Supporting Information

for

Novel azocoumarin derivatives synthesis and characterization

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Table S1. Solubility of azocumarin derivatives in different solvents (2 mg of the compound in 1ml of solvent).

Sample	H_2O		THF		$CHCl_3$		DMF		CH_3OH	
	room temp.	boiling temp.	room temp.	boiling temp.	room temp.	boiling temp.	room temp.	boiling temp.	room temp.	boiling temp.
6-a	–	+/-	+/-	+/-	+/-	+/-	+	+	+/-	+/-
6-b	–	–	+/-	+/-	+/-	+/-	+	+	+/-	+/-
6-c	–	+/-	+/-	+/-	+/-	+/-	+	+	+/-	+/-
6-d	–	+/-	+/-	+/-	+/-	+/-	+	+	+/-	+/-
6-e	–	–	+/-	+/-	+/-	+/-	+	+	+/-	+/-
6-f	–	–	+/-	+/-	+/-	+/-	+/-	+	+/-	+/-
6-g	+/-	+/-	+/-	+/-	+/-	+/-	+/-	+	+/-	+/-
6-h	–	+/-	+/-	+/-	+	+	+/-	+	+/-	+/-
6-i	–	+/-	+/-	+/-	+	+	+/-	+	+/-	+/-

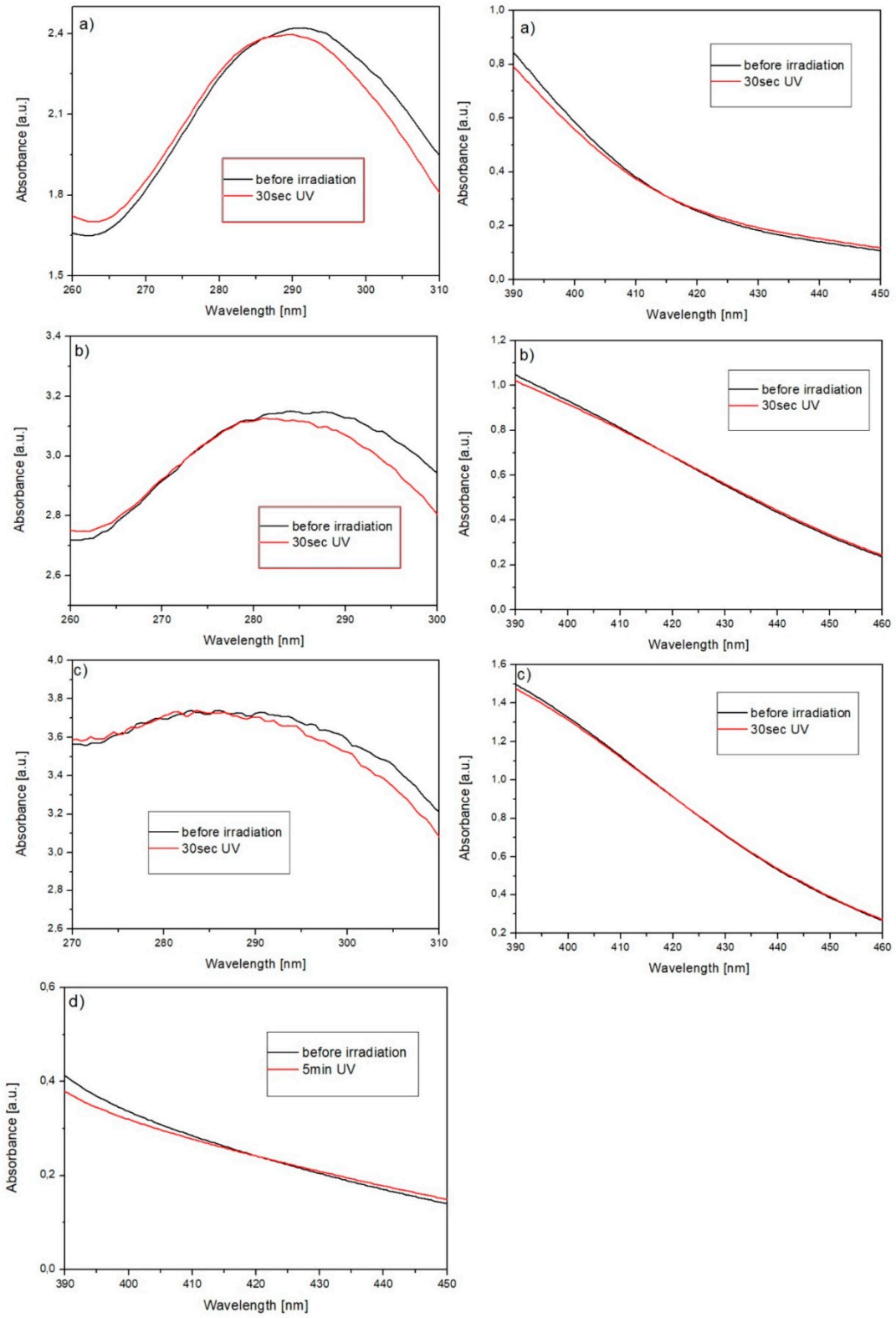


Figure S1. UV-vis spectra of **6b** registered before and after irradiation (λ=365nm, 2.9 W, 30s) in (a) chloroform, (b) ethanol, (c) DMF, and (d) polystyrene.

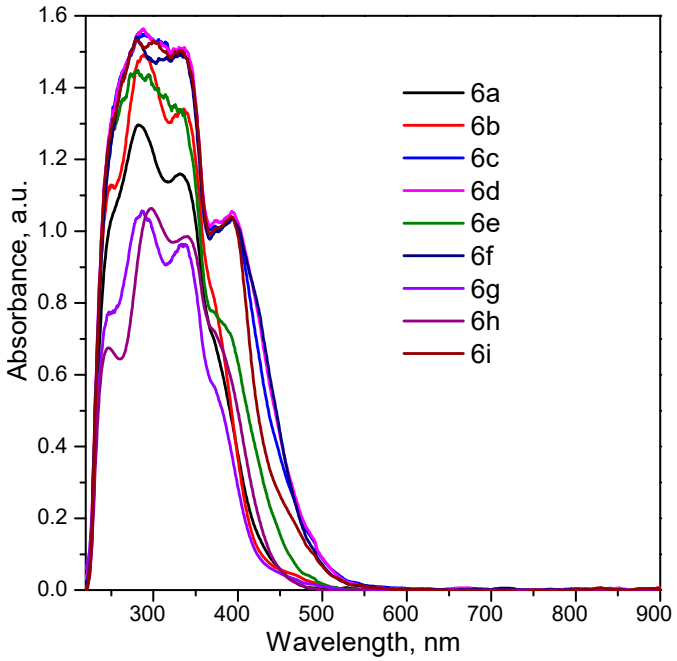


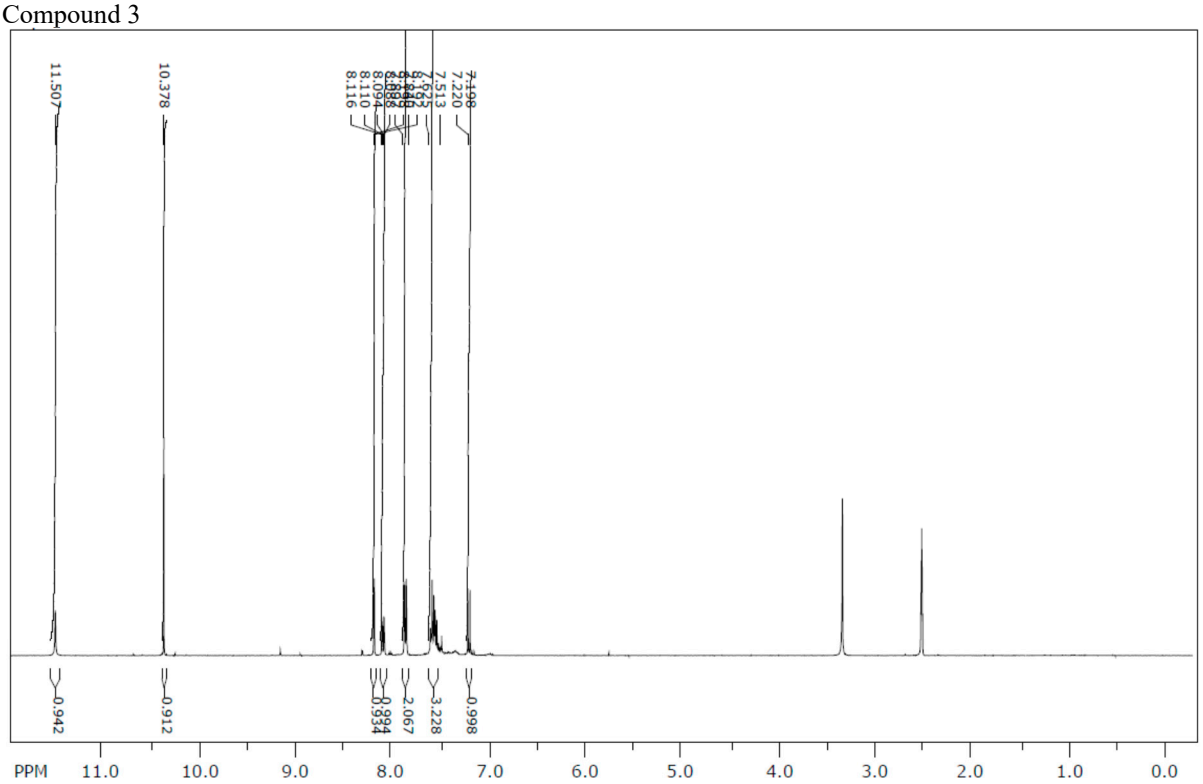
Figure S2. Absorbance spectra of compound 6a-6i in DCM

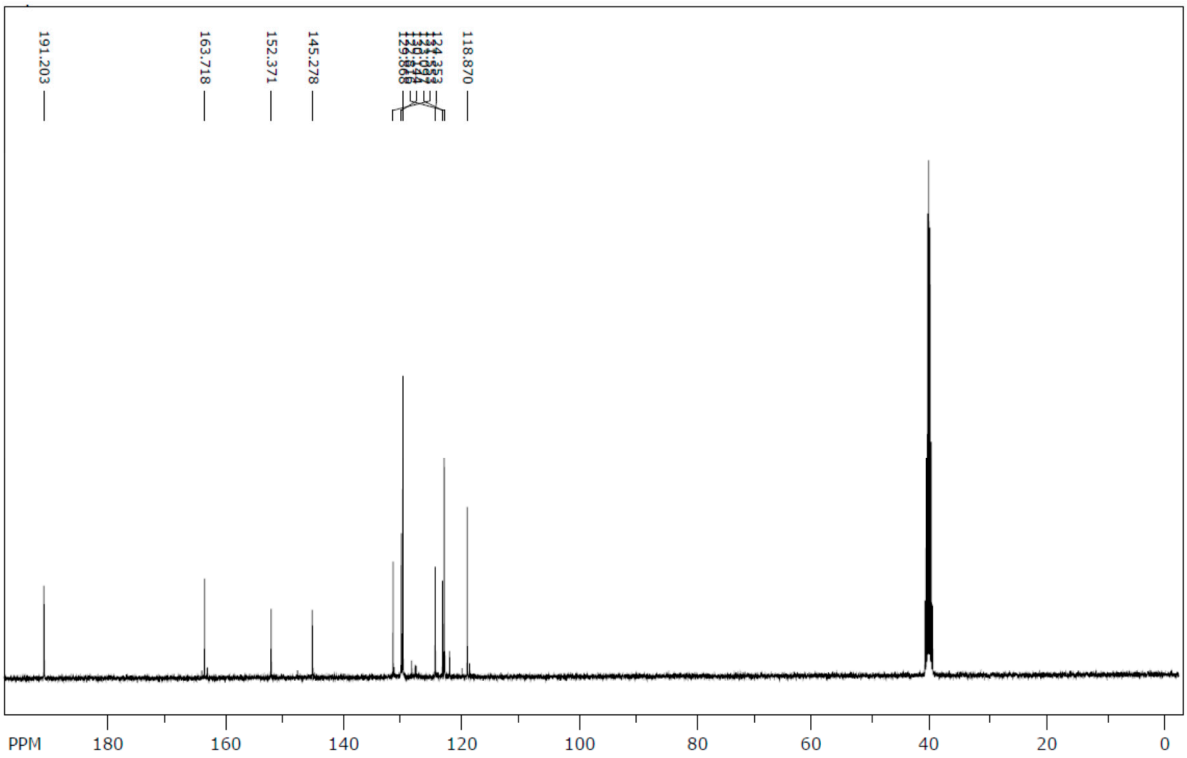
Table S2. Content of *cis*-isomer directly after the 5 min of UV-light irradiation, and time of *cis* to *trans* transformation of dyes in polystyrene matrix.

Code	**Isosbestic points [nm]**	**Content of *cis* isomer (%)**	**Time of *cis*-*trans* conversion [days]**
6a+PS	418	13	8
6b+PS	420	14	8
6c+PS	421	13	>8
6d+PS	424	11	>8
6f+PS	419	14	7
6g+PS	410	14	>8
6h+PS	437	7	7
6i+PS	407	22	>8

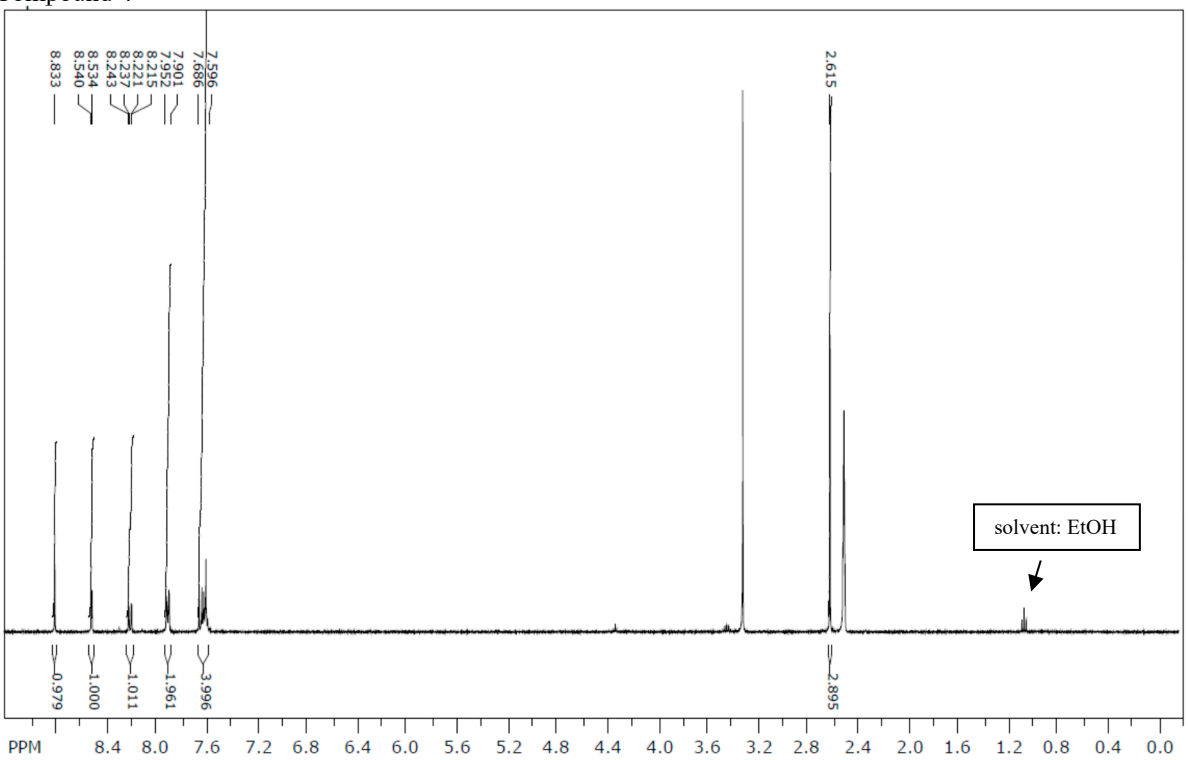
^{1}H, ^{13}C NMR and HRMS spectra of compounds **3-5**, **6a-6i** and additional DEPT-135, COSY, NOESY, HMBC, HSQC spectra for compound **6g**.

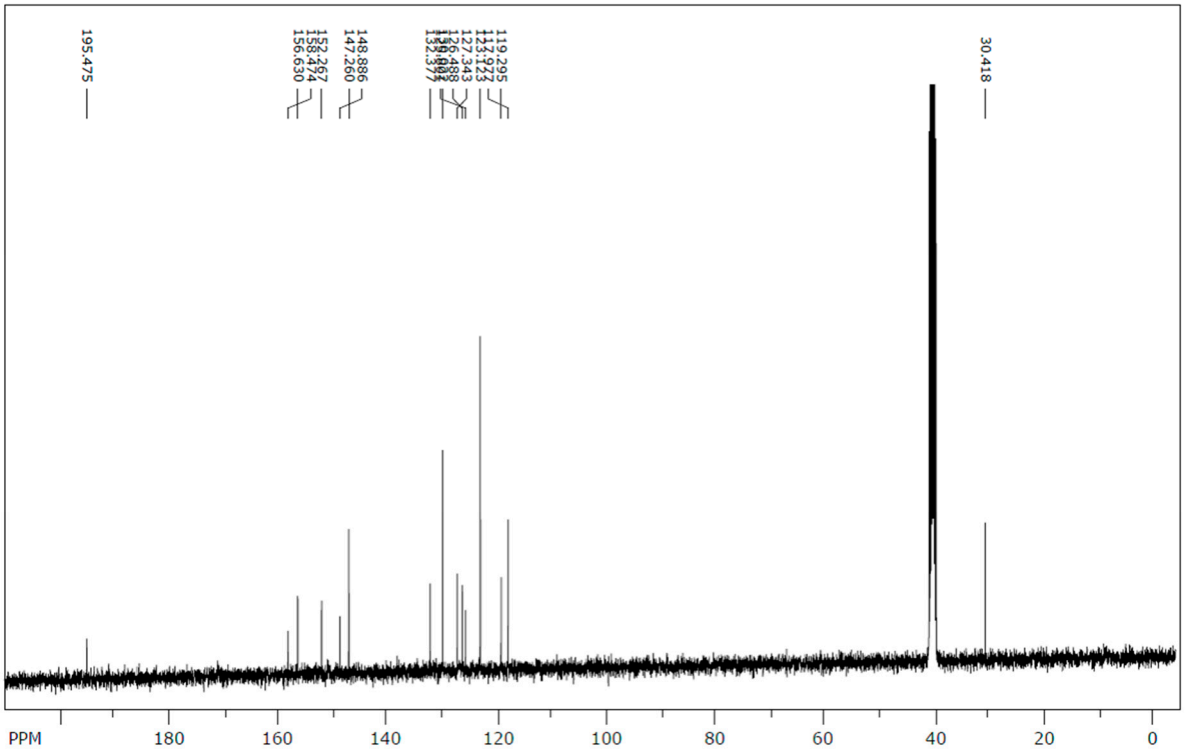
Compound 3


11.507
10.378
8.116
8.110
8.094
7.513
7.220
0.942
0.912
0.994
2.067
3.228
0.998
PPM
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

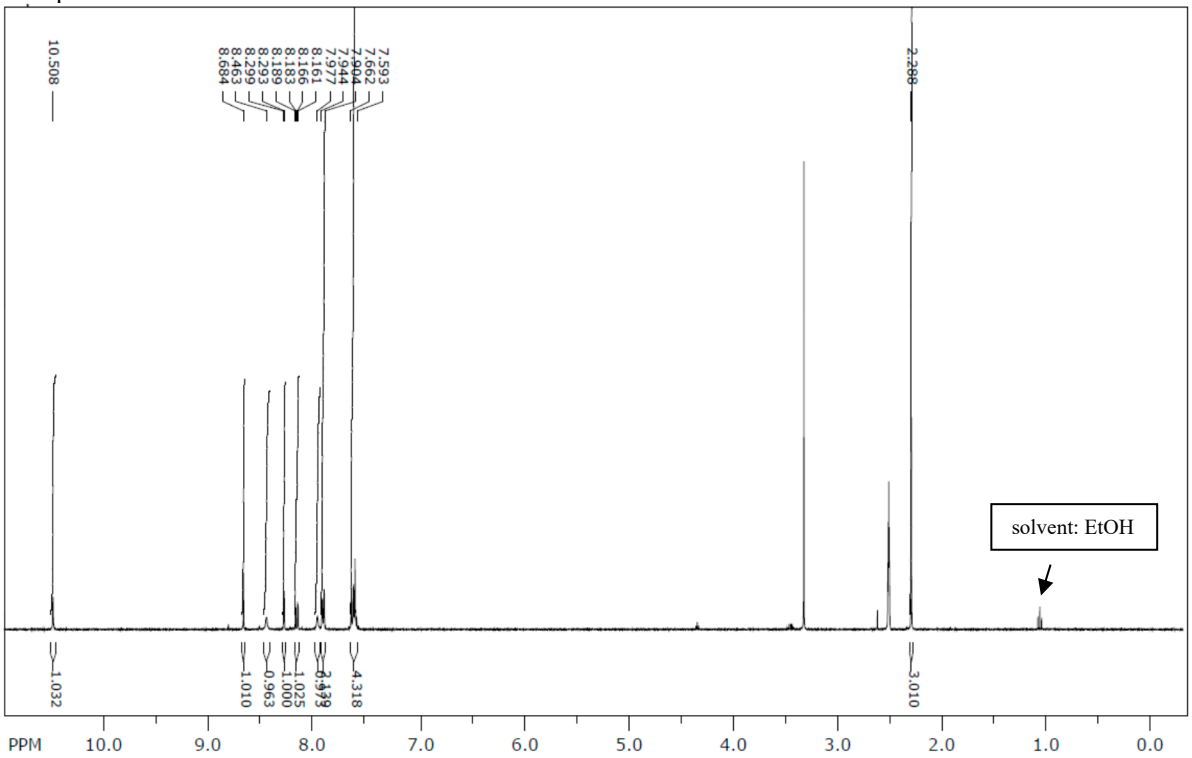

191.203
163.718
152.371
145.278
118.870
PPM
180
160
140
120
100
80
60
40
20
0

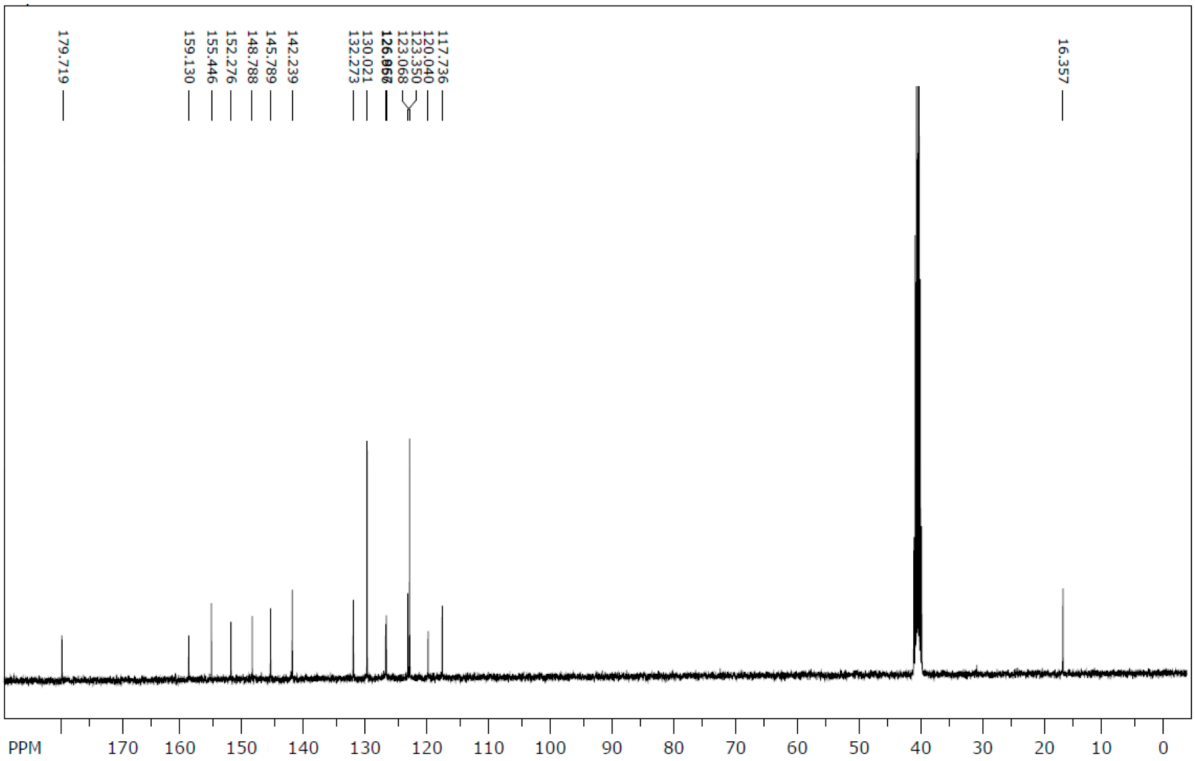
Compound 4


8.833
8.540
8.534
8.243
8.237
8.221
8.215
7.952
7.901
7.686
7.596
2.615
solvent: EtOH
0.979
1.000
1.011
1.961
3.996
2.895
PPM
8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0

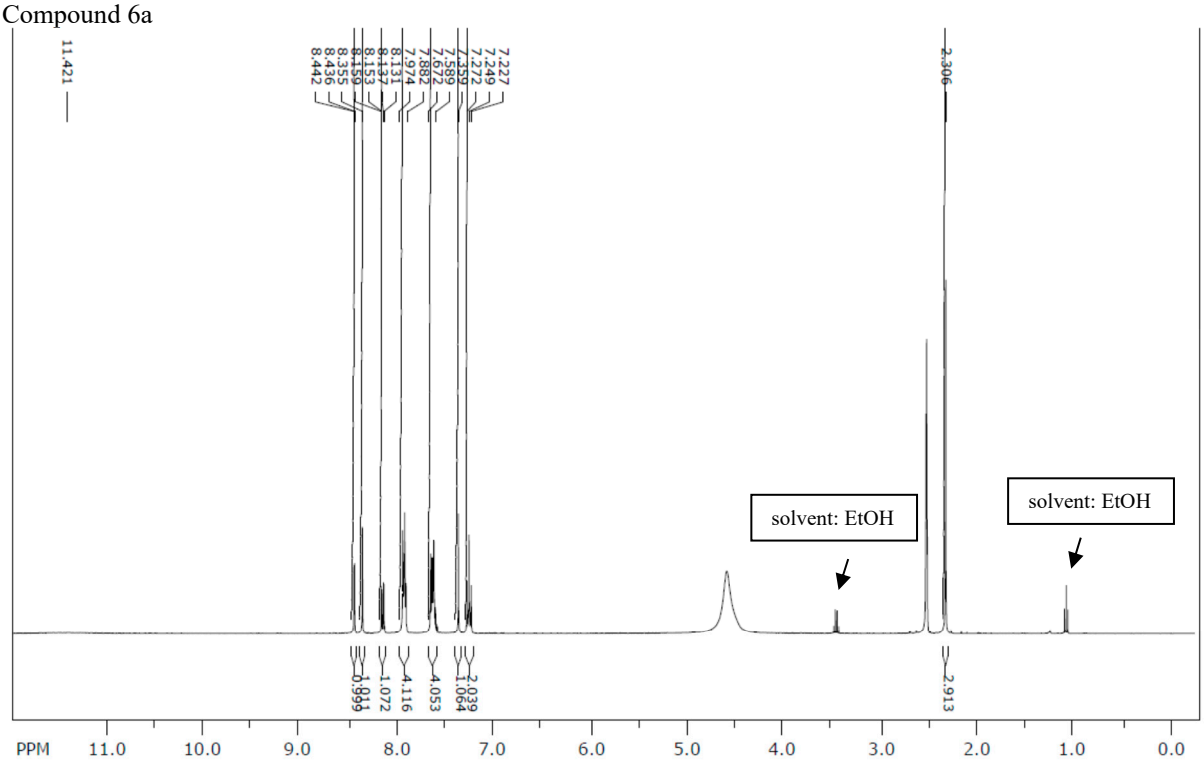

195.475
156.630
158.474
152.267
147.260
148.886
132.377
127.343
123.123
119.295
30.418
PPM
180 160 140 120 100 80 60 40 20 0

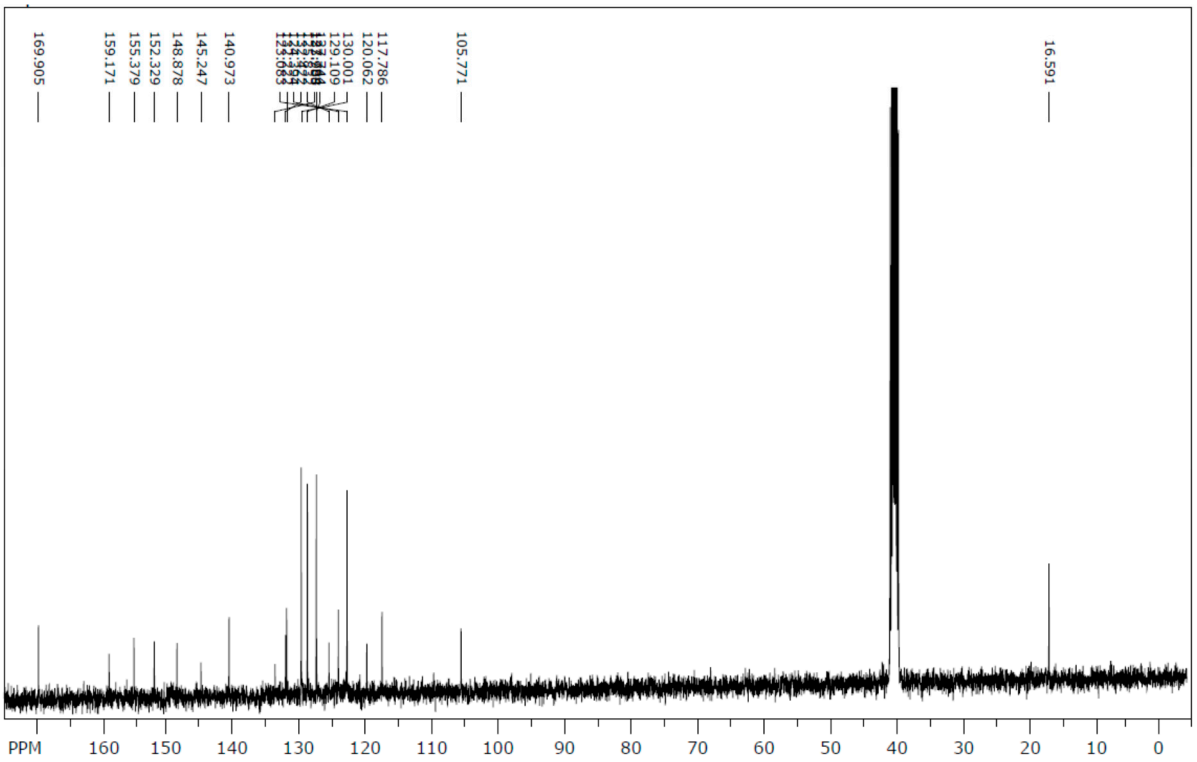
Compound 5


10.508
8.684
8.463
8.299
8.283
8.183
8.166
8.161
7.977
7.944
7.904
7.662
7.593
2.288
solvent: EtOH
1.032
1.010
0.963
1.000
1.025
4.318
3.010
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


179.719
159.130
155.446
152.276
148.788
145.789
142.239
132.273
130.021
126.866
123.350
123.068
120.040
117.736
16.357
PPM
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound 6a


11.421
8.442
8.435
8.355
8.159
8.153
8.137
8.131
7.974
7.882
7.672
7.589
7.359
7.272
7.249
7.227
2.306
solvent: EtOH
solvent: EtOH
0.999
1.041
1.072
4.116
4.053
1.064
2.039
2.913
PPM
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


169.905
159.171
155.379
152.329
148.878
145.247
140.973
130.001
129.109
120.062
117.786
105.771
16.591
PPM
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150
140
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100
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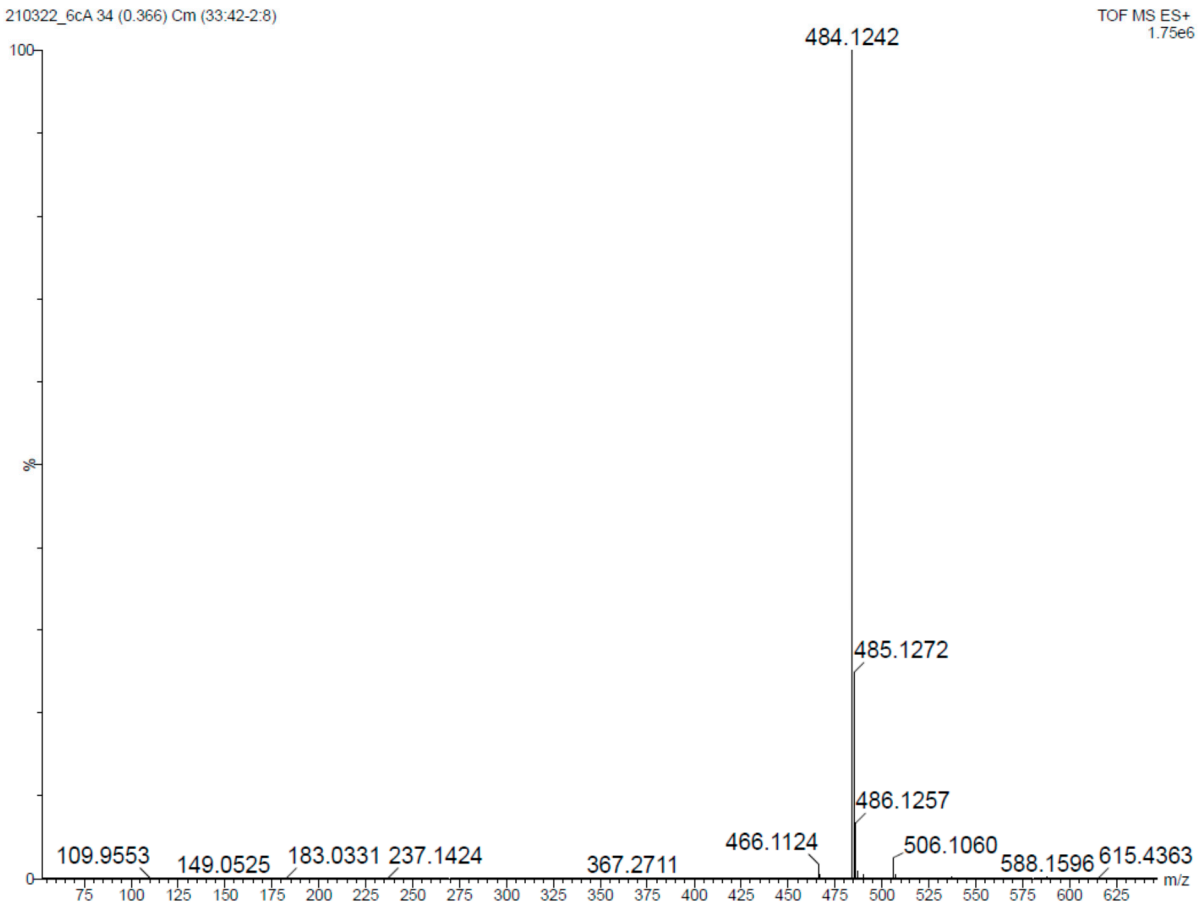
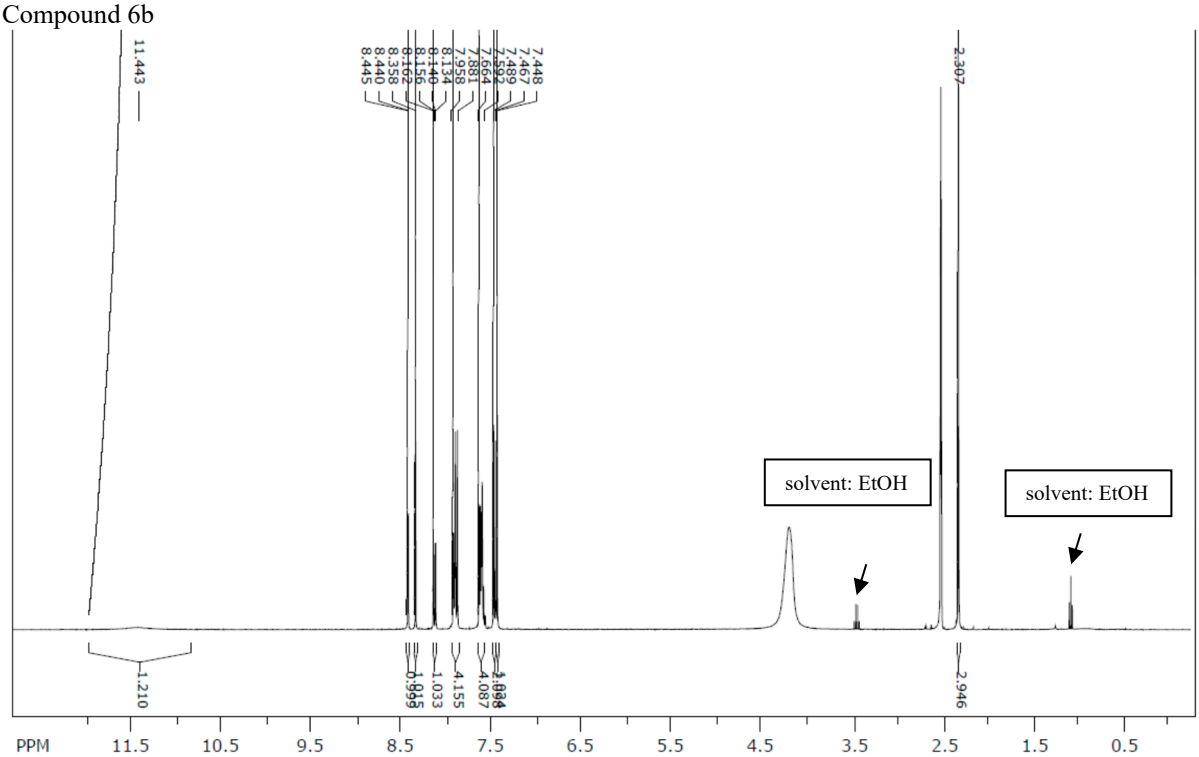
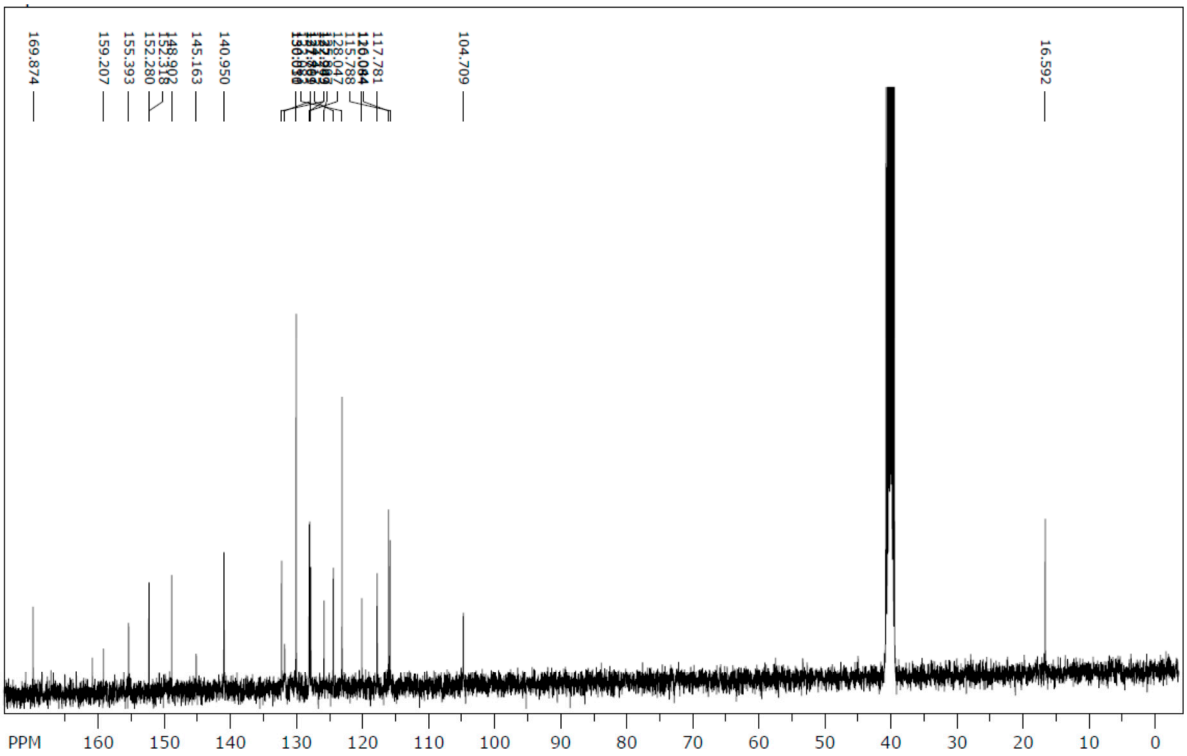
60
50
40
30
20
10
0


210322_6cA 34 (0.366) Cm (33:42-2:8)
TOF MS ES+
1.75e6
484.1242
485.1272
486.1257
109.9553
149.0525
183.0331
237.1424
367.2711
466.1124
506.1060
588.1596
615.4363
m/z

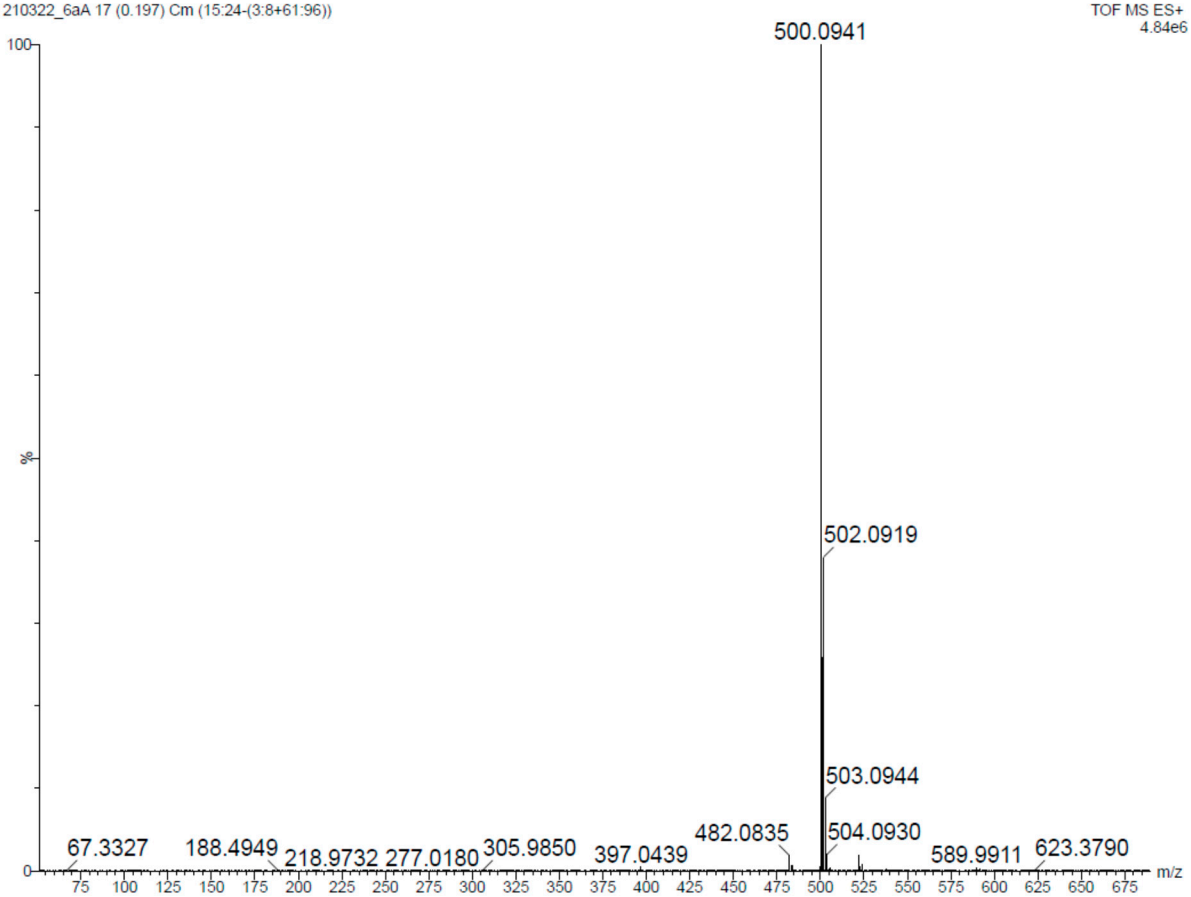
Compound 6b


solvent: EtOH
solvent: EtOH
PPM

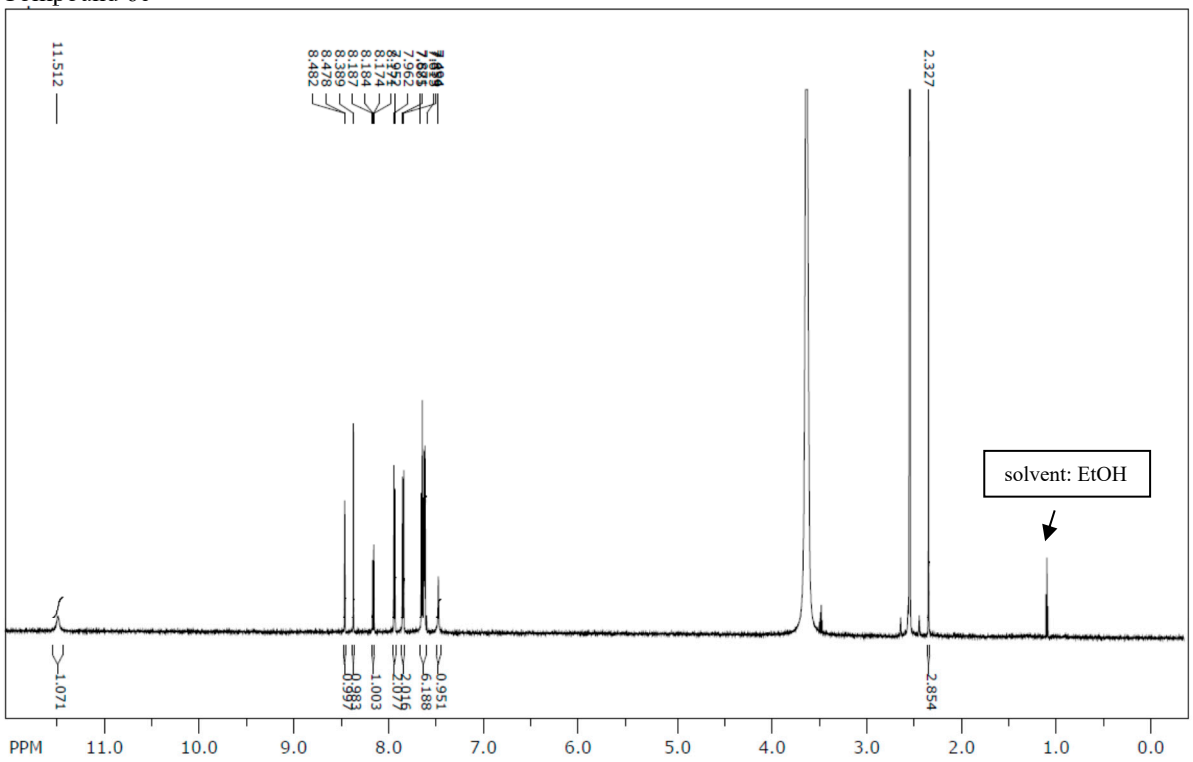


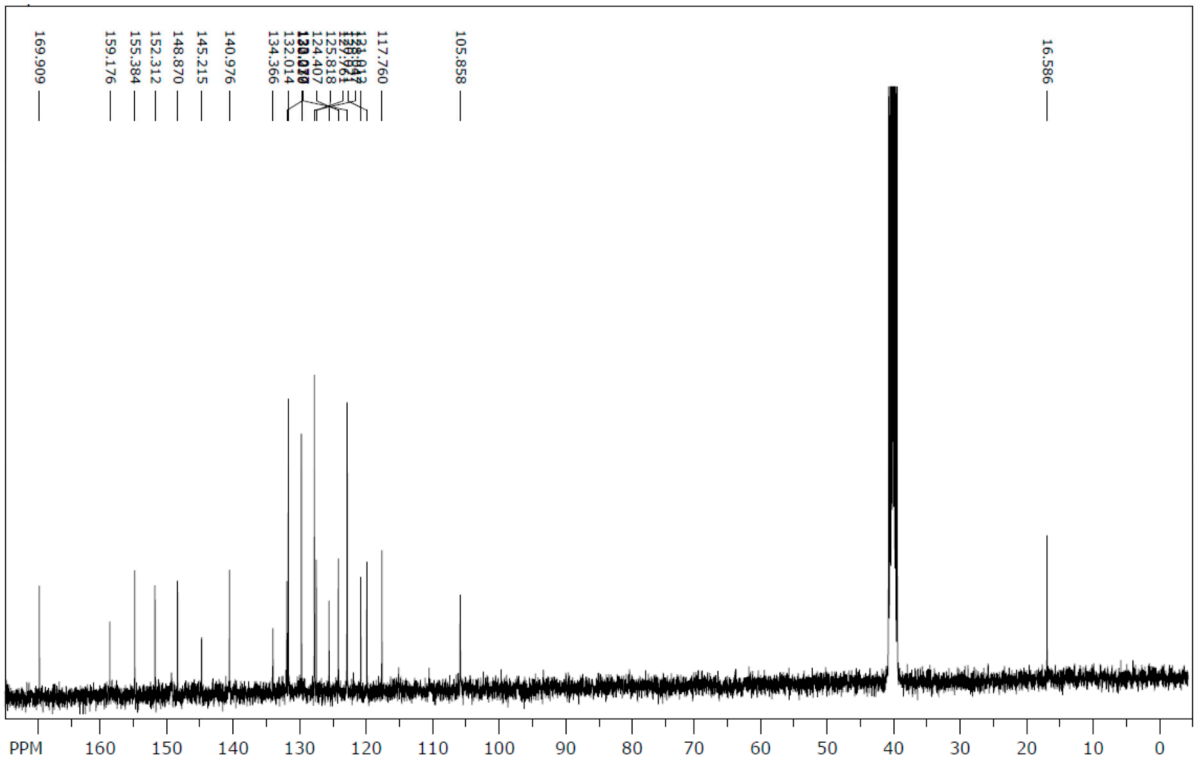
210322_6aA 17 (0.197) Cm (15:24-(3:8+61:96))

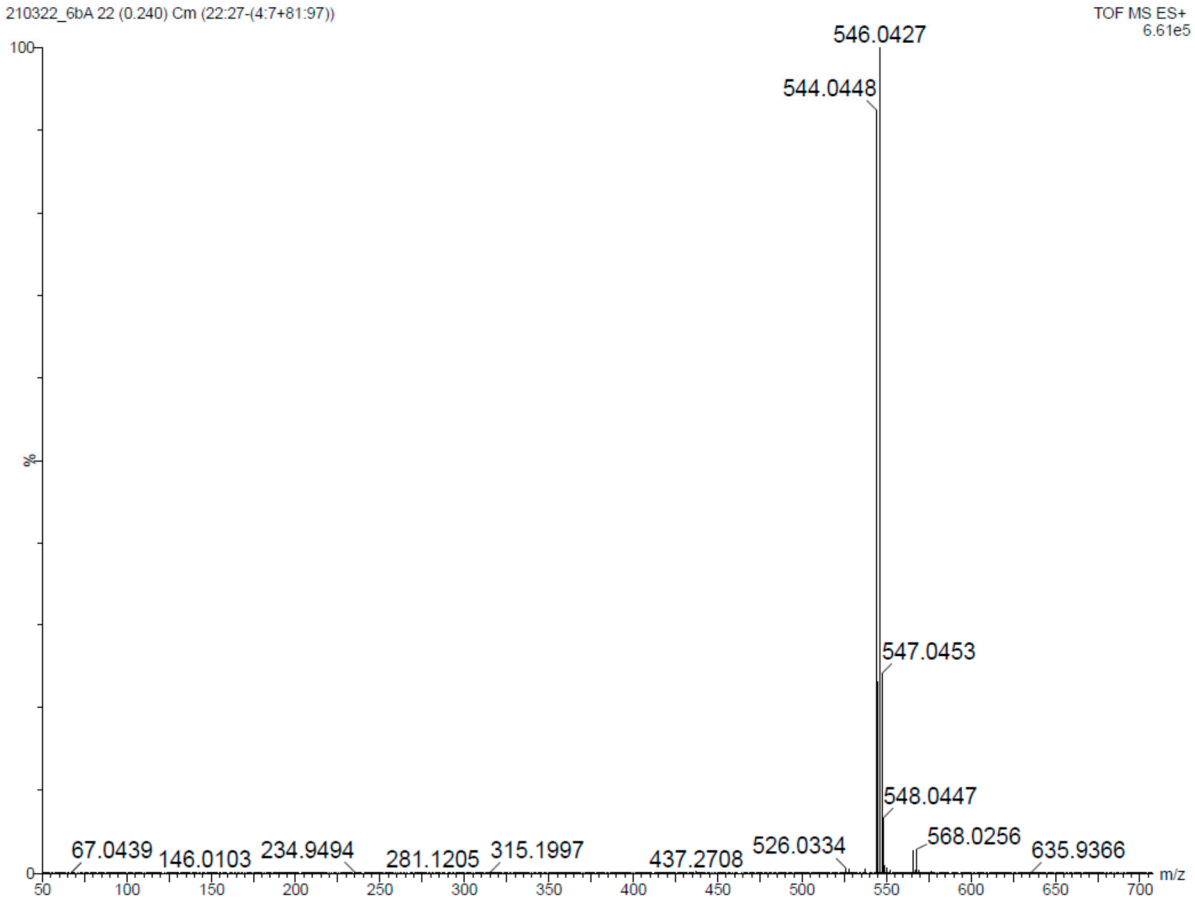
TOF MS ES+
4.84e6



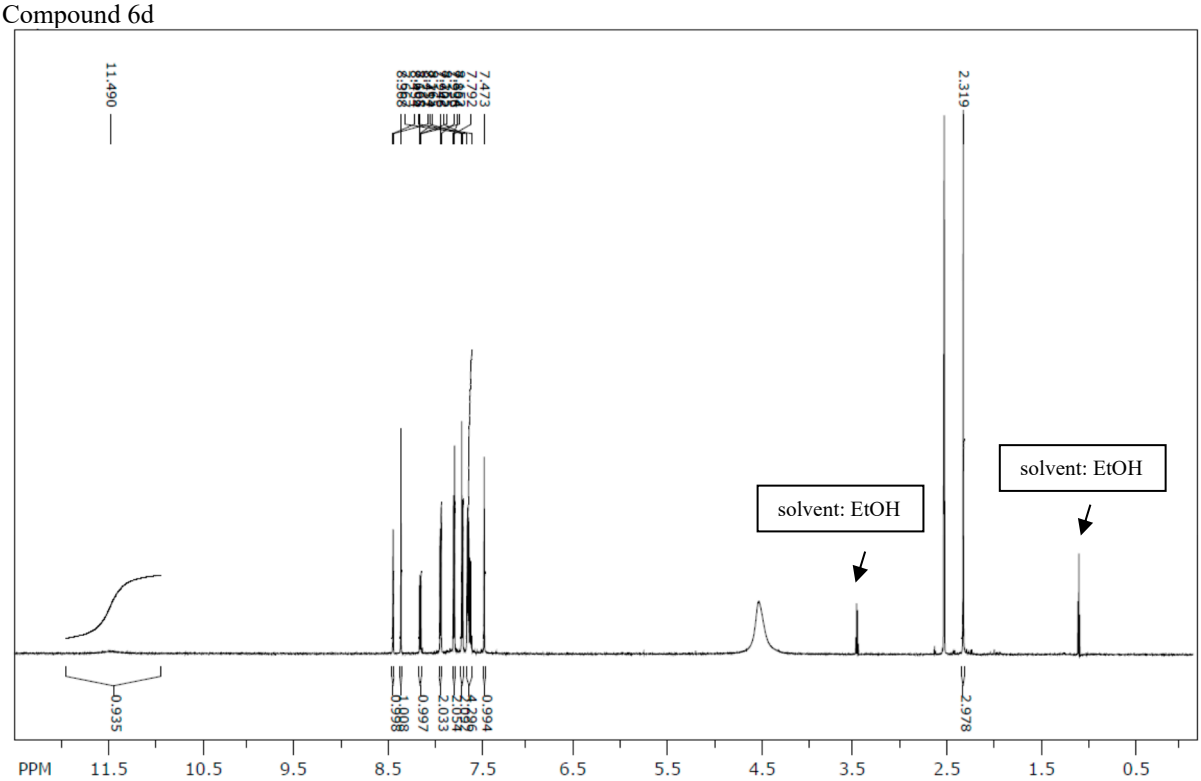
Compound 6c

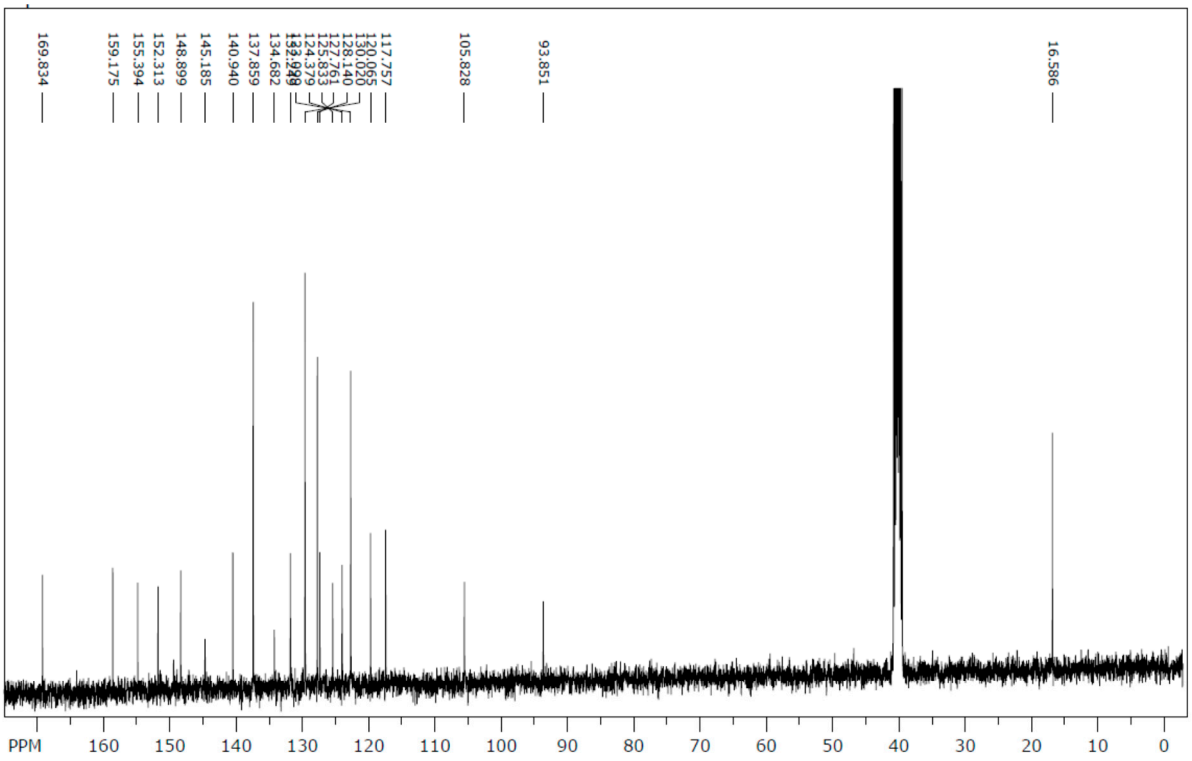

11.512
8.482
8.478
8.389
8.187
8.184
8.174
7.962
2.327
solvent: EtOH
1.071
0.997
0.983
1.003
2.015
6.188
0.951
2.854
PPM
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

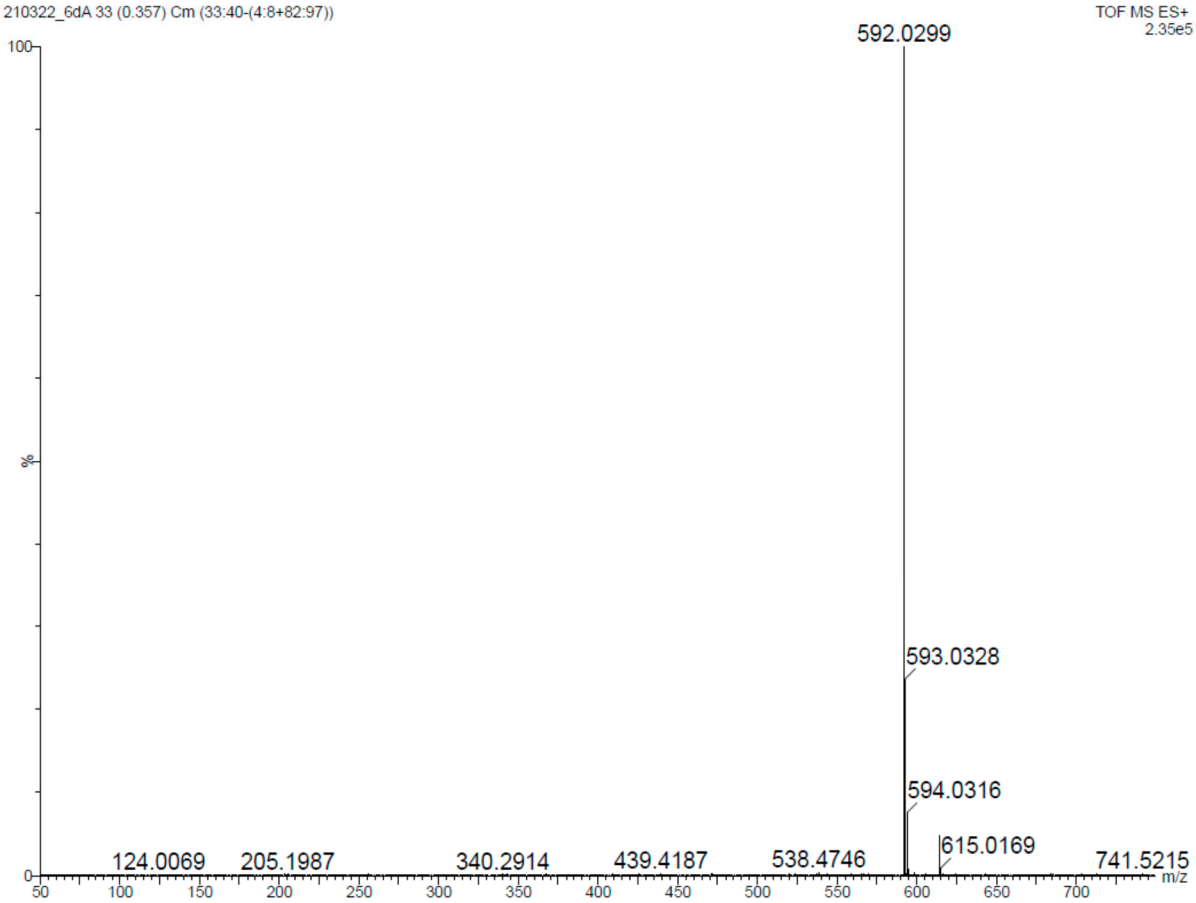

169.909
159.176
155.384
152.312
148.870
145.215
140.976
134.366
132.014
124.407
125.818
117.760
105.858
16.586
PPM
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


210322_6bA 22 (0.240) Cm (22:27-(4:7+81:97))
TOF MS ES+
6.61e5
546.0427
544.0448
547.0453
548.0447
568.0256
635.9366
67.0439
146.0103
234.9494
281.1205
315.1997
437.2708
526.0334
m/z

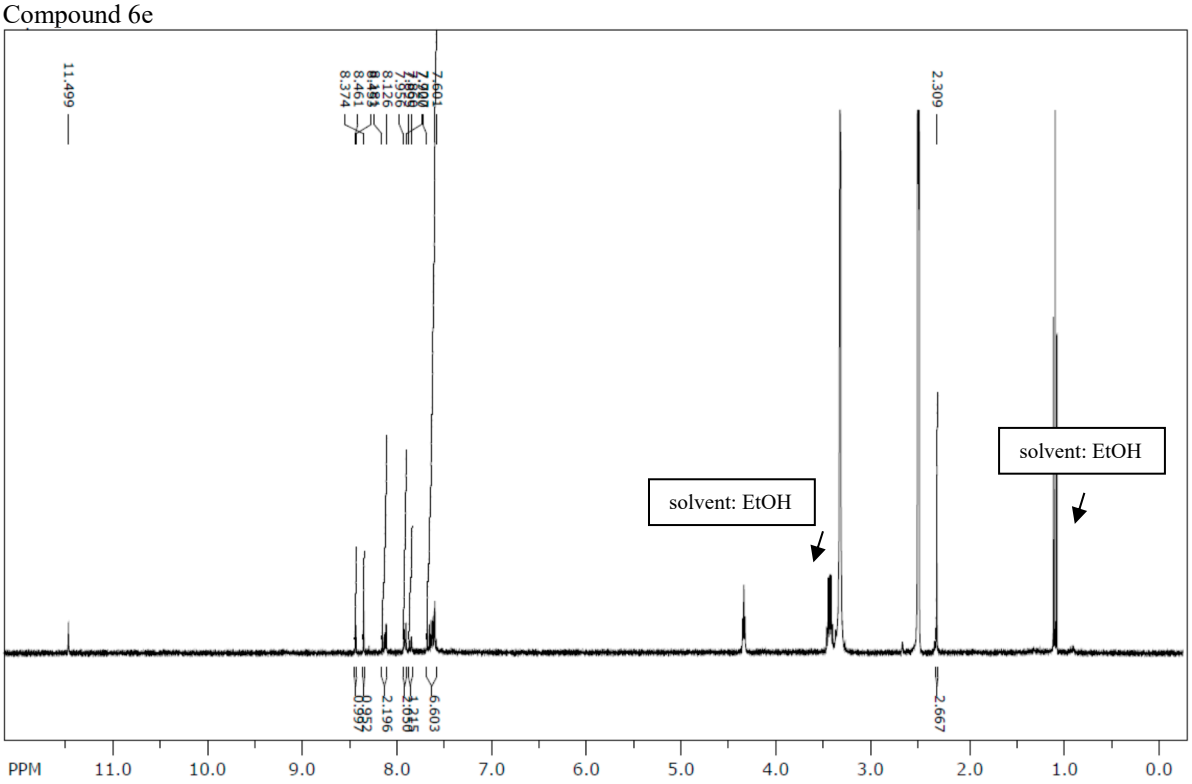
Compound 6d

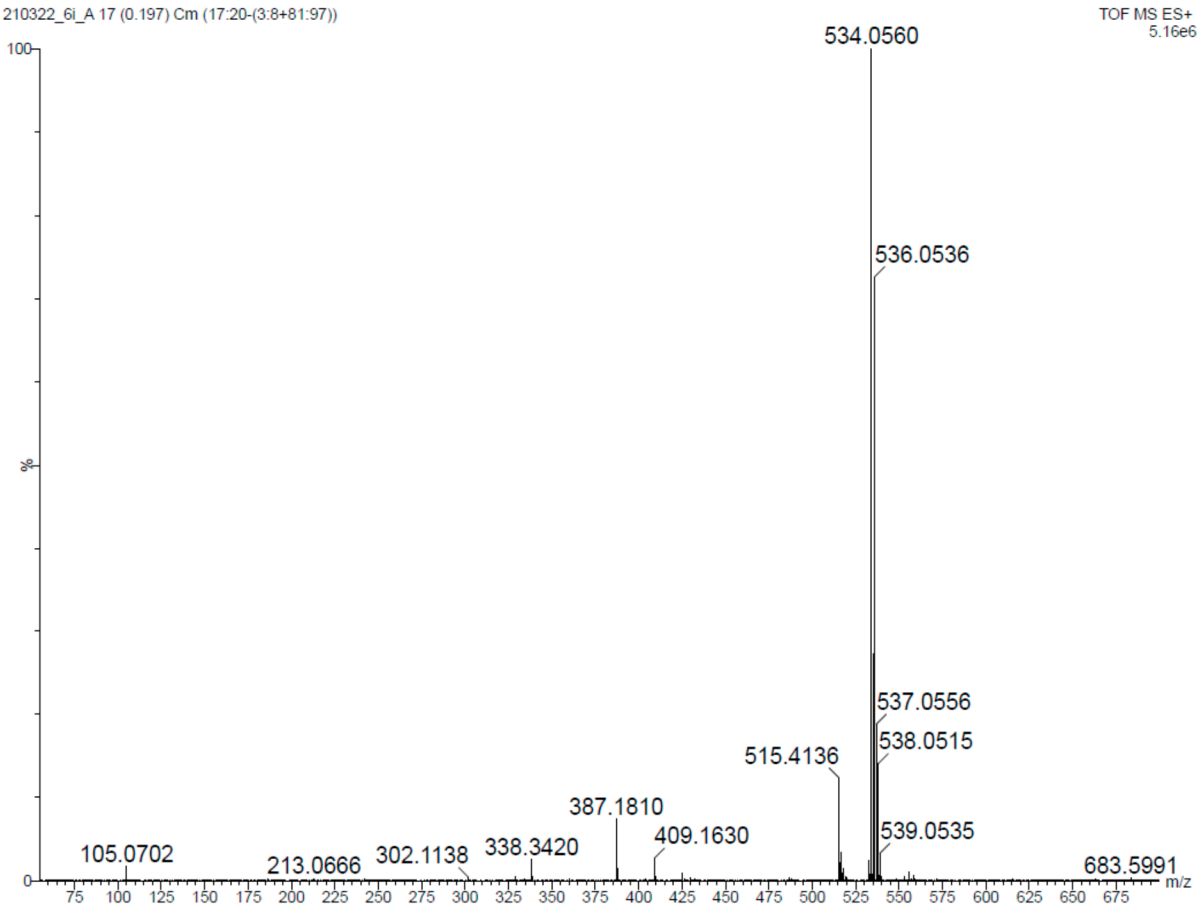

solvent: EtOH
solvent: EtOH
PPM


169.834
159.175
155.394
152.313
148.899
145.185
140.940
137.859
134.682
132.249
124.379
117.757
105.828
93.851
16.586
PPM
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

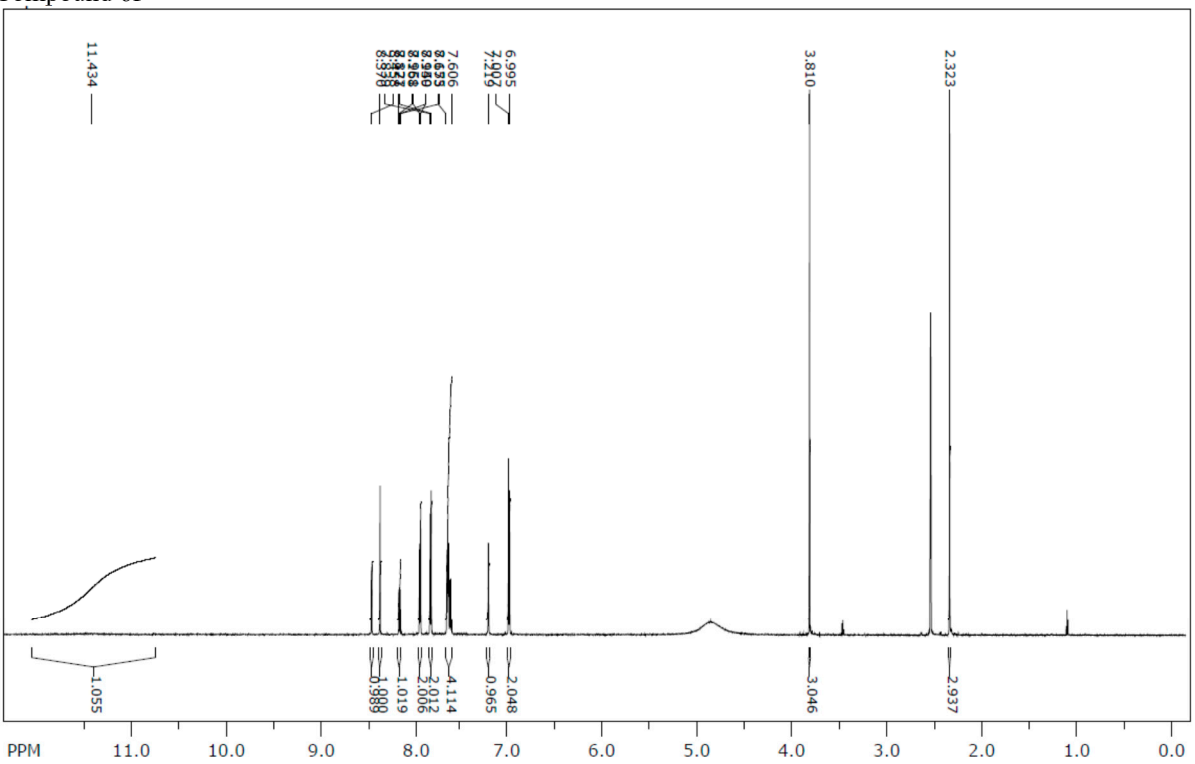

210322_6dA 33 (0.357) Cm (33:40-(4:8+82:97))
TOF MS ES+
2.35e5
592.0299
593.0328
594.0316
615.0169
124.0069
205.1987
340.2914
439.4187
538.4746
741.5215
100
%
0
m/z

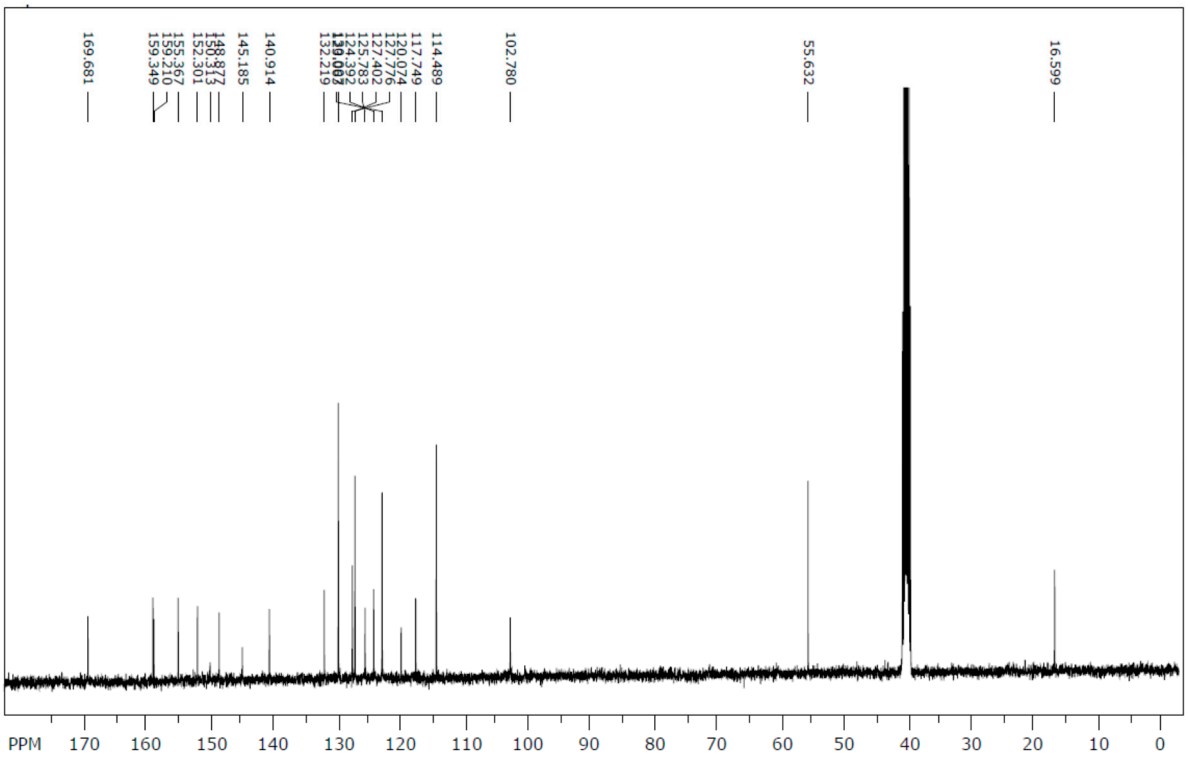
Compound 6e

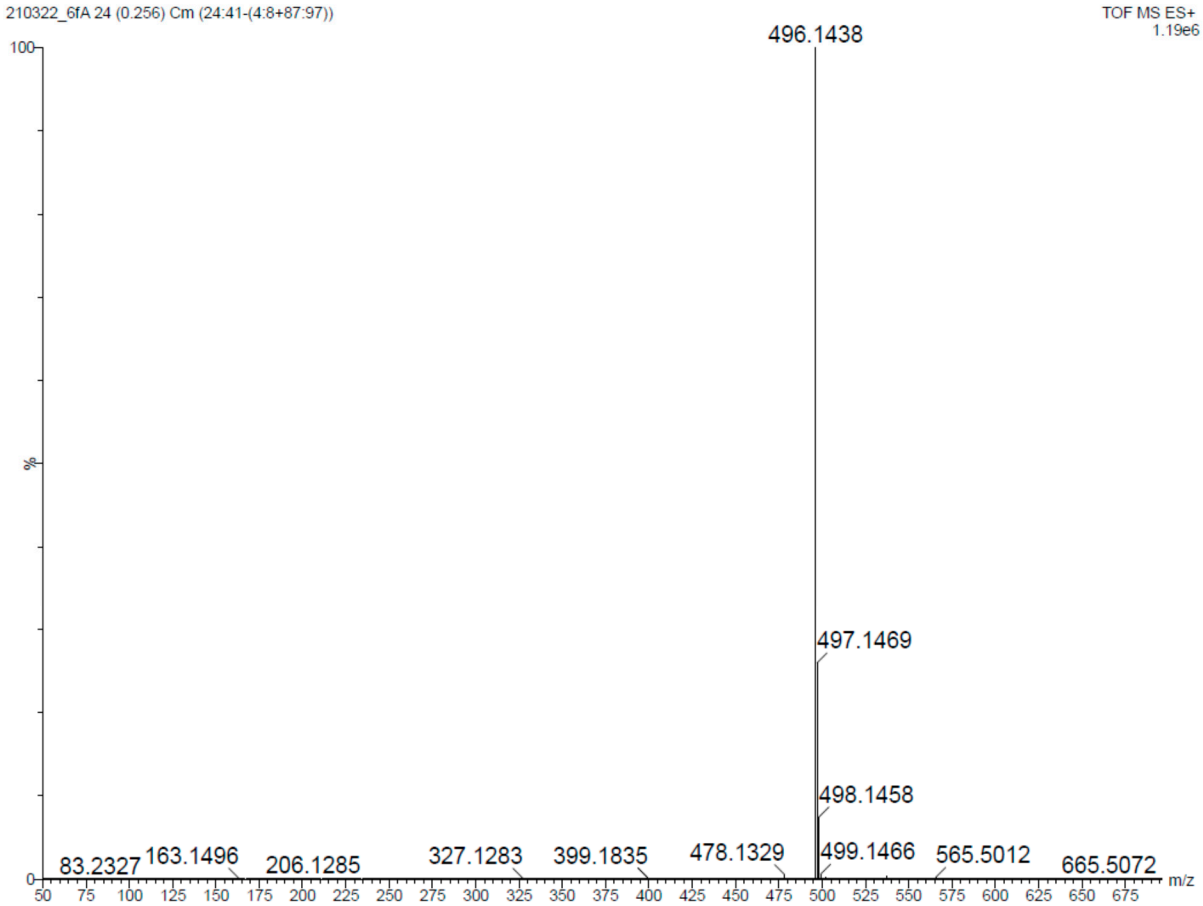

11.499
8.374
8.461
8.126
7.601
2.309
solvent: EtOH
solvent: EtOH
0.997
2.196
6.603
2.667
PPM
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


210322_6i_A 17 (0.197) Cm (17:20-(3:8+81:97))
TOF MS ES+
5.16e6
100
%
0
534.0560
536.0536
537.0556
538.0515
539.0535
515.4136
387.1810
409.1630
338.3420
302.1138
213.0666
105.0702
683.5991
m/z
75
100
125
150
175
200
225
250
275
300
325
350
375
400
425
450
475
500
525
550
575
600
625
650
675

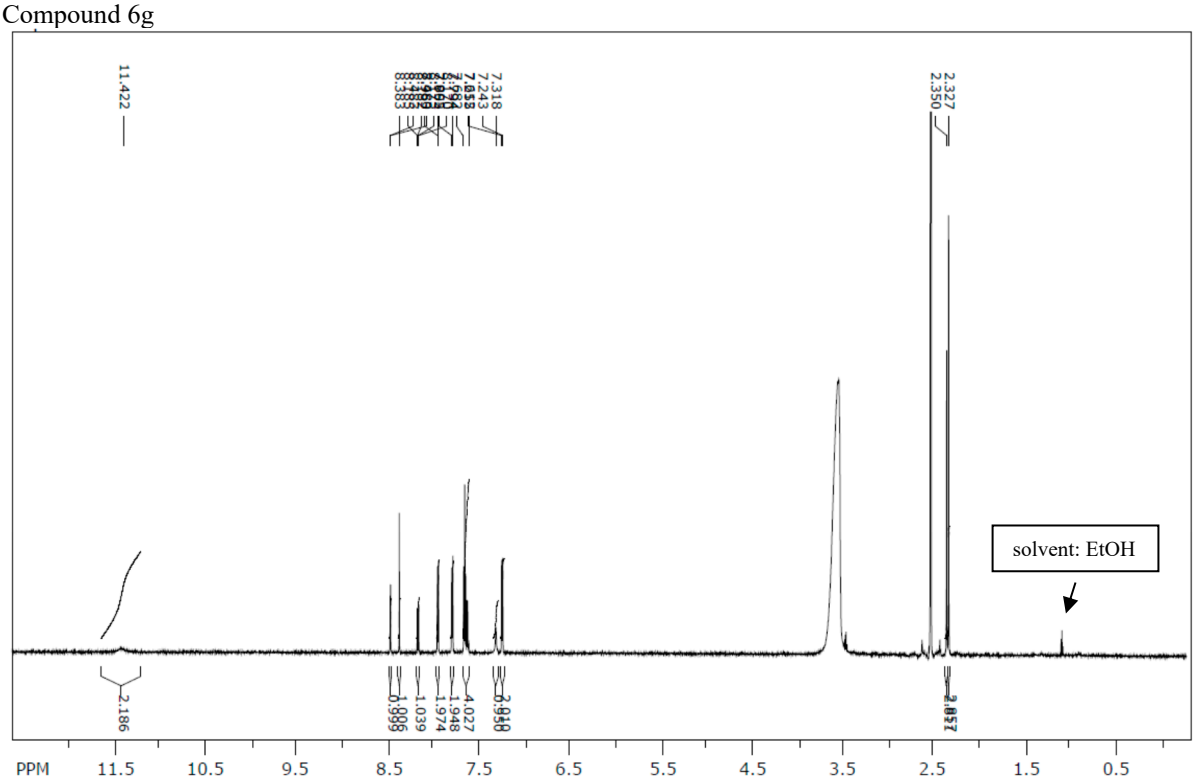
Compound 6f

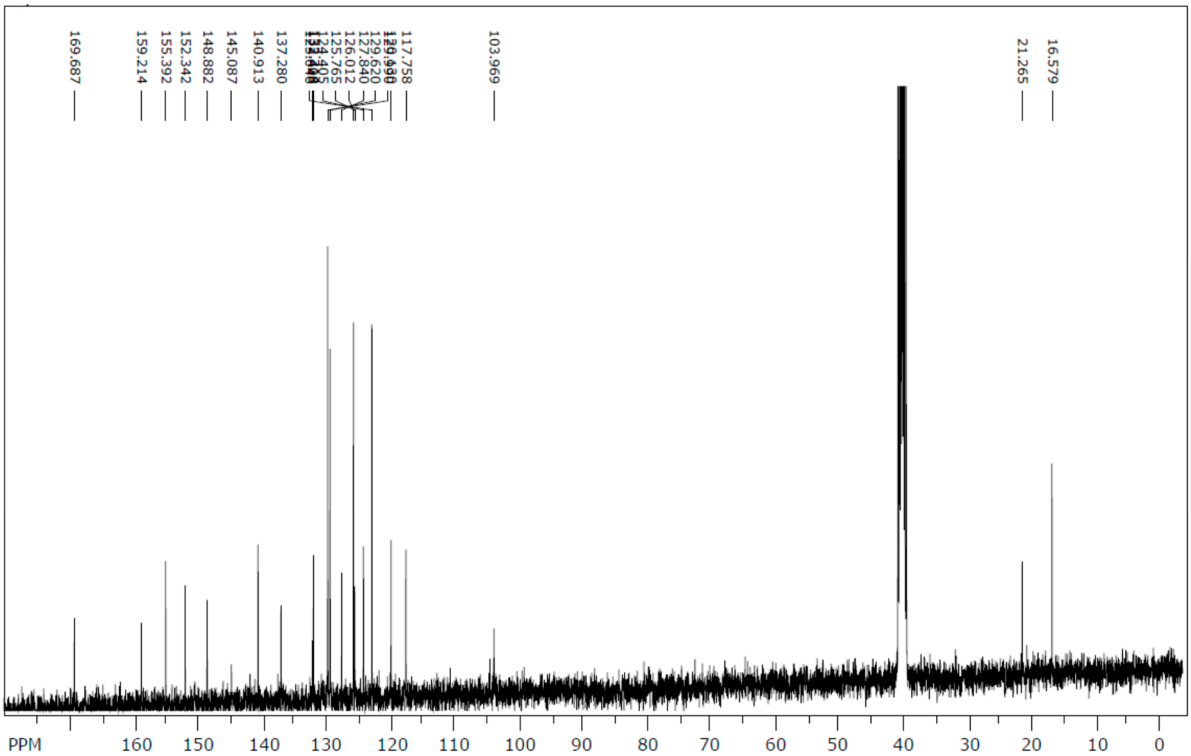

11.434
8.370
7.606
7.219
7.207
6.995
3.810
2.323
1.055
0.989
1.000
1.019
2.006
2.012
4.114
0.965
2.048
3.046
2.937
PPM
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


169.681
159.349
155.110
155.367
152.301
148.877
145.185
140.914
132.219
130.067
129.974
127.405
125.783
124.392
117.749
114.489
102.780
55.632
16.599
PPM
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

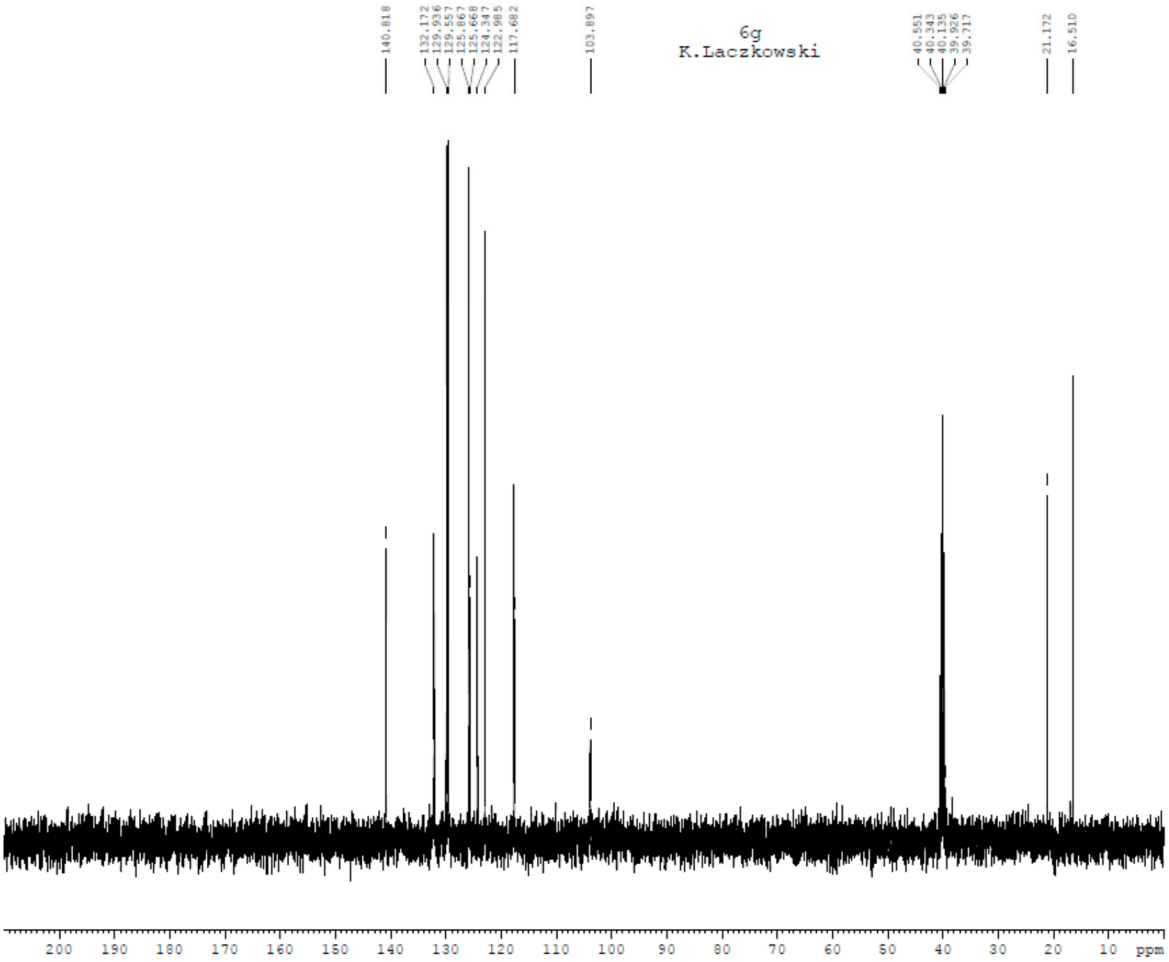

210322_6fA 24 (0.256) Cm (24:41-(4:8+87:97))
TOF MS ES+
1.19e6
496.1438
497.1469
498.1458
499.1466
83.2327
163.1496
206.1285
327.1283
399.1835
478.1329
565.5012
665.5072
%
m/z

Compound 6g

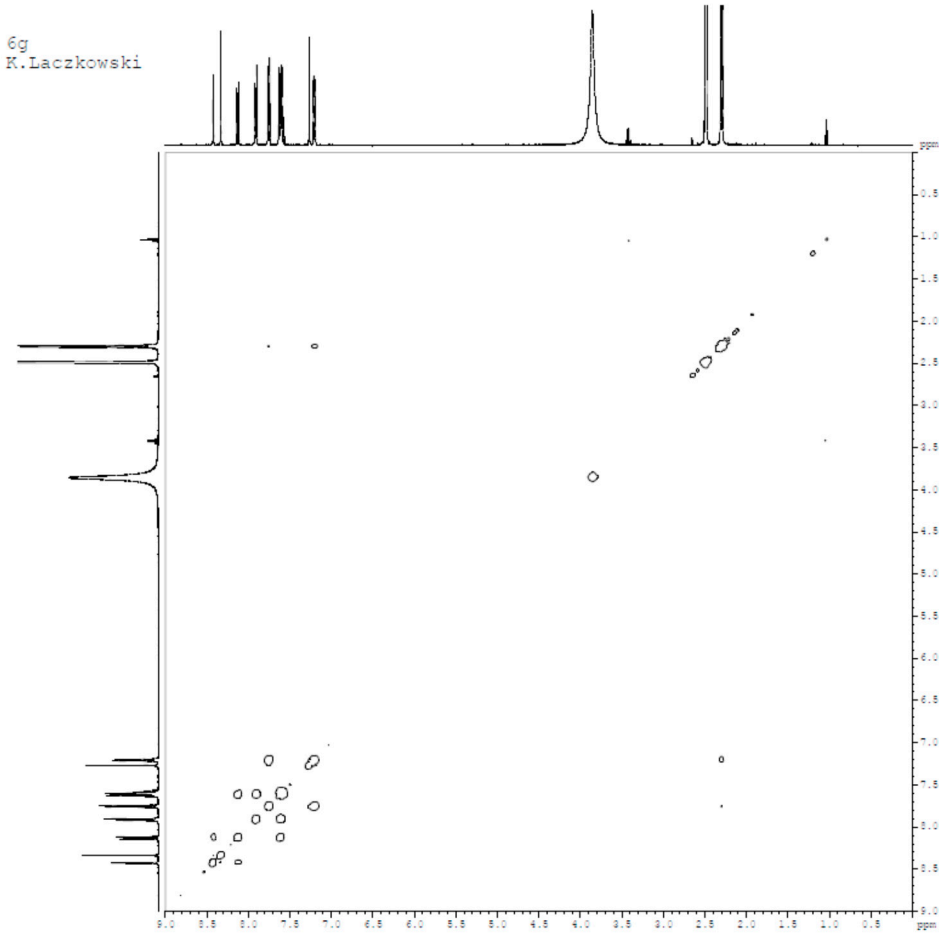

solvent: EtOH
PPM


169.687
159.214
155.392
152.342
148.882
145.087
140.913
137.280
117.758
103.969
21.265
16.579
PPM
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

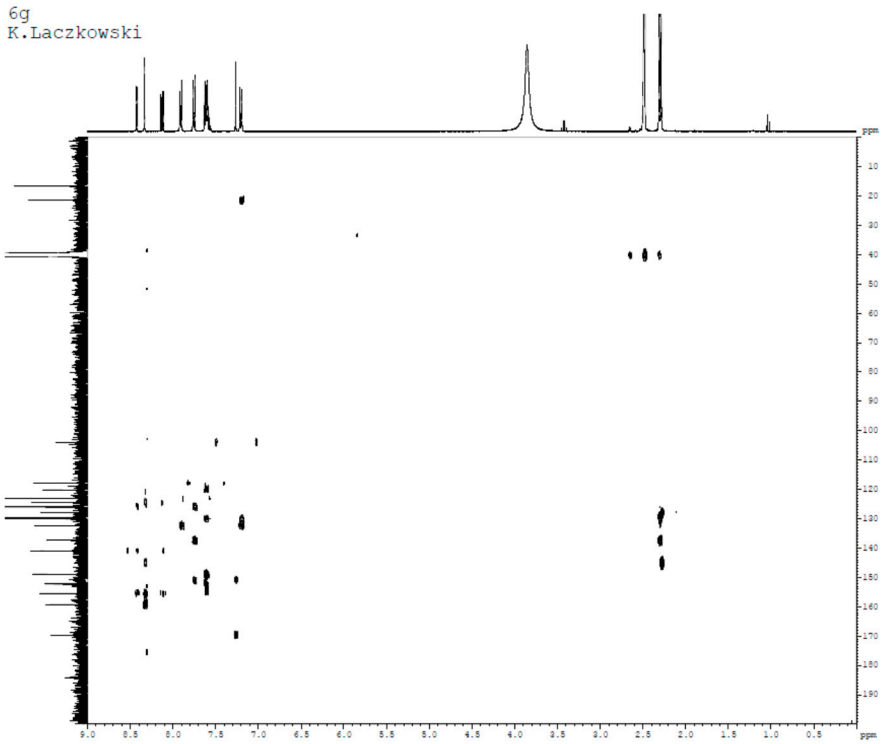
DEPT-135


140.818
132.172
129.936
129.557
125.867
125.668
124.347
122.985
117.682
103.897
6g
K.Laczkowski
40.551
40.343
40.135
39.926
39.717
21.172
16.510
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

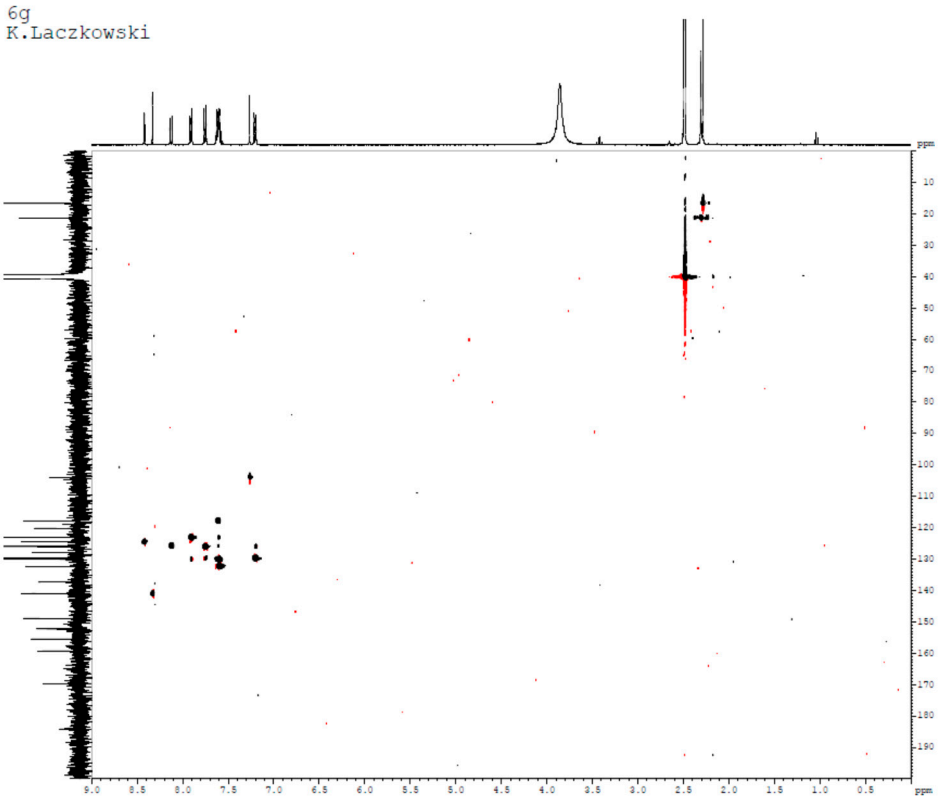
COSY



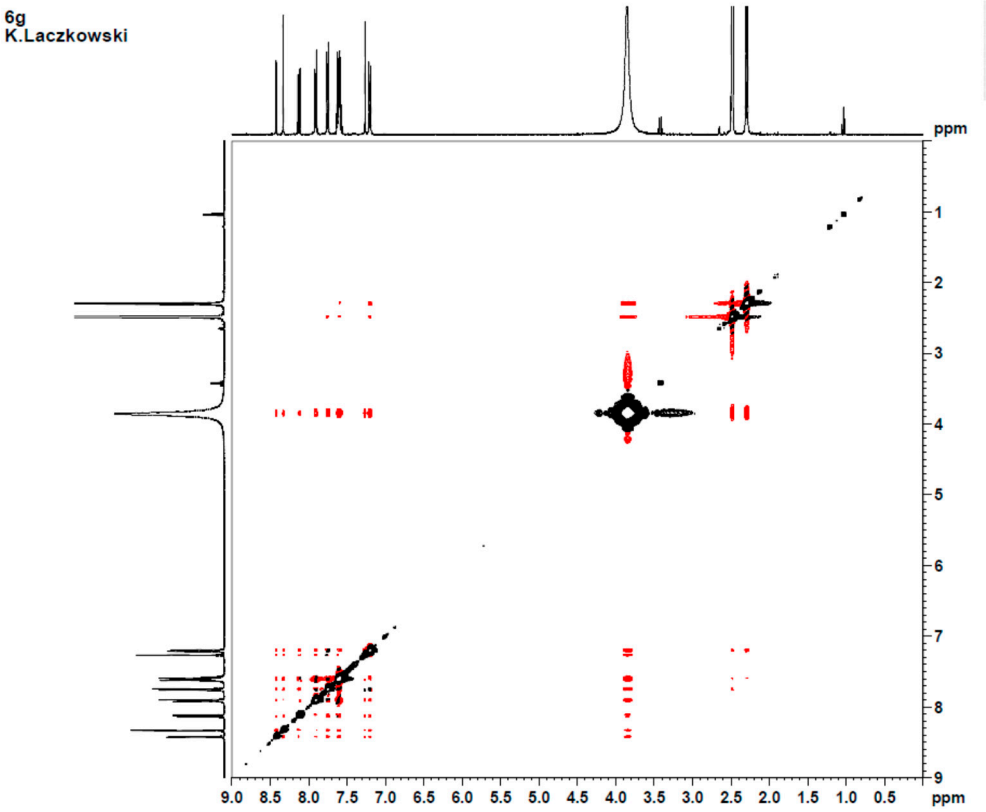
HMBC

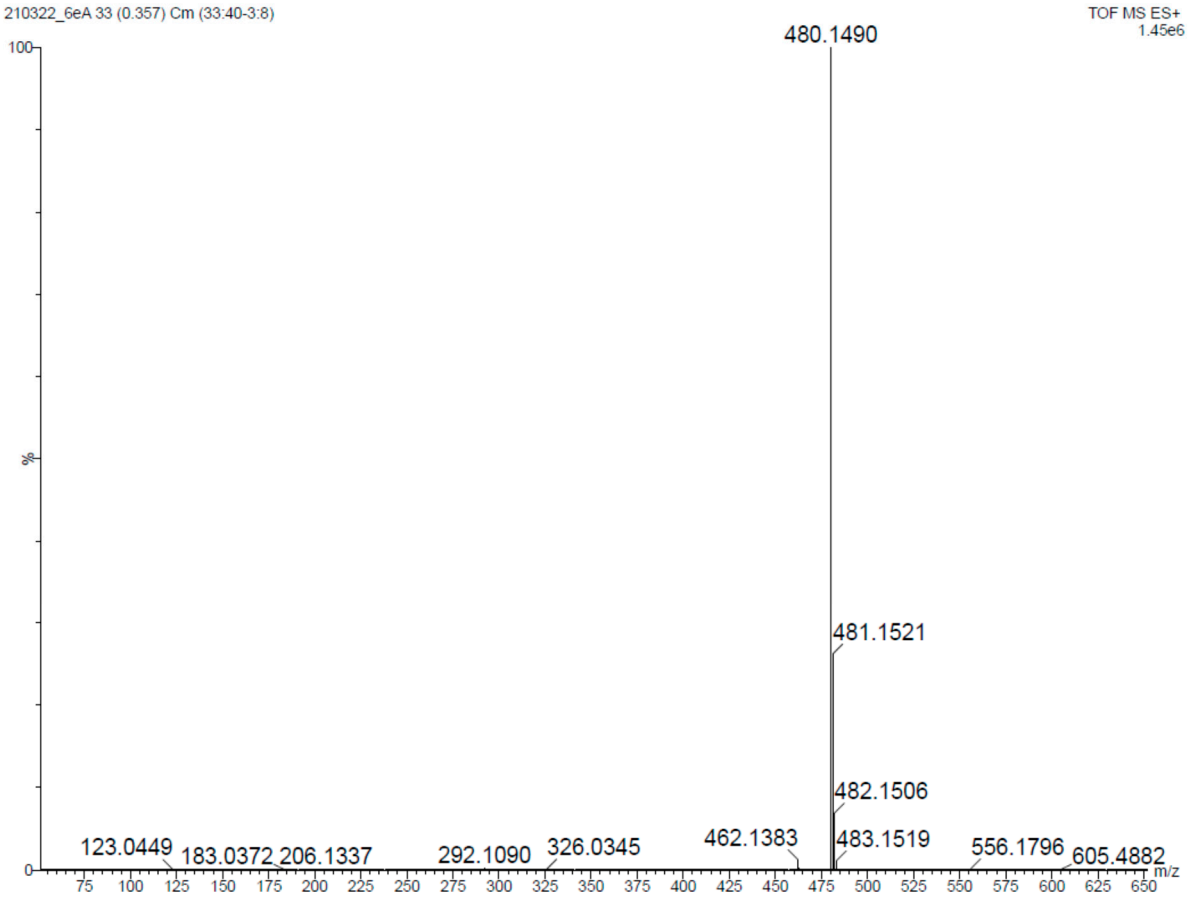


HSQC

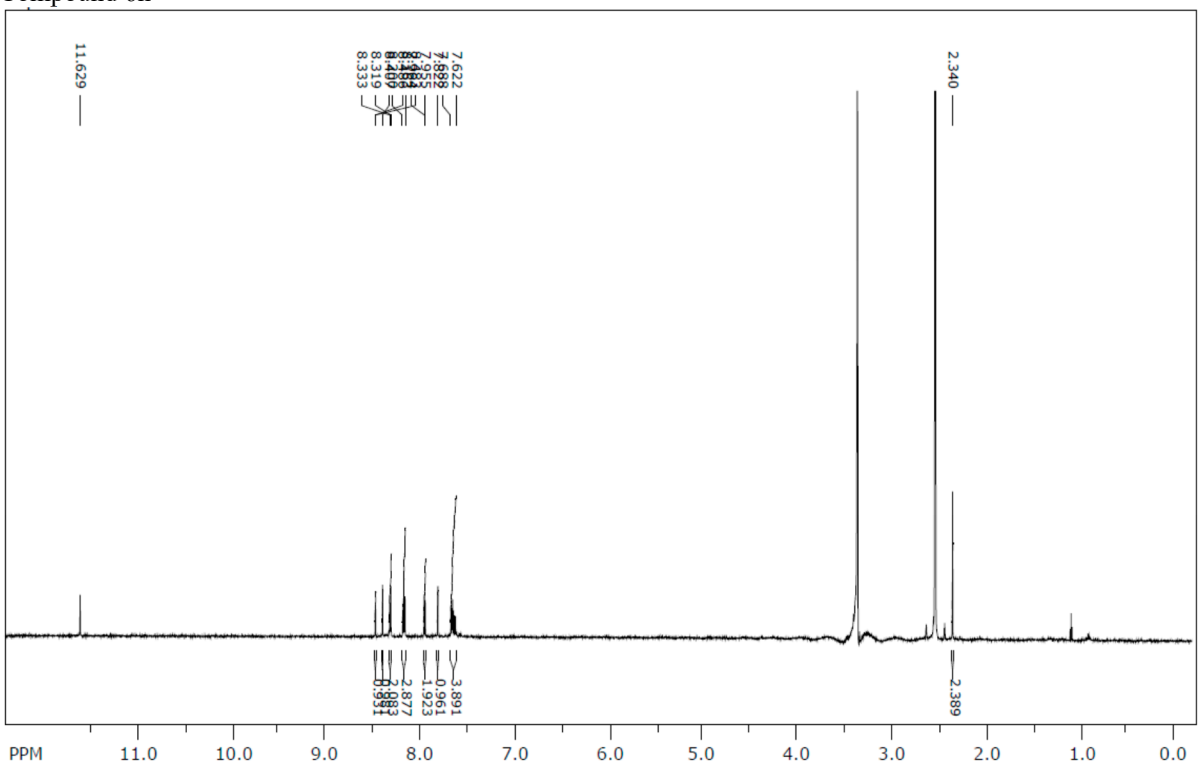

6g
K.Laczkowski
ppm

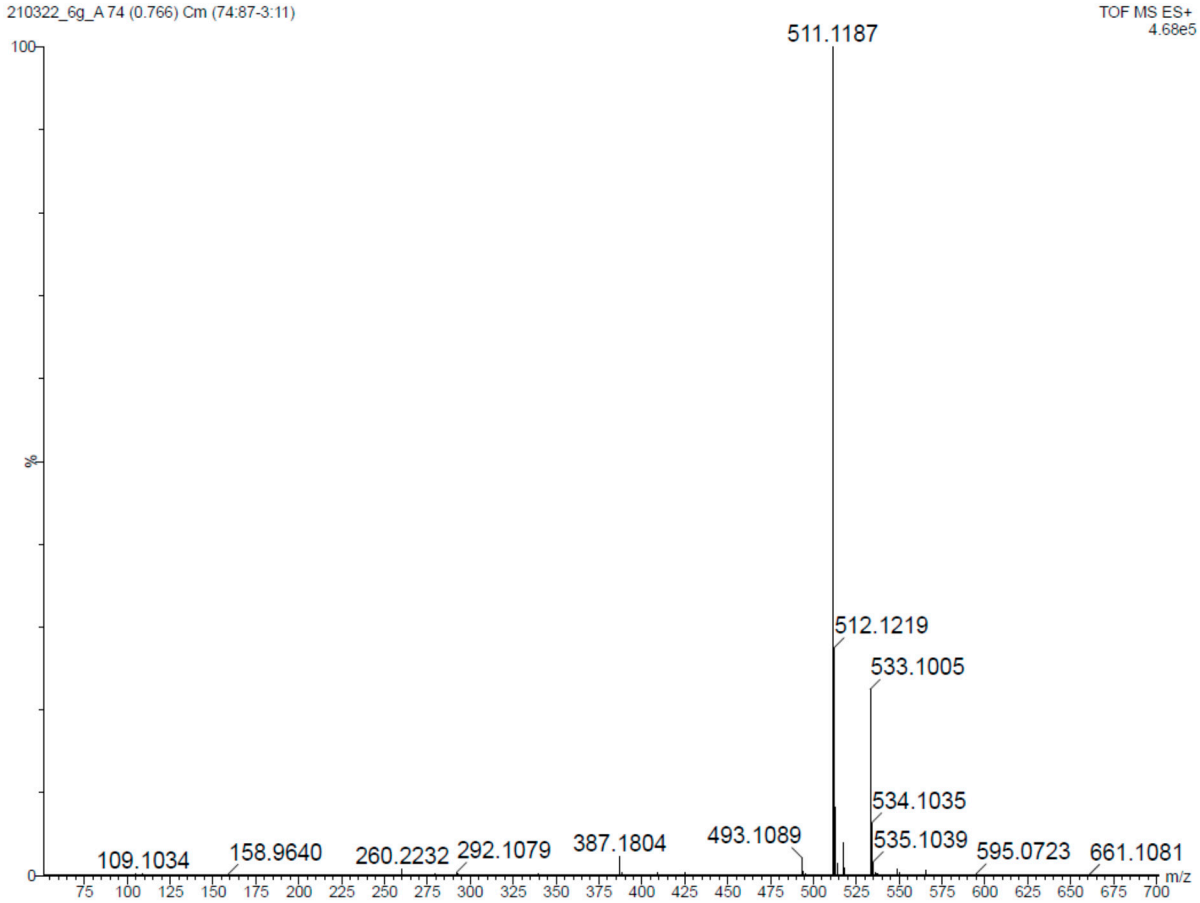
NOESY


6g
K.Laczkowski
ppm
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm

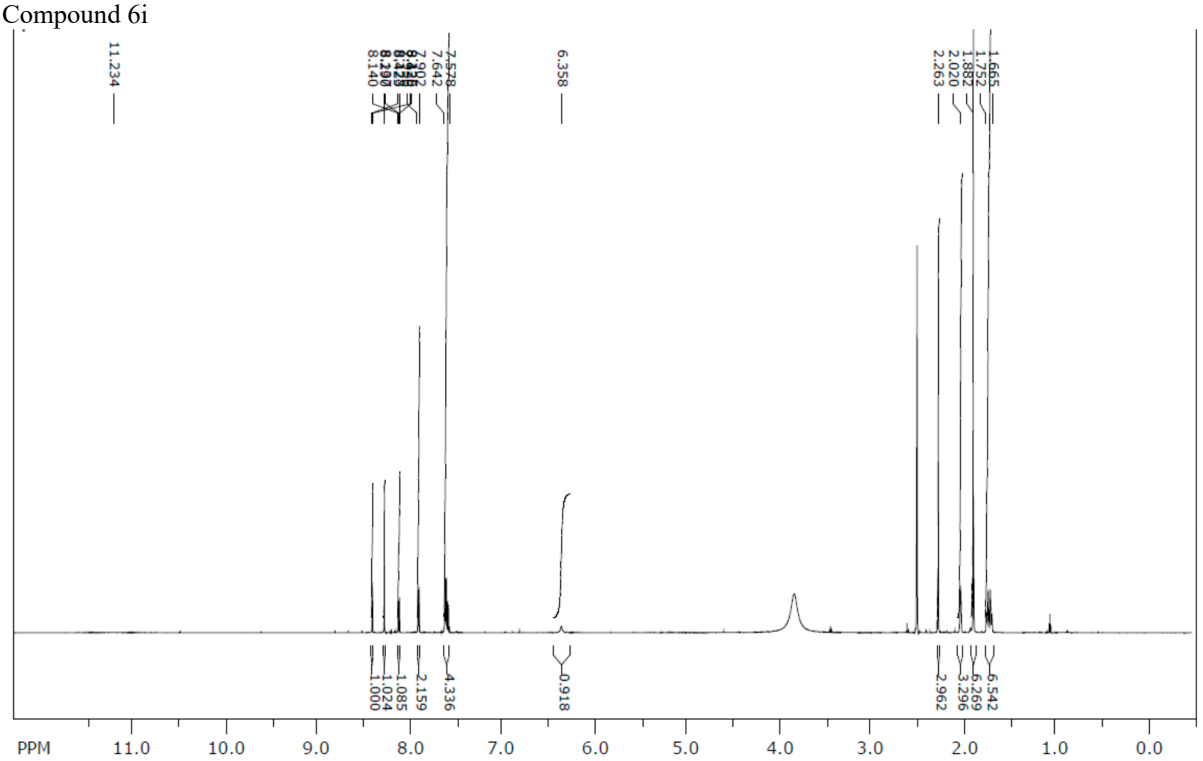

210322_6eA 33 (0.357) Cm (33:40-3:8)
TOF MS ES+
1.45e6
480.1490
481.1521
482.1506
483.1519
123.0449
183.0372
206.1337
292.1090
326.0345
462.1383
556.1796
605.4882
%
m/z

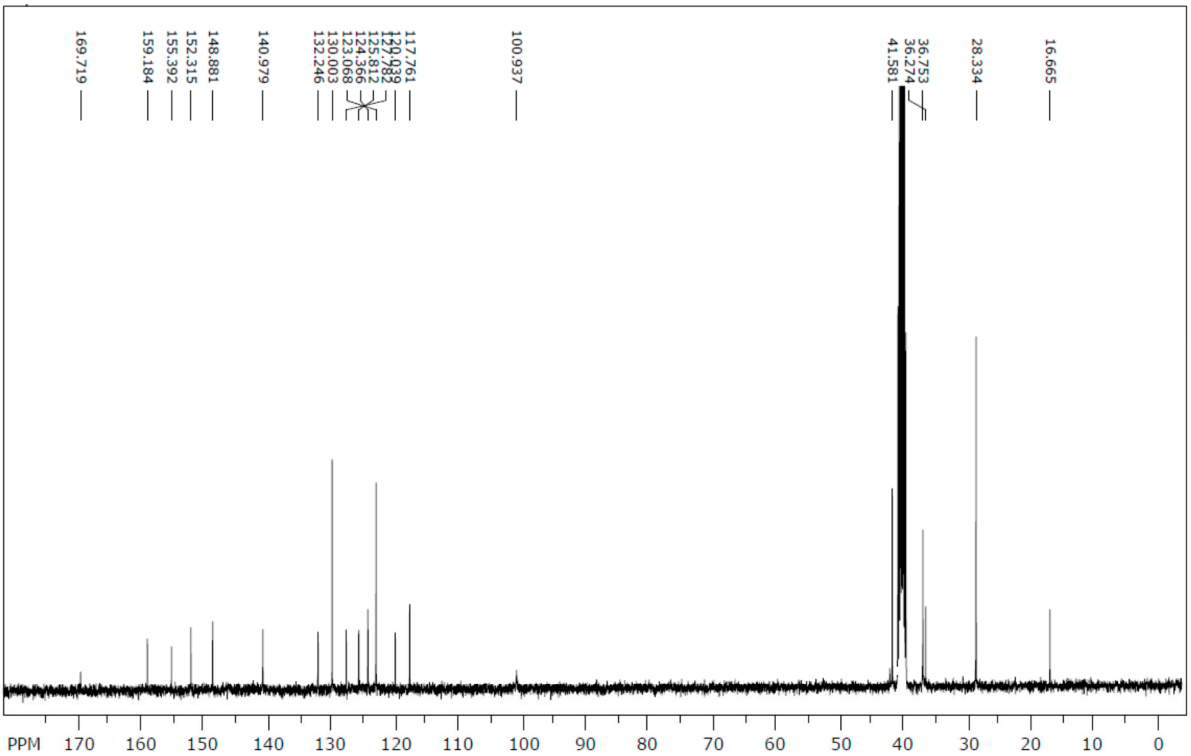
Compound 6h

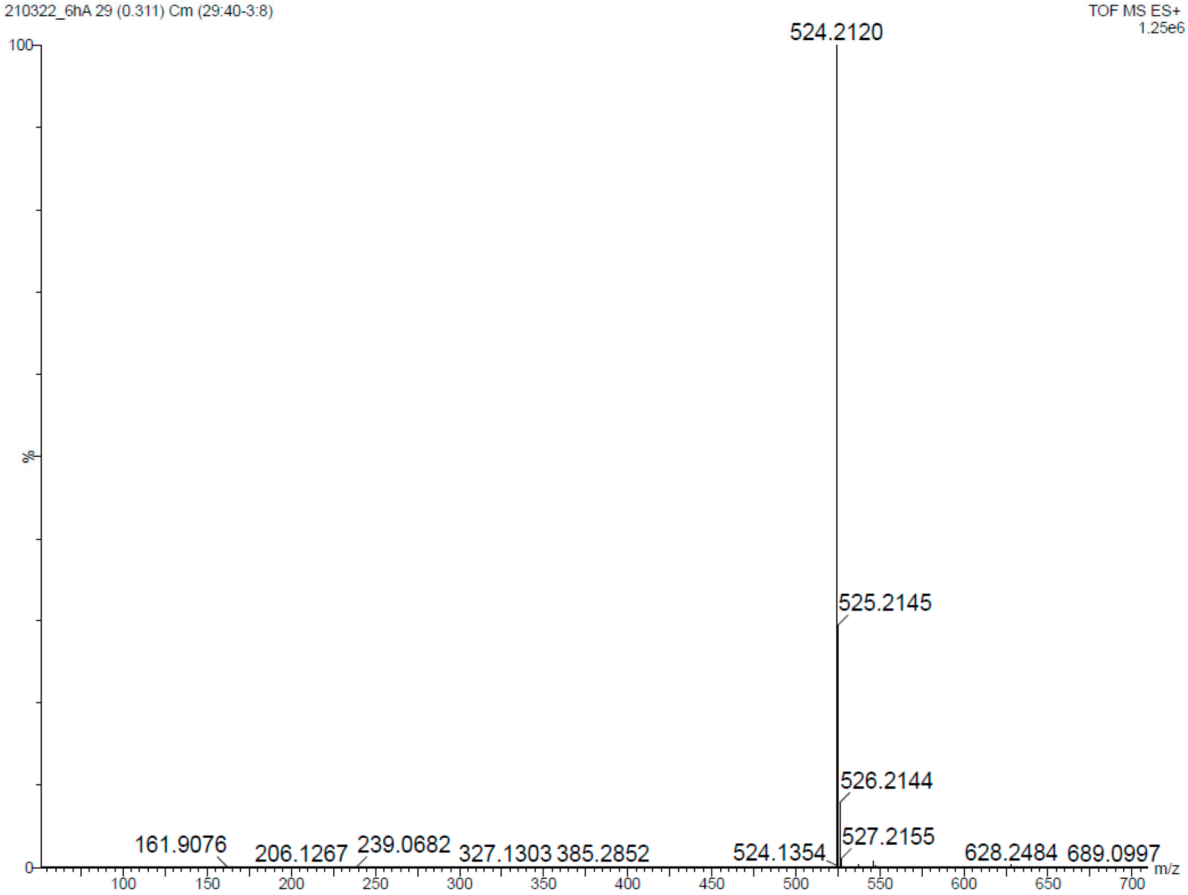

11.629
8.333
8.319
7.622
2.340
3.891
0.961
1.923
2.877
2.389
PPM


210322_6g_A 74 (0.766) Cm (74:87-3:11)
TOF MS ES+
4.68e5
511.1187
512.1219
533.1005
534.1035
535.1039
109.1034
158.9640
260.2232
292.1079
387.1804
493.1089
595.0723
661.1081
m/z

Compound 6i


11.234
8.140
7.642
7.578
6.358
2.263
2.020
1.882
1.752
1.665
1.000
1.024
1.085
2.159
4.336
0.918
2.962
3.296
6.269
6.542
PPM


169.719
159.184
155.392
152.315
148.881
140.979
132.246
130.003
123.068
124.366
117.761
100.937
41.581
36.753
36.274
28.334
16.665
PPM 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


210322_6hA 29 (0.311) Cm (29:40-3:8)
TOF MS ES+
1.25e6
524.2120
525.2145
526.2144
527.2155
161.9076
206.1267
239.0682
327.1303
385.2852
524.1354
628.2484
689.0997
100
%
0
100 150 200 250 300 350 400 450 500 550 600 650 700
m/z