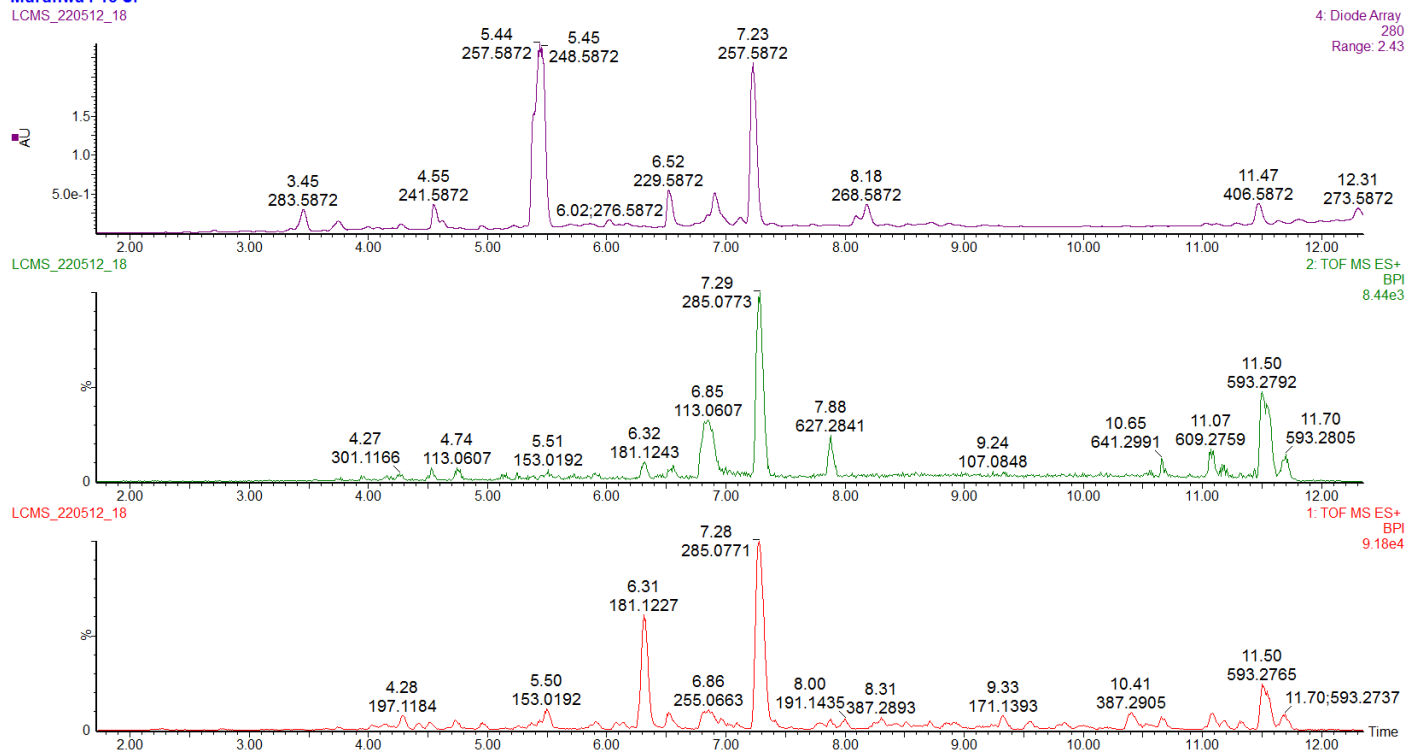


Requested: Murunwa Madzinga
 c/o Prof Namrita Lall
 University of Pretoria
 Report No: MurunwaMadzinga_UP_220607
 Instrument: Waters Synapt G2, ESI probe, ESI Pos/Neg, Cone Voltage 15 V

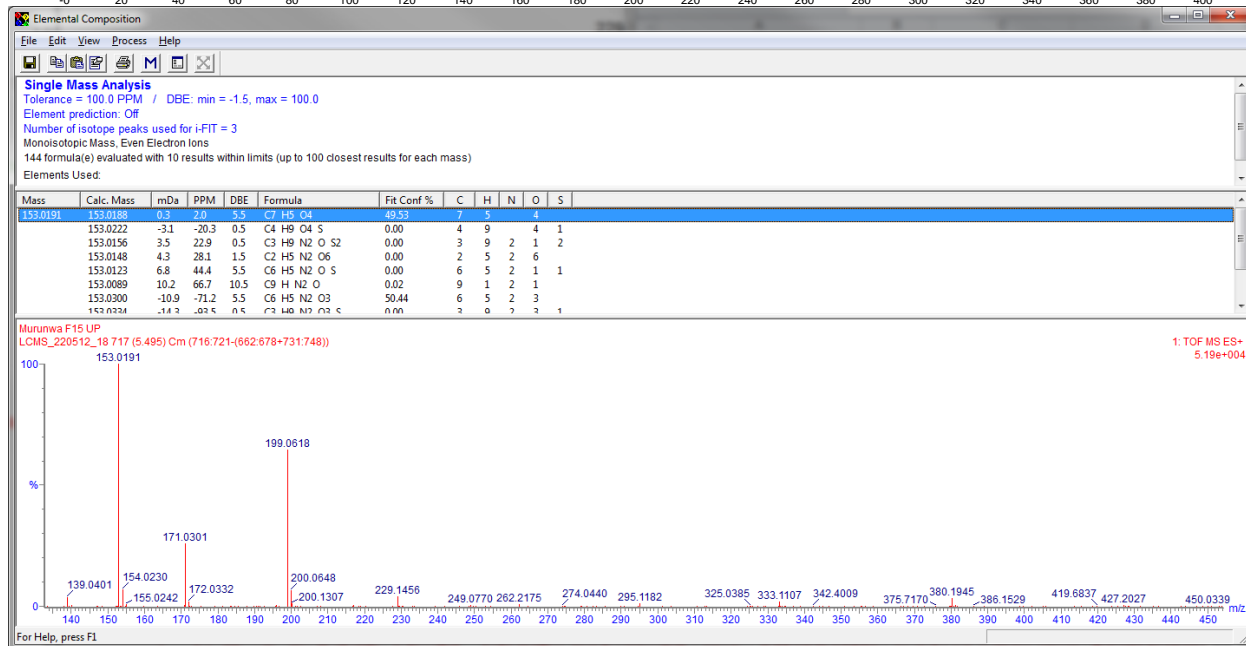
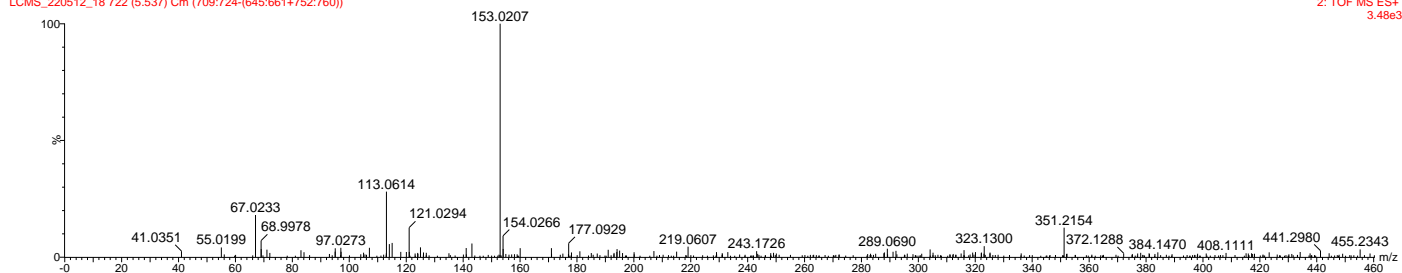
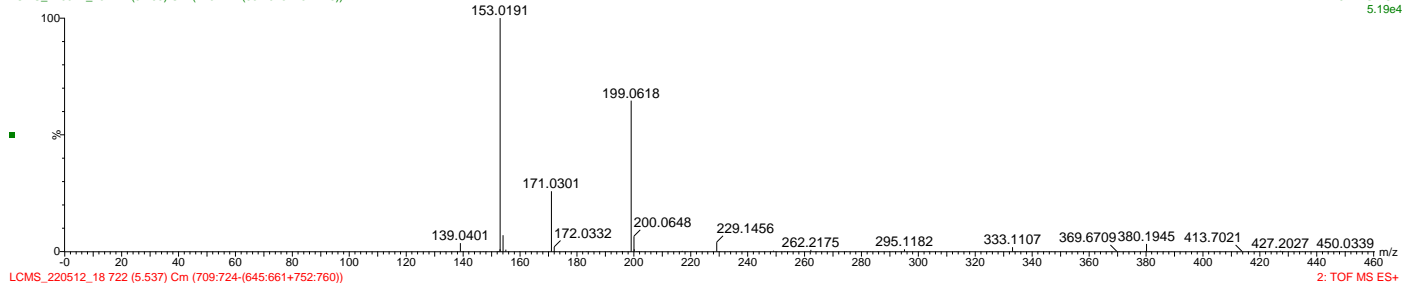
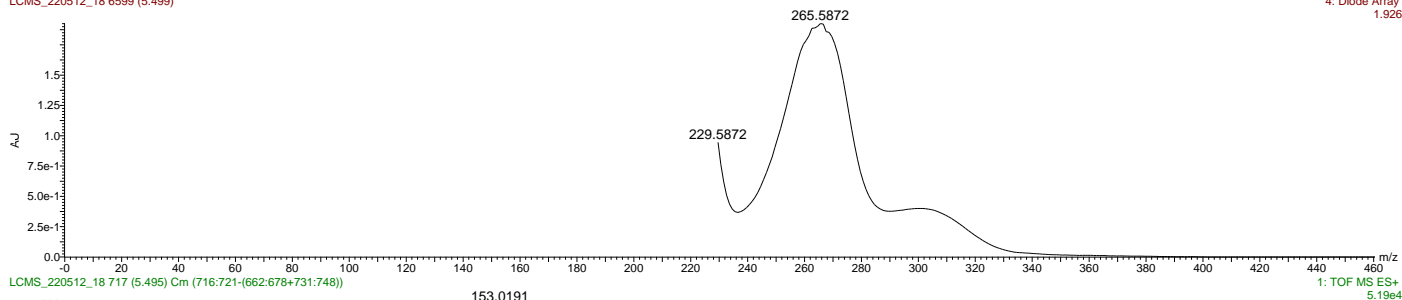
Murunwa F15 UP
 LCMS_220512_18



MS Unit

JC Smuts building., Private Bag X1, Matieland, 7602, South Africa

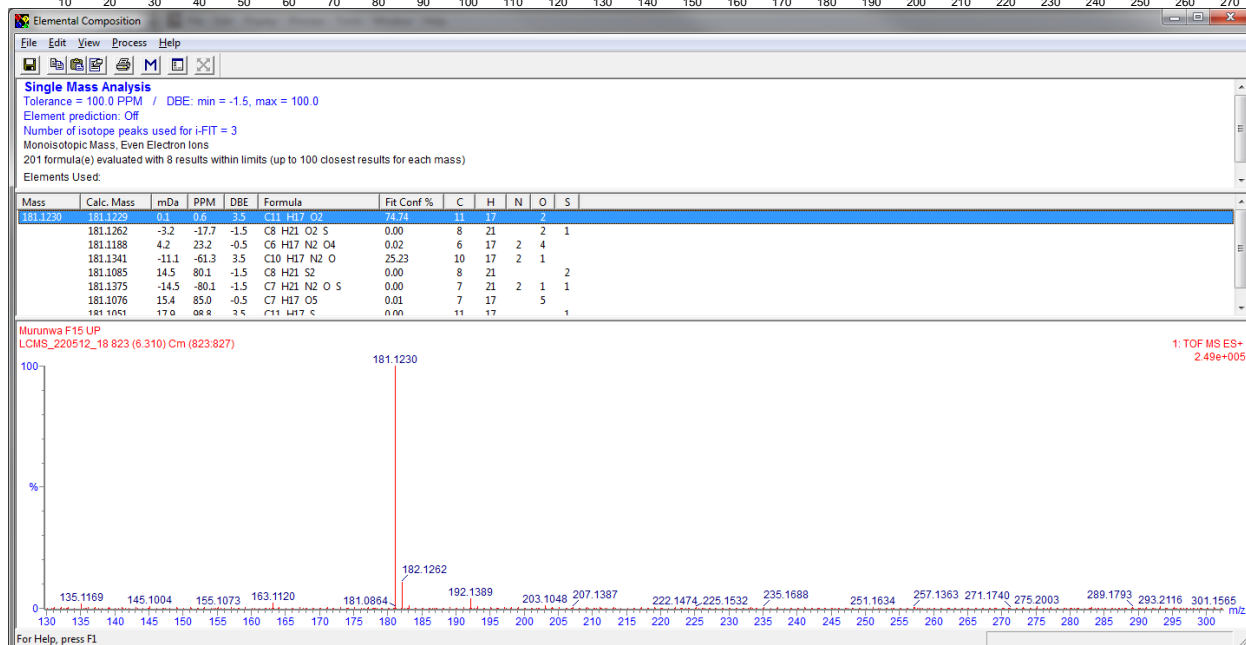
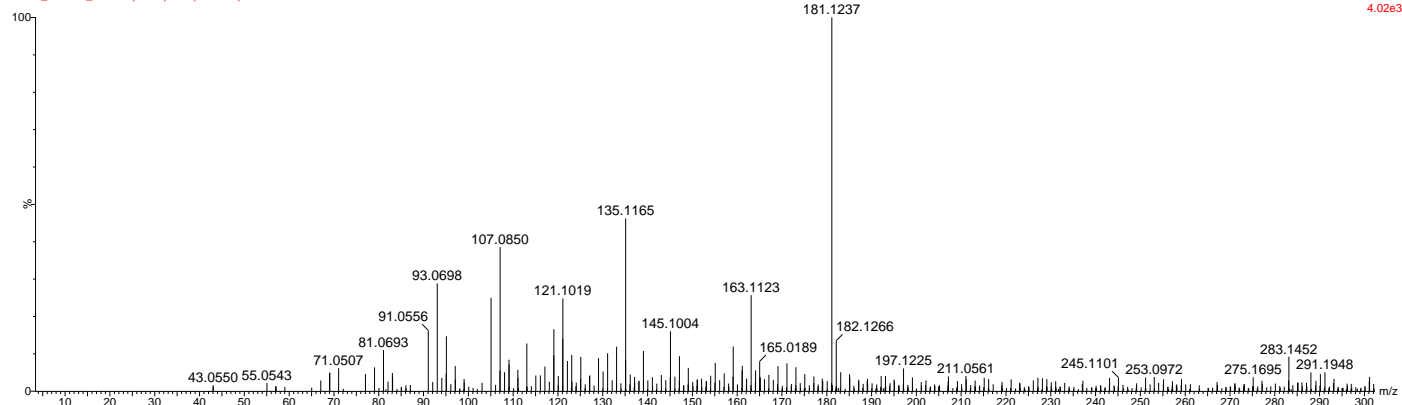
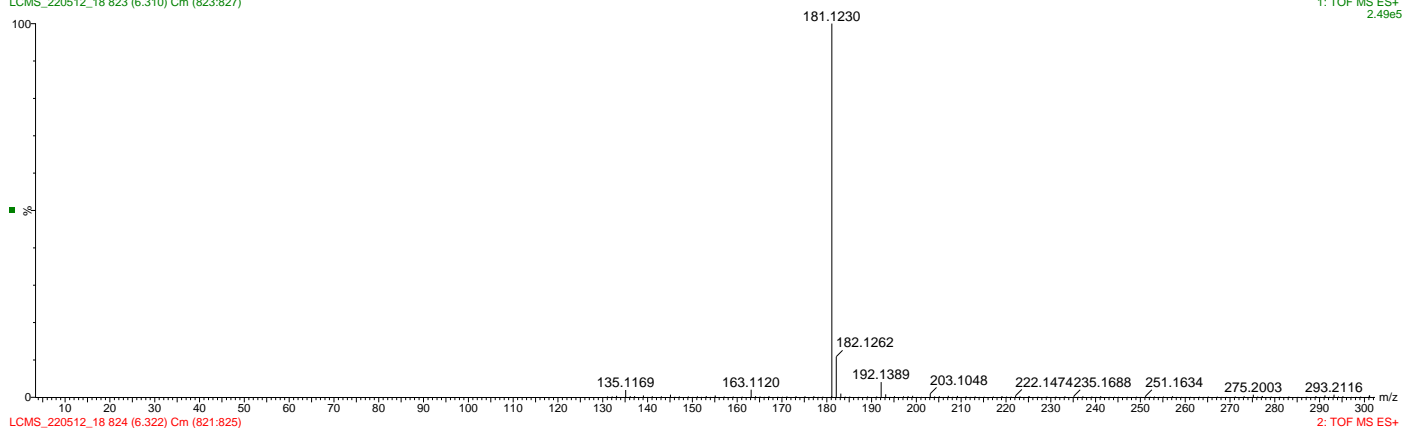
Tel: +27 21 808 5825 Fax: +27 21 808 5863 lcms@sun.ac.za www.sun.ac.za/caf



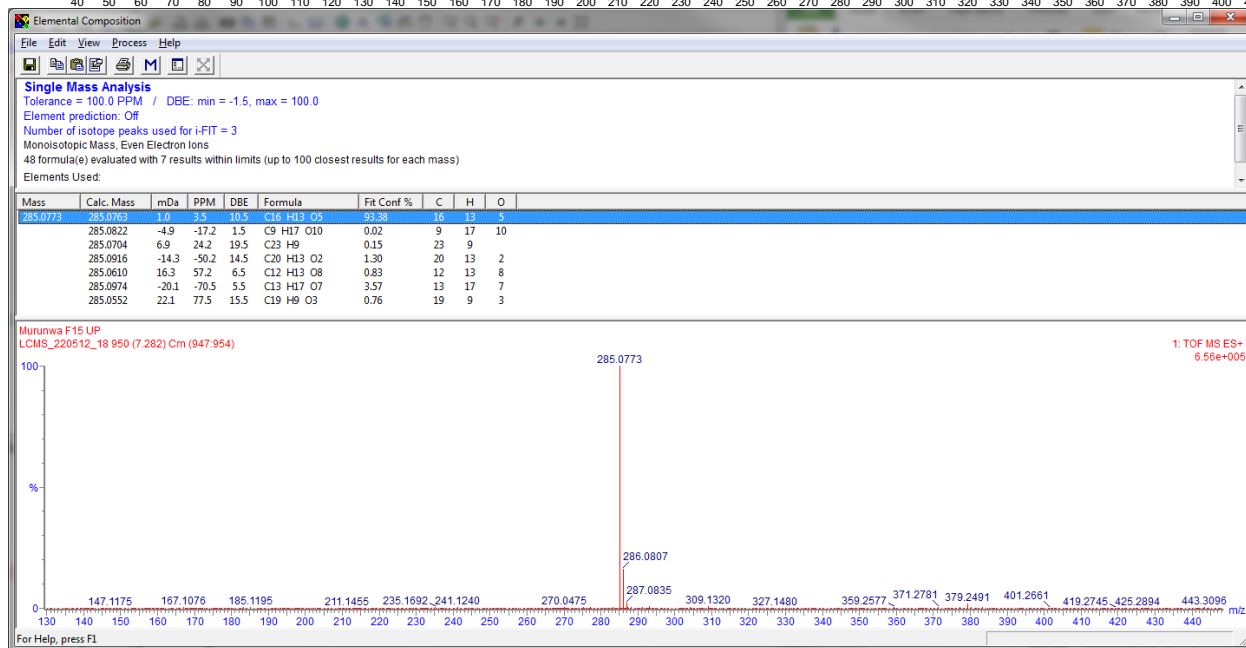
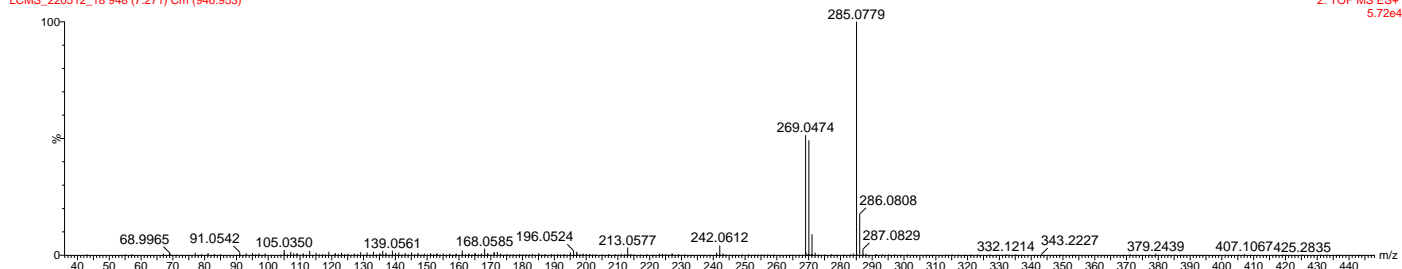
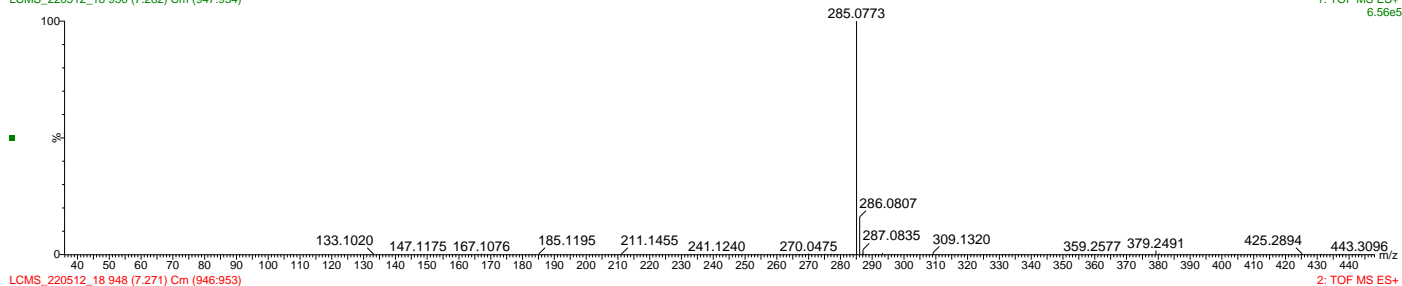
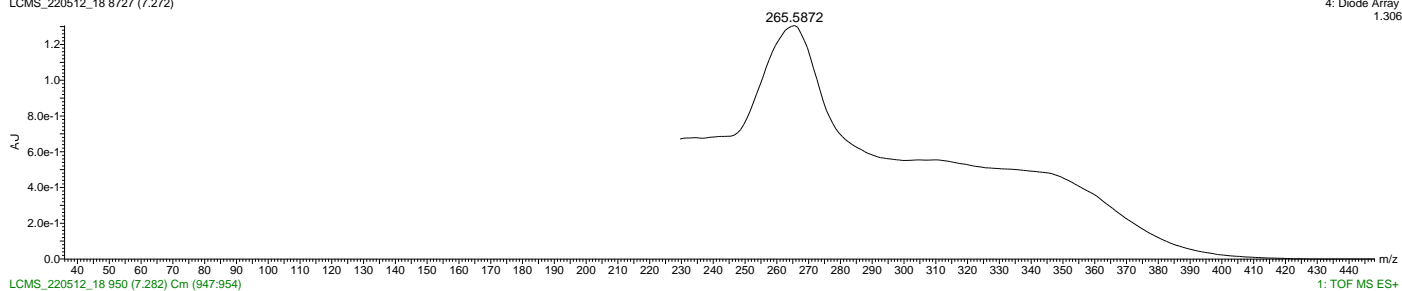
Gentisic/Protocatechuic acid

Murunwa F15 UP

LCMS_220512_18 823 (6.310) Cm (823:827)

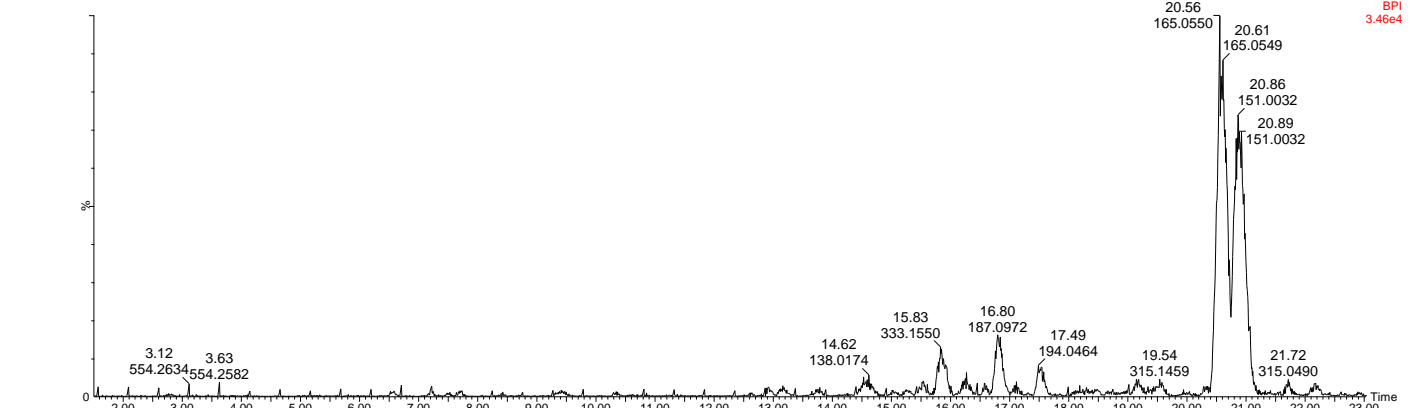
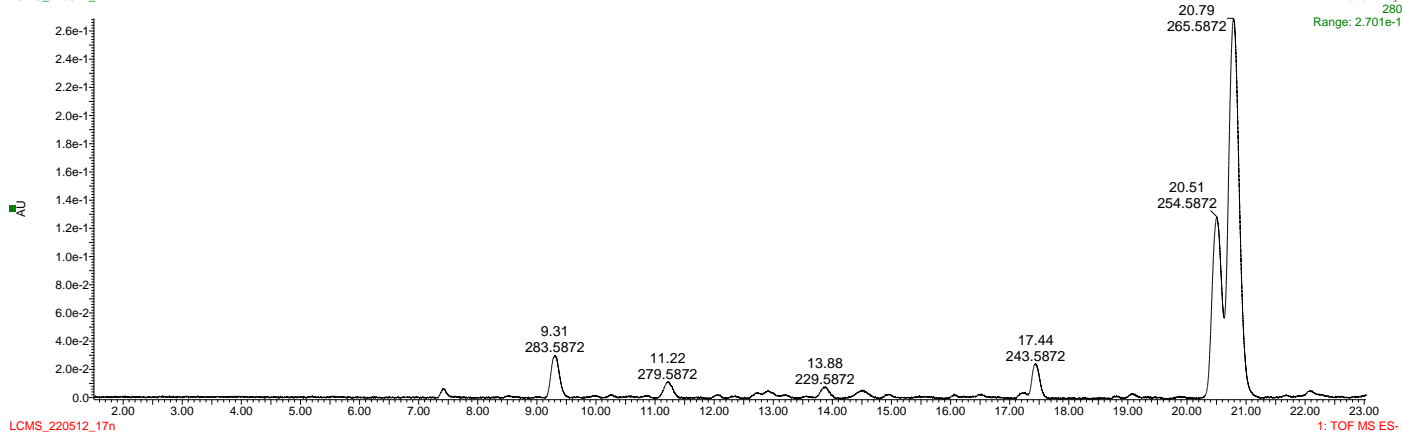


Unknown, no UV absorbance at 280nm

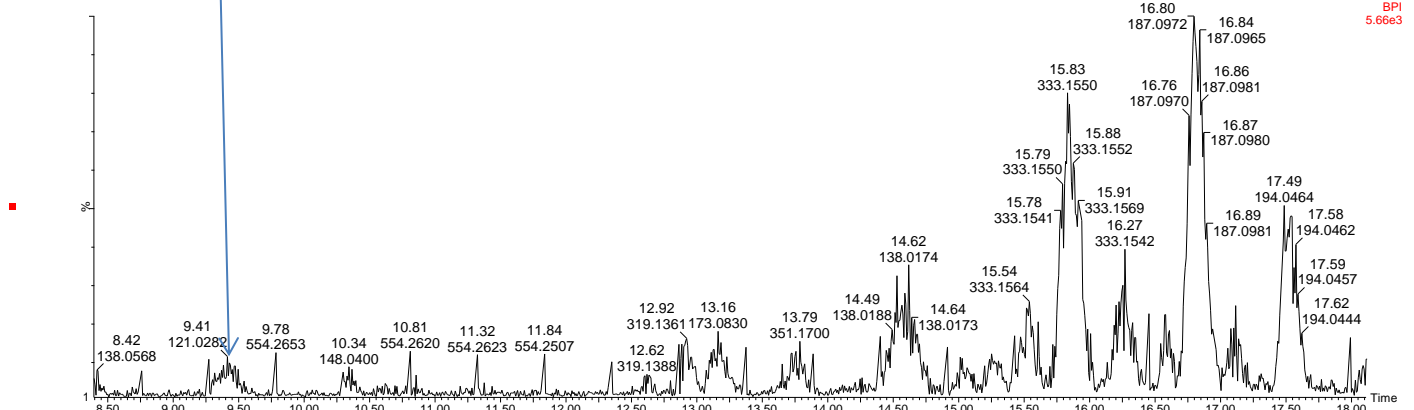
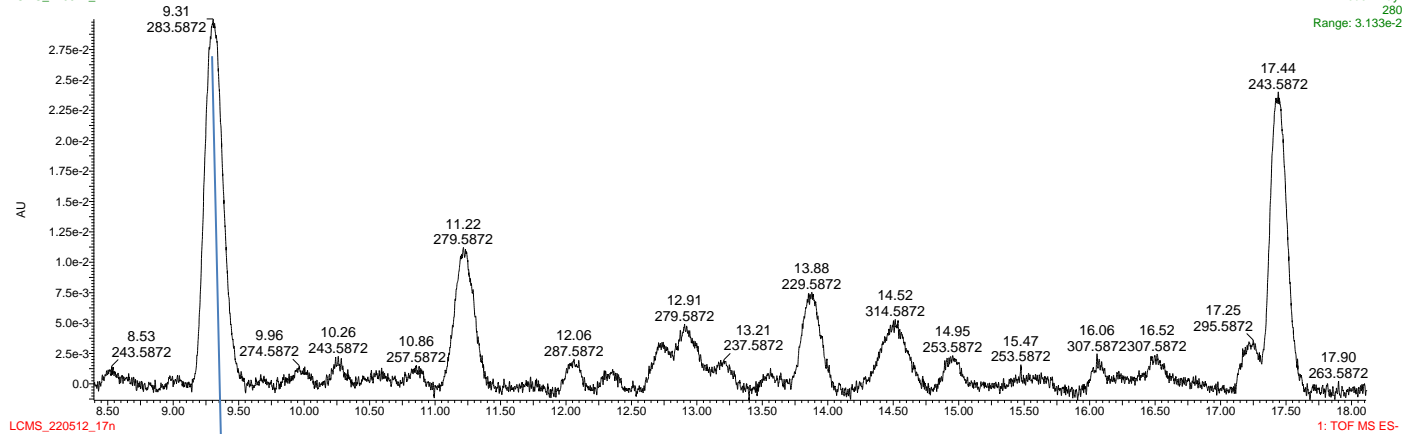


Sakuranetin tentative ID

Murunwa F15 UP
LCMS_220512_17n



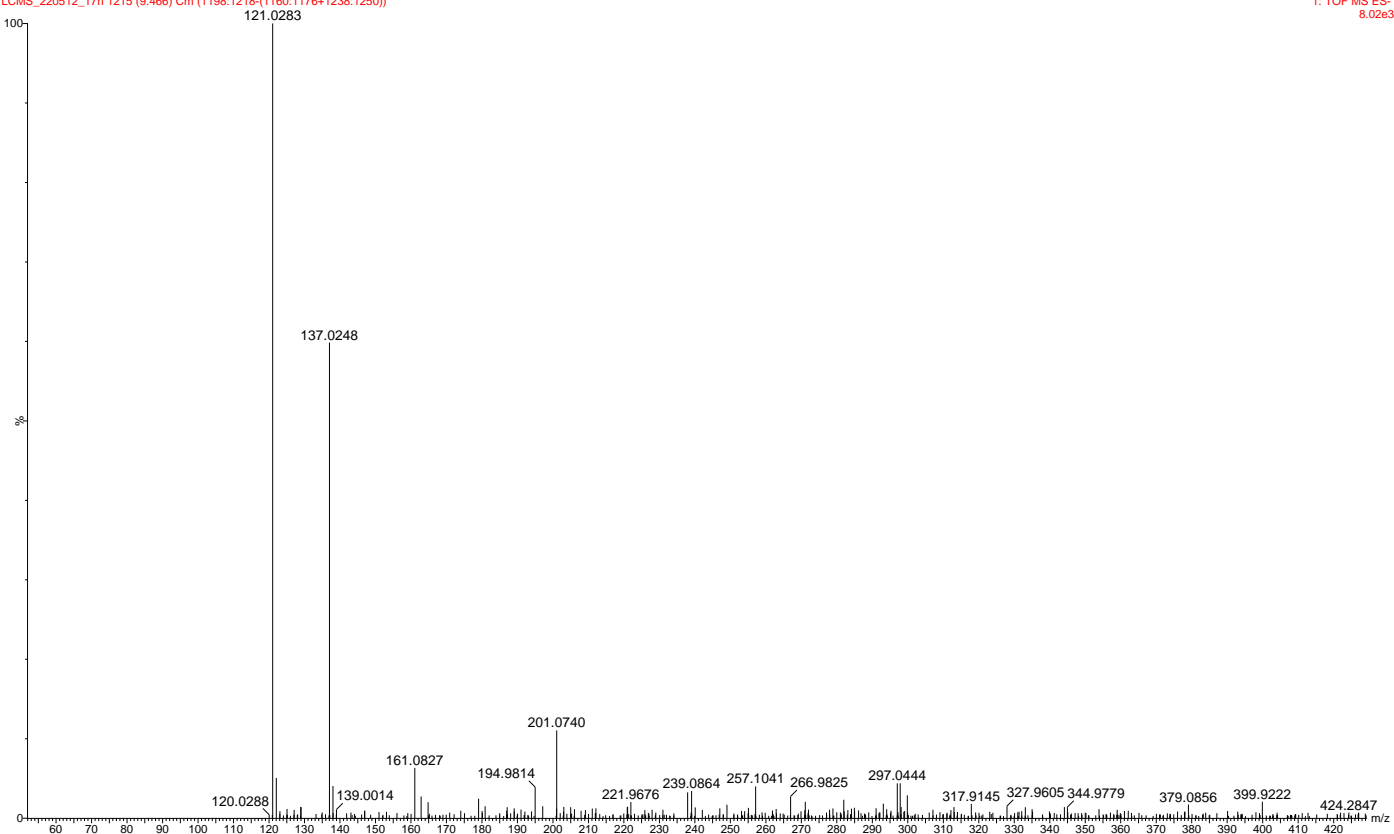
Murunwa F15 UP
LCMS_220512_17n



Murunwa F15 UP

LCMS_220512_17n 1215 (9.466) Cm (1198:1218-(1160:1176+1238:1250))

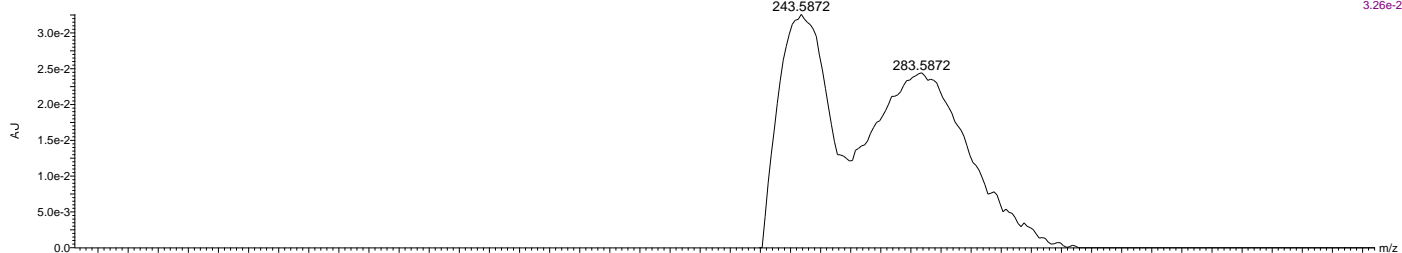
1: TOF MS ES-
8.02e3



Murunwa F15 UP

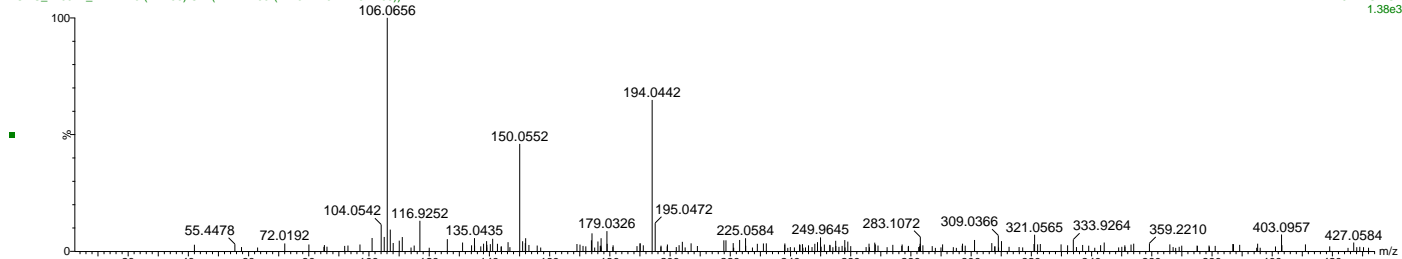
LCMS_220512_17n 20922 (17.437)

4: Diode Array
3.26e-2



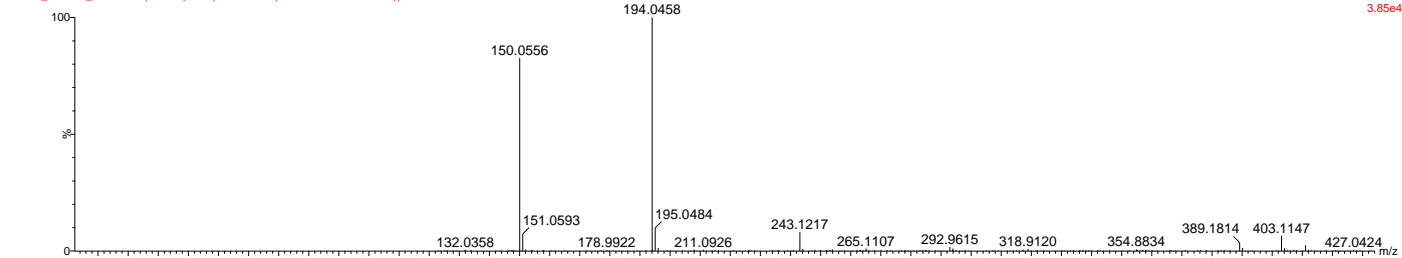
LCMS_220512_17n 2245 (17.483) Cm (2244:2255-(2223:2226+2279:2289))

2: TOF MS ES-
1.38e3



LCMS_220512_17n 2245 (17.479) Cm (2245:2263-(2211:2225+2283:2298))

1: TOF MS ES-
3.85e4



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):

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 insoluble and unstable molecules. The cost is the same as for LCMS analysis.

Standard Terms and Conditions

1. Ownership of the data and/or samples provided by the client shall remain so vested.
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.
5. Data files will not be kept for longer than one week after delivery of the results to the Client.
6. (Please advise the laboratory staff within one week after results have been received if any additional analysis or processing of data is required. It remains the responsibility of our Clients to make proper backups of data.)
7. SU and all its employees shall in no event be liable for loss of profits or for incidental, special or consequential damages, whether direct or indirect, arising out of or in connection with the use of the Analysis Report.
8. In the event of gross negligence on the side of SU, SU shall only be liable for the contract value.
9. SU does not warrant or make any representations regarding the use, validity, accuracy, or reliability of the Analysis Report.
10. SU shall be under no obligation to disclose proprietary analysis methodologies.