Compound Spectrum SmartFormula Report

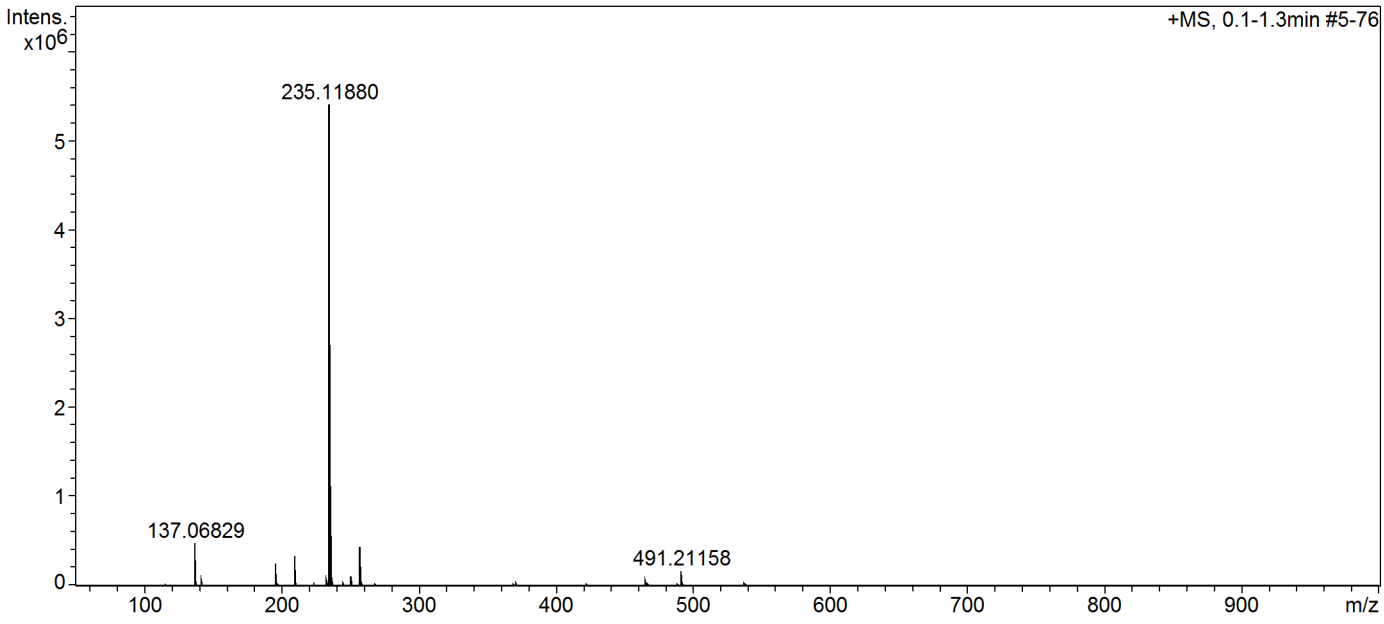
Analysis Info

Analysis Name	D:\Data\AC\AHP\Conrads\CC-273-2-ESI-pos-1.d	Acquisition Date	1/19/2022 9:49:29 AM
Method	ESI-kleine Massen - 2.m	Operator	tof user
Sample Name	CC-273-2-pos-1	Instrument	maXis II 1828979.22385
Comment	MeCN		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

+MS, 0.1-1.3min #5-76



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#	m/z	Res.	S/N	I	I %	FWHM
1	116.14319	27875	441.6	16927	0.3	0.00417
2	137.06829	29593	12606.0	478280	8.9	0.00463
3	138.07159	28765	677.1	25707	0.5	0.00480
4	142.13364	29561	2055.0	75595	1.4	0.00481
5	143.13695	29758	163.7	5978	0.1	0.00481
6	170.16489	33293	188.8	6683	0.1	0.00511
7	184.18053	34555	334.5	11758	0.2	0.00533
8	185.11447	33147	267.9	9416	0.2	0.00558
9	196.18049	33673	7049.8	247658	4.6	0.00583
10	197.18375	33166	839.7	29481	0.5	0.00595
11	198.19613	34187	609.0	21382	0.4	0.00580
12	210.17099	34133	9669.3	337259	6.2	0.00616
13	211.17410	33510	1072.3	37373	0.7	0.00630
14	217.10431	35776	185.3	6391	0.1	0.00607
15	224.09450	34828	1153.7	39597	0.7	0.00643
16	224.21174	36076	538.6	18491	0.3	0.00621
17	226.09153	35302	378.8	12922	0.2	0.00640
18	233.10290	35775	1759.2	60638	1.1	0.00652
19	234.10772	25313	247.7	8564	0.2	0.00925
20	235.11880	24833	156134.6	5403803	100.0	0.00947
21	235.20836	69535	1693.4	58605	1.1	0.00338
22	235.27343	21938	2377.6	82286	1.5	0.01072
23	235.29315	50021	1381.3	47807	0.9	0.00470
24	235.30598	77996	309.7	10718	0.2	0.00302
25	235.32346	77022	719.4	24897	0.5	0.00306
26	235.33875	106668	228.9	7921	0.1	0.00221
27	235.35293	77412	252.8	8749	0.2	0.00304
28	235.37836	75859	1255.4	43448	0.8	0.00310
29	235.39228	77242	241.4	8355	0.2	0.00305
30	235.40253	81867	168.4	5829	0.1	0.00288
31	235.42893	57424	1182.0	40902	0.8	0.00410
32	235.46810	59498	527.8	18262	0.3	0.00396
33	235.48910	101501	1224.0	42351	0.8	0.00232
34	235.49556	62807	1182.0	40898	0.8	0.00375
35	236.12166	33207	32468.8	1123227	20.8	0.00711
36	237.12392	29443	2682.9	92770	1.7	0.00805
37	238.12635	27118	199.4	6892	0.1	0.00878
38	242.28377	35752	224.0	7719	0.1	0.00678
39	245.17561	37371	944.4	32454	0.6	0.00656
40	247.19125	36272	360.4	12337	0.2	0.00681
41	251.14738	35991	3131.2	106526	2.0	0.00698
42	252.15052	35447	358.0	12159	0.2	0.00711
43	257.10040	35896	13070.5	441506	8.2	0.00716
44	258.10354	35957	1641.7	55306	1.0	0.00718
45	261.13107	33951	361.2	12037	0.2	0.00769
46	264.23172	36246	255.6	8435	0.2	0.00729
47	268.16771	39295	229.7	7512	0.1	0.00682
48	269.17537	37941	521.6	17029	0.3	0.00709
49	269.67699	36404	187.4	6110	0.1	0.00741
50	273.07430	37621	244.3	7904	0.1	0.00726
51	326.16044	40008	265.4	8312	0.2	0.00815
52	342.07776	39724	265.7	8212	0.2	0.00861
53	346.19790	40497	275.0	8460	0.2	0.00855
54	349.19745	39112	354.7	10898	0.2	0.00893
55	356.13463	41098	258.3	7884	0.1	0.00867
56	369.07583	41972	514.9	15804	0.3	0.00879
57	369.12981	40870	204.6	6279	0.1	0.00903
58	371.17938	39954	1345.5	41296	0.8	0.00929
59	372.18242	38785	254.7	7826	0.1	0.00960
60	373.20862	38030	235.5	7211	0.1	0.00981
61	422.22899	42091	959.6	28058	0.5	0.01003
62	423.23206	41306	244.2	7132	0.1	0.01025

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63	465.19840	42087	2318.6	65149	1.2	0.01105
64	466.20404	36564	1113.5	31229	0.6	0.01275
65	467.21232	35738	597.6	16729	0.3	0.01307
66	489.27503	43302	1032.5	28134	0.5	0.01130
67	490.27815	42323	366.0	9959	0.2	0.01158
68	491.21158	42069	6104.7	165967	3.1	0.01168
69	492.21449	40699	1541.3	41867	0.8	0.01209
70	493.21761	36319	251.0	6809	0.1	0.01358
71	501.17496	44133	437.0	11697	0.2	0.01136
72	537.34374	43827	1573.9	40881	0.8	0.01226
73	538.34685	43247	564.7	14654	0.3	0.01245
74	633.25896	44891	250.6	5804	0.1	0.01411
75	759.15538	47299	427.9	8173	0.2	0.01605