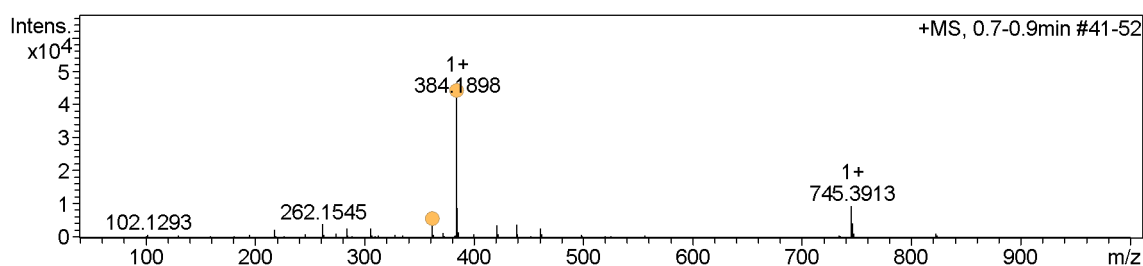




Sample-ID	pazrjk_PhedaA_05	Lab	C13
Submitter	Rafal Kopiasz (pazrjk)	Supervisor	Cameron Alexander (pczca1)
Analysis Name	pazrjk_PhedaA_05_643562_52_01_124541	Acquisition Date	2/3/2023 3:42:50 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #41-52



#	m/z	I %
1	218.2124	5.3
2	262.1545	9.4
3	274.2737	2.6
4	284.1377	6.2
5	306.1453	6.6
6	362.2069	8.3
7	372.1874	3.2
8	384.1898	100.0
9	385.1921	21.5
10	386.1942	3.5
11	400.1638	2.4
12	421.2817	8.7
13	422.2843	2.4
14	439.1044	9.1
15	440.1057	2.3
16	461.0848	6.5
17	745.3913	22.7
18	746.3940	10.3
19	747.3968	2.6
20	822.2860	2.9

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 C₁₉H₂₇N₃O₄ **Adduct(s):** H, Na, NH₄, C₃H₅N₂, radical

#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	362.2069	362.2074	1.40	0.0144	C ₁₉ H ₂₈ N ₃ O ₄	M+H	1.0078
1	384.1898	384.1894	1.10	0.0043	C ₁₉ H ₂₇ N ₃ NaO ₄	M+Na	22.9898

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