Atmospheric secondary organic aerosols (SOA) are complex mixtures of chemicals that affect climate and pose considerable health risks in urban areas. Processes that form organic aerosols and dissolve them in cloud droplets remain either completely unknown or very poorly characterized. The goal of this research is to combine for the first time a novel experimental molecular analysis of organic aerosols with a powerful computational approach, capable of predicting all possible chemical reactions between the organic aerosol compounds. This unique marriage of experimental and computational techniques will significantly improve our understanding of the evolution of organic aerosols and dissolved organic matter in the environment.

High Resolution Mass Spectrometry – Nizkorodov Group

Isoprene is the most important source of SOA. The recently developed high resolution electrospray mass spectrometer makes identifying the composition of SOA possible.

Detailed analysis reveals that SOA contains thousands of individual compounds. Most of the compounds are large (oligomeric), highly oxidized and functionalized. Comparing our molecular formula assignments to predictions made by chemoinformatics will identify reactions that produce SOA.

In Silico Reaction Pathway Generation – Baldi Group

Computational combinatorial chemistry has been applied to drug discovery and materials science. Similar techniques can be utilized to elicit reaction pathways for SOA.

Given initial isoprene oxidation products and a set of plausible reaction transforms, we recursively generate all possible products from application of the reaction rules. Intelligent filtering methods limit oligomer size and avoid redundant calculation.

Predicted products are matched with experimental results. The chain of applied transforms used to generate products will provide insight into the reaction pathways of SOA.