Characterization of bio-oils derived from biomass pyrolysis using liquid chromatography hyphenated with 18 T FTICR mass spectrometer

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Résumé

Lignocellulosic biomass is the most abundant renewable feedstock and can be used to produce bio-oils through pyrolysis processes. Depending on the treatment and feedstocks used, the bio-oils obtained present very different molecular properties, influencing their upgrading process into biofuels. As they are highly complex mixtures their characterization at the molecular level is generally done by direct introduction FTICR MS yielding loss of isomeric information and loss of information through ionization discrimination. In this work we evaluated the performances of a new 18 T FTICR platform coupled to reverse phase liquid chromatography for the characterization of bio-oils.

Chromatographic analyses were performed with an ultra-high performance liquid chromatography (UHPLC) system (Thermo Vanquish), on two different types of reversed-phase columns: an ACQUITY UPLC HSS T3 (100 × 2.1 mm, 1.8 μm) and an ACQUITY Premier BEH C18 (100 × 2.1 mm, 1.7 μm). Experiments were carried out on an 18 T FTICR prototype (Bruker timsMRMS), equipped with a electrospray ionization (ESI), and an atmospheric pressure chemical ionization (APCI) source, both in positive ion mode. The new generation cart was described previously (1). Data processing was carried out using PyC2MC software. We first performed a comparative study using RPLC-HRMS in ESI(+) and APCI(+) modes, which provided an initial overview of oxygenated molecules in bio-oils thanks to a pool of 37 standards. The analysis of different bio-oil batches by RPLC-MS enabled the comparison of molecular family evolution using van Krevelen diagrams. Following this initial screening, LC-FTICR was used to take advantage of its ultra-high resolution with 1 s transient providing 1 million of resolution and sub-ppm mass accuracy, and enabling more precise molecular assignments. The increased resolution provided deeper insights into bio-oil composition, resolving additional molecular overlaps and refining the characterization of complex mixtures.

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