Supporting Information

Khellinoflavanone, a Semisynthetic Derivative of Khellin, Overcomes Benzo[a]pyrene Toxicity in Human Normal and Cancer Cells that Express CYP1A1

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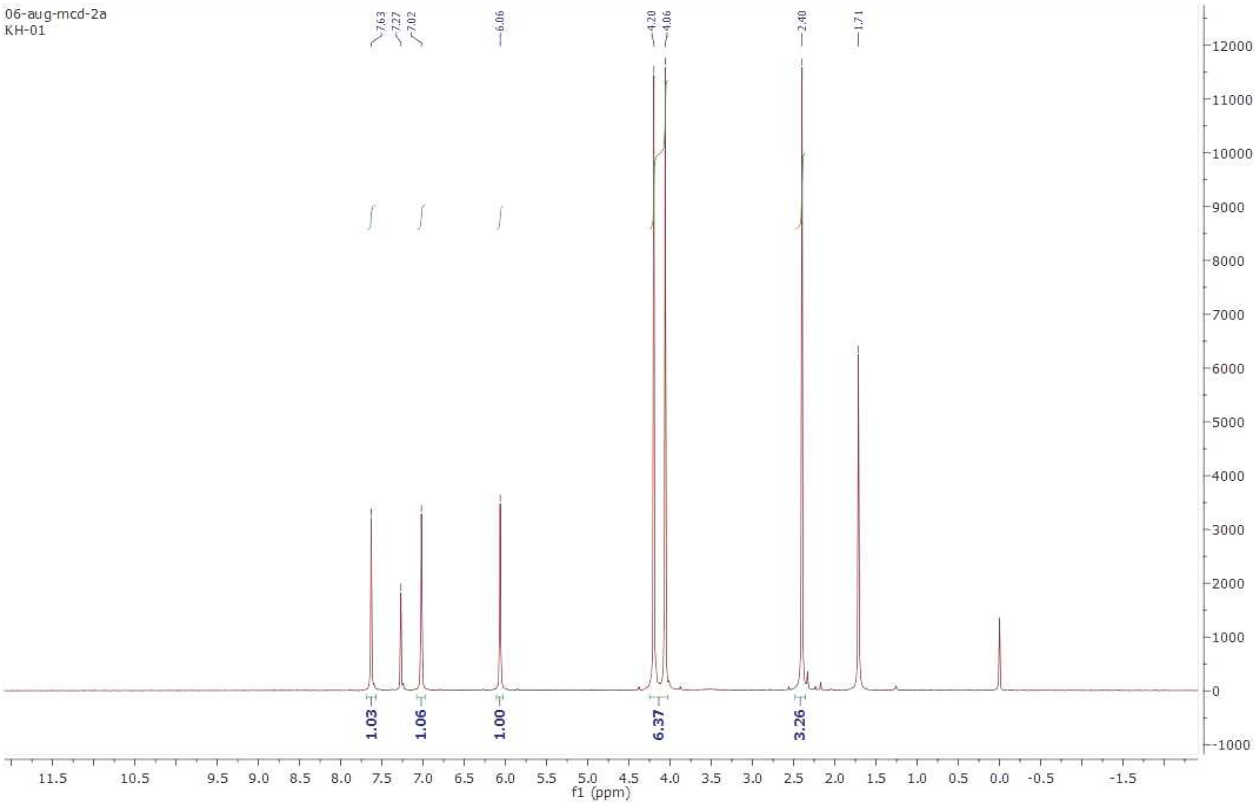
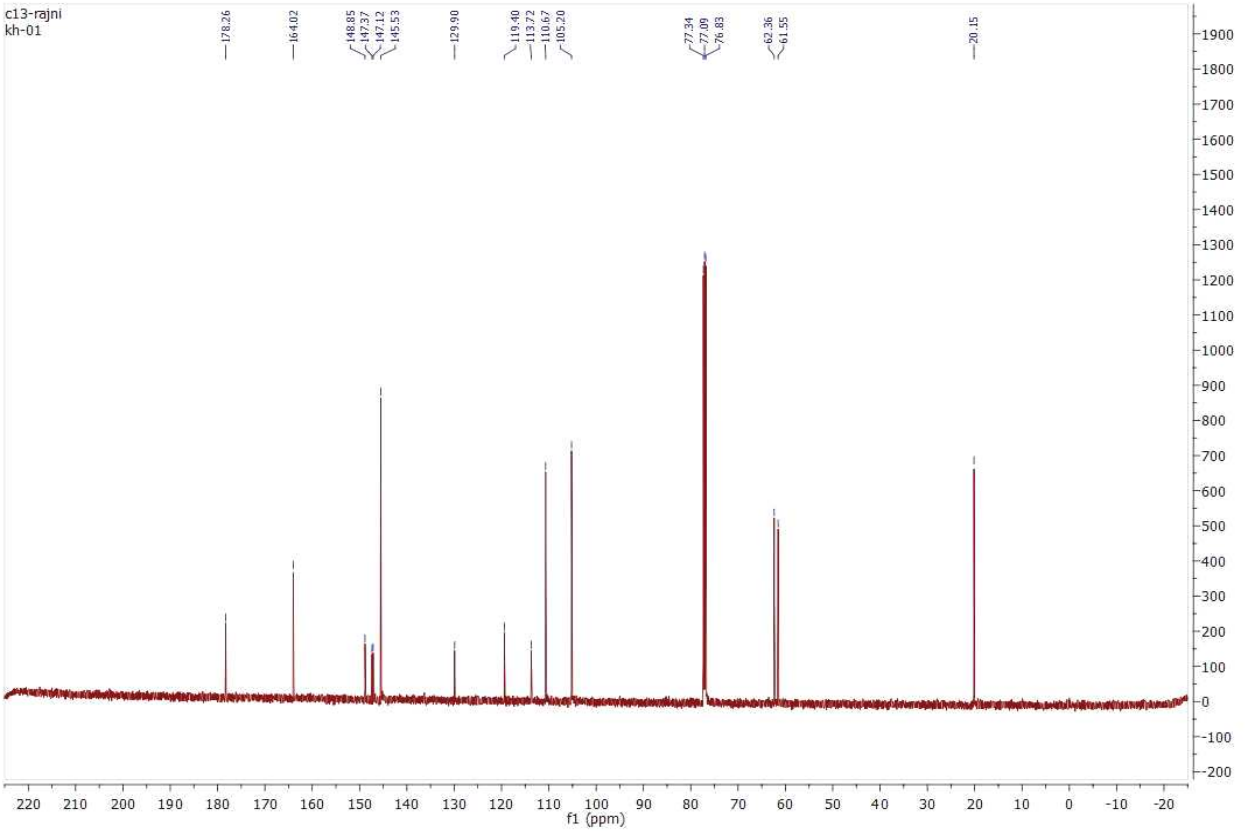
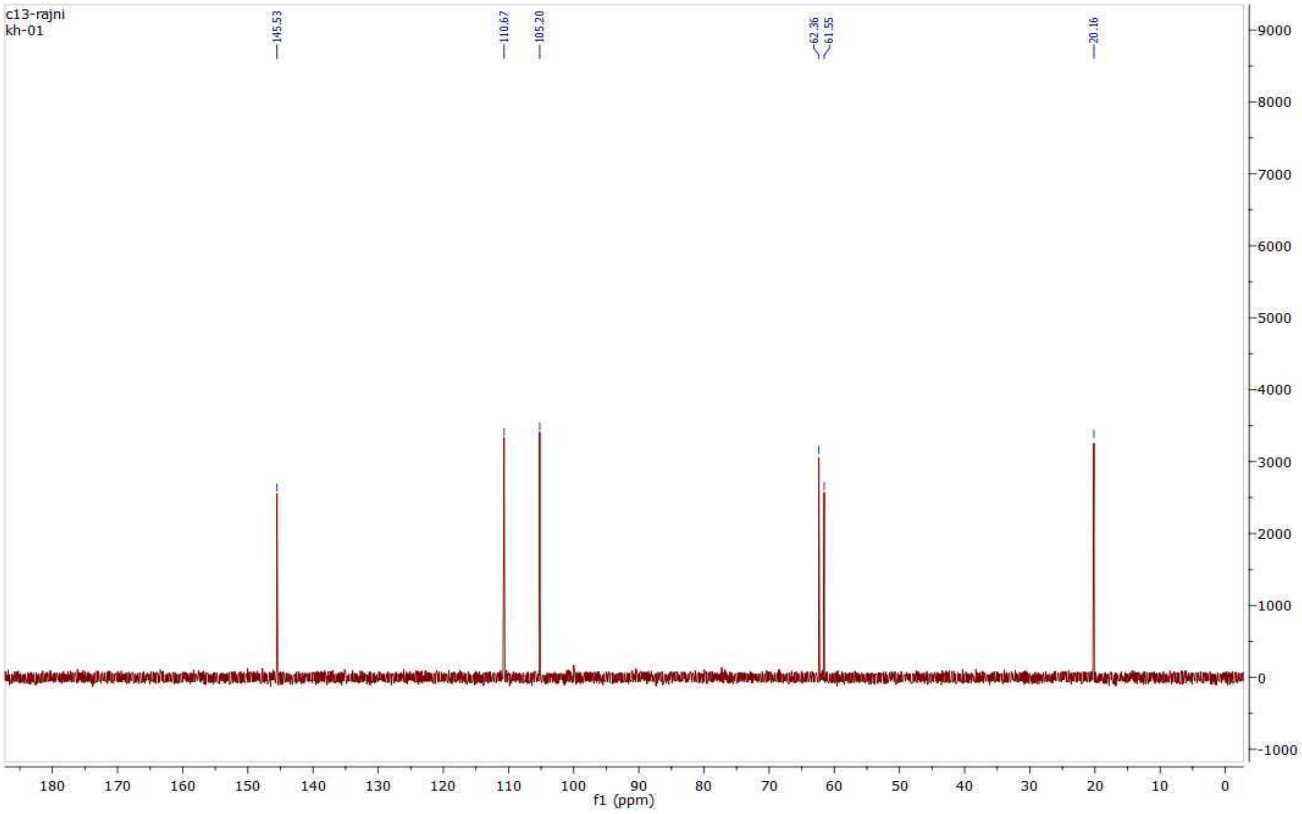
Section S1. Scan copies of ^{1}H NMR and ^{13}C spectra of all compounds

Figure S1.1. ^{1}H, ^{13}C and DEPT-135 NMR of **1** in $CDCl_3$






c13-rajni
kh-01
145.53
110.67
105.20
62.36
61.55
20.16
9000
8000
7000
6000
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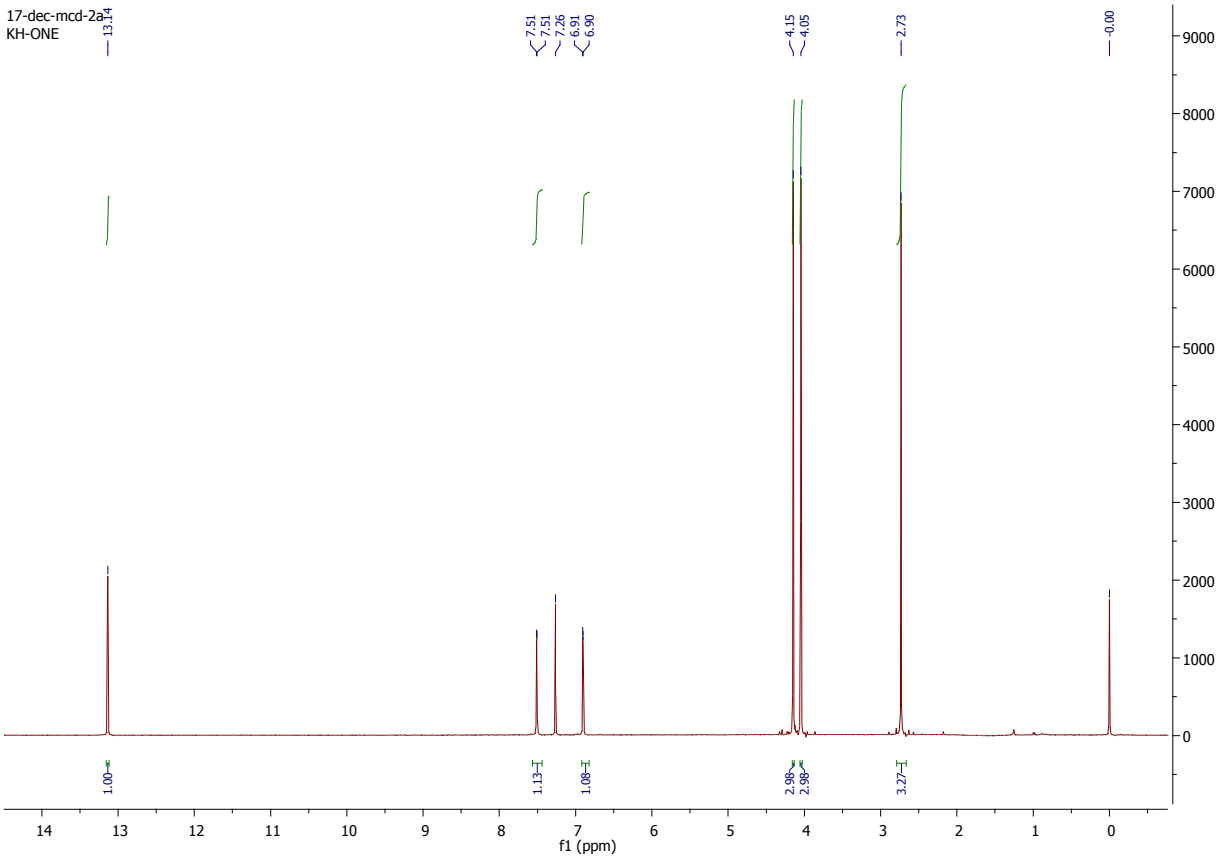
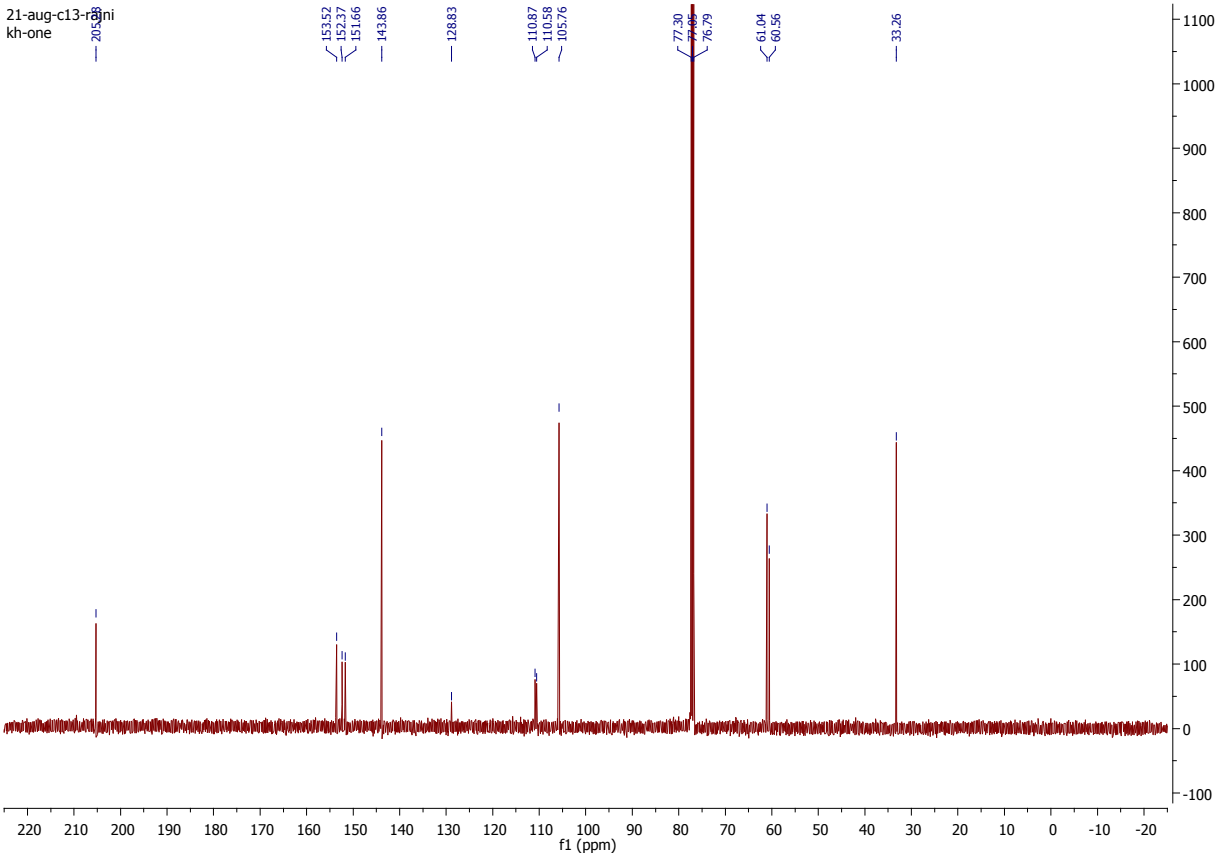
2000
1000
0
-1000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Figure S1.2. ^{1}H, ^{13}C and DEPT-135 NMR of **2** in $CDCl_3$





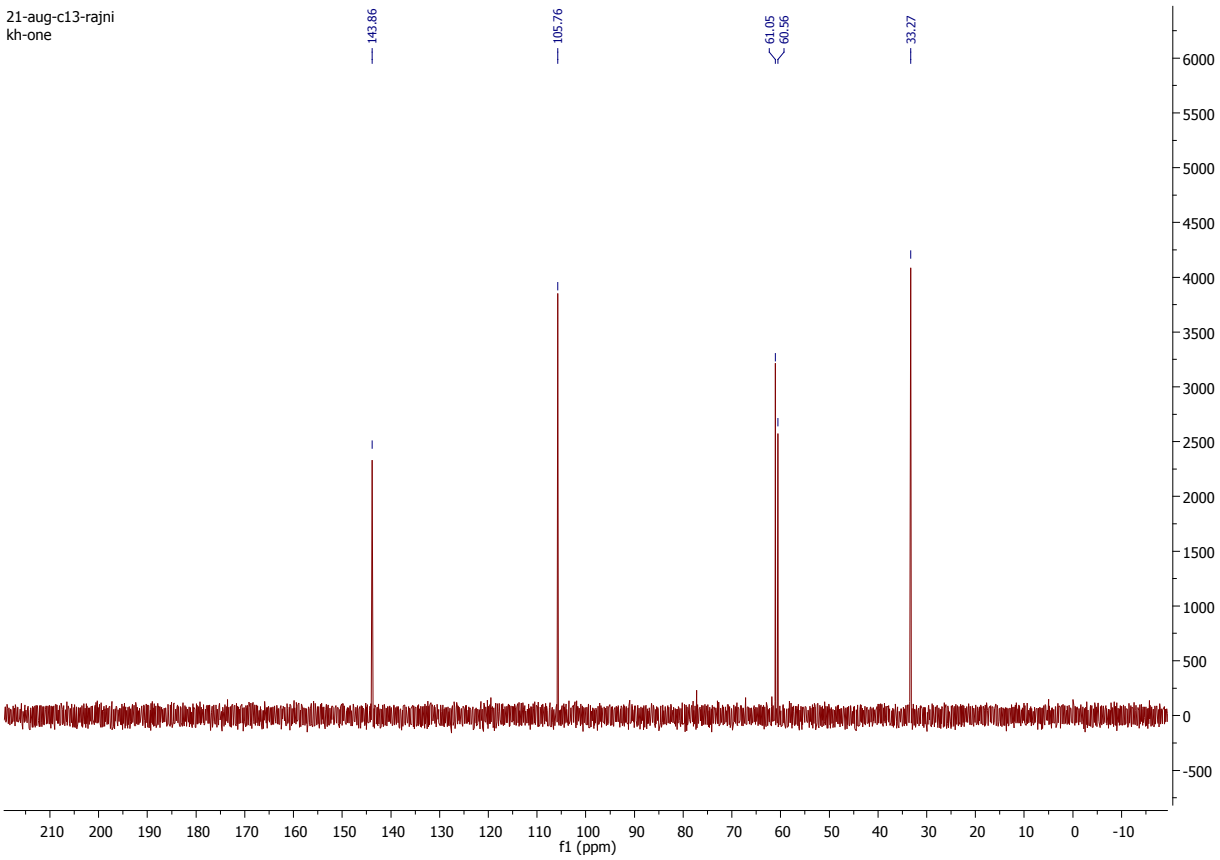
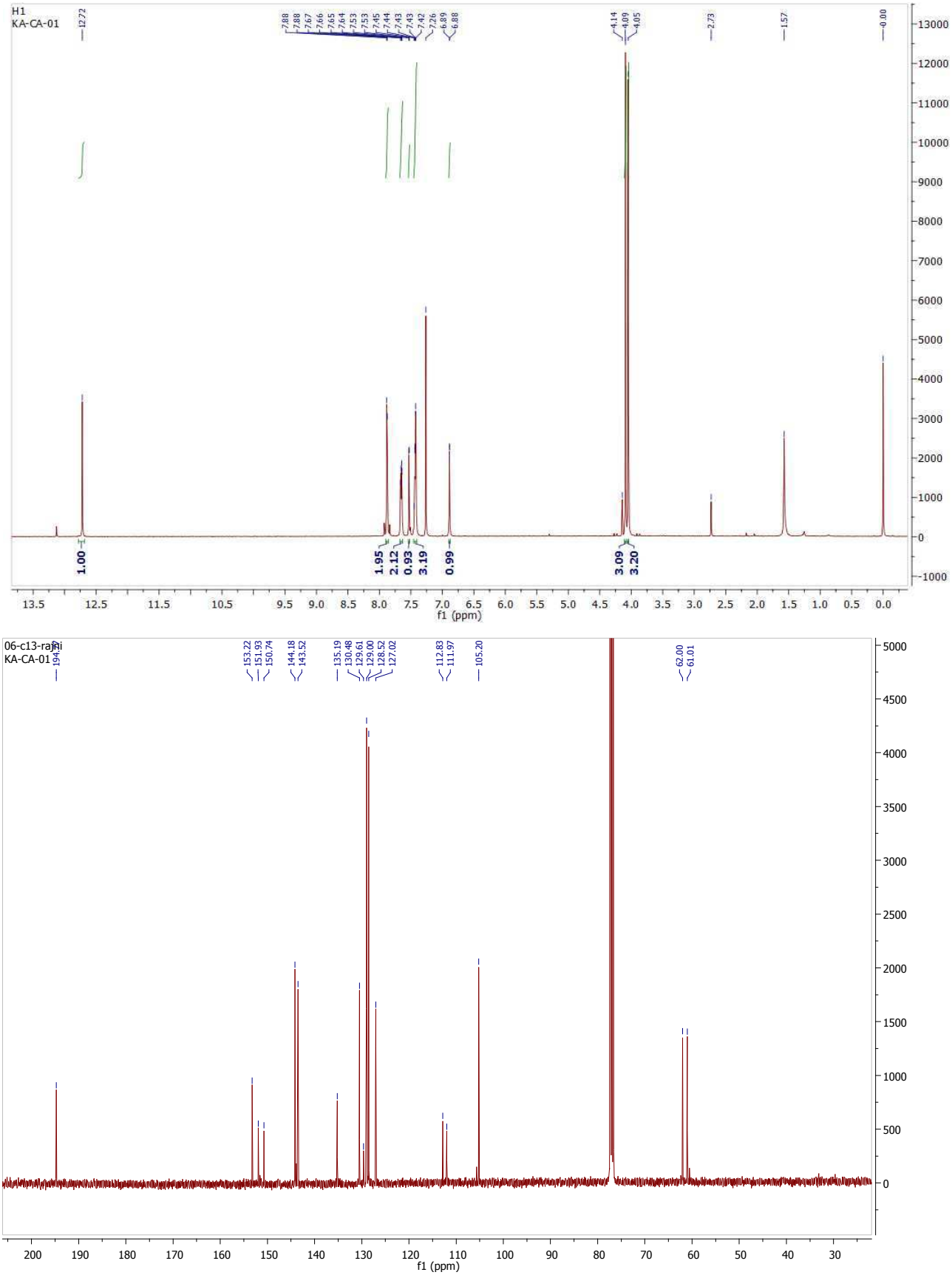

21-aug-c13-rajni
kh-one
143.86
105.76
61.05
60.56
33.27
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Figure S1.3. ^{1}H, ^{13}C and DEPT-135 NMR of **3a** in $CDCl_3$



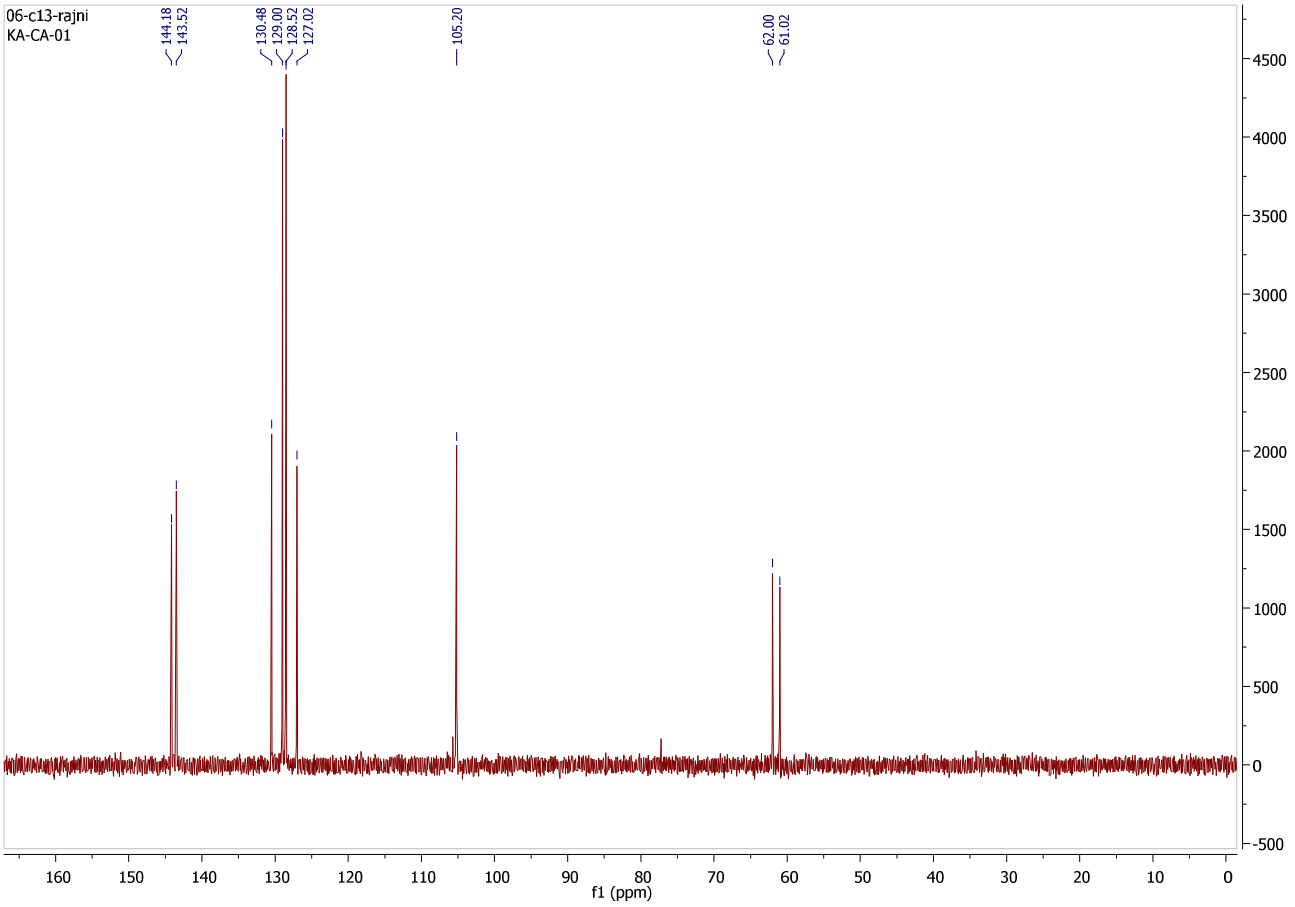
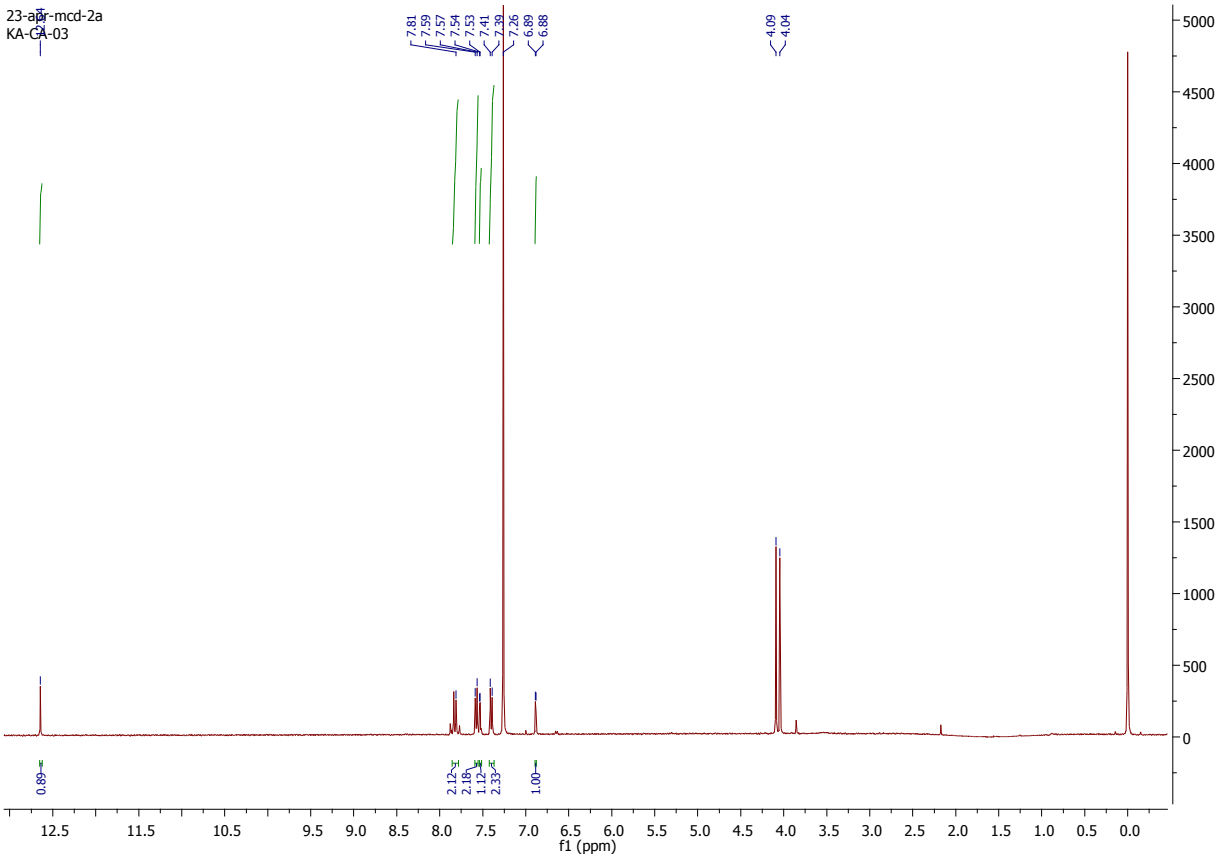
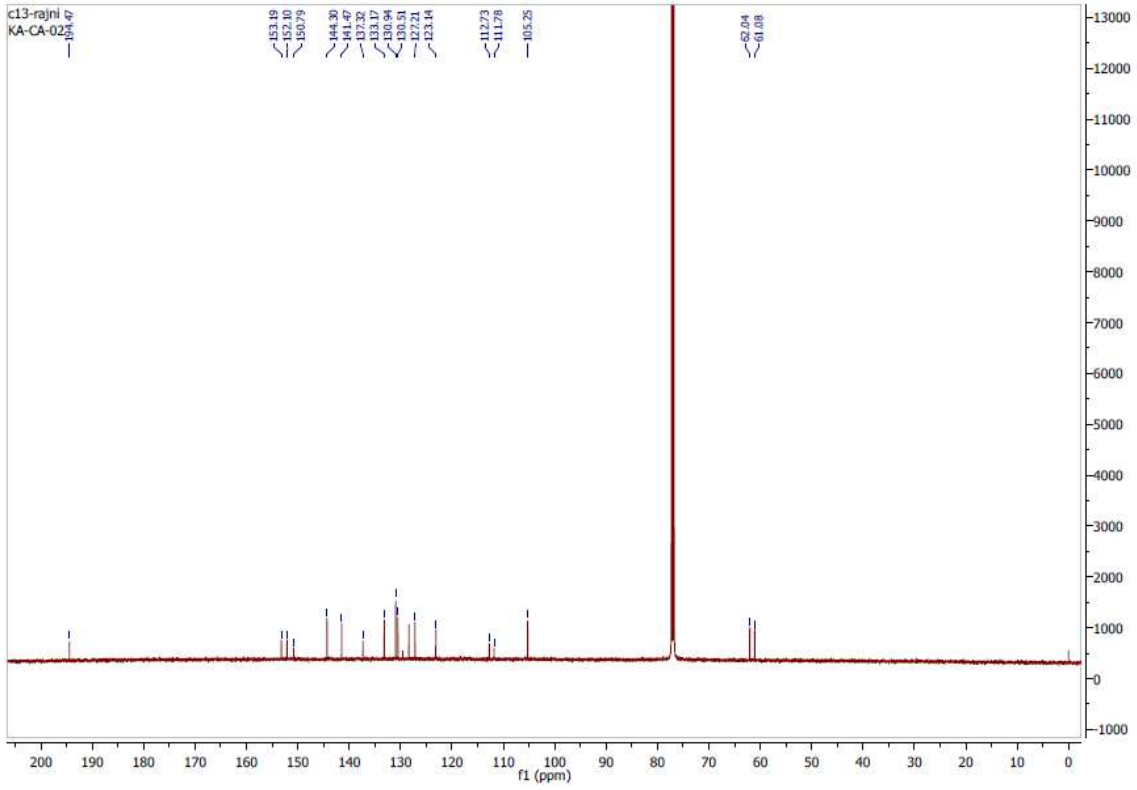

06-c13-rajni
KA-CA-01
144.18
143.52
130.48
129.00
128.52
127.02
105.20
62.00
61.02
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Figure S1.4. ^{1}H, ^{13}C and DEPT-135 NMR of **3b** in $CDCl_3$





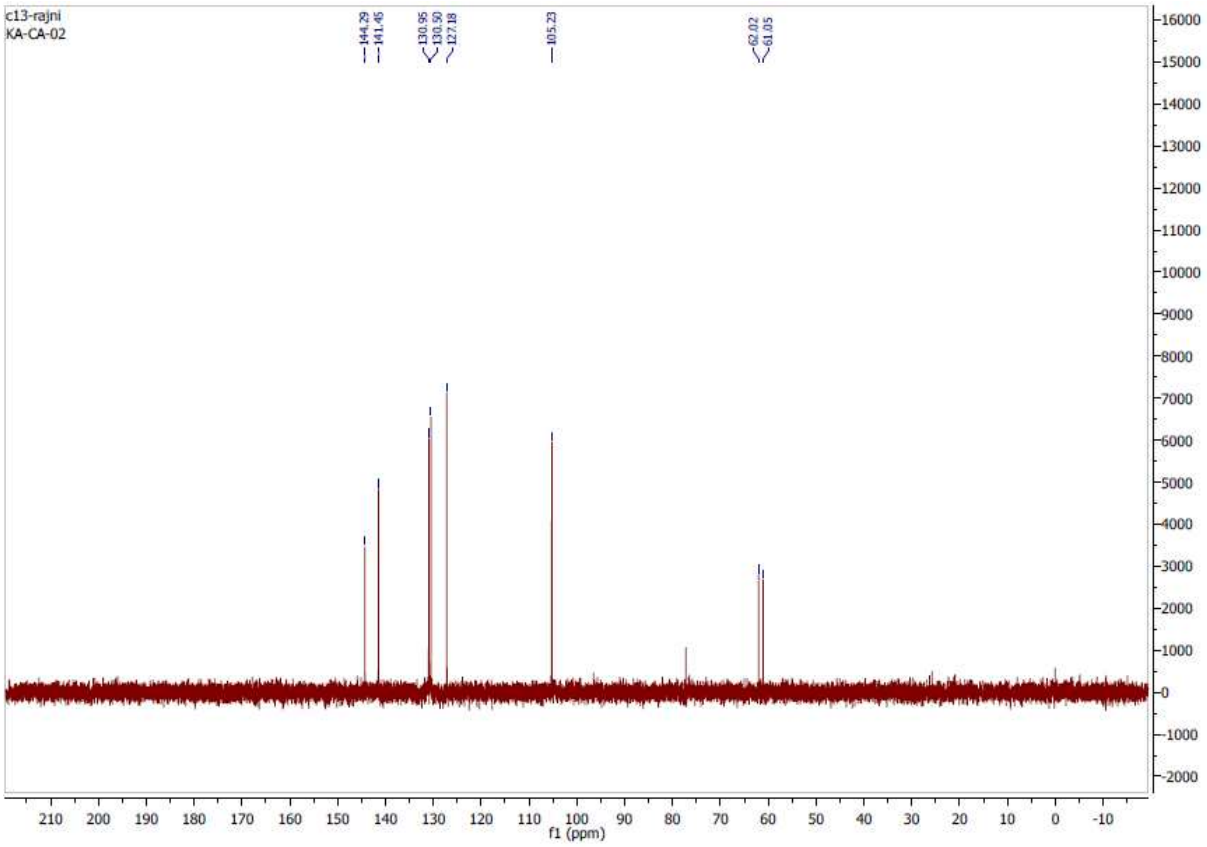
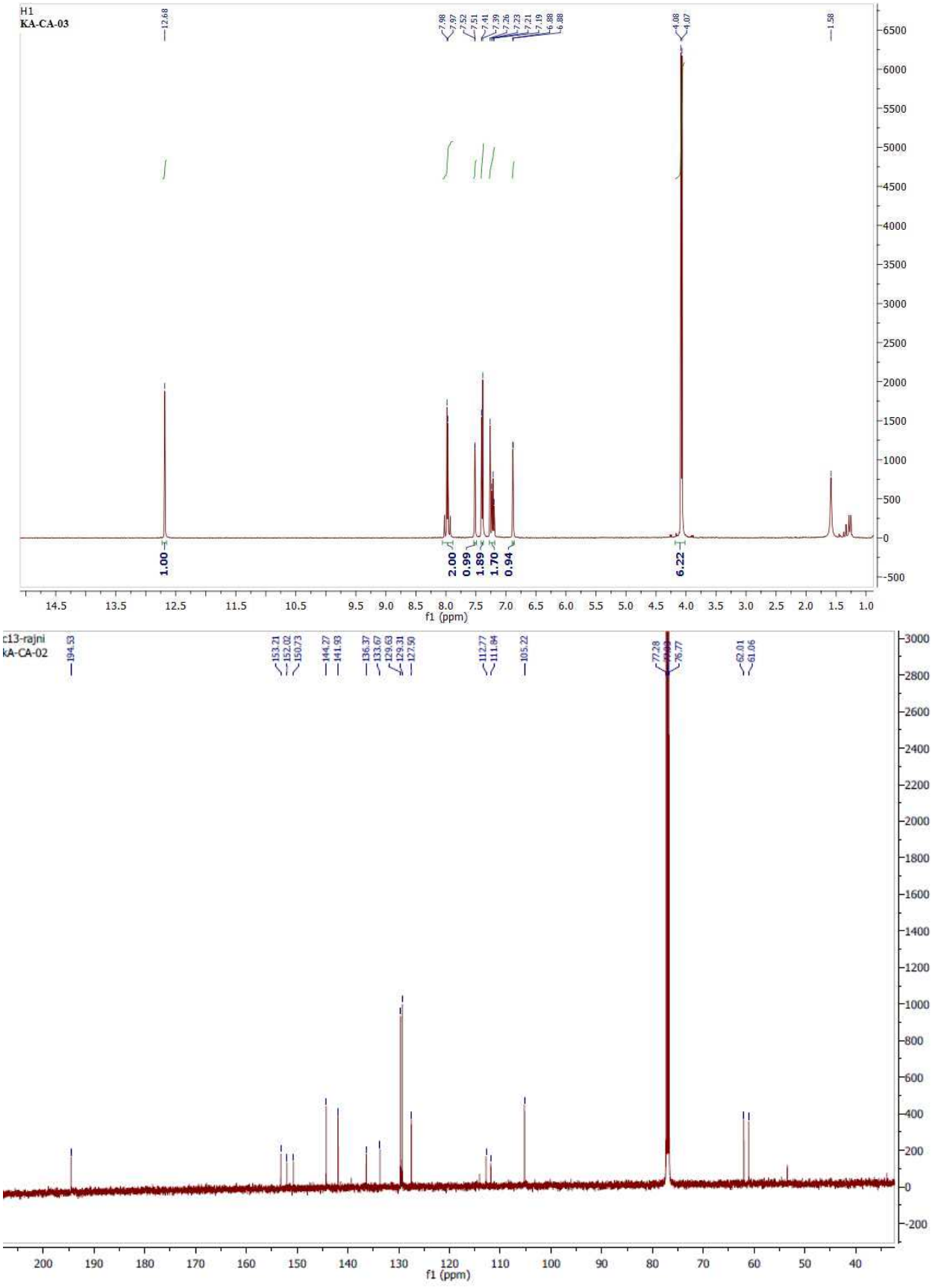

c13-rajni
KA-CA-02
144.29
141.45
130.95
130.50
127.18
105.23
62.02
61.05
f1 (ppm)

Figure S1.5. ^{1}H, ^{13}C and DEPT-135 NMR of **3c** in $CDCl_3$



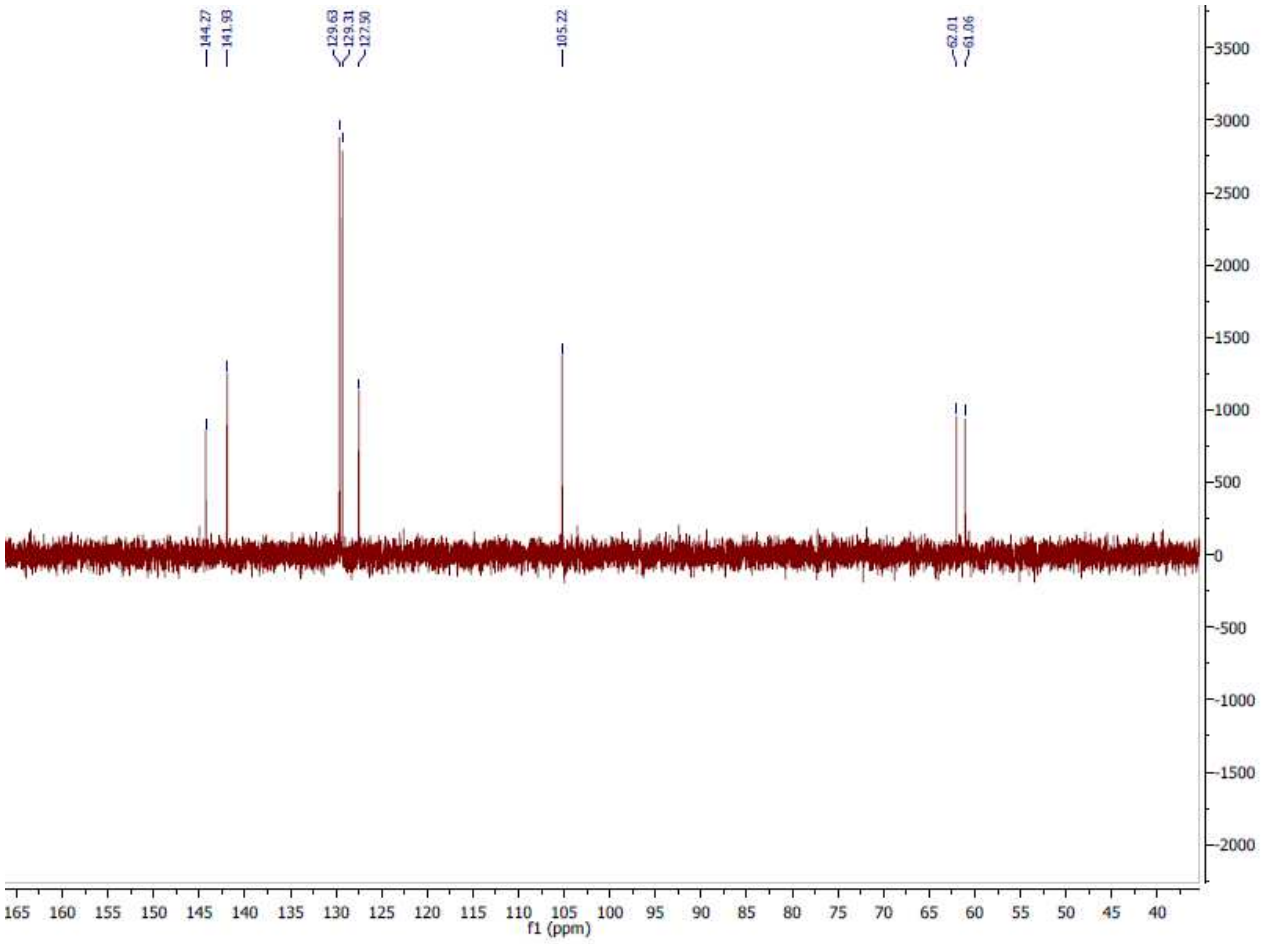
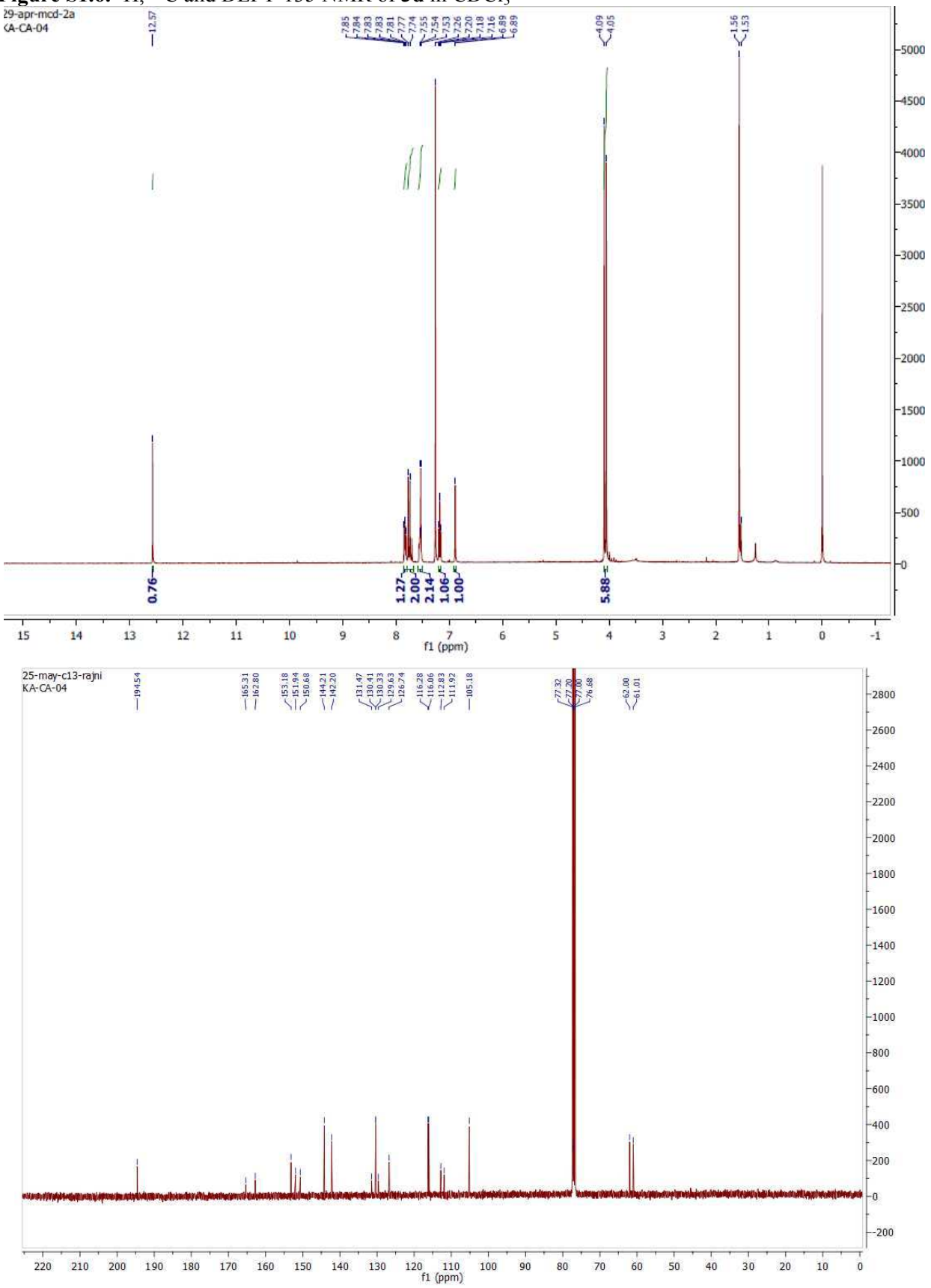

144.27
141.93
129.63
129.31
127.90
105.22
62.01
61.06
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

Figure S1.6. ^{1}H, ^{13}C and DEPT-135 NMR of **3d** in $CDCl_3$



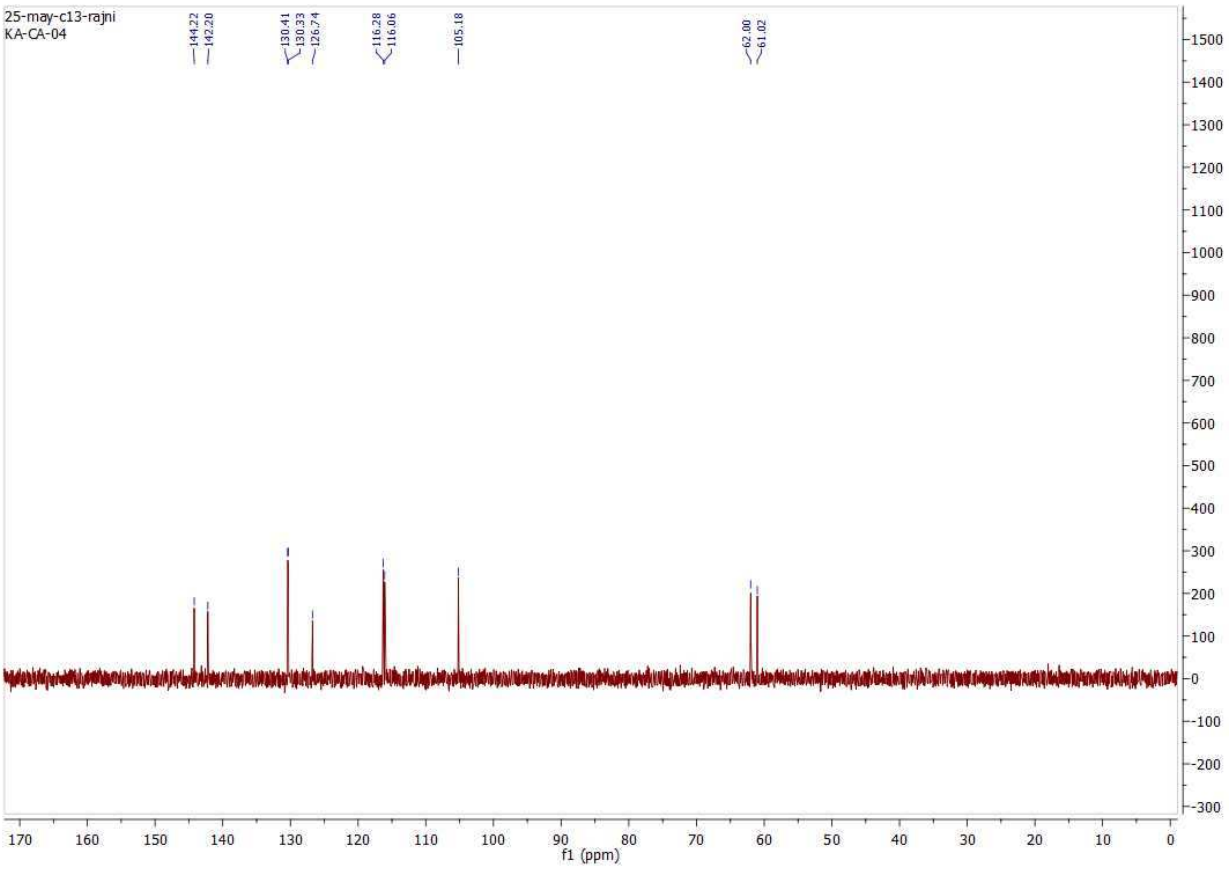
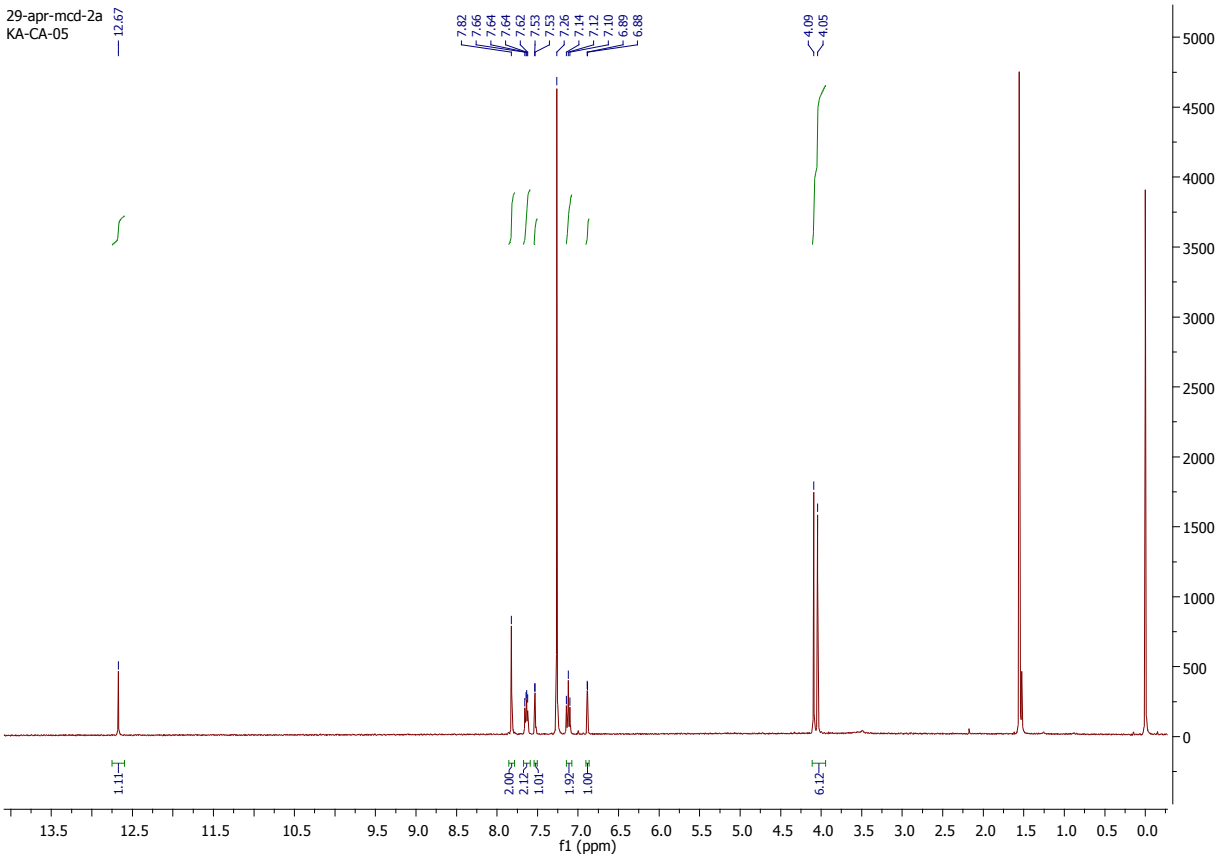
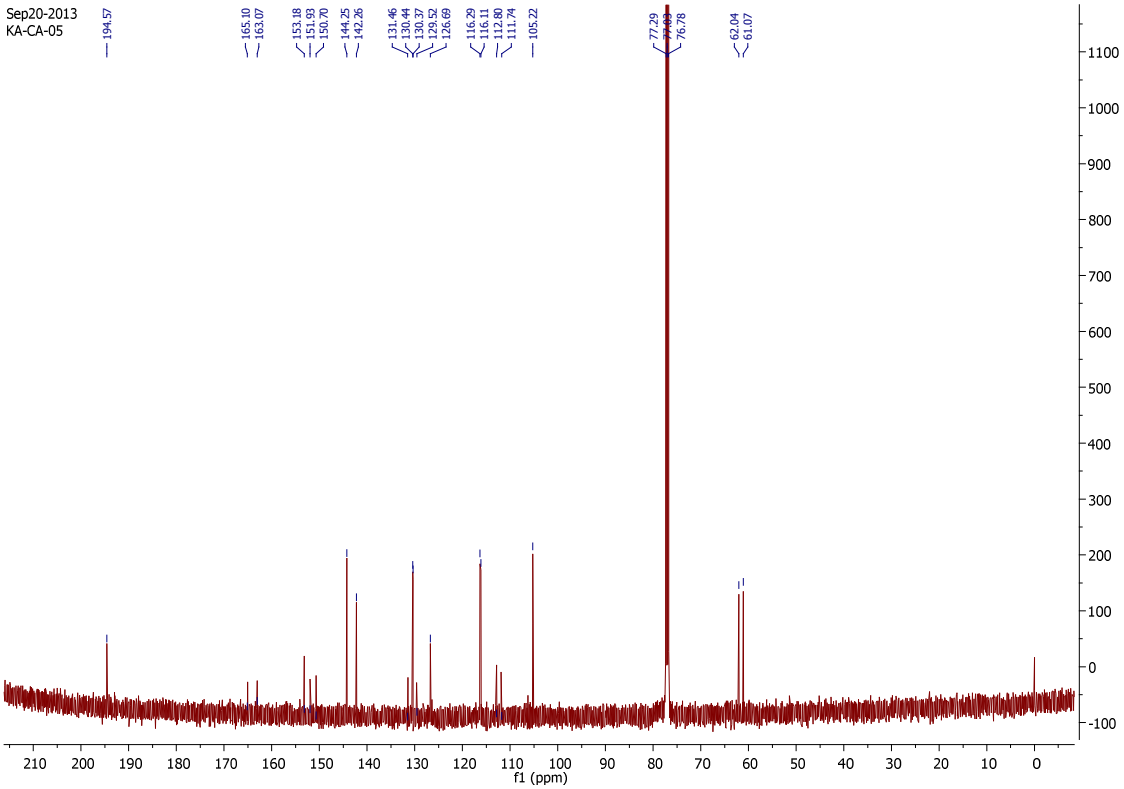

25-may-c13-rajni
KA-CA-04
144.22
142.20
130.41
130.33
126.74
116.28
116.06
105.18
62.00
61.02
f1 (ppm)

Figure S1.7. ^{1}H, ^{13}C and DEPT-135 NMR of **3e** in $CDCl_3$





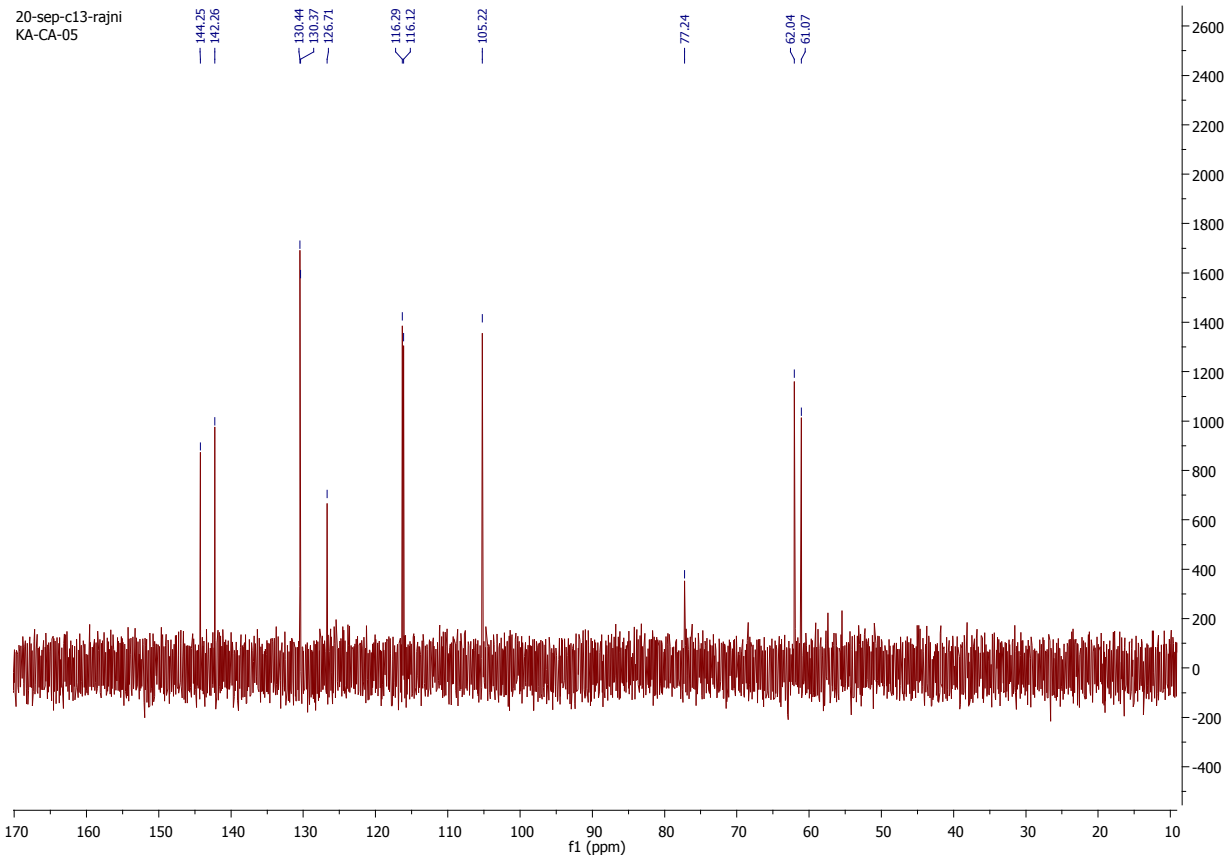
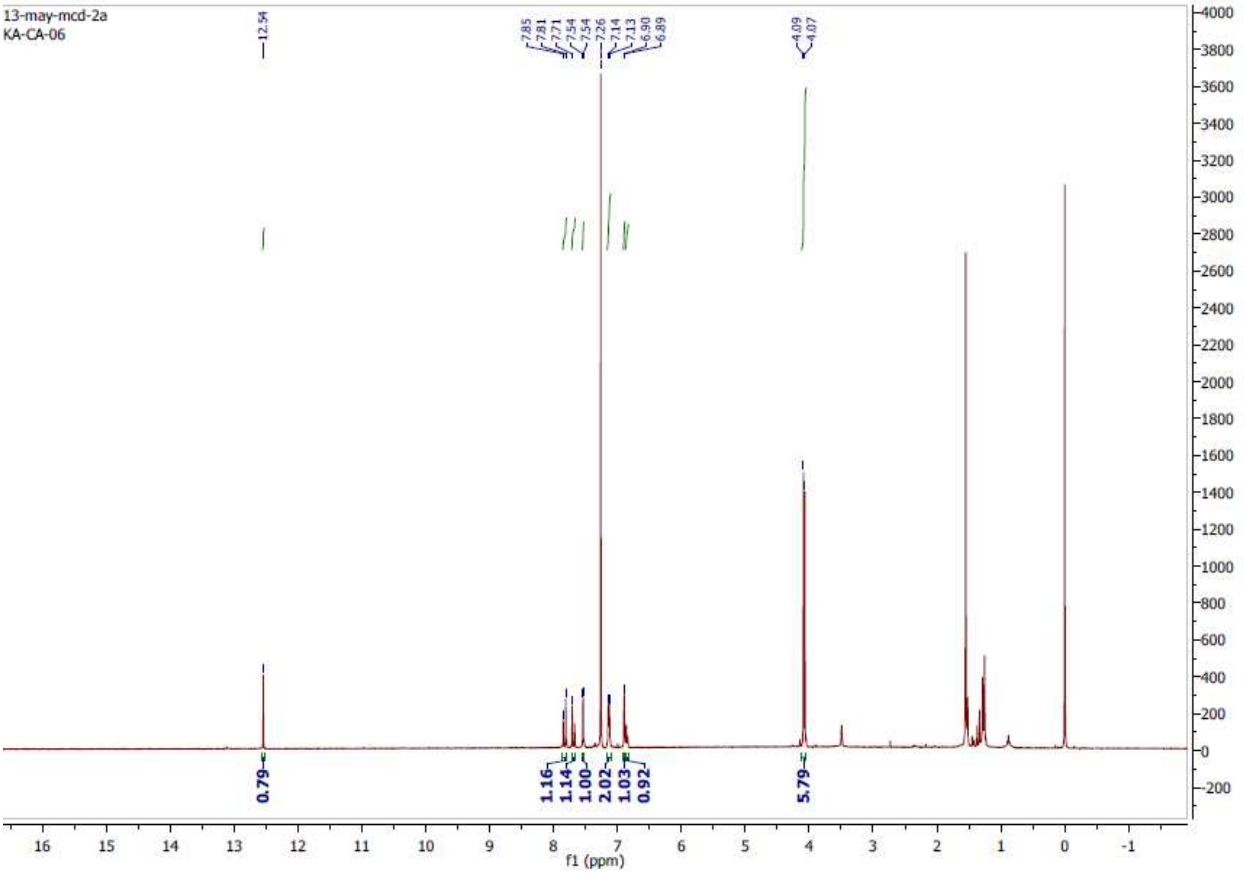
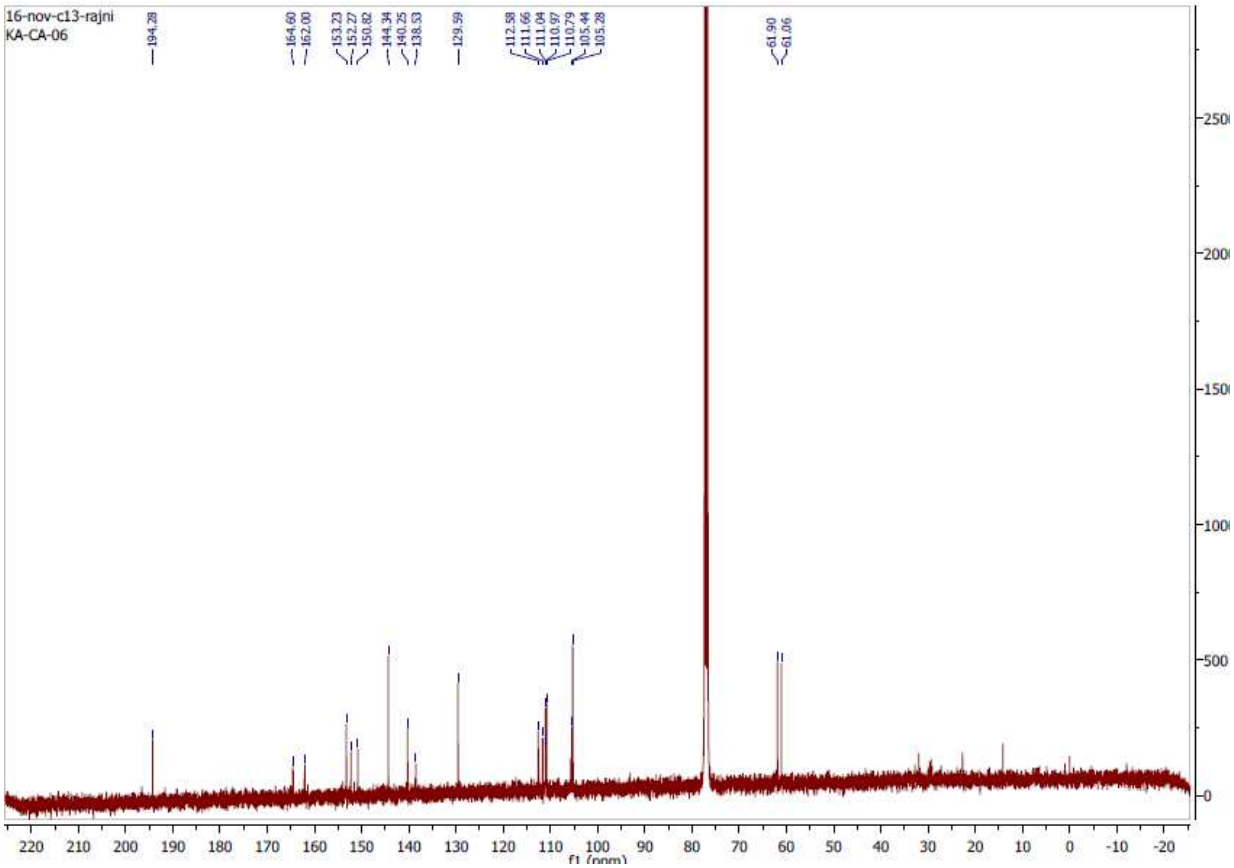

20-sep-c13-rajni
KA-CA-05
144.25
142.26
130.44
130.37
126.71
116.29
116.12
105.22
77.24
62.04
61.07
f1 (ppm)

Figure S1.8. ^{1}H, ^{13}C and DEPT-135 NMR of **3f** in $CDCl_3$





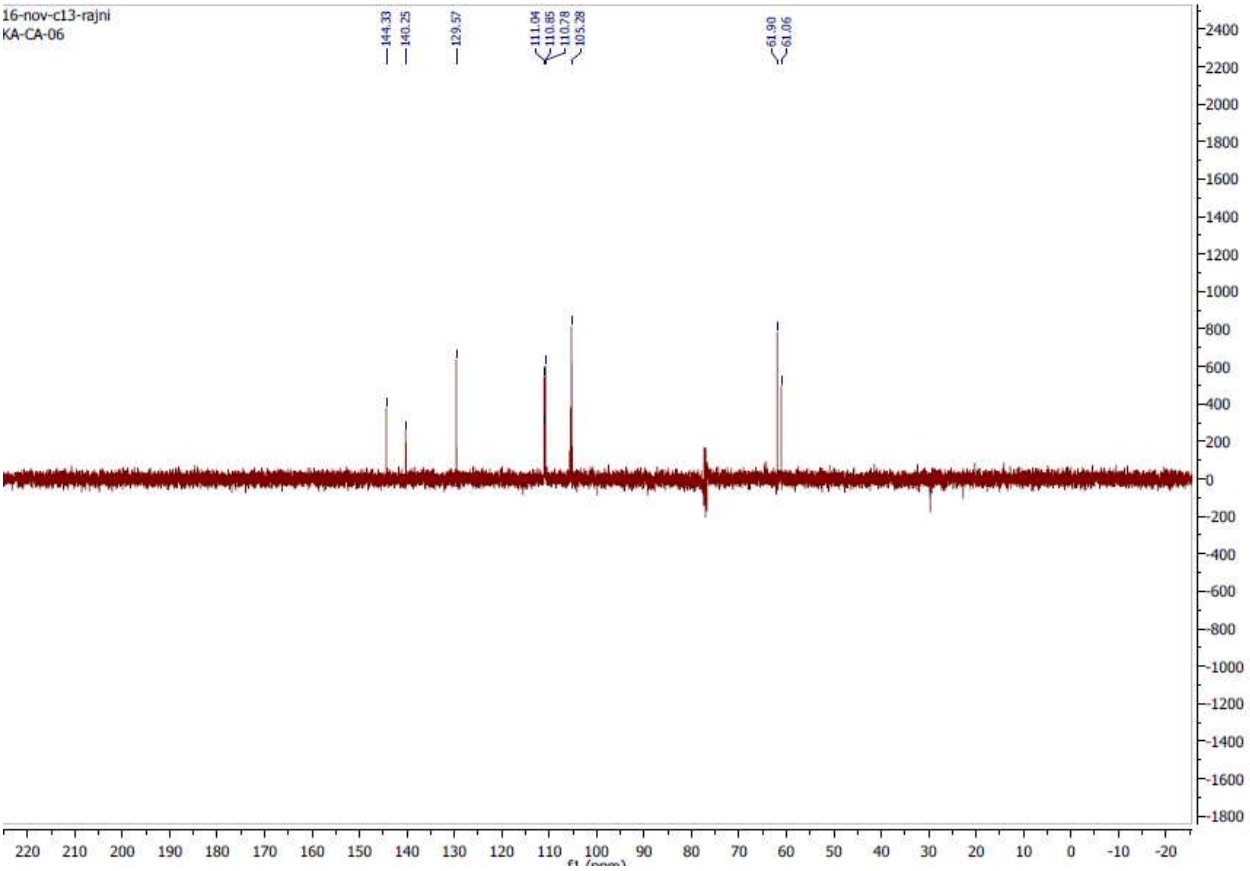
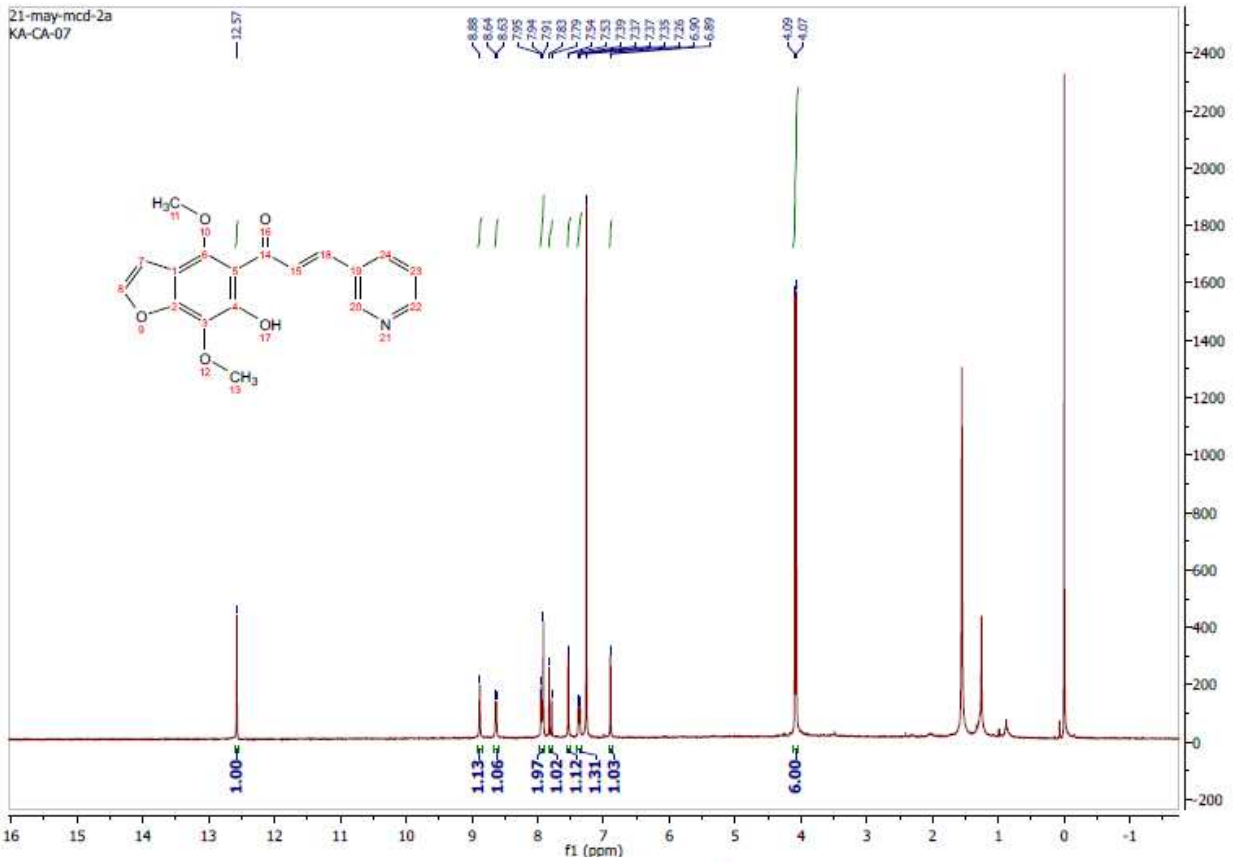
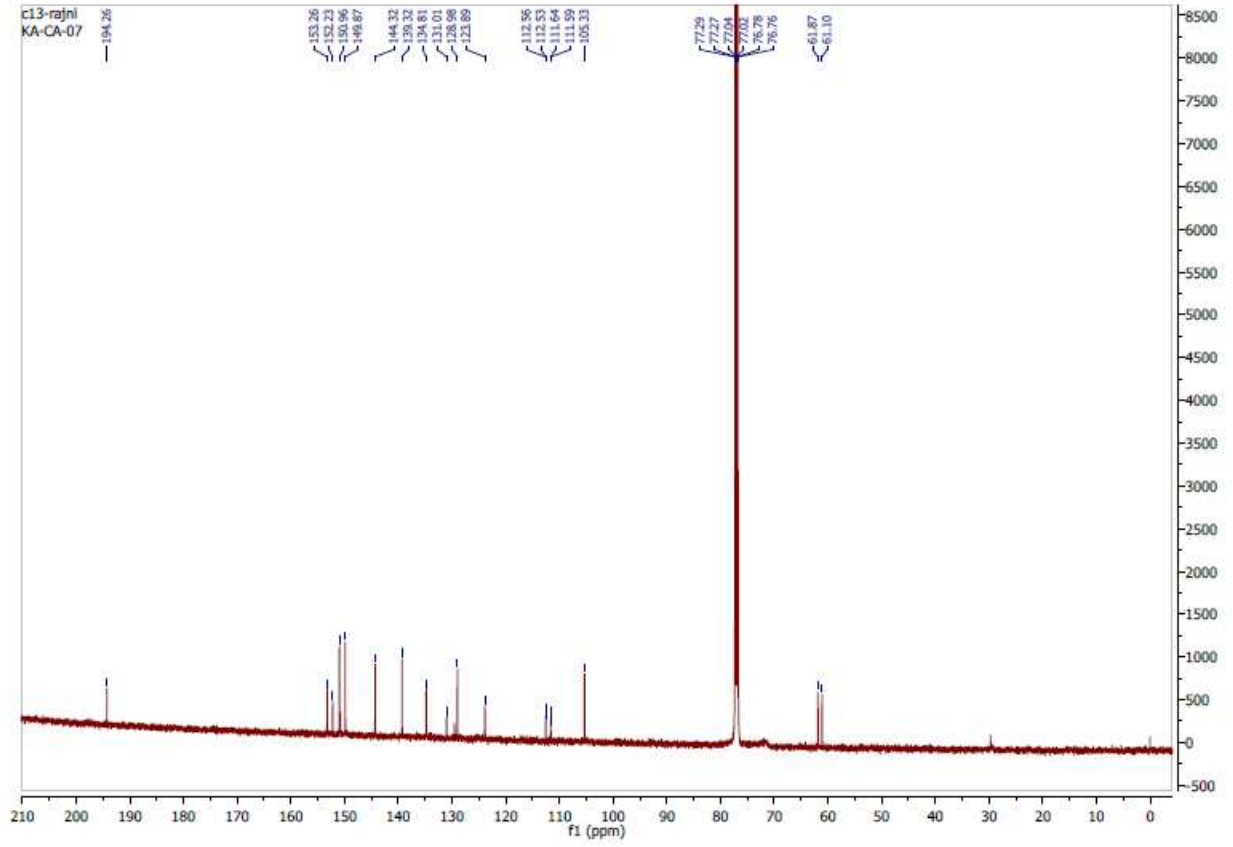

16-nov-c13-rajni
KA-CA-06
144.33
140.25
129.57
111.04
110.85
110.78
105.28
61.90
61.06
f1 (ppm)

Figure S1.9. ^{1}H, ^{13}C and DEPT-135 NMR of **3g** in $CDCl_3$





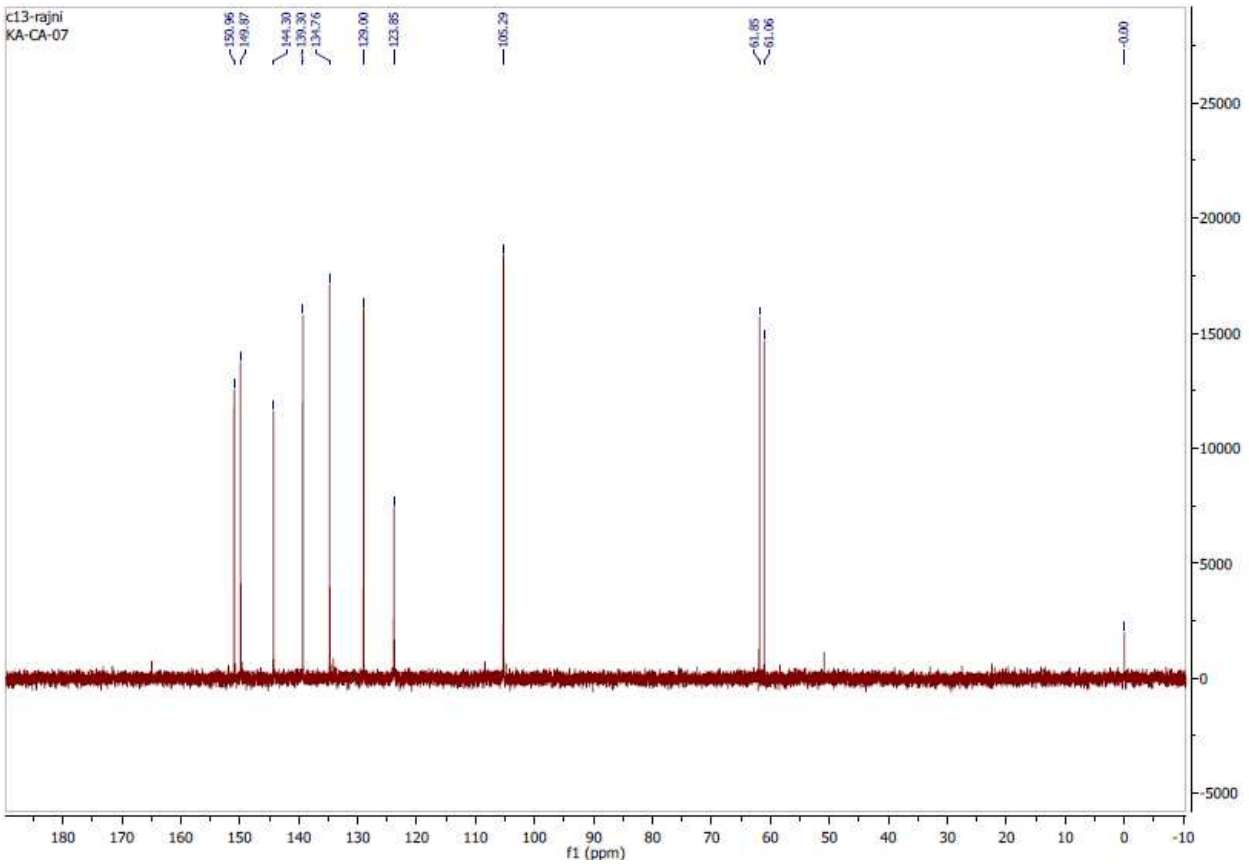
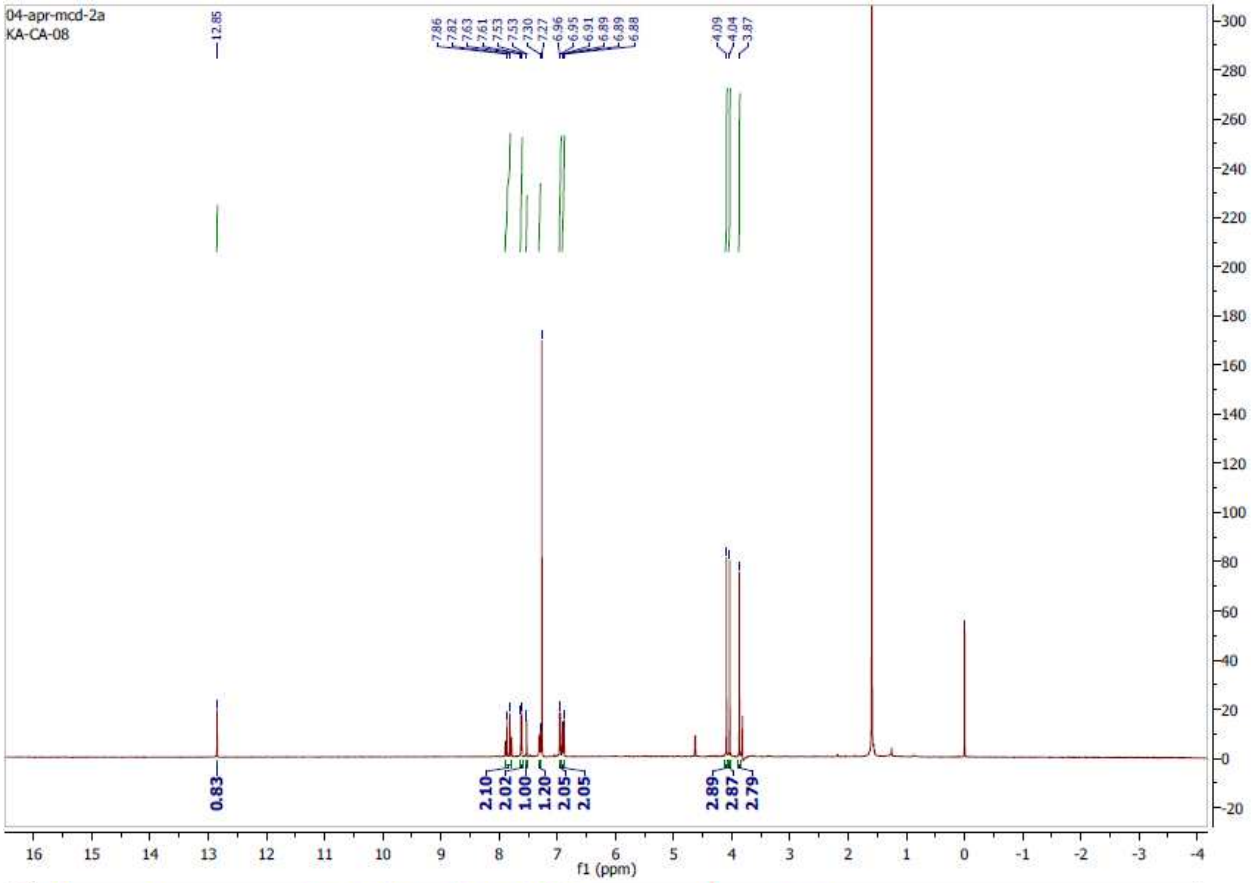
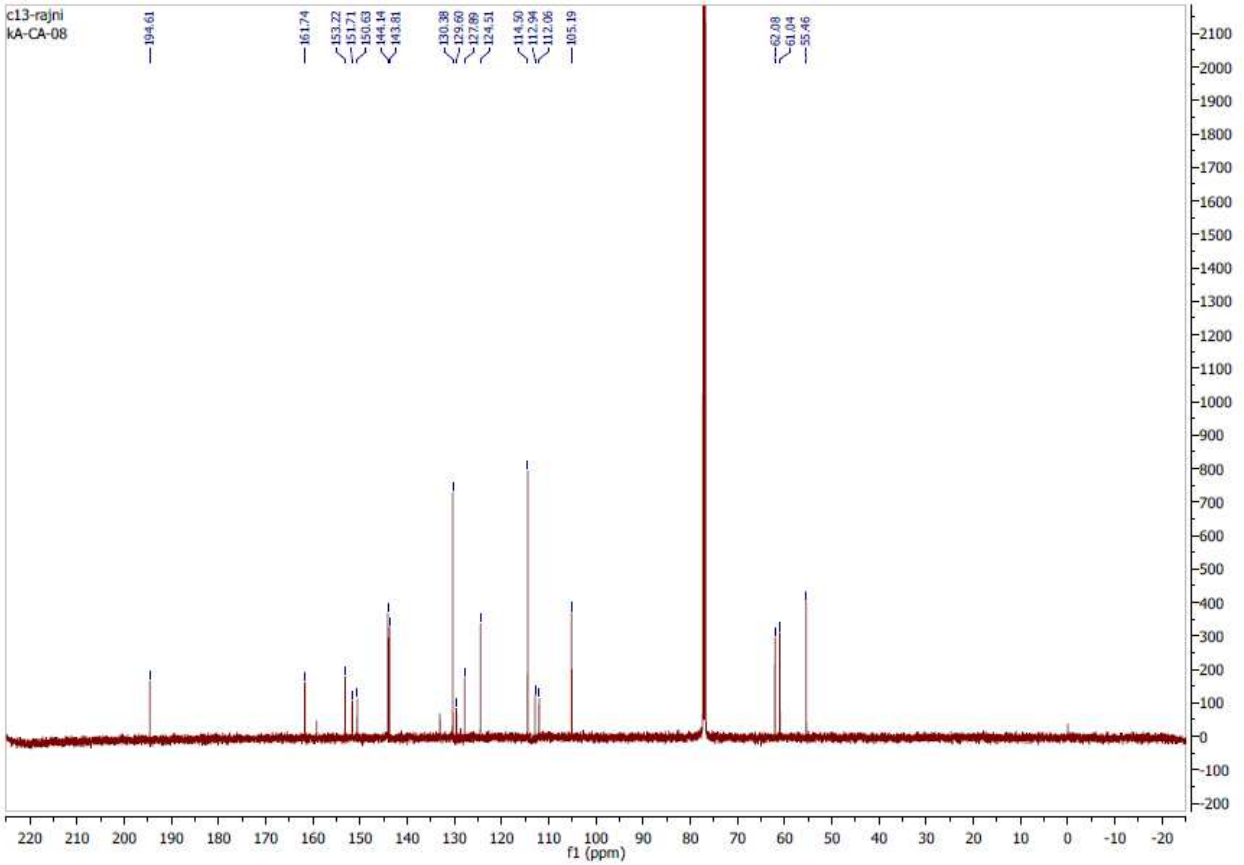

c13-rajni
KA-CA-07
150.96
149.87
144.30
139.30
134.76
129.00
123.85
105.29
61.85
61.06
0.00
25000
20000
15000
10000
5000
0
-5000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Figure S1.10. ^{1}H, ^{13}C and DEPT-135 NMR of **3h** in $CDCl_3$





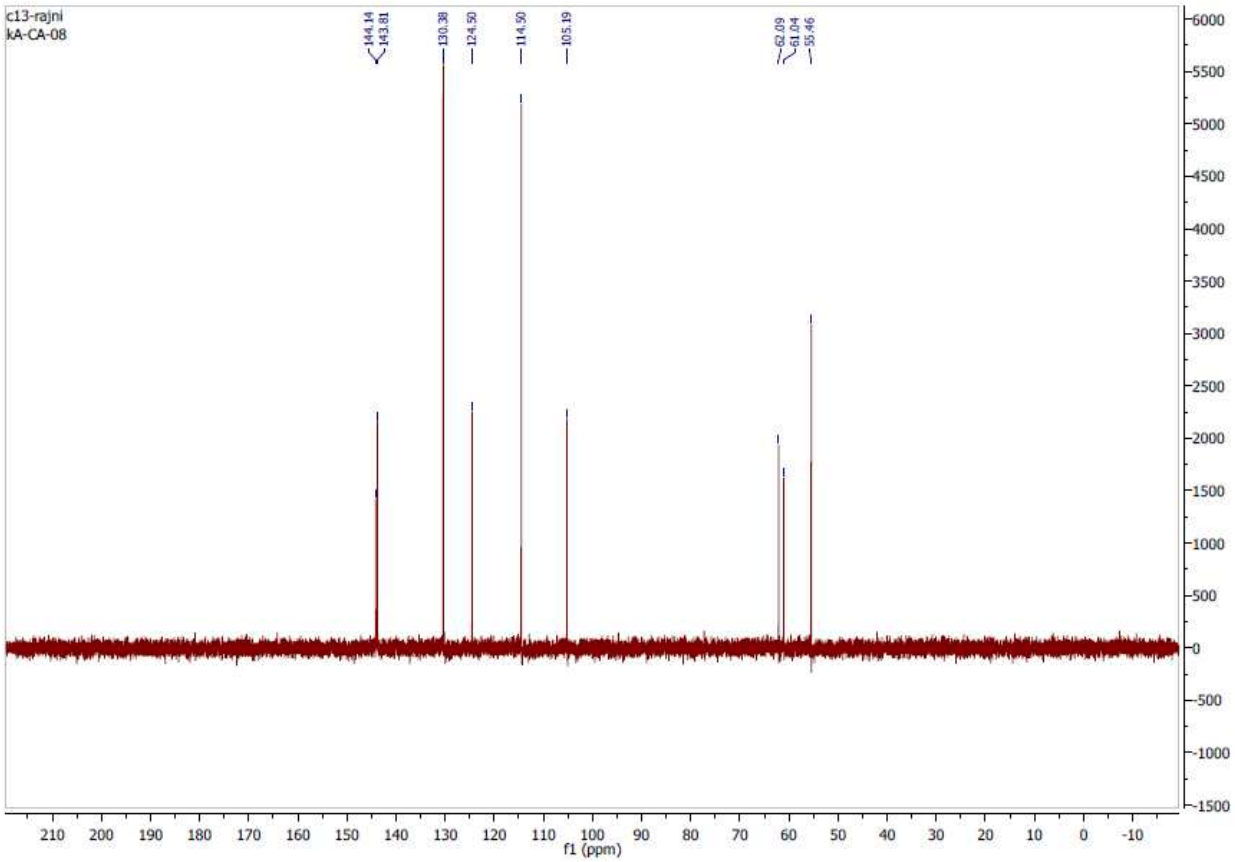
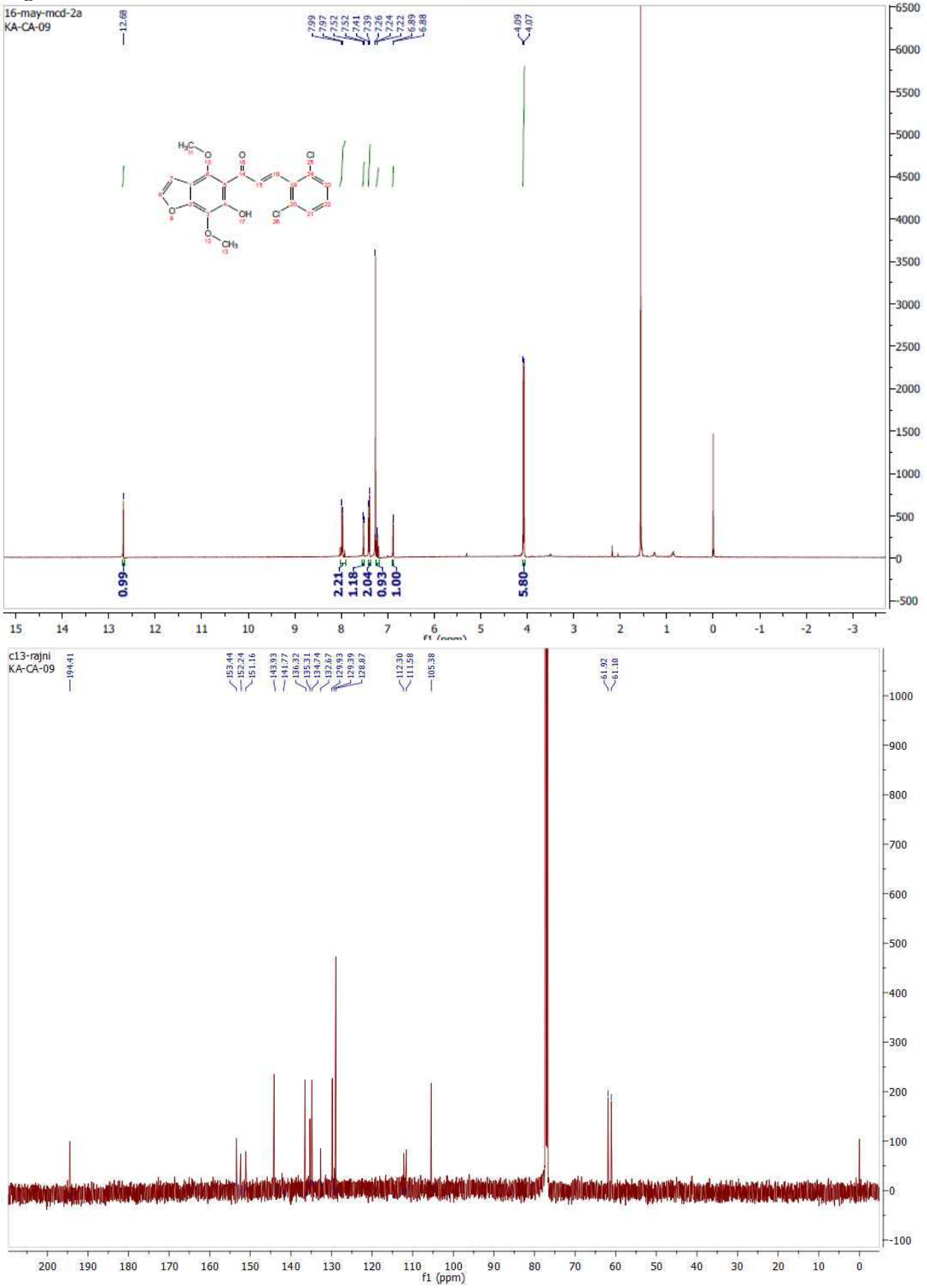

c13-rajni
kA-CA-08
144.14
143.81
130.38
124.50
114.50
105.19
62.09
61.04
55.46
f1 (ppm)

Figure S1.11. ^{1}H, ^{13}C and DEPT-135 NMR of **3i** in $CDCl_3$



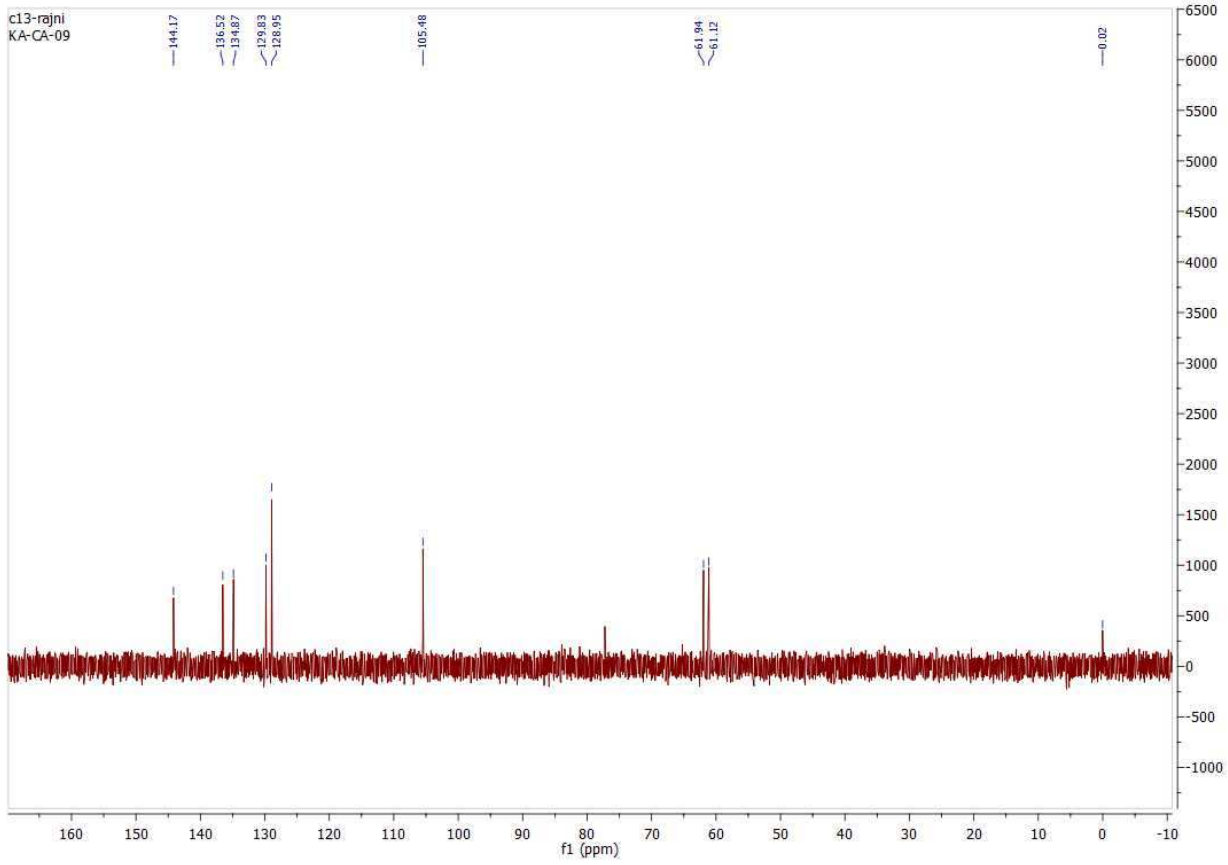
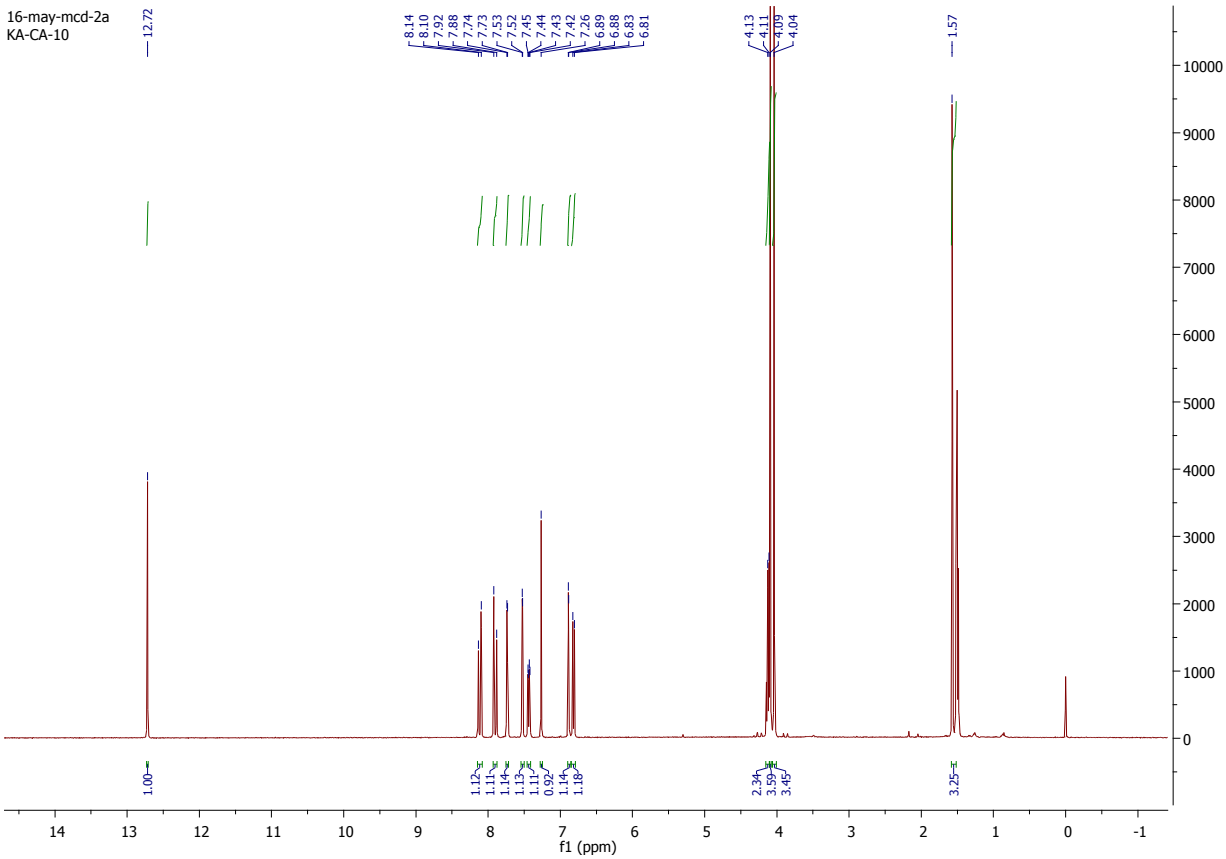
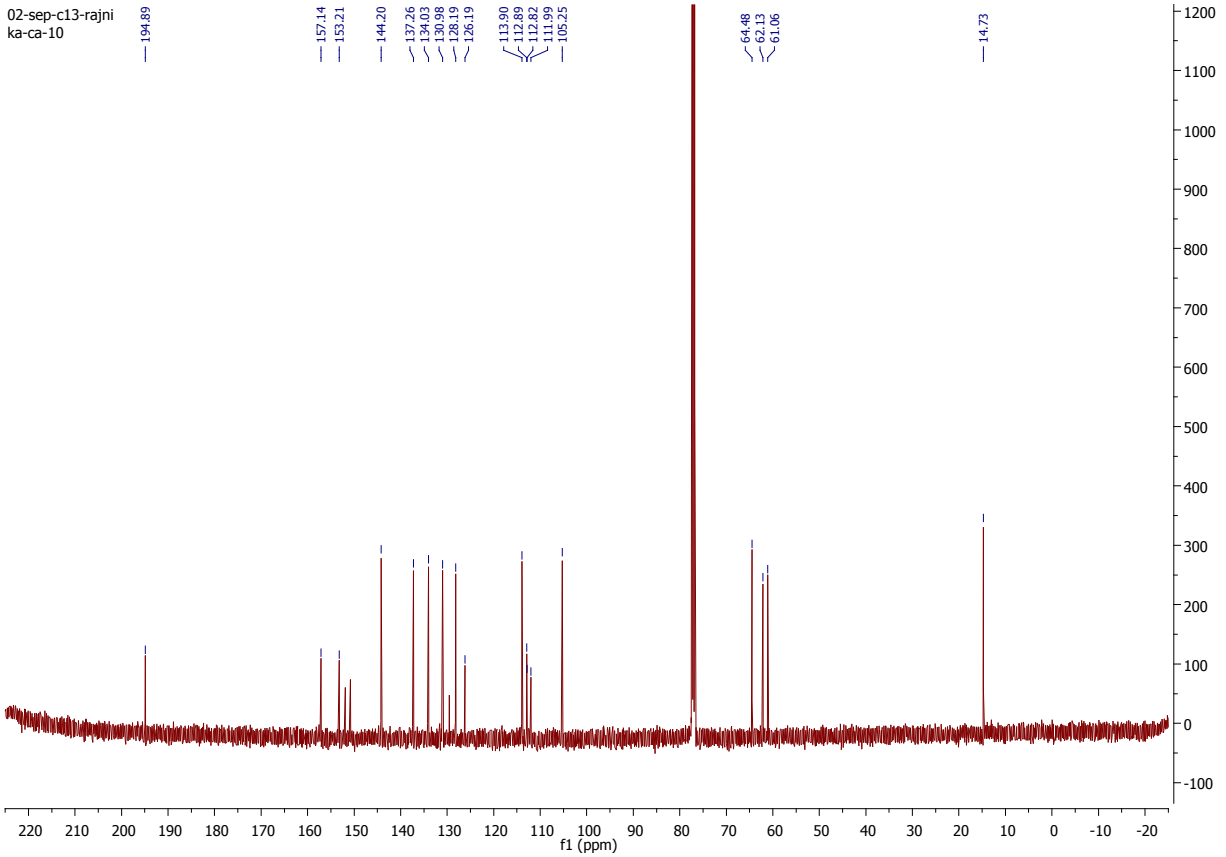

c13-rajni
KA-CA-09
144.17
136.52
134.87
129.83
128.95
105.48
61.94
61.12
0.02
f1 (ppm)

Figure S1.12. ^{1}H, ^{13}C and DEPT-135 NMR of **3j** in $CDCl_3$





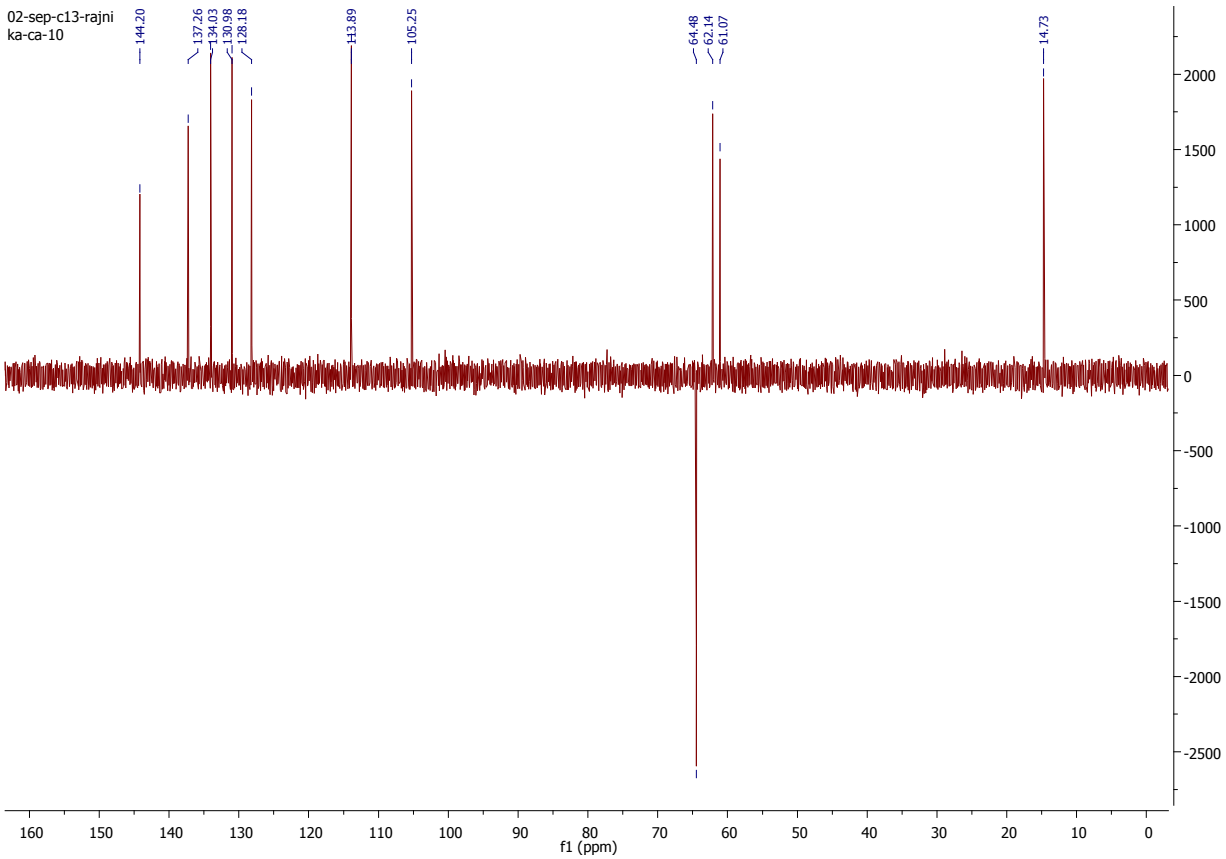
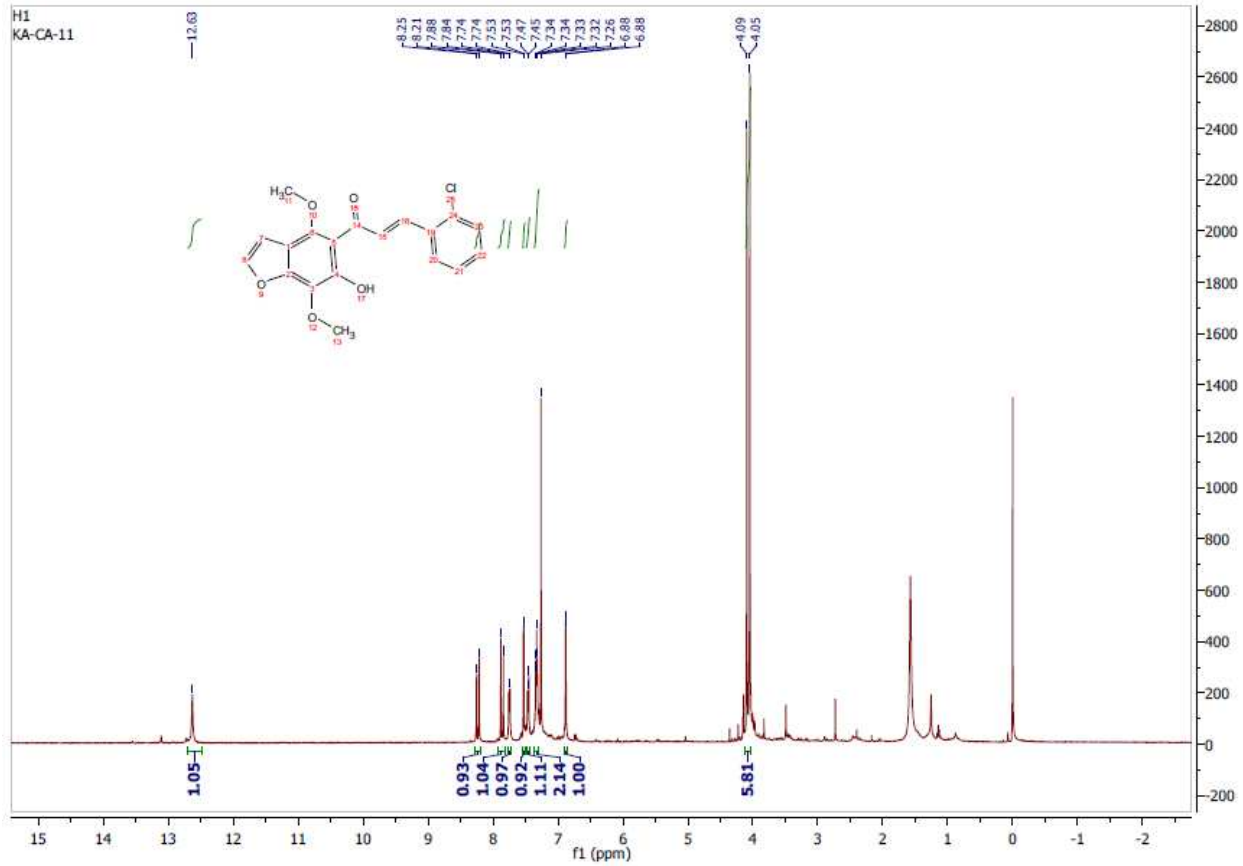
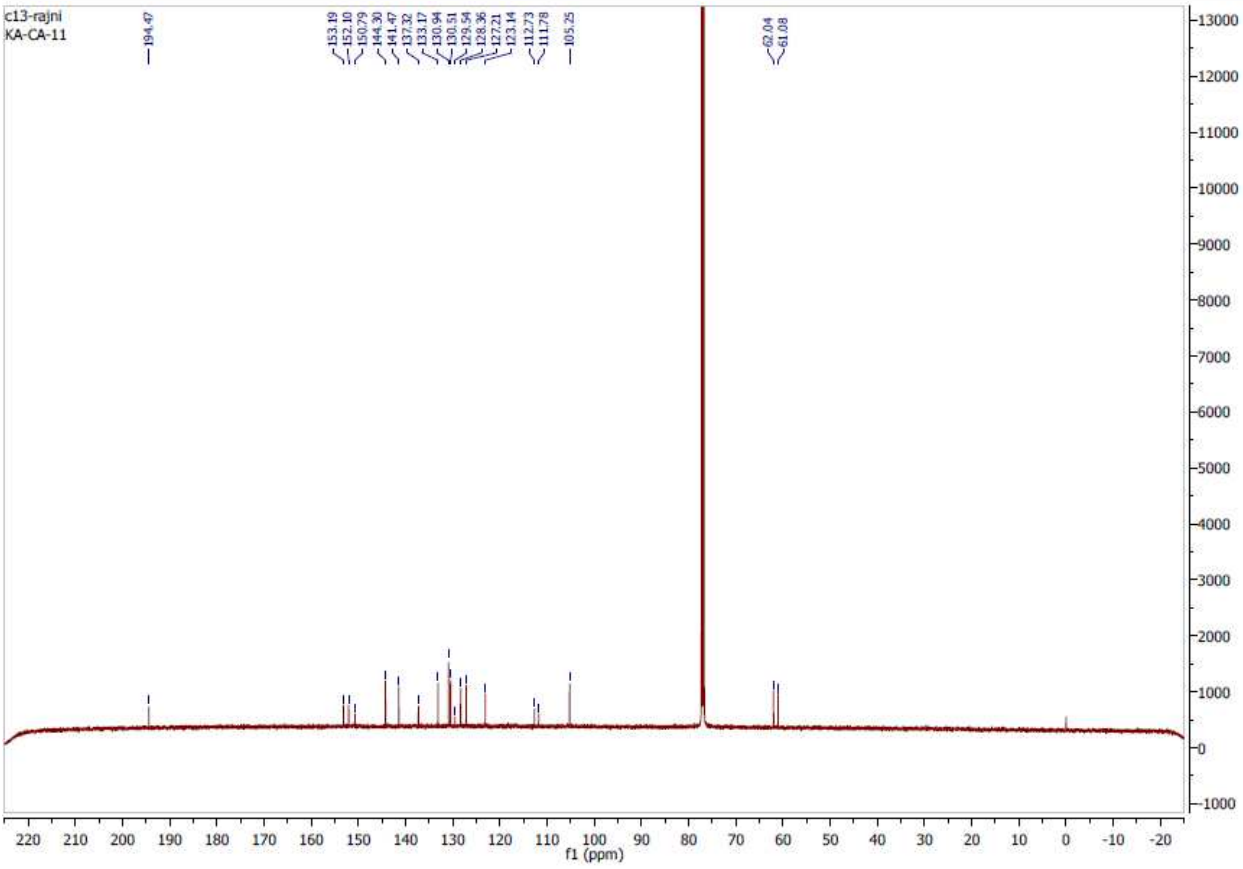

02-sep-c13-rajni
ka-ca-10
144.20
137.26
134.03
130.98
128.18
113.89
105.25
64.48
62.14
61.07
14.73
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Figure S1.13. ^{1}H, ^{13}C and DEPT-135 NMR of **3k** in $CDCl_3$





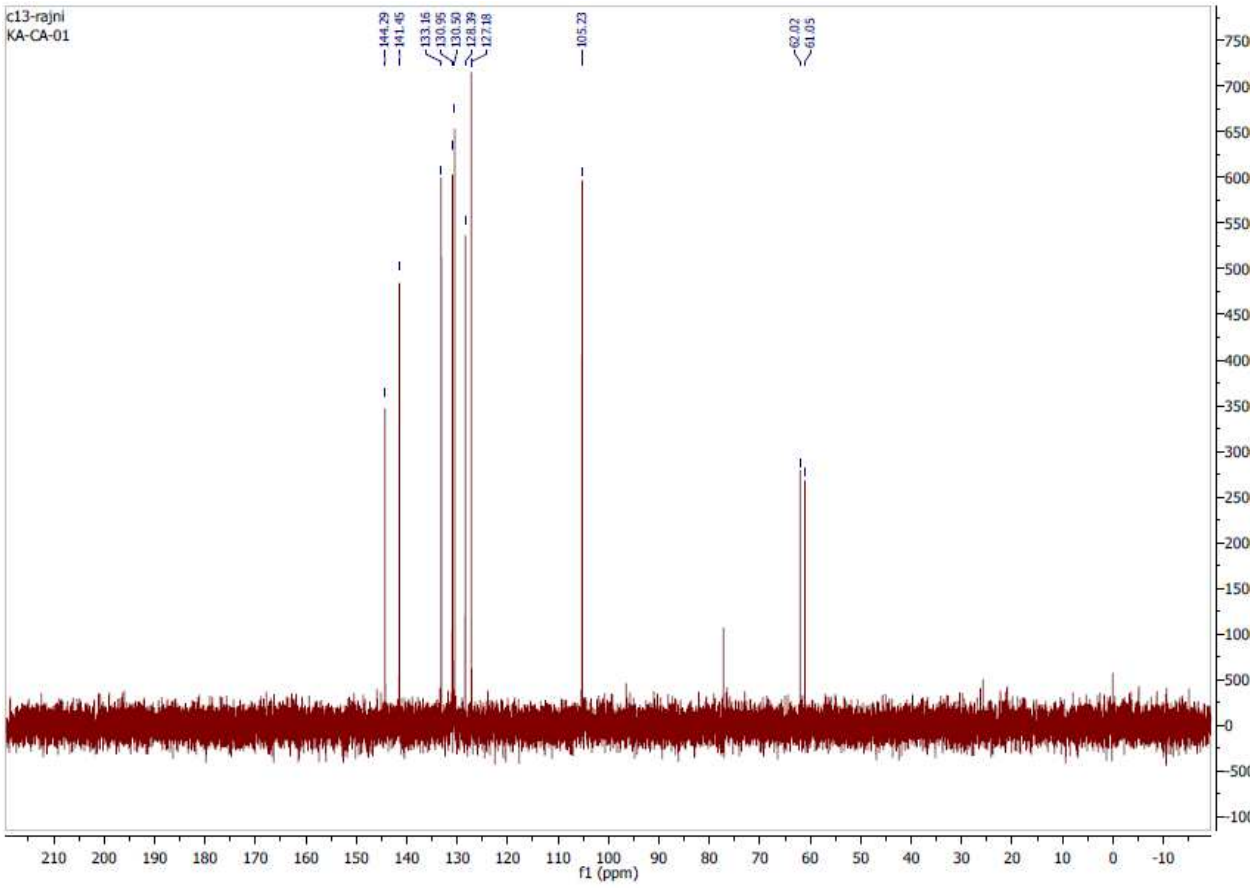
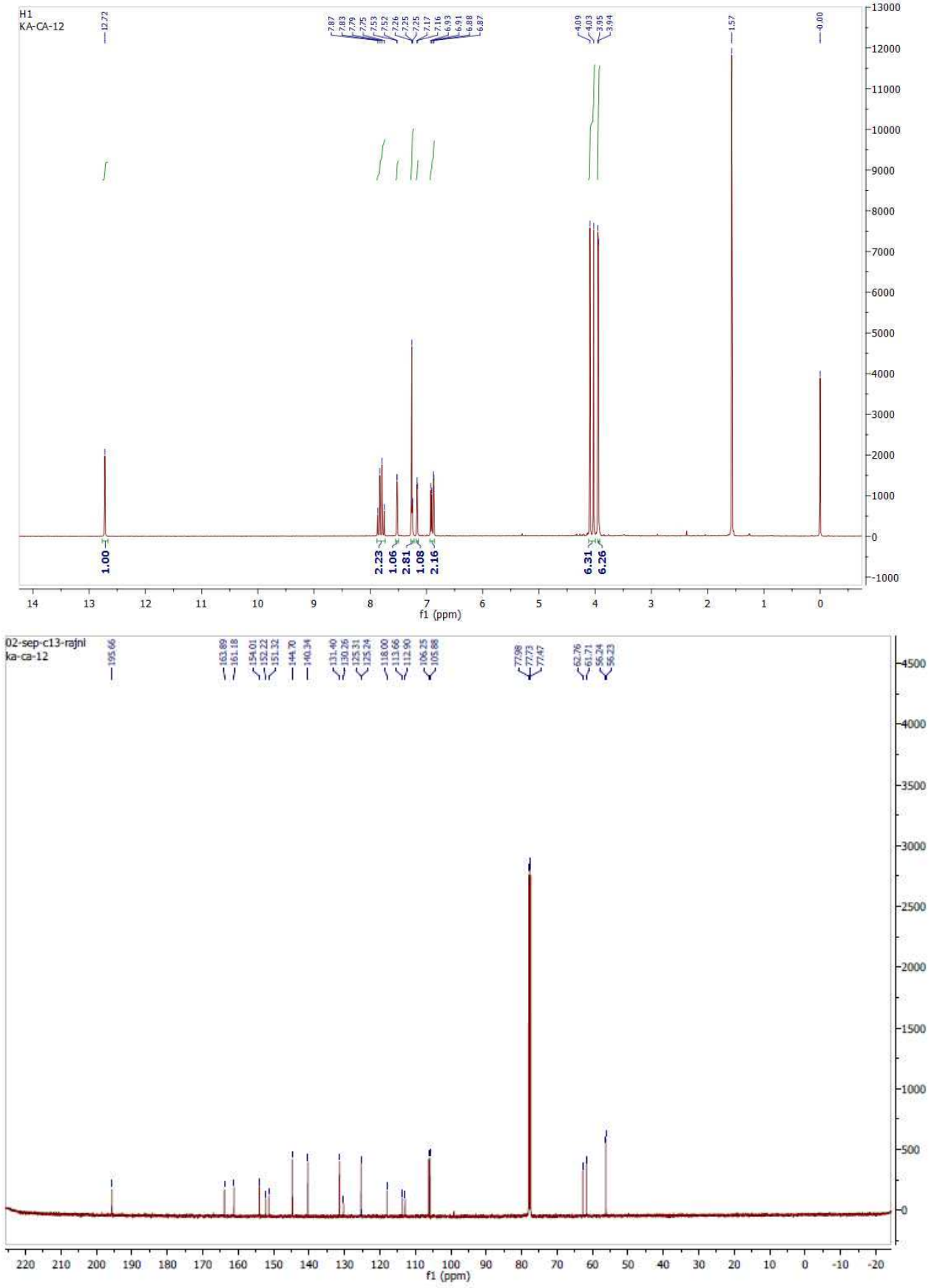

c13-rajni
KA-CA-01
144.29
141.45
133.16
130.95
130.50
128.39
127.18
105.23
62.02
61.05
f1 (ppm)

Figure S1.14. ^{1}H, ^{13}C and DEPT-135 NMR of **3l** in $CDCl_3$



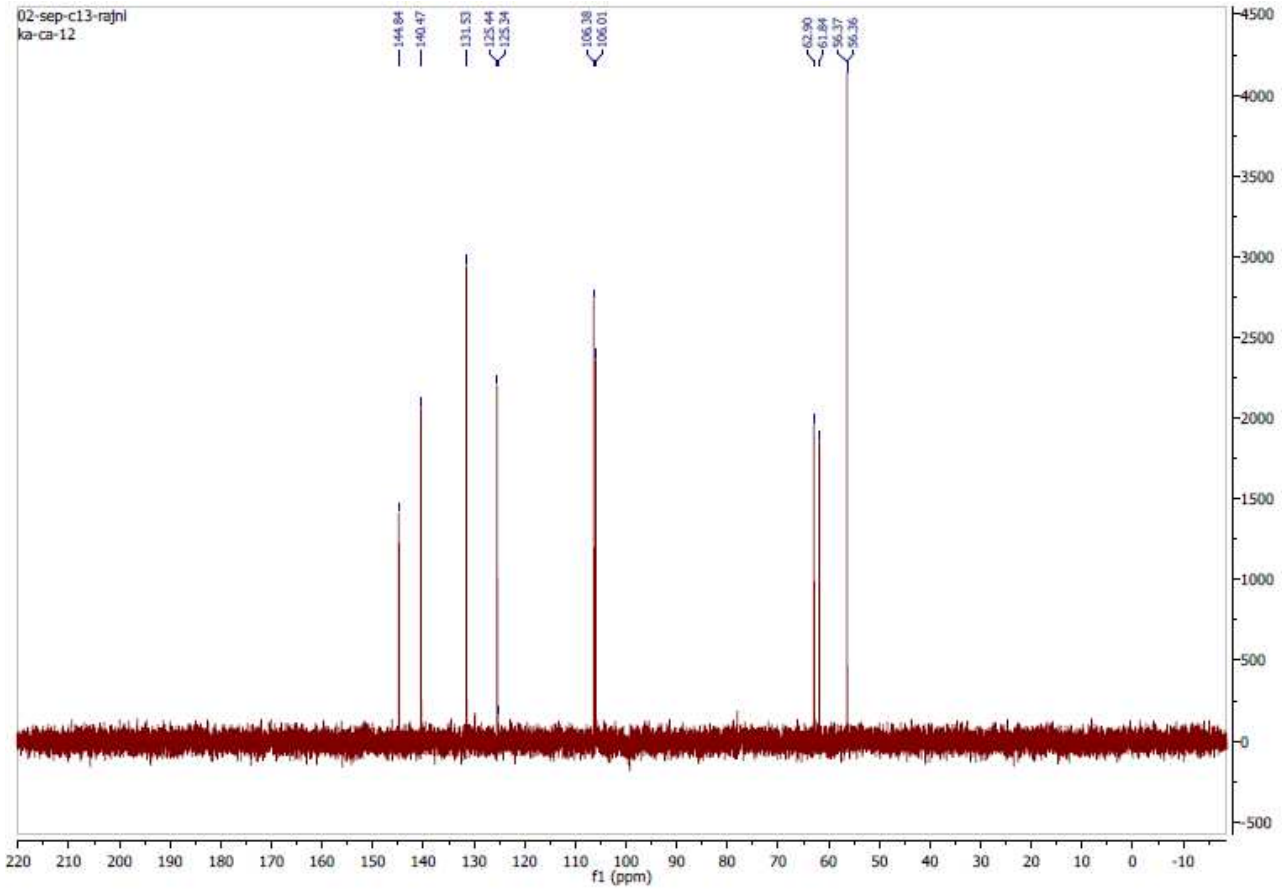
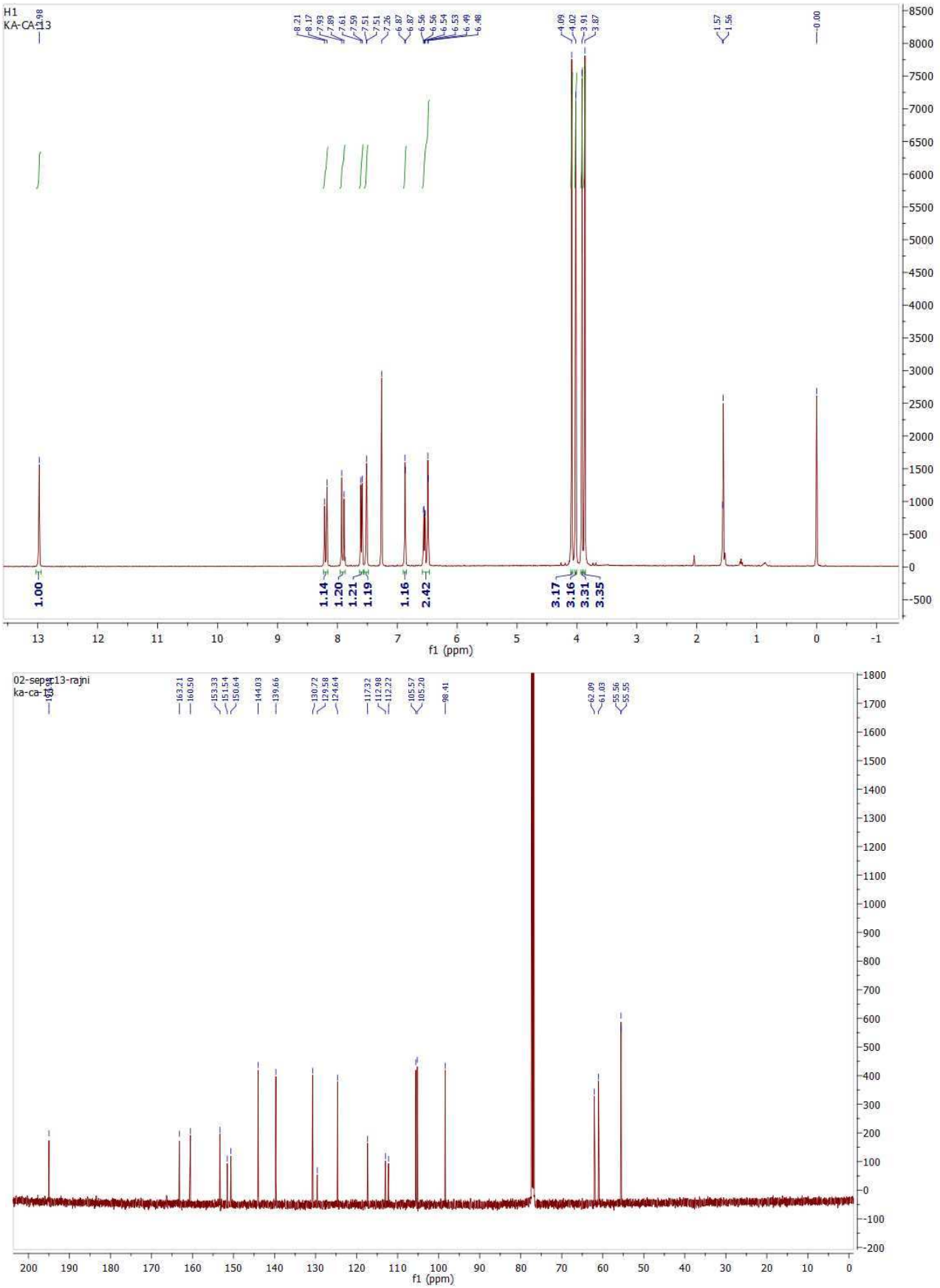

02-sep-c13-rajni
ka-ca-12
144.84
140.47
131.53
125.44
125.34
106.38
106.01
62.90
61.84
56.37
56.36
f1 (ppm)

Figure S1.15. ^{1}H, ^{13}C and DEPT-135 NMR of **3m** in $CDCl_3$



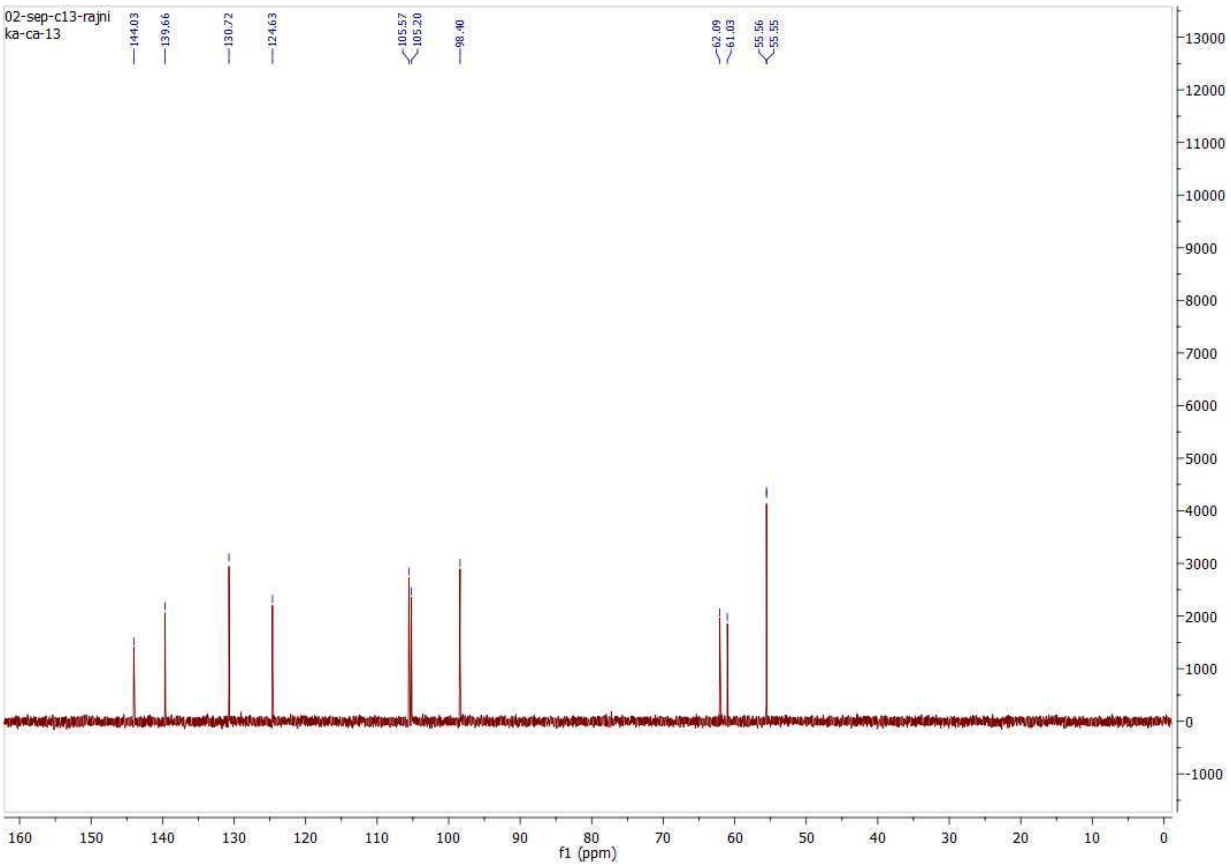
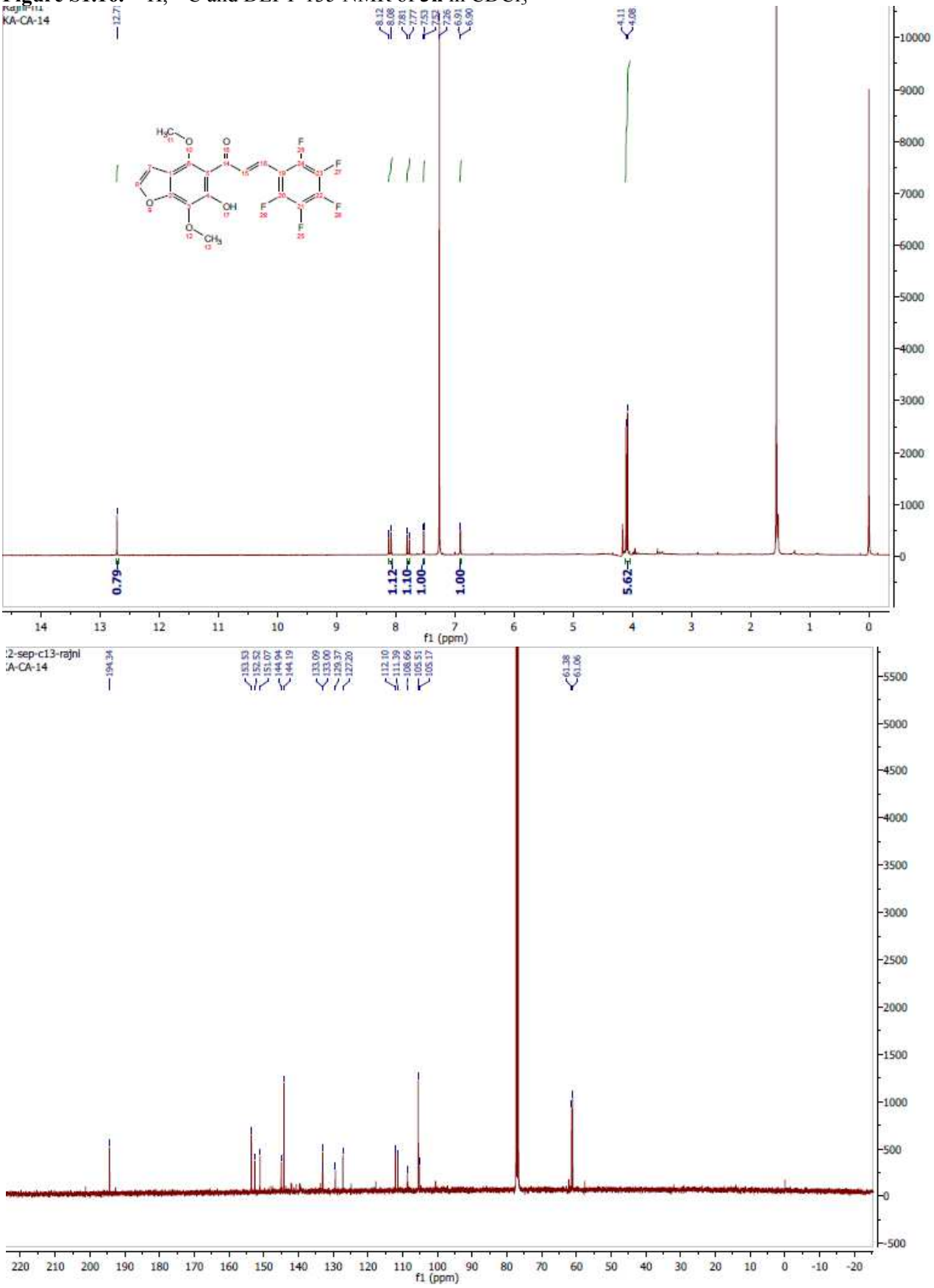

02-sep-c13-rajni
ka-ca-13
144.03
139.66
130.72
124.63
105.57
105.20
98.40
62.09
61.03
55.56
55.55
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Figure S1.16. ^{1}H, ^{13}C and DEPT-135 NMR of **3n** in $CDCl_3$



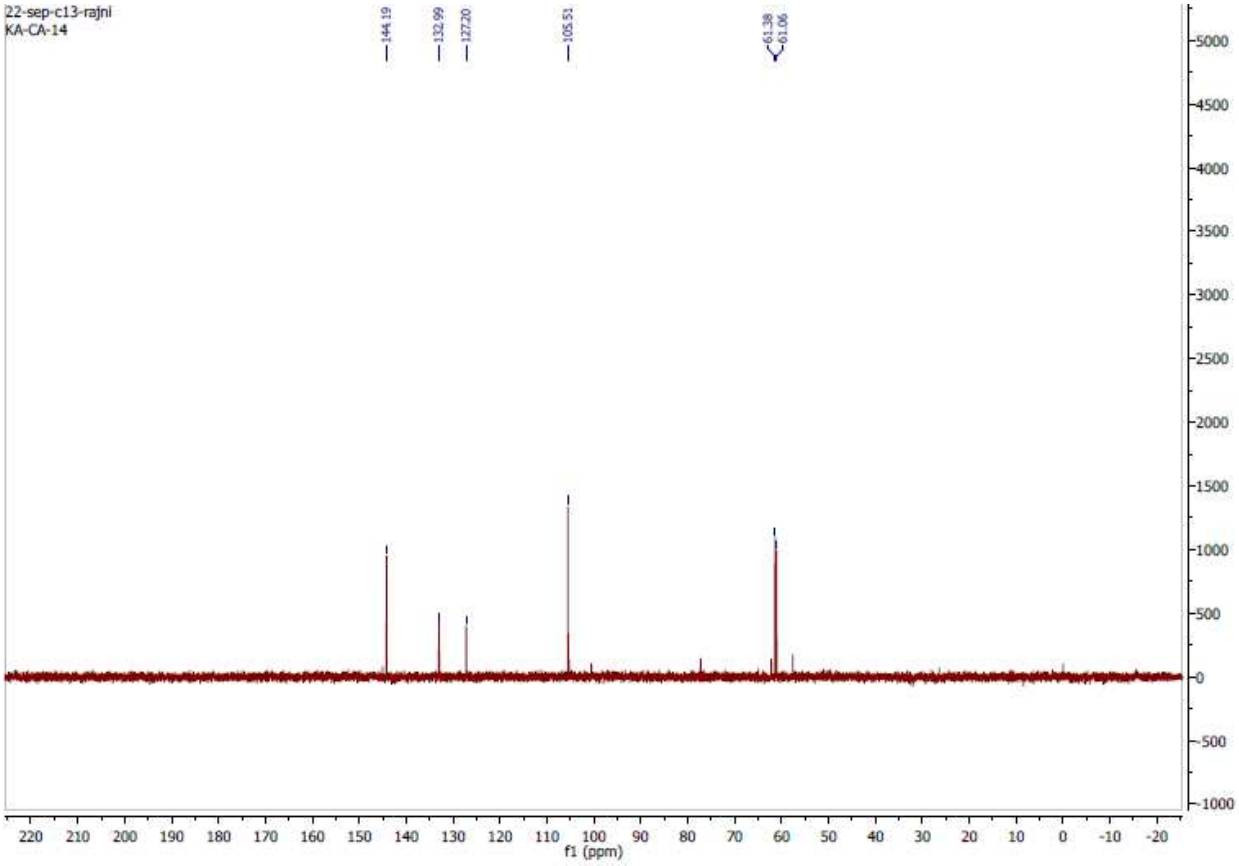
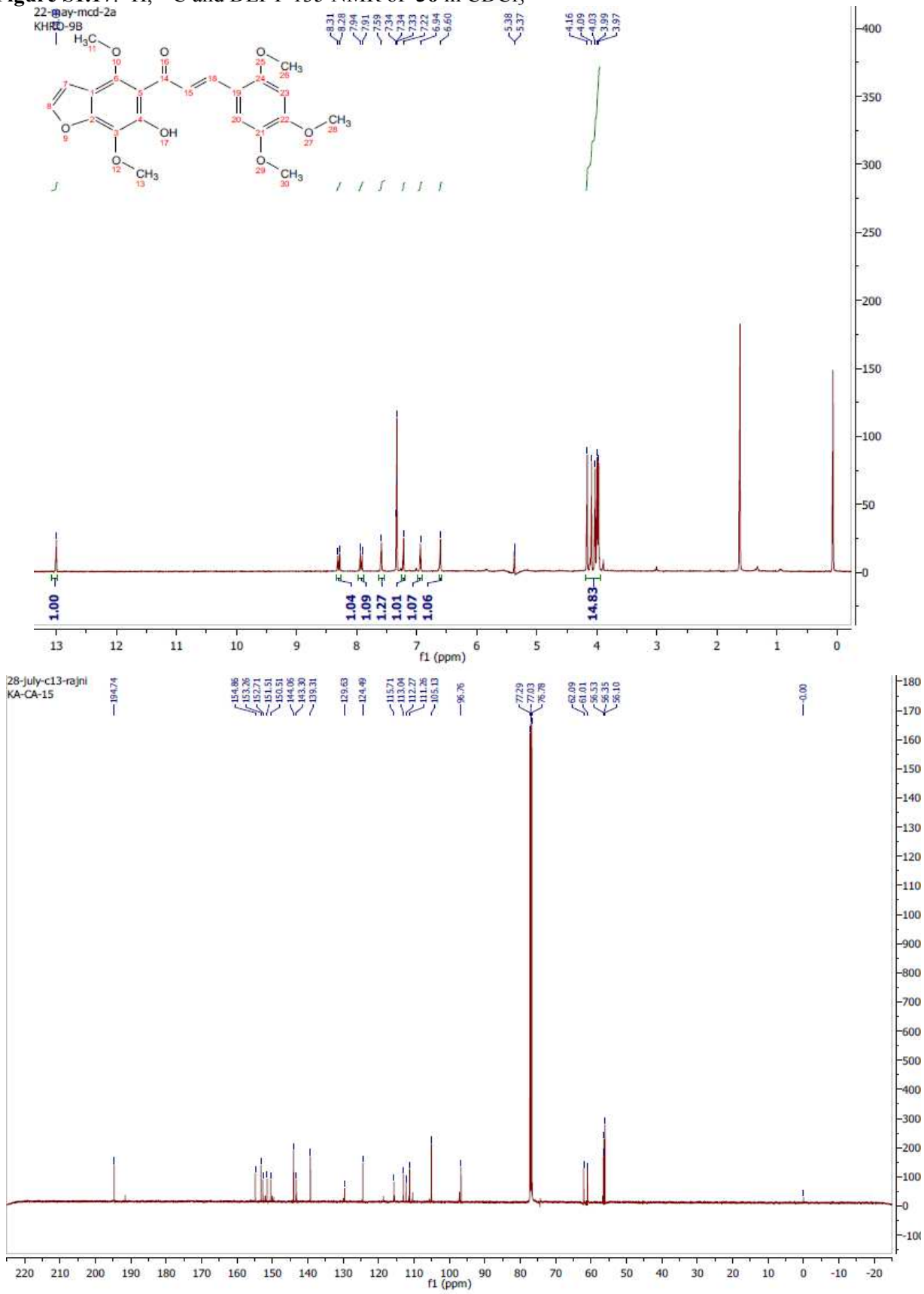

22-sep-c13-rajni
KA-CA-14
144.19
132.99
127.20
105.51
61.38
61.06
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

Figure S1.17. ^{1}H, ^{13}C and DEPT-135 NMR of **3o** in $CDCl_3$



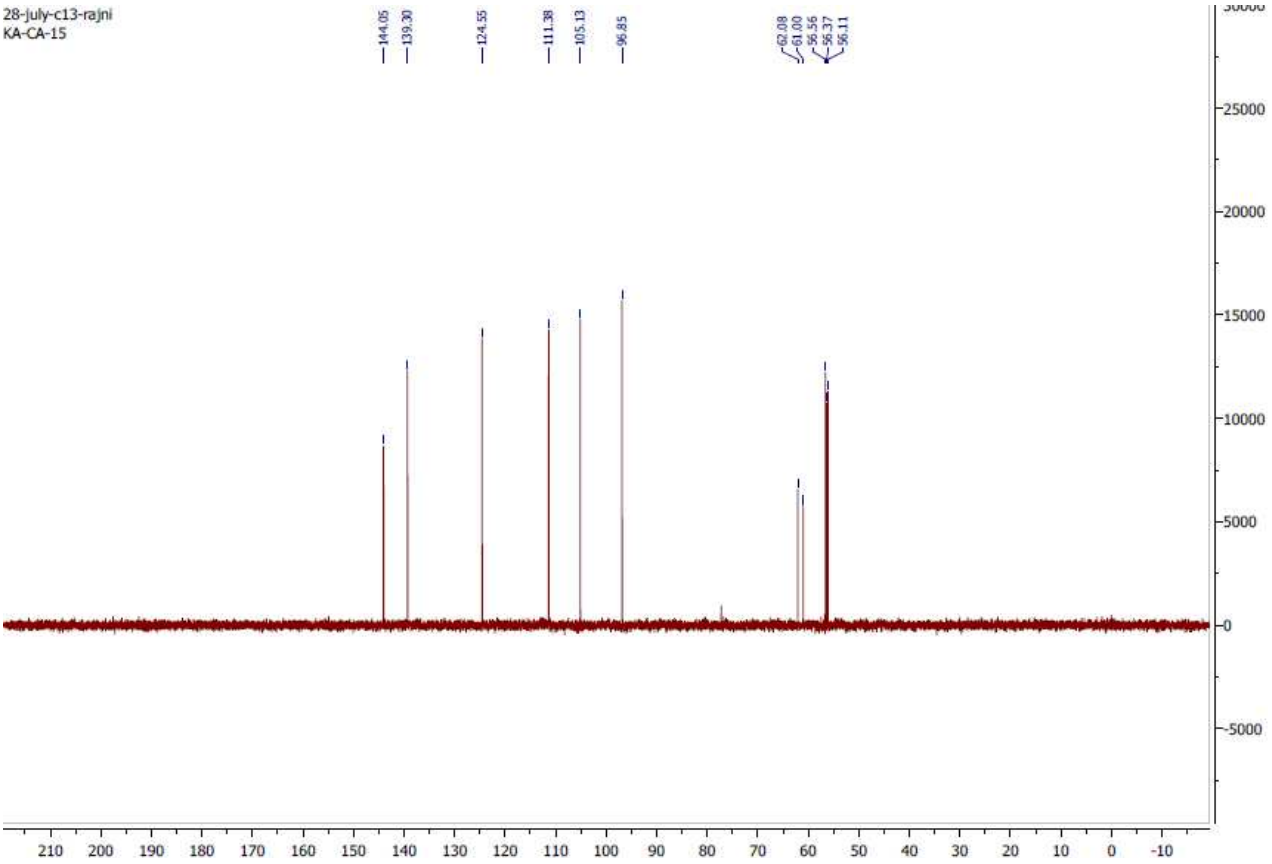
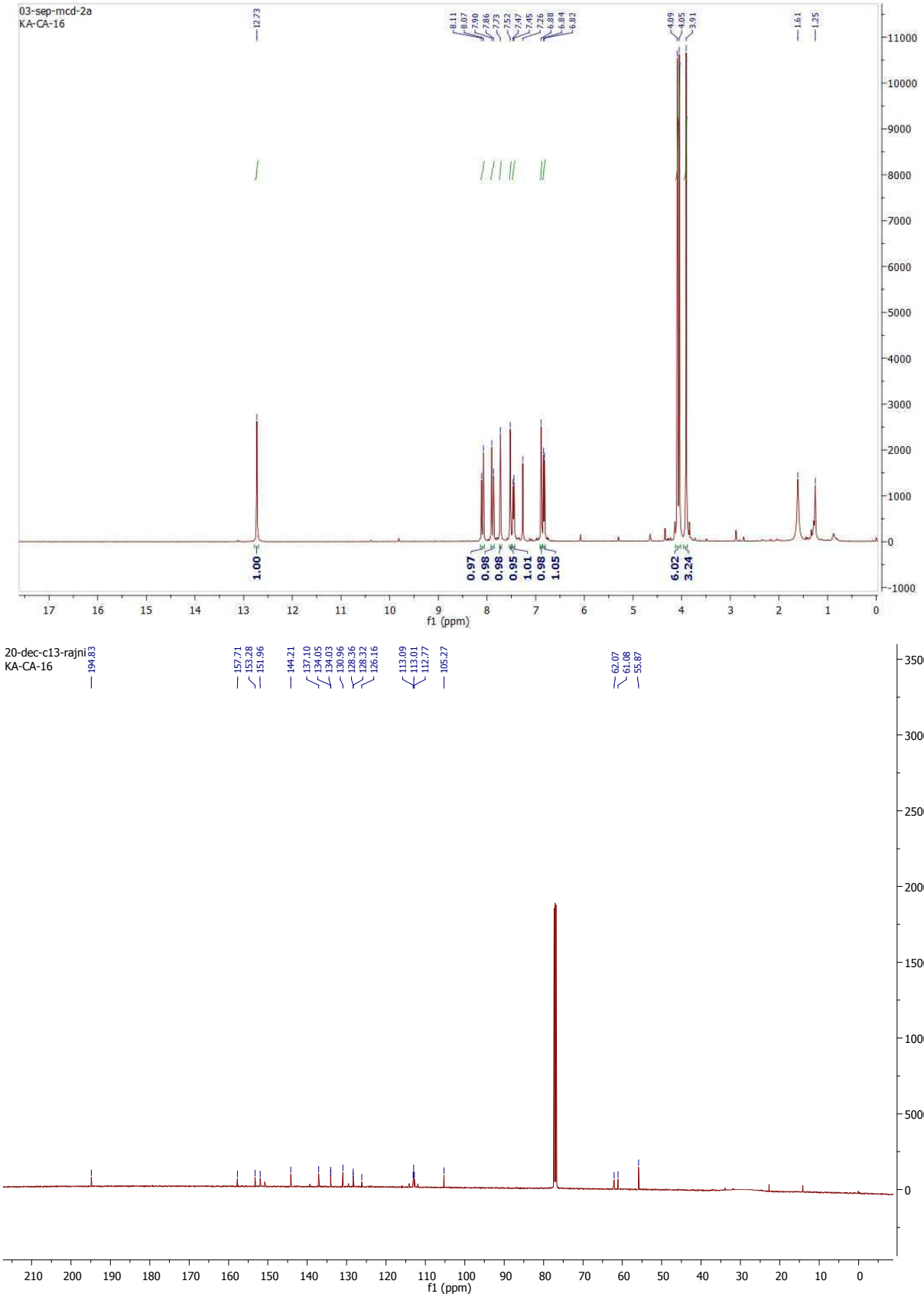

28-july-c13-rajni
KA-CA-15
144.05
139.30
124.55
111.38
105.13
96.85
62.08
61.00
56.56
56.37
56.11
25000
20000
15000
10000
5000
0
-5000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

Figure S1.18. ^{11}H, ^{13}C and DEPT-135 NMR of **3p** in $CDCl_3$



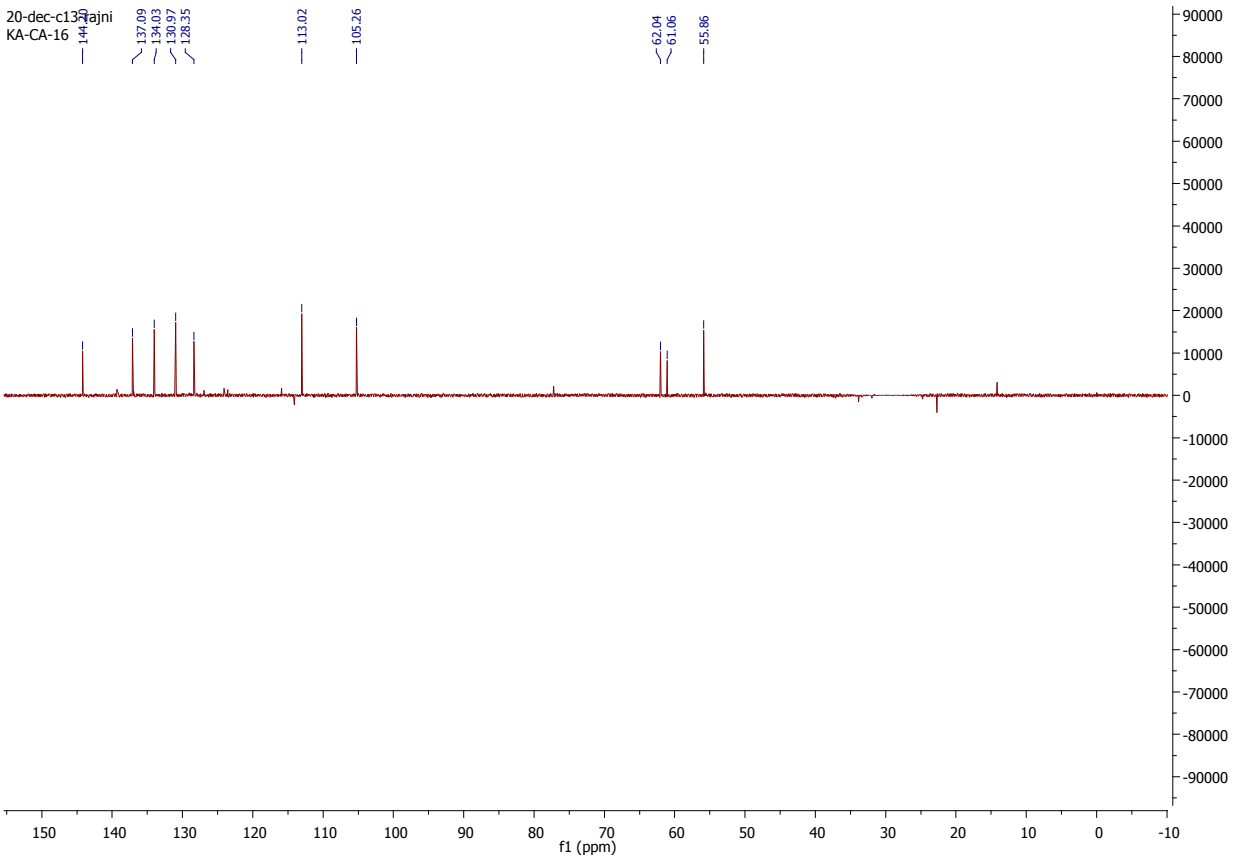
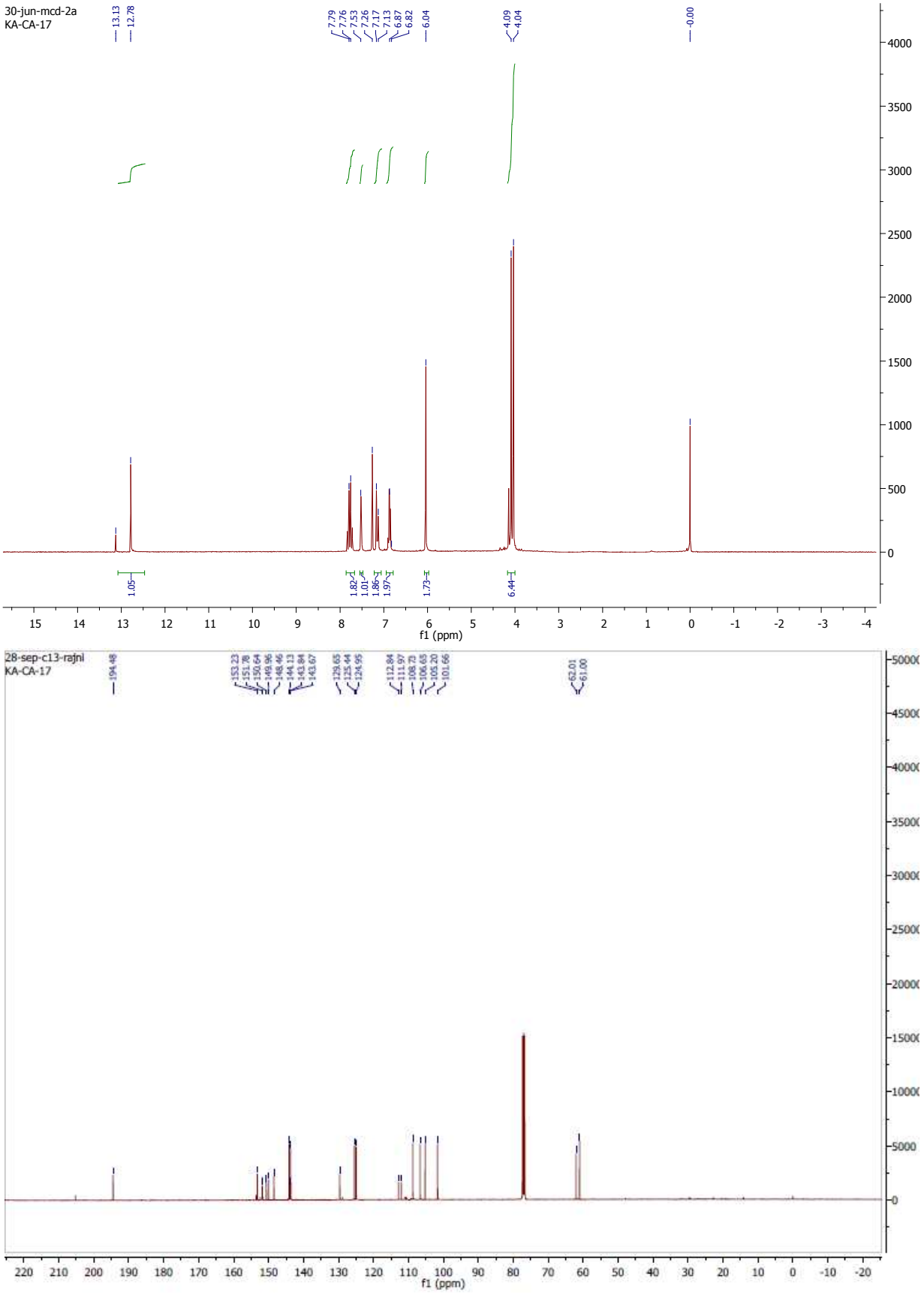

20-dec-c13-rajni
KA-CA-16
144.50
137.09
134.03
130.97
128.35
113.02
105.26
62.04
61.06
55.86
f1 (ppm)

Figure S1.19. ^{1}H, ^{13}C and DEPT-135 NMR of **3q** in $CDCl_3$



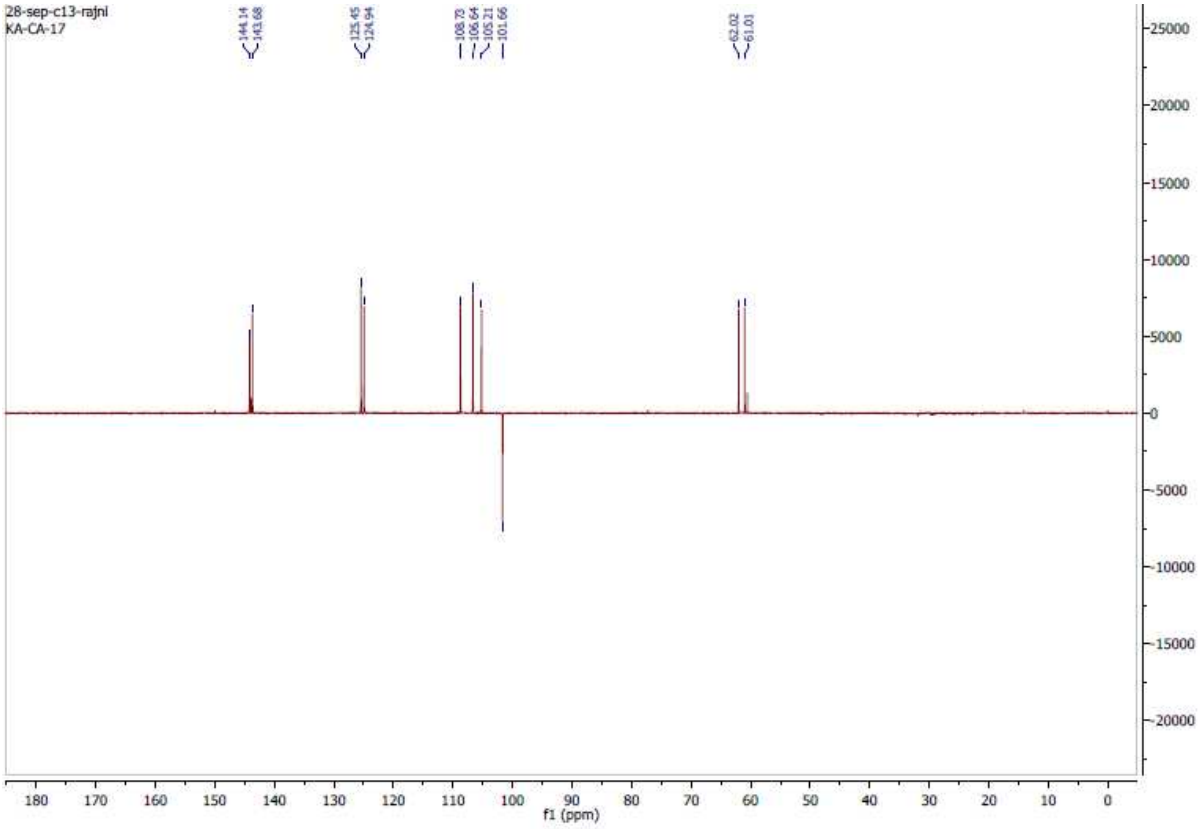
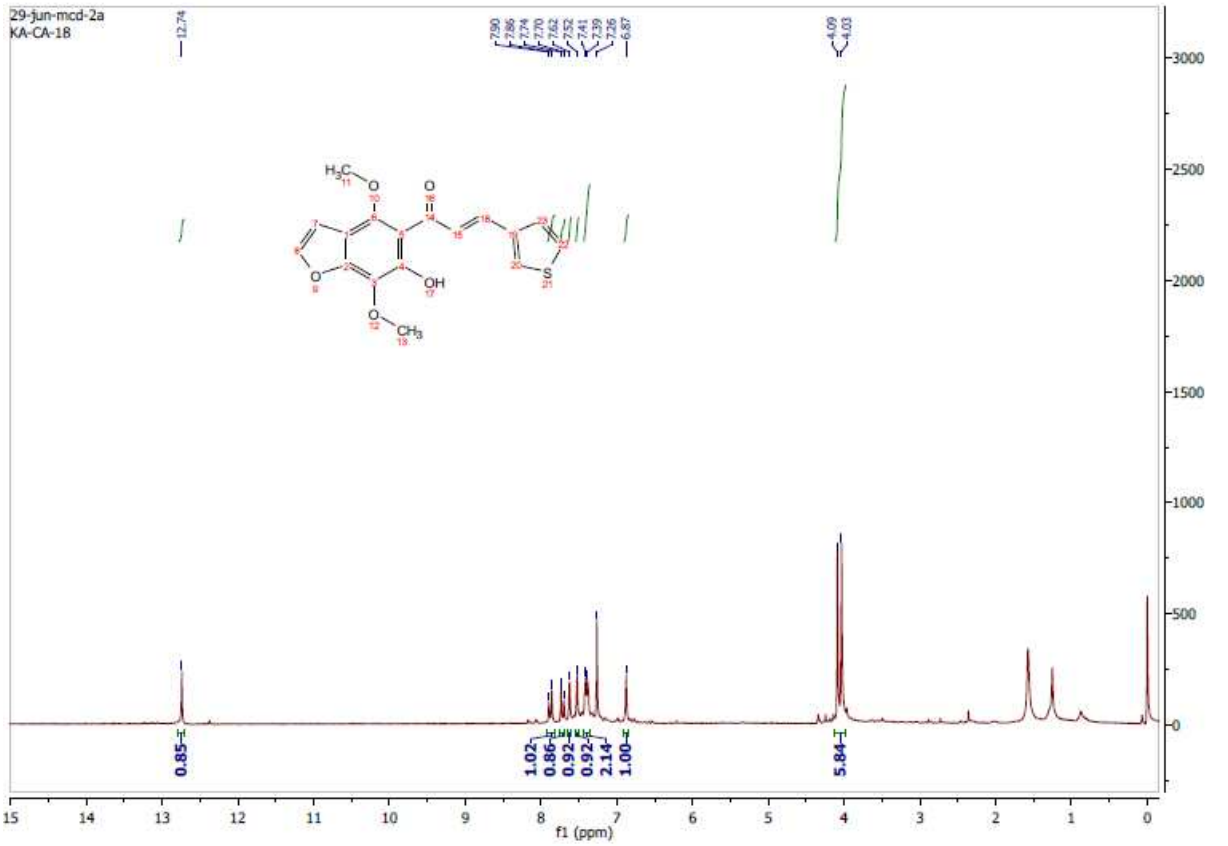
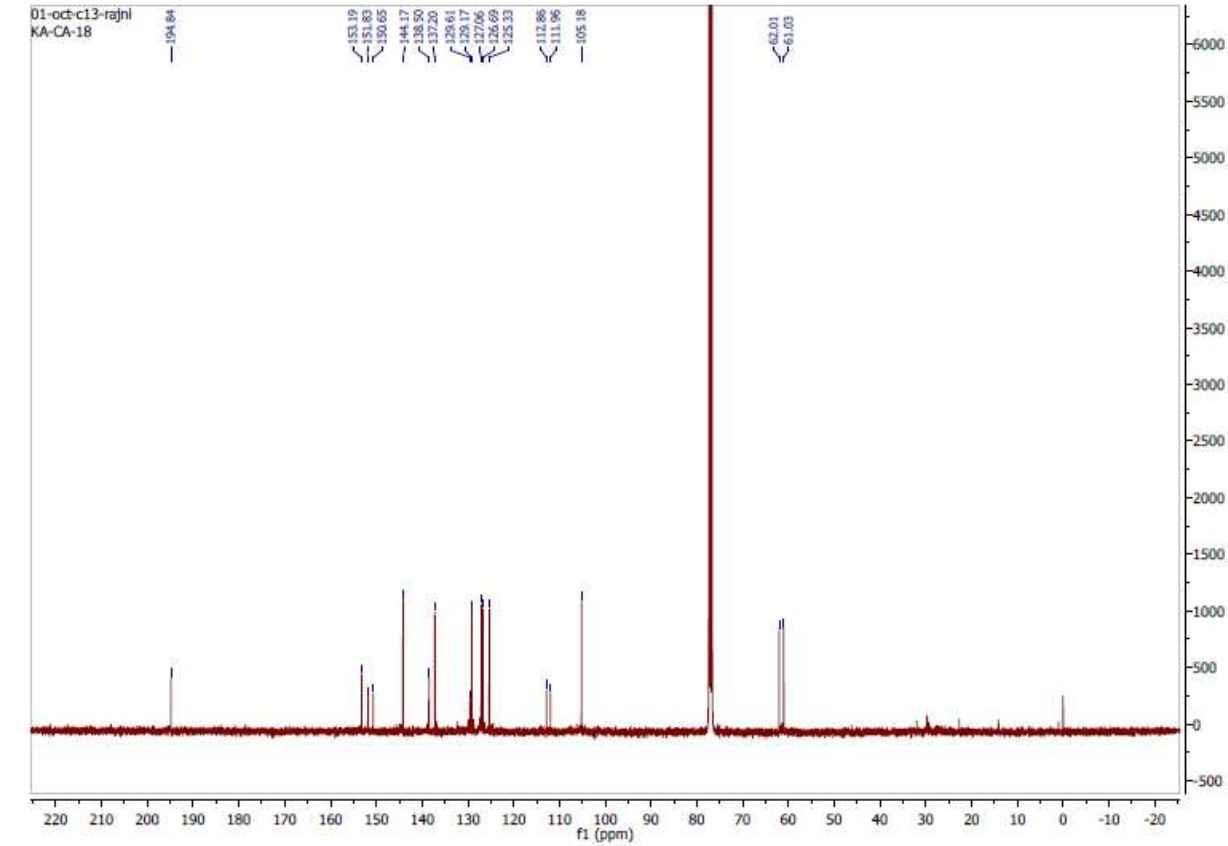

28-sep-c13-rajni
KA-CA-17
144.14
143.68
125.45
124.94
108.73
106.64
105.21
101.66
62.02
61.01
25000
20000
15000
10000
5000
0
5000
10000
15000
20000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Figure S1.20. ^{1}H, ^{13}C and DEPT-135 NMR of **3r** in $CDCl_3$





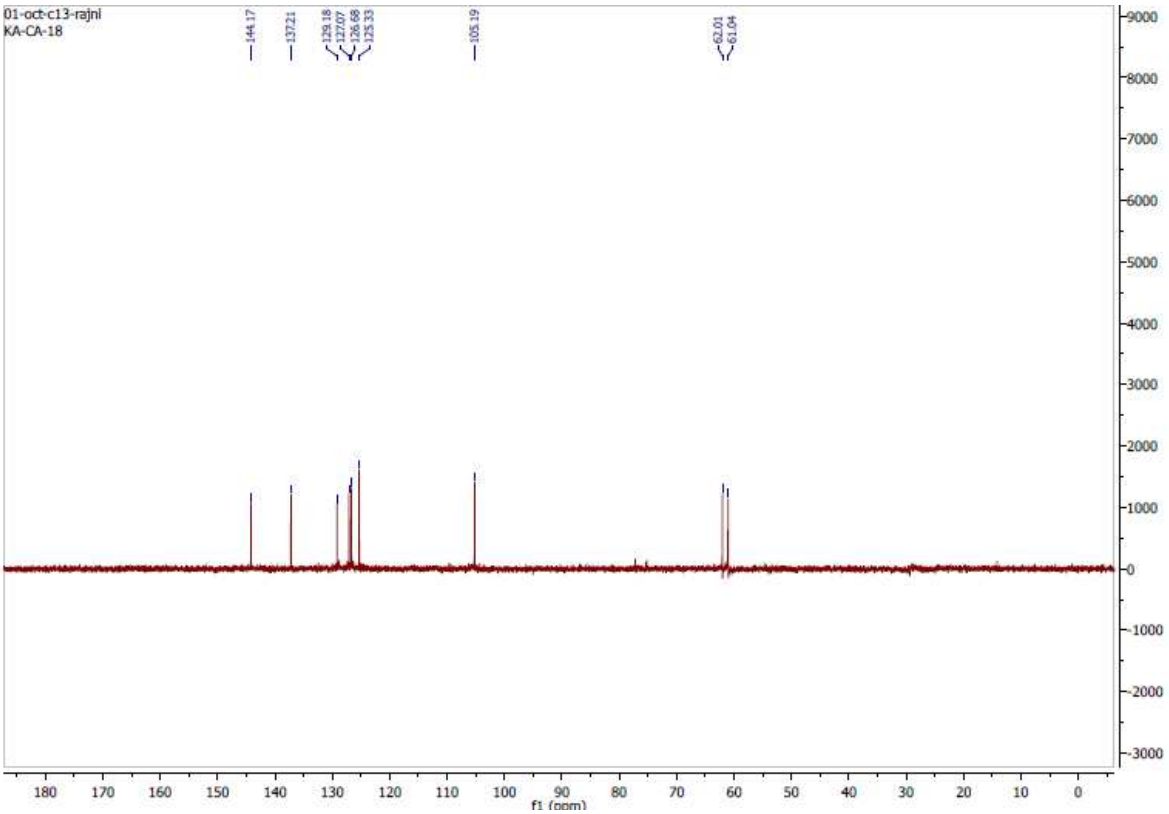
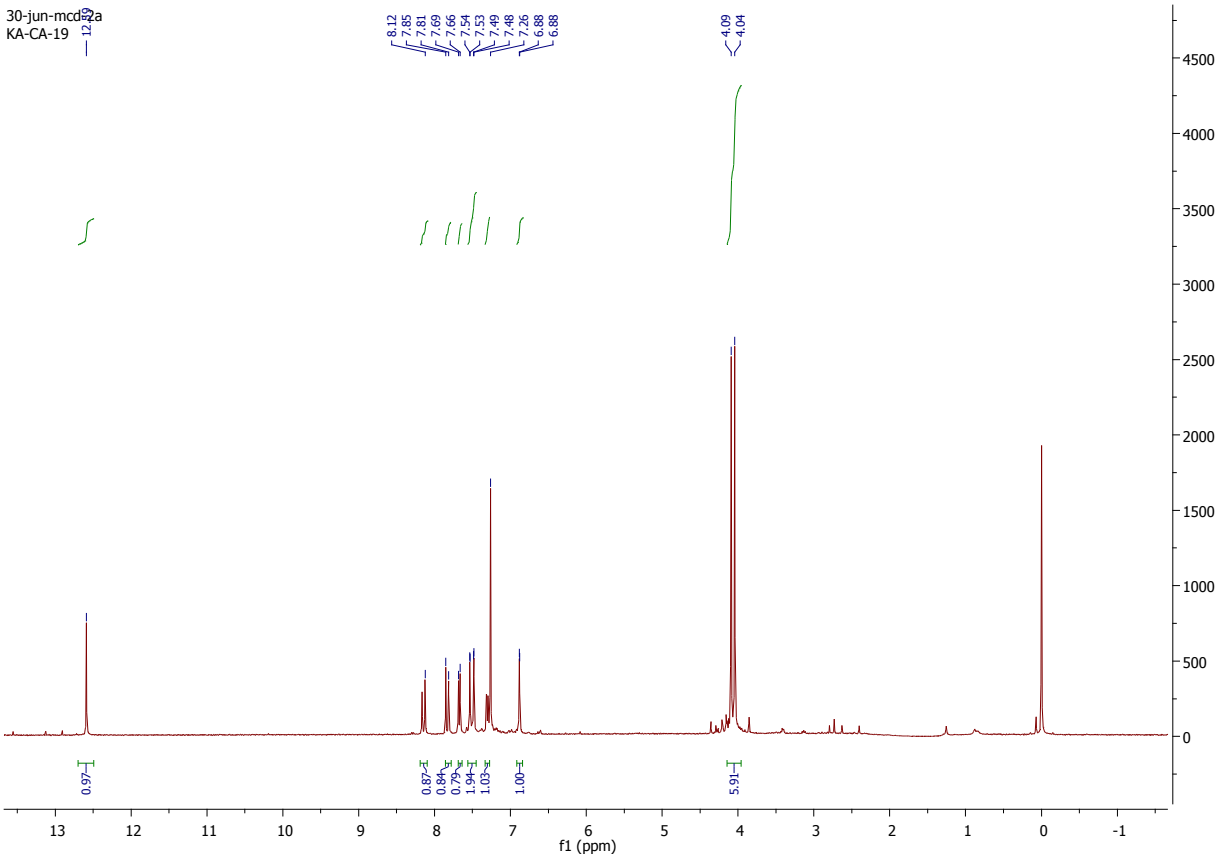
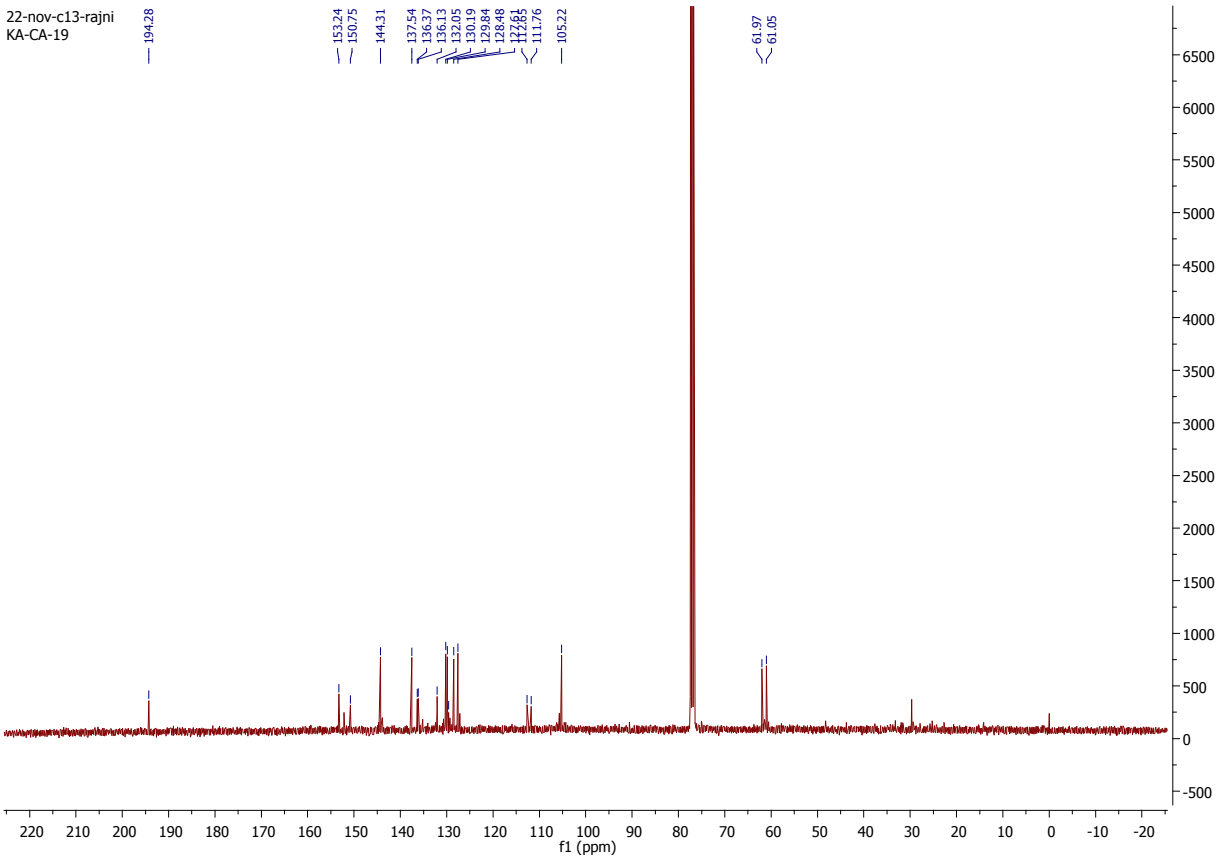

01-oct-c13-rajni
KA-CA-18
144.17
137.21
129.18
127.07
126.68
125.33
105.19
62.01
61.04
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Figure S1.21. ^{1}H, ^{13}C and DEPT-135 NMR of **3s** in $CDCl_3$





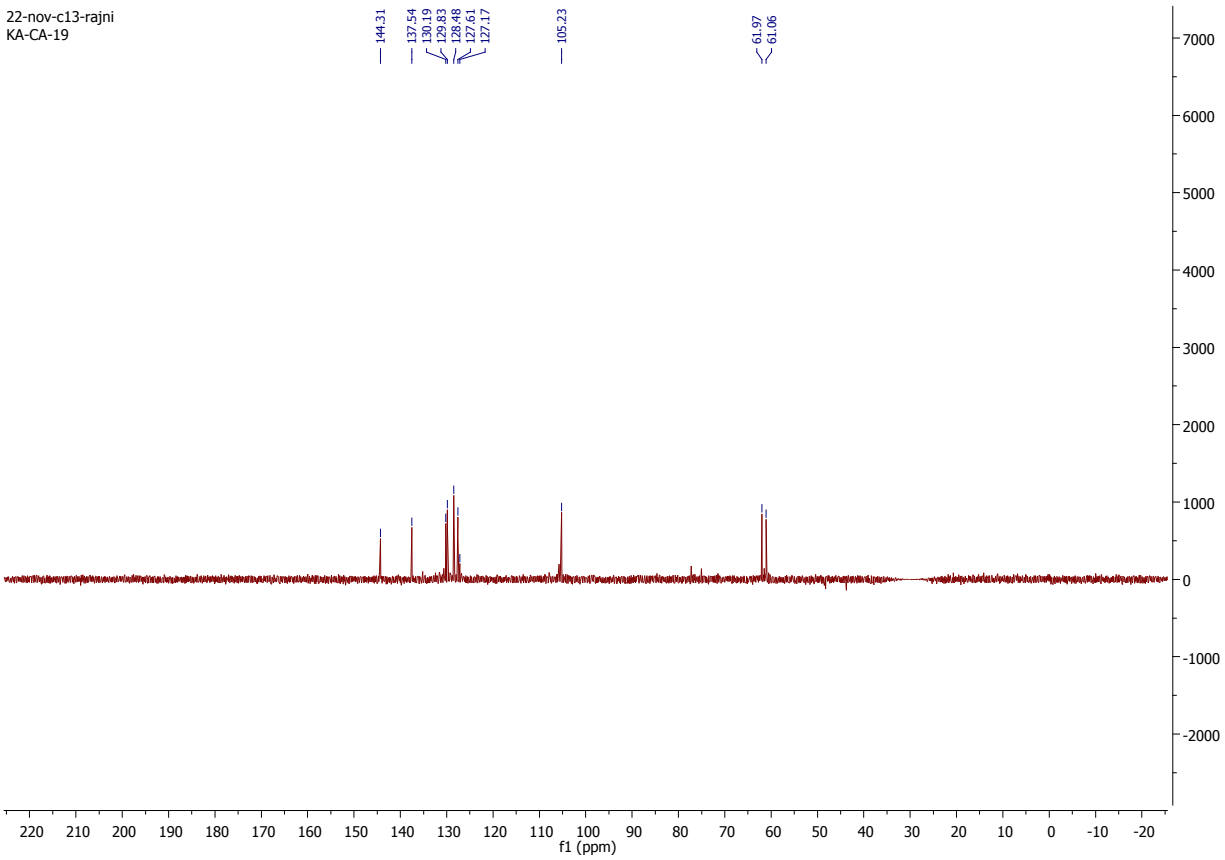
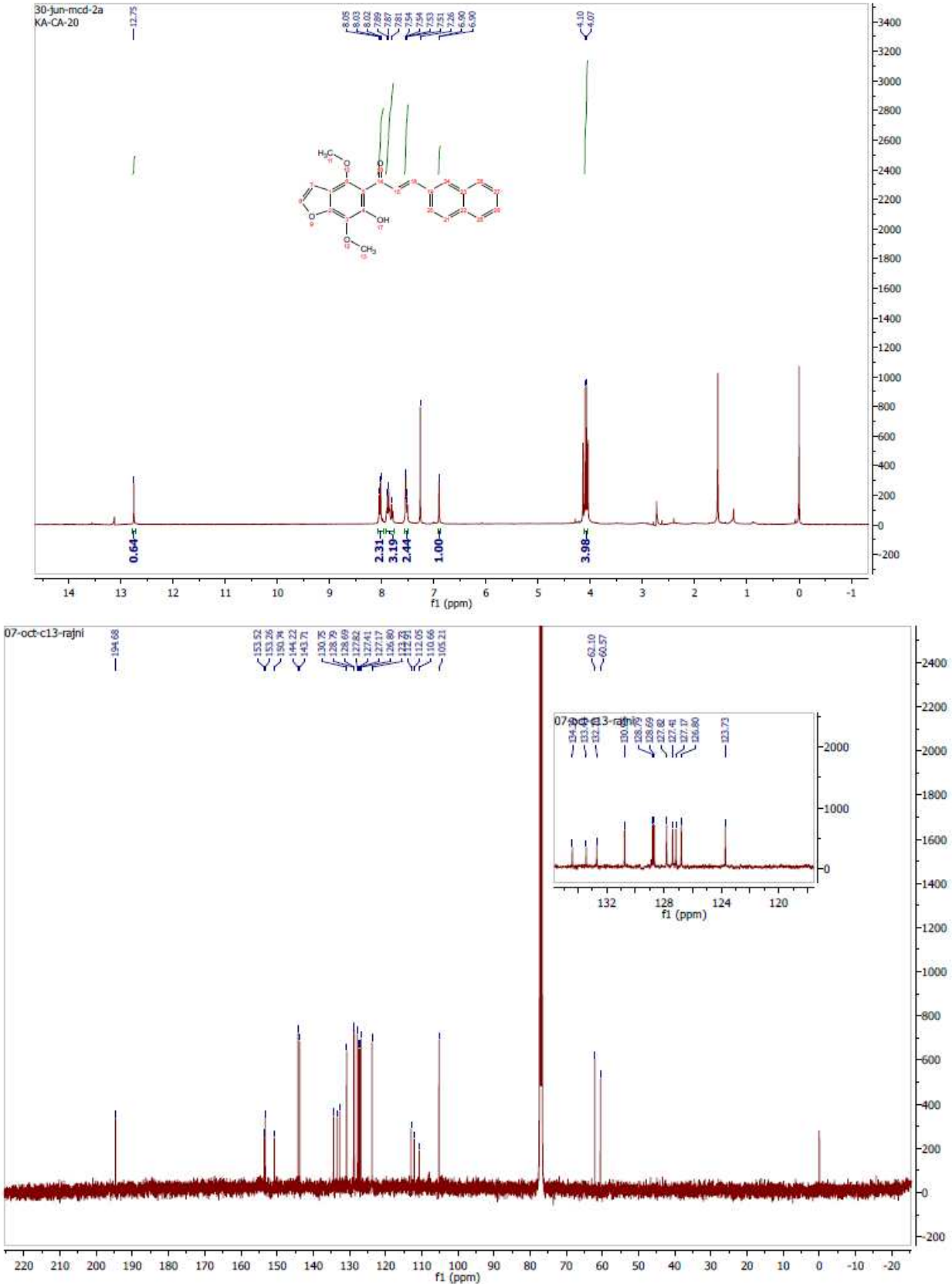

22-nov-c13-rajni
KA-CA-19
144.31
137.54
130.19
129.83
128.48
127.61
127.17
105.23
61.97
61.06
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

Figure S1.22. ^{1}H, ^{13}C and DEPT-135 NMR of **3t** in $CDCl_3$



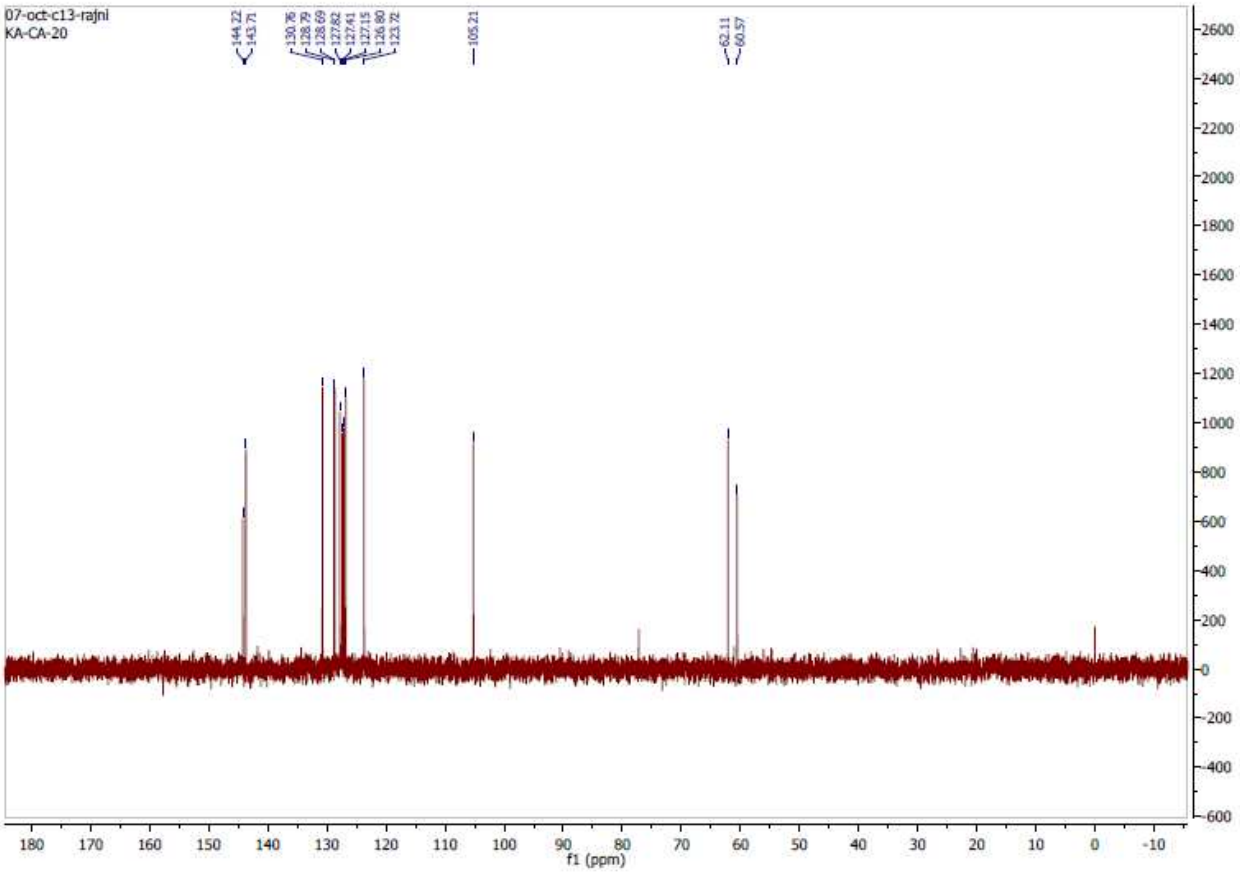
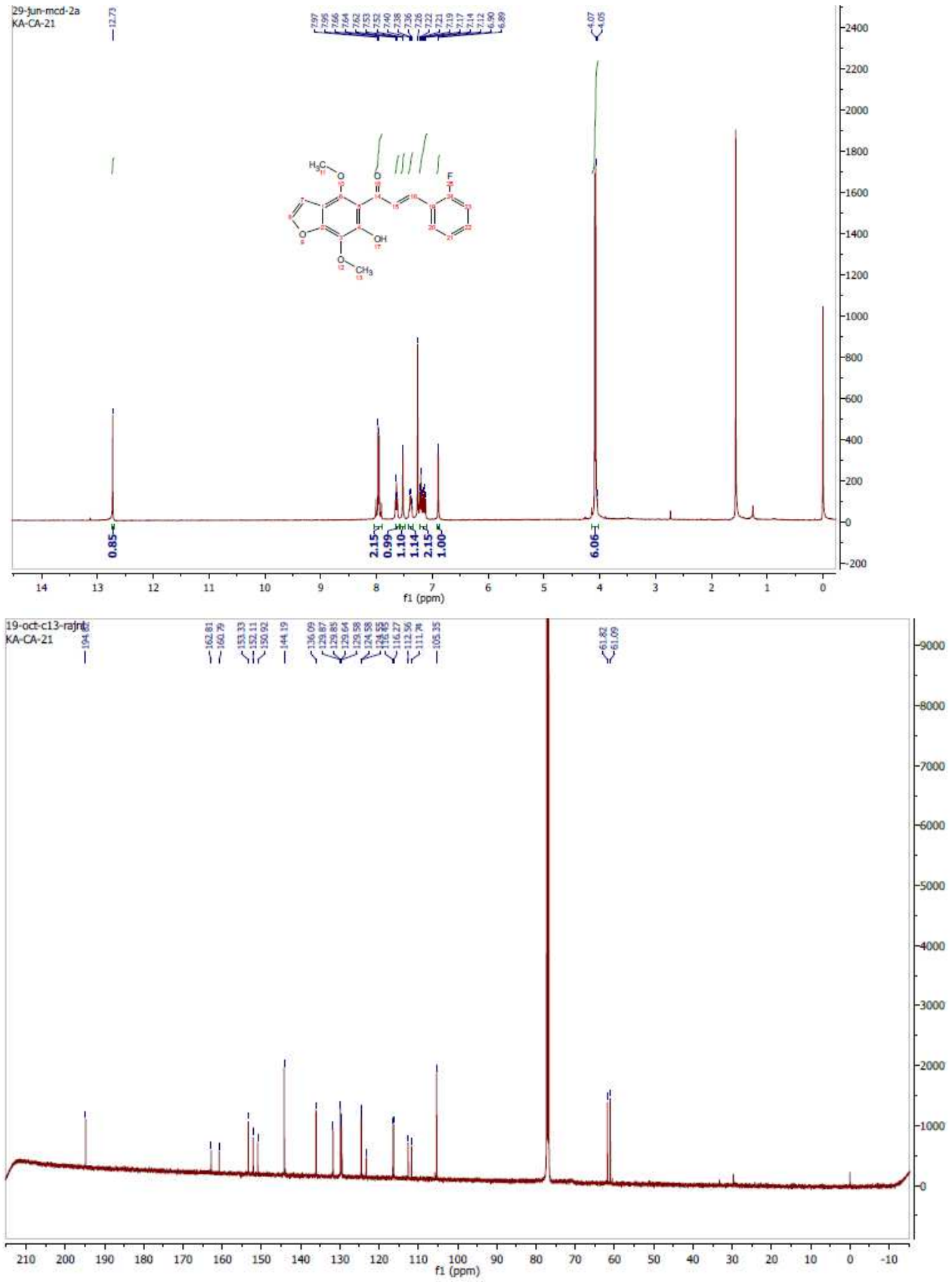

07-oct-c13-rajni
KA-CA-20
144.22
143.71
130.76
128.79
128.69
127.82
127.41
127.15
126.80
123.72
105.21
62.11
60.57
f1 (ppm)

Figure S1.23. ^{1}H, ^{13}C and DEPT-135 NMR of **3u** in $CDCl_3$



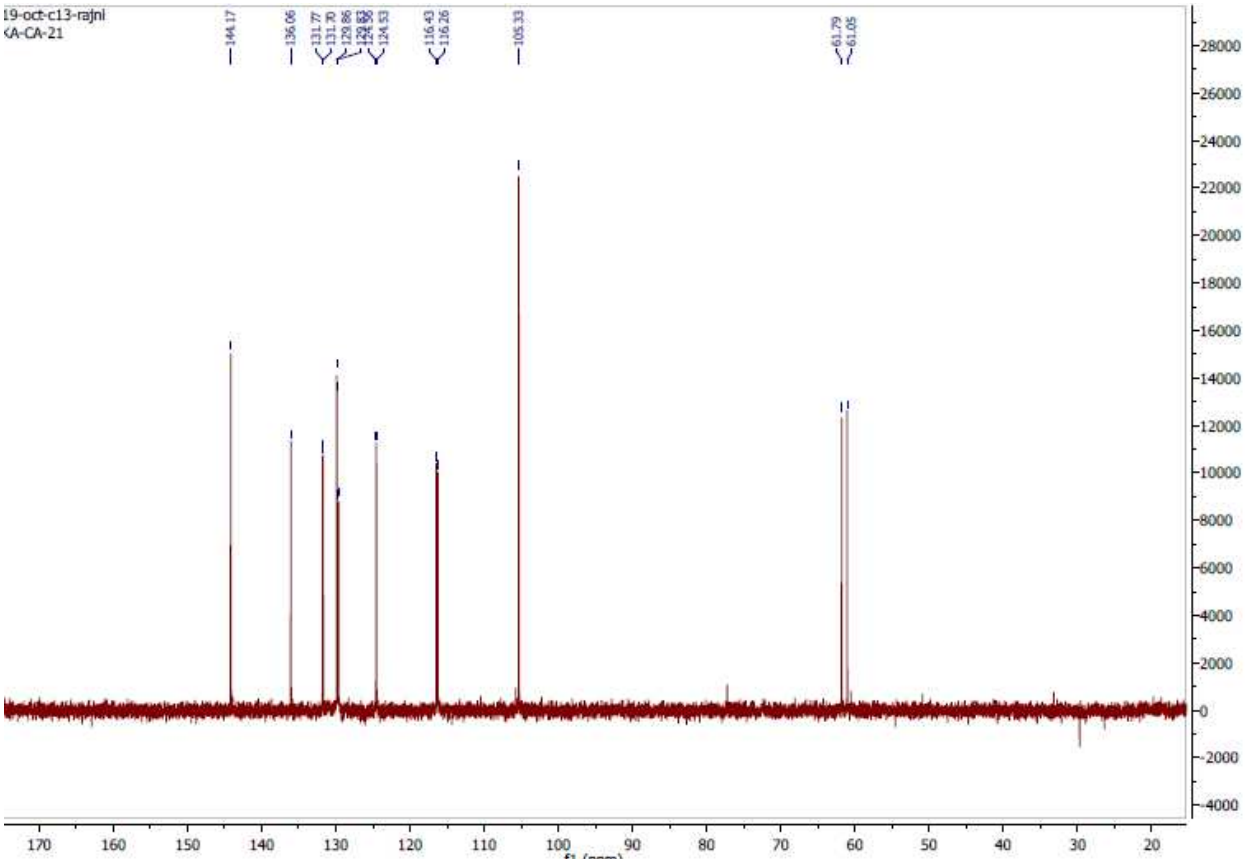
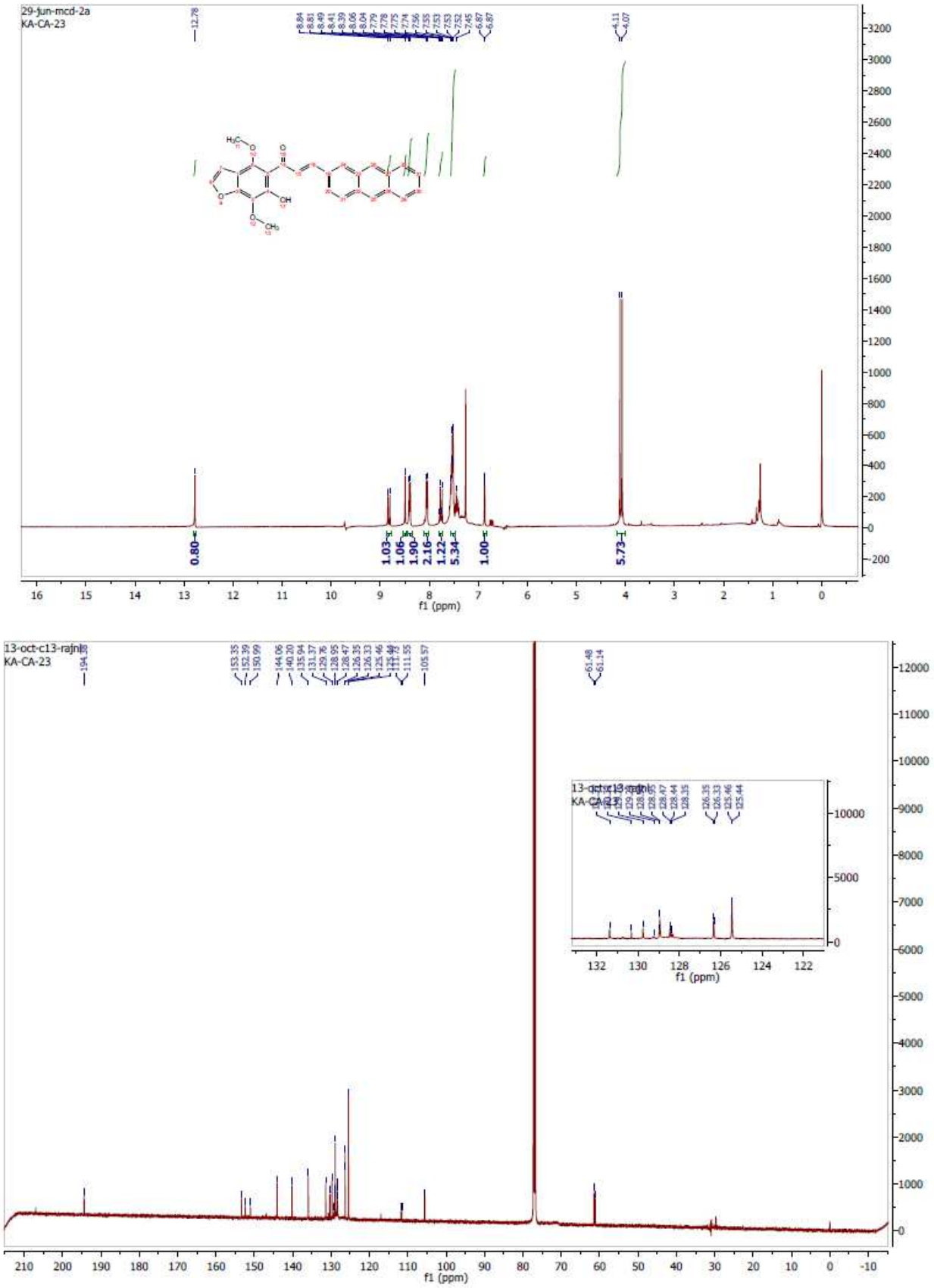

19-oct-c13-rajni
<A-CA-21
144.17
136.06
131.77
131.70
129.86
124.53
116.43
116.26
105.33
61.79
61.05
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
-4000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20

Figure S1.24. ^{1}H, ^{13}C and DEPT-135 NMR of **3v** in $CDCl_3$



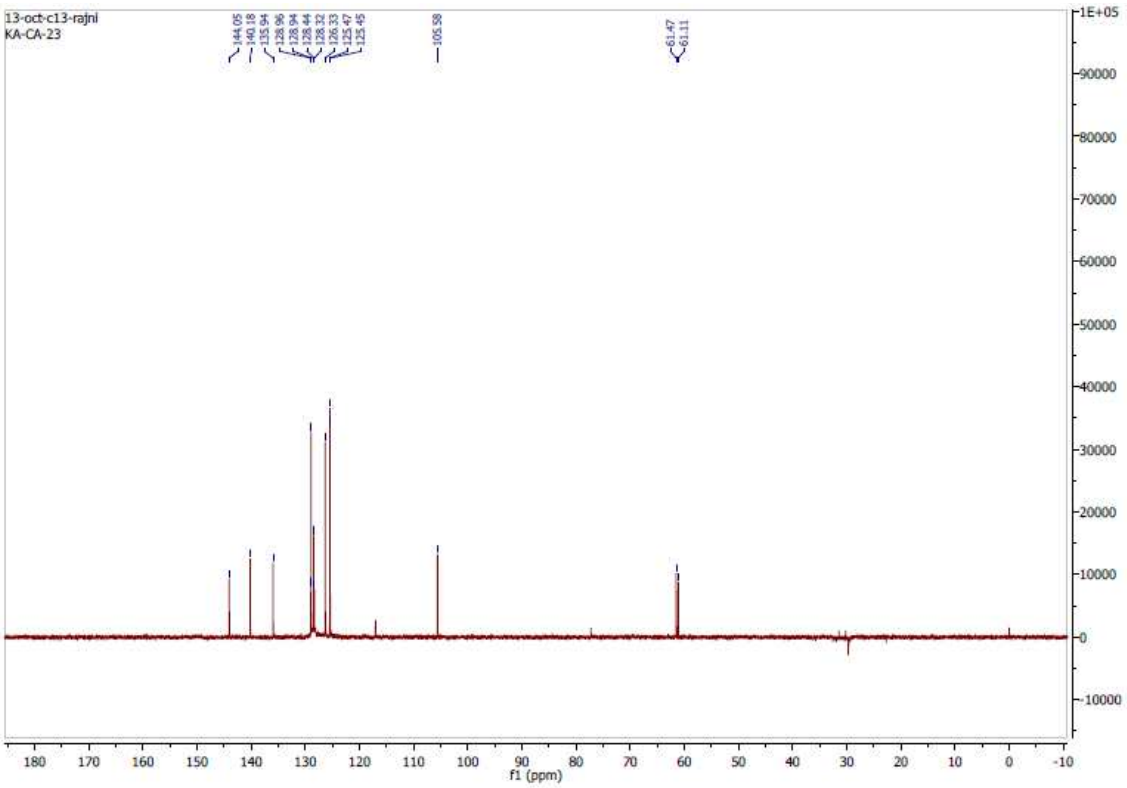
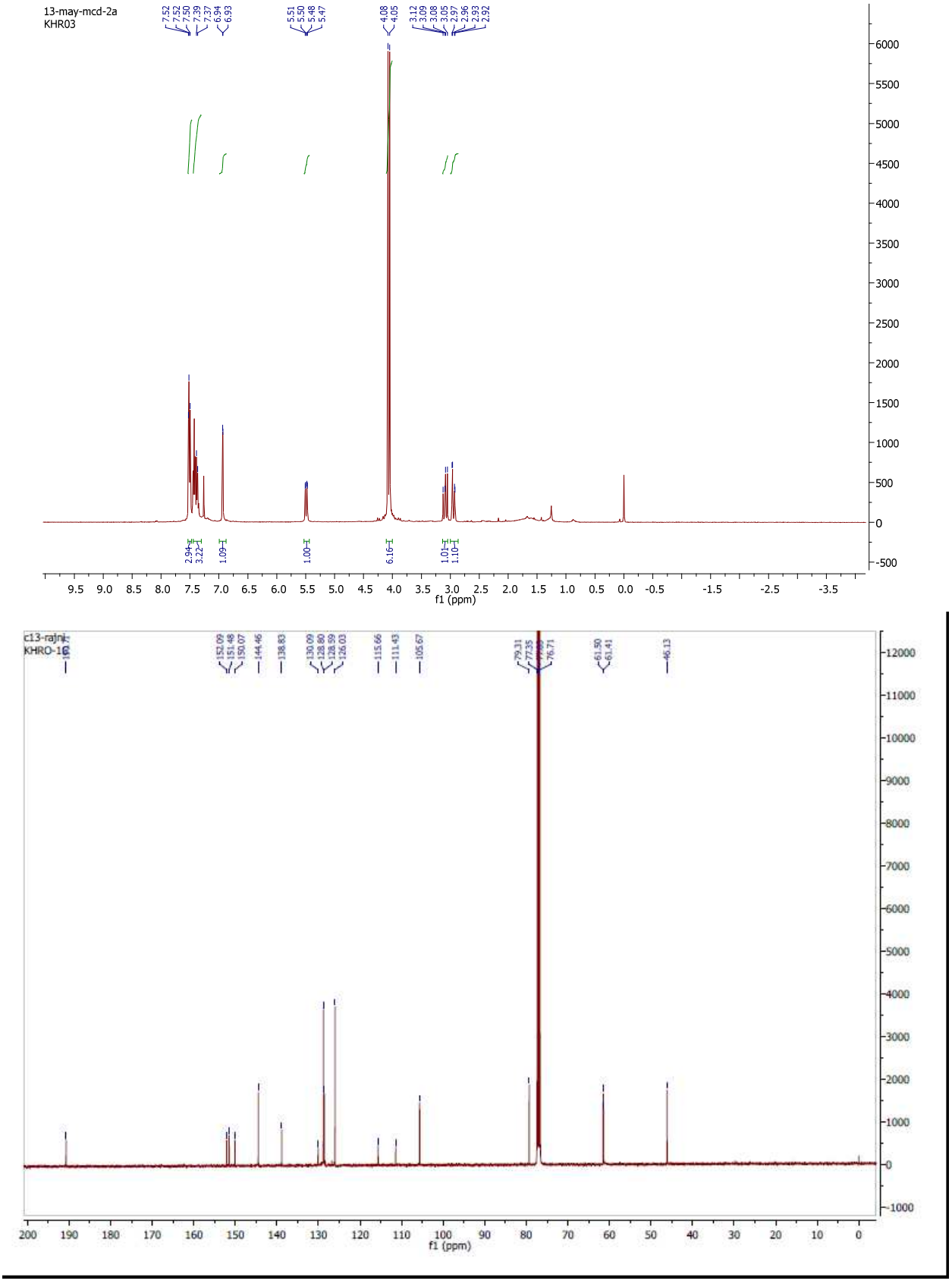

13-oct-c13-rajni
KA-CA-23
144.05
140.18
135.94
128.96
128.94
128.44
128.32
126.33
125.47
125.45
105.58
61.47
61.11
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Figure S1.25. ^{1}H, ^{13}C and DEPT-135 NMR of **4a** in $CDCl_3$



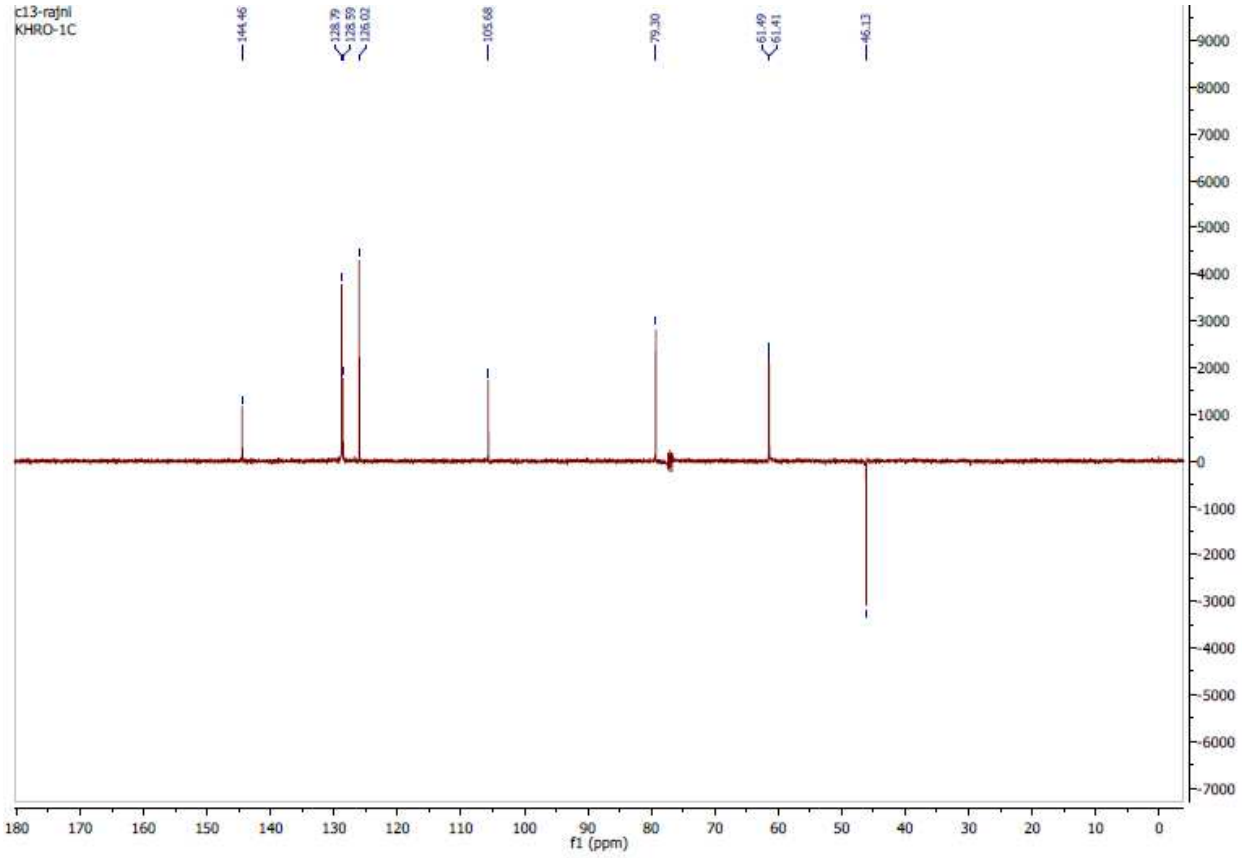
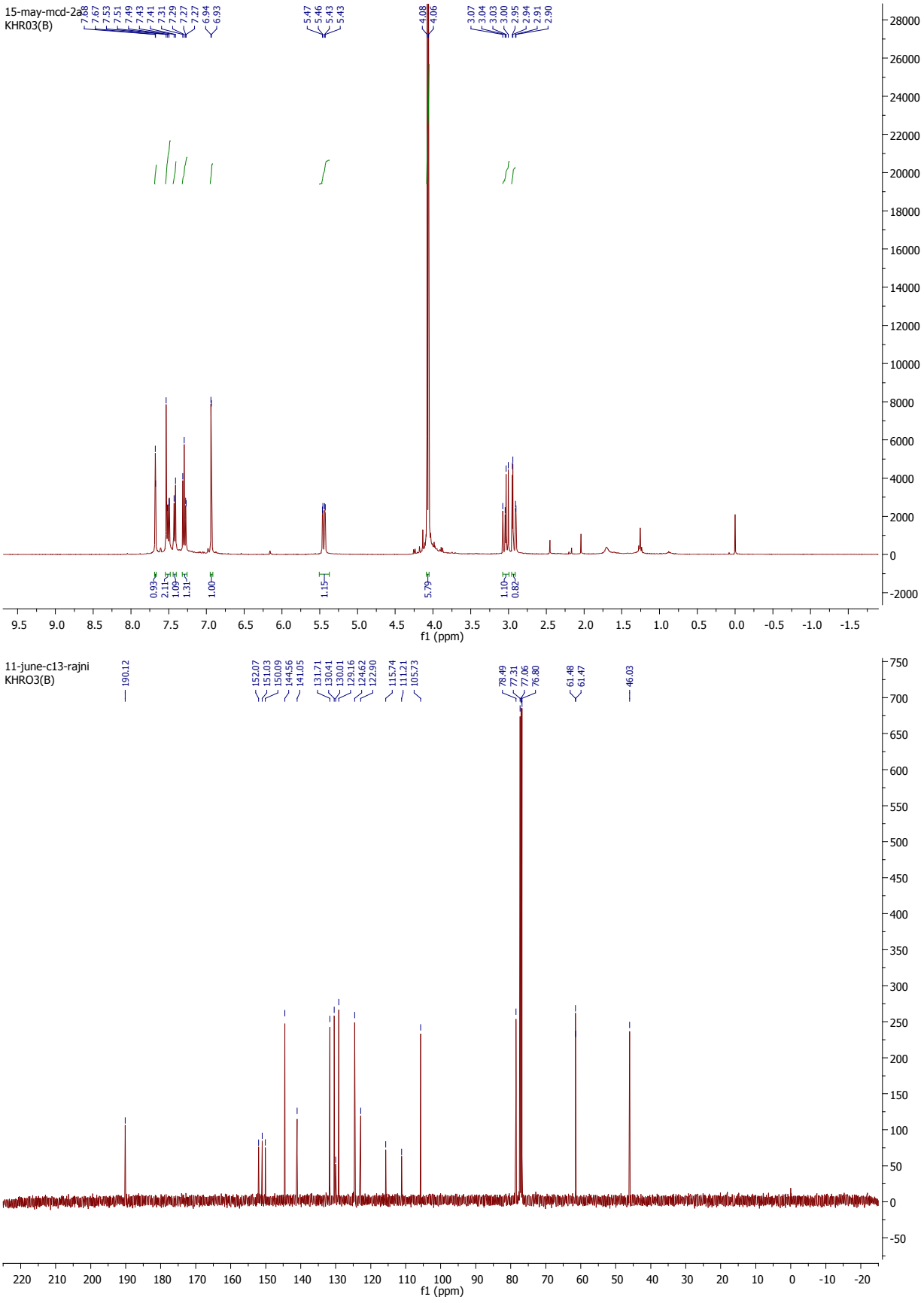

c13-rajni
KHRO-1C
144.46
128.79
128.59
126.02
105.68
79.30
61.49
61.41
46.13
f1 (ppm)

Figure S1.26. ^{1}H, ^{13}C, DEPT-135 NMR and HPLC of **4b** in $CDCl_3$



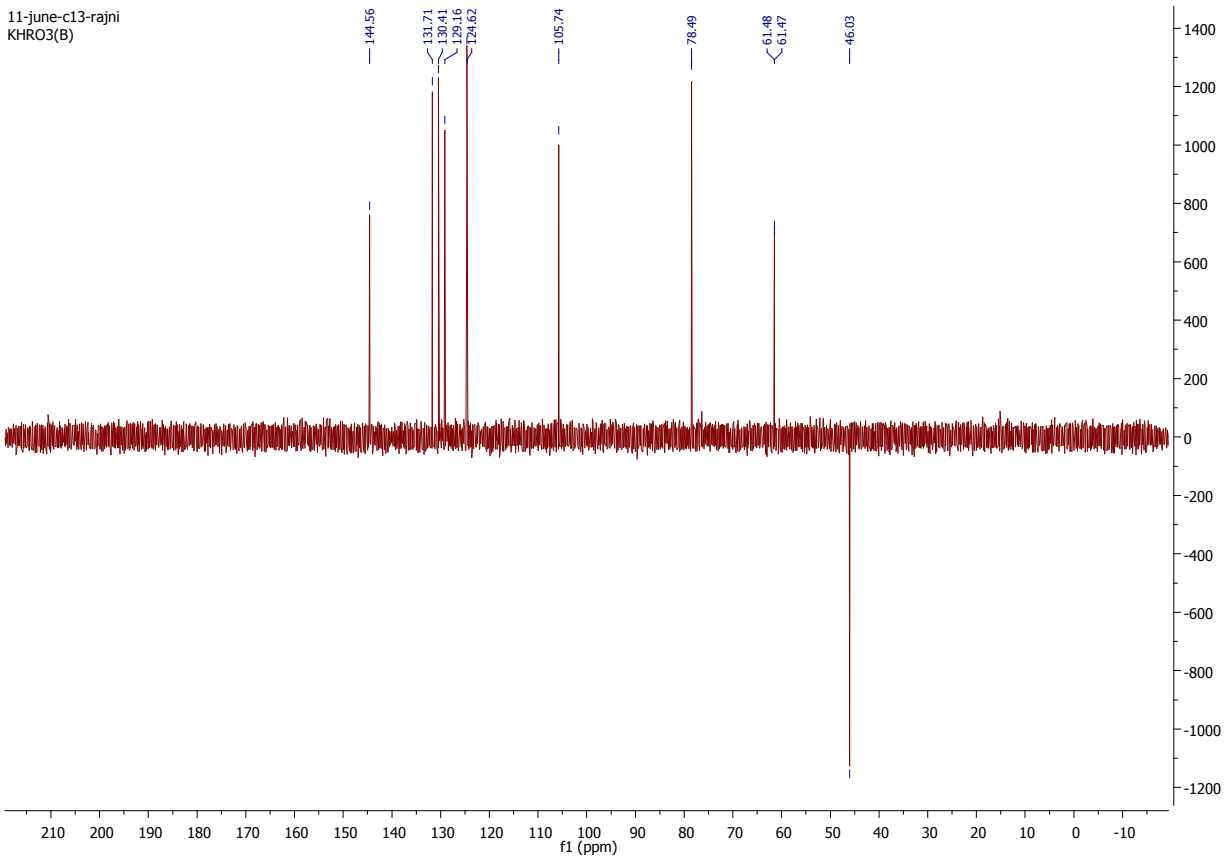
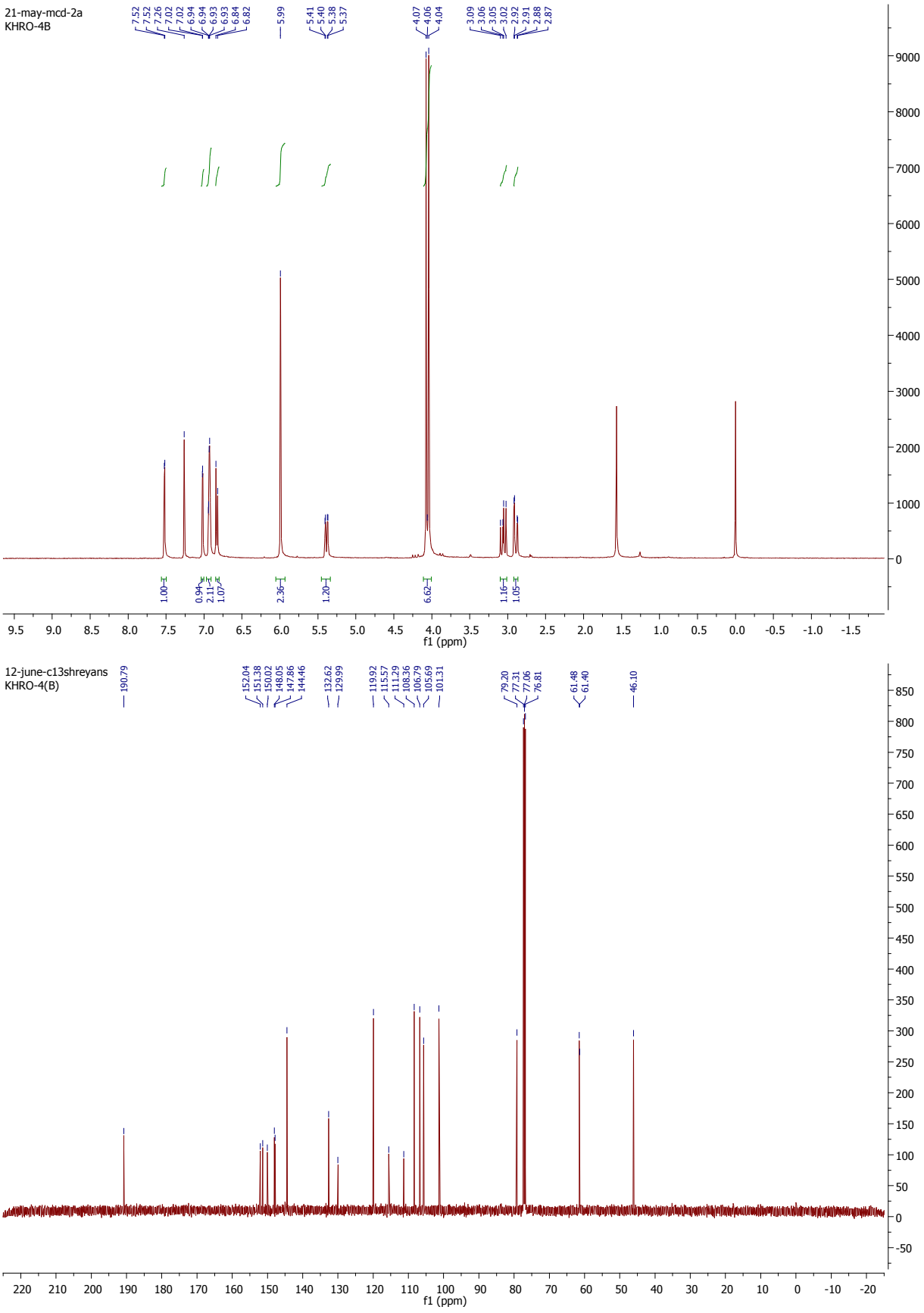

11-june-c13-rajni
KHRO3(B)
144.56
131.71
130.41
129.16
124.62
105.74
78.49
61.48
61.47
46.03
f1 (ppm)

Figure S1.27. ^{1}H, ^{13}C and DEPT-135 NMR of **4c** in $CDCl_3$



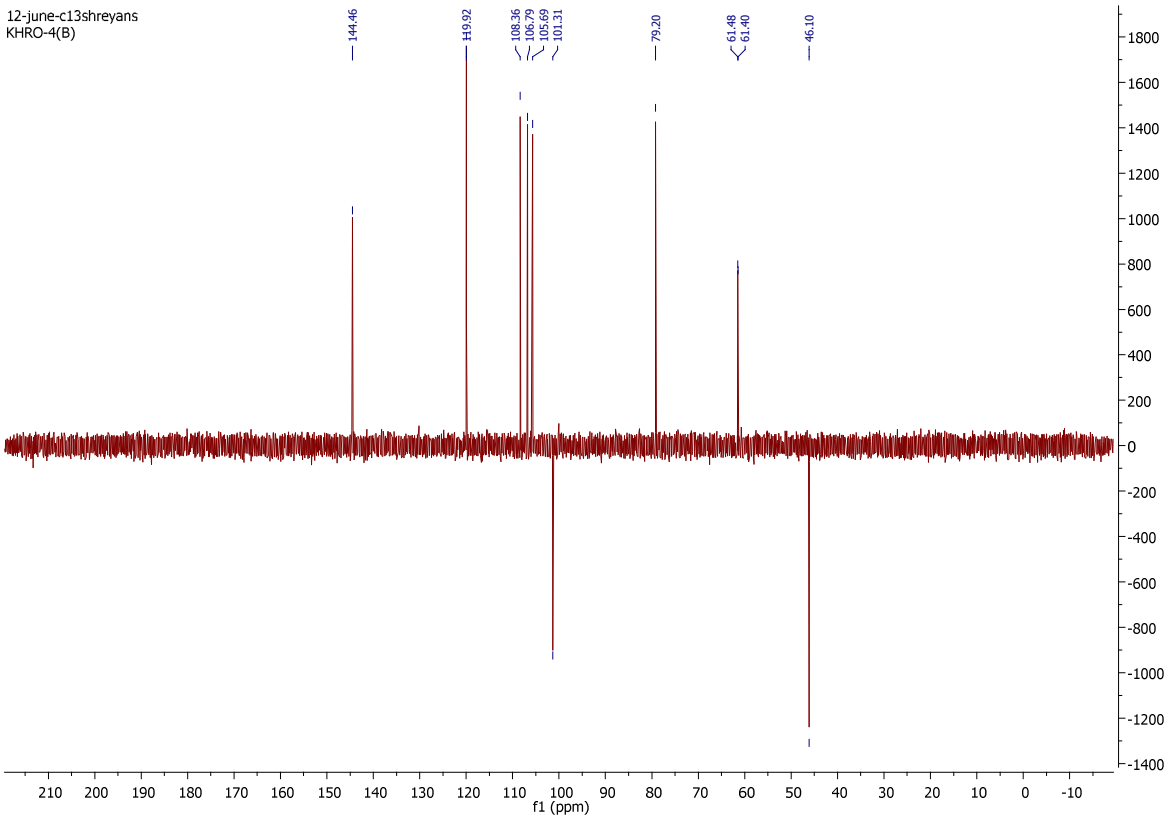
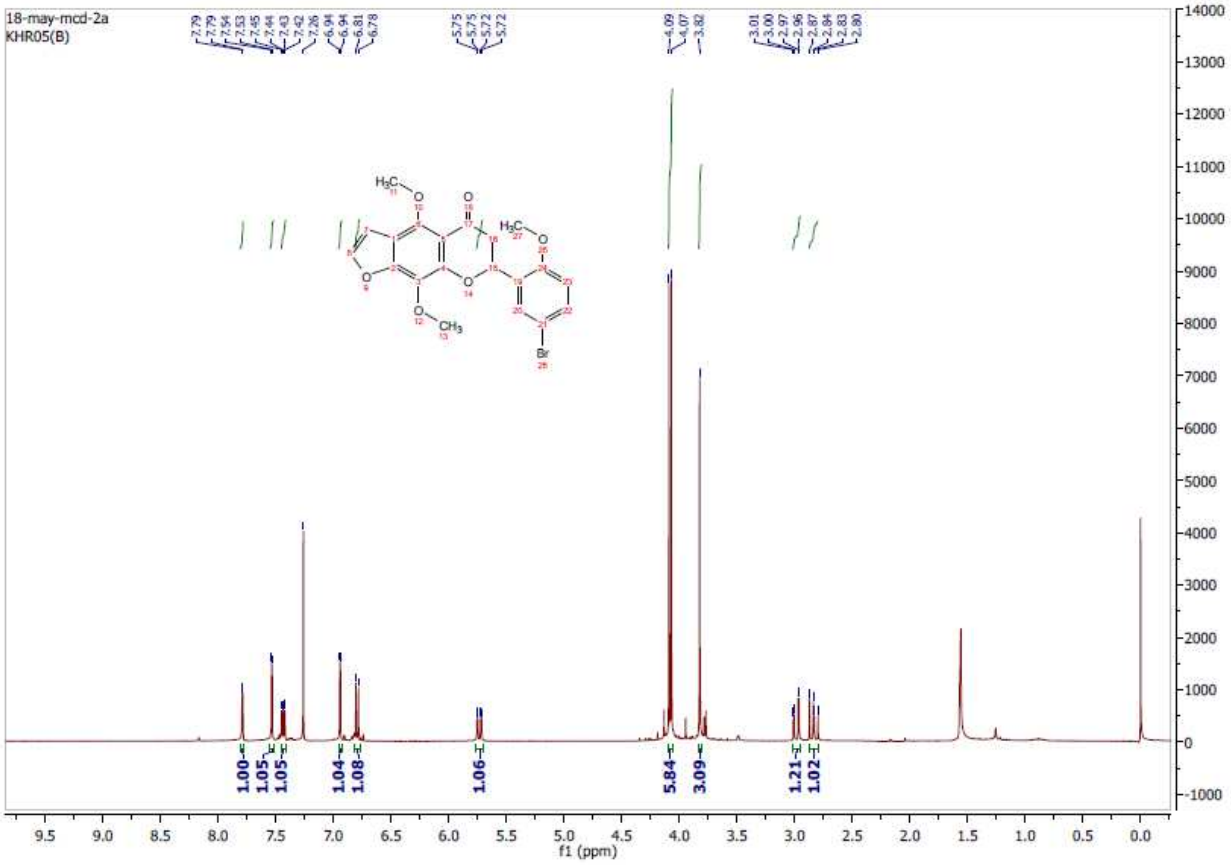
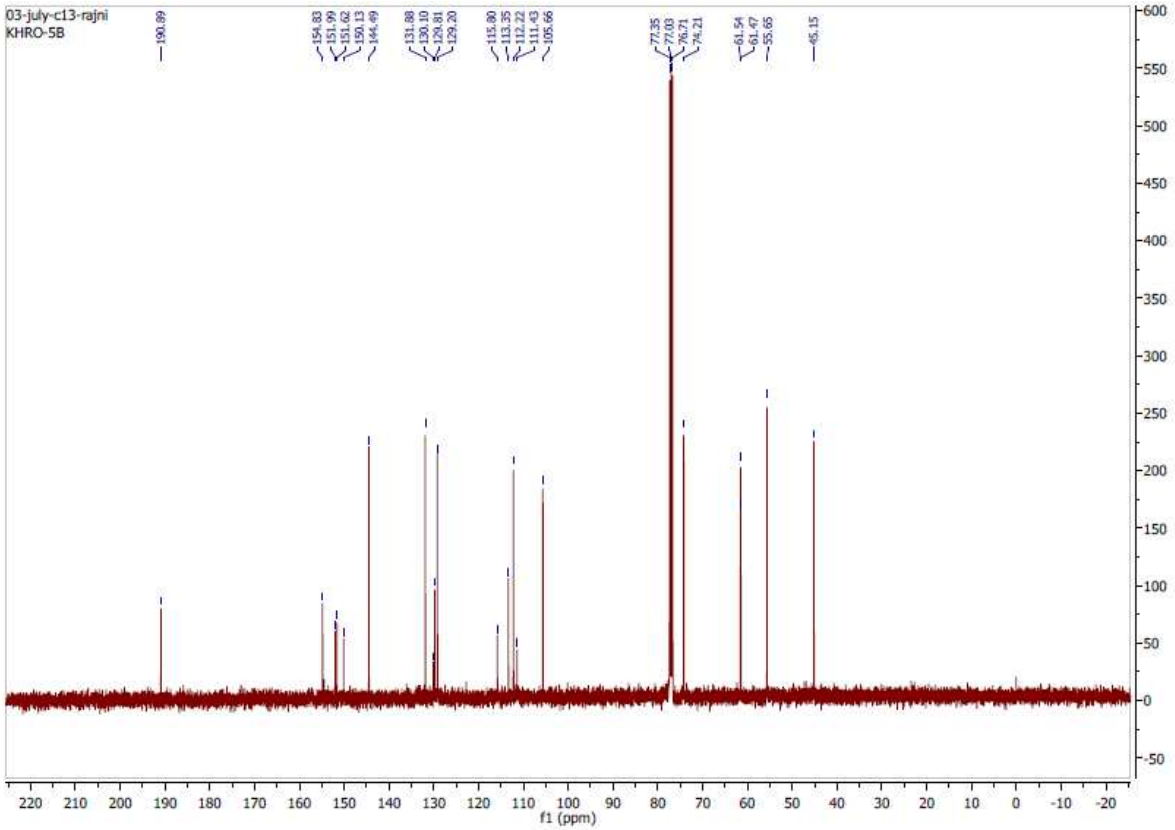

12-june-c13shreyans
KHRO-4(B)
144.46
119.92
108.36
106.79
105.69
101.31
79.20
61.48
61.40
46.10
f1 (ppm)

Figure S1.28. ^{1}H, ^{13}C, DEPT-135 NMR and HPLC of **4d** in $CDCl_3$





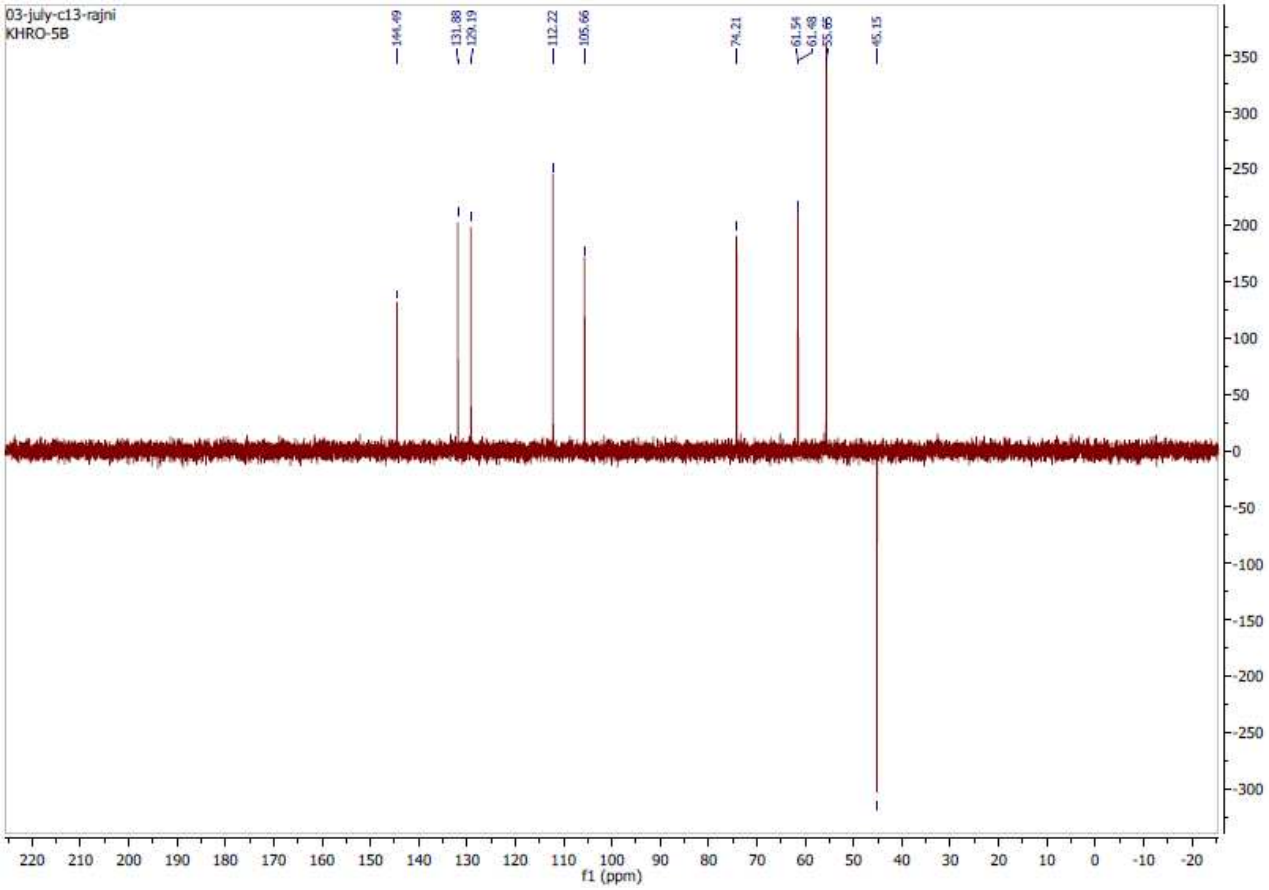
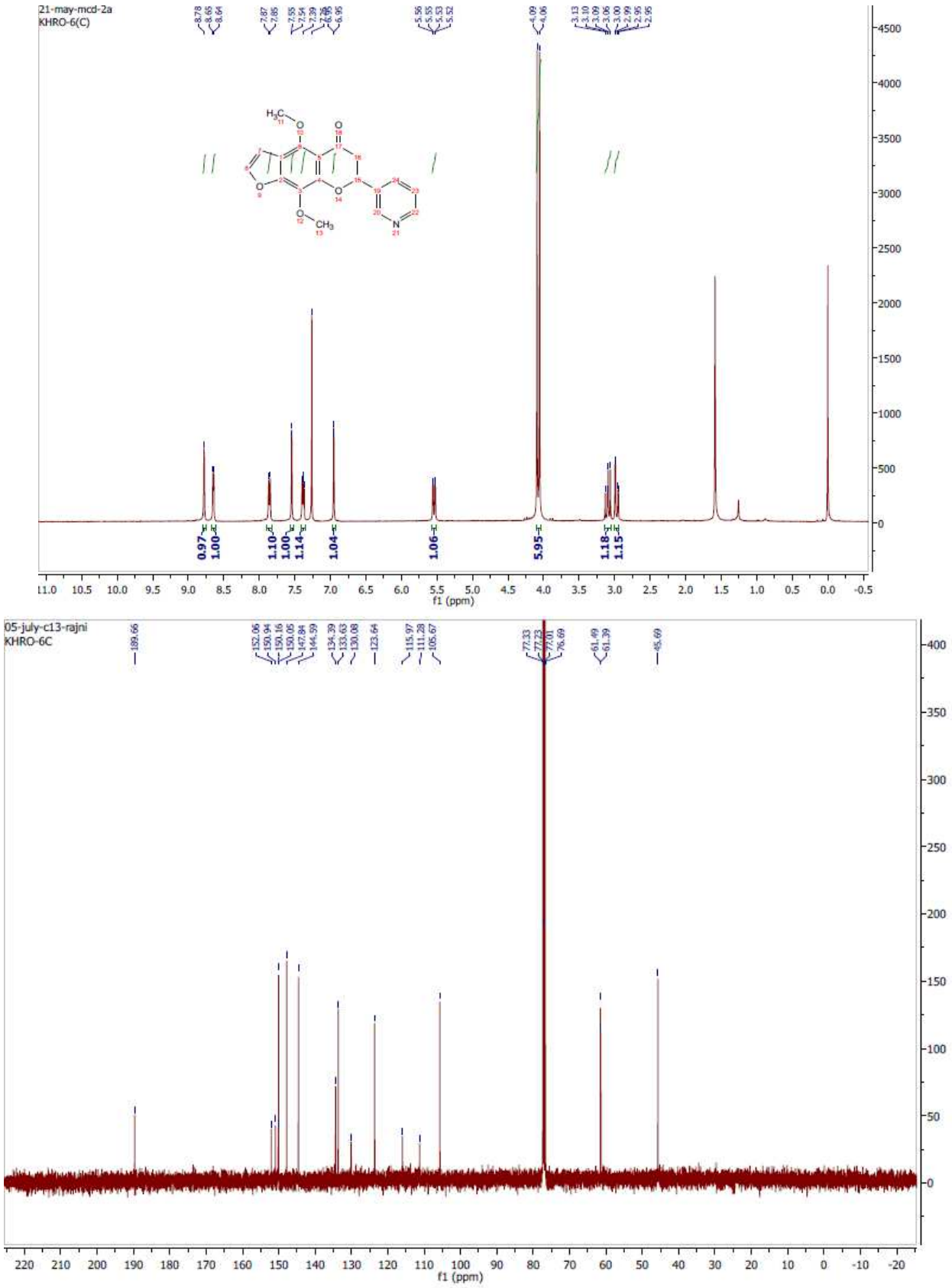

03-july-c13-rajni
KHRO-5B
144.49
131.88
129.19
112.22
105.66
74.21
61.54
61.48
55.65
45.15
f1 (ppm)

Figure S1.29. ^{1}H, ^{13}C, DEPT-135 NMR and HPLC of **4e** in $CDCl_3$



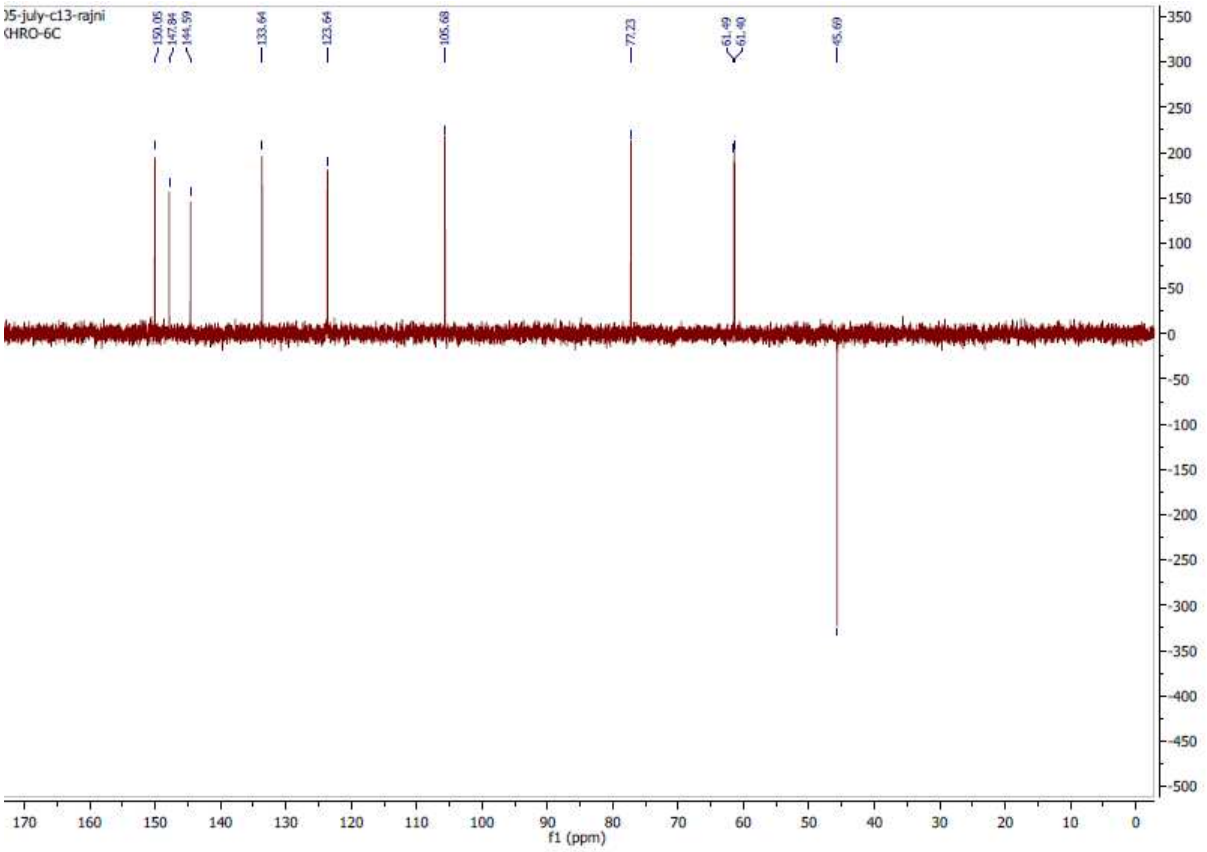
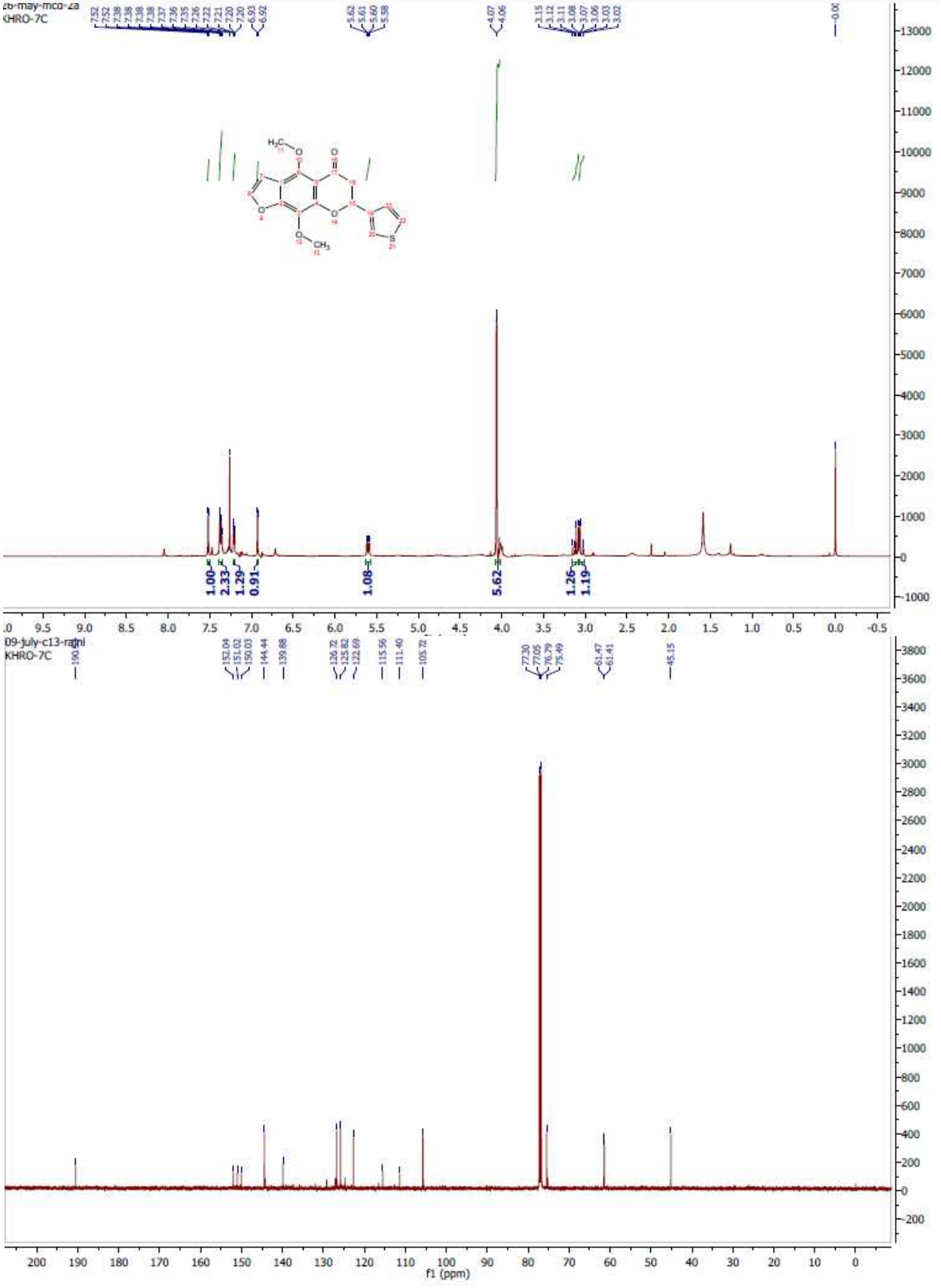

)5-july-c13-rajni
CHRO-6C
150.05
147.84
144.59
133.64
123.64
105.68
77.23
61.49
61.40
45.69
f1 (ppm)

Figure S1.30. ^{1}H, ^{13}C and DEPT-135 NMR of **4f** in $CDCl_3$



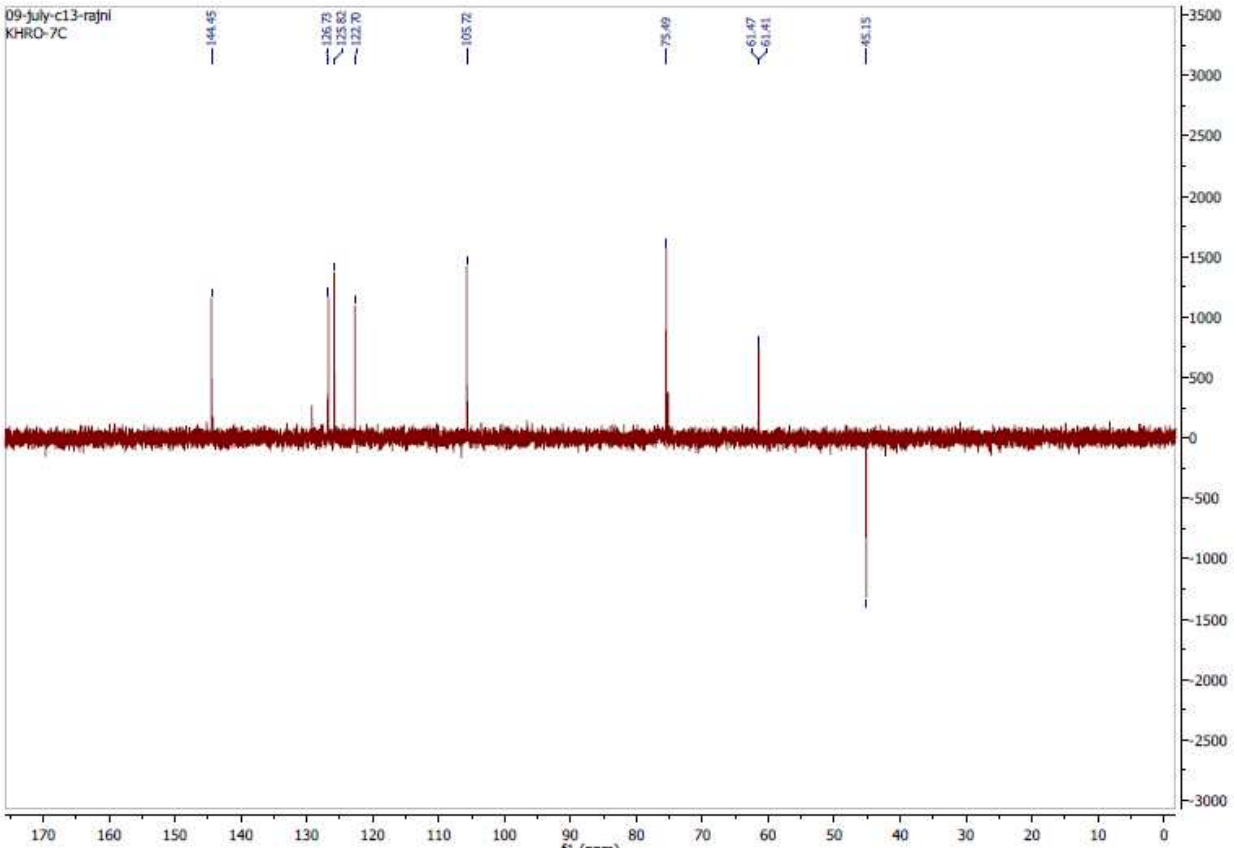
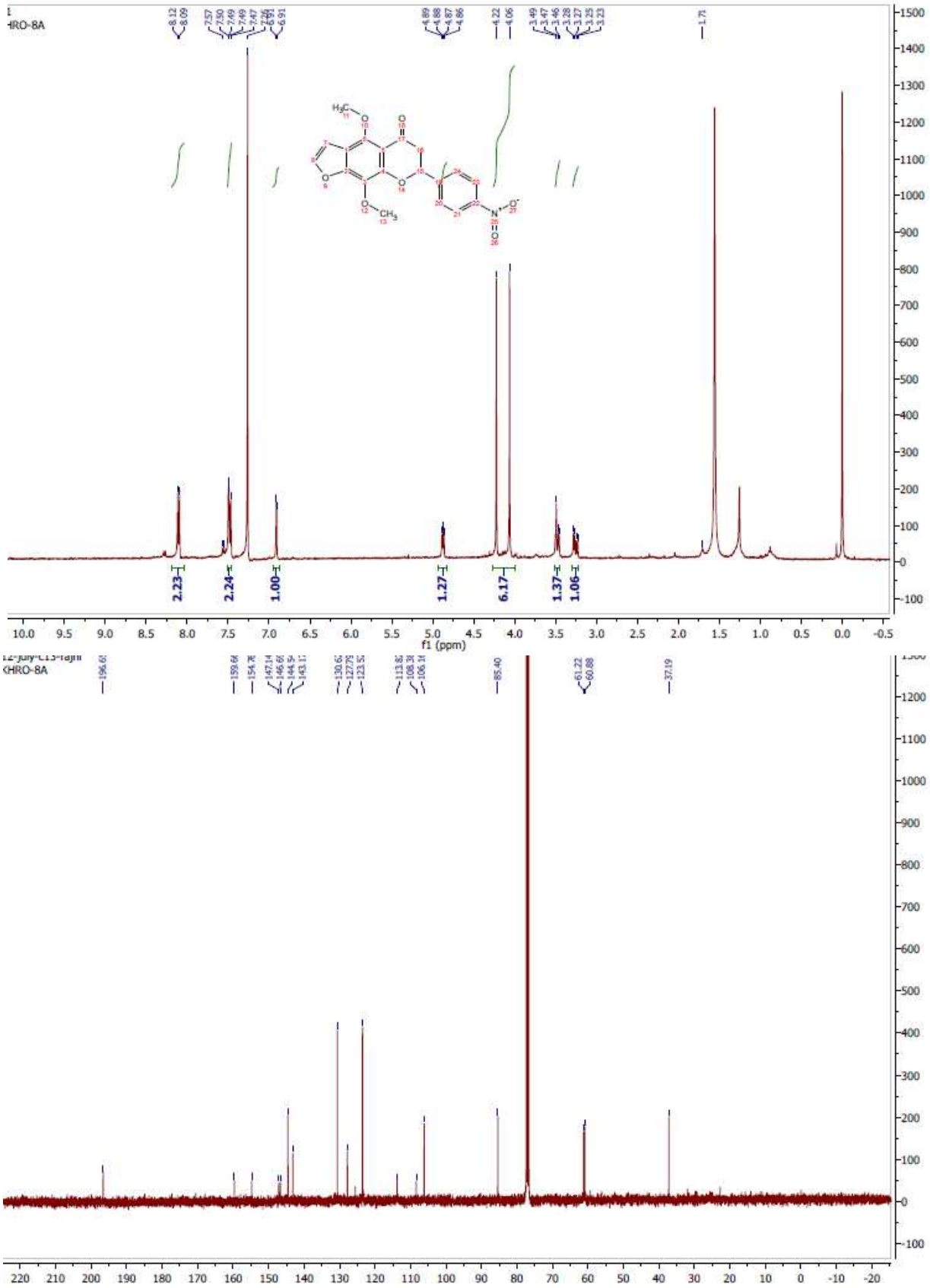

09-July-c13-rajni
KHRO-7C
144.45
126.73
125.62
122.70
105.72
75.49
61.47
61.41
45.15

Figure S1.31. ^{1}H, ^{13}C and DEPT-135 NMR of **4g** in $CDCl_3$



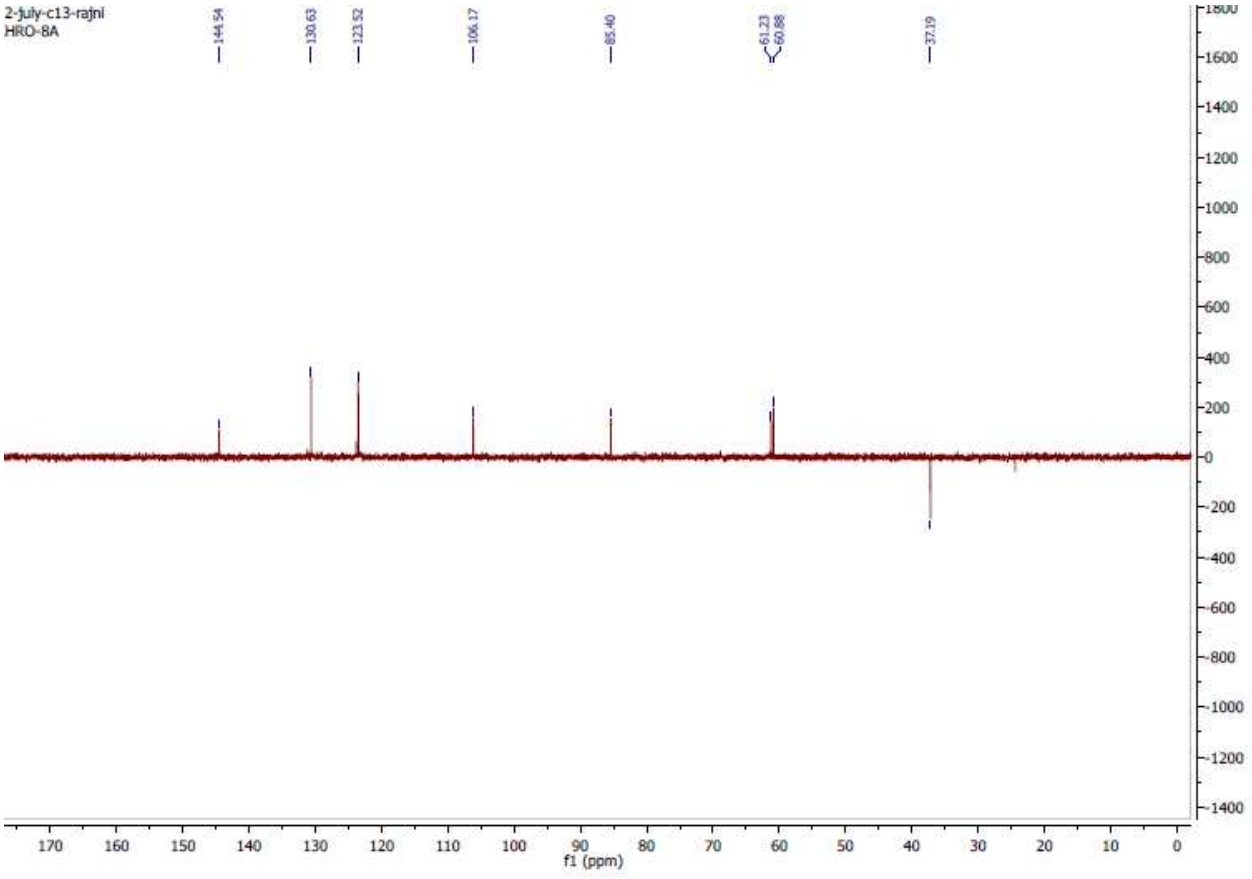
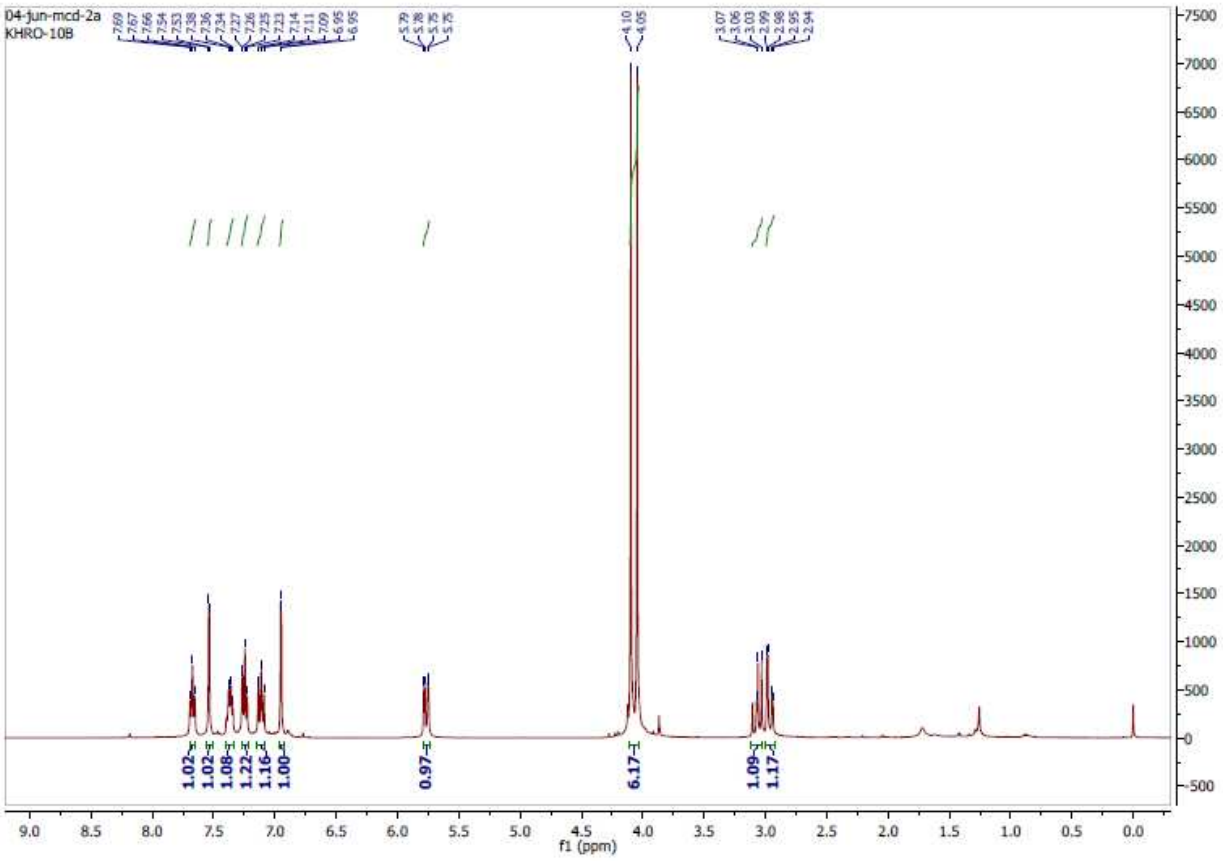
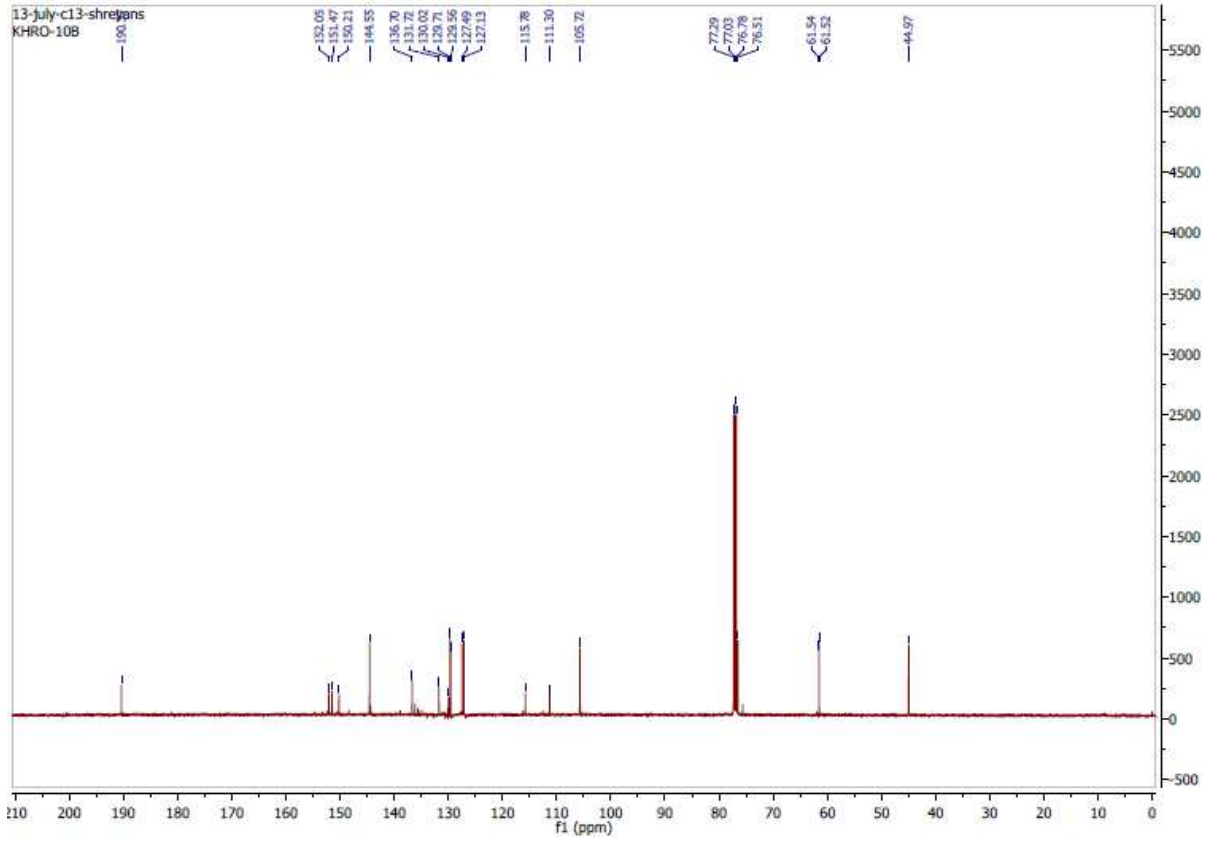

2-july-c13-rajnl
HRO-8A
144.54
130.63
123.52
106.17
85.40
61.23
60.88
37.19
f1 (ppm)

Figure S1.32. ^{1}H, ^{13}C and DEPT-135 NMR of **4h** in $CDCl_3$





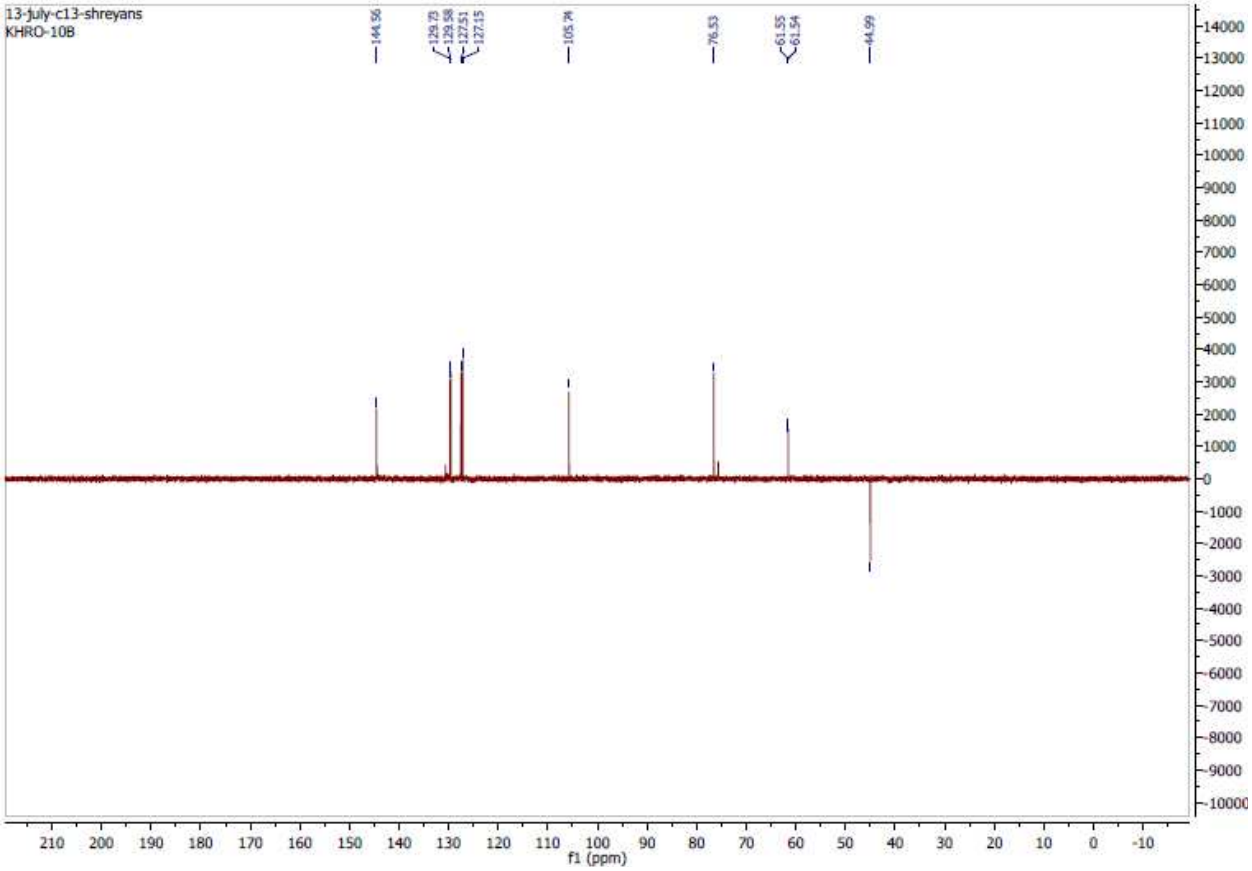
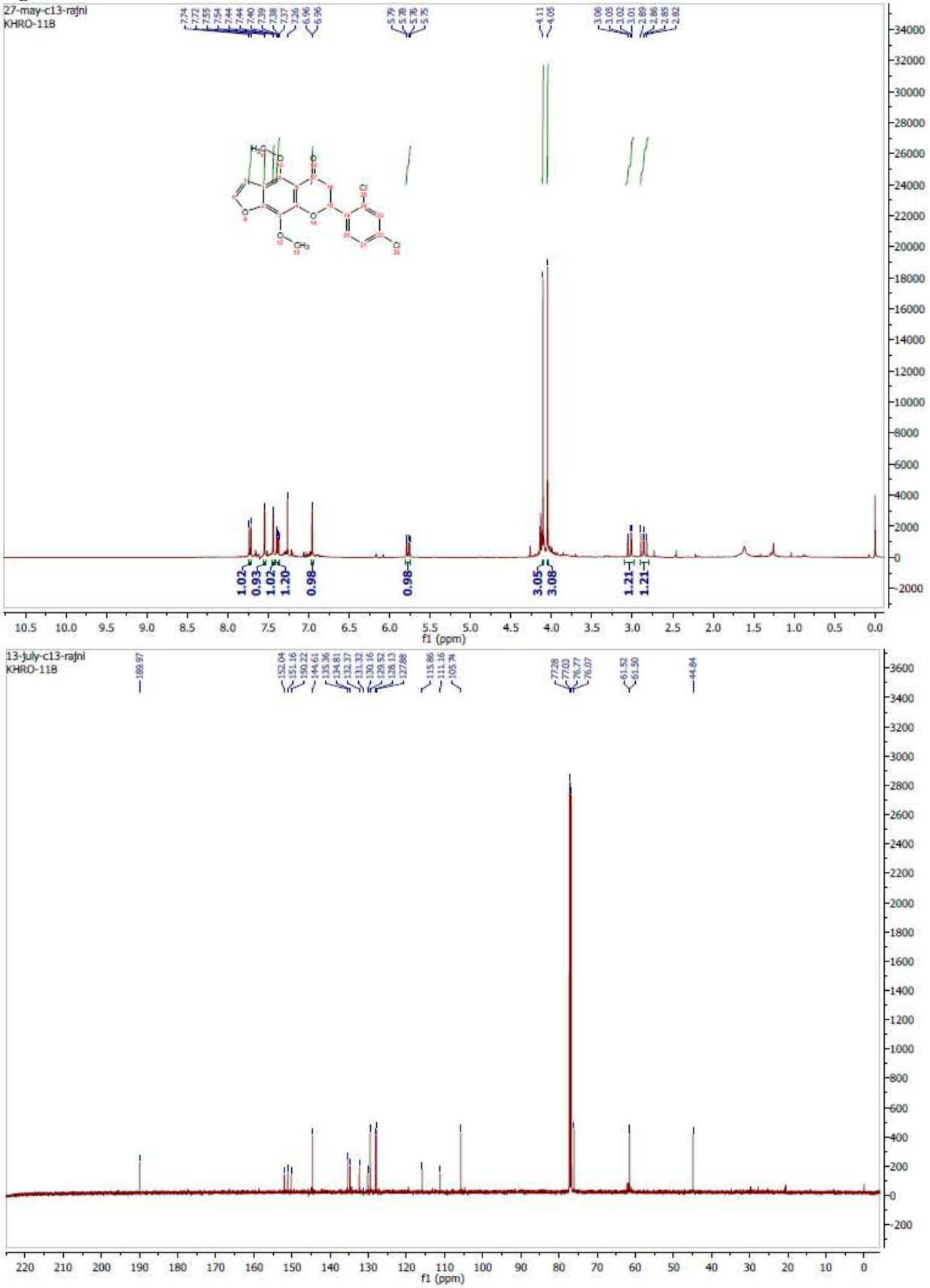

13-july-c13-shreyans
KHRO-10B
144.56
129.73
129.58
127.51
127.15
105.74
76.53
61.55
61.54
44.99
f1 (ppm)

Figure S1.33. ^{1}H, ^{13}C and DEPT-135 NMR of **4i** in $CDCl_3$



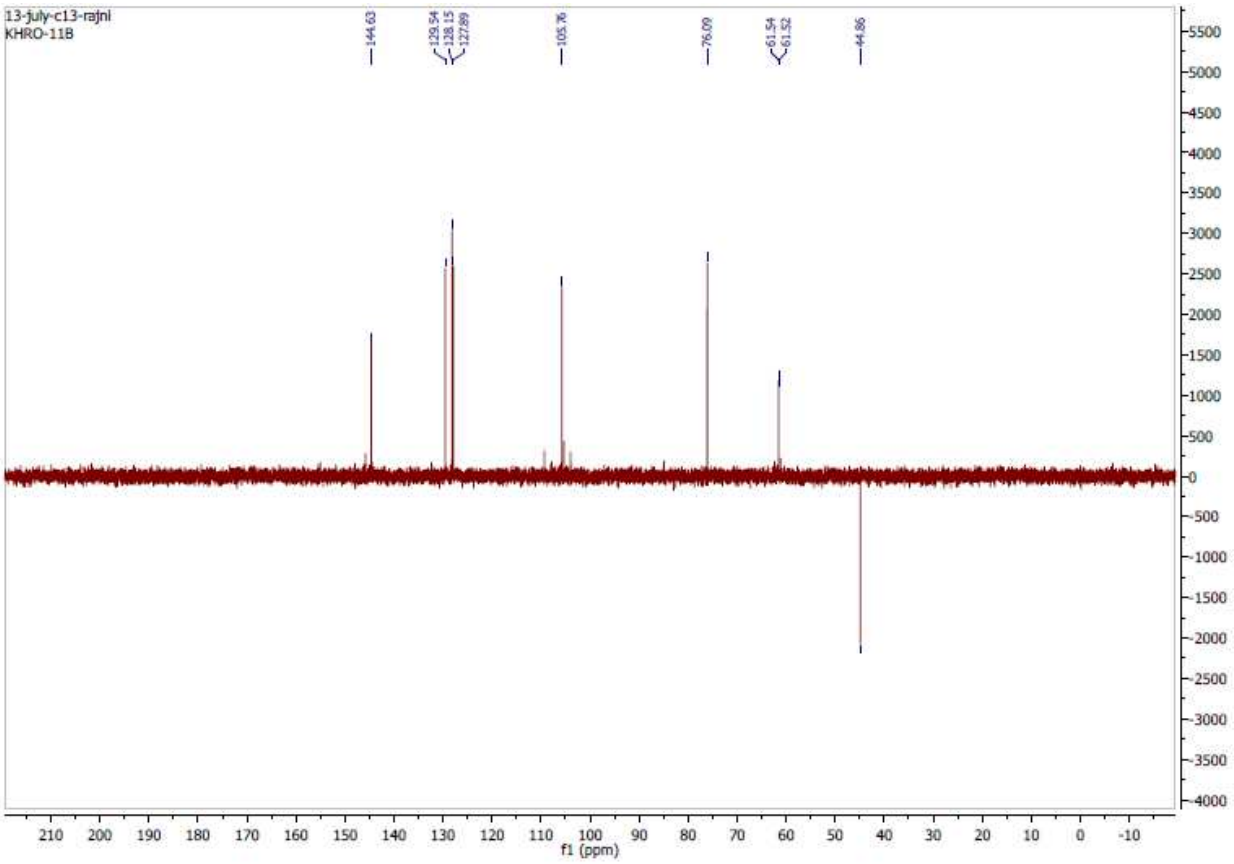
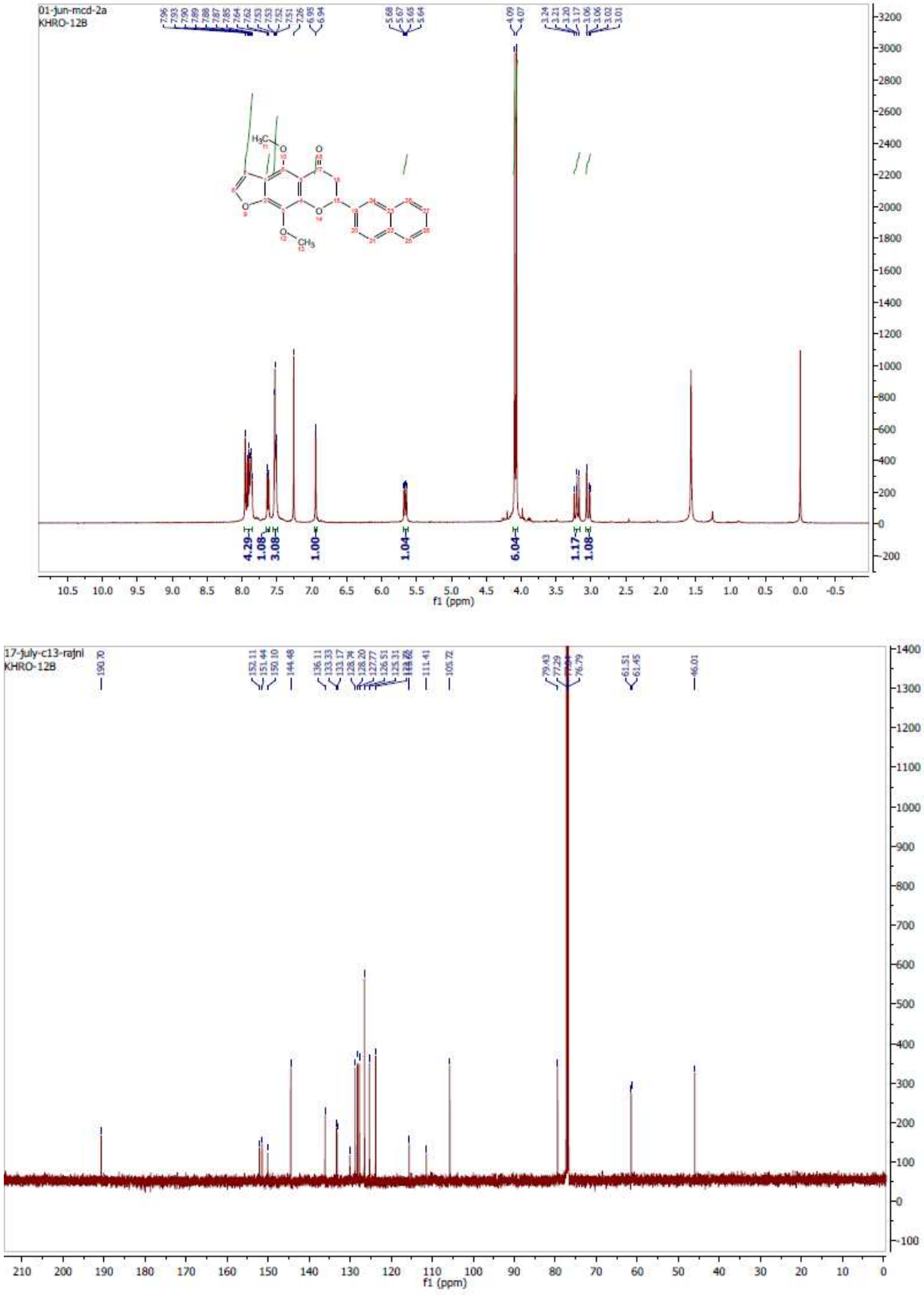

13-july-c13-rajni
KHRO-11B
144.63
129.54
128.15
127.89
105.76
76.09
61.54
61.52
44.86
f1 (ppm)

Figure S1.34. ^{1}H, ^{13}C and DEPT-135 NMR of **4j** in $CDCl_3$



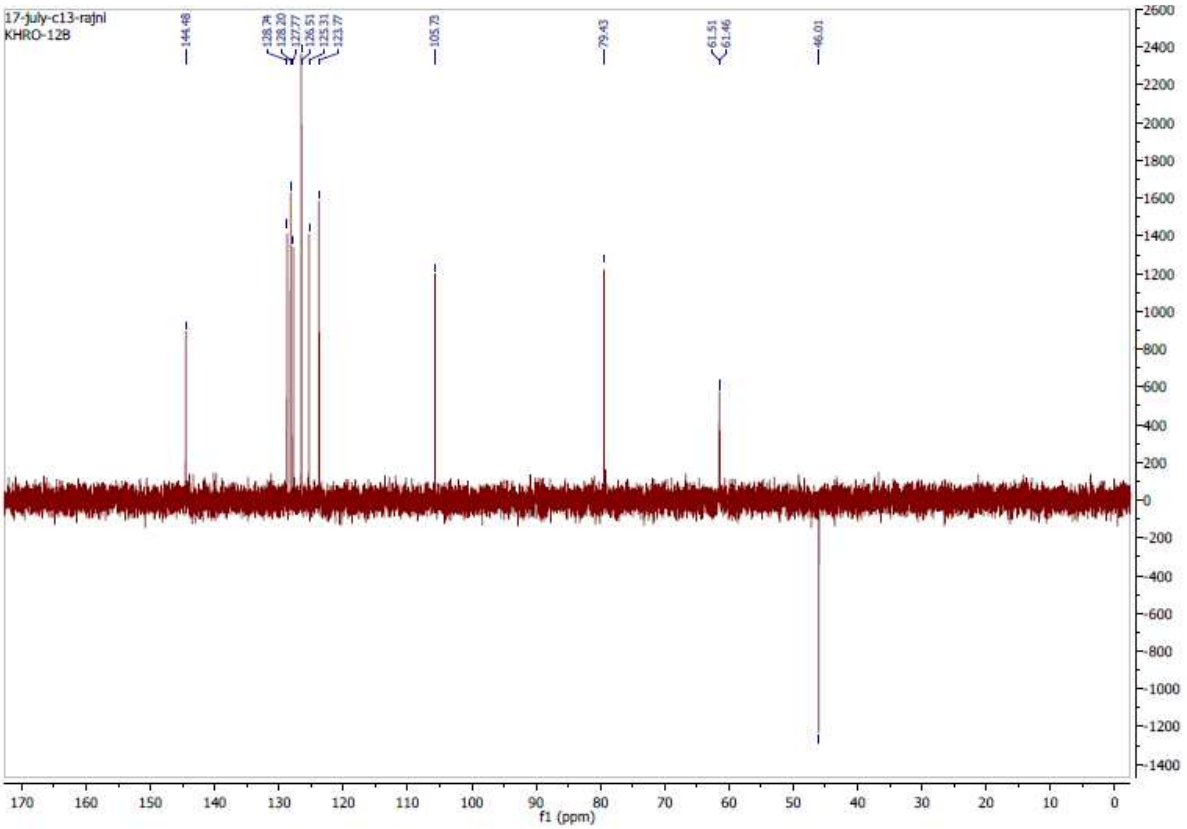
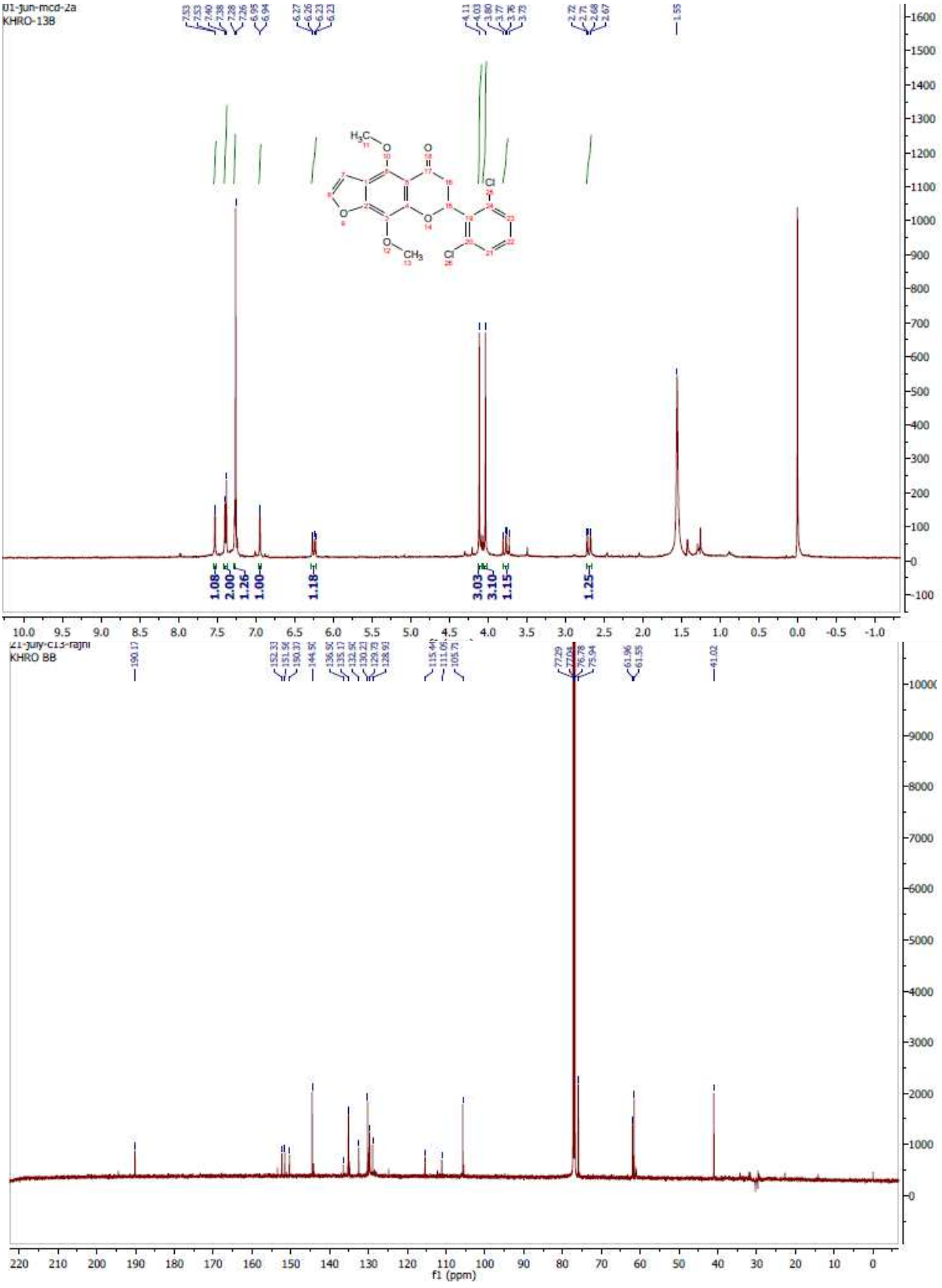

17-july-c13-rajni
KHRO-12B
144.48
128.74
128.20
127.77
126.51
125.31
123.77
105.73
79.43
61.51
61.46
46.01
f1 (ppm)

Figure S1.35. ^{1}H, ^{13}C and DEPT-135 NMR of **4k** in $CDCl_3$



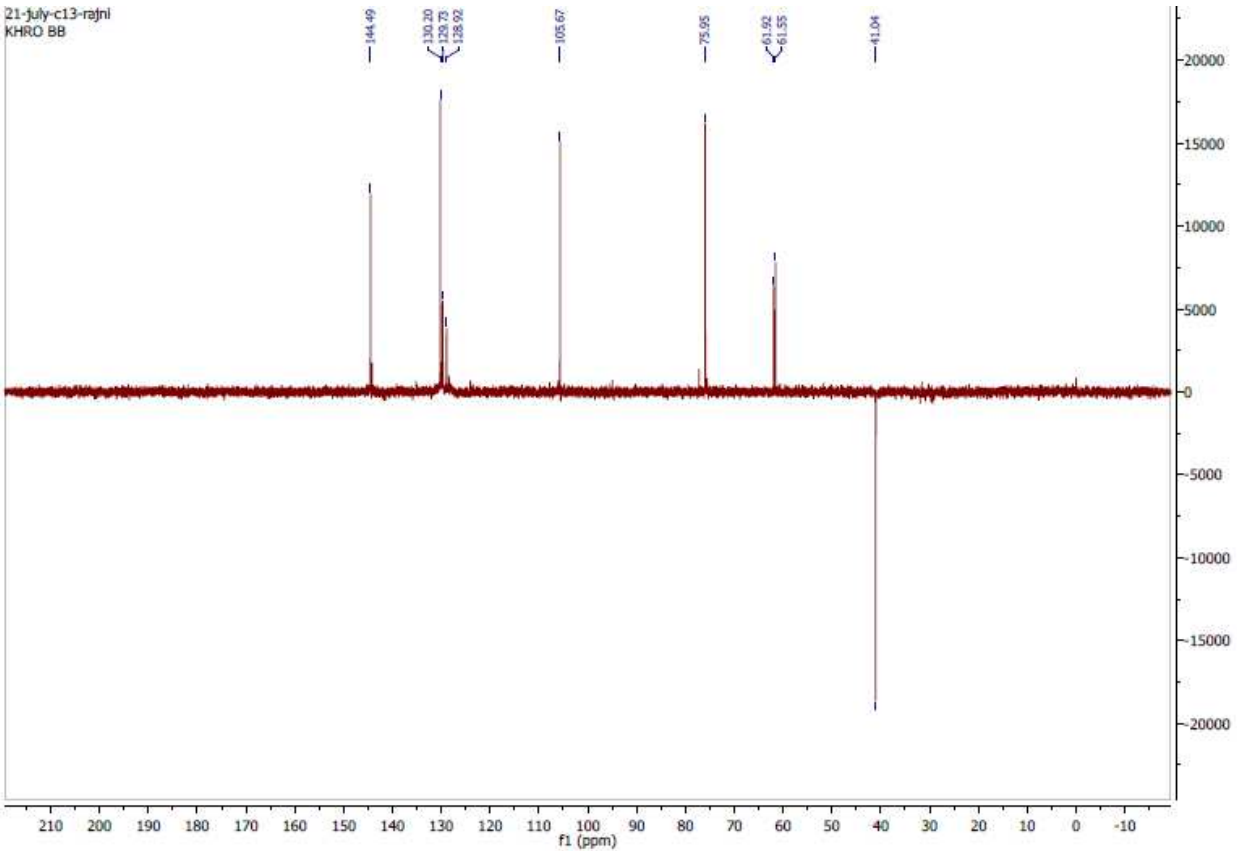
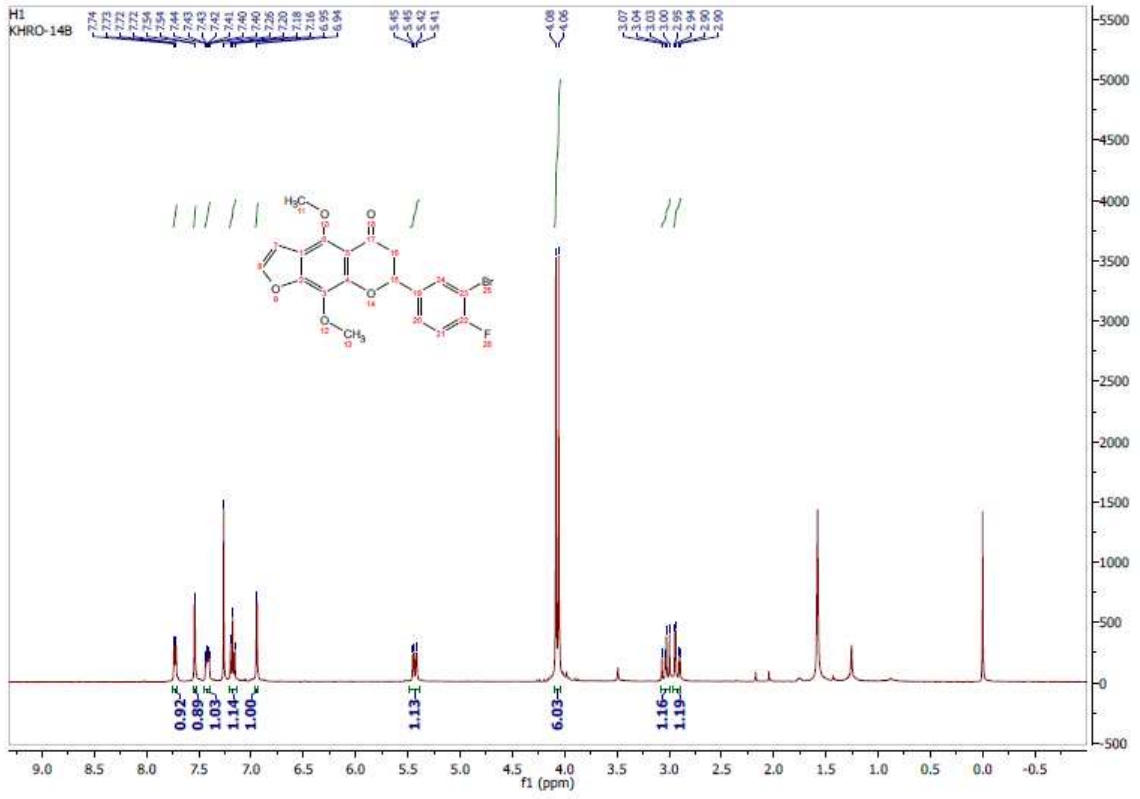
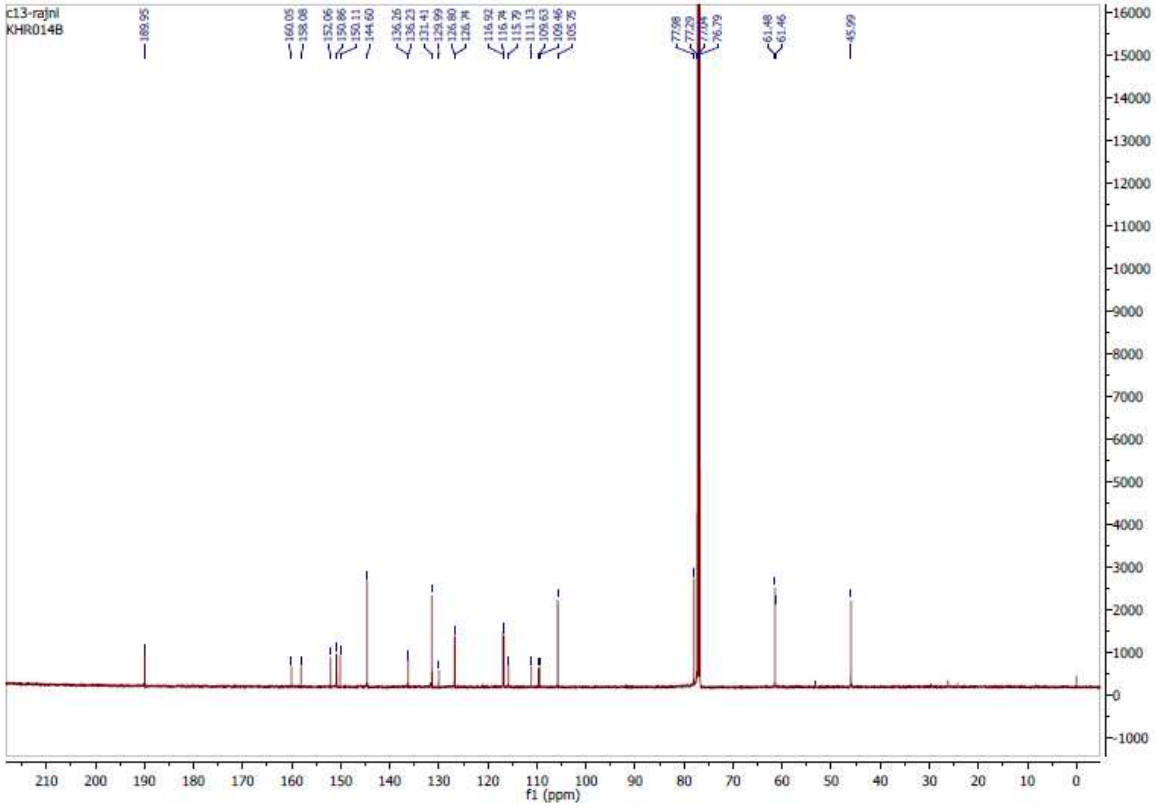

21-july-c13-rajni
KHRO BB
144.49
130.20
129.73
128.92
105.67
75.95
61.92
61.55
41.04
20000
15000
10000
5000
0
-5000
-10000
-15000
-20000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Figure S1.36. ^{1}H, ^{13}C and DEPT-135 NMR of **4l** in $CDCl_3$





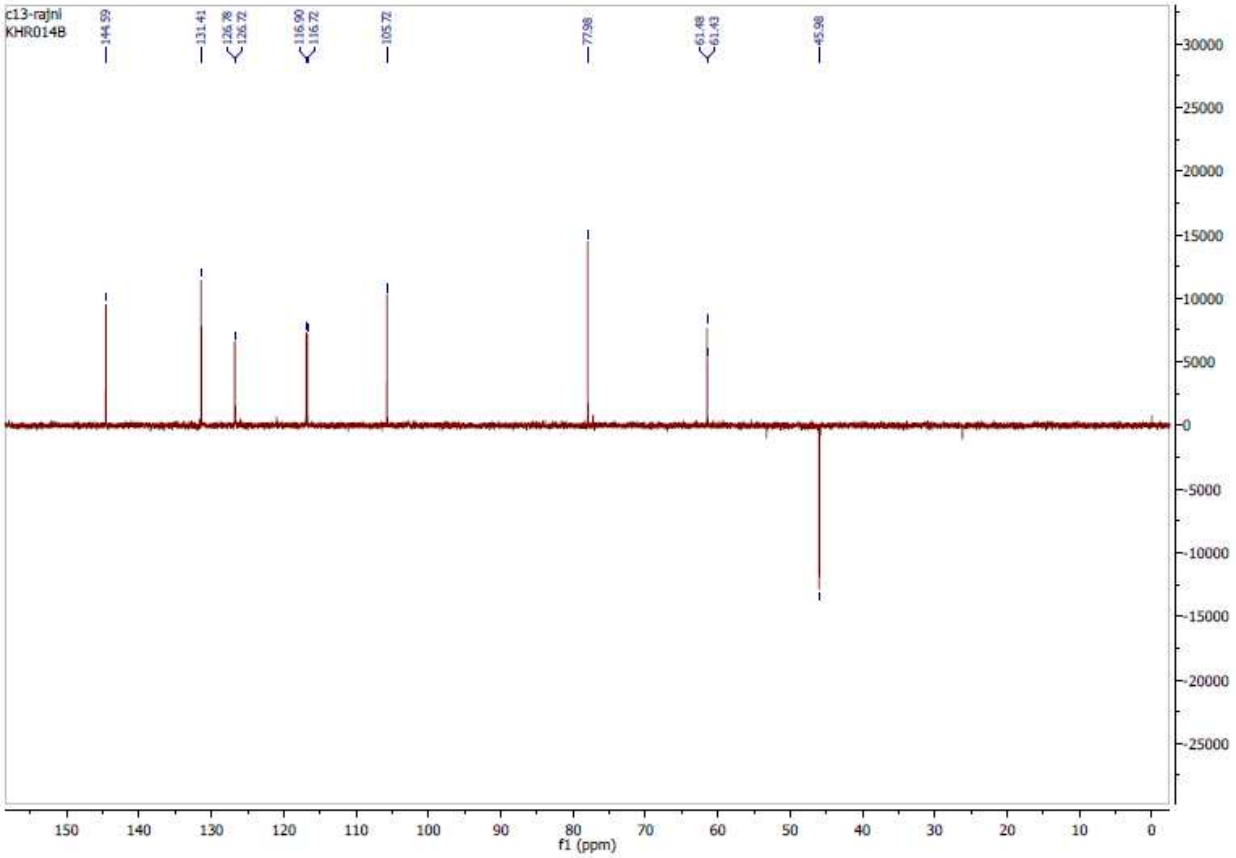
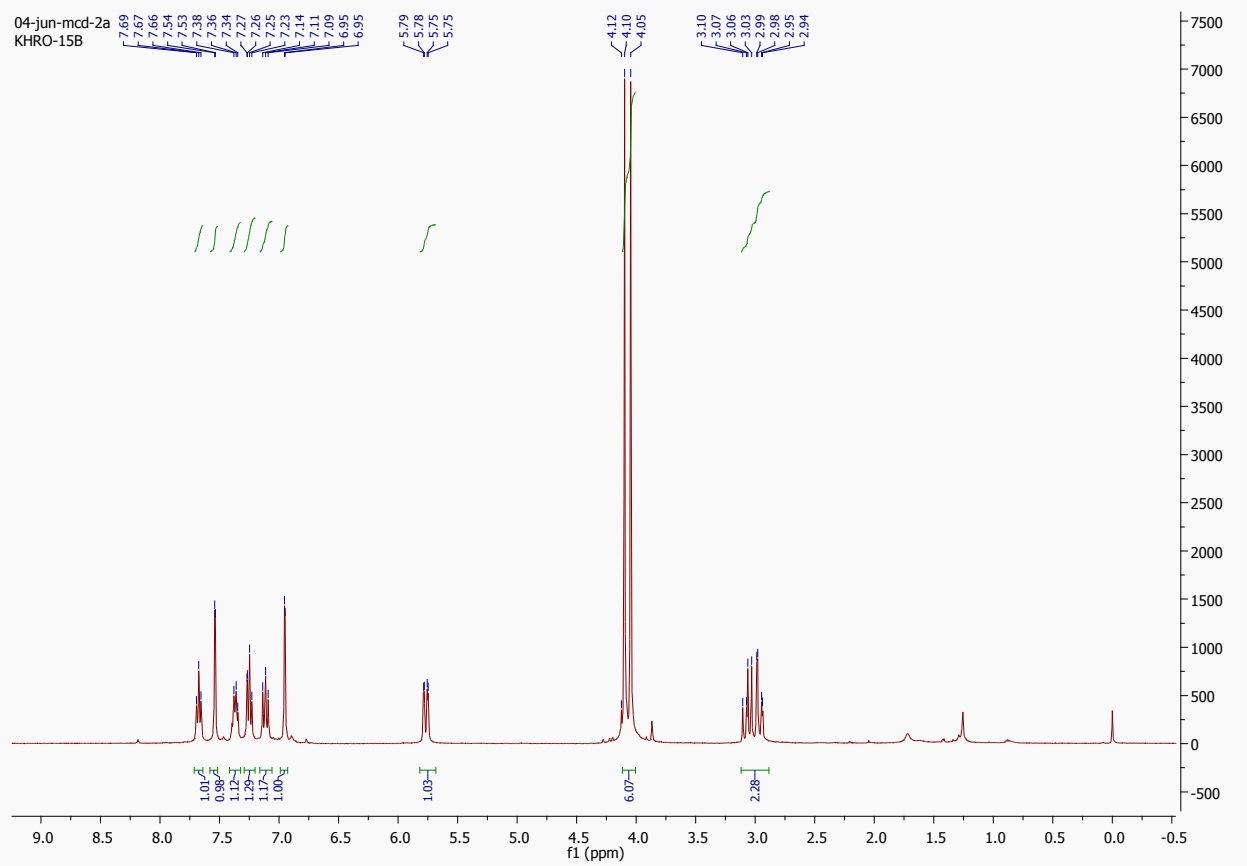
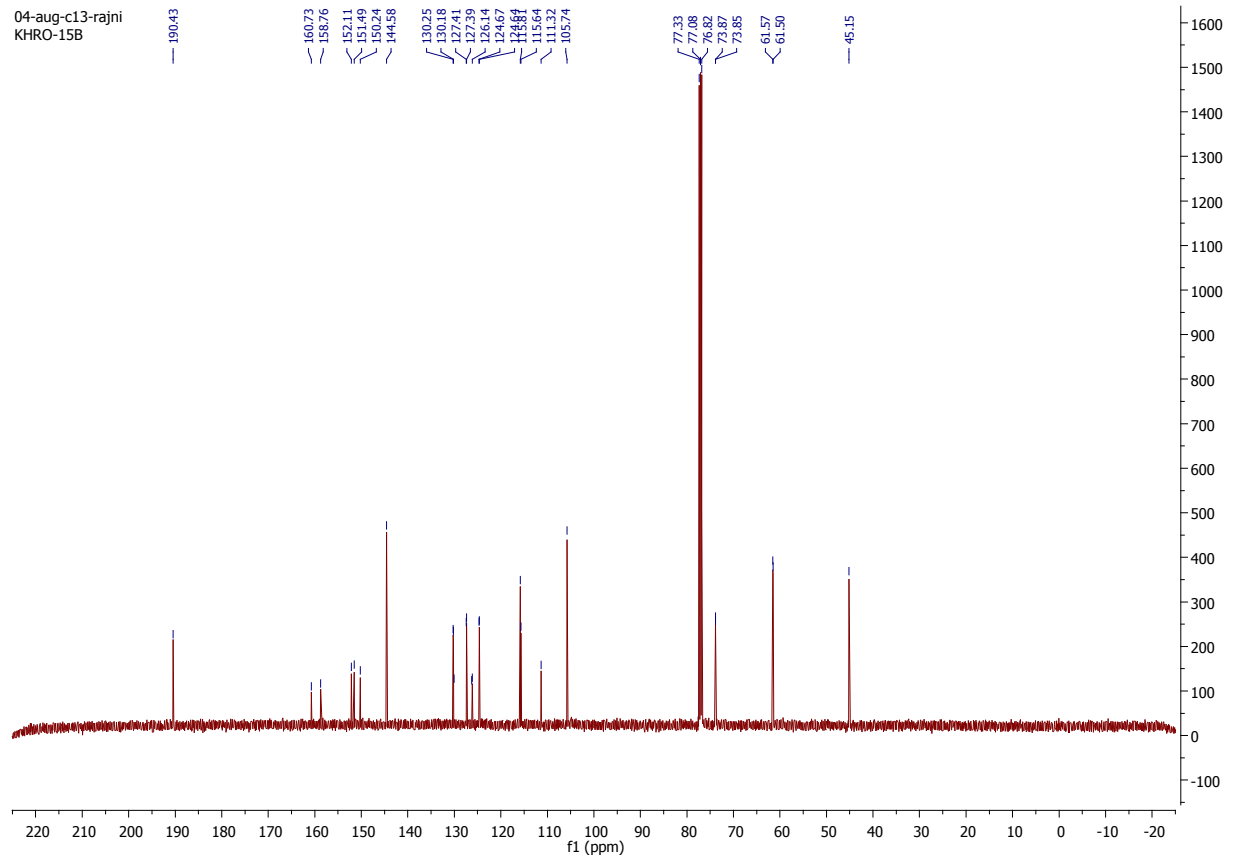

c13-rajni
KHR014B
144.59
131.41
126.78
126.72
116.90
116.72
105.72
77.98
61.48
61.43
45.98
30000
25000
20000
15000
10000
5000
0
-5000
-10000
-15000
-20000
-25000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Figure S1.37. ^{1}H, ^{13}C and DEPT-135 NMR of **4m** in $CDCl_3$





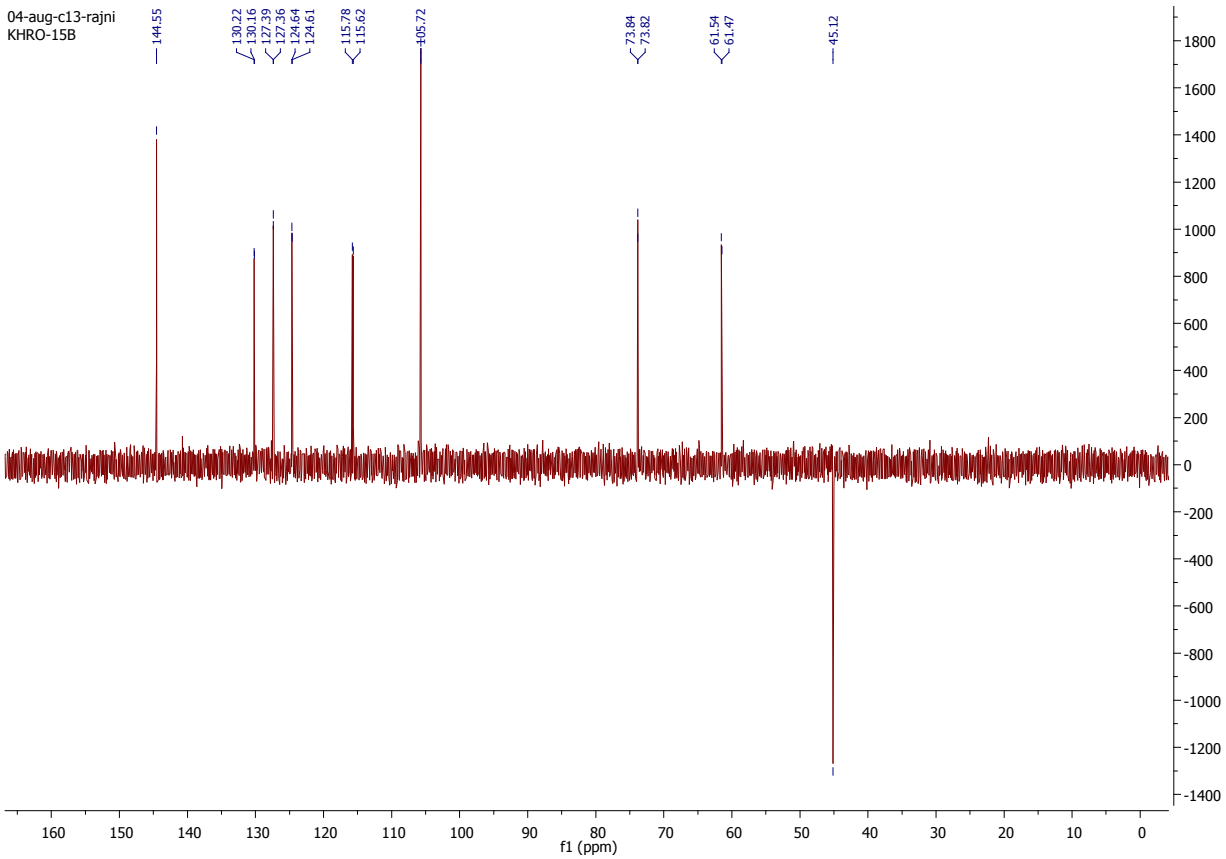
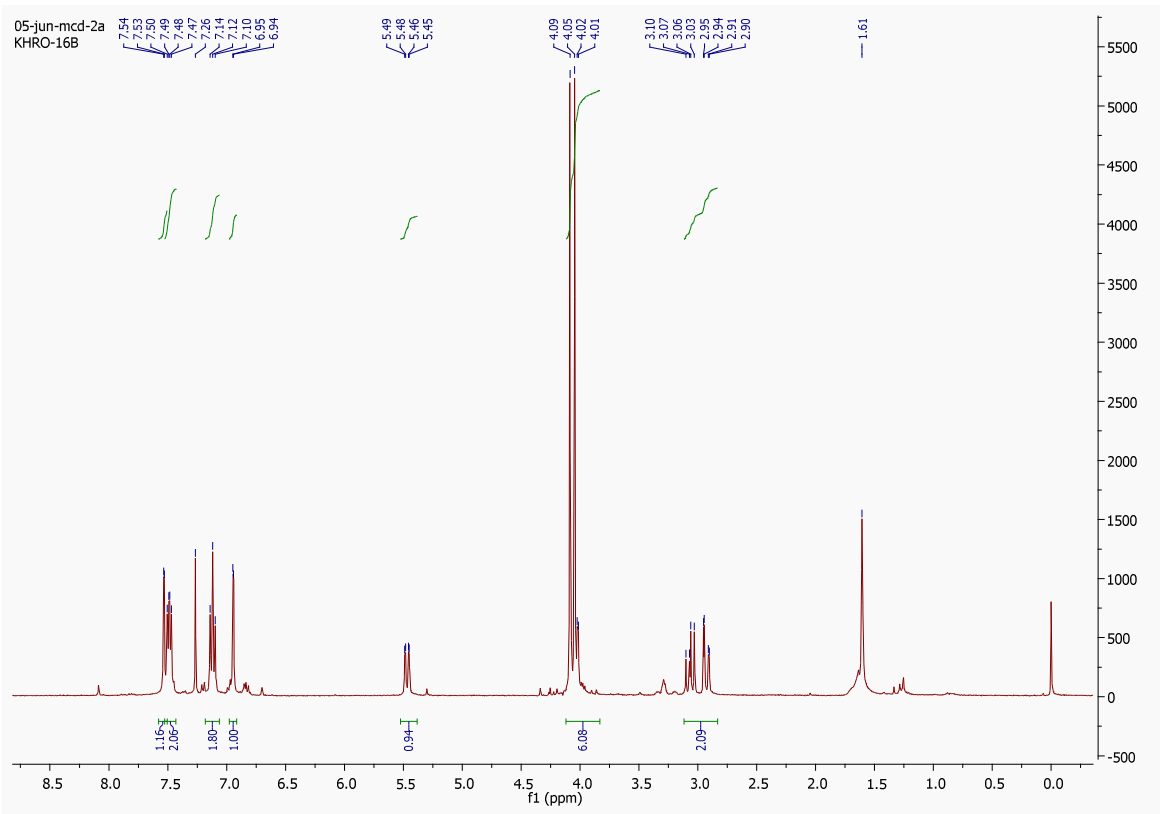
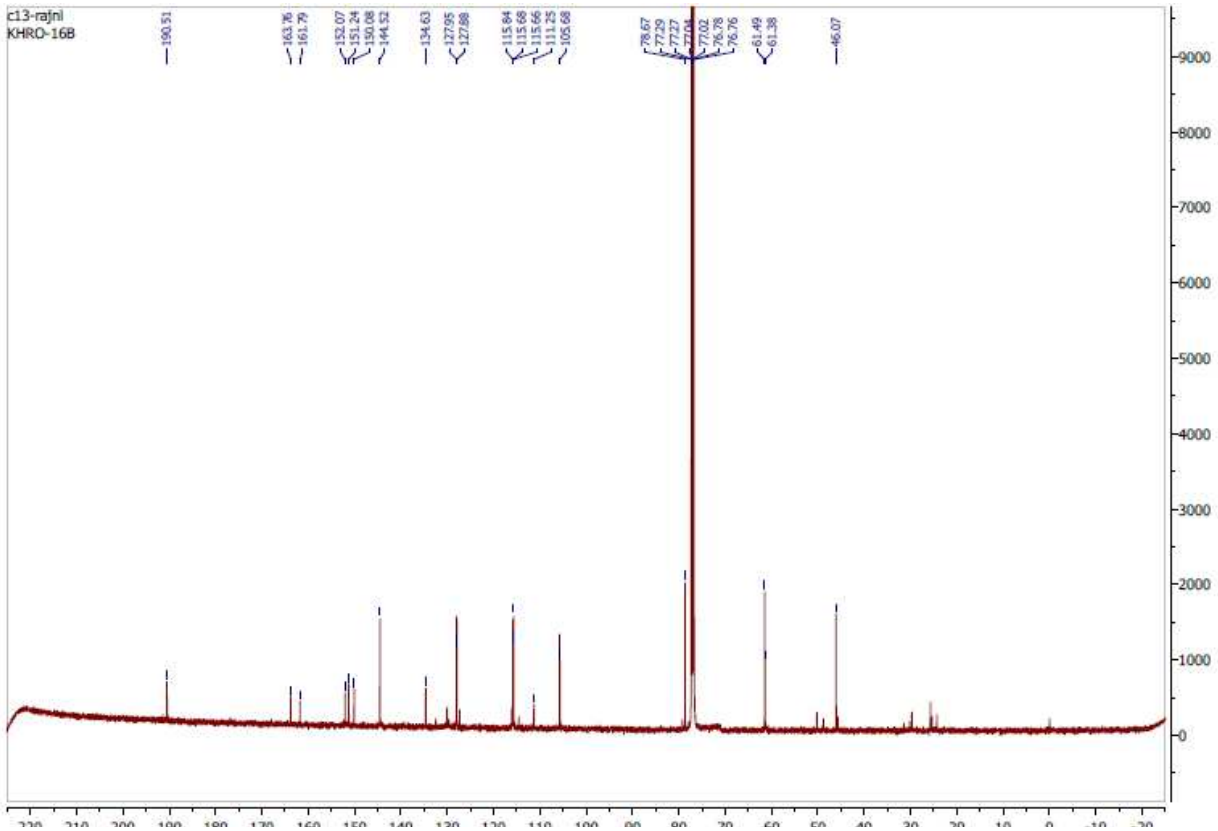

04-aug-c13-rajni
KHRO-15B
144.55
130.22
130.16
127.39
127.36
124.64
124.61
115.78
115.62
105.72
73.84
73.82
61.54
61.47
45.12
f1 (ppm)

Figure S1.38. ^{1}H, ^{13}C and DEPT-135 NMR of **4n** in $CDCl_3$





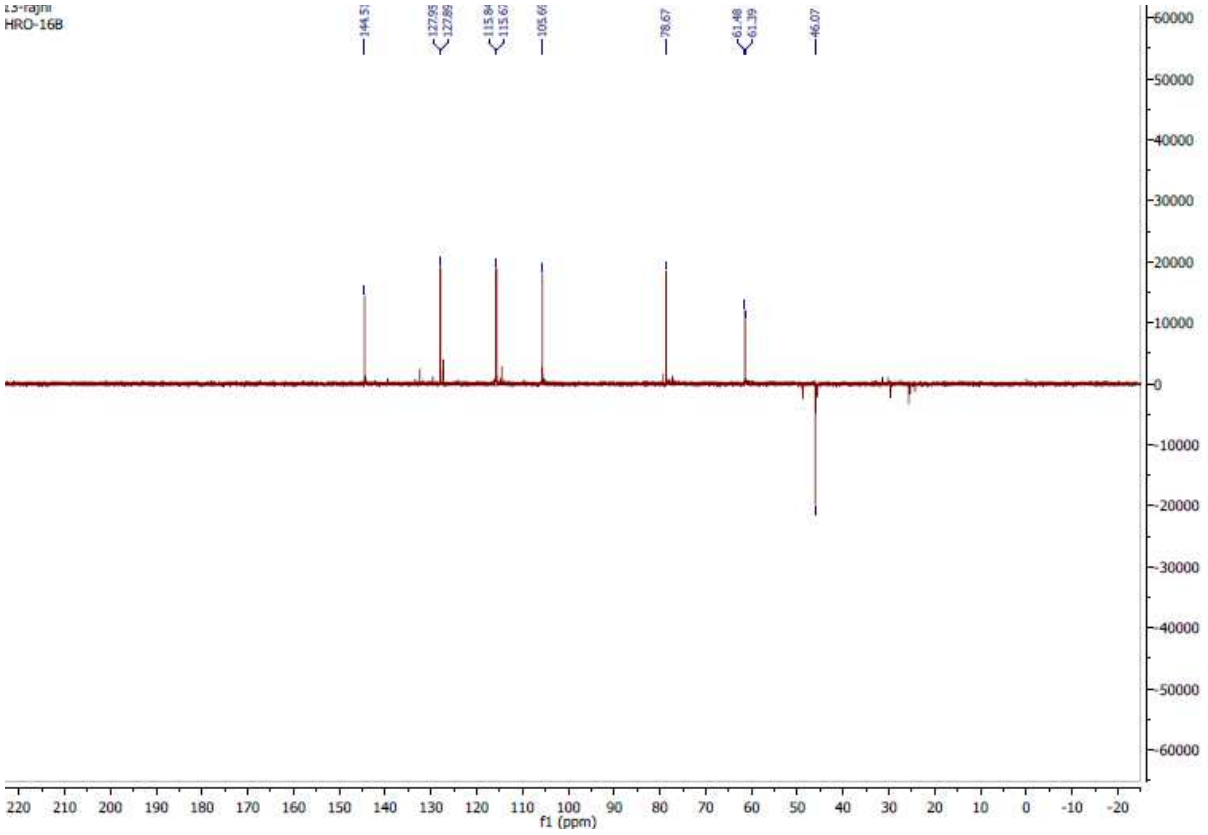
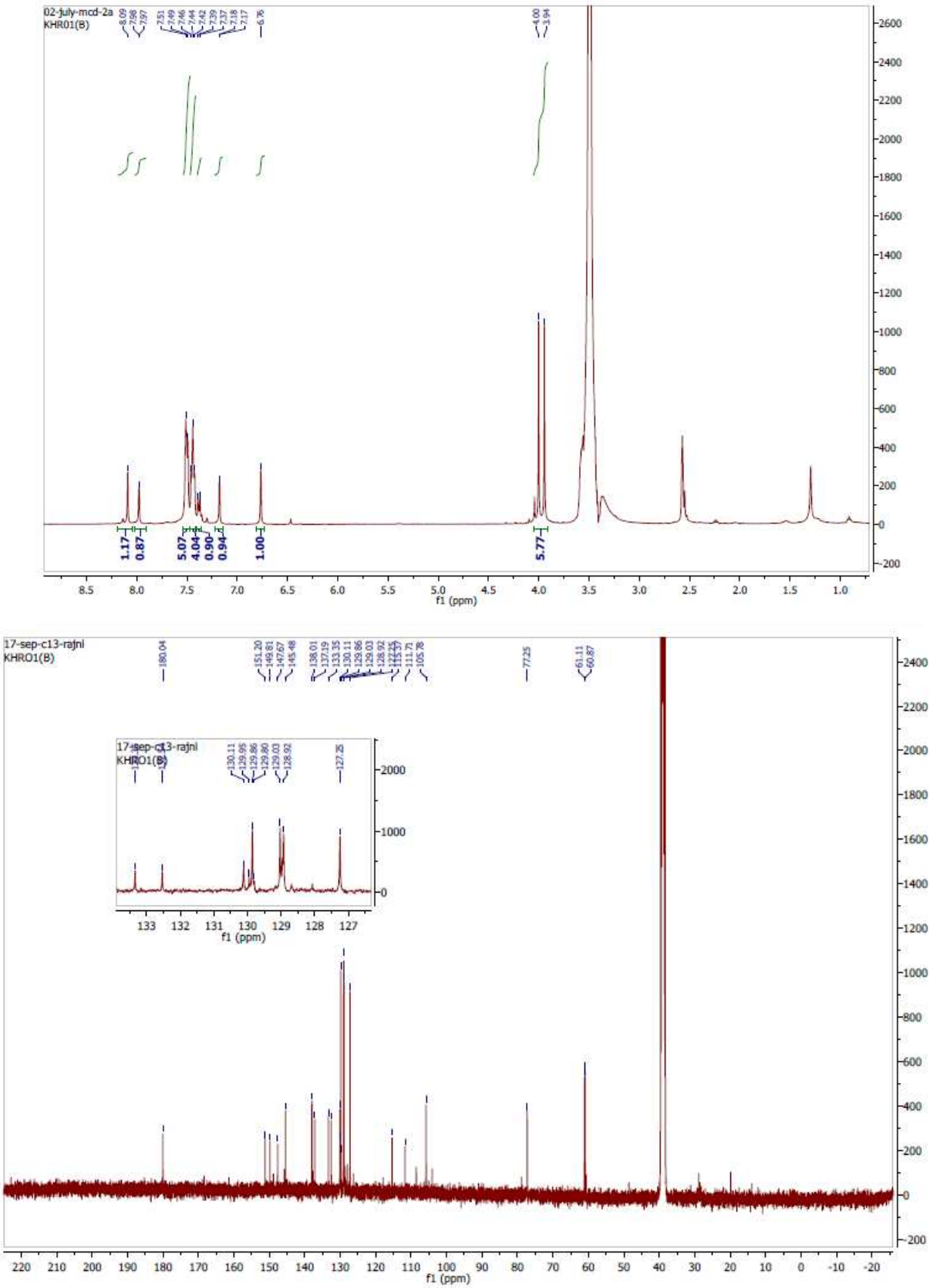

HRO-16B
144.51
127.95
127.89
115.84
115.61
105.66
78.67
61.48
61.39
46.07
60000
50000
40000
30000
20000
10000
0
10000
20000
30000
40000
50000
60000
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

Figure S1.39. ^{1}H, ^{13}C and DEPT-135 NMR of **4o** in $CDCl_3$



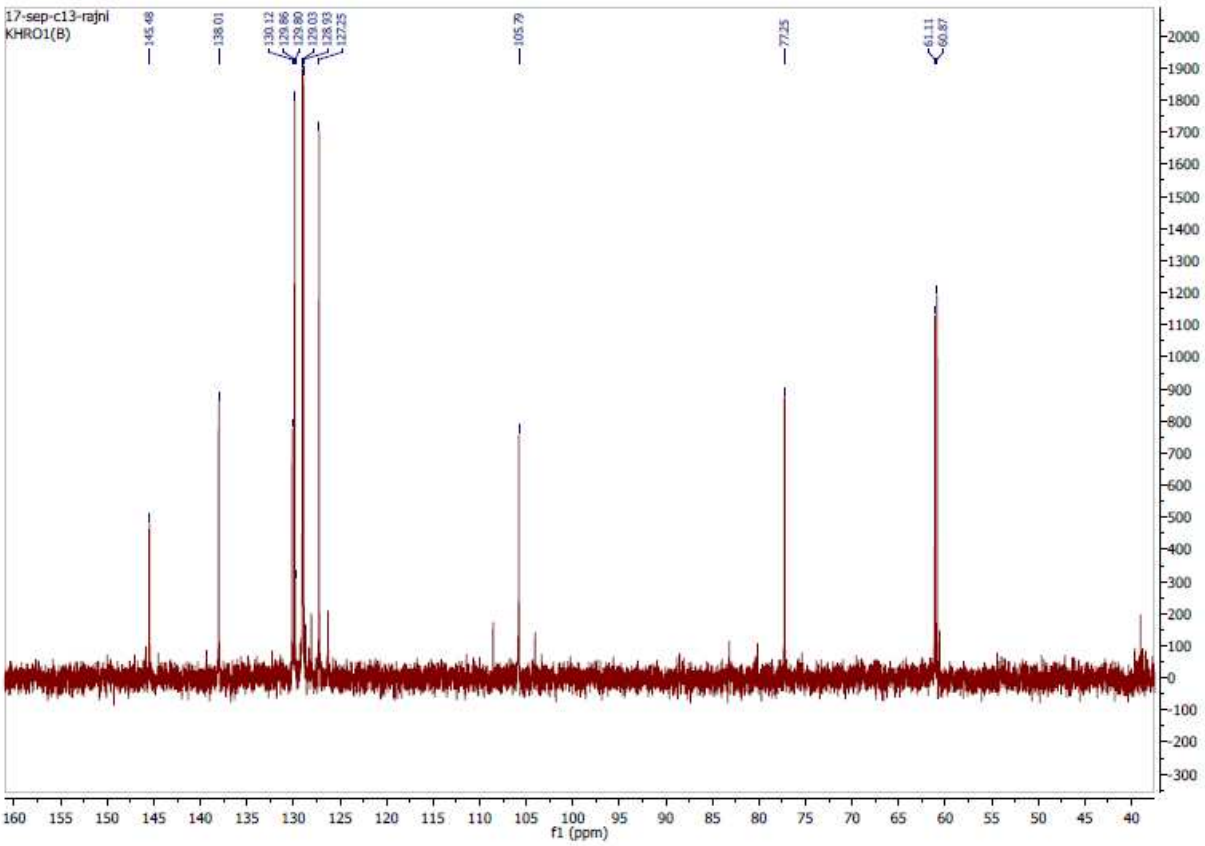
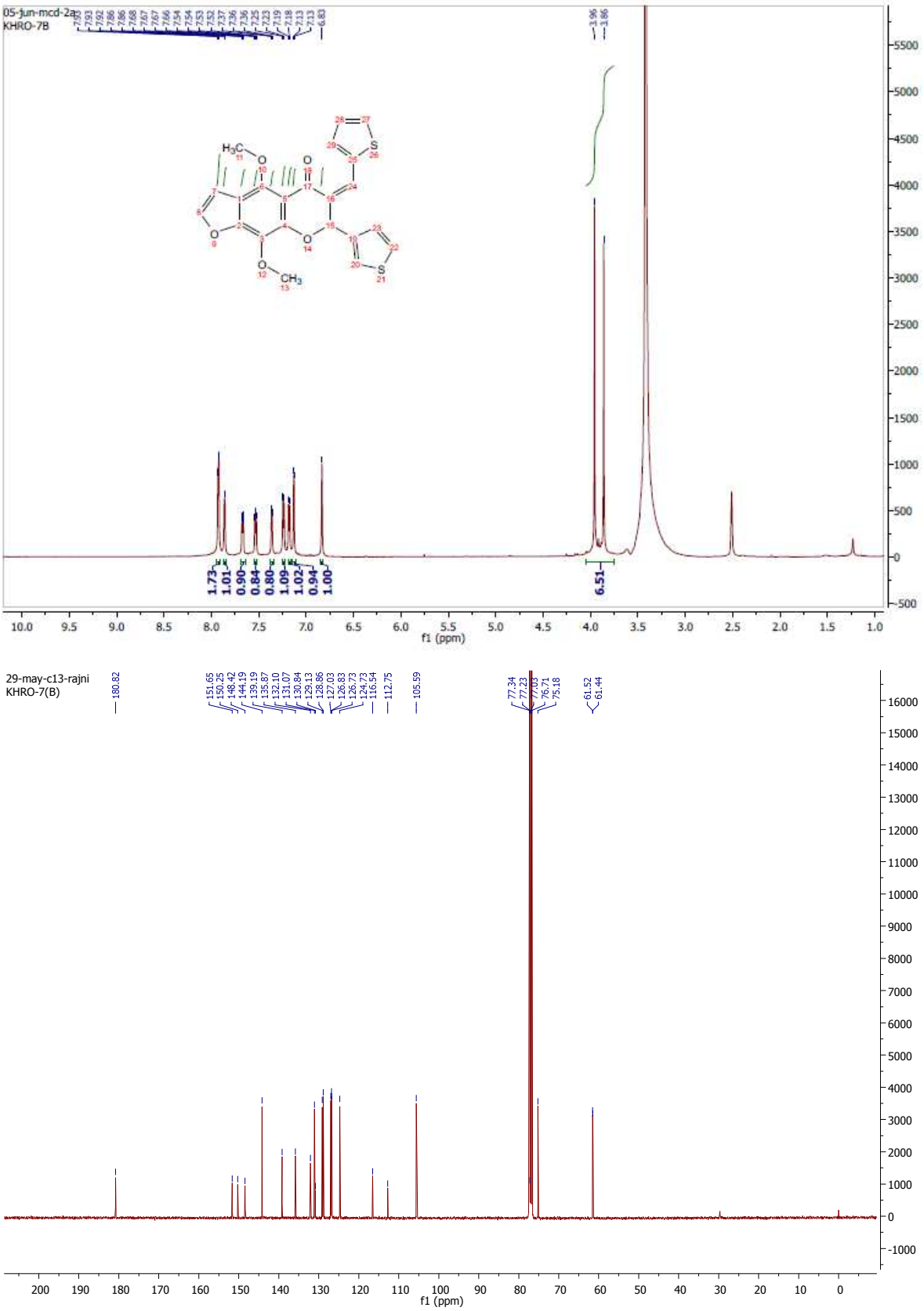
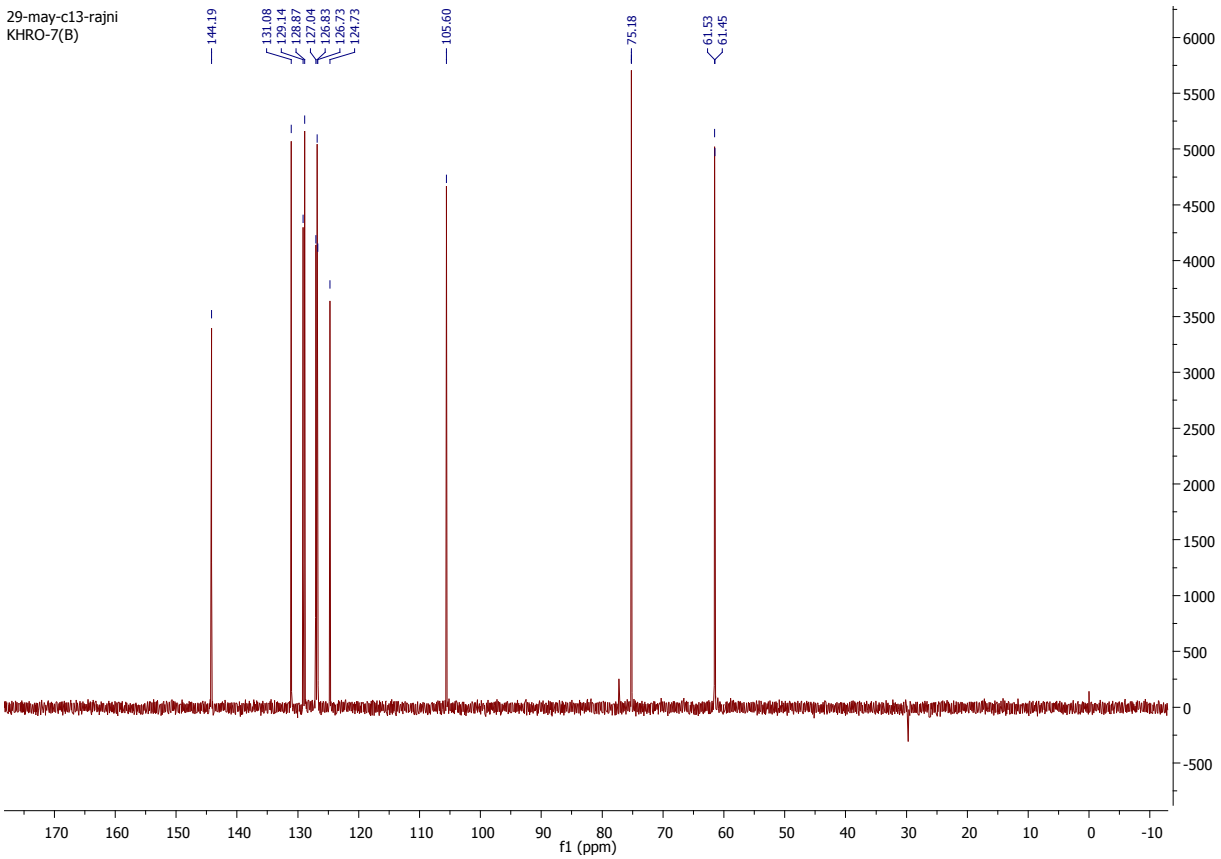

17-sep-c13-rajni
KHRO1(B)
145.48
138.01
130.12
129.86
129.80
129.03
128.93
127.25
105.79
77.25
61.11
60.87
f1 (ppm)

Figure S1.40. ^{1}H, ^{13}C and DEPT-135 NMR of **4p** in $CDCl_3$




29-may-c13-rajni
KHRO-7(B)
144.19
131.08
129.14
128.87
127.04
126.83
126.73
124.73
105.60
75.18
61.53
61.45
f1 (ppm)