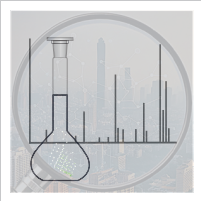
doi:10.2533/chimia.2025.363 Chimia 79 (2025) 363



Highlights of Analytical Sciences in Switzerland

Division of Analytical Sciences

A Division of the Swiss Chemical Society

Tracing Aerosol Sources *via* Measurements and Data Mining

Kaspar R. Daellenbach* and Lubna Dada

*Correspondence: Dr. K. R. Daellenbach, E-mail: kaspar.daellenbach@psi.ch
PSI Center for Energy and Environmental Sciences, Paul Scherrer Institute, CH-5232 Villigen

Keywords: Air pollution · Air quality · Mass spectrometry · Megacity · Source apportionment

Every breath we take contains countless aerosol particles – some more harmful than others, depending on their origin and processing through the atmosphere. To support efforts in mitigating pollution, particles are traced back to their emission sources, a process akin to searching for the invisible within a sea of invisibles.

But how is this done? One approach involves collecting particles and analyzing their chemical and molecular composition using advanced mass spectrometers (Fig. 1). These instruments generate spectra – unique 'fingerprints' that reveal particles' molecular information. Due to atmospheric complexity, air samples contain diverse particles that evolve chemically over time. Data mining techniques are used to identify patterns in their temporal behaviour and spectral composition, refining the separation of the different sources. By further comparing atmospheric measurements to controlled laboratory experiments, specific emission sources within a collected air sample are determined.

Fig. 1. Combining detailed molecular and chemical composition measurements with data mining techniques allows for source and process identification of air pollutants. (Image generated from https://firefly.adobe.com/, last access 10.02.2025).

In our study, we measured aerosol molecular composition in central Beijing using a mass spectrometer over several months including the COVID lockdown period, capturing seasonal variability and periods of reduced urban activity. Results show that in winter, organic aerosols from solid-fuel emissions dominate, both from local sources and long-range transport from the Beijing-Tianjin-Hebei Plain and mountainous areas west of the city. In summer, atmospherically formed so-called 'secondary' organic aerosols from aromatic emissions – likely originating from the Xi'an-Shanghai-Beijing corridor – become the main contributors. While biogenic secondary organic aerosols appear in small amounts, our methods can still detect them. We confirmed source identification by comparing spectra with chamber experiments, revealing interactions between biogenic and anthropogenic emissions (Fig. 2). Beijing is one example of many where severe pollution affects a large population. Our transferable approaches have been, and currently are being applied there to support efforts in improving air quality. **A comprehensive identification and quantification of aerosol particle sources requires the integration of long-term measurements, chamber experiments, and data mining techniques.**

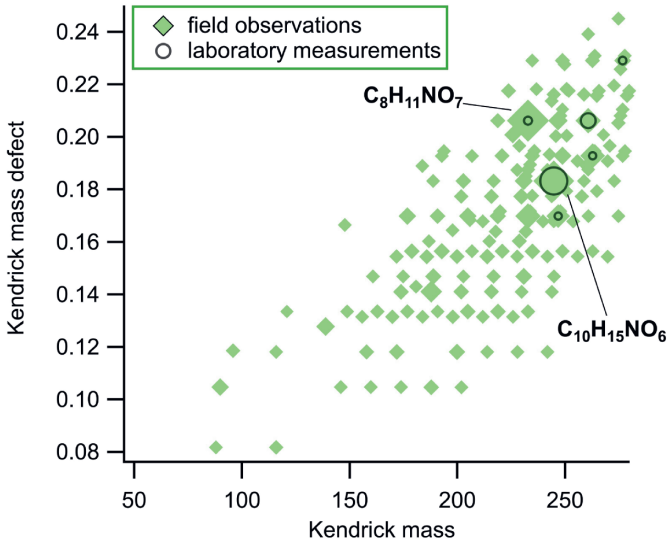


Fig. 2. Comparison of the nighttime biogenic secondary aerosol mass spectrum from Beijing measurements with those from chamber experiments simulating biogenic-anthropogenic interactions (limonene and nitrogen oxides). Marker sizes represent the relative abundance of each molecule. Figure adapted from ref. [1].

[1] K. R. Daellenbach, J. Cai, S. Hakala, L. Dada, C. Yan, W. Du, L. Yao, F. Zheng, J. Ma, F. Ungeheuer, A. L. Vogel, D. Stolzenburg, Y. Hao, Y. Liu, F. Bianchi, G. Uzu, J.-L. Jaffrezo, D. R. Worsnop, N. M. Donahue, M. Kulmala, *Nat. Geosci.* **2024**, *17*, 747, https://doi.org/10.1038/s41561-024-01493-3.

Can you show us your analytical highlight?
Please contact: Dr. Veronika R. Meyer, Unterstrasse 58, CH-9000 St. Gallen
Tel.: +41 71 222 16 81, E-mail: analytical_highlights@chimia.ch