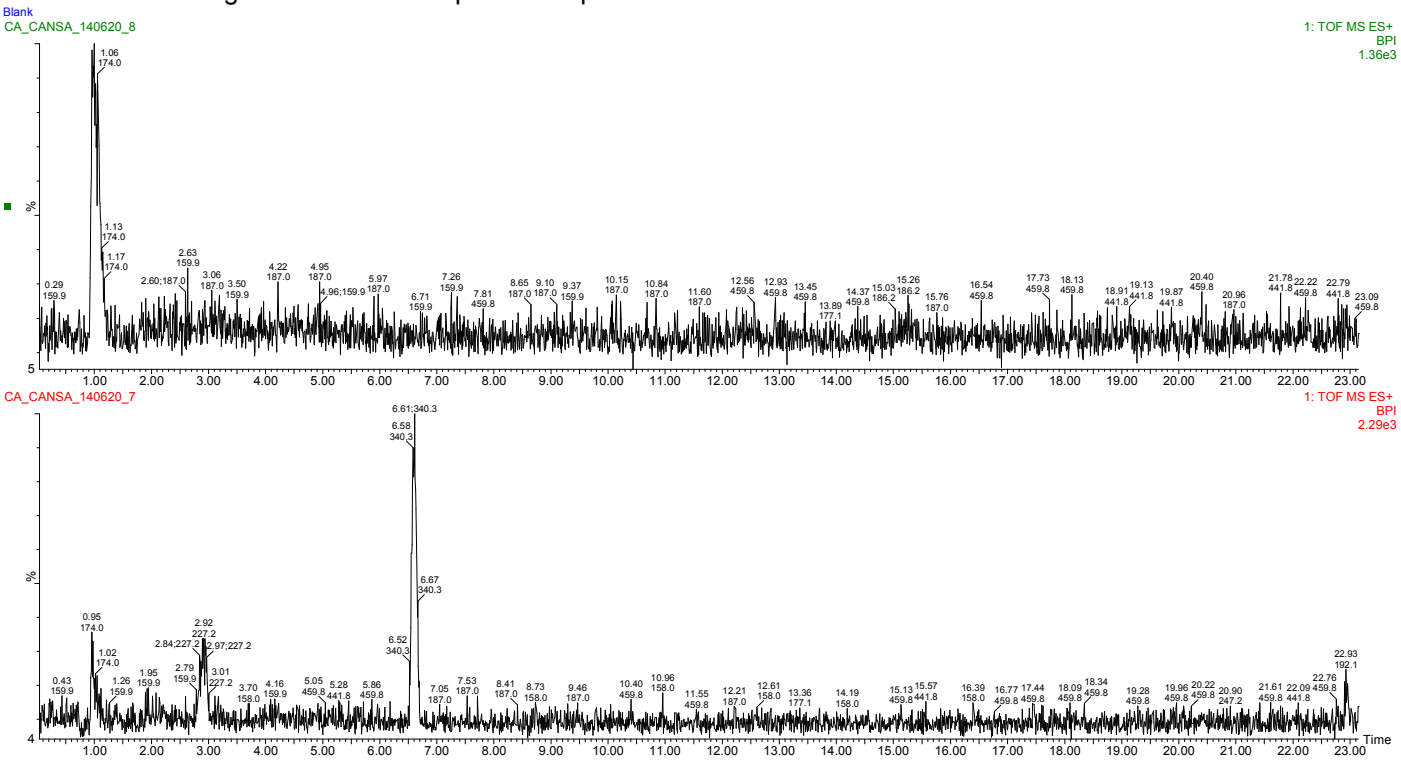
Requested: C. Albrecht (CANSA)
Report No: CA_CANSA_140626
Instrument: Waters Synapt G2
Introduction: Waters UPLC Source: Electrospray positive

Samples: The supplied water sample was concentrated 1000 fold on a SPE C18 cartridge and injected onto the LCMS system.

Solvent A1: 1% formic acid
Solvent B1: acetonitrile
Column:Waters BEH C18, 2.1x100mm, 1.7um

Total ion chromatogram of Blank on top and sample at the bottom



Helpful hints in interpreting MS results from Masslynx data

1. The ionization mode is indicated in the top right hand corner of spectra:

ESMS and LCMS lab (more suitable for non-volatile compounds):

ES+ = Electrospray positive: Typically a M+H or M+Na ion is observed
ES-= Electrospray negative: Only used for molecules that can be negatively charged like phenols and carboxylic acids, typically a M-H or M+Cl is observed

APCI = Atmospheric pressure chemical ionization: A softer technique for non-polar molecules – rarely used

GCMS (more suitable for smaller and volatile compounds):

MS Unit
JC Smuts building., Private Bag X1, Matieland, 7602, South Africa
Tel: +27 21 808 5825 Fax: +27 21 808 5863 lcms@sun.ac.za www.sun.ac.za/caf

EI = Electron impact, this is a harsher ionization technique. A fragmentation pattern and M^+ is sometimes observed

2. The retention time is given on the top left hand corner of a spectrum after the file name in brackets for GCMS and LCMS results.

3. Only the TOF instruments (GCT and Synapt) are capable of High resolution, samples should be pure and free of salts and buffers. Most journals require that the ppm deviation from the theoretical mass should be less than 5 ppm or in the case of very small molecules it should differ by less than 2 mDa. The iFit Confidence % gives an indication of how well the isotope pattern correlates to the theoretical pattern.

4. Advanced MS analysis techniques (MSMS, ion mobility and high resolution LCMS and LCMSMS analysis) require day bookings.

5. Mass spectrometry is not a universal technique, especially the atmospheric ionization techniques (ESI and APCI) give no representation of the purity of compounds: different compounds have different ionization potentials under different conditions.

6. ASAP probe: This is a solids technique that uses APCI to ionize molecules from the tip of a melting point tube. This technique is labour intensive and time consuming and will only be used as last resort for unsoluble and unstable molecules. The cost is the same as for LCMS analysis.

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2. All data and/or samples provided by the Client will be treated as confidential.
3. The Analysis Report prepared by SU shall become the property of the Client after payment.
4. Although the greatest care is taken by SU during analysis, SU accepts no responsibility for the loss of any work, samples or data provided by the Client.
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