A software tool (Orbitool) for analyzing online Orbitrap mass spectrometry data and its applications
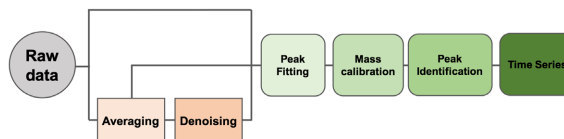
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The Orbitrap Fourier Transform mass spectrometry (MS) has been proven to be a promising new-generation technique for online analysis in geochemistry. Coupled with chemical ionization and other inlets, Orbitrap MS can measure gaseous precursors and particulate matters with a substantially greater mass resolving power than other widely used online mass spectrometers in atmospheric sciences.

Trace compounds in the real atmosphere usually correspond to low signals in online measurements, posing a major challenge to their detection using mass spectrometric approaches. On one hand, we have improved the signal-to-noise ratio of online Orbitrap MS and hence its sensitivity to trace compounds by increasing the number of microscans (transients) (Cai et al., 2022). On the other hand, the identification of trace compounds usually requires spectral averaging, which can further decrease the noise of the averaged spectra.

To respond to the need for averaging long-term online data measured by Orbitrap MS and provide other convenient functions, we have developed an open-source software tool (Orbitool, https://orbitrap.catalyse.cnrs.fr, continuously being updated) (Cai et al., 2021). Orbitool is capable of averaging raw data across files while improving mass accuracy, distinguishing signal peaks against noise peaks, assigning chemical compounds and their isotopes via peak fitting, and exporting time series and mass defect plots. A noise reduction procedure in Orbitool can separate signal peaks from noise peaks and greatly reduce computational and storage expenses.

We have used Orbitool to analyze chemical ionization Orbitrap data from both laboratory experiments on ozonolysis of monoterpenes and ambient measurements in polluted megacities. These applications show that Orbitool can automatically assign hundreds to thousands of molecular formulae as well as their isotopes with high accuracy.

Reference

[1] Cai, R. et al. (2021) Orbitool: A software tool for analyzing online Orbitrap mass spectrometry data. *Atmospheric Measurement Techniques* 14, 2377–2387, doi:10.5194/amt-2020-267.

[2] Cai, R. et al. (2022) Improving the Sensitivity of Fourier Transform Mass Spectrometer (Orbitrap) for Online Measurements of Atmospheric Vapors. *Analytical Chemistry* 94, 15746-15753, doi:10.1021/acs.analchem.2c03403.