

# Unraveling the structural complexity of Dissolved Organic Matter: isomeric diversity

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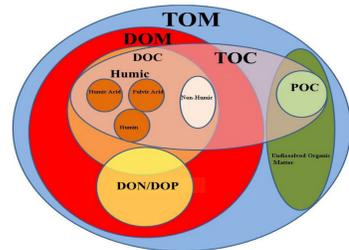
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## Goal

Examine the analytical advantages of using Trapped Ion Mobility Spectrometry-Fourier transform Ion Cyclotron Resonance-Mass Spectrometry (TIMS-FTICR-MS) and FT-ICR MS/MS to address the isomeric complexity of DOM samples collected from Pantanal (PAN) National Park (Brazil).



Figure 1. Pantanal National Park, Brazil



T. Pagano, M. Bida and J. E. Kenny, Water, 2014, 6, 2862.

DOM plays a significant role by controlling light attenuation, influencing metal speciation and bioavailability, and serving as a source of nutrients.

## References

- L. V. Tose, P. Benigni, D. Leyva, A. Sundberg, C. E. Ramirez, M. E. Ridgeway, M. A. Park, W. Romão, R. Jaffé and F. Fernandez-Lima, *Rapid Communications in Mass Spectrometry*, 2018, **32**, 1287-1295.
- D. Leyva, L. Valadares, J. Porter, J. Wolff, R. Jaffé and F. Fernandez-Lima, *Faraday Discussions*, 2019, DOI: 10.1039/C8FD00221E.

## Research Methodology

### TIMS-FTICR MS Analysis

Experiments were performed on a custom built TIMS-FT-ICR MS 7T Solarix spectrometer (Bruker Daltonics Inc., MA).

### TIMS-FTICR MS/MS Analysis

Fragmentation studies were performed using quadrupole isolation at nominal mass and typical CID energies of 15-20 eV.

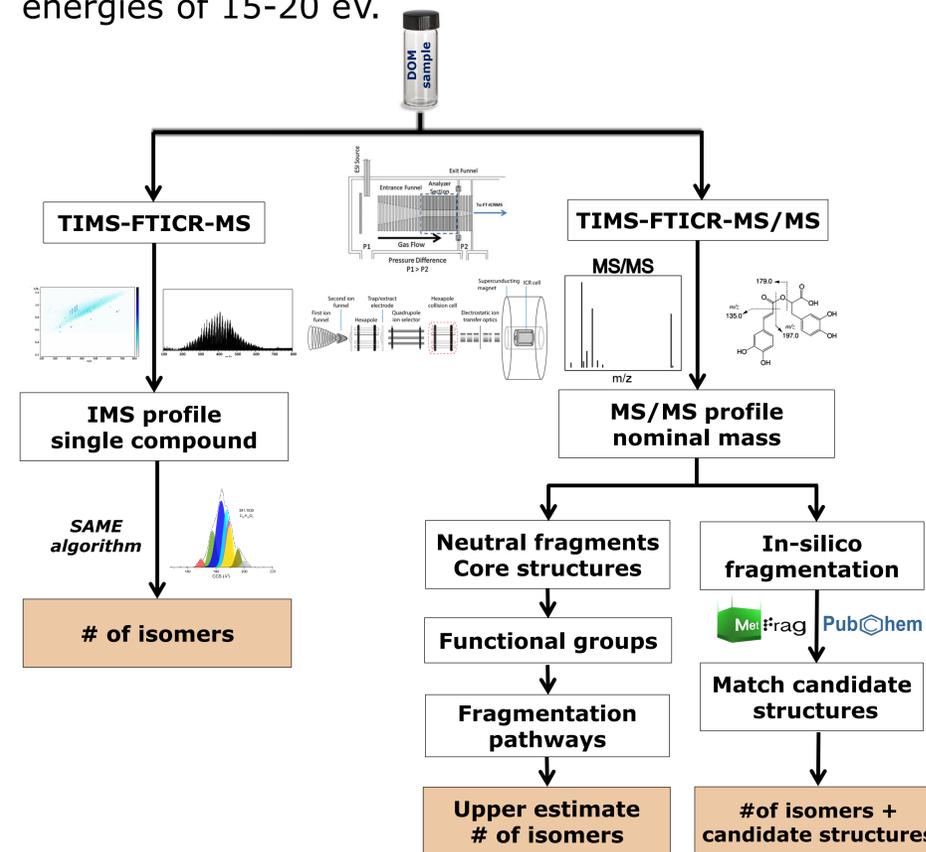


Figure 2. Workflow used to estimate the number of isomers in PAN sample

## Results

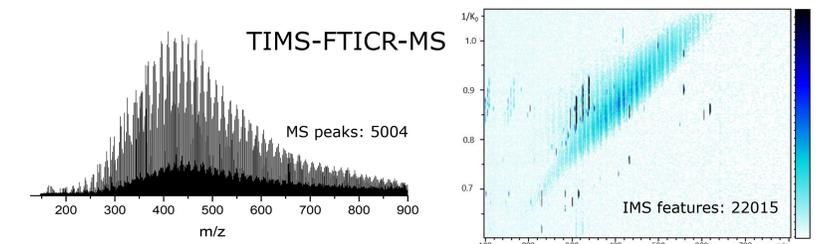


Figure 3. MS and 2D-IMS contour plots of PAN sample

**3,066 compounds based on formula  $C_xH_yN_{0-3}O_{0-19}S_{0-1}$**

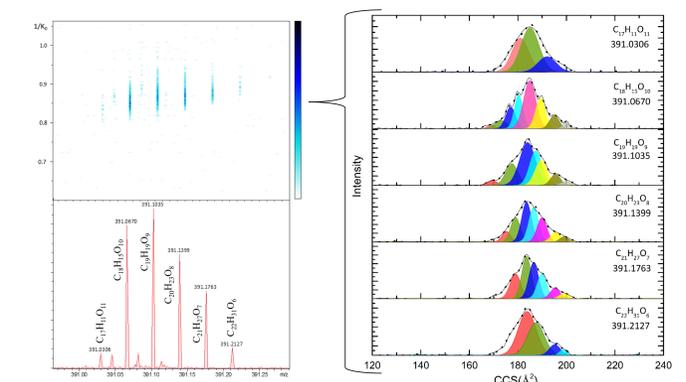


Figure 4. 2D-IMS-MS, MS and IMS projections at nominal mass 391 m/z.

**Average of 6-10 isomers per chemical formula**

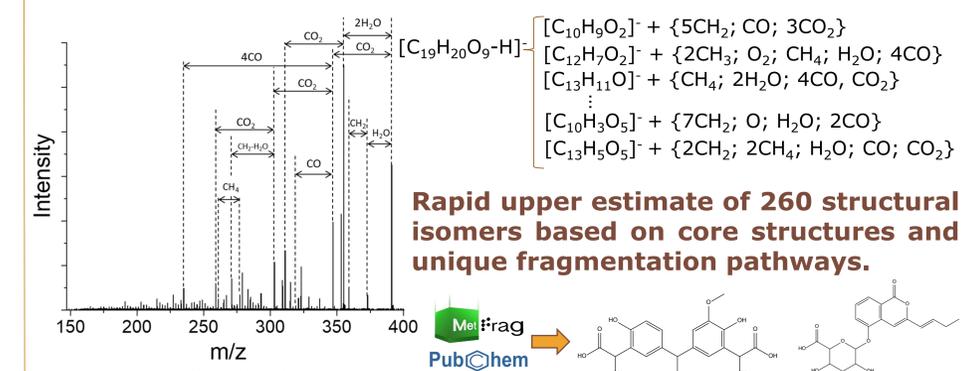


Figure 5. FTICR-MS/MS profile of 391 m/z precursor ions.

**96 candidate isomeric structures (1mDa tolerance)**



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