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NMR Aerosolomics: A Convenient Route to Organic Aerosol Analysis

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Aerosolomics provides complex evaluation of aerosol composition and compound concentration [1]. It is exploiting metabolomic approach, which is applied to aerosol samples. In our laboratory an NMR method for organic aerosol analysis was developed and tested. The method is focused on water soluble organic compounds (WSOC), which is the least examined group of organic aerosols. In NMR metabolomic approach library ^1H spectra of individual compounds are fitted into the complex ^1H spectrum of a mixture and are subsequently subtracted. This is allowed by the employment of ChenomX software. Since ChenomX is originally a metabolomics software, WSOC are being added to its database continuously. The database currently consists of 120 substances.

Collection of aerosol samples in a high volume cascade impactor together with a special preparation of the sample increased number of identified compounds in every analysed sample. The high volume cascade impactor collects atmospheric aerosols into six stages according to the particle size. Therefore variances in WSOC composition between different particle size samples were found. In this work we present mainly summer 2015 collection of real atmospheric aerosols from Prague – Suchbát.

Major differences were observed in the fraction of carbohydrates and sugar alcohols. Carbohydrate derivatives were found mainly in bigger particle size samples (2.24–4.56 μm and 4.56–20.00 μm). Other groups of WSOC (mono- and dicarboxylic acids, hydroxycarboxylic acids, oxocarboxylic acids, aromatic compounds or amines) were also thoroughly examined and the results are discussed in this work. The abundance of certain groups of WSOC and the presence of a marker compound can indicate the origin of the aerosol particles.



References

1. Ruiz-Jimenez, J.; Parshintsev, J.; Hartonen, K.; Riekkola, M. L.; Petaja, T.; Virkkula, A.; Kulmala, M. Aerosolomics profiling: application to biogenic and anthropogenic samples. In *Aerosol Science 109*, Finnish Center of Excellency (FCoE) in physics, chemistry, biology and meteorology of atmospheric composition and climate change, Kuopio, Finland, 17–19 May, 2010

