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Supplement of

Contrasting organic aerosol molecular composition between the urban and agricultural environment of the Po Valley

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Contents

S1 Calculations

S1.1 Normalized-Signal Intensity (nSI)

In order to take into account the ionization efficiency and ion transmission variability between positive and negative ionization mode and to compare the time serie, we choose to scale the signal intensity of each individual compound detected in each sample by the maximum signal intensity detected over the whole time serie taking into account the ionization mode.
Let us call $SI_{c,pol,d}$ the signal intensity of compound *c* detected in polarization mode *pol* on a sample collected on day *d* and let us call $MAX(SI_{pol})$ the maximum SI within the entire dataset detected in *pol*. Then:

$$nSI_{c,d} = \frac{SI_{c,pol,d}}{MAX(SI_{pol})} \tag{S1}$$

As a consequence, the normalized-Total Signal Intensity (*nTSI*) of the sample collected on day *d* is:

$$nTSI_d = \sum_{c=1}^{C} nSI \tag{S2}$$

S1.2 Residuals contribution calculation

Let us indicate $nSI_{MI,c,d}$ the normalized signal intensity (nSI) for compound *c* detected by the HPLC-HESI-HRMS system on the $PM_{2.5}$ sample collected at Milan (MI) on day *d*. Similarly, $nSI_{SKI,c,d}$ is the nSI for compund *c* detected on the sample collected on the same day *d* at Schivenoglia (SKI).
Then:

$$Residuals_{c,d} = nSI_{MI,c,d} - nSI_{SKI,c,d} \tag{S3}$$

Positive *Residuals* means that $nSI_{c,d}$ is higher at MI, whereas negative *Residuals* indicates higher $nSI_{c,d}$ at SKI. To evaluate the relative contribution amount of compound c detected with higher intensity at the site where it is higher (*site*) to the nTSI on day d, we calculate:

$$Contribution = \frac{Residuals_{c,d}}{nTSI_{site,d}} \times 100 \tag{S4}$$

S2 Supplement figures

S2.1 Map of North of Italy

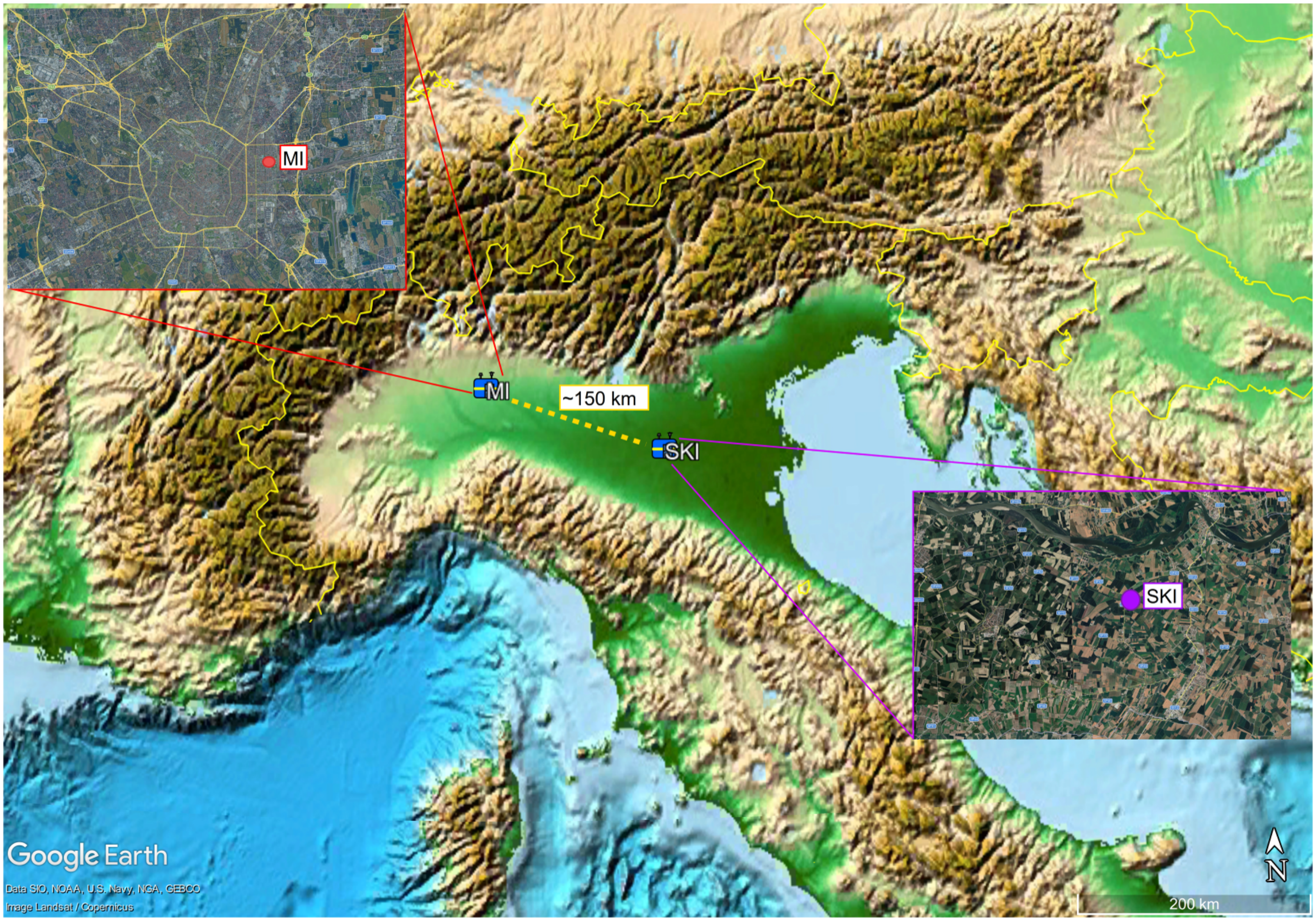


Figure S1. Map of Northern Italy. The Po Valley area is clearly visible, including the orography that often prevent incoming air masses able to abate the high aerosol concentrations that affect the basin. In the map the location of the two sampling sites considered in this work are also shown: MI (the urban background site) and SKI (the rural–agricultural background site). Layer background: ©Google Earth using imagery by Landsat/Copernicus. Topography dat set used by ETOPO1 1 Arc-Minute Global Relief Model (Amante and Eakins, 2009), NOAA National Geophysical Data Center.

S2.2 Brown carbon-related compounds

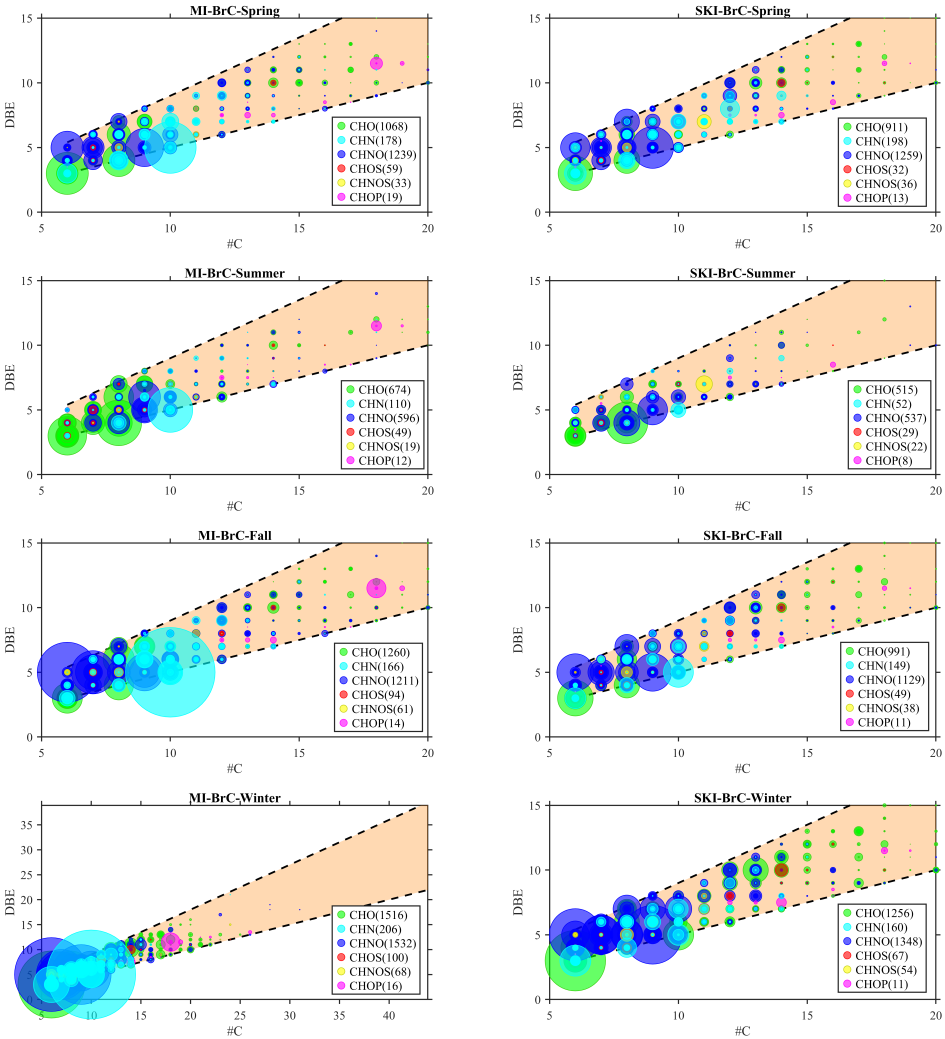


Figure S2. Seasonal fingerprints of BrC-related compounds for MI (left) and SKI (right) sites. The plots highlight the molecular variability between the two environments over the seasons.

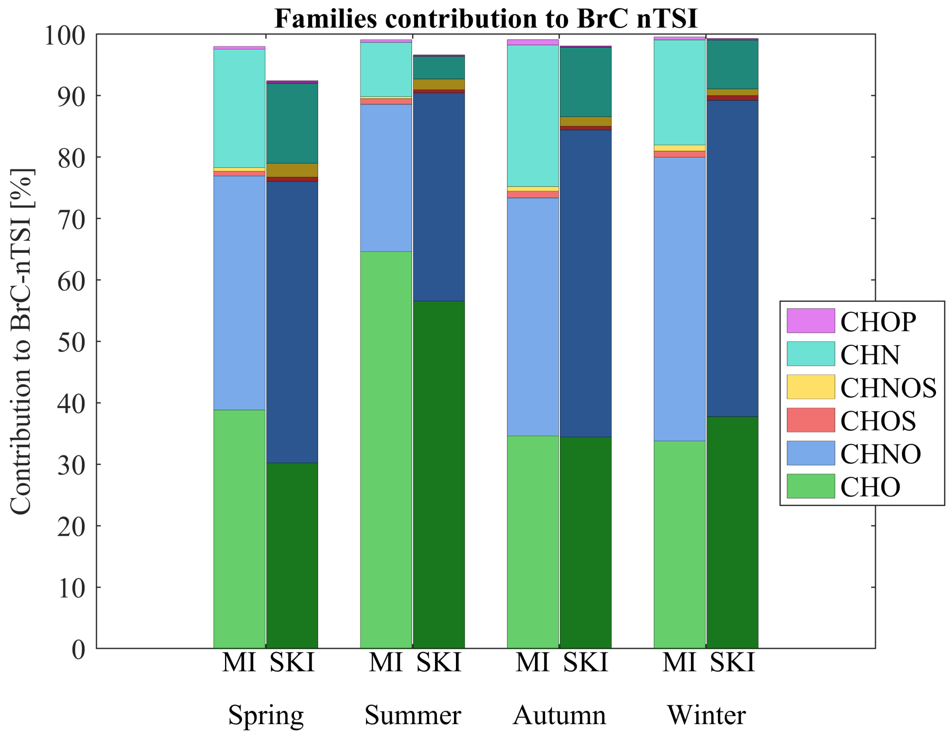


Figure S3. Contribution of the compound families related to BrC nTSI. The residual contribution (not shown) is due to compounds belonging to the "Other" group.

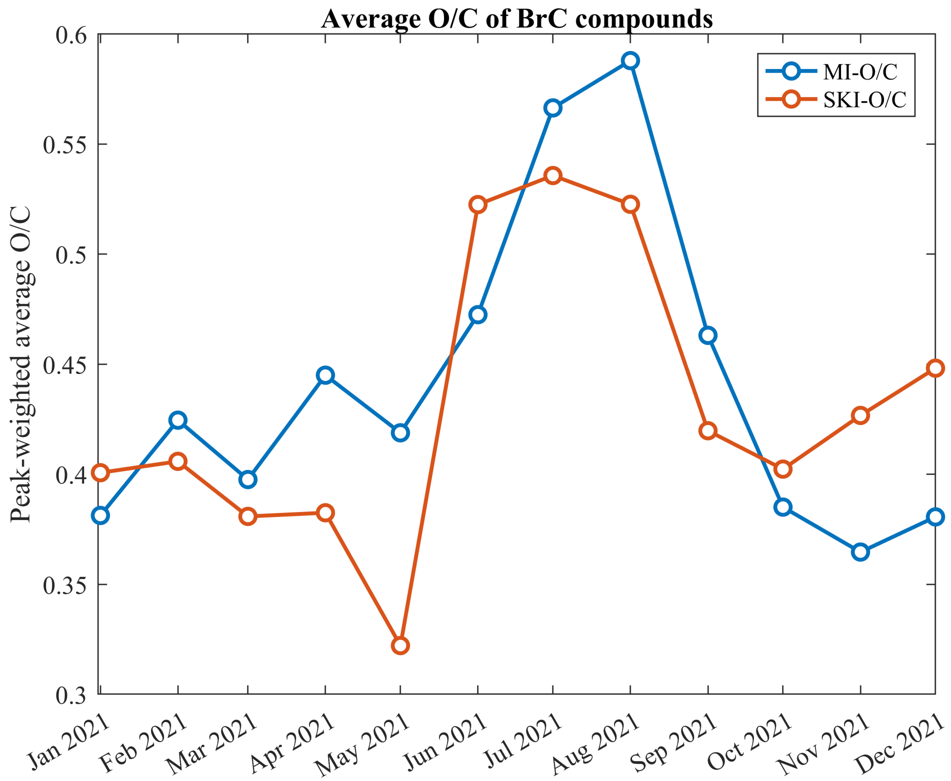
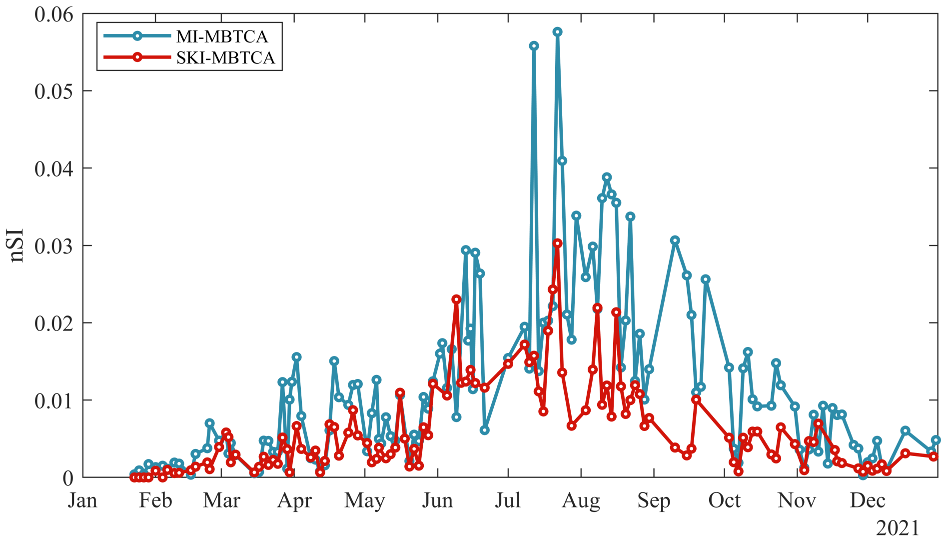


Figure S4. Peak-weighted average of O/C for BrC-related compounds. The monthly average suggests a stronger oxidation regime during summer.

S2.3 Time serie of confirmed compounds



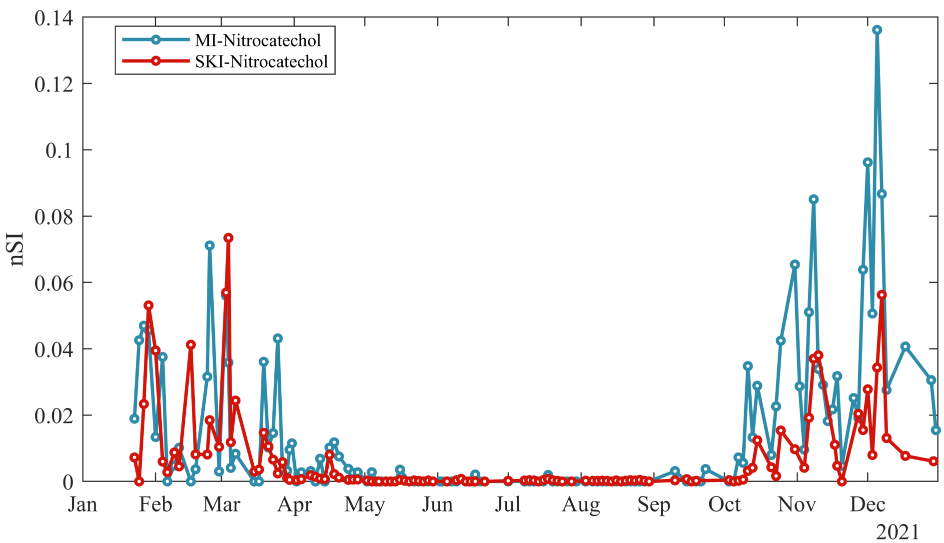


Figure S5. Time series of L1 identification confidence compounds for biogenic (MBTCA, upper plot) and anthropogenic (nitrocatechol, lower plot) SOA at MI and SKI sites.

S2.4 Clustergrams

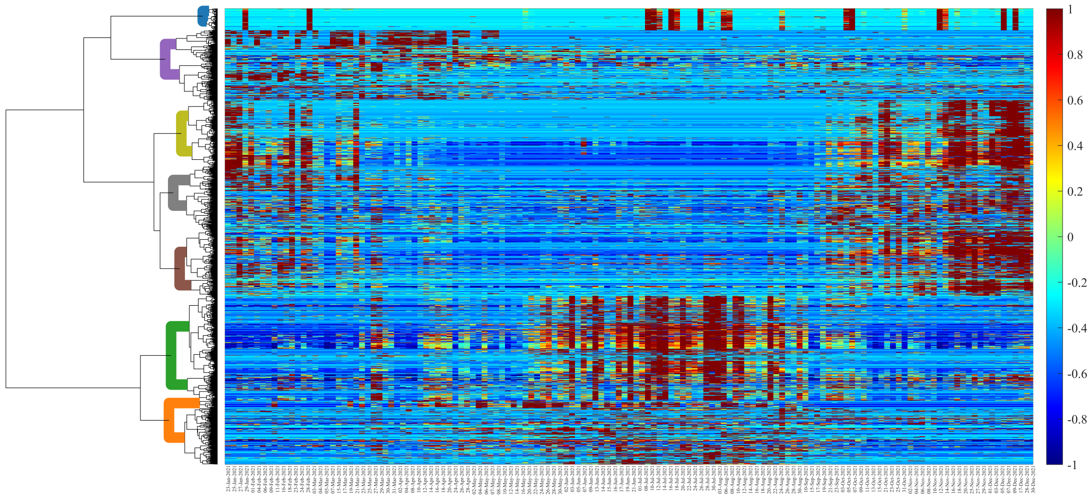


Figure S6. Graphic result of the hierarchical clustering performed on MI dataset. Warmer colors indicate higher values after standardization over the time series of each individual compound. The assigned clusters are marked with the same colors showed in Figure 3 in the main text.

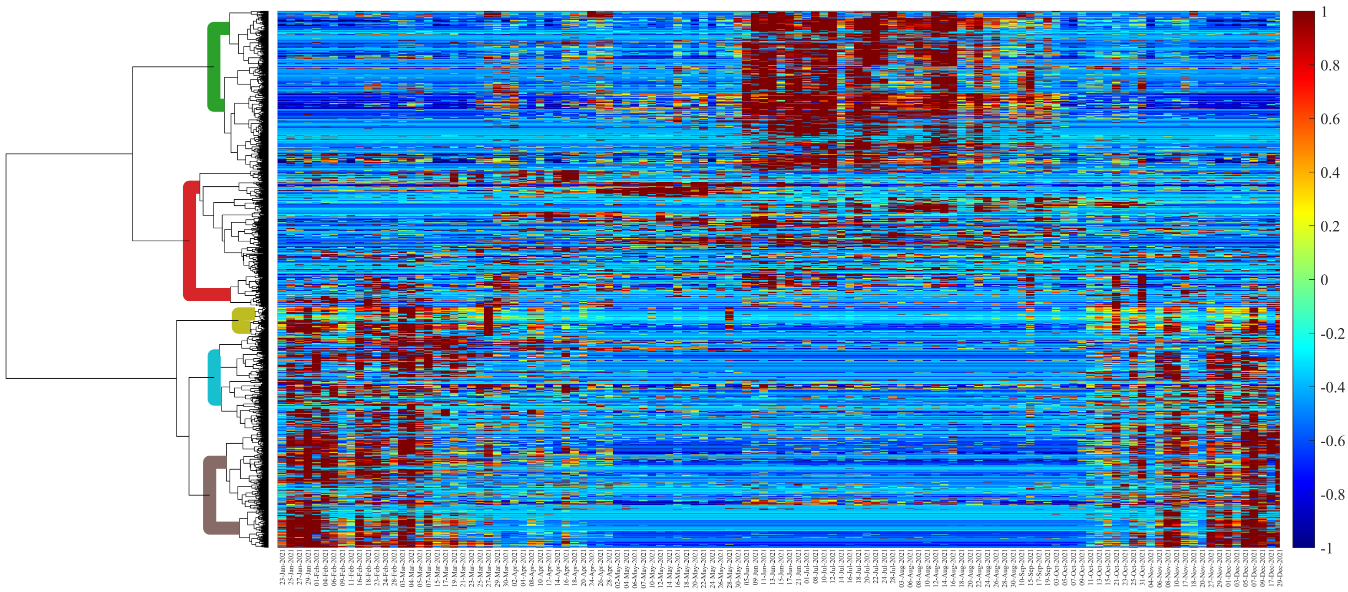


Figure S7. Graphic result of the hierarchical clustering performed on SKI dataset. Warmer colors indicate higher values after standardization over the time series of each individual compound. The assigned clusters are marked with the same colors showed in Figure 3 in the main text.

S2.5 Clusters molecular fingerprints

In this section we show the molecular fingerprint of each cluster. We chose to graphically described the clusters' characteristics based on their retention time (a proxy for the polarity of the molecules) against their calculated molecular weight (left plots), their H/C ratio against O/C ratio with the Van Krevelen diagram (center) and their average OS_C against the number of carbon in the Kroll plot (right). Within these plots, each feature is colored based on the molecular class and the size of the bullet is proportional to its nSI considering as null value all SI below the threshold after blank correction.

S2.5.1 Clusters molecular fingerprints - MI site

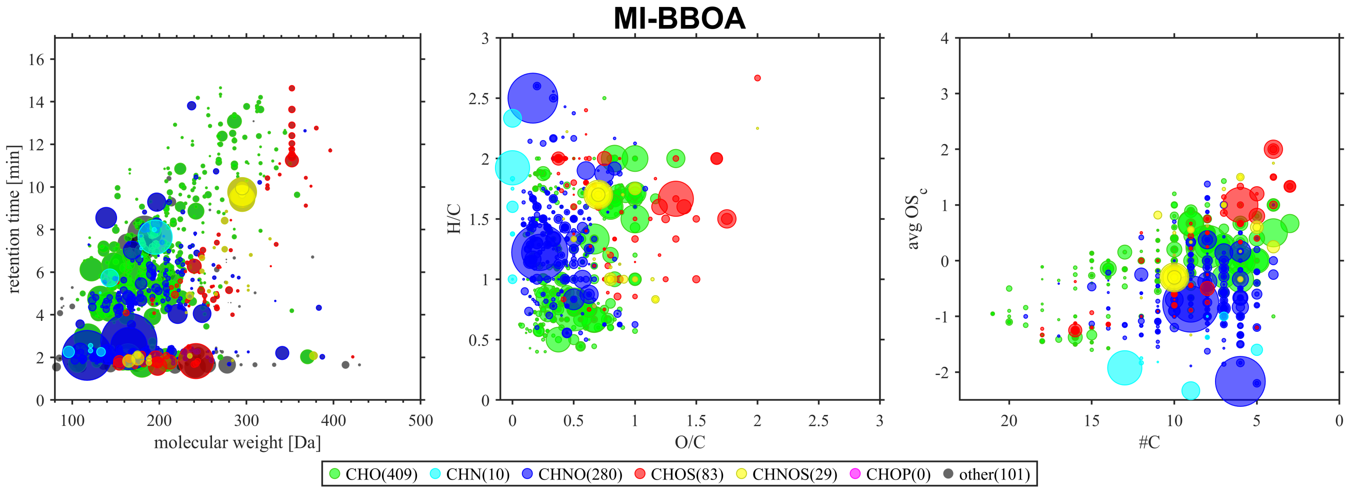


Figure S8. Molecular fingerprint of biomass burning organic aerosols at MI (MI-BBOA).

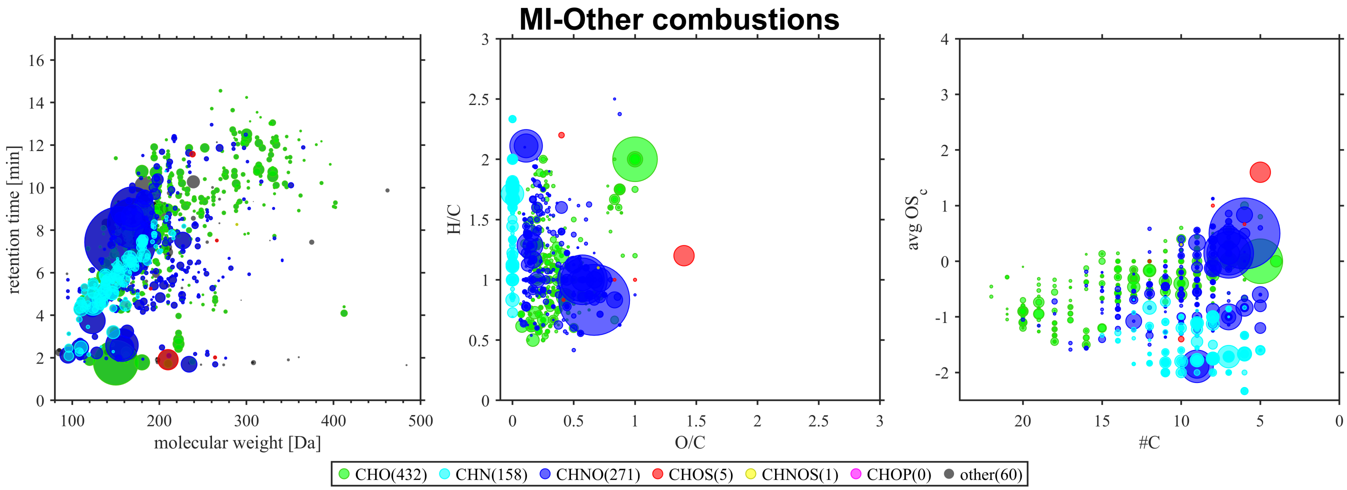


Figure S9. Molecular fingerprint of other combustion related features at MI (MI-Other combustion).

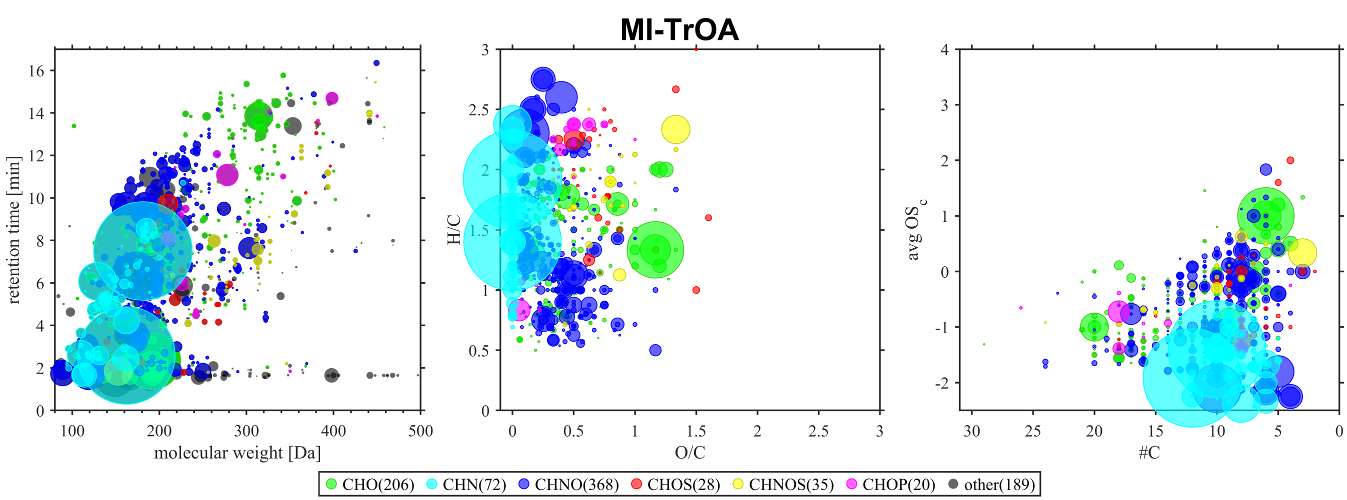


Figure S10. Molecular fingerprint of traffic organic aerosols at MI (MI-TrOA).

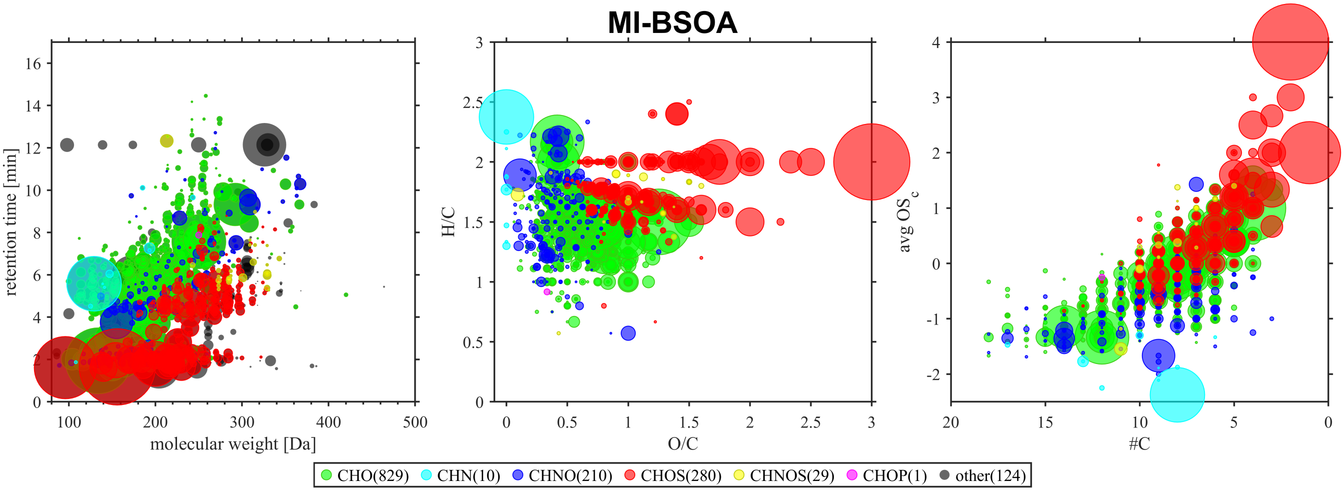


Figure S11. Molecular fingerprint of biogenic organic aerosols at MI (MI-BSOA).

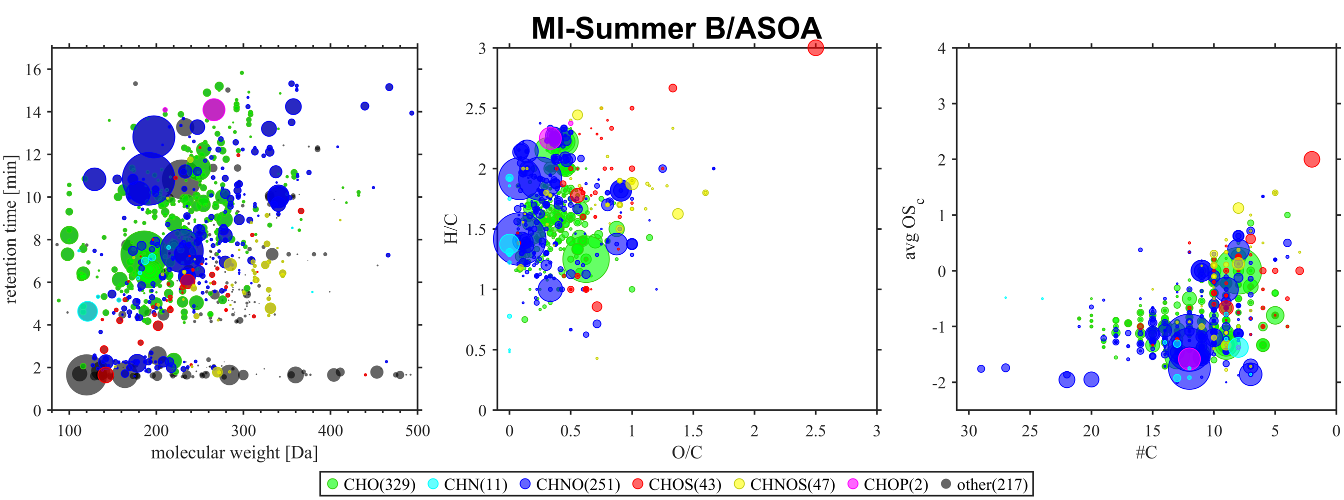


Figure S12. Molecular fingerprint of summertime mixed biogenic and anthropogenic aerosols at MI (MI-Summer B/ASOA).

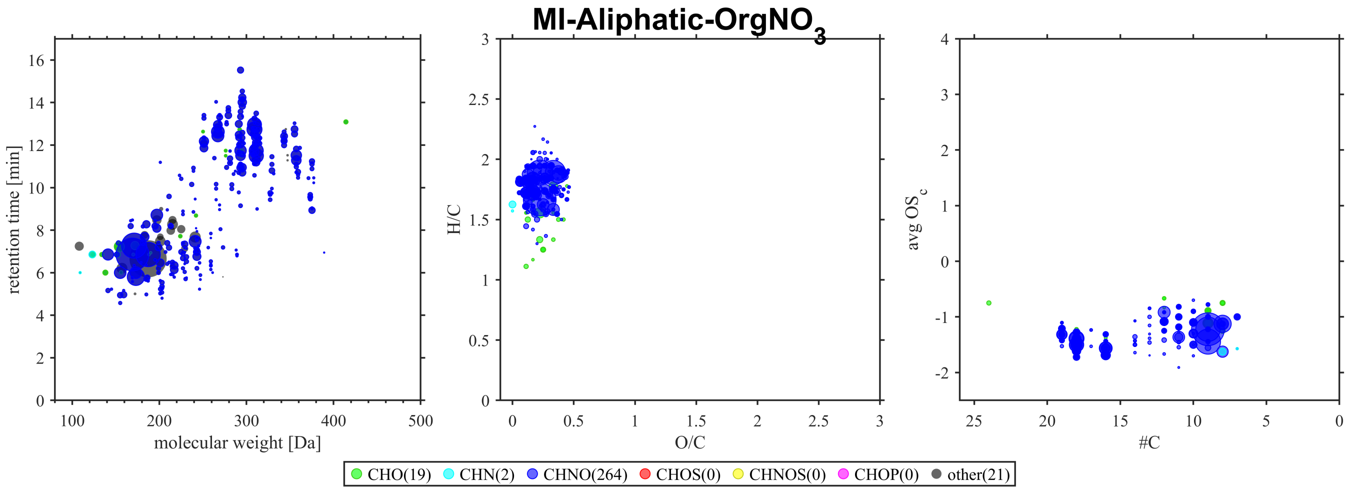


Figure S13. Molecular fingerprint of aliphatic organo-nitrate aerosols at MI (MI-OrgNO$_3$).

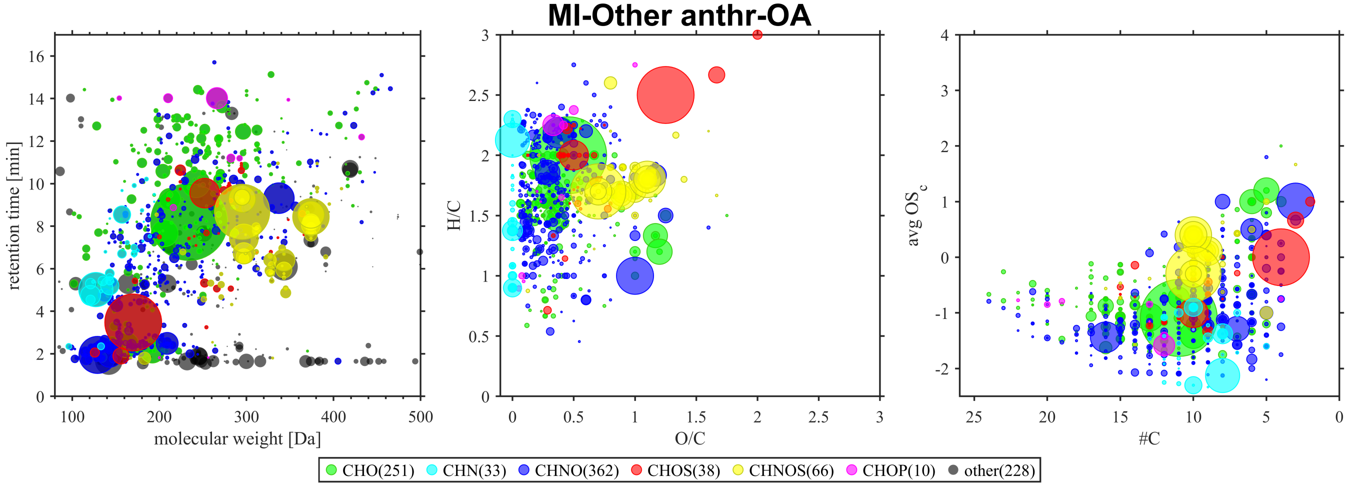


Figure S14. Molecular fingerprint of other anthropogenic organic aerosols at MI (MI-Other anthr-OA).

S2.5.2 Clusters molecular fingerprints - SKI site

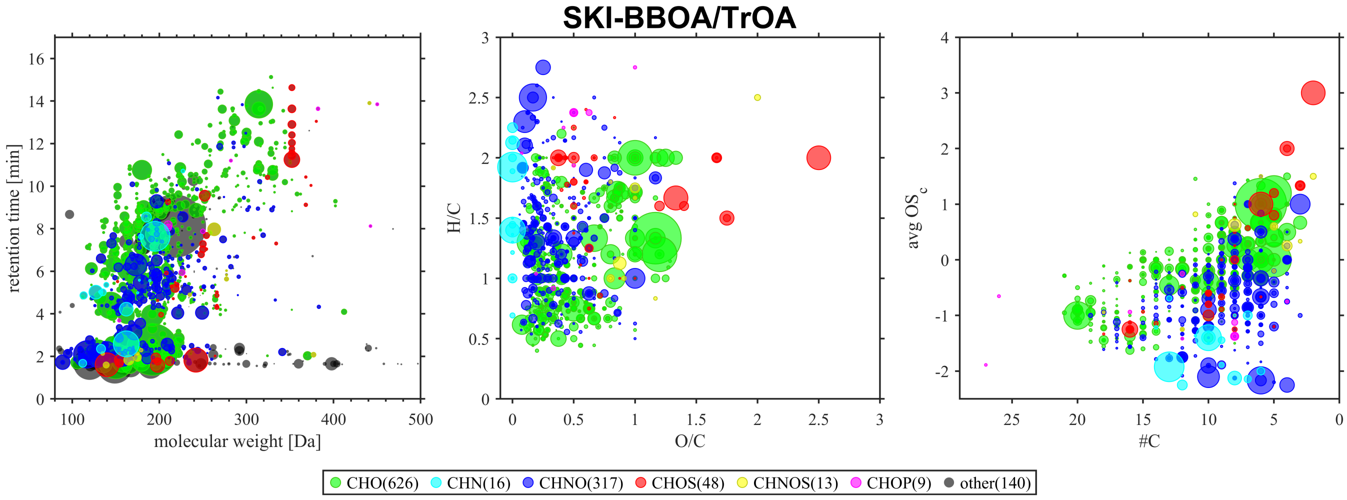


Figure S15. Molecular fingerprint of mixed biomass burning and traffic related organic aerosols at SKI (SKI-BBOA/TrOA).

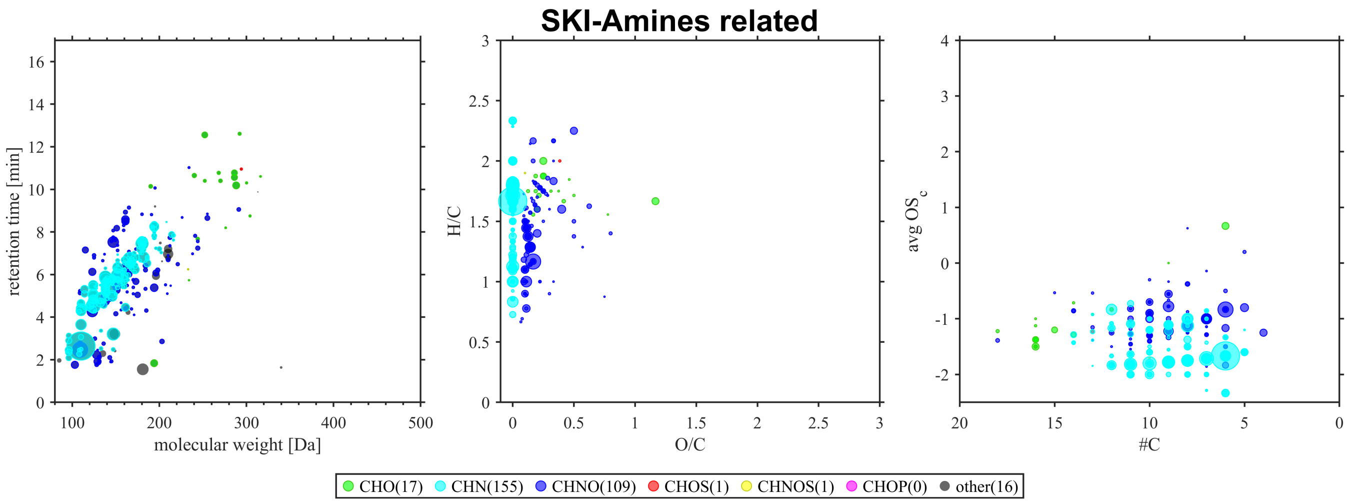


Figure S16. Molecular fingerprint of amines related organic aerosols at SKI (SKI-Amines related).

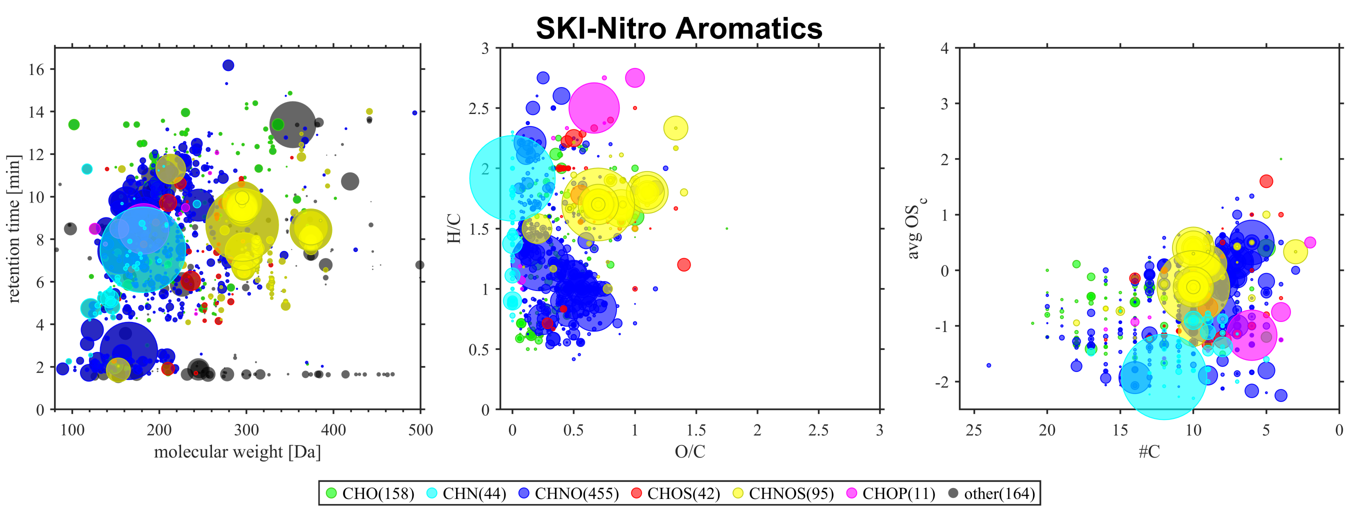


Figure S17. Molecular fingerprint of nitro-aromatic related organic aerosols at SKI (SKI-Nitro Aromatics).

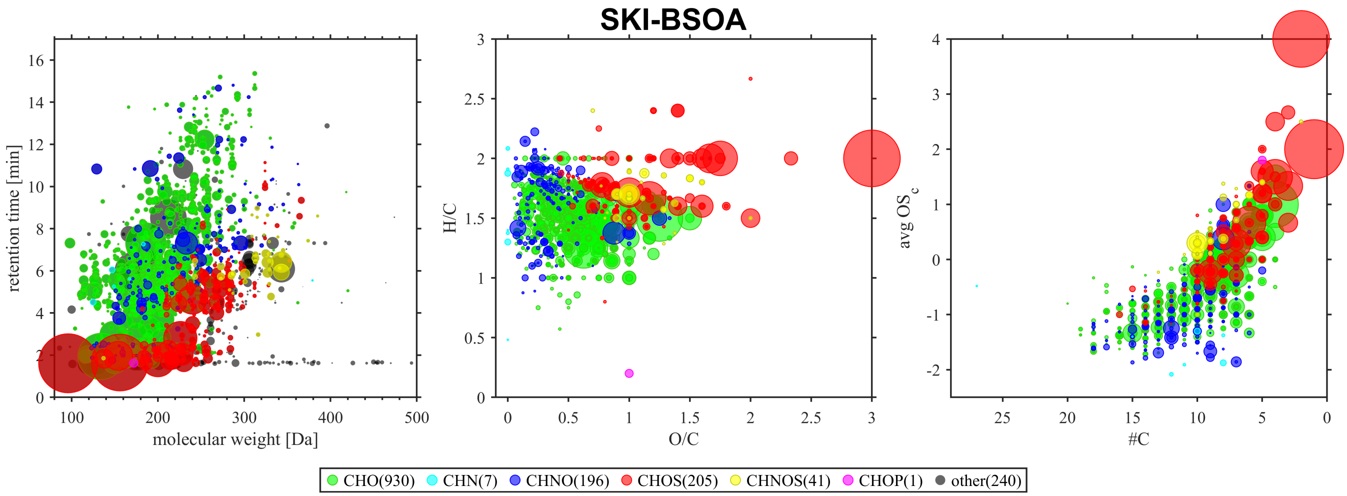


Figure S18. Molecular fingerprint of biogenic organic aerosols at SKI (SKI-BSOA).

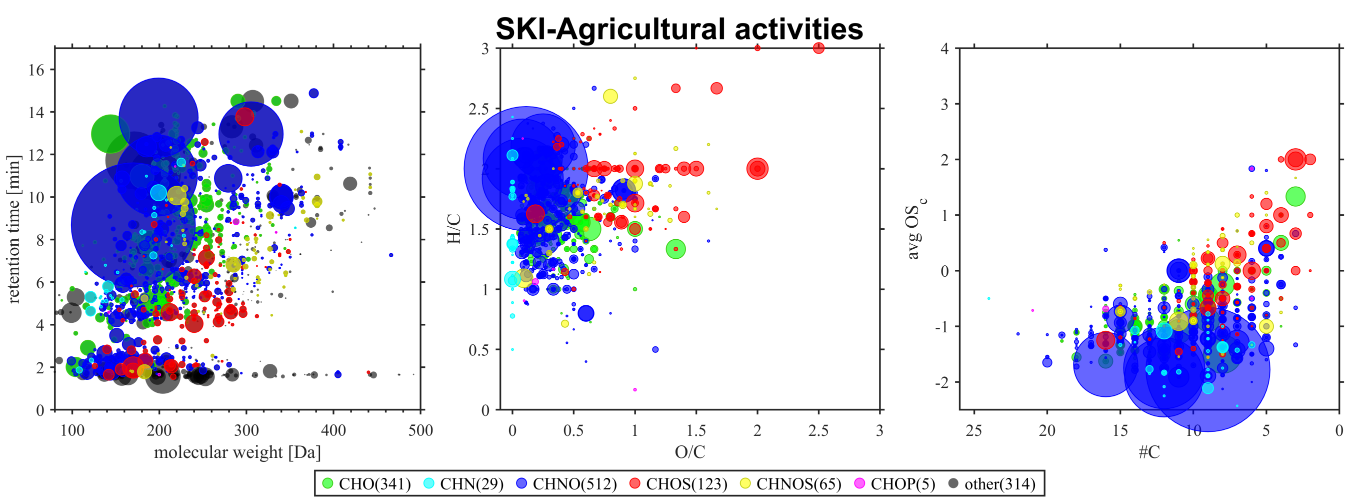


Figure S19. Molecular fingerprint of features linked to agricultural activities at SKI (SKI-Agricultural activities).

S2.6 Site-specific compound fingerprints

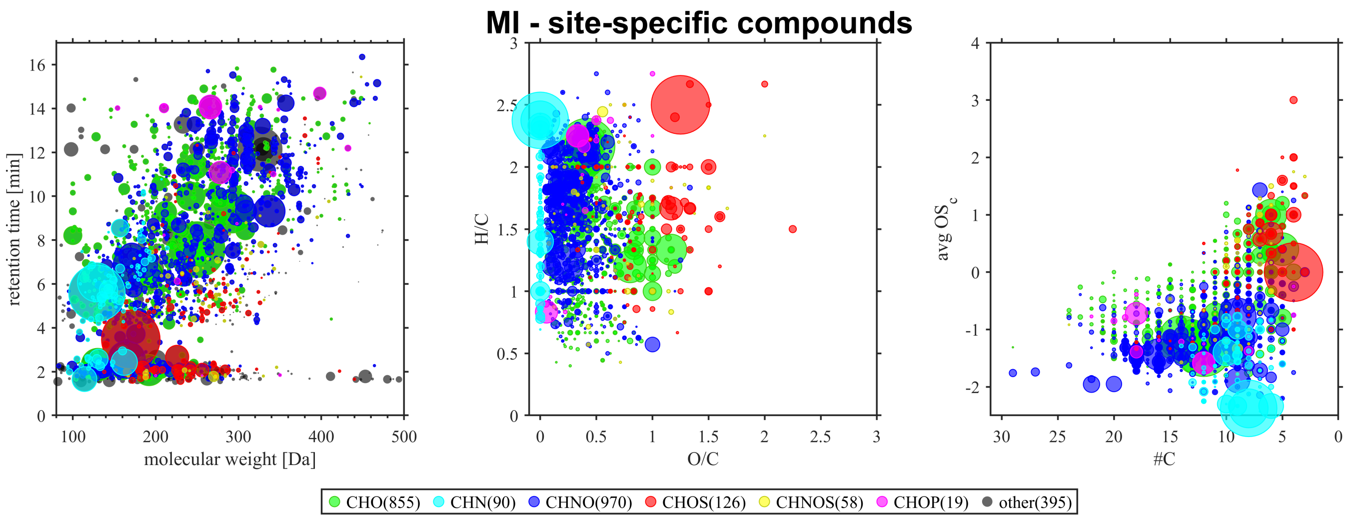


Figure S20. Molecular fingerprint of site-specific compounds detected at MI site and classified with the HCA.

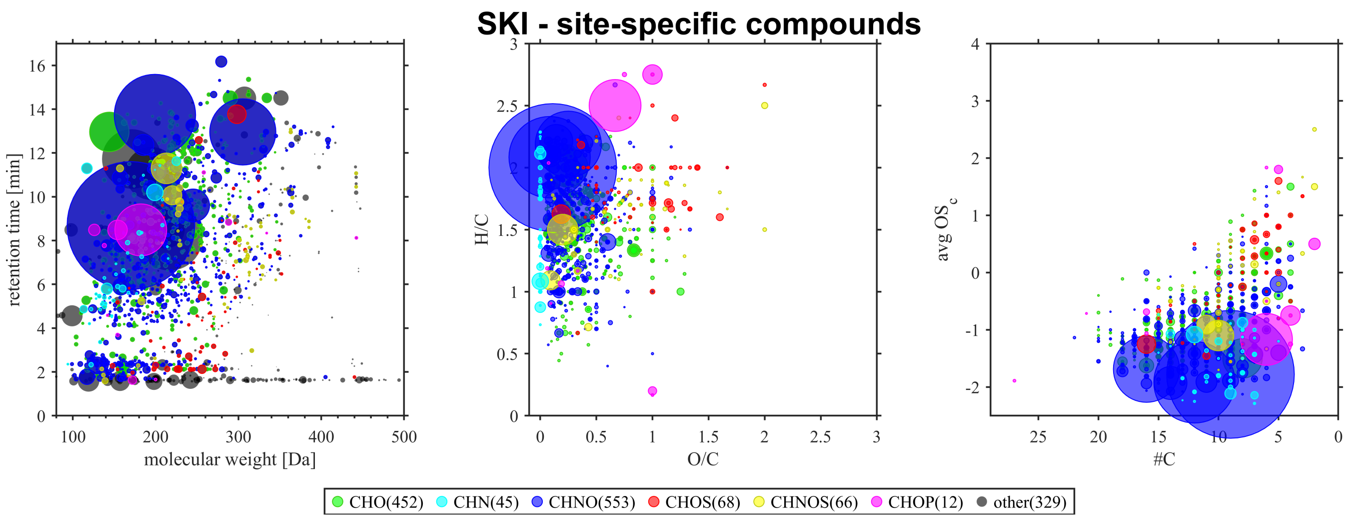


Figure S21. Molecular fingerprint of site-specific compounds detected at SKI site and classified with the HCA.

S2.7 Occurrence of similar samples

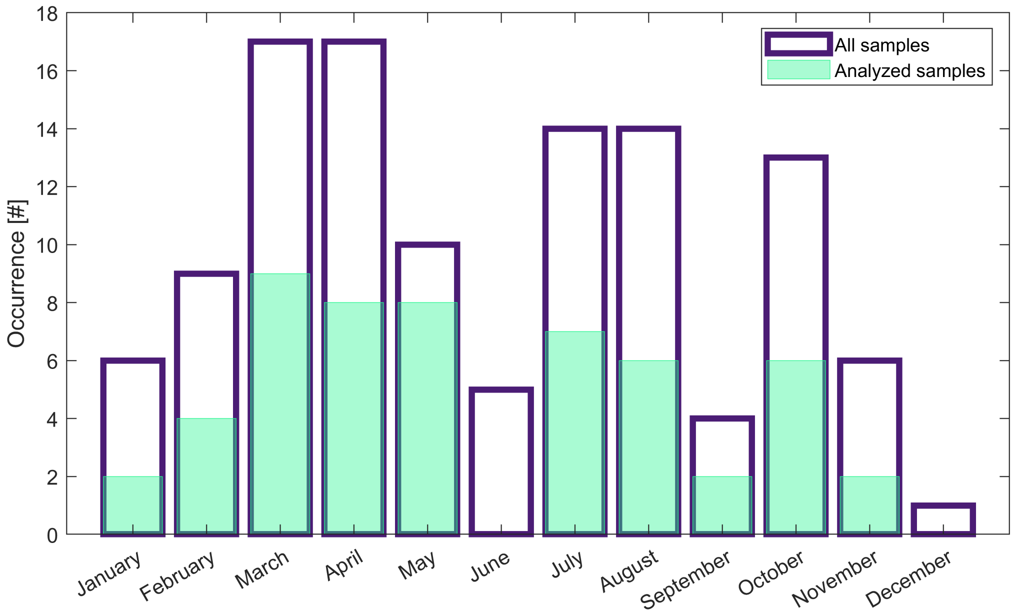


Figure S22. Frequency histogram of samples (collected on the same day in 2021) that meet the criteria to be defined as ‘similar samples,’ grouped by month. The blue bars represent the entire dataset of samples collected throughout the year, whereas the green bars indicate the pairs of samples that were actually extracted and analyzed in this study.

S2.8 Fingerprint of potential BrC features

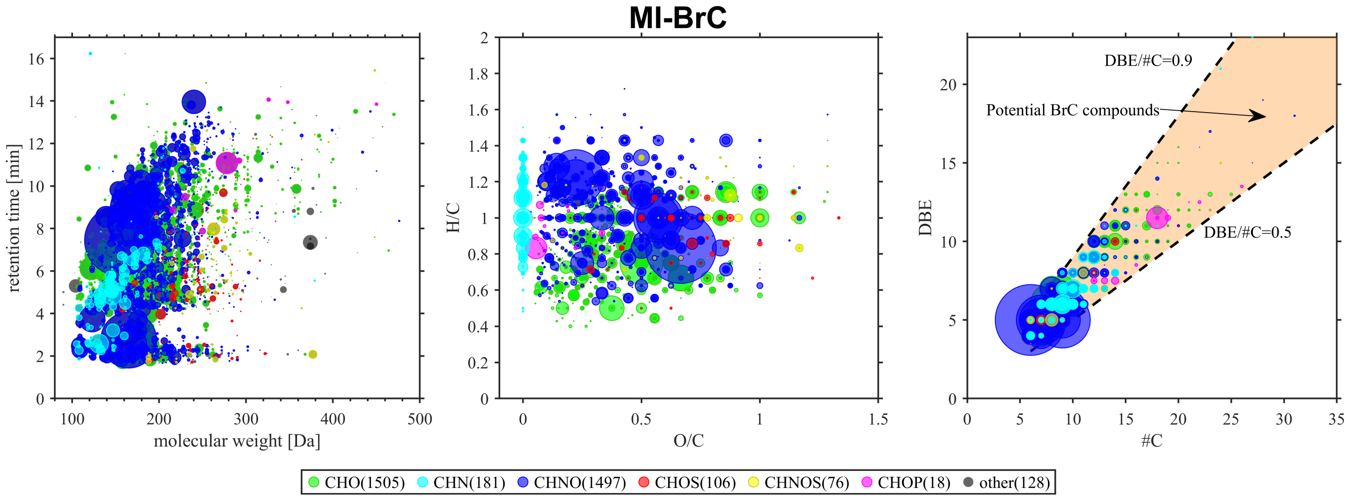


Figure S23. Molecular fingerprints of potential BrC-related compounds detected and classified at MI site.

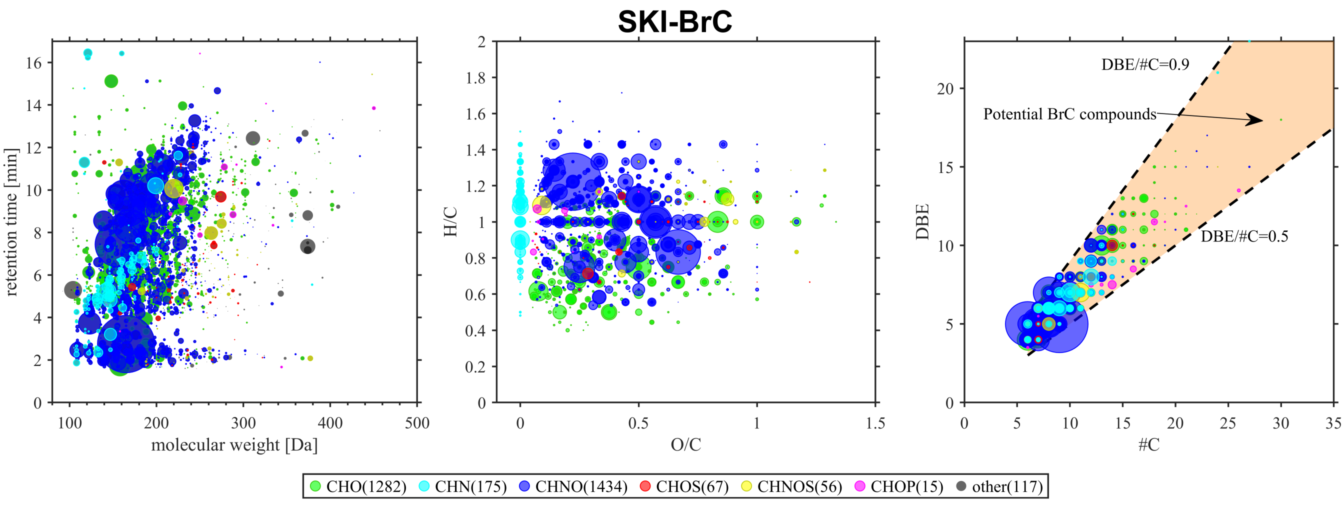


Figure S24. Molecular fingerprints of potential BrC-related compounds detected and classified at SKI site.

S2.9 Attribution of potential BrC features at both sites

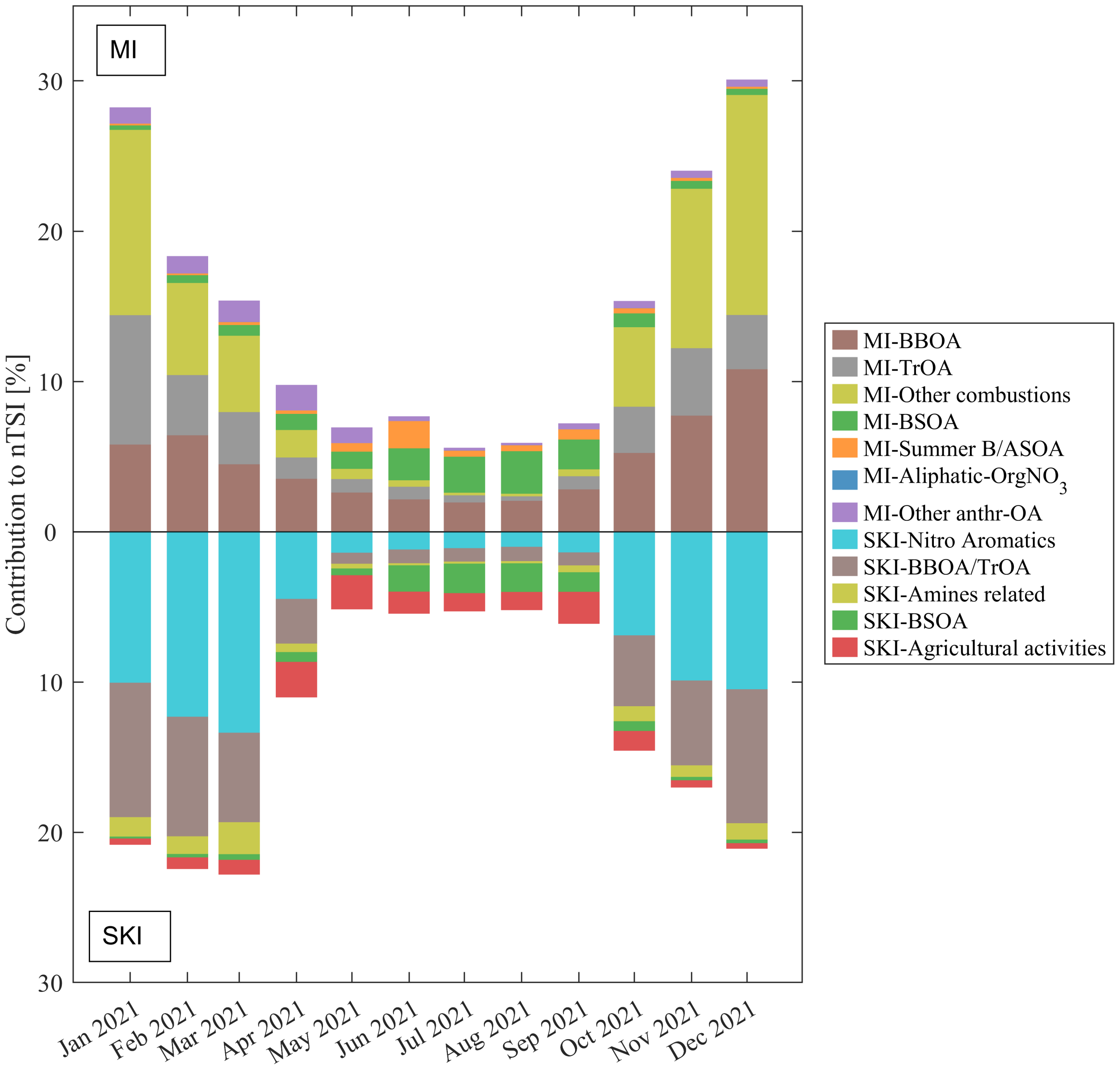


Figure S25. Contribution to nTSI due to features identified as potential BrC-related compounds.

S2.10 Aerosol Ångstrom Exponent for pair samples

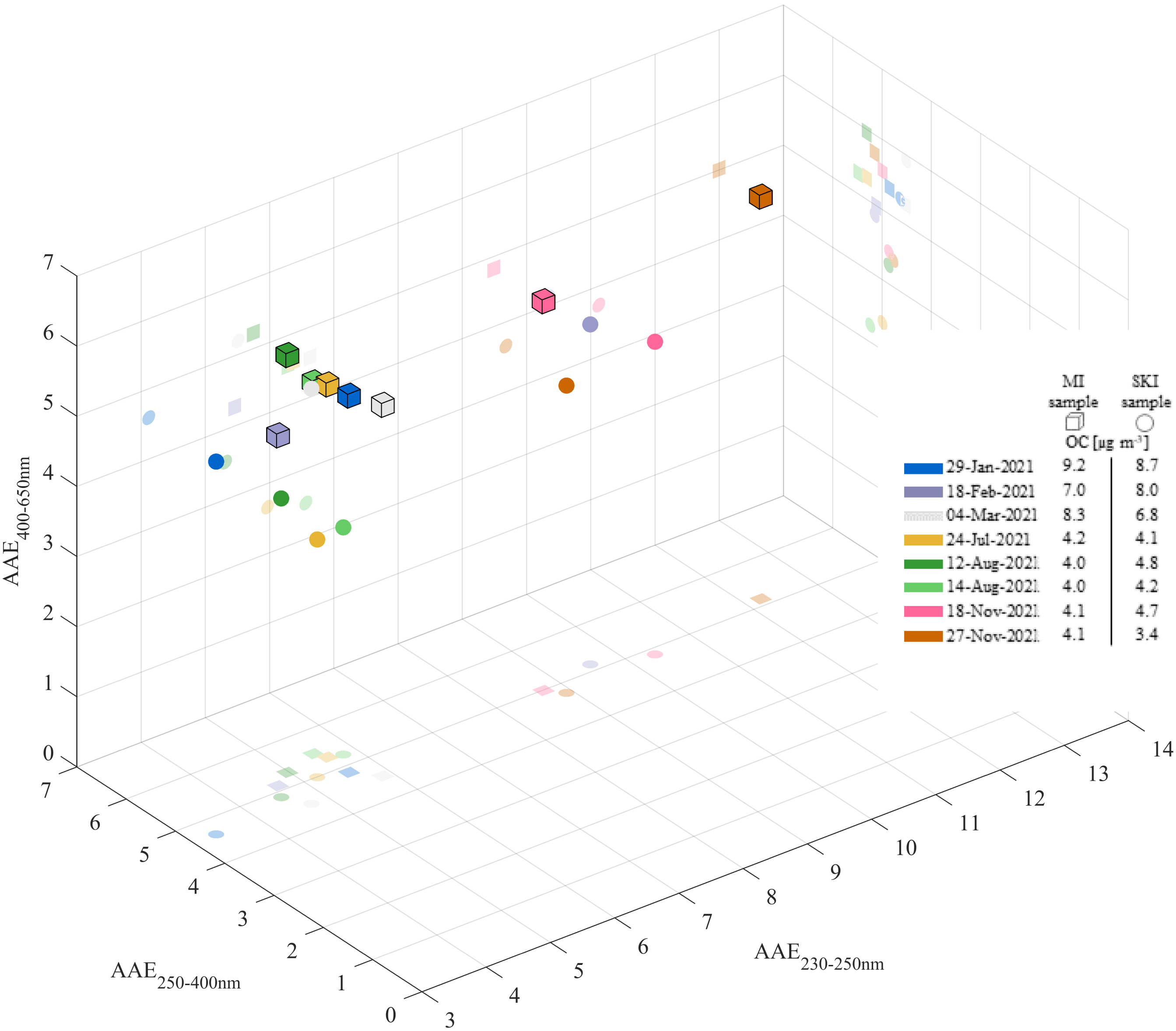


Figure S26. AAE for pairs of samples with similar OC concentrations and contribution to $PM_{2.5}$. OC concentrations are shown in the legend. Same colors indicates samples collected on the same days whereas the shape refers to the collection site: MI (cubes) or SKI (spheres). The marker projections make it easier to appreciate the distances between the points across the three planes, and they are oriented toward the reader.

S3 Compound Discoverer workflows

Table S1. Workflow of the non-target software Compound Discoverer 3.3.2.31 - negative ionization mode data

Processing node	Parameter	Settings
Select Spectra		
	1. Spectrum Properties Filter:	
		Lower RT Limit: 0
		Upper RT Limit: 16.5
		First Scan: 0
		Last Scan: 0
		Ignore Specified Scans: (not specified)
		Lowest Charge State: 0
		Highest Charge State: 0
		Min. Precursor Mass: 50 Da
		Max. Precursor Mass: 5000 Da
		Total Intensity Threshold: 10000
		Minimum Peak Count: 1
	2. Scan Event Filters:	
		Mass Analyzer: Is FTMS
		MS Order: Is MS2, MS1
		Activation Type: Is HCD
		Min. Collision Energy: 0
		Max. Collision Energy: 1000
		Scan Type: Any
		Polarity Mode: Is -
	3. Peak Filters:	
		S/N Threshold (FT-only): 5
	4. Replacements for Unrecognized Properties:	
		Unrecognized Charge Replacements: 1
		Unrecognized Mass Analyzer Replacements: ITMS
		Unrecognized MS Order Replacements: MS2
		Unrecognized Activation Type Replacements: HCD
		Unrecognized Polarity Replacements: -
		Unrecognized MS Resolution@200 Replacements: 60000
		Unrecognized MSn Resolution@200 Replacements: 30000
	5. General Settings:	
		Precursor Selection: Use MS1 Precursor
		Use Isotope Pattern in Precursor Reevaluation: True
		Provide Profile Spectra: Automatic
		Store Chromatograms: False
Align Retention Times		
	1. General Settings:	
		Alignment Model: Adaptive curve
		Alignment Fallback: Use Linear Model
		Maximum Shift [min]: 0.2
		Shift Reference File: True
		Mass Tolerance: 5 ppm

continued on next page

Processing node	Parameter	Settings
		Remove Outlier: True
Detect Compounds		
	1. General Settings:	
		Mass Tolerance [ppm]: 2 ppm
		Min. Peak Intensity: 10000
		Min. [#] Scans per Peak: 5
		Use Most Intense Isotope Only: False
	2. Trace Detection:	
		Max. Number of Gaps to Correct: 2
		Min. Number of Adjacent Non-Zeros: 2
	3. Peak Detection:	
		Chromatographic S/N Threshold: 1.5
		Remove Baseline: False
		Gap Ratio Threshold: 0.35
		Max. Peak Width [min]: 2
		Min. Relatiive Valley Depth: 0.2
	4. Isotope Pattern Detection:	
		Group Isotopes for: Br, Cl
		Use Peak Quality for Isotope Grouping: True
		Filter out Features with Bad Peaks Only: True
		Zig-Zag Index Threshold: 0.2
		Jaggedness Threshold: 0.4
		Modality Threshold: 0.9
		Remove Potentially False Positive Isotopes: True
	5. Compound Detection:	
		Ions: [2M-H]-1; [M-H]-1
		Base Ions: [M-H]-1
		Remove Singlets: True
	6. AcquireX Settings:	
		Detect Persistent Background Ions: False
Group Compounds		
	1. General Settings:	
		Mass Tolerance: 2 ppm
		RT Tolerance [min]: 0.2
		Align Peaks: False
		Preferred Ions: [M-H]-1
		Area Integration: All Ions
	2. Peak Rating Contributions:	
		Area Contribution: 3
		CV Contribution: 1
		FWHM to Base Contribution: 5
		Jaggedness Contribution: 5
		Modality Contribution: 5
		Zig-Zag Index Contribution: 5
	3. Peak Rating Filter:	

continued on next page

Processing node	Parameter	Settings
		Peak Rating Threshold: 4
		Number of Files: 4
Fill Gaps		
	1. General Settings:	
		Mass Tolerance: 2 ppm
		S/N Threshold: 1.5
		Use Real Peak Detection: True
		Apply Restrictive Gap Filling: True
Mark Background Compounds		
	1. General Settings:	
		Max. Sample/Blank: 5
		Max. Blank/Sample: 0
		Hide Background: False
Assign Compound Annotations		
	1. General Settings:	
		Mass Tolerance: 2 ppm
	2. Data Sources:	
		Data Source #1: Predicted Compositions
		Data Source #2: mzVault Search
		Data Source #3: mzCloud Search
		Data Source #4: ChemSpider Search
	3. Scoring Rules:	
		Use mzLogic: True
		Use Spectral Distance: True
		SFit Threshold: 20
		SFit Range: 20
	4. Reprocessing:	
		Clear Names: False
Search Neutral Losses		
	1. General Settings:	
		C_2H_3 (C2 H3, 27.02)
		$C_2H_3O_2$ (C2 H3 O2, 59.01)
		C_2H_4N (C2 H4 N, 42.03)
		C_2H_5 (C2 H5, 29.04)
		C_2H_5O (C2 H5 O, 45.03)
		C_2H_5OH (C2 H6 O, 46.04)
		C_2H_6 (C2 H6, 30.05)
		C_3H_7 (C3 H7, 43.05)
		C_4H_{10} (C4 H10, 58.08)
		C_4H_7 (C4 H7, 55.05)
		C_4H_8 (C4 H8, 56.06)
		C_4H_9 (C4 H9, 57.07)
		C_6H_6 (C6 H6, 78.05)
		$C_6H_6CH_3$ (C7 H9, 93.07)
		C_6H_6O (C6 H6 O, 94.04)

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Processing node	Parameter	Settings
		C_6H_7N (C6 H7 N, 93.06) CH_2 (C H2, 14.02) $CH_2C{=}O$ (C2 H2 O, 42.01) CH_3 (C H3, 15.02) $CH_3CH{=}CH_2$ (C3 H6, 42.05) CH_3CO (C2 H3 O, 43.02) CH_3COOH (C2 H4 O2, 60.02) CH_3O (C H3 O, 31.02) CH_3OH (C H4 O, 32.03) CH_4 (C H4, 16.03) CH_5O (C H5 O, 33.03) CO (C O, 27.99) CO_2 (C O2, 43.99) $CONH_2$ (C H2 N O, 44.01) $H_2C{=}CH_2$ (C2 H4, 28.03) $H_2C{=}O$ (C H2 O, 30.01) H_2O (H2 O, 18.01) H_2S (H2 S, 33.99) H_2SO_4 (H2 O4 S, 97.97) HCCH (C2 H2, 26.02) HCl (H Cl, 35.98) HCN (C H N, 27.01) HNO_3 (H N O3, 63.00) HS (H S, 32.98) HSO_4 (H O4 S, 96.96) NH_3 (H3 N, 17.03) NO (N O, 30.00) NO_2 (N O2, 45.99) NO_3 (N O3, 61.99) OH (H O, 17.00) S (S, 31.97) SO (O S, 47.97) SO_2 (O2 S, 63.96)
	2. High Acc. Mass Tolerance: 2.5 mmu 3. Low Acc. Mass Tolerance: 0.5 Da 4. S/N Threshold: 3 5. Use DIA Scans for Search: False	
Search mzCloud		
	1. General Settings:	
		Compound Classes: All Precursor Mass Tolerance: 5 ppm FT Fragment Mass Tolerance: 5 ppm IT Fragment Mass Tolerance: 0.4 Da Library: Autoprocessed; Reference

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Processing node	Parameter	Settings
		Post Processing: Recalibrated
		Max. # Results: 10
		Annotate Matching Fragments: False
		Search MSn Tree: False
	2. DDA Search:	
		Identity Search: HighChem HighRes
		Match Activation Type: True
		Match Activation Energy: Match with Tolerance
		Activation Energy Tolerance: 20
		Apply Intensity Threshold: True
		Similarity Search: Similarity Reverse
		Match Factor Threshold: 60
	3. DIA Search:	
		Use DIA Scans for Search: False
		Max. Isolation Width [Da]: 500
		Match Activation Type: False
		Match Activation Energy: Any
		Activation Energy Tolerance: 100
		Apply Intensity Threshold: False
		Match Factor Threshold: 20
Predict Compositions		
	1. Prediction Settings:	
		Mass Tolerance: 2 ppm
		Min. Element Counts: C H
		Max. Element Counts: C_{90} H_{190} Br_3 Cl_4 N_4 O_{20} P S_3
		Min. RDBE: 0
		Max. RDBE: 40
		Min. H/C: 0.1
		Max. H/C: 3.5
		Max. # Candidates: 10
		Max. # Internal Candidates: 200
	2. Pattern Matching:	
		Intensity Tolerance [%]: 10
		Intensity Threshold [%]: 0.1
		S/N Threshold: 3
		Min. Spectral Fit [%]: 30
		Min. Pattern Cov. [%]: 90
		Use Dynamic Recalibration: True
	3. Fragments Matching:	
		Use Fragments Matching: True
		Mass Tolerance: 10 ppm
		S/N Threshold: 5
Search mzVault		
	1. Search Settings:	
		mzVault Library: *add libraries created with mzVault*
		Max. # Results: 10
		Match Factor Threshold: 50

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Processing node	Parameter	Settings
		Search Algorithm: HighChem HighRes Match Analyzer Type: True IT Fragment Mass Tolerance: 0.4 Da FT Fragment Mass Tolerance: 10 ppm Use Retention Time: True Precursor Mass Tolerance: 10 ppm Apply Intensity Threshold: True Match Ionization Method: True Ion Activation Energy Tolerance: 20 Match Ion Activation Energy: Match with Tolerance Match Ion Activation Type: True Compound Classes: All Remove Precursor Ion: True RT Tolerance [min]: 3

Table S2. Workflow of the non-target software Compound Discoverer 3.3.2.31 - positive ionization mode data

Processing node	Parameter	Settings
Select Spectra		
	1. Spectrum Properties Filter:	
		Lower RT Limit: 0
		Upper RT Limit: 16.5
		First Scan: 0
		Last Scan: 0
		Ignore Specified Scans: (not specified)
		Lowest Charge State: 0
		Highest Charge State: 0
		Min. Precursor Mass: 50 Da
		Max. Precursor Mass: 5000 Da
		Total Intensity Threshold: 10000
		Minimum Peak Count: 1
	2. Scan Event Filters:	
		Mass Analyzer: Is FTMS
		MS Order: Is MS2, MS1
		Activation Type: (not specified)
		Min. Collision Energy: 0
		Max. Collision Energy: 1000
		Scan Type: Any
		Polarity Mode: Is +
		MS1 Mass Range: (not specified)
	FAIMS CV: (not specified)	3. Peak Filters:
		S/N Threshold (FT-only): 1.5
	4. Replacements for Unrecognized Properties:	
		Unrecognized Charge Replacements: 1
		Unrecognized Mass Analyzer Replacements: ITMS
		Unrecognized MS Order Replacements: MS2
		Unrecognized Activation Type Replacements: CID
		Unrecognized Polarity Replacements: +
		Unrecognized MS Resolution@200 Replacements: 60000
		Unrecognized MSn Resolution@200 Replacements: 30000
	5. General Settings:	
		Precursor Selection: Use MS1 Precursor
		Use Isotope Pattern in Precursor Reevaluation: True
		Provide Profile Spectra: Automatic
		Store Chromatograms: False
Align Retention Times		
	1. General Settings:	
		Alignment Model: Adaptive curve
		Alignment Fallback: Use Linear Model
		Maximum Shift [min]: 0.2
		Shift Reference File: True

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Processing node	Parameter	Settings
		Mass Tolerance: 5 ppm
		Remove Outlier: True
Detect Compounds		
	1. General Settings:	
		Mass Tolerance [ppm]: 2 ppm
		Min. Peak Intensity: 100000
		Min. [#] Scans per Peak: 5
		Use Most Intense Isotope Only: True
	2. Trace Detection:	
		Max. Number of Gaps to Correct: 2
		Min. Number of Adjacent Non-Zeros: 2
	3. Peak Detection:	
		Chromatographic S/N Threshold: 1.5
		Remove Baseline: False
		Gap Ratio Threshold: 0.35
		Max. Peak Width [min]: 1
		Min. Relatiive Valley Depth: 0.1
	4. Isotope Pattern Detection:	
		Group Isotopes for: Br, Cl
		Use Peak Quality for Isotope Grouping: True
		Filter out Features with Bad Peaks Only: True
		Zig-Zag Index Threshold: 0.2
		Jaggedness Threshold: 0.4
		Modality Threshold: 0.9
		Remove Potentially False Positive Isotopes: True
	5. Compound Detection:	
		Ions: [2M+H]+1; [M+H]+1; [2M+Na]+1; [M+Na]+1
		Base Ions: [M+H]+1
		Remove Singlets: True
	6. AcquireX Settings:	
		Detect Persistent Background Ions: False
Group Compounds		
	1. General Settings:	
		Mass Tolerance: 2 ppm
		RT Tolerance [min]: 0.2
		Align Peaks: False
		Preferred Ions: [M+H]+1; [M+Na]+1
		Area Integration: All Ions
	2. Peak Rating Contributions:	
		Area Contribution: 3
		CV Contribution: 1
		FWHM to Base Contribution: 5
		Jaggedness Contribution: 5
		Modality Contribution: 5
		Zig-Zag Index Contribution: 5

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Processing node	Parameter	Settings
	3. Peak Rating Filter:	
		Peak Rating Threshold: 4 Number of Files: 4
Fill Gaps		
	1. General Settings:	
		Mass Tolerance: 2 ppm S/N Threshold: 1.5 Use Real Peak Detection: True Apply Restrictive Gap Filling: True
Mark Background Compounds		
	1. General Settings:	
		Max. Sample/Blank: 5 Max. Blank/Sample: 0 Hide Background: False
Assign Compound Annotations		
	1. General Settings:	
		Mass Tolerance: 2 ppm
	2. Data Sources:	
		Data Source #1: Predicted Compositions Data Source #2: mzCloud Search
	3. Scoring Rules:	
		Use mzLogic: True Use Spectral Distance: True SFit Threshold: 20 SFit Range: 20
	4. Reprocessing:	
		Clear Names: False
Search mzCloud		
	1. General Settings:	
		Compound Classes: All Precursor Mass Tolerance: 5 ppm FT Fragment Mass Tolerance: 5 ppm IT Fragment Mass Tolerance: 0.4 Da Library: Autoprocessed; Reference Post Processing: Recalibrated Max. # Results: 10 Annotate Matching Fragments: False Search MSn Tree: False
	2. DDA Search:	
		Identity Search: HighChem HighRes Match Activation Type: True Match Activation Energy: Match with Tolerance Activation Energy Tolerance: 20 Apply Intensity Threshold: True Similarity Search: Similarity Forward

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Processing node	Parameter	Settings
		Match Factor Threshold: 80
	3. DIA Search:	
		Use DIA Scans for Search: False
		Max. Isolation Width [Da]: 500
		Match Activation Type: False
		Match Activation Energy: Any
		Activation Energy Tolerance: 100
		Apply Intensity Threshold: False
		Match Factor Threshold: 20
Search Neutral Losses		
	1. General Settings:	
		C_2H_3 (C2 H3, 27.02)
		$C_2H_3O_2$ (C2 H3 O2, 59.01)
		C_2H_4N (C2 H4 N, 42.03)
		C_2H_5 (C2 H5, 29.04)
		C_2H_5O (C2 H5 O, 45.03)
		C_2H_5OH (C2 H6 O, 46.04)
		C_2H_6 (C2 H6, 30.05)
		C_3H_7 (C3 H7, 43.05)
		C_4H_{10} (C4 H10, 58.08)
		C_4H_7 (C4 H7, 55.05)
		C_4H_8 (C4 H8, 56.06)
		C_4H_9 (C4 H9, 57.07)
		C_6H_6 (C6 H6, 78.05)
		$C_6H_6CH_3$ (C7 H9, 93.07)
		C_6H_6O (C6 H6 O, 94.04)
		C_6H_7N (C6 H7 N, 93.06)
		CH_2 (C H2, 14.02)
		$CH_2C{=}O$ (C2 H2 O, 42.01)
		CH_3 (C H3, 15.02)
		$CH_3CH{=}CH_2$ (C3 H6, 42.05)
		CH_3CO (C2 H3 O, 43.02)
		CH_3COOH (C2 H4 O2, 60.02)
		CH_3O (C H3 O, 31.02)
		CH_3OH (C H4 O, 32.03)
		CH_4 (C H4, 16.03)
		CH_5O (C H5 O, 33.03)
		CO (C O, 27.99)
		CO_2 (C O2, 43.99)
		$CONH_2$ (C H2 N O, 44.01)
		$H_2C{=}CH_2$ (C2 H4, 28.03)
		$H_2C{=}O$ (C H2 O, 30.01)
		H_2O (H2 O, 18.01)
		H_2S (H2 S, 33.99)
		H_2SO_4 (H2 O4 S, 97.97)
		HCCH (C2 H2, 26.02)
		HCl (H Cl, 35.98)

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Processing node	Parameter	Settings
		HCN (C H N, 27.01)
		HNO_3 (H N O3, 63.00)
		HS (H S, 32.98)
		HSO_4 (H O4 S, 96.96)
		NH_3 (H3 N, 17.03)
		NO (N O, 30.00)
		NO_2 (N O2, 45.99)
		NO_3 (N O3, 61.99)
		OH (H O, 17.00)
		S (S, 31.97)
		SO (O S, 47.97)
		SO_2 (O2 S, 63.96)
	2. High Acc. Mass Tolerance: 2.5 mmu	
	3. Low Acc. Mass Tolerance: 0.5 Da	
	4. S/N Threshold: 3	
	5. Use DIA Scans for Search: False	
Predict Compositions		
	1. Prediction Settings:	
		Mass Tolerance: 2 ppm
		Min. Element Counts: C H
		Max. Element Counts: C_{90} H_{190} Br_3 Cl_4 N_4 O_{20} S_3 P
		Min. RDBE: 0
		Max. RDBE: 40
		Min. H/C: 0.1
		Max. H/C: 3.5
		Max. # Candidates: 10
		Max. # Internal Candidates: 200
	2. Pattern Matching:	
		Intensity Tolerance [%]: 10
		Intensity Threshold [%]: 0.1
		S/N Threshold: 3
		Min. Spectral Fit [%]: 30
		Min. Pattern Cov. [%]: 90
		Use Dynamic Recalibration: True
	3. Fragments Matching:	
		Use Fragments Matching: True
		Mass Tolerance: 10 ppm
		S/N Threshold: 5

References

Amante, C. and Eakins, B. W.: ETOPO1 1 Arc-Minute Global Relief Model: Procedures Data Sources and Analysis, https://doi.org/doi:10.7289/V5C8276M, 2009.