# Decoding the structural features of fine urban organic aerosols by two-dimensional NMR: comparison between water and alkaline soluble components

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Decoding the structural features of the organic matter present in the fine atmospheric aerosols has remained an important goal for the atmospheric research community. This Organic Aerosol (OA) fraction covers a huge variety of molecular structures with different physicochemical properties and sources. The lack of knowledge regarding the inherent complexity of their chemical nature is still nowadays one of the major impairments, not only to an improved understanding of atmospheric organic matter chemistry and composition, but also to predict how these compounds affect the climate system, atmospheric processes, and human health.

In this study, a combination of two-dimensional nuclear magnetic resonance (2D NMR) techniques, namely $^{1}H-^{1}H$ Homonuclear Correlation Spectroscopy (COSY), $^{1}H-^{13}C$ Heteronuclear Single Quantum Coherence (HSQC), and $^{1}H-^{13}C$ Heteronuclear Multiple Bond Correlation (HMBC), were used to identify the main structures and functional groups present in Water-soluble and Alkaline-soluble Organic Matter (WSOM and ASOM, respectively), sequentially extracted from fine urban aerosols collected during different seasons. The use of such high-resolution NMR techniques improves the spectral resolution and provides a deeper and comprehensive insight into the C-H backbone of the organic compounds present in atmospheric aerosols. Moreover, the spectral data and structural features of WSOM and ASOM organic fraction (e.g., Figure 1) was used to build a NMR fingerprinting database of the most atmospherically-relevant structures, in order to assist the identification of the main aerosol sources and formation mechanisms, as well as their variability over seasons.

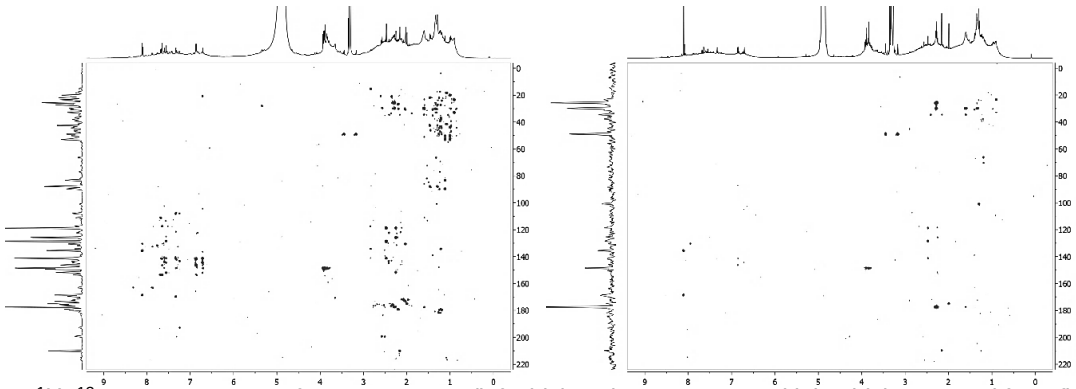

**Figure 1.** $^{1}H-^{13}C$ HMBC spectra of WSOM extract (left side) and ASOM extract (right side) extracted from fine urban aerosols collected in winter.

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