Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information for:

Synthesis of 4-aryl-1,2,3-triazolyl appended natural coumarin-related compounds with antiproliferative, radical scavenging activities and intracellular ROS production modification

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Contents

Fig. S1 Radical scavenging capacity (RSC) of compounds **16a–16e, 17a–17e, 18a–18e, 19a–19d, 20a–20d** and reference compounds umbelliferone and esculetin at 0.2mM after 30 min and 60 min of incubation.

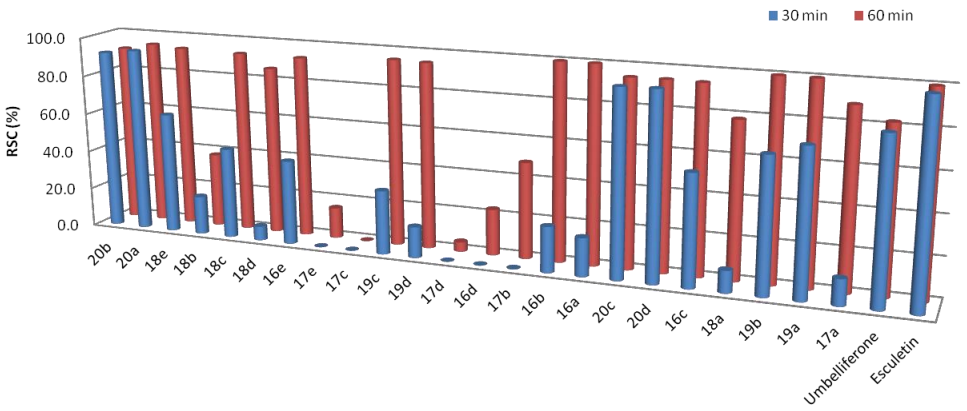


Fig. S2 Cyclic voltammograms obtained for compounds **16a–16e**

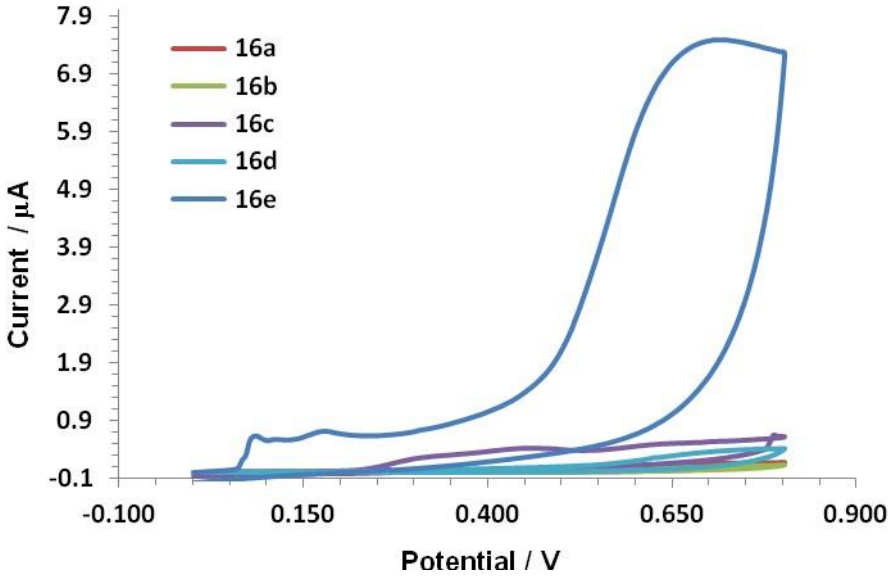


Fig. S3 Cyclic voltammograms obtained for compounds **17a–17e**

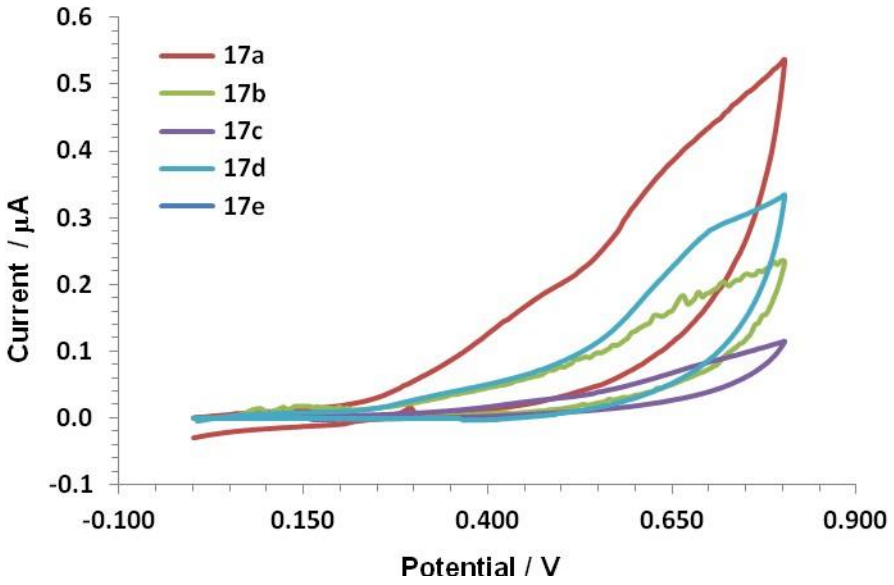


Fig. S4 Cyclic voltammograms obtained for compounds **18a–18e**

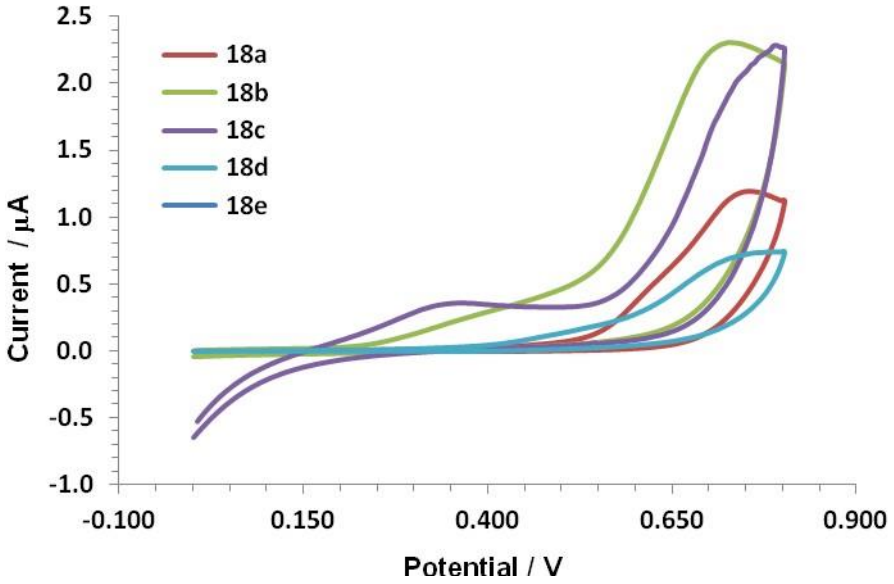


Fig. S5 Cyclic voltammograms obtained for compounds **19a–19e**

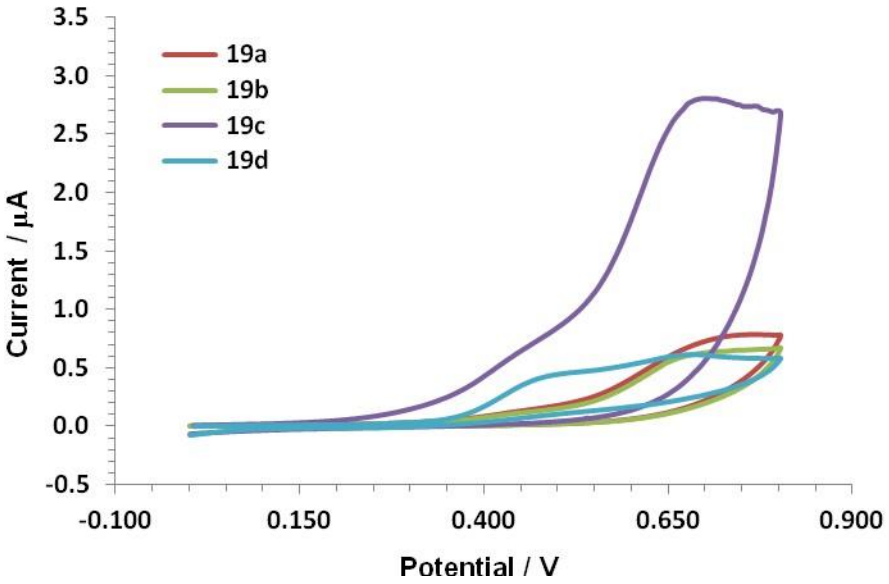


Fig. S6 ROS detection of compd **20d**; cells were treated with 1 x 10^{-4} M compound **20d** for 1h and analyzed by flow cytometry. Histogram overlays show fluorescence patterns for control (blue) and ecsuletin (red) compared to **20d** shown in green.

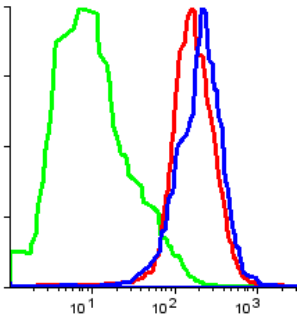
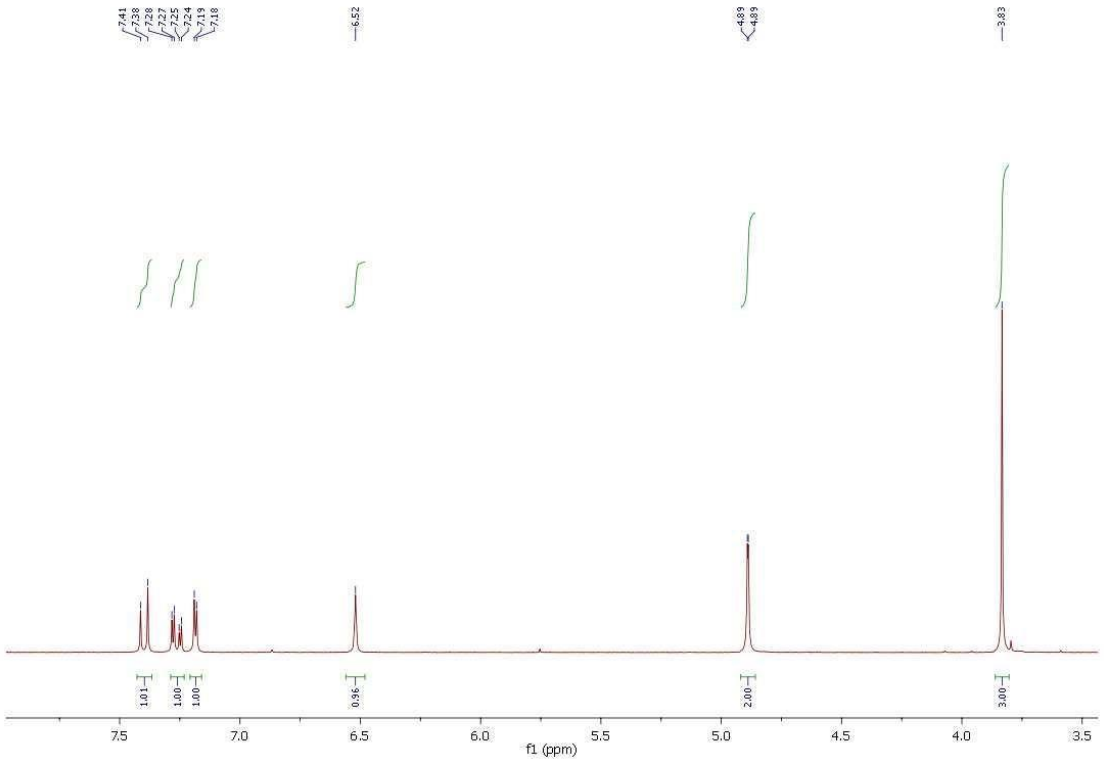


Fig. S7 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **12**

a)



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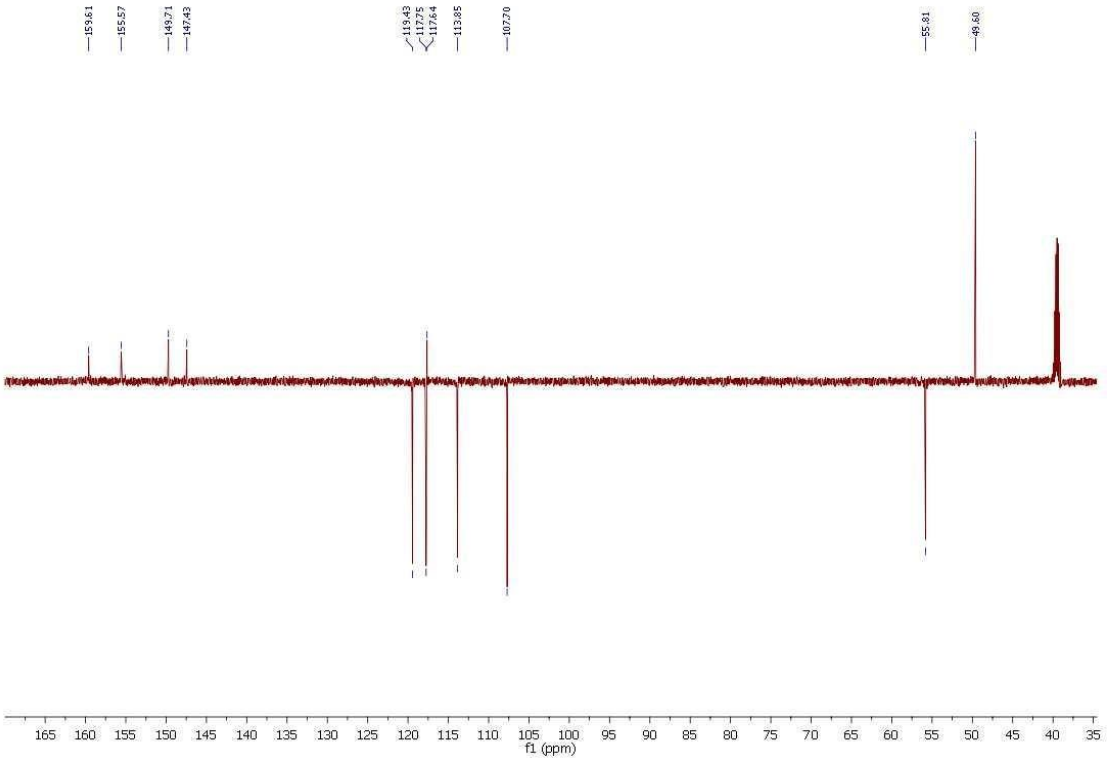

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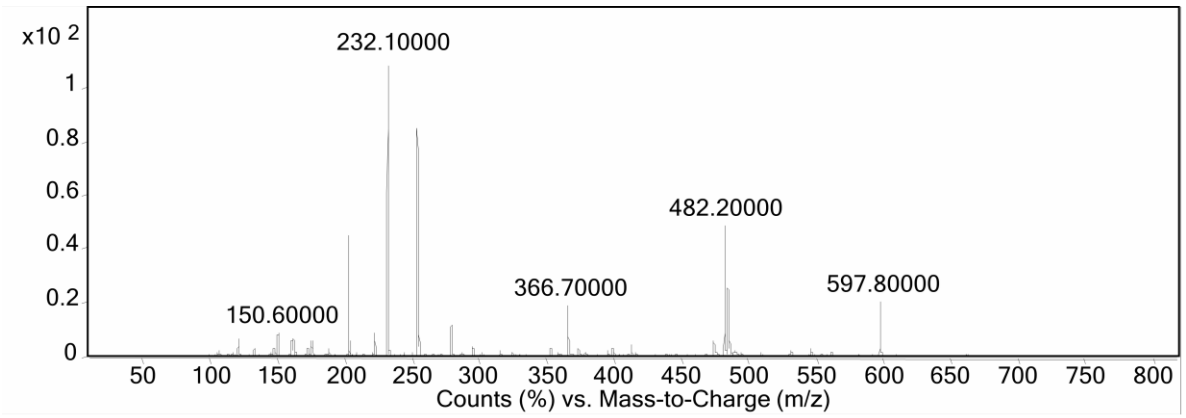
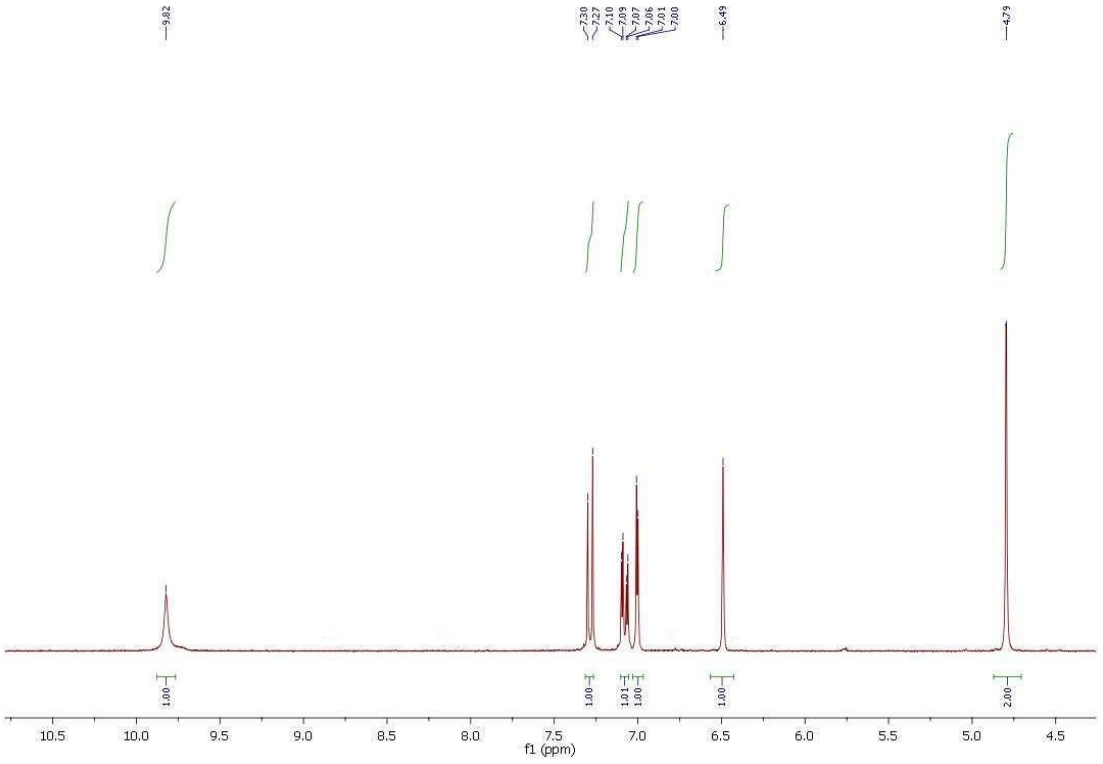
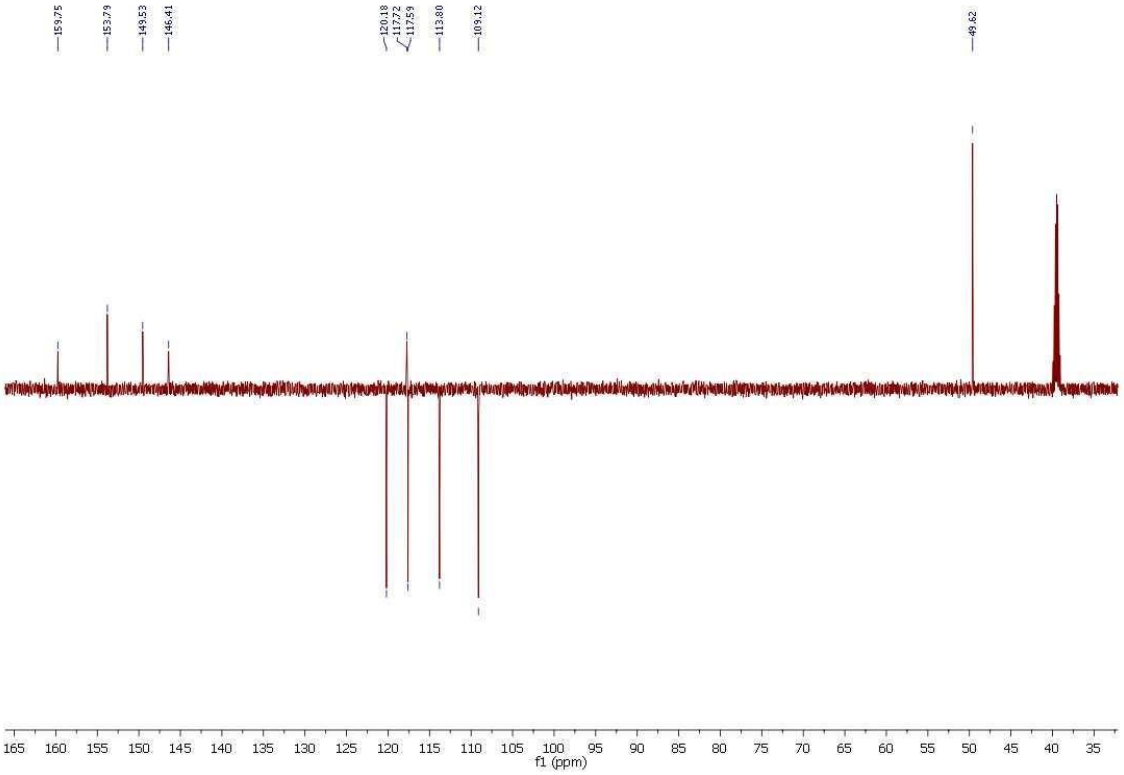


Fig. S8 a) ^{1}H NMR and b) ^{13}C NMR of compd. **14**

a)



b)


159.75
153.79
149.53
146.41
120.18
117.72
117.59
113.80
109.12
49.62
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

c)

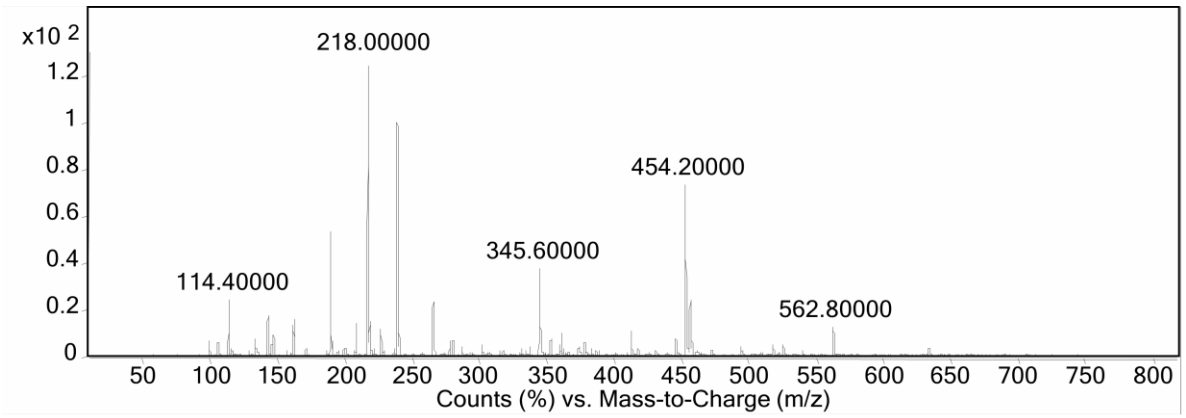
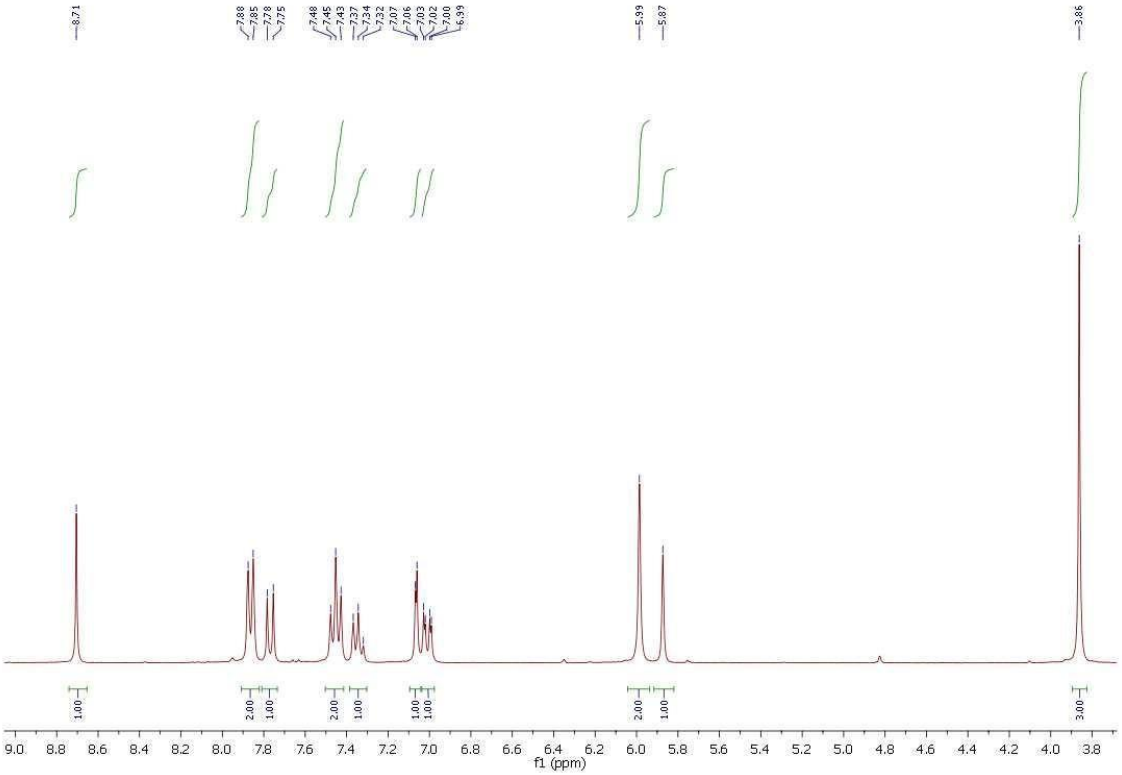
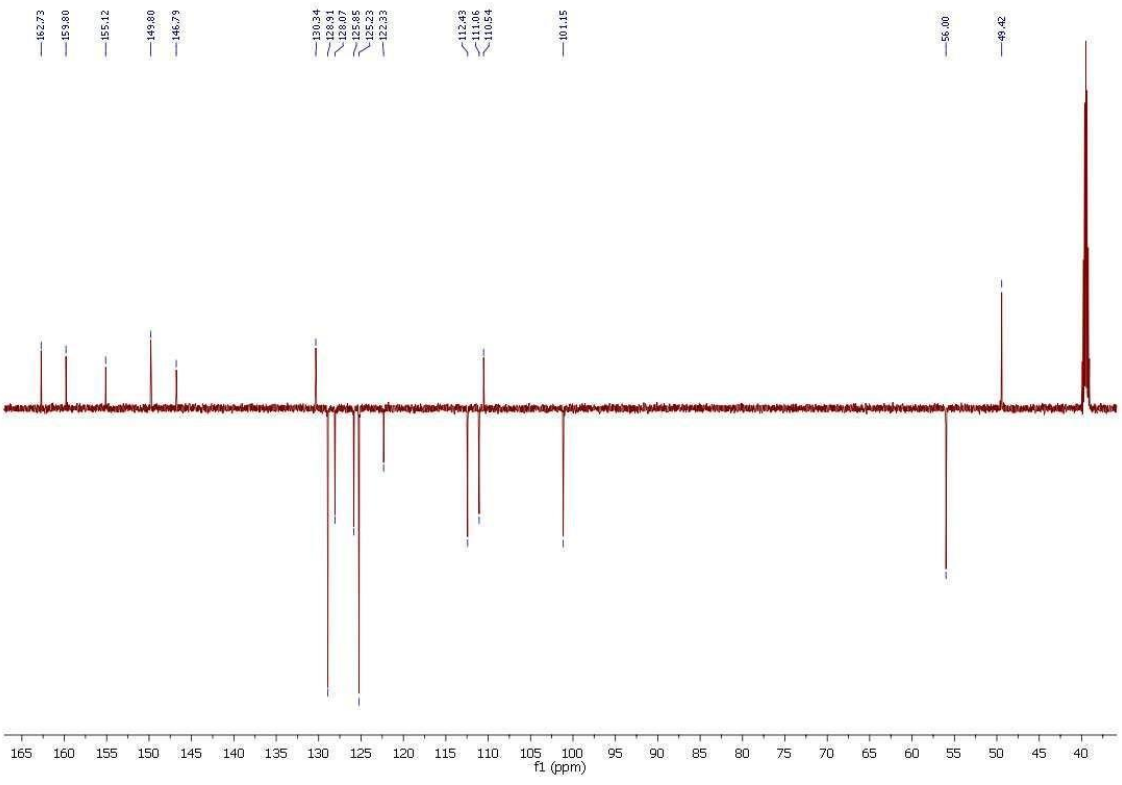

x10 2
1.2
1
0.8
0.6
0.4
0.2
0
218.00000
454.20000
345.60000
114.40000
562.80000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S9 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **16a**

a)



b)



c)

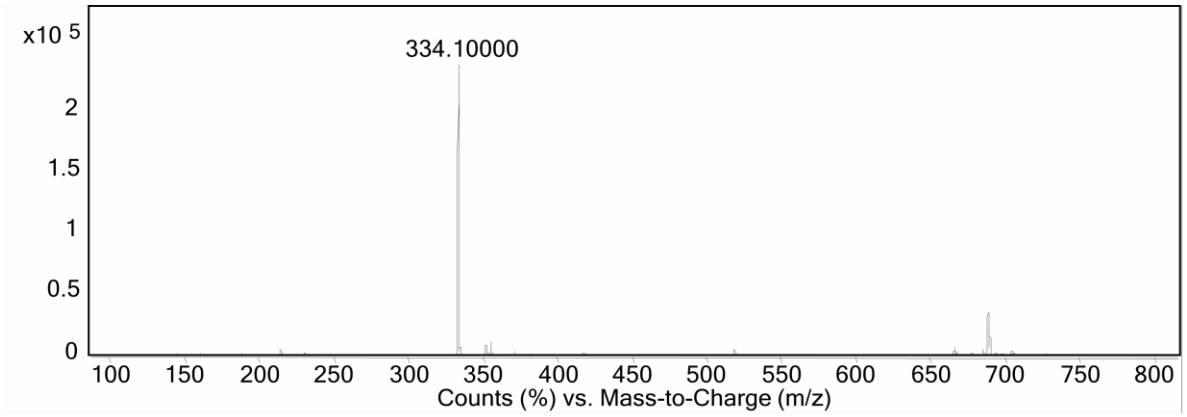
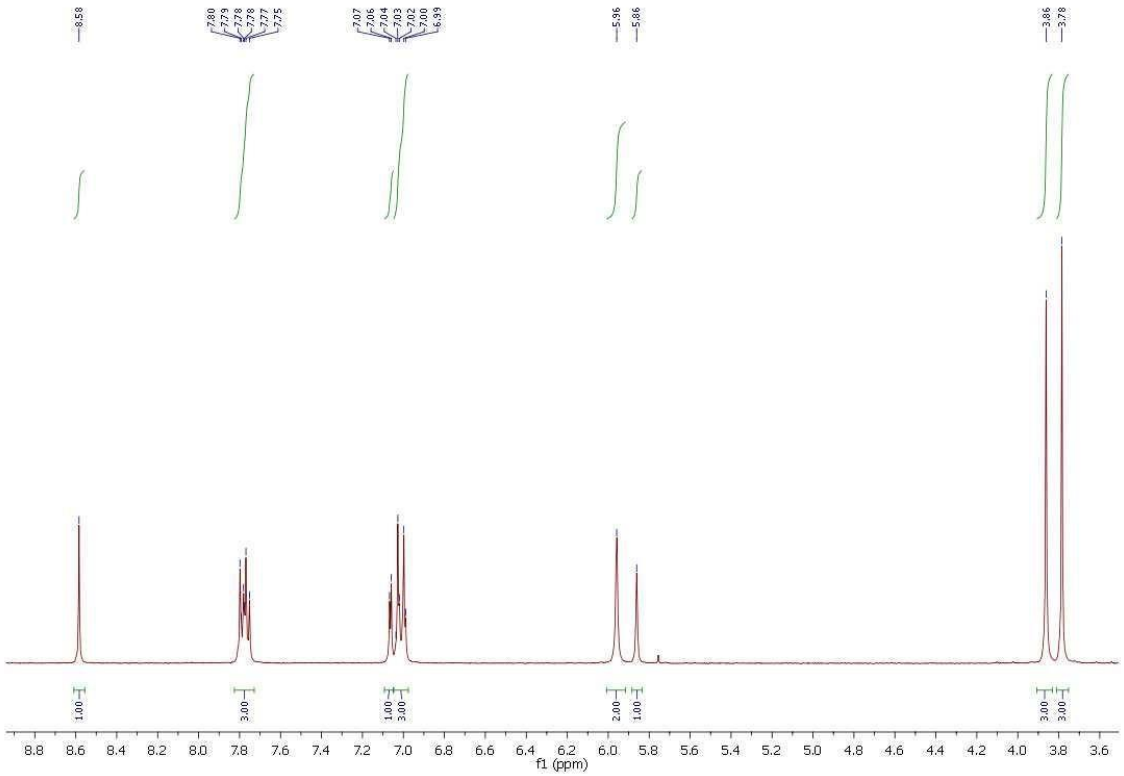


Fig. S10 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **16b**

a)



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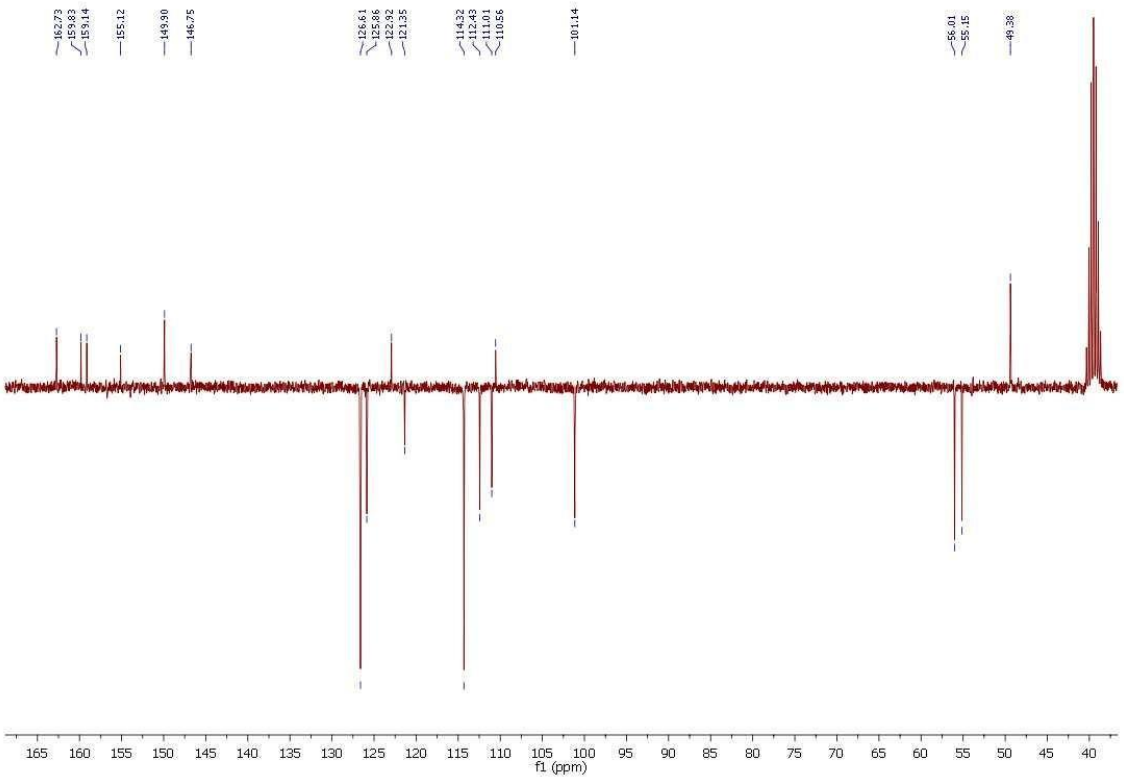

162.73
159.83
159.14
155.12
149.90
146.75
126.61
125.86
122.92
121.35
114.32
112.43
111.01
110.56
101.14
56.01
55.15
49.38
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

c)

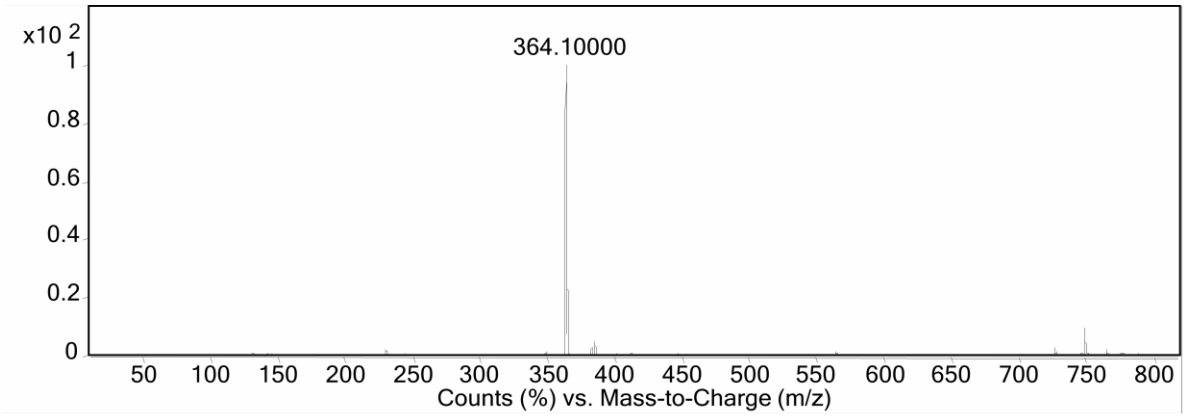
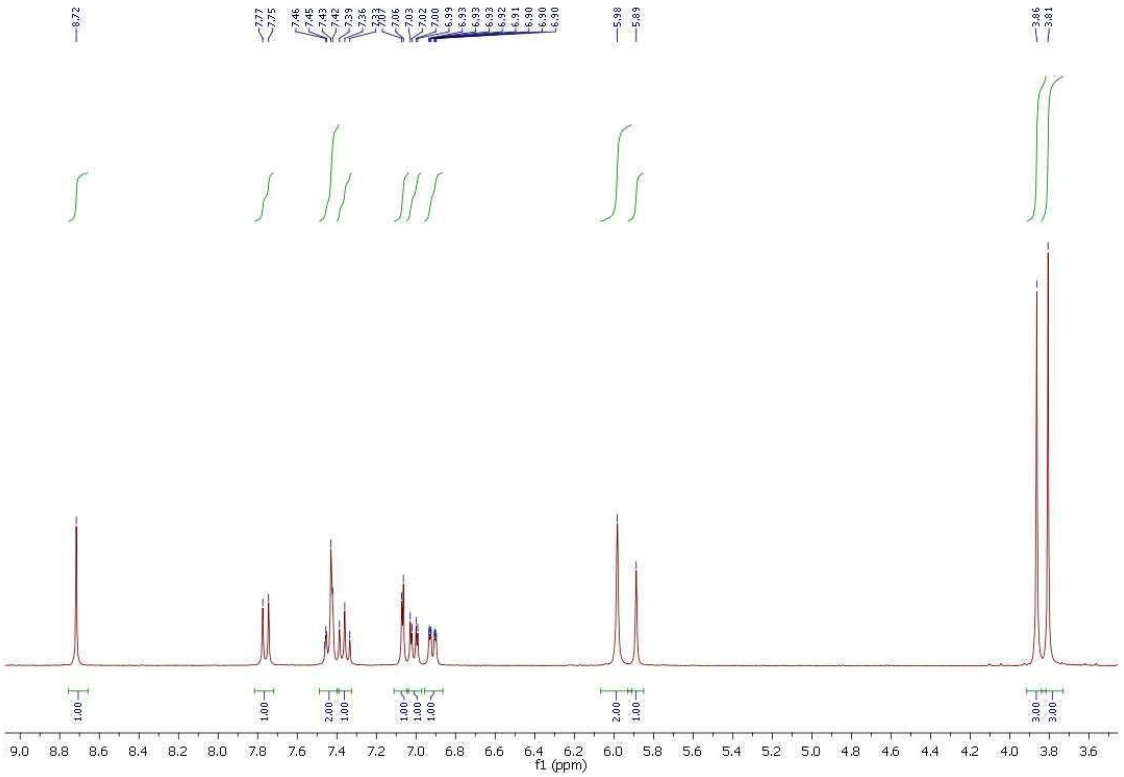
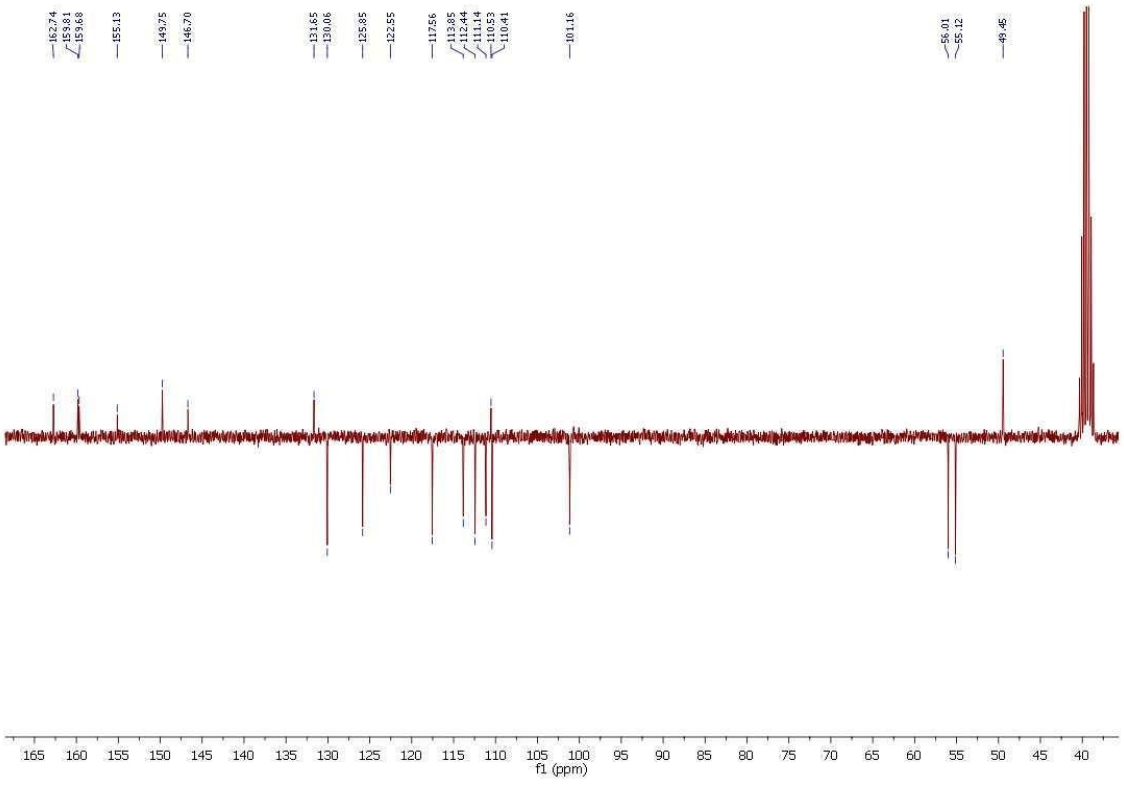

x10 2
1
0.8
0.6
0.4
0.2
0
364.10000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S11 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **16c**

a)



b)



c)

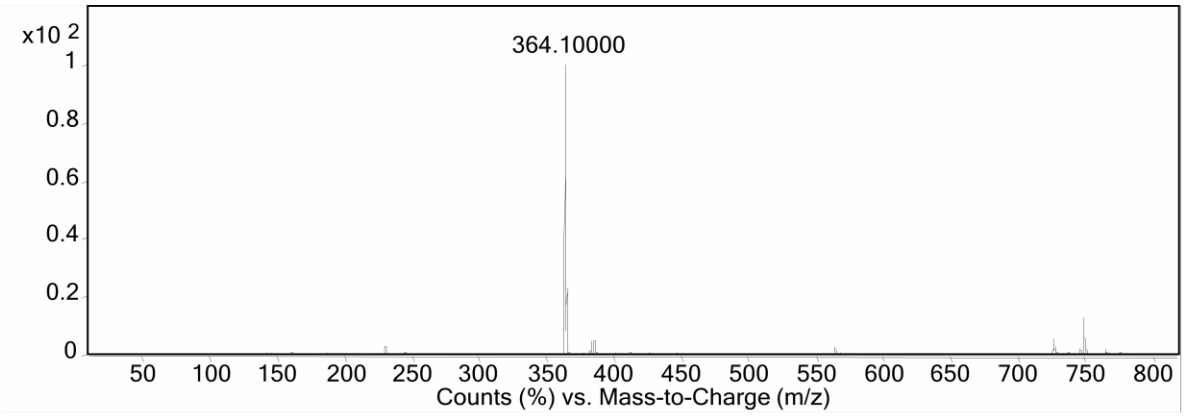
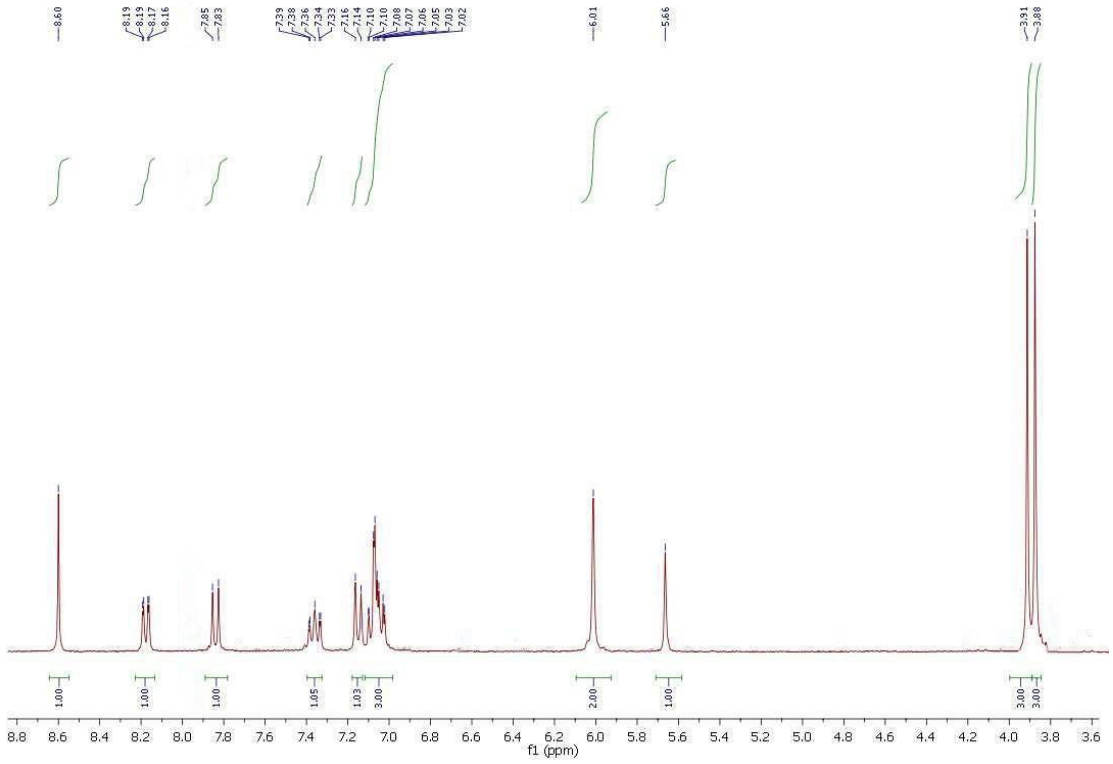


Fig. S12 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **16d**

a)



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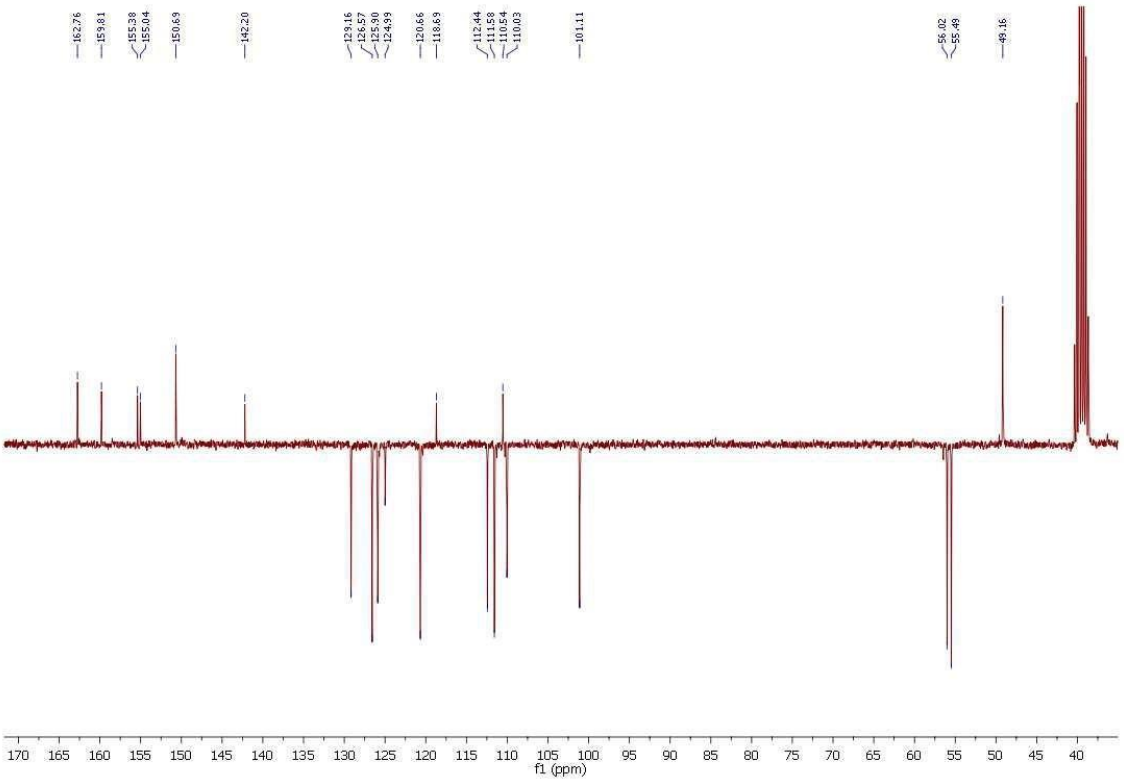

162.76
159.81
155.38
155.04
150.69
142.20
129.16
126.57
125.90
124.99
120.66
118.69
112.44
111.58
110.54
110.03
101.11
56.02
55.49
49.16
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

c)

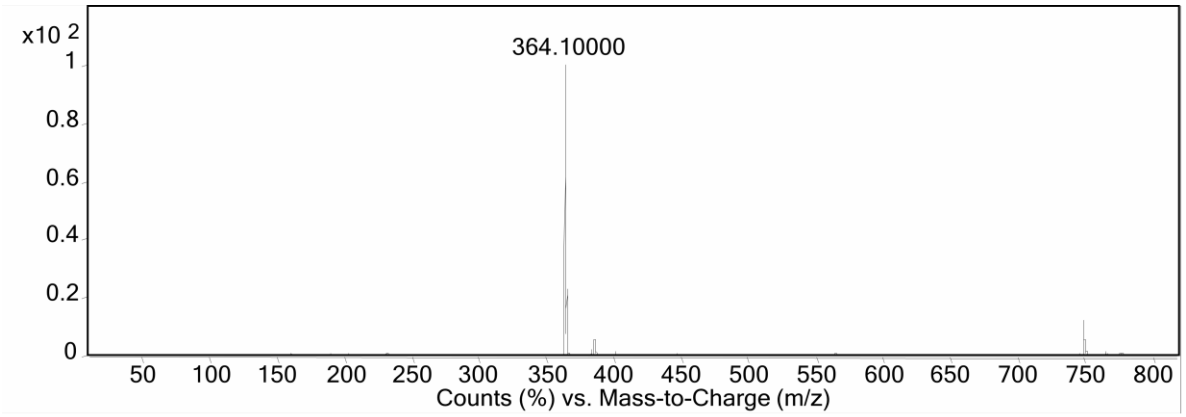
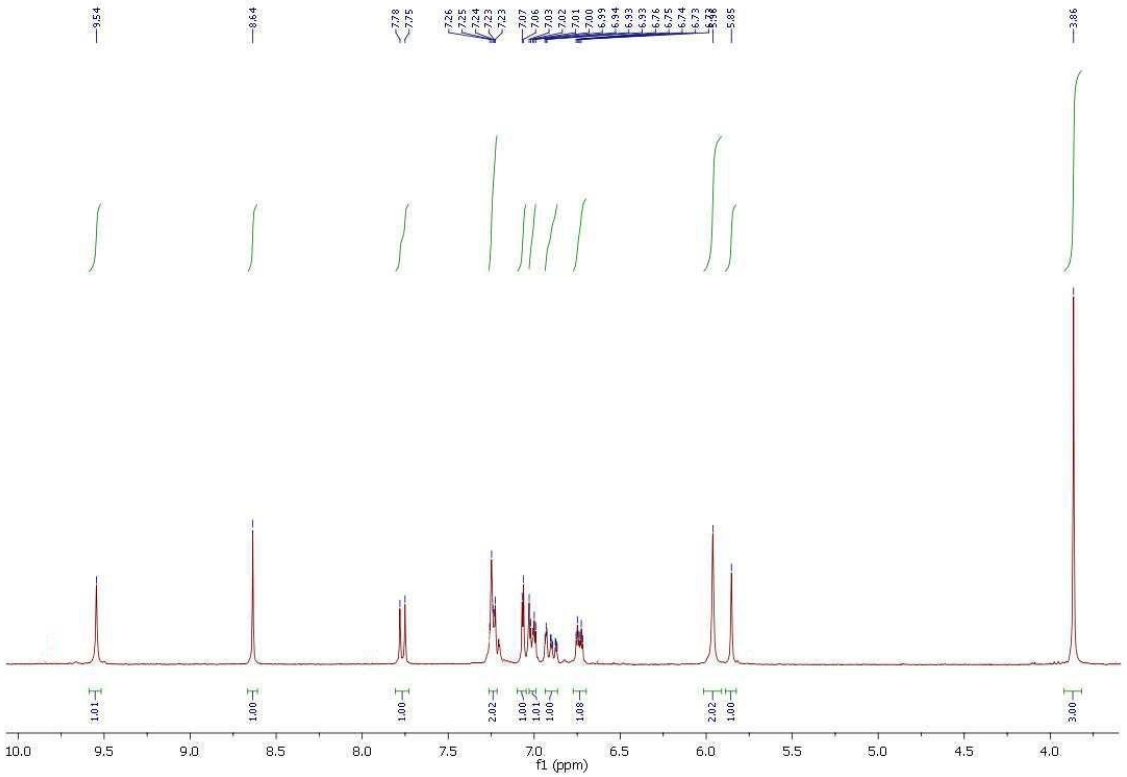
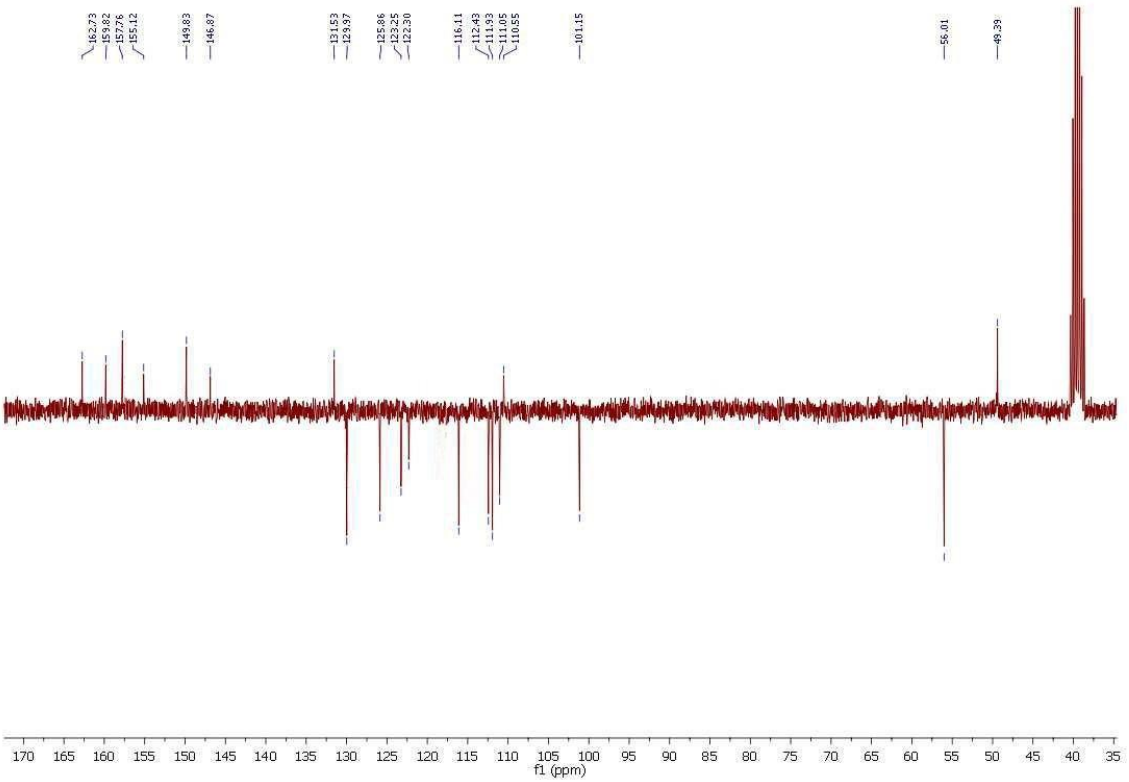

x10 2
1
0.8
0.6
0.4
0.2
0
364.10000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S13 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **16e**

a)



b)



c)

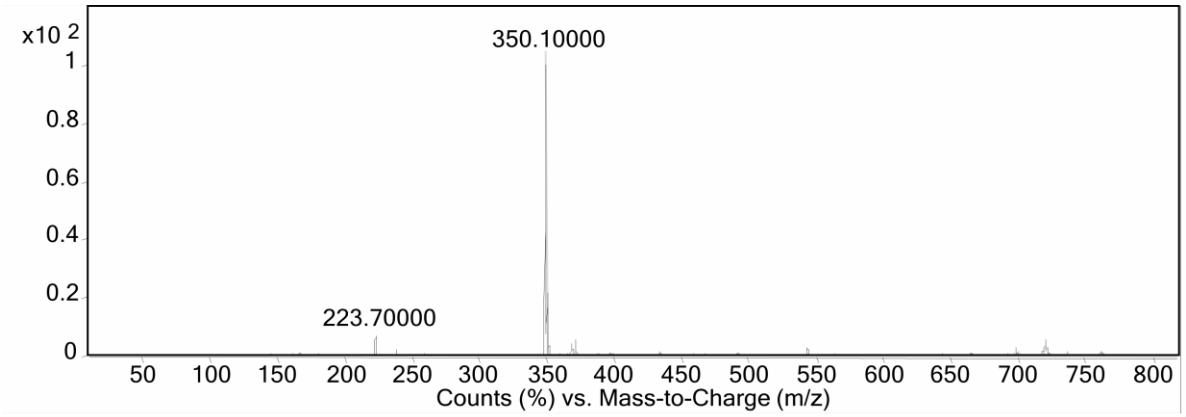
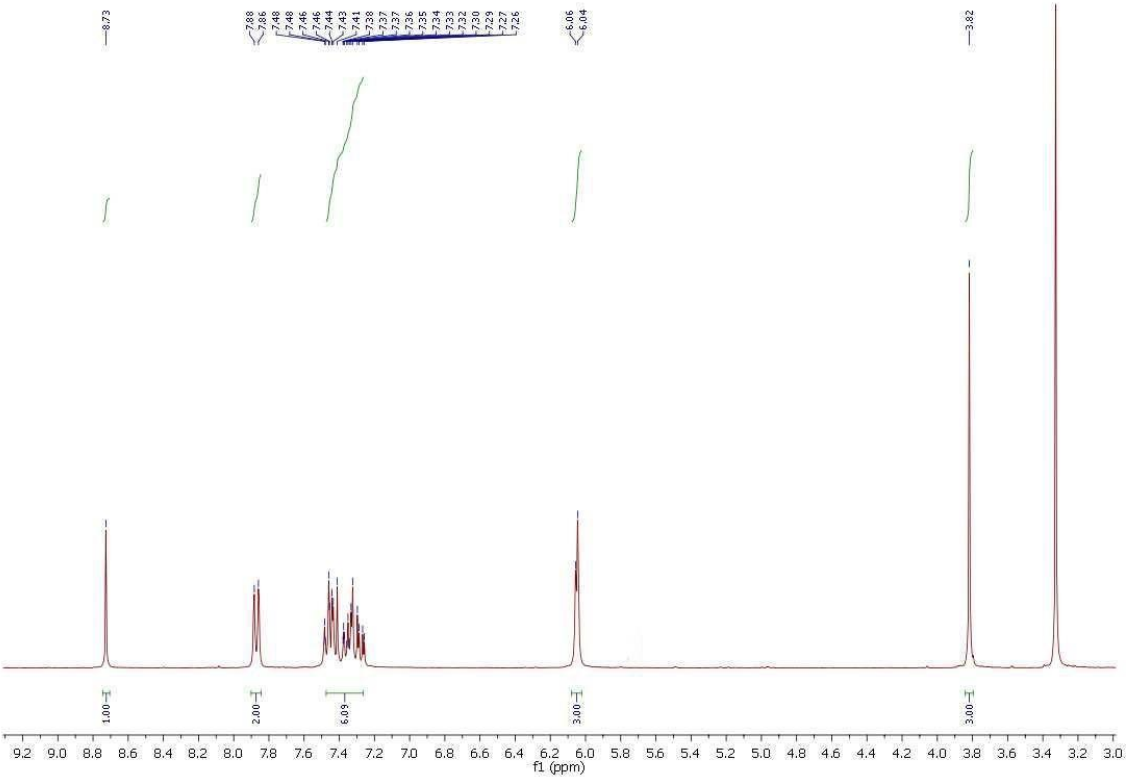


Fig. S14 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **17a**

a)



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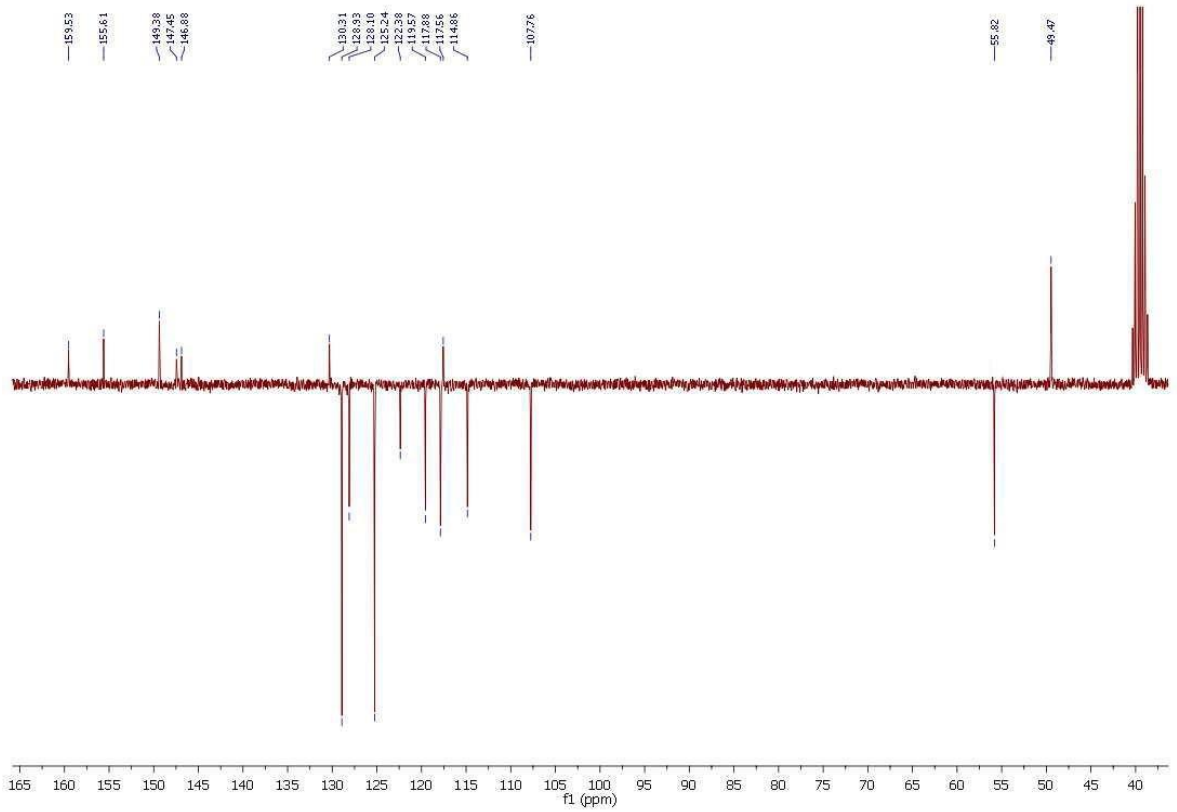

153.53
155.61
149.38
147.45
146.88
130.31
128.93
128.10
125.24
122.38
119.57
117.88
117.56
114.86
107.76
55.82
49.47
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

c)

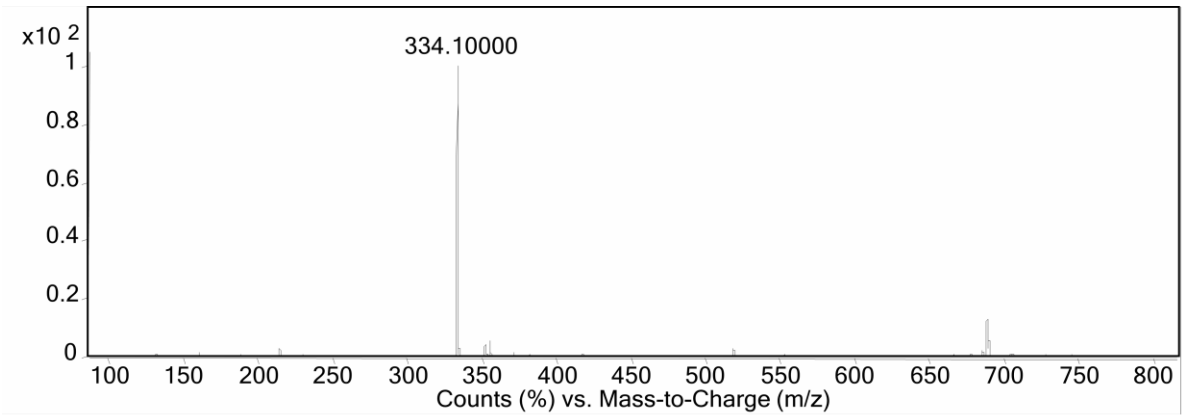
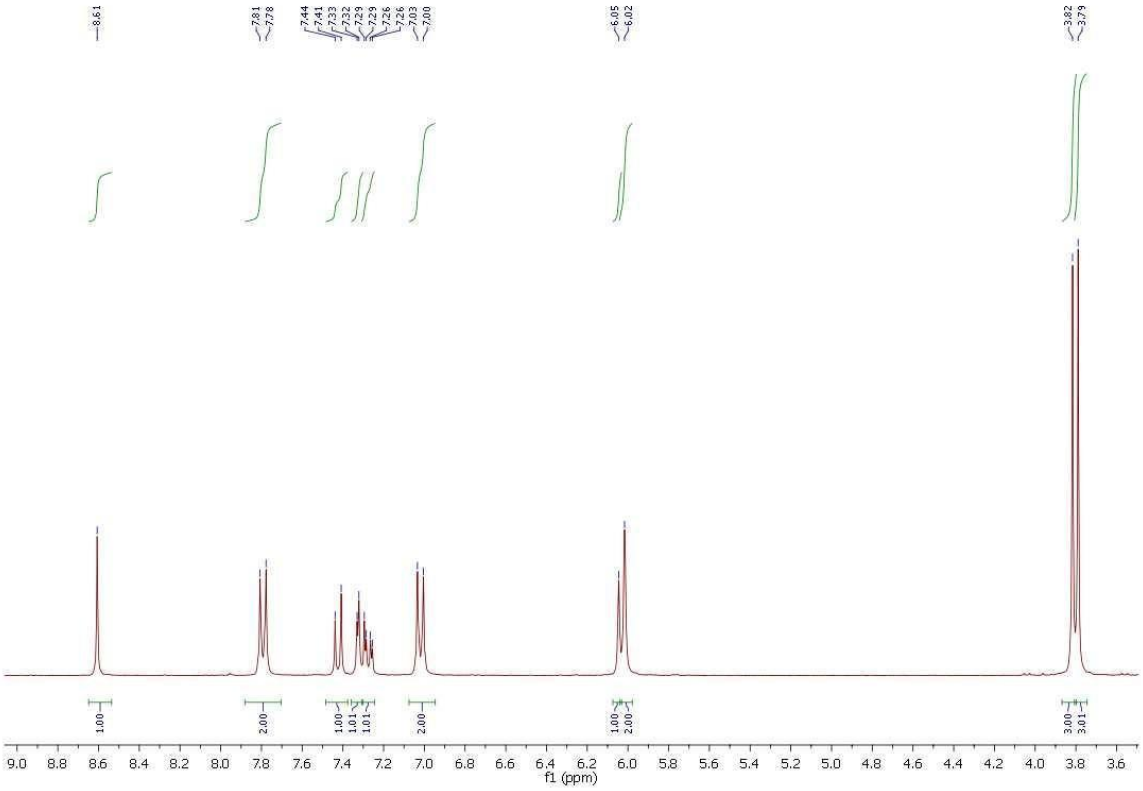
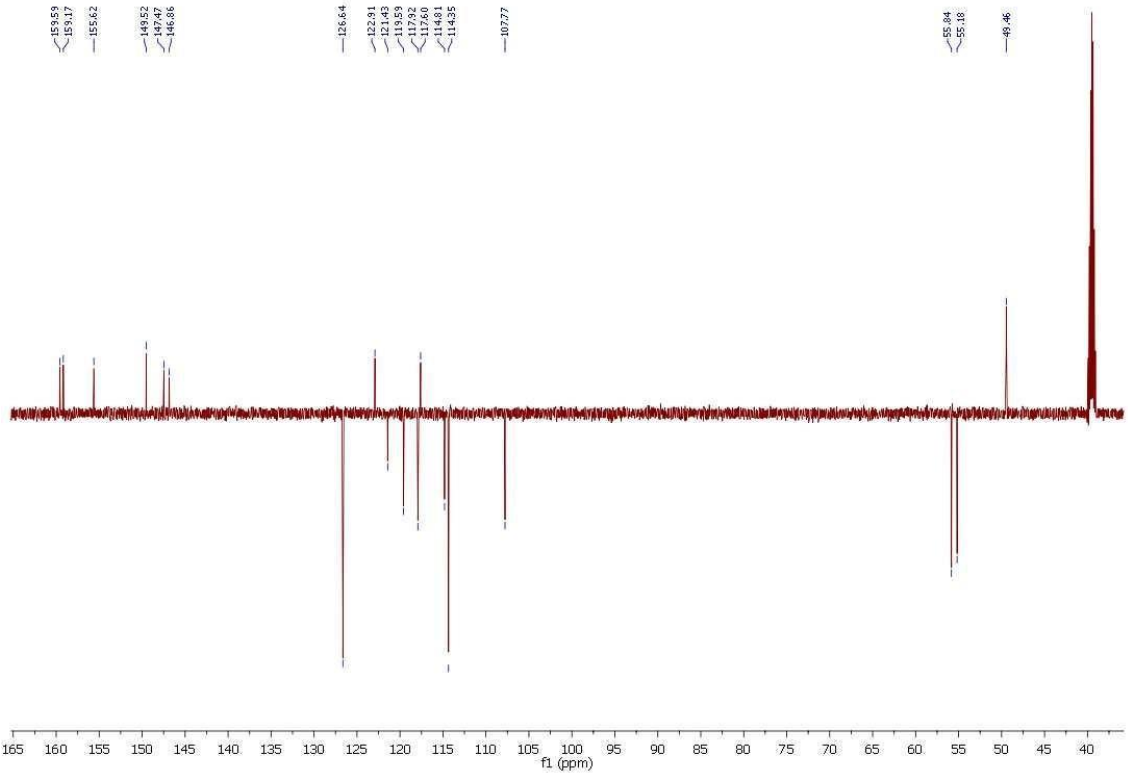

x10 2
1
0.8
0.6
0.4
0.2
0
334.10000
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S15 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **17b**

a)



b)



c)

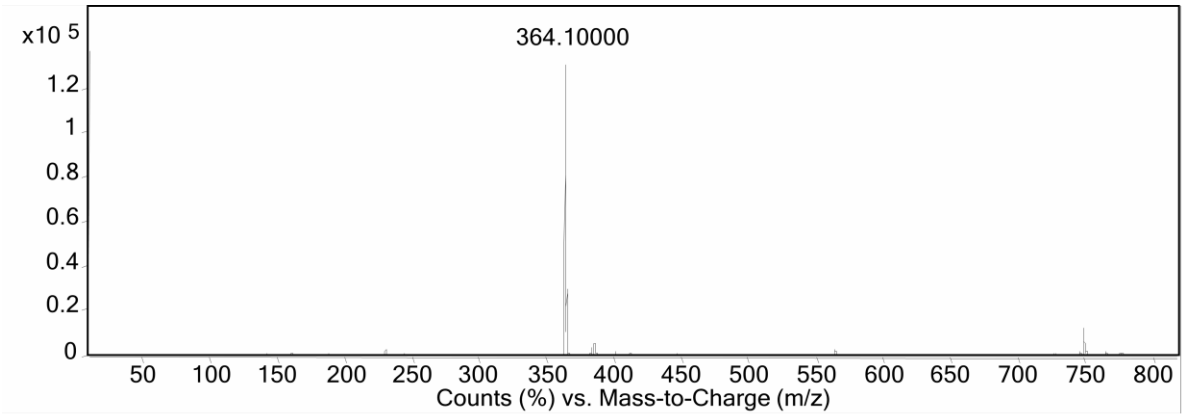
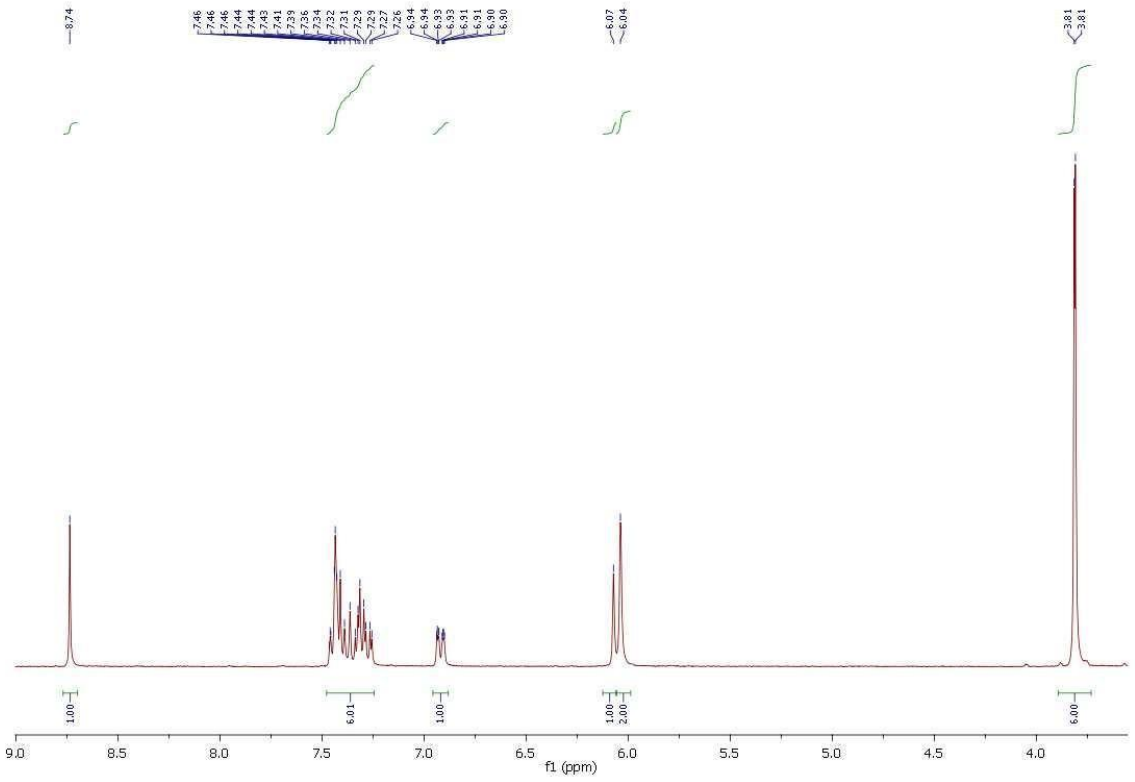


Fig. S16 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **17c**

a)



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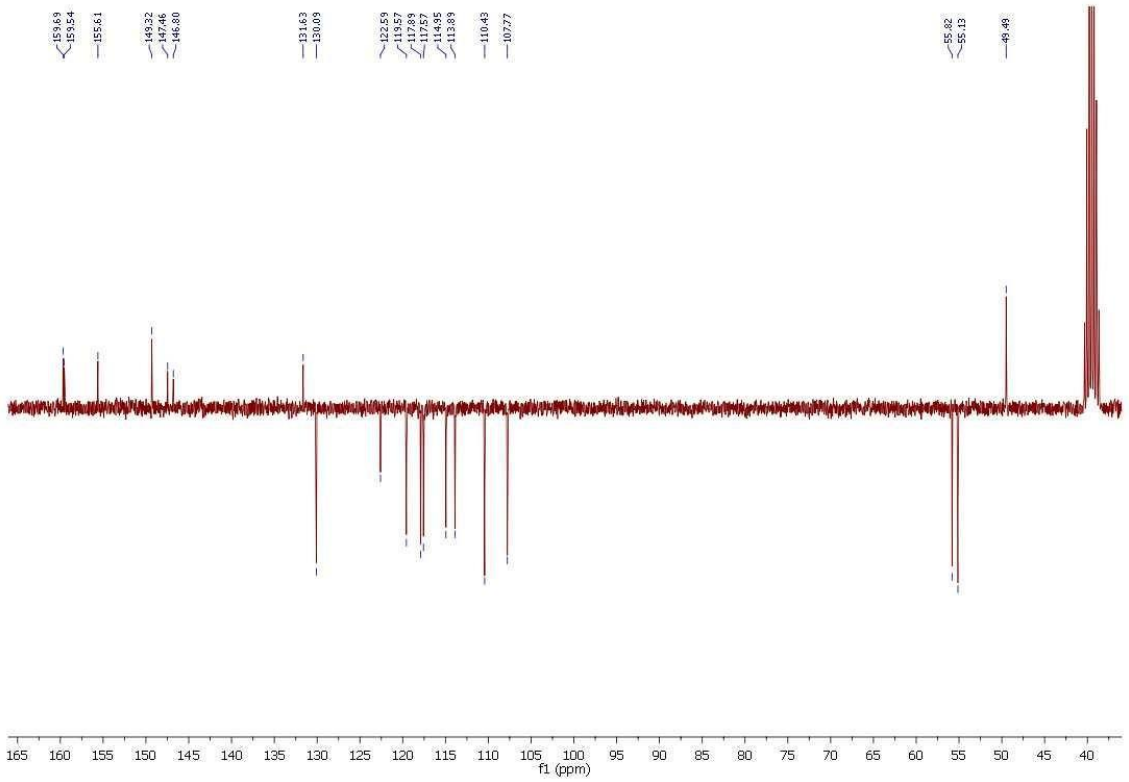

159.69
159.54
155.61
149.32
147.46
146.80
131.63
130.09
122.59
119.57
117.89
117.57
114.95
113.89
110.43
107.77
55.82
55.13
49.49
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

c)

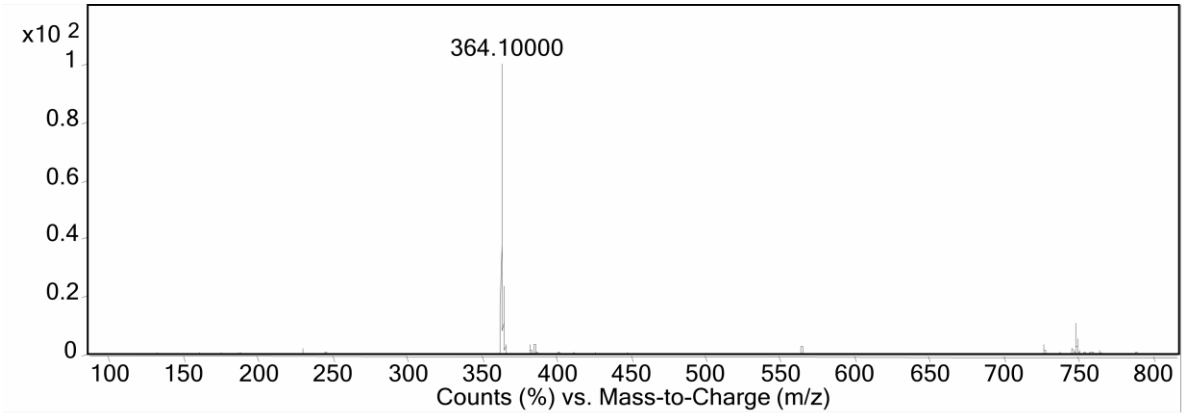
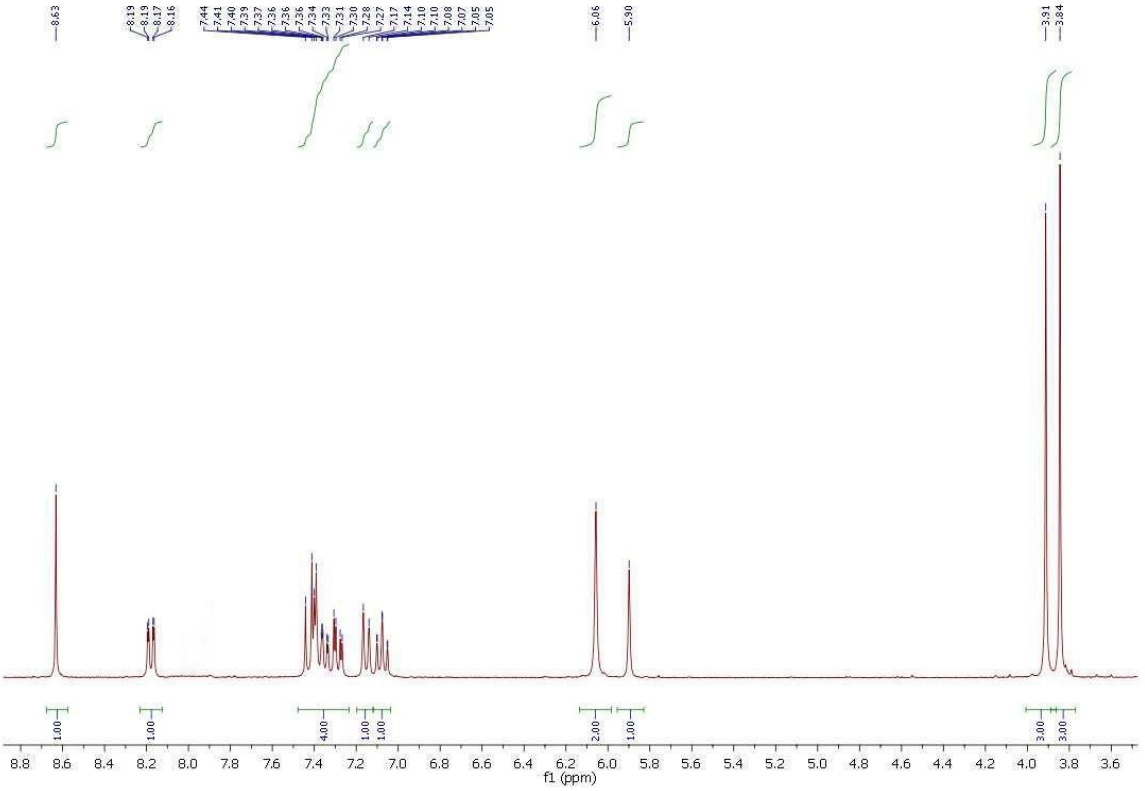
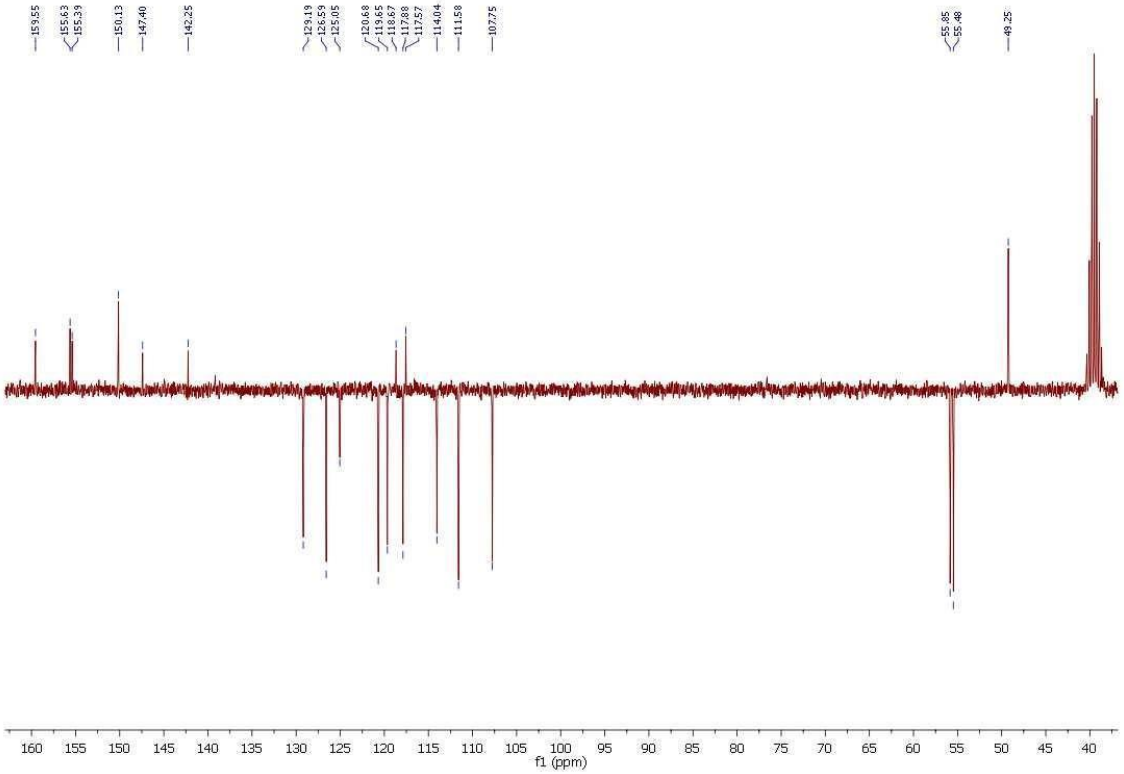

x10 2
1
0.8
0.6
0.4
0.2
0
364.10000
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S17 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **17d**

a)



b)



c)

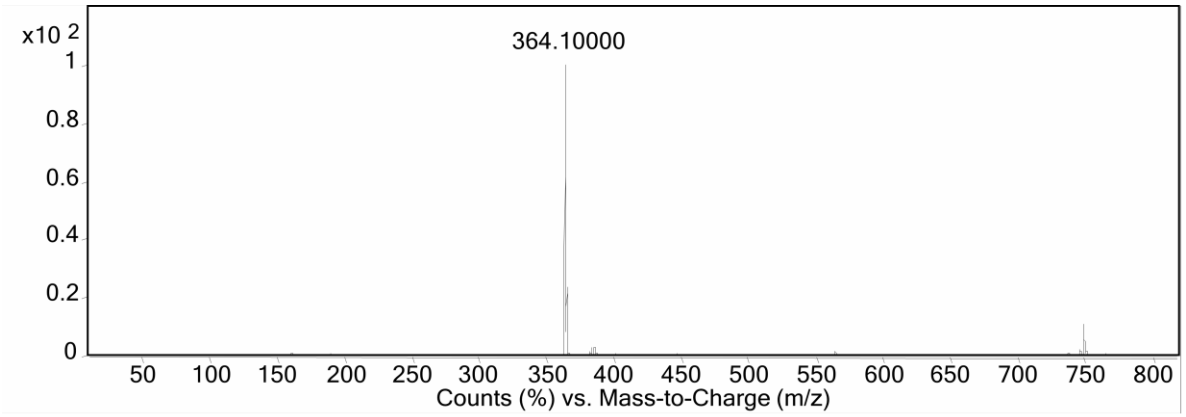
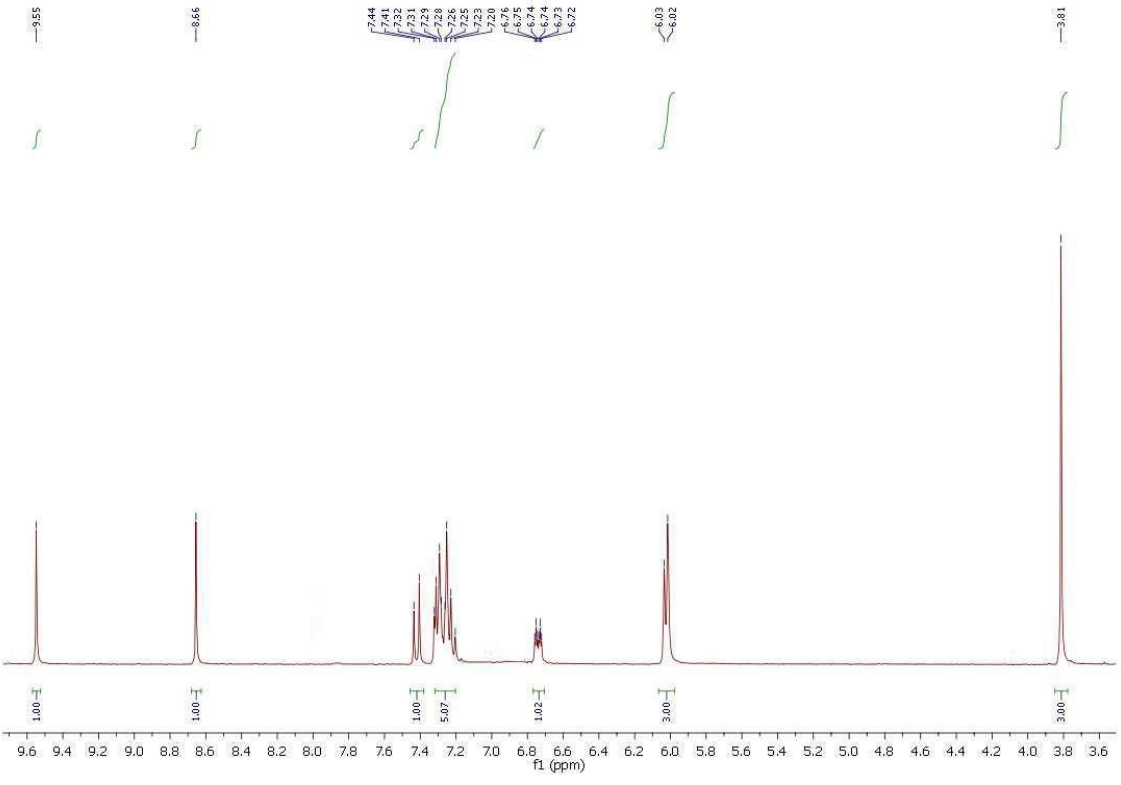
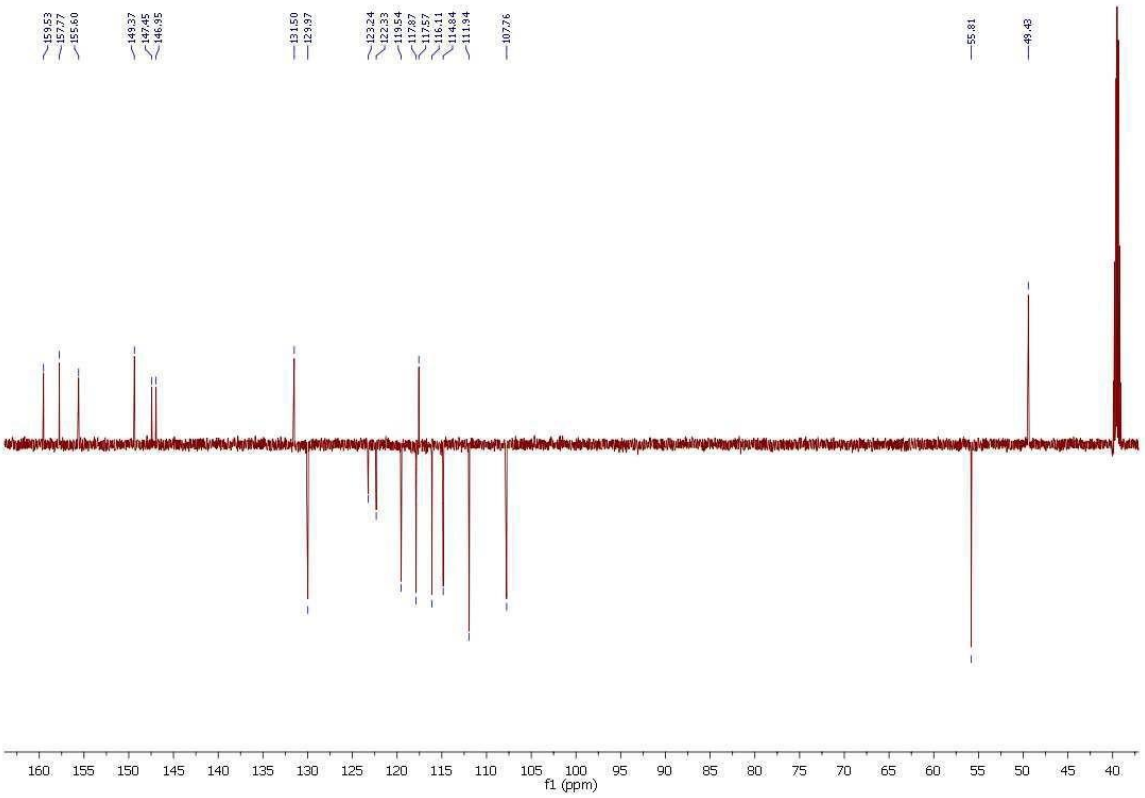


Fig. S18 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **17e**

a)



b)


159.53
157.77
155.60
149.37
147.45
146.95
131.50
129.97
123.24
122.33
119.54
117.87
117.57
116.11
114.84
111.94
107.76
55.81
49.48
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

c)

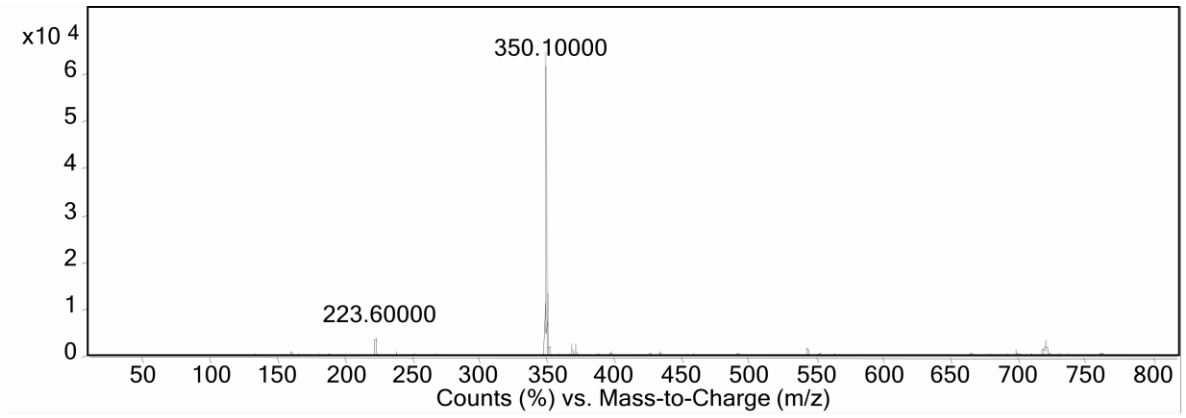
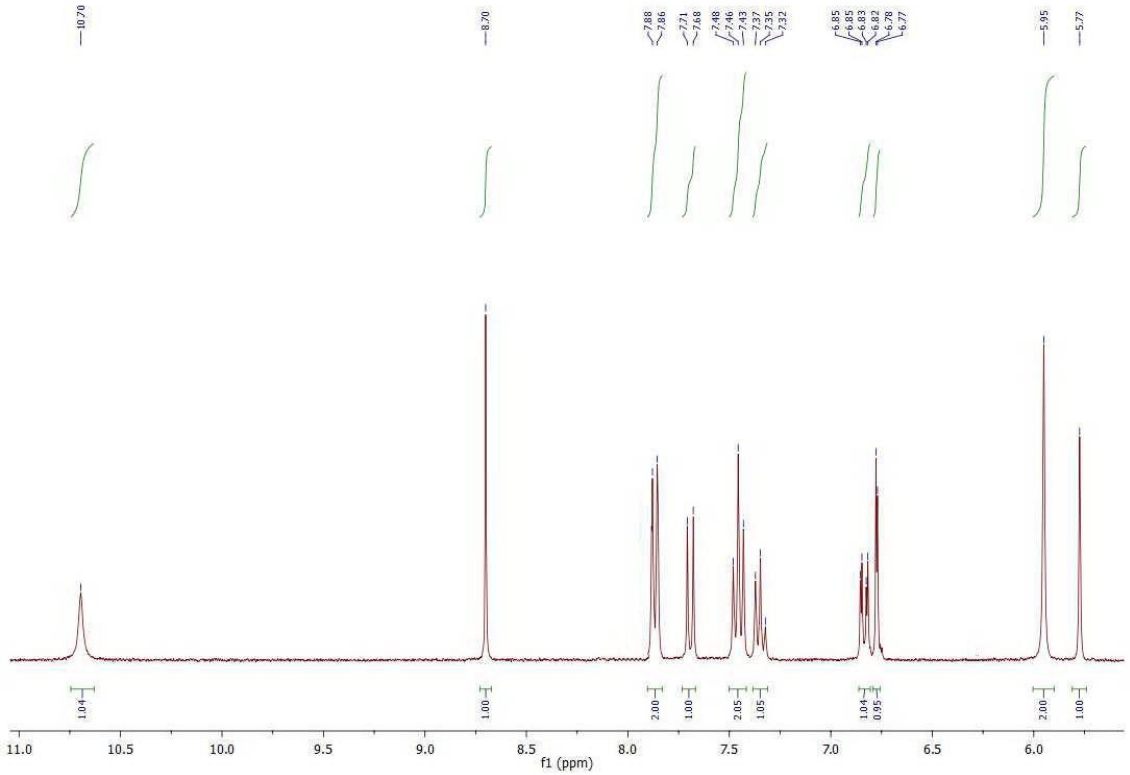
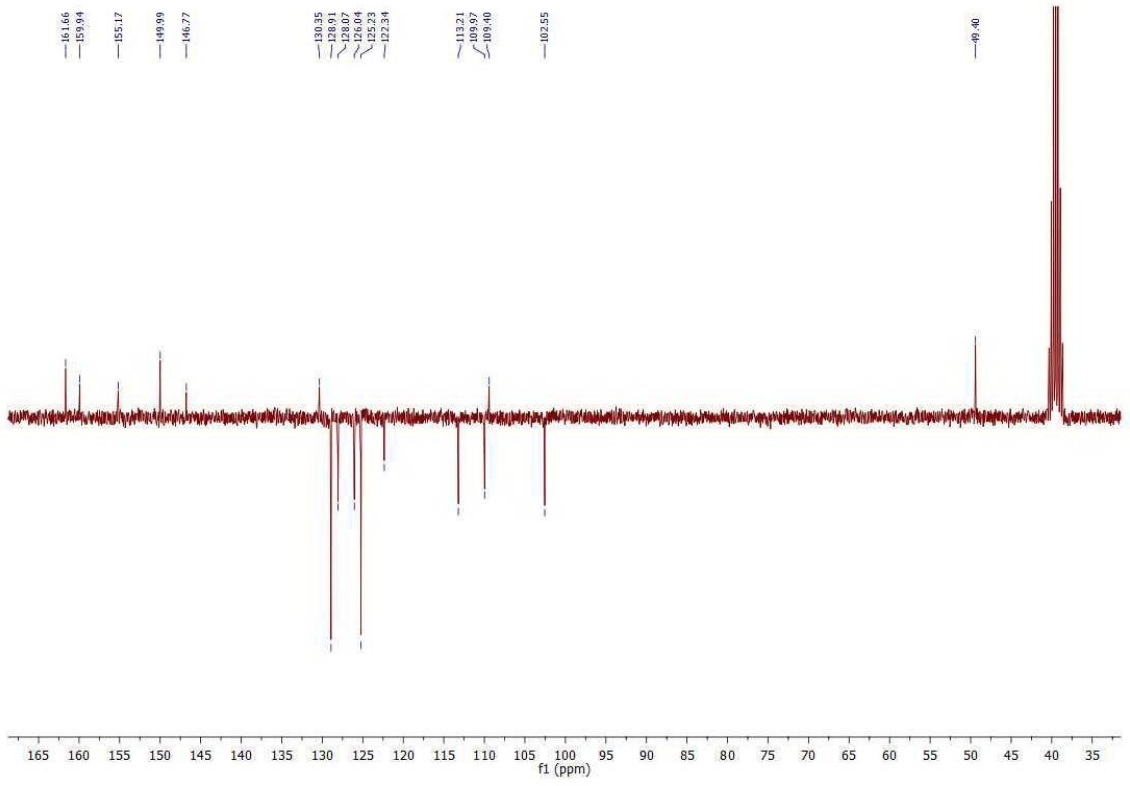

x10 4
6
5
4
3
2
1
0
350.10000
223.60000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S19 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **18a**

a)



b)



c)

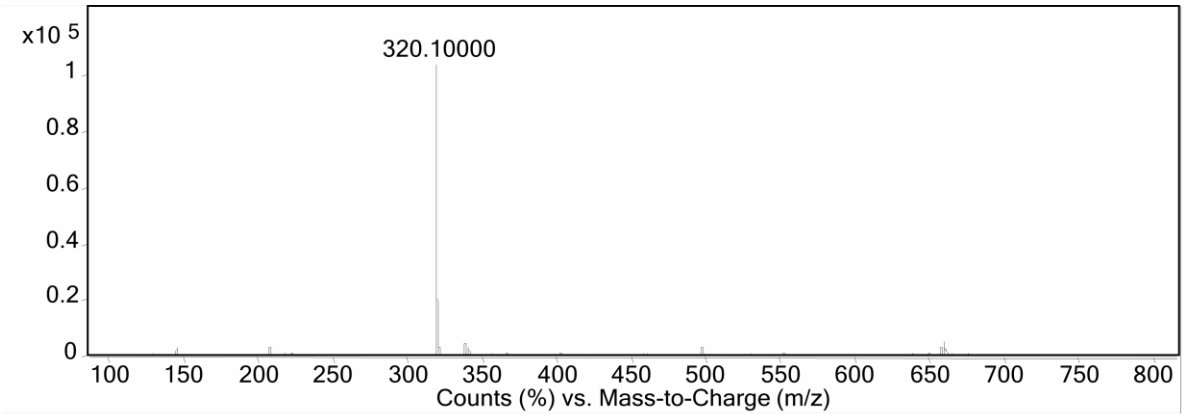
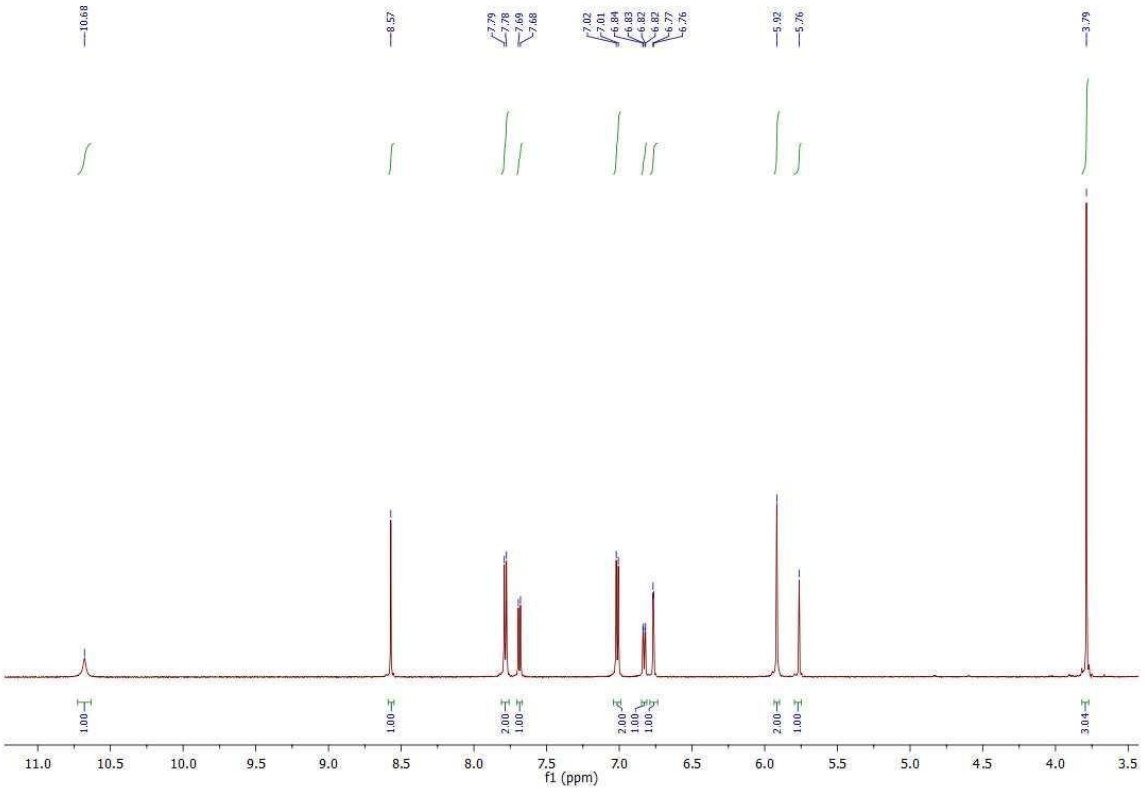
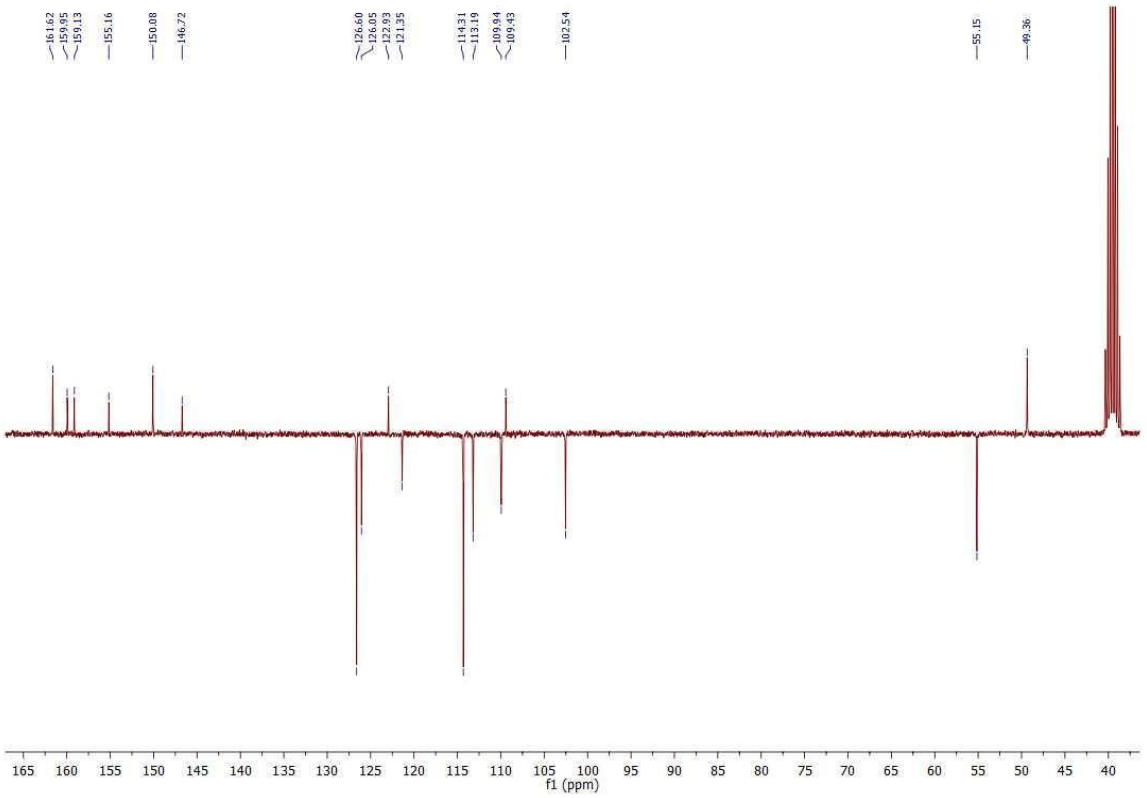


Fig. S20 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **18b**

a)



b)


161.62
159.95
159.13
155.16
150.08
146.72
126.60
126.05
122.93
121.35
114.31
113.19
109.94
109.43
102.54
55.15
49.36
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

c)

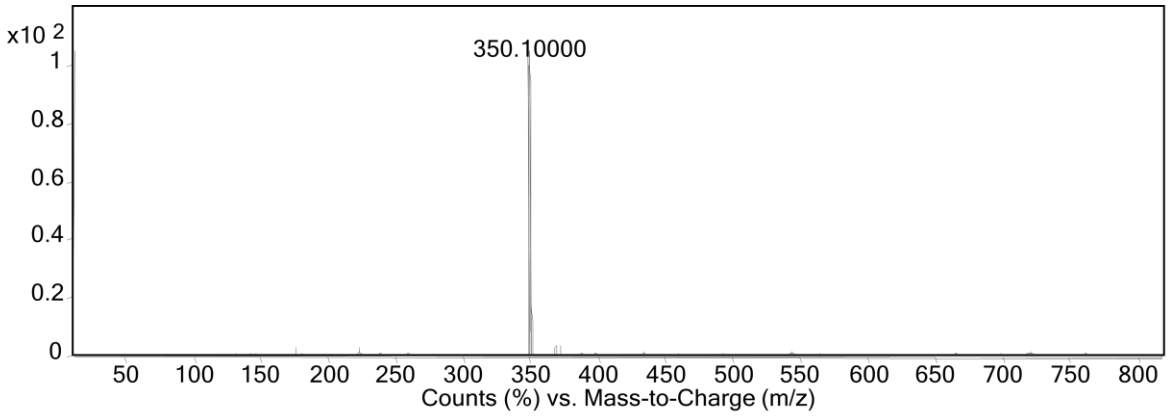
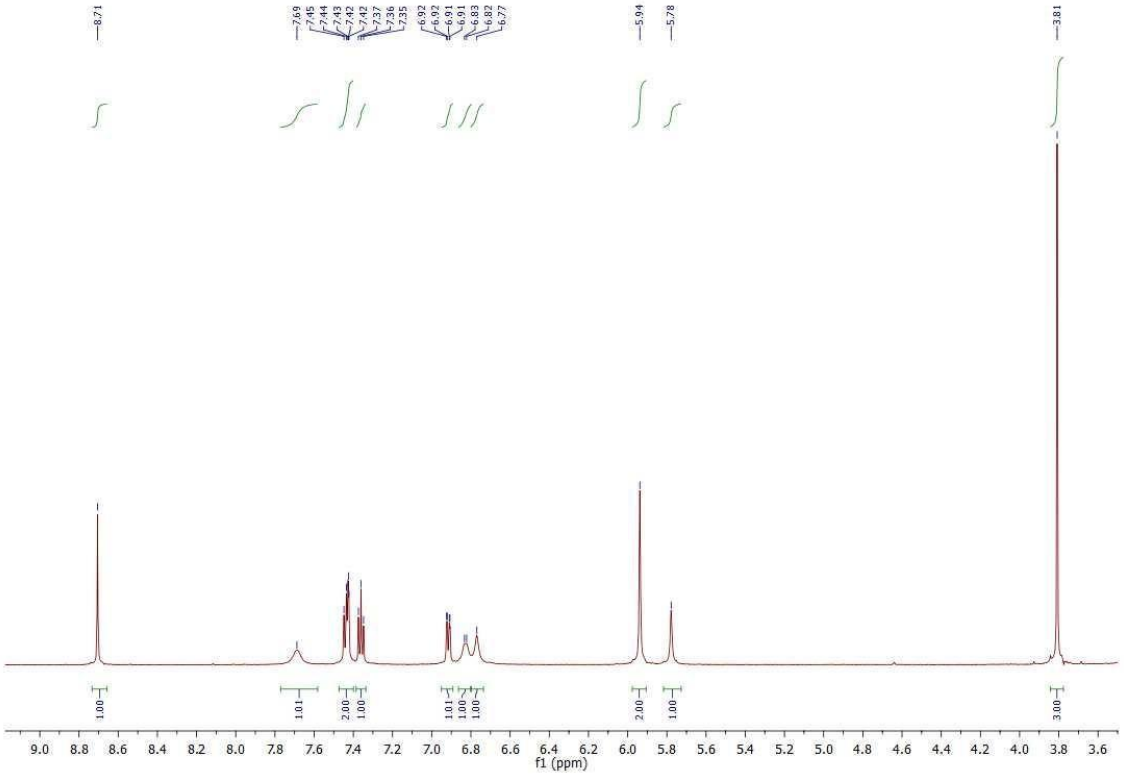
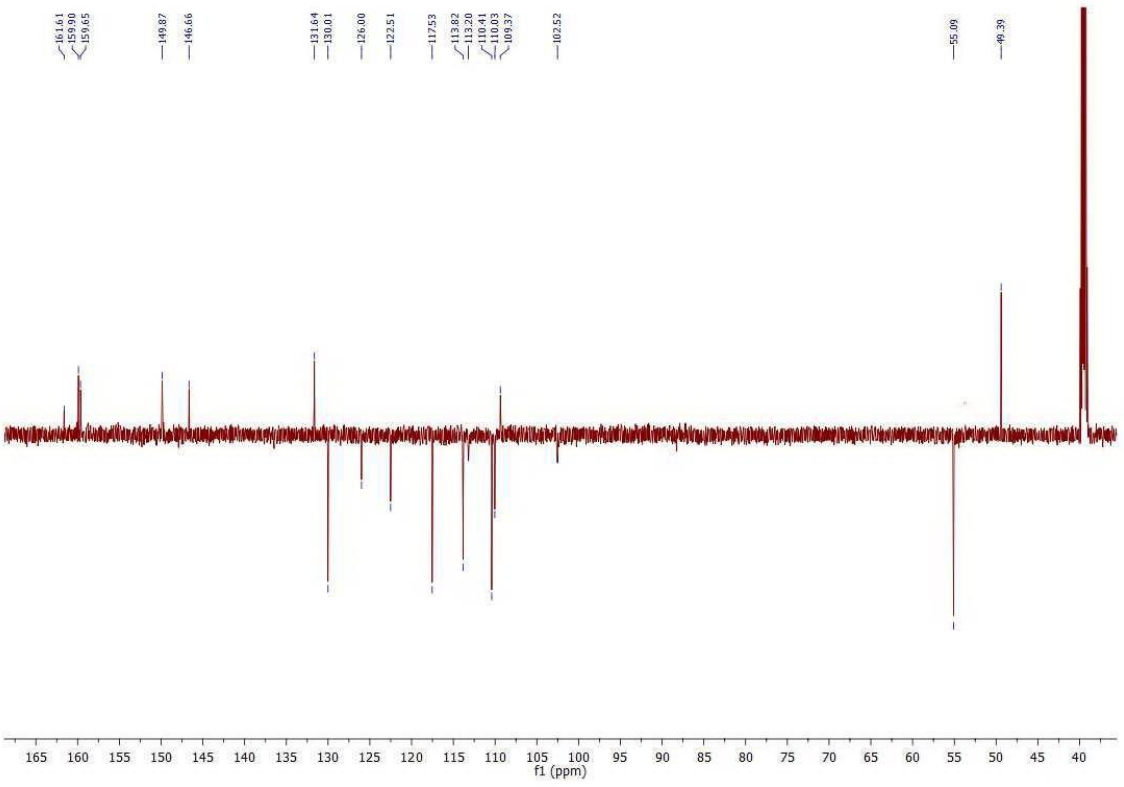

x10 2
1
0.8
0.6
0.4
0.2
0
350.10000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S21 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **18c**

a)



b)



c)

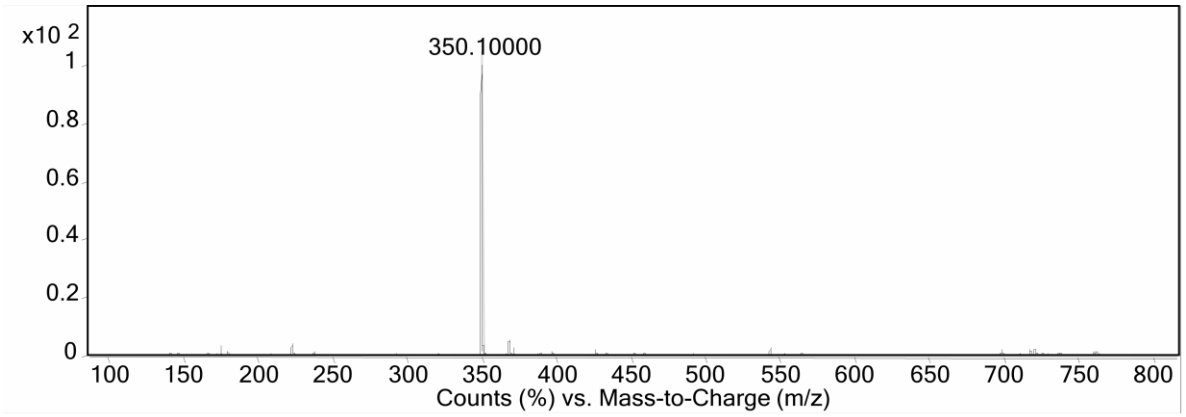
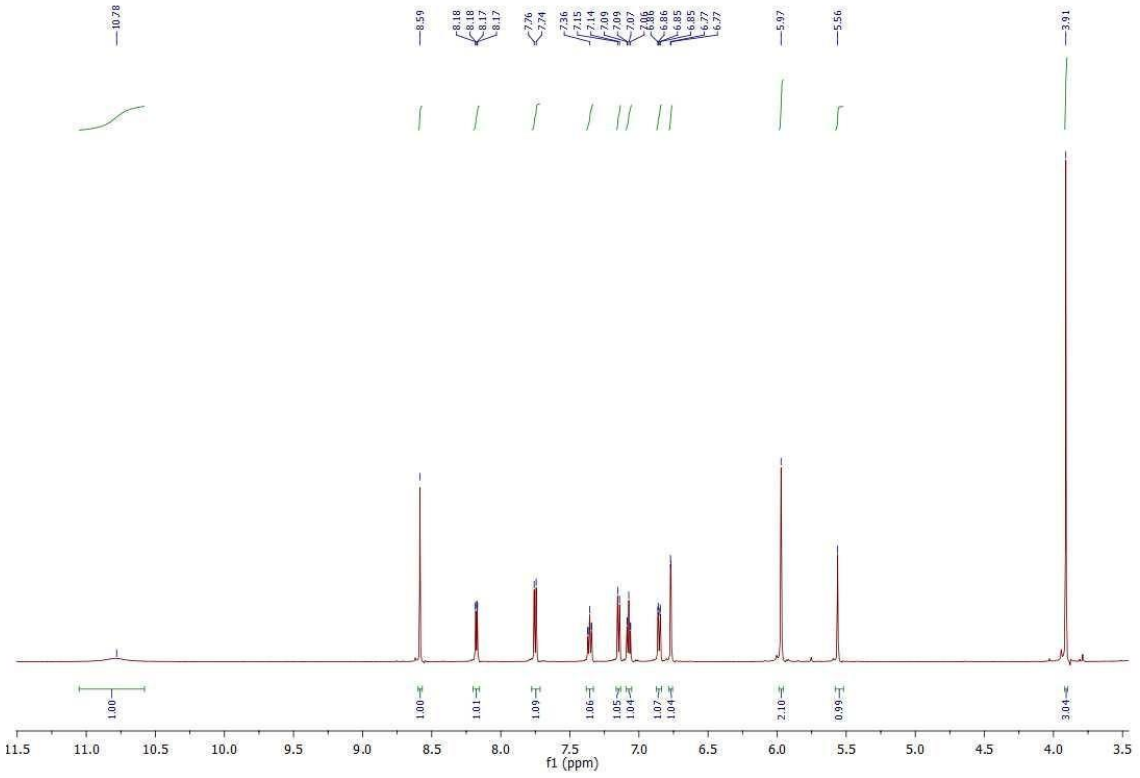
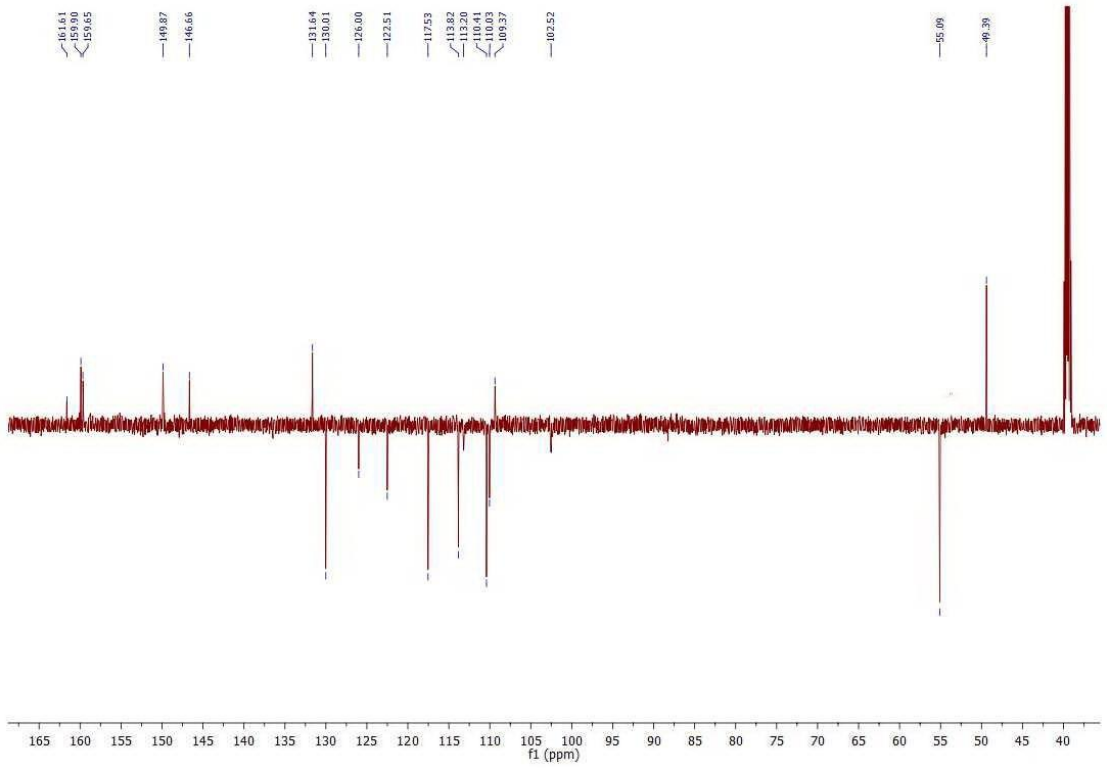


Fig. S22 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **18d**

a)



b)


161.61
159.90
159.65
149.87
146.66
131.64
130.01
126.00
122.51
117.53
113.82
113.20
110.41
110.03
105.37
102.52
55.09
49.39
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

c)

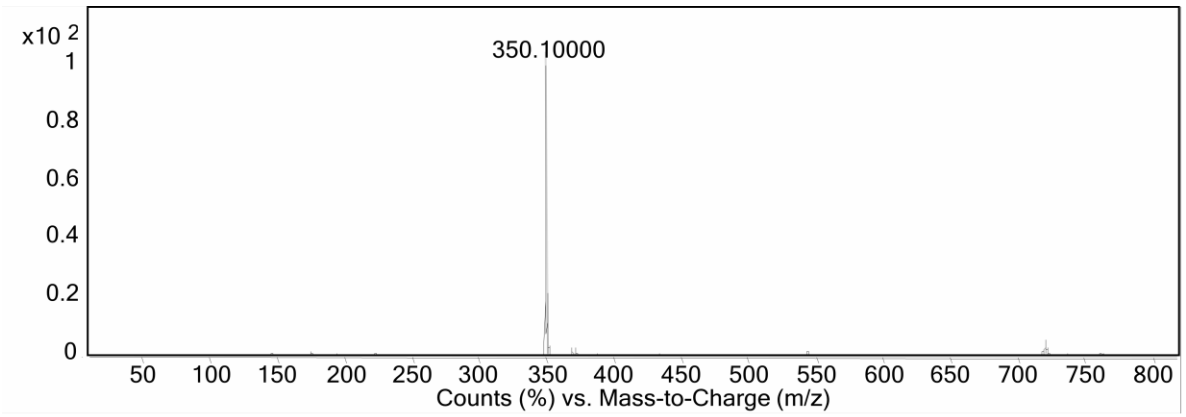
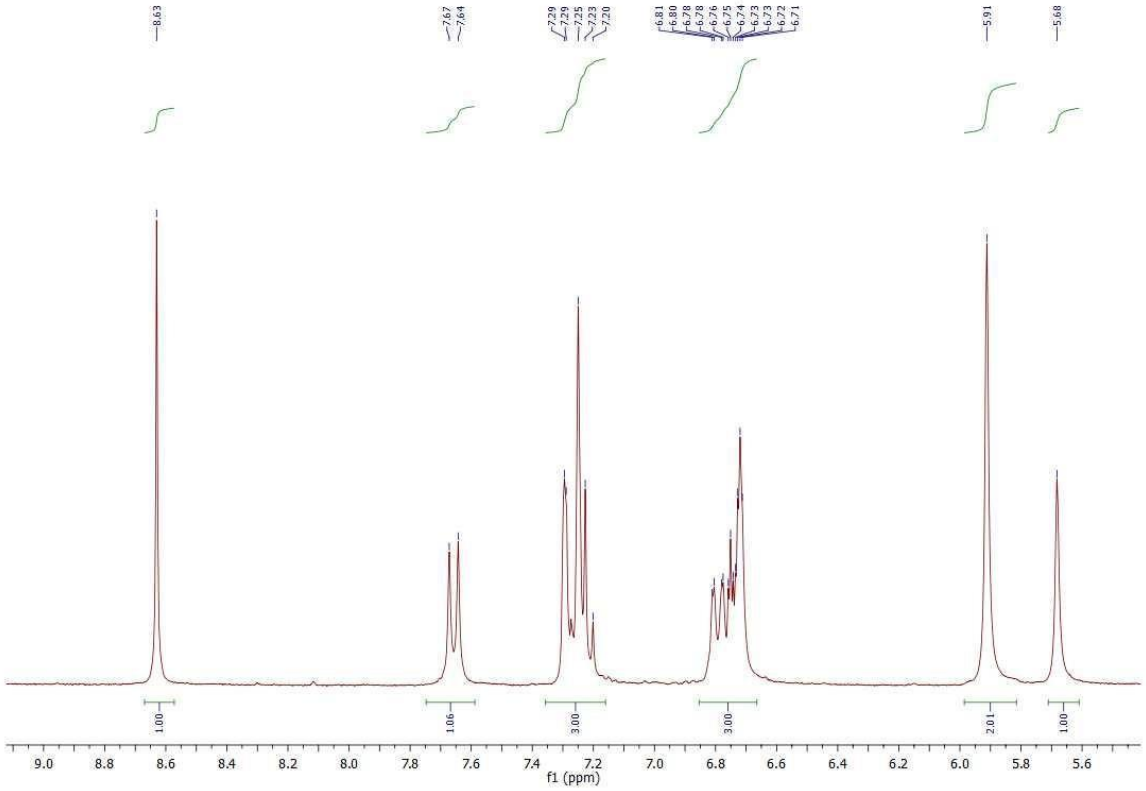
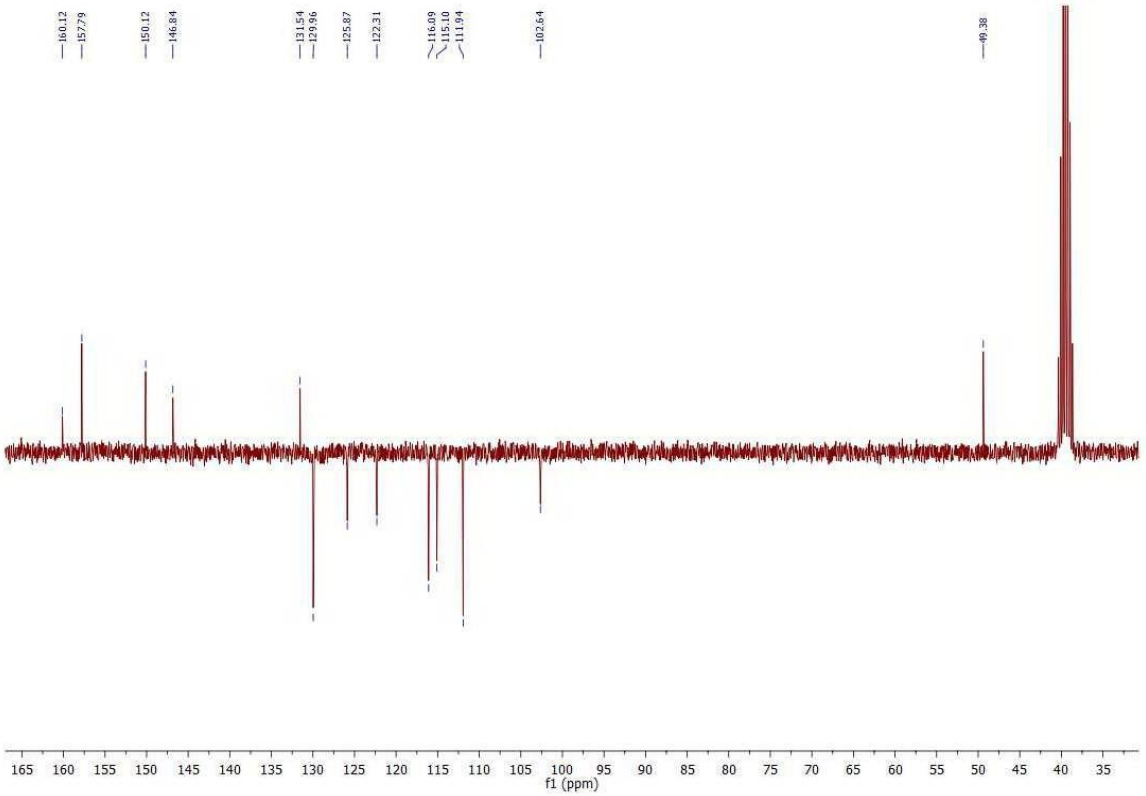

x10 2
1
0.8
0.6
0.4
0.2
0
350.10000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S23 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **18e**

a)



b)



c)

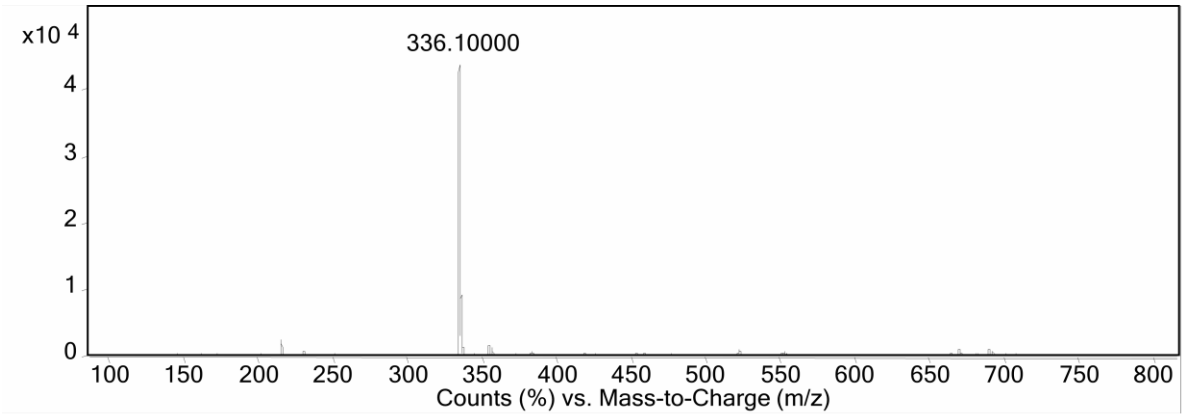
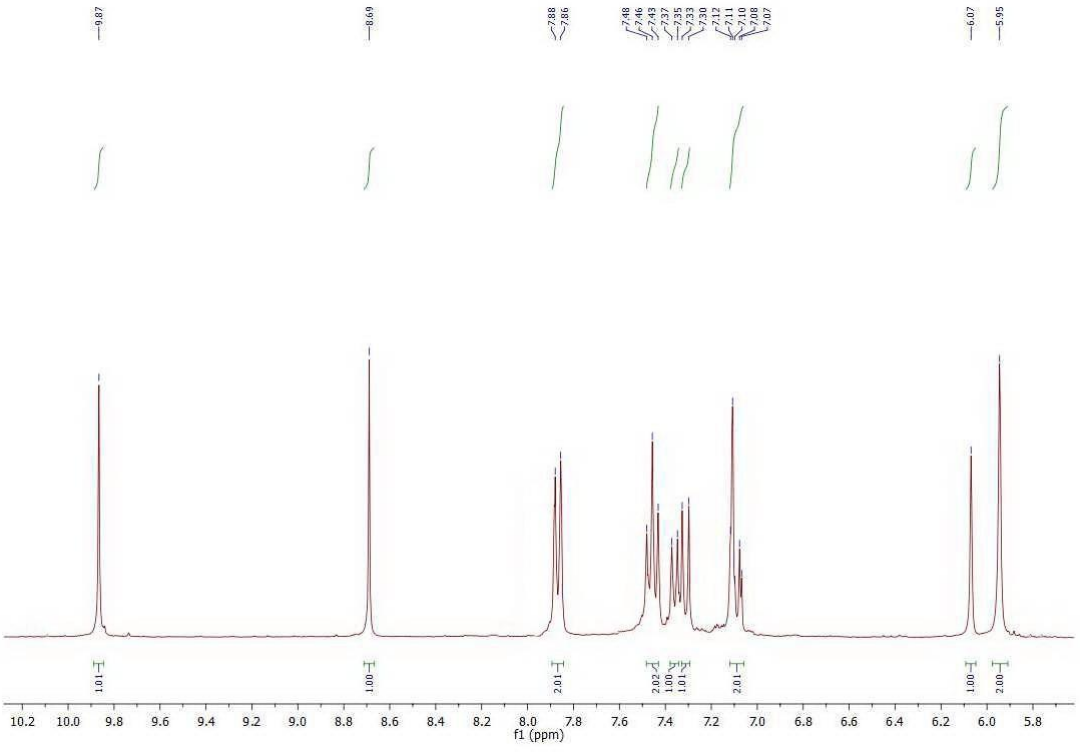
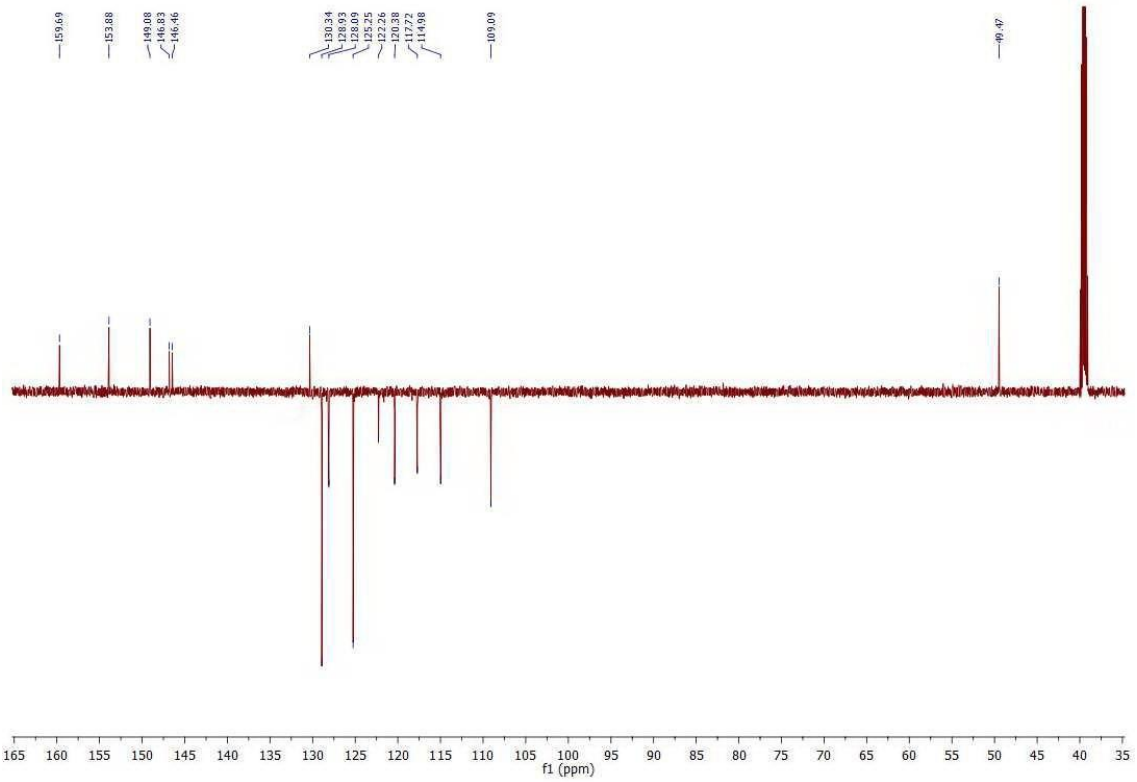


Fig. S24 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **19a**

a)



b)


159.69
153.88
149.08
146.83
146.46
130.34
128.93
128.09
125.25
122.26
120.38
117.72
114.98
109.09
49.47
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

c)

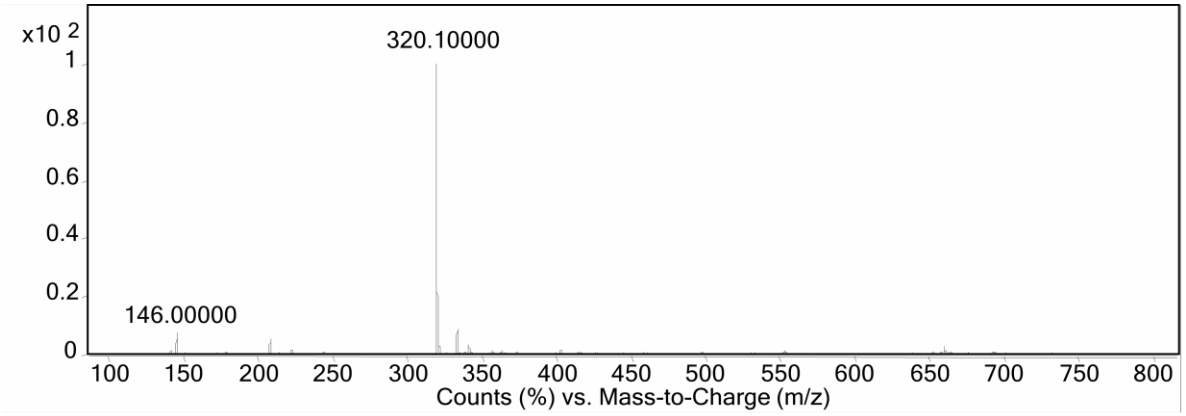
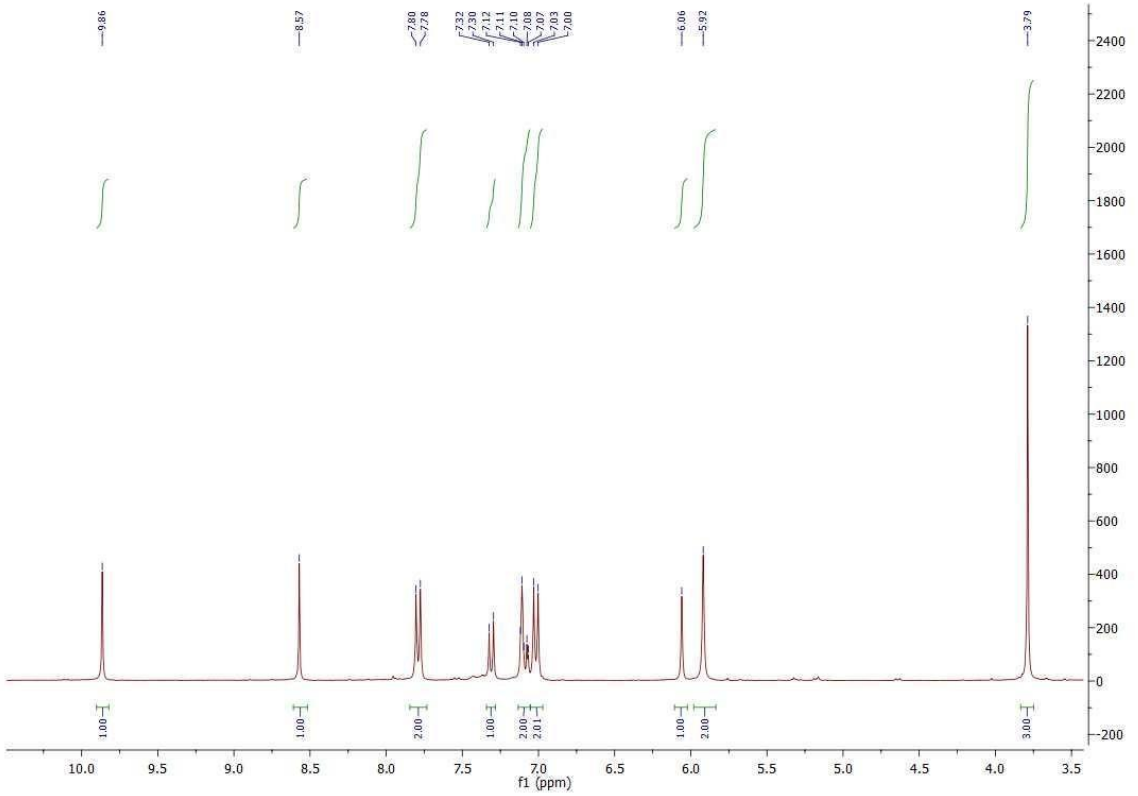
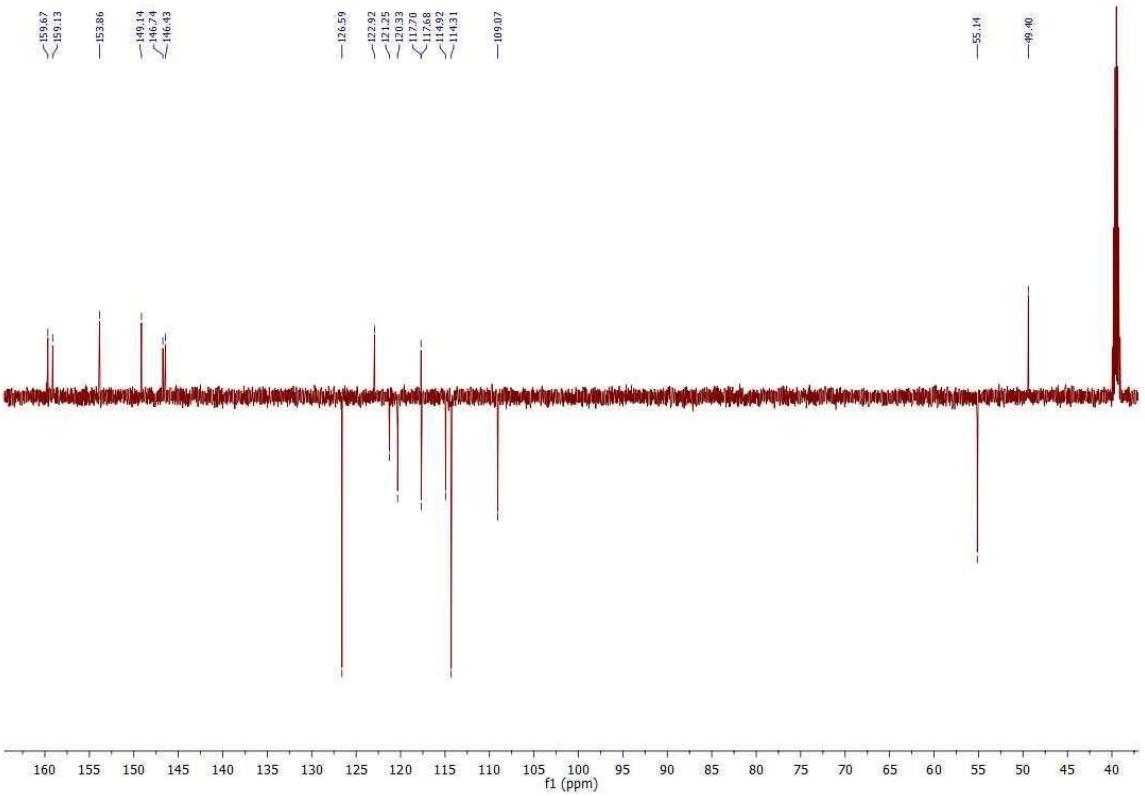

x10 2
1
0.8
0.6
0.4
0.2
0
320.10000
146.00000
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S25 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **19b**

a)



b)



c)

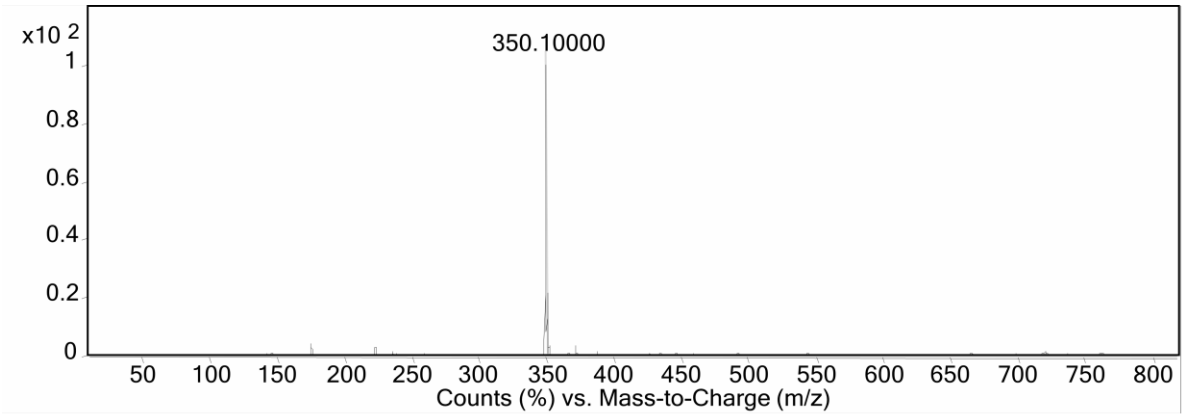
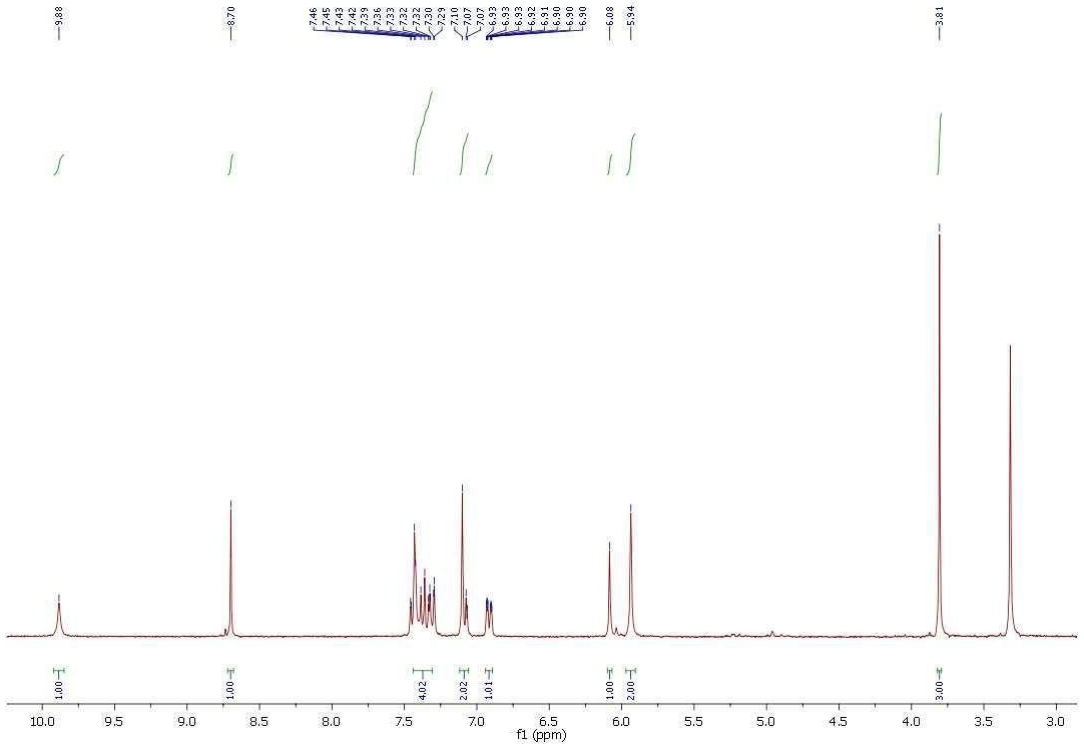
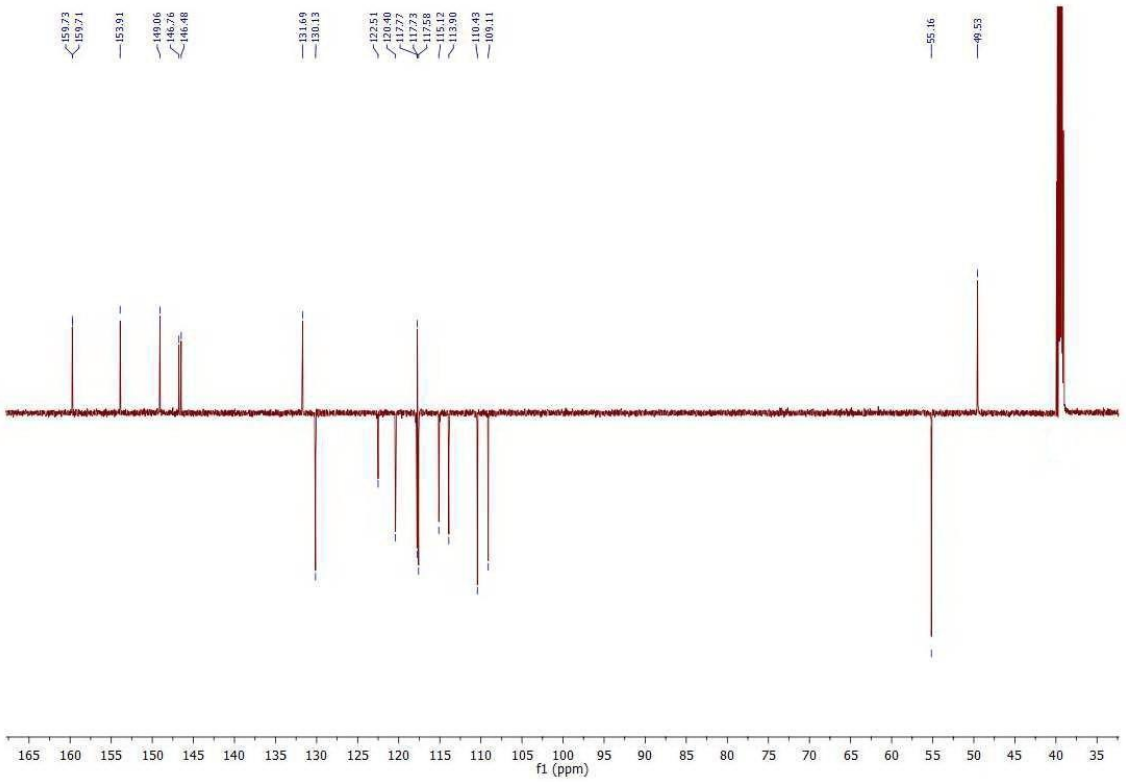


Fig. S26 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **19c**

a)



b)


159.73
159.71
153.91
149.06
146.76
146.48
131.69
130.13
122.51
120.40
117.77
117.73
117.58
115.12
113.90
110.43
109.11
55.16
49.53
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

c)

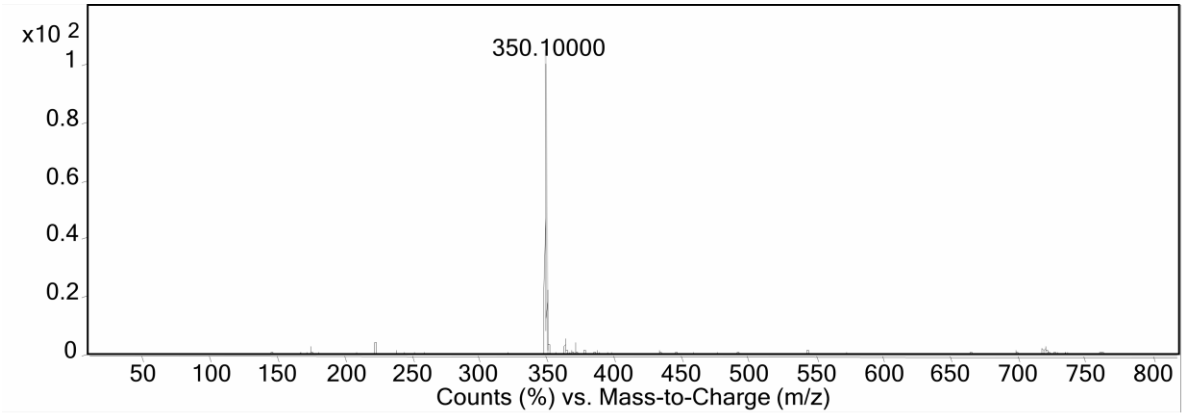
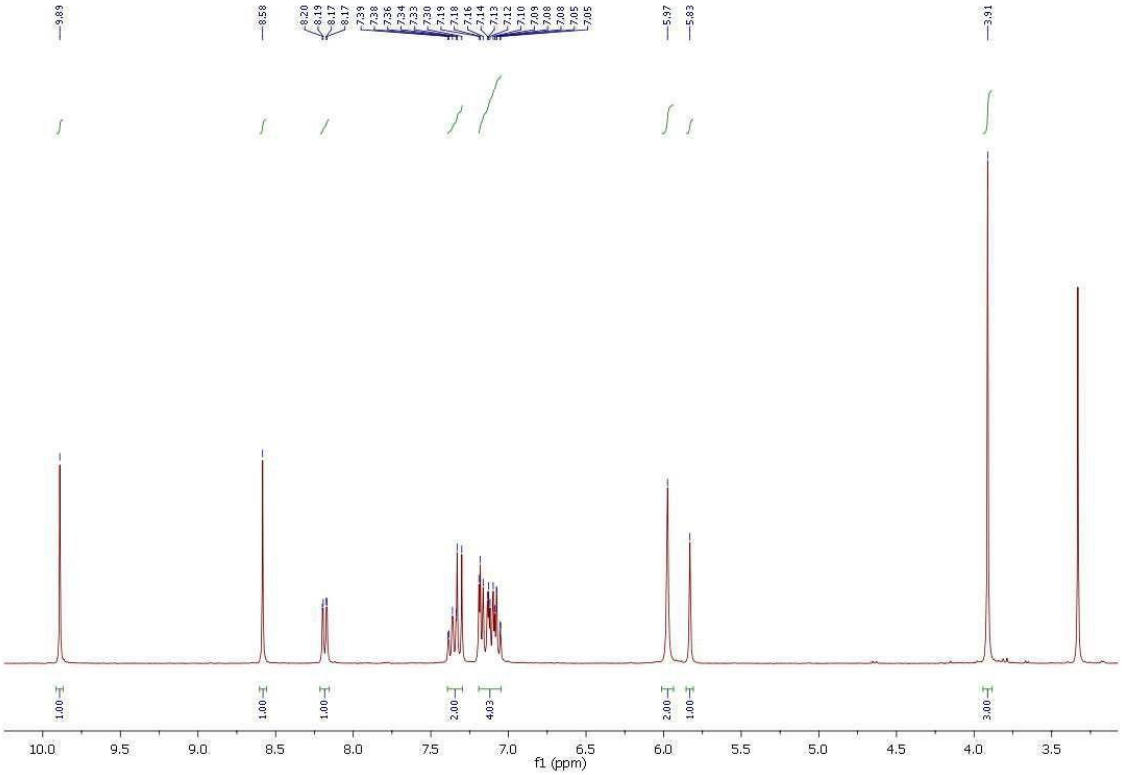
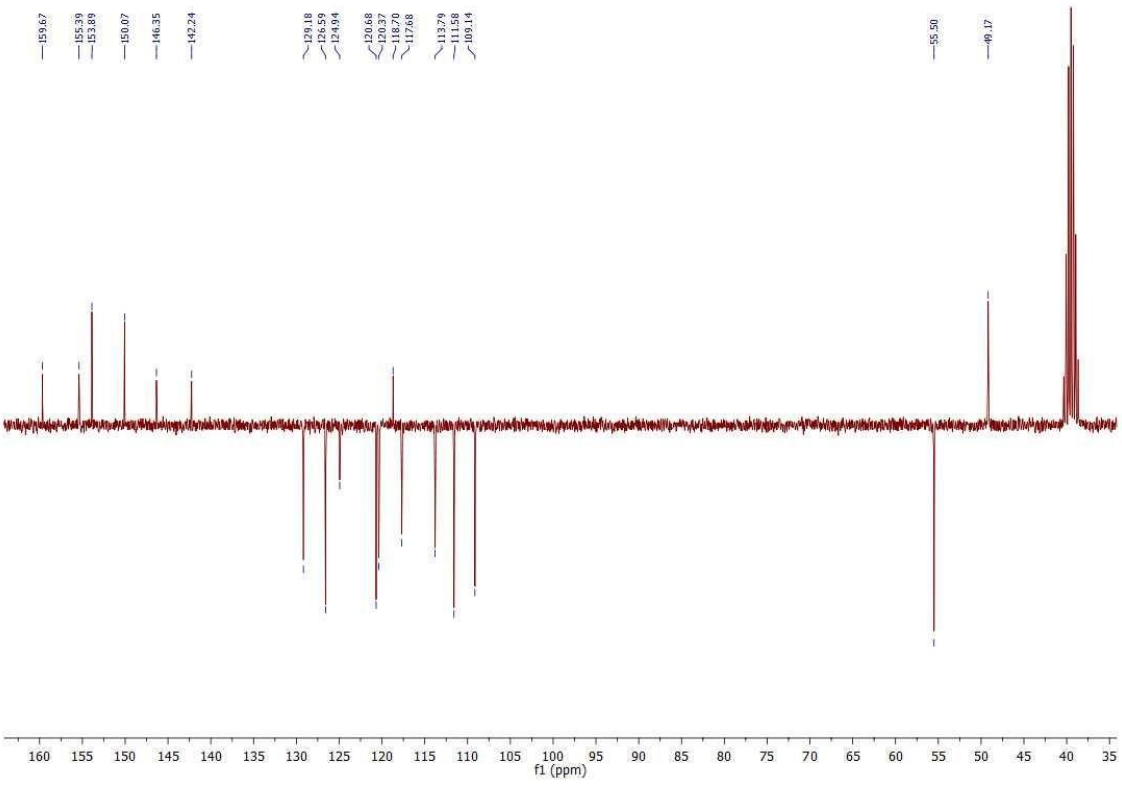

x10 2
1
0.8
0.6
0.4
0.2
0
350.10000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S27 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **19d**

a)



b)



c)

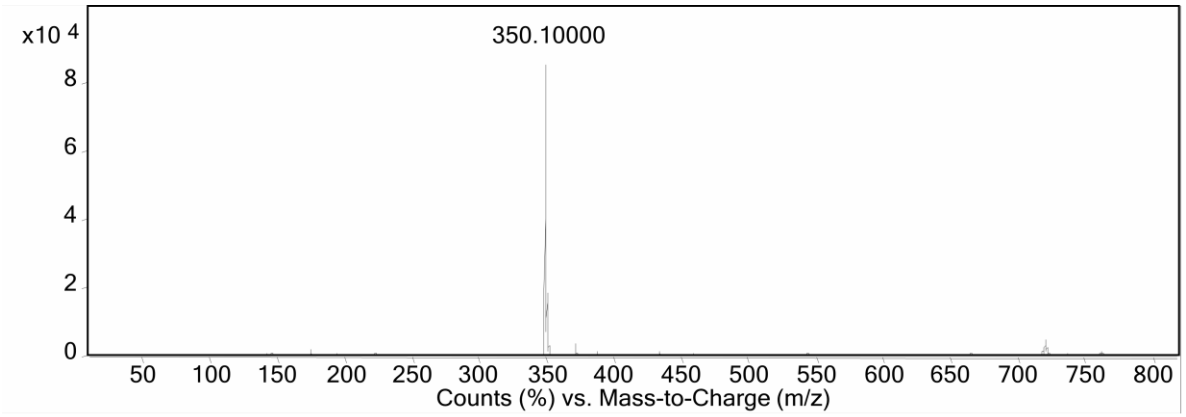
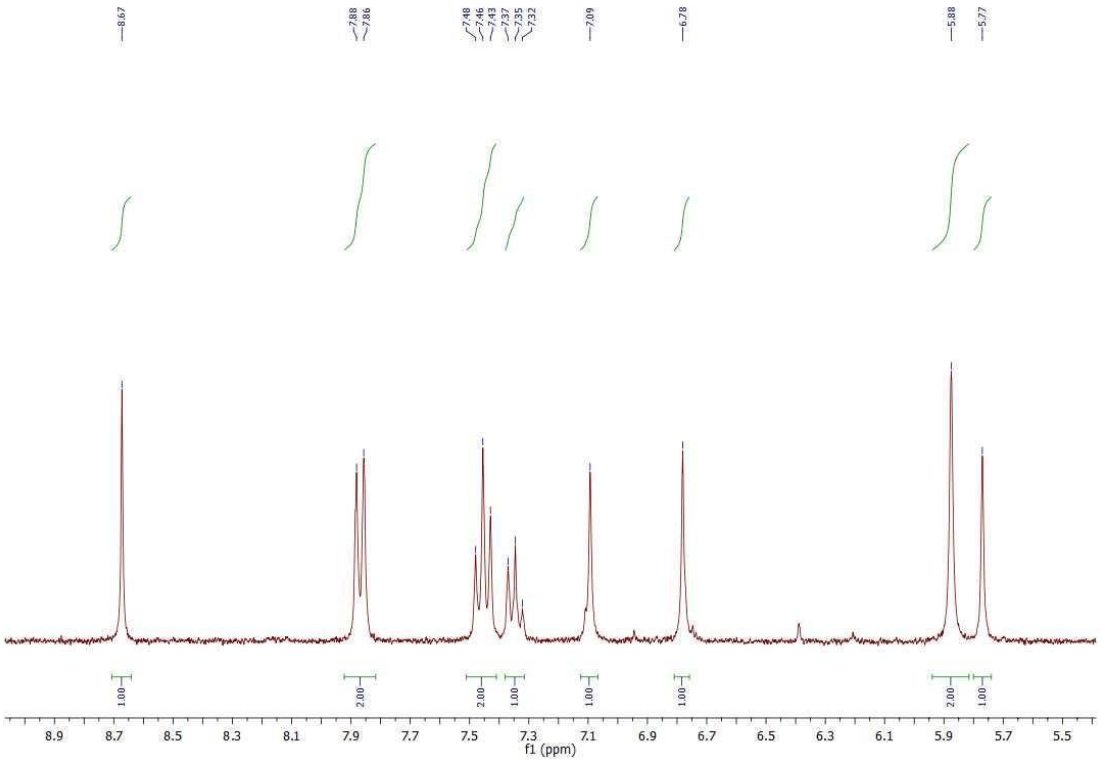
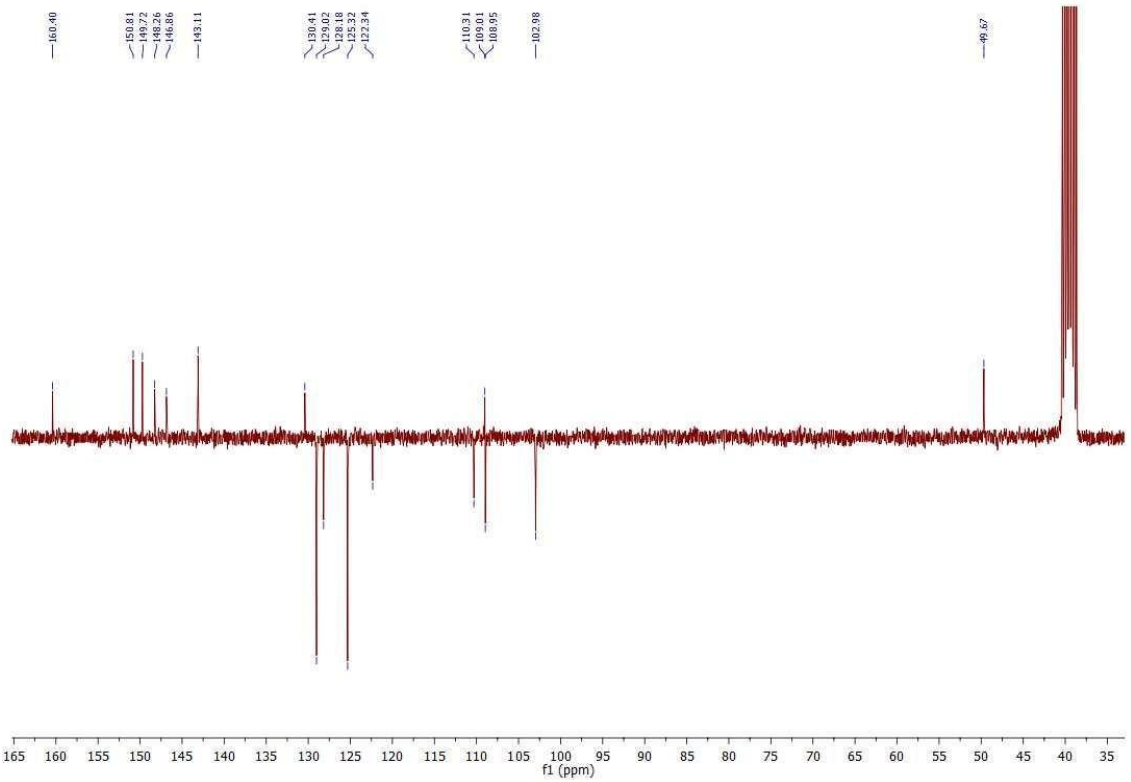


Fig. S28 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **20a**

a)



b)


160.40
150.81
149.72
148.26
146.86
143.11
130.41
129.02
126.18
125.32
122.34
110.31
109.01
108.95
102.98
49.67
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

c)

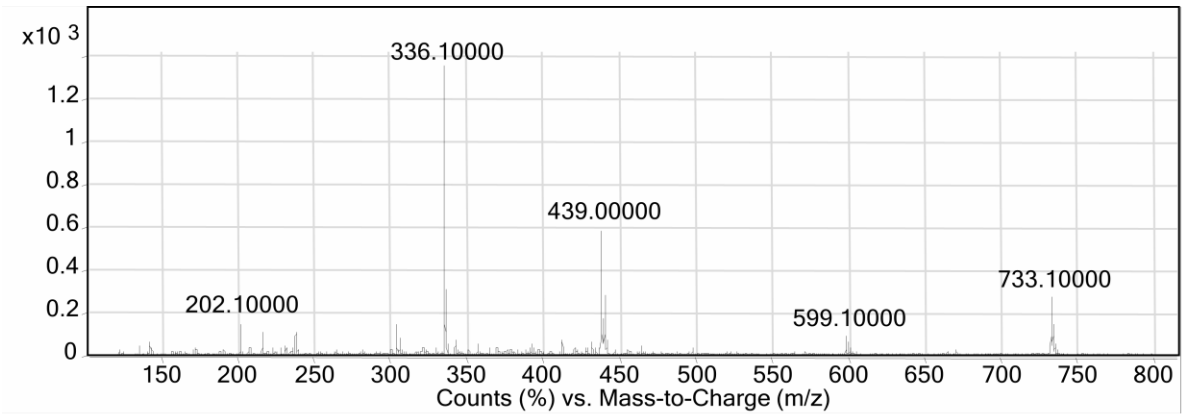
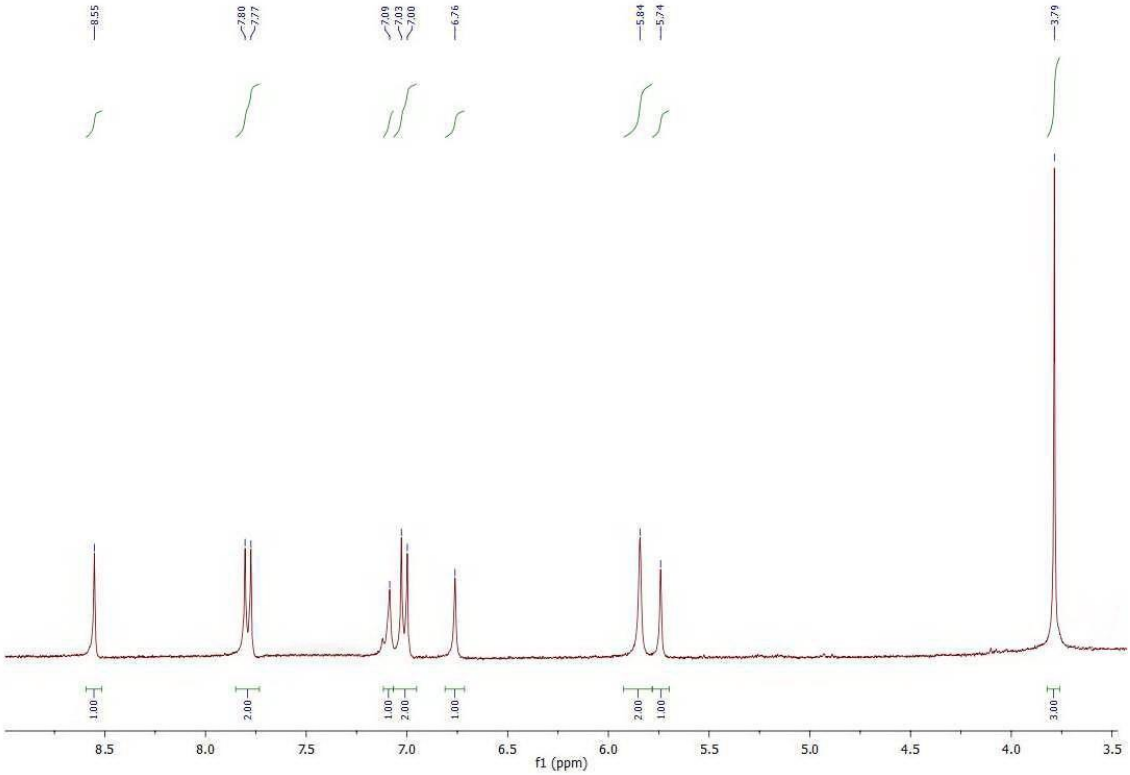
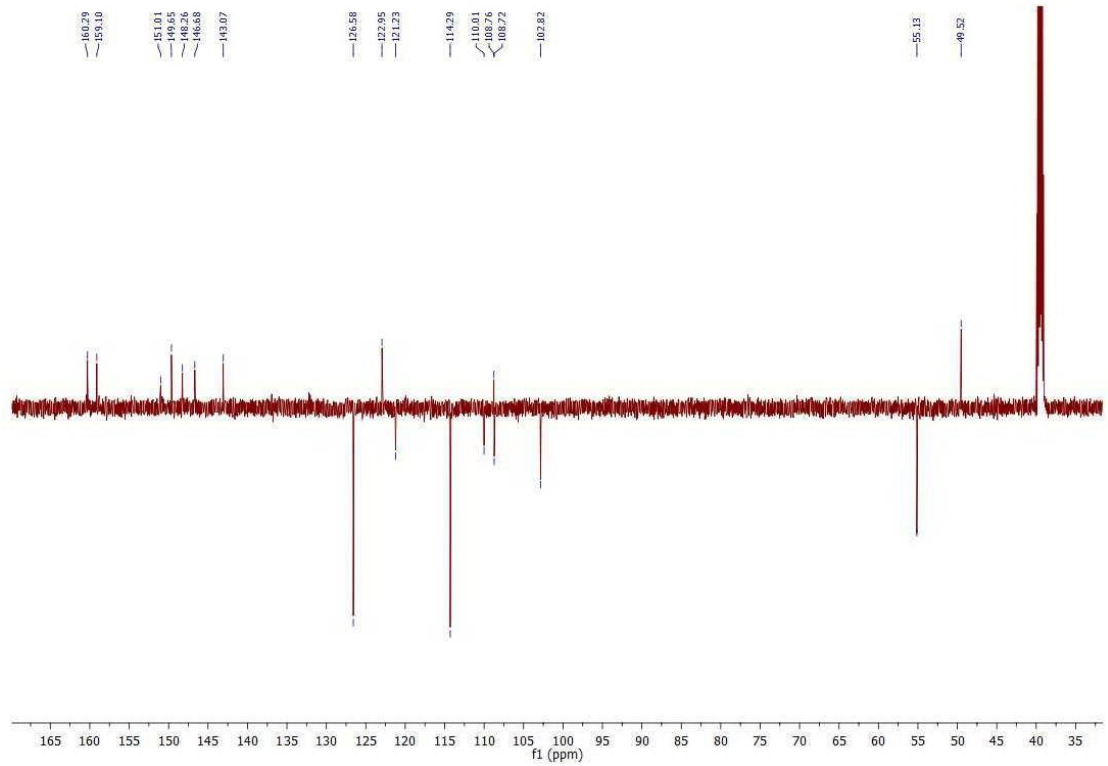

x10 3
1.2
1
0.8
0.6
0.4
0.2
0
336.10000
439.00000
202.10000
599.10000
733.10000
150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S29 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **20b**

a)



b)



c)

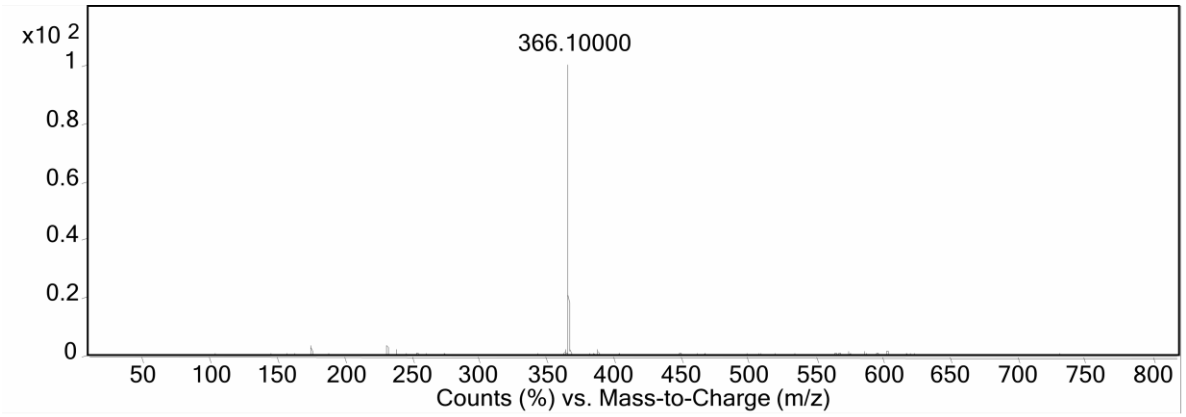
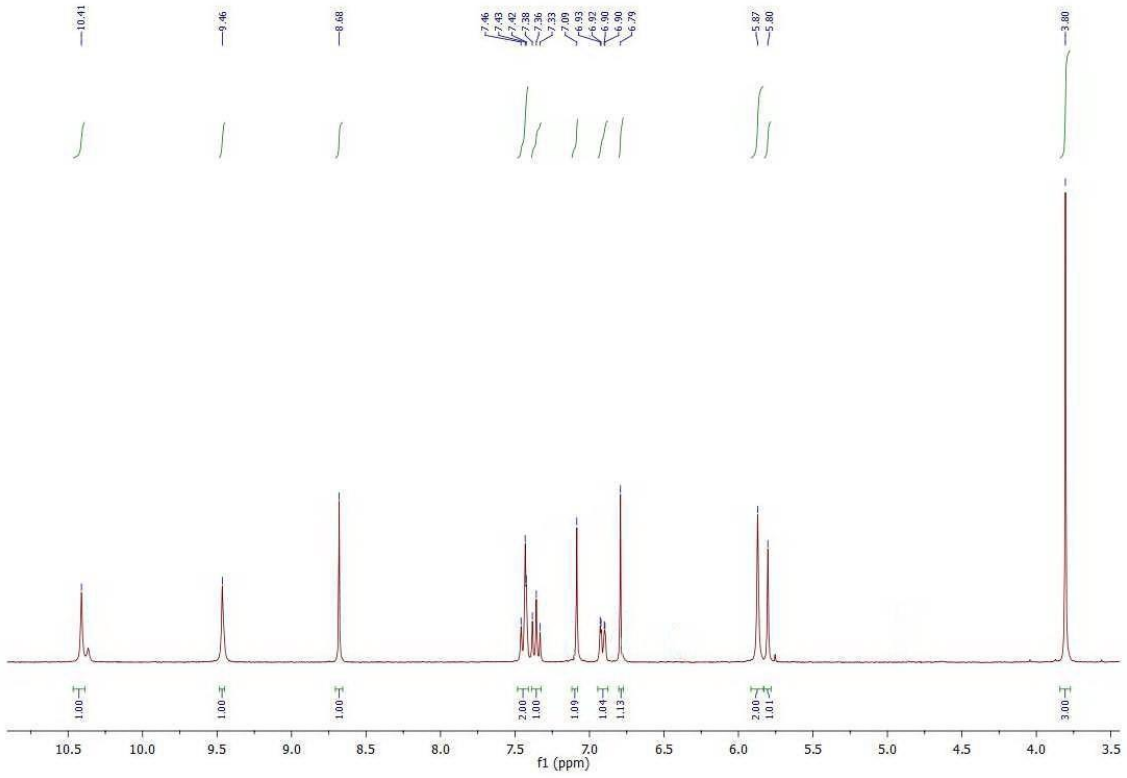
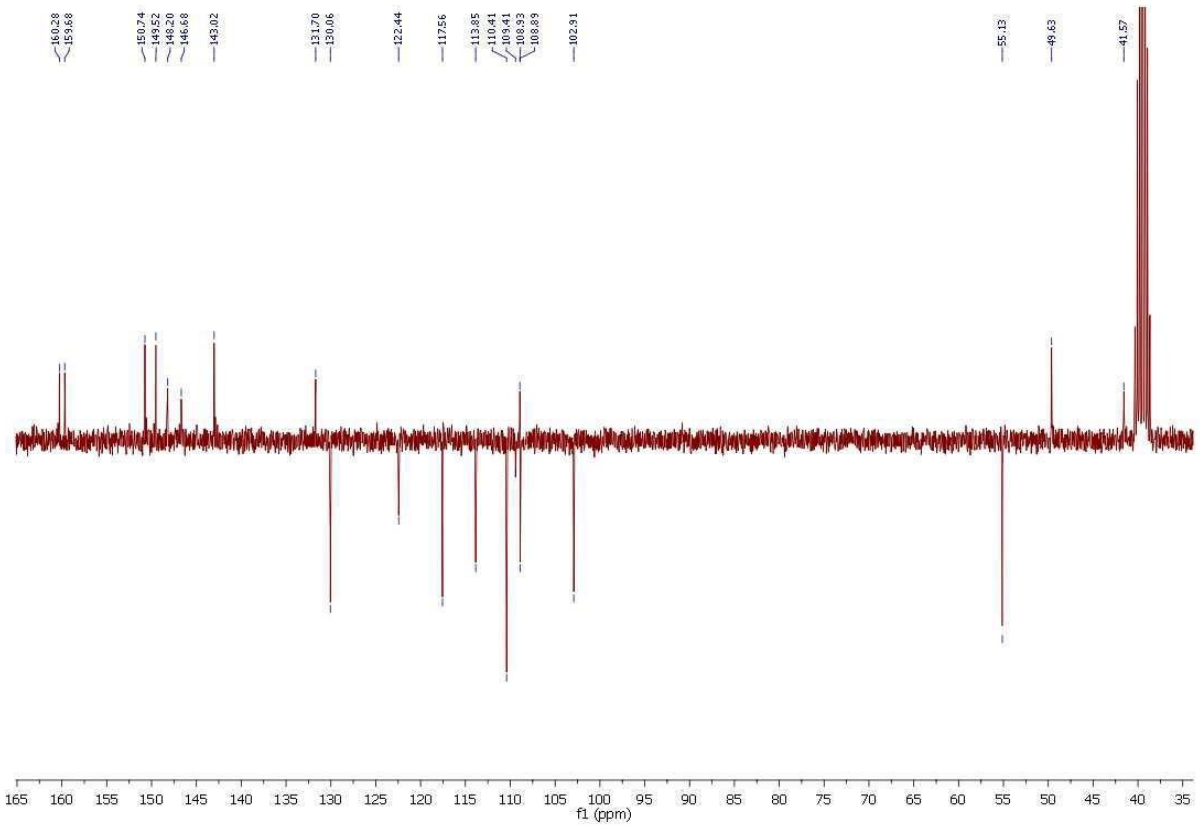


Fig. S30 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **20c**

a)



b)


160.28
153.68
150.74
149.52
148.20
146.88
143.02
131.70
130.06
122.44
117.56
113.85
110.41
109.41
108.33
108.89
102.91
55.13
49.63
41.57
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

c)

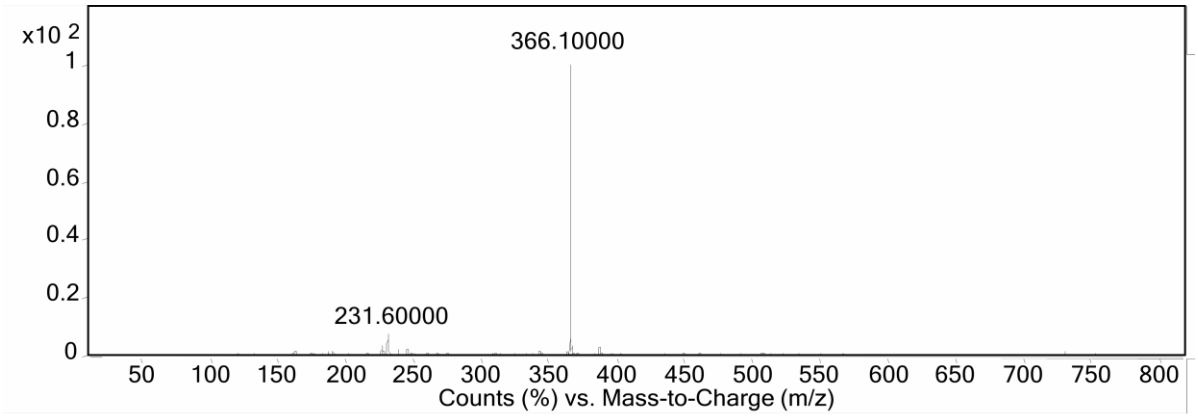
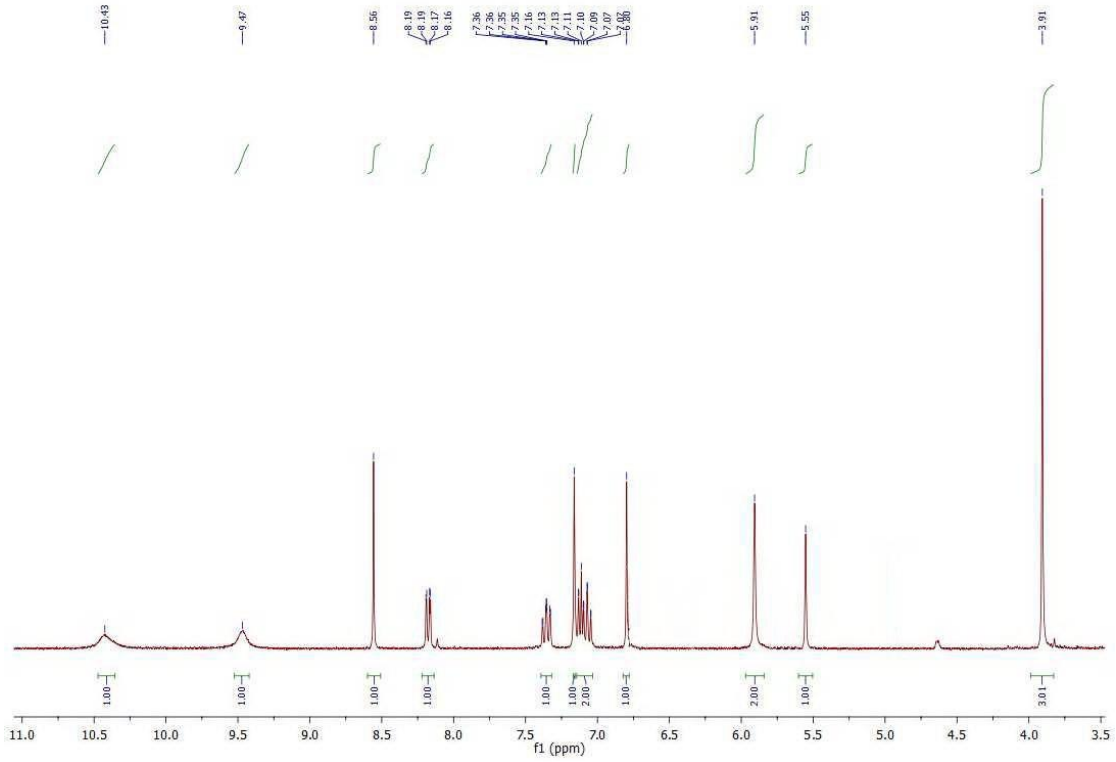
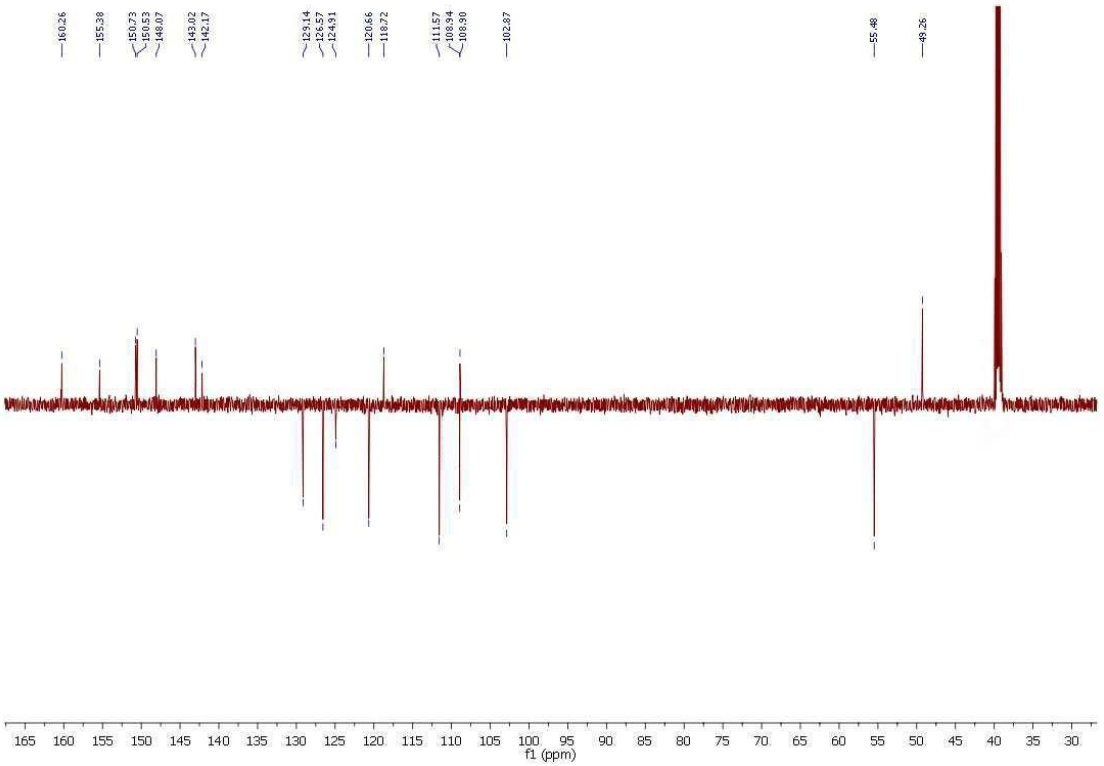

x10 2
1
0.8
0.6
0.4
0.2
0
366.10000
231.60000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)

Fig. S31 a) ^{1}H NMR, b) ^{13}C NMR and c) MS of compd. **20d**

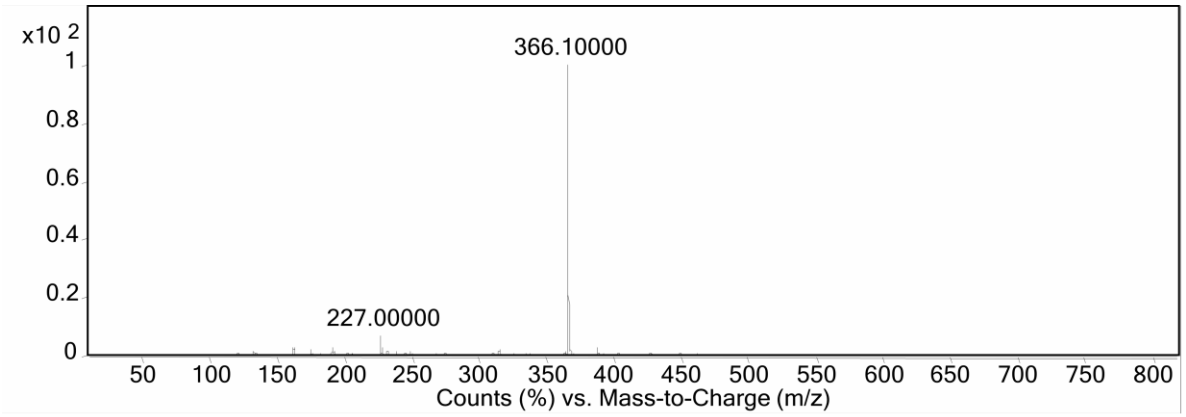
a)



b)



c)


x10 2
1
0.8
0.6
0.4
0.2
0
366.10000
227.00000
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800
Counts (%) vs. Mass-to-Charge (m/z)