



## **Understanding the toxicological potential of aerosol organic compounds using informatics based screening**

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Exposure to atmospheric particulate matter is responsible for both short-term and long-term adverse health effects. So far, all efforts spent in achieving a systematic epidemiological evidence of specific aerosol compounds determining the overall aerosol toxicity were unsuccessful. The results of the epidemiological studies apparently conflict with the laboratory toxicological analyses which have highlighted very different chemical and toxicological potentials for speciated aerosol compounds. Speciation remains a problem, especially for organic compounds: it is impossible to conduct screening on all possible molecular species. At the same time, research on toxic compounds risks to be biased towards the already known compounds, such as PAHs and dioxins.

In this study we present results from an initial assessment of the use of *in silico* methods (i.e. (Q)SAR, read-across) to predict toxicity of atmospheric organic compounds including evaluation of applicability of a variety of popular tools (e.g. OECD QSAR Toolbox) for selected endpoints (e.g. genotoxicity). Compounds are categorised based on the need of new experimental data for the development of *in silico* approaches for toxicity prediction covering this specific chemical space, namely the atmospheric aerosols. Whilst only an initial investigation, we present recommendations for continuation of this work.