

Next generation solutions to ensure healthy water resources for future generations

'Omic' and chemical fingerprinting methodologies using ultrahigh-resolution mass spectrometry for geochemistry and healthy waters

(GWF Pillars 1 &2)



Next Generation Solutions to Ensure Healthy Water Resources for Future Generations

Paul D. Jones, (PI), Northern Ecosystem Toxicology Initiative Chair, School of Environment and Sustainability and Toxicology Centre, uSask

John P. Giesy (co-PI), CRC in Environmental Toxicology, Department of Veterinary Biomedical Sciences and Toxicology Centre, uSask

Tim Davis (Collaborator), NOAA/Bowling Green State University

John Pomeroy (Collaborator), uSask

Research Partners: Buffalo Pound and Prince Albert Water Treatment Plants

Technical Partner: Thermo Scientific

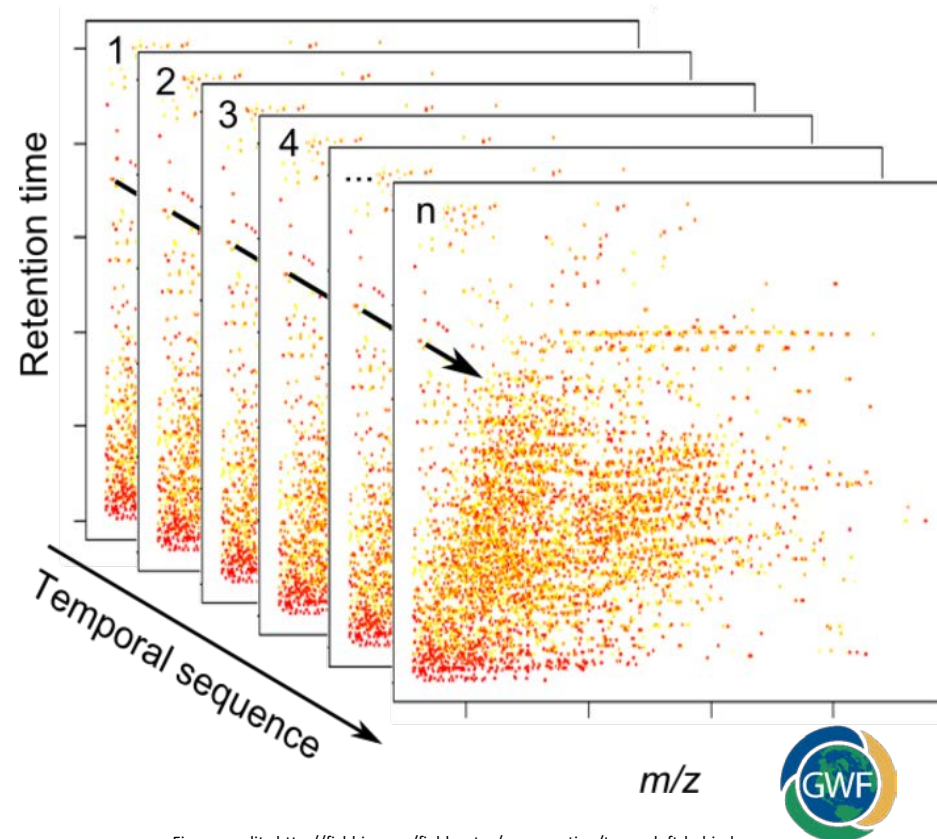


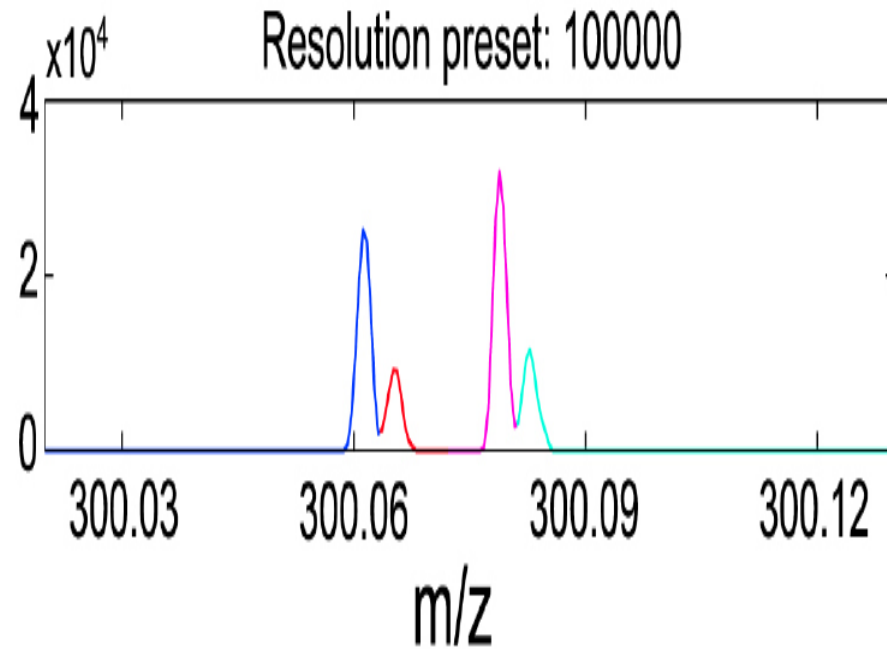
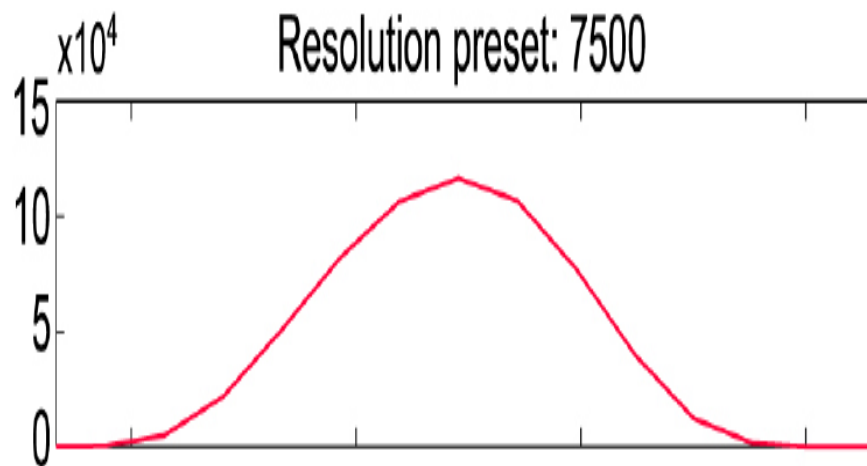
Figure credit <http://fishbio.com/field-notes/conservation/traces-left-behind>



Why Does Resolution Matter ??



Why Does Resolution Matter ??



Orbitrap

Mass Range

m/z 50-6,000

Max Resolving Power

250,000 @ m/z 200

Max Scan Rate

Up to 25 Hz @ 17,500 Res m/z 200

Mass Accuracy

Internal: < 1 ppm RMS

External: < 3 ppm RMS

Accuracy < 1 mmu, for reference the mass of an e⁻ is 0.55 mmu (0.00055 mass units)

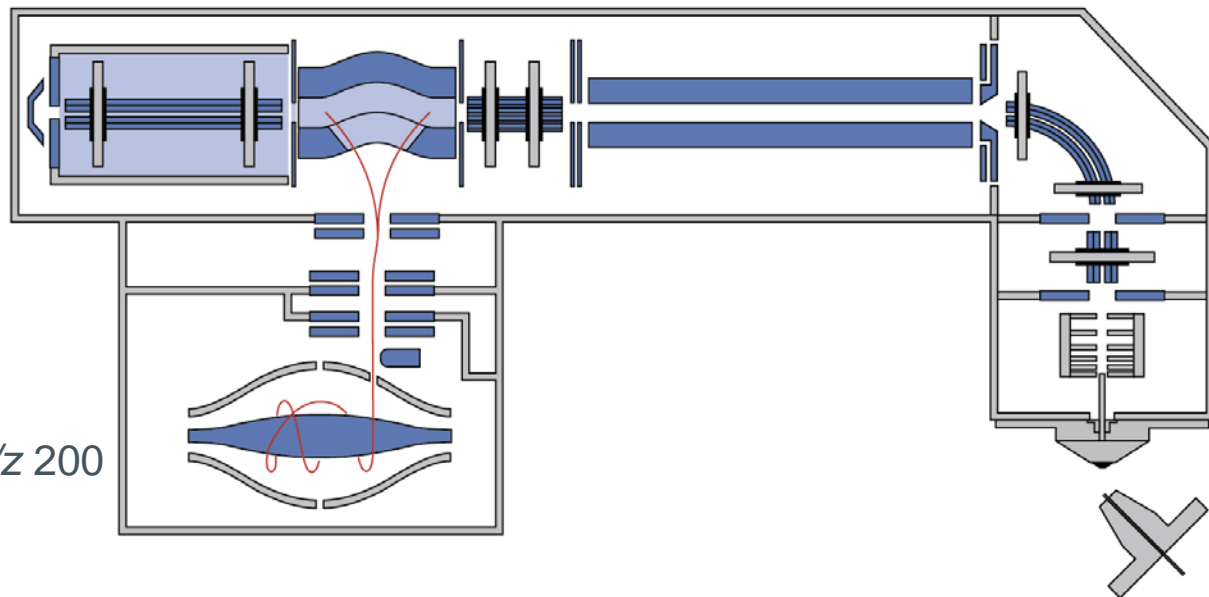
Sensitivity

Full MS: 500 fg Bupirone on column S/N 100:1

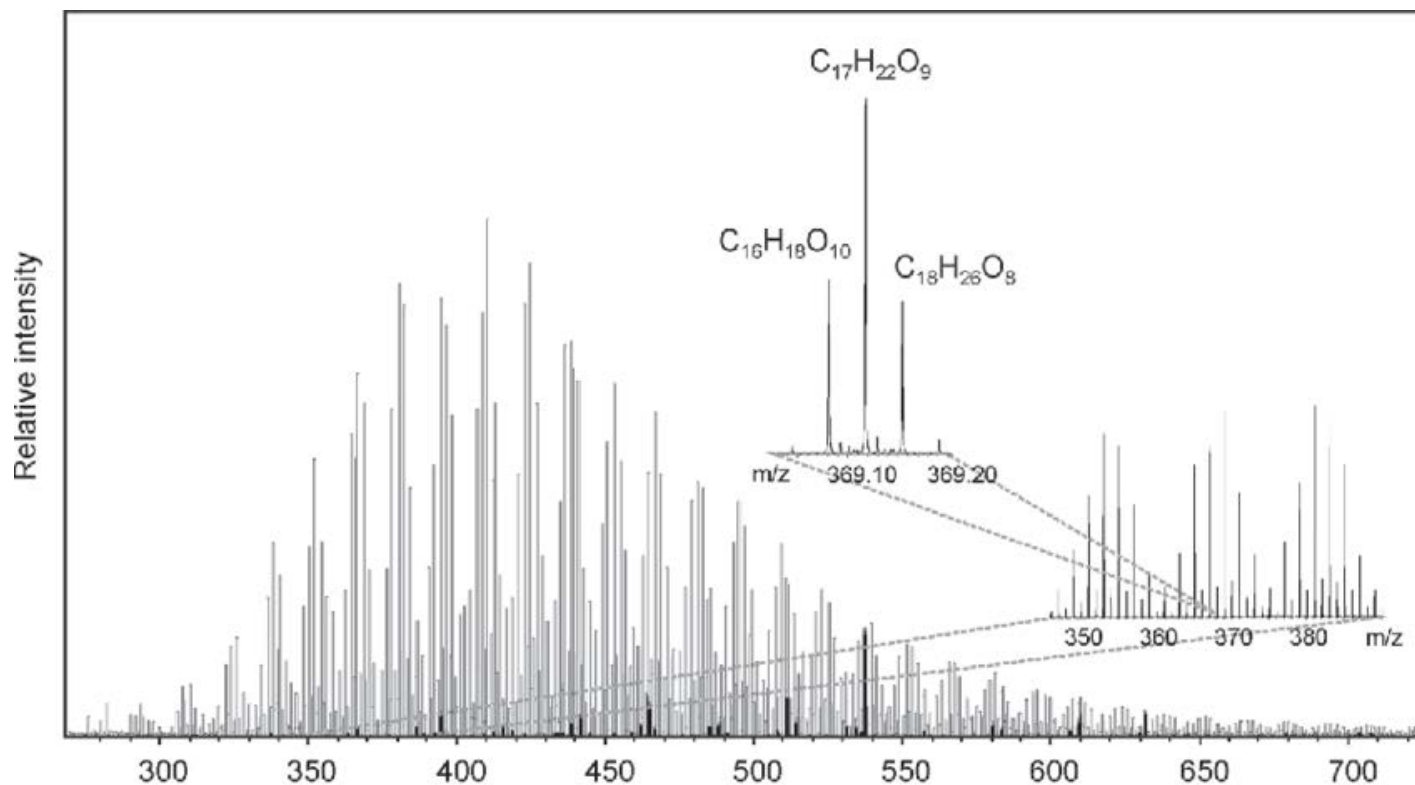
SIM: 50 fg Bupirone on column S/N 100:1

Polarity Switching

1 full cycle in < 1 sec (1 full scan +ve mode and 1 full scan -ve mode at 35,000 resolution)

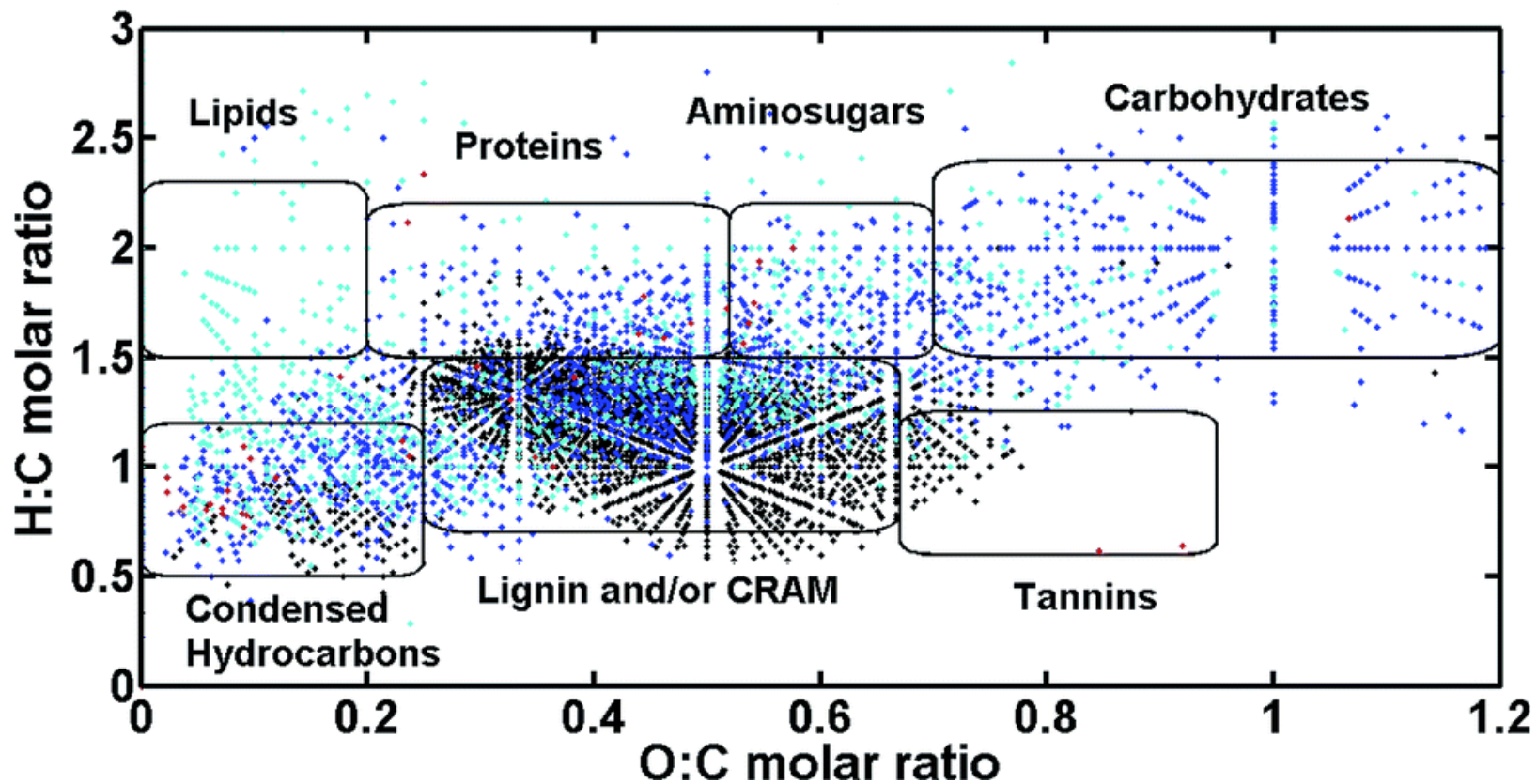


Why Does Mass Resolution Do Matter ??



Can assign a formula to every 'feature' – we know its chemical make up

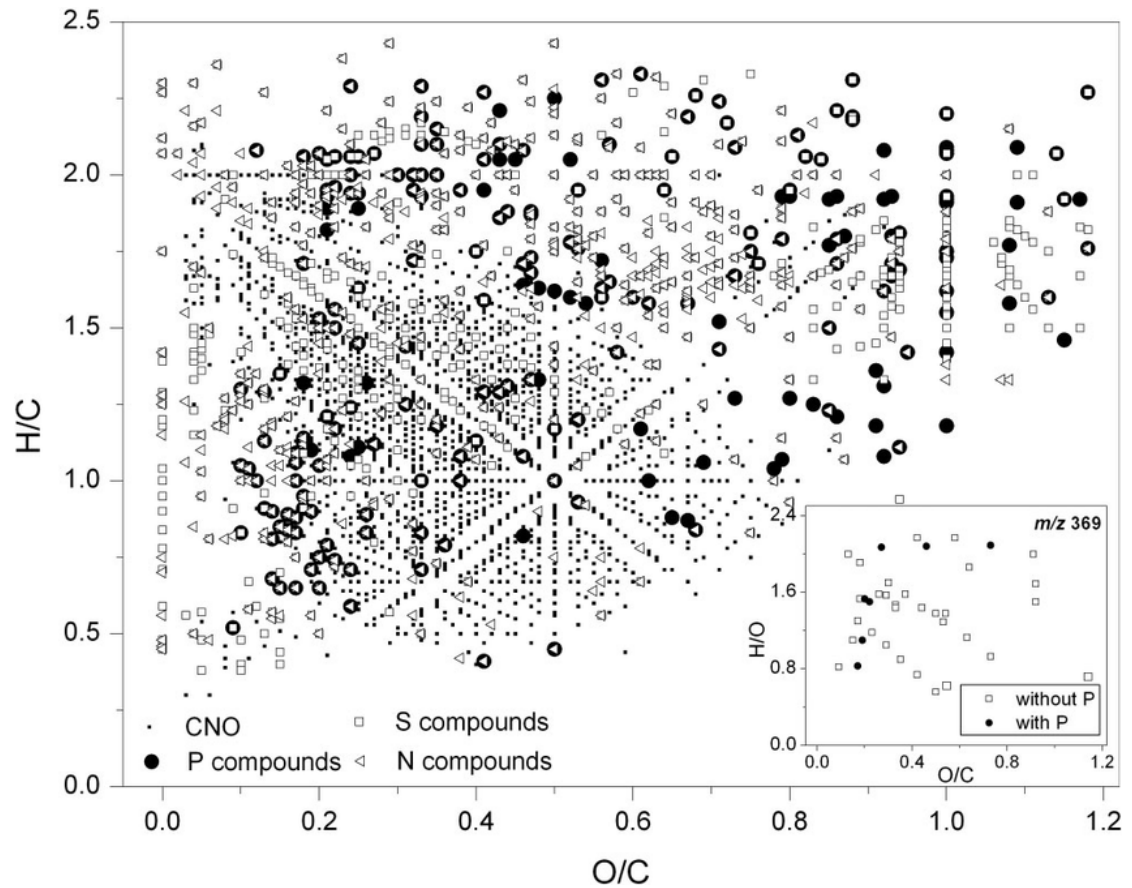
Van Krevelin Diagram – Dissolved Organic Matter



lignin/CRAM (carboxyl-rich alicyclic molecules)

Van Krevelin Diagram – Dissolved Organic Matter

- S – metal ligand binding
- P – P availability
- Cl – persistent organic pollutants



Priority Project Focus

Chemical fingerprinting

- contaminant sources
- Data pipelines for untargeted screening and quantification
- *In silico* data archiving (c.f. water sample archiving) for subsequent 'historical' interrogation

Natural products

- lake metabolism
- chemical signals of algal community health

DOM characterization

- Organic matter sources
- Impacts on nutrient and contaminant cycling and availability

Progress to date

Project management:

- Equipment installed

HQP Recruitment:

Postdoctoral Fellow - recruiting

PhD – recruiting

Research:

- Testing and validating methods for
 - Volatiles in water
 - Solid Phase Microextraction (SPME) from water
 - Organic/Inorganic mercury determination

Collaborations with other projects ?

Established linkages to:

- Next Generation Solutions to Ensure Healthy Water Resources for Future Generations
- Sub-Arctic Metal Mobility Study (SAMMS) PI Brent Wolfe. OM characterization



Potential linkages :

- Co-Creation of Indigenous Water Quality Tools. Dr. Dawn Martin-Hill, McMaster University (Years 4-7)
- Northern Water Futures



Core needs and contributions to the core ?

Providing Instrumentation:

- Ultra-High Resolution Mass Spectrometry

Core Needs:

- Knowledge Mobilization Team – assistance in structuring and delivery of KM
- Computer Science Team – supporting unknown identification and data pipelines
- Data Team – Management of very large chemical data sets

We can support people wanting to collaborate to apply chemical fingerprinting technologies for water characterization and quality assessment.



Q Exactive Orbitrap - Workhorse

Mass Range

m/z 50-6,000

Max Resolving Power

140,000 @ m/z 200

Max Scan Rate

Up to 20 Hz @ 15,00 Res m/z 200

Mass Accuracy

Internal: < 1 ppm RMS

External: < 3 ppm RMS

under defined conditions

Sensitivity

Full MS: 500 fg Bupirone on column S/N 100:1

SIM: 50 fg Bupirone on column S/N 100:1

Polarity Switching

1 full cycle in <1 sec (1 full +ve and 1 full -ve scan at 35,000 resolution)



Q Exactive HF OrbiTrap – High Mass, High Resolution

Mass Range

m/z 50-8,000

Max Resolving Power

250,000 @ m/z 200

Max Scan Rate

Up to 40 Hz @ 7,500 Res m/z 200

Mass Accuracy

Internal: < 1 ppm RMS
External: < 3 ppm RMS
under defined conditions

High Mass Functionality

Extended Mass range
High mass configuration
Intact Protein Analysis (Mr >1,000,000)



Q Exactive GC – the Newest Dimension

Mass Range

m/z 30–3000

Max Resolving Power

120,000 @ m/z 272

Max Scan Rate

Up to 25 Hz at resolution setting of 15,000
@ m/z 272 under defined conditions

Mass Accuracy

Internal: <1 ppm RMS
External: <3 ppm RMS
under conditions defined in 1 μ L, 100 fg/ μ L
octafluoronaphthalene EI Full MS installation
specification

Robotic Sample Handling

Solid Phase Micro-extraction
Headspace analysis (volatiles, taste and odor)

