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Non-Target Analyses of organic compounds in ice cores using HPLC-ESI-UHRMS

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To study the global climatic and environmental changes it is necessary to know the environmental and especially atmospheric conditions of the past. By analysing climate archives, such as for example ice cores, unique environmental information can be obtained. In contrast to the well-established analysis of inorganic species in ice cores, organic compounds have been analysed in ice cores to a much smaller extent. Because of current analytical limitations it has become commonplace to focus on "total organic carbon" measurements or specific classes of organic molecules, as no analytical methods exist that can provide a broad characterization of the organic material present[1]. On the one hand, it is important to focus on already known atmospheric markers in ice cores and to quantify, where possible, in order to compare them to current conditions. On the other hand, unfortunately a wealth of information is lost when only a small fraction of the organic material is examined. However, recent developments in mass spectrometry in respect to higher mass resolution and mass accuracy enable a new approach to the analysis of complex environmental samples.

The qualitative characterization of the complex mixture of water soluble organic carbon (WSOC) in the ice using high-resolution mass spectrometry allows for novel insights concerning the composition and possible sources of aerosol derived WSOC deposited at glacier sites. By performing a non-target analysis of an ice core from the Swiss Alps using previous enrichment by solid-phase extraction (SPE) and high performance liquid chromatography coupled to electrospray ionization and ultra-high resolution mass spectrometry (HPLC-ESI-UHRMS) 475 elemental formulas distributed onto 659 different peaks were detected. The elemental formulas were classified according to their elemental composition into CHO-, CHON-, CHOS-, CHONS-containing compounds and "others". Several methods for the analysis of complex data sets of high resolution mass spectrometry were applied to the results of the non-target analysis. By various classifications in Van Krevelen plots[2], amino acids and degradation products of proteins as well as degradation products of lignins have been determined as the main components of the ice core. Furthermore, the majority of WSOC molecular formulas identified in this non-target analysis had molar H/C and O/C ratios similar to mono- and di-carboxylic acids and SOAs[3]. Studies of the carbon oxidation state as a metric for describing the chemistry of atmospheric organic aerosol showed that a majority of the elemental formulas can be associated with the combustion of biomass as a major source of the WSOC[4].

References:

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