

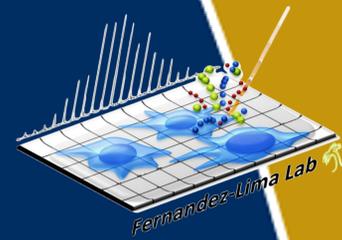
Chemical formula and structural level characterization of Dissolved Organic Matter by TIMS-FT-ICR MS/MS

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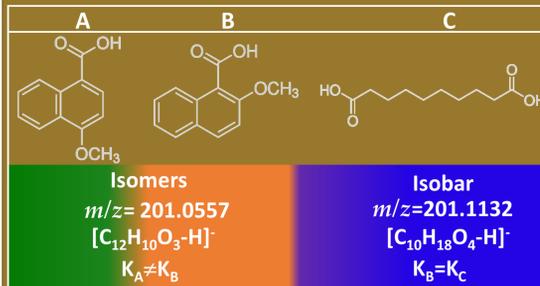


Introduction

- The analysis of complex mixtures (e.g. Dissolved Organic Matter) is challenging among other aspects because its isomeric complexity.
- Traditional MS/MS experiments (1 Da window) co-isolate multiple precursors biasing the structural elucidation of single compounds.
- In this study, we mobility selected and isolated single mass peaks in the ICR cell by CHEF and shot ejections of isobars following SORI-CID fragmentation. Potential chemical structures were generated based on unambiguous fragmentation patterns.

Experimental

Standards



A DOM sample collected from Pantanal National Park, Brazil was also studied.

Instrumentation and methods

- Custom built 7T Solarix ESI-TIMS-FT-ICR MS (TIMS nonlinear stepping scan function mode (mobility resolving power ~ 100))
- q-CID ($\Delta m/z = 1$ Da) and CHEF-SORI-CID ($\Delta m/z = 36$ mDa).

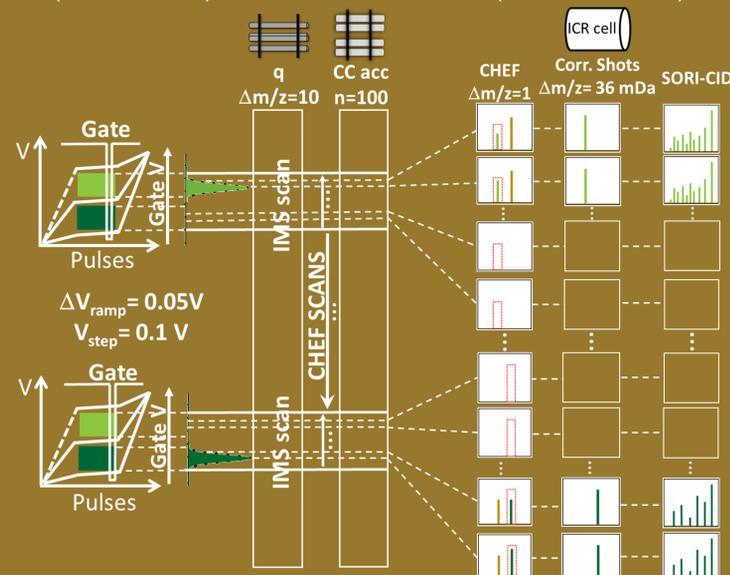


Figure 1. Event sequence during in-cell ESI-TIMS-FT-ICR MSMS

ESI-TIMS-FT-ICR MSMS of standards

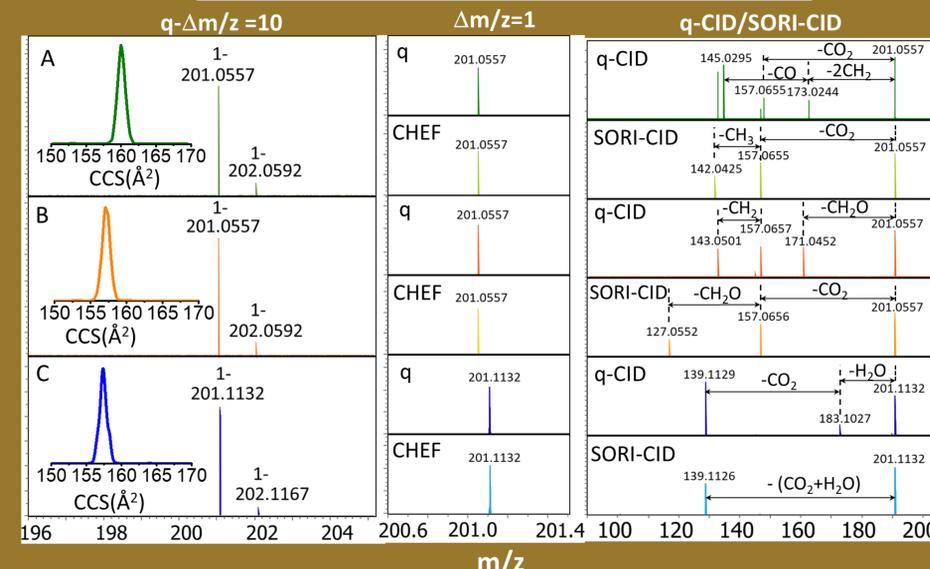


Figure 2. Mobility selected q-CID and CHEF-SORI-CID of individual standards (A, B and C). Notice that isomeric species A and B are mobility separated (inset IMS profiles) and the isobaric species C (bottom row) can be isolated in the ICR cell though it cannot be separated from B (middle row) in the IMS domain.

ESI-TIMS-FT-ICR MSMS of the standards mixture

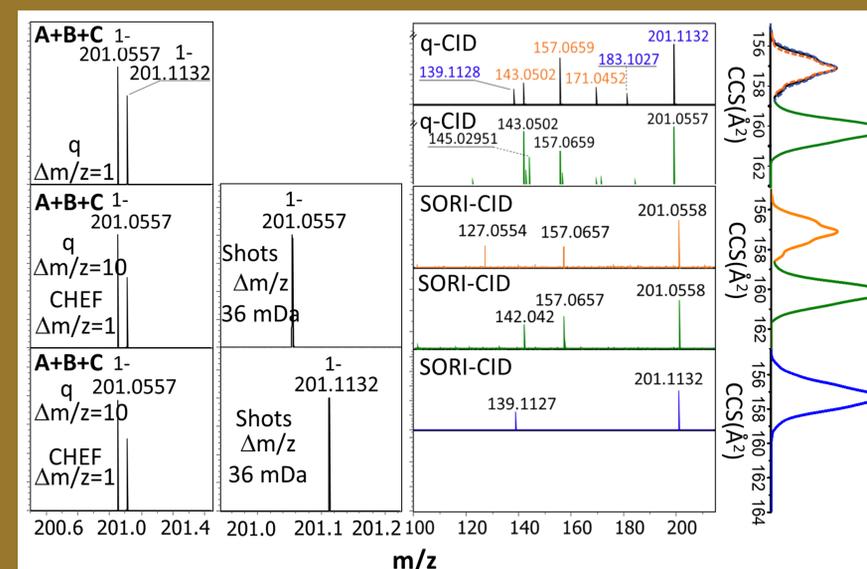
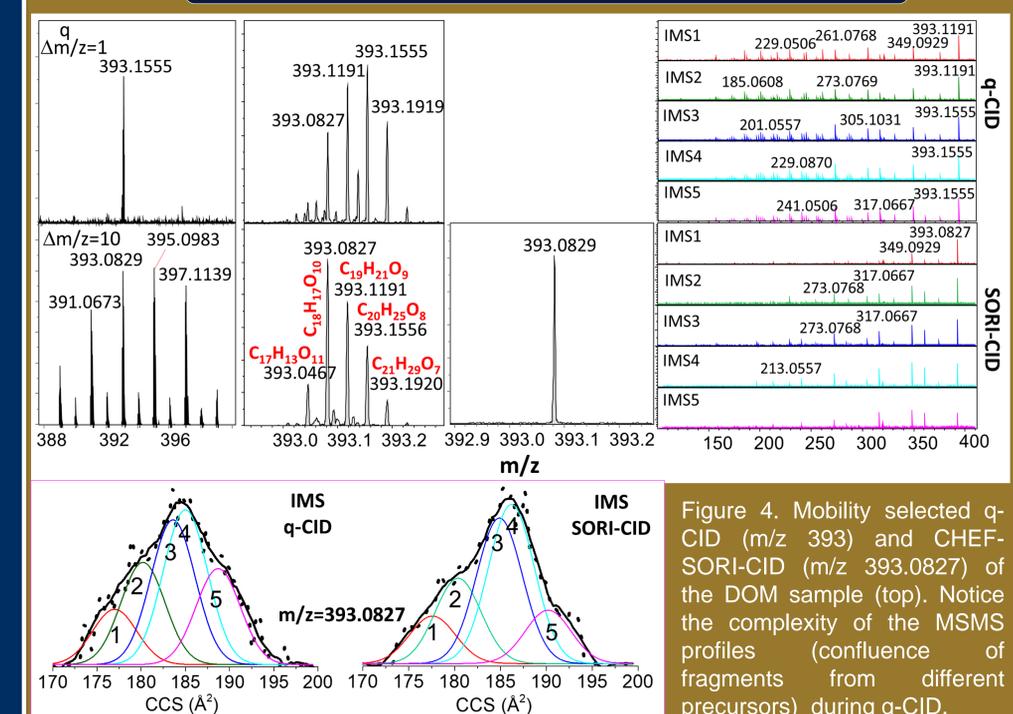


Figure 3. Mobility selected q-CID and CHEF-SORI-CID of the standards mixture. Notice that with traditional TIMS-CID experiments, even with mobility separated A and B, it is not possible to distinguish the isobar (C) from (B) in the mixture (top row). Conversely, each standard can be unambiguously identified after combining TIMS with single peak isolation in the ICR.

ESI-TIMS-FT-ICR MSMS of a DOM sample



IMS profiles of the ion $[C_{18}H_{18}O_{10}-H]^-$ with five annotated IMS bands.

Potential isomeric structures for $C_{18}H_{18}O_{10}$

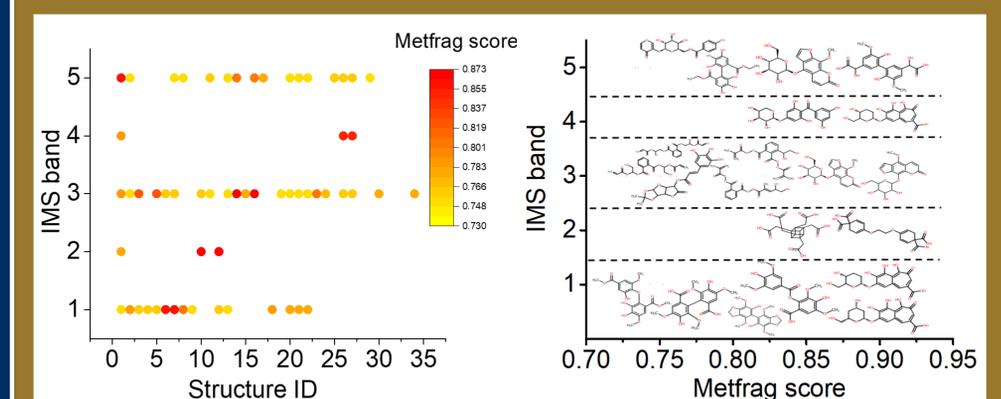


Figure 4. Distribution of isomeric candidates structures identified during in-silico fragmentation (Metfrag) of the precursor ion $[C_{18}H_{18}O_{10}-H]^-$ using the generated MSMS data (SORI-CID) per assigned IMS band. Structures are assigned based on the Metfrag scoring system (left). Potential isomeric structures of the compound $C_{18}H_{18}O_{10}$ correlated with each assigned IMS band (right).