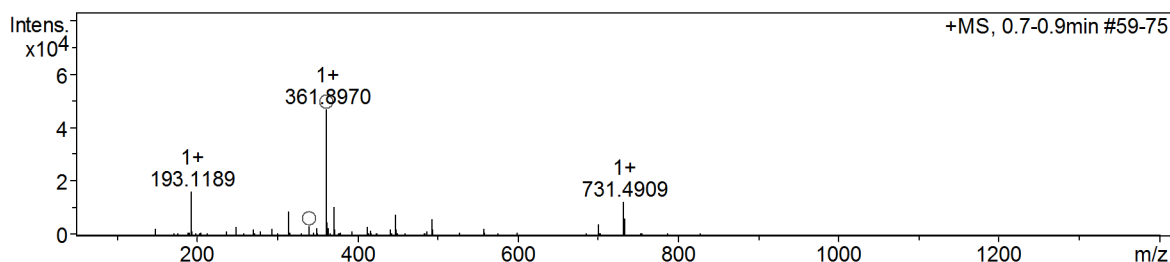




Sample-ID	m_cal_556_sm	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_556_sm_527155_25_01_24255.d	Acquisition Date	6/2/2016 11:05:07 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	149.1278	5.5
2	193.1189	34.6
3	249.1768	6.8
4	293.1719	5.3
5	314.9509	18.9
6	339.9152	7.6
7	349.2341	5.9
8	361.8970	100.0
9	362.9002	10.4
10	363.8951	5.9
11	371.2168	22.5
12	413.1056	6.1
13	413.2681	6.8
14	447.3450	16.7
15	448.3487	4.9
16	493.3998	12.6
17	557.3486	5.1
18	700.8006	8.8
19	731.4909	26.6
20	732.4951	13.8

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		C8 H6 I1 N1 O4 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	339.9152	339.9135	5.00	0.0063	C8H7INO4S	M+H	1.0078
1	361.8970	361.8954	4.40	0.0022	C8H6INNaO4S	M+Na	22.9898

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