

Tech Transfer: EnviroOrg and PetroOrg Chemical Analysis Software



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Recent advances in ion cyclotron resonance mass spectrometry (ICR-MS) have dramatically increased the quantity and quality of data obtained from complex mixtures. The goal of ICR-MS is to identify the molecular formula for each constituent in a complex mixture of chemicals. However, more compositional information results in a severe data processing "bottleneck", because the data process workflow is an interdisciplinary, highly complex, and time-consuming process. Clearly one of the major research challenges in this area is how to strategize data reduction techniques and molecular formula attribution for a wide variety of mixtures, including natural organic matter (NOM), petroleum, biofuels, lipids, and metabolites.

MagLab-developed software packages (PetroOrg and EnviroOrg) simplify and automate complex chemical mixture data analysis to provide high-throughput, accurate, and customizable data visualization. The software is offered commercially and has grown to support • ion mobility mass spectrometry, • lipids analysis, • automated multivariate analysis (principal component analysis and hierarchical cluster analysis), • liquid chromatography mass spectrometry (LC-MS), and • batch processing of analyses.

Facilities: Ion Cyclotron Resonance

Citation: 1) *Polar Lipid Composition of Biodiesel Algae Candidates Nannochloropsis oculata and Haematococcus pluvialis from Nano Liquid Chromatography Coupled with Negative Electrospray Ionization 14.5 T Fourier Transform Ion Cyclotron Resonance Mass Spectrometry* Liu, P.; Corilo, Y. and Marshall, A.G., **Energy & Fuels**, **30**, 10, 8270–8276 (2016), 2) *Calculation of the Total Sulfur Content in Crude Oils by Positive-Ion Atmospheric Pressure Photoionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry* Corilo, Y.E.; Rowland, S.M. and Rodgers, R.P., **Energy & Fuels**, **30**, 3962–3966 (2016), 3) *Oil Spill Source Identification by Principal Component Analysis of Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectra* Corilo, Y.E.; Podgorski, D.C.; McKenna, A.M.; Lemkau, K.L.; Reddy, C.M.; Marshall, A.G. and Rodgers, R.P., **Analytical Chemistry**, **85**, 19, 9064–9069 (2013)



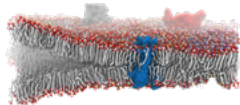
Natural Organic Matter



Petroleum



Bio Fuels



Lipids

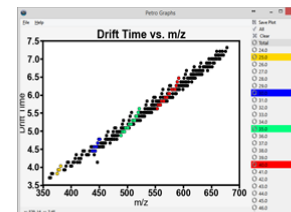
Software Development

- Intelligent Molecular Formula Assignments
- Ion Mobility Support (Synapt Waters)
- Batch process and LC-MS support

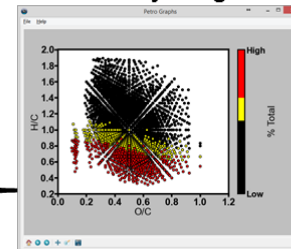


FT-ICR MS Data Processing

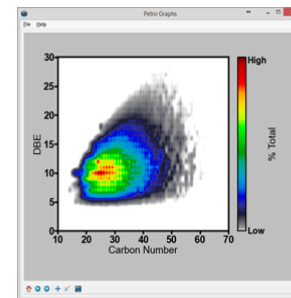
- Comprehensive Visualization tools
- Smart data reduction
- Embedded Chemometric Tools



Ion Mobility Diagrams



NOM Diagrams



Petroleomics Diagrams