NMR AEROSOLOMICS: AN OVERVIEW

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NMR Aerosolomics offers a different analysis approach of water-soluble organic compounds (WSOCs) from complex aerosol mixtures, inspired by the profiling of substances in metabolomics. To this end, an extensive library of compounds commonly found in atmospheric aerosols was created. The method was evaluated on a set of 21 samples of aerosol particulate matter ($PM_{2.5}$ and PM_{10}) collected in summer 2008 and winter 2009 at a Prague suburban site. Approximately 60 compounds were identified in each sample. Three compounds were identified for the first time in atmospheric aerosols and the presence of four other theoretically predicted species was confirmed. In total, the number of identified compounds reached 79. The concentration values of the identified compounds were then used for statistical analysis. A clear differentiation between summer and winter samples was obtained, while separation by particle size was indicated only in the group of summer samples. Univariate statistical analysis revealed which compounds were responsible for the group separation, and possible sources for these compounds were suggested.[1]

In addition, the method was used in WSOC analysis of size-resolved aerosol particles collected by a 6-stage high-volume cascade impactor collected during summer and winter resulting in four sample series. In each sample, 31-45 compounds were identified, for a total of 73 compounds. Distribution profiles were used to reveal associations between individual compounds and to identify associations with probable sources. The results were supported by multivariate statistical analysis.[2]

Unlike other methods used for the analysis of WSOC in atmospheric aerosols, NMR aerosolomics allows the simultaneous determination of several groups of WSOC. The method offers great potential for source apportionment, which is an important issue in contemporary aerosol science.

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