KairosMS: A solution for complex mixture data analysis and visualisation

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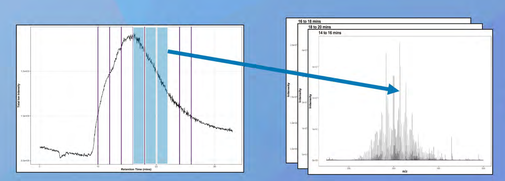
Introduction

- Coupling of Fourier transform mass spectrometry such as Fourier transform ion cyclotron resonance (FTICR) or Orbitrap, with chromatography can provide further insights for complex mixtures such as petroleum, dissolved organic matter and bio oils
- Chromatography is required to separate isomers while high resolution mass spectrometry is required to resolve co-eluting components
- Challenges exist in processing resultant large datasets (tens of gigabytes), and the accurate identification of extracted ion chromatograms (EICs)
- KairosMS is presented as a tool that addresses many of the issues of hyphenated data processing, while incorporating interactive data analysis and visualisation

Old Workflow

Manually extract a mass spectrum for a window of 2-5 minutes → Compositional assignment in third party software



→ Data analysis and visualisation per slice

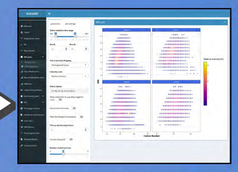
New Workflow

Extracted mass list from instrument vendor software → **KairosMS**: Data processed, Optional recalibration, Export mass list → Compositional assignment in third party software → **KairosMS**: Assignments merged with processed data → Data Analysis and interactive visualisation

Raw file: ~30 GB
Extracted mass list: ~160MB

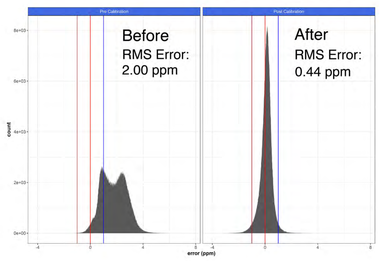
1 - 5 min processing time
Exported mass list: ~100 KB

Final file: ~100MB

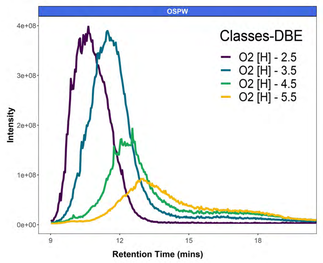


Gas Chromatography (GC) APCI FTICR MS of OSPW

Oil sands process water (OSPW) is a by product of the oil sands industry in Alberta, Canada



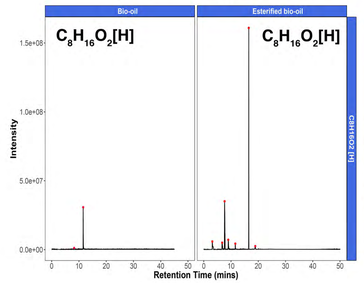
Automatic recalibration process



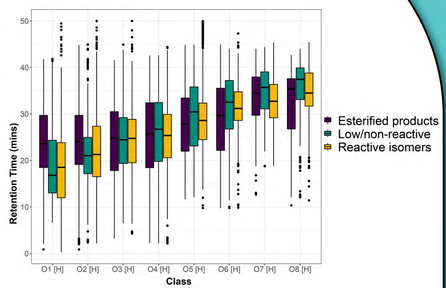
Extracted ion chromatograms (EICs) can be produced for individual ions, homologous series, or entire heteroatom classes

Gas Chromatography (GC) APCI FTICR MS of Bio-Oils

Bio-Oil Upgraded Bio-Oil



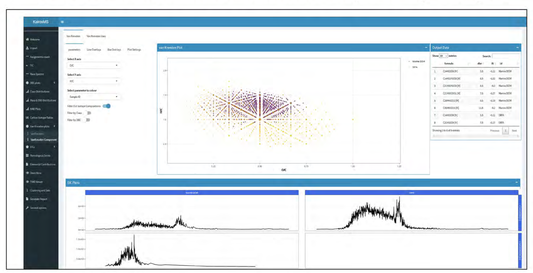
Comparison of EICs from two samples



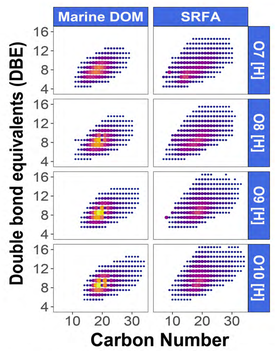
Matching of isomers between samples

Liquid Chromatography (LC) ESI Orbitrap MS of DOM

Marine dissolved organic matter (DOM) and Suwanee River fulvic acid (SRFA) sample



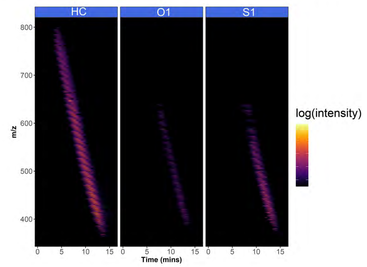
Interactive van Krevelen plot
Comparison of multiple data sets
(hyphenated or direct infusion data)



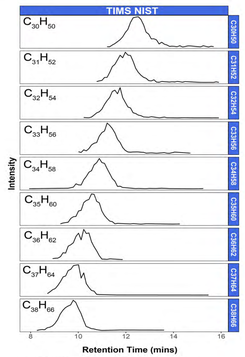
Generation of multiple plots by class: DBE vs carbon number

TIMS APPI FTICR MS of NIST Crude Oil

Trapped ion mobility spectrometry (TIMS)



m/z vs time plot for different classes
$1/K_0$ and CCS values can also be plotted



EIC visualisation
Filtering by DBE and carbon number

KairosMS Capabilities

- Import and compare multiple samples
- Interactive plots and data filtering by retention time, carbon number, DBE and class
- EIC targeting and visualisation
- Automated principal component analysis (PCA)
- Quantification by area under EIC curves
- All graphics and plot data easily exported
- Hyphenated and direct infusion compatible
- Ongoing rapid development of features

Conclusions

- Improved and accelerated workflow for hyphenated high resolution mass spectrometry data
- Rapid processing, recalibration, and visualisation of data
- Graphics and plot data are interactive and exportable
- Application can be run on a laptop or hosted on a server
- We have used KairosMS with GC, LC and TIMS for both FTICR and Orbitrap data
- KairosMS has been demonstrated here with petroleomics, bio-oils and environmental samples but could also be applied to other sample types

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