

SUPPORTING INFORMATION

Isomeric Separation and Structural Characterization of Acids in Petroleum by Ion Mobility Mass Spectrometry

Priscila M. Lalli,^{†,‡} Yuri E. Corilo,^{†,‡} Steven M. Rowland,^{†,‡} Alan G. Marshall,^{†,§} and Ryan P. Rodgers^{*,†,‡,§}

[†]National High Magnetic Field Laboratory, Florida State University, 1800 East Paul Dirac Drive, Tallahassee, Florida 32310

[‡]Florida State University Future Fuels Institute, 1800 East Paul Dirac Drive, Tallahassee, Florida 32310

[§]Department of Chemistry and Biochemistry, Florida State University, 95 Chieftain Way, Tallahassee, Florida, 32306

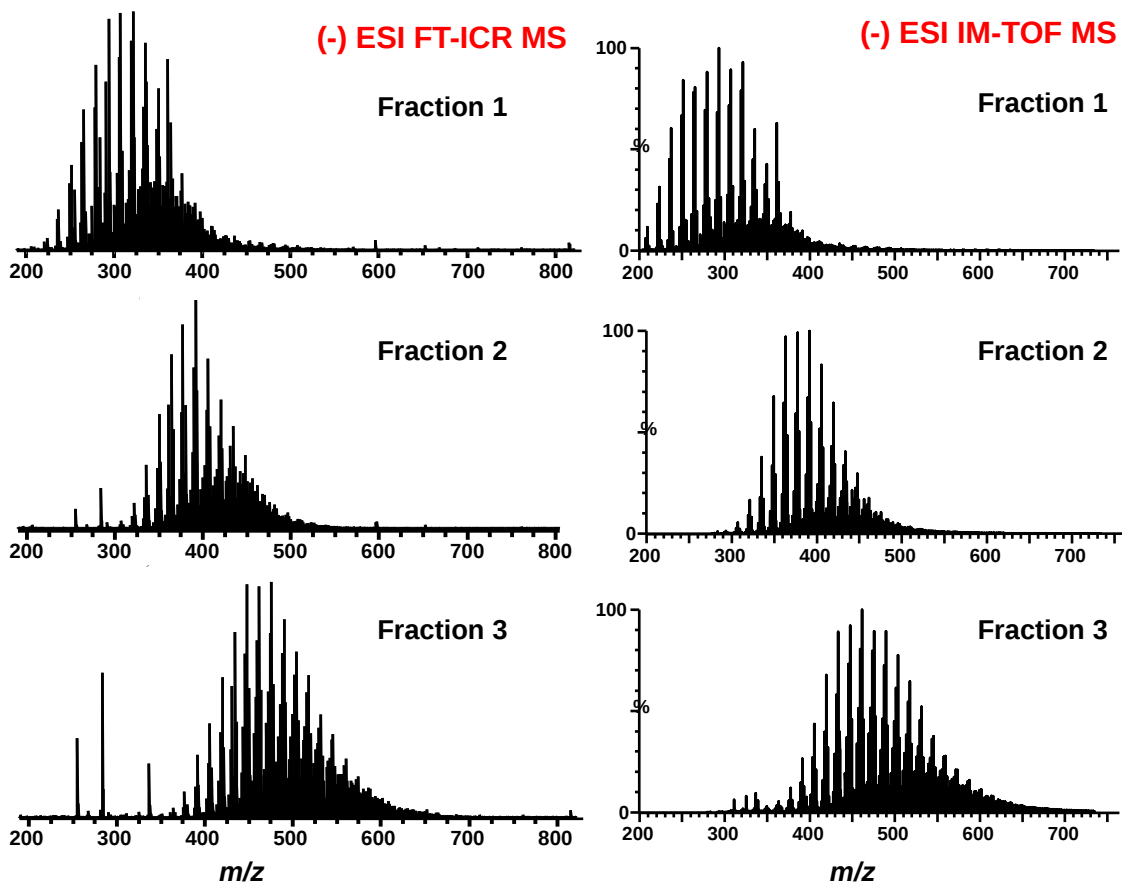


Figure S1. (-) ESI FT-ICR (left) and (-) ESI IM-TOF mass spectra for the three MAPS acid fractions.

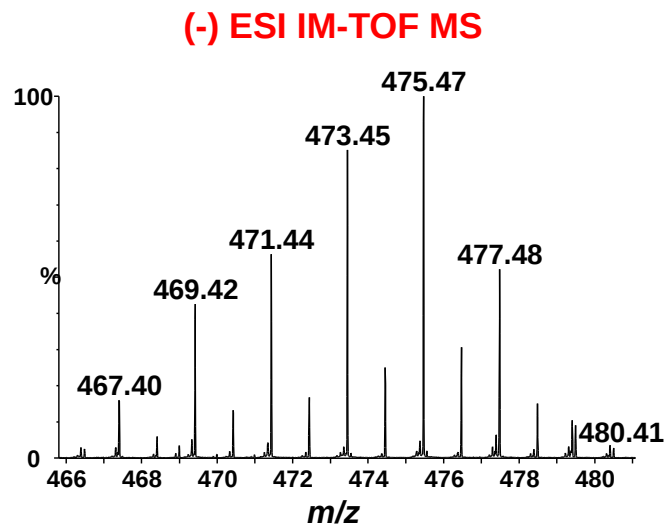
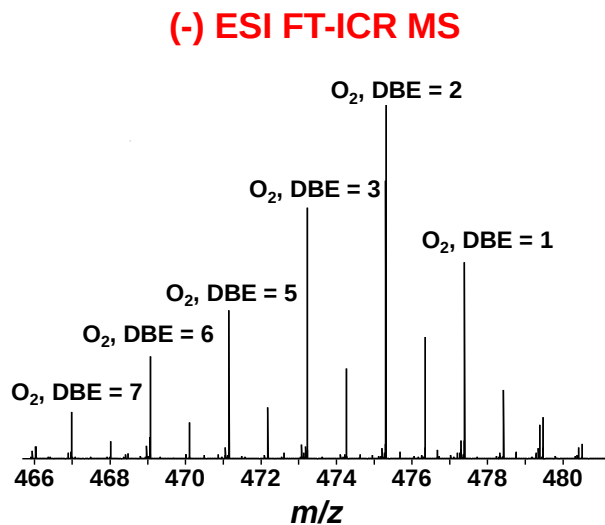


Figure S2. Mass scale-expanded segment of (-) ESI FT-ICR and (-) ESI IM-TOF mass spectra for Acid Fraction 3.

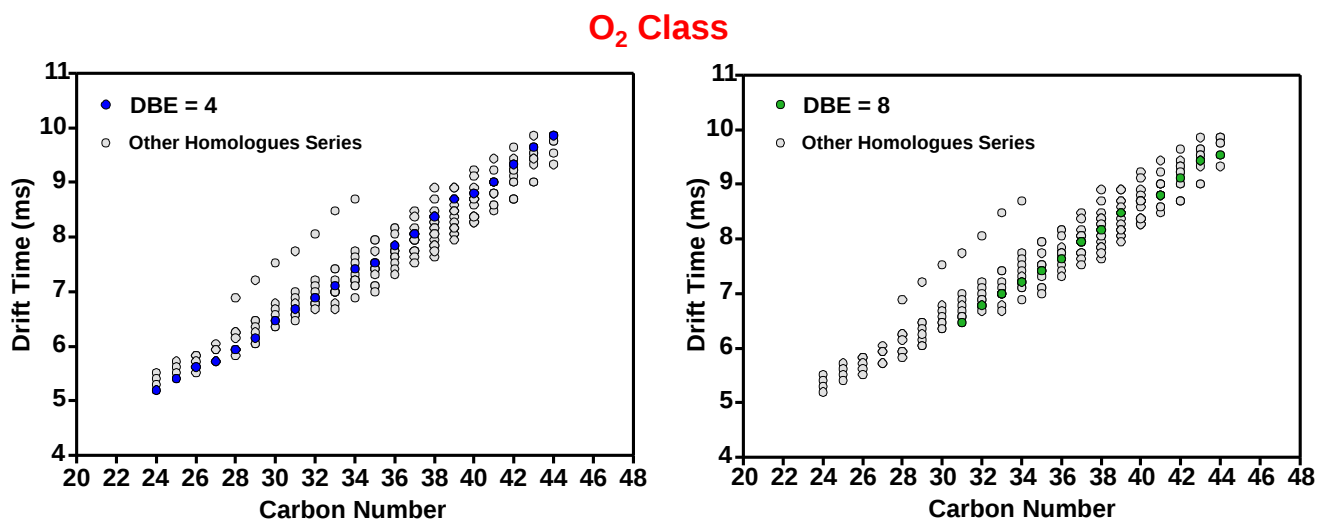


Figure S3. Drift time vs. carbon number for O₂ species in Acid Fraction 3. Ions of DBE = 4 (left) and DBE = 8 (right) are highlighted in blue and green, whereas the remaining O₂ species appear in light gray.

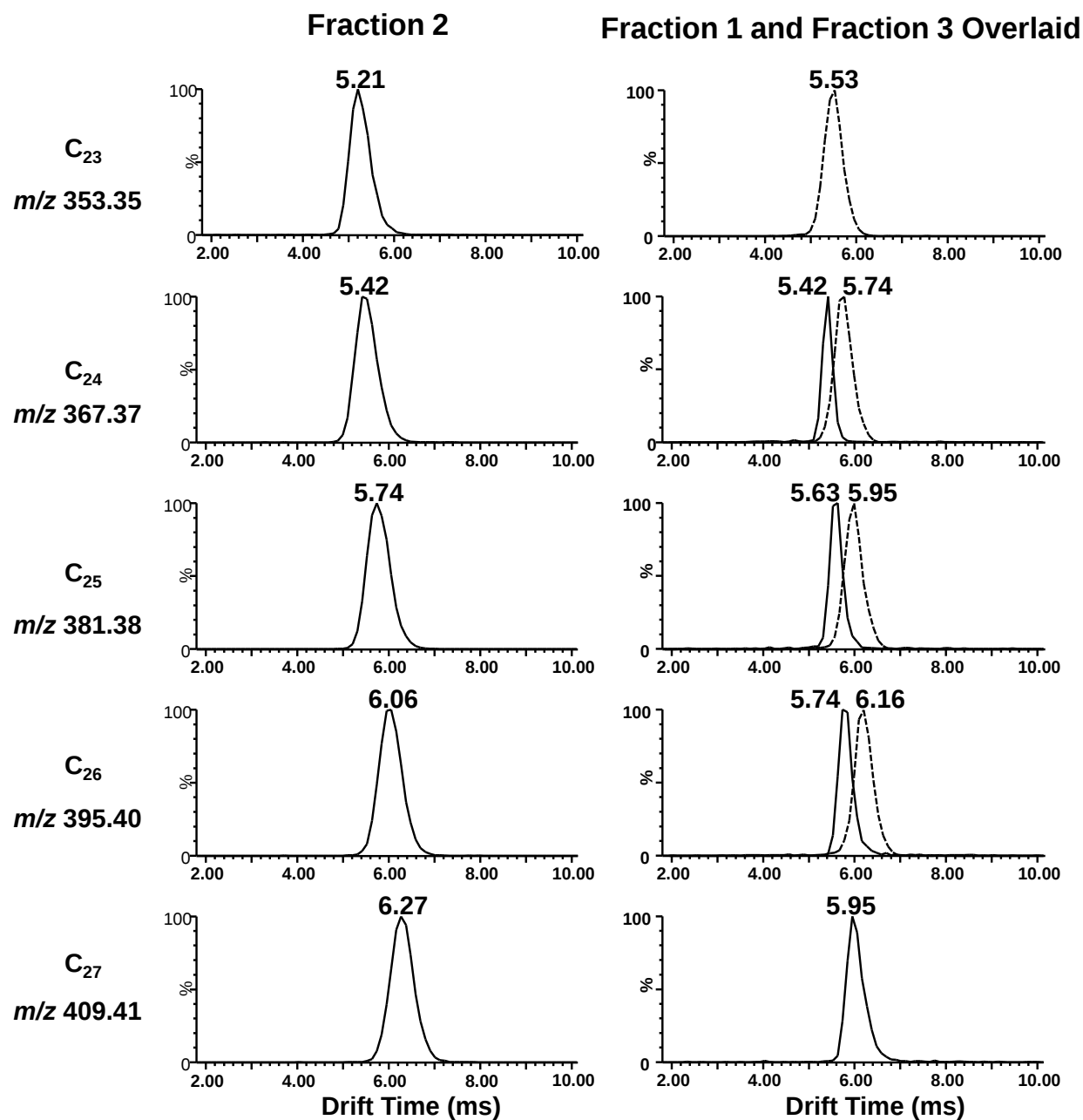


Figure S4. Mobiligrams extracted for O₂ species of DBE = 1 from Fraction 2 (left) and overlaid mobiligrams from Fraction 1 (solid line) and Fraction 3 (dashed line) (right).