

Multiple Mass Analysis: 5 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 80.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

33660 formula(e) evaluated with 53 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 N: 0-5 O: 0-5 1H: 0-100 2H: 0-10

DCI-CH4

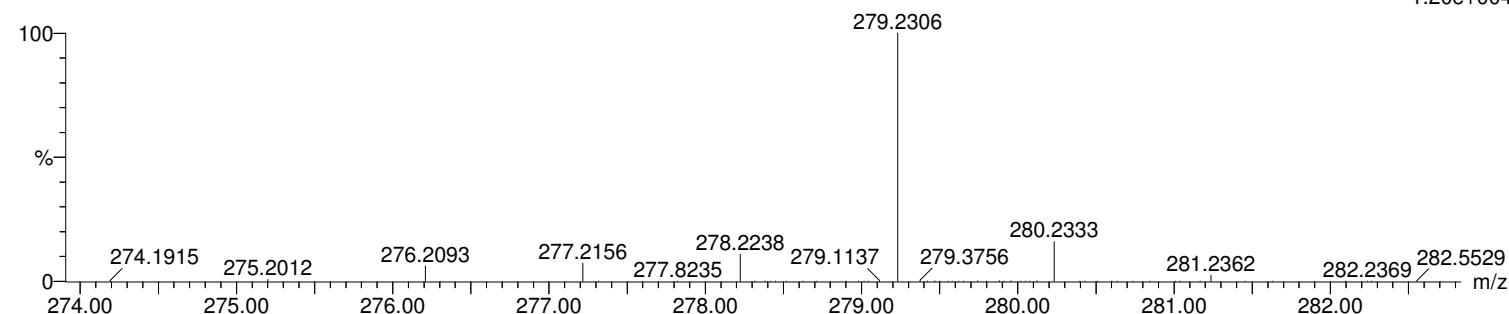
GCT Premier CAB109

09-Jun-202210:03:58

20220609-J-amide-D6 16 (0.267) Cm (16:22-84:91x5.000)

TOF MS CI+

1.20e+004



Minimum: 5.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
276.2093	6.04	276.2093	0.0	0.0	8.5	429812.6	C17 N2 O 1H14 2H7
		276.2092	0.1	0.4	1.5	1314410.3	C8 N5 O5 1H10 2H10
		276.2095	-0.2	-0.7	8.5	242236.7	C15 N5 1H14 2H6
		276.2097	-0.4	-1.4	3.0	27476.7	C14 N O4 1H20 2H5
		276.2089	0.4	1.4	5.0	926.4	C18 O2 1H28
		276.2099	-0.6	-2.2	3.0	27297.8	C12 N4 O3 1H20 2H4
		276.2084	0.9	3.3	3.5	108229.9	C12 N4 O3 1H18 2H5
		276.2082	1.1	4.0	3.5	108572.7	C14 N O4 1H18 2H6
		276.2080	1.3	4.7	9.0	430235.3	C15 N5 1H12 2H7
		277.2156	0.0	0.0	8.5	798406.0	C17 N2 O 1H13 2H8
277.2156	7.24	277.2154	0.2	0.7	5.0	6517.4	C16 N3 O 1H27
		277.2158	-0.2	-0.7	8.5	511597.1	C15 N5 1H13 2H7
		277.2160	-0.4	-1.4	3.0	129014.0	C14 N O4 1H19 2H6
		277.2152	0.4	1.4	5.0	6627.1	C18 O2 1H27 2H
		277.2162	-0.6	-2.2	3.0	128590.8	C12 N4 O3 1H19 2H5
		277.2147	0.9	3.2	3.5	288625.7	C12 N4 O3 1H17 2H6
		277.2145	1.1	4.0	3.5	289236.2	C14 N O4 1H17 2H7
		277.2168	-1.2	-4.3	4.5	6488.5	C18 O2 1H29
		277.2143	1.3	4.7	9.0	799034.4	C15 N5 1H11 2H8
		278.2238	0.0	0.0	2.5	192499.5	C14 N O4 1H20 2H6
278.2238	10.87	278.2236	0.2	0.7	8.0	763219.4	C15 N5 1H14 2H7
		278.2240	-0.2	-0.7	2.5	191874.0	C12 N4 O3 1H20 2H5
		278.2234	0.4	1.4	8.0	1190987.1	C17 N2 O 1H14 2H8
		278.2232	0.6	2.2	4.5	6675.6	C16 N3 O 1H28
		278.2230	0.8	2.9	4.5	6823.5	C18 O2 1H28 2H
		278.2246	-0.8	-2.9	4.0	6644.6	C18 O2 1H30
		278.2249	-1.1	-4.0	0.5	2332191.5	C8 N5 O5 1H12 2H10
		278.2250	-1.2	-4.3	7.5	762423.3	C17 N2 O 1H16 2H7
		278.2225	1.3	4.7	3.0	430575.7	C12 N4 O3 1H18 2H6
		278.2252	-1.4	-5.0	7.5	429614.0	C15 N5 1H16 2H6
279.2306	100.00	279.2303	0.3	1.1	2.5	3929073.0	C12 N4 O3 1H19 2H6
		279.2309	-0.3	-1.1	4.0	106.6	C18 O2 1H29 2H
		279.2311	-0.5	-1.8	4.0	40.7	C16 N3 O 1H29
		279.2301	0.5	1.8	2.5	3937624.3	C14 N O4 1H19 2H7
		279.2299	0.7	2.5	8.0	10879695.0	C15 N5 1H13 2H8
		279.2313	-0.7	-2.5	7.5	10870610.0	C17 N2 O 1H15 2H8
		279.2297	0.9	3.2	8.0	15652099.0	C17 N2 O 1H13 2H9
		279.2315	-0.9	-3.2	7.5	6965196.0	C15 N5 1H15 2H7
		279.2295	1.1	3.9	4.5	186.2	C16 N3 O 1H27 2H
		279.2317	-1.1	-3.9	2.0	1755816.8	C14 N O4 1H21 2H6
280.2333	15.89	279.2319	-1.3	-4.7	2.0	1750266.5	C12 N4 O3 1H21 2H5
		279.2293	1.3	4.7	4.5	299.3	C18 O2 1H27 2H2
		280.2333	0.0	0.0	0.0	29.5	C11 N5 O3 1H28 2H
		280.2333	0.0	0.0	3.5	2472853.3	C14 N O4 1H14 2H10
		280.2335	-0.2	-0.7	3.5	2470235.3	C12 N4 O3 1H14 2H9

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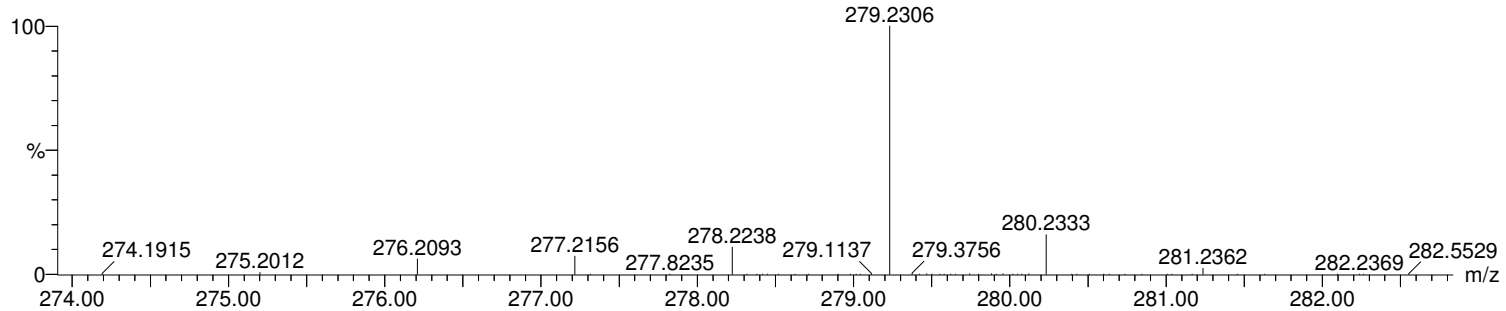
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TOF MS CI+
1.20e+004



Minimum: 5.00 -1.5

Maximum: 100.00 1.4 5.0 80.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula				
		280.2331	0.2	0.7	0.0	32.0	C13	N2	O4	1H28	2H2
		280.2327	0.6	2.1	5.5	69846.5	C16	N3	O	1H22	2H4
		280.2340	-0.7	-2.5	5.0	10.4	C18	O2	1H24	2H4	
		280.2325	0.8	2.9	5.5	70270.5	C18	O2	1H22	2H5	
		280.2342	-0.9	-3.2	5.0	5.8	C16	N3	O	1H24	2H3
		280.2320	1.3	4.6	4.0	3361959.3	C12	N4	O3	1H12	2H10
		280.2346	-1.3	-4.6	8.5	3358703.3	C15	N5	1H10	2H10	
		280.2347	-1.4	-5.0	-0.5	40.5	C13	N2	O4	1H30	2H