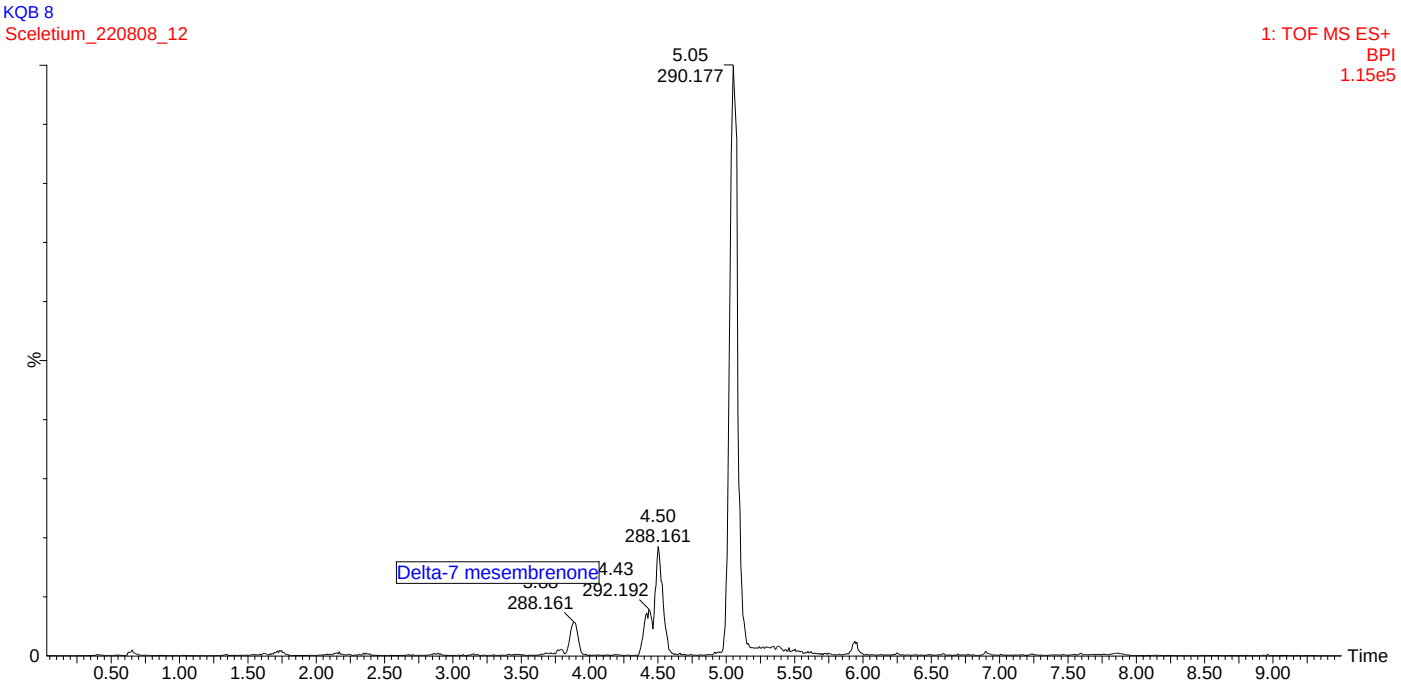
Requested: Lizande Kellerman
Report No: LK_Kellquin_Sceletium_220809
Instrument: Waters Synapt G2, ESI probe, ESI Pos, Cone Voltage 15 V

Sample preparation: 0.5 g accurately weighed out and extracted with 10 ml methanol. After centrifugation, two dilutions were performed- 10x and 100x in glass vials ready for analysis by lcms.

Total ion chromatogram:



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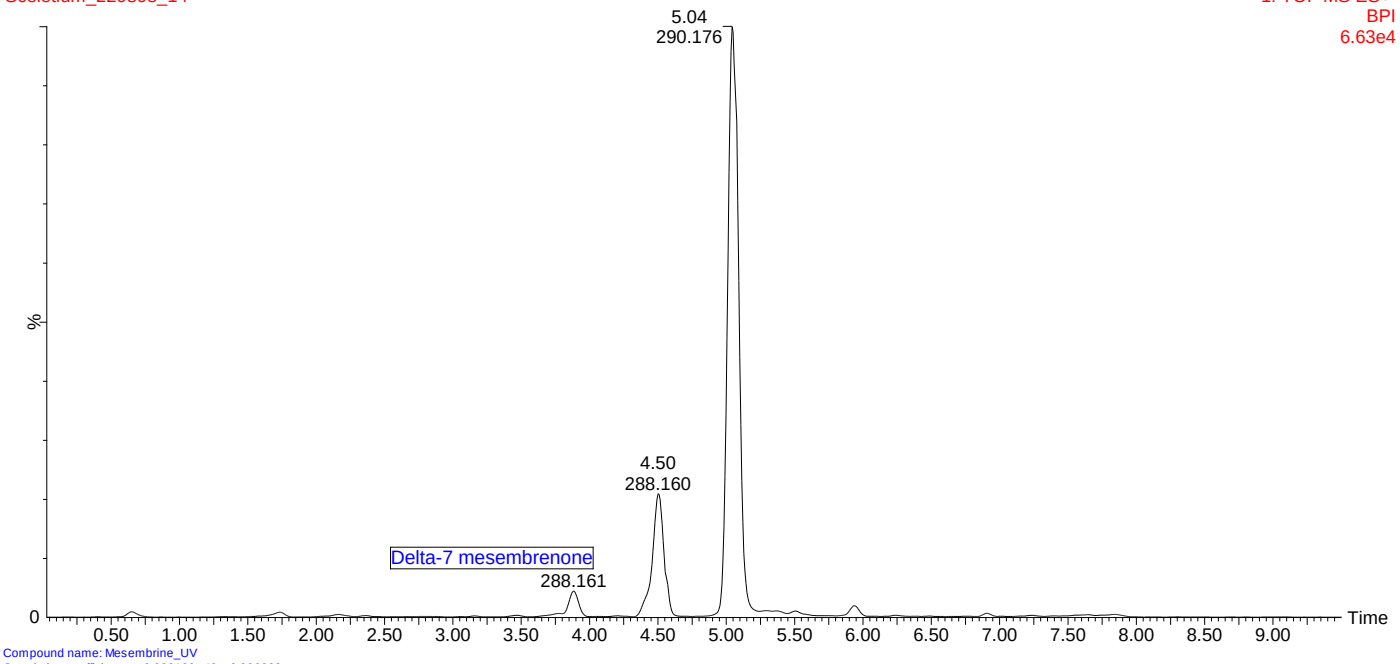
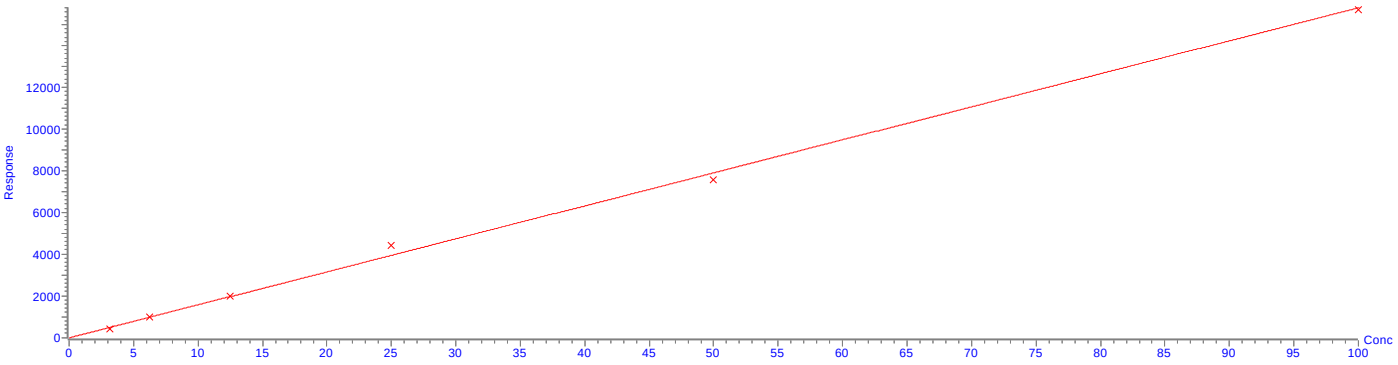
KQB 12
Sceletium_220808_14

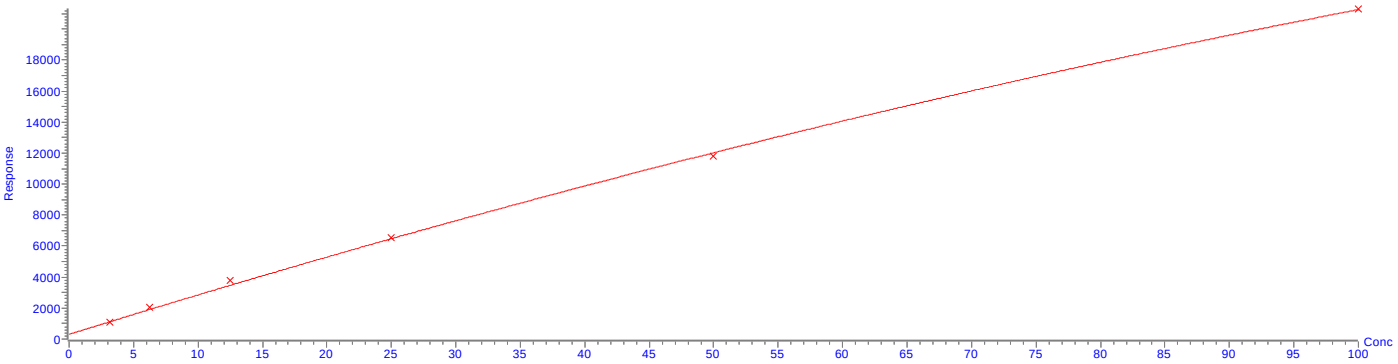
1: TOF MS ES+
BPI
6.63e4



Compound name: Mesembrine_UV
Correlation coefficient: r = 0.998190, r^2 = 0.996383
Calibration curve: 158.363 * x + -22.9333
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



Compound name: Mesembrine
Coefficient of Determination: R^2 = 0.999196
Calibration curve: -0.496776 * x^2 + 259.133 * x + 308.25
Response type: External Std, Area
Curve type: 2nd Order, Origin: Include, Weighting: Null, Axis trans: None



Results:

Quantify Sample Summary Report

Printed Tue Aug 09 12:31:12 2022

Sample Name: Sceletium_220808_12 Sample ID: KQB 8

	#	Name	Trace	RT	Conc. mg/kg	% (m/m)
1	1	delta-7-mesembrenone	288	3.65	400.00	0.04
2	2	Mesembrenol	290			0.00
3	3	Mesembranol	292	4.43	747.16	0.07
4	4	Mesembrenone	288	4.51	1254.10	0.13
5	5	Mesembrine	290	5.05	7208.51	0.72
7	7	Sceletium_A4_1	325	5.51	65.55	0.01
8	8	Epimesembranol	292	5.31	478.13	0.05
9	9	Sceletium A4 _2	325			0.00
10	10	O-Demethylmesembrenone	274	3.47	35.60	0.00
11	11	O-Demethylmesembrine	276	3.92	46.28	0.00
12	12	Dehydrojoubertamine	262	5.17	16.58	0.00
13	13	O-acetylmesembrenol	332			0.00
14	14	Epimesembrenol	290			0.00
					Total	1.03

Quantify Sample Summary Report

Printed Tue Aug 09 12:31:12 2022

Sample Name: Sceletium_220808_14 Sample ID: KQB 12

	#	Name	Trace	RT	Conc. mg/kg	% (m/m)
1	1	delta-7-mesembrenone	288	3.56	221.00	0.02
2	2	Mesembrenol	290			0.00
3	3	Mesembranol	292	4.43	255.65	0.03
4	4	Mesembrenone	288	4.5	1118.71	0.11
5	5	Mesembrine	290	5.04	5803.08	0.58
7	7	Sceletium_A4_1	325	5.51	59.73	0.01
8	8	Epimesembranol	292	5.3	216.69	0.02
9	9	Sceletium A4 _2	325			0.00
10	10	O-Demethylmesembrenone	274	3.46	23.42	0.00
11	11	O-Demethylmesembrine	276	3.92	33.51	0.00
12	12	Dehydrojoubertamine	262	5.18	25.08	0.00
13	13	O-acetylmesembrenol	332			0.00
14	14	Epimesembrenol	290			0.00
					Total	0.78

Conclusion

Results are expressed as a relative concentration to the response of mesembrine.

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

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