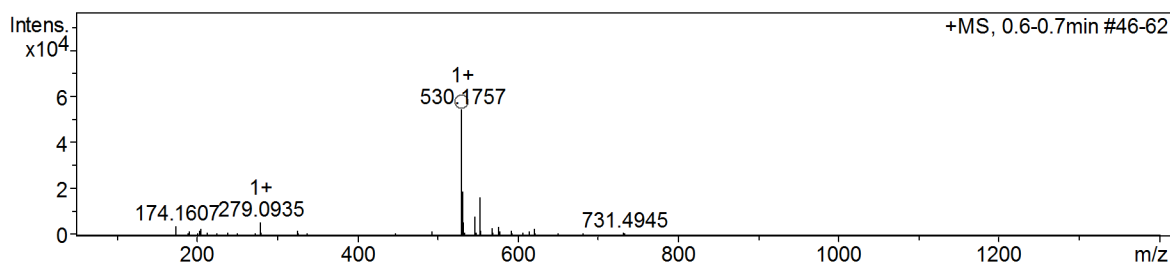




Sample-ID	m_cal_665	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_665_524781_1_01_21535.d	Acquisition Date	4/22/2016 5:13:44 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.7min #46-62



#	m/z	I %
1	174.1607	7.6
2	204.0277	3.5
3	205.0244	5.1
4	279.0935	10.4
5	326.2106	4.0
6	493.3998	2.8
7	530.1757	100.0
8	531.1783	35.0
9	532.1784	10.9
10	546.1479	15.4
11	547.1499	5.9
12	552.1578	30.5
13	553.1604	11.0
14	554.1590	3.4
15	568.1305	5.7
16	576.2247	7.0
17	577.2255	2.8
18	592.1463	3.6
19	614.1305	2.9
20	620.1447	5.1

Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C32 H29 N1 O3 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	530.1757	530.1760	0.50	0.0067	C32H29NNaO3S	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF