Design, Synthesis and Docking Study of Novel Coumarin Ligands as Potential Selective Acetylcholinesterase Inhibitors

Fatih Sonmez[1,*], Belma Zengin Kurt[2], Isil Gazioglu[2], Livia Basile[3,**], Aydan Dag [2], Valentina Cappello[3], Tiziana Ginex[4], Mustafa Kucukislamoglu[5] and Salvatore Guccione[3]

[1]*Sakarya University, Pamukova Vocational High School, 54900, Sakarya, TURKEY*

[2]*Bezmialem Vakif University, Faculty of Pharmacy, Department of Analytical and Pharmaceutical Chemistry, 34093, Istanbul, TURKEY*

[3]*Department of Drug Sciences, University of Catania, Viale A. Doria 6 Ed. 2, Città Universitaria, I- 95125, Catania, ITALY*

[4]*Molecular Modelling Laboratory, Department of Food Science, University of Parma, Parco Area delle Scienze 17/A, Parma 43124, ITALY*

[5]*Sakarya University, Faculty of Arts and Science, Department of Chemistry, 54055, Sakarya, TURKEY*

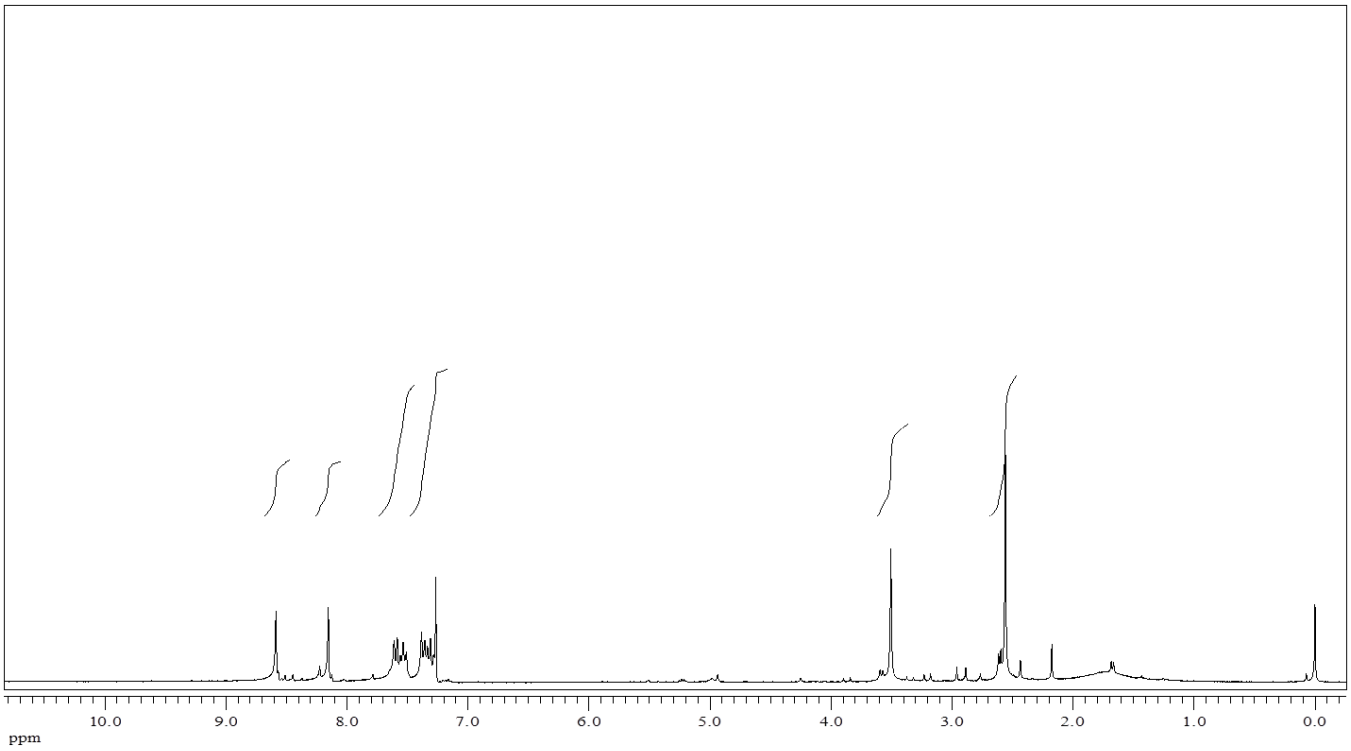
* Corresponding authors. Tel.: +90-264-2953378, fax: +90-264-2953679 (F. Sonmez); e-mail addresses: fsonmez@sakarya.edu.tr (F. Sonmez).

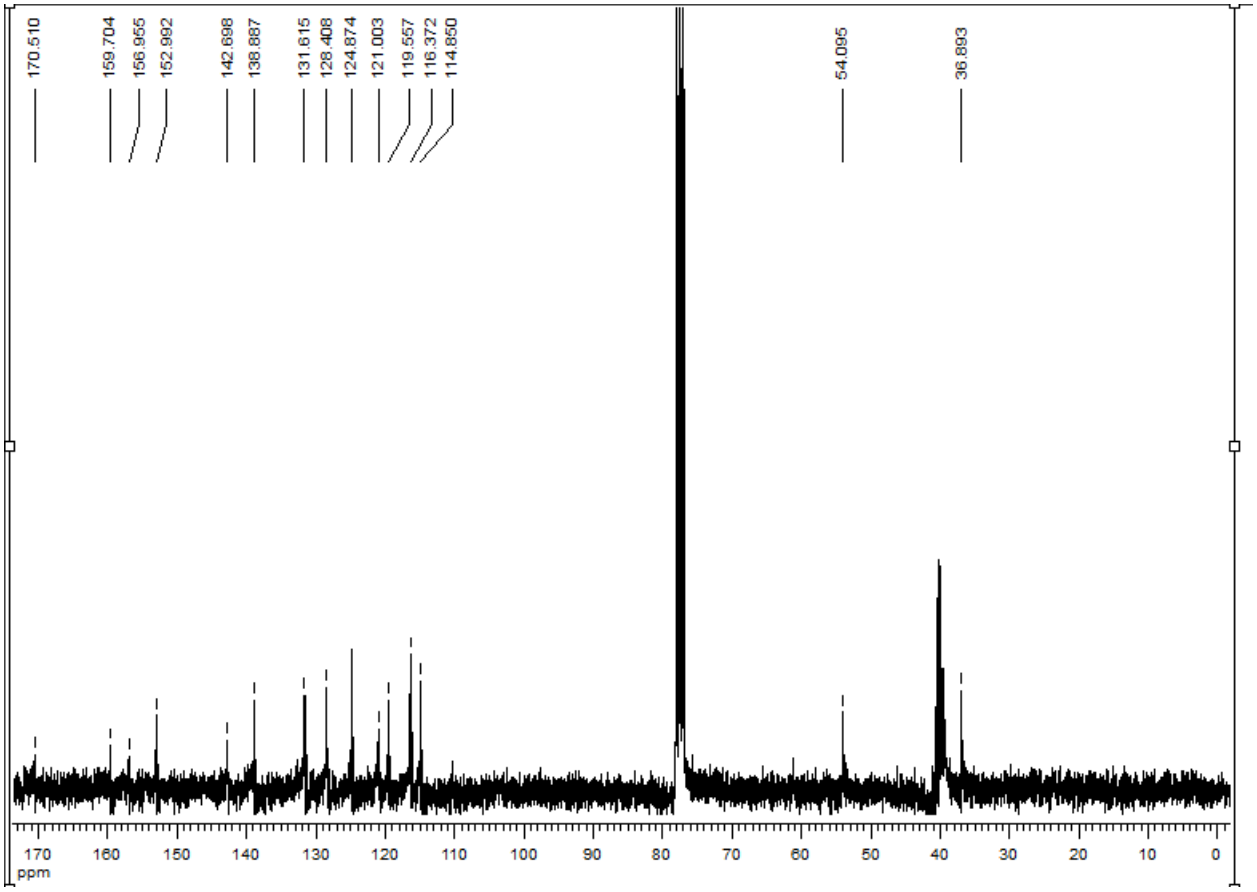
** Corresponding authors. Tel.: +39-095-7384020; e-mail addresses: basilelivia@gmail.com, liviabasile@unict.it (L. Basile).

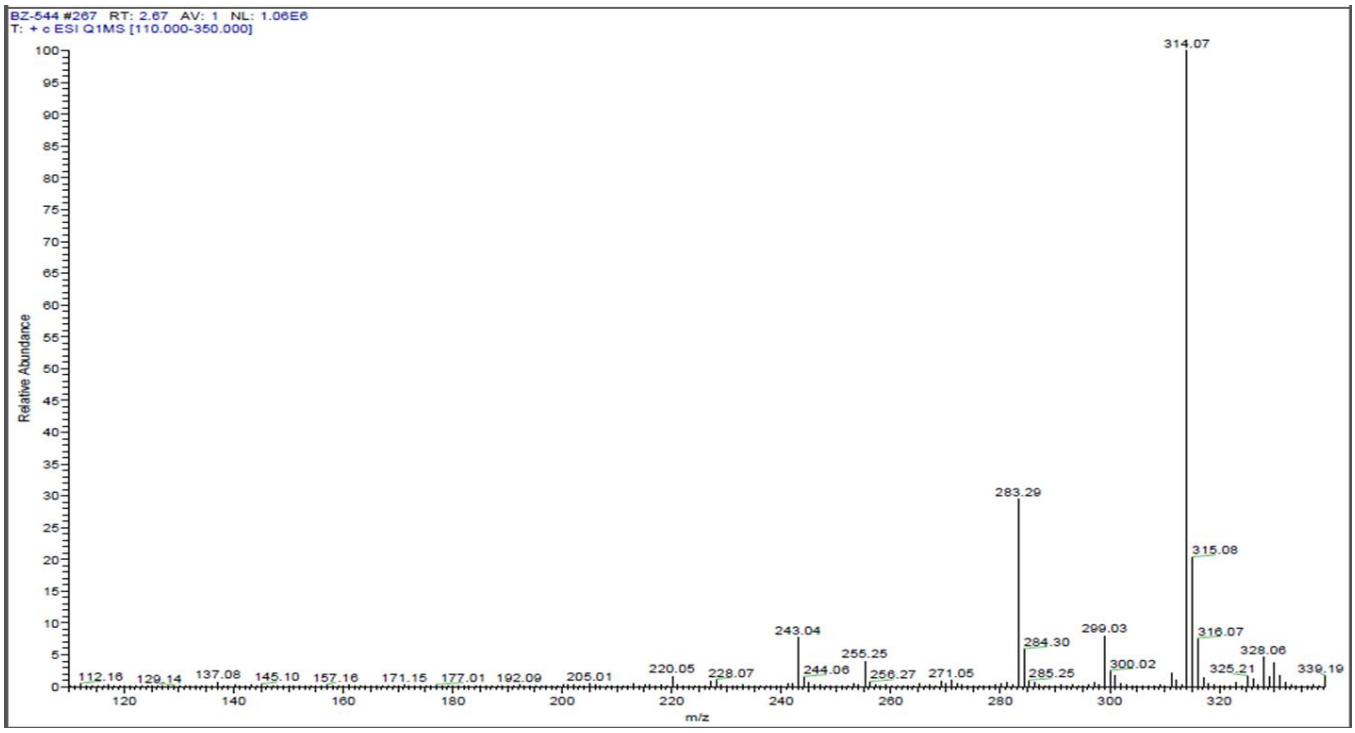
SUPPLEMANTARY MATERIALS

^{1}H and ^{13}C NMR and MS spectra of **6a-t** …… 2-31

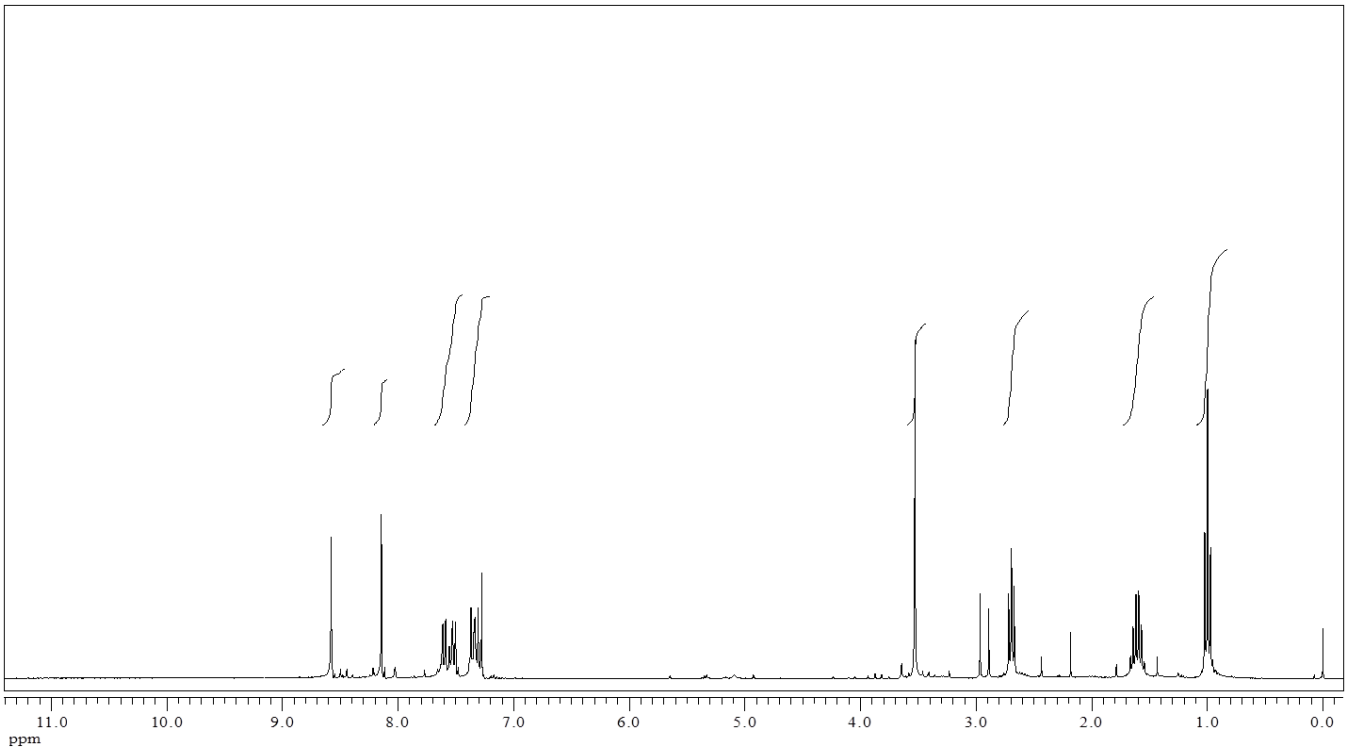
S1: ^{1}H and ^{13}C NMR and MS spectra of **6a**

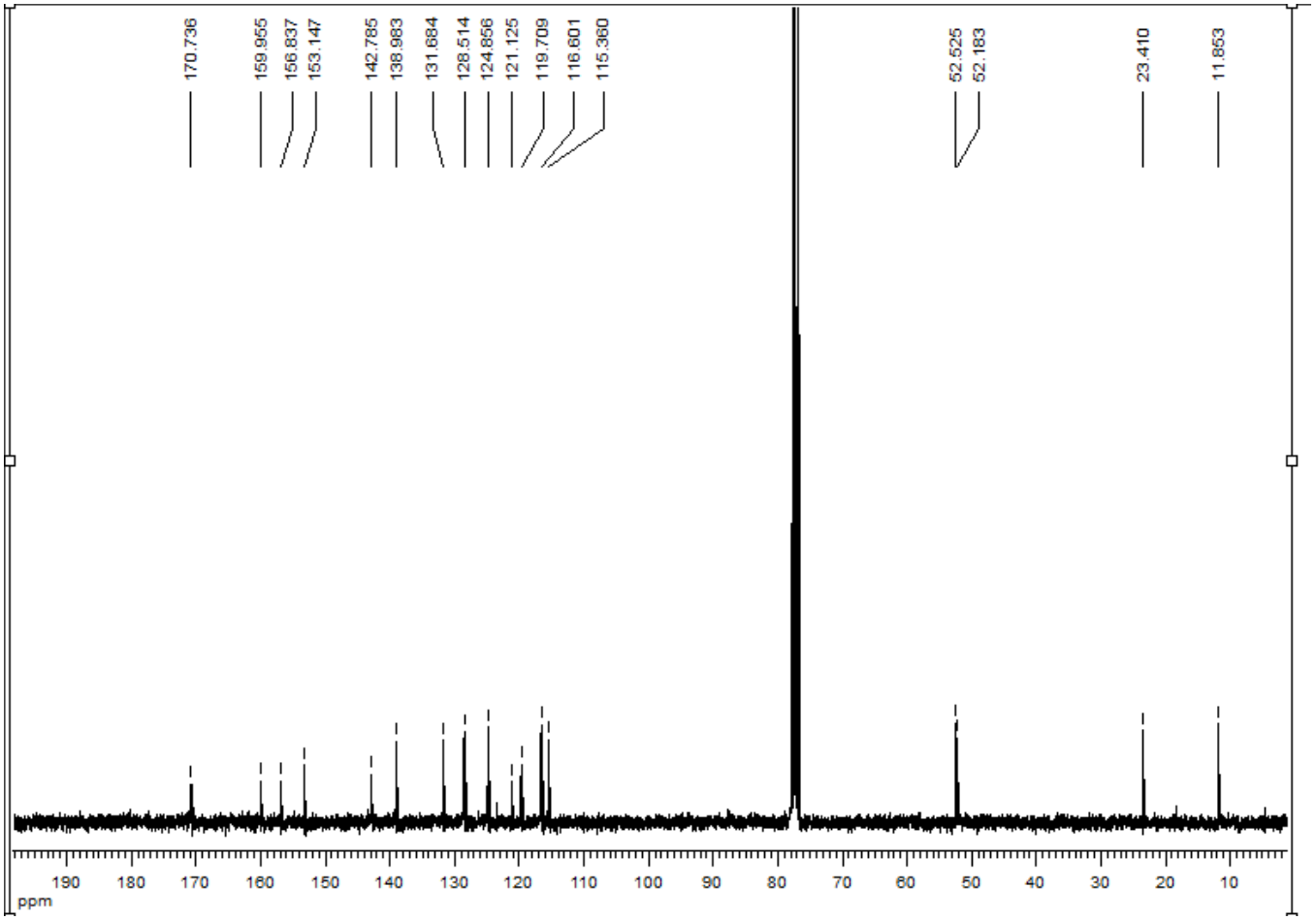


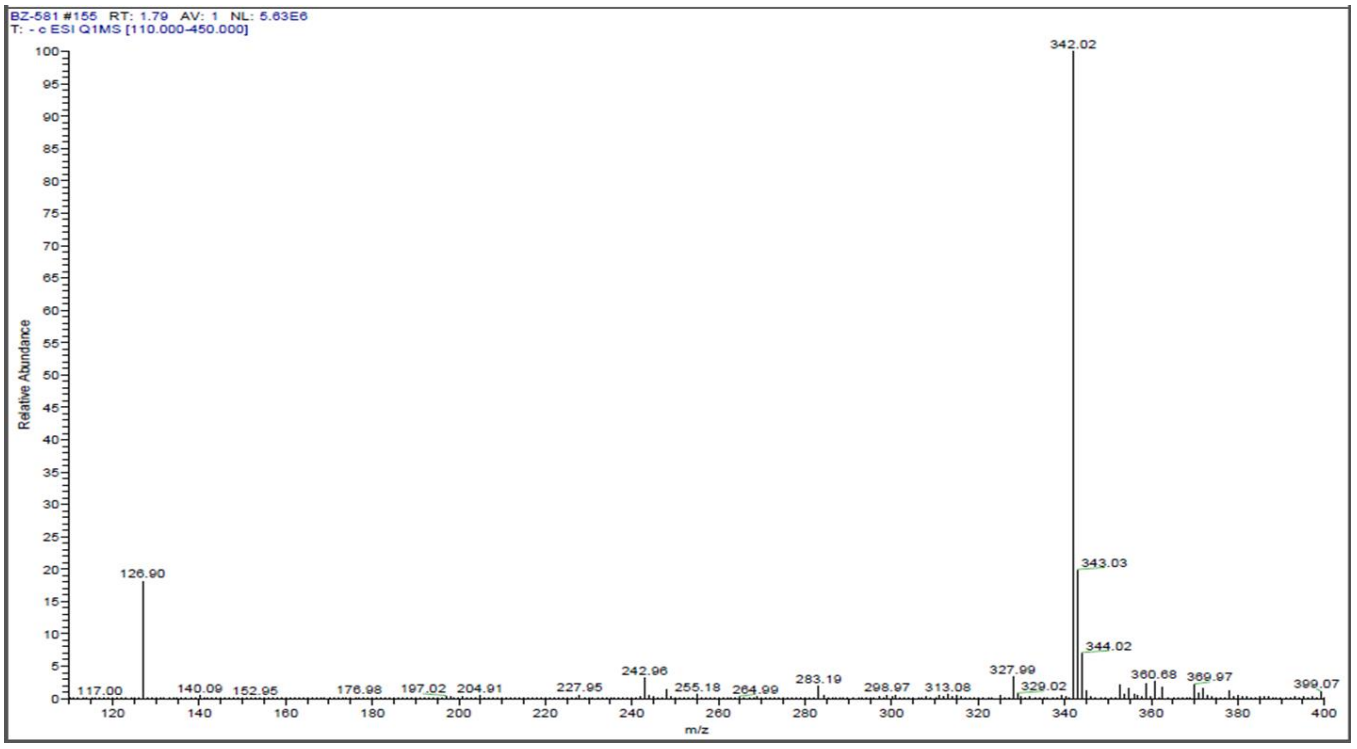




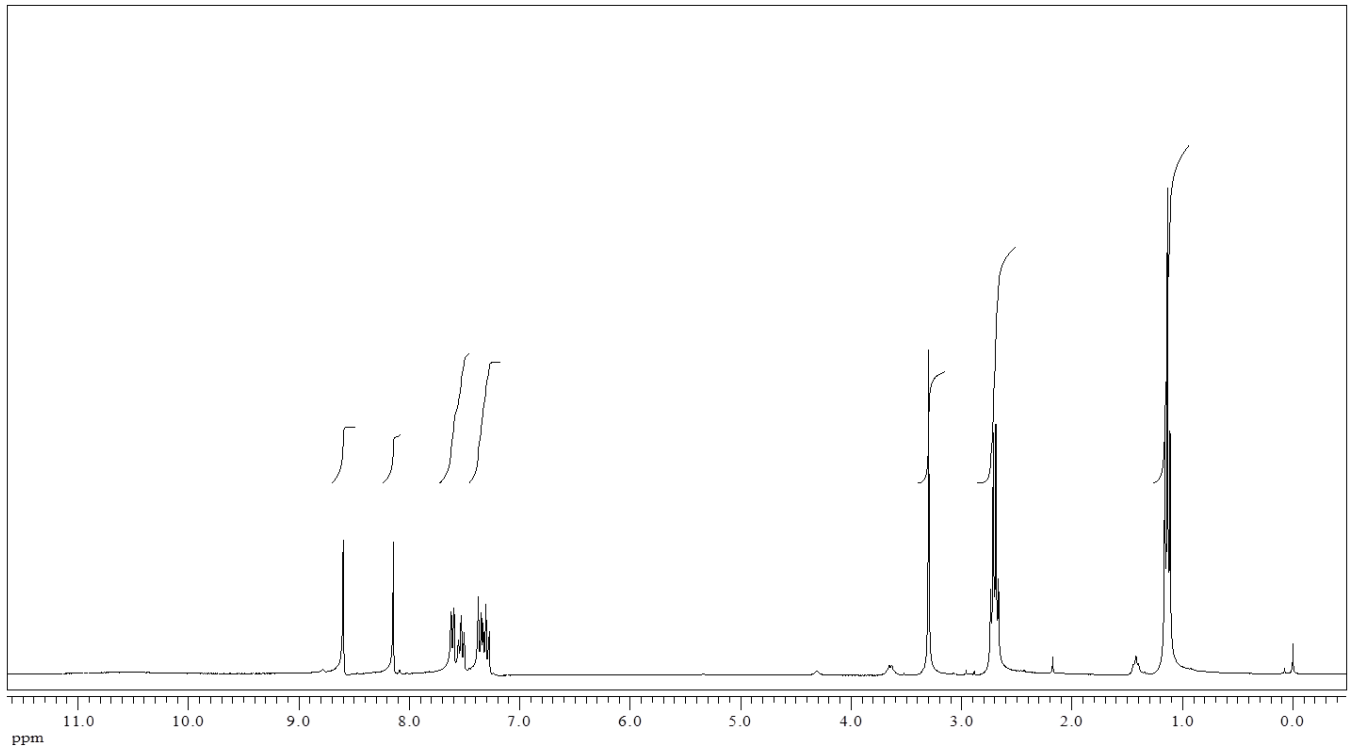
S2: ^{1}H and ^{13}C NMR and MS spectra of **6b**

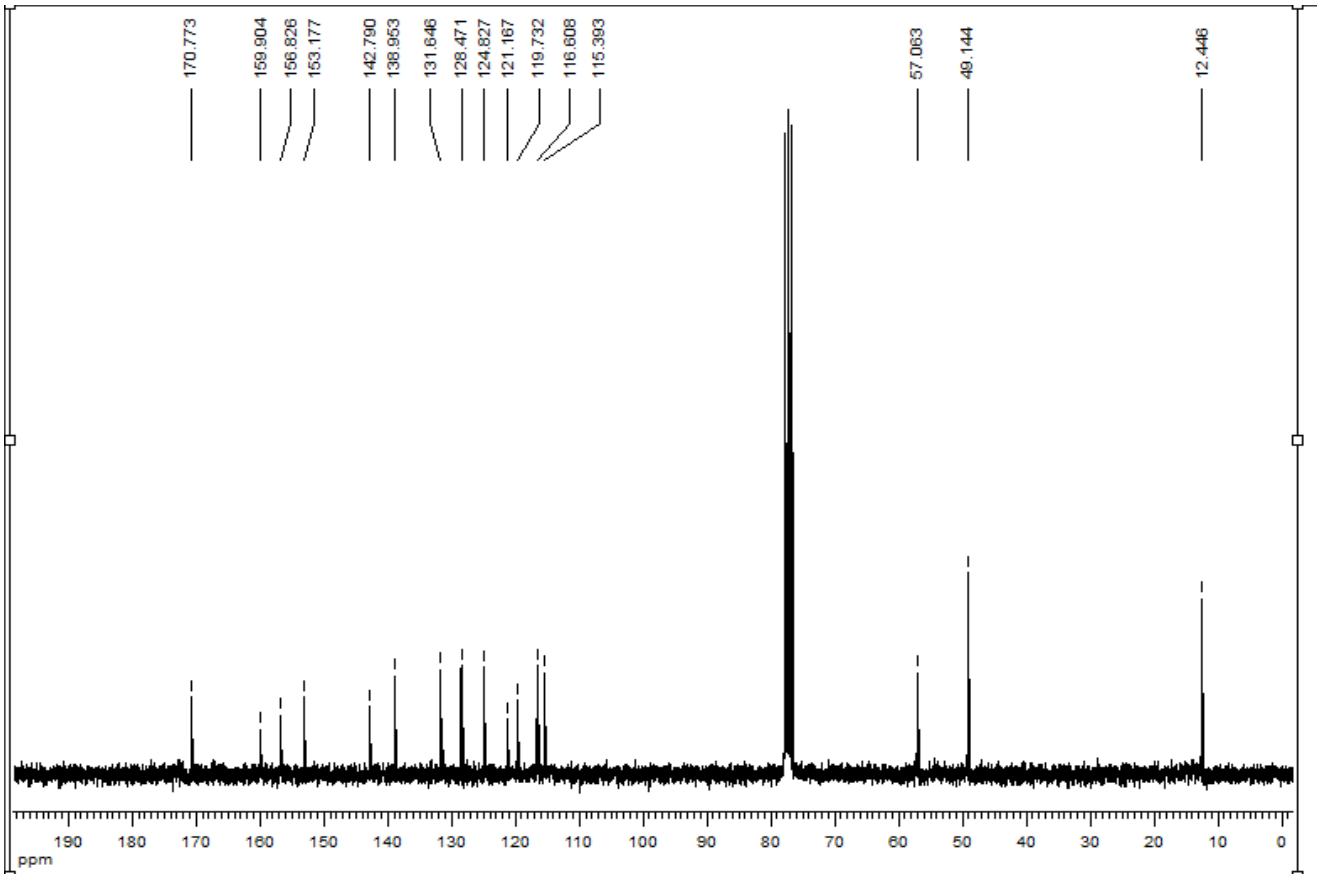


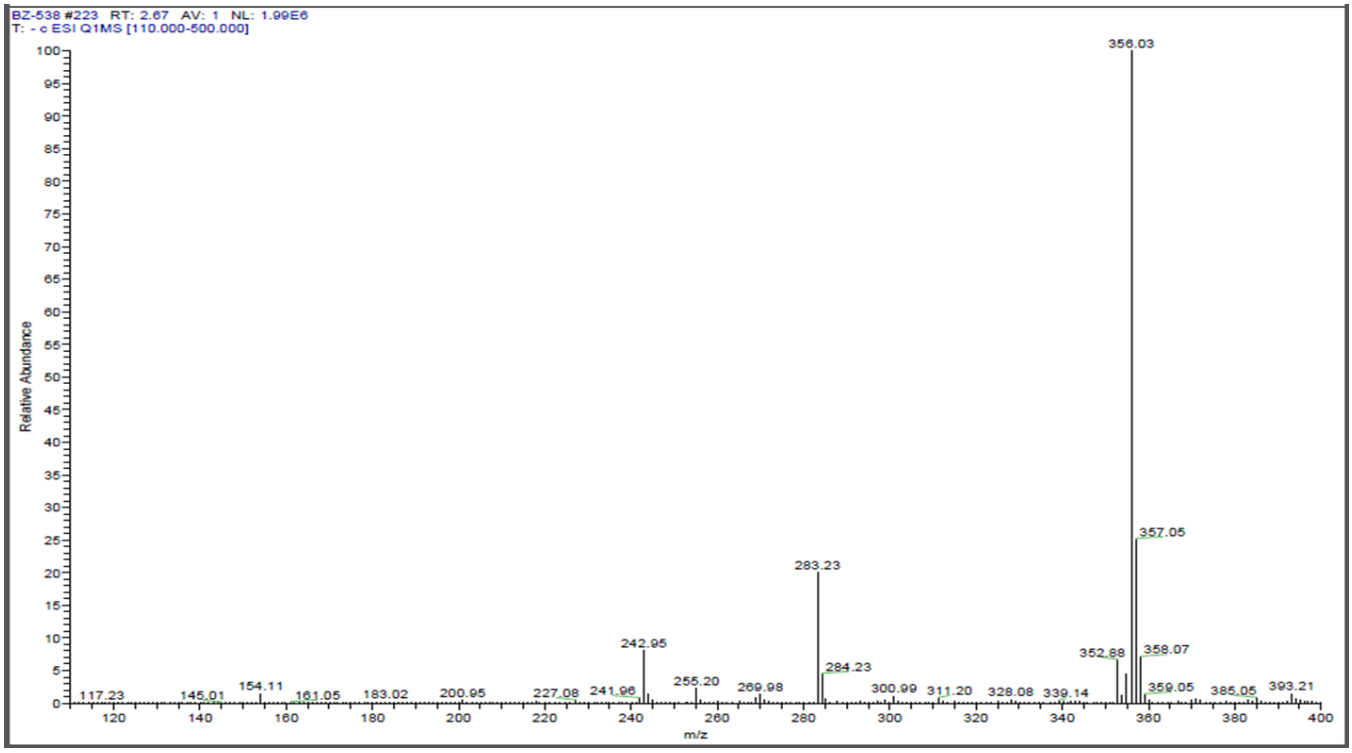

170.736
159.955
156.837
153.147
142.785
138.983
131.684
128.514
124.856
121.125
119.709
116.601
115.360
52.525
52.183
23.410
11.853
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


BZ-581 #155 RT: 1.79 AV: 1 NL: 5.63E6
T: - c ESI Q1MS [110.000-450.000]
Relative Abundance
m/z
342.02
343.03
344.02
126.90
117.00
140.09
152.95
176.98
197.02
204.91
227.95
242.96
255.18
264.99
283.19
298.97
313.08
327.99
329.02
360.68
369.97
399.07

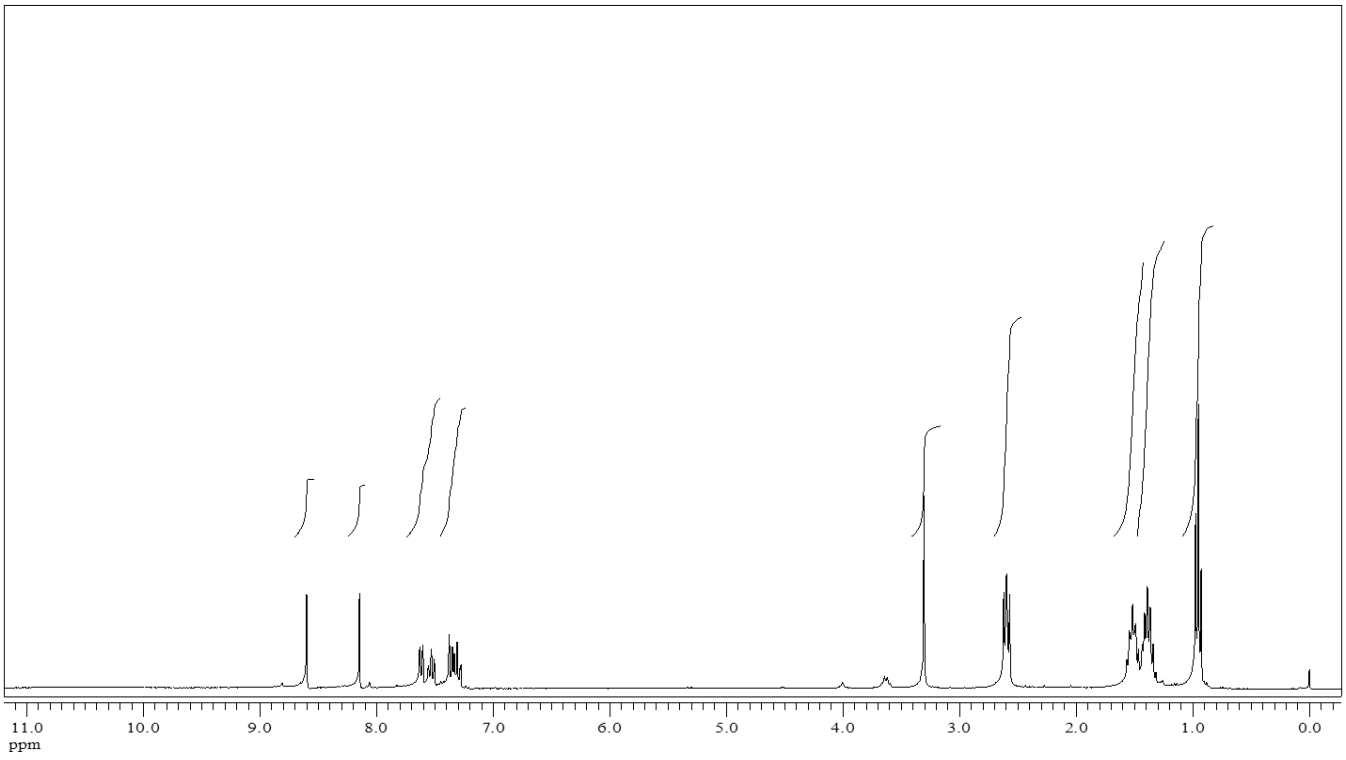
S3: [1] H and [13]C NMR and MS spectra of **6c**

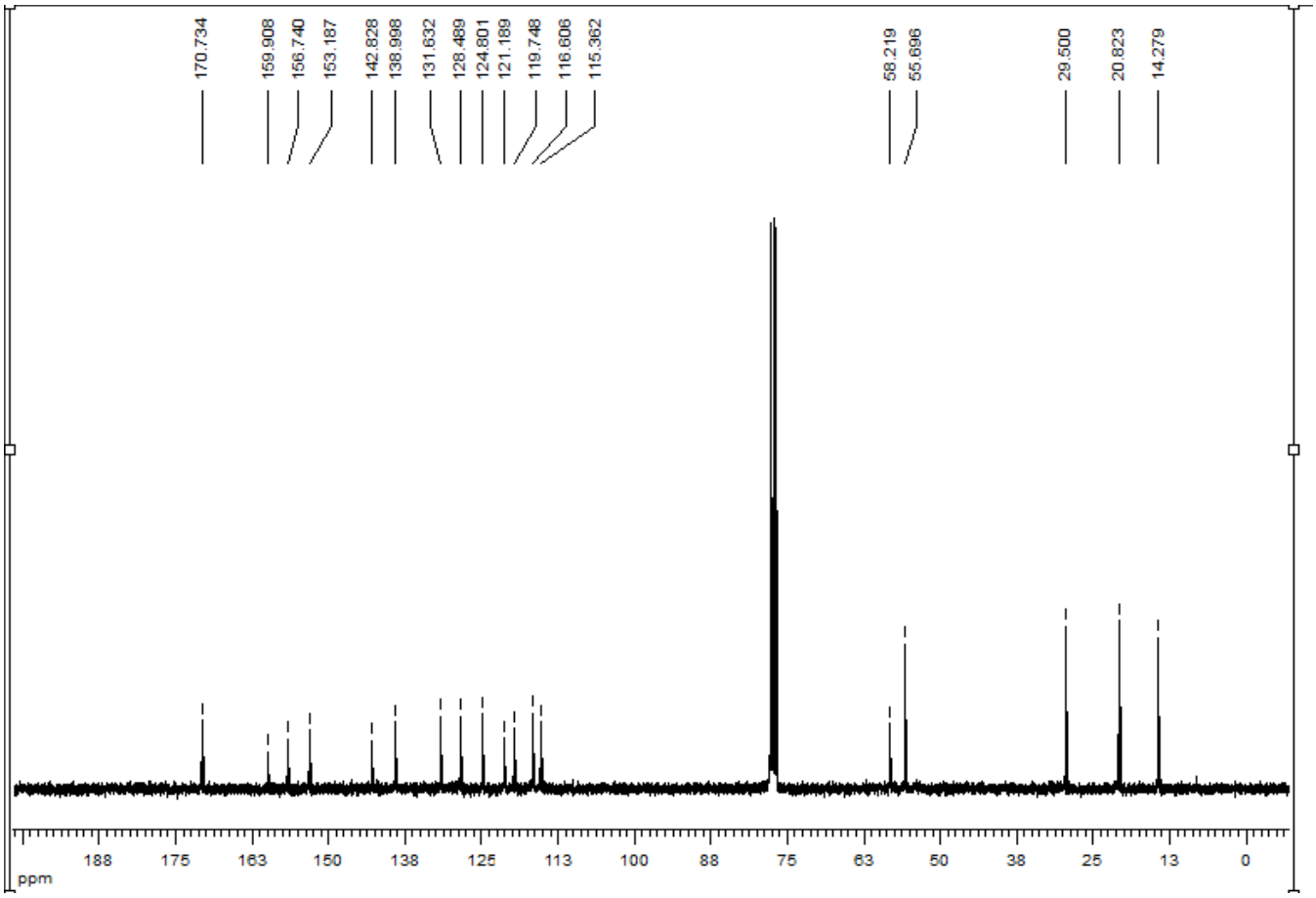


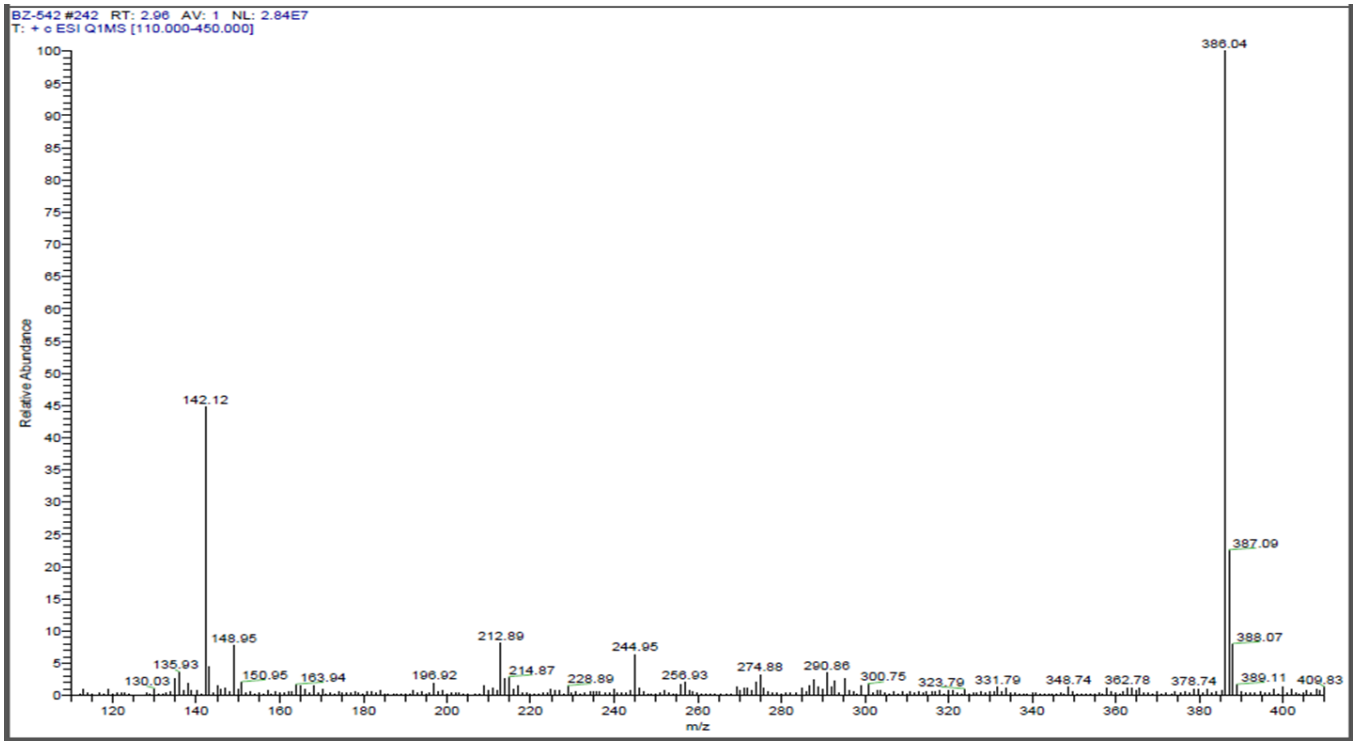




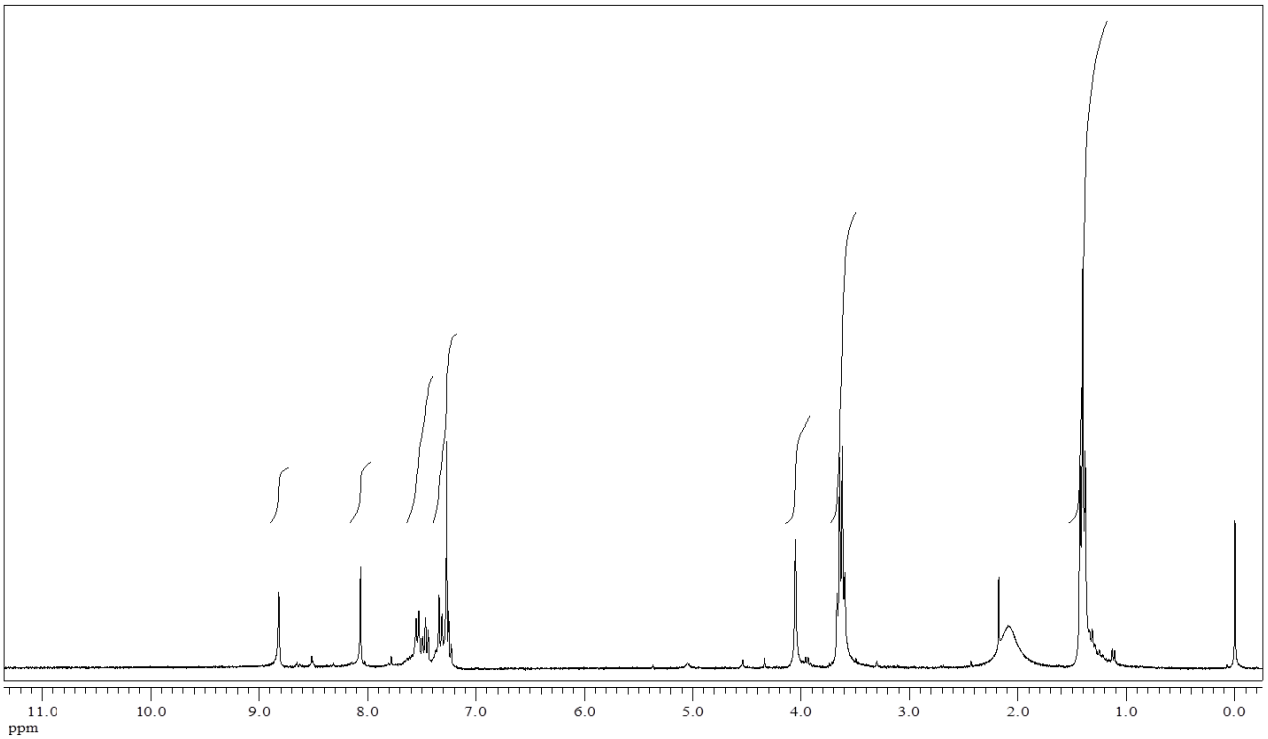
S4: [1] H and [13]C NMR and MS spectra of **6d**

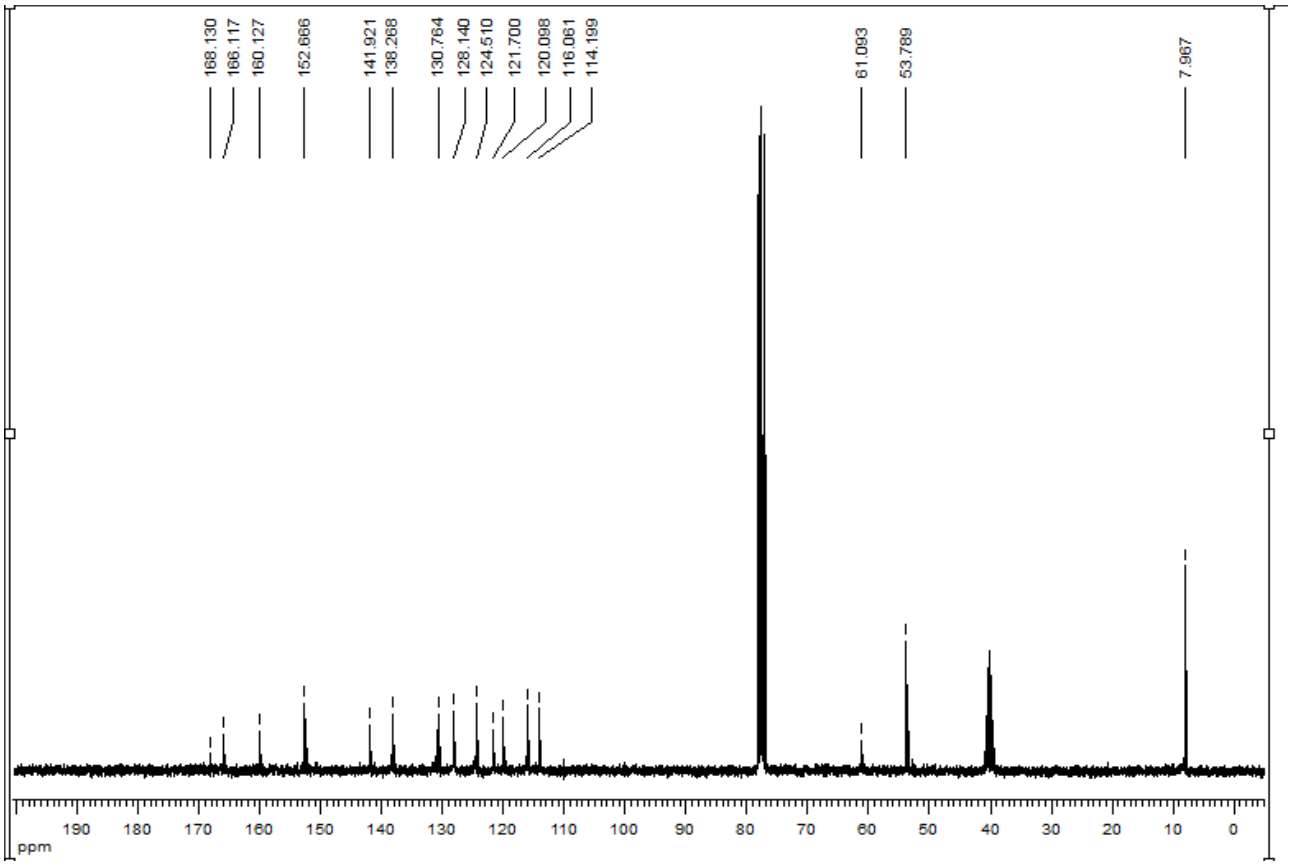


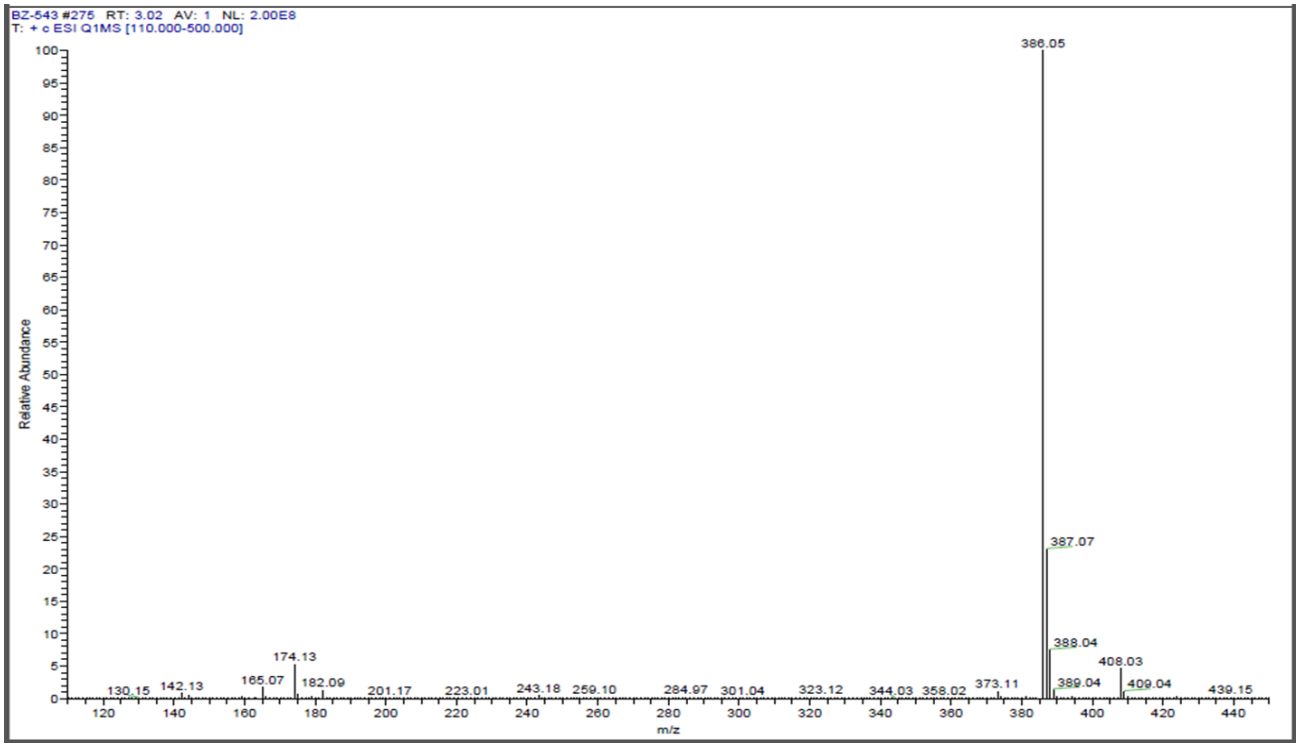

170.734
159.908
156.740
153.187
142.828
138.998
131.632
128.489
124.801
121.189
119.748
116.606
115.362
58.219
55.696
29.500
20.823
14.279
188
175
163
150
138
125
113
100
88
75
63
50
38
25
13
0
ppm


BZ-542 #242 RT: 2.96 AV: 1 NL: 2.84E7
T: + c ESI Q1MS [110.000-450.000]
Relative Abundance
m/z
386.04
387.09
388.07
389.11
409.83
142.12
148.95
135.93
130.03
150.95
163.94
196.92
212.89
214.87
228.89
244.95
256.93
274.88
290.86
300.75
323.79
331.79
348.74
362.78
378.74

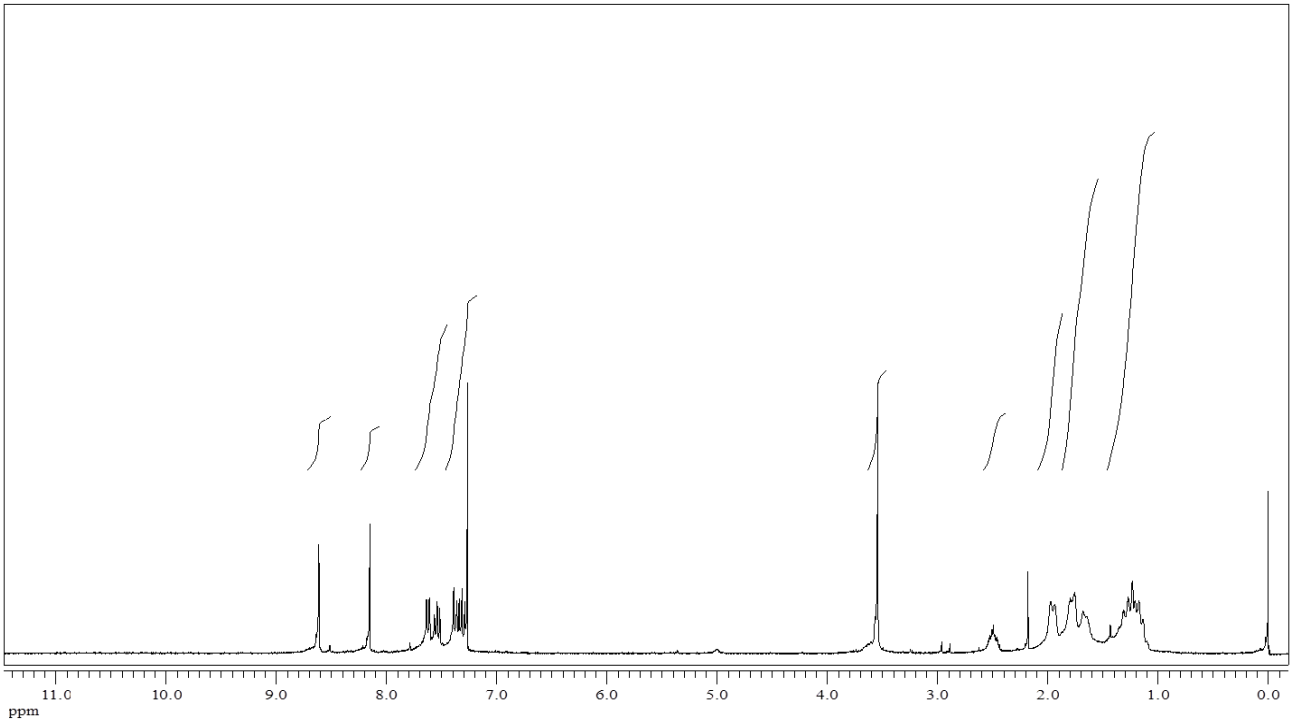
S5: ^{1}H and ^{13}C NMR and MS spectra of **6e**

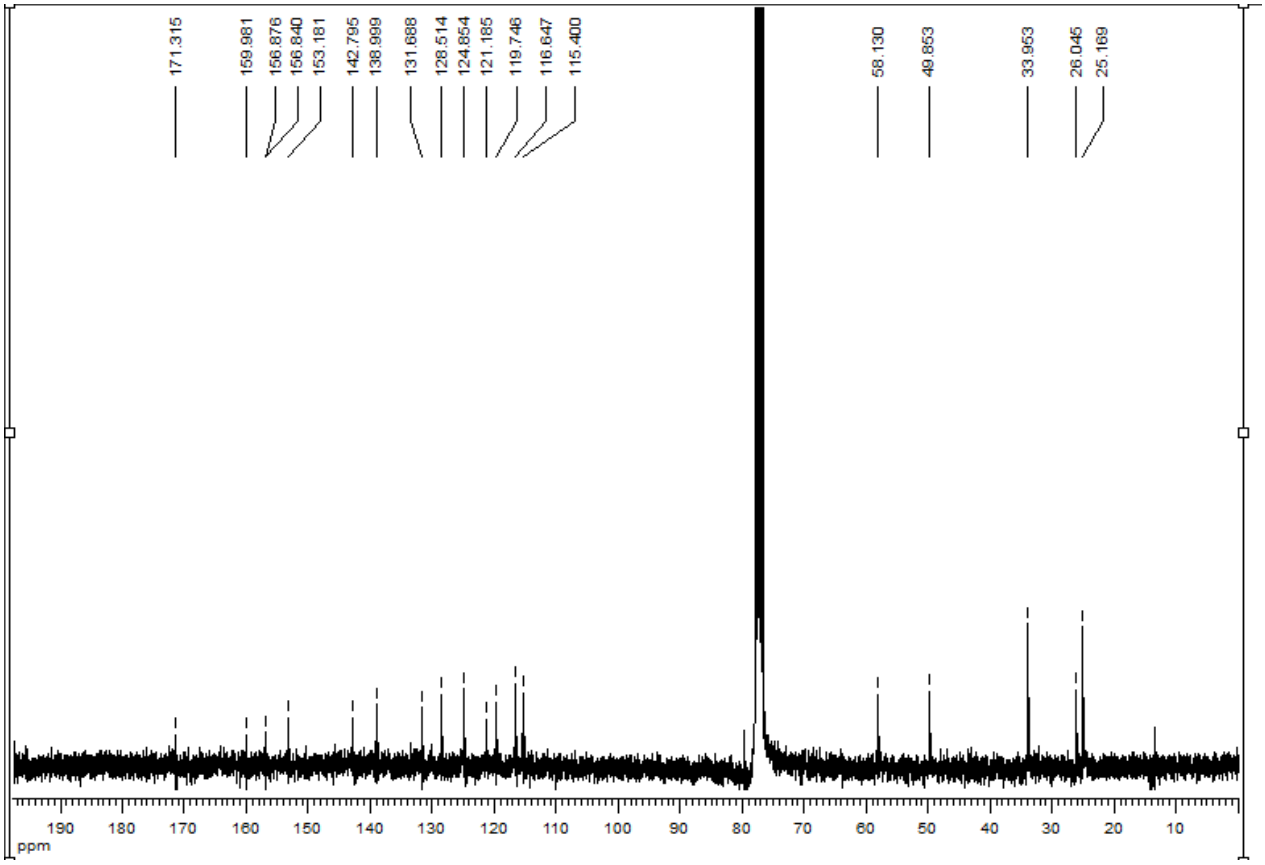


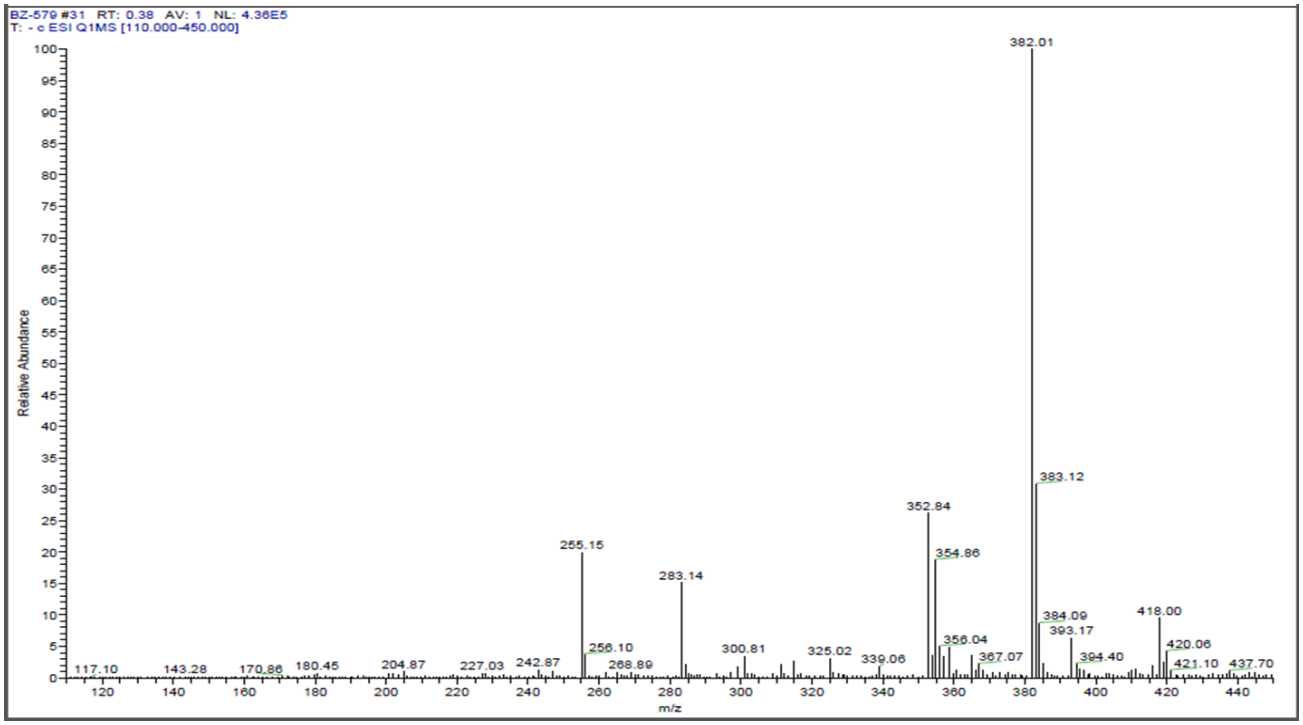




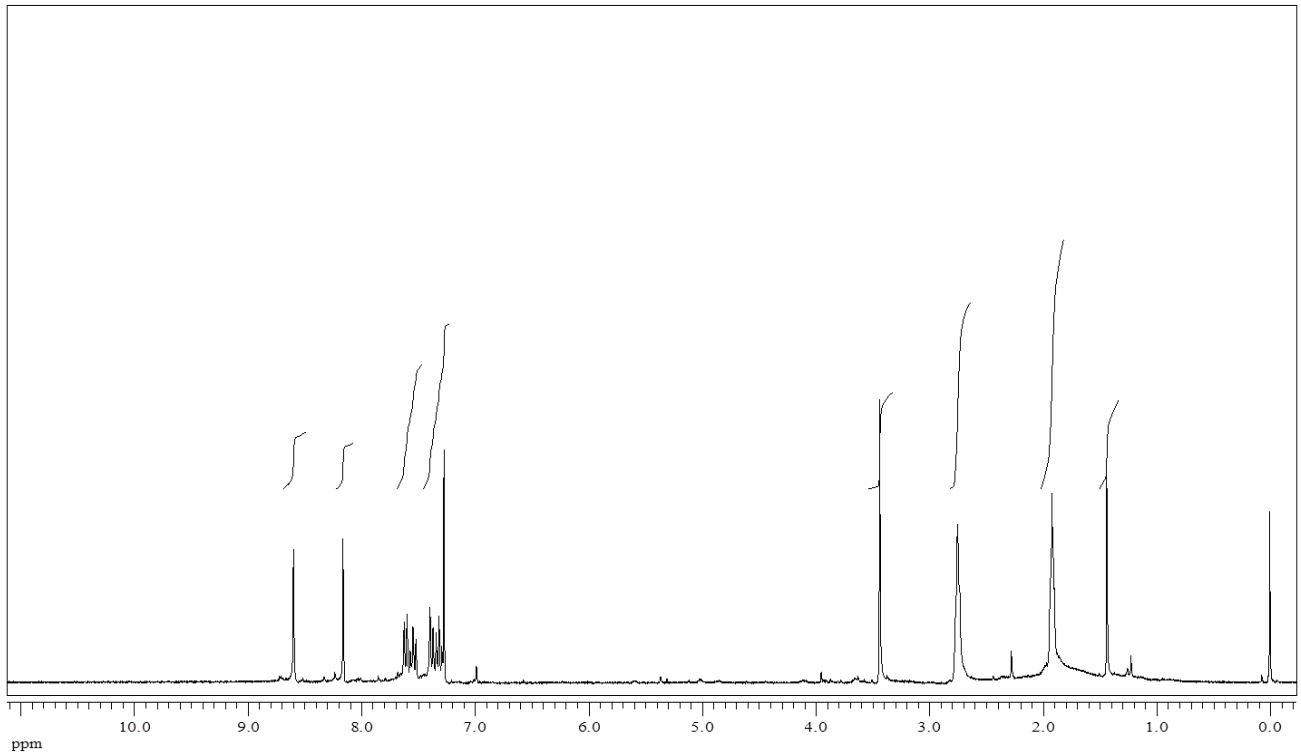
S6: ^{1}H and ^{13}C NMR and MS spectra of **6f**

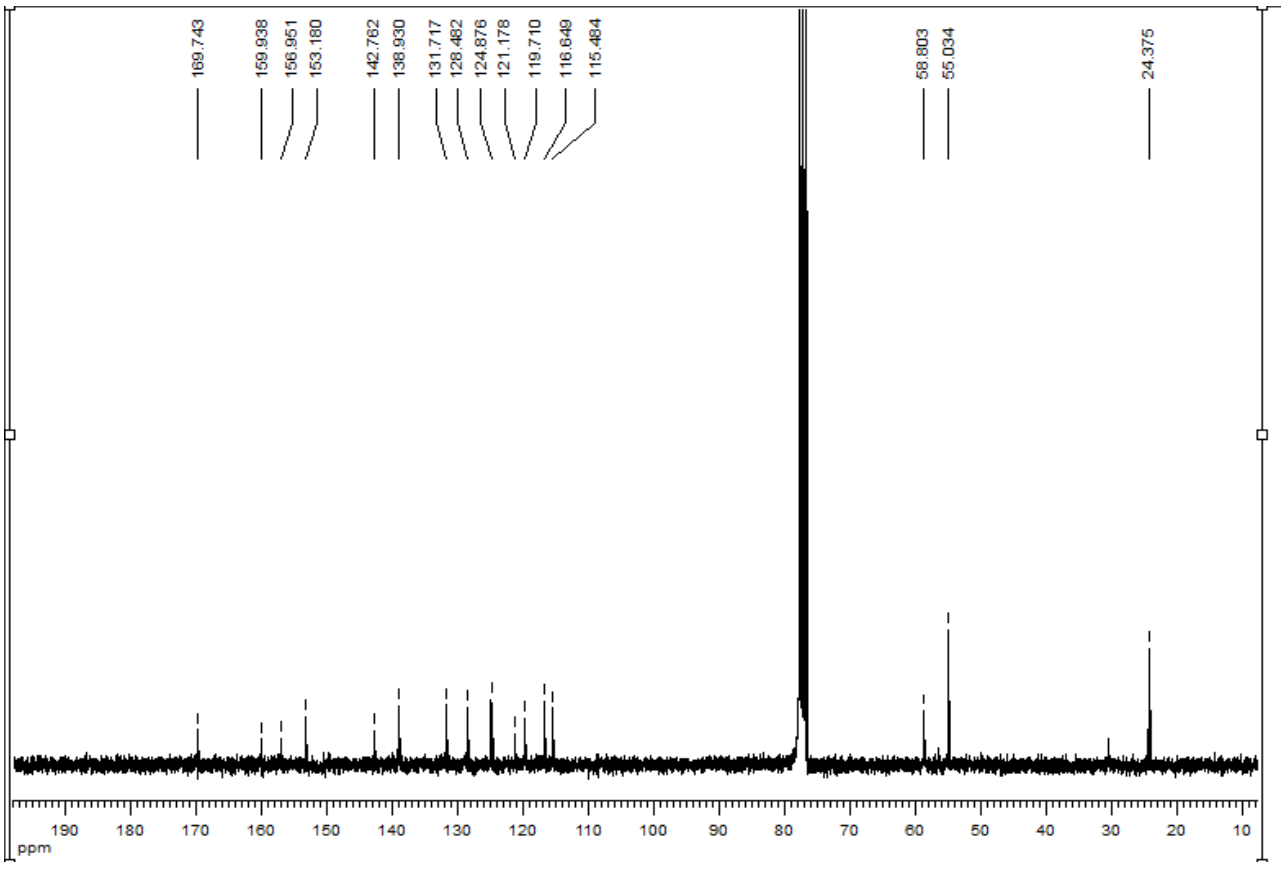


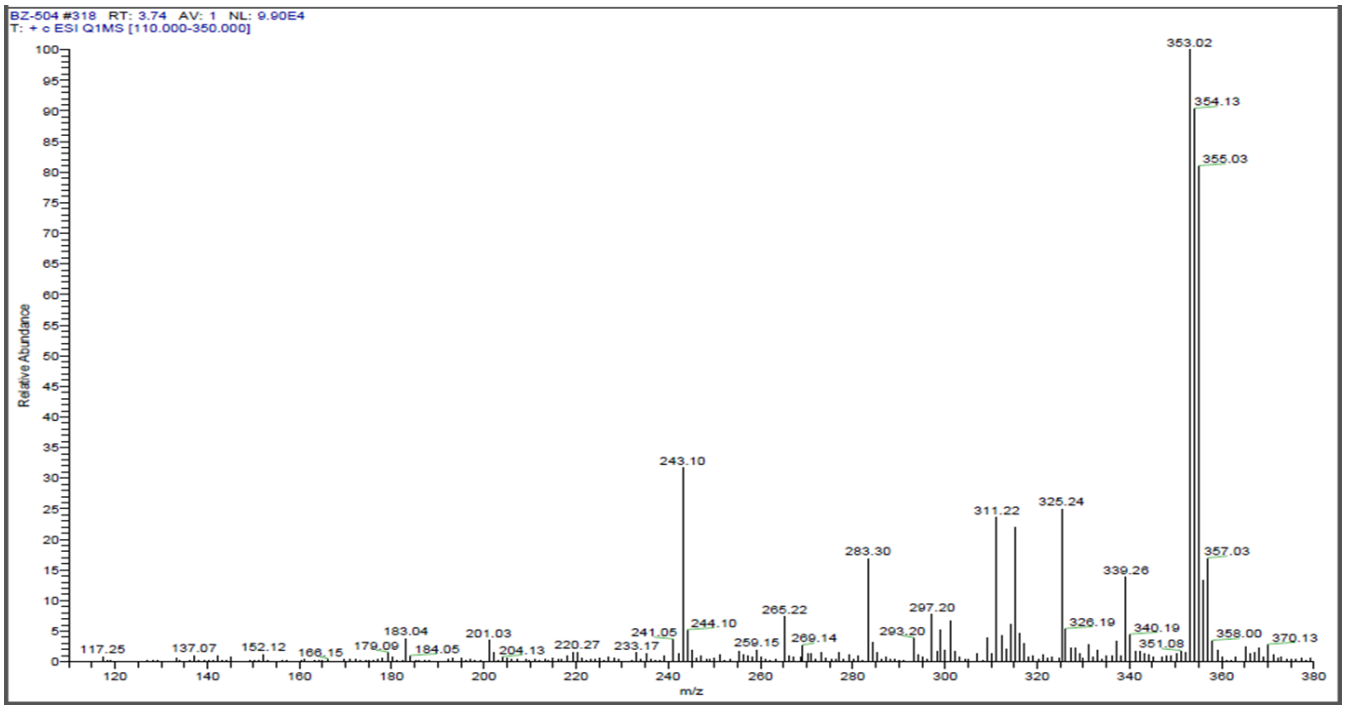

171.315
159.981
156.876
156.840
153.181
142.795
138.999
131.688
128.514
124.854
121.185
119.746
116.647
115.400
58.130
49.853
33.953
26.045
25.169
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


BZ-579 #31 RT: 0.38 AV: 1 NL: 4.36E5
T: - c ESI Q1MS [110.000-450.000]
Relative Abundance
m/z
382.01
383.12
352.84
354.86
255.15
283.14
384.09
393.17
418.00
420.06
356.04
367.07
394.40
421.10
437.70
256.10
268.89
300.81
325.02
339.06
117.10
143.28
170.86
180.45
204.87
227.03
242.87

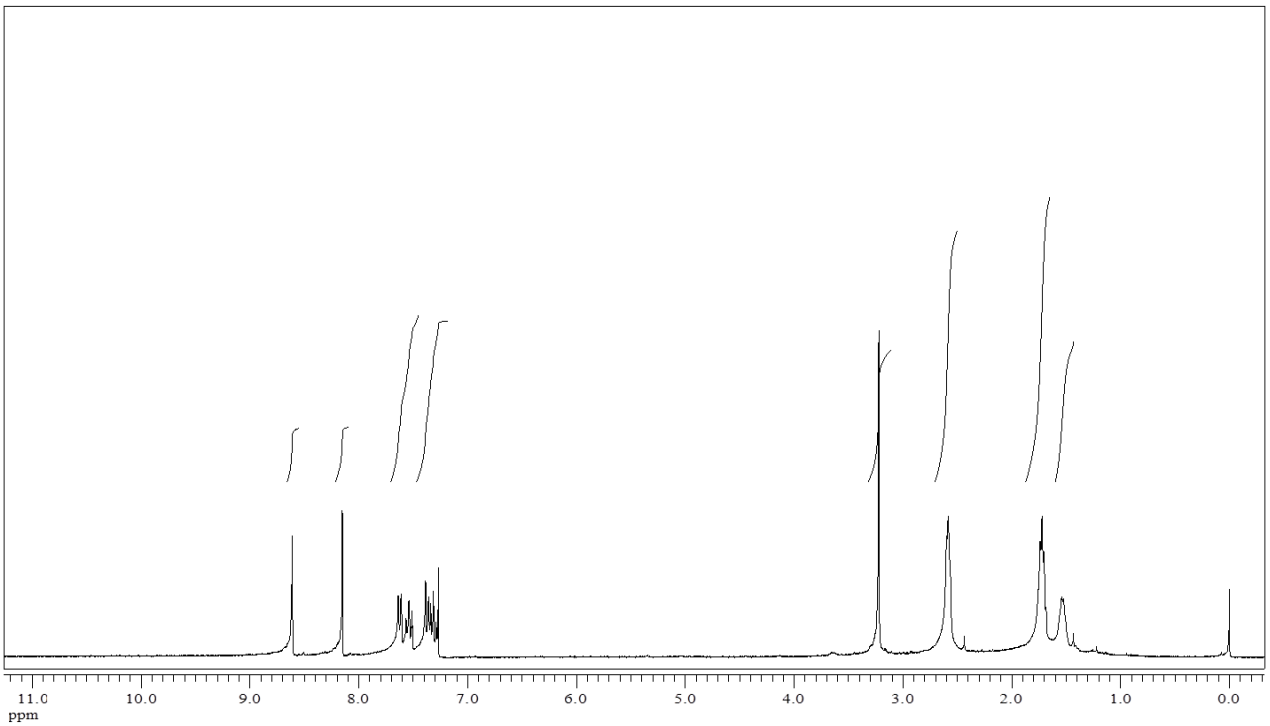
S7: ^{1}H and ^{13}C NMR and MS spectra of **6g**

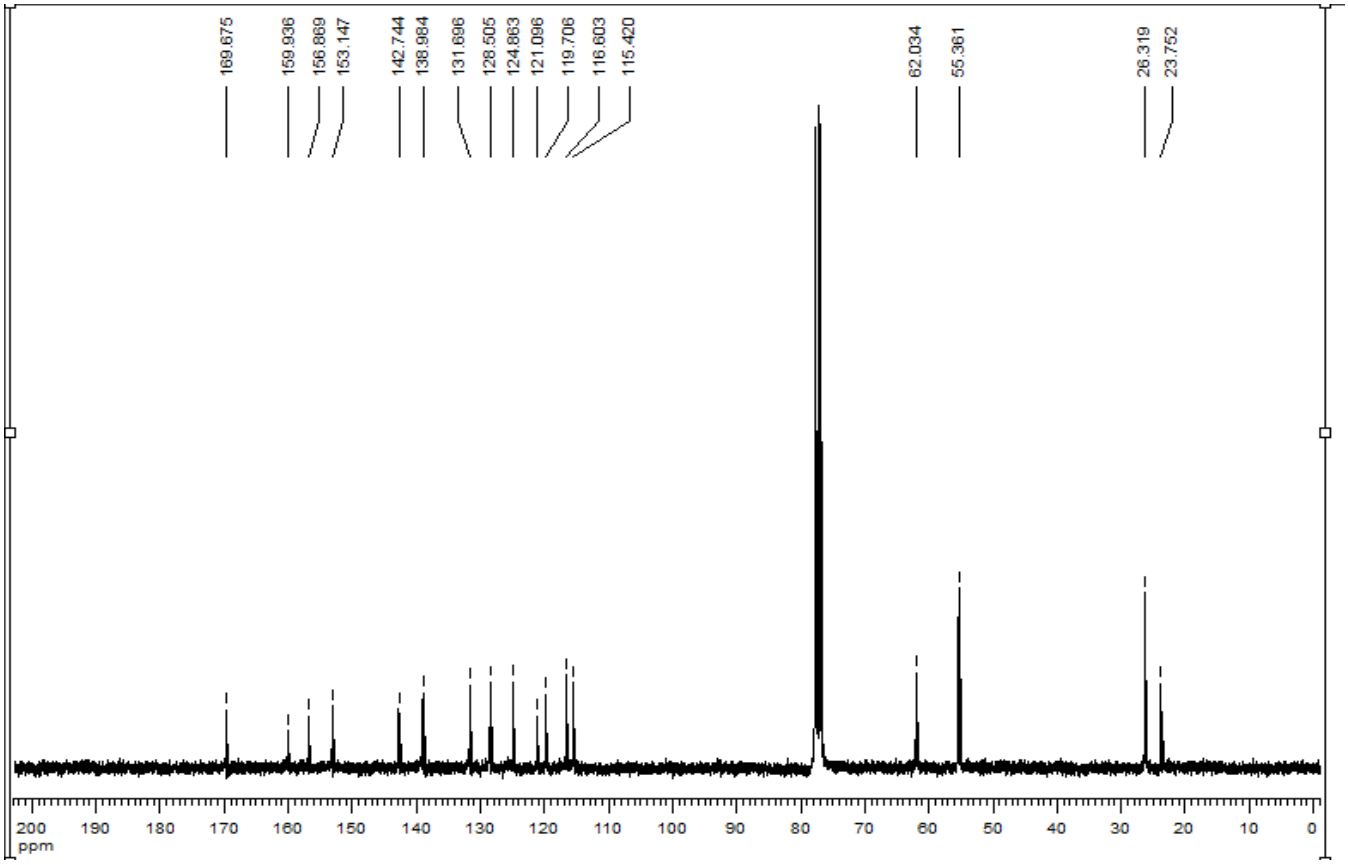


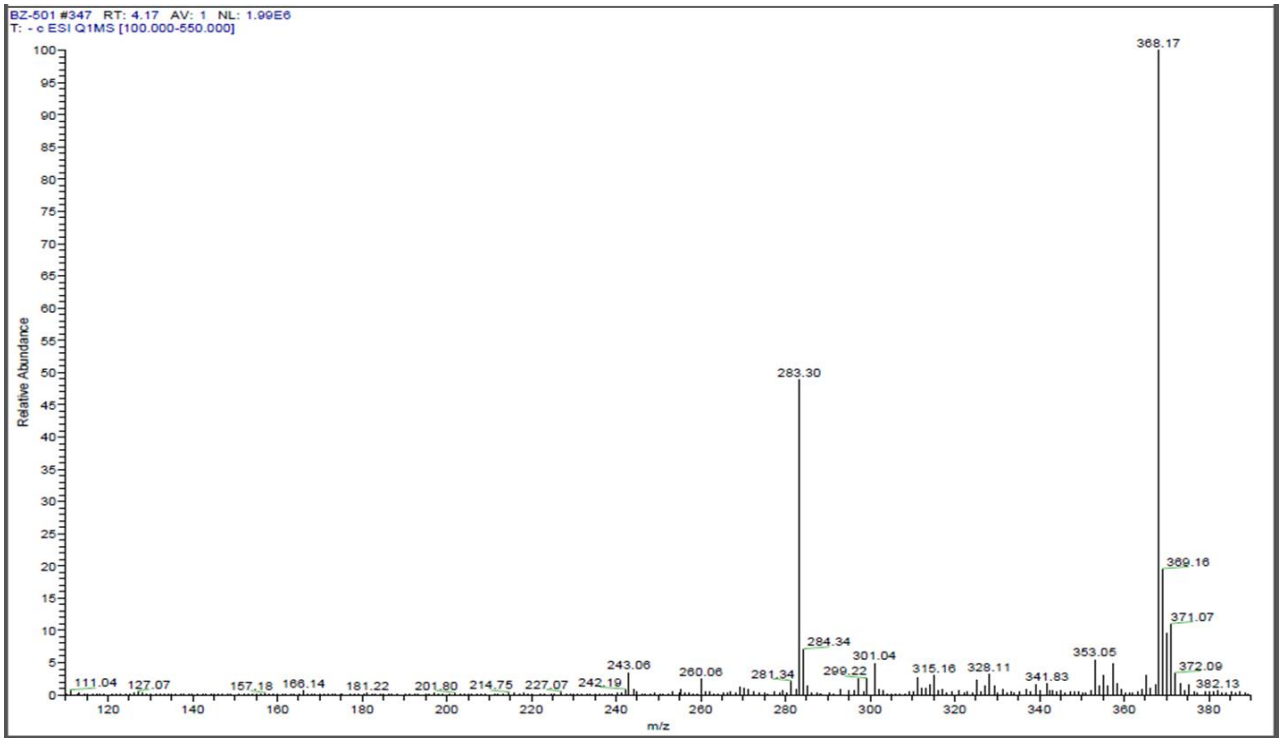




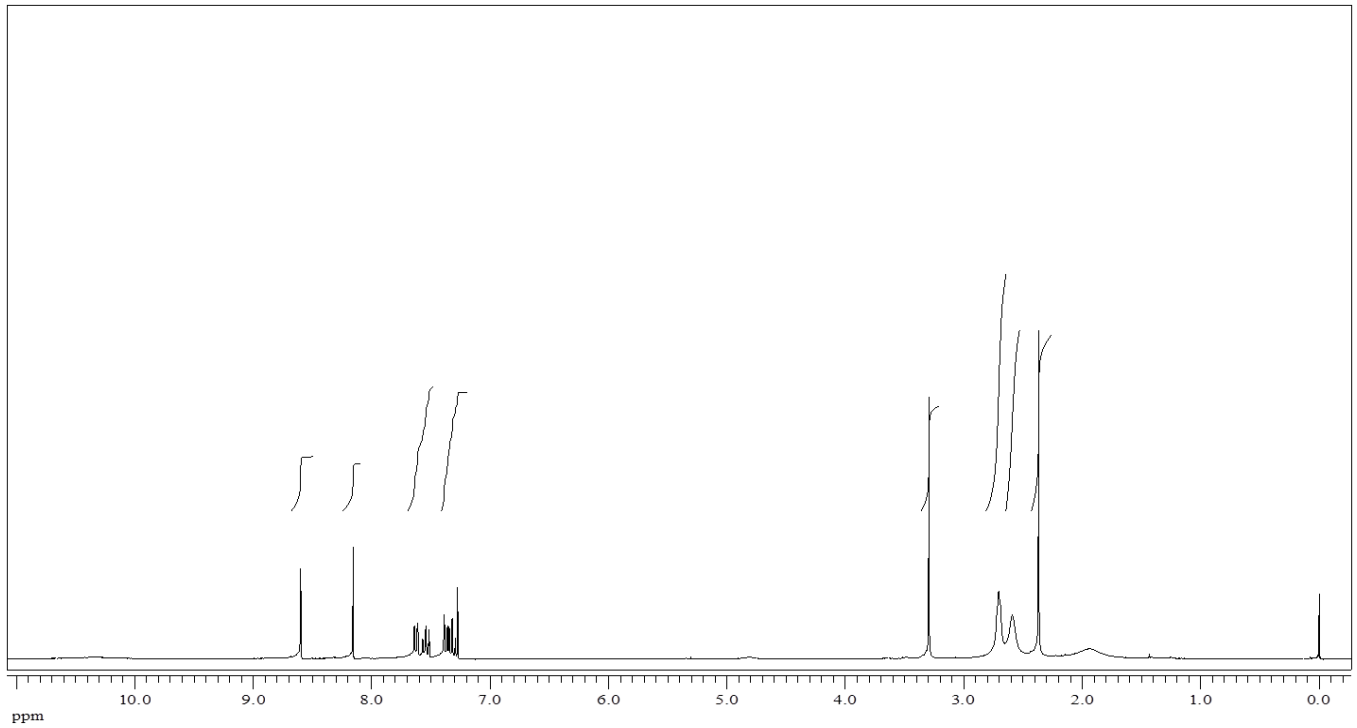
S8: [1] H and [13]C NMR and MS spectra of **6h**

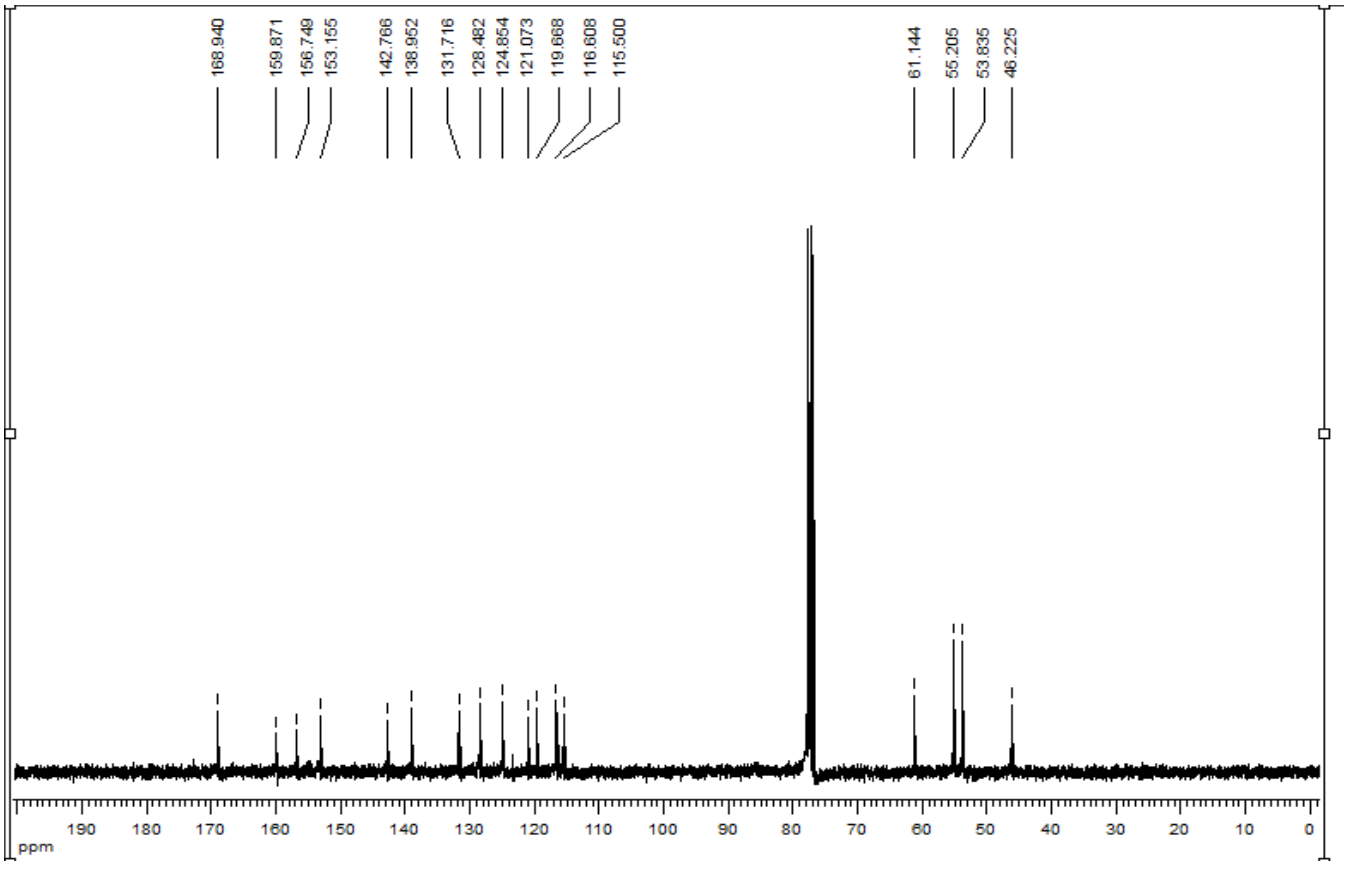


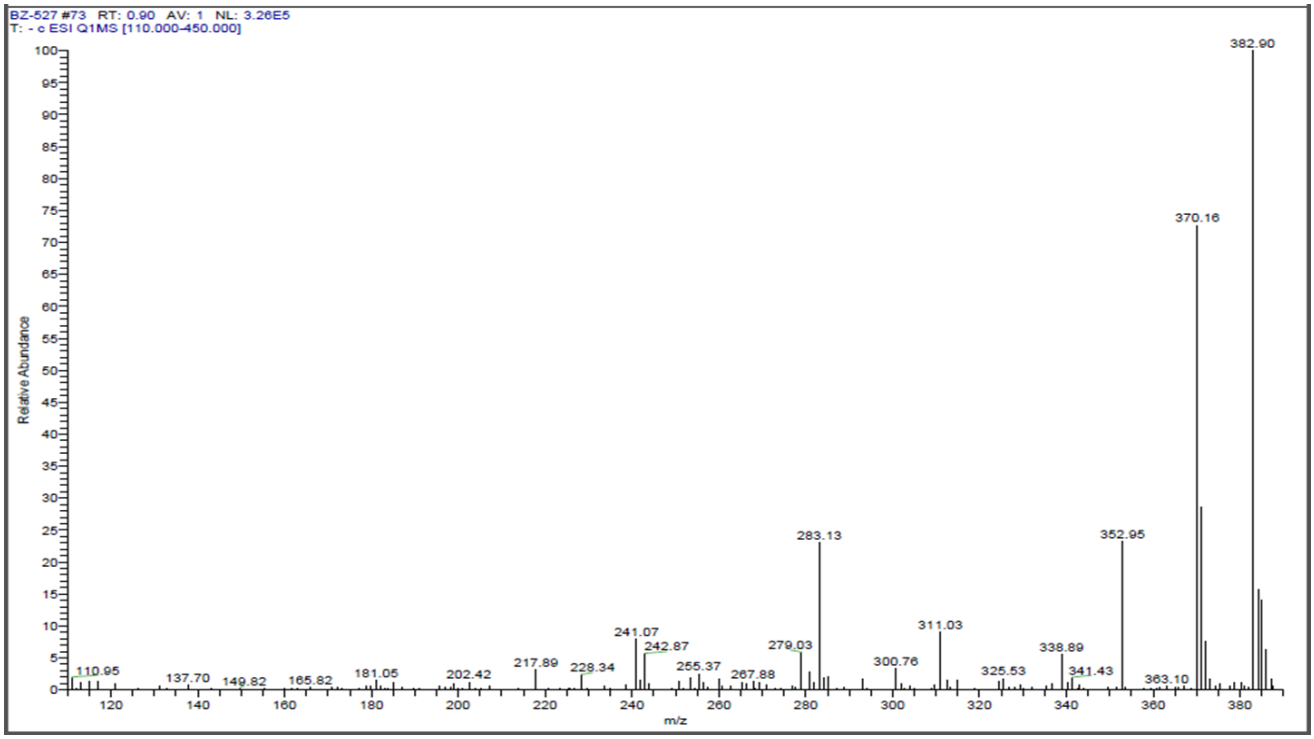

169.675
159.936
156.869
153.147
142.744
136.984
131.696
128.505
124.863
121.096
119.706
116.603
115.420
62.034
55.361
26.319
23.752
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


BZ-501 #347 RT: 4.17 AV: 1 NL: 1.99E6
T: - c ESI Q1MS [100.000-550.000]
Relative Abundance
m/z
368.17
283.30
369.16
371.07
284.34
301.04
299.22
243.06
260.06
281.34
315.16
328.11
353.05
341.83
372.09
382.13
111.04
127.07
157.18
166.14
181.22
201.80
214.75
227.07
242.19

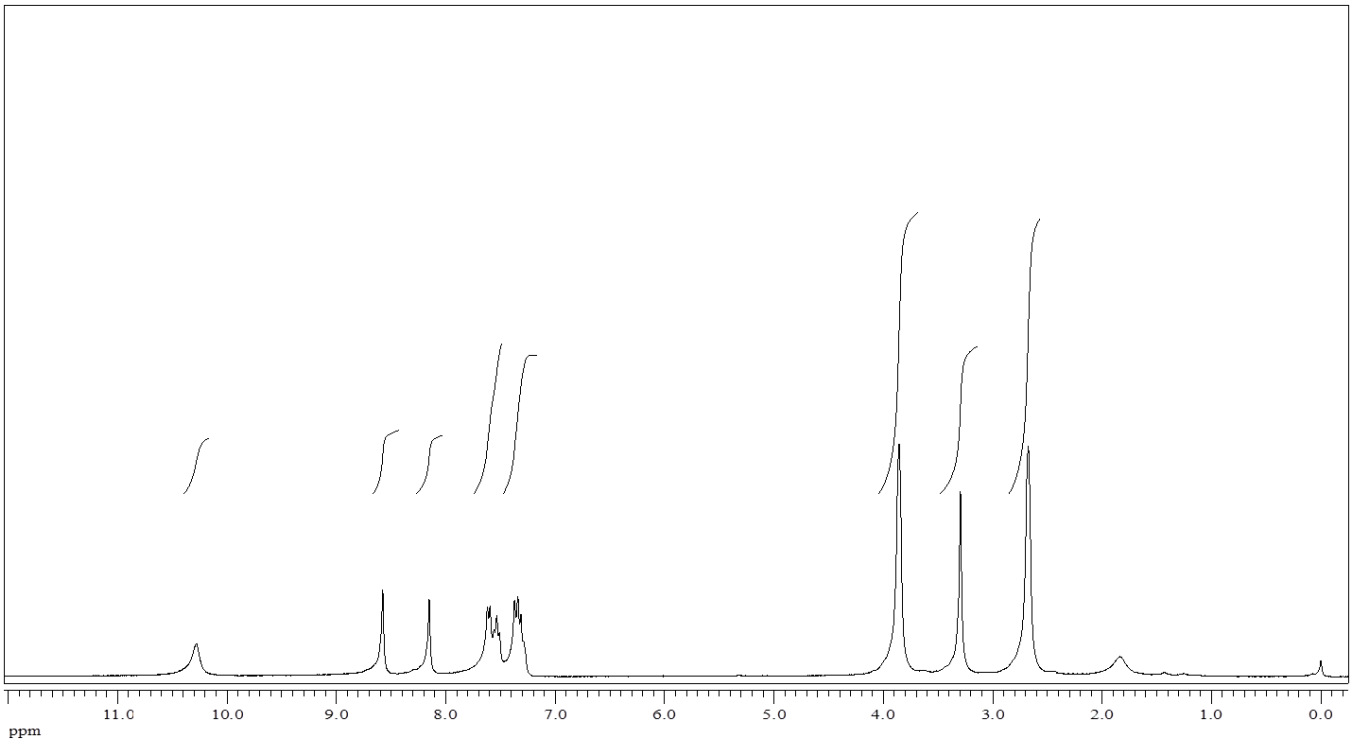
S9: ^{1}H and ^{13}C NMR and MS spectra of **6i**

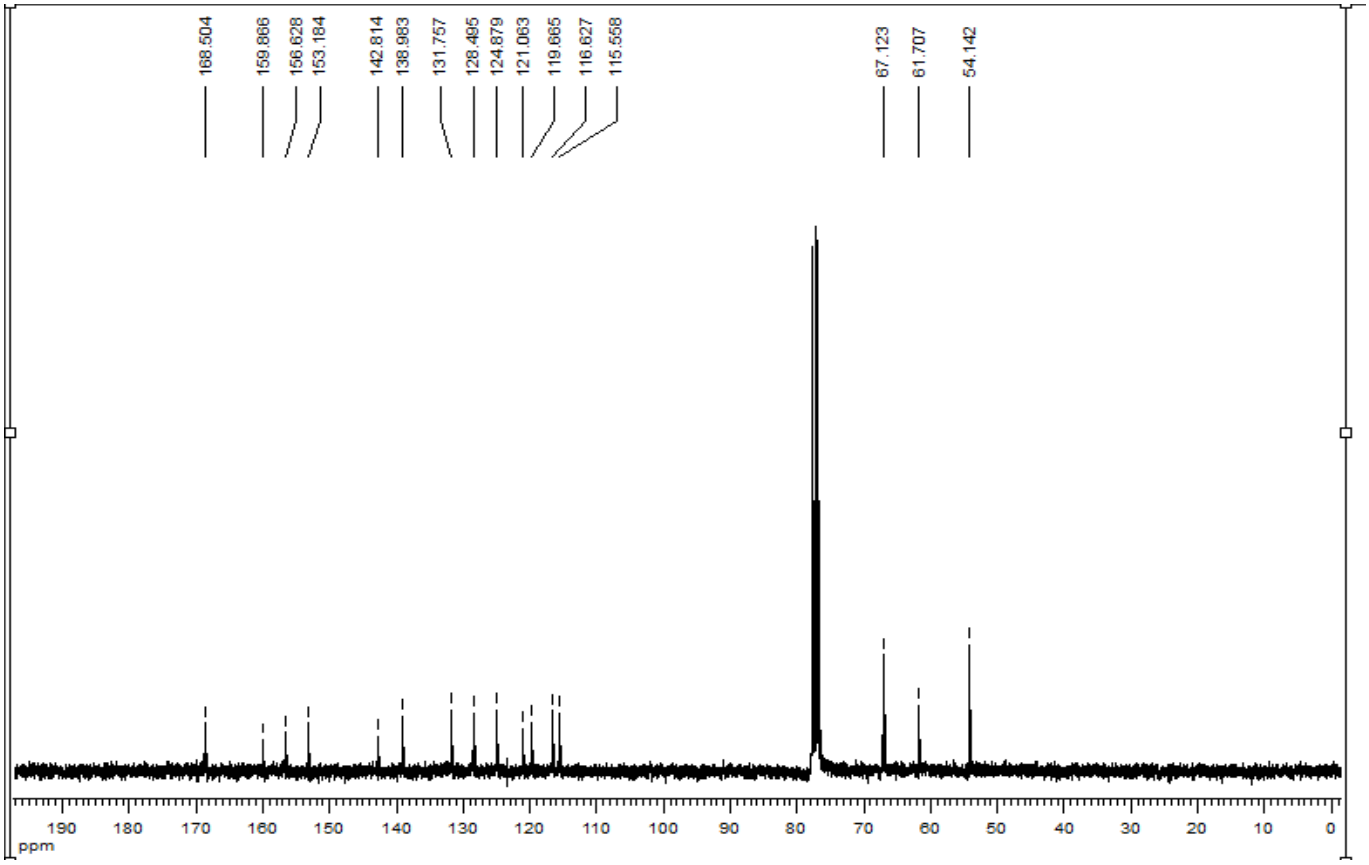


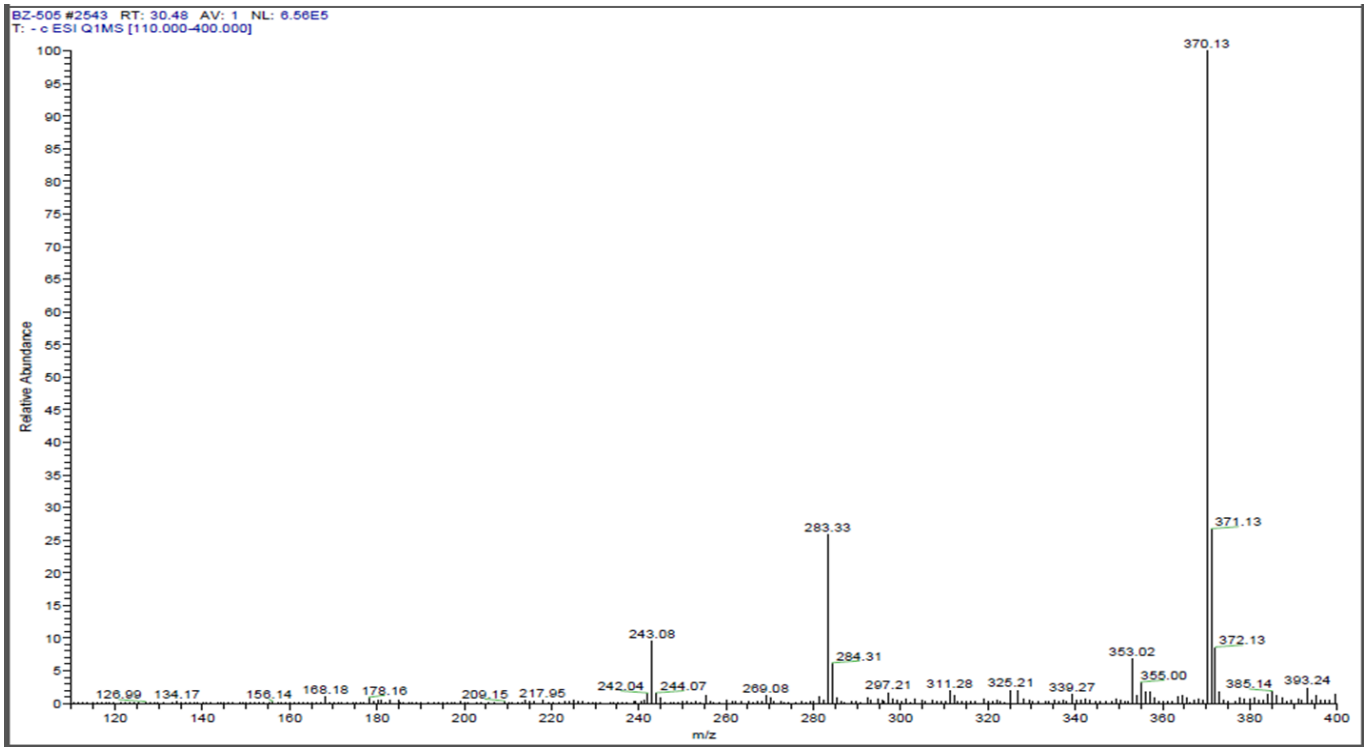




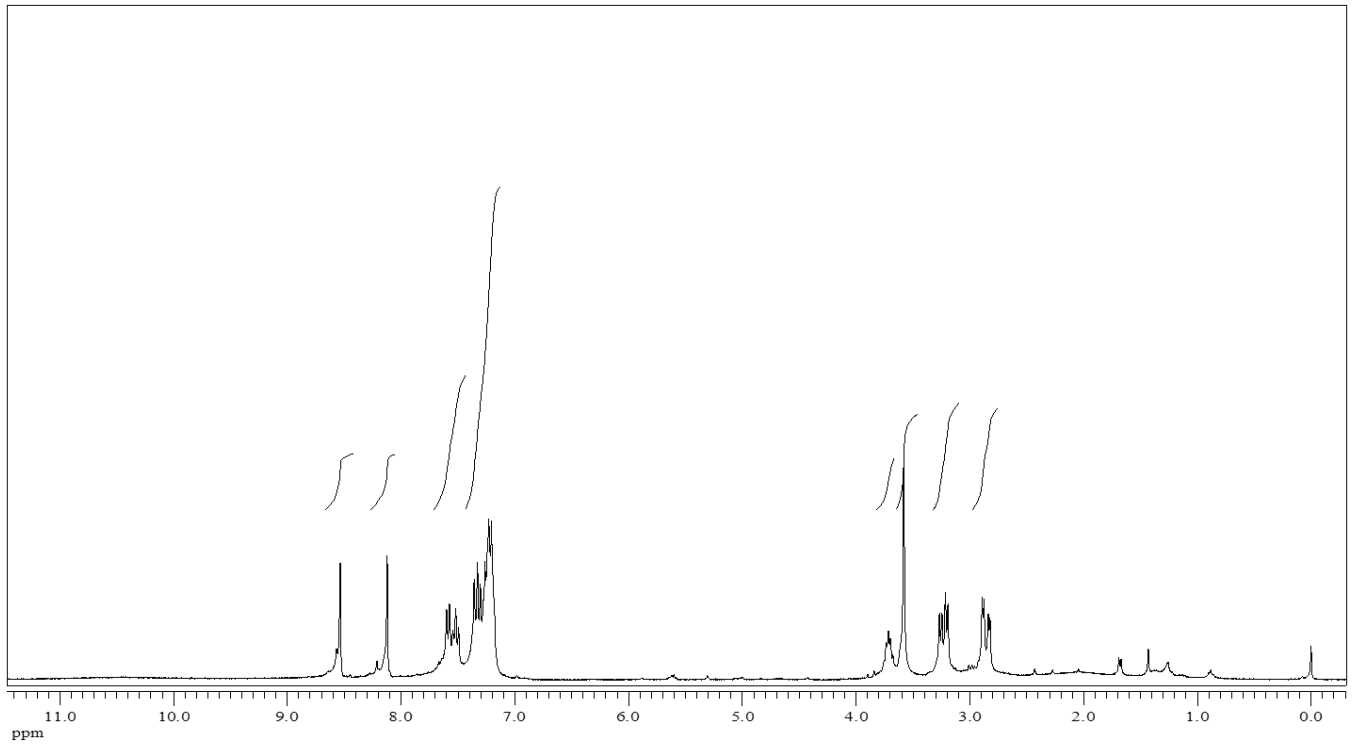
S10: ^{1}H and ^{13}C NMR and MS spectra of **6j**

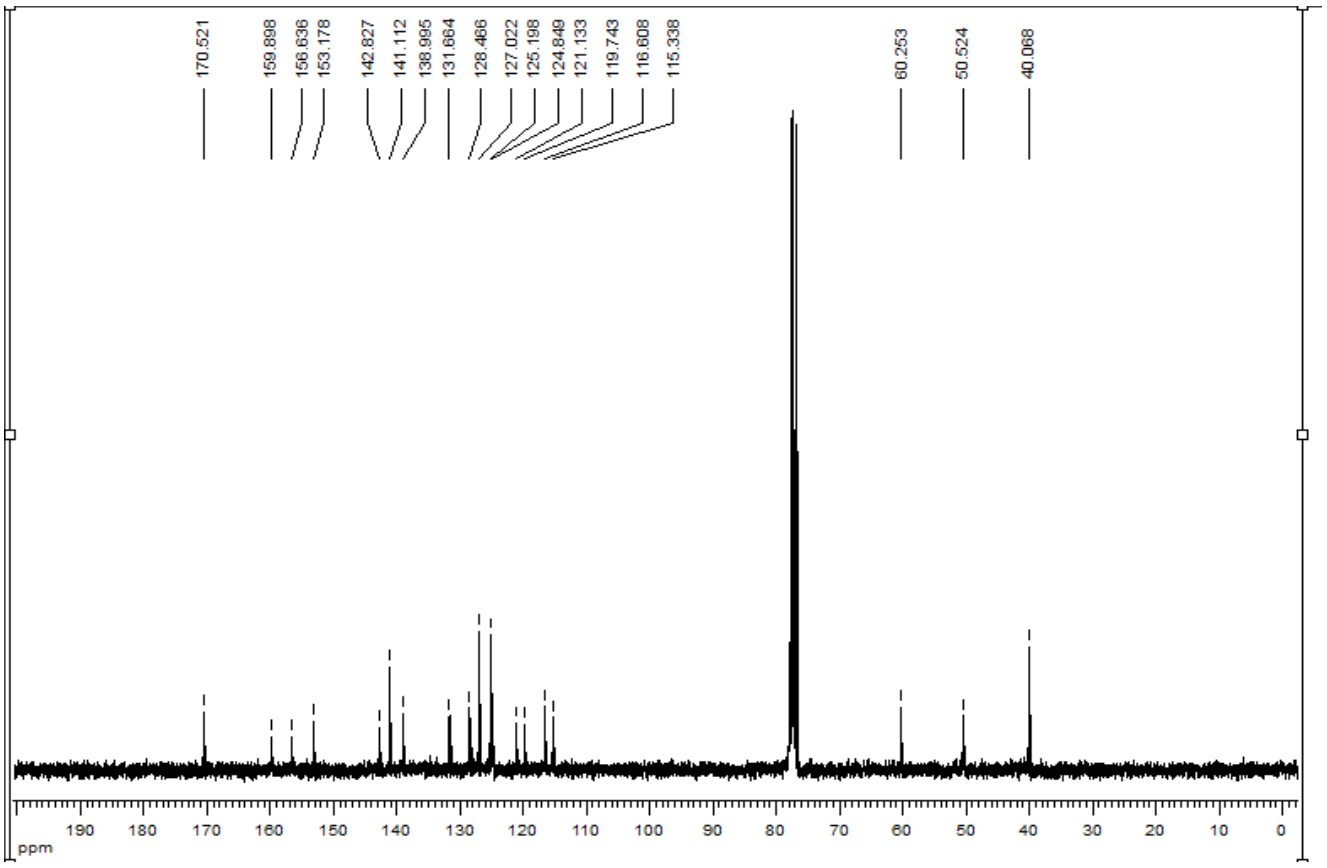


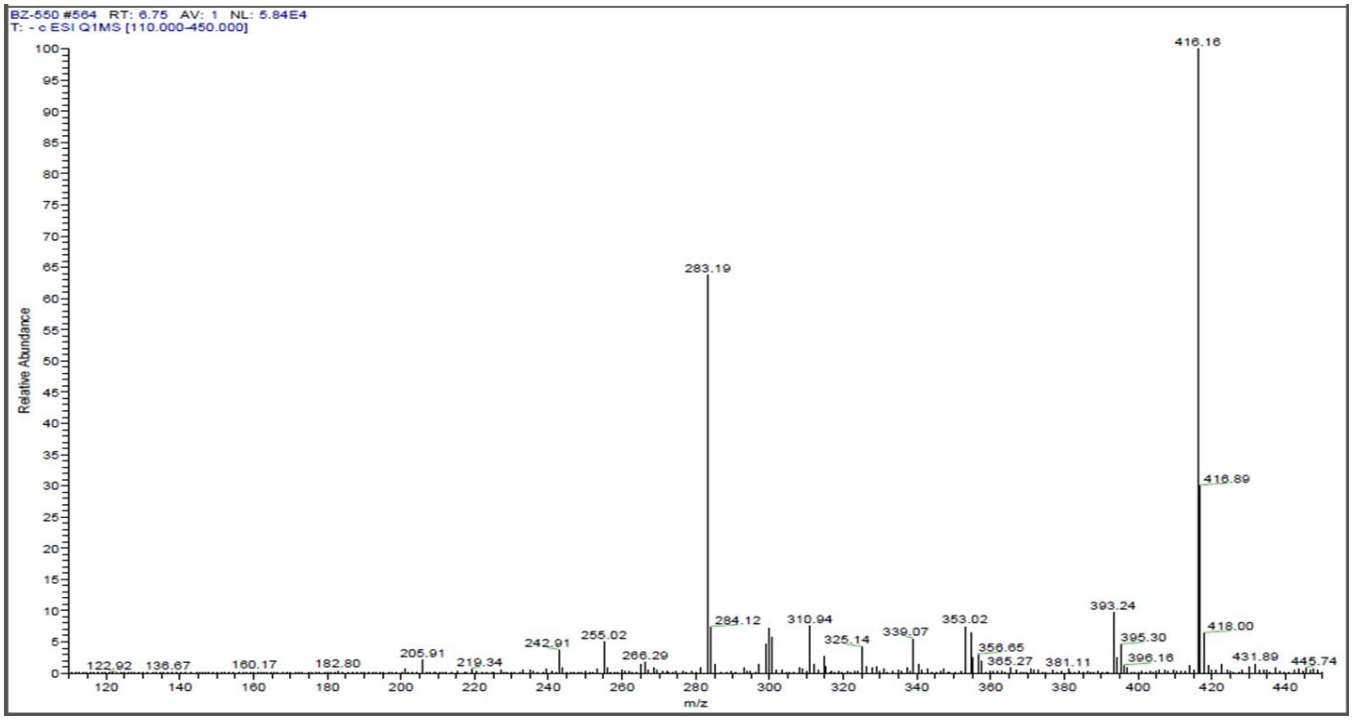

168.504
159.866
156.628
153.184
142.814
138.983
131.757
128.495
124.879
121.063
119.665
116.627
115.558
67.123
61.707
54.142
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


BZ-505 #2543 RT: 30.48 AV: 1 NL: 6.56E5
T: - c ESI Q1MS [110.000-400.000]
Relative Abundance
m/z
370.13
371.13
372.13
283.33
284.31
243.08
242.04
244.07
269.08
297.21
311.28
325.21
339.27
353.02
355.00
385.14
393.24
126.99
134.17
156.14
168.18
178.16
209.15
217.95

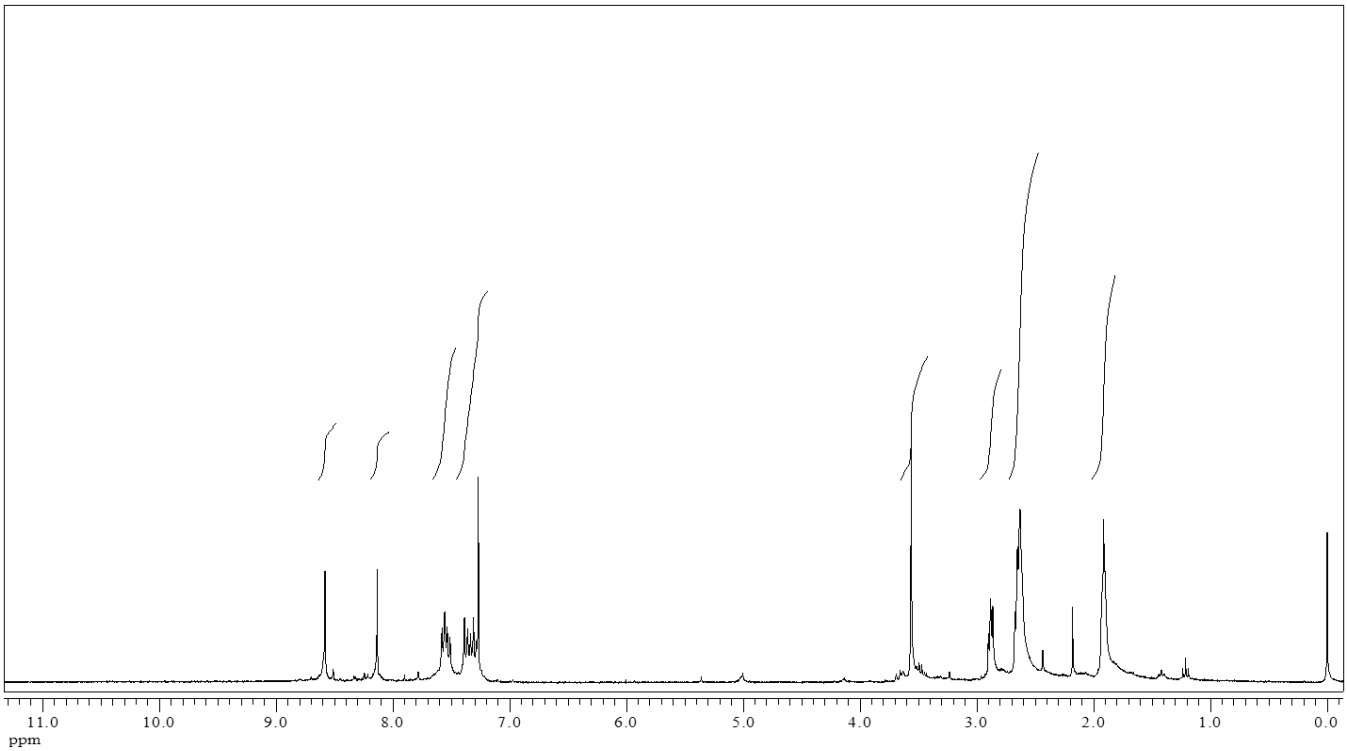
S11: ^{1}H and ^{13}C NMR and MS spectra of **6k**

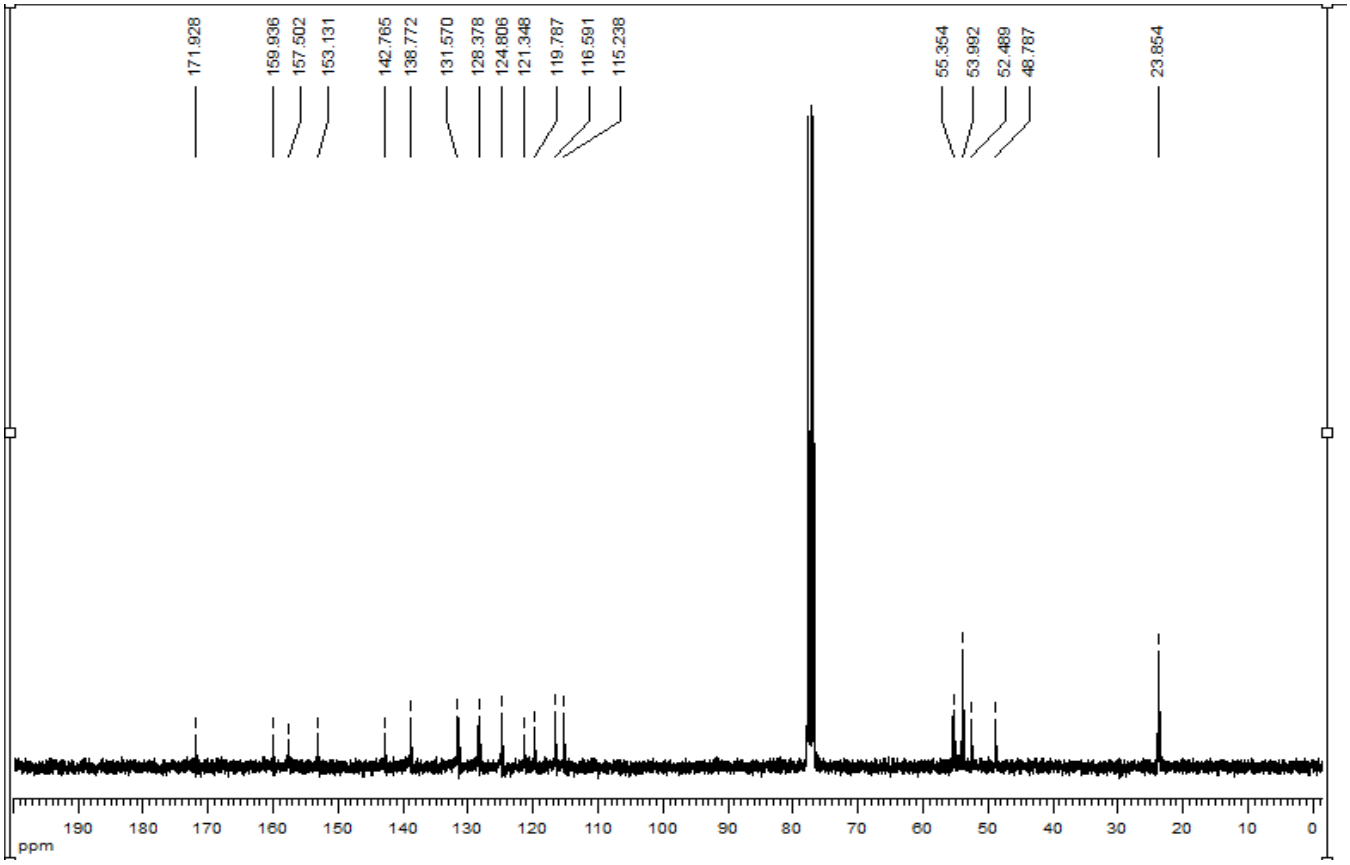


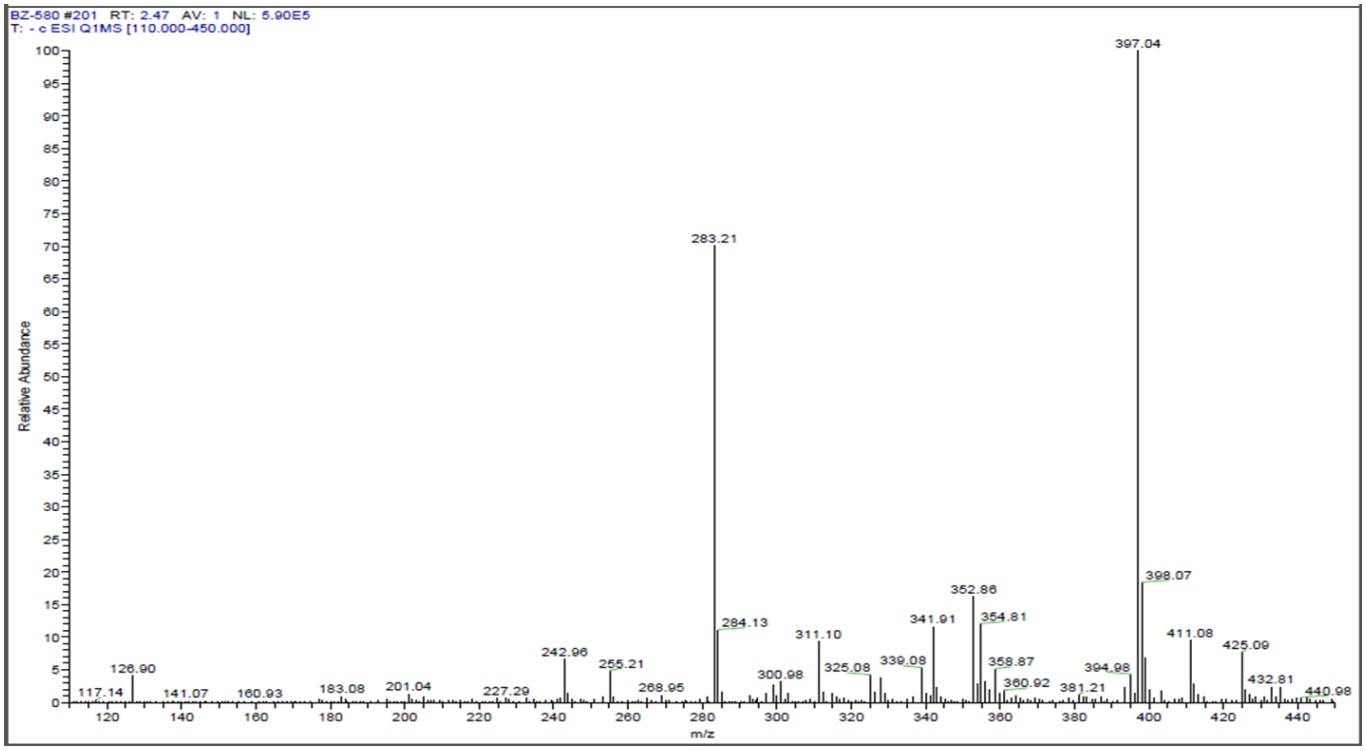




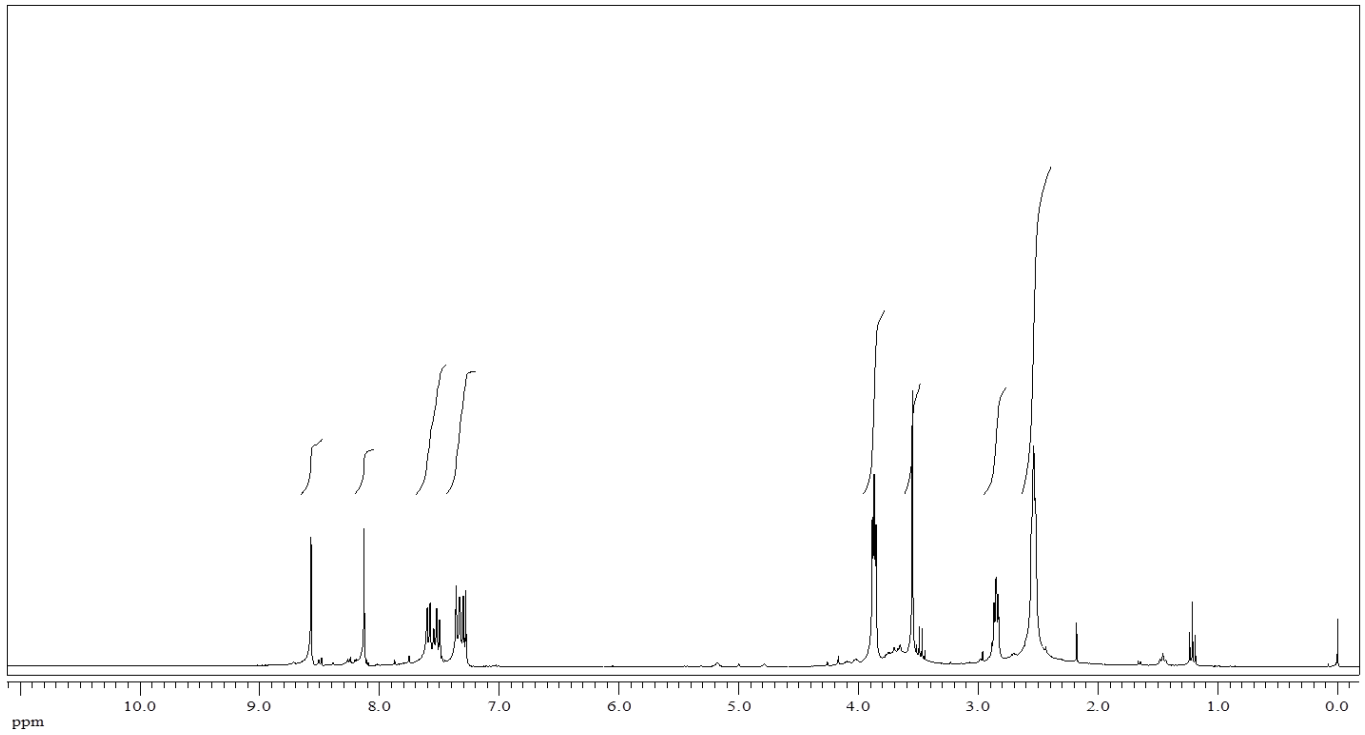
S12: [1] H and [13]C NMR and MS spectra of **6l**

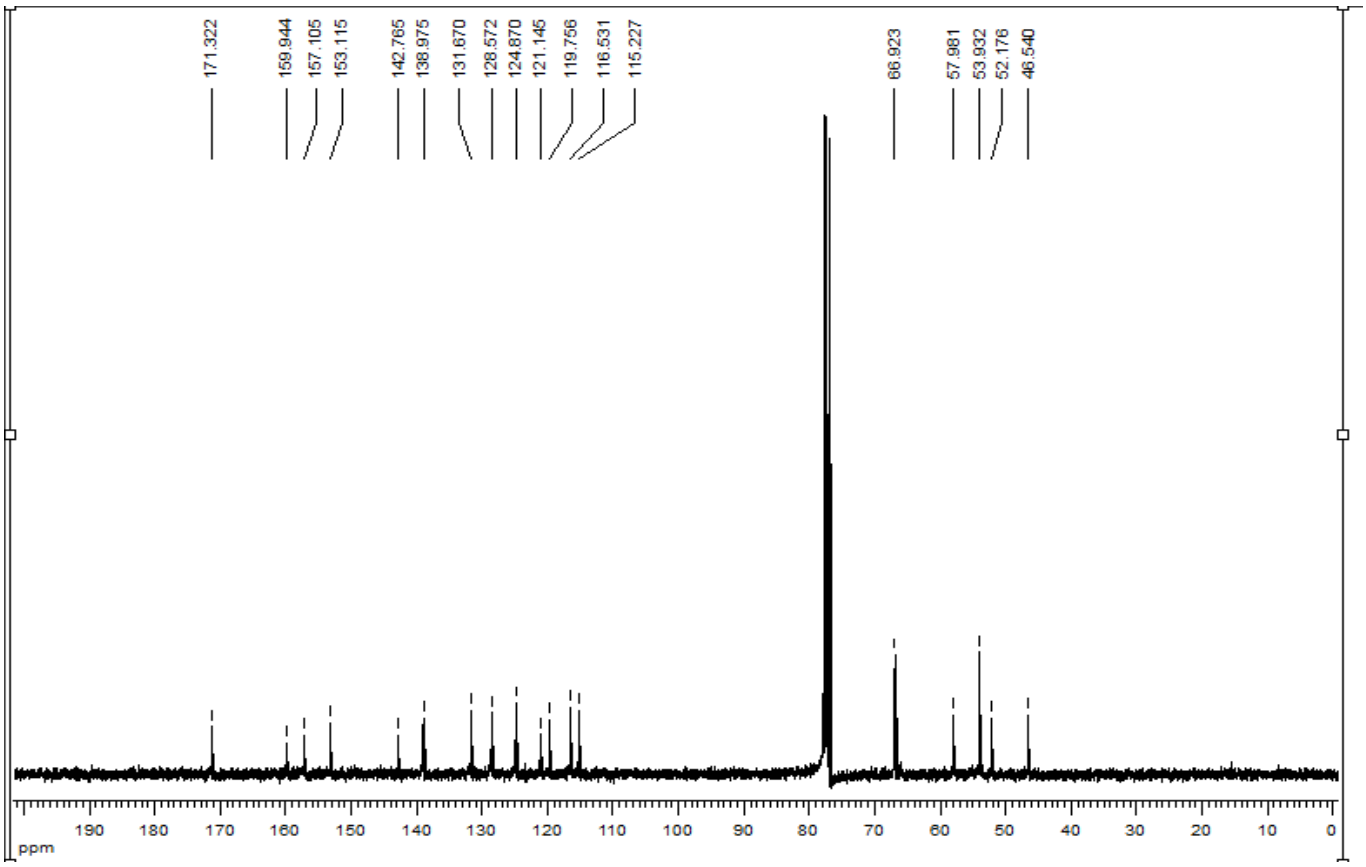


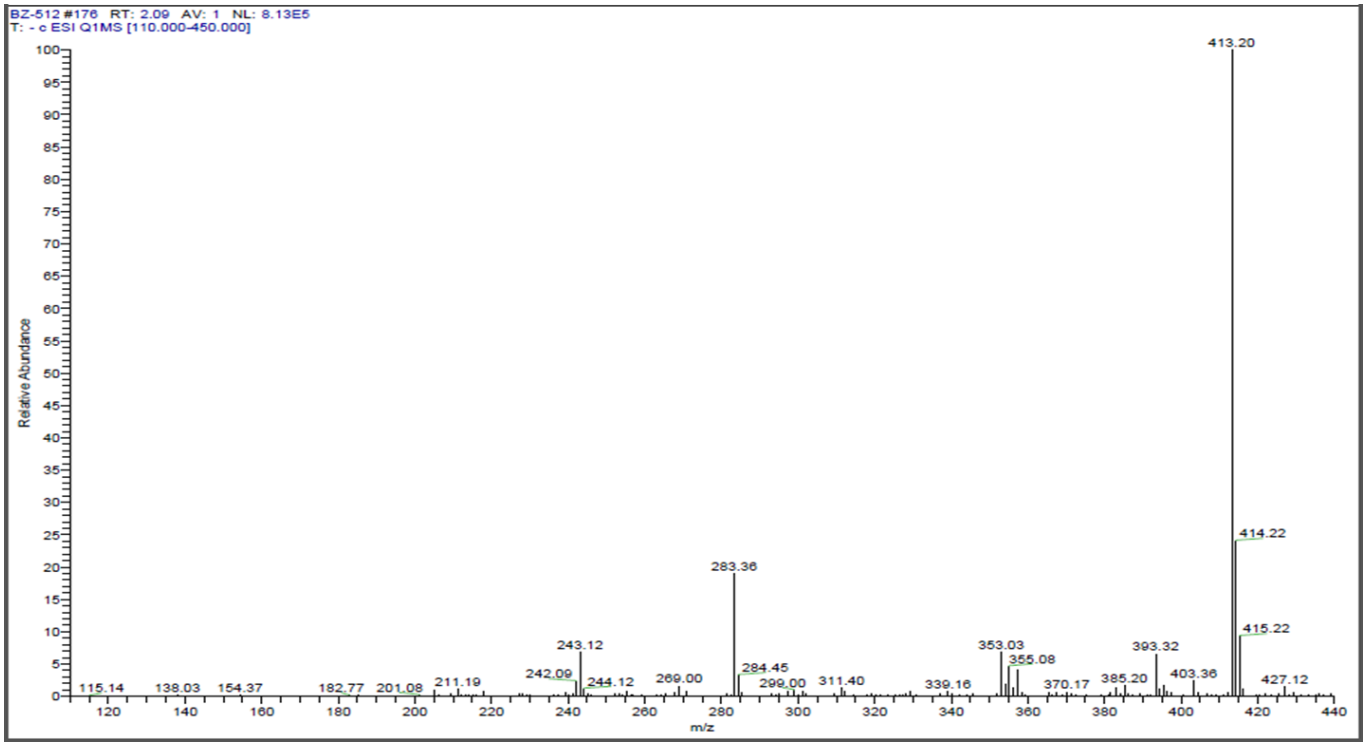

171.928
159.936
157.502
153.131
142.765
138.772
131.570
128.378
124.806
121.348
119.787
116.591
115.238
55.354
53.992
52.489
48.787
23.854
ppm


BZ-580 #201 RT: 2.47 AV: 1 NL: 5.90E5
T: - c ESI Q1MS [110.000-450.000]
Relative Abundance
m/z
397.04
283.21
398.07
352.86
354.81
341.91
284.13
311.10
411.08
425.09
242.96
255.21
339.08
325.08
358.87
394.98
432.81
126.90
300.98
360.92
381.21
440.98
117.14
141.07
160.93
183.08
201.04
227.29
268.95

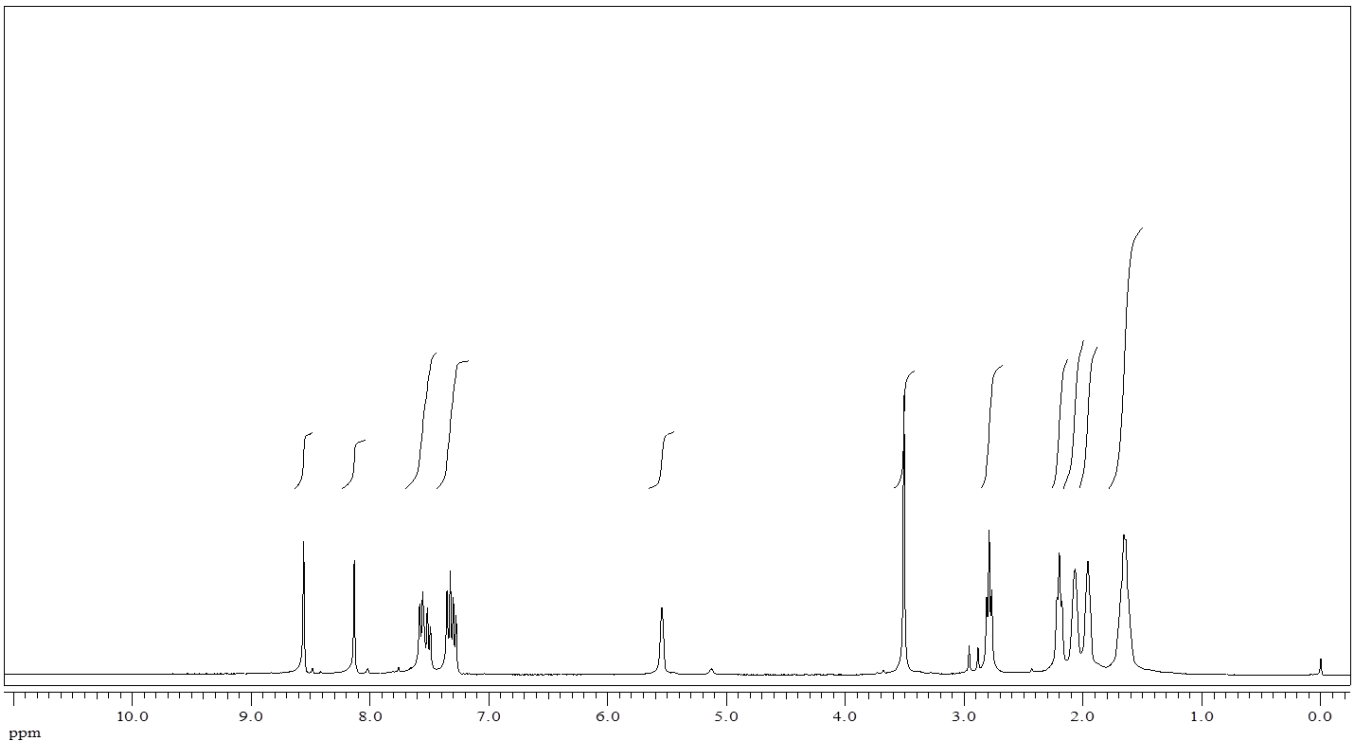
S13: ^{1}H and ^{13}C NMR and MS spectra of **6m**

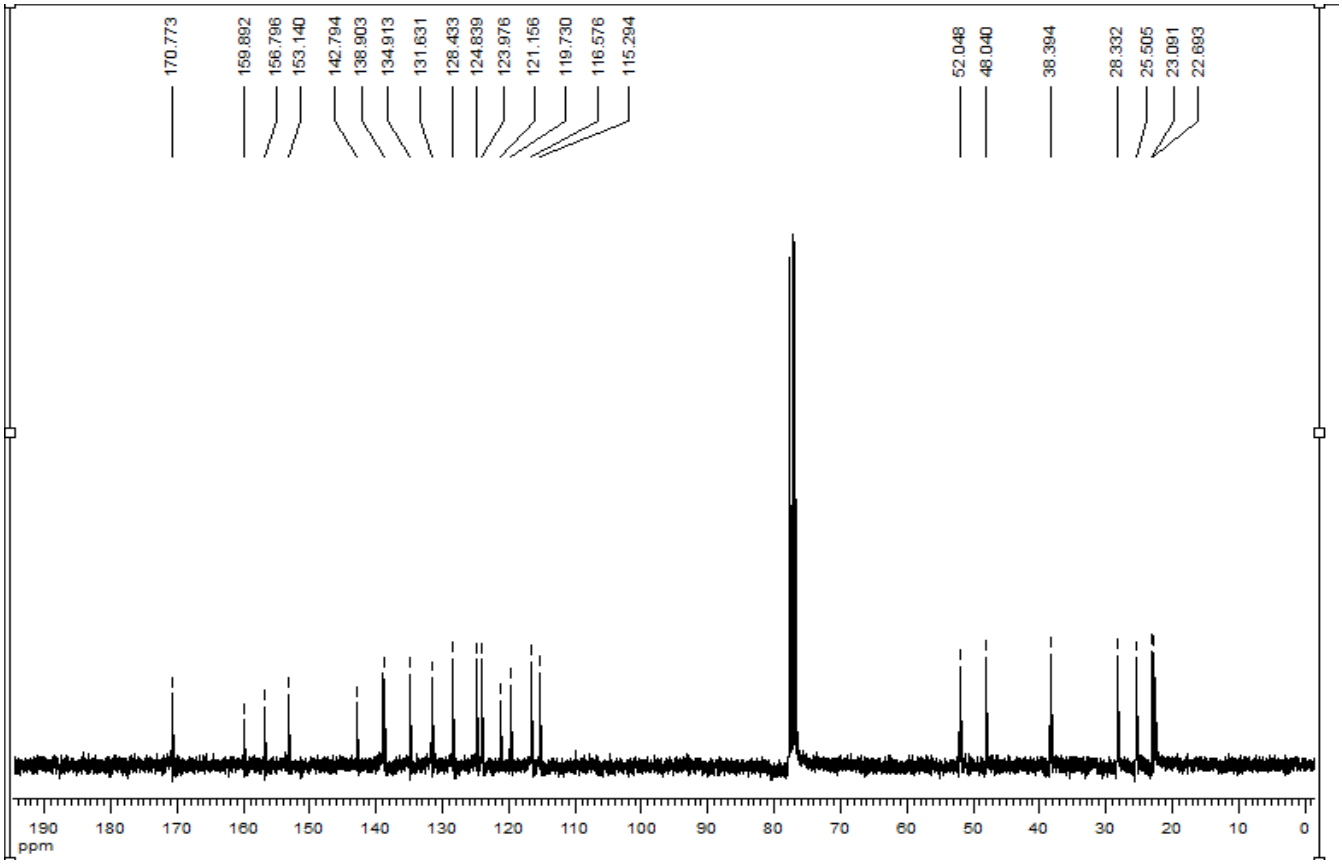


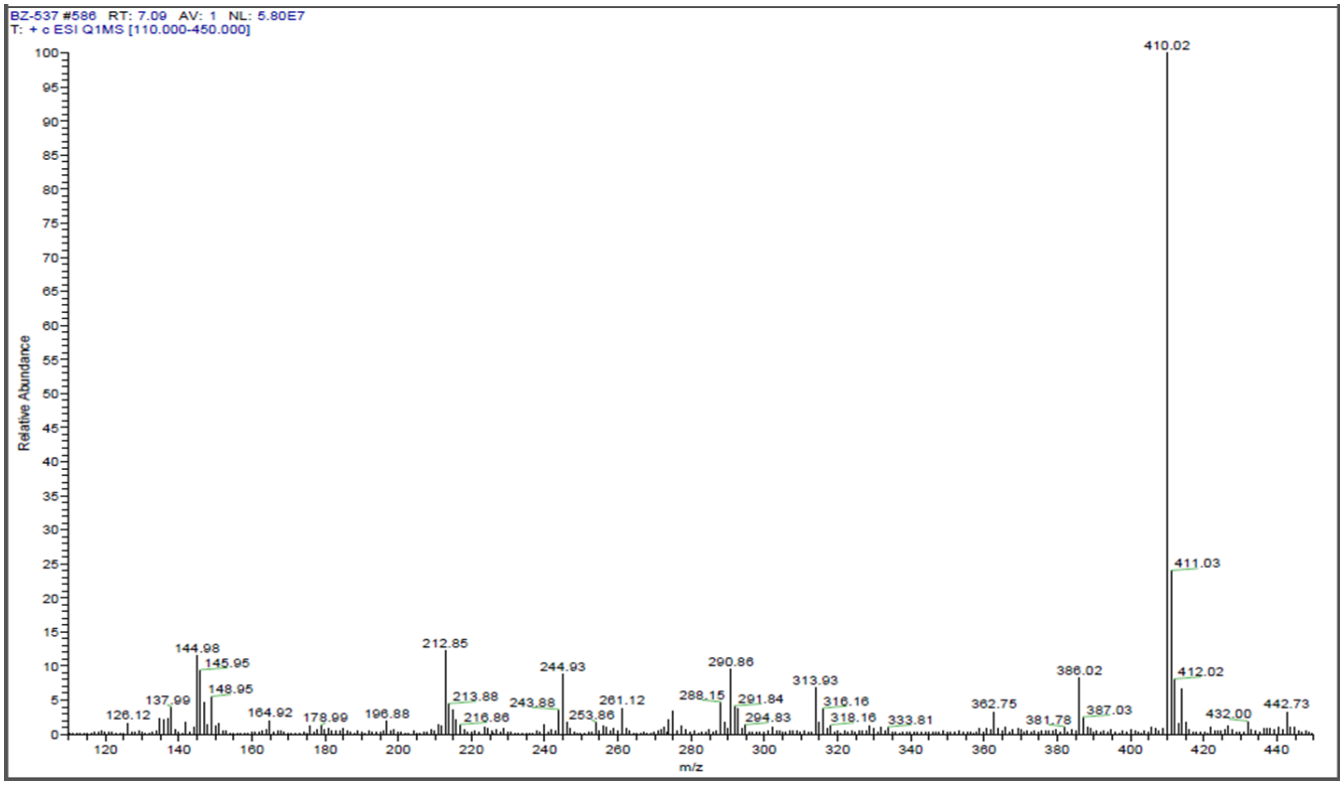




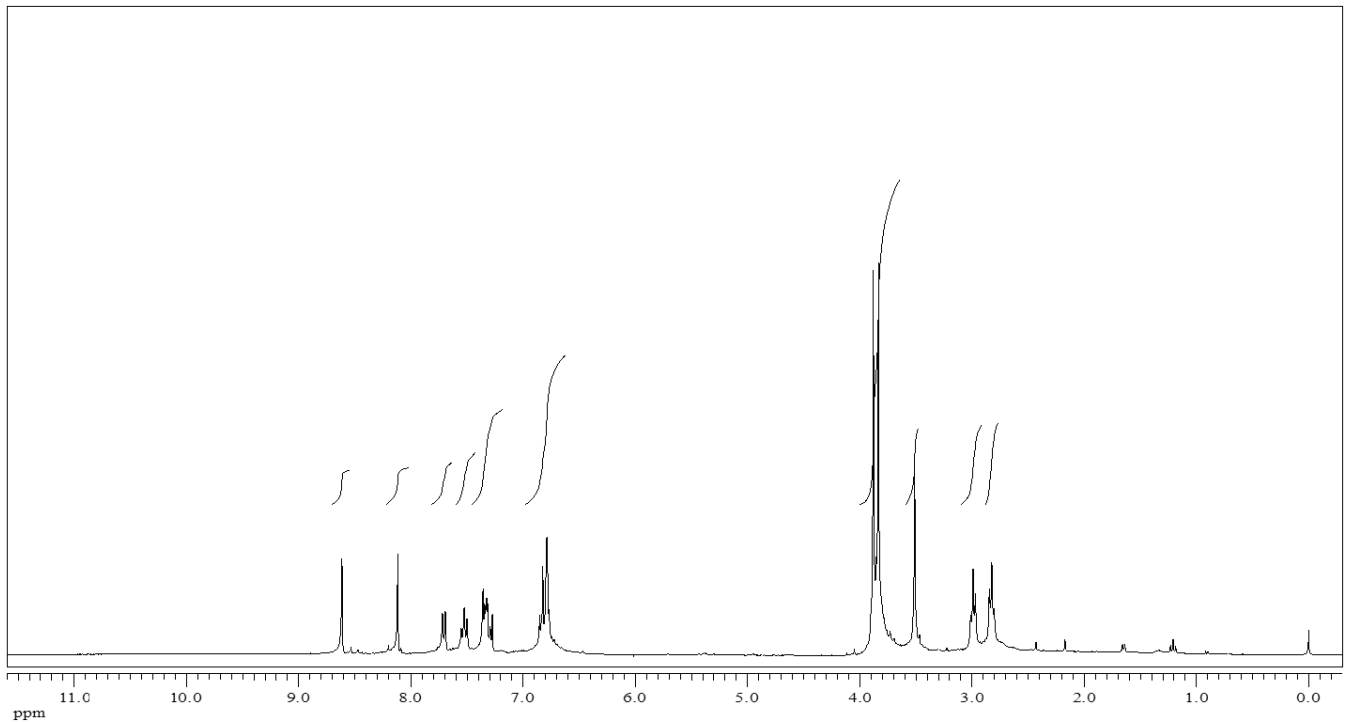
S14: [1] H and [13]C NMR and MS spectra of **6n**

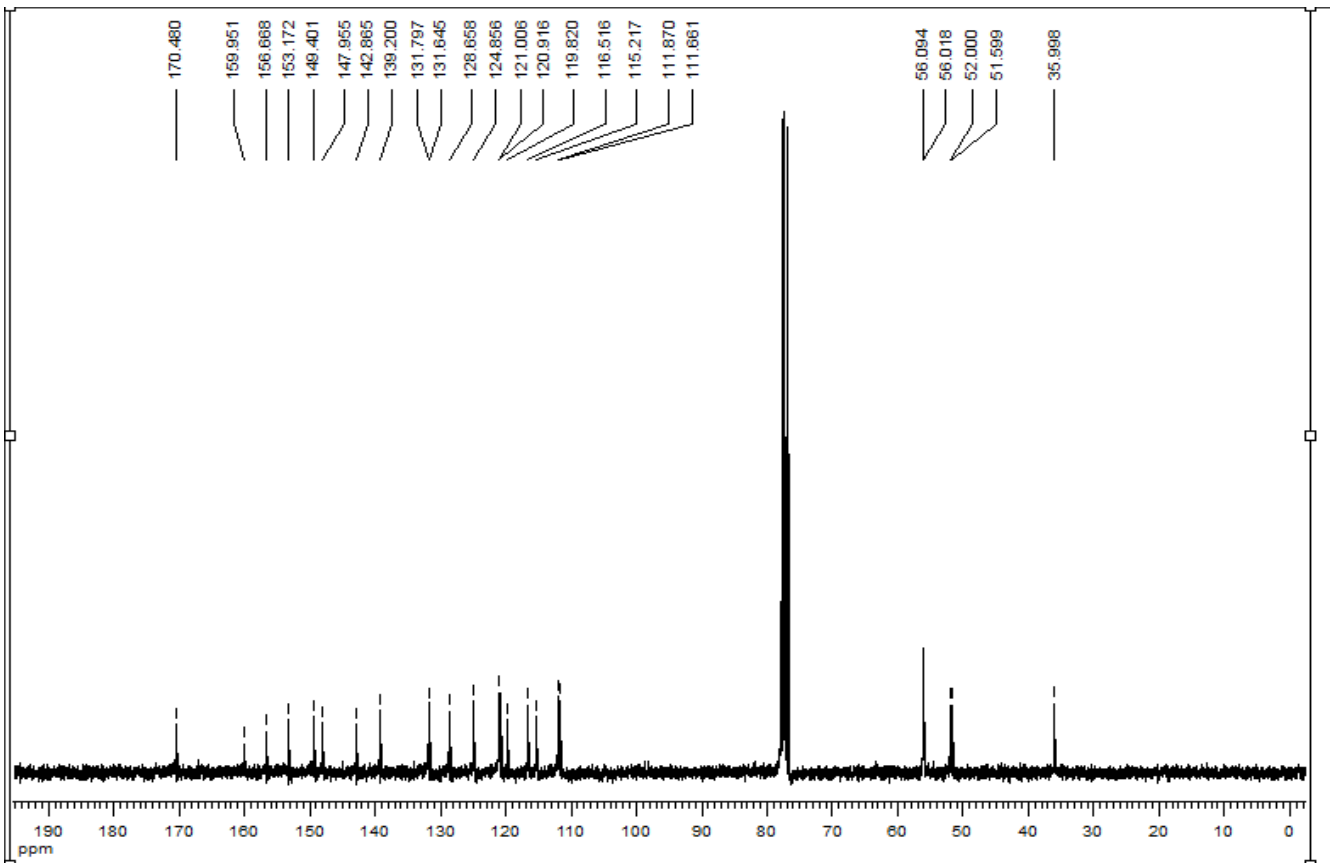


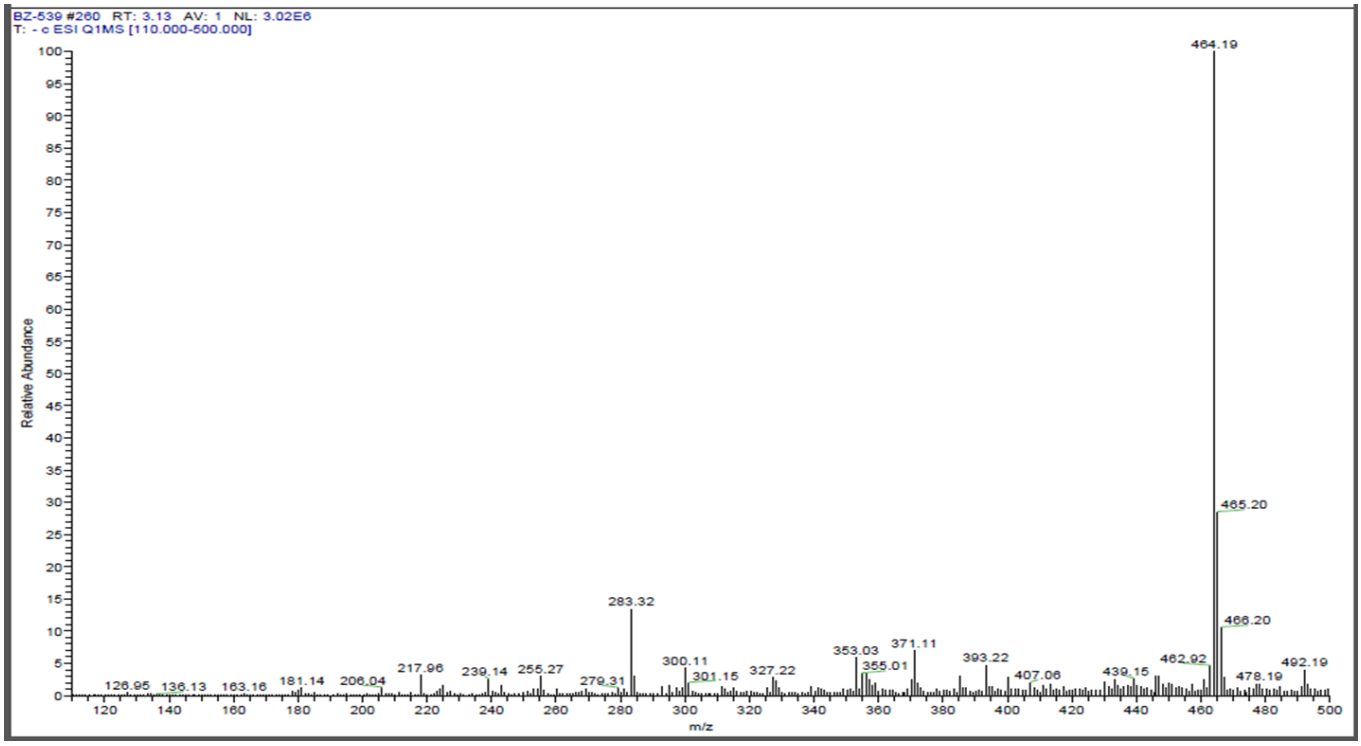

170.773
159.892
156.796
153.140
142.794
138.903
134.913
131.631
126.433
124.839
123.976
121.156
119.730
116.576
115.294
52.048
48.040
38.394
28.332
25.505
23.091
22.693
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


BZ-537 #586 RT: 7.09 AV: 1 NL: 5.80E7
T: + c ESI Q1MS [110.000-450.000]
Relative Abundance
m/z
410.02
411.03
412.02
144.98
145.95
148.95
137.99
126.12
164.92
178.99
196.88
212.85
213.88
216.86
243.88
244.93
253.86
261.12
288.15
290.86
291.84
294.83
313.93
316.16
318.16
333.81
362.75
381.78
386.02
387.03
432.00
442.73

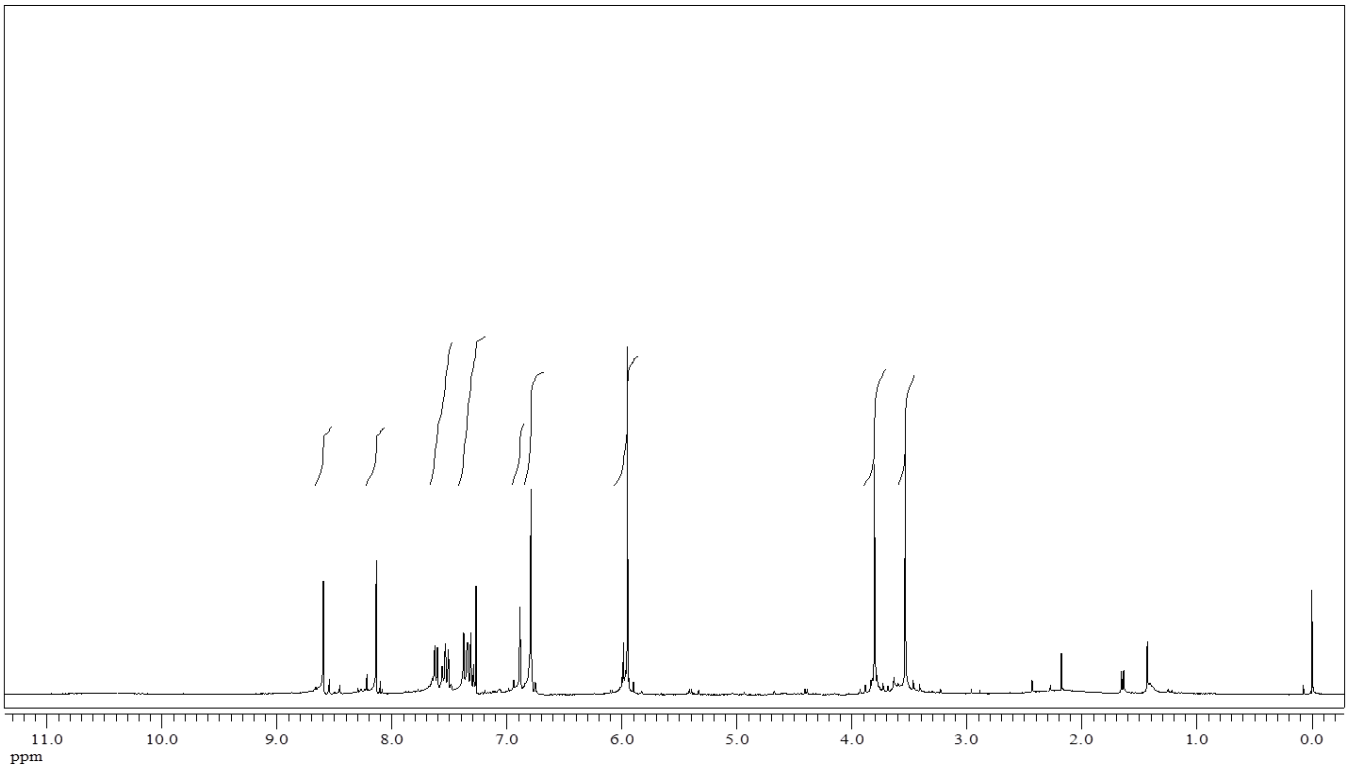
S15: ^{1}H and ^{13}C NMR and MS spectra of **6o**

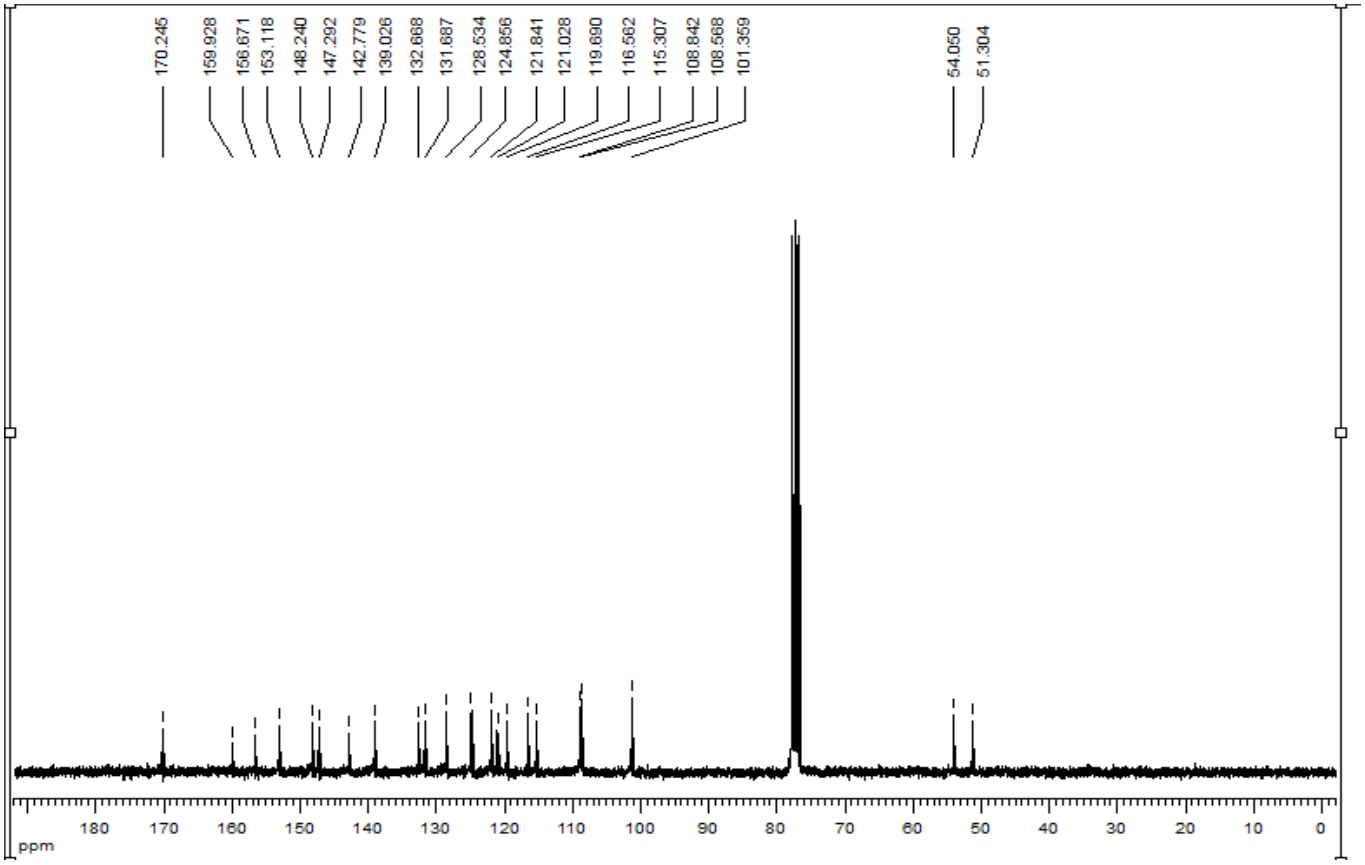


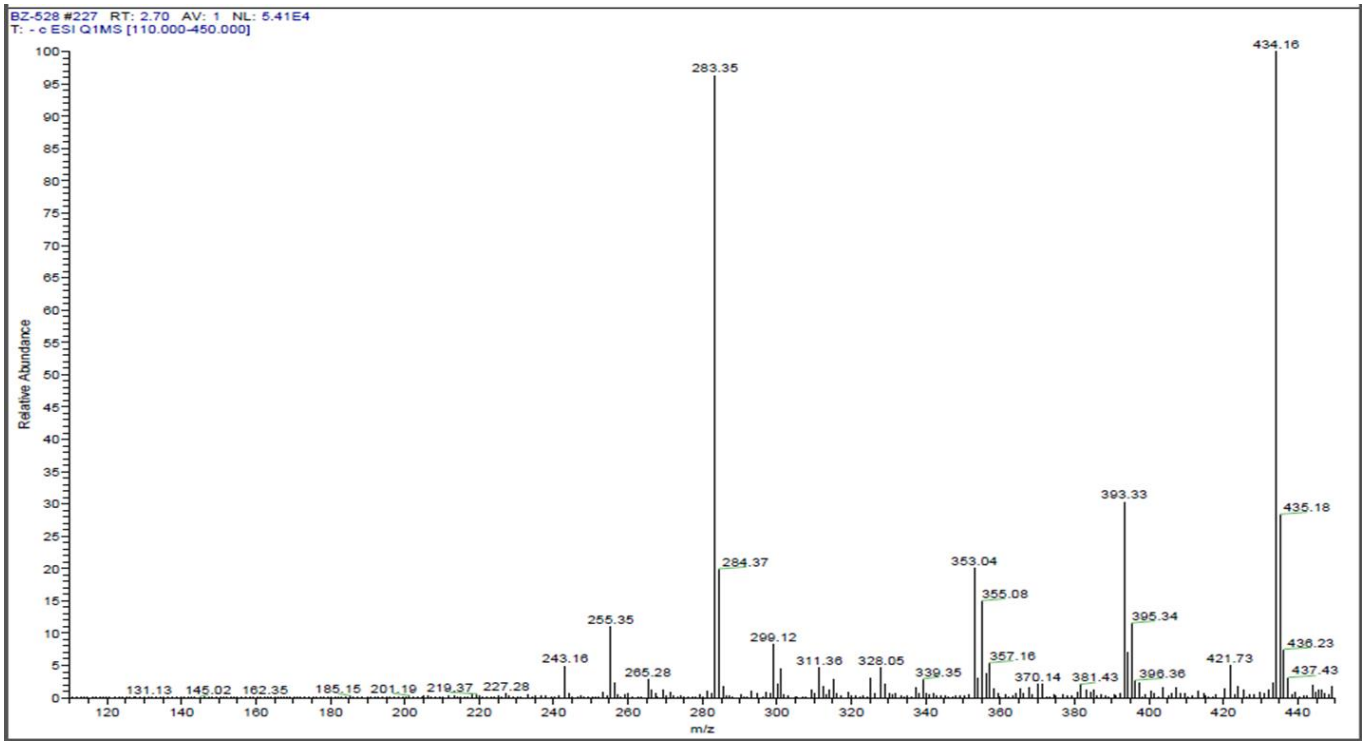




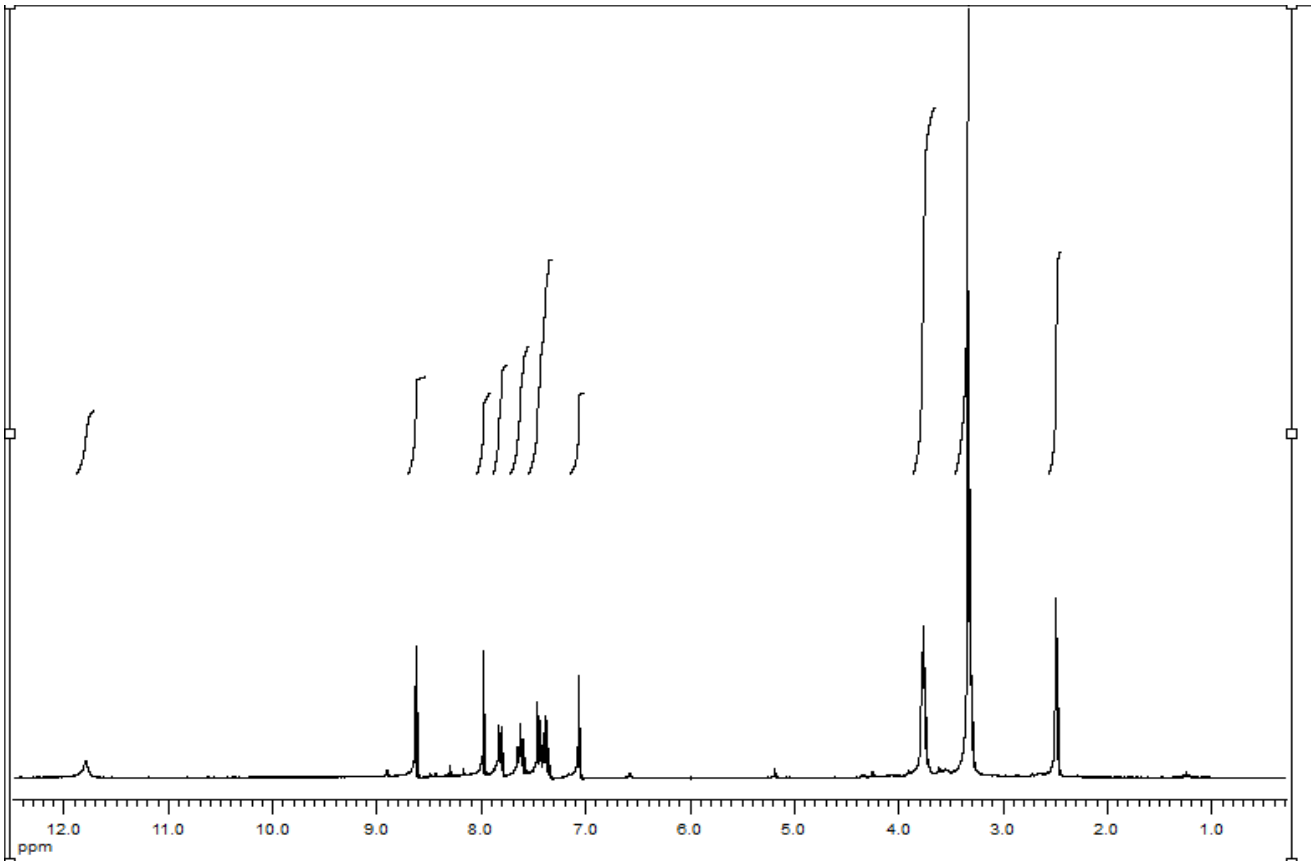
S16: [1] H and [13]C NMR and MS spectra of **6p**

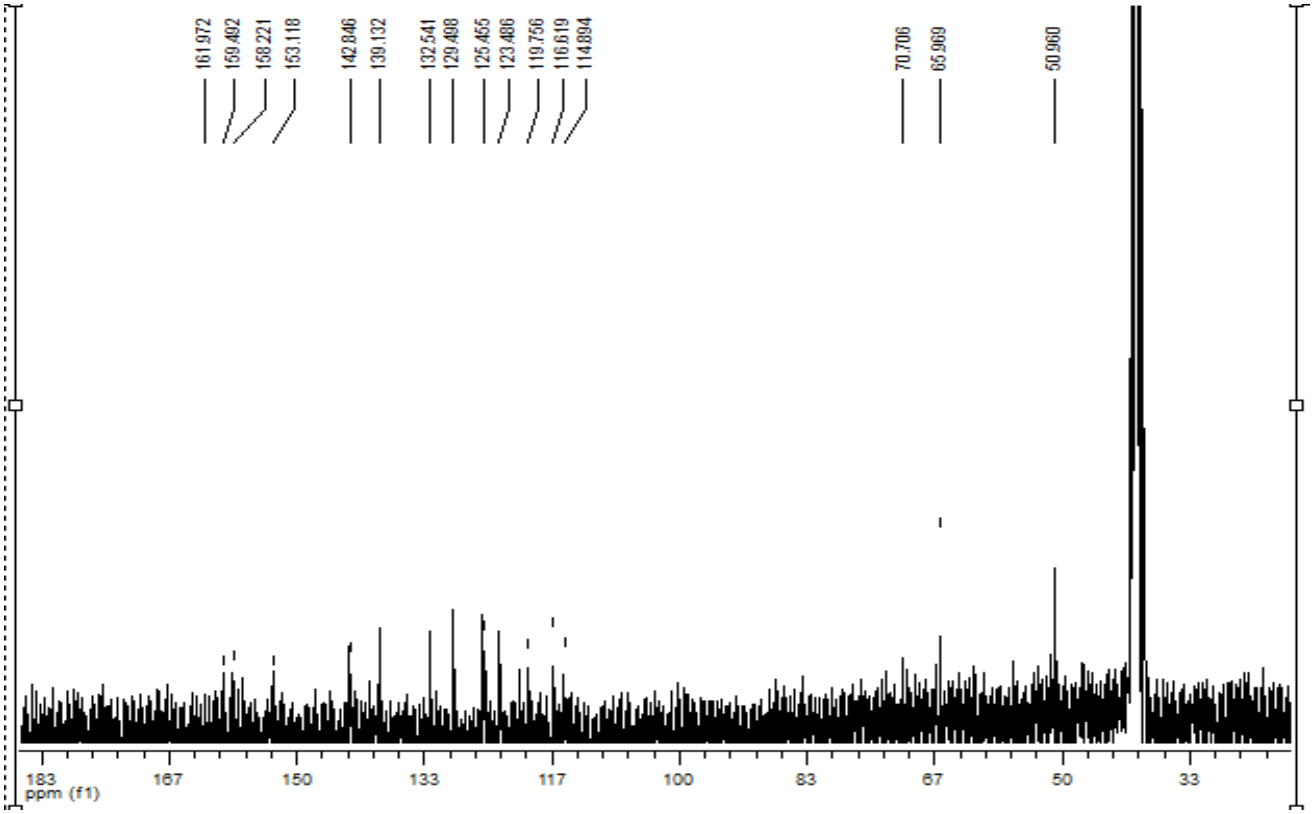


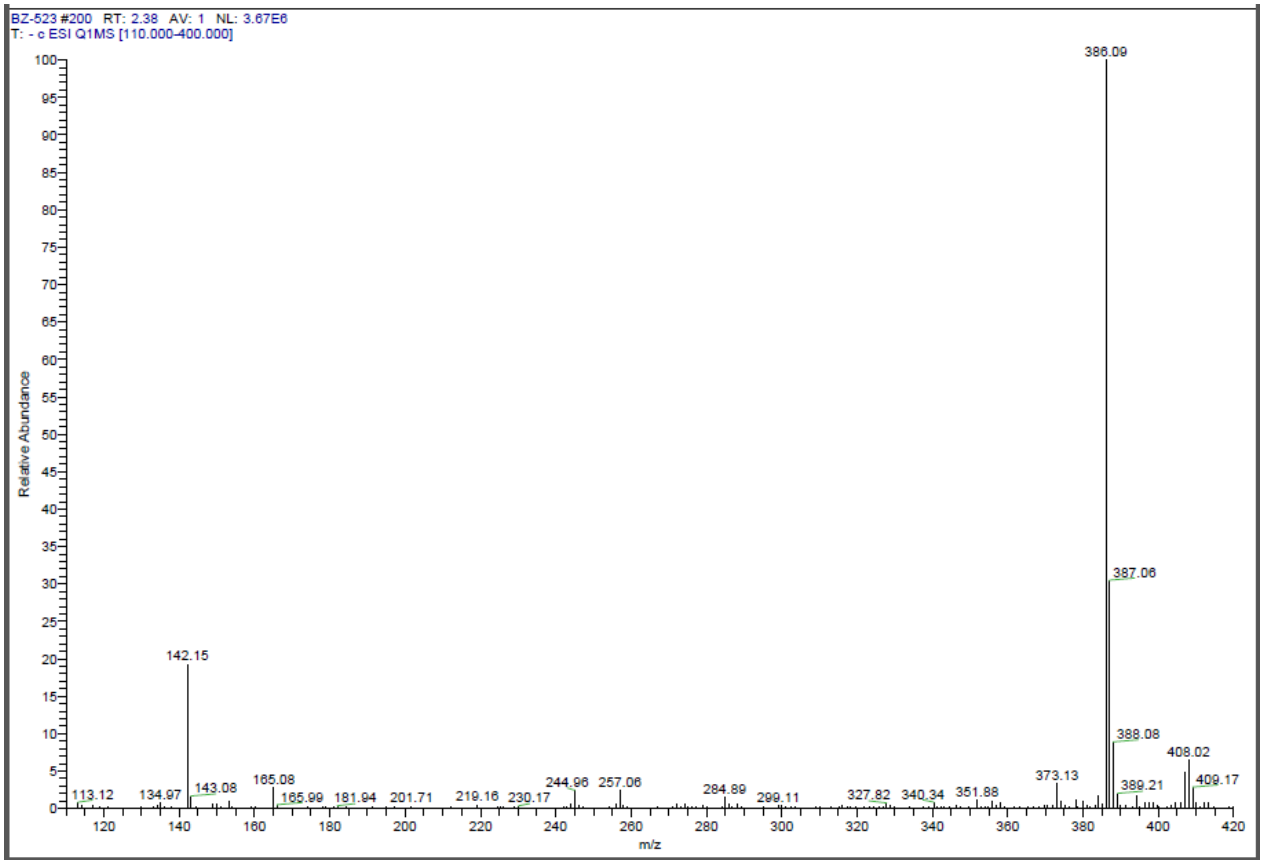

170.245
159.928
156.671
153.118
148.240
147.292
142.779
139.026
132.668
131.687
128.534
124.856
121.841
121.028
119.690
116.562
115.307
108.842
108.568
101.359
54.050
51.304
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


BZ-528 #227 RT: 2.70 AV: 1 NL: 5.41E4
T: - c ESI Q1MS [110.000-450.000]
Relative Abundance
m/z
434.16
283.35
435.18
284.37
393.33
353.04
355.08
395.34
299.12
436.23
357.16
255.35
243.16
311.36
328.05
339.35
265.28
370.14
381.43
396.36
421.73
437.43
131.13
145.02
162.35
185.15
201.19
219.37
227.28

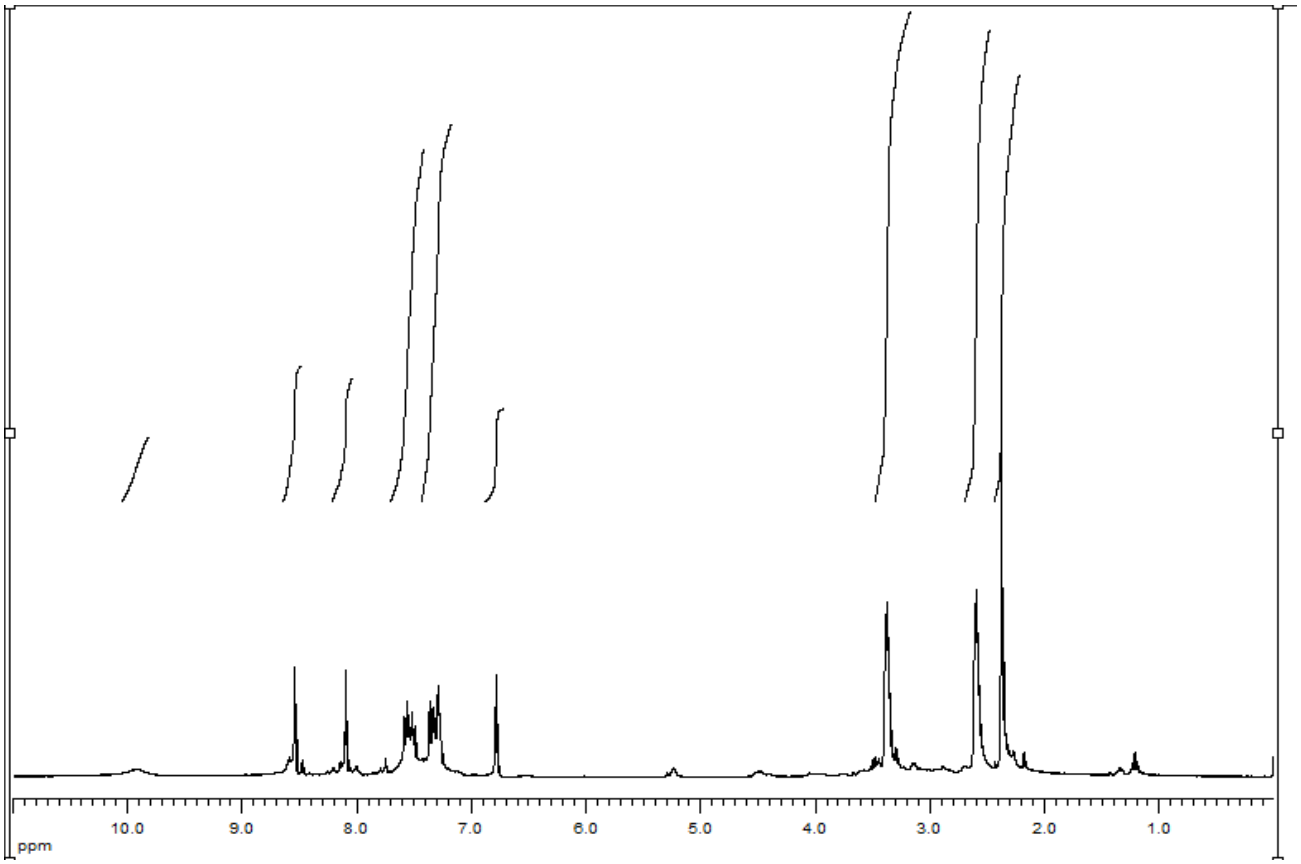
S17: ^{1}H and ^{13}C NMR and MSspectra of **6q**

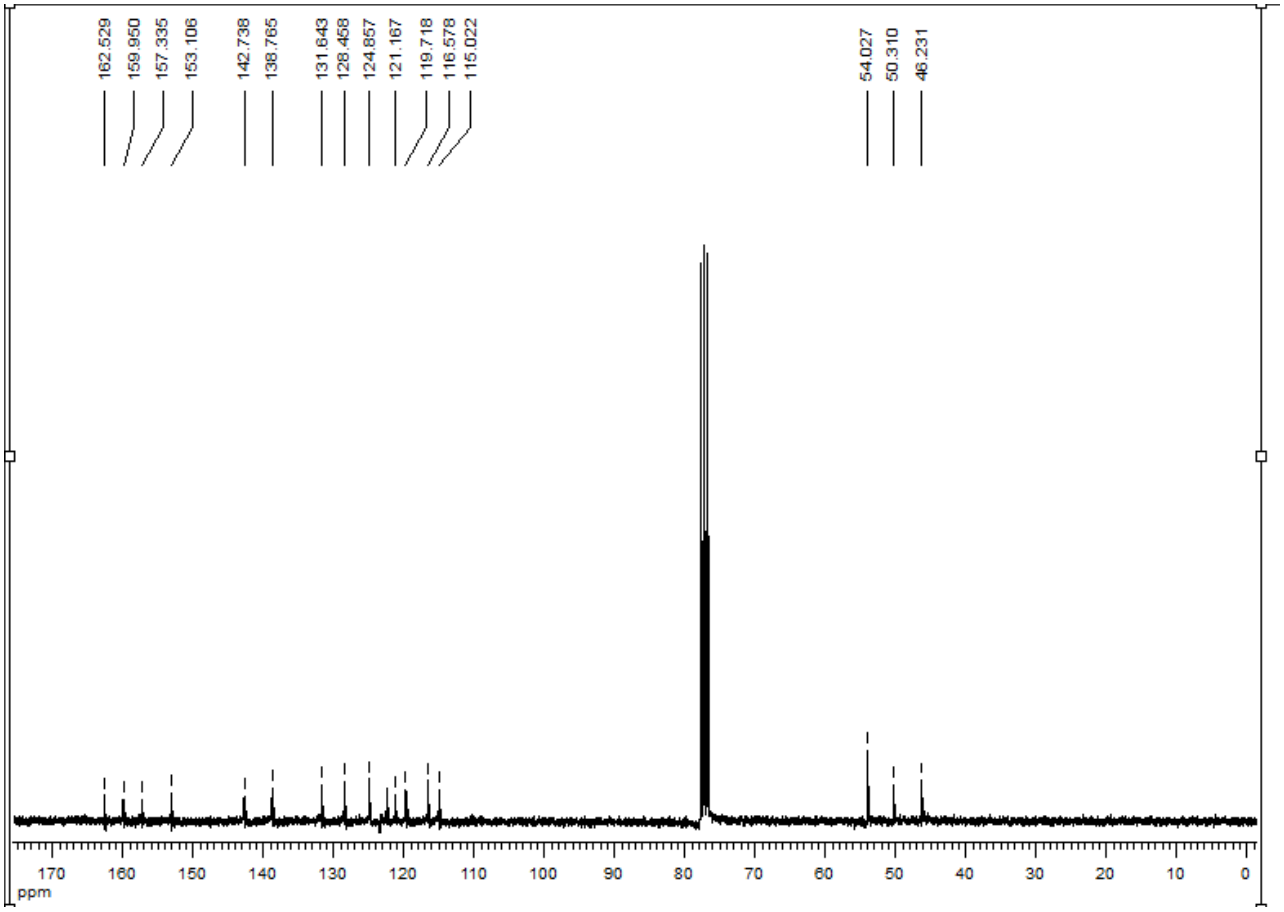


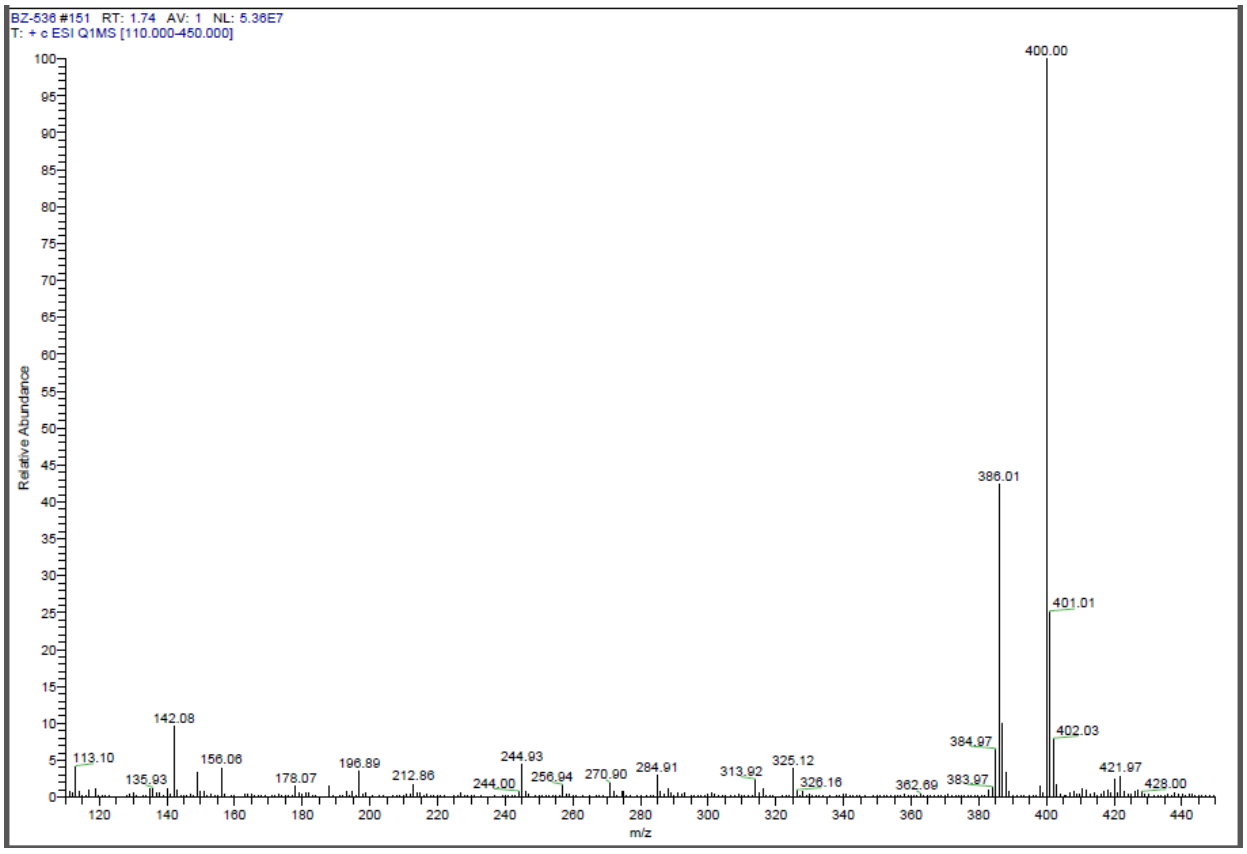




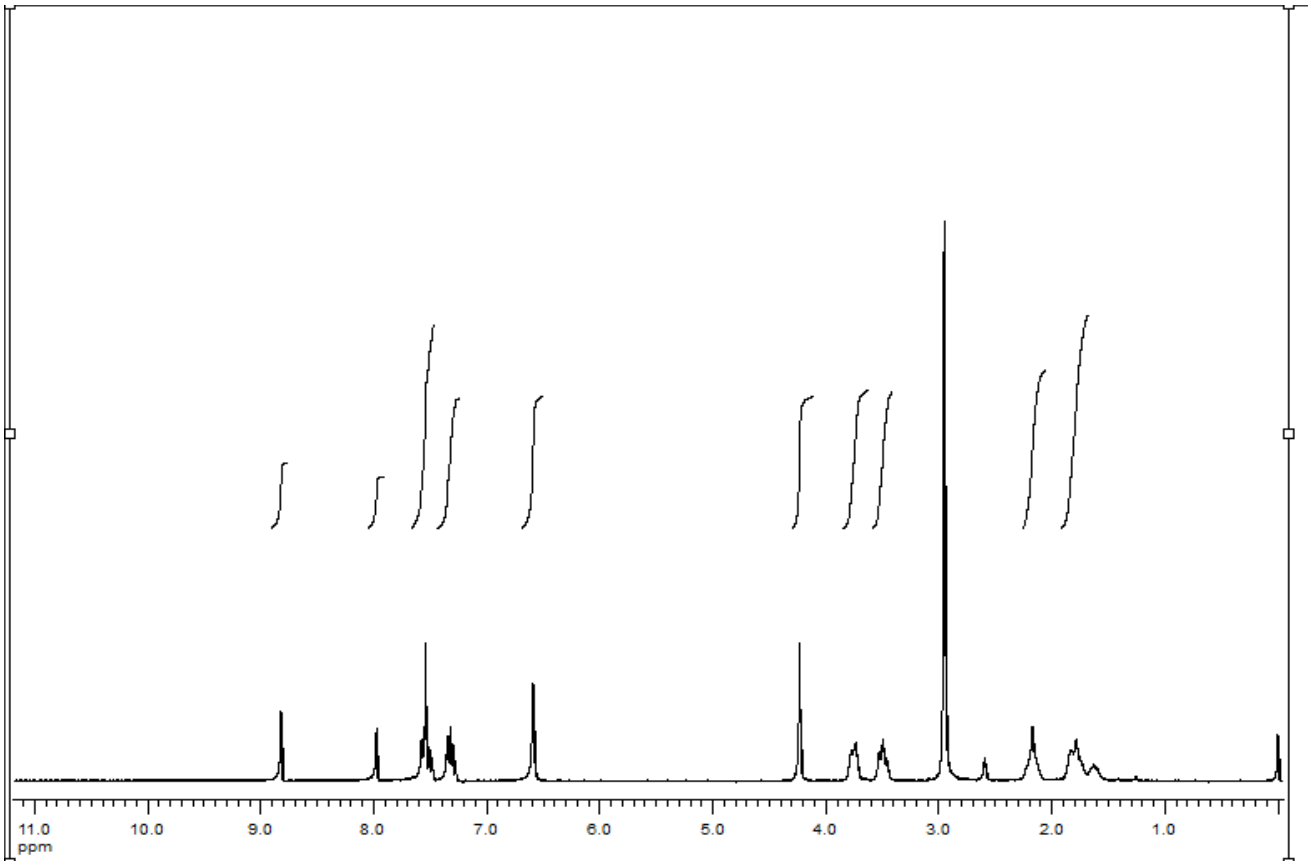
S18: ^{1}H and ^{13}C NMR and MS spectra of **6r**

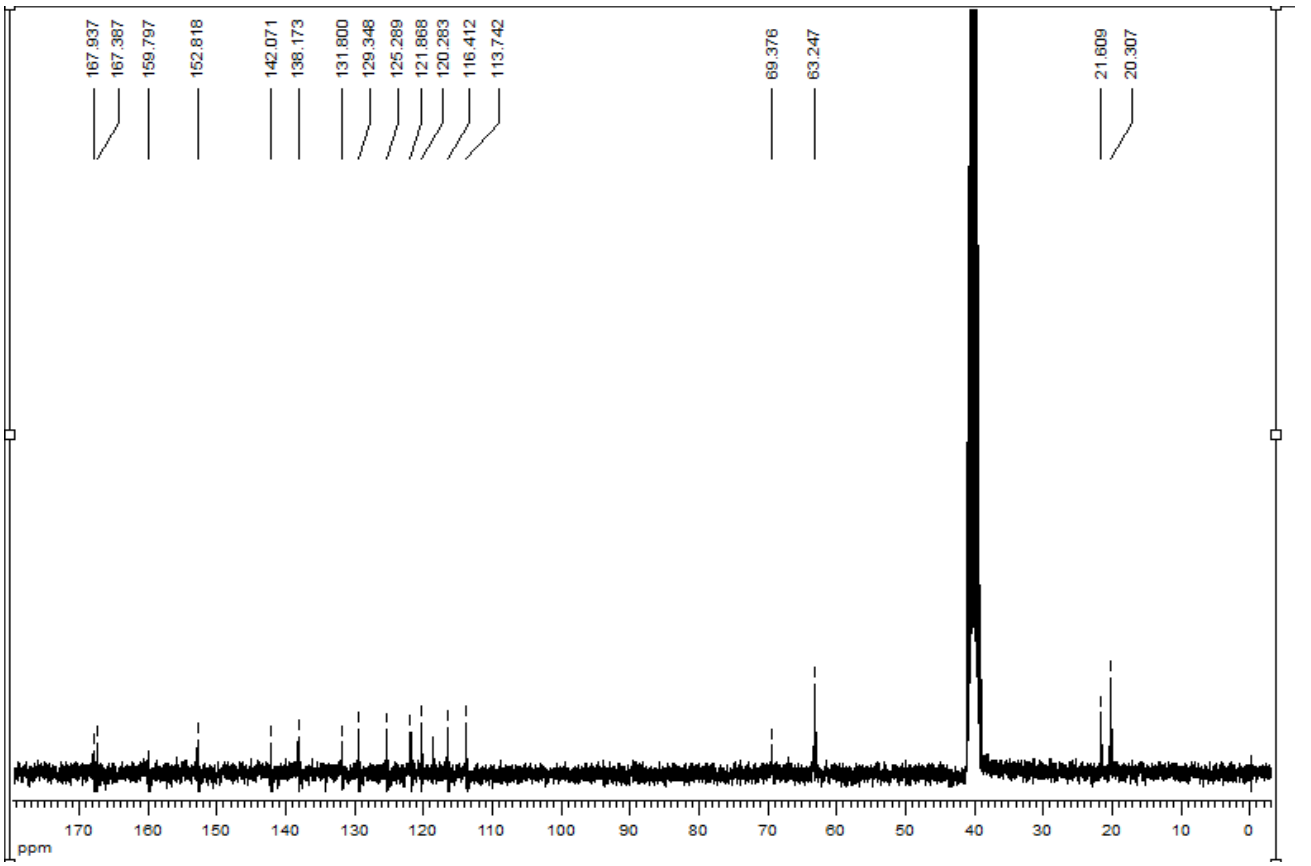


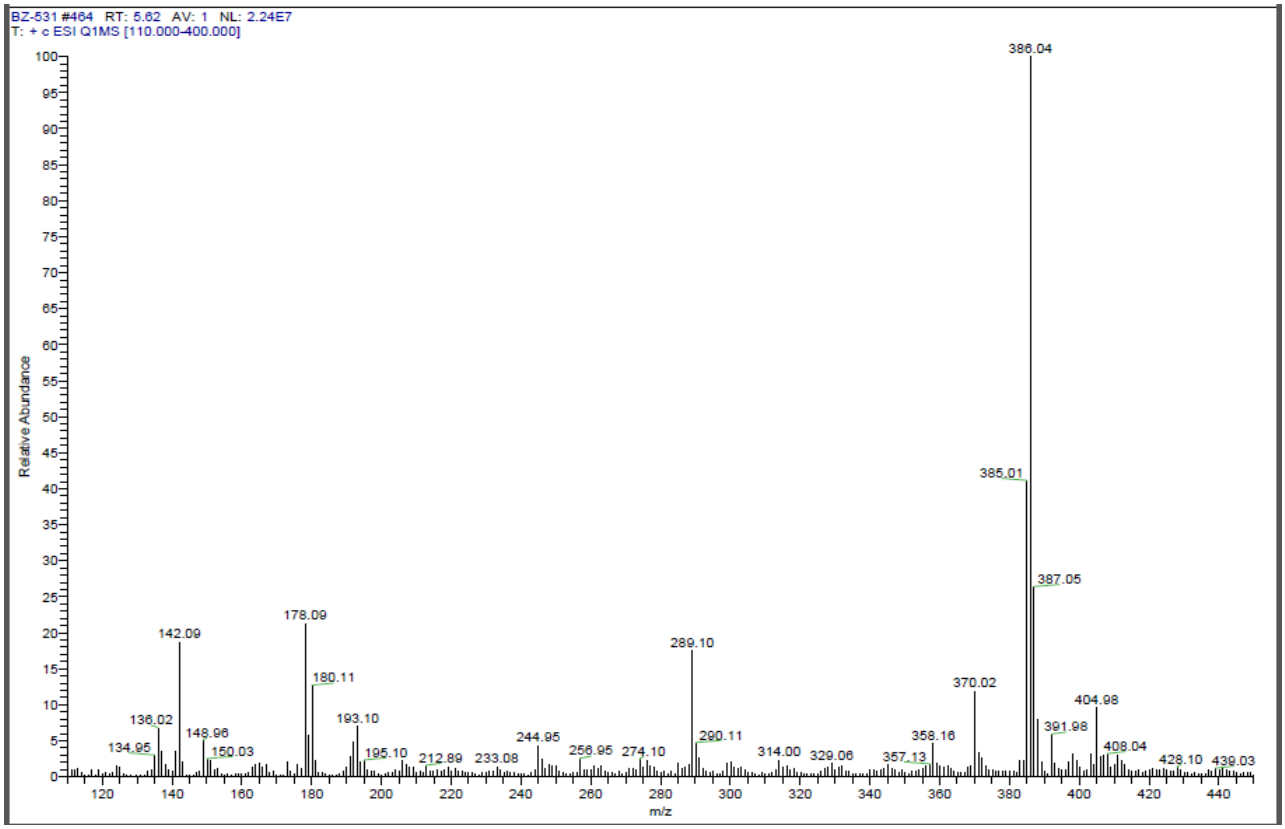

162.529
159.950
157.335
153.106
142.738
138.765
131.643
128.458
124.857
121.167
119.718
116.578
115.022
54.027
50.310
46.231
ppm


BZ-536 #151 RT: 1.74 AV: 1 NL: 5.36E7
T: + c ESI Q1MS [110.000-450.000]
Relative Abundance
m/z
400.00
386.01
401.01
402.03
142.08
113.10
156.06
135.93
178.07
196.89
212.86
244.93
244.00
256.94
270.90
284.91
313.92
325.12
326.16
362.69
383.97
384.97
421.97
428.00

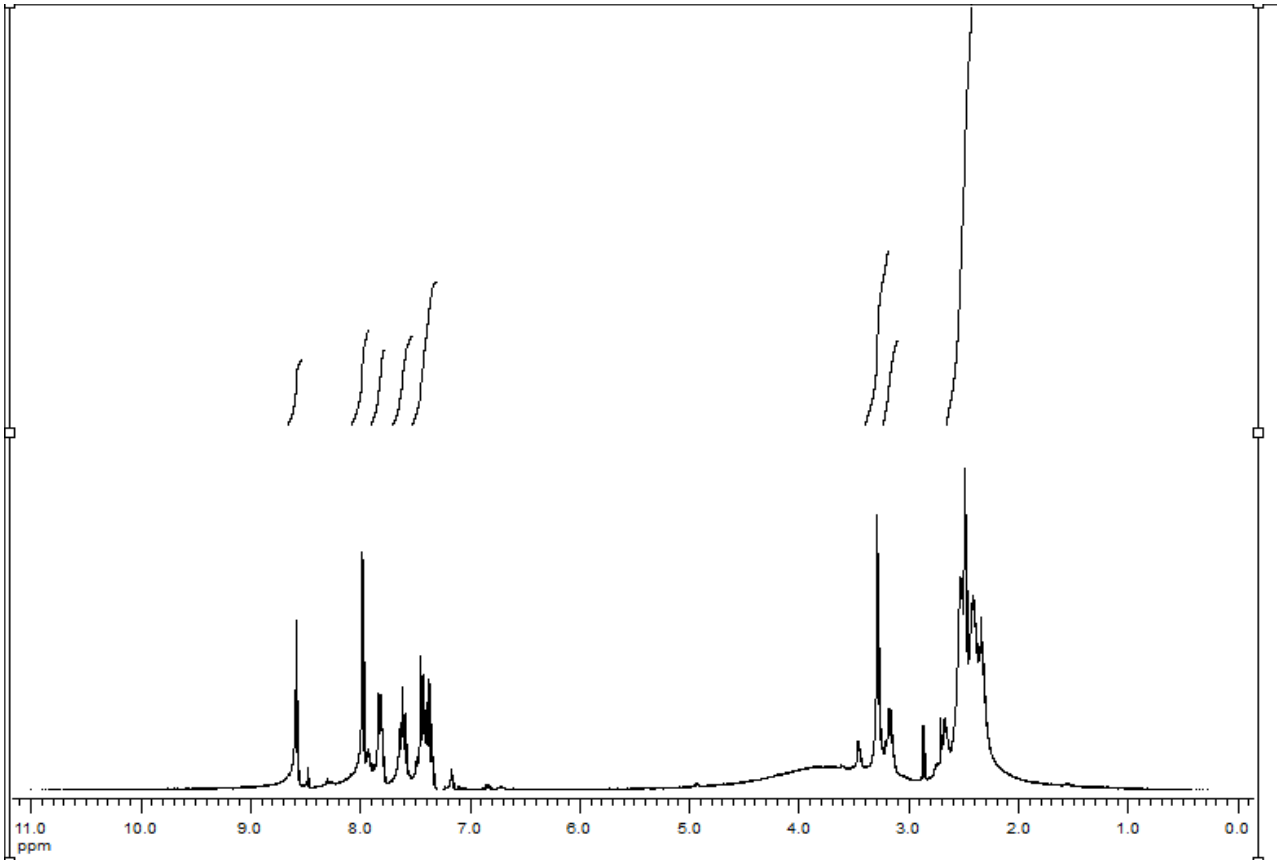
S19: ^{1}H and ^{13}C NMR and MS spectra of **6s**

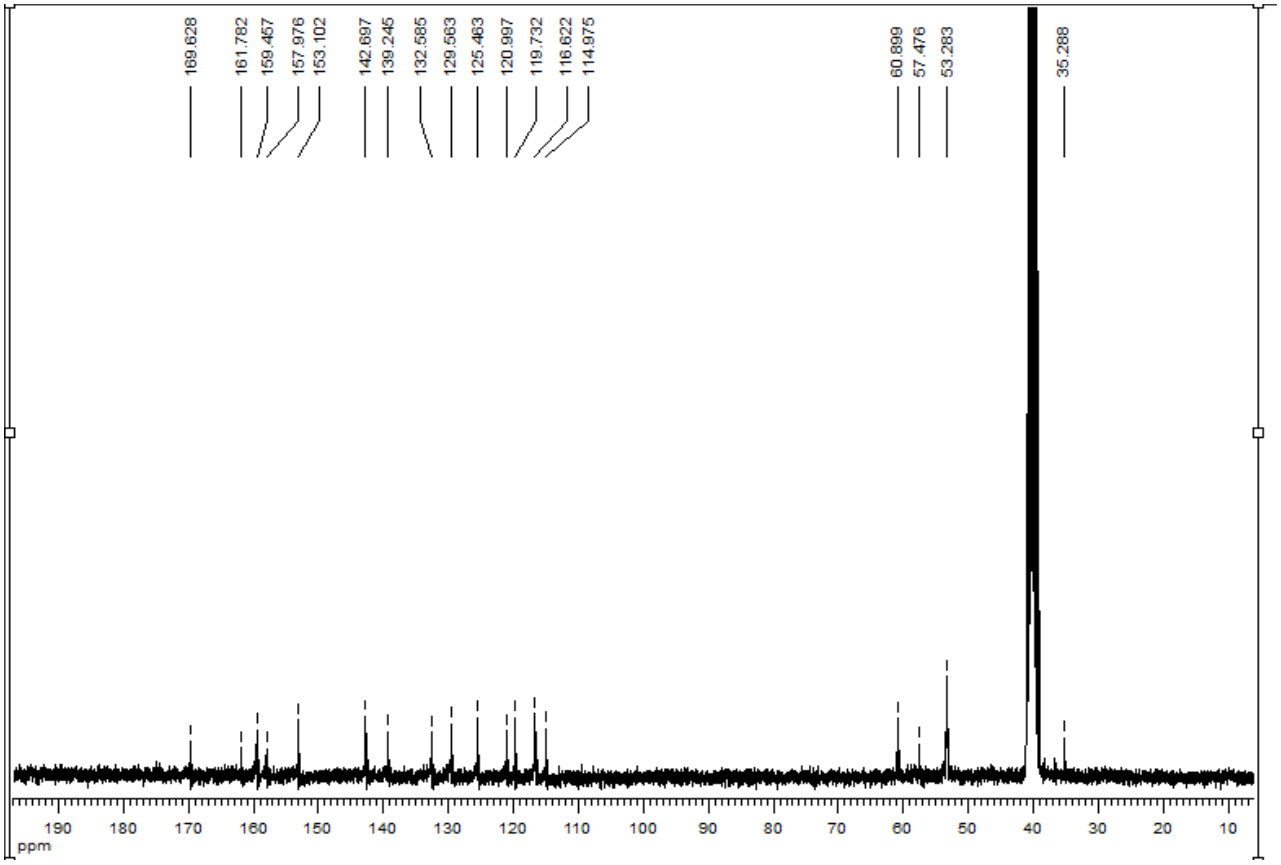


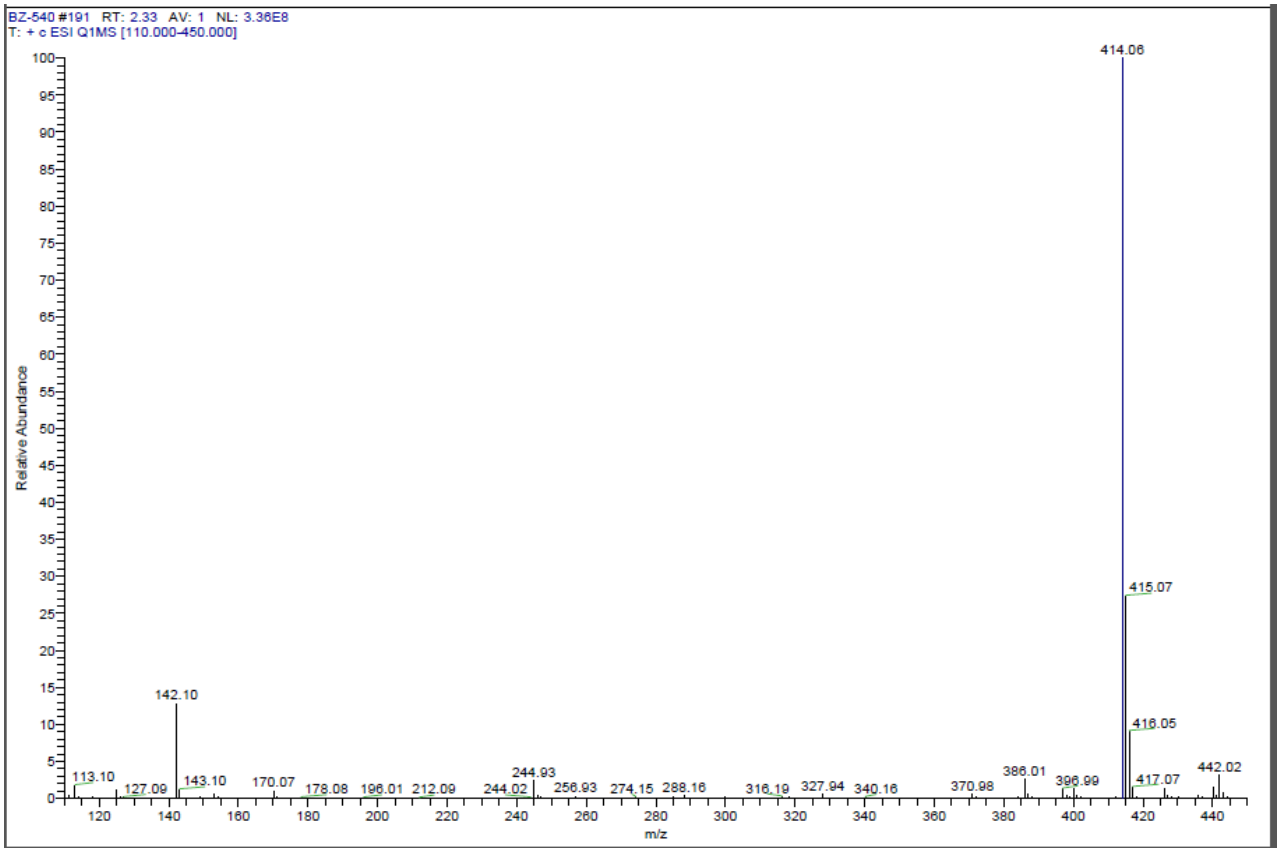




S20: ^{1}H and ^{13}C NMR and MS spectra of **6t**




169.628
161.782
159.457
157.976
153.102
142.697
139.245
132.585
129.563
125.463
120.997
119.732
116.622
114.975
60.899
57.476
53.283
35.288
ppm


BZ-540 #191 RT: 2.33 AV: 1 NL: 3.36E8
T: + c ESI Q1MS [110.000-450.000]
Relative Abundance
m/z
414.06
415.07
416.05
417.07
442.02
142.10
113.10
127.09
143.10
170.07
178.08
196.01
212.09
244.93
244.02
256.93
274.15
288.16
316.19
327.94
340.16
370.98
386.01
396.99