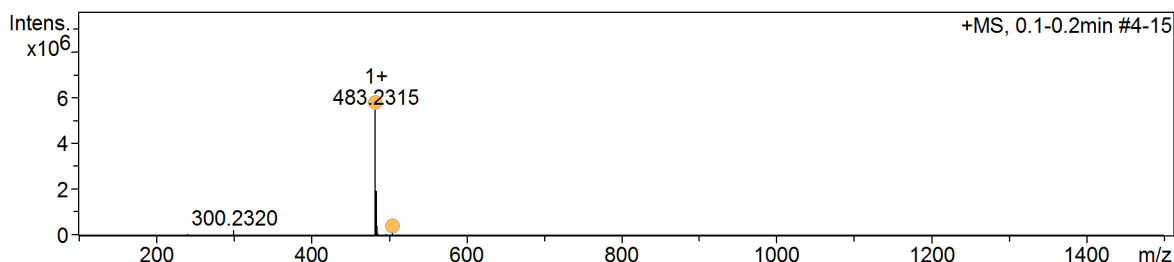




Sample-ID	b_pa1_16_050	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_050_523179_GB6_01_623.d	Acquisition Date	3/30/2016 3:08:31 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.1-0.2min #4-15



#	m/z	I %
1	222.1850	0.5
2	224.2006	0.3
3	240.1956	1.4
4	258.1617	0.3
5	296.2371	0.3
6	300.2320	4.4
7	301.2353	0.9
8	316.2268	0.6
9	483.2315	100.0
10	483.3929	0.9
11	483.5093	0.8
12	483.9331	0.3
13	484.2342	35.7
14	485.2325	8.6
15	486.2328	1.8
16	487.2340	0.2
17	497.2464	1.4
18	498.2495	0.3
19	505.2128	1.8
20	506.2159	0.5

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		C27 H34 N2 O4 S1				Adduct(s):	H, Na, NH4, radical
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	483.2315	483.2312	0.70	0.0234	C27H35N2O4S	M+H	1.0078
1	505.2128	505.2131	0.70	0.0425	C27H34N2NaO4S	M+Na	22.9898

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