | 182.0579 | 2.30 | 5 | 1.11 | 0.44 |
| C7H4O5N1 | 183.0168 | 1.29 | 6 | 0.71 | 0.71 |
| C7H4O5N1 | 183.0168 | 2.94 | 6 | 0.71 | 0.71 |
| C7H4O5N1 | 183.0168 | 3.26 | 6 | 0.71 | 0.71 |
| C6H4O4N3 | 183.0280 | 4.93 | 6 | 0.83 | 0.67 |
| C8H8O4N1 | 183.0532 | 3.33 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 3.41 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 3.51 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 4.18 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 5.70 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 5.99 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 6.53 | 5 | 1.13 | 0.50 |
| C8H8O4N1 | 183.0532 | 7.05 | 5 | 1.13 | 0.50 |
| C6H3O5N2 | 184.0120 | 6.31 | 6 | 0.67 | 0.83 |
| C5H11O5S1 | 184.0405 | 0.52 | 0 | 2.40 | 1.00 |
| C7H6O5N1 | 185.0324 | 2.44 | 5 | 1.00 | 0.71 |
| C7H6O5N1 | 185.0324 | 2.62 | 5 | 1.00 | 0.71 |
| C7H6O5N1 | 185.0324 | 3.30 | 5 | 1.00 | 0.71 |
| C10H5O2N2 | 186.0429 | 3.50 | 9 | 0.60 | 0.20 |
| C8H11O6 | 204.0634 | 0.60 | 3 | 1.50 | 0.75 |
| C8H9O5 | 186.0528 | 3.04 | 4 | 1.25 | 0.63 |
| C9H13O4 | 186.0892 | 2.85 | 3 | 1.56 | 0.44 |
| C9H13O4 | 186.0892 | 2.95 | 3 | 1.56 | 0.44 |
| C7H7O6 | 188.0321 | 0.46 | 4 | 1.14 | 0.86 |
| C8H11O5 | 188.0685 | 0.85 | 3 | 1.50 | 0.63 |
| C8H11O5 | 188.0685 | 1.27 | 3 | 1.50 | 0.63 |

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| C8H11O5 | 188.0685 | 1.93 | 3 | 1.50 | 0.63 |
| C8H11O5 | 188.0685 | 2.45 | 3 | 1.50 | 0.63 |
| C8H11O5 | 188.0685 | 2.78 | 3 | 1.50 | 0.63 |
| C8H11O5 | 188.0685 | 1.47 | 3 | 1.50 | 0.63 |
| C10H6O3N1 | 189.0426 | 7.74 | 8 | 0.70 | 0.30 |
| C9H5O3N2 | 190.0378 | 2.75 | 8 | 0.67 | 0.33 |
| C7H9O6 | 190.0477 | 0.77 | 3 | 1.43 | 0.86 |
| C7H9O6 | 190.0477 | 0.99 | 3 | 1.43 | 0.86 |
| C8H13O5 | 190.0841 | 2.26 | 2 | 1.75 | 0.63 |
| C9H17O4 | 190.1205 | 2.86 | 1 | 2.00 | 0.44 |
| C6H7O7 | 192.0270 | 0.38 | 3 | 1.33 | 1.17 |
| C10H7O4 | 192.0423 | 2.40 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.10 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 3.28 | 7 | 0.80 | 0.40 |
| C10H7O4 | 192.0423 | 7.00 | 7 | 0.80 | 0.40 |
| C7H11O6 | 192.0634 | 0.39 | 2 | 1.71 | 0.86 |
| C9H6O4N1 | 193.0375 | 3.48 | 7 | 0.78 | 0.44 |
| C9H6O4N1 | 193.0375 | 3.66 | 7 | 0.78 | 0.44 |
| C9H6O4N1 | 193.0375 | 6.79 | 7 | 0.78 | 0.44 |
| C9H6O4N1 | 193.0375 | 7.17 | 7 | 0.78 | 0.44 |
| C9H6O4N1 | 193.0375 | 7.26 | 7 | 0.78 | 0.44 |
| C9H5O5 | 194.0215 | 0.82 | 7 | 0.67 | 0.56 |
| C9H5O5 | 194.0215 | 2.61 | 7 | 0.67 | 0.56 |
| C9H5O5 | 194.0215 | 2.77 | 7 | 0.67 | 0.56 |
| C8H7O7 | 216.0270 | 0.35 | 5 | 1.00 | 0.88 |
| C10H9O4 | 194.0579 | 3.65 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.80 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 3.95 | 6 | 1.00 | 0.40 |
| C10H9O4 | 194.0579 | 6.40 | 6 | 1.00 | 0.40 |
| C8H17O3S1 | 194.0977 | 5.21 | 0 | 2.25 | 0.38 |
| C8H4O5N1 | 195.0168 | 3.15 | 7 | 0.63 | 0.63 |
| C9H8O4N1 | 195.0532 | 3.96 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 4.76 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 5.01 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 6.34 | 6 | 1.00 | 0.44 |
| C9H8O4N1 | 195.0532 | 6.63 | 6 | 1.00 | 0.44 |
| C6H9O8S1 | 242.0096 | 0.47 | 2 | 1.67 | 1.33 |
| C9H7O5 | 196.0372 | 2.50 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 2.74 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.27 | 6 | 0.89 | 0.56 |
| C9H7O5 | 196.0372 | 3.39 | 6 | 0.89 | 0.56 |
| C6H11O5S1 | 196.0405 | 0.85 | 1 | 2.00 | 0.83 |
| C6H11O5S1 | 196.0405 | 1.02 | 1 | 2.00 | 0.83 |
| C8H7O4N2 | 196.0484 | 3.19 | 6 | 1.00 | 0.50 |
| C13H7O2 | 196.0524 | 4.90 | 10 | 0.62 | 0.15 |
| C13H7O2 | 196.0524 | 7.17 | 10 | 0.62 | 0.15 |
| C13H7O2 | 196.0524 | 7.53 | 10 | 0.62 | 0.15 |
| C7H15O4S1 | 196.0769 | 5.16 | 0 | 2.29 | 0.57 |
| C8H6O5N1 | 197.0324 | 3.26 | 6 | 0.88 | 0.63 |
| C8H6O5N1 | 197.0324 | 4.31 | 6 | 0.88 | 0.63 |

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| C8H6O5N1 | 197.0324 | 4.71 | 6 | 0.88 | 0.63 |
| C9H10O4N1 | 197.0688 | 7.57 | 5 | 1.22 | 0.44 |
| C9H10O4N1 | 197.0688 | 7.77 | 5 | 1.22 | 0.44 |
| C8H5O6 | 198.0164 | 0.90 | 6 | 0.75 | 0.75 |
| C8H5O6 | 198.0164 | 1.23 | 6 | 0.75 | 0.75 |
| C8H5O6 | 198.0164 | 3.09 | 6 | 0.75 | 0.75 |
| C7H5O5N2 | 198.0277 | 7.42 | 6 | 0.86 | 0.71 |
| C10H13O4 | 198.0892 | 2.65 | 4 | 1.40 | 0.40 |
| C10H13O4 | 198.0892 | 3.75 | 4 | 1.40 | 0.40 |
| C7H4O6N1 | 199.0117 | 2.67 | 6 | 0.71 | 0.86 |
| C7H4O6N1 | 199.0117 | 3.42 | 6 | 0.71 | 0.86 |
| C8H8O5N1 | 199.0481 | 2.50 | 5 | 1.13 | 0.63 |
| C8H8O5N1 | 199.0481 | 2.83 | 5 | 1.13 | 0.63 |
| C8H8O5N1 | 199.0481 | 4.26 | 5 | 1.13 | 0.63 |
| C6H3O6N2 | 200.0069 | 4.24 | 6 | 0.67 | 1.00 |
| C7H5O5S1 | 201.9936 | 0.63 | 5 | 0.86 | 0.71 |
| C9H13O5 | 202.0841 | 2.50 | 3 | 1.56 | 0.56 |
| C9H13O5 | 202.0841 | 2.64 | 3 | 1.56 | 0.56 |
| C9H13O5 | 202.0841 | 2.69 | 3 | 1.56 | 0.56 |
| C10H17O4 | 202.1205 | 2.89 | 2 | 1.80 | 0.40 |
| C10H4O2N1S1 | 203.0041 | 0.52 | 9 | 0.50 | 0.20 |
| C11H8O3N1 | 203.0582 | 8.06 | 8 | 0.82 | 0.27 |
| C5H3O1N2S3 | 203.9486 | 0.30 | 5 | 0.80 | 0.20 |
| C8H11O6 | 204.0634 | 0.67 | 3 | 1.50 | 0.75 |
| C7H7O6N6 | 272.0505 | 2.33 | 7 | 1.14 | 0.86 |
| C9H15O5 | 204.0998 | 2.57 | 2 | 1.78 | 0.56 |
| C9H15O5 | 204.0998 | 2.77 | 2 | 1.78 | 0.56 |
| C10H6O4N1 | 205.0375 | 3.12 | 8 | 0.70 | 0.40 |
| C10H5O5 | 206.0215 | 3.15 | 8 | 0.60 | 0.50 |
| C11H9O4 | 206.0579 | 3.19 | 7 | 0.91 | 0.36 |
| C9H4O5N1 | 207.0168 | 3.19 | 8 | 0.56 | 0.56 |
| C9H4O5N1 | 207.0168 | 3.93 | 8 | 0.56 | 0.56 |
| C10H8O4N1 | 207.0532 | 4.56 | 7 | 0.90 | 0.40 |
| C10H8O4N1 | 207.0532 | 4.89 | 7 | 0.90 | 0.40 |
| C10H8O4N1 | 207.0532 | 7.65 | 7 | 0.90 | 0.40 |
| C10H7O5 | 208.0372 | 2.27 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.37 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.54 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.72 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.84 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.94 | 7 | 0.80 | 0.50 |
| C10H7O5 | 208.0372 | 2.97 | 7 | 0.80 | 0.50 |
| C7H11O7 | 208.0583 | 0.37 | 2 | 1.71 | 1.00 |
| C5H6O6N1S1 | 208.9994 | 0.38 | 3 | 1.40 | 1.20 |
| C9H6O5N1 | 209.0324 | 3.99 | 7 | 0.78 | 0.56 |
| C9H6O5N1 | 209.0324 | 4.08 | 7 | 0.78 | 0.56 |
| C10H10O4N1 | 209.0688 | 7.56 | 6 | 1.10 | 0.40 |
| C9H5O6 | 210.0164 | 1.09 | 7 | 0.67 | 0.67 |
| C9H5O6 | 210.0164 | 1.94 | 7 | 0.67 | 0.67 |
| C9H5O6 | 210.0164 | 2.23 | 7 | 0.67 | 0.67 |

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| C9H5O6 | 210.0164 | 2.54 | 7 | 0.67 | 0.67 |
| C6H9O6S1 | 210.0198 | 0.90 | 2 | 1.67 | 1.00 |
| C8H7O6N2 | 228.0382 | 7.60 | 6 | 1.00 | 0.75 |
| C7H13O5S1 | 210.0562 | 1.93 | 1 | 2.00 | 0.71 |
| C7H13O5S1 | 210.0562 | 2.51 | 1 | 2.00 | 0.71 |
| C8H17O4S1 | 210.0926 | 7.16 | 0 | 2.25 | 0.50 |
| C8H4O6N1 | 211.0117 | 2.58 | 7 | 0.63 | 0.75 |
| C9H8O5N1 | 211.0481 | 3.15 | 6 | 1.00 | 0.56 |
| C9H8O5N1 | 211.0481 | 7.01 | 6 | 1.00 | 0.56 |
| C6H11O6S1 | 212.0355 | 0.96 | 1 | 2.00 | 1.00 |
| C6H11O6S1 | 212.0355 | 1.59 | 1 | 2.00 | 1.00 |
| C6H11O6S1 | 212.0355 | 0.97 | 1 | 2.00 | 1.00 |
| C8H7O5N2 | 212.0433 | 7.92 | 6 | 1.00 | 0.63 |
| C13H7O3 | 212.0473 | 7.09 | 10 | 0.62 | 0.23 |
| C8H6O6N1 | 213.0273 | 2.66 | 6 | 0.88 | 0.75 |
| C8H6O6N1 | 213.0273 | 3.42 | 6 | 0.88 | 0.75 |
| C8H6O6N1 | 213.0273 | 3.72 | 6 | 0.88 | 0.75 |
| C8H5O5S1 | 213.9936 | 1.59 | 6 | 0.75 | 0.63 |
| C7H5O6N2 | 214.0226 | 3.55 | 6 | 0.86 | 0.86 |
| C7H5O6N2 | 214.0226 | 4.84 | 6 | 0.86 | 0.86 |
| C7H5O6N2 | 214.0226 | 7.12 | 6 | 0.86 | 0.86 |
| C7H5O6N2 | 214.0226 | 7.27 | 6 | 0.86 | 0.86 |
| C12H5O4 | 214.0266 | 5.50 | 10 | 0.50 | 0.33 |
| C6H13O6S1 | 214.0511 | 0.38 | 0 | 2.33 | 1.00 |
| C10H13O5 | 214.0841 | 2.51 | 4 | 1.40 | 0.50 |
| C10H13O5 | 214.0841 | 2.81 | 4 | 1.40 | 0.50 |
| C10H13O5 | 214.0841 | 2.88 | 4 | 1.40 | 0.50 |
| C11H17O4 | 214.1205 | 4.43 | 3 | 1.64 | 0.36 |
| C11H17O4 | 214.1205 | 6.76 | 3 | 1.64 | 0.36 |
| C12H8O3N1 | 215.0582 | 7.86 | 9 | 0.75 | 0.25 |
| C12H8O3N1 | 215.0582 | 8.10 | 9 | 0.75 | 0.25 |
| C4H7O8S1 | 215.9940 | 0.32 | 1 | 2.00 | 2.00 |
| C12H7O4 | 216.0423 | 3.86 | 9 | 0.67 | 0.33 |
| C12H7O4 | 216.0423 | 4.06 | 9 | 0.67 | 0.33 |
| C12H7O4 | 216.0423 | 4.46 | 9 | 0.67 | 0.33 |
| C10H15O5 | 216.0998 | 2.91 | 3 | 1.60 | 0.50 |
| C10H15O5 | 216.0998 | 3.02 | 3 | 1.60 | 0.50 |
| C12H10O3N1 | 217.0739 | 8.22 | 8 | 0.92 | 0.25 |
| C8H9O5S1 | 218.0249 | 1.42 | 4 | 1.25 | 0.63 |
| C16H9O1 | 218.0732 | 8.36 | 12 | 0.63 | 0.06 |
| C9H13O6 | 218.0790 | 1.33 | 3 | 1.56 | 0.67 |
| C9H13O6 | 218.0790 | 3.01 | 3 | 1.56 | 0.67 |
| C8H11O7 | 220.0583 | 0.38 | 3 | 1.50 | 0.88 |
| C8H11O7 | 220.0583 | 0.47 | 3 | 1.50 | 0.88 |
| C10H6O5N1 | 221.0324 | 3.47 | 8 | 0.70 | 0.50 |
| C10H6O5N1 | 221.0324 | 4.18 | 8 | 0.70 | 0.50 |
| C10H6O5N1 | 221.0324 | 5.86 | 8 | 0.70 | 0.50 |
| C11H9O5 | 222.0528 | 2.71 | 7 | 0.91 | 0.45 |
| C11H9O5 | 222.0528 | 2.90 | 7 | 0.91 | 0.45 |
| C11H9O5 | 222.0528 | 2.96 | 7 | 0.91 | 0.45 |

| | | | | | |
|---|---|---|---|---|---|
| C11H9O5 | 222.0528 | 3.06 | 7 | 0.91 | 0.45 |
| C11H9O5 | 222.0528 | 3.16 | 7 | 0.91 | 0.45 |
| C12H13O4 | 222.0892 | 7.48 | 6 | 1.17 | 0.33 |
| C12H7O5N2 | 260.0433 | 8.04 | 10 | 0.67 | 0.42 |
| C10H8O5N1 | 223.0481 | 5.94 | 7 | 0.90 | 0.50 |
| C8H3O6N2 | 224.0069 | 4.16 | 8 | 0.50 | 0.75 |
| C10H7O6 | 224.0321 | 2.31 | 7 | 0.80 | 0.60 |
| C10H7O6 | 224.0321 | 2.43 | 7 | 0.80 | 0.60 |
| C10H7O6 | 224.0321 | 2.87 | 7 | 0.80 | 0.60 |
| C10H7O6 | 224.0321 | 3.02 | 7 | 0.80 | 0.60 |
| C10H7O6 | 224.0321 | 3.07 | 7 | 0.80 | 0.60 |
| C14H7O3 | 224.0473 | 7.57 | 11 | 0.57 | 0.21 |
| C8H15O5S1 | 224.0718 | 2.82 | 1 | 2.00 | 0.63 |
| C9H19O4S1 | 224.1082 | 7.64 | 0 | 2.22 | 0.44 |
| C9H5O7 | 226.0114 | 1.06 | 7 | 0.67 | 0.78 |
| C9H5O7 | 226.0114 | 2.88 | 7 | 0.67 | 0.78 |
| C7H13O6S1 | 226.0511 | 2.22 | 1 | 2.00 | 0.86 |
| C7H13O6S1 | 226.0511 | 2.45 | 1 | 2.00 | 0.86 |
| C7H13O6S1 | 226.0511 | 2.48 | 1 | 2.00 | 0.86 |
| C14H9O3 | 226.0630 | 7.13 | 10 | 0.71 | 0.21 |
| C14H9O3 | 226.0630 | 7.26 | 10 | 0.71 | 0.21 |
| C8H4O7N1 | 227.0066 | 4.09 | 7 | 0.63 | 0.88 |
| C9H8O6N1 | 227.0430 | 2.99 | 6 | 1.00 | 0.67 |
| C9H8O6N1 | 227.0430 | 3.38 | 6 | 1.00 | 0.67 |
| C13H8O3N1 | 227.0582 | 8.23 | 10 | 0.69 | 0.23 |
| C7H3O7N2 | 228.0019 | 4.07 | 7 | 0.57 | 1.00 |
| C8H7O6N2 | 228.0382 | 4.69 | 6 | 1.00 | 0.75 |
| C11H15O5 | 228.0998 | 3.02 | 4 | 1.45 | 0.45 |
| C12H19O4 | 228.1362 | 6.64 | 3 | 1.67 | 0.33 |
| C6H2O7N3 | 228.9971 | 4.09 | 7 | 0.50 | 1.17 |
| C5H10O7N1S1 | 229.0256 | 2.74 | 1 | 2.20 | 1.40 |
| C12H6O4N1 | 229.0375 | 7.99 | 10 | 0.58 | 0.33 |
| C12H6O4N1 | 229.0375 | 8.06 | 10 | 0.58 | 0.33 |
| C13H10O3N1 | 229.0739 | 8.12 | 9 | 0.85 | 0.23 |
| C13H10O3N1 | 229.0739 | 8.20 | 9 | 0.85 | 0.23 |
| C8H5O4S2 | 229.9707 | 0.30 | 6 | 0.75 | 0.50 |
| C8H5O6S1 | 229.9885 | 2.52 | 6 | 0.75 | 0.75 |
| C10H13O6 | 230.0790 | 2.30 | 4 | 1.40 | 0.60 |
| C10H13O6 | 230.0790 | 2.71 | 4 | 1.40 | 0.60 |
| C10H13O6 | 230.0790 | 2.82 | 4 | 1.40 | 0.60 |
| C11H17O5 | 230.1154 | 3.21 | 3 | 1.64 | 0.45 |
| C11H17O5 | 230.1154 | 3.42 | 3 | 1.64 | 0.45 |
| C12H8O4N1 | 231.0532 | 7.44 | 9 | 0.75 | 0.33 |
| C10H15O6 | 232.0947 | 3.05 | 3 | 1.60 | 0.60 |
| C11H6O5N1 | 233.0324 | 7.22 | 9 | 0.64 | 0.45 |
| C10H5O5N2 | 234.0277 | 7.61 | 9 | 0.60 | 0.50 |
| C12H9O5 | 234.0528 | 3.19 | 8 | 0.83 | 0.42 |
| C12H11O5 | 236.0685 | 3.15 | 7 | 1.00 | 0.42 |
| C9H15O5S1 | 236.0718 | 2.66 | 2 | 1.78 | 0.56 |
| C10H5O3S2 | 237.9758 | 0.53 | 8 | 0.60 | 0.30 |

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|---|---|---|---|---|---|
| C7H9O7S1 | 238.0147 | 0.44 | 3 | 1.43 | 1.00 |
| C11H9O6 | 238.0477 | 2.85 | 7 | 0.91 | 0.55 |
| C11H9O6 | 238.0477 | 3.01 | 7 | 0.91 | 0.55 |
| C12H13O5 | 238.0841 | 3.42 | 6 | 1.17 | 0.42 |
| C12H13O5 | 238.0841 | 3.54 | 6 | 1.17 | 0.42 |
| C12H13O5 | 238.0841 | 3.58 | 6 | 1.17 | 0.42 |
| C9H17O5S1 | 238.0875 | 3.17 | 1 | 2.00 | 0.56 |
| C10H21O4S1 | 238.1239 | 7.95 | 0 | 2.20 | 0.40 |
| C14H8O3N1 | 239.0582 | 8.22 | 11 | 0.64 | 0.21 |
| C10H7O7 | 240.0270 | 2.65 | 7 | 0.80 | 0.70 |
| C8H13O9S1 | 286.0359 | 0.38 | 2 | 1.75 | 1.13 |
| C7H11O7S1 | 240.0304 | 0.90 | 2 | 1.71 | 1.00 |
| C14H7O4 | 240.0423 | 3.97 | 11 | 0.57 | 0.29 |
| C14H7O4 | 240.0423 | 7.13 | 11 | 0.57 | 0.29 |
| C14H7O4 | 240.0423 | 7.28 | 11 | 0.57 | 0.29 |
| C8H15O6S1 | 240.0668 | 2.76 | 1 | 2.00 | 0.75 |
| C8H15O6S1 | 240.0668 | 2.99 | 1 | 2.00 | 0.75 |
| C13H6O4N1 | 241.0375 | 7.83 | 11 | 0.54 | 0.31 |
| C7H13O7S1 | 242.0460 | 0.57 | 1 | 2.00 | 1.00 |
| C9H9O6N2 | 242.0539 | 6.82 | 6 | 1.11 | 0.67 |
| C14H9O4 | 242.0579 | 5.07 | 10 | 0.71 | 0.29 |
| C14H9O4 | 242.0579 | 7.48 | 10 | 0.71 | 0.29 |
| C8H4O8N1 | 243.0015 | 2.89 | 7 | 0.63 | 1.00 |
| C6H12O7N1S1 | 243.0413 | 3.46 | 1 | 2.17 | 1.17 |
| C11H15O6 | 244.0947 | 2.83 | 4 | 1.45 | 0.55 |
| C11H15O6 | 244.0947 | 2.90 | 4 | 1.45 | 0.55 |
| C12H19O5 | 244.1311 | 3.83 | 3 | 1.67 | 0.42 |
| C12H19O5 | 244.1311 | 3.94 | 3 | 1.67 | 0.42 |
| C12H19O5 | 244.1311 | 4.37 | 3 | 1.67 | 0.42 |
| C9H9O6S1 | 246.0198 | 2.88 | 5 | 1.11 | 0.67 |
| C9H9O8 | 246.0376 | 0.38 | 5 | 1.11 | 0.89 |
| C11H17O6 | 246.1103 | 4.39 | 3 | 1.64 | 0.55 |
| C8H3O4N6 | 248.0294 | 3.13 | 10 | 0.50 | 0.50 |
| C10H17O6S1 | 266.0824 | 2.99 | 2 | 1.80 | 0.60 |
| C7H5O8S1 | 249.9783 | 2.59 | 5 | 0.86 | 1.14 |
| C10H17O5S1 | 250.0875 | 3.09 | 2 | 1.80 | 0.50 |
| C14H4O2N1S1 | 251.0041 | 2.66 | 13 | 0.36 | 0.14 |
| C11H7O7 | 252.0270 | 2.75 | 8 | 0.73 | 0.64 |
| C8H11O7S1 | 252.0304 | 0.38 | 3 | 1.50 | 0.88 |
| C8H11O7S1 | 252.0304 | 0.62 | 3 | 1.50 | 0.88 |
| C9H15O6S1 | 252.0668 | 2.60 | 2 | 1.78 | 0.67 |
| C9H15O6S1 | 252.0668 | 3.91 | 2 | 1.78 | 0.67 |
| C9H15O6S1 | 252.0668 | 4.10 | 2 | 1.78 | 0.67 |
| C10H19O5S1 | 252.1031 | 7.01 | 1 | 2.00 | 0.50 |
| C11H23O4S1 | 252.1395 | 8.19 | 0 | 2.18 | 0.36 |
| C8H13O7S1 | 254.0460 | 1.05 | 2 | 1.75 | 0.88 |
| C8H13O7S1 | 254.0460 | 2.32 | 2 | 1.75 | 0.88 |
| C10H9O6N2 | 254.0539 | 7.80 | 7 | 1.00 | 0.60 |
| C9H17O6S1 | 254.0824 | 3.19 | 1 | 2.00 | 0.67 |
| C9H17O6S1 | 254.0824 | 3.54 | 1 | 2.00 | 0.67 |

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|---|---|---|---|---|---|
| C10H11O6N2 | 256.0695 | 8.04 | 6 | 1.20 | 0.60 |
| C14H23O4 | 256.1675 | 7.86 | 3 | 1.71 | 0.29 |
| C6H5O6N6 | 258.0349 | 0.55 | 7 | 1.00 | 1.00 |
| C12H17O6 | 258.1103 | 2.89 | 4 | 1.50 | 0.50 |
| C12H4O6N1 | 259.0117 | 3.87 | 11 | 0.42 | 0.50 |
| C6H12O8N1S1 | 259.0362 | 1.44 | 1 | 2.17 | 1.33 |
| C8H8O7N1S1 | 263.0100 | 3.61 | 5 | 1.13 | 0.88 |
| C10H15O6S1 | 264.0668 | 3.14 | 3 | 1.60 | 0.60 |
| C12H9O5S1 | 266.0249 | 3.34 | 8 | 0.83 | 0.42 |
| C8H11O8S1 | 268.0253 | 0.62 | 3 | 1.50 | 1.00 |
| C9H15O7S1 | 268.0617 | 2.15 | 2 | 1.78 | 0.78 |
| C9H15O7S1 | 268.0617 | 2.23 | 2 | 1.78 | 0.78 |
| C9H15O7S1 | 268.0617 | 2.50 | 2 | 1.78 | 0.78 |
| C9H15O7S1 | 268.0617 | 2.61 | 2 | 1.78 | 0.78 |
| C13H5O1N6S1 | 294.0324 | 2.35 | 14 | 0.46 | 0.08 |
| C16H15O4 | 272.1049 | 8.15 | 9 | 1.00 | 0.25 |
| C13H23O4N2 | 272.1736 | 2.33 | 3 | 1.85 | 0.31 |
| C7H14O8N1S1 | 273.0518 | 2.70 | 1 | 2.14 | 1.14 |
| C14H9O4S1 | 274.0300 | 7.09 | 10 | 0.71 | 0.29 |
| C9H8O7N1S1 | 275.0100 | 3.72 | 6 | 1.00 | 0.78 |
| C9H8O7N1S1 | 275.0100 | 4.22 | 6 | 1.00 | 0.78 |
| C9H3O5N6 | 276.0243 | 2.86 | 11 | 0.44 | 0.56 |
| C9H5O5N6 | 278.0400 | 3.01 | 10 | 0.67 | 0.56 |
| C10H15O7S1 | 280.0617 | 2.48 | 3 | 1.60 | 0.70 |
| C10H15O7S1 | 280.0617 | 2.69 | 3 | 1.60 | 0.70 |
| C8H11O9S1 | 284.0202 | 0.42 | 3 | 1.50 | 1.13 |
| C9H15O8S1 | 284.0566 | 2.50 | 2 | 1.78 | 0.89 |
| C15H21O8 | 330.1315 | 3.08 | 5 | 1.47 | 0.53 |
| C8H14O8N1S1 | 285.0518 | 2.99 | 2 | 1.88 | 1.00 |
| C15H9O6 | 286.0477 | 3.51 | 11 | 0.67 | 0.40 |
| C8H16O8N1S1 | 287.0675 | 2.90 | 1 | 2.13 | 1.00 |
| C8H16O8N1S1 | 287.0675 | 2.94 | 1 | 2.13 | 1.00 |
| C13H25O5S1 | 294.1501 | 7.60 | 1 | 2.00 | 0.38 |
| C13H25O5S1 | 294.1501 | 7.72 | 1 | 2.00 | 0.38 |
| C10H16O7N1S1 | 295.0726 | 4.71 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 6.33 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 6.61 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 6.85 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 7.02 | 3 | 1.70 | 0.70 |
| C10H16O7N1S1 | 295.0726 | 7.25 | 3 | 1.70 | 0.70 |
| C9H14O8N1S1 | 297.0518 | 2.82 | 3 | 1.67 | 0.89 |
| C9H14O8N1S1 | 297.0518 | 2.92 | 3 | 1.67 | 0.89 |
| C9H14O8N1S1 | 297.0518 | 3.27 | 3 | 1.67 | 0.89 |
| C7H6O7N7 | 301.0407 | 3.04 | 8 | 1.00 | 1.00 |
| C9H18O8N1S1 | 301.0831 | 3.40 | 1 | 2.11 | 0.89 |
| C5H9O11N2S1 | 306.0005 | 2.61 | 2 | 2.00 | 2.20 |
| C10H16O8N1S1 | 311.0675 | 3.52 | 3 | 1.70 | 0.80 |
| C10H18O8N1S1 | 313.0831 | 3.09 | 2 | 1.90 | 0.80 |
| C10H18O8N1S1 | 313.0831 | 3.40 | 2 | 1.90 | 0.80 |
| C17H13O6 | 314.0790 | 7.97 | 11 | 0.82 | 0.35 |

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|---|---|---|---|---|---|
| C19H21O4 | 314.1518 | 7.71 | 9 | 1.16 | 0.21 |
| C9H16O9N1S1 | 315.0624 | 2.54 | 2 | 1.89 | 1.00 |
| C8H11O11S1 | 316.0100 | 0.38 | 3 | 1.50 | 1.38 |
| C6H3O12N4 | 323.9826 | 2.59 | 7 | 0.67 | 2.00 |
| C10H16O9N1S1 | 327.0624 | 2.54 | 3 | 1.70 | 0.90 |
| C10H16O9N1S1 | 327.0624 | 2.83 | 3 | 1.70 | 0.90 |
| C10H18O9N1S1 | 329.0781 | 2.70 | 2 | 1.90 | 0.90 |
| C20H25O4 | 330.1831 | 7.61 | 8 | 1.30 | 0.20 |
| C11H19O10N2 | 340.1118 | 6.81 | 3 | 1.82 | 0.91 |
| C6H1O9N2S3 | 341.8922 | 0.27 | 7 | 0.33 | 1.50 |
| C10H16O10N1S1 | 343.0573 | 2.69 | 3 | 1.70 | 1.00 |
| C10H16O10N1S1 | 343.0573 | 2.88 | 3 | 1.70 | 1.00 |
| C16H31O6S1 | 352.1920 | 7.88 | 1 | 2.00 | 0.38 |
| C16H31O6S1 | 352.1920 | 8.10 | 1 | 2.00 | 0.38 |
| C7H20O10N7 | 363.1350 | 8.04 | 1 | 3.00 | 1.43 |
| C10H17O11N2S1 | 374.0631 | 3.16 | 3 | 1.80 | 1.10 |
| C10H17O11N2S1 | 374.0631 | 3.33 | 3 | 1.80 | 1.10 |
| C10H17O11N2S1 | 374.0631 | 3.68 | 3 | 1.80 | 1.10 |
| C10H17O11N2S1 | 374.0631 | 3.88 | 3 | 1.80 | 1.10 |
| C10H17O11N2S1 | 374.0631 | 4.56 | 3 | 1.80 | 1.10 |
| C20H17O8 | 386.1002 | 8.21 | 12 | 0.90 | 0.40 |
| C10H16O11N1S2 | 391.0243 | 3.09 | 3 | 1.70 | 1.10 |
| C20H17O9 | 402.0951 | 7.44 | 12 | 0.90 | 0.45 |
| C18H33O8S1 | 410.1974 | 8.19 | 2 | 1.89 | 0.44 |
| C10H16O13N3S1 | 419.0482 | 7.61 | 4 | 1.70 | 1.30 |
| C8H5O7N6S4 | 425.9181 | 0.27 | 9 | 0.75 | 0.88 |

Table S3.2.6 Molecular formulas of organic compounds detected in GZ in ESI+ mode.

| Formula [M+H]/[M+Na] | Neutral mass (Da) | RT (min) | DBE | H/C | O/C |
|---|---|---|---|---|---|
| C3H7O5N2 | 150.0277 | 0.28 | 2 | 2.00 | 1.67 |
| C6H11O2N2 | 142.0742 | 0.37 | 3 | 1.67 | 0.33 |
| C6H13O5 | 164.0685 | 0.36 | 1 | 2.00 | 0.83 |
| C8H12N1 | 121.0891 | 1.47 | 4 | 1.38 | 0.00 |
| C7H8N3 | 133.0640 | 0.38 | 6 | 1.00 | 0.00 |
| C7H12O1N3 | 153.0902 | 0.33 | 4 | 1.57 | 0.14 |
| C7H11O2N2 | 154.0742 | 0.43 | 4 | 1.43 | 0.29 |
| C7H16N1 | 113.1204 | 1.00 | 1 | 2.14 | 0.00 |
| C6H15N2 | 114.1157 | 1.24 | 1 | 2.33 | 0.00 |
| C6H15N2 | 114.1157 | 1.50 | 1 | 2.33 | 0.00 |
| C6H9O2N2 | 140.0586 | 0.38 | 4 | 1.33 | 0.33 |
| C7H7N2 | 118.0531 | 0.49 | 6 | 0.86 | 0.00 |
| C7H7N2 | 118.0531 | 0.76 | 6 | 0.86 | 0.00 |
| C6H6N3 | 119.0483 | 0.35 | 6 | 0.83 | 0.00 |
| C6H6N3 | 119.0483 | 2.76 | 6 | 0.83 | 0.00 |
| C8H10N1 | 119.0735 | 0.39 | 5 | 1.13 | 0.00 |
| C5H14O2N1 | 119.0946 | 0.32 | 0 | 2.60 | 0.40 |
| C7H9N2 | 120.0687 | 0.38 | 5 | 1.14 | 0.00 |
| C7H9N2 | 120.0687 | 0.58 | 5 | 1.14 | 0.00 |

| | | | | | |
|---|---|---|---|---|---|
| C10H15N2 | 162.1157 | 0.39 | 5 | 1.40 | 0.00 |
| C8H12N1 | 121.0891 | 0.76 | 4 | 1.38 | 0.00 |
| C8H12N1 | 121.0891 | 0.85 | 4 | 1.38 | 0.00 |
| C8H12N1 | 121.0891 | 1.49 | 4 | 1.38 | 0.00 |
| C7H11N2 | 122.0844 | 0.46 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.48 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.49 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.93 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 0.99 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.02 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.05 | 4 | 1.43 | 0.00 |
| C7H11N2 | 122.0844 | 1.15 | 4 | 1.43 | 0.00 |
| C7H10O1N1 | 123.0684 | 0.55 | 4 | 1.29 | 0.14 |
| C8H10N3 | 147.0796 | 0.38 | 6 | 1.13 | 0.00 |
| C5H9N4 | 124.0749 | 0.39 | 4 | 1.60 | 0.00 |
| C7H13N2 | 124.1000 | 0.39 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 0.56 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 0.70 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 0.89 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 0.99 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.31 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.86 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 1.97 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.09 | 3 | 1.71 | 0.00 |
| C7H13N2 | 124.1000 | 2.38 | 3 | 1.71 | 0.00 |
| C6H8O2N1 | 125.0477 | 0.38 | 4 | 1.17 | 0.33 |
| C6H8O2N1 | 125.0477 | 1.21 | 4 | 1.17 | 0.33 |
| C5H7O2N2 | 126.0429 | 0.44 | 4 | 1.20 | 0.40 |
| C7H15N2 | 126.1157 | 0.83 | 2 | 2.00 | 0.00 |
| C7H15N2 | 126.1157 | 1.50 | 2 | 2.00 | 0.00 |
| C8H18N1 | 127.1361 | 1.13 | 1 | 2.13 | 0.00 |
| C3H9O3N2S1 | 152.0256 | 0.28 | 1 | 2.67 | 1.00 |
| C7H16O1N1 | 129.1154 | 0.38 | 1 | 2.14 | 0.14 |
| C8H20N1 | 129.1517 | 2.54 | 0 | 2.38 | 0.00 |
| C8H7N2 | 130.0531 | 1.01 | 7 | 0.75 | 0.00 |
| C5H11O2N2 | 130.0742 | 0.33 | 2 | 2.00 | 0.40 |
| C4H10O2N3 | 131.0695 | 0.33 | 2 | 2.25 | 0.50 |
| C9H10N1 | 131.0735 | 0.39 | 6 | 1.00 | 0.00 |
| C9H10N1 | 131.0735 | 0.46 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 0.62 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.31 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 1.64 | 6 | 1.00 | 0.00 |
| C8H9N2 | 132.0687 | 2.15 | 6 | 1.00 | 0.00 |
| C7H8N3 | 133.0640 | 1.56 | 6 | 1.00 | 0.00 |
| C9H18O6N1S1 | 267.0777 | 3.73 | 2 | 1.89 | 0.67 |
| C8H7O2 | 134.0368 | 3.10 | 6 | 0.75 | 0.25 |
| C7H7O1N2 | 134.0480 | 0.57 | 6 | 0.86 | 0.14 |
| C7H7O1N2 | 134.0480 | 2.71 | 6 | 0.86 | 0.14 |
| C6H6O1N3 | 135.0433 | 0.37 | 6 | 0.83 | 0.17 |
| C8H10O1N1 | 135.0684 | 0.37 | 5 | 1.13 | 0.13 |

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|---|---|---|---|---|---|
| C8H13N2 | 136.1000 | 0.70 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 0.83 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 1.32 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.09 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.38 | 4 | 1.50 | 0.00 |
| C8H13N2 | 136.1000 | 2.47 | 4 | 1.50 | 0.00 |
| C7H8O2N1 | 137.0477 | 0.38 | 5 | 1.00 | 0.29 |
| C10H13N2 | 160.1000 | 0.39 | 6 | 1.20 | 0.00 |
| C8H12O1N1 | 137.0841 | 0.51 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 0.91 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.15 | 4 | 1.38 | 0.13 |
| C8H12O1N1 | 137.0841 | 1.29 | 4 | 1.38 | 0.13 |
| C12H12O2N1 | 201.0790 | 2.53 | 8 | 0.92 | 0.17 |
| C7H11O1N2 | 138.0793 | 0.38 | 4 | 1.43 | 0.14 |
| C7H11O1N2 | 138.0793 | 0.58 | 4 | 1.43 | 0.14 |
| C8H15N2 | 138.1157 | 1.27 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.48 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.57 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 1.77 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.03 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.15 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.29 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.47 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.61 | 3 | 1.75 | 0.00 |
| C8H15N2 | 138.1157 | 2.77 | 3 | 1.75 | 0.00 |
| C6H6O3N1 | 139.0269 | 0.37 | 5 | 0.83 | 0.50 |
| C6H6O3N1 | 139.0269 | 0.59 | 5 | 0.83 | 0.50 |
| C7H10O2N1 | 139.0633 | 0.38 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 0.67 | 4 | 1.29 | 0.29 |
| C7H10O2N1 | 139.0633 | 0.83 | 4 | 1.29 | 0.29 |
| C5H10N5 | 139.0858 | 0.39 | 4 | 1.80 | 0.00 |
| C8H14O1N1 | 139.0997 | 0.38 | 3 | 1.63 | 0.13 |
| C9H18N1 | 139.1361 | 1.79 | 2 | 1.89 | 0.00 |
| C8H17N2 | 140.1313 | 1.31 | 2 | 2.00 | 0.00 |
| C8H17N2 | 140.1313 | 2.43 | 2 | 2.00 | 0.00 |
| C6H8O3N1 | 141.0426 | 0.43 | 4 | 1.17 | 0.50 |
| C7H12O2N1 | 141.0790 | 0.34 | 3 | 1.57 | 0.29 |
| C6H7O4 | 142.0266 | 0.54 | 4 | 1.00 | 0.67 |
| C5H7O3N2 | 142.0378 | 0.39 | 4 | 1.20 | 0.60 |
| C6H11O2N2 | 142.0742 | 0.39 | 3 | 1.67 | 0.33 |
| C10H10N1 | 143.0735 | 1.41 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 1.78 | 7 | 0.90 | 0.00 |
| C10H10N1 | 143.0735 | 2.21 | 7 | 0.90 | 0.00 |
| C6H9O4 | 144.0423 | 0.69 | 3 | 1.33 | 0.67 |
| C5H9O3N2 | 144.0535 | 0.33 | 3 | 1.60 | 0.60 |
| C9H9N2 | 144.0687 | 1.26 | 7 | 0.89 | 0.00 |
| C9H9N2 | 144.0687 | 2.43 | 7 | 0.89 | 0.00 |
| C7H11O4N2 | 186.0641 | 0.36 | 4 | 1.43 | 0.57 |
| C9H8O1N1 | 145.0528 | 0.90 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 2.25 | 7 | 0.78 | 0.11 |

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|---|---|---|---|---|---|
| C9H8O1N1 | 145.0528 | 2.32 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 3.15 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 3.24 | 7 | 0.78 | 0.11 |
| C9H8O1N1 | 145.0528 | 2.40 | 7 | 0.78 | 0.11 |
| C6H12O3N1 | 145.0739 | 0.33 | 2 | 1.83 | 0.50 |
| C6H12O3N1 | 145.0739 | 0.64 | 2 | 1.83 | 0.50 |
| C10H12N1 | 145.0891 | 1.61 | 6 | 1.10 | 0.00 |
| C7H16O2N1 | 145.1103 | 0.36 | 1 | 2.14 | 0.29 |
| C5H7O5 | 146.0215 | 0.39 | 3 | 1.20 | 1.00 |
| C4H7O4N2 | 146.0328 | 0.33 | 3 | 1.50 | 1.00 |
| C9H7O2 | 146.0368 | 2.29 | 7 | 0.67 | 0.22 |
| C9H7O2 | 146.0368 | 3.07 | 7 | 0.67 | 0.22 |
| C9H7O2 | 146.0368 | 2.67 | 7 | 0.67 | 0.22 |
| C8H7O1N2 | 146.0480 | 2.63 | 7 | 0.75 | 0.13 |
| C5H11O3N2 | 146.0691 | 0.32 | 2 | 2.00 | 0.60 |
| C9H11N2 | 146.0844 | 0.48 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.06 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.21 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.29 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.35 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.44 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.53 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.76 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 1.87 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.30 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.39 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.53 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.60 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.75 | 6 | 1.11 | 0.00 |
| C9H11N2 | 146.0844 | 2.86 | 6 | 1.11 | 0.00 |
| C8H10N3 | 147.0796 | 0.49 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 0.55 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 0.67 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 2.26 | 6 | 1.13 | 0.00 |
| C8H10N3 | 147.0796 | 2.77 | 6 | 1.13 | 0.00 |
| C6H14O3N1 | 147.0895 | 0.32 | 1 | 2.17 | 0.50 |
| C10H14N1 | 147.1048 | 2.38 | 5 | 1.30 | 0.00 |
| C9H9O2 | 148.0524 | 2.97 | 6 | 0.89 | 0.22 |
| C8H9O1N2 | 148.0637 | 0.78 | 6 | 1.00 | 0.13 |
| C8H9O1N2 | 148.0637 | 3.25 | 6 | 1.00 | 0.13 |
| C9H13N2 | 148.1000 | 2.36 | 5 | 1.33 | 0.00 |
| C7H8O1N3 | 149.0589 | 0.38 | 6 | 1.00 | 0.14 |
| C5H12O4N1 | 149.0688 | 0.33 | 1 | 2.20 | 0.80 |
| C6H8N5 | 149.0701 | 0.50 | 6 | 1.17 | 0.00 |
| C9H12O1N1 | 149.0841 | 3.20 | 5 | 1.22 | 0.11 |
| C6H16O3N1 | 149.1052 | 0.32 | 0 | 2.50 | 0.50 |
| C10H16N1 | 149.1204 | 2.53 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 2.67 | 4 | 1.50 | 0.00 |
| C10H16N1 | 149.1204 | 2.81 | 4 | 1.50 | 0.00 |
| C8H7O3 | 150.0317 | 2.65 | 6 | 0.75 | 0.38 |

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|---|---|---|---|---|---|
| C5H8O2N2Na1 | 128.0586 | 0.37 | 3 | 1.60 | 0.40 |
| C6H7O1N4 | 150.0542 | 0.55 | 6 | 1.00 | 0.17 |
| C9H11O2 | 150.0681 | 2.94 | 5 | 1.11 | 0.22 |
| C8H11O1N2 | 150.0793 | 0.46 | 5 | 1.25 | 0.13 |
| C9H15N2 | 150.1157 | 1.52 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.26 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.55 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.80 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 2.89 | 4 | 1.56 | 0.00 |
| C9H15N2 | 150.1157 | 1.64 | 4 | 1.56 | 0.00 |
| C8H10O2N1 | 151.0633 | 0.74 | 5 | 1.13 | 0.25 |
| C8H10O2N1 | 151.0633 | 1.76 | 5 | 1.13 | 0.25 |
| C11H17O1N2 | 192.1263 | 0.40 | 5 | 1.45 | 0.09 |
| C9H14O1N1 | 151.0997 | 0.52 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 0.69 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 1.06 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.37 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.49 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 2.66 | 4 | 1.44 | 0.11 |
| C9H14O1N1 | 151.0997 | 0.79 | 4 | 1.44 | 0.11 |
| C8H9O3 | 152.0473 | 2.65 | 5 | 1.00 | 0.38 |
| C7H9O2N2 | 152.0586 | 0.45 | 5 | 1.14 | 0.29 |
| C8H13O3N2 | 184.0848 | 0.46 | 4 | 1.50 | 0.38 |
| C7H9O2N2 | 152.0586 | 0.48 | 5 | 1.14 | 0.29 |
| C7H9O2N2 | 152.0586 | 0.51 | 5 | 1.14 | 0.29 |
| C7H9O2N2 | 152.0586 | 0.79 | 5 | 1.14 | 0.29 |
| C9H17N2 | 152.1313 | 2.23 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.34 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.41 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.54 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.63 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.75 | 3 | 1.78 | 0.00 |
| C9H17N2 | 152.1313 | 2.86 | 3 | 1.78 | 0.00 |
| C7H8O3N1 | 153.0426 | 0.56 | 5 | 1.00 | 0.43 |
| C7H8O3N1 | 153.0426 | 1.06 | 5 | 1.00 | 0.43 |
| C7H8O3N1 | 153.0426 | 2.61 | 5 | 1.00 | 0.43 |
| C6H8O2N3 | 153.0538 | 0.41 | 5 | 1.17 | 0.33 |
| C8H12O2N1 | 153.0790 | 0.38 | 4 | 1.38 | 0.25 |
| C8H12O2N1 | 153.0790 | 0.99 | 4 | 1.38 | 0.25 |
| C6H7O3N2 | 154.0378 | 2.86 | 5 | 1.00 | 0.50 |
| C7H11O2N2 | 154.0742 | 0.47 | 4 | 1.43 | 0.29 |
| C7H11O2N2 | 154.0742 | 0.58 | 4 | 1.43 | 0.29 |
| C5H11N6 | 154.0967 | 0.71 | 4 | 2.00 | 0.00 |
| C7H10O3N1 | 155.0582 | 0.44 | 4 | 1.29 | 0.43 |
| C11H13N2 | 172.1000 | 2.77 | 7 | 1.09 | 0.00 |
| C7H9O4 | 156.0423 | 0.75 | 4 | 1.14 | 0.57 |
| C10H9N2 | 156.0687 | 1.64 | 8 | 0.80 | 0.00 |
| C8H11O4N2 | 198.0641 | 0.38 | 5 | 1.25 | 0.50 |
| C6H12O2N3 | 157.0851 | 0.38 | 3 | 1.83 | 0.33 |
| C11H12N1 | 157.0891 | 2.54 | 7 | 1.00 | 0.00 |

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|---|---|---|---|---|---|
| C11H12N1 | 157.0891 | 2.71 | 7 | 1.00 | 0.00 |
| C7H11O4 | 158.0579 | 2.75 | 3 | 1.43 | 0.57 |
| C7H11O4 | 158.0579 | 2.79 | 3 | 1.43 | 0.57 |
| C10H11N2 | 158.0844 | 1.88 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.41 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.48 | 7 | 1.00 | 0.00 |
| C10H11N2 | 158.0844 | 2.66 | 7 | 1.00 | 0.00 |
| C6H8O3N1 | 141.0426 | 0.38 | 4 | 1.17 | 0.50 |
| C6H10O4N1 | 159.0532 | 0.64 | 3 | 1.50 | 0.67 |
| C7H14O3N1 | 159.0895 | 0.35 | 2 | 1.86 | 0.43 |
| C11H15O3N2 | 222.1004 | 0.36 | 6 | 1.27 | 0.27 |
| C11H14N1 | 159.1048 | 2.54 | 6 | 1.18 | 0.00 |
| C10H9O2 | 160.0524 | 3.82 | 7 | 0.80 | 0.20 |
| C9H9O1N2 | 160.0637 | 2.37 | 7 | 0.89 | 0.11 |
| C10H13N2 | 160.1000 | 2.41 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.58 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.67 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.78 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.88 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 2.98 | 6 | 1.20 | 0.00 |
| C10H13N2 | 160.1000 | 3.07 | 6 | 1.20 | 0.00 |
| C6H12O4N1 | 161.0688 | 0.33 | 2 | 1.83 | 0.67 |
| C10H12O1N1 | 161.0841 | 0.60 | 6 | 1.10 | 0.10 |
| C9H12N3 | 161.0953 | 1.20 | 6 | 1.22 | 0.00 |
| C11H16N1 | 161.1204 | 2.89 | 5 | 1.36 | 0.00 |
| C9H7O3 | 162.0317 | 2.52 | 7 | 0.67 | 0.33 |
| C9H7O3 | 162.0317 | 2.64 | 7 | 0.67 | 0.33 |
| C10H15N2 | 162.1157 | 0.49 | 5 | 1.40 | 0.00 |
| C5H10O5N1 | 163.0481 | 0.33 | 2 | 1.80 | 1.00 |
| C8H10O1N3 | 163.0746 | 0.48 | 6 | 1.13 | 0.13 |
| C6H14O4N1 | 163.0845 | 0.32 | 1 | 2.17 | 0.67 |
| C7H10N5 | 163.0858 | 0.65 | 6 | 1.29 | 0.00 |
| C10H14O1N1 | 163.0997 | 0.61 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 0.74 | 5 | 1.30 | 0.10 |
| C10H14O1N1 | 163.0997 | 0.82 | 5 | 1.30 | 0.10 |
| C8H5O4 | 164.0110 | 1.08 | 7 | 0.50 | 0.50 |
| C8H5O4 | 164.0110 | 2.72 | 7 | 0.50 | 0.50 |
| C4H9O5N2 | 164.0433 | 0.33 | 2 | 2.00 | 1.25 |
| C9H9O3 | 164.0473 | 3.06 | 6 | 0.89 | 0.33 |
| C9H9O3 | 164.0473 | 3.36 | 6 | 0.89 | 0.33 |
| C8H9O2N2 | 164.0586 | 0.39 | 6 | 1.00 | 0.25 |
| C7H9O1N4 | 164.0698 | 0.80 | 6 | 1.14 | 0.14 |
| C8H16O5N1 | 205.0950 | 0.81 | 2 | 1.88 | 0.63 |
| C7H9O1N4 | 164.0698 | 0.89 | 6 | 1.14 | 0.14 |
| C9H13O1N2 | 164.0950 | 0.44 | 5 | 1.33 | 0.11 |
| C10H17N2 | 164.1313 | 2.54 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.63 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.77 | 4 | 1.60 | 0.00 |
| C10H17N2 | 164.1313 | 2.85 | 4 | 1.60 | 0.00 |
| C8H8O3N1 | 165.0426 | 1.25 | 6 | 0.88 | 0.38 |

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|---|---|---|---|---|---|
| C8H8O3N1 | 165.0426 | 3.20 | 6 | 0.88 | 0.38 |
| C9H12O2N1 | 165.0790 | 0.39 | 5 | 1.22 | 0.22 |
| C9H12O2N1 | 165.0790 | 0.62 | 5 | 1.22 | 0.22 |
| C10H16O1N1 | 165.1154 | 2.64 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 2.68 | 4 | 1.50 | 0.10 |
| C10H16O1N1 | 165.1154 | 2.77 | 4 | 1.50 | 0.10 |
| C12H17N2 | 188.1313 | 3.14 | 6 | 1.33 | 0.00 |
| C8H7O4 | 166.0266 | 2.57 | 6 | 0.75 | 0.50 |
| C8H5O3 | 148.0160 | 2.58 | 7 | 0.50 | 0.38 |
| C9H13N2 | 148.1000 | 0.38 | 5 | 1.33 | 0.00 |
| C10H19N2 | 166.1470 | 2.70 | 3 | 1.80 | 0.00 |
| C10H19N2 | 166.1470 | 2.86 | 3 | 1.80 | 0.00 |
| C10H19N2 | 166.1470 | 3.04 | 3 | 1.80 | 0.00 |
| C8H10O3N1 | 167.0582 | 0.40 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 0.70 | 5 | 1.13 | 0.38 |
| C8H10O3N1 | 167.0582 | 2.78 | 5 | 1.13 | 0.38 |
| C10H18O3N1 | 199.1208 | 0.38 | 3 | 1.70 | 0.30 |
| C10H18O3N1 | 199.1208 | 0.38 | 3 | 1.70 | 0.30 |
| C9H14O2N1 | 167.0946 | 0.68 | 4 | 1.44 | 0.22 |
| C9H14O2N1 | 167.0946 | 2.53 | 4 | 1.44 | 0.22 |
| C9H14O2N1 | 167.0946 | 2.75 | 4 | 1.44 | 0.22 |
| C11H5O2 | 168.0211 | 3.86 | 10 | 0.36 | 0.18 |
| C4H9O7 | 168.0270 | 2.65 | 1 | 2.00 | 1.75 |
| C11H9N2 | 168.0687 | 2.22 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.51 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.73 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 2.90 | 9 | 0.73 | 0.00 |
| C11H9N2 | 168.0687 | 3.01 | 9 | 0.73 | 0.00 |
| C9H13O3 | 168.0786 | 2.61 | 4 | 1.33 | 0.33 |
| C8H13O2N2 | 168.0899 | 0.39 | 4 | 1.50 | 0.25 |
| C8H10O2N1 | 151.0633 | 0.52 | 5 | 1.13 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.74 | 4 | 1.50 | 0.25 |
| C8H13O2N2 | 168.0899 | 0.85 | 4 | 1.50 | 0.25 |
| C7H8O4N1 | 169.0375 | 0.34 | 5 | 1.00 | 0.57 |
| C11H8O1N1 | 169.0528 | 2.90 | 9 | 0.64 | 0.09 |
| C8H12O3N1 | 169.0739 | 0.58 | 4 | 1.38 | 0.38 |
| C8H12O3N1 | 169.0739 | 0.75 | 4 | 1.38 | 0.38 |
| C8H11O4 | 170.0579 | 0.84 | 4 | 1.25 | 0.50 |
| C8H11O4 | 170.0579 | 1.94 | 4 | 1.25 | 0.50 |
| C8H11O4 | 170.0579 | 2.38 | 4 | 1.25 | 0.50 |
| C8H11O4 | 170.0579 | 2.41 | 4 | 1.25 | 0.50 |
| C11H11N2 | 170.0844 | 2.68 | 8 | 0.91 | 0.00 |
| C8H15O2N2 | 170.1055 | 0.38 | 3 | 1.75 | 0.25 |
| C8H15O2N2 | 170.1055 | 0.43 | 3 | 1.75 | 0.25 |
| C8H15O2N2 | 170.1055 | 0.46 | 3 | 1.75 | 0.25 |
| C8H15O2N2 | 170.1055 | 2.23 | 3 | 1.75 | 0.25 |
| C11H10O1N1 | 171.0684 | 1.79 | 8 | 0.82 | 0.09 |
| C11H10O1N1 | 171.0684 | 2.43 | 8 | 0.82 | 0.09 |
| C9H18O4N1 | 203.1158 | 0.38 | 2 | 1.89 | 0.44 |
| C12H14N1 | 171.1048 | 2.98 | 7 | 1.08 | 0.00 |

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|---|---|---|---|---|---|
| C12H14N1 | 171.1048 | 3.14 | 7 | 1.08 | 0.00 |
| C11H9O2 | 172.0524 | 3.25 | 8 | 0.73 | 0.18 |
| C8H13O4 | 172.0736 | 2.27 | 3 | 1.50 | 0.50 |
| C8H13O4 | 172.0736 | 2.45 | 3 | 1.50 | 0.50 |
| C8H13O4 | 172.0736 | 2.50 | 3 | 1.50 | 0.50 |
| C8H13O4 | 172.0736 | 3.05 | 3 | 1.50 | 0.50 |
| C7H13O3N2 | 172.0848 | 0.33 | 3 | 1.71 | 0.43 |
| C11H13N2 | 172.1000 | 2.67 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.74 | 7 | 1.09 | 0.00 |
| C11H13N2 | 172.1000 | 2.84 | 7 | 1.09 | 0.00 |
| C5H4O4N1S1 | 172.9783 | 0.28 | 5 | 0.60 | 0.80 |
| C7H12O4N1 | 173.0688 | 0.41 | 3 | 1.57 | 0.57 |
| C6H12O3N3 | 173.0800 | 0.33 | 3 | 1.83 | 0.50 |
| C11H12O1N1 | 173.0841 | 2.57 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.63 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.77 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.88 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 2.96 | 7 | 1.00 | 0.09 |
| C11H12O1N1 | 173.0841 | 3.03 | 7 | 1.00 | 0.09 |
| C10H24O1N1 | 173.1780 | 2.74 | 0 | 2.30 | 0.10 |
| C6H11O4N2 | 174.0641 | 0.33 | 3 | 1.67 | 0.67 |
| C11H15N2 | 174.1157 | 2.77 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 2.84 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 2.93 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 3.02 | 6 | 1.27 | 0.00 |
| C11H15N2 | 174.1157 | 3.32 | 6 | 1.27 | 0.00 |
| C5H6O4N1S1 | 174.9939 | 0.37 | 4 | 1.00 | 0.80 |
| C6H10O5N1 | 175.0481 | 0.38 | 3 | 1.50 | 0.83 |
| C7H14O4N1 | 175.0845 | 0.33 | 2 | 1.86 | 0.57 |
| C7H14O4N1 | 175.0845 | 0.43 | 2 | 1.86 | 0.57 |
| C7H14O4N1 | 175.0845 | 1.26 | 2 | 1.86 | 0.57 |
| C11H14O1N1 | 175.0997 | 1.25 | 6 | 1.18 | 0.09 |
| C10H14N3 | 175.1109 | 2.50 | 6 | 1.30 | 0.00 |
| C10H9O3 | 176.0473 | 3.15 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.32 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.42 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.72 | 7 | 0.80 | 0.30 |
| C10H9O3 | 176.0473 | 3.87 | 7 | 0.80 | 0.30 |
| C9H9O2N2 | 176.0586 | 0.79 | 7 | 0.89 | 0.22 |
| C6H13O4N2 | 176.0797 | 0.32 | 2 | 2.00 | 0.67 |
| C9H8O3N1 | 177.0426 | 2.72 | 7 | 0.78 | 0.33 |
| C9H12O1N3 | 177.0902 | 0.61 | 6 | 1.22 | 0.11 |
| C9H7O4 | 178.0266 | 2.22 | 7 | 0.67 | 0.44 |
| C10H11O3 | 178.0630 | 3.80 | 6 | 1.00 | 0.30 |
| C10H15O1N2 | 178.1106 | 0.51 | 5 | 1.40 | 0.10 |
| C11H19N2 | 178.1470 | 3.08 | 4 | 1.64 | 0.00 |
| C13H10N1 | 179.0735 | 2.89 | 10 | 0.69 | 0.00 |
| C13H13N2 | 196.1000 | 3.17 | 9 | 0.92 | 0.00 |
| C13H10N1 | 179.0735 | 3.32 | 10 | 0.69 | 0.00 |
| C13H10N1 | 179.0735 | 4.02 | 10 | 0.69 | 0.00 |

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|---|---|---|---|---|---|
| C13H10N1 | 179.0735 | 3.42 | 10 | 0.69 | 0.00 |
| C10H14O2N1 | 179.0946 | 0.39 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.43 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.48 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.57 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.70 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.88 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 0.95 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 1.05 | 5 | 1.30 | 0.20 |
| C10H14O2N1 | 179.0946 | 1.97 | 5 | 1.30 | 0.20 |
| C9H13O2N2 | 180.0899 | 2.76 | 5 | 1.33 | 0.22 |
| C11H21N2 | 180.1626 | 3.31 | 3 | 1.82 | 0.00 |
| C11H21N2 | 180.1626 | 3.37 | 3 | 1.82 | 0.00 |
| C5H9O1N3Na1S1 | 159.0466 | 5.09 | 3 | 1.80 | 0.20 |
| C8H8O4N1 | 181.0375 | 0.35 | 6 | 0.88 | 0.50 |
| C5H12O6N1 | 181.0586 | 0.37 | 1 | 2.20 | 1.20 |
| C9H12O3N1 | 181.0739 | 0.47 | 5 | 1.22 | 0.33 |
| C9H8O1N1 | 145.0528 | 0.87 | 7 | 0.78 | 0.11 |
| C9H12O3N1 | 181.0739 | 2.55 | 5 | 1.22 | 0.33 |
| C9H12O3N1 | 181.0739 | 2.87 | 5 | 1.22 | 0.33 |
| C6H16O5N1 | 181.0950 | 0.34 | 0 | 2.50 | 0.83 |
| C10H16O2N1 | 181.1103 | 0.48 | 4 | 1.50 | 0.20 |
| C9H16O1N3 | 181.1215 | 0.39 | 4 | 1.67 | 0.11 |
| C12H24N1 | 181.1830 | 3.28 | 2 | 1.92 | 0.00 |
| C12H11N2 | 182.0844 | 2.81 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 2.93 | 9 | 0.83 | 0.00 |
| C12H11N2 | 182.0844 | 2.97 | 9 | 0.83 | 0.00 |
| C10H15O3 | 182.0943 | 2.46 | 4 | 1.40 | 0.30 |
| C10H15O3 | 182.0943 | 2.58 | 4 | 1.40 | 0.30 |
| C10H15O3 | 182.0943 | 2.70 | 4 | 1.40 | 0.30 |
| C10H15O3 | 182.0943 | 3.08 | 4 | 1.40 | 0.30 |
| C10H15O3 | 182.0943 | 3.16 | 4 | 1.40 | 0.30 |
| C10H15O3 | 182.0943 | 4.34 | 4 | 1.40 | 0.30 |
| C9H15O2N2 | 182.1055 | 0.38 | 4 | 1.56 | 0.22 |
| C9H15O2N2 | 182.1055 | 0.89 | 4 | 1.56 | 0.22 |
| C11H23N2 | 182.1783 | 3.20 | 2 | 2.00 | 0.00 |
| C11H23N2 | 182.1783 | 3.25 | 2 | 2.00 | 0.00 |
| C11H23N2 | 182.1783 | 3.35 | 2 | 2.00 | 0.00 |
| C8H10O4N1 | 183.0532 | 0.40 | 5 | 1.13 | 0.50 |
| C5H14O4N1S1 | 183.0565 | 0.33 | 0 | 2.60 | 0.80 |
| C7H10O3N3 | 183.0644 | 0.38 | 5 | 1.29 | 0.43 |
| C13H14N1 | 183.1048 | 3.14 | 8 | 1.00 | 0.00 |
| C12H9O2 | 184.0524 | 3.47 | 9 | 0.67 | 0.17 |
| C9H13O4 | 184.0736 | 2.71 | 4 | 1.33 | 0.44 |
| C9H13O4 | 184.0736 | 2.83 | 4 | 1.33 | 0.44 |
| C8H13O3N2 | 184.0848 | 0.48 | 4 | 1.50 | 0.38 |
| C12H13N2 | 184.1000 | 3.14 | 8 | 1.00 | 0.00 |
| C10H17O3 | 184.1099 | 3.21 | 3 | 1.60 | 0.30 |
| C10H17O3 | 184.1099 | 3.52 | 3 | 1.60 | 0.30 |
| C9H17O2N2 | 184.1212 | 0.36 | 3 | 1.78 | 0.22 |

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|---|---|---|---|---|---|
| C12H12O1N1 | 185.0841 | 2.49 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.65 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.78 | 8 | 0.92 | 0.08 |
| C12H12O1N1 | 185.0841 | 2.91 | 8 | 0.92 | 0.08 |
| C9H16O3N1 | 185.1052 | 0.40 | 3 | 1.67 | 0.33 |
| C13H16N1 | 185.1204 | 3.22 | 7 | 1.15 | 0.00 |
| C13H16N1 | 185.1204 | 3.24 | 7 | 1.15 | 0.00 |
| C12H28N1 | 185.2143 | 4.12 | 0 | 2.25 | 0.00 |
| C8H11O5 | 186.0528 | 0.64 | 4 | 1.25 | 0.63 |
| C7H9O2N6 | 208.0709 | 1.58 | 7 | 1.14 | 0.29 |
| C9H15O4 | 186.0892 | 2.84 | 3 | 1.56 | 0.44 |
| C9H15O4 | 186.0892 | 2.94 | 3 | 1.56 | 0.44 |
| C9H15O4 | 186.0892 | 2.97 | 3 | 1.56 | 0.44 |
| C12H15N2 | 186.1157 | 2.93 | 7 | 1.17 | 0.00 |
| C12H15N2 | 186.1157 | 3.05 | 7 | 1.17 | 0.00 |
| C12H15N2 | 186.1157 | 3.15 | 7 | 1.17 | 0.00 |
| C8H19O1N4 | 186.1481 | 1.64 | 2 | 2.25 | 0.13 |
| C12H14O1N1 | 187.0997 | 2.83 | 7 | 1.08 | 0.08 |
| C8H13O5 | 188.0685 | 0.84 | 3 | 1.50 | 0.63 |
| C6H7O3N6 | 210.0501 | 1.95 | 7 | 1.00 | 0.50 |
| C9H17O4 | 188.1049 | 3.72 | 2 | 1.78 | 0.44 |
| C8H16O4N1 | 189.1001 | 0.47 | 2 | 1.88 | 0.50 |
| C8H16O4N1 | 189.1001 | 2.31 | 2 | 1.88 | 0.50 |
| C10H11O2N2 | 190.0742 | 0.54 | 7 | 1.00 | 0.20 |
| C10H11O2N2 | 190.0742 | 2.45 | 7 | 1.00 | 0.20 |
| C8H11O5N2 | 214.0590 | 0.37 | 5 | 1.25 | 0.63 |
| C5H10O5N3 | 191.0542 | 0.28 | 3 | 1.80 | 1.00 |
| C10H10O3N1 | 191.0582 | 3.16 | 7 | 0.90 | 0.30 |
| C9H10O2N3 | 191.0695 | 0.37 | 7 | 1.00 | 0.22 |
| C7H14O5N1 | 191.0794 | 0.33 | 2 | 1.86 | 0.71 |
| C9H5O5 | 192.0059 | 1.95 | 8 | 0.44 | 0.56 |
| C6H8O7Na1 | 192.0270 | 0.38 | 3 | 1.33 | 1.17 |
| C10H9O4 | 192.0423 | 2.94 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.10 | 7 | 0.80 | 0.40 |
| C10H9O4 | 192.0423 | 3.17 | 7 | 0.80 | 0.40 |
| C7H9O1N6 | 192.0760 | 2.73 | 7 | 1.14 | 0.14 |
| C9H8O4N1 | 193.0375 | 2.37 | 7 | 0.78 | 0.44 |
| C10H12O3N1 | 193.0739 | 0.38 | 6 | 1.10 | 0.30 |
| C14H12N1 | 193.0891 | 3.26 | 10 | 0.79 | 0.00 |
| C12H20O1N1 | 193.1467 | 2.68 | 4 | 1.58 | 0.08 |
| C9H7O5 | 194.0215 | 1.32 | 7 | 0.67 | 0.56 |
| C13H11N2 | 194.0844 | 2.99 | 10 | 0.77 | 0.00 |
| C11H15O3 | 194.0943 | 3.22 | 5 | 1.27 | 0.27 |
| C10H15O2N2 | 194.1055 | 1.57 | 5 | 1.40 | 0.20 |
| C10H15O2N2 | 194.1055 | 2.94 | 5 | 1.40 | 0.20 |
| C12H23N2 | 194.1783 | 6.84 | 3 | 1.83 | 0.00 |
| C12H23N2 | 194.1783 | 4.27 | 3 | 1.83 | 0.00 |
| C13H10O1N1 | 195.0684 | 6.93 | 10 | 0.69 | 0.08 |
| C10H14O3N1 | 195.0895 | 0.40 | 5 | 1.30 | 0.30 |
| C10H14O3N1 | 195.0895 | 0.56 | 5 | 1.30 | 0.30 |

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| C10H14O3N1 | 195.0895 | 1.07 | 5 | 1.30 | 0.30 |
| C10H14O3N1 | 195.0895 | 1.17 | 5 | 1.30 | 0.30 |
| C13H26N1 | 195.1987 | 3.34 | 2 | 1.92 | 0.00 |
| C10H13O4 | 196.0736 | 2.80 | 5 | 1.20 | 0.40 |
| C9H13O3N2 | 196.0848 | 0.43 | 5 | 1.33 | 0.33 |
| C13H13N2 | 196.1000 | 3.05 | 9 | 0.92 | 0.00 |
| C13H13N2 | 196.1000 | 3.20 | 9 | 0.92 | 0.00 |
| C11H17O3 | 196.1099 | 3.39 | 4 | 1.45 | 0.27 |
| C10H17O2N2 | 196.1212 | 2.24 | 4 | 1.60 | 0.20 |
| C10H17O2N2 | 196.1212 | 2.58 | 4 | 1.60 | 0.20 |
| C12H24O1N1 | 197.1780 | 2.59 | 2 | 1.92 | 0.08 |
| C12H7O3 | 198.0317 | 3.87 | 10 | 0.50 | 0.25 |
| C10H15O4 | 198.0892 | 2.90 | 4 | 1.40 | 0.40 |
| C10H15O4 | 198.0892 | 2.94 | 4 | 1.40 | 0.40 |
| C10H15O4 | 198.0892 | 3.14 | 4 | 1.40 | 0.40 |
| C9H15O3N2 | 198.1004 | 0.46 | 4 | 1.56 | 0.33 |
| C13H15N2 | 198.1157 | 2.98 | 8 | 1.08 | 0.00 |
| C8H14O3N3 | 199.0957 | 0.33 | 4 | 1.63 | 0.38 |
| C13H14O1N1 | 199.0997 | 2.72 | 8 | 1.00 | 0.08 |
| C13H14O1N1 | 199.0997 | 2.90 | 8 | 1.00 | 0.08 |
| C10H18O3N1 | 199.1208 | 0.41 | 3 | 1.70 | 0.30 |
| C12H9O3 | 200.0473 | 4.41 | 9 | 0.67 | 0.25 |
| C8H13O4N2 | 200.0797 | 0.33 | 4 | 1.50 | 0.50 |
| C10H20O4N1 | 217.1314 | 2.37 | 2 | 1.90 | 0.40 |
| C10H17O4 | 200.1049 | 2.56 | 3 | 1.60 | 0.40 |
| C10H17O4 | 200.1049 | 3.41 | 3 | 1.60 | 0.40 |
| C13H17N2 | 200.1313 | 3.16 | 7 | 1.23 | 0.00 |
| C8H12O5N1 | 201.0637 | 0.36 | 4 | 1.38 | 0.63 |
| C12H12O2N1 | 201.0790 | 1.01 | 8 | 0.92 | 0.17 |
| C12H12O2N1 | 201.0790 | 2.45 | 8 | 0.92 | 0.17 |
| C10H20O3N1 | 201.1365 | 0.36 | 2 | 1.90 | 0.30 |
| C12H11O3 | 202.0630 | 3.10 | 8 | 0.83 | 0.25 |
| C12H11O3 | 202.0630 | 3.56 | 8 | 0.83 | 0.25 |
| C11H11O2N2 | 202.0742 | 2.65 | 8 | 0.91 | 0.18 |
| C8H15O4N2 | 202.0954 | 0.33 | 3 | 1.75 | 0.50 |
| C13H19N2 | 202.1470 | 3.10 | 6 | 1.38 | 0.00 |
| C15H10N1 | 203.0735 | 3.30 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.13 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.21 | 12 | 0.60 | 0.00 |
| C15H10N1 | 203.0735 | 7.61 | 12 | 0.60 | 0.00 |
| C8H14O5N1 | 203.0794 | 0.60 | 3 | 1.63 | 0.63 |
| C9H18O4N1 | 203.1158 | 2.86 | 2 | 1.89 | 0.44 |
| C13H18O1N1 | 203.1310 | 2.77 | 6 | 1.31 | 0.08 |
| C8H12O6Na1 | 204.0634 | 2.34 | 3 | 1.50 | 0.75 |
| C8H9O1N6 | 204.0760 | 2.54 | 8 | 1.00 | 0.13 |
| C9H17O5 | 204.0998 | 2.62 | 2 | 1.78 | 0.56 |
| C12H17O1N2 | 204.1263 | 0.62 | 6 | 1.33 | 0.08 |
| C15H12N1 | 205.0891 | 2.78 | 11 | 0.73 | 0.00 |
| C7H7O2N6 | 206.0552 | 1.97 | 8 | 0.86 | 0.29 |
| C11H11O4 | 206.0579 | 3.03 | 7 | 0.91 | 0.36 |

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| C11H11O4 | 206.0579 | 3.40 | 7 | 0.91 | 0.36 |
| C12H19O1N2 | 206.1419 | 2.53 | 5 | 1.50 | 0.08 |
| C10H22O4Na1 | 206.1518 | 3.61 | 0 | 2.20 | 0.40 |
| C11H14O3N1 | 207.0895 | 0.54 | 6 | 1.18 | 0.27 |
| C11H14O3N1 | 207.0895 | 0.99 | 6 | 1.18 | 0.27 |
| C12H18O2N1 | 207.1259 | 2.43 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.46 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.56 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.61 | 5 | 1.42 | 0.17 |
| C12H18O2N1 | 207.1259 | 2.74 | 5 | 1.42 | 0.17 |
| C11H18O1N3 | 207.1372 | 2.40 | 5 | 1.55 | 0.09 |
| C9H14O4Na1 | 186.0892 | 2.95 | 3 | 1.56 | 0.44 |
| C14H13N2 | 208.1000 | 3.14 | 10 | 0.86 | 0.00 |
| C9H20O5Na1 | 208.1311 | 2.47 | 0 | 2.22 | 0.56 |
| C10H12O4N1 | 209.0688 | 0.39 | 6 | 1.10 | 0.40 |
| C14H12O1N1 | 209.0841 | 7.60 | 10 | 0.79 | 0.07 |
| C7H16O6N1 | 209.0899 | 0.38 | 1 | 2.14 | 0.86 |
| C9H7O6 | 210.0164 | 1.06 | 7 | 0.67 | 0.67 |
| C6H7O3N6 | 210.0501 | 1.32 | 7 | 1.00 | 0.50 |
| C7H11O2N6 | 210.0865 | 2.63 | 6 | 1.43 | 0.29 |
| C14H15N2 | 210.1157 | 3.40 | 9 | 1.00 | 0.00 |
| C14H14N2Na1 | 210.1157 | 7.23 | 9 | 1.00 | 0.00 |
| C11H19O2N2 | 210.1368 | 2.63 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 2.93 | 4 | 1.64 | 0.18 |
| C11H19O2N2 | 210.1368 | 2.97 | 4 | 1.64 | 0.18 |
| C6H14O1N1S3 | 211.0159 | 0.77 | 1 | 2.17 | 0.17 |
| C6H14O7N1 | 211.0692 | 0.36 | 1 | 2.17 | 1.17 |
| C13H14N3 | 211.1109 | 3.03 | 9 | 1.00 | 0.00 |
| C5H5O4N6 | 212.0294 | 0.49 | 7 | 0.80 | 0.80 |
| C13H13O1N2 | 212.0950 | 2.45 | 9 | 0.92 | 0.08 |
| C11H17O4 | 212.1049 | 2.87 | 4 | 1.45 | 0.36 |
| C11H17O4 | 212.1049 | 3.00 | 4 | 1.45 | 0.36 |
| C10H17O3N2 | 212.1161 | 3.11 | 4 | 1.60 | 0.30 |
| C14H16O1N1 | 213.1154 | 2.75 | 8 | 1.07 | 0.07 |
| C14H16O1N1 | 213.1154 | 3.03 | 8 | 1.07 | 0.07 |
| C8H11O5N2 | 214.0590 | 0.37 | 5 | 1.25 | 0.63 |
| C10H15O5 | 214.0841 | 2.67 | 4 | 1.40 | 0.50 |
| C10H15O5 | 214.0841 | 2.81 | 4 | 1.40 | 0.50 |
| C13H14O2N1 | 215.0946 | 2.43 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 2.61 | 8 | 1.00 | 0.15 |
| C13H14O2N1 | 215.0946 | 2.96 | 8 | 1.00 | 0.15 |
| C8H12O6N1 | 217.0586 | 0.38 | 4 | 1.38 | 0.75 |
| C12H12O3N1 | 217.0739 | 0.70 | 8 | 0.92 | 0.25 |
| C9H16O5N1 | 217.0950 | 0.38 | 3 | 1.67 | 0.56 |
| C7H11O6N2 | 218.0539 | 0.35 | 4 | 1.43 | 0.86 |
| C12H11O4 | 218.0579 | 3.15 | 8 | 0.83 | 0.33 |
| C8H15O5N2 | 218.0903 | 0.33 | 3 | 1.75 | 0.63 |
| C8H9O2N6 | 220.0709 | 2.73 | 8 | 1.00 | 0.25 |
| C8H9O2N6 | 220.0709 | 2.77 | 8 | 1.00 | 0.25 |
| C12H17O2N2 | 220.1212 | 0.33 | 6 | 1.33 | 0.17 |

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| C8H16O6N1 | 221.0899 | 0.47 | 2 | 1.88 | 0.75 |
| C8H16O6N1 | 221.0899 | 0.76 | 2 | 1.88 | 0.75 |
| C13H20O2N1 | 221.1416 | 2.75 | 5 | 1.46 | 0.15 |
| C13H20O2N1 | 221.1416 | 2.86 | 5 | 1.46 | 0.15 |
| C13H20O2N1 | 221.1416 | 2.88 | 5 | 1.46 | 0.15 |
| C7H7O3N6 | 222.0501 | 1.47 | 8 | 0.86 | 0.43 |
| C10H16O4Na1 | 200.1049 | 2.91 | 3 | 1.60 | 0.40 |
| C12H15O4 | 222.0892 | 7.48 | 6 | 1.17 | 0.33 |
| C7H14O7N1 | 223.0692 | 0.38 | 2 | 1.86 | 1.00 |
| C10H14O3N3 | 223.0957 | 0.38 | 6 | 1.30 | 0.30 |
| C8H18O6N1 | 223.1056 | 0.39 | 1 | 2.13 | 0.75 |
| C14H9O3 | 224.0473 | 7.31 | 11 | 0.57 | 0.21 |
| C9H14O5Na1 | 202.0841 | 2.64 | 3 | 1.56 | 0.56 |
| C9H14O5Na1 | 202.0841 | 2.69 | 3 | 1.56 | 0.56 |
| C9H11O5N2 | 226.0590 | 0.38 | 6 | 1.11 | 0.56 |
| C12H23O2N2 | 226.1681 | 1.50 | 3 | 1.83 | 0.17 |
| C12H23O2N2 | 226.1681 | 2.34 | 3 | 1.83 | 0.17 |
| C7H3O1N5Na1S1 | 205.0058 | 0.77 | 9 | 0.43 | 0.14 |
| C14H14O2N1 | 227.0946 | 2.70 | 9 | 0.93 | 0.14 |
| C15H18O1N1 | 227.1310 | 3.09 | 8 | 1.13 | 0.07 |
| C11H17O5 | 228.0998 | 3.03 | 4 | 1.45 | 0.45 |
| C10H17O4N2 | 228.1110 | 0.38 | 4 | 1.60 | 0.40 |
| C10H16O5N1 | 229.0950 | 0.38 | 4 | 1.50 | 0.50 |
| C14H16O2N1 | 229.1103 | 2.83 | 8 | 1.07 | 0.14 |
| C6H9O3N2S3 | 251.9697 | 0.30 | 4 | 1.33 | 0.50 |
| C17H11O1 | 230.0732 | 8.33 | 13 | 0.59 | 0.06 |
| C17H11O1 | 230.0732 | 8.44 | 13 | 0.59 | 0.06 |
| C6H11O4N6 | 230.0764 | 0.31 | 5 | 1.67 | 0.67 |
| C9H15O5N2 | 230.0903 | 0.33 | 4 | 1.56 | 0.56 |
| C14H19O1N2 | 230.1419 | 2.98 | 7 | 1.29 | 0.07 |
| C13H14O3N1 | 231.0895 | 2.69 | 8 | 1.00 | 0.23 |
| C11H22O4N1 | 231.1471 | 2.78 | 2 | 1.91 | 0.36 |
| C15H22O1N1 | 231.1623 | 3.14 | 6 | 1.40 | 0.07 |
| C9H6O6Na1 | 210.0164 | 1.95 | 7 | 0.67 | 0.67 |
| C16H9O2 | 232.0524 | 7.64 | 13 | 0.50 | 0.13 |
| C14H21O1N2 | 232.1576 | 0.33 | 6 | 1.43 | 0.07 |
| C4H5O5N1Na1S2 | 210.9609 | 0.29 | 3 | 1.25 | 1.25 |
| C14H20O2N1 | 233.1416 | 2.90 | 6 | 1.36 | 0.14 |
| C13H19O2N2 | 234.1368 | 0.32 | 6 | 1.38 | 0.15 |
| C16H27O3 | 266.1882 | 8.06 | 4 | 1.63 | 0.19 |
| C6H6O3N1S3 | 234.9432 | 0.37 | 5 | 0.83 | 0.50 |
| C7H7O5N3Na1 | 213.0386 | 0.60 | 6 | 1.00 | 0.71 |
| C8H14O7N1 | 235.0692 | 0.38 | 3 | 1.63 | 0.88 |
| C14H22O2N1 | 235.1572 | 2.94 | 5 | 1.50 | 0.14 |
| C14H22O2N1 | 235.1572 | 3.00 | 5 | 1.50 | 0.14 |
| C11H9O6 | 236.0321 | 2.41 | 8 | 0.73 | 0.55 |
| C7H9O3N3Na1S1 | 215.0365 | 0.60 | 5 | 1.29 | 0.43 |
| C11H12O5N1 | 237.0637 | 0.38 | 7 | 1.00 | 0.45 |
| C12H8O4Na1 | 216.0423 | 3.89 | 9 | 0.67 | 0.33 |
| C8H11O3N6 | 238.0814 | 2.65 | 7 | 1.25 | 0.38 |

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|---|---|---|---|---|---|
| C8H11O3N6 | 238.0814 | 2.82 | 7 | 1.25 | 0.38 |
| C10H16O5Na1 | 216.0998 | 2.93 | 3 | 1.60 | 0.50 |
| C11H15O4N2 | 238.0954 | 0.38 | 6 | 1.27 | 0.36 |
| C13H19N2 | 202.1470 | 3.11 | 6 | 1.38 | 0.00 |
| C7H9O4N6 | 240.0607 | 2.69 | 7 | 1.14 | 0.57 |
| C12H21O3N2 | 240.1474 | 2.68 | 4 | 1.67 | 0.25 |
| C8H12O7Na1 | 220.0583 | 0.38 | 3 | 1.50 | 0.88 |
| C14H11O4 | 242.0579 | 5.09 | 10 | 0.71 | 0.29 |
| C12H19O5 | 242.1154 | 2.91 | 4 | 1.50 | 0.42 |
| C13H23O4 | 242.1518 | 7.49 | 3 | 1.69 | 0.31 |
| C10H14O6N1 | 243.0743 | 0.38 | 5 | 1.30 | 0.60 |
| C14H17O2N2 | 244.1212 | 3.14 | 8 | 1.14 | 0.14 |
| C10H16O6N1 | 245.0899 | 2.69 | 4 | 1.50 | 0.60 |
| C9H14O7N1 | 247.0692 | 0.38 | 4 | 1.44 | 0.78 |
| C12H16O6N1 | 269.0899 | 0.38 | 6 | 1.25 | 0.50 |
| C15H21O3 | 248.1412 | 7.38 | 6 | 1.33 | 0.20 |
| C14H21O2N2 | 248.1525 | 0.32 | 6 | 1.43 | 0.14 |
| C16H11O3 | 250.0630 | 7.63 | 12 | 0.63 | 0.19 |
| C8H15O5N2S1 | 250.0623 | 7.64 | 3 | 1.75 | 0.63 |
| C8H15O5N2S1 | 250.0623 | 7.64 | 3 | 1.75 | 0.63 |
| C16H11O3 | 250.0630 | 7.65 | 12 | 0.63 | 0.19 |
| C11H16O5Na1 | 228.0998 | 2.88 | 4 | 1.45 | 0.45 |
| C12H20O4Na1 | 228.1362 | 2.81 | 3 | 1.67 | 0.33 |
| C13H19O3N2 | 250.1317 | 0.32 | 6 | 1.38 | 0.23 |
| C8H14O8N1 | 251.0641 | 0.38 | 3 | 1.63 | 1.00 |
| C11H15O5N2 | 254.0903 | 0.38 | 6 | 1.27 | 0.45 |
| C13H23O3N2 | 254.1630 | 2.76 | 4 | 1.69 | 0.23 |
| C16H22N3 | 255.1735 | 7.23 | 8 | 1.31 | 0.00 |
| C11H18O6N1 | 259.1056 | 0.39 | 4 | 1.55 | 0.55 |
| C12H14O5Na1 | 238.0841 | 3.42 | 6 | 1.17 | 0.42 |
| C9H14O8N1 | 263.0641 | 0.38 | 4 | 1.44 | 0.89 |
| C14H21O3N2 | 264.1474 | 0.32 | 6 | 1.43 | 0.21 |
| C9H16O8N1 | 265.0798 | 0.38 | 3 | 1.67 | 0.89 |
| C12H15O5N2 | 266.0903 | 0.38 | 7 | 1.17 | 0.42 |
| C16H29O3 | 268.2038 | 7.83 | 3 | 1.75 | 0.19 |
| C16H29O3 | 268.2038 | 8.49 | 3 | 1.75 | 0.19 |
| C5H4O4N1S4 | 268.8945 | 0.29 | 5 | 0.60 | 0.80 |
| C11H13O4N2 | 236.0797 | 0.38 | 7 | 1.09 | 0.36 |
| C18H11O3 | 274.0630 | 7.95 | 14 | 0.56 | 0.17 |
| C10H16O8N1 | 277.0798 | 0.38 | 4 | 1.50 | 0.80 |
| C8H15O7N4 | 278.0862 | 7.71 | 4 | 1.75 | 0.88 |
| C14H19O4N2 | 278.1267 | 0.32 | 7 | 1.29 | 0.29 |
| C12H23O6 | 262.1416 | 3.45 | 2 | 1.83 | 0.50 |
| C6H4O6N1S3 | 280.9122 | 0.29 | 6 | 0.50 | 1.00 |
| C14H23O4N2 | 282.1580 | 2.87 | 5 | 1.57 | 0.29 |
| C14H21O6 | 284.1260 | 3.07 | 5 | 1.43 | 0.43 |
| C16H29O4 | 284.1988 | 7.91 | 3 | 1.75 | 0.25 |
| C10H18O8Na1 | 266.1002 | 2.92 | 2 | 1.80 | 0.80 |
| C12H26O6Na1 | 266.1729 | 2.76 | 0 | 2.17 | 0.50 |
| C15H19O4N2 | 290.1267 | 0.32 | 8 | 1.20 | 0.27 |

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|---|---|---|---|---|---|
| C5H7O10N1Na1S1 | 272.9791 | 0.28 | 3 | 1.40 | 2.00 |
| C15H22O3N1S1 | 295.1242 | 2.52 | 6 | 1.40 | 0.20 |
| C6H6O7N1S3 | 298.9228 | 0.29 | 5 | 0.83 | 1.17 |
| C12H22O7Na1 | 278.1366 | 2.89 | 2 | 1.83 | 0.58 |
| C4H7O12N4 | 301.9982 | 2.63 | 4 | 1.50 | 3.00 |
| C14H26O6N1 | 303.1682 | 7.75 | 3 | 1.79 | 0.43 |
| C10H21O8N1Na1 | 283.1267 | 3.12 | 1 | 2.10 | 0.80 |
| C6H6O4N5S3 | 306.9504 | 0.28 | 7 | 0.83 | 0.67 |
| C7H18O7N7 | 311.1189 | 2.95 | 3 | 2.43 | 1.00 |
| C16H23O5N2 | 322.1529 | 0.38 | 7 | 1.38 | 0.31 |
| C16H23O5N2 | 322.1529 | 0.47 | 7 | 1.38 | 0.31 |
| C16H23O5N2 | 322.1529 | 0.48 | 7 | 1.38 | 0.31 |
| C8H15O10N4 | 326.0710 | 8.50 | 4 | 1.75 | 1.25 |
| C13H27O2N6S1 | 330.1838 | 7.61 | 4 | 2.00 | 0.15 |
| C18H34O5N1 | 343.2359 | 3.24 | 3 | 1.83 | 0.28 |
| C20H44O5N1 | 377.3141 | 8.42 | 0 | 2.15 | 0.25 |
| C23H26O7Na1 | 414.1679 | 8.30 | 11 | 1.13 | 0.30 |
| C24H52O6N1 | 449.3716 | 8.68 | 0 | 2.13 | 0.25 |

# **C.** Supplementary material to chapter 4

## “Molecular characterization and source prediction of atmospheric particulate organosulfates using ultrahigh resolution mass spectrometry

Table S4.3.1: List of the molecular formulas of OS and nitrooxy-OS generated from smog chamber experiments.

| Molecular Weight (MW) | Formula | precursor | Ref. |
|---|---|---|---|
| 139.9779437 | C2H4O5S | isoprene | Surratt et al., 2007 |
| 153.9935937 | C3H6O5S | isoprene | Surratt et al., 2007 |
| 155.9728583 | C2H4O6S | isoprene | Surratt et al., 2007 |
| 169.9885083 | C3H6O6S | isoprene | Surratt et al., 2007 |
| 199.9990729 | C4H8O7S | isoprene | Surratt et al., 2007 |
| 211.9990729 | C5H8O7S | isoprene | Surratt et al., 2007 |
| 214.0147229 | C5H10O7S | isoprene | Surratt et al., 2007 |
| 216.0303729 | C5H12O7S | isoprene | synthesized |
| 302.0307667 | C8H14O10S | isoprene | Surratt et al., 2007 |
| 332.0777167 | C10H20O10S | isoprene | Surratt et al., 2007 |
| 334.0933667 | C10H22O10S | isoprene | Surratt et al., 2007 |
| 452.1563605 | C15H32O13S | isoprene | Surratt et al., 2007 |
| 224.0354583 | C7H12O6S | α-pinene | Surratt et al., 2007 |
| 227.9939875 | C5H8O8S | α-pinene | Surratt et al., 2007 |
| 238.0511083 | C8H14O6S | α-pinene | Surratt et al., 2007 |
| 248.0718437 | C10H16O5S | α-pinene | Surratt et al., 2007 |
| 250.0874937 | C10H18O5S | α-pinene | Surratt et al., 2007 |
| 266.0824083 | C10H18O6S | α-pinene | Surratt et al., 2007 |
| 280.0616729 | C10H16O7S | α-pinene | Surratt et al., 2007 |
| 282.0773229 | C10H18O7S | α-pinene | Surratt et al., 2007 |
| 298.0722375 | C10H18O8S | α-pinene | Surratt et al., 2007 |
| 240.0303729 | C7H12O7S | limonene | Surratt et al., 2007 |
| 250.0511083 | C9H14O6S | limonene | Surratt et al., 2007 |
| 252.0667583 | C9H16O6S | limonene | Surratt et al., 2007 |
| 268.0616729 | C9H16O7S | limonene | Surratt et al., 2007 |

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|---|---|---|---|
| 280.0616729 | C10H16O7S | limonene | Surratt et al., 2007 |
| 282.0773229 | C10H18O7S | limonene | Surratt et al., 2007 |
| 254.0460229 | C8H14O7S | α-terpinene | Surratt et al., 2007 |
| 266.0824083 | C10H18O6S | α-terpinene | Surratt et al., 2007 |
| 280.0616729 | C10H16O7S | α-terpinene | Surratt et al., 2007 |
| 282.0773229 | C10H18O7S | α-terpinene | Surratt et al., 2007 |
| 330.0443082 | C10H18O8S | α-terpinene | Surratt et al., 2007 |
| 284.0565875 | C9H16O8S | α-terpinene | Surratt et al., 2007 |
| 284.0929729 | C10H20O7S | α-terpinene | Surratt et al., 2007 |
| 280.0616729 | C10H16O7S | γ-terpinene | Surratt et al., 2007 |
| 250.0511083 | C9H14O6S | terpinolene | Surratt et al., 2007 |
| 250.0874937 | C10H18O5S | terpinolene | Surratt et al., 2007 |
| 266.0824083 | C10H18O6S | terpinolene | Surratt et al., 2007 |
| 282.0773229 | C10H18O7S | terpinolene | Surratt et al., 2007 |
| 284.0929729 | C10H20O7S | terpinolene | Surratt et al., 2007 |
| 298.0722375 | C10H18O8S | terpinolene | Surratt et al., 2007 |
| 250.0874937 | C10H18O5S | β-pinene | Surratt et al., 2007 |
| 264.0667583 | C10H16O6S | β-pinene | Surratt et al., 2007 |
| 280.0616729 | C10H16O7S | β-pinene | Surratt et al., 2007 |
| 282.0773229 | C10H18O7S | β-pinene | Surratt et al., 2007 |
| 284.0929729 | C10H20O7S | β-pinene | Surratt et al., 2007 |
| 252.0667583 | C9H16O6S | β-caryophyllene | Chan et al., 2011 |
| 304.1344437 | C14H24O5S | β-caryophyllene | Chan et al., 2011 |
| 318.1500937 | C15H26O5S | β-caryophyllene | Chan et al., 2011 |
| 320.1293583 | C14H24O6S | β-caryophyllene | Chan et al., 2011 |
| 334.1086229 | C14H22O7S | β-caryophyllene | Chan et al., 2011 |
| 334.1450083 | C15H26O6S | β-caryophyllene | Chan et al., 2011 |
| 348.1242729 | C15H24O7S | β-caryophyllene | Chan et al., 2011 |
| 350.1035375 | C14H22O8S | β-caryophyllene | Chan et al., 2011 |
| 350.1399229 | C15H26O7S | β-caryophyllene | Chan et al., 2011 |
| 352.1191875 | C14H24O8S | β-caryophyllene | Chan et al., 2011 |
| 364.1191875 | C15H24O8S | β-caryophyllene | Chan et al., 2011 |

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|---|---|---|---|
| 364.1555729 | C16H28O7S | β-caryophyllene | Chan et al., 2011 |
| 380.1504875 | C16H28O8S | β-caryophyllene | Chan et al., 2011 |
| 210.0561937 | C7H14O5S | dodecane | Riva et al., 2016 |
| 238.0874937 | C9H18O5S | dodecane | Riva et al., 2016 |
| 252.1031437 | C10H20O5S | cyclodecane | Riva et al., 2016 |
| 266.0824083 | C10H18O6S | cyclodecane | Riva et al., 2016 |
| 268.0616729 | C9H16O7S | decalin | Riva et al., 2016 |
| 270.0773229 | C9H18O7S | decalin | Riva et al., 2016 |
| 280.0616729 | C10H16O7S | cyclodecane | Riva et al., 2016 |
| 280.1344437 | C12H24O5S | dodecane | Riva et al., 2016 |
| 286.0722375 | C9H18O8S | decalin | Riva et al., 2016 |
| 296.0565875 | C10H16O8S | decalin | Riva et al., 2016 |
| 298.0722375 | C10H18O8S | decalin | Riva et al., 2016 |
| 210.0925791 | C8H18SO4 | octyl OS | commercial available |
| 266.1551791 | C12H26SO4 | dodecyl OS | commercial available |
| 258.0198083 | C10H10O6S | naphthalene | Riva et al., 2015 |
| 274.0147229 | C10H10O7S | naphthalene | Riva et al., 2015 |
| 276.0303729 | C10H12O7S | naphthalene | Riva et al., 2015 |
| 232.0405437 | C9H12O5S | 2-methylnaphthalene | Riva et al., 2015 |
| 288.0303729 | C11H12O7S | 2-methylnaphthalene | Riva et al., 2015 |
| 290.0460229 | C11H14O7S | 2-methylnaphthalene | Riva et al., 2015 |
| 202.0299791 | C8H10S1O4 | benzene | synthesized |
| 216.0456291 | C9H12S1O4 | benzene | synthesized |
| 202.0299791 | C8H10S1O4 | benzene | synthesized |
| 173.9986791 | C6H6S1O4 | benzene | synthesized |
| 188.0143291 | C7H8S1O4 | benzene | synthesized |
| 216.0456291 | C9H12S1O4 | benzene | synthesized |
| 245.0205365 | C5H11NO8S | isoprene | Surratt et al., 2007 |
| 261.0154511 | C5H11NO9S | isoprene | Surratt et al., 2007 |
| 306.0005293 | C5H10N2O11S | isoprene | Surratt et al., 2007 |
| 347.0158449 | C8H13NO12S | isoprene | Surratt et al., 2007 |
| 295.0725719 | C10H17NO7S | α-pinene | Surratt et al., 2007 |

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|---|---|---|---|
| 311.0674865 | C10H17NO8S | α-pinene | Surratt et al., 2007 |
| 340.0576501 | C10H16N2O9S | α-pinene | Surratt et al., 2007 |
| 343.0573157 | C10H17NO10S | α-pinene | Surratt et al., 2007 |
| 356.0525647 | C10H16N2O10S | α-pinene | Surratt et al., 2007 |
| 297.0518365 | C9H15NO8S | limonene | Surratt et al., 2007 |
| 313.0467511 | C9H15NO9S | limonene | Surratt et al., 2007 |
| 327.0624011 | C10H17NO9S | limonene | Surratt et al., 2007 |
| 329.0780511 | C10H19NO9S | limonene | Surratt et al., 2007 |
| 331.0573157 | C9H17NO10S | limonene | Surratt et al., 2007 |
| 374.0631293 | C10H18N2O11S | limonene | Surratt et al., 2007 |
| 390.0580439 | C10H18N2O12S | limonene | Surratt et al., 2007 |
| 295.0725719 | C10H17NO7S | α-terpinene | Surratt et al., 2007 |
| 311.0674865 | C10H17NO8S | α-terpinene | Surratt et al., 2007 |
| 343.0573157 | C10H17NO10S | α-terpinene | Surratt et al., 2007 |
| 374.0631293 | C10H18N2O11S | α-terpinene | Surratt et al., 2007 |
| 311.0674865 | C10H17NO8S | γ-terpinene | Surratt et al., 2007 |
| 374.0631293 | C10H18N2O11S | γ-terpinene | Surratt et al., 2007 |
| 295.0725719 | C10H17NO7S | terpinolene | Surratt et al., 2007 |
| 327.0624011 | C10H17NO9S | terpinolene | Surratt et al., 2007 |
| 374.0631293 | C10H18N2O11S | terpinolene | Surratt et al., 2007 |
| 295.0725719 | C10H17NO7S | β-pinene | Surratt et al., 2007 |
| 311.0674865 | C10H17NO8S | β-pinene | Surratt et al., 2007 |
| 327.0624011 | C10H17NO9S | β-pinene | Surratt et al., 2007 |
| 343.0573157 | C10H17NO10S | β-pinene | Surratt et al., 2007 |
| 363.1351719 | C15H25NO7S | β-caryophyllene | Chan et al., 2011 |
| 383.1250011 | C14H25NO9S | β-caryophyllene | Chan et al., 2011 |
| 327.0624011 | C10H17NO9S | decalin | Riva et al., 2016 |
| 321.0154511 | C10H11NO9S | naphthalene | Riva et al., 2015 |
| 218.9837573 | C6H5NO6S | 2-methylnaphthalene | Riva et al., 2015 |

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

**Peer-reviewed publications:**

Wang K., Zhang, Y., Huang, R. J., Cao, J. J., and Hoffmann, T.: UHPLC- Orbitrap mass spectrometric characterization of organic aerosol from a central European city (Mainz, Germany) and a Chinese megacity (Beijing), *Atmos. Environ.*, *https://doi.org/10.1016/j.atmosenv.2018. 06.036*, **2018**.

Wang K., Zhang, Y., Huang, R. J., Cao, J. J., Kampf, C., Cheng, Y. F., Pöschl, U., and Hoffmann T.: *Molecular characterization of organic aerosols in three cities at the northeast, central east and southeast of China using UHPLC- Orbitrap mass spectrometry, Atmos. Chem. Phys.*, in preparation, **2018**.

Wang K., Zhang, Y., Huang, R. J., Cao, J. J., Kampf, C., Cheng, Y. F., Pöschl, U., Glasius, M. and Hoffmann T.: *Molecular characterization and source prediction of atmospheric particulate organosulfates using ultrahigh resolution mass spectrometry, Atmos. Chem. Phys.*, in preparation, **2018**.

Huang, R. J., Yang, L., Cao, J. J., Chen, Y., Chen, Q., Li, Y. J., Duan, J., Zhu, C. S., Dai, W. T., Wang, K., Lin, C. S., Ni, H. Y., Corbin, J. C., Wu, Y. F., Zhang, R., J., Tie, X. X., Hoffmann, T., O'Dowd, C. D., and Dusek, U.: Brown carbon aerosol in urban Xi'an, Northwest China: the composition and light absorption properties, *Environ. Sci. Technol.*, doi: 10.1021/acs.est.8b02386, **2018**.

Huang, R. J., Cao, J. J., Chen, Y., Yang, L., Shen, J. C.., You, Q. H., Wang, K., Lin, C. S., Gao, B., Li, Y. J., Hoffmann, T., O'Dowd, C. D., Bilde, M., and Glasius, M.: Organosulfates in atmospheric aerosol: synthesis and quantitative analysis of PM2.5 from Xi'an, Northwest China, *Atmos. Meas. Tech., https://doi.org/10.5194/amt-11-3447-2018*, **2018**.

**Presentations:**

Wang K., Huang, R. J., and Hoffmann, T.: Ultrahigh resolution mass spectrometric characterization of organic aerosol from European and Chinese cities, *European Geosciences Union, General Assembly*, Vienna, Austria, April 2016, (post presentation).

Wang K., Huang, R. J., Cao, J. J., Kampf, C., Cheng, Y. F., Pöschl, U., and Hoffmann T.: Molecular characterization of organic aerosol from European and Chinese cities: an ultrahigh resolution mass spectrometry study, *European Aerosol Conference*, Tours, France, September 2016, (post presentation).

Wang K., Huang, R. J., Cao, J. J., Kampf, C., Cheng, Y. F., Pöschl, U., and Hoffmann T.: Molecular characterization of organosulfates from European and Chinese cities by ultrahigh resolution mass spectrometry., *European Aerosol Conference*, Zurich, Switzerland, September 2017, (post presentation).

Wang K., and Hoffmann T.: Orbitrap coupled with UHPLC applied for organic aerosol analysis, *Ultrahigh Resolution Mass Spectrometry and Data Interpretation Workshop*, Paris, France, June, 2017, (oral presentation).

# **E.** Acknowledgements

# **F.** Curriculum vitae