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DECODING ORGANIC MATTER COMPLEXITY THROUGH HYPHENATED CHROMATOGRAPHY AND ION MOBILITY ON AN 18 T TIMS–FTICR PLATFORM

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Complex organic matter such as bio-oils from lignocellulosic biomass pyrolysis and natural dissolved organic matter (DOM) consists of highly heterogeneous and oxygen-rich molecular mixtures. This chemical complexity leads to challenges in processing, storage, reactivity, and environmental behavior, and necessitates advanced analytical approaches to resolve compositional and structural diversity. Fourier-transform ion cyclotron resonance mass spectrometry (FTICR MS) is widely used for molecular-level characterization of such mixtures; however, direct infusion alone provides limited information on isomeric diversity. The integration of chromatographic and ion mobility separations therefore represents a critical step toward a more comprehensive characterization.
In this work, reverse-phase liquid chromatography (RPLC) and gated trapped ion mobility spectrometry (gTIMS) were coupled to an 18 T FTICR MS (Bruker timsMRMS) to investigate upgraded bio-oils and to demonstrate the broader applicability of this multidimensional approach to complex organic matter such as DOM.1 Bio-oil samples derived from catalytic fast pyrolysis of lignocellulosic biomass and subjected to extended hydrotreatment were analyzed by direct infusion, RPLC-FTICR MS, and gTIMS-FTICR MS. Direct infusion provided ultra-high mass resolution and accurate molecular formula assignment, revealing marked decreases in oxygen content and aromaticity during upgrading.

Keywords
Organic matter, bio-oils, FTICR, Ion mobility, Chromatography