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Novel method for the untargeted molecular reconstruction of secondary organic aerosols in ice cores.

Content

Ice cores have been widely studied and characterized for trace elements, major ions, water stable isotopes and black carbon. However, the organic fraction, which constitutes up to 20-70% of today's particulate matter, has been often overlooked, mainly due to its low concentration in the ice and subsequent analytical limitations (e.g. high instrumental limits of detection), but also because of its complex composition including thousands of molecules. In the past decade, thanks to the availability of progressively more sensitive instruments and reliable sample preparation procedures, first studies on organics in ice cores have been published to evaluate, for example, the impact of anthropogenic pollution on the environment since the Industrial Revolution. However, since these studies targeted specific molecules, a large organic fraction remains unknown and uncharacterized. Today, high-resolution mass spectrometry offers unprecedented opportunities to overcome this knowledge gap, offering the opportunity to qualitatively characterize a larger spectrum of molecules.

The sample preparation methodology and the instrumental set-up are critical to define the organic molecule class that will be addressed. In this study, we developed a method that provides high SPE recoveries in addition to high instrumental sensitivity for the analysis of secondary organic aerosols (SOA) and wildfire tracers in ice matrices. The method was tested for selected SOA (pinic acid) and organic biomass burning proxies (syringaldehyde, syringic acid, p-hydroxybenzoic acid, vanillic acid and vanillin) and applied to a Belukha ice core drilled in the Siberian Altai in 2018, to provide the first-time untargeted SOA reconstruction over the period that covers both pre-industrial and industrial times. Further, thanks to the application of state-of-the-art machine learning algorithms, we provide the semi-quantification of a selection of molecules, offering new strategies for future untargeted organics reconstructions in ice cores.

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