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NMR AEROSOLOMICS AS A TOOL TO DISTINGUISH VARIOUS TYPES OF AEROSOL SAMPLES

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Atmospheric aerosols are a small but very important part of the Earth's atmosphere. The proportion of inorganic and organic compounds in aerosol particles seems to be equal on average [1]. While the inorganic composition of aerosols is well explored, knowledge about the organic part is still very limited. It is well known that the major part of organic aerosol compounds is represented by polar, water-soluble organic compounds (WSOC) [1]. NMR spectroscopy was for the purpose of aerosol chemistry "discovered" only recently [2]. Nevertheless, NMR has undergone rapid development and sensitivity gain of late.

Aerosolomics provides complex evaluation of aerosol composition and compound concentration [3]. It is exploiting metabolomic approach, which is applied to aerosol samples. In NMR aerosolomics the assignment of dominant signals is based on precise chemical shift of the compound which enables identification of organic compounds in given aerosol sample. For this purpose, a comprehensive library of high-res ¹H NMR spectra of organic compounds that are known to be present in aerosol particles is essential. Such a library was built and is extended continuously.

In the recent study, the summer and winter aerosol samples were analyzed using NMR aerosolomics approach. The samples were collected in Prague-Suchbát during summer 2008 and winter 2009 in two different particle size fractions – PM_{2.5} and PM₁₀. Around 50 compounds were identified in each aerosol spectrum owing to the comprehensive library. The profile of 86 identified compounds, which were identified in the samples altogether, served as an input data for statistical analysis. Multivariate statistical analysis clearly discriminates the two groups studied. Furthermore, it is possible to determine the most significant compounds.

References

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