Supplementary material for:

Synthesis and *in vitro* antiproliferative and antibacterial activity of new thiazolidine-2,4-dione derivatives

Nazar Trotsko[a], Agata Przekora[b], Justyna Zalewska[b], Grażyna Ginalska[b], Agata Paneth[a], Monika Wujec[a]

[a]*Department of Organic Chemistry, Faculty of Pharmacy, Medical University of Lublin, Chodźki 4A, 20-093 Lublin, Poland*

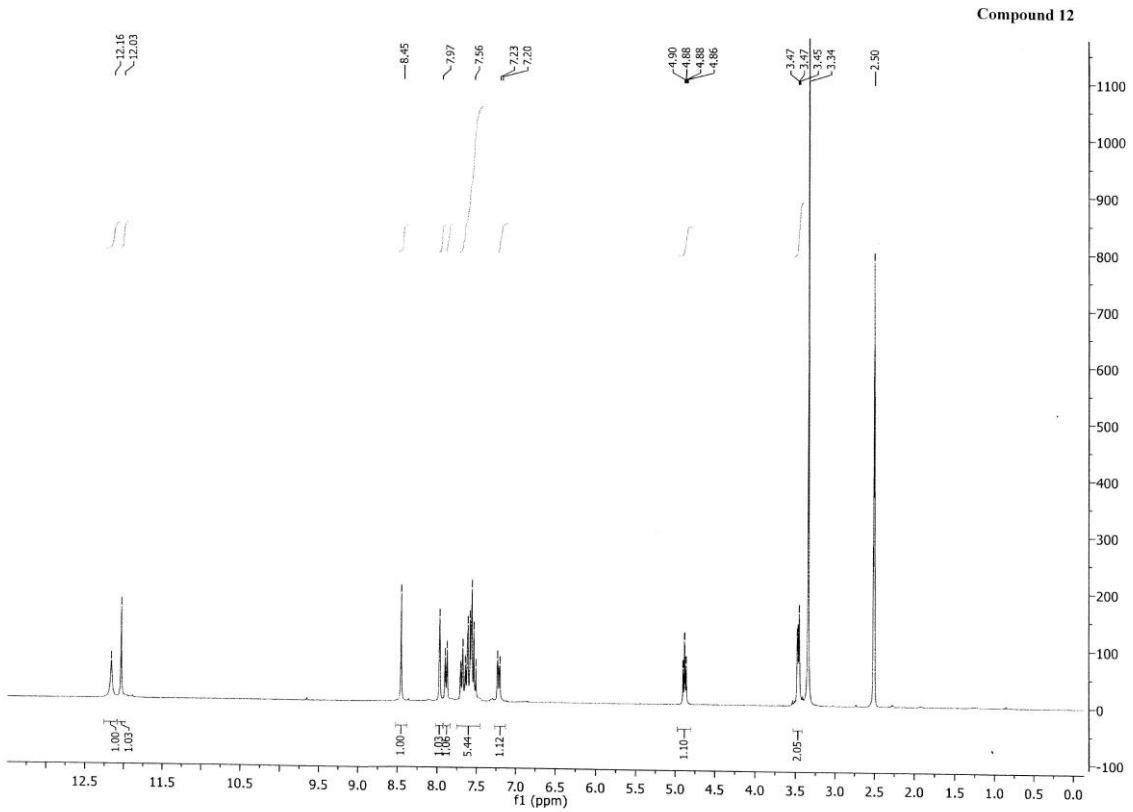
[b]*Department of Biochemistry and Biotechnology, Faculty of Pharmacy, Medical University of Lublin, Chodźki 1, 20-093 Lublin, Poland*

Contents:

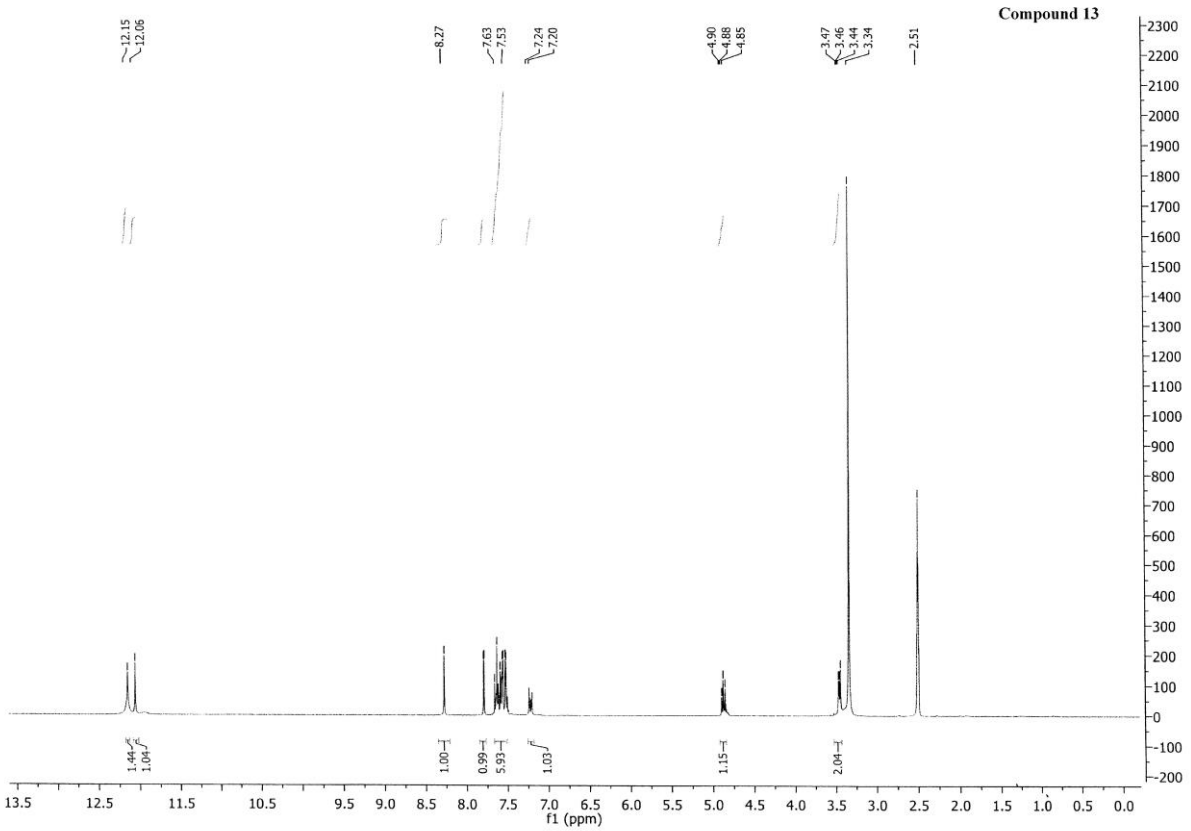
1. ^{1}H NMR spectra for compounds (**12-28**) ……2-18
2. ^{13}C NMR spectra for compounds (**12-28**)……19-35
3. MS spectra for compounds (**12-28**)……..36-52

^{1}H NMR spectra for compounds (12-28)

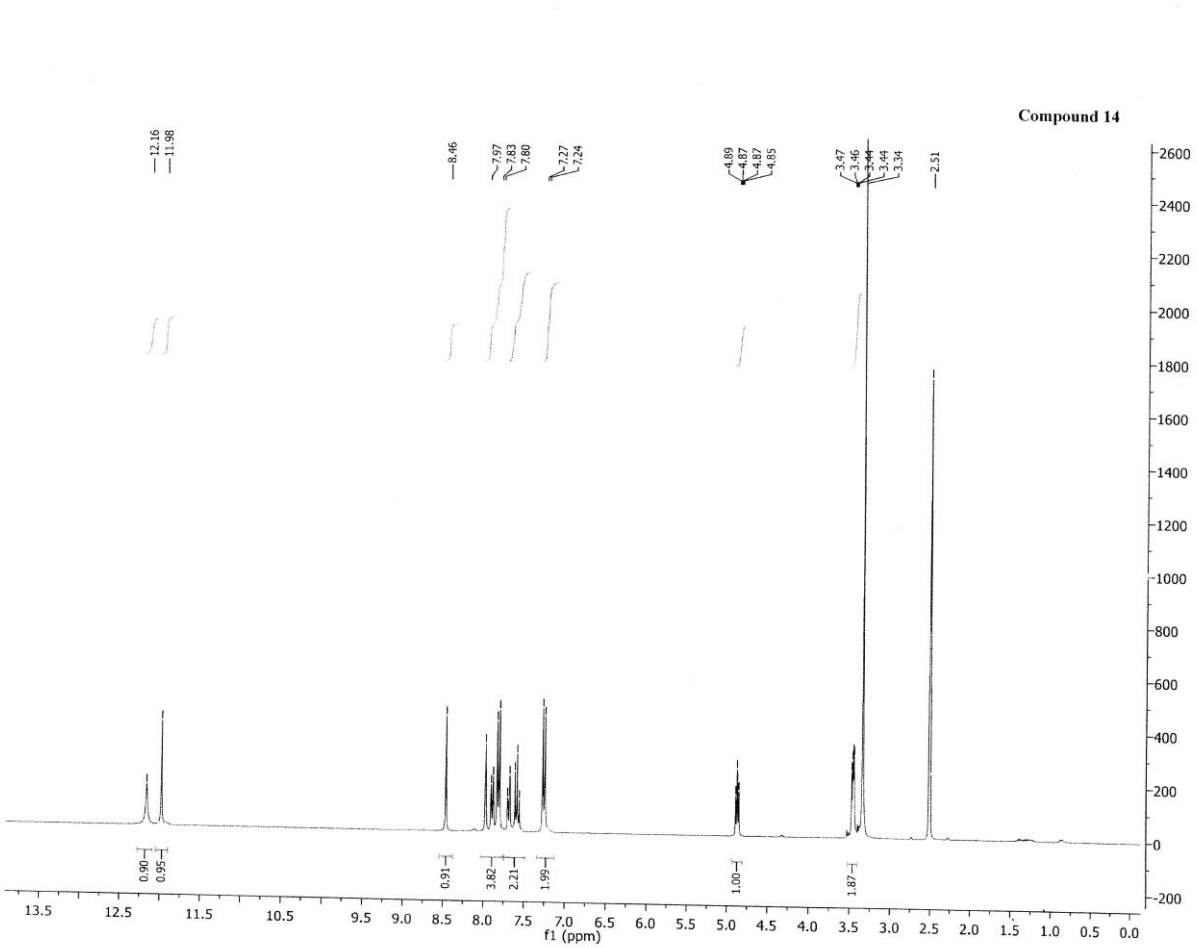
	ppm	Hz	Intensity
1	3.45	1035.8	162.0
2	2.50	751.7	785.7
3	12.03	3612.4	159.5
4	8.45	2537.3	188.4
5	7.97	2392.0	145.9
6	7.90	2371.5	78.1
7	7.87	2363.8	90.7
8	7.70	2311.6	55.9
9	7.67	2303.5	94.1
10	7.64	2294.0	65.9
11	7.61	2284.1	134.3
12	7.58	2276.0	143.9
13	7.56	2269.8	197.7
14	7.53	2261.7	124.1
15	7.51	2253.9	59.4
16	7.23	2171.0	74.5
17	7.20	2161.8	64.7
18	4.90	1471.1	63.0
19	4.88	1465.7	111.3
20	4.88	1464.5	88.3
21	4.86	1459.0	69.5
22	3.47	1043.1	120.9
23	3.47	1040.5	127.8
24	3.34	1002.0	2664.0
25	12.16	3650.9	65.8



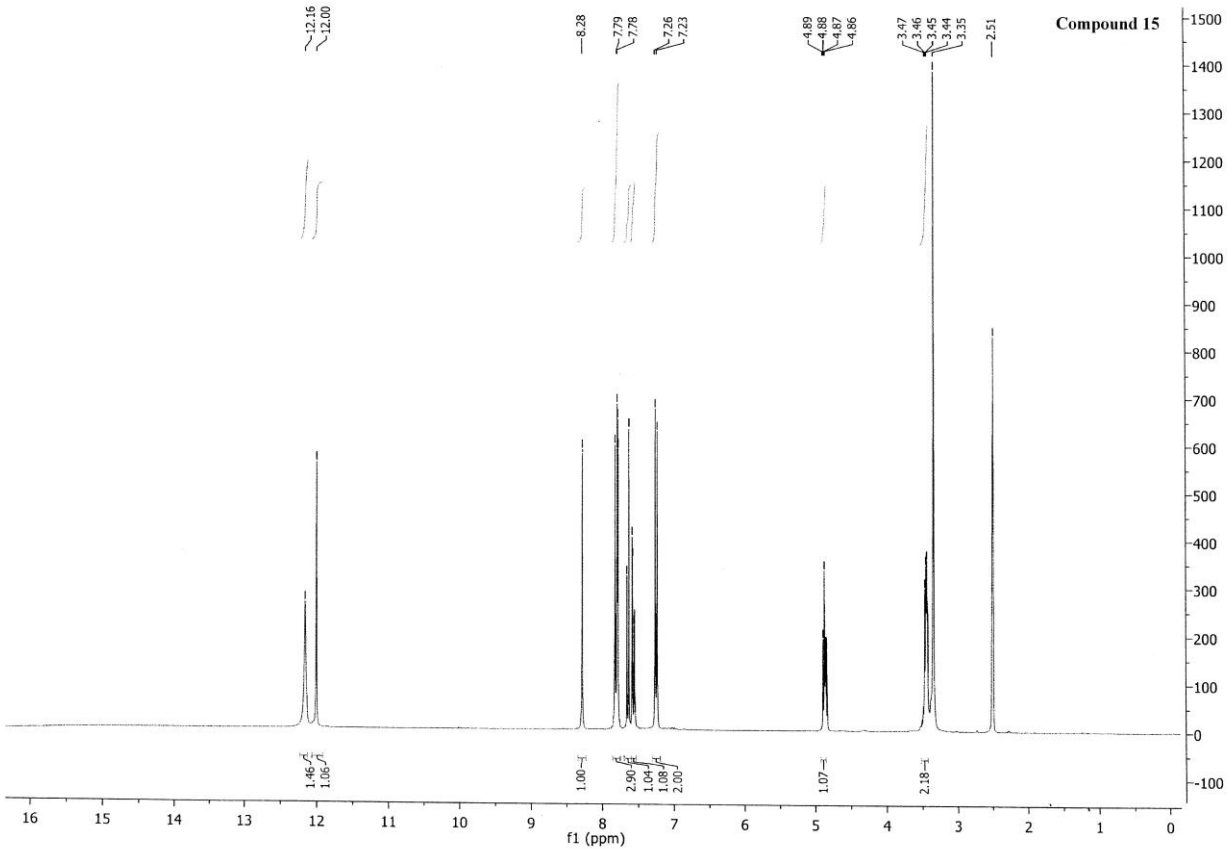
	ppm	Hz	Intensity
1	7.79	2336.9	184.7
2	3.44	1034.1	155.0
3	3.34	1002.1	1766.1
4	12.06	3618.9	170.5
5	8.27	2483.8	198.1
6	7.66	2298.2	106.2
7	12.15	3647.1	140.4
8	7.59	2278.0	146.7
9	7.56	2269.8	179.9
10	7.56	2267.9	184.4
11	7.53	2259.3	186.7
12	7.52	2256.8	178.5
13	7.24	2172.7	61.4
14	7.20	2161.5	47.1
15	4.90	1469.6	62.7
16	4.88	1464.1	119.8
17	4.85	1457.3	91.1
18	3.47	1041.3	117.8
19	3.46	1039.2	118.8
20	2.51	752.1	722.3
21	7.63	2290.0	228.6
22	7.79	2338.8	181.3



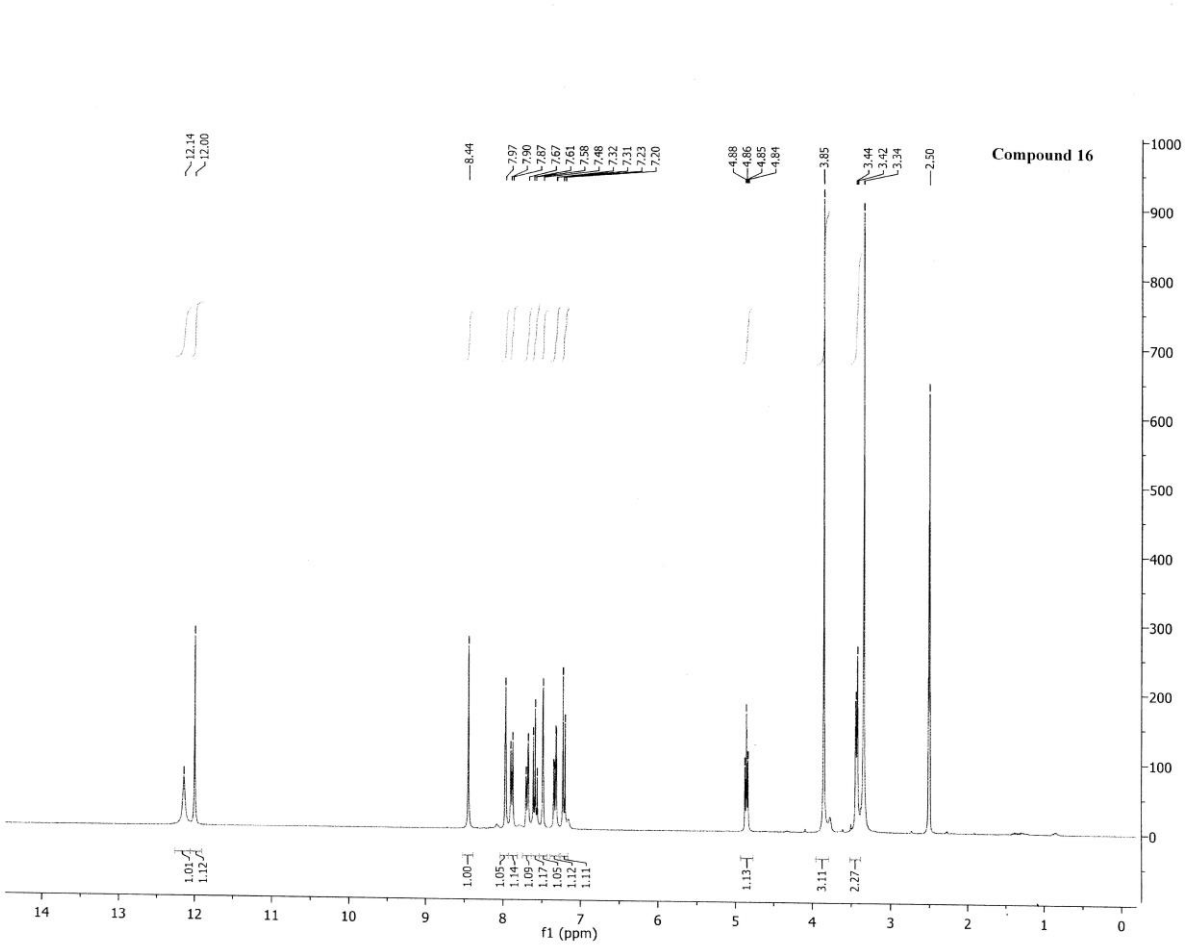
	ppm	Hz	Intensity
1	3.44	1032.3	305.6
2	2.51	752.1	1734.0
3	11.98	3595.8	389.5
4	8.46	2539.9	428.2
5	7.97	2392.5	328.7
6	7.90	2371.8	175.4
7	7.88	2364.1	206.2
8	7.83	2349.8	412.5
9	7.80	2341.2	454.8
10	7.70	2311.2	128.5
11	7.67	2303.1	210.2
12	7.61	2283.5	225.1
13	7.58	2275.7	290.4
14	7.55	2267.8	121.5
15	7.27	2181.7	463.7
16	7.24	2173.2	433.9
17	4.89	1468.3	151.5
18	4.87	1463.0	249.8
19	4.87	1461.5	201.9
20	4.85	1456.2	167.7
21	3.47	1041.1	247.1
22	3.46	1037.2	289.6
23	3.44	1034.1	316.0
24	3.34	1001.3	4134.0
25	12.16	3650.4	151.0



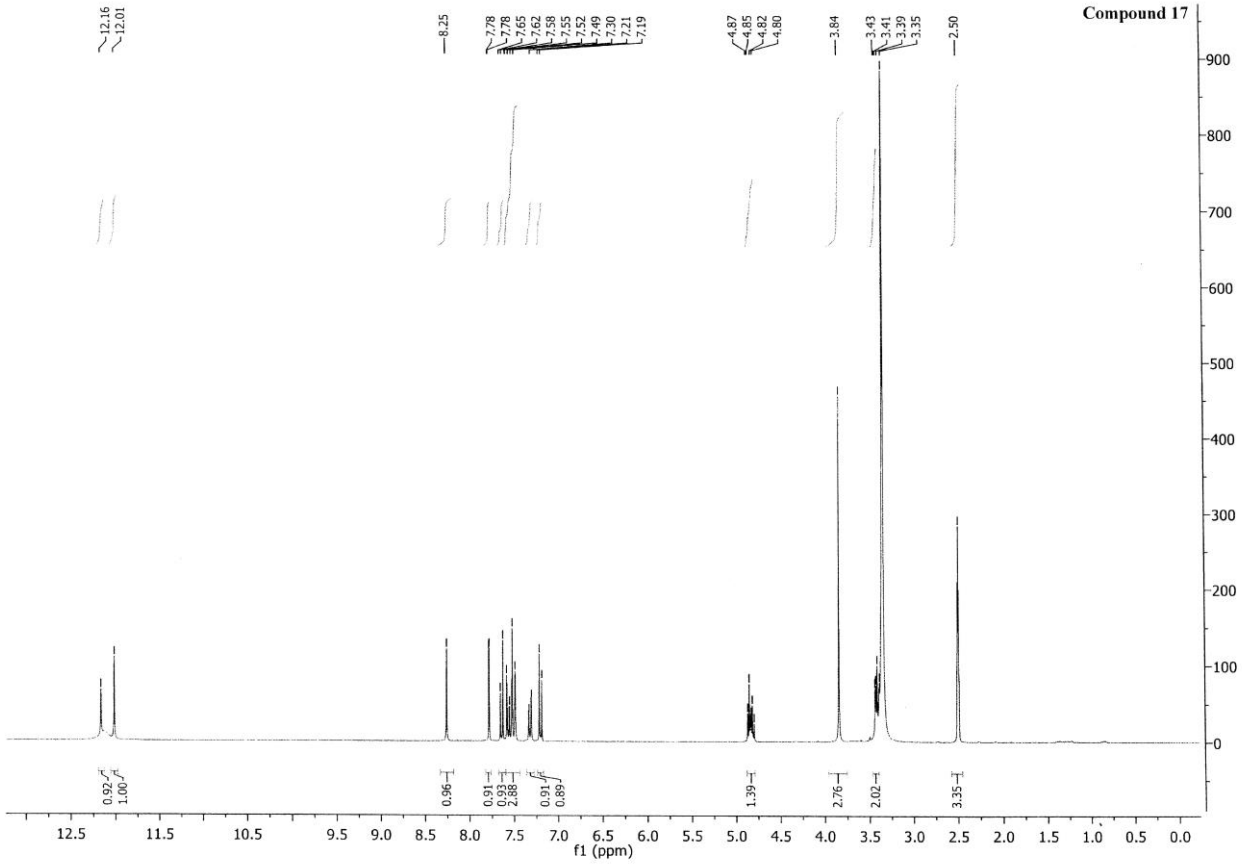
	ppm	Hz	Intensity
1	3.44	1032.4	359.2
2	2.51	752.2	830.1
3	12.00	3602.5	558.5
4	8.28	2485.9	588.4
5	7.82	2348.0	599.3
6	7.79	2339.3	684.9
7	7.78	2336.8	652.7
8	7.78	2334.8	589.9
9	7.66	2298.7	323.1
10	7.63	2290.4	633.3
11	7.58	2276.7	405.9
12	7.58	2274.8	360.9
13	7.56	2268.5	219.7
14	7.23	2171.6	627.6
15	4.86	1459.2	178.4
16	3.47	1041.9	299.4
17	7.55	2266.6	232.2
18	7.26	2180.3	675.0
19	4.89	1469.1	193.8
20	4.88	1463.9	336.1
21	4.87	1462.1	244.6
22	3.46	1037.5	347.5
23	3.45	1034.9	356.8
24	3.35	1005.3	1385.4
25	12.16	3649.1	264.0



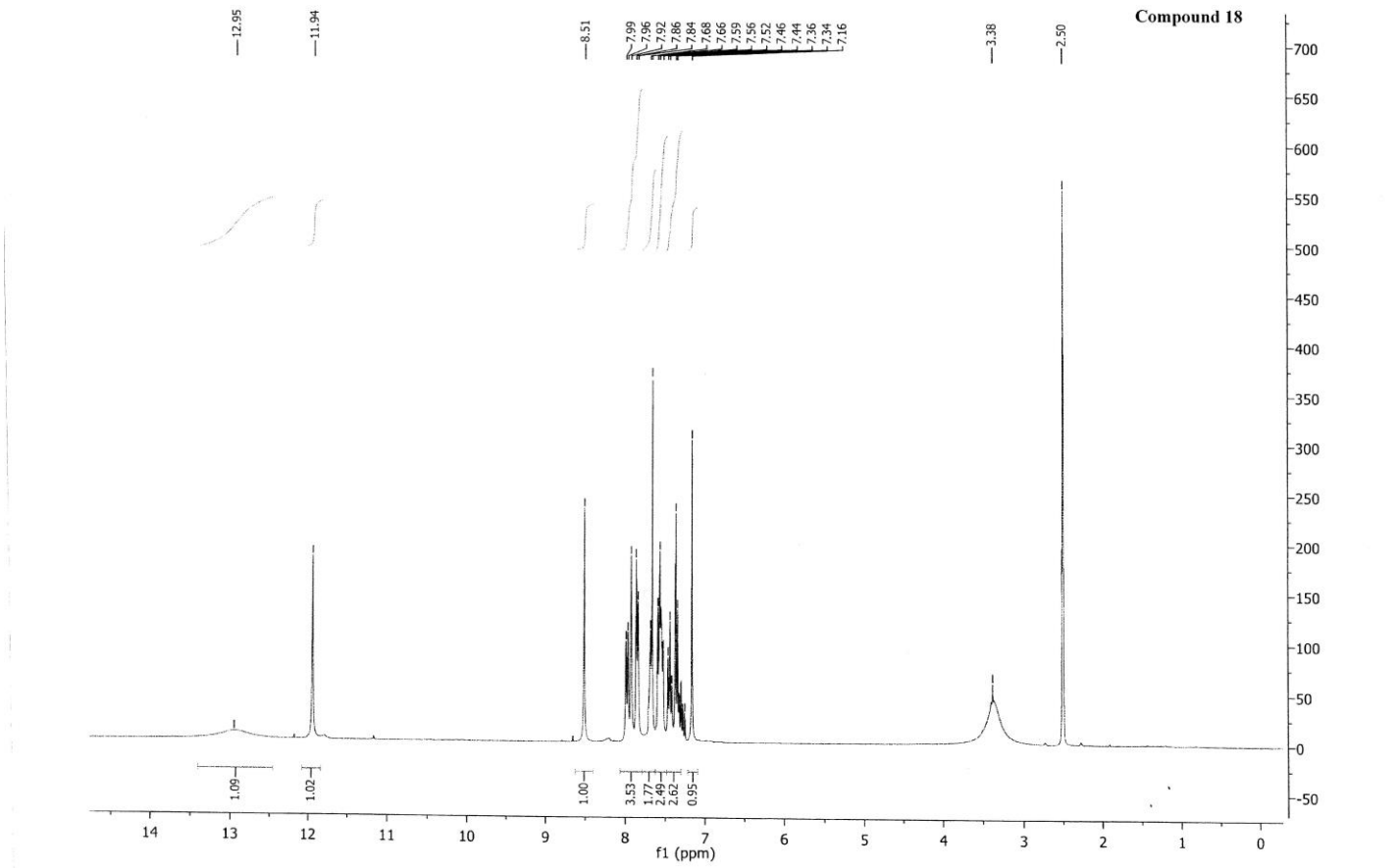
	ppm	Hz	Intensity
1	3.34	1003.1	894.7
2	4.84	1451.7	101.9
3	12.00	3601.5	272.3
4	8.44	2534.5	263.2
5	7.97	2391.1	203.4
6	7.90	2370.8	112.5
7	7.87	2363.0	125.1
8	7.70	2311.4	76.0
9	7.67	2302.6	124.0
10	7.61	2283.6	132.6
11	7.58	2275.8	172.7
12	7.56	2267.9	74.1
13	7.48	2245.8	202.8
14	7.34	2204.5	87.2
15	7.34	2203.0	83.5
16	7.32	2196.2	135.1
17	7.31	2194.8	131.6
18	7.23	2169.0	219.5
19	3.42	1026.7	254.7
20	4.88	1463.7	92.7
21	4.86	1458.3	169.4
22	12.14	3644.0	69.6
23	3.85	1156.1	913.6
24	3.44	1033.6	175.6
25	3.44	1031.8	189.0
26	2.50	751.7	636.2
27	7.20	2160.9	151.4
28	4.85	1457.2	132.6



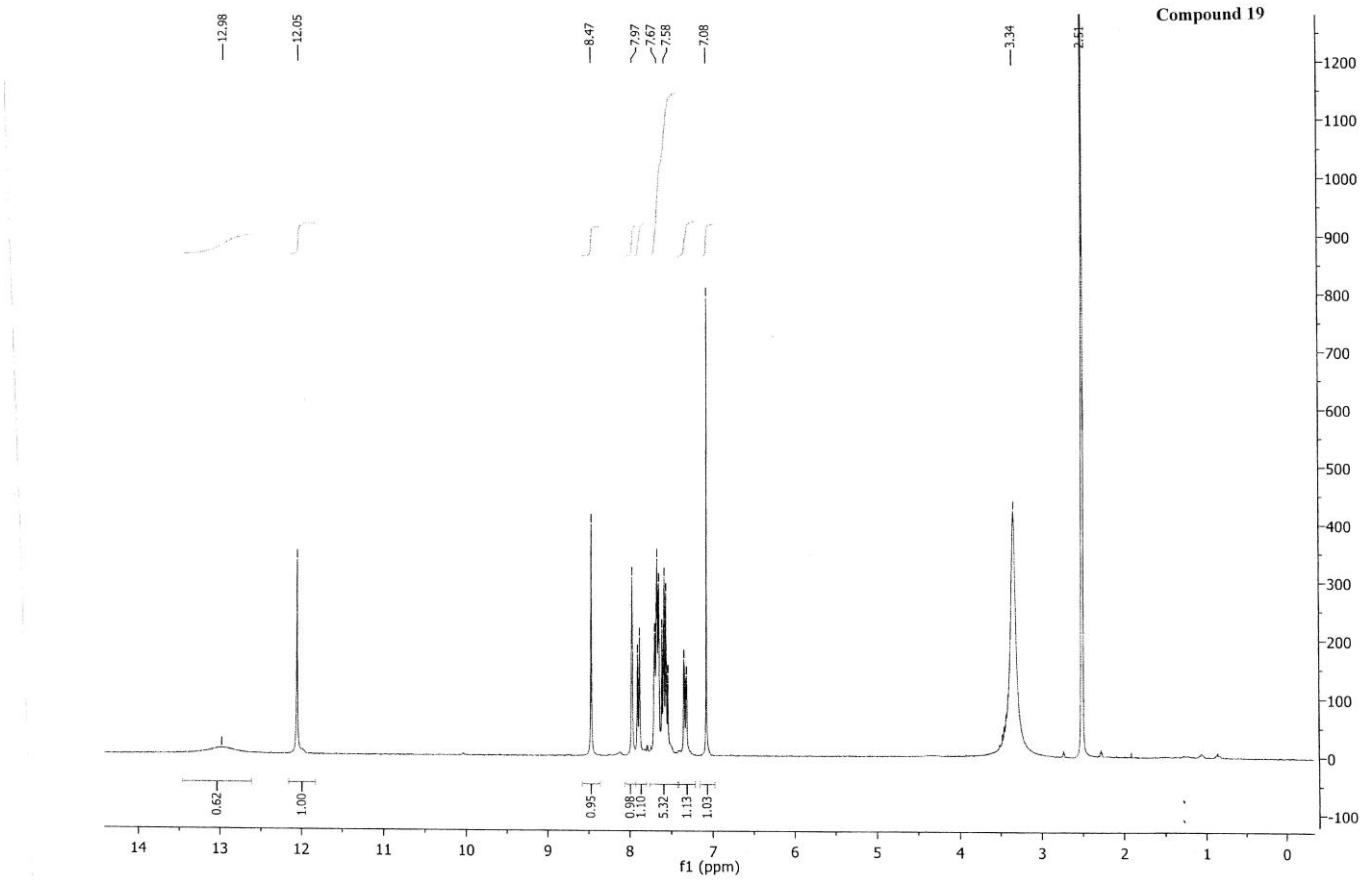
	ppm	Hz	Intensity
1	3.35	1005.3	884.7
2	4.80	1439.7	25.2
3	12.01	3606.0	110.8
4	8.25	2477.8	122.3
5	7.78	2336.0	120.3
6	7.78	2334.1	122.6
7	7.65	2296.3	64.6
8	7.62	2288.1	133.4
9	7.58	2275.9	87.8
10	7.55	2265.7	47.3
11	7.52	2257.0	149.1
12	7.49	2247.7	92.5
13	7.33	2200.2	37.3
14	7.30	2191.9	56.4
15	7.21	2165.1	115.6
16	3.39	1016.7	78.7
17	4.87	1461.6	39.0
18	4.85	1456.3	76.9
19	12.16	3650.9	67.8
20	3.84	1152.9	456.7
21	3.44	1031.6	70.7
22	3.43	1029.4	75.5
23	3.41	1024.5	101.3
24	2.50	750.4	285.3
25	7.19	2157.0	81.7
26	4.82	1446.2	49.2



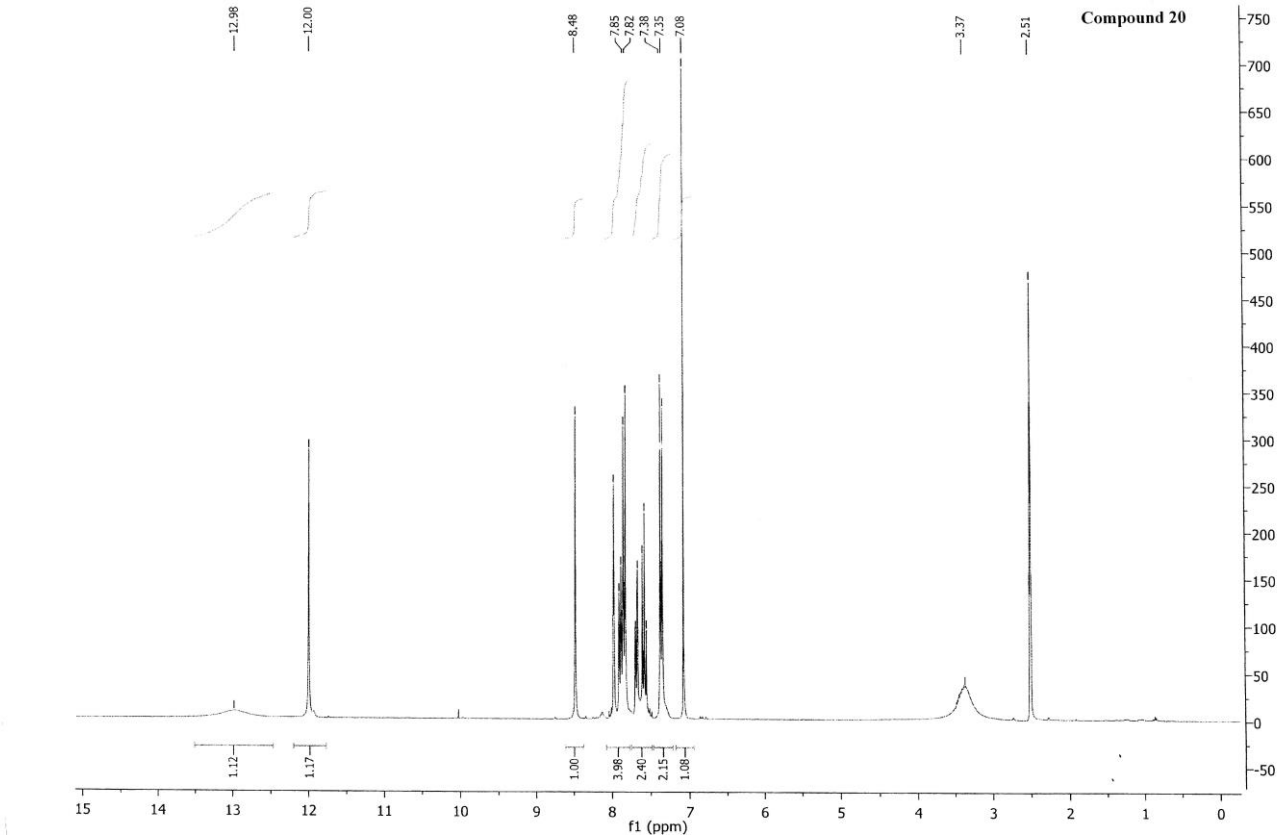
	ppm	Hz	Intensity
1	7.34	2204.8	132.5
2	3.38	1015.6	61.4
3	11.94	3585.3	183.5
4	8.51	2555.4	234.0
5	7.99	2398.2	101.2
6	7.96	2390.8	109.8
7	7.92	2378.4	186.4
8	7.86	2359.8	183.1
9	7.84	2351.9	140.6
10	7.68	2306.0	111.8
11	7.66	2299.1	365.1
12	7.36	2210.6	229.6
13	7.16	2150.2	302.9
14	7.59	2278.1	134.4
15	2.50	751.7	556.5
16	7.52	2258.0	92.5
17	7.56	2270.3	191.1
18	7.41	2225.5	57.5
19	7.25	2176.6	30.0
20	7.46	2240.3	85.3
21	7.44	2232.8	120.8
22	12.95	3887.7	8.7



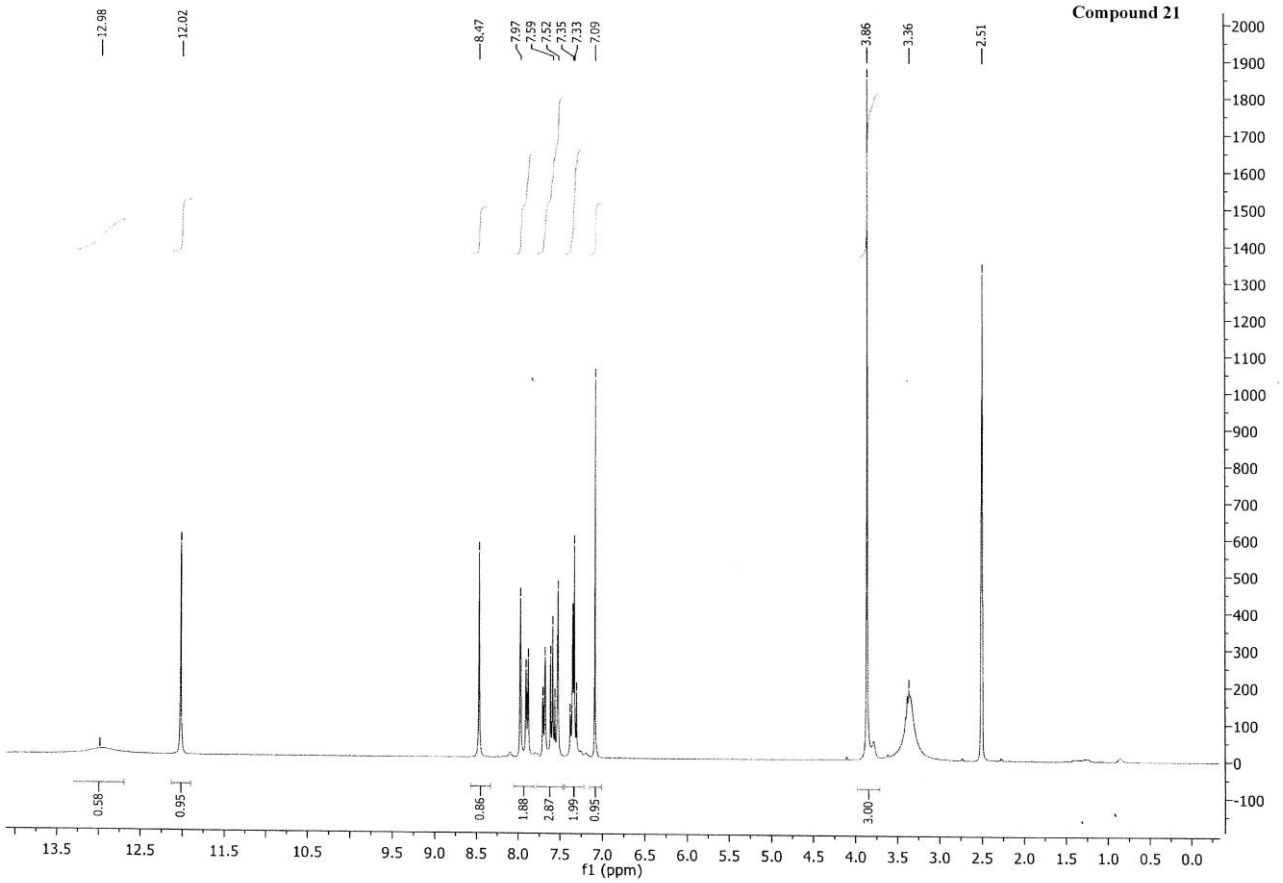
	ppm	Hz	Intensity
1	7.08	2124.3	789.8
2	2.51	752.1	2012.6
3	12.05	3617.7	332.4
4	8.47	2541.3	397.1
5	7.97	2392.9	306.1
6	7.90	2372.4	172.7
7	7.88	2364.7	201.7
8	7.70	2310.4	208.9
9	7.61	2284.1	216.0
10	7.58	2276.3	305.3
11	7.65	2295.9	295.7
12	7.56	2270.6	278.4
13	7.67	2302.5	337.7
14	7.59	2278.3	207.4
15	7.56	2268.7	175.0
16	7.54	2262.8	138.4
17	7.34	2204.8	164.4
18	7.31	2195.5	135.9
19	3.34	1003.1	423.6
20	12.98	3895.7	9.9



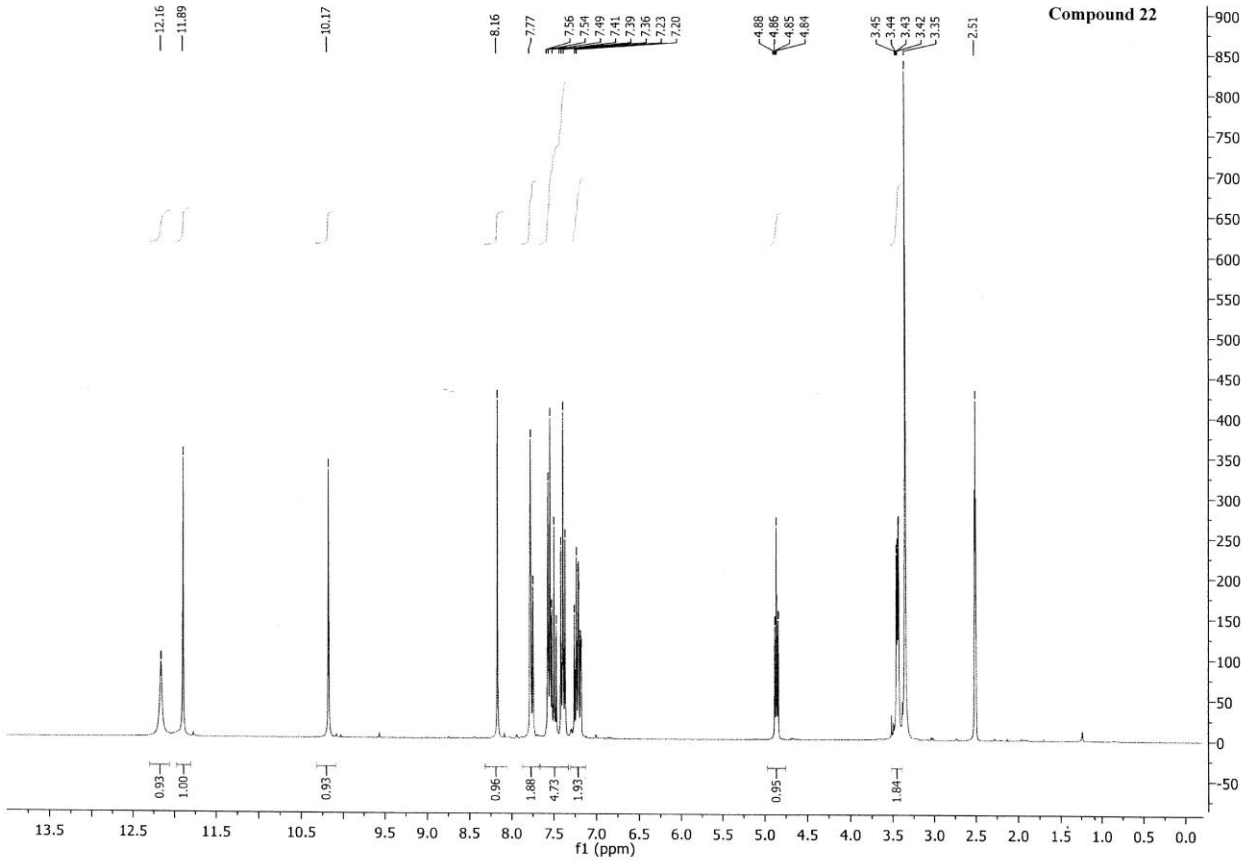
	ppm	Hz	Intensity
1	7.08	2123.9	695.1
2	2.51	752.0	470.1
3	12.00	3601.3	287.3
4	8.48	2545.1	324.0
5	7.97	2393.5	251.5
6	7.91	2373.0	135.2
7	7.88	2365.3	163.2
8	7.85	2357.0	313.1
9	7.82	2348.3	347.1
10	7.69	2309.6	95.4
11	7.67	2301.5	159.5
12	7.60	2282.8	175.7
13	7.58	2275.0	220.7
14	7.55	2267.1	95.9
15	7.38	2214.0	358.9
16	7.35	2205.4	333.1
17	3.37	1010.8	37.6
18	12.98	3896.9	9.3



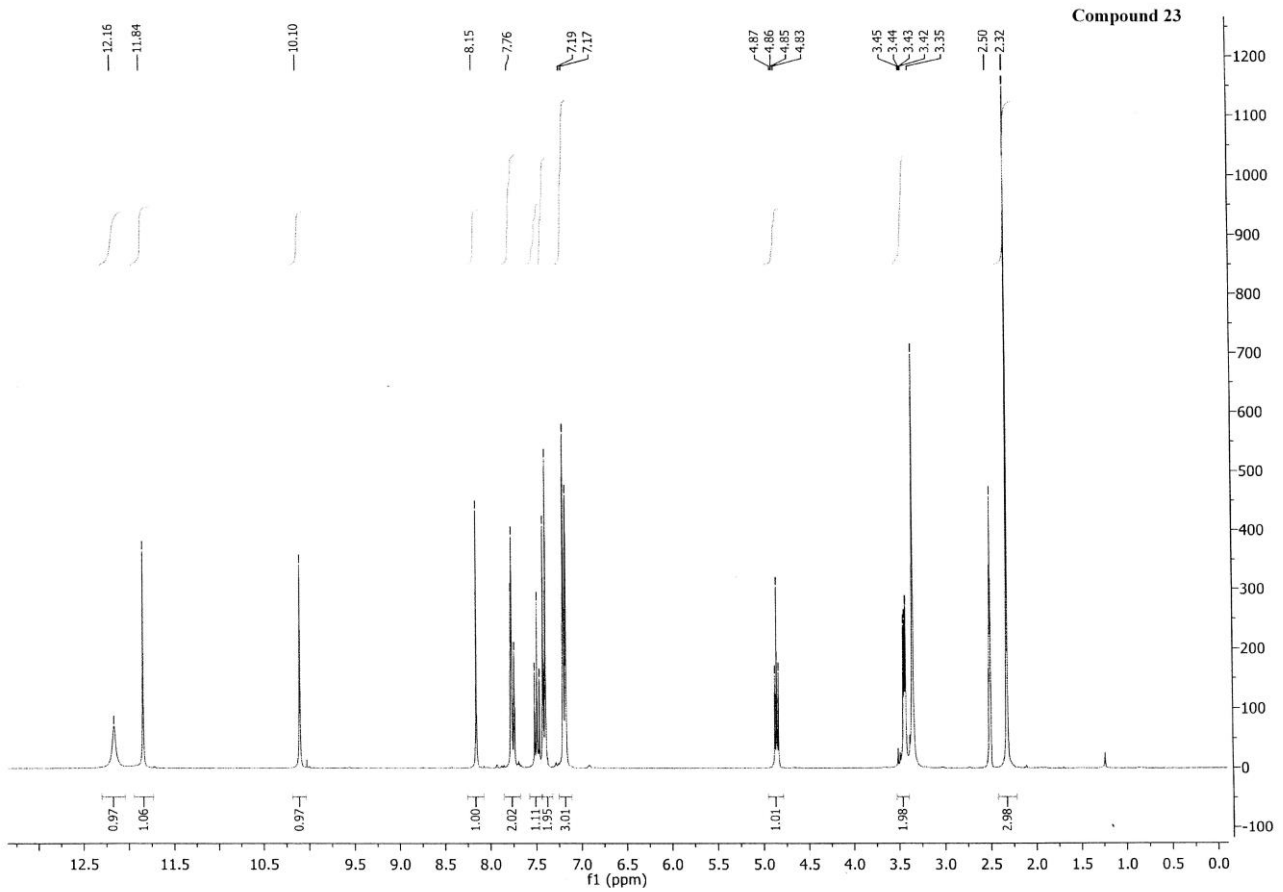
	ppm	Hz	Intensity
1	7.30	2192.1	177.2
2	3.86	1159.7	1848.6
3	12.02	3608.0	573.2
4	8.47	2541.2	554.4
5	7.97	2392.9	430.3
6	7.90	2372.7	237.9
7	7.88	2365.0	266.6
8	7.70	2312.4	163.4
9	7.68	2304.3	271.2
10	7.61	2284.9	274.9
11	7.59	2277.1	355.1
12	7.56	2269.2	159.0
13	7.52	2258.2	451.1
14	7.38	2214.6	119.3
15	7.35	2206.2	390.0
16	7.09	2127.6	1029.7
17	2.51	752.1	1323.8
18	3.36	1009.3	192.3
19	7.33	2200.3	575.1
20	12.98	3897.8	14.1



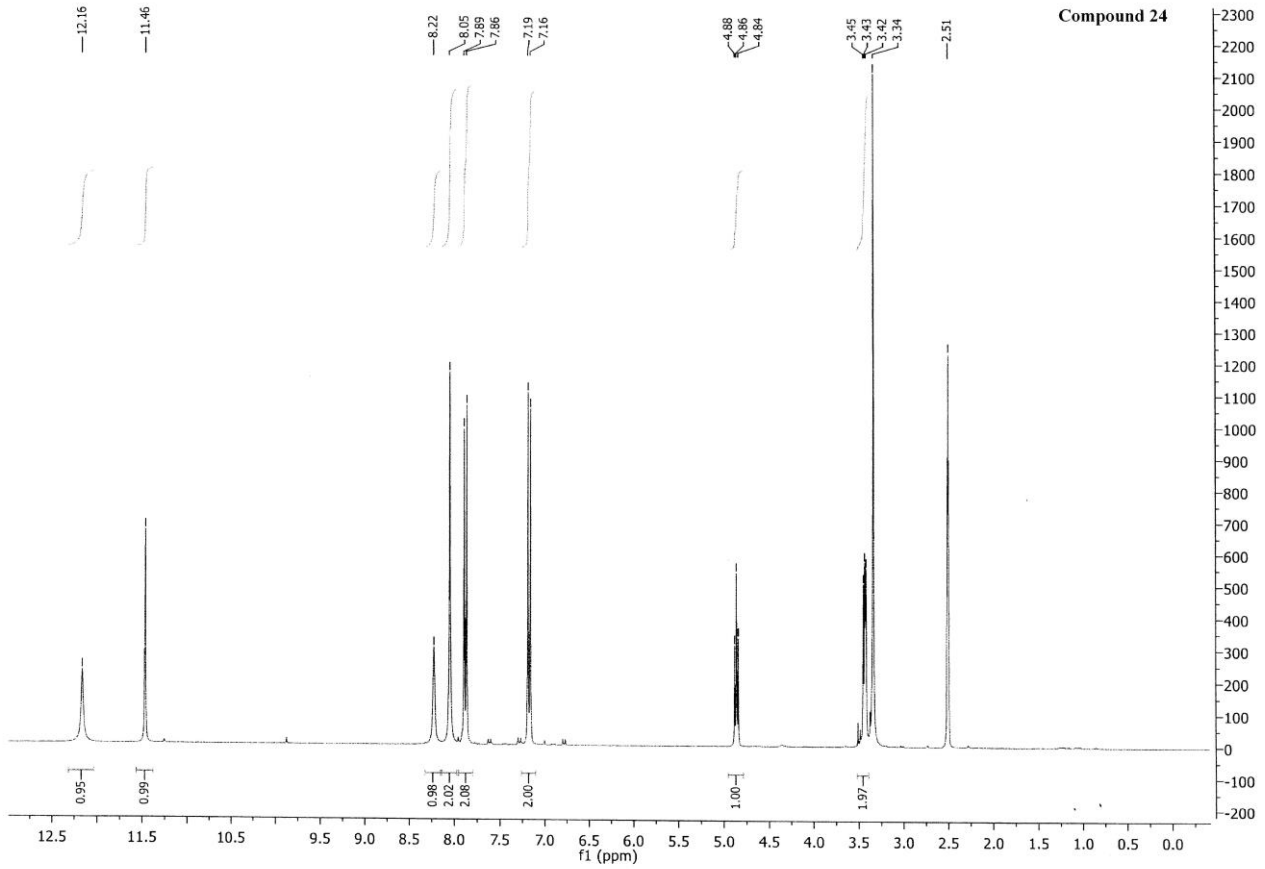
	ppm	Hz	Intensity
1	3.35	1004.8	829.9
2	8.16	2450.3	420.3
3	3.42	1028.1	265.7
4	12.16	3650.3	92.9
5	7.78	2334.7	277.4
6	7.77	2332.8	371.3
7	7.74	2324.0	189.0
8	7.56	2270.1	317.9
9	7.54	2262.6	398.2
10	7.52	2256.0	159.8
11	7.49	2248.1	262.8
12	7.46	2240.3	140.1
13	7.41	2224.4	237.6
14	7.39	2216.8	405.7
15	7.36	2208.8	247.1
16	7.25	2176.2	153.6
17	7.23	2168.8	225.1
18	7.20	2162.5	204.5
19	7.20	2160.3	182.0
20	4.88	1463.7	140.2
21	4.85	1456.9	167.2
22	7.17	2152.2	110.9
23	4.84	1451.6	147.0
24	7.18	2155.4	122.2
25	4.86	1458.4	263.3
26	3.45	1036.4	229.8
27	3.44	1033.2	237.9
28	3.43	1029.5	263.3
29	2.51	752.1	421.9
30	11.89	3570.3	346.7
31	10.17	3053.3	333.1



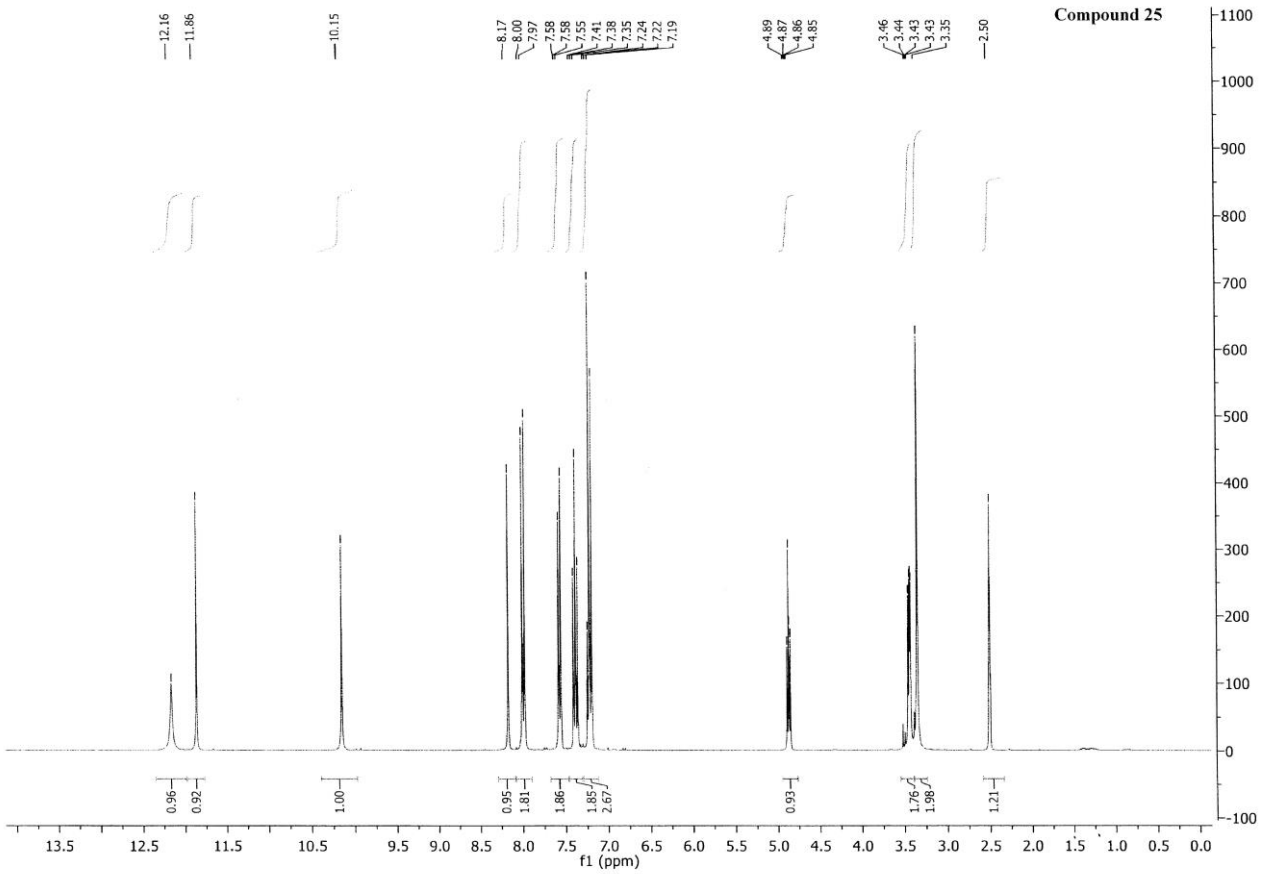
	ppm	Hz	Intensity
1	3.35	1004.6	700.2
2	2.32	696.1	1151.6
3	11.84	3554.6	366.1
4	10.10	3031.7	342.7
5	8.15	2446.5	434.8
6	7.77	2332.5	294.2
7	7.76	2330.5	390.8
8	7.73	2321.8	195.8
9	7.51	2254.5	160.7
10	7.48	2246.5	279.2
11	7.46	2238.7	150.4
12	7.42	2226.8	408.9
13	7.39	2218.5	522.2
14	4.87	1463.1	155.9
15	4.85	1456.3	178.3
16	7.17	2151.5	461.3
17	4.83	1451.1	160.7
18	7.19	2159.7	564.7
19	4.86	1457.9	304.8
20	3.45	1035.7	240.8
21	3.44	1032.5	249.7
22	3.43	1028.8	273.6
23	3.42	1027.3	271.5
24	2.50	751.9	458.7
25	12.16	3651.3	72.3



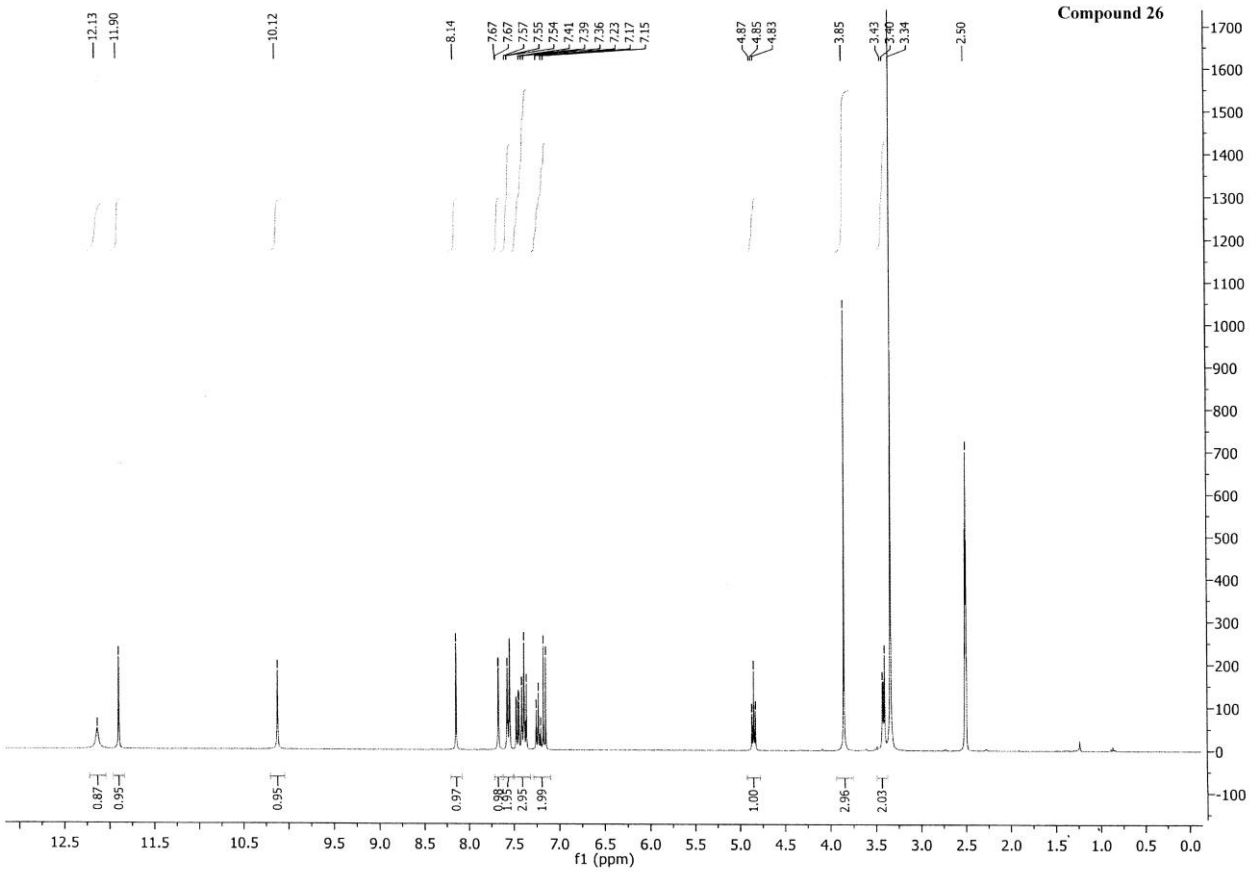
	ppm	Hz	Intensity
1	3.42	1025.8	555.7
2	8.05	2415.9	1166.7
3	2.51	752.3	1233.6
4	7.89	2368.4	990.0
5	3.34	1002.5	2108.2
6	8.22	2468.2	303.8
7	7.86	2359.7	1063.7
8	7.19	2157.5	1104.4
9	7.16	2148.8	1052.6
10	4.88	1465.4	313.9
11	4.86	1460.2	540.0
12	4.84	1453.3	337.5
13	3.45	1035.1	506.4
14	3.43	1030.9	575.2
15	11.46	3440.7	667.3
16	12.16	3649.6	228.2



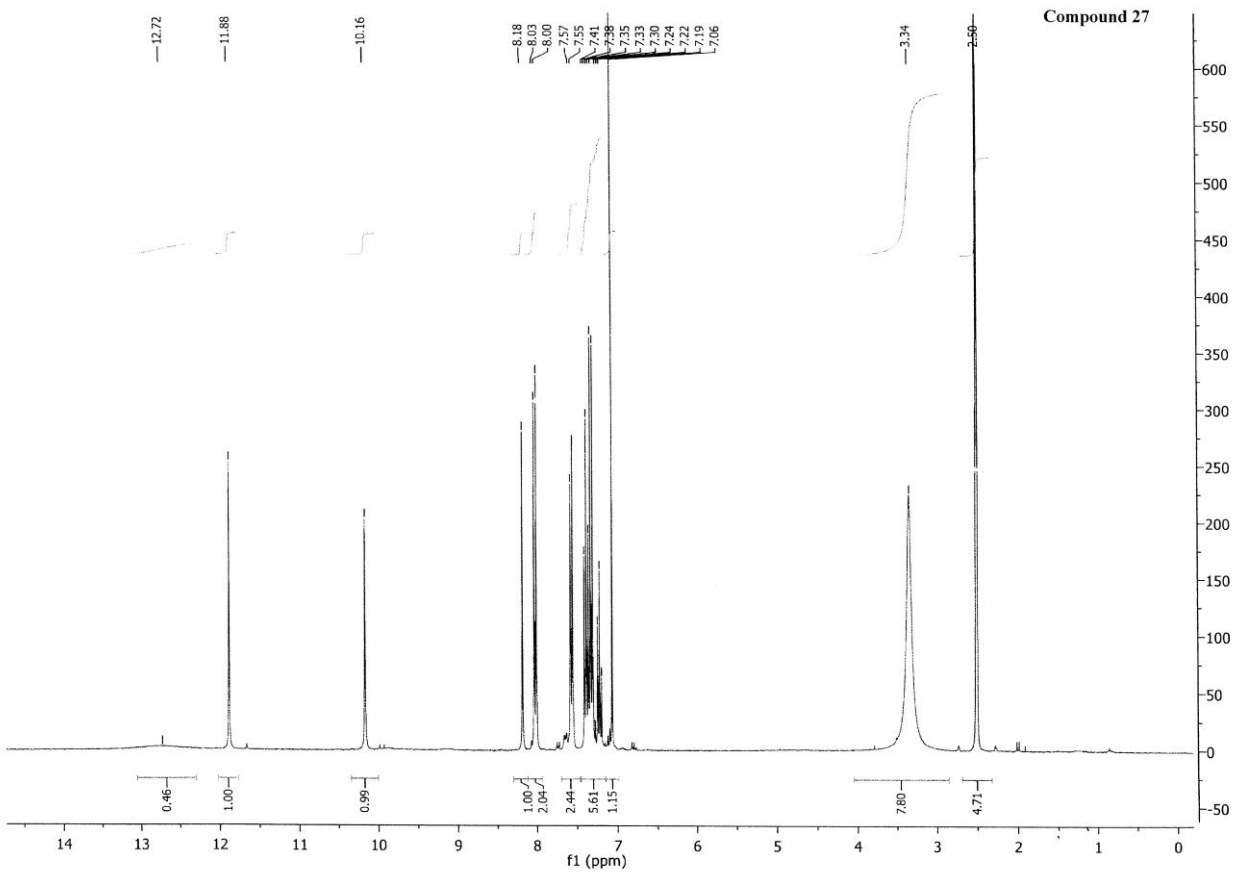
	ppm	Hz	Intensity
1	4.86	1460.0	185.4
2	2.50	751.9	369.0
3	11.86	3561.1	372.8
4	10.15	3046.2	307.6
5	8.17	2451.6	414.1
6	8.00	2402.3	470.2
7	7.97	2393.5	496.8
8	7.22	2167.0	703.1
9	7.24	2173.8	177.7
10	3.44	1033.5	256.4
11	7.58	2275.4	255.6
12	7.38	2215.5	436.8
13	7.35	2207.5	274.7
14	7.55	2266.7	409.1
15	3.35	1005.2	621.5
16	3.43	1028.3	250.8
17	7.41	2223.1	258.8
18	3.46	1037.6	232.0
19	7.58	2274.1	342.4
20	4.87	1461.8	300.6
21	7.19	2158.3	557.9
22	3.43	1030.6	260.8
23	4.85	1454.8	167.0
24	4.89	1467.0	155.6
25	12.16	3651.3	100.7



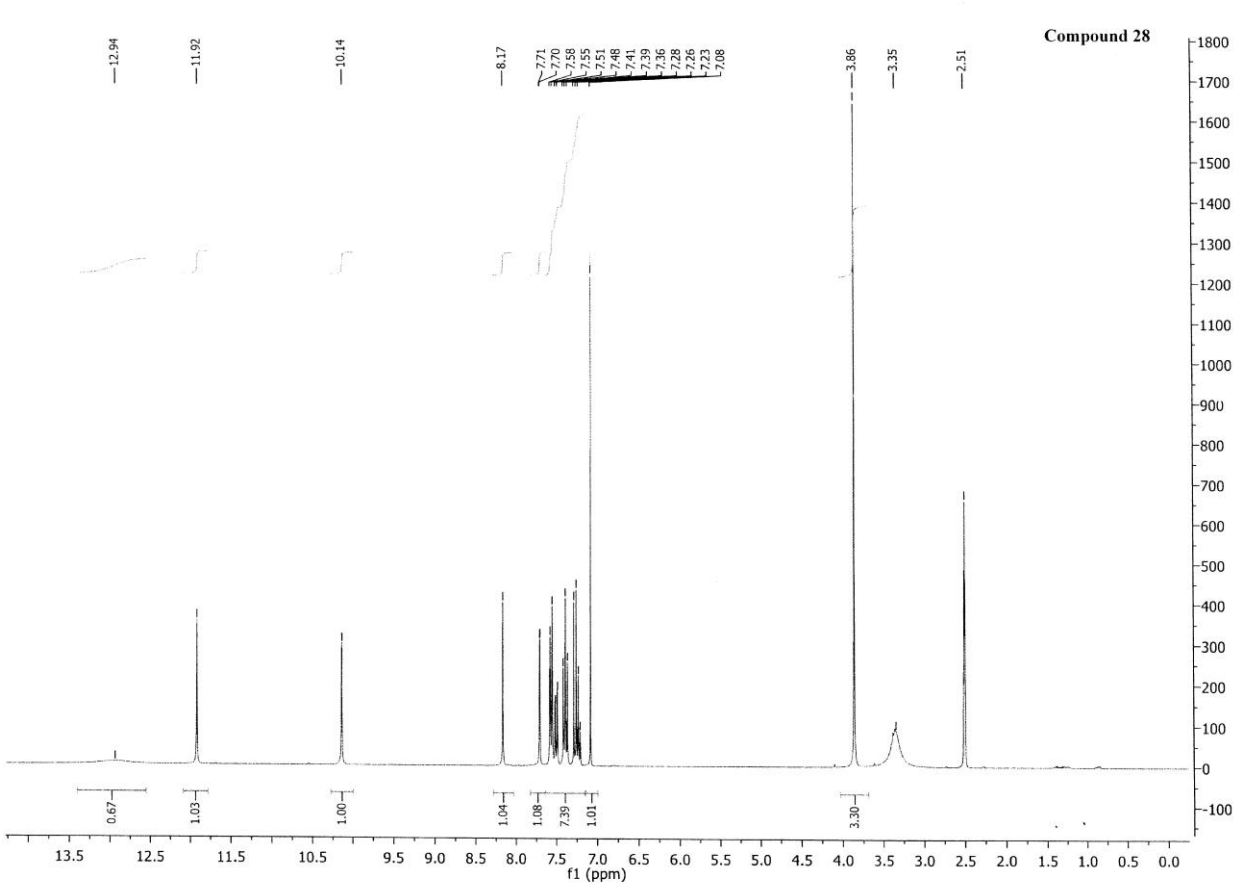
	ppm	Hz	Intensity
1	3.40	1021.8	223.7
2	2.50	751.7	702.2
3	11.90	3570.8	214.6
4	10.12	3037.9	184.2
5	8.14	2444.7	248.6
6	7.67	2303.5	190.5
7	7.67	2301.7	192.4
8	7.57	2272.7	191.6
9	7.55	2265.3	236.7
10	7.54	2264.6	222.5
11	7.47	2243.7	101.2
12	7.47	2242.0	94.2
13	7.45	2235.4	116.2
14	7.44	2233.7	112.0
15	7.41	2224.7	147.0
16	7.39	2217.2	251.5
17	7.36	2209.1	154.3
18	7.25	2176.7	94.3
19	7.23	2169.4	133.6
20	7.20	2162.0	53.6
21	7.17	2153.2	244.2
22	7.15	2145.0	218.2
23	4.87	1461.2	86.1
24	4.85	1455.6	185.7
25	4.83	1449.1	92.3
26	3.85	1155.4	1035.8
27	3.43	1028.6	161.1
28	3.34	1001.9	1898.0
29	12.13	3642.2	48.8



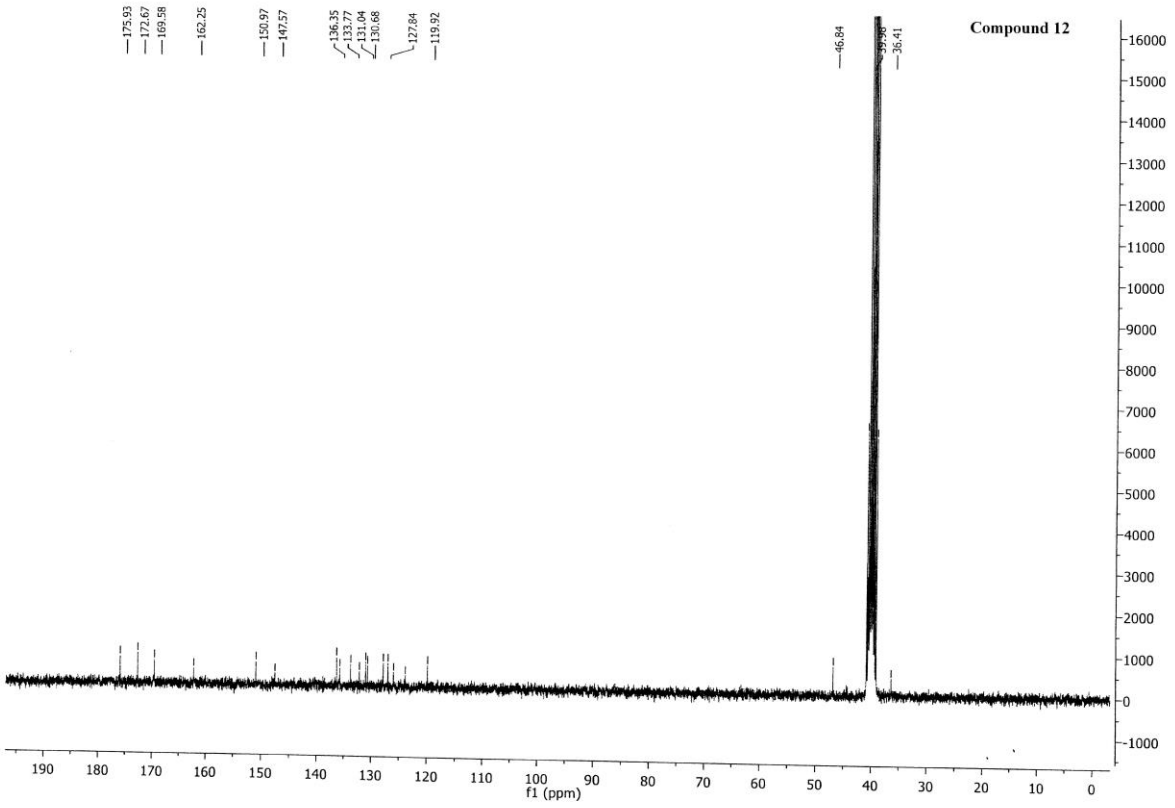
	ppm	Hz	Intensity
1	7.06	2120.0	757.8
2	2.50	751.8	850.6
3	11.88	3564.9	252.7
4	10.16	3050.8	202.7
5	8.18	2454.8	280.2
6	8.03	2410.5	306.5
7	8.00	2401.7	330.2
8	7.57	2273.4	234.2
9	7.55	2265.3	265.8
10	7.41	2223.0	170.1
11	7.38	2215.5	291.5
12	7.35	2207.4	189.0
13	7.33	2200.3	364.6
14	7.30	2191.6	356.7
15	7.24	2173.9	108.4
16	7.22	2166.5	157.3
17	7.19	2159.2	63.6
18	3.34	1003.6	224.8
19	12.72	3819.2	2.8

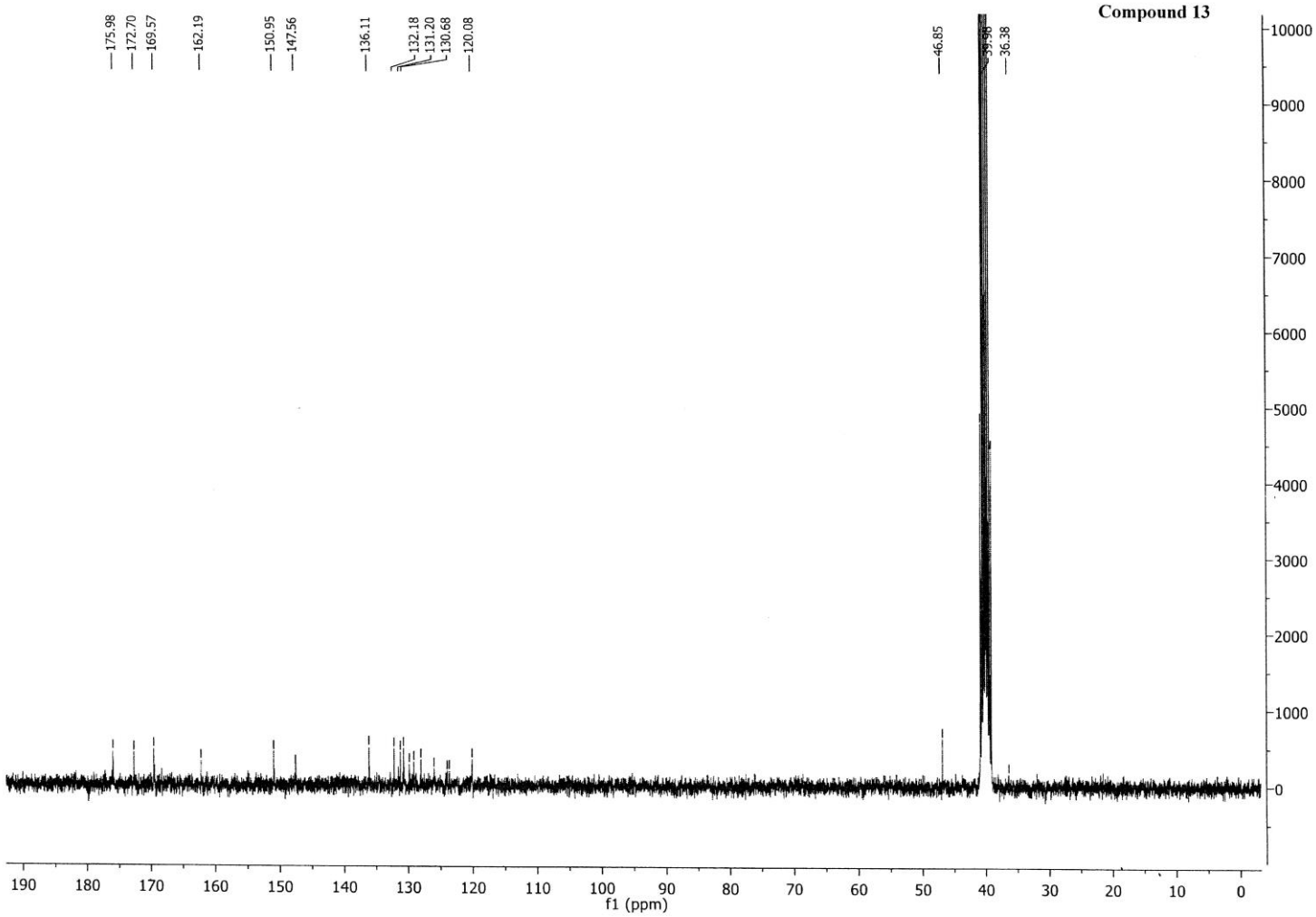


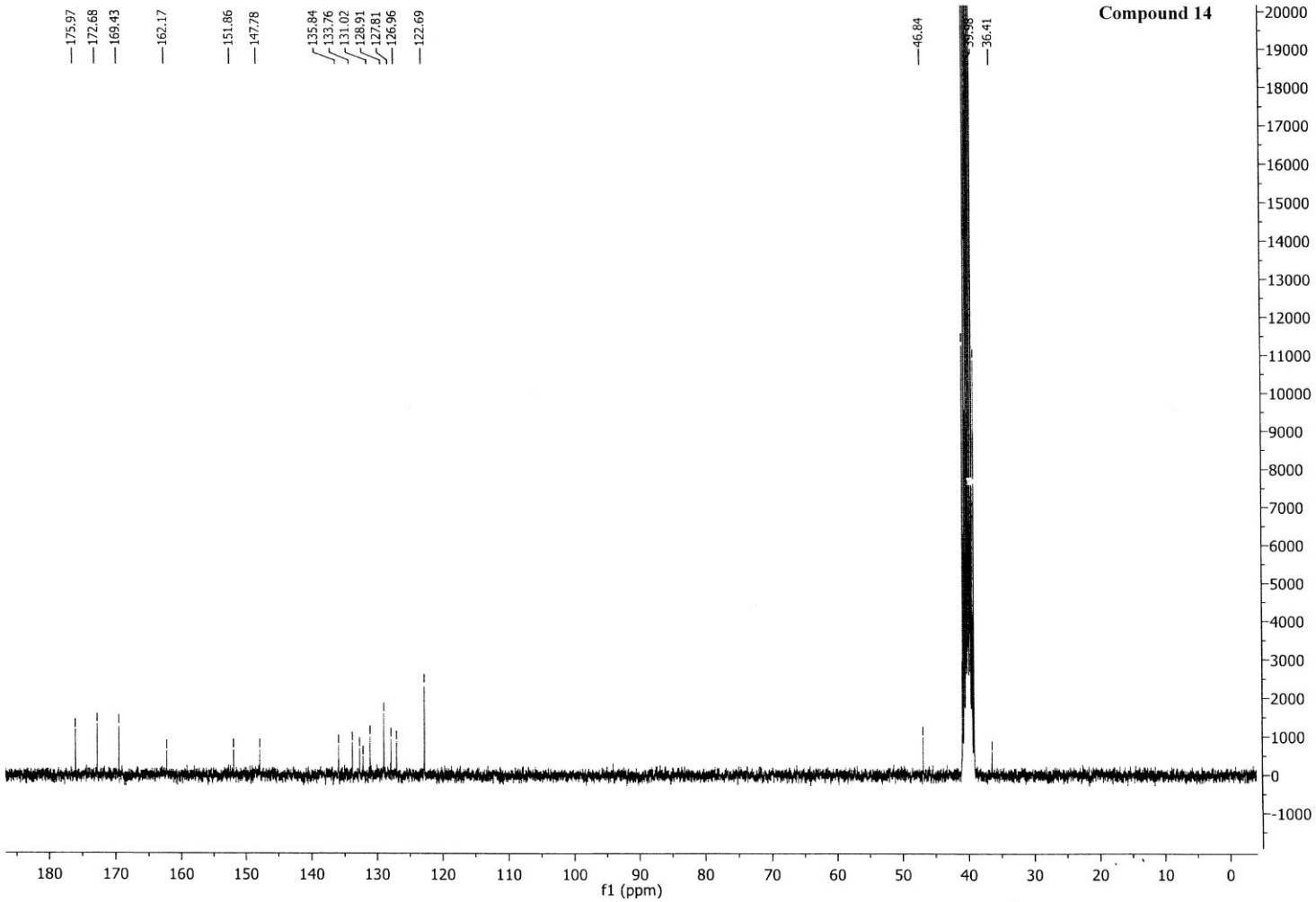
	ppm	Hz	Intensity
1	3.86	1158.9	1647.6
2	2.51	752.1	660.1
3	11.92	3577.5	355.1
4	10.14	3042.9	299.7
5	8.17	2451.0	402.6
6	7.71	2313.9	310.7
7	7.70	2312.2	312.5
8	7.58	2274.4	319.0
9	7.55	2266.9	393.1
10	7.51	2254.7	150.4
11	7.48	2246.4	182.5
12	7.41	2225.6	241.2
13	7.39	2218.1	413.6
14	7.36	2210.0	254.8
15	7.28	2186.6	404.4
16	7.26	2178.4	435.0
17	7.23	2170.1	222.0
18	7.20	2162.7	85.5
19	7.08	2125.5	1218.2
20	3.35	1004.9	90.1
21	12.94	3883.3	6.9

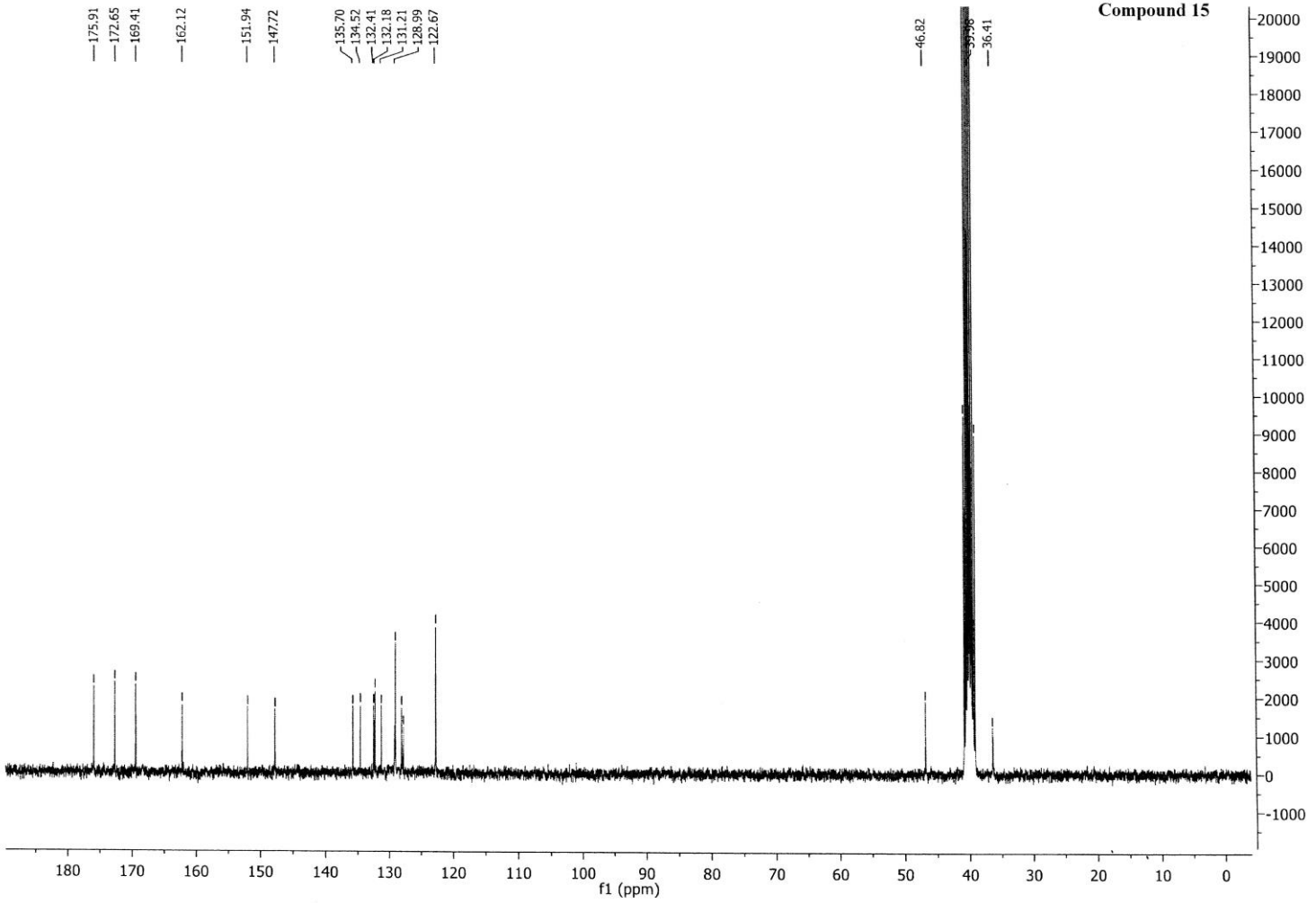


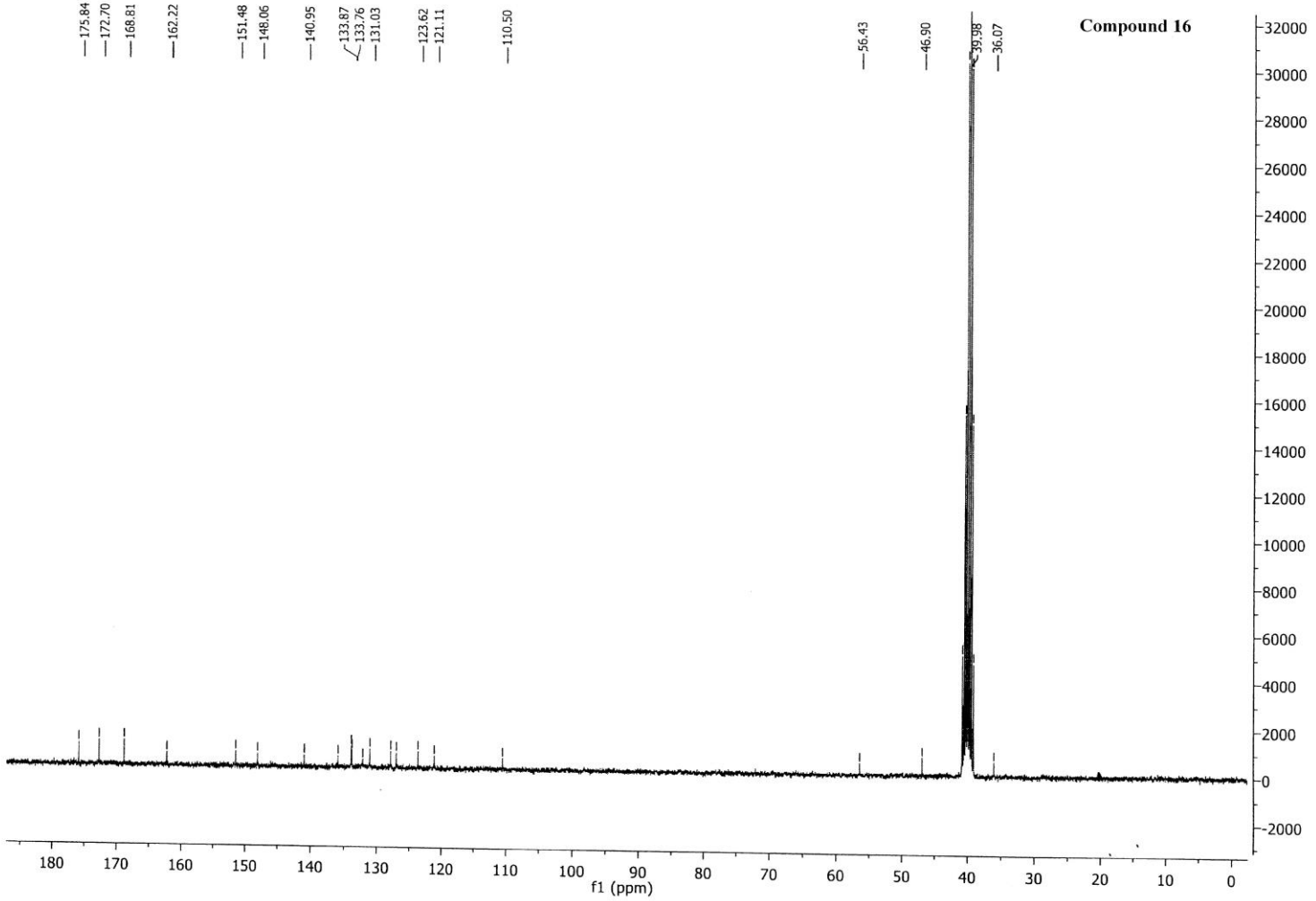
^{13}C NMR spectra for compounds (12-28)

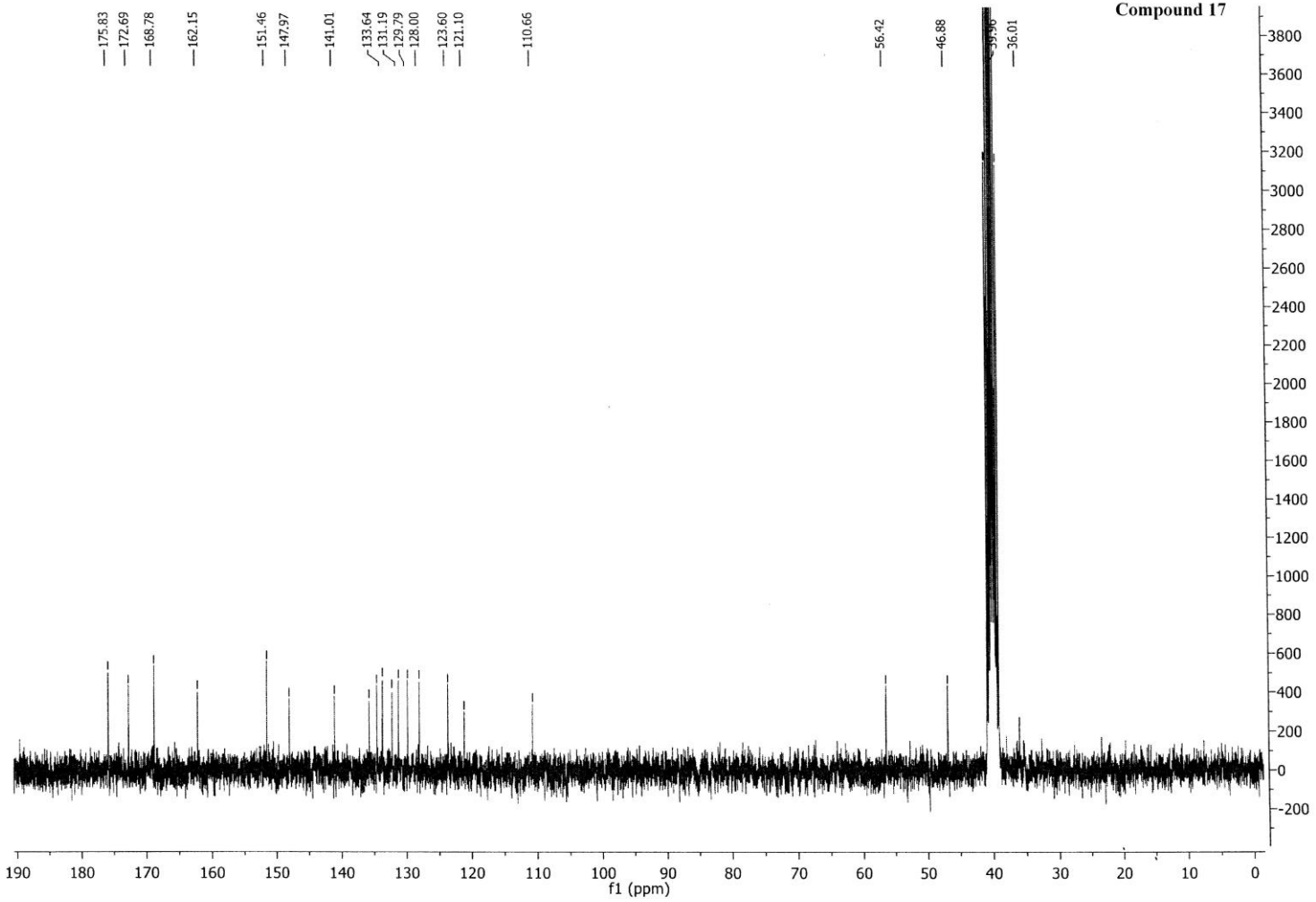


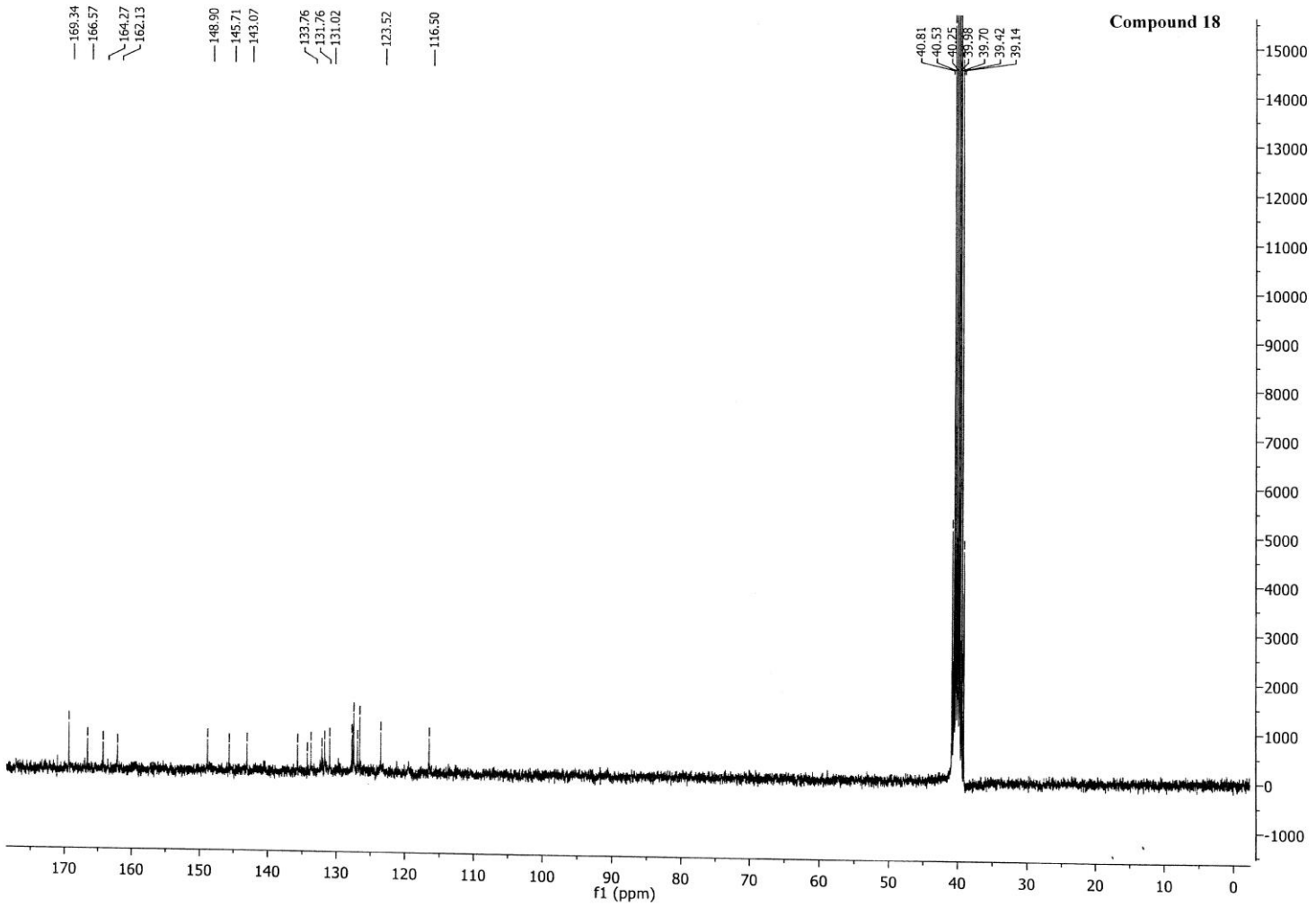

Compound 13
175.98
172.70
169.57
162.19
150.95
147.56
136.11
132.18
131.20
130.68
120.08
46.85
39.98
36.38
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

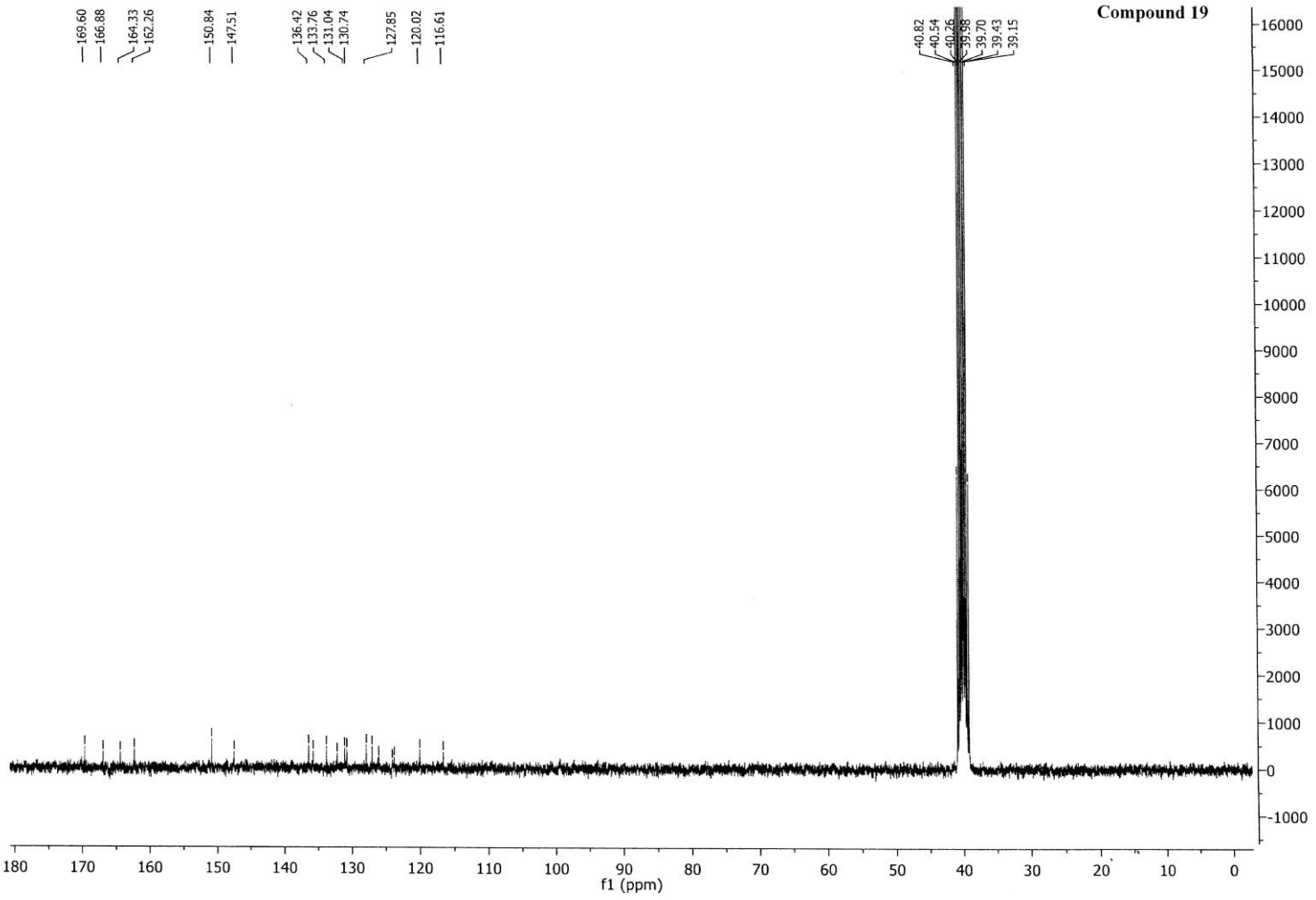

Compound 14
175.97
172.68
169.43
162.17
151.86
147.78
135.84
133.76
131.02
128.91
127.81
126.96
122.69
46.84
39.98
36.41
f1 (ppm)

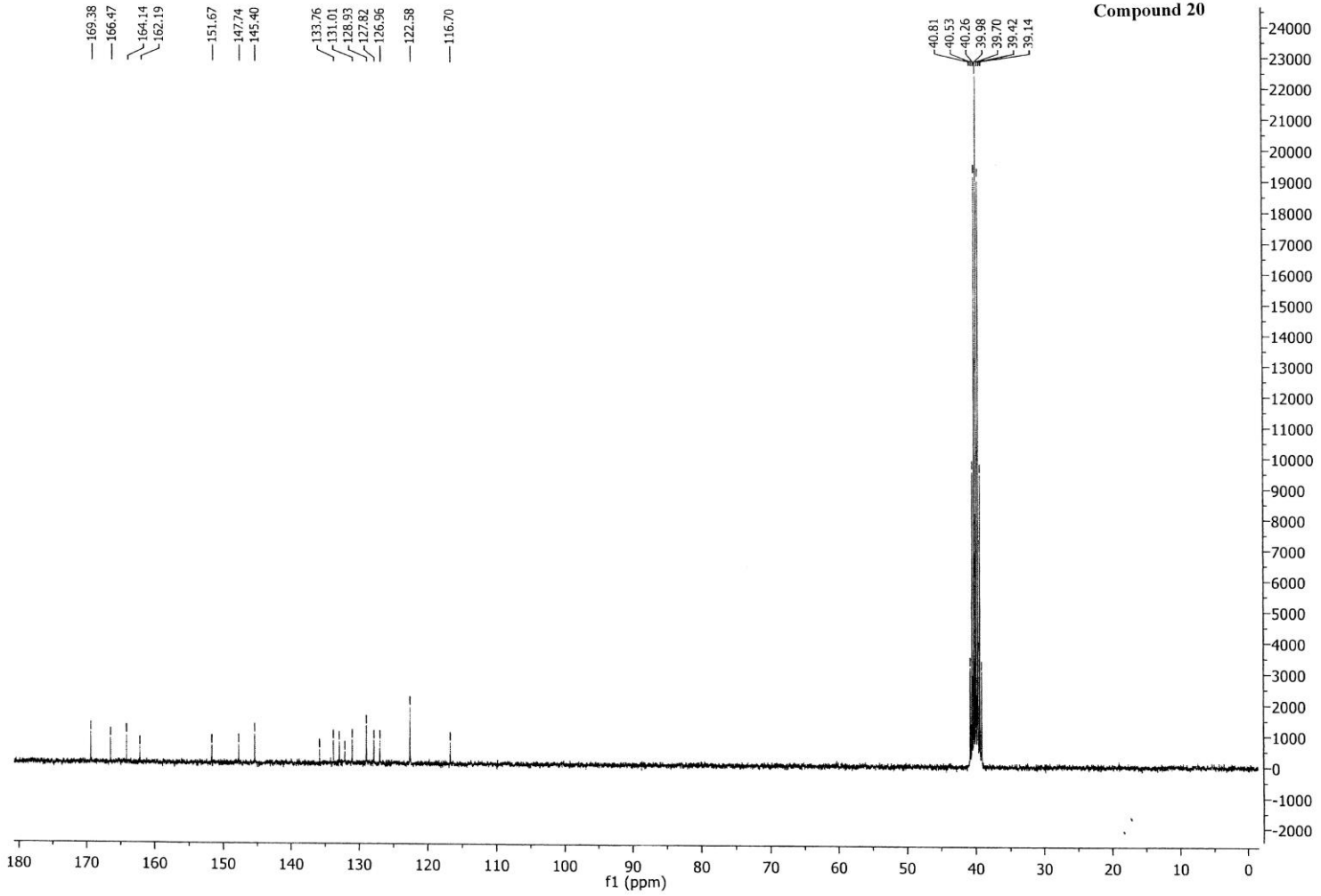

Compound 15
175.91
172.65
169.41
162.12
151.94
147.72
135.70
134.52
132.41
132.18
131.21
128.99
122.67
46.82
33.58
36.41
f1 (ppm)

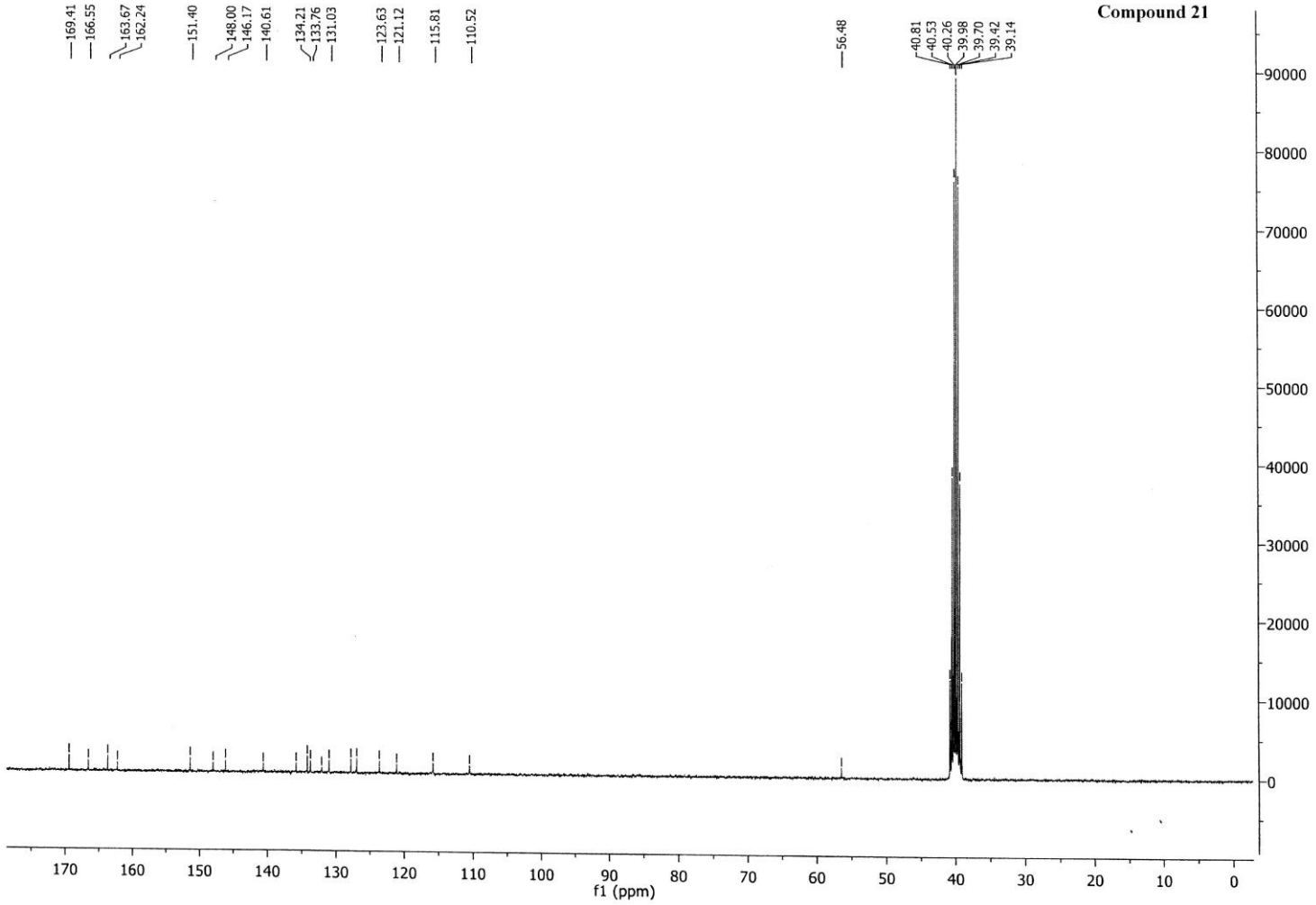

Compound 16
175.84
172.70
168.81
162.22
151.48
148.06
140.95
133.87
133.76
131.03
123.62
121.11
110.50
56.43
46.90
39.98
36.07
f1 (ppm)

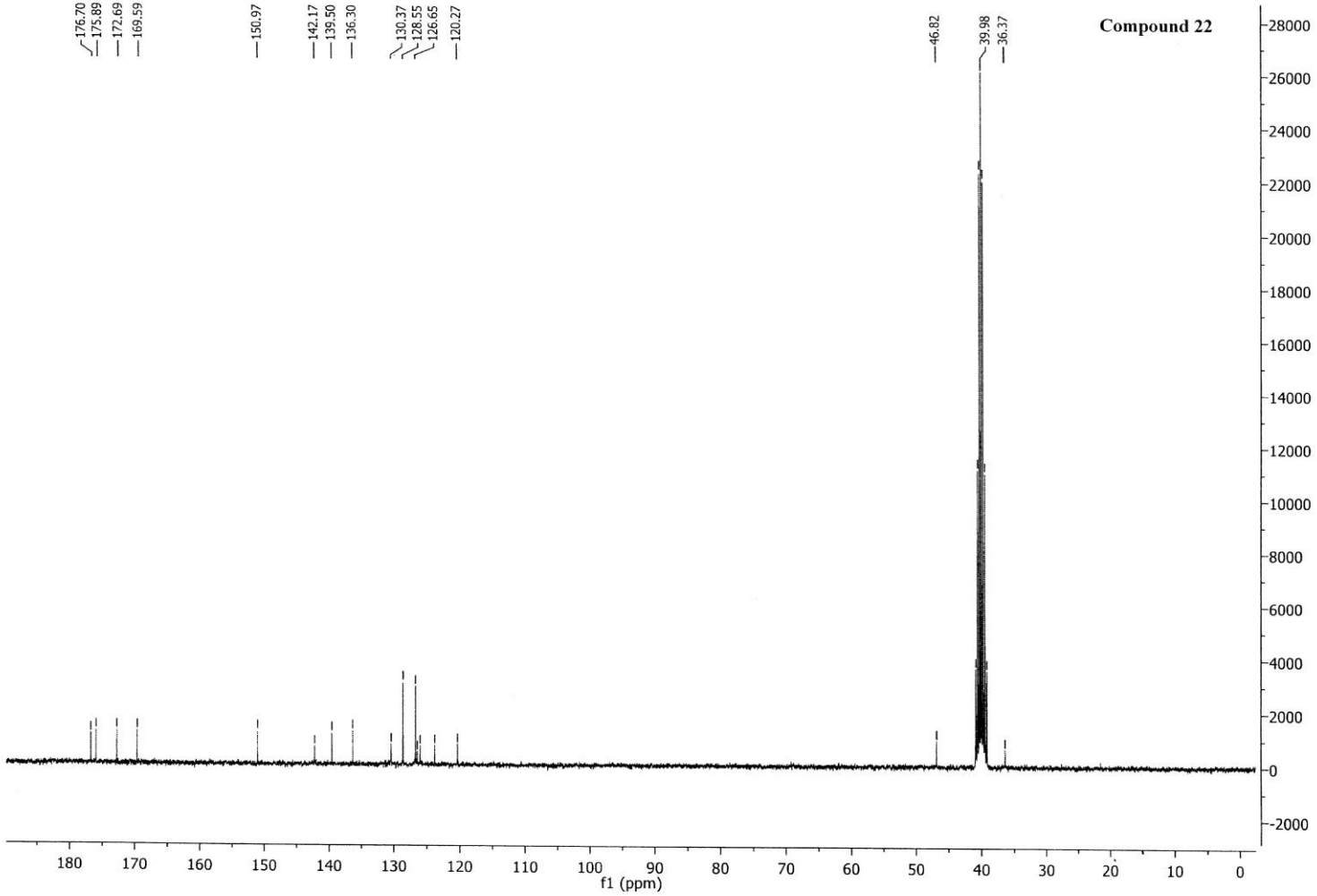

Compound 17
175.83
172.69
168.78
162.15
151.46
147.97
141.01
133.64
131.19
129.79
128.00
123.60
121.10
110.66
56.42
46.88
39.96
36.01
f1 (ppm)

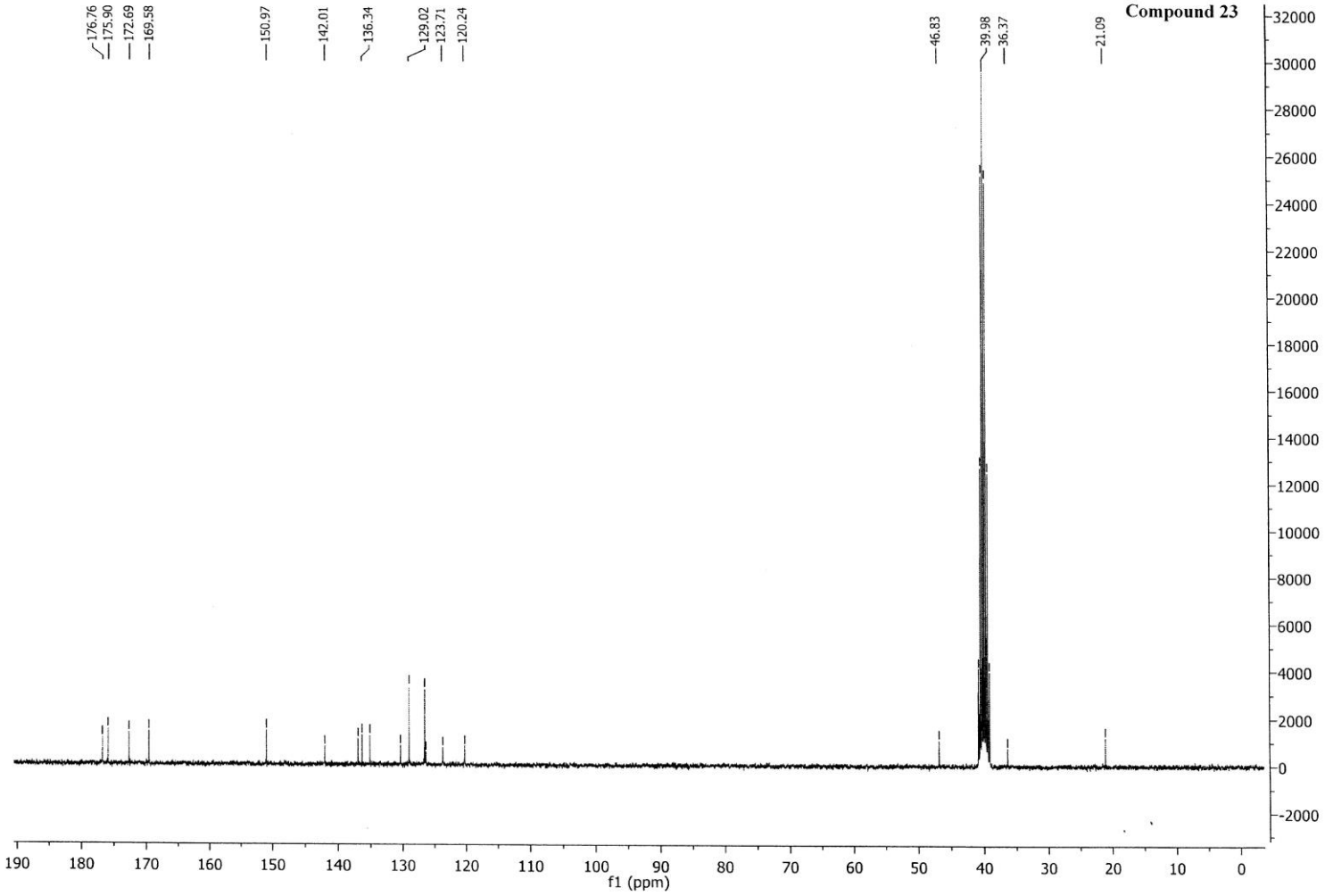

Compound 18
169.34
166.57
164.27
162.13
148.90
145.71
143.07
133.76
131.76
131.02
123.52
116.50
40.81
40.53
40.25
39.98
39.70
39.42
39.14
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

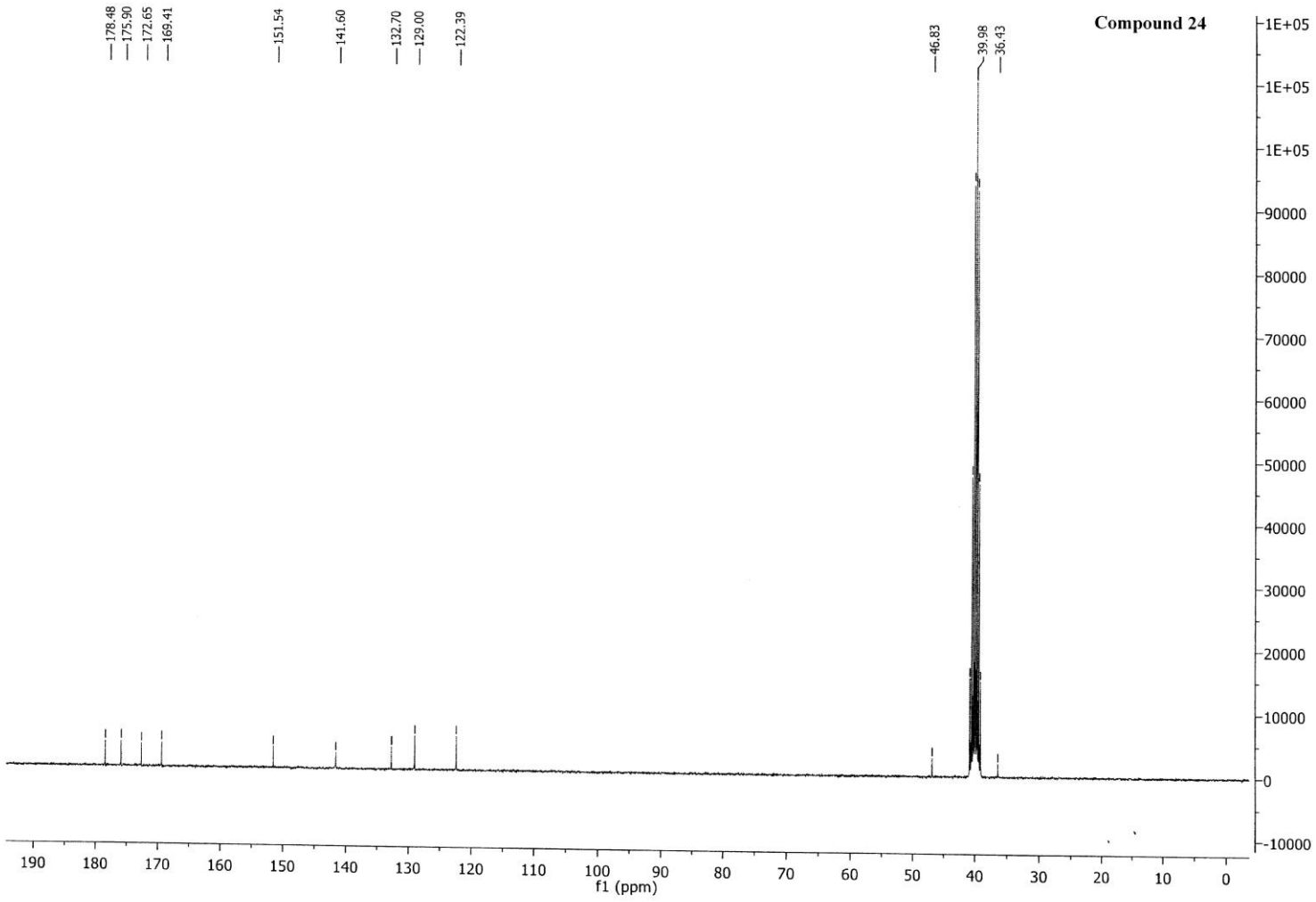

Compound 19
169.60
166.88
164.33
162.26
150.84
147.51
136.42
133.76
131.04
130.74
127.85
120.02
116.61
40.82
40.54
40.26
39.98
39.70
39.43
39.15
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

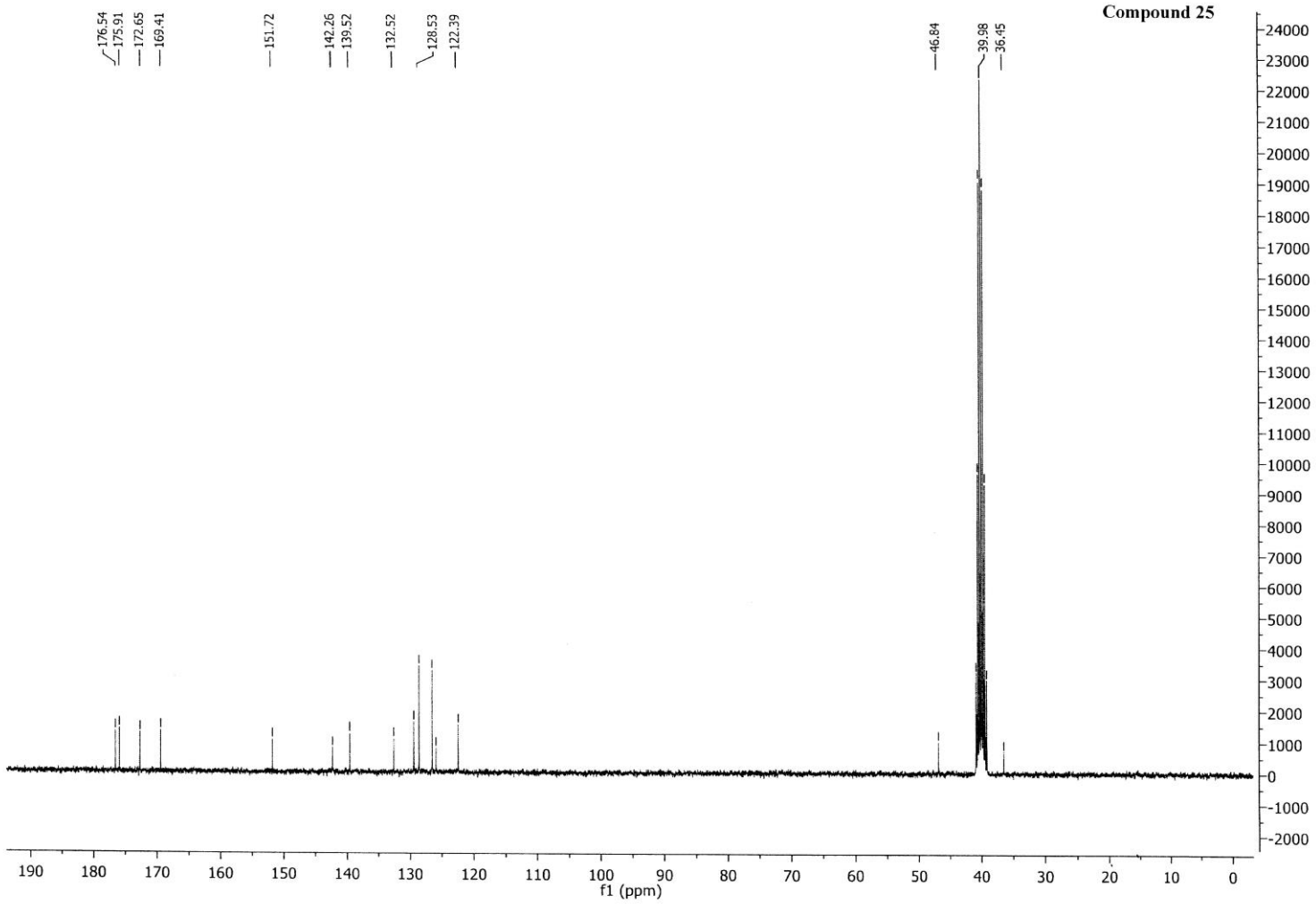

Compound 20
169.38
166.47
164.14
162.19
151.67
147.74
145.40
133.76
131.01
128.93
127.82
126.96
122.58
116.70
40.81
40.53
40.26
39.98
39.70
39.42
39.14
f1 (ppm)

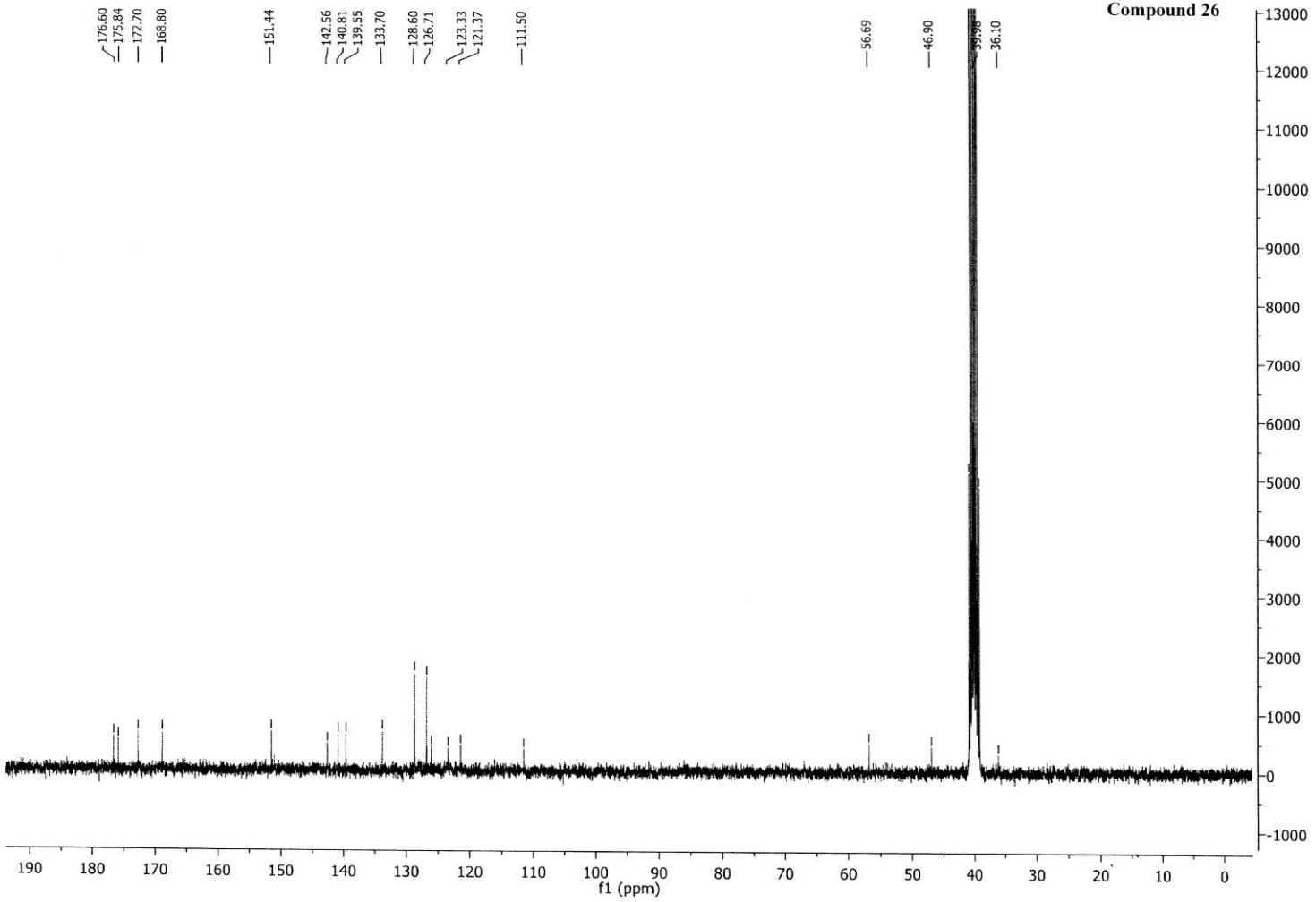

Compound 21
169.41
166.55
163.67
162.24
151.40
148.00
146.17
140.61
134.21
133.76
131.03
123.63
121.12
115.81
110.52
56.48
40.81
40.53
40.26
39.98
39.70
39.42
39.14
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

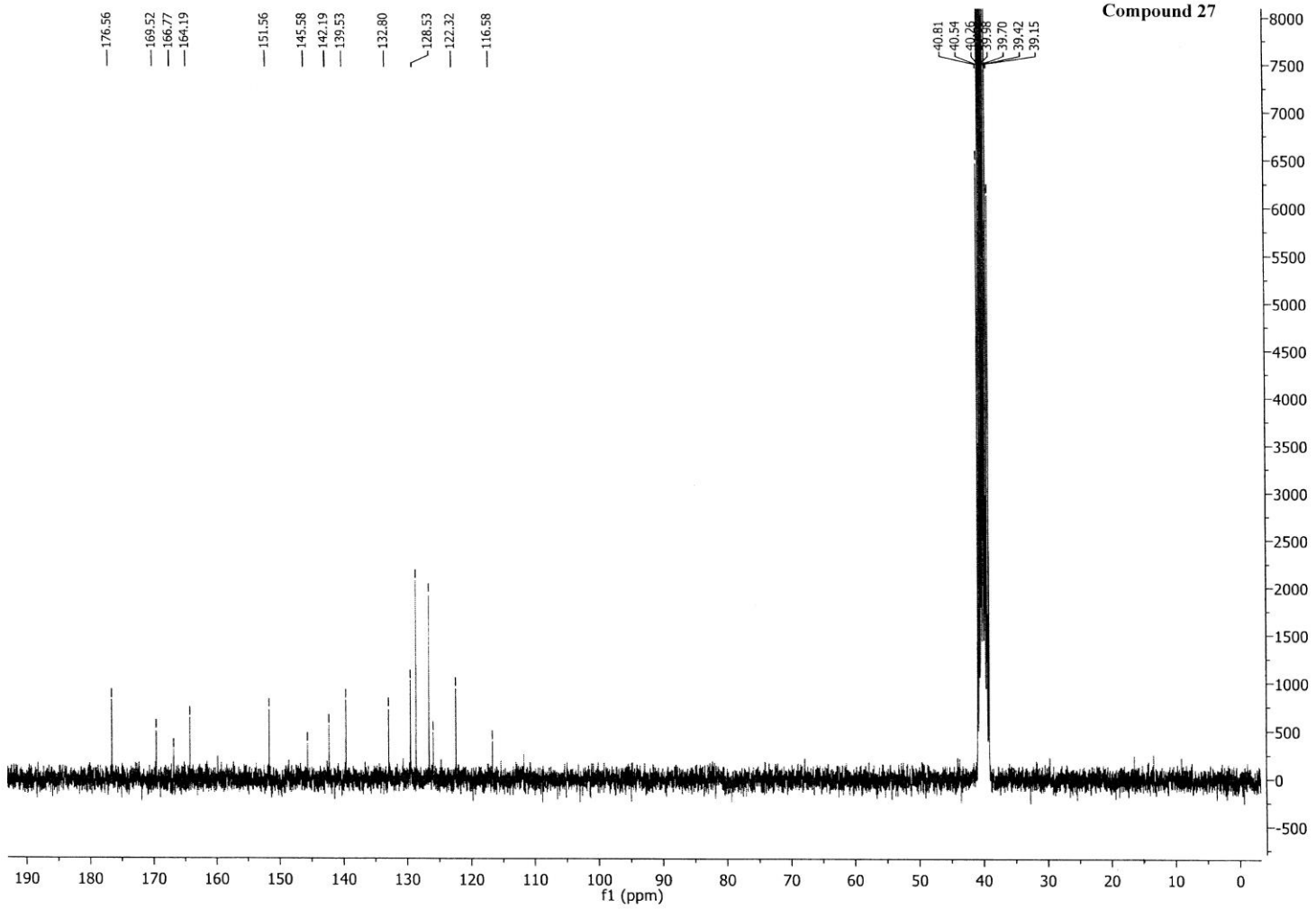

Compound 22
176.70
175.89
172.69
169.59
150.97
142.17
139.50
136.30
130.37
128.55
126.65
120.27
46.82
39.98
36.37
f1 (ppm)

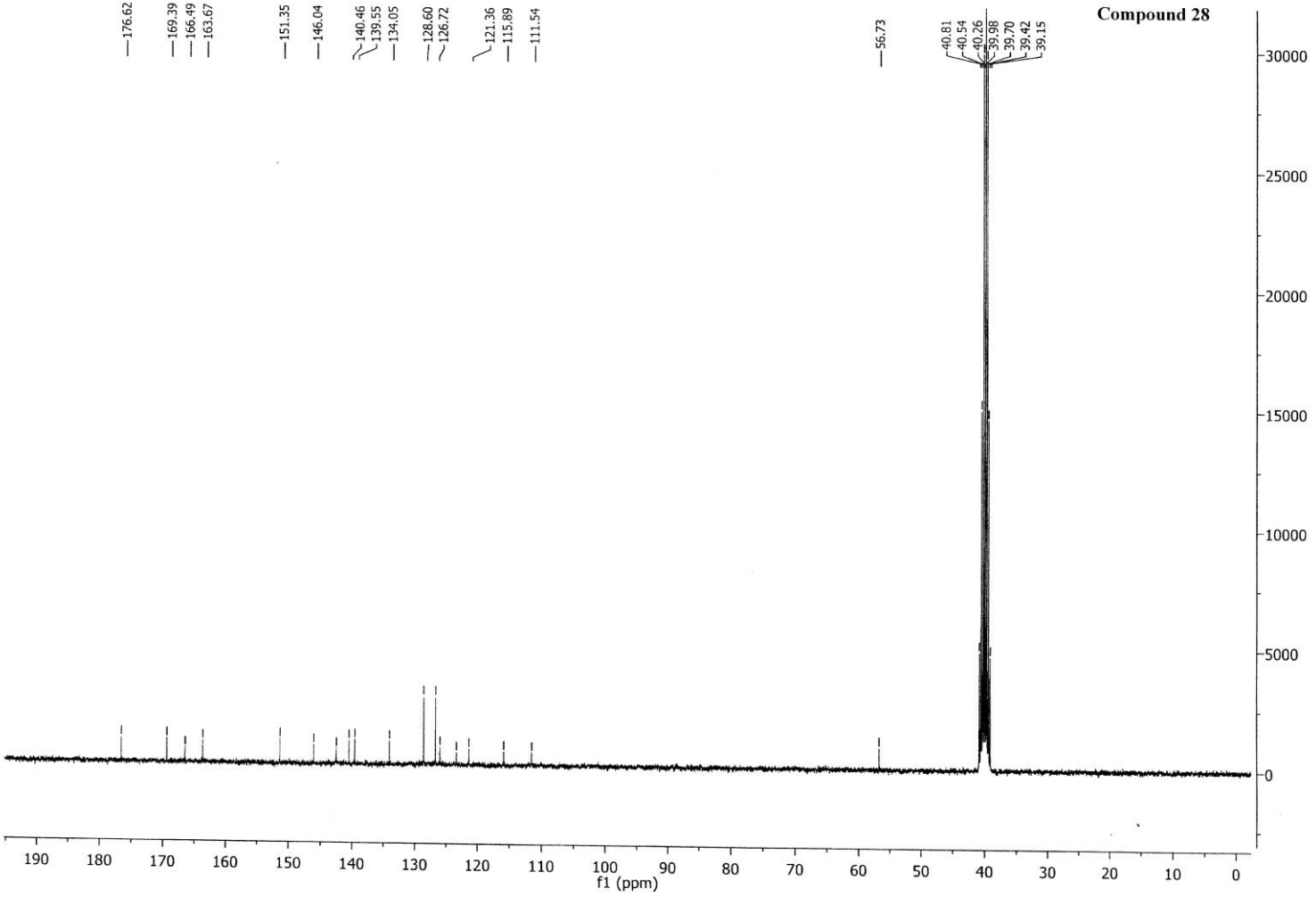

Compound 23
176.76
175.90
172.69
169.58
150.97
142.01
136.34
129.02
123.71
120.24
46.83
39.98
36.37
21.09
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Compound 24
178.48
175.90
172.65
169.41
151.54
141.60
132.70
129.00
122.39
46.83
39.98
36.43
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

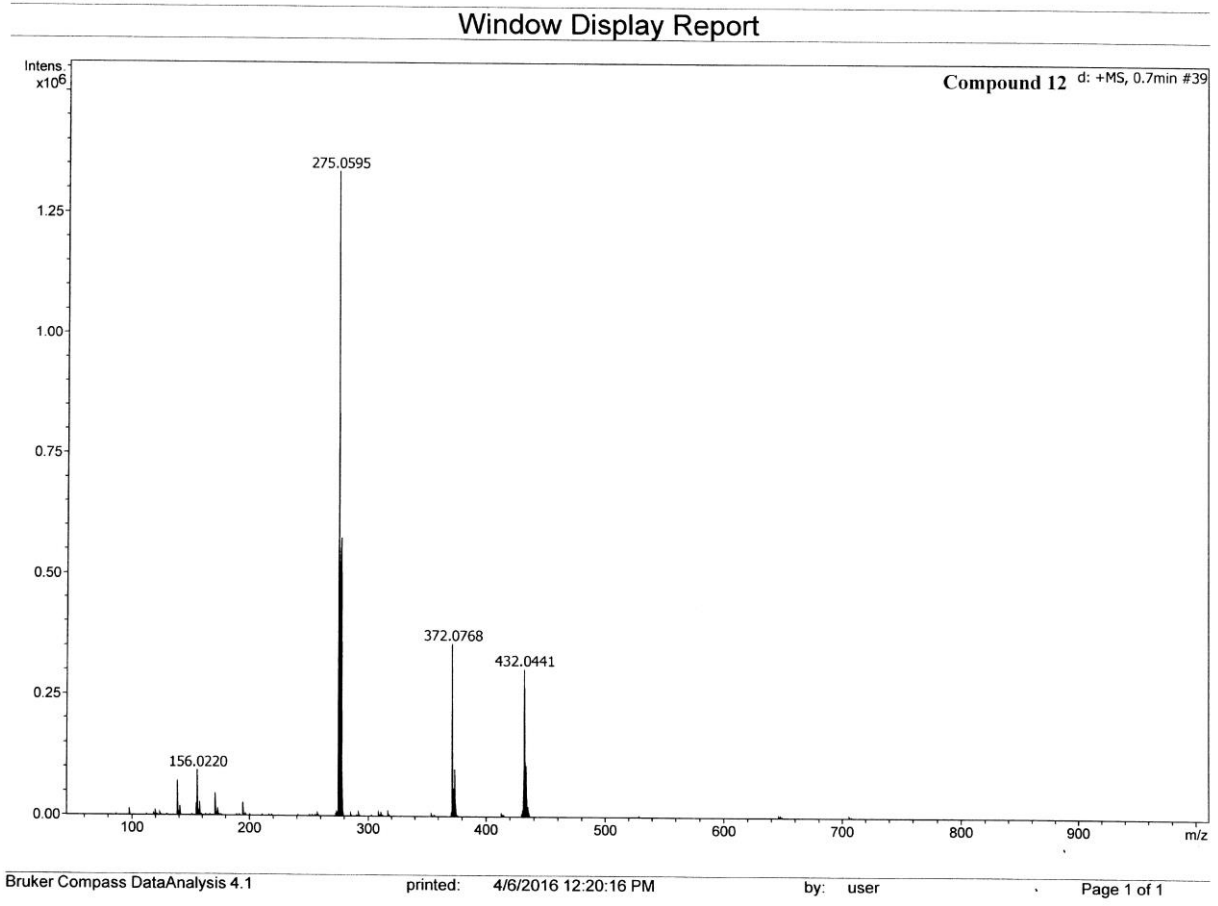

Compound 25
176.54
175.91
172.65
169.41
151.72
142.26
139.52
132.52
128.53
122.39
46.84
39.98
36.45
f1 (ppm)


Compound 26
176.60
175.84
172.70
168.80
151.44
142.56
140.81
139.55
133.70
128.60
126.71
123.33
121.37
111.50
56.69
46.90
39.98
36.10
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

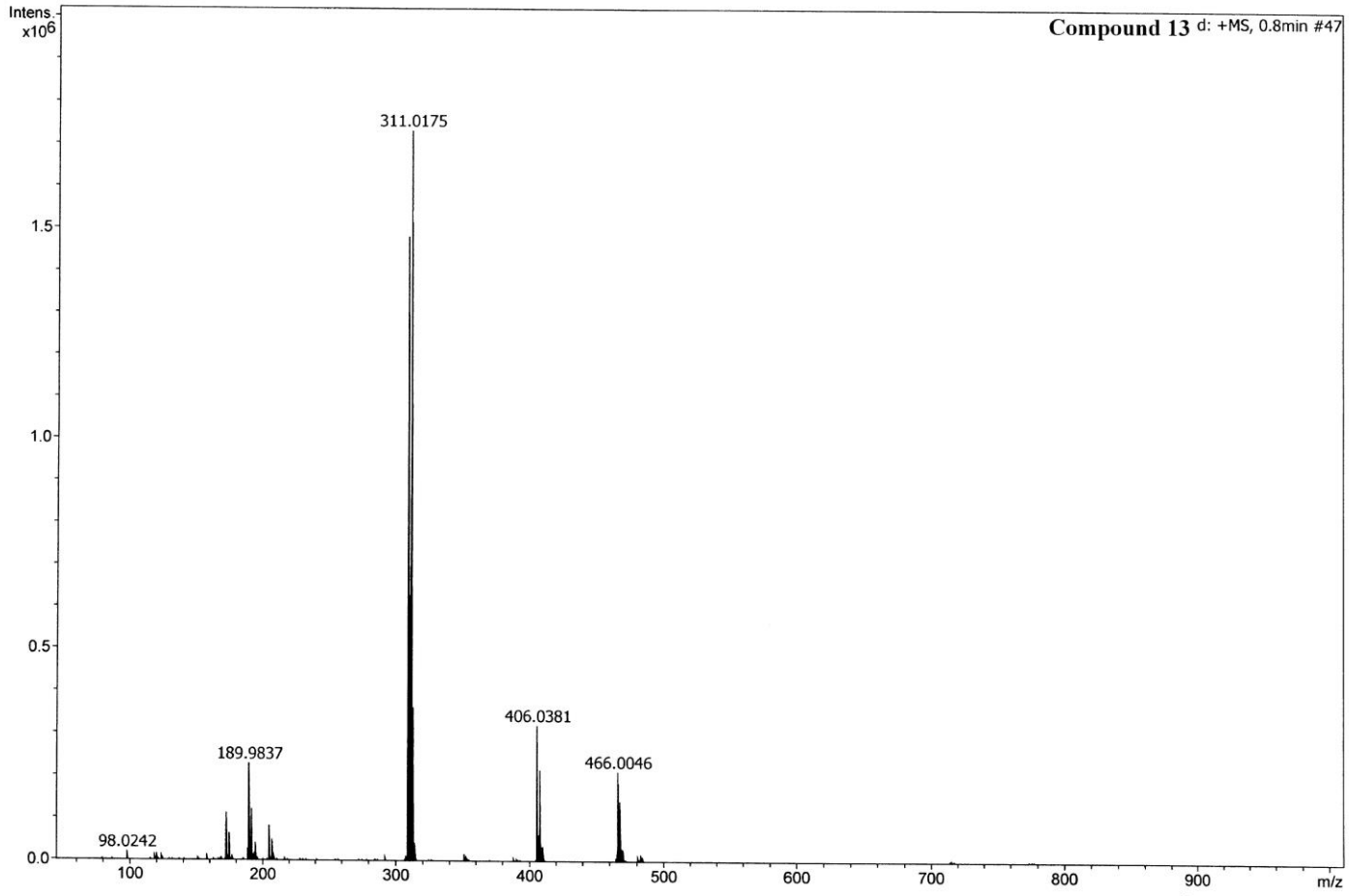

Compound 27
176.56
169.52
166.77
164.19
151.56
145.58
142.19
139.53
132.80
128.53
122.32
116.58
40.81
40.54
40.26
39.98
39.70
39.42
39.15
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Compound 28
176.62
169.39
166.49
163.67
151.35
146.04
140.46
139.55
134.05
128.60
126.72
121.36
115.89
111.54
56.73
40.81
40.54
40.26
39.98
39.70
39.42
39.15
30000
25000
20000
15000
10000
5000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

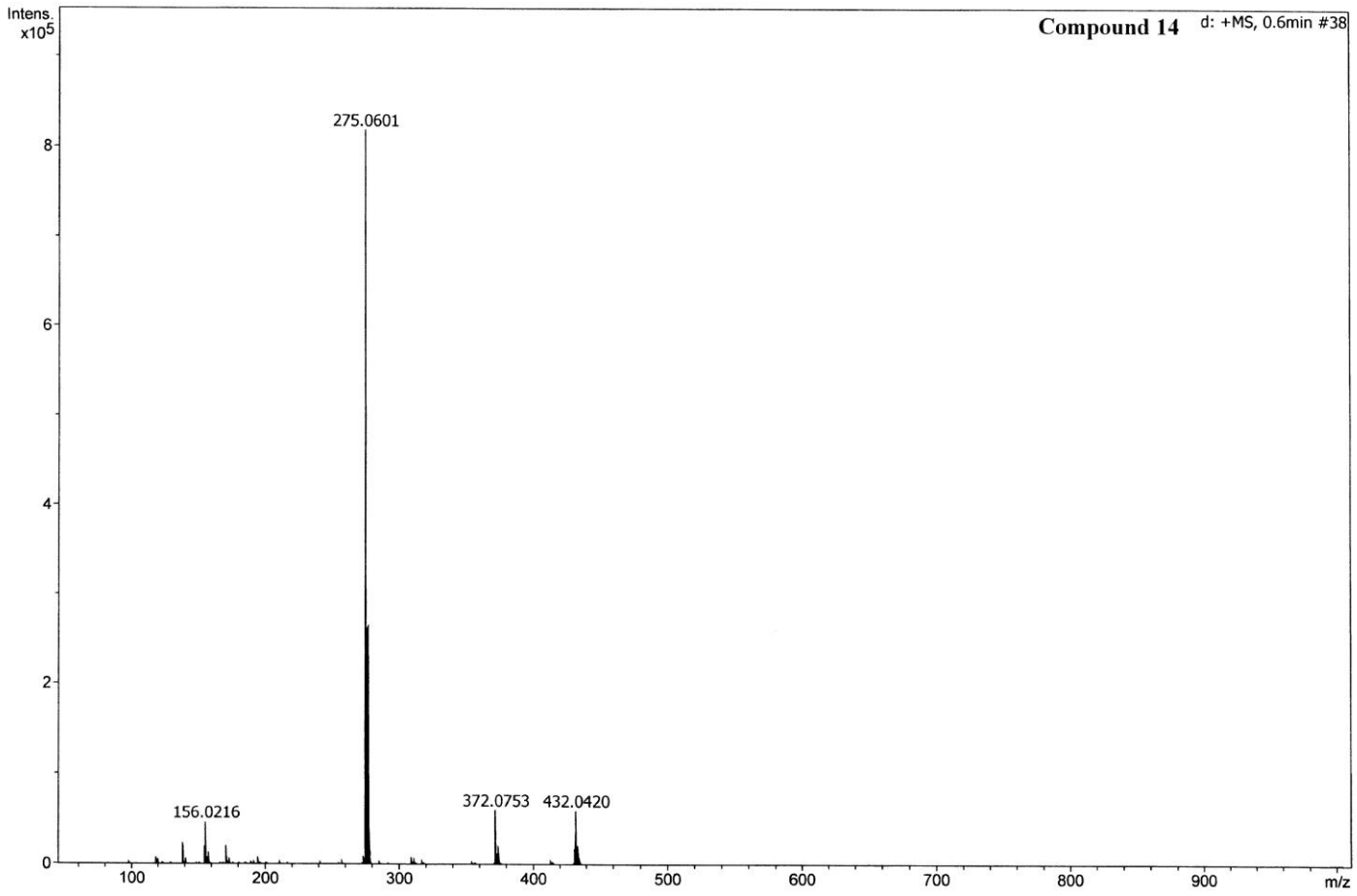
MS spectra for compounds (12-28)



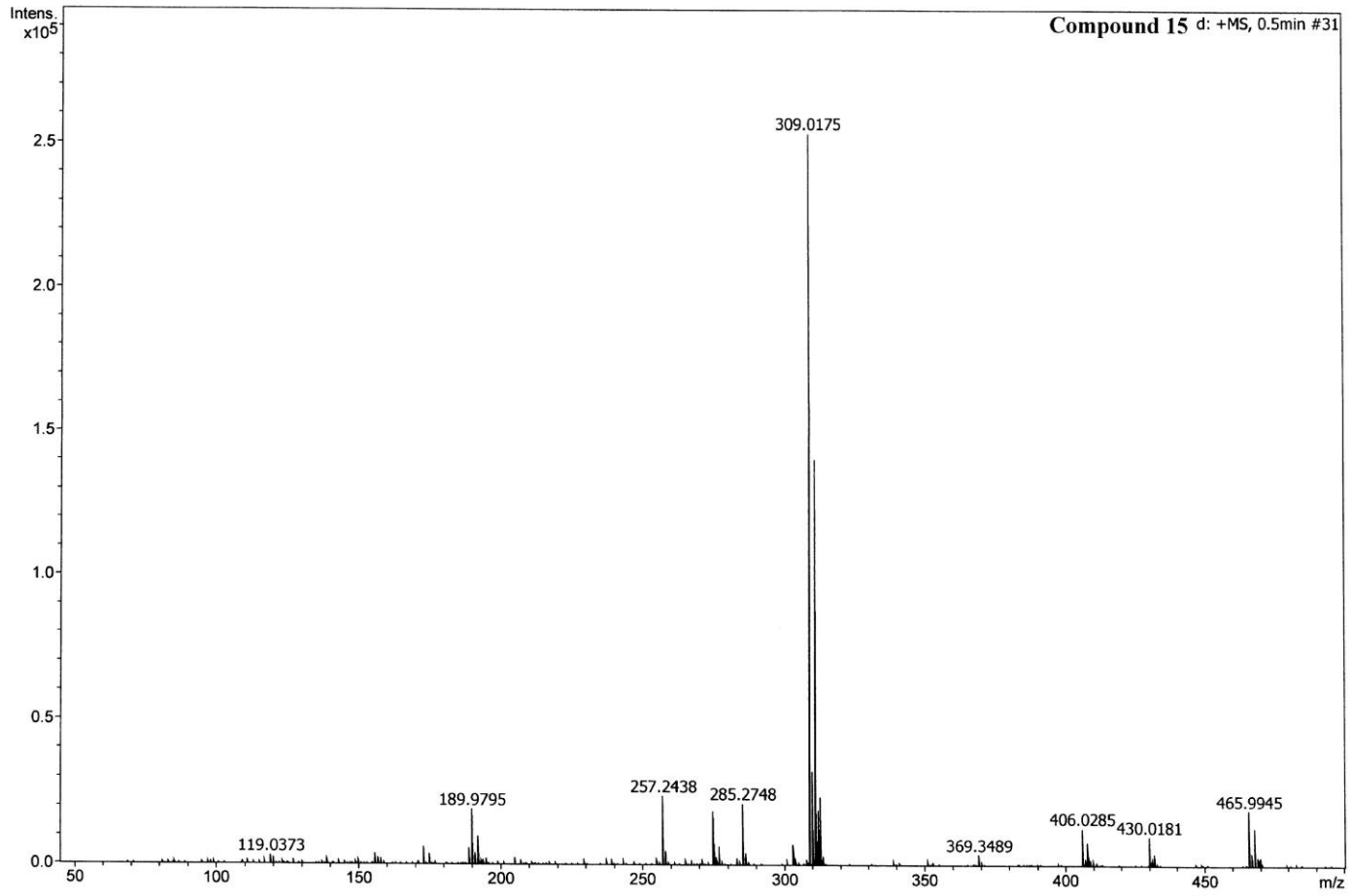
Window Display Report



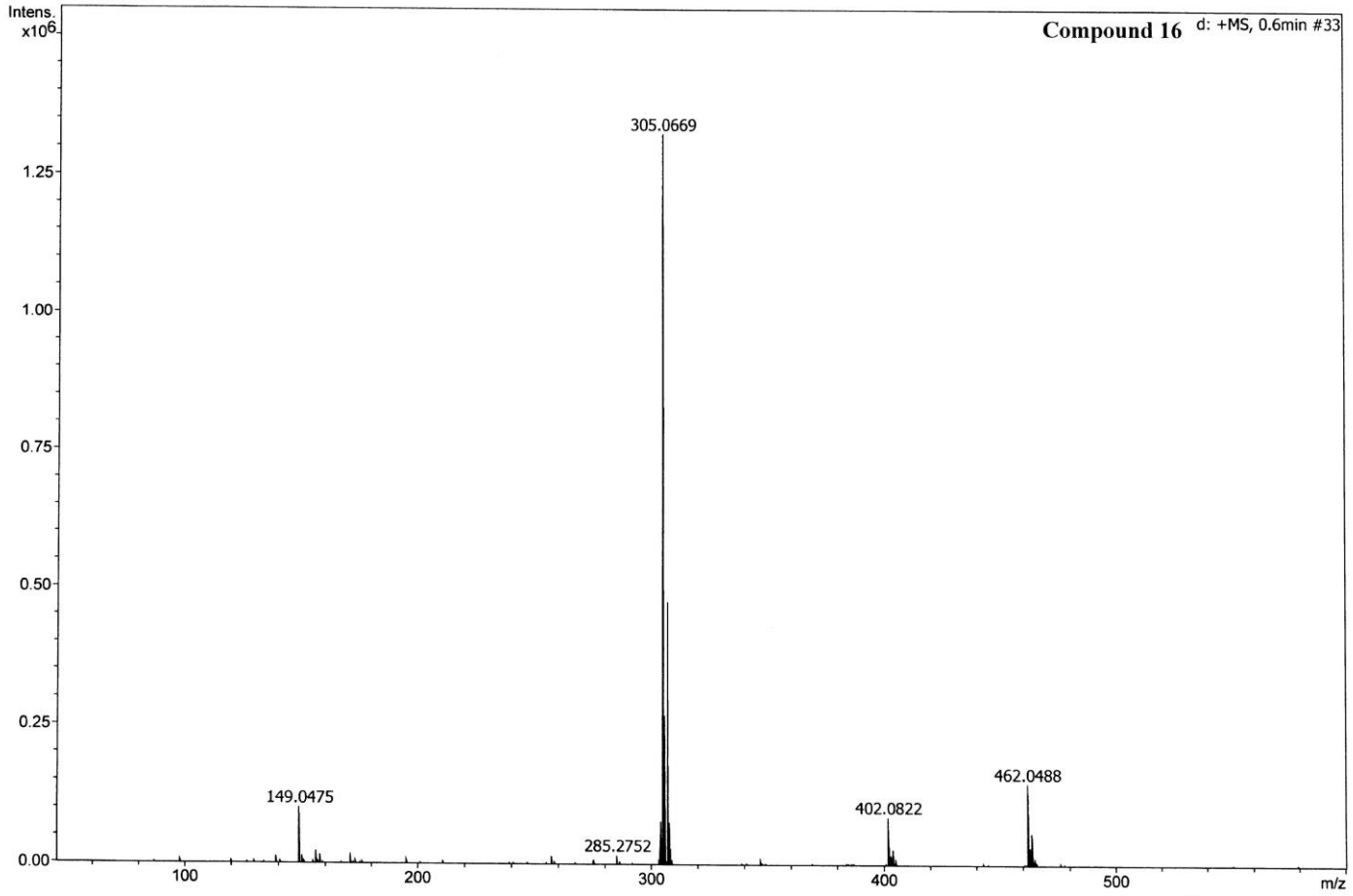
Window Display Report



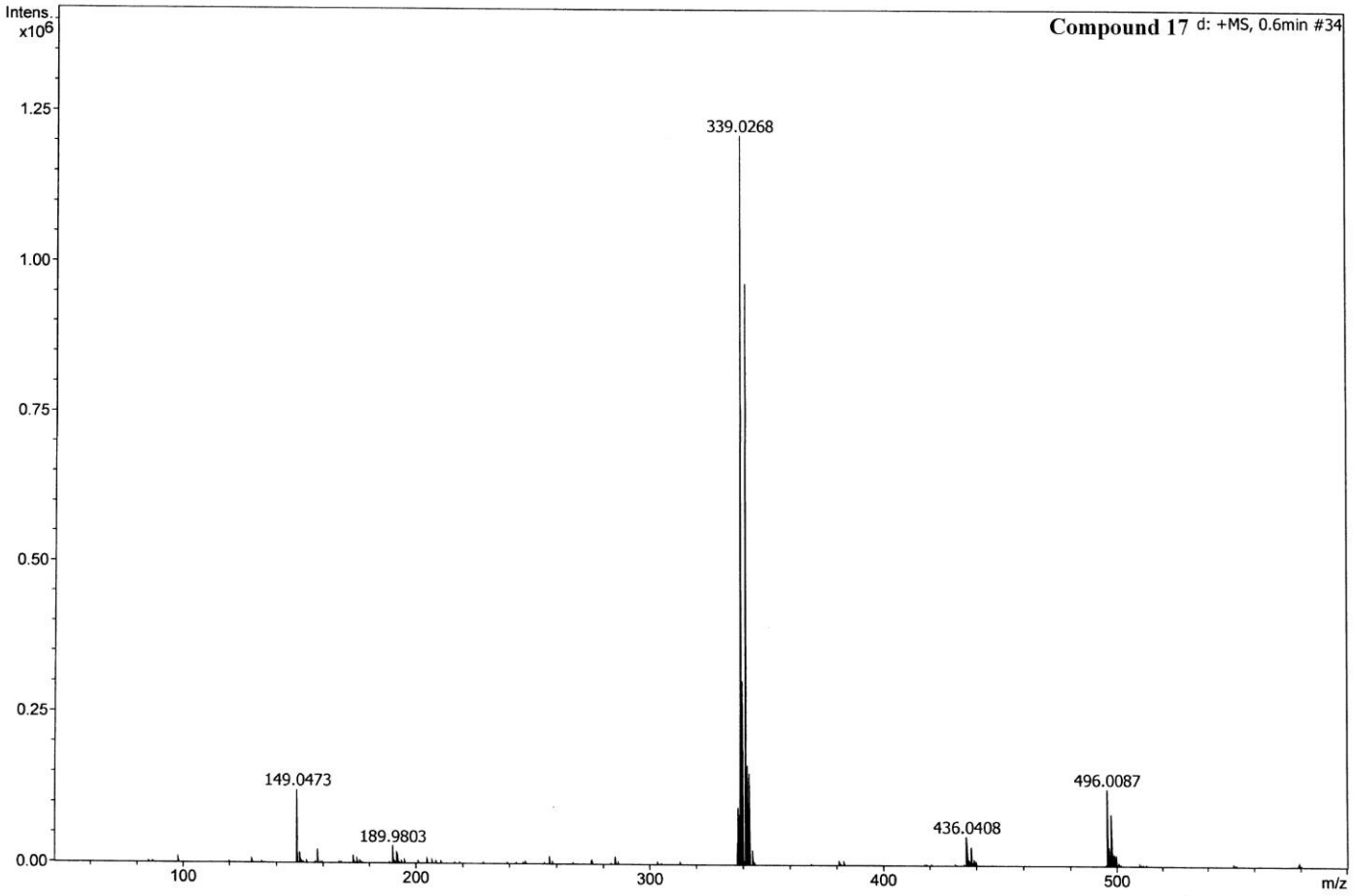
Window Display Report



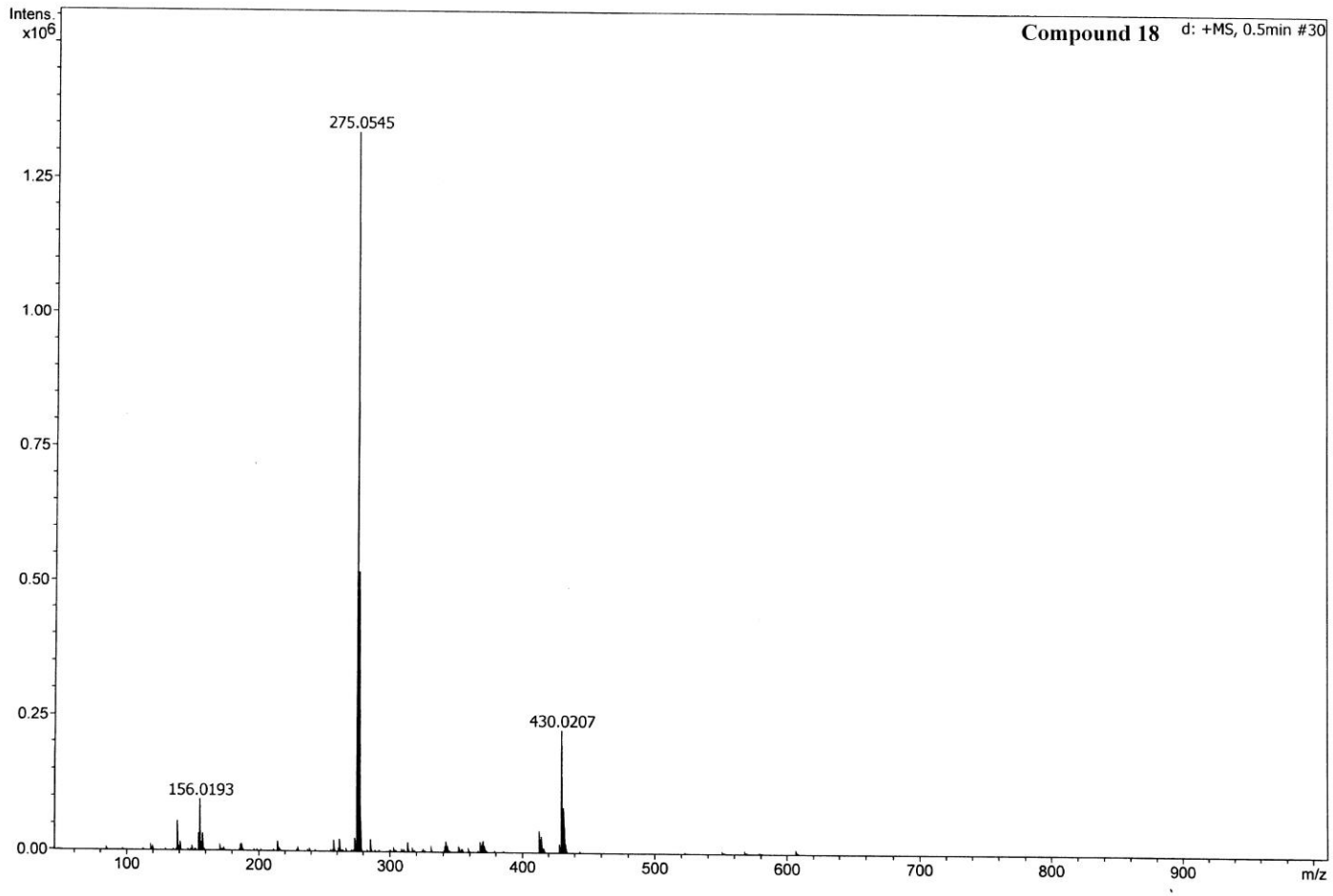
Window Display Report



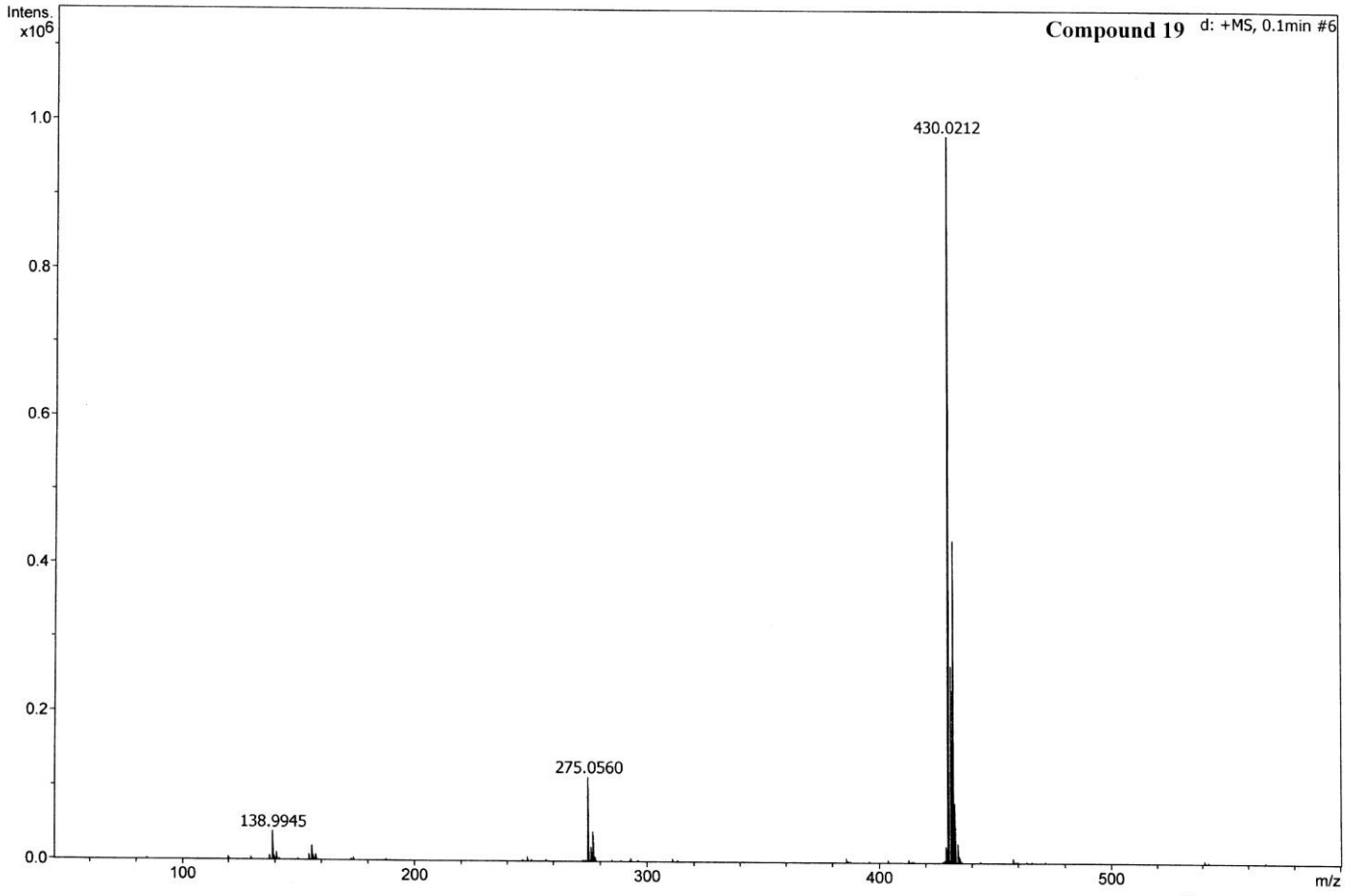
Window Display Report



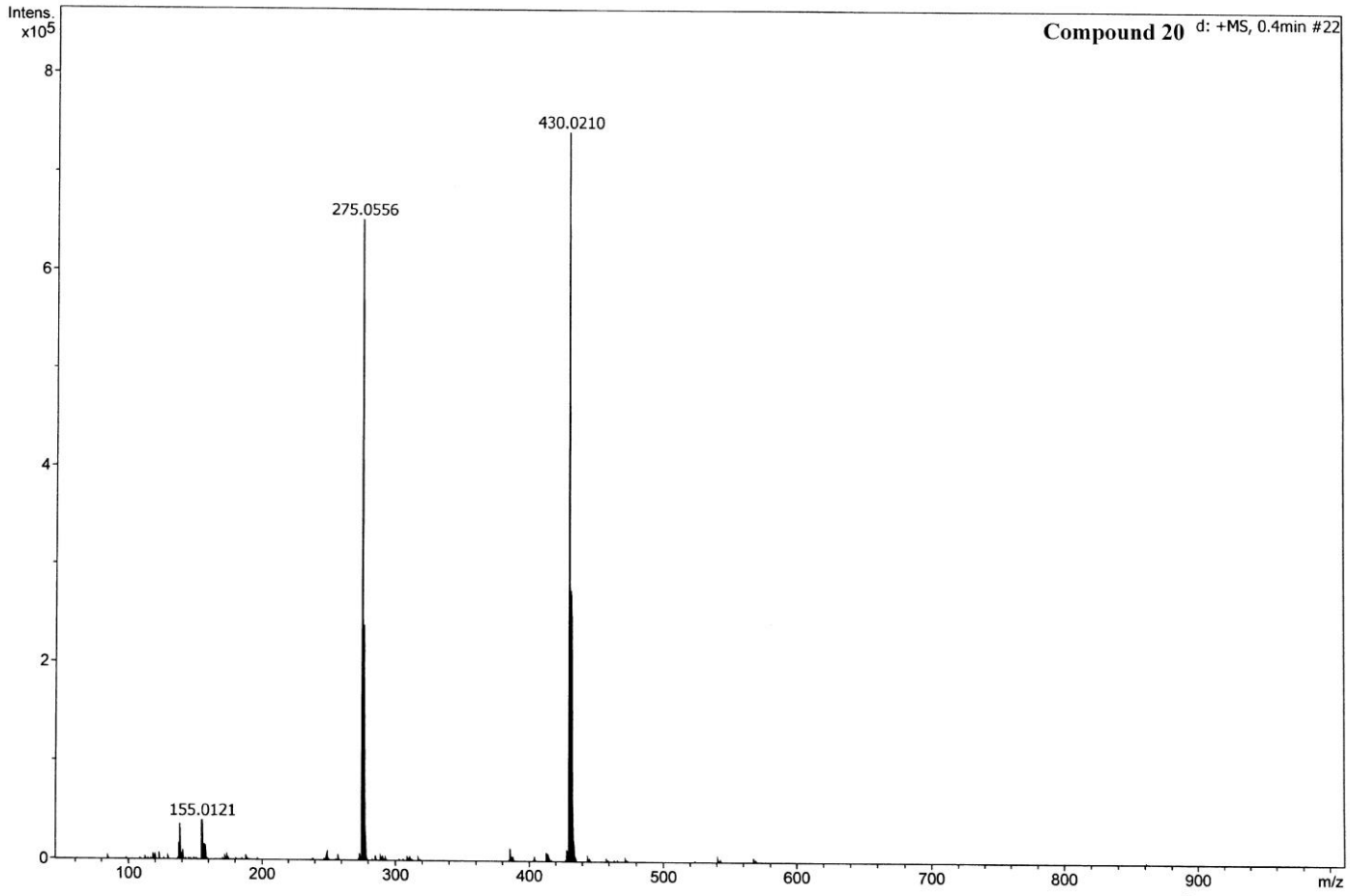
Window Display Report



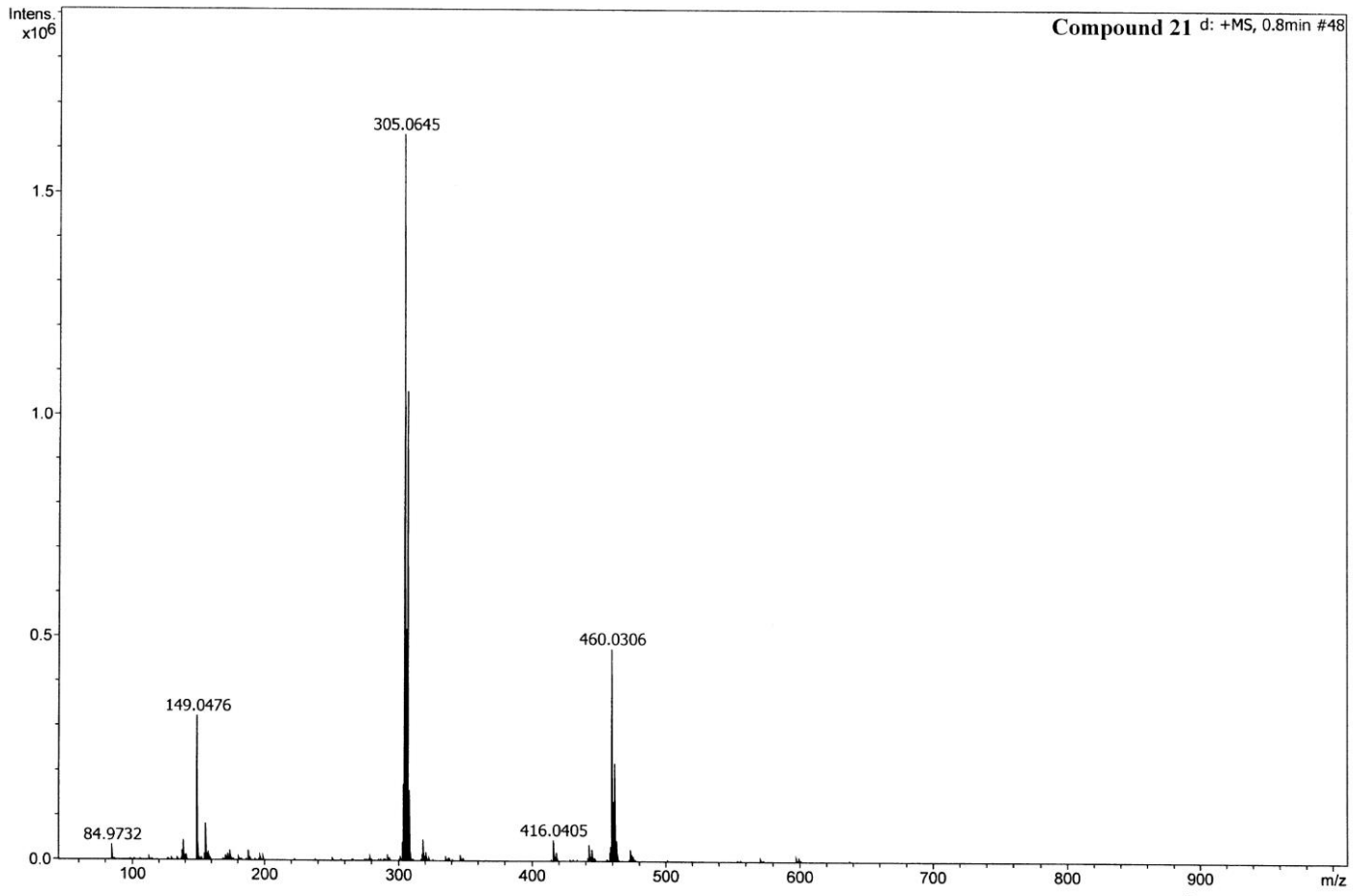
Window Display Report

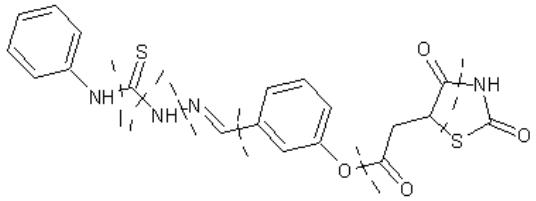


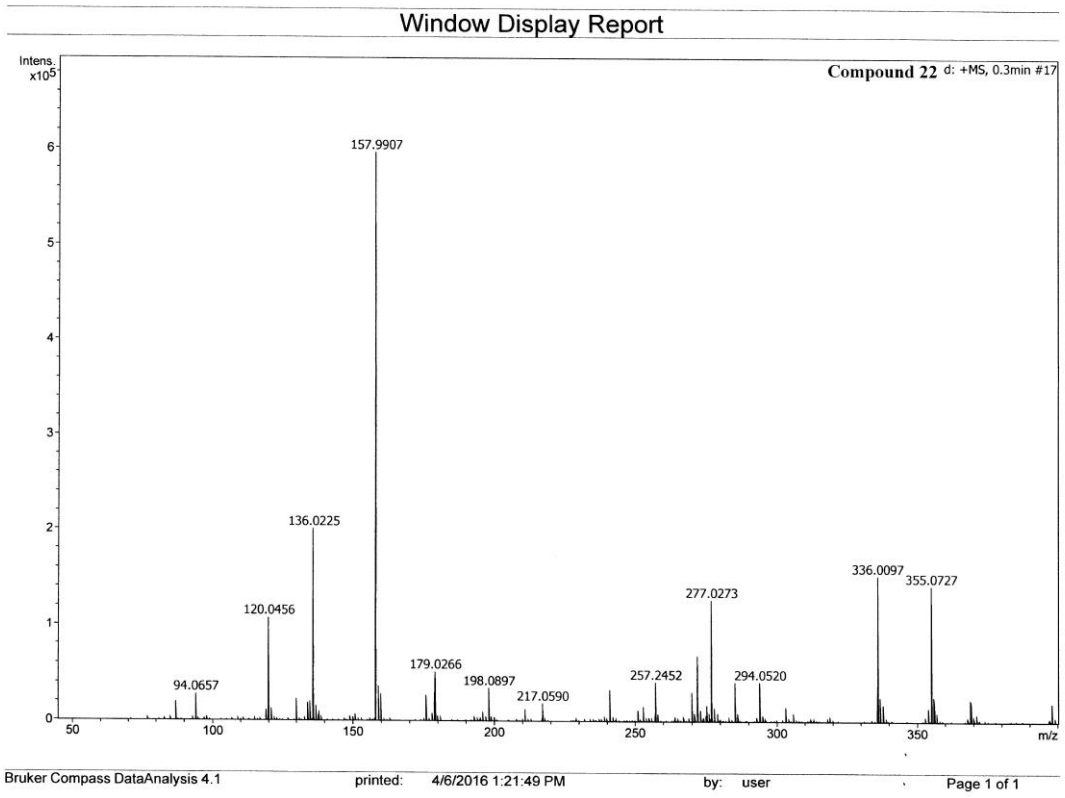
Window Display Report



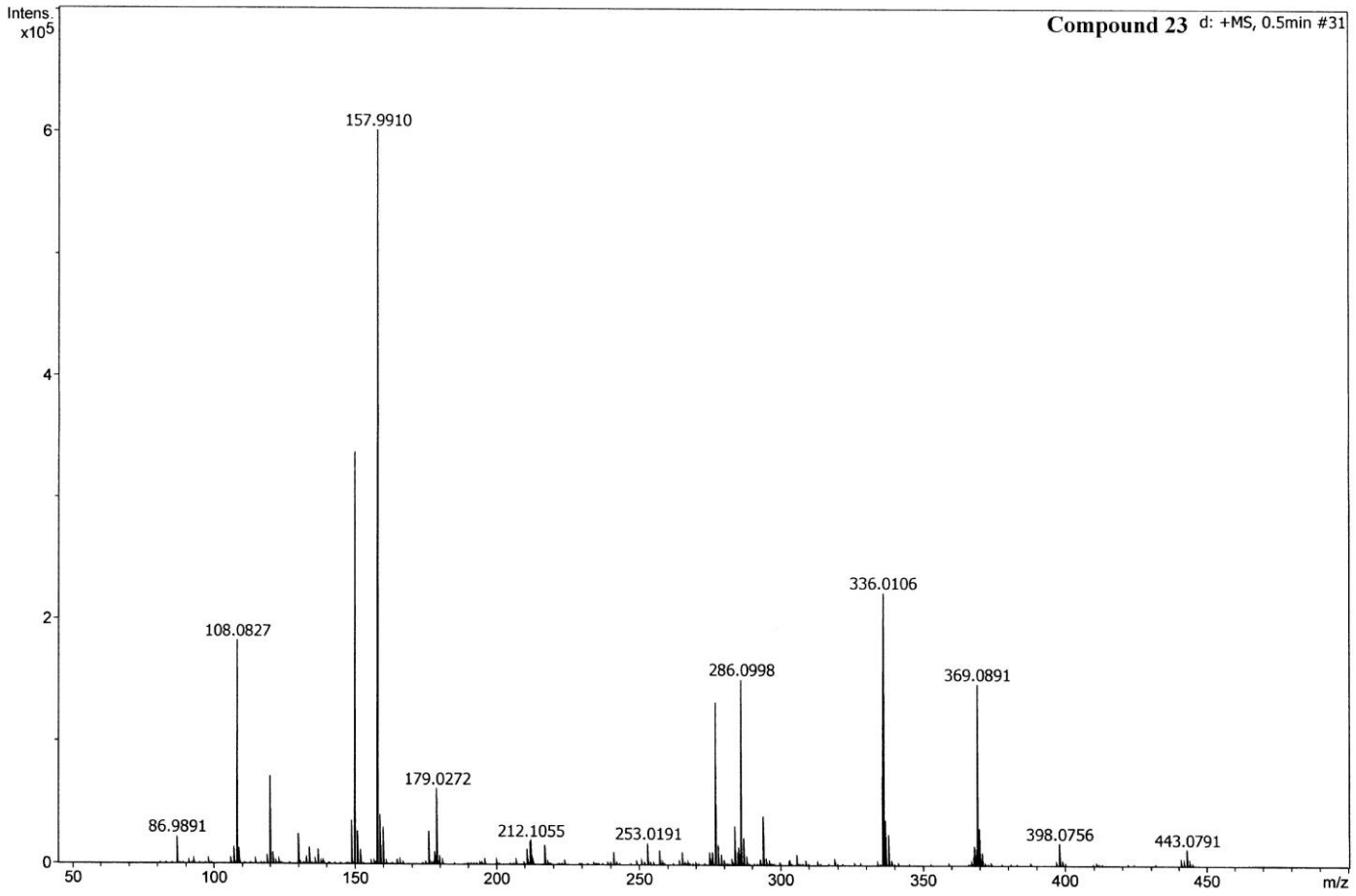
Window Display Report



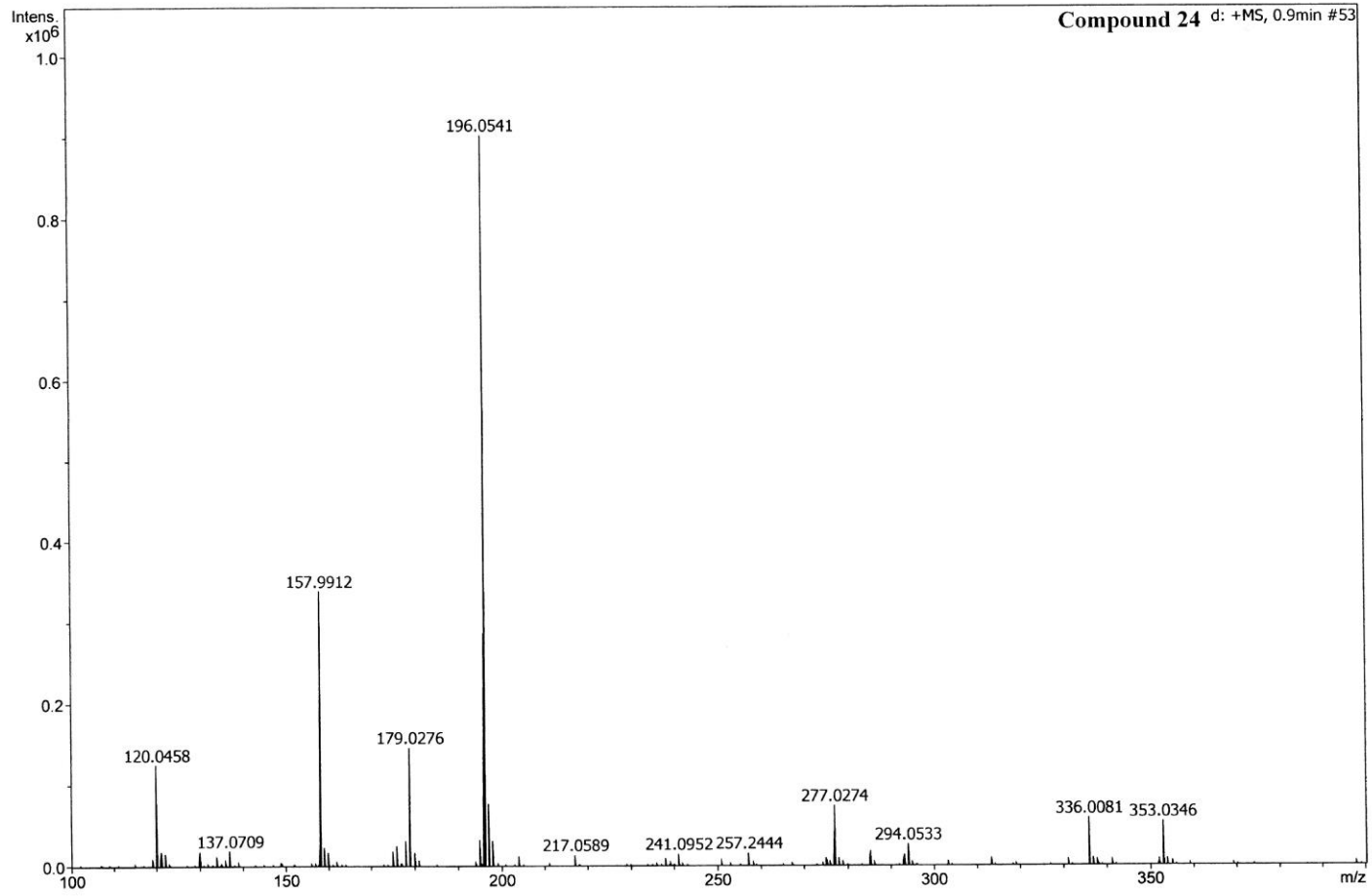

S
NH
NH
N
O
NH
O
S
O
O

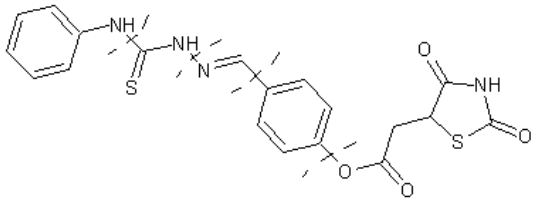

Window Display Report
Intens.
x10^5
Compound 22 d: +MS, 0.3min #17
157.9907
136.0225
120.0456
94.0657
179.0266
198.0897
217.0590
257.2452
277.0273
294.0520
336.0097
355.0727
m/z
Bruker Compass DataAnalysis 4.1
printed: 4/6/2016 1:21:49 PM
by: user
Page 1 of 1

Window Display Report

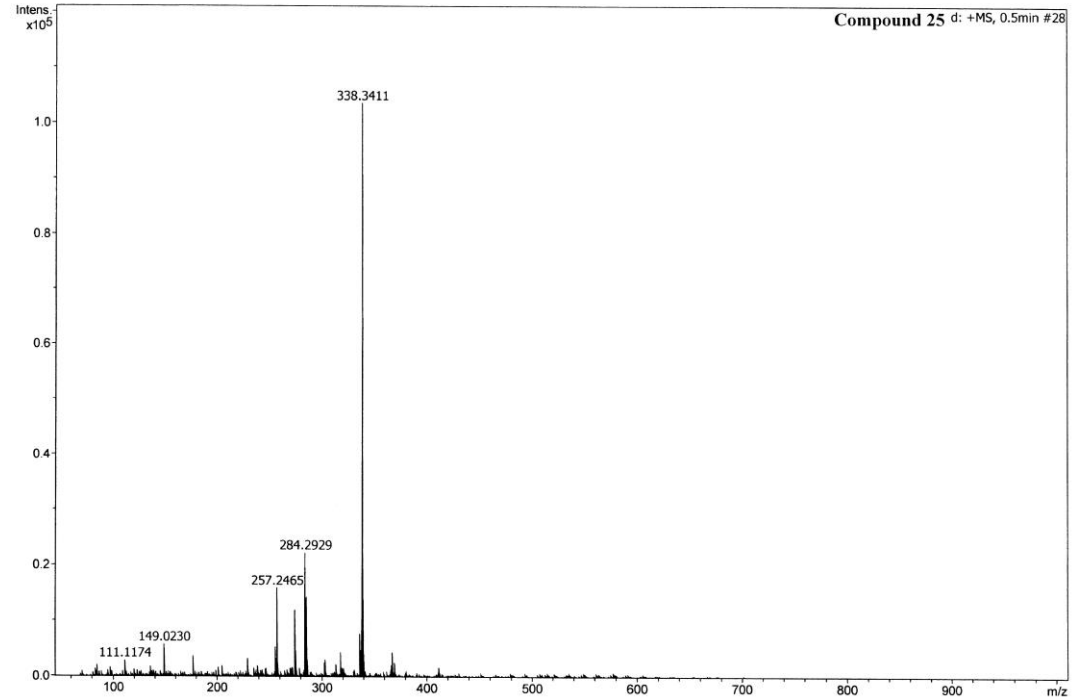


Window Display Report



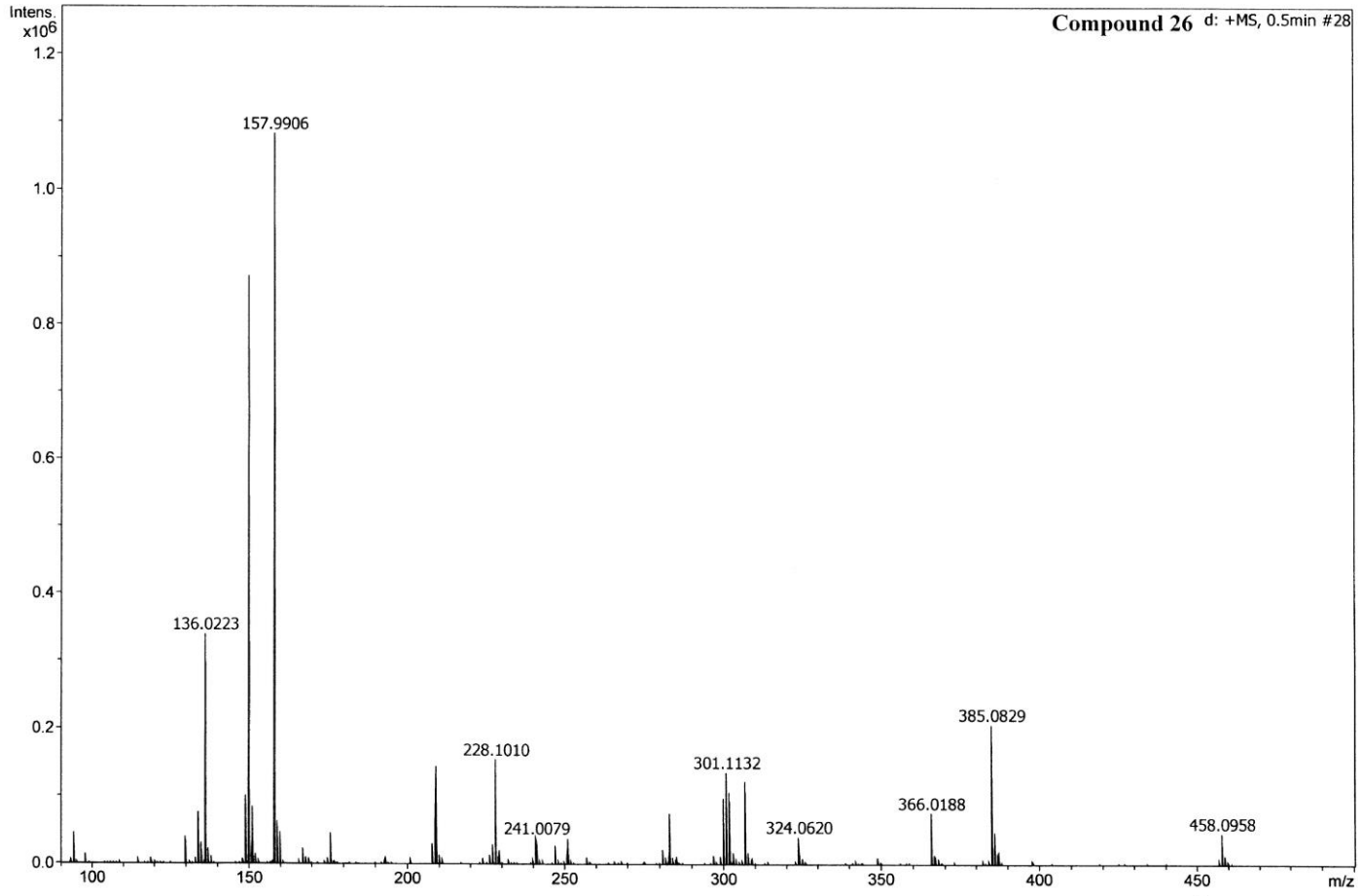


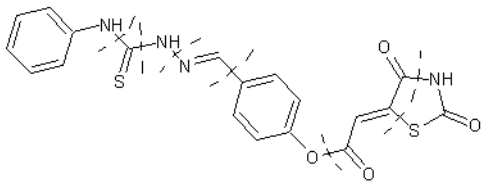
Window Display Report



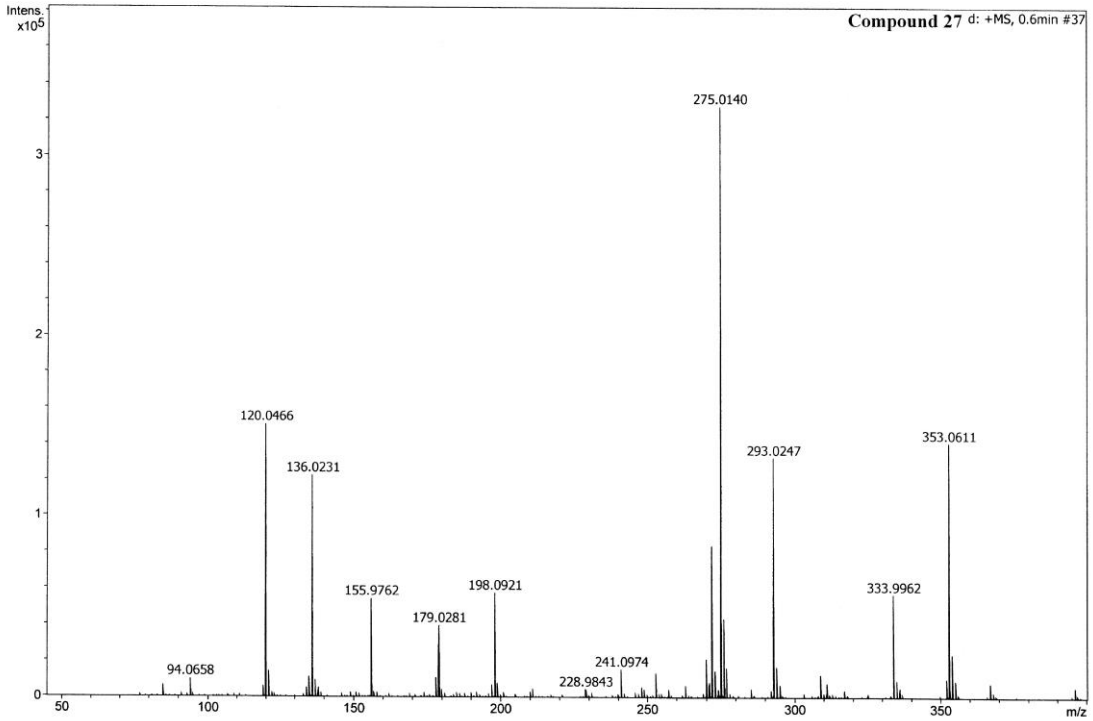
Bruker Compass DataAnalysis 4.1 printed: 4/6/2016 1:12:54 PM by: user Page 1 of 1

Window Display Report

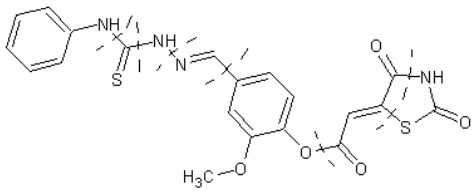




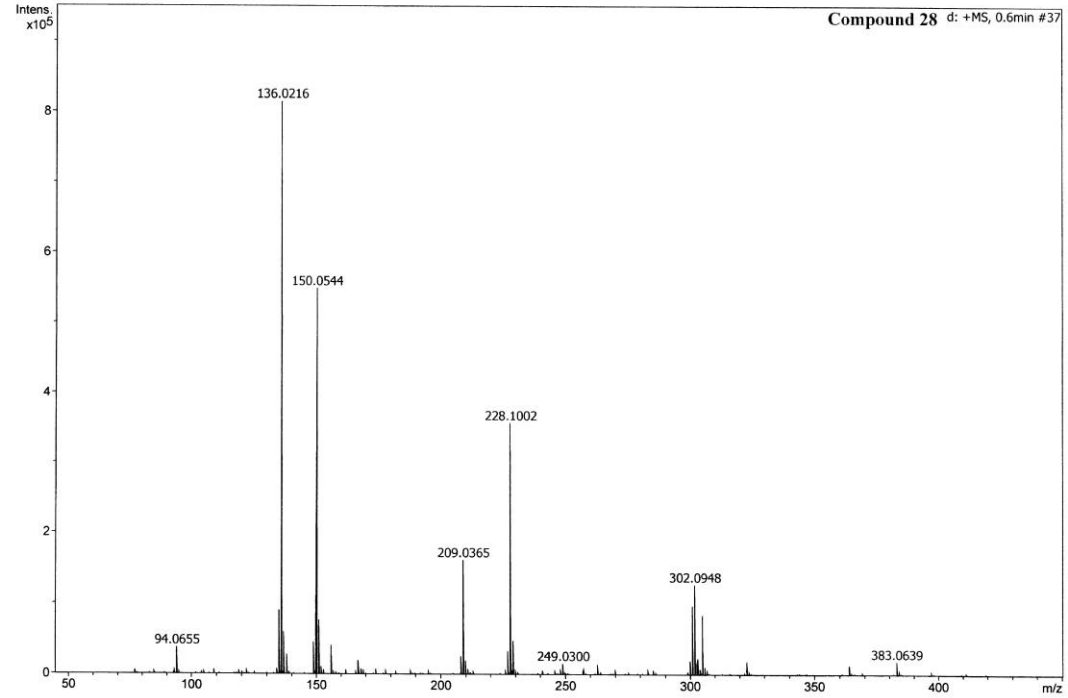
Window Display Report



Bruker Compass DataAnalysis 4.1 printed: 4/6/2016 12:16:54 PM by: user Page 1 of 1



Window Display Report



Bruker Compass DataAnalysis 4.1 printed: 4/6/2016 1:53:51 PM by: user Page 1 of 1