Novel structural MS-based elucidation methods for the analysis of complex environmental samples

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Goal

- Use Trapped Ion Mobility Spectrometry coupled to FT-ICR MS for the characterization of a complex mixture.
- Develop theoretical tools to compliment the experimental workflow, enabling structural elucidation of unknown structures.

Instrumentation

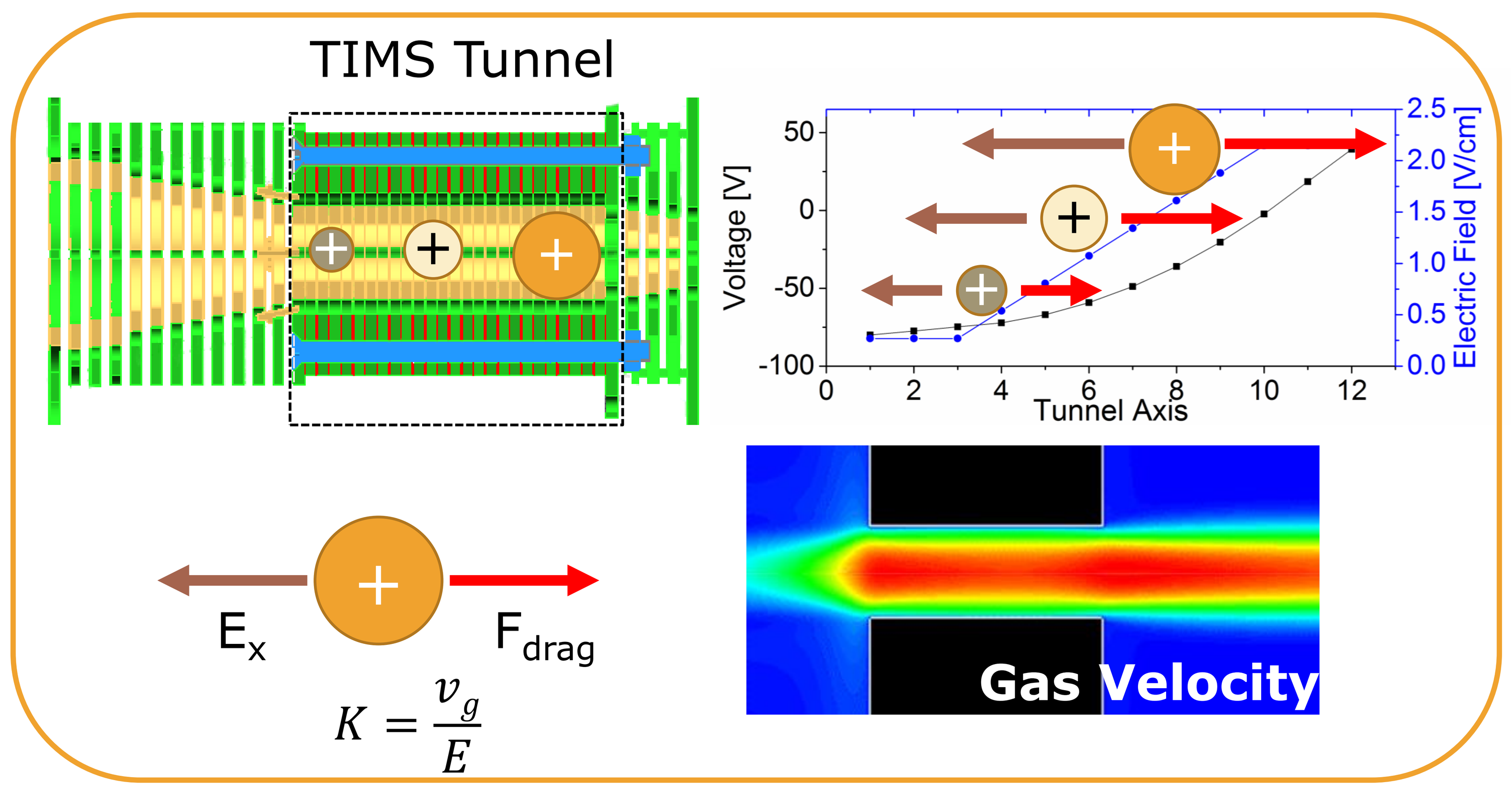
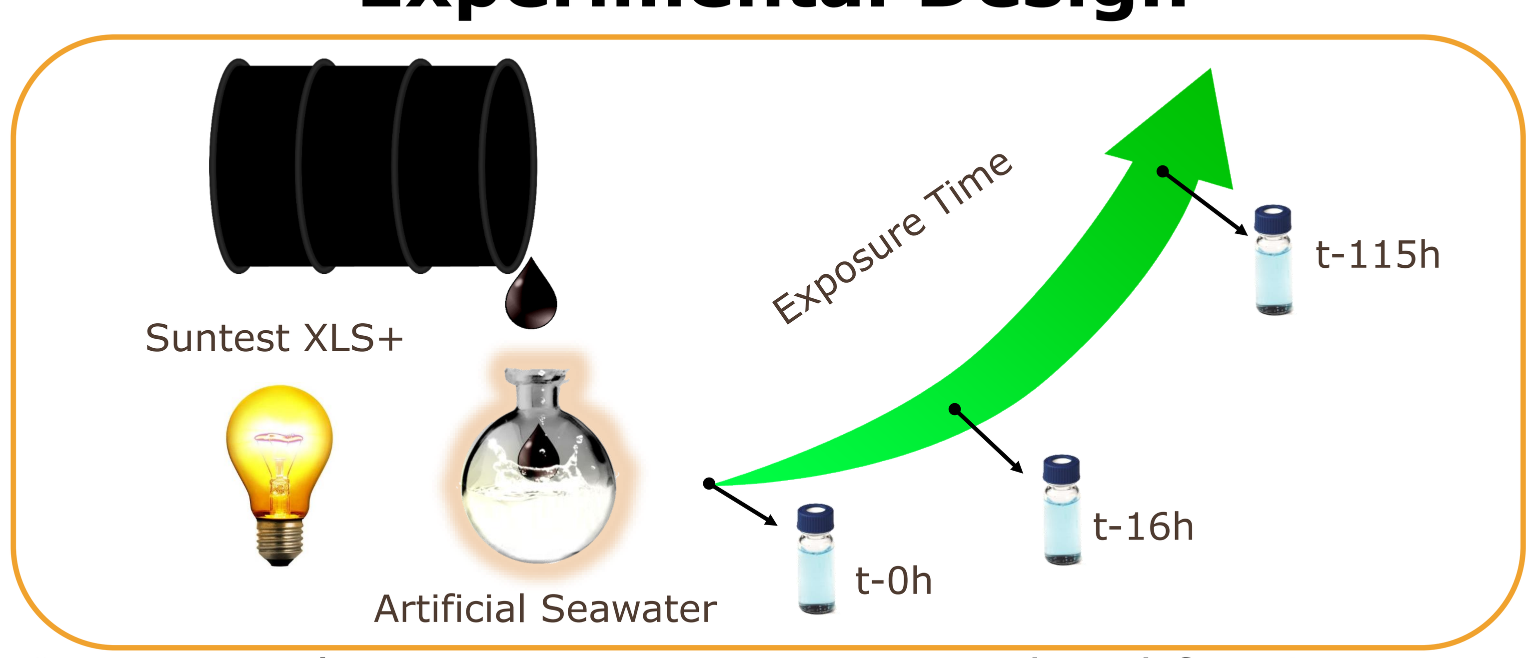


Figure 1. Diagram and principles of separation of Trapped Ion Mobility Spectrometry

Experimental Design



Generate a low energy water accommodated fraction, expose it to solar light, and collect fractions at 16 and 115h.

Results

- Samples were analyzed with atmospheric pressure laser ionization TIMS-FT-ICR MS to characterize the aromatic components.

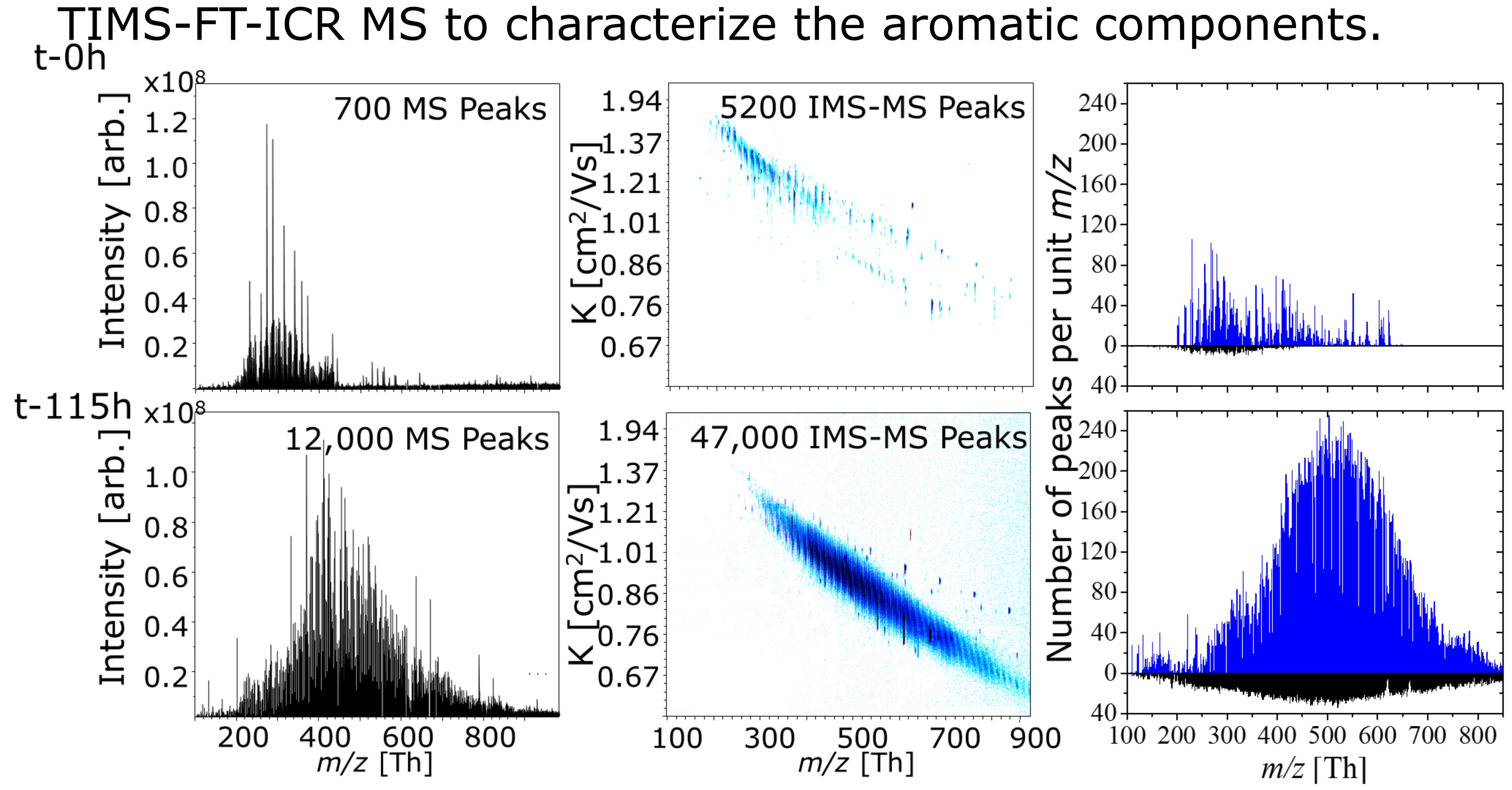


Figure 2. Mass spectrum, 2D TIMS-FT-ICR MS spectrum and number of peaks measured per unit *m/z* by MS (black) and IMS-MS (blue) of the WAF at 0 and 115 hours. Note the change in complexity over time

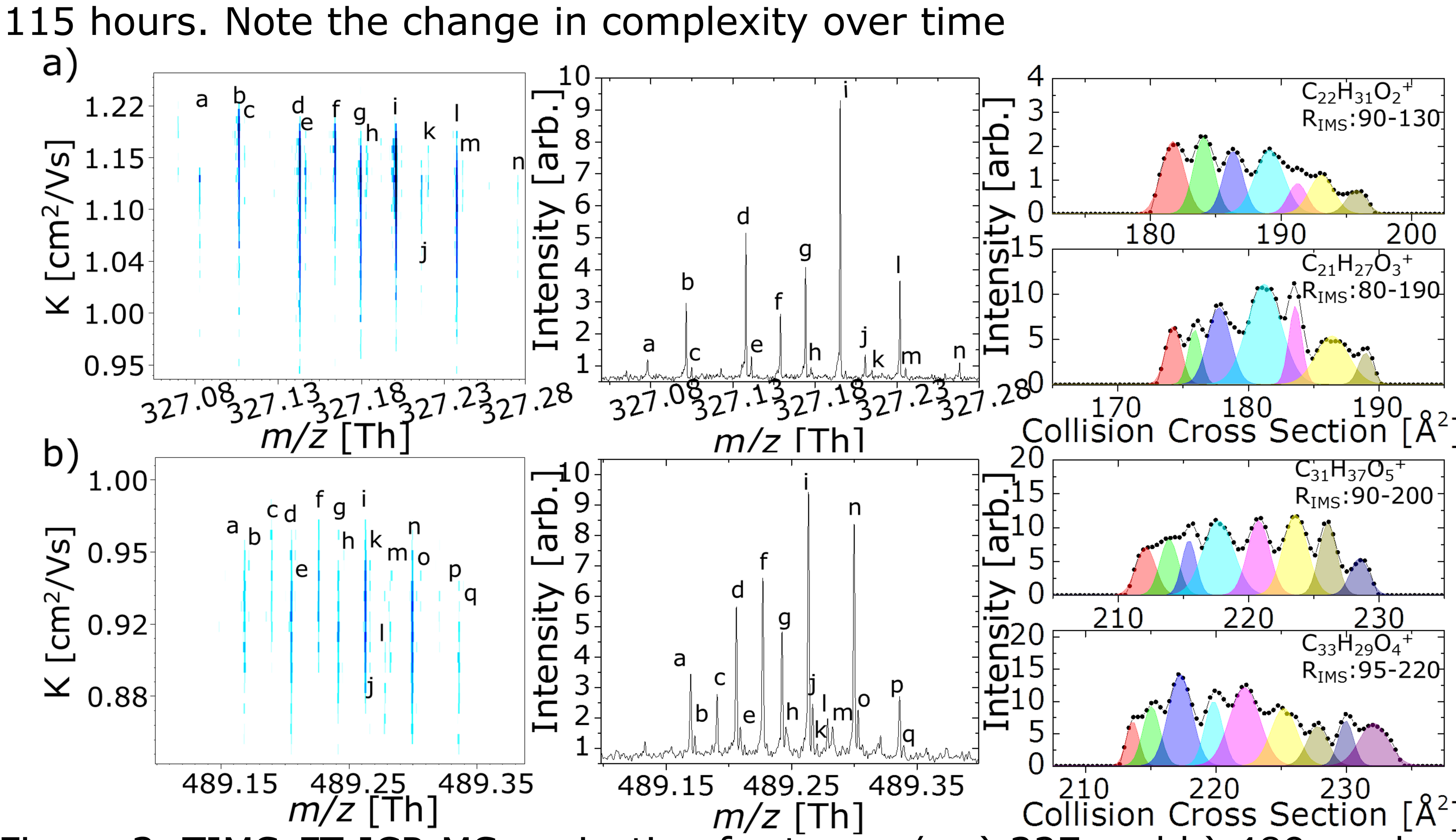


Figure 3. TIMS-FT-ICR MS projection for two *m/z* a) 327 and b) 489, and mobility features for selected chemical formulas. Note the isomeric complexity.

Results

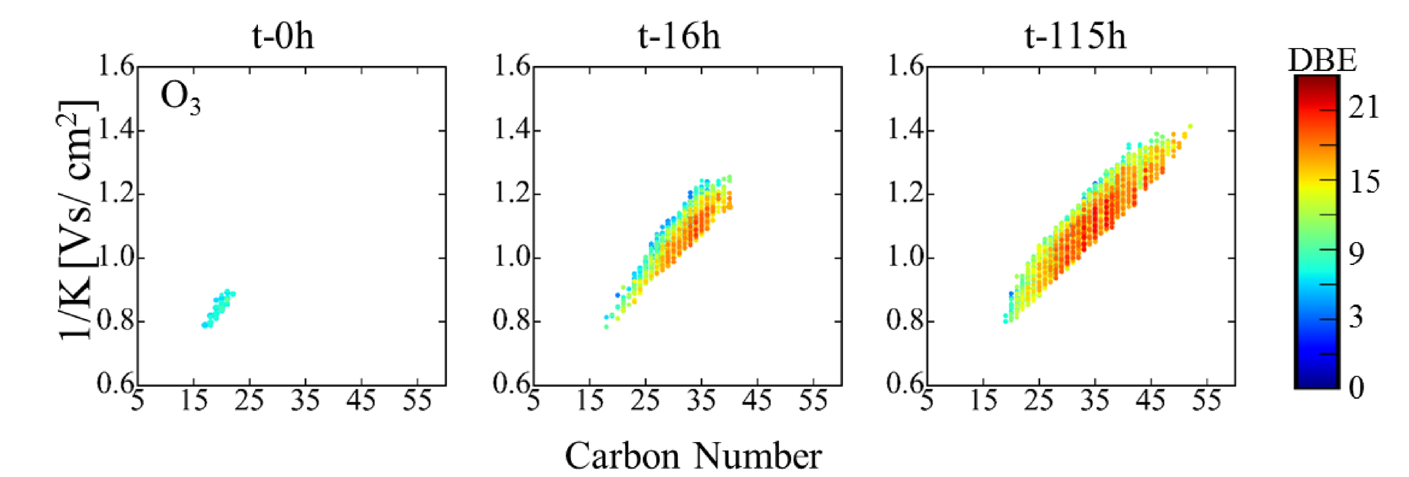


Figure 4. Change in carbon number vs mobility distribution for the O_3 class over time.

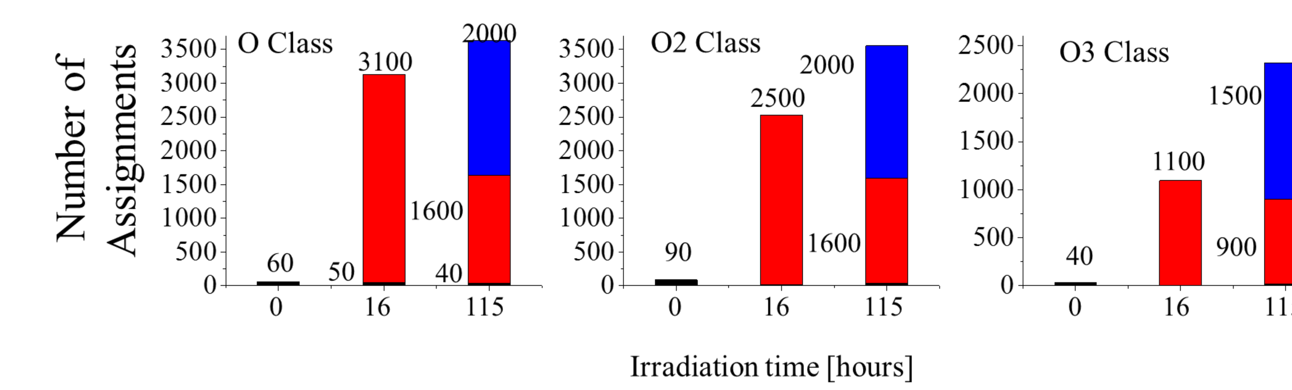
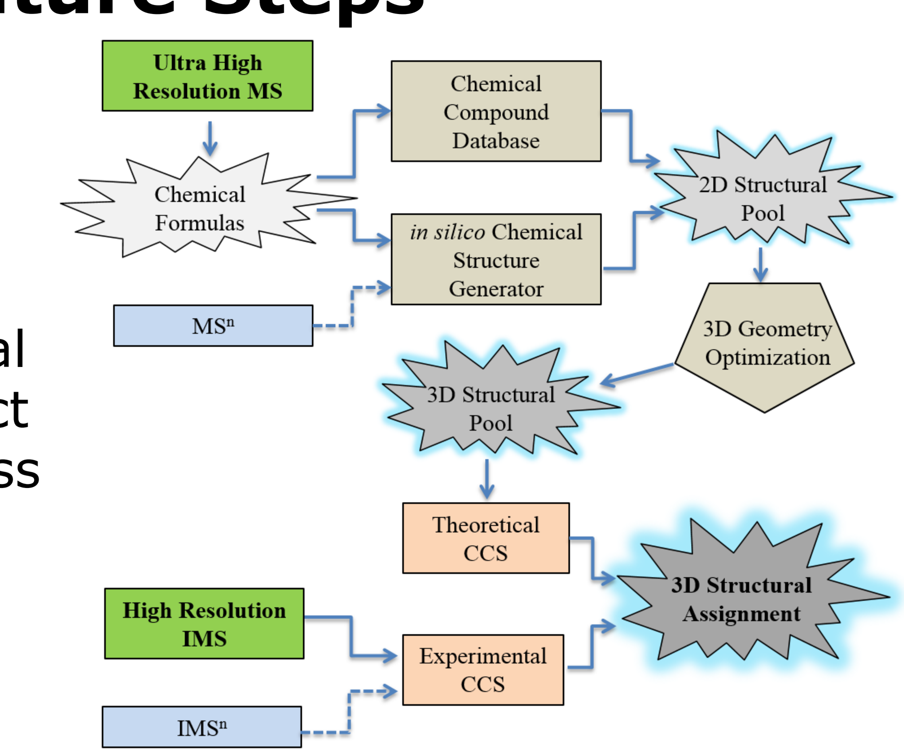


Figure 5. Number of identification at t-0h (black), t-16h (red) and t-115h (blue) for the O_{1-3} classes.

Future Steps

Figure 6. Workflow for unsupervised structural assignment using exact mass and collision cross section information.



Conclusions

- Exposure of the LEWAF to sunlight results in an increase in the number of molecules observed in the spectrum.
- TIMS-FT-ICR MS is able to separate the isobaric and isomeric complexity of the LEWAF
- The LEWAF is a chemically dynamic system that undergoes significant changes in composition over time.

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