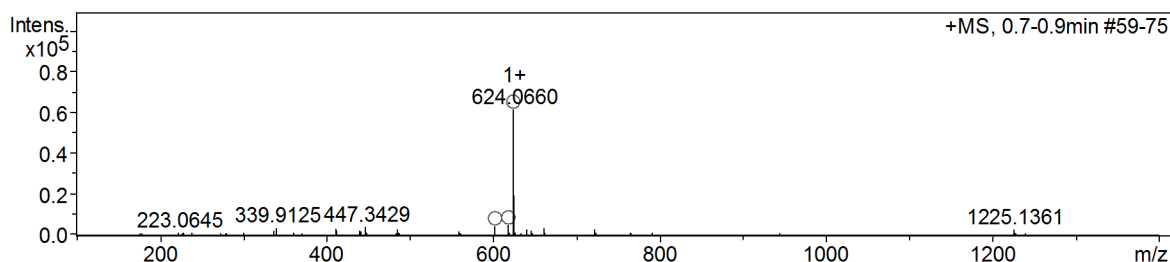




Sample-ID	m_cal_556	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_556_517792_22_01_13861.d	Acquisition Date	1/28/2016 10:44:13 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	337.0747	3.8
2	339.9125	6.3
3	411.0932	5.4
4	413.2660	4.0
5	439.9424	3.4
6	441.2965	2.9
7	447.3429	6.6
8	485.1113	4.4
9	559.1300	3.3
10	602.0834	7.3
11	619.1111	8.2
12	624.0660	100.0
13	625.0695	32.0
14	626.0686	10.0
15	640.0418	4.5
16	646.0487	3.6
17	661.1584	6.4
18	722.5260	4.3
19	1225.1361	4.4
20	1226.1409	2.6

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		C28 H28 I1 N1 O4 S1				Adduct(s): H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	602.0834	602.0857	3.70	0.0124	C28H29INO4S	M+H	1.0078
1	624.0660	624.0676	2.50	0.0013	C28H28INNaO4S	M+Na	22.9898
1	619.1111	619.1122	1.70	0.0542	C28H32IN2O4S	M+H4N	18.0344

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