New water-soluble, toxic tracers of wood burning identified in fine brown carbon aerosol using a non-target approach

Vinh Nguyen[1], Bartłomiej Witkowski[1*], Tomasz Gierczak[1]

[1]University of Warsaw, Faculty of Chemistry, al. Żwirki i Wigury 101, 02-089 Warsaw, Poland

Correspondence to: Bartłomiej Witkowski (bwitk@chem.uw.edu.pl)

Abstract. The molecular composition of water-soluble fine (PM_3) brown carbon aerosol (BrC_{aq}) generated by the combustion of wood was studied with ultra-performance liquid chromatography coupled with electrospray ionization time-of-flight mass spectrometry (UPLC-ESI-ToF/MS) using a non-target analysis (NTA) workflow. The NTA analysis workflow based on MS-DIAL and MS-FINDER showed the best performance of the five software tested. Structures of 361 out of the 420 water-soluble organics in BrC were tentatively identified for the first time. The total emission of fine, water-soluble BrC_{aq} was approx. 1 g per kg of wood burned, comparable with the emission factors of some semi-volatile organics from open biomass burning. Potential precursors of aqueous secondary organic aerosols ($_{aq}$SOAs) and toxic molecules were selected among the newly identified molecules.

The newly identified harmful tracers of fine BrC included plant and wood care products, alkaloids, and fungal metabolites. Fungal metabolites were also identified among the potential precursors of $_{aq}$SOAs with high Henry's law constant values, alongside natural compounds occurring in roots and leaves, diterpenoids, flavonoids, anthraquinones, and coumarins. The release of these natural and man-made compounds is possible during wildfires and domestic uses of biomass. The atmospheric lifetimes calculated for the newly identified precursors of $_{aq}$SOAs showed that natural dyes, bacterial and fungal metabolites, and (aromatic) glucosides can undergo aqueous OH oxidation in cloud water. Such molecules can produce low-volatility products without decomposing due to their large carbon backbones. Many new potential chromophores were also identified in BrC, including natural dyes and molecules with conjugated double bonds and aromatic rings.

1 Introduction

Biomass is organic material from plants and animals and often refers to non-fossil fuels, like wood, pellets, and straw. Biomass is used around the globe for generating heat and energy, including domestic and industrial uses (Antar et al., 2021; Tomlin, 2021). Over 3 billion people use solid (bio)fuels for cooking and heating, which globally accounts for 41% of households (Amegah and Jaakkola, 2016). Open biomass burning (BB) is also widespread in some regions due to cultural and economic practices (Admasie et al., 2018). Furthermore, the use of biomass aims to limit the reliance of the energy sector on nonrenewable fossil fuels and to decrease the net emissions of greenhouse gases (GHG) (Tomlin, 2021). At the same time, the large-scale use of biomass as a renewable, carbon-neutral fuel in power and heating plants remains debatable (Stubenrauch and Garske, 2023).

Open BB includes burning crop residues (Hartner et al., 2024b), vegetation fires intensified by man-made climate change (Jones et al., 2024). Around the globe, more frequent and widespread wildfires pose a serious threat to humans, infrastructure, and ecosystems. In the 2023-2024 fire season, the global area burned is estimated at 3.9×10^6 km^2, causing many fatalities and billions of dollars in damages in the US, Canada, the EU, and Asia (Jones et al., 2024).

In addition to direct exposure effects, open BB emits large amounts of pollutants, which can affect areas far from the source (Jones et al., 2024; Laskin et al., 2025). BB is a major global source of methane (5-15%), CO (30-50%), NO_x (20%), anthropogenic CO_2 (18%), and the second-largest source of non-methane volatile organic compounds (VOCs) (Pan et al., 2020). Furthermore, BB is the major source of black carbon (BC) and primary organic aerosols, accounting for 57±2% and 87±2% of the global emissions, respectively (Andreae, 2019; Jiang et al., 2024). BC and organic aerosols, including also light absorbing aerosols, the so-called brown carbon (BrC) emitted by BB, account for up to 70% of the total emission of fine particulate matter ($PM_{2.5}$) into the atmosphere (Jiang et al., 2024; Yadav and Devi, 2019).

BB pollutants, including GHGs and fine PM, affect the air quality and climate and harm human health (Jiang et al., 2024). All fine PMs influence the hydrological cycle by initiating the formation of clouds and ice crystals (Bellouin et al., 2020). Fine aerosols, including biogenic secondary organic aerosols (BSOAs) (Tsigaridis and Kanakidou, 2018), also scatter light, thereby reducing the amount of radiation reaching the Earth's surface (Kahn et al., 2023). Unlike most BSOAs, BC and BrC absorb the incoming solar radiation, exhibiting positive radiative forcing, which increases global temperature (Laskin et al., 2025).

Due to its high atmospheric abundance, BC is the second largest contributor to man-made radiative forcing (Matsui et al., 2018). The contribution of BrC to the direct radiative forcing of BC is likely substantial, but the estimates vary between 20 and 70% (Laskin et al., 2025). BC absorbs light from infrared (IR) down to the ultraviolet (UV) region, whereas BrC exhibits a much narrower (wavelength-dependent) absorption in the UV-Vis region of the electromagnetic spectrum (Saleh, 2020; Laskin et al., 2025).

The radiative forcing of BrC estimated by global models varies from 0.03 to 0.57 W m^{-2} (Li et al., 2023). This uncertainty is, in part, due to incomplete data about the sources, formation mechanisms, atmospheric transformations, light absorbance, and chemical composition of BrC (Li et al., 2023). For this reason, identifying the pollutants emitted from combustion sources has

been the subject of extensive research (Li et al., 2023; Young et al., 2021a). Thousands of unique molecules contribute to BrC aerosols, including saccharides, halogenated, nitrated, and halogenated phenols, polycyclic aromatic hydrocarbons, terpenoids, resin acids, dioxins, alkanes, oxygenated and aromatic, and organosulfur compounds etc. (Divisekara et al., 2023; Young et al., 2021a; Brege et al., 2021a). At the same time, most of these compounds remain unidentified because a comprehensive, molecular-level characterization of BrC presents a considerable analytical challenge (Brege et al., 2021a; Divisekara et al., 2023; Laskin et al., 2025).

Furthermore, the chemical composition of BrC is not only forbiddingly complex but also evolves during transport and chemical processing (the so-called chemical aging) in the atmosphere (Moise et al., 2015; Laskin et al., 2025). Formation and evolution of BrC in the atmosphere involve various gas, aqueous, and multiphase reactions, such as chemical aging by UV radiation and inorganic radicals (Zhao et al., 2015). Particularly, the currently poorly characterized (photo)chemical processing of BB emissions in atmospheric hydrometeors largely influences the composition, light absorption, and toxicological and physicochemical properties of BrC (Wong et al., 2019; Choudhary et al., 2023). For instance, the aqueous oxidation of BrC by OH initially enhanced the UV-Vis absorbance but led to bleaching following prolonged exposure (Lei et al., 2025; Hems et al., 2020). However, due to the limited data on the water-soluble organic compounds (WSOCs) emitted by BB, our understanding of the climate and health effects of BrC remains incomplete (Li et al., 2023).

This work aimed to study the WSOCs in fine BrC (BrC_{aq}) emitted by the pyrolysis of woody biomass, focusing on toxic molecules and those with high Henry's law constant (H, M/atm) values. The latter group can dissolve in atmospheric hydrometeors and undergo further chemical processing, resulting in (light-absorbing) aqueous secondary organic aerosols ($_{aq}$SOAs) (Lei et al., 2025; Go et al., 2024). $_{aq}$SOAs are likely important but still poorly characterized compounds of fine atmospheric PM (Su et al., 2020).

In the work presented, to gain detailed, molecular-level insights into the composition of BrC_{aq}, analyses were carried out with ultra-performance liquid chromatography coupled with electrospray ionization time-of-flight mass spectrometry (UPLC-ESI-ToF/MS) using a non-target analysis (NTA) workflow. NTA identifies (annotates) unknown compounds based on the high-resolution mass spectrometry (HR-MS) data using databases and *in-silico* fragmentation prediction (Hulleman et al., 2023; Vosough et al., 2024). Therefore, NTA is a promising approach for resolving the molecular complexity of BrC (Laskin et al., 2025). This work presents the first application of NTA in analyzing BrC_{aq} generated by wood pyrolysis (Divisekara et al., 2023; Young et al., 2021a; Hartner et al., 2024b).

The immense amounts of data generated by the modern LC/MS and GC/MS instruments require advanced processing algorithms, involving deconvolution, feature detection, and annotation (Hohrenk et al., 2020b). Over the past decade, there has been a considerable increase in the availability of software for HR-MS data mining (Hohrenk et al., 2020b). However, the number of features extracted and identified in NTA largely depends on the data processing workflow (Hohrenk et al., 2020b; Wartmann et al., 2024). For this reason, several NTA workflows were tested in this work, including competitive Fragmentation Modeling for Metabolite Identification (CFM-ID) (Wang et al., 2021), Metaboanalyst (Pang et al., 2024), Global Natural Products Social Molecular Networking (GNPS) (Aron et al., 2020), MS-DIAL, MS-FINDER (Tsugawa et al.,

2015b), and MZmine (Schmid et al., 2023), using a mixture of model BB pollutants. Afterward, the best-performing workflow was used to analyze BrC_{aq}.

Here, BrC was generated in the N_2 atmosphere in a new, custom-designed combustor. Wood pyrolysis was conducted to simulate combustion conditions during vegetation fires, as oxygen is absent inside logs and in the deeper zones of the fire (Chen and Bond, 2010; Sekimoto et al., 2018; Divisekara et al., 2023; Gao et al., 2024). The composition of BrC_{aq} was compared with the previously published data, and >360 tracers of wood pyrolysis were tentatively identified for the first time. Several WSOCs in BrC_{aq} with high H values and toxicities (LD_{50}) were also first identified in this work.

Additionally, quantitative analysis was performed with LC/MS using surrogate standards to identify the major components of BrC_{aq} (Pieke et al., 2017). Quantitative results obtained using surrogate standards, a total organic carbon (TOC) analyzer, and the gravimetric method showed that estimating relative ionization efficiencies for WSOCs in BrC_{aq} yielded reasonably accurate results.

2. Experimental section

Materials and reagents are listed in Section S1 in the Supplementary Information (SI).

2.1 Biomass combustor and fine particle collection

A diagram of the newly constructed biomass combustor is shown in Fig. 1

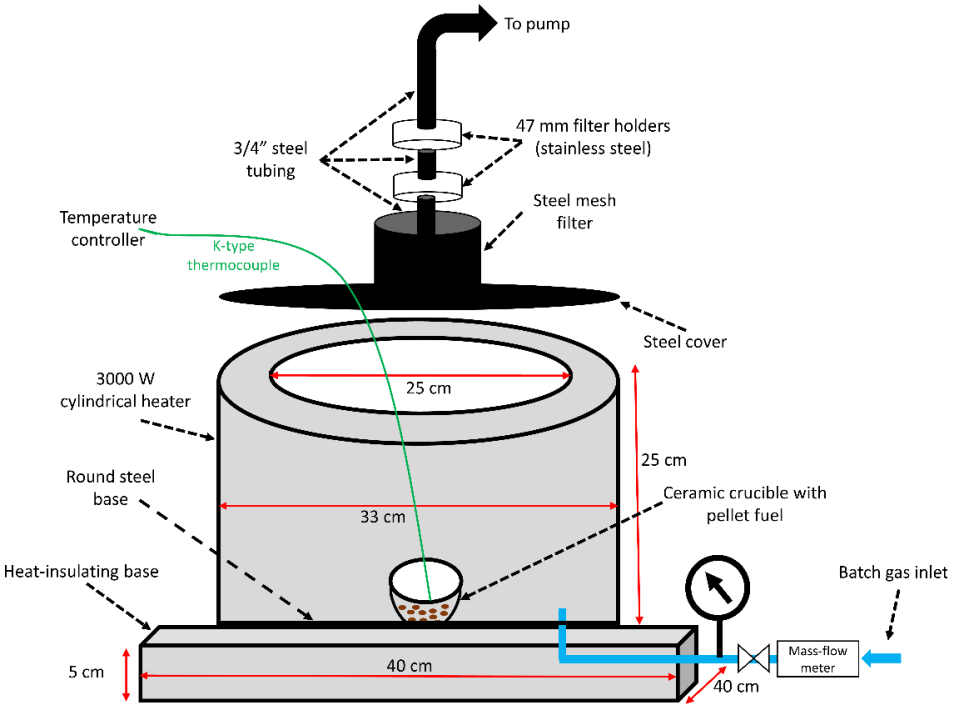


Figure 1: Diagram of the biomass combustor

The combustor consisted of a 3 kW cylindrical resistance heater with a round steel base that was placed on top of a heat-insulating board – Fig. 1. The heater was secured to the base with heatproof cement, and surrounded by a 5-cm thick layer of fireproof insulation. The outer wall of the combustor was a steel cylinder with an additional layer of a heat-reflecting mat. The combustor base was equipped with the bath gas inlet, which ran inside the insulating board – Fig. 1. A controller was used to adjust the combustion temperature within ± 5ºC. Pellets were placed in a ceramic crucible with a K-type thermocouple connected to the temperature controller and inserted in the middle of the fuel stack. The flow of batch gas and the pumping speed were adjusted with manual valves, and the pressure inside the combustor was 1 atm.

Mixed wood pellets (25 g) were heated at 350°C for 2 hours, and the bath gas flow (N_2) was maintained at 1.5 L/min. The stream from the combustor cooled down to approx. 80 ºC before reaching the sampling assembly. First, the emissions passed through a stainless steel mesh filter (mesh size 0.5 mm - 50 µm, Fig. 1) to remove coarse particles. Afterward, two 47 mm filters were used; the first filter (hydrophobic PTFE, pore size 3 µm, Fluoropore, FSLW07400) was followed by a second PTFE-coated glass microfiber filter (EMFAB TX40H120-WW, Pallflex, aerosol retention 99.95%). During sampling, both filter assemblies were kept at 80 ºC using a heating sleeve (10 cm I.D., not included in Fig. 1) to avoid condensation of water and other semi-volatiles.

Before sampling, filters were placed in a desiccator with dry molecular sieves for 24 hours. Particles collected on the second filter (PM_3) were extracted using 2 mL of water via mechanical agitation and filtered through a 0.22 µm PTFE filter before analysis. The extracts were diluted tenfold before LC/MS analysis to prevent ion source contamination and minimize matrix effects on the semi-quantitative results (see Section 2.5).

2.2 Liquid chromatography coupled to mass spectrometry

Analyses were performed using the Q-TOF LCMS-9030 system (Shimadzu) using an Acquity HSS-T3 column (Waters, 100 mm × 2.1 mm, 1.8 µm). The mobile phase consisted of 0.1% formic acid in water (eluent A) and 0.1% formic acid in ACN (eluent B); the injection volume was 2 µL. The mobile phase flow rate was 0.25 mL/min, and the column temperature was 30°C. The gradient elution program involved adjusting the amount of eluent B as follows: initially, 5% for 10 minutes, then linear increase to 25% over 5–22 minutes; held at 25% for 13 minutes, then linear increase to 95% over 35-39 minutes, held at 95% for 5 minutes, then linear decrease to 5% over 1 minute, and held at 5% for 5 minutes. The total analysis time was 50 minutes.

The mass spectrometer was equipped with an electrospray ion (ESI) source, operating in positive or negative ionization modes. The nebulizing, drying, and heating gas flows were set at 3.0 L/min, 10 L/min, and 10 L/min, respectively. The interface temperature was 300°C. The TOF mass resolving power was approx. 45,000. Spectra were collected in the data-dependent acquisition (DDA) mode; 100 – 600 m/z (precursor selection, even time 1 s), 40-600 m/z (product ion scan, even time 0.1 s), number of dependent events 3, intensity threshold 3000, delay time 1 s, charge state 1. Each sample was analyzed six times, at positive and negative ionization modes utilizing three collision energy (CE, V) values: 0-7 V for (low), 10±5 V (medium),

and 17±5 V (high), and the CE spread was 5 V. After adjusting the DDA conditions using BrC filter extracts, a quality MS and MS/MS spectra were obtained for approx. 4000 features, which is comparable with similar, combustion-related samples (Brege et al., 2021b; Divisekara et al., 2023; Young et al., 2021b; Graham et al., 2002a).

2.3 Mass spectrometric data processing workflows

The raw data files were first processed with MS-DIAL or MZmine (Fig. 2). First, the workflows based on MS-FINDER, CFM-ID, Metaboanalyst, GNPS, and MZmine were tested using 59 model compounds. These molecules were selected to mimic the molecular composition of water-soluble BrC emitted by BB based on previously published results and standards availability (Tables S1 and S2), and included derivatives of cinnamic acid, nitrophenols, and polycarboxylic, furoic, and fatty acids. The final workflow, used for analyzing BrC_{aq}, was based on MS-DIAL and MS-FINDER.

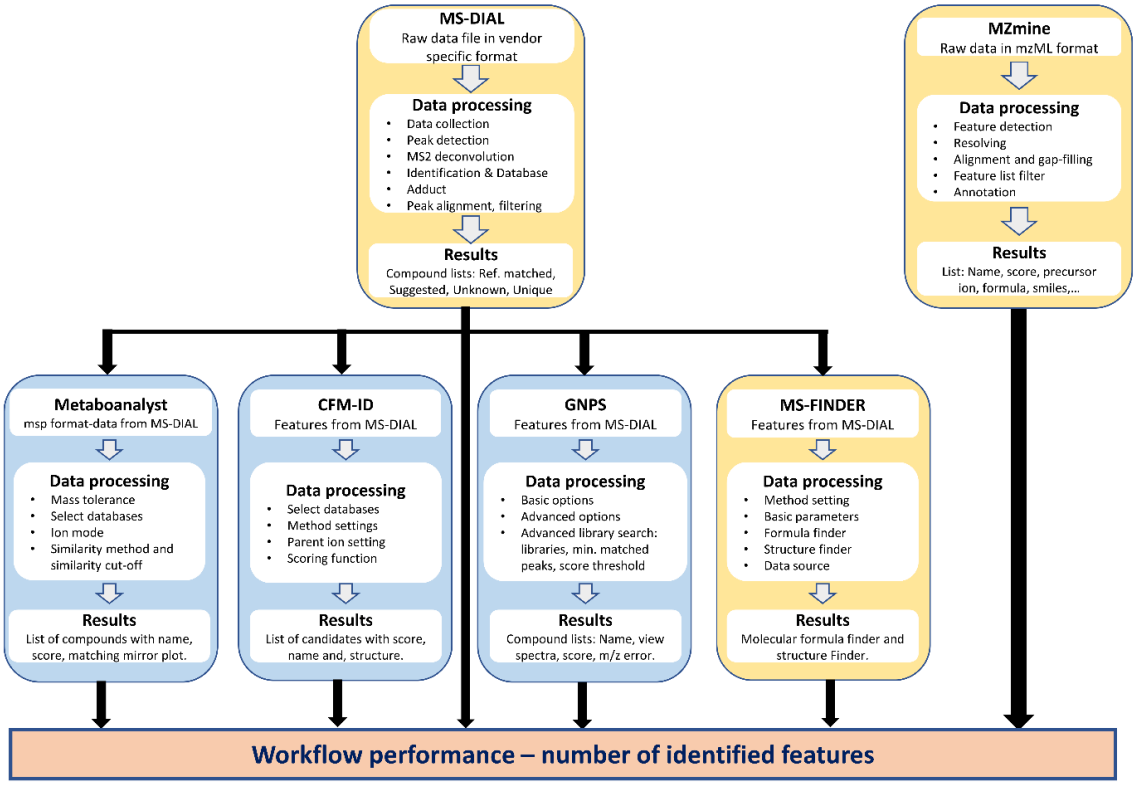


Figure 2. The MS data processing software was tested in this work. All data processing was performed with a Dell Vostro 3020T desktop PC equipped with an Intel Core i7-13700 CPU, 1TB SSD drive, and 64 GB of 3200 MHz DDR4 RAM.

The same MS databases, including internal and user-uploaded libraries, were used in workflows based on MS-DIAL, MS-FINDER, and MZmine; GNPS allows user-defined databases, while the other web-based platforms (MetaboAnalyst and CFM-ID) are limited to pre-selected MS libraries – Table S6 (Lai et al., 2018; Vaniya et al., 2017; Mona, 2024; Ms-Dial, 2024; Tsugawa et al., 2015b). Workflows based on MZmine, GNPS, MetaboAnalyst, and CFM-ID are described in Section S3.1.

2.3.1 MS-DIAL

MS-DIAL (v5.3.240617) was used for the raw data processing, spectra deconvolution, and feature extraction and annotation – Fig. 3.

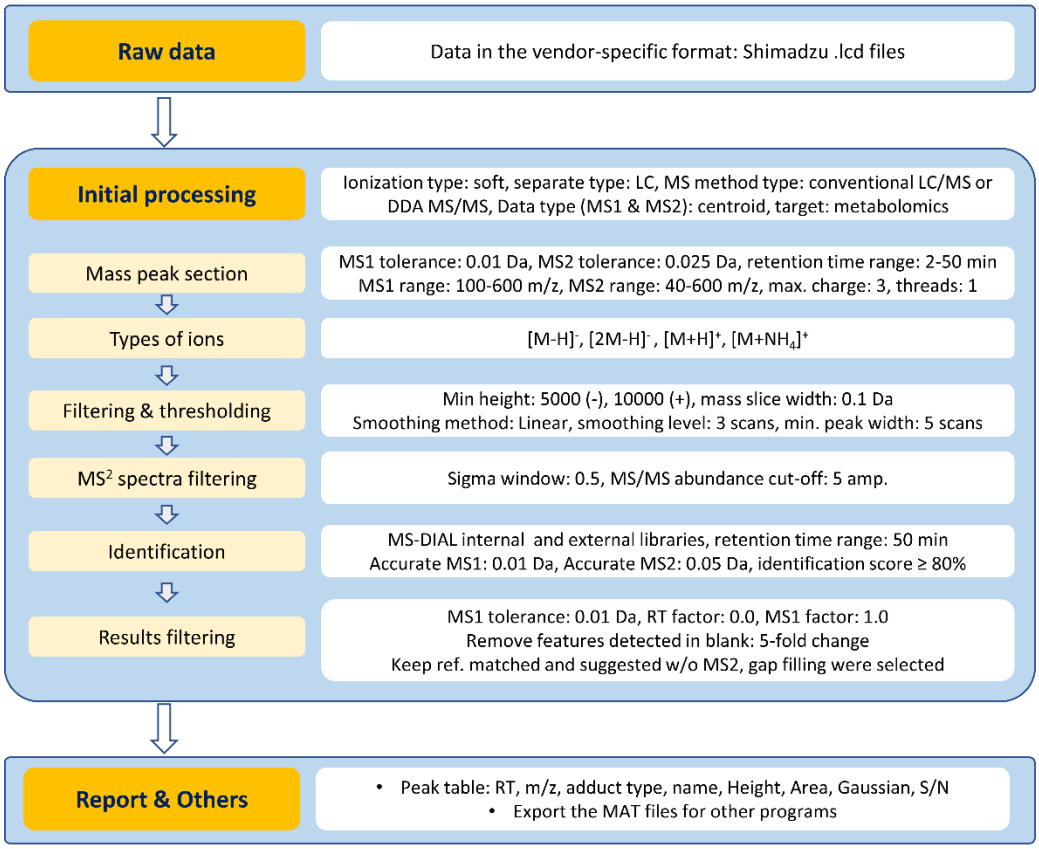


Figure 3. MS-DIAL workflow

The identification criteria included retention time, precursor *m/z*, isotopic ratio, and MS/MS spectra (Fig. 3). MS/MS spectra were indispensable for feature annotation and distinguishing isomers. Here, the compound with the highest total score above 80% was assigned to each focus peak (Tsugawa et al., 2015a). In cases where DDA lacked MS/MS spectra, the MS/MS similarity value was zero, and the structure was proposed based on the MS1 score. The scoring approach implemented in MS-DIAL is described in more detail in section S3.1.5).

The Microsoft Access Table (MAT) file, which included both MS and MS/MS spectra exported from MS-DIAL, was used as input data for MS-FINDER, CFM-ID, GNPS, and MetaboAnalyst but not MZmine (Fig. 2). Features not annotated by MS-DIAL were further analyzed using MS-FINDER (Section 2.3.2).

2.3.2 MS-FINDER

MS-FINDER v3.61 (Fig. 4) is a highly versatile tool for predicting formulas, annotating fragments, and elucidating structures. In addition to the internal libraries embedded in MS-FINDER, an in-silico MS/MS spectra predictor was used. Assigned structures were ranked based on their scoring.

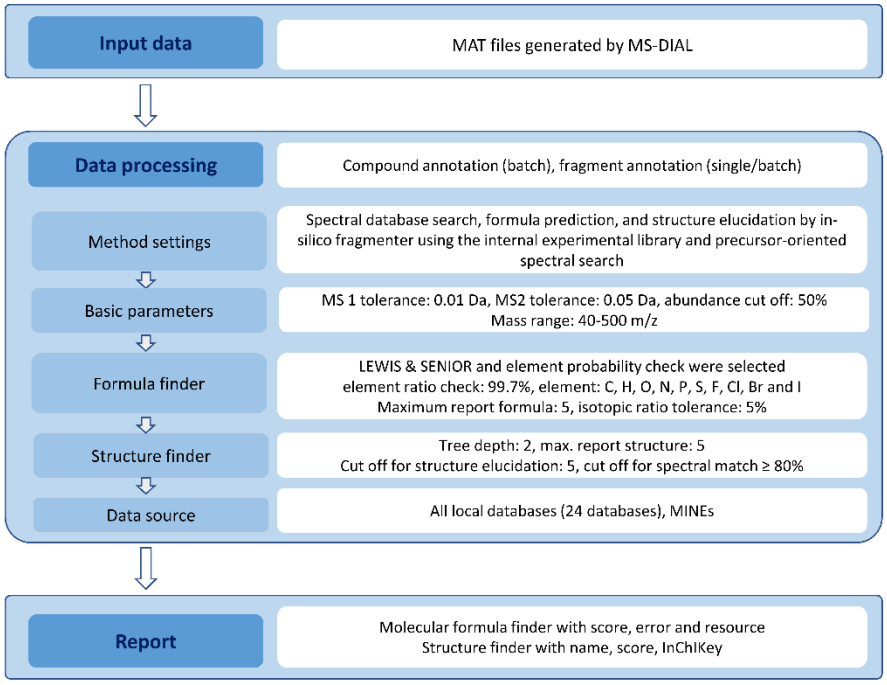


Figure 4. MS-FINDER workflow

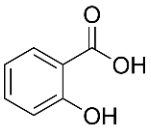
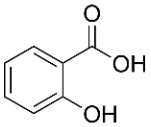
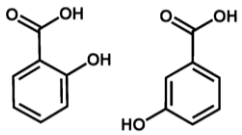
In MS-FINDER, the formula candidates were considered based on mass error, isotopic ratio, product ions annotation, neutral-loss ions annotation, and database score (Fig. 4). Structural candidates were ranked using a weighted scoring system, integrating bond dissociation energies, mass similarities, fragment linkages, and, most importantly, nine hydrogen rearrangement rules during bond cleavages. The final molecular structure rankings were determined using a combined formula and structure scores (Tsugawa et al., 2016; Blaženović et al., 2018).

2.4 Confidence levels in annotation

Confidence levels in NTA are showcased in Table 1 (Schymanski et al., 2014).

Table 1. Confidence levels in the NTA workflow

Confidence level	Required data	Classification	Description	Example

1	MS spectra, MS/MS spectra, library MS/MS spectra, and retention time matching	*Confirmed with authentic standard*	Input spectra matched with reference spectra by MS-DIAL with a retention time confirmation	
2	MS spectra, MS/MS spectra, library MS/MS spectra matching	*Reference matched*	Input spectra matched with reference spectra by MS-DIAL	
3	MS, MS/MS, experimental data	*Suggested structure*	From MS-DIAL, and MS-FINDER with MS/MS spectra	 *o-* *m-*
4	MS isotope/adduct	*Suggested formula*	From MS-DIAL with MS spectra	$C_7H_6O_3$
5	MS	*Unknowns*	With MS spectra and an unknown compound with MS/MS spectra	*m/z* 137.0228

For the features annotated at least level 4 (elemental formula assignment), the van Krevelen diagram, Kendrick mass defects, double-bound equivalents (DBE), and average carbon oxidation states (OS_c) were calculated – Section S4 (Kroll et al., 2011).

2.5 Semi-qualitative analyses with surrogate standards

Surrogate standards were used to quantify organic compounds detected in filter extracts; this approach assumes that closely eluting compounds have similar response factors (RFs) (Pieke et al., 2017). Five surrogate standards were used in each ionization mode, with retention times from 2 to 40 min (Table S3), covering the elution window for WSOCs detected in BrC_{aq}. Working standards were prepared in ($MeOH/H_2O$, 1:1, v/v) with concentrations from 0.001 to 0.05 mg/L.

RFs for surrogate standards were calculated with eq. I.

$$RF_{Surrogate} = \frac{A_{Surrogate}}{C_{Surrogate}} \quad \text{(I)}$$

In eq. I, $RF_{Surrogate}$ represents the ratio between the peak area $A_{Surrogate}$ and the concentration ($C_{\mathrm{Surrogate}}$, mg/L) of the surrogate standards. The analyte concentrations were calculated using eq. II (Pieke et al., 2017).

$$C_{unknown}\left(\frac{mg}{L}\right) = \frac{A_{unknown}}{RF_{closest\ surrogate}} \quad \text{(II)}$$

In eq. II, $RF_{\text{closest ST}}$ is the response factor of surrogate standards with the retention time closest to the analyte, and $A_{unknown}$ is the chromatographic peak area of the unknown compound. $C_{unknown}$ is the concentration of the analyte in mg/L. In eq. II, the total concentration of WSOCs in the filter extracts was calculated as the sum of concentrations of the individual analytes. Due to the use of surrogate standards, a 50% uncertainty was imposed for all concentrations obtained with eq. II (Kruve, 2019; Evans et al., 2024b; Malm et al., 2021; Pieke et al., 2017). For compounds detected in BrC_{aq}, this value is consistent with the results obtained using authentic and surrogate standards (Table S4). Furthermore, the imposed 50% uncertainty exceeds the matrix effects observed for most surrogate standards (Table S5). To prevent introducing a positive bias into the quantitative data, molecules detected in both ionization modes were identified by comparing annotation results, and their average concentrations were used to estimate the amount of BrC_{aq}.

The total (Σ_{LCMS}) and individual amounts of WSOCs emitted were derived with eq. III.

$$\sum_{LCMS}\left(\frac{g}{kg}\right) = \frac{\sum C_{unknown} \times DF \times V_{total}}{\Delta m_{fuel}} \quad \text{(III)}$$

In eq. III, $\Sigma C_{unknown}$ is the sum of analytes (mg/L) from eq. II, DF is the dilution factor, V_{total} is the total volume of extraction solvent (2 mL), Δm_{fuel} is the decrease in the mass of pellets (g) corrected for the water content (8.0%).

2.6 Total organic carbon analysis

Analyses were conducted using a Shimadzu TOC-5050A analyzer with an ASI-5000A autosampler. The instrument was calibrated with the standard solution of 4-nitrophenol and glucose between 4 and 40 (mgC/L). A squared linear coefficient of determination (R^2) of 0.9996 was obtained, and the RF values for the two standards were practically identical.

Samples were diluted with water to a ca. 20 mgC/L and filtered through a 0.22 μm PTFE syringe filter. Before injection, 50 μL of 2M HCl was added to each sample, followed by sparging with O_2 for 2 minutes. The injection volume was 21 μL, and each sample was injected three times, which yielded a precision <1%.

$$\Sigma_{TOC}\left(\frac{g}{kg}\right) = \frac{C_{TOC} \times DF \times V_{total}}{\Delta m_{fuel}} \times \frac{1}{0.625} \quad \text{(IV)}$$

In eq. IV, C_{TOC} is the measured concentration of TOC (mgC/L), DF is the dilution factor, V_{total} is the total volume of extraction solvent (2 mL), Δm_{fuel} is the fuel mass (g) corrected for the water content (8.0%) and, 0.625 ± 0.144 (2σ) is the factor used to convert mgC/L units to mg/L. This conversion factor was the average carbon content of the analytes detected with LC-ToF/MS and the main source of the uncertainty of the TOC measurements.

2.7 Gravimetric analyses

Aqueous samples (0.4 mL) were filtered through a 0.22 μm PTFE filter and evaporated to dryness at 30°C using a centrifugal vacuum evaporator (Labconco, model no. 7810033). Afterward, the dried residues were placed in a desiccator for 24 hours to

remove the leftover moisture. This procedure yielded ≥1 mg of residue, which was weighed using an analytical microbalance (Radwag, model no.XA52.5Y).

The amount of BrC_{aq} emitted was calculated with eq. V.

$$TC_{grav}\left(\frac{g}{kg}\right) = \frac{(m_{residue} - m_{blank}) * V_{total}}{V_{use} * \Delta m_{fuel}} \quad \text{(V)}$$

In eq. V, $m_{residue}$ is the mass of the residue after evaporation (mg), m_{blank} is the mass of the blank (mg), V_{total} is the total volume of extraction solvent (2 mL), V_{use} is the volume of extract used for evaporation (0.4 mL), and Δm_{fuel} is the fuel mass (g) corrected for the water content (8.0%).

2.8 Henry's law constants and toxicity estimates

Acute toxicity, measured as LD_{50} (mg/kg), was estimated using the VEGA-QSAR regression model (KNN, v. 1.0.0). Henry's Law values (M/atm) were estimated using OPERA, v.1.0.1 model (Mansouri et al., 2021; Mansouri et al., 2018).

Eq. VI and VII were used to derive the total toxicity and H scores for individual compounds in BrC_{aq}.

$$H\ score\ (arb) = H \times emission\ factor\ (LC/MS) \quad \text{(VI)}$$

$$LD_{50}\ score\ (arb) = \frac{1}{LD_{50}} \times emission\ factor\ (LC/MS) \quad \text{(VII)}$$

Using eq. VI and VII, the candidates for $_{aq}$SOAs precursors and the most harmful molecules, were identified by considering their properties and amounts emitted.

2.9 Quality and control measurements

Blank filters were prepared without the fuel (Section 2.1). The extract from the blank filter was then used to correct the TOC and LC-MS analysis results. After each experiment, the combustor was cleaned by heating the chamber to 550°C and flushing with air (5.0 L/min) for 1 hour to oxidize the residues. The sampling assembly was sonicated in detergent, rinsed with distilled water and organic solvent, and dried in the oven.

3. Results and discussion

3.1 Non-target workflow selection

Workflows (Sections 2.3 and S3.1) were evaluated using model compounds – Fig. 5.

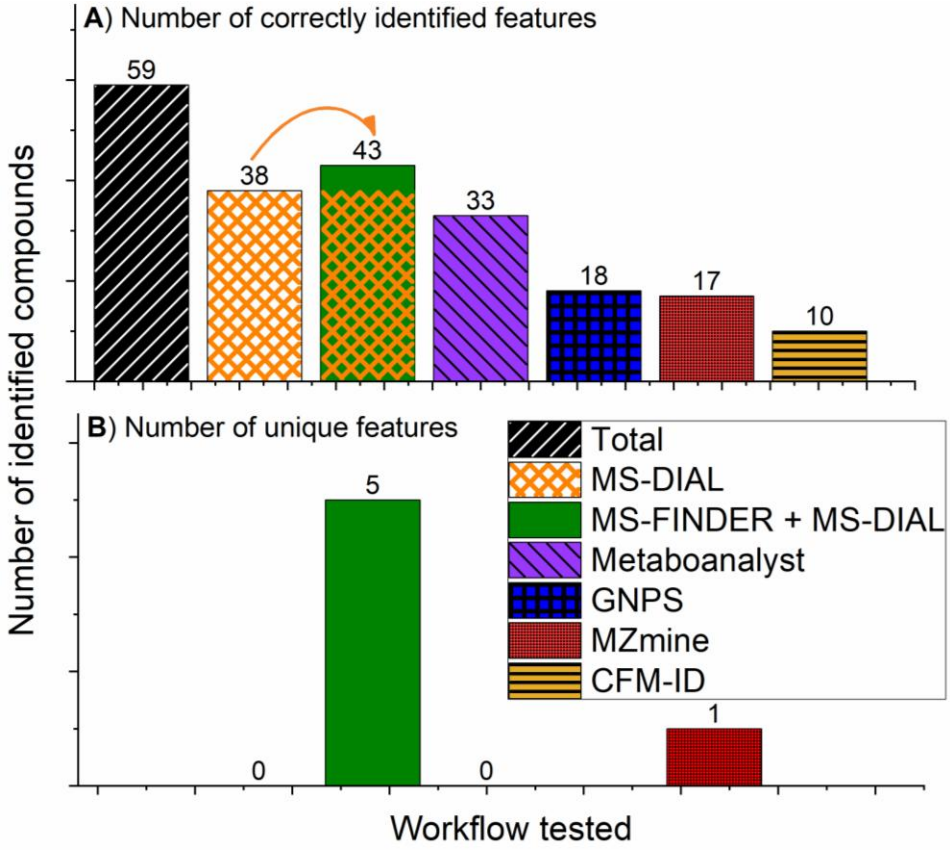


Figure 5. Workflow performance evaluation with the standard mixture of 59 model compounds (Table S1). Number of correctly identified analytes (A) and number of analytes identified only by a given software (B).

The optimal workflow, combining MS-DIAL and MS-FINDER, correctly identified 73% of standards (Fig. 2), similar to earlier studies (Young et al., 2021a; Black et al., 2021). The combination of MS-DIAL and MS-FINDER also annotated 5 unique features not recognized by any other workflow, whereas MZmine annotated only one unique analyte – Fig. 5.

In addition to searching MS databases, MS-FINDER identifies unknown compounds using *silico* fragmentation algorithms (Blaženović et al., 2018). The performance of the combined workflow (Fig. 5) is attributed to the accurate prediction (simulation) of the fragmentation spectra in MS-FINDER (Tsugawa et al., 2016; Su et al., 2023). While MS-DIAL excelled in reproducibility and peak picking, MS-FINDER demonstrated a robust capability to identify unknown BB pollutants (Wartmann et al., 2024; Mallmann et al., 2023).

Despite using different peak-picking parameters (Fig. 3 and Fig. S1), the number of features extracted by MZmine and MS-DIAL was very similar. While MZmine extracted more features than MS-DIAL, it is not necessarily an indicator of higher data quality (Rivera-Pérez and Garrido Frenich, 2024). MZmine enhanced the accuracy with noise filter and duplicate peak filter (Heuckeroth et al., 2024b), while MS-DIAL highlighted interference reduction using its "blank filtering" capability,

currently absent in MZmine (Heuckeroth et al., 2024a). These functions made MS-DIAL well-suited for NTA, further complemented by the user-friendly interface.

MZmine successfully identified only 29% of standards, despite using the same databases as MS-DIAL and MS-FINDER (Table S6), consistent with earlier findings (Wartmann et al., 2024). Such a result is attributed to differences in mass peak-picking algorithms, which largely impacted the accuracy of extracted *m/z* values. In MZmine, mass detection was performed via the exact mass algorithm using the full width at half maximum paradigm to determine peak centers and extract *m/z* values and intensities (Hohrenk et al., 2020a). On the other hand, MS-DIAL employed peak detection algorithms rooted in a linearly weighted smoothing average, regarding retention time and accurate mass (Tsugawa et al., 2014). This process was based on differential calculus principles and noise estimations, forming the backbone of MS-DIAL peak detection methodology (Tsugawa et al., 2015a).

All web-based platforms, MetaboAnalyst, GNPS, and CFM-ID utilize measured and predicted spectra in their matching functions. MetaboAnalyst correctly identified 33 standards, while GNPS and CFM-ID identified only 18 and 10 out of 59 standards, respectively (Fig. 5).

In most MS data mining programs, MS/MS fragments are transformed into vectors. The cosine value, representing the angle between the input and reference vectors from databases, is used to quantify their similarity (Li et al., 2021b). The MetaboAnalyst platform integrates similarity scores in a single value derived neither from the vector direction (dot-product) nor the vector magnitude (entropy) (Pang et al., 2024). In MS-DIAL, the similarity score is based on a combination of dot-product (also used in MetaboAnalyst) and secondary input spectra. The secondary input spectra remove fragments that did not appear in the reference spectra of the candidate compound. It decreases the impact of unwanted fragments derived from isotopic and background noise (Tsugawa et al., 2015a). Consequently, for the selected standards (Section S1), the accuracy of the results generated by MS-DIAL and MetaboAnalyst is higher than the other tested programs (Fig. 5) (Tsugawa et al., 2015a).

Databases embedded in CFM-ID contain nearly nine million spectra, but most are simulated (Table S6) (Databases, 2024). Since CFM-ID identified only 10 standards (Fig. 5), the accuracy of these prediction algorithms was somewhat insufficient (Bremer et al., 2022). Another drawback of the CFM-ID is the requirement to provide three fragmentation spectra for each unknown compound, acquired at low, medium, and high CE to enhance the identification accuracy, which greatly prolongs the analysis time (Chao et al., 2020). Nevertheless, simulating MS/MS spectra with machine learning is a promising approach to identifying “known unknowns” via *in-silico* fragmentation and “unknown unknowns” in non-target identification (Bremer et al., 2022; Russo et al., 2024)

3.2 General characteristics of fine BrC_{aq}

The combined workflow (MS-DIAL and MS-FINDER) exhibited the best performance and was used to analyze the composition of BrC_{aq}. Analysis of BrC_{aq} yielded 4086 features; this number was reduced to 2121 features annotated at least at level 4 (elemental formula assignment, Table 1). These features were categorized based on their elemental composition - Fig. 6

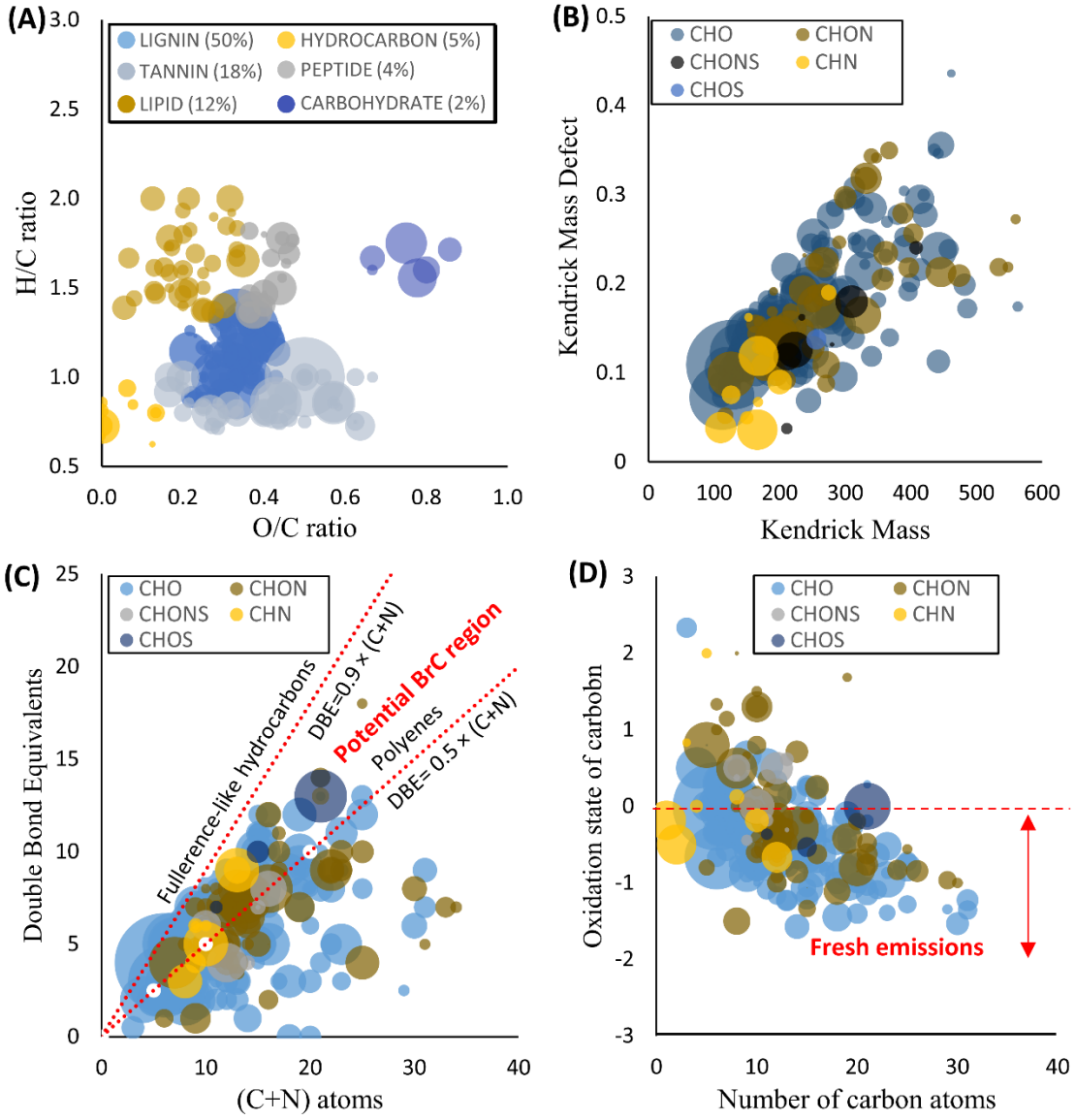


Figure 6. The van Krevelen Diagram (A), Kendrick Mass Defect (B), DBE vs (C+N) atoms (C), and OS_c vs C atoms (D) plots for unique molecular compounds of water-soluble particulate matter identified by MS-DIAL and MS-FINDER. The combination of symbols C, H, O, N, and S refers to the molecules composed of the listed elements. The size of the circles corresponds to the relative concentrations in the aqueous extracts obtained with LC/MS using surrogate standards (Section 2.5). These general characteristics (Section S4) of water-extractable BrC were comparable to those of the surrogate standards used to evaluate the NTA workflows (Table S2).

The van Krevelen diagram (Fig. 6A) revealed the clustering of O/C and H/C ratios between 0.2-0.4 and 0.7-1.3, respectively, corresponding to molecules derived from lignins and tannins (D'andrilli et al., 2015; Hartner et al., 2024b), which were the most abundant in BrC_{aq}, both number and concentration-wise - Fig. 6 (Laszakovits and Mackay, 2021; Moschos et al., 2024b). Similar results were previously reported for the ambient and chamber-generated BB aerosols (Fleming et al., 2018; Evans et al., 2024a). Furthermore, a Kendrick Mass Defect plot (Fig. 6B) revealed a homolog series of CHON, CHO, and CHONS molecules with molecular weights between 150 and 300 Da, similar to organic aerosols emitted by dung and brushwood burning (Fleming et al., 2018).

Highly oxidized $C_xH_yO_{3\text{-}6}$ compounds with $C_xH_yO_4$ formulas were the most frequently detected, constituting 73% of 96 annotated features detected with (-ESI). On the other hand, nitrogen-containing organic compounds, such as $C_xH_yNO_{2\text{-}4}$, and $C_xH_yN_z$, were predominantly observed in positive ion mode, accounting for approximately 38% of all detected compounds - Fig. 6 (Ma et al., 2024; Li et al., 2024).

Double-bond equivalent (DBE) values (Fig. 6C), reflecting the degree of unsaturation, ranged from 4–6 for lignin pyrolysis products, 7–8 for coumarins, and 10–12 for stilbenes and flavonoids (Moschos et al., 2024b; Koch and Dittmar, 2006). In Fig. 6C, 60% of (–ESI) and 40% of (+ESI) candidates fell within the potential BrC chromophores region, positioned between the lines for conjugated polyenes and linear fullerene-like hydrocarbons (Tang et al., 2020; Lin et al., 2018; Siemens et al., 2022; Moschos et al., 2024b; Sun et al., 2024). The chromophore candidates were primarily lignin-like CHO molecules, followed by nitrogen-containing CHON compounds, previously identified in wood-burning BrC (Fleming et al., 2018; Evans et al., 2024a). The BrC_{aq} exhibited the carbon oxidation state (OS_c) values ranging from -2 to 1 (Fig. 6D), consistent with observations in organic aerosols within Earth's atmosphere (Moschos et al., 2024b; Kroll et al., 2011). Furthermore, for approximately 83 % of the annotated compounds, the OS_c was between -2 and 0, characteristic of unaged emissions (Nihill et al., 2023). Hence, the general characteristics and oxidation state of BrC_{aq} corresponded to the unaged OAs emitted by BB (Moschos et al., 2024b; Fleming et al., 2018; Smith et al., 2009; Song et al., 2018; Li et al., 2024).

3.3. Quantitative and qualitative analyses of fine BrC_{aq}

Quantitative analyses of the water-extractable fraction of fine BrC were performed with LC-MS using surrogate standards (Section 2.5), TOC (Section 2.6), and gravimetric analysis (Section 2.7) – Fig. 7.

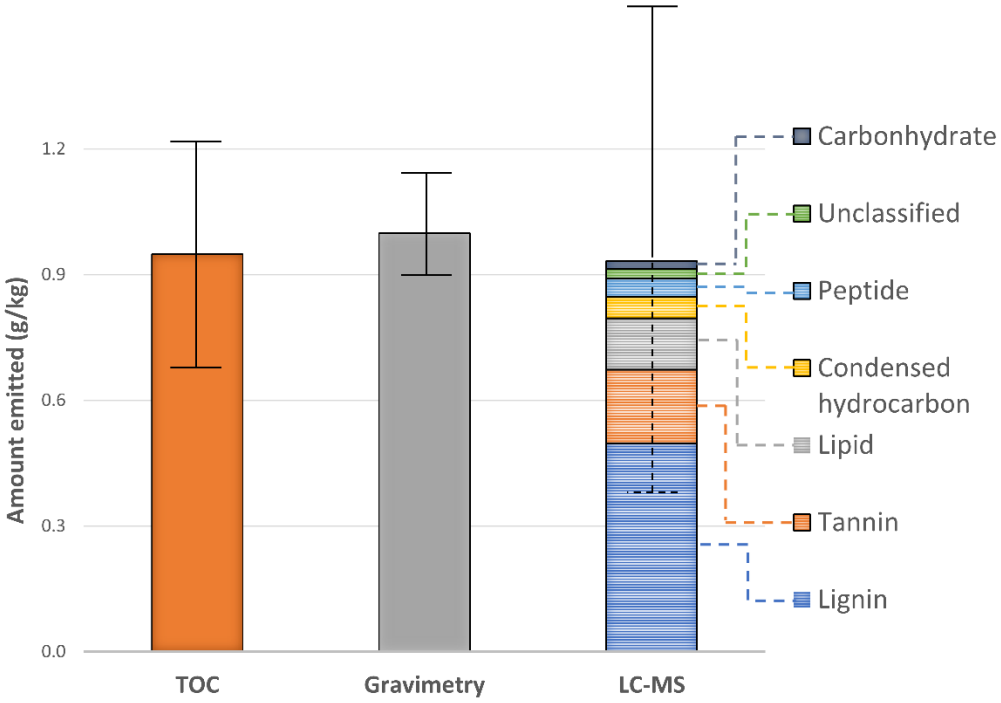


Figure 7. The total concentration of BrC_{aq} (PM3) generated by pyrolysis of wood pellets at 350°C measured with LC-MS (Σ_{LCMS}), TOC (Σ_{TOC}), and gravimetry (Σ_{grav}). The data presented are provided in Table S10.

The WSOCs detected in BrC_{aq} were classified as fatty and carboxylic acids, alkanes and aliphatic hydrocarbons, aromatic compounds, peptides, and polypeptides (Fig. 7) based on their general characteristics derived from elemental composition – Fig. 6 (Smith et al., 2009; Merel, 2023; Zherebker et al., 2024). BrC_{aq} was dominated by pyrolysis products of lignin and tannins, followed by lipids, peptides, hydrocarbons, condensed hydrocarbons, and carbohydrates (Seo et al., 2020; Shahid et al., 2019; Divisekara et al., 2023; Smith et al., 2020; Noblet et al., 2024; Hartner et al., 2024c; Kawamoto, 2017).

An excellent agreement between the Σ_{LCMS}, Σ_{TOC}, and Σ_{grav} was obtained, but the first two values are largely implied by uncertainties - Fig. 7. Moreover, the values of Σ_{TOC} and Σ_{grav} may be affected by the loss of some volatile organics during sparging with O_2 (Section 2.6) and drying under vacuum (Section 2.7) and, such molecules were shown to contribute to BrC (Sinha et al., 2023; Priestley et al., 2024). Furthermore, the value of Σ_{grav} may include fine soot (not removed by the 0.22 µm filter, Section 2.7) and water-soluble inorganics, which can contribute 8.9-21% to fine BrC (Yadav et al., 2023; Trubetskaya, 2022). Nevertheless, the results (Fig. 7) indicate that the semi-qualitative analysis with LC/MS (Section 2.5) reasonably estimated the total concentration of BrC_{aq} (Seo et al., 2020; Shahid et al., 2019; Divisekara et al., 2023; Smith et al., 2020; Noblet et al., 2024; Hartner et al., 2024c; Evans et al., 2024b).

The total emission of polar, water-soluble organics from wood pyrolysis at 350°C, representing the (oxygen-depleted) smoldering conditions, was ca. 1 g/kg of fuel burned (Fig. 7). The values derived for individual WSOCs (mg/kg) were derived with eq. III (Section 2.5) pertains solely to the water-soluble fraction of fine BrC and should be regarded as a rough estimate

of the actual emission factors (EFs) (Pokhrel et al., 2021). Nevertheless, the amounts of individual WSOCs emitted (Tables S8 and S9) are comparable with the EFs (mg/kg) range reported for the minor BB pollutants, including semi-volatile organics (Akagi et al., 2011), indicating a significant contribution of water-soluble organics to BB emissions.

3.4 Molecular composition and properties of the fine, water-soluble brown carbon

The BrC_{aq} sampled from the combustor was analyzed in DDA mode, and the detected features were annotated by MS-DIAL and MS-FINDER – Fig. 8

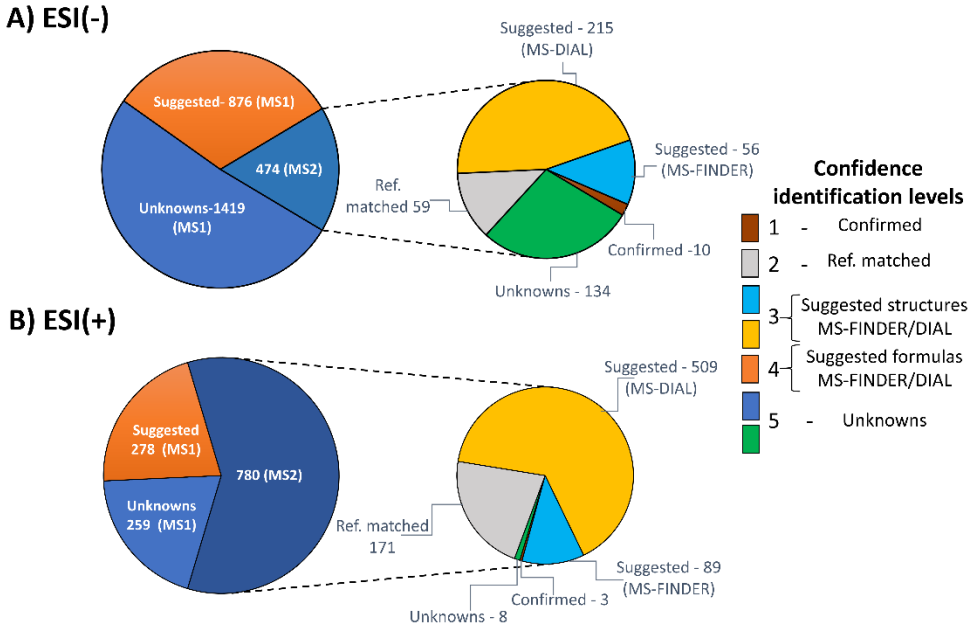


Figure 8. The number of features extracted and identified by MS-DIAL and MS-FINDER in fine BrC generated by pyrolysis of woody biomass at 350°C; negative (A) and positive (B) ionization modes. All compounds identified in both ionization modes are listed in Tables S8 and S9.

The extracted features were first annotated at level 4 (elemental formula assignment) based on the MS1 spectra. At this stage, 51% (-ESI) and 20% (+ESI) of features were denoted as unknowns – Fig. 8. Subsequently, MS2 spectra were further analyzed, and 12% (-ESI) and 59% (+ESI) of total features were annotated at least at level 3. Furthermore, confidence level 4, or higher, was obtained for 44% and 80% of the detected features in negative and positive ionization modes, respectively (Yang et al., 2023; Schymanski et al., 2014). MS databases for positive ion mode contained over 326,000 records compared to 53,337 records in negative mode (Table S6), which likely enhanced the annotation results for (+ESI) – Fig. 8 (Ng, 2021). Hence, the database plays a critical role in the structural elucidation of NTA, but currently, the number of (freely available) MS/MS databases focused on environmental pollutants is limited (Ng, 2021).

Major WSOCs detected in BrC_{aq} were tentatively identified using NTA – Fig. 9.

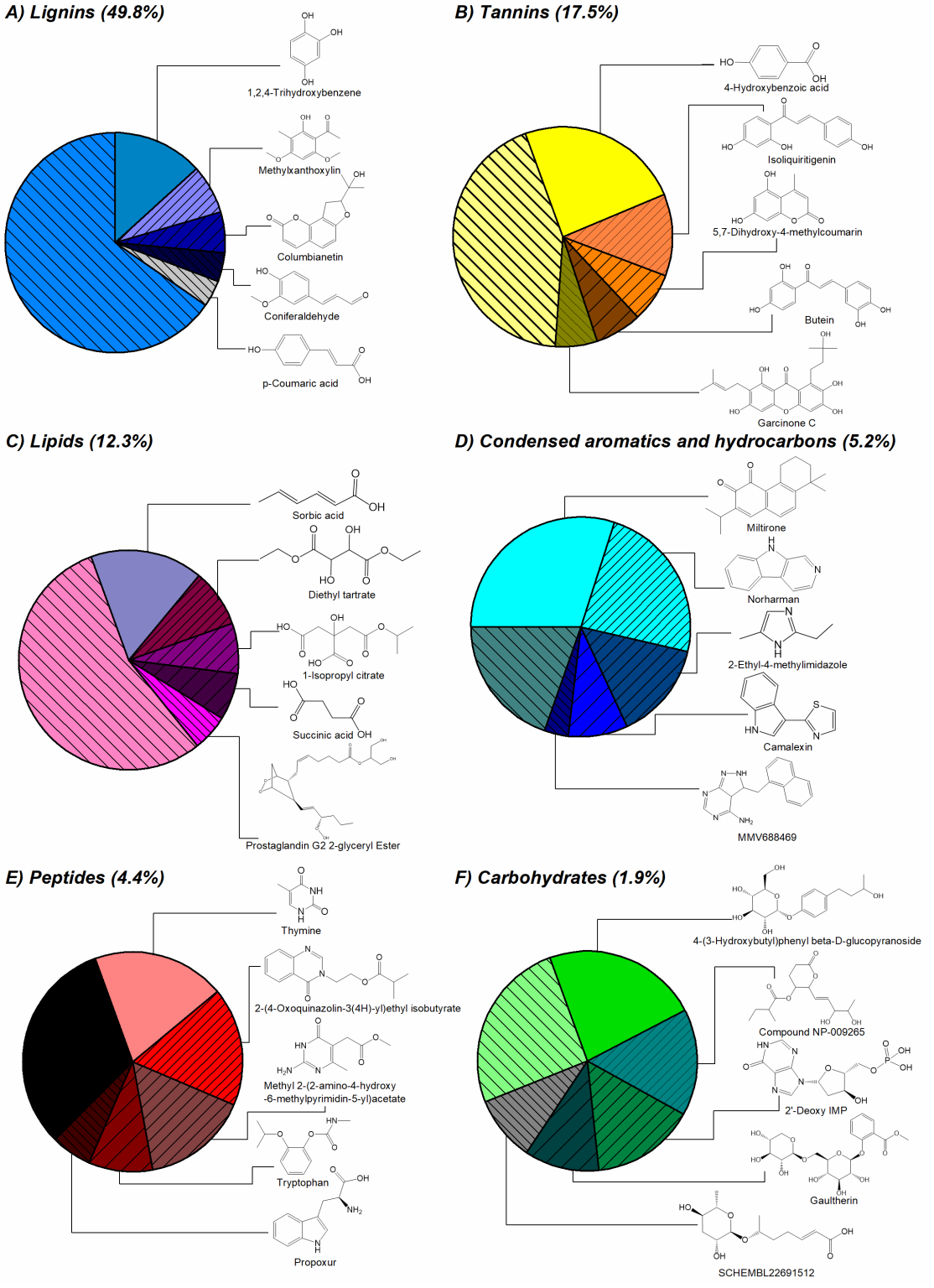

A) Lignins (49.8%)
1,2,4-Trihydroxybenzene
Methylxanthoxylin
Columbianetin
Coniferaldehyde
p-Coumaric acid
B) Tannins (17.5%)
4-Hydroxybenzoic acid
Isoliquiritigenin
5,7-Dihydroxy-4-methylcoumarin
Butein
Garcinone C
C) Lipids (12.3%)
Sorbic acid
Diethyl tartrate
1-Isopropyl citrate
Succinic acid
Prostaglandin G2 2-glyceryl Ester
D) Condensed aromatics and hydrocarbons (5.2%)
Miltirone
Norharman
2-Ethyl-4-methylimidazole
Camalexin
MMV688469
E) Peptides (4.4%)
Thymine
2-(4-Oxoquinazolin-3(4H)-yl)ethyl isobutyrate
Methyl 2-(2-amino-4-hydroxy
-6-methylpyrimidin-5-yl)acetate
Tryptophan
Propoxur
F) Carbohydrates (1.9%)
4-(3-Hydroxybutyl)phenyl beta-D-glucopyranoside
Compound NP-009265
2'-Deoxy IMP
Gaultherin
SCHEMBL22691512

Figure 9. Tentatively assigned structures of the most abundant WSOCs in BrC_{aq}, classified as derivatives and pyrolysis products of lignins (A), tannins (B), lipids (C), condensed aromatics and hydrocarbons (D), peptides (E), and carbohydrates (F). Detected compounds were assigned to these groups based on assigned elemental formulas (confidence level 4 in Table 1) as presented in Fig. 6. Unlabeled areas correspond to unidentified molecules in each group. Only five major components from each group are shown, and all structural assignments via NTA and identification confidence levels 1 to 3 are listed in Tables S8 and S9.

The major tracers of BB identified include phenols and methoxyphenols originating from lignin and tannin pyrolysis (Figs. 9A-B) (Li et al., 2021a; Hartner et al., 2024a; Wan et al., 2019). As previously reported, products derived from aromatic alcohols sinapyl, coniferyl, and p-coumaryl constituted 53.4% of WSOCs generated by the combustion of lignin (Fleming et al., 2018; Kawamoto, 2017; Simoneit, 2002). Furthermore, mono and poly-carboxylic acids, including succinic, glutaric, adipic, sorbic, and azelaic acids (Hu and Yu, 2013; Narukawa et al., 1999), were identified as major compounds in the lipid fraction (Fig. 9C), consistent with the polar semi-volatile organic compounds from laboratory-generated BB emissions and fine particles collected at an urban location (Sengupta et al., 2020; Hu and Yu, 2013; Shen et al., 2022). Condensed aromatics and hydrocarbons, peptides, and carbohydrates were minor components of BrC_{aq} (Figs. 9D-F). While some studies reported higher emissions of these molecules, their contribution varies considerably depending on the pyrolysis temperature (Zhang et al., 2024; Oros et al., 2006; Chang et al., 2024).

Structures of 361 out of the 420 WSOCs detected in BrC_{aq} were tentatively identified for the first time (Tables S8 and S9). Of the 50 most abundant molecules in BrC_{aq} (Table S11) identified at least at level 3 (Table 1), 28% were previously detected in ambient and laboratory-generated (light-absorbing) OAs (Yee et al., 2013; Sengupta et al., 2020; Divisekara, 2023; Moschos et al., 2024b; Fleming et al., 2020; Oros et al., 2006; Graham et al., 2002b; Hartner et al., 2024a; Bianco et al., 2016; Oros and Simoneit, 2001; Chan et al., 2020).

These (newly) identified structures were used to estimate H and LD_{50} values (Section 2.8) listed in Tables S12 and S13. The estimated properties exhibited almost no correlation with the elemental composition and the general characteristics of WSOCs annotated at least at level 4 (Table 1), including the number of O, N, C, and S atoms and N/O ratio for each molecule (Table S14). Statistically significant (p value<0.05), but weak ($r= 0.561$) correlation was observed between H values and the number of oxygen atoms. Hence, the properties of polar (complex) molecules in BrC_{aq} cannot be even roughly constrained using simple parameters derived from HR-MS measurements, and more sophisticated models, such as quantitative structure-activity relationships (QSARs), are necessary (Mansouri et al., 2021; Mansouri et al., 2018).

3.5 Potential precursors of $_{aq}$SOAs in fine BrC_{aq}

Because some structural assignments were ambiguous, which is inevitable in NTA (Hulleman et al., 2023; Hohrenk et al., 2020b), the list of potential $_{aq}$SOAs precursors with the 50 highest H scores (Table S12) was further refined - Fig. 10.

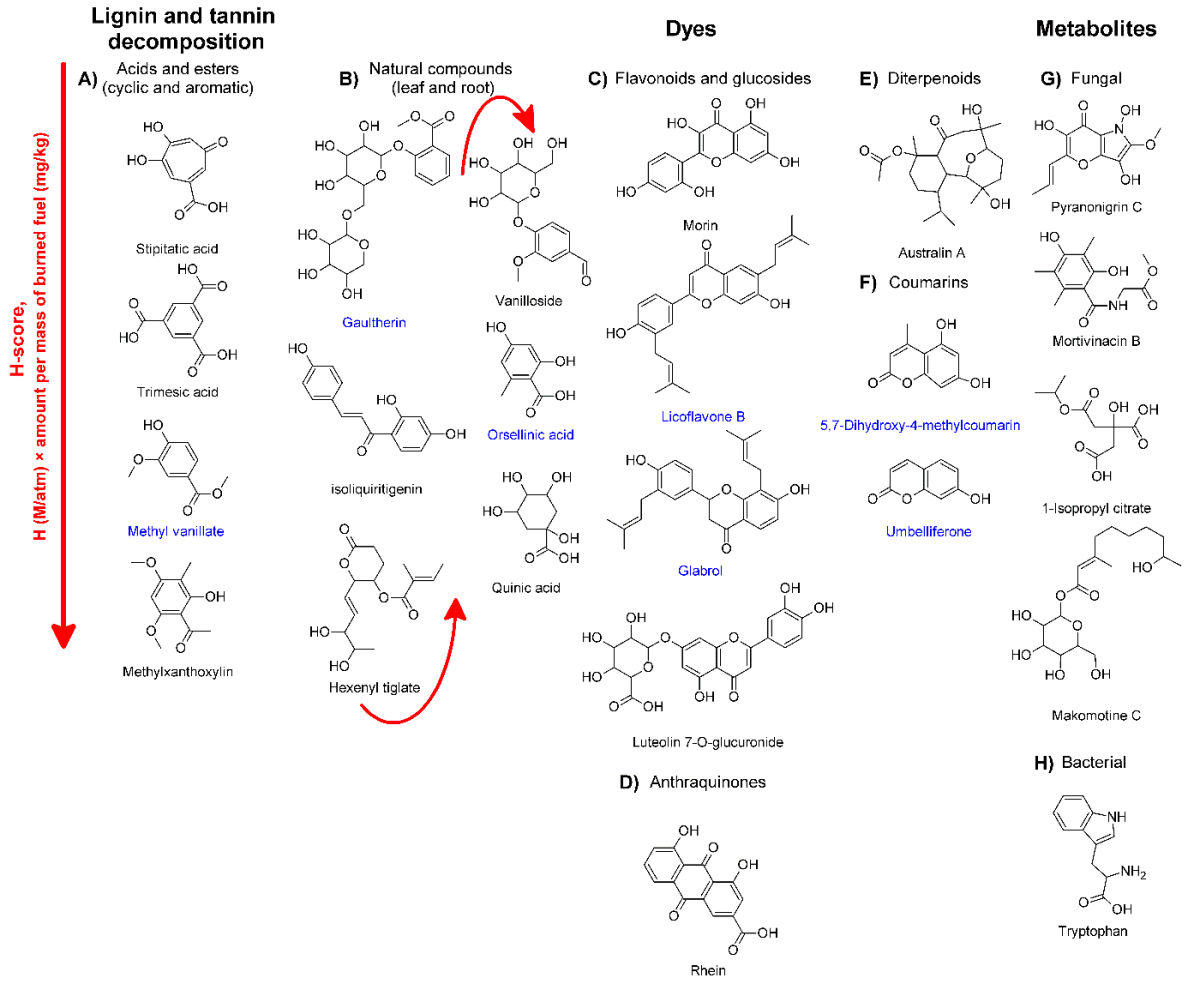


Figure 10. Newly identified potential precursors of $_{aq}$SOAs with the highest H scores (eq. VI in Section 2.8). The structures shown were assigned at levels 2 and 3, with names shown in black and blue, respectively. Identification levels in NTA are showcased in Table 1; the lower is better. Seven out of twenty-two compounds shown were identified at the 2nd level, the highest possible confidence without using authentic standards.

The newly identified $_{aq}$SOAs precursor candidates included cyclic and aromatic acids and esters, which can be classified as typical BB tracers (Fig. 10A) (Laskin et al., 2025; Wan et al., 2019). Furthermore, relatively large quantities of natural compounds present in roots and leaves (Fig. 10B), and natural dyes, including flavonoids (aglycones and glucosides, Fig. 10C) and anthraquinones (Fig. 10D), and coumarins (Fig. 10E) were also identified (Lin et al., 2016; Moschos et al., 2024a; Laskin et al., 2025; Huang et al., 2022). In addition to high solubility in water, natural dyes substantially contribute to the BrC absorption between 300 and 370 nm (Laskin et al., 2025; Zhou et al., 2021). Moreover, one diterpenoid (Fig. 10E) and several fungal and bacterial metabolites (Figs. 10G and H) were detected (Laskin et al., 2025; Wei et al., 2019).

Molecules shown in Fig. 10 (or their analogs) can be obtained from commercial suppliers and serve as model precursors for investigating the combustion-related $_{aq}$SOAs. To date, such studies have focused primarily on (nitrated) phenols (Lei et al., 2025; Jiang et al., 2021; Hems and Abbatt, 2018; Witkowski et al., 2022). Hence, studying these newly identified WSOCs can shed new light on the formation and evolution of light-absorbing OAs in the atmospheric hydrometeors, even if they only serve as proxies of ambient BrC (Hems et al., 2020; Liu et al., 2020; Laskin et al., 2025). The atmospheric lifetimes of the compounds shown in Fig. 10 due to the reaction with OH (the major daytime atmospheric oxidant) are further discussed in Section 4.

3.6 Toxic compounds identified in fine BrC_{aq}

The newly identified molecules with the highest LD_{50} scores (Table S13) are shown in Fig. 11

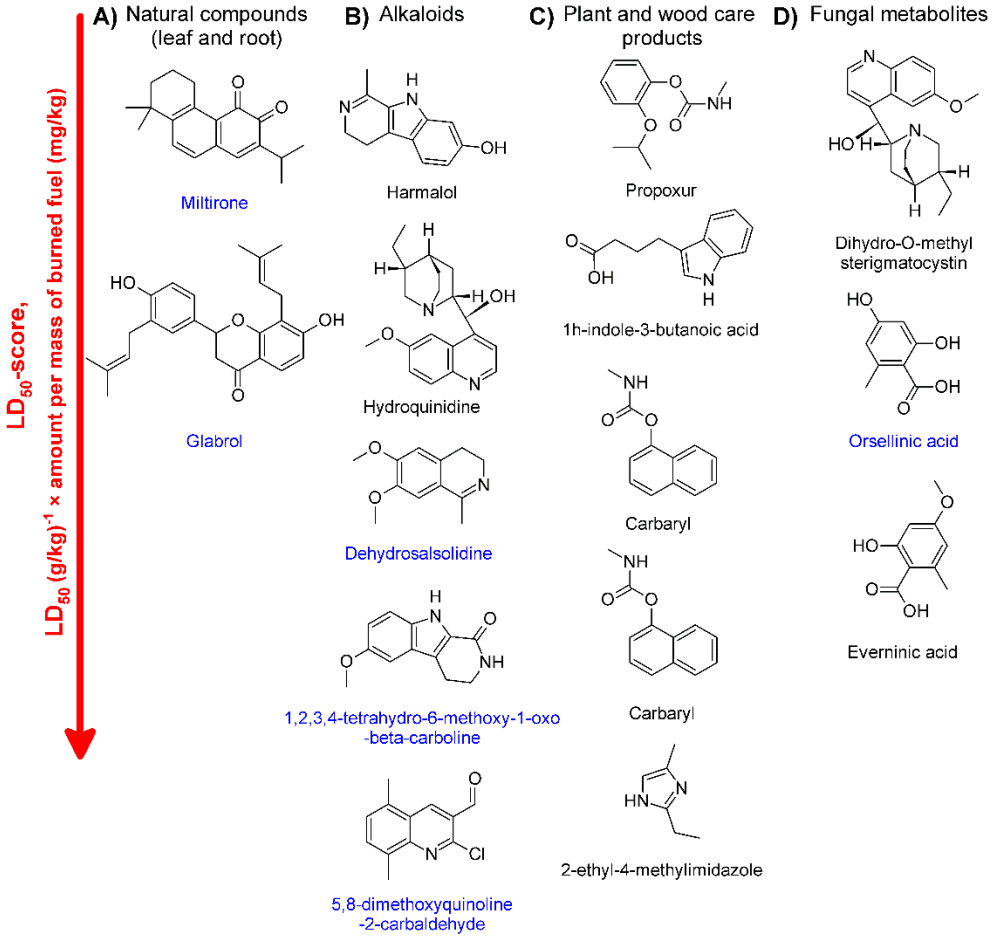


Figure 11. Newly identified, harmful components of BrC_{aq} with the highest LD_{50} scores (eq. VII in Section 2.8). The structures shown were assigned at levels 2 and 3, with names shown in black and blue, respectively. Identification levels in NTA are showcased in Table 1; the lower is better. Six out of fifteen compounds shown were identified at the 2nd level, the highest possible confidence without using authentic standards.

Of the 50 WSOCs with the highest LD_{50} scores, 32 were classified as moderately ($50<LD_{50}<500$) toxic, and harmful ($500<LD_{50}<2000$), with five highly toxic (LD_{50} <50) molecules – Table S13 (Gadaleta et al., 2019). Several N-containing compounds were identified among the toxic components of BrC_{aq} (Fig. 11) (Pflieger and Kroflič, 2017; Majewska et al., 2021). However, no correlation of the LD_{50} values with the number of N atoms or N/O ratios (Table S14) underscores that such general classifications can be unreliable and more sophisticated methods are needed to evaluate whether or not a given pollutant is harmful (Young et al., 2021a; Khan et al., 2021). The newly identified WSOCs included natural compounds (Fig. 11A), particularly alkaloids (Fig. 11B), which were seldom identified as (harmful) BB tracers (Young et al., 2021a; Nizkorodov et al., 2011).

Furthermore, plant and wood care products (Fig. 11C) and fungal metabolites (Fig. 11D) were detected in a toxic fraction of BrC_{aq} (Laskin et al., 2025; Wei et al., 2019; Růžičková et al., 2021). The release of insecticides from commercial pellet fuel was previously observed at low-temperature pyrolysis (here, 350°C was used – Section 2.1), which is insufficient to decompose such molecules (Růžičková et al., 2021). Forest protection with man-made chemicals and the production of wood pellets from different waste materials contribute to releasing these toxic WSOCs (Růžičková et al., 2021; Cesprini et al., 2021; Alakoski et al., 2016). Furthermore, the raw material for wood pellets usually contains between 70 and 95% tree wood and thus can include other kinds of forest biomass (Cesprini et al., 2021), but secondary contamination during storage (e.g., fungal growth) is also possible (Alakoski et al., 2016). In vegetation fires, properties cannot be controlled, but the current wood pellet quality standards do not consider the organic (micro)pollutants (Cesprini et al., 2021; Alakoski et al., 2016).

3.7 Atmospheric implications

The chemical aging of BB aerosols is connected with the formation and evolution (bleaching) of BrC (Wong et al., 2019; Zhao et al., 2015; Choudhary et al., 2023; Witkowski et al., 2022). Therefore, the lifetimes of potential $_{aq}$SOA precursors shown in Fig.10 due to reaction with OH were estimated with eq. VIII (Sarang et al., 2021).

$$\tau = \frac{1}{\left(\frac{k_{OH_{gas}}}{H_{OH}^{cc}} + k_{OH_{aq}} H_{BrC}^{cc} \omega\right)[OH]_{aq}} \qquad (VIII)$$

In eq. VIII, τ is the overall gas and aqueous phase lifetime due to the reaction with OH. The equilibrium concentrations of individual BrC_{aq} and OH in both phases are derived using the dimensionless H_{OH}^{cc} and H_{BrC}^{cc} values (Sander, 2015), and liquid water content (LWC, ω, unit m^3/m^3). The bimolecular reaction rate coefficients ($k_{OH_{gas,}}$ and $k_{OH_{aq}}$ – Table S15) at 298K were estimated with *py*SiRC model (Sanches-Neto et al., 2021).

The lifetimes estimated with eq. VIII for the potential precursors of $_{aq}$SOAs (Fig. 10) cover a wide range of values from less than one minute to several hours – Fig. 12A.

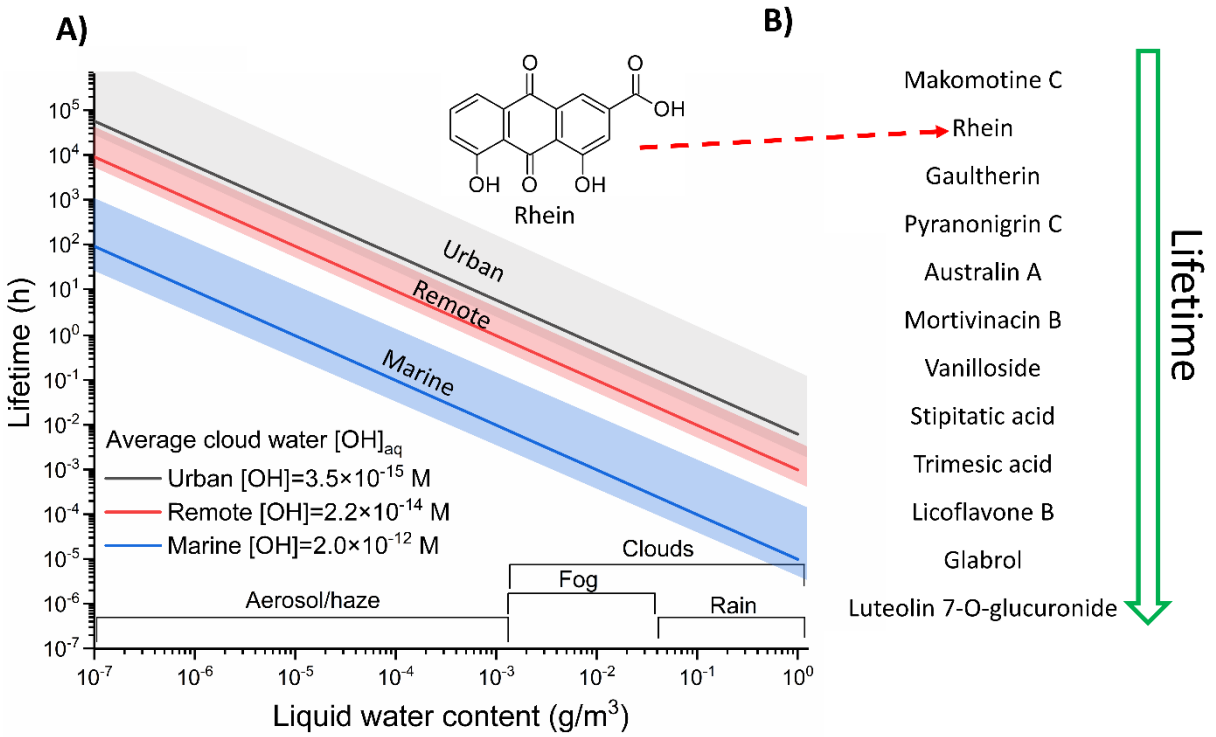


Figure 12. A - estimated τ values (eq. VIII) for anthraquinone rhein due to the reaction with OH in different atmospheric hydrometeors, shaded areas represent the highest and lowest $[OH]_{aq}$. Only one sample plot is shown because the same profiles were obtained for all compounds listed in Table S12 (molecules with the highest H scores). B - the potential precursors of $_{aq}$SOAs with the shortest lifetimes are listed.

Considering the aqueous processing of BB emissions in the atmosphere, continental (urban and remote) cloud-water processing is the most relevant, with marine scenarios being feasible following long-range transport (Che et al., 2022; Laskin et al., 2025). The τ values for all compounds with high H scores (Table S12) were affected by liquid water even in urban clouds, with the lowest $[OH]_{aq}$ (Fig. 12A). An estimated time of air-parcel interaction with the cloud is very long (18h) (Herrmann et al., 2015), but the cloud droplet lifetimes are < 1 min (Kumar et al., 2013; Paulson et al., 2019). The estimated τ values also do not consider aqueous sources of OH, primarily Fenton (like) reactions, which can increase $[OH]_{aq}$ by several orders of magnitude (Kuang et al., 2020; Paulson et al., 2019).

Under these assumptions, of all potential precursors (Table S12), the most reactive molecules and those emitted in the highest quantities were selected (Fig. 12B). Thus, these newly identified WSOCs (Fig. 10) will likely undergo aqueous OH oxidation under realistic atmospheric conditions. Analyzing the yields of $_{aq}$SOAs from these precursors would require a separate investigation. However, compounds with large carbon backbones (Fig. 10) will likely yield low-volatility products following a reaction with OH without decomposing, at least during the early stages of oxidation (Fig. 12) (Herraiz and Galisteo, 2015).

4. Conclusions

This work revealed new, water-soluble tracers of wood combustion in fine, water-soluble BrC, including insecticides, wood-care products, and bacterial and fungal metabolites. The release of these compounds is possible during vegetation fires and domestic uses of wood and pellet fuel, contributing to the adverse health effects of open and domestic BB. Furthermore, in the case of vegetation fires, even 70% of the fuel is consumed under oxygen-depleted and smoldering conditions (Akagi et al., 2011), likely favoring the release of polar, water-soluble organics, such as the molecule newly identified in this work (Chen and Bond, 2010). Global, annual emissions from open BB (not including domestic uses) were estimated at ca. 2600 TgC, including 18.6 Tg of particle-bound organic carbon (Liu et al., 2024). At the same time, very little data is still available about the EF of the polar, higher-molecular-weight WSOCs emitted by open BB, even though such molecules are released during combustion and pyrolysis without decomposing (Li et al., 2021a). This work revealed that the amount of water-soluble organics emitted under oxygen-depleted conditions may be comparable to the EFs of non-polar, lower-molecular-weight BB tracers. Such molecules can form light-absorbing SOAs following oxidation reactions in different hydrometeors and contribute to the adverse health effects of BB emissions

Studying the light-absorbing properties of BrC_{aq} was beyond the scope of this work; however, new potential chromophores, including natural dyes and molecules with conjugated double bonds and aromatic rings, were also identified (Tables S8-S9). The results presented provide new insights into the structures of BrC chromophores (Laskin et al., 2025)

Data availability. The raw data can be obtained by contacting the corresponding author.

Author contributions. BW designed the study, developed the methodology, and analyzed the data. VN carried out the experiments, optimized the methodology, and processed the raw data. TG supervised the experiments, analyzed the data. All authors contributed to the interpretation of the results and contributed to manuscript writing and editing.

*Competing interests***.** The authors declare that they have no conflicts of interest

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