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Deciphering Complex Organic Mixtures with Very-High Resolution Tandem Mass Spectrometry: A Case Study on Intermediate and Semi-Volatile Organic Compounds from Oil Sands Processing

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We present the design and initial testing of our offline system for the detailed characterization of complex mixtures of gas- and aerosol-phase organic compounds. Offline samples of compounds with 7 or more carbon atoms are analyzed using a thermal desorption-gas chromatography system connected to both a very-high resolution, chemical ionization, tandem mass spectrometer and an electron ionization quadrupole mass spectrometer. The sampled complex mixtures of organic compounds are comprehensively speciated by carbon number and compound class, with resolution of major isomers. We also present the results of a laboratory experiment that realistically simulates the processing of oil sands, which has been shown to cause SOA formation downwind of extraction and processing operations in Alberta. We compare the distribution of chemical compound classes and volatility in a preliminary assessment of their relative potential for secondary organic aerosol formation.