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EnviroNote News

EnviroNote 1122 – September 2022

Introducing the QToF Discovery Suite

There is a new chemical registered for use approximately once every six seconds.[1] These chemicals are often untested with respect to their environmental impact and could be recognised as hazards in the future. With such a rapidly changing chemical landscape it can be difficult to keep up.

What is QToF-MS?

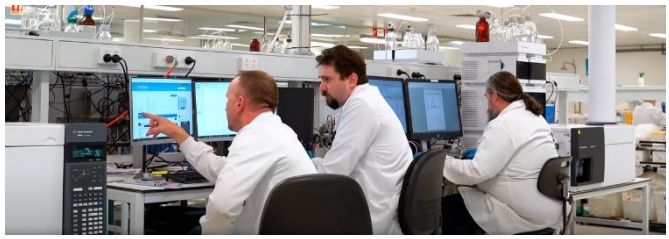
QToF-MS, or 'quadrupole time-of-flight mass spectrometry' is a powerful analytical tool for comprehensive sample characterisation and discovery of new compounds in complex samples. It combines the separating power of liquid or gas chromatography with high resolution, accurate mass tandem mass spectrometry to discriminate between closely related structures and identify previously unknown compounds in complex samples.

Structure elucidation and tentative compound identification is based on highly accurate mass determination – up to four decimal places – and multiple lines of evidence, including retention time, isotope profile, fragmentation pattern and adduct formation. Targeted Screening, Suspect Screening ("Known Unknowns") and Non-Targeted Analysis (NTA) ("Unknown Unknowns") workflows compare the mass spectral fingerprint of a sample to an authentic reference material (if available); to commercial or in-house spectral libraries created from experimental data (e.g. NIST[2]); and/or comparison to large, open-source databases containing thousands of entries, such as the NORMAN Suspect Exchange List[3], or US EPA CompTox Chemicals Dashboard.[4] Results are reported with confidence levels of 2 or 3 on the Schymanski scale.[5] This can be increased to level 1 (the highest confidence) if compared to an authentic reference material.

Our Laboratory

Our Emerging Contaminants laboratory in Brisbane houses state-of-the-art instrumentation, including an Agilent Infinity LC coupled to a 6545 QToF-MS, and an Agilent 7250 GC-QToF-MS. Our highly trained Emerging Contaminants team have a combined 50 years' experience in analytical methods development and mass spectrometry.

Eurofins' QToF Discovery Suite uses cutting-edge technology to expand your contaminated land assessment toolkit.



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What Can QToF-MS Do for You?

- ✓ **Comprehensive sample characterisation**
  Generic extraction protocols and unbiased data collection capture information on the whole sample
- ✓ **Explore the unknown**
  Screen for thousands of compounds in a single test without the need for expensive standards or reference materials. Discover new compounds, metabolites or detect emerging contaminants of concern
- ✓ **Expand your PFAS analysis**
  Complement your existing targeted analysis by exploring PFAS precursors and 'dark matter'.
- ✓ **Retain data, not samples!**
  Digital Data Archiving allows retrospective analysis without the need to re-extract and reanalyse samples

QToF Discovery Suite

Since the launch of the first commercial instrument nearly 25 years ago, QToF-MS has largely remained in the domain of research laboratories. Eurofins is proud to bring this technology to the commercial market in an affordable and accessible format. The QToF-MS Discovery Suite consists of five new test suites tailored to the contaminated land sector:

1. PFAS Characterisation (Compact): Screen for legacy per- and polyfluoroalkyl substances (PFAS), precursors and dead end products in water, soil, sediment and aqueous film-forming foams (AFFF). Suspect screening of high-resolution data against a library containing ~100 PFAS compounds, created from authentic reference materials. Use this test for site investigations, simple source tracking, AFFF characterisation, or precursor identification.

2. PFAS Characterisation (Comprehensive): Need to dig a little deeper? Have a complex site investigation? Our comprehensive PFAS characterisation uses multiple sample extraction strategies to capture anionic, cationic and zwitterionic compounds.[5] Data is screened against a large database containing >5000 PFAS and related compounds, and your report contains an interpretative analysis of your PFAS profile from our expert team.

3. Contaminant Screening: Suspect screening of sediment, soil, water and air samples for thousands of contaminants including pharmaceuticals and personal care products; forensic compounds, toxins, drugs and their metabolites; pesticides, industrial chemicals and surfactants; petrochemicals; food flavours and fragrances; human and plant metabolites

4. Targeted Screening & Product Verification:
Identify suspect contaminants, confirm active constituents, or investigate potential product failures in consumer products or impacted environmental samples. Unequivocal compound identification (confidence level 1)[6] and quantitative data can be provided on request.

5. Environmental Forensics: Work with our team of highly experienced analytical chemists to design and execute a bespoke workflow for your most complex samples. We can provide technical guidance on sampling design and analysis and summarise the results in a custom report tailored to you.

LEARN MORE! – CLICK TO REGISTER FOR OUR WEBINAR

or Email EmergingContaminantsAUS@eurofins.com

References:
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[2] NIST Mass Spectrometry Data Center. Available: https://chemdata.nist.gov/dokuwiki/doku.php
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[4] https://comptox.epa.gov/dashboard/
[5] Nickerson et al. (2020) Environ Sci Technol. 54(8):4952-62. DOI: 10.1021/acs.est.0c00792
[6] Schymanski, E.L *et al*. (2014) Environ Sci Technol 48: 2097-98. DOI: 10.1021/es5002105

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