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Supporting Information

A Bioinspired Catalytic Aerobic Oxidative C–H Functionalization of Primary Aliphatic Amines: Synthesis of 1,2-Disubstituted Benzimidazoles

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Supporting Information

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I. General considerations

^1H NMR and 1D proton decoupled ^{13}C NMR spectra were recorded in CDCl_3 on a Bruker AC-300 spectrometer operating at 300 MHz and 75 MHz, respectively. Chemical shifts δ are given in ppm relative to TMS and coupling constants J , in Hertz. The measurements were carried out using the standard pulse-sequences. The carbon type (methyl, methylene, methine, or quaternary) was determined by DEPT experiments. High-resolution mass spectra (HRMS) were performed on a Bruker maXis mass spectrometer operating in the positive ion mode. Chemicals were commercial products of the highest available purity and were used as supplied.

The following compounds are known with analytical data reported in the literature: benzimidazole **4a**^[1-3]; benzimidazole **4b**^[2]; benzimidazole **4d**^[2]; benzimidazole **4g**^[2]; benzimidazole **4h**^[2]; benzimidazole **4k**^[3]; benzimidazole **4q**^[4]; benzimidazole **4s**^[5]; benzimidazole **4t**^[6]; benzimidazole **4u**^[3]; benzimidazole **4v**^[7]

II. Analytical data for known compounds for which NMR data are not reported

Benzimidazole 4c.^[8] ^1H NMR (300 MHz, CDCl_3 , 25°C, TMS): δ = 1.35 (s, 9H, CH_3), 7.28 (m, 2H, Ar), 7.35-7.40 (m, 5H, Ar), 7.55-7.58 (m, 5H, Ar), 7.95 (d, J = 8 Hz, 1H, Ar); ^{13}C NMR (75 MHz, CDCl_3 , 25°C, TMS): δ = 31.2 (3 x CH_3), 34.8 (Cq), 110.4 (CH, Ar), 119.7 (CH, Ar), 122.9 (CH, Ar), 123.2 (CH, Ar), 125.3 (2 x CH, Ar), 126.9 (Cq), 127.6 (2 x CH, Ar), 128.6 (CH, Ar), 129.1 (2 x CH, Ar), 129.9 (2 x CH, Ar), 137.2 (Cq), 137.3 (Cq), 143.0 (Cq), 152.4 (Cq), 152.7 (Cq); HRMS (ESI+) m/z calcd for $\text{C}_{23}\text{H}_{22}\text{N}_2$ $[\text{M}+\text{H}]^+$ 327.1856, Found 327.1856.

Benzimidazole 4e.^[9] ^1H NMR (300 MHz, CDCl_3 , 25°C, TMS): δ = 3.66 (s, 6H, 2 x CH_3), 6.49 (m, 1H, Ar), 6.78 (m, 2H, Ar), 7.26-7.28 (m, 2H, Ar), 7.33-7.36 (m, 3H, Ar), 7.50-7.53 (m, 3H, Ar), 7.95 (d, J = 8 Hz, 1H, Ar); ^{13}C NMR (75 MHz, CDCl_3 , 25°C, TMS): δ = 55.3 (2 x CH_3), 102.7 (CH, Ar), 107.2 (2 x CH, Ar), 110.5 (CH, Ar), 119.9 (CH, Ar), 123.1 (CH, Ar), 123.5 (CH, Ar), 127.5 (2 x CH, Ar), 128.6 (CH, Ar), 129.9 (2 x CH, Ar), 131.5, (Cq), 137.1 (Cq), 137.3 (Cq), 142.8 (Cq), 152.1 (Cq), 160.5 (2 x Cq); HRMS (ESI+) m/z calcd for $\text{C}_{21}\text{H}_{18}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 331.1441, Found 331.1441.

Benzimidazole 4f.^[10] ^1H NMR (300 MHz, CDCl_3 , 25°C, TMS): δ = 3.65 (m, 2H, NH, D_2O exchanged), 6.60 (d, J = 8.55 Hz, 2H, Ar), 7.25-7.43 (m, 7H, Ar), 7.53-7.56 (m, 3H, Ar), 7.90 (d, J = 7.9 Hz, 1H, Ar); ^{13}C NMR (75 MHz, CDCl_3 , 25°C, TMS): δ = 110.5 (CH, Ar), 115.4 (CH, Ar), 115.7 (CH, Ar), 119.8 (CH, Ar), 123.2 (CH, Ar), 123.5 (CH, Ar), 126.09 (CH, Ar), 126.13 (CH, Ar), 127.4 (CH, Ar), 128.8 (CH, Ar), 130.0 (CH, Ar), 131.4 (CH, Ar), 131.5 (CH, Ar), 136.8 (Cq), 137.2 (Cq), 142.8 (Cq), 151.4

(Cq), 161.8 (Cq), 165.1 (Cq); HRMS (ESI+) m/z calcd for $C_{19}H_{15}N_3$ $[M+H]^+$ 286.1344, Found 286.1347.

Benzimidazole 4j.^[9] 1H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 7.23-7.55 (m, 12H, Ar), 7.89-7.94 (m, 2H, Ar), 8.05 (d, J = 8.7 Hz, 1H, Ar), 8.18 (m, 1H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$, 25°C, TMS): δ = 110.7 (CH, Ar), 120.2 (CH, Ar), 123.1 (CH, Ar), 123.5 (CH, Ar), 124.6 (CH, Ar), 125.9 (CH, Ar), 126.3 (CH, Ar), 126.5 (2 x CH, Ar), 126.7 (CH, Ar), 127.7 (Cq), 128.1 (CH, Ar), 128.3 (CH, Ar), 129.5 (3 x CH, Ar), 130.0 (CH, Ar), 132.2 (Cq), 133.6 (Cq), 136.1 (Cq), 136.4 (Cq), 143.2 (Cq), 151.9 (Cq); HRMS (ESI+) m/z calcd for $C_{23}H_{16}N_2$ $[M+H]^+$ 321.1386, Found 321.1387.

Benzimidazole 4l.^[11] 1H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 6.21 (d, J = 3.4 Hz, 1H, furyl), 6.4 (m, 1H, furyl), 7.13 (d, J = 7.8 Hz, 1H, furyl), 7.25-7.40 (m, 2H, Ar), 7.44-7.47 (m, 2H, Ar), 7.52-7.53 (m, 1H, Ar), 7.62-7.63 (m, 3H, Ar), 7.92 (d, J = 8.0 Hz, 1H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$, 25°C, TMS): δ = 110.2 (CH, Ar), 111.5 (CH, Ar), 112.2 (CH, Ar), 119.9 (CH, Ar), 123.1 (CH, Ar), 123.6 (CH, Ar), 128.0 (2 x CH, Ar), 129.5 (CH, Ar), 130.0 (2 x CH, Ar), 136.4 (Cq), 137.2 (Cq), 142.9 (Cq), 144.2 (2 x CH, Ar), 144.5 (Cq); HRMS (ESI+) m/z calcd for $C_{17}H_{12}N_2O$ $[M+H]^+$ 261.1028, Found 261.1035.

Benzimidazole 4m.^[12] 1H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 1.22-1.97 (m, 10H, cyclohexyl), 2.73-2.78 (m, 1H, cyclohexyl), 7.10 (d, J = 8 Hz, 1H, Ar), 7.22 (t, J = 8 Hz, 1H, Ar), 7.31 (d, J = 8 Hz, 1H, CH, Ar), 7.40 (m, 2H, Ar), 7.61-7.64 (m, 3H, Ar), 7.86 (d, J = 7.9 Hz, 1H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$, 25°C, TMS): δ = 25.7 (CH_2), 26.2 (2 x CH_2), 32.0 (2 x CH_2), 36.2 (CH), 110.1 (CH, Ar), 119.1 (CH, Ar), 122.4 (CH, Ar), 122.5 (CH, Ar), 127.6 (2 x CH, Ar), 129.0 (CH, Ar), 130.0 (2 x CH, Ar), 136.0 (Cq), 136.4 (Cq), 142.3 (Cq), 159.3 (Cq); HRMS (ESI+) m/z calcd for $C_{19}H_{20}N_2$ $[M+H]^+$ 277.1705, Found 277.1693.

Benzimidazole 4n.^[13] 1H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ = 1.05-1.10 (m, 2H, cyclopropyl), 1.37-1.40 (m, 2H, cyclopropyl), 1.90 (m, 1H, cyclopropyl), 7.18-7.20 (m, 2H, Ar), 7.25-7.29 (m, 1H, Ar), 7.50-7.54 (m, 3H, Ar), 7.60-7.62 (m, 2H, Ar), 7.77 (d, J = 7.9 Hz, 1H, Ar); ^{13}C NMR (75 MHz, $CDCl_3$, 25°C, TMS): δ = 8.3 (CH), 9.6 (2 x CH_2), 109.7 (CH, Ar), 118.8 (CH, Ar), 122.2 (CH, Ar), 122.4 (CH, Ar), 127.4 (2 x CH, Ar), 128.7 (CH, Ar), 129.9 (2 x CH, Ar), 136.0 (Cq), 136.5 (Cq), 142.4 (Cq), 156.9 (Cq); HRMS (ESI+) m/z calcd for $C_{16}H_{14}N_2$ $[M+H]^+$ 235.1235, Found 235.1228.

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IV. Analytical data for new compounds

Benzimidazole 4i. Colorless crystal (recrystallized from petroleum ether) m.p. 120-124°C; ¹H NMR (300 MHz, CDCl₃, 25°C, TMS): δ = 7.28-7.35 (m, 3H, Ar), 7.41-7.53 (m, 8H, Ar), 7.98 (d, *J* = 9.0 Hz, 1H, Ar); ¹³C NMR (75 MHz, CDCl₃, 25°C, TMS): δ = 110.7 (CH, Ar), 120.3 (CH, Ar), 123.2 (CH, Ar), 123.9 (CH, Ar), 126.6 (2 x CH, Ar), 127.2 (CH, Ar), 128.4 (CH, Ar), 128.8 (CH, Ar), 129.6 (2 x CH, Ar), 129.8 (CH, Ar), 133.3 (Cq), 135.0 (Cq), 135.8 (Cq), 135.9 (Cq), 136.5 (Cq), 142.8 (Cq), 149.4 (Cq); HRMS (ESI+) *m/z* calcd for C₁₉H₁₂Cl₂N₂ [M+H]⁺ 339.0450. Found 339.0450.

Benzimidazole 4o. Colorless crystal (recrystallized from petroleum ether): m.p. 80-84°C; ¹H NMR (300 MHz, CDCl₃, 25°C, TMS): δ = 3.10-3.30 (m, 4H, 2 x CH₂), 7.13-7.36 (m, 10H, Ar), 7.57 (m, 3H, Ar), 7.88 (d, *J* = 7.9 Hz, 1H, Ar); ¹³C NMR (75 MHz, CDCl₃, 25°C, TMS): δ = 29.8 (CH₂), 34.2 (CH₂), 110.2 (CH, Ar), 119.1 (CH, Ar), 122.6 (CH, Ar), 122.8 (CH, Ar), 126.3 (CH, Ar), 127.4 (2 x CH, Ar), 128.4 (2 x CH, Ar), 128.5 (2 x CH, Ar), 129.0 (CH, Ar), 129.9 (2 x CH, Ar), 135.7 (Cq), 136.4 (Cq), 140.8 (Cq), 142.2 (Cq), 154.3 (Cq); HRMS (ESI+) *m/z* calcd for C₂₁H₁₈N₂ [M+H]⁺ 299.1548. Found 299.1548.

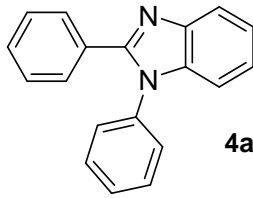
Benzimidazole 4p. Pale yellow oil: ¹H NMR (300 MHz, CDCl₃, 25°C, TMS): δ = 0.85-0.89 (t, *J* = 7.0 Hz, 3H, *n*-octyl), 1.25-1.40 (m, 8H, *n*-octyl), 1.76-7.86 (m, 2H, *n*-octyl), 2.78-2.83 (t, *J* = 7.0 Hz, 2H, *n*-octyl), 7.10 (d, *J* = 7.5 Hz, 1H, Ar), 7.20 (t, *J* = 7.5 Hz, 1H, Ar), 7.3 (t, *J* = 7.0 Hz, 1H, Ar), 7.36 (d, *J* = 7 Hz, 2H, Ar), 7.57 (m, 3H, Ar), 7.82 (d, *J* = 7.0 Hz, 1H, Ar); ¹³C NMR (75 MHz, CDCl₃, 25°C, TMS): δ = 14.1 (CH₃), 22.6 (CH₂), 27.7 (CH₂), 27.8 (CH₂), 28.9 (CH₂), 29.3 (CH₂), 31.6 (CH₂), 109.9 (CH, Ar), 119.1 (CH, Ar), 122.3 (CH, Ar), 122.5 (CH, Ar), 127.4 (2 x CH, Ar), 128.9 (CH, Ar), 129.9 (2 x CH, Ar), 136.1 (Cq), 136.5 (Cq), 142.6 (Cq), 155.4 (Cq); HRMS (ESI+) *m/z* calcd for C₂₀H₂₄N₂ [M+H]⁺ 293.2018. Found 293.2018.

Benzimidazole 4r. Colorless crystal (recrystallized from petroleum ether) : m.p. 120-124°C, ¹H NMR (300 MHz, CDCl₃, 25°C, TMS): δ = 0.96 (d, *J* = 6.6 Hz, 6H, isobutyl),

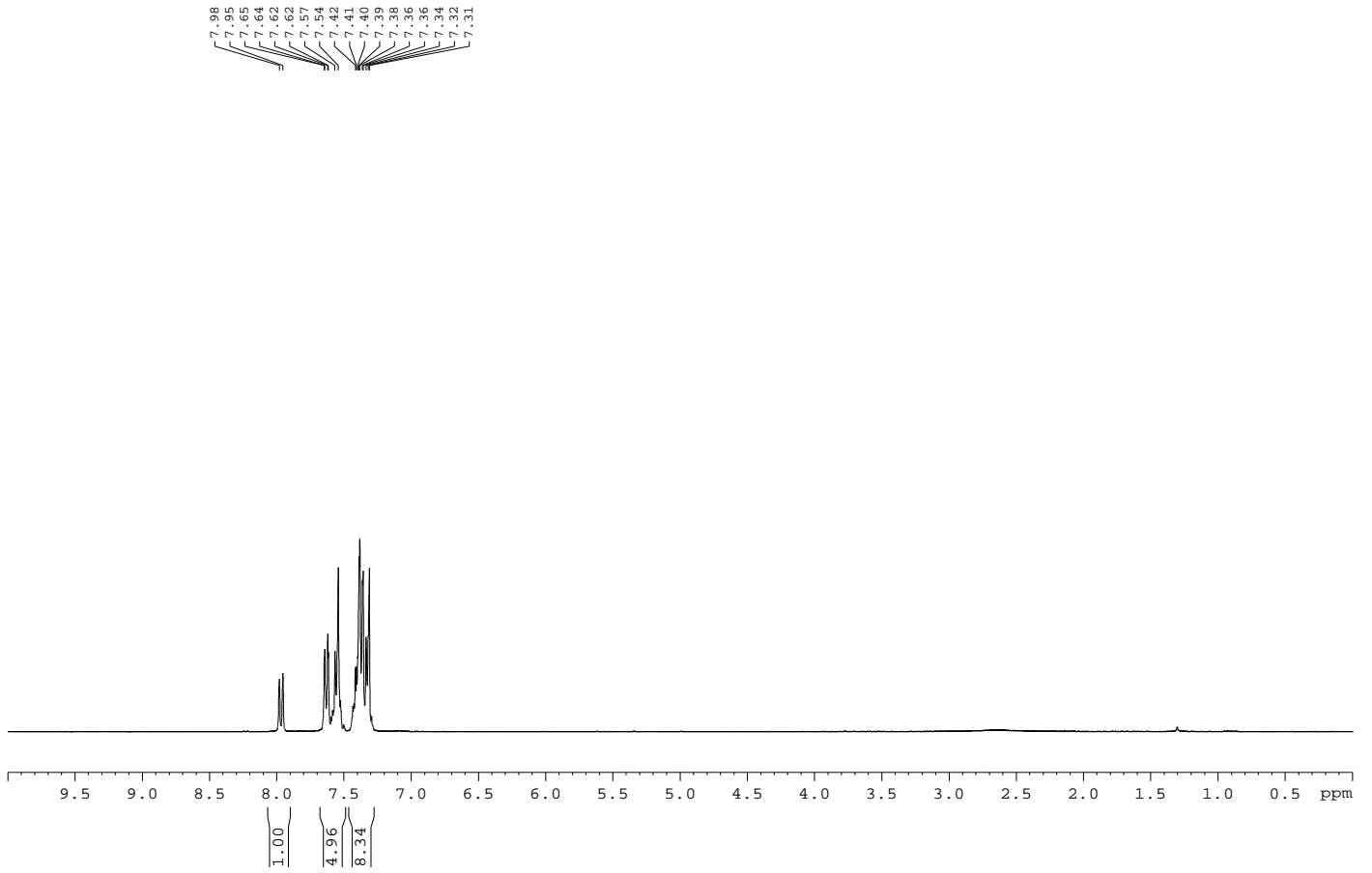
2.20-2.29 (m, 1H, isobutyl), 2.73-2.76 (d, $J = 6.6$ Hz, 2H, isobutyl), 7.15 (d, $J = 7.9$ Hz, 1H, Ar), 7.25 (t, $J = 7.1$ Hz, 1H, CH, Ar), 7.35 (m, 1H, Ar), 7.4 (d, $J = 7.1$ Hz, 2H, Ar), 7.58-7.64 (m, 3H, Ar), 7.85 (d, $J = 7.9$ Hz, 1H, Ar) ; ^{13}C NMR (75 MHz, CDCl_3 , 25°C , TMS): $\delta = 22.5$ (2 x CH_3) , 28.0 (CH, isobutyl), 36.4 (CH_2), 110.1 (CH, Ar), 119.0 (CH, Ar), 122.5 (CH, Ar), 122.7 (CH, Ar), 127.6 (2 x CH, Ar), 129.0 (CH, Ar), 130.0 (2 x CH, Ar), 136.0 (Cq), 136.4 (Cq), 142.1 (Cq), 154.6 (Cq); HRMS (ESI+) m/z calcd for $\text{C}_{17}\text{H}_{18}\text{N}_2$ $[\text{M}+\text{H}]^+$ 251.1548. Found 251.1560.

Benzimidazole 4w. Colorless crystal (recrystallized from petroleum ether) : mp $92-96^\circ\text{C}$ ^1H NMR (300 MHz, CDCl_3 , 25°C , TMS): $\delta = 1.04-1.10$ (m, 2H, cyclopropyl), 1.34-1.39 (m, 2H, cyclopropyl), 1.85 (m, 1H, cyclopropyl), 7.12-7.30 (m, 3H, Ar), 7.45 (d, $J = 8.6$ Hz, 2H, Ar), 7.58 (d, $J = 8.6$ Hz, 2H, Ar), 7.75 (d, $J = 7.9$ Hz, 1H, Ar) ; ^{13}C NMR (75 MHz, CDCl_3 , 25°C , TMS): $\delta = 8.3$ (CH), 9.7 (2 x CH_2), 109.4 (CH, Ar), 119.0 (CH, Ar), 122.5 (CH, Ar), 122.7 (CH, Ar), 128.6 (2 x CH, Ar), 130.1 (2 x CH, Ar), 134.52 (Cq), 134.55 (Cq), 136.3 (Cq), 142.4 (Cq), 156.6 (Cq); HRMS (ESI+) m/z calcd for $\text{C}_{16}\text{H}_{13}\text{ClN}_2$ $[\text{M}+\text{H}]^+$ 269.0846. Found 269.0841.

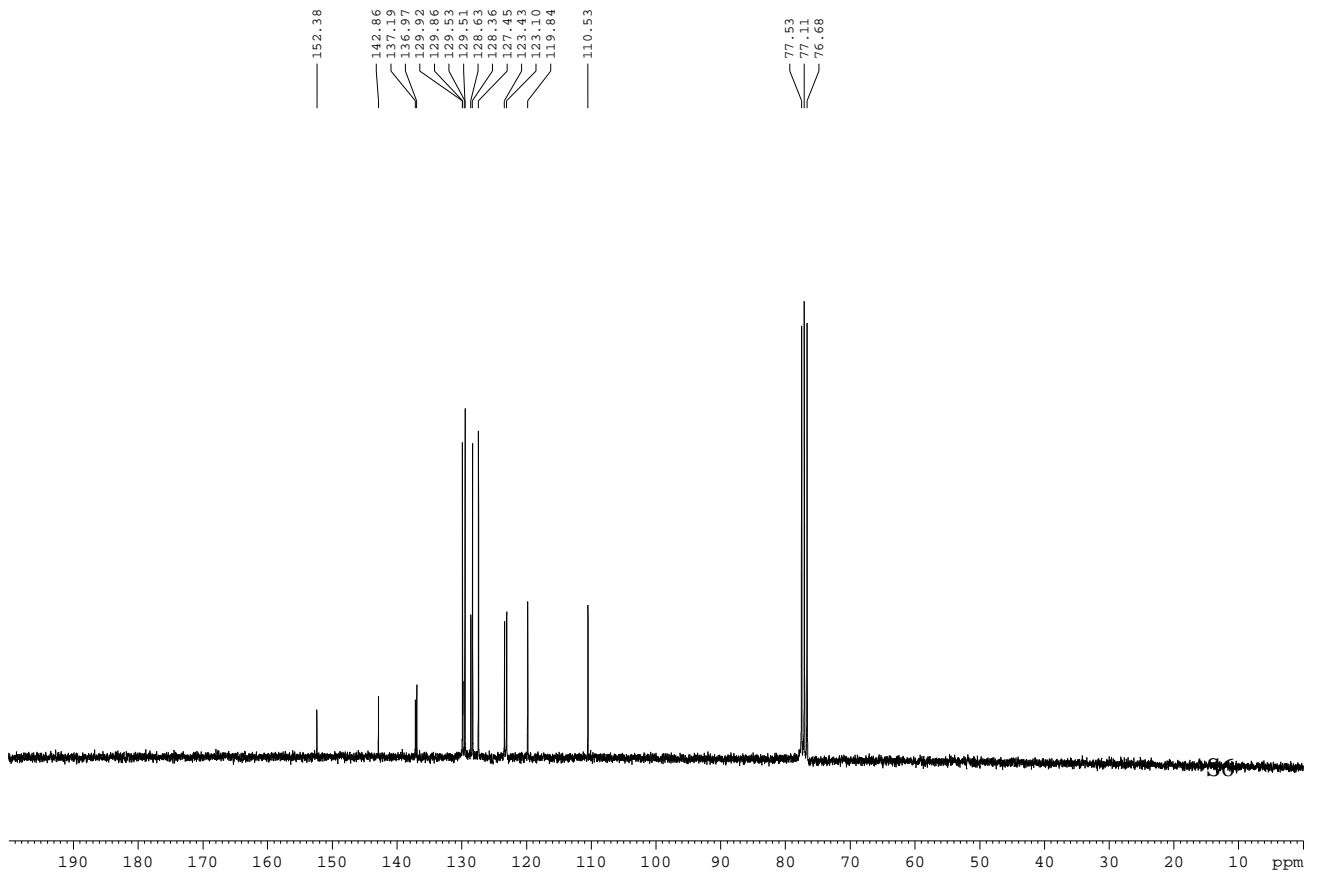
V.High field ^1H NMR spectra and 1D proton-decoupled ^{13}C NMR spectra for all compounds 4a-w (see next page)

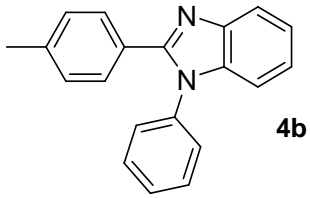


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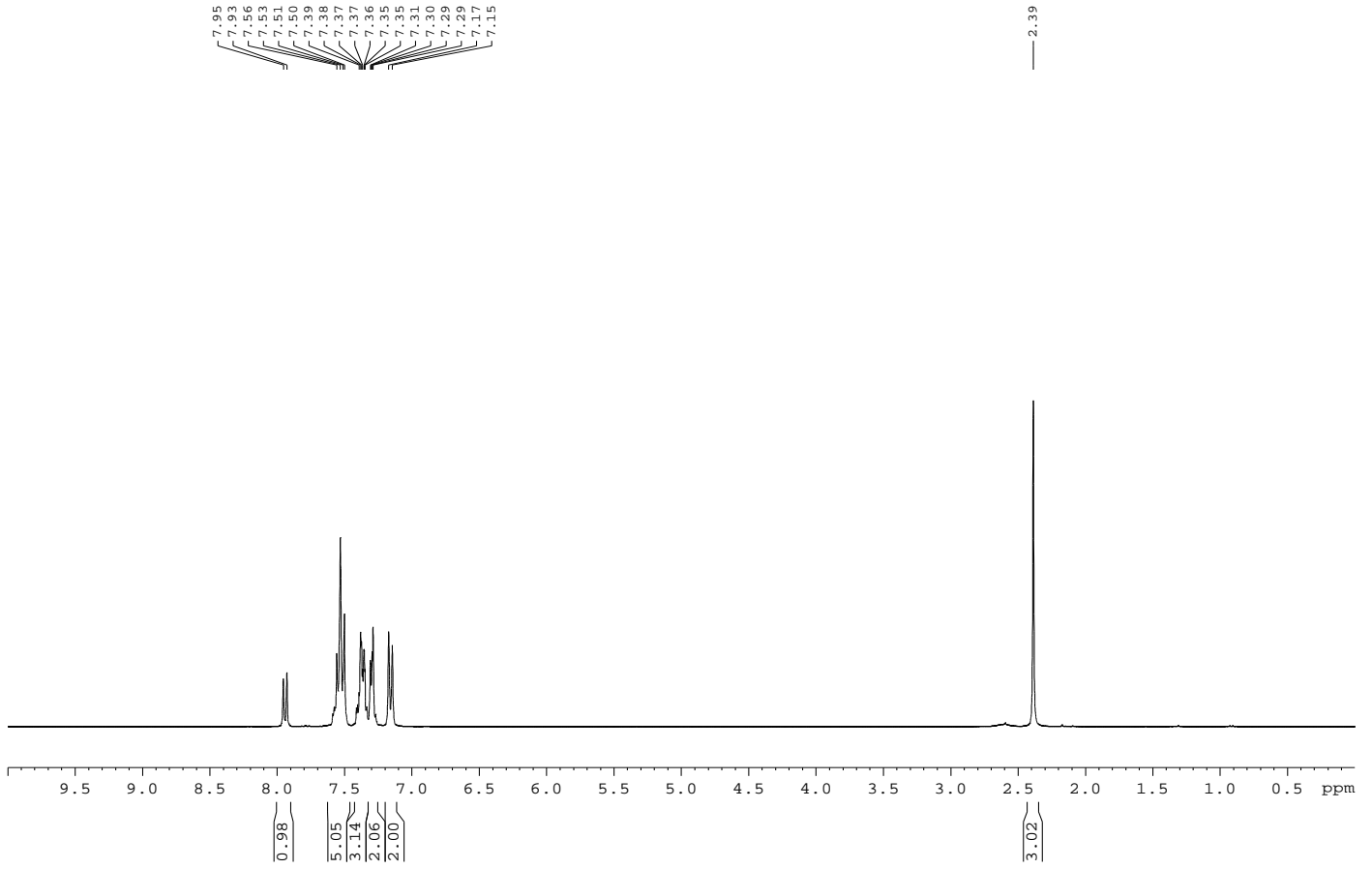


Proton-decoupled carbon NMR spectrum

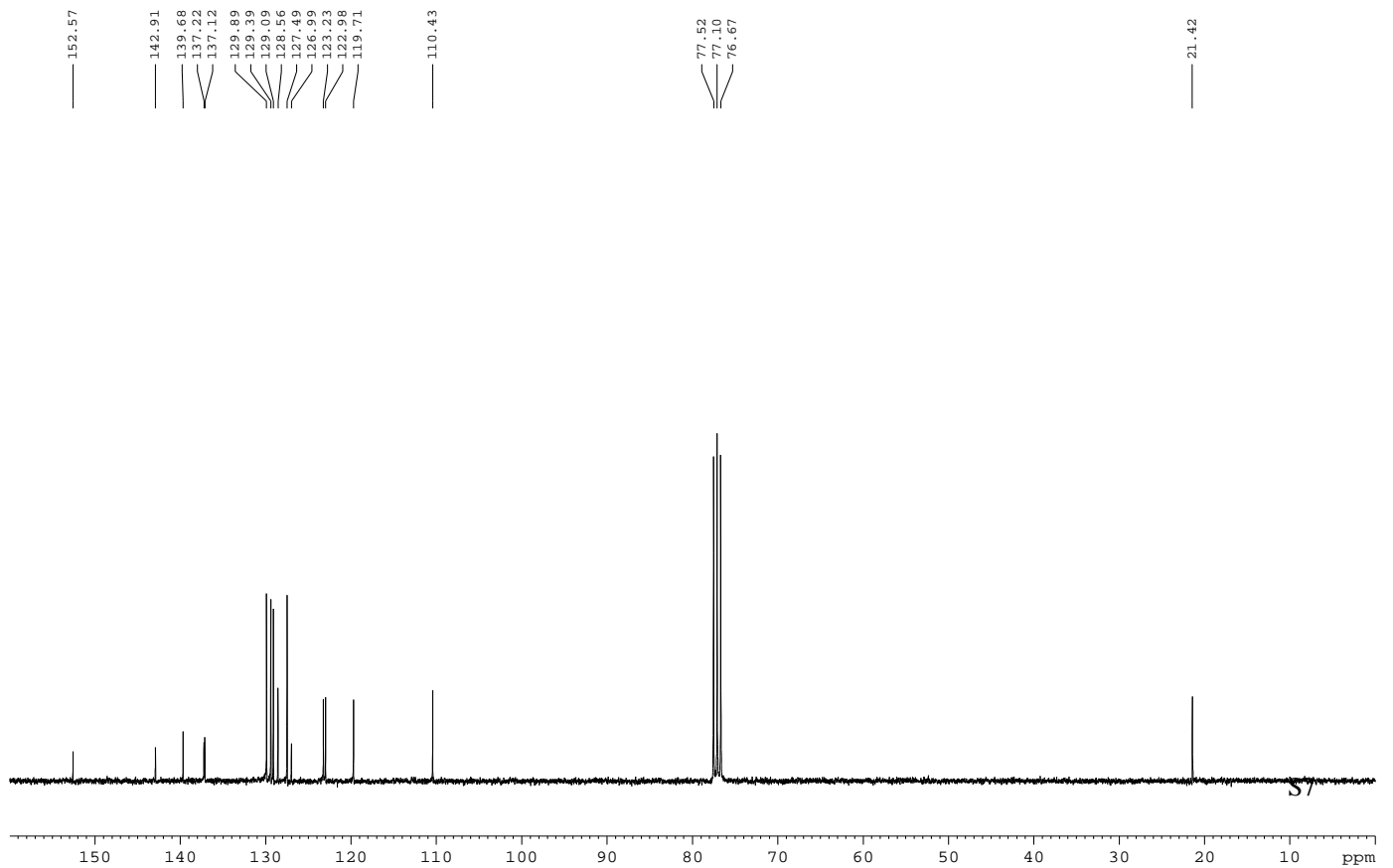


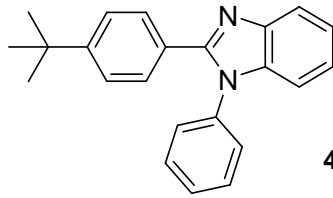


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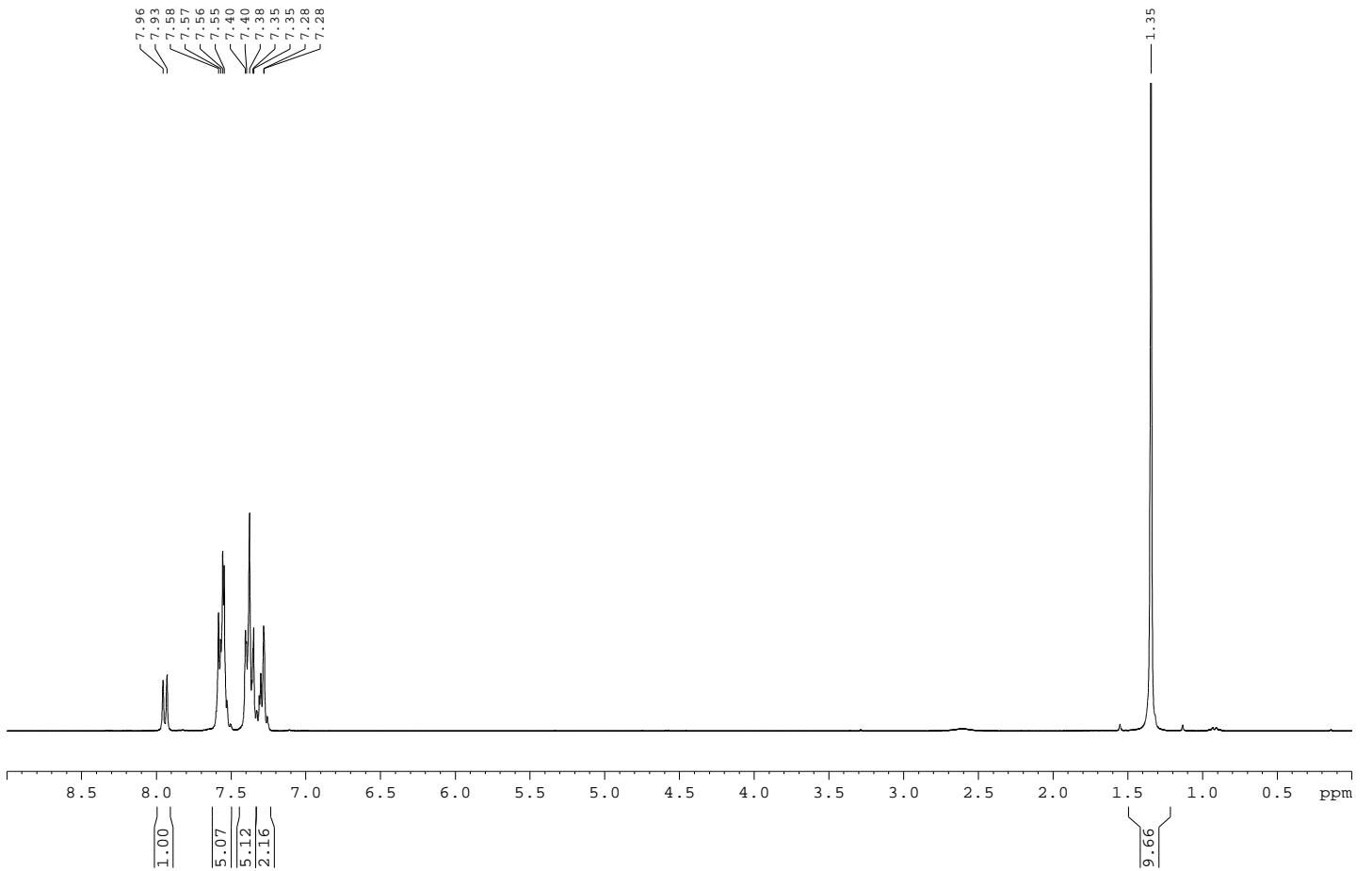


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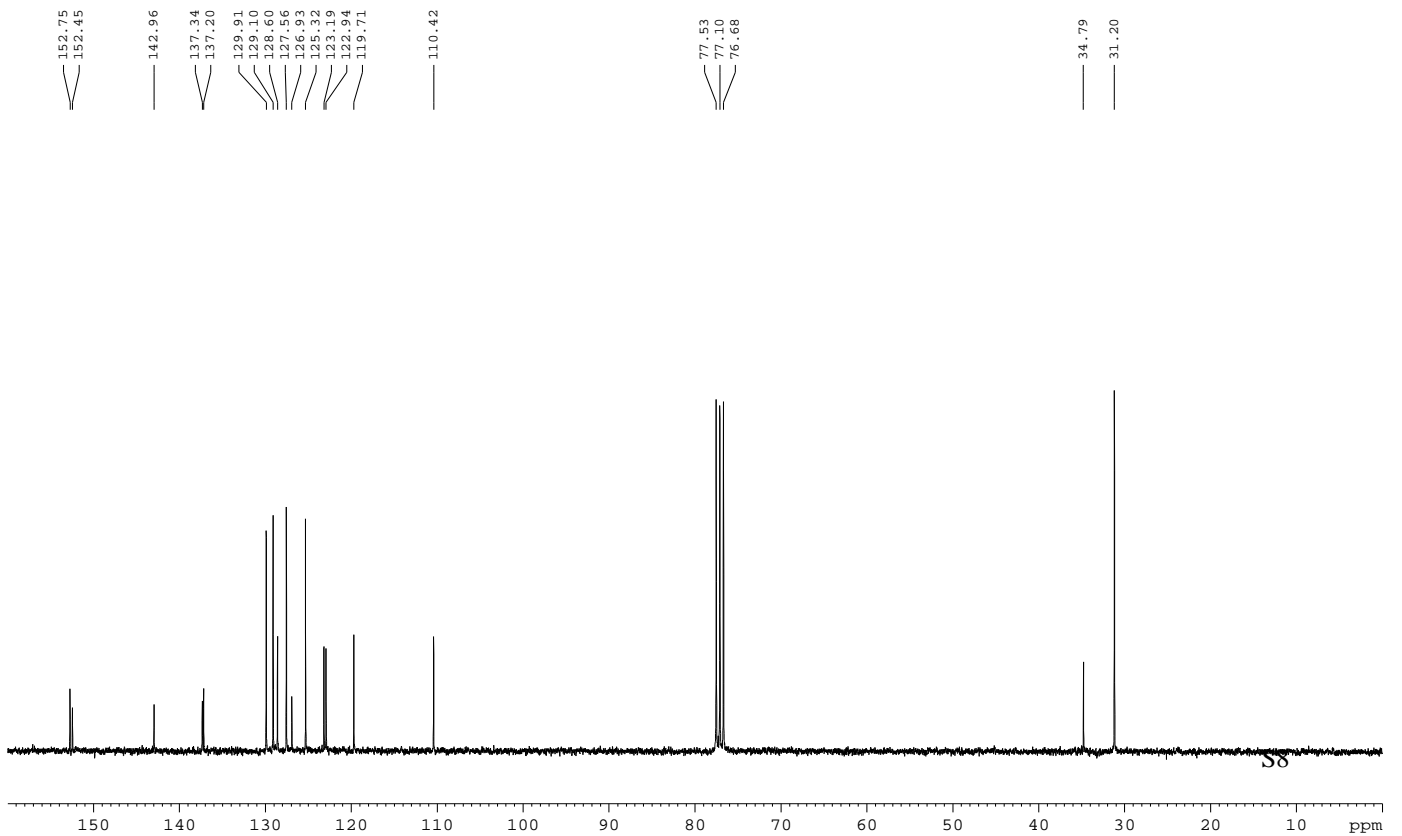


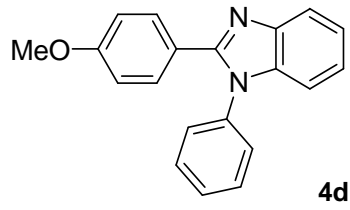


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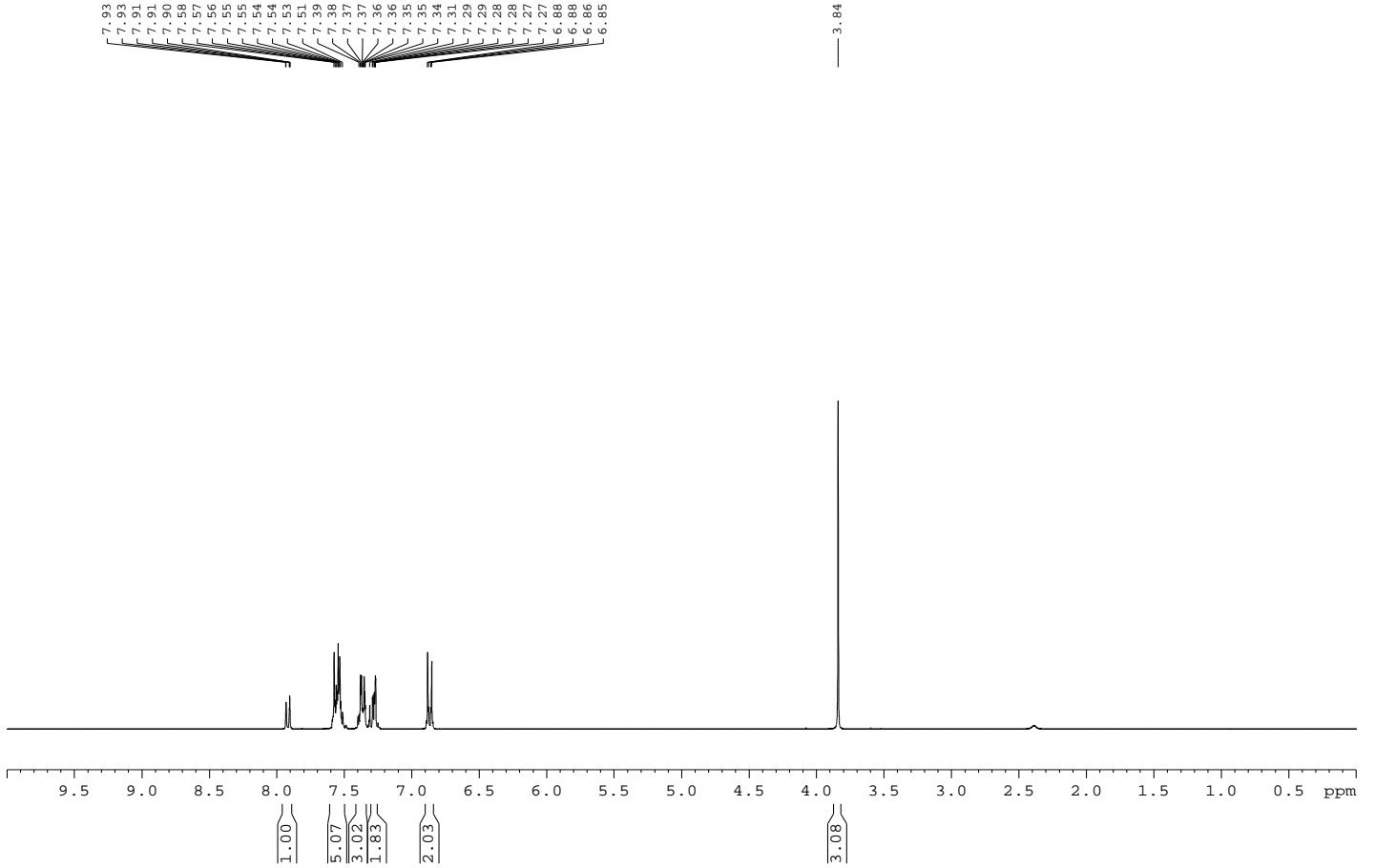


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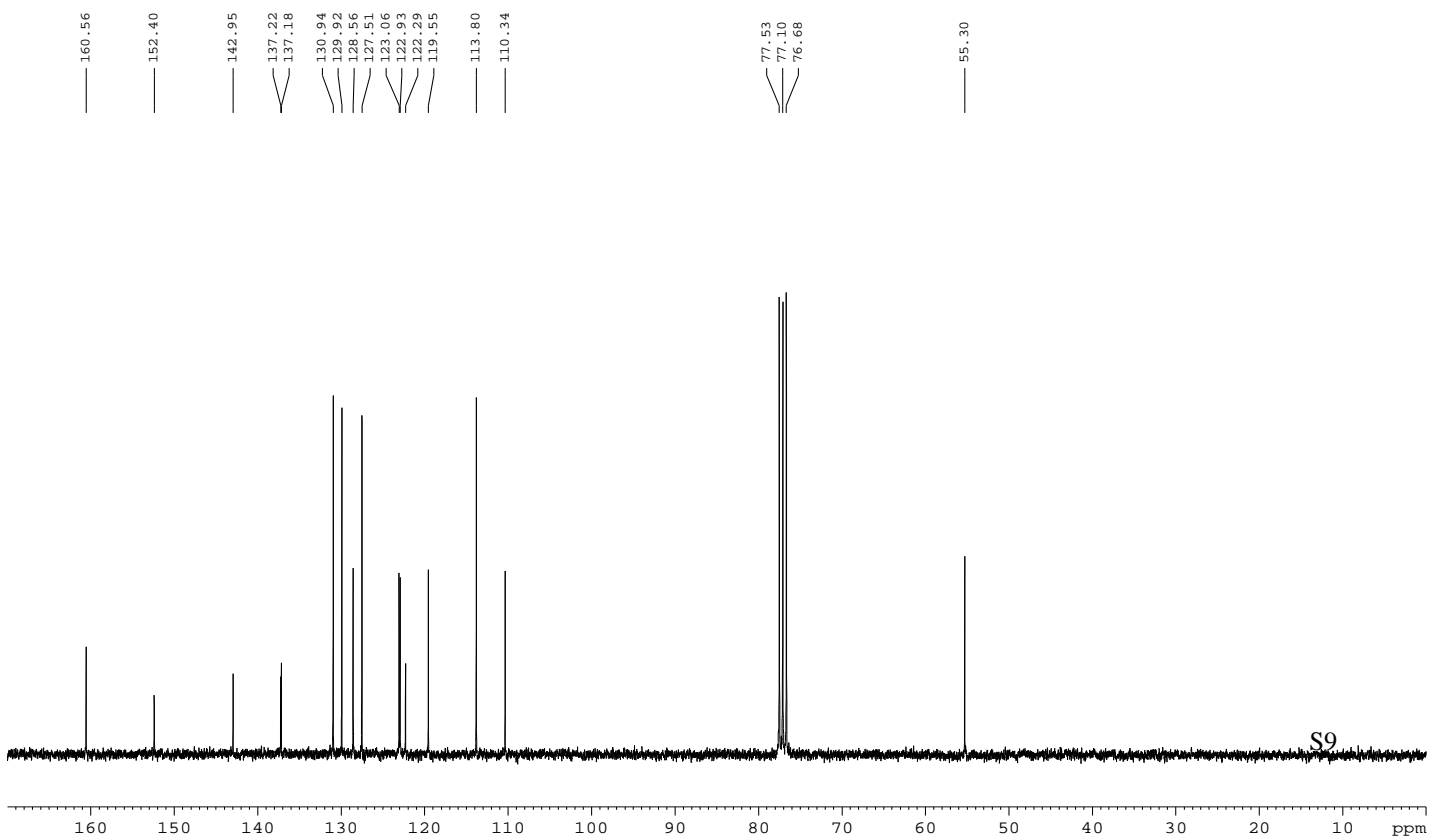


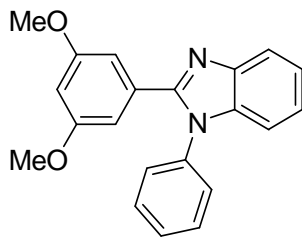


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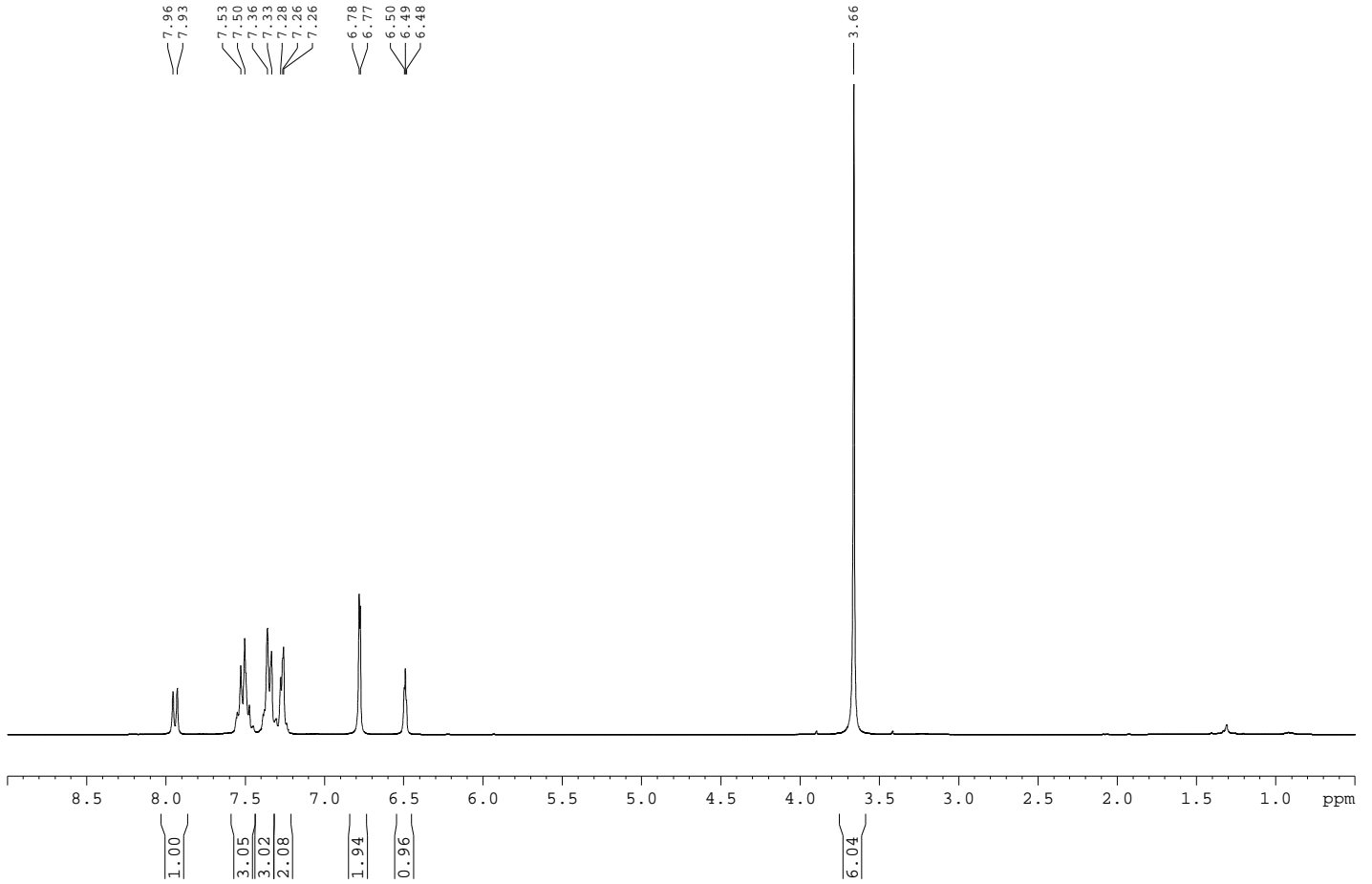
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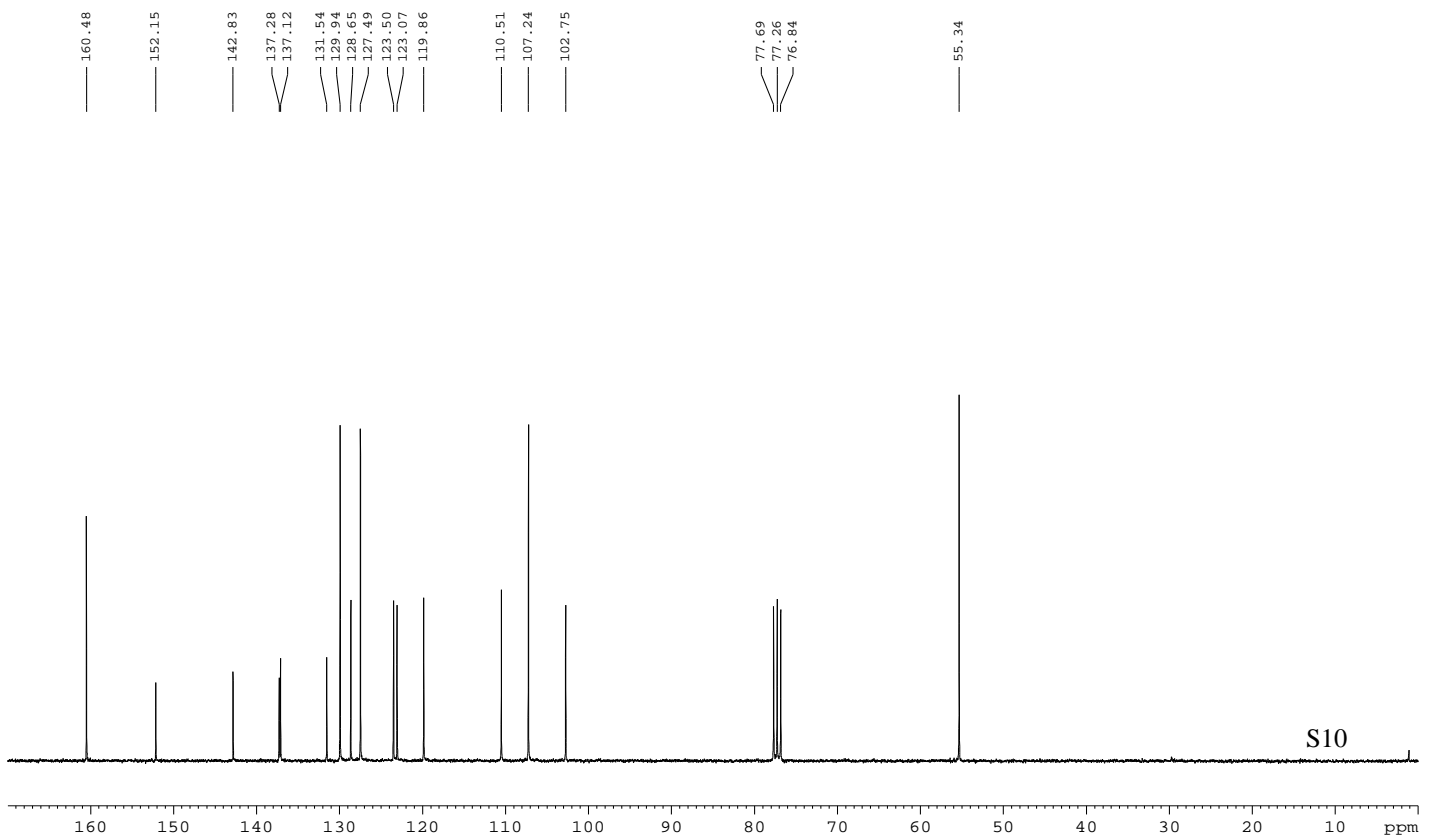


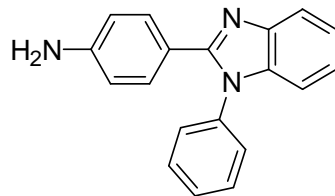
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1D proton NMR spectrum



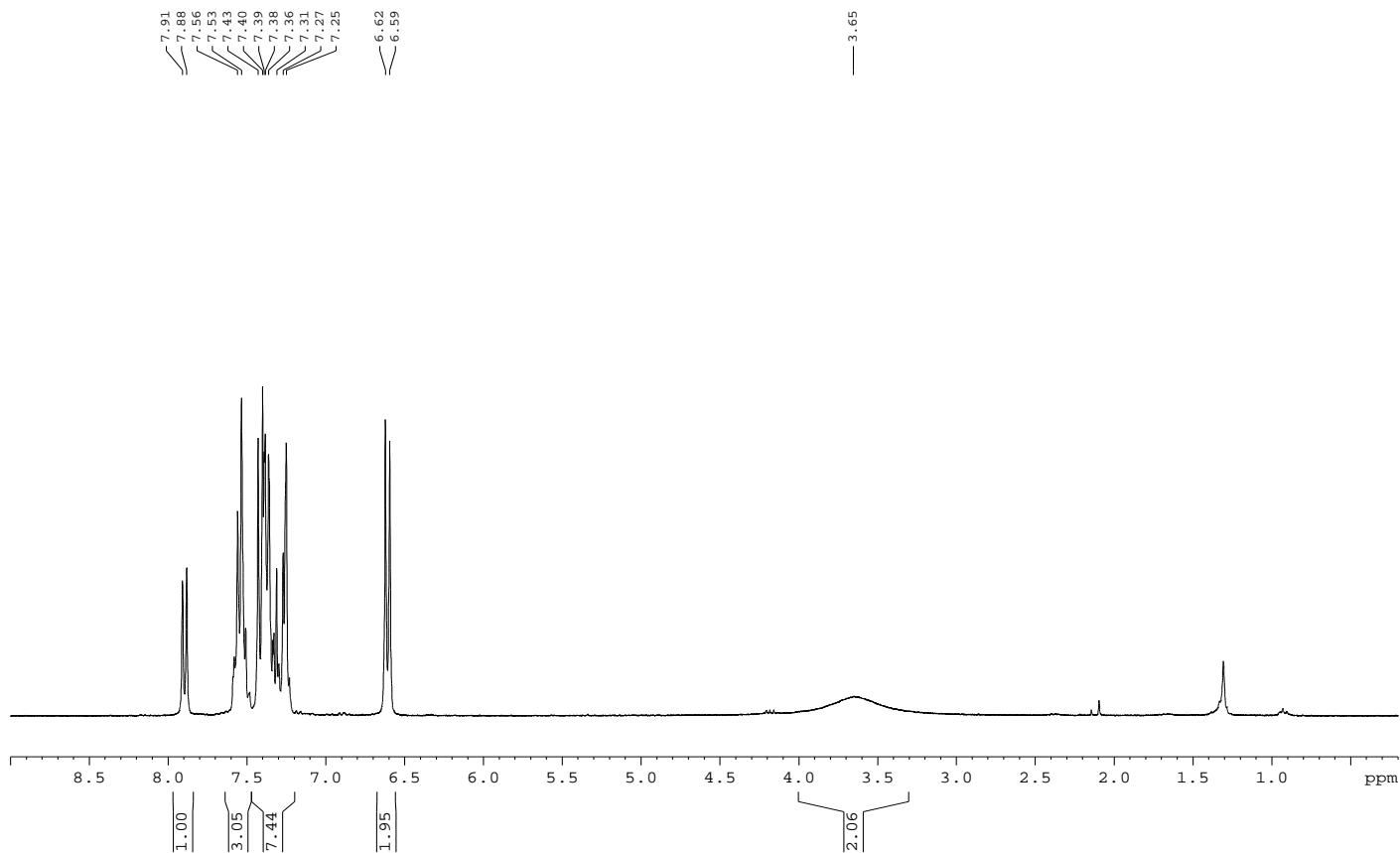
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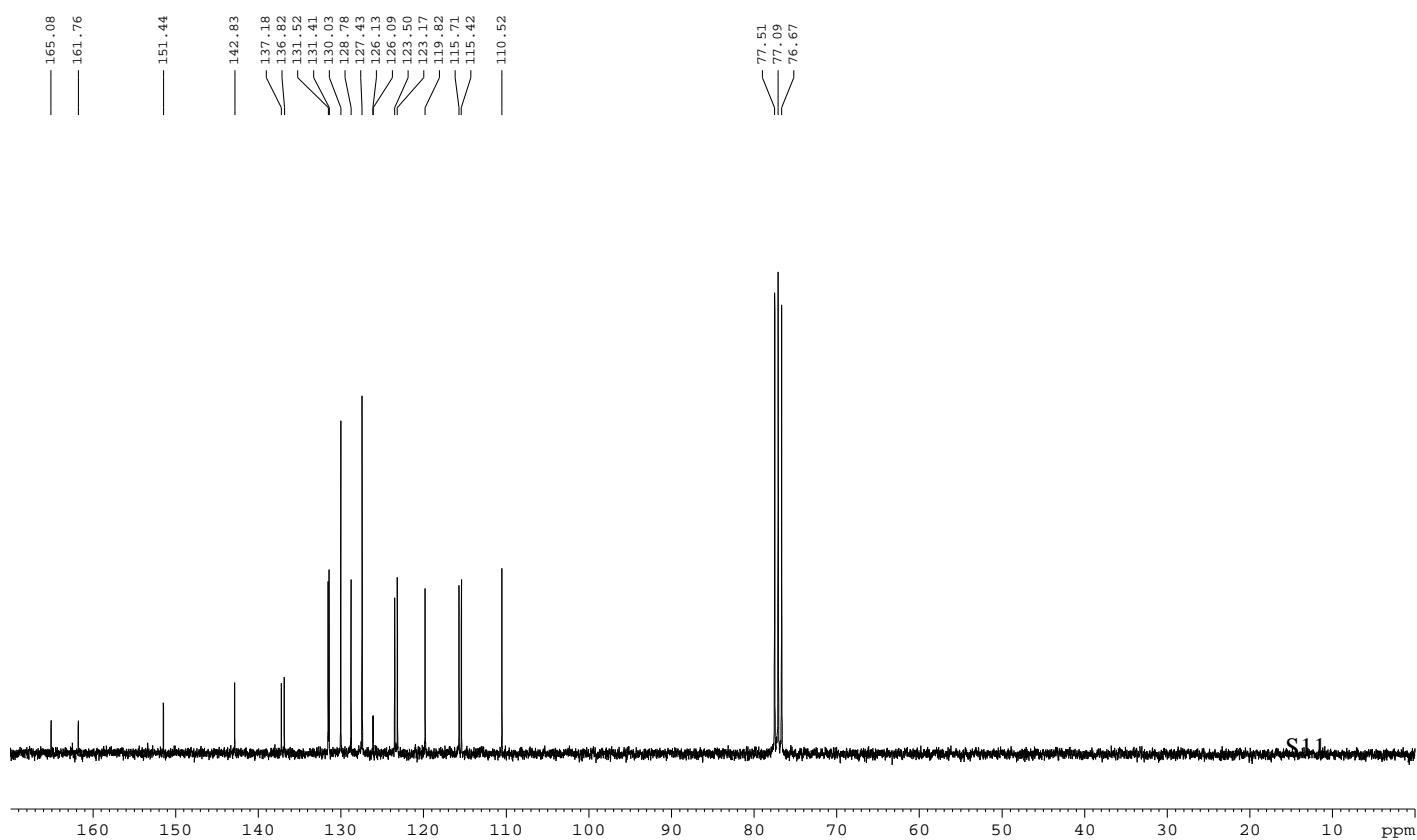


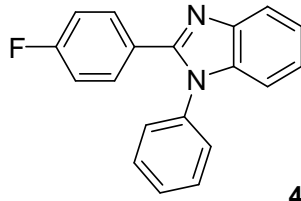
1D proton NMR spectrum

4f



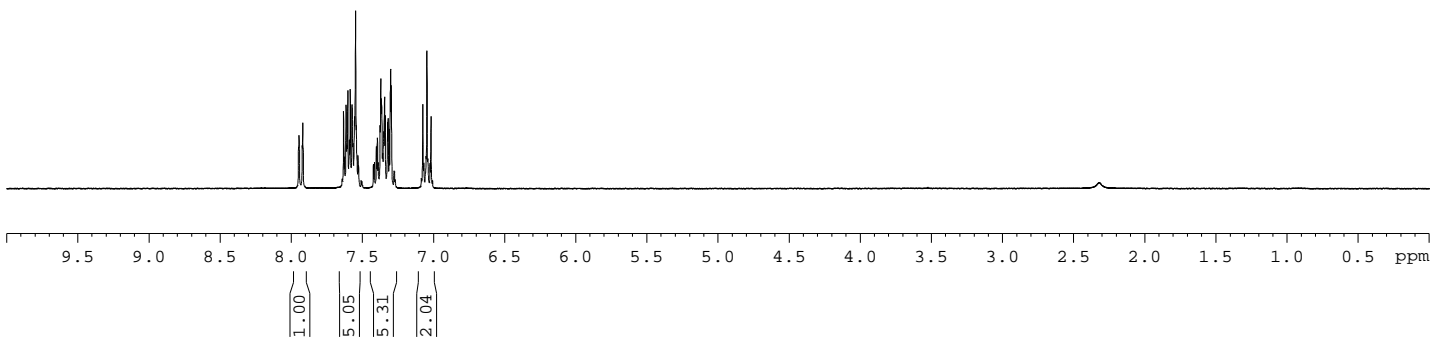
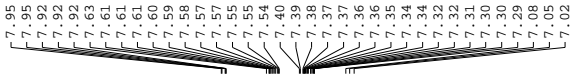
Proton-decoupled carbon NMR spectrum



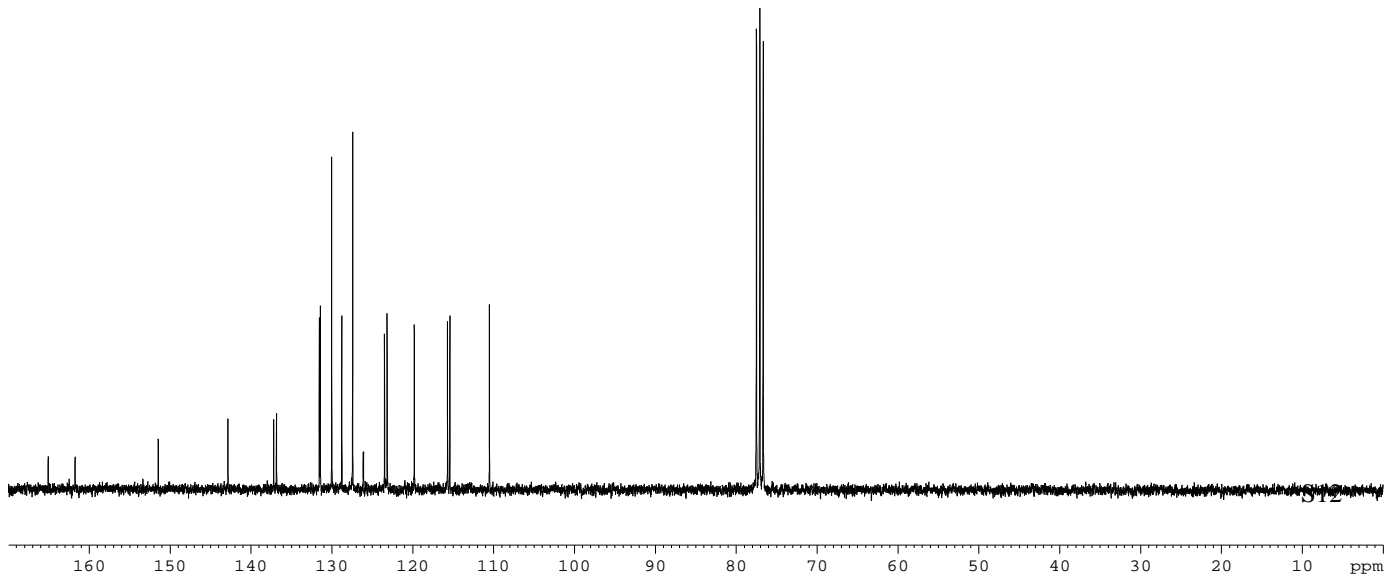
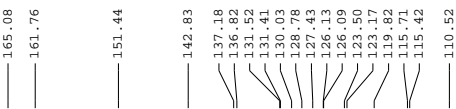


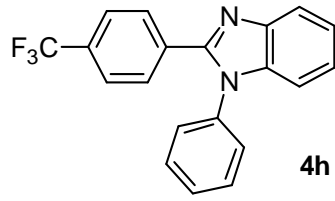
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1D proton NMR spectrum

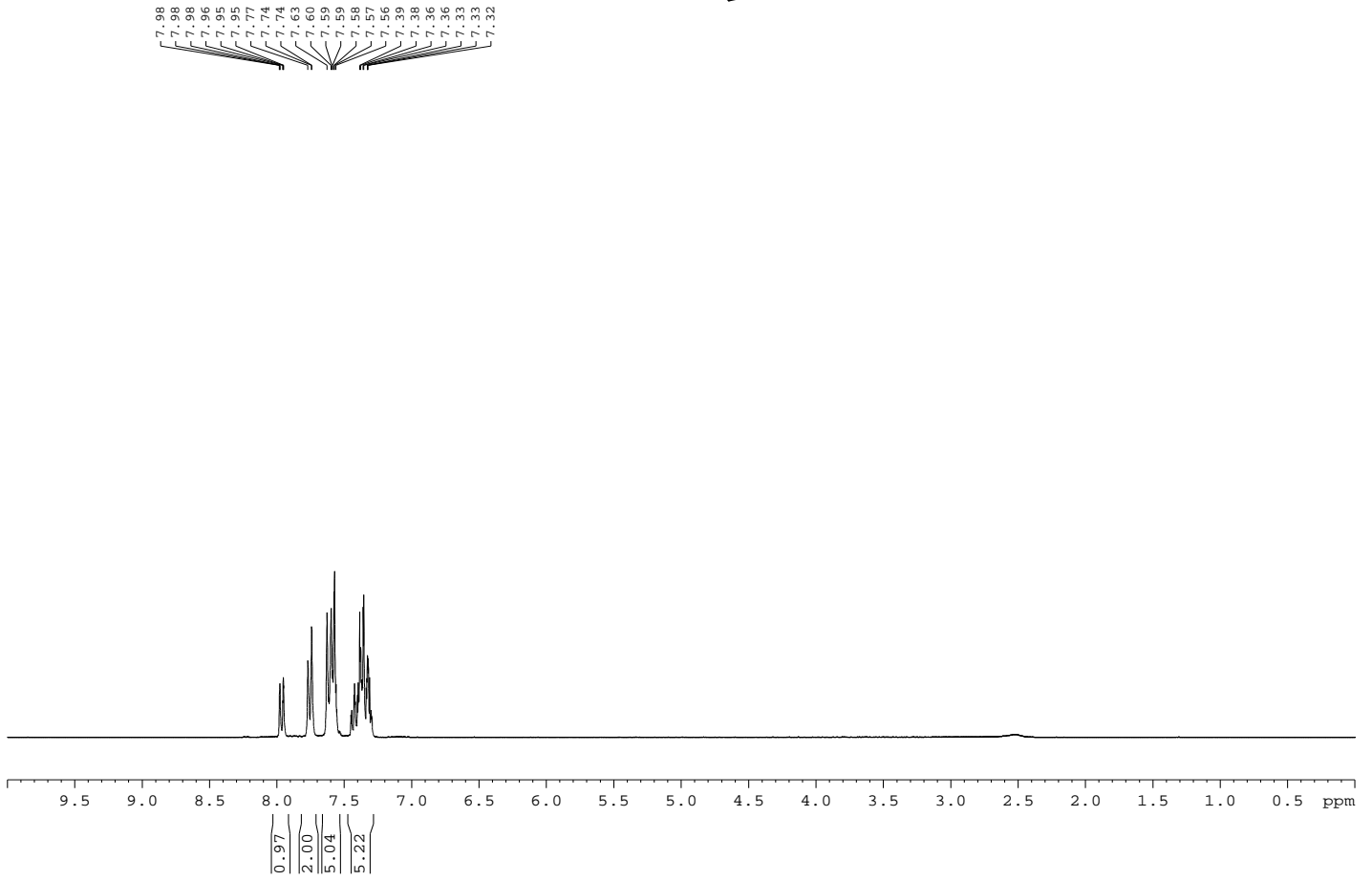


Proton-decoupled carbon NMR spectrum

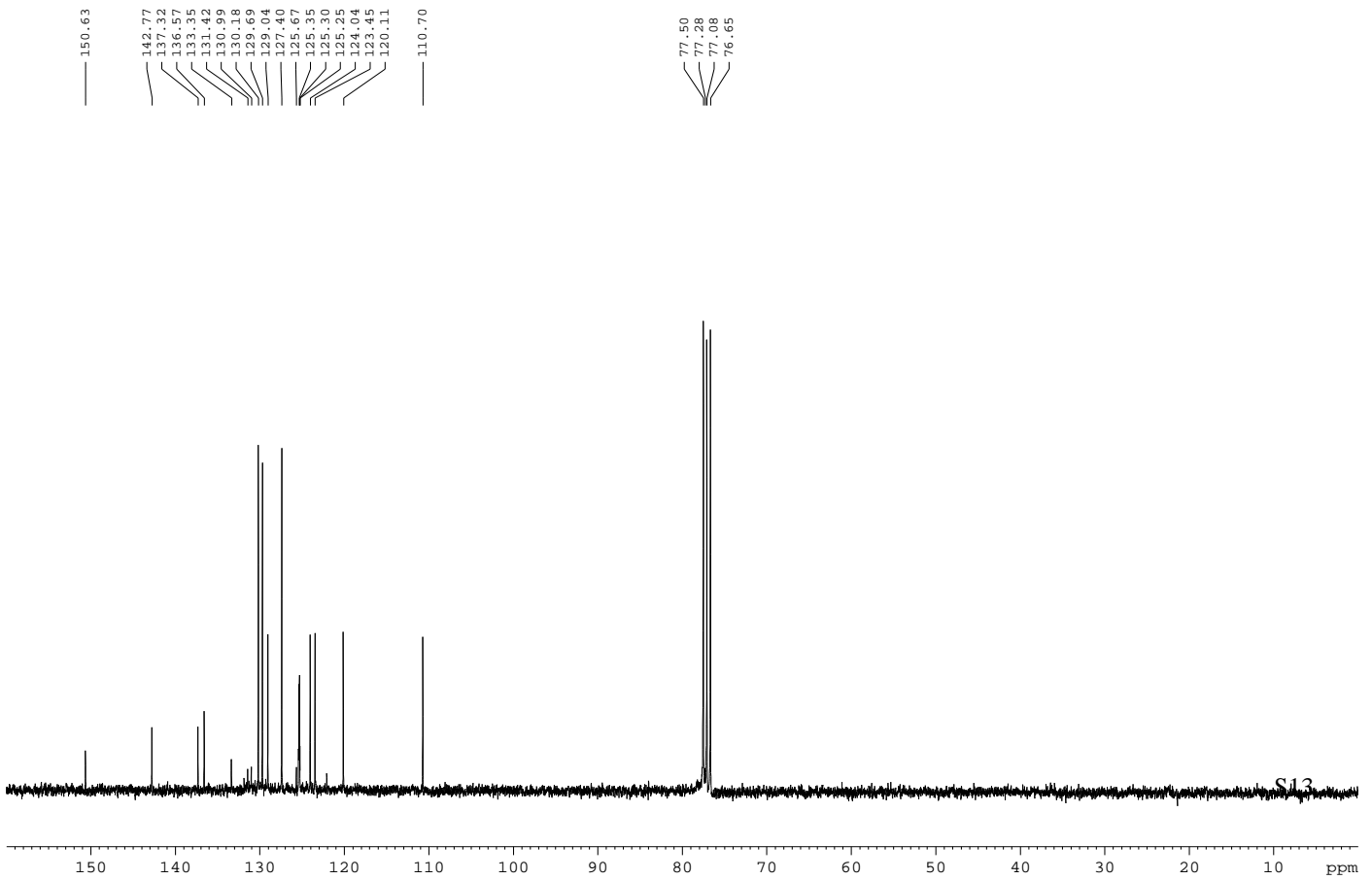


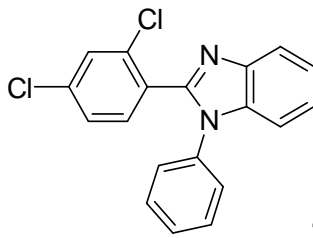


1D proton NMR spectrum



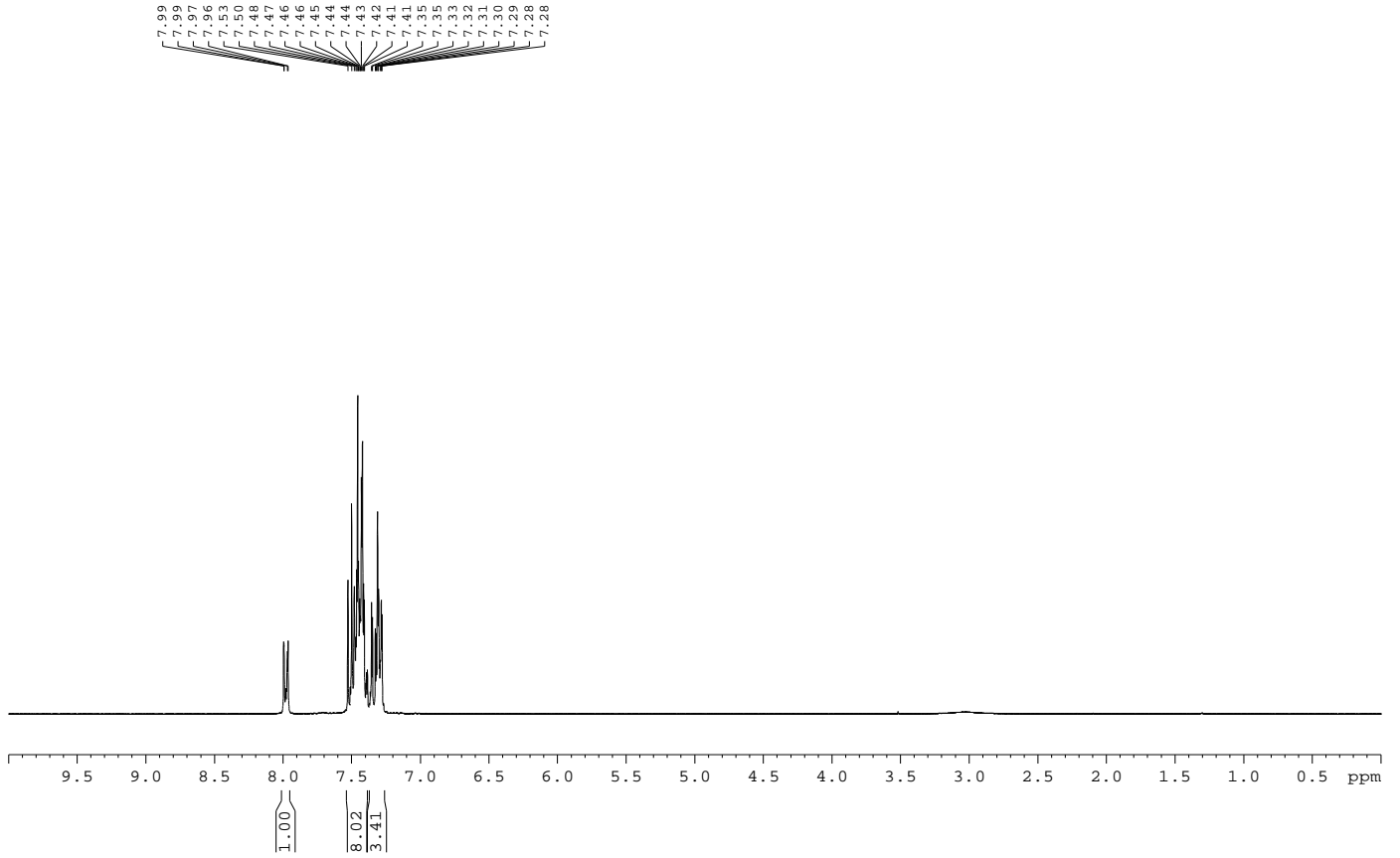
Proton-decoupled carbon NMR spectrum



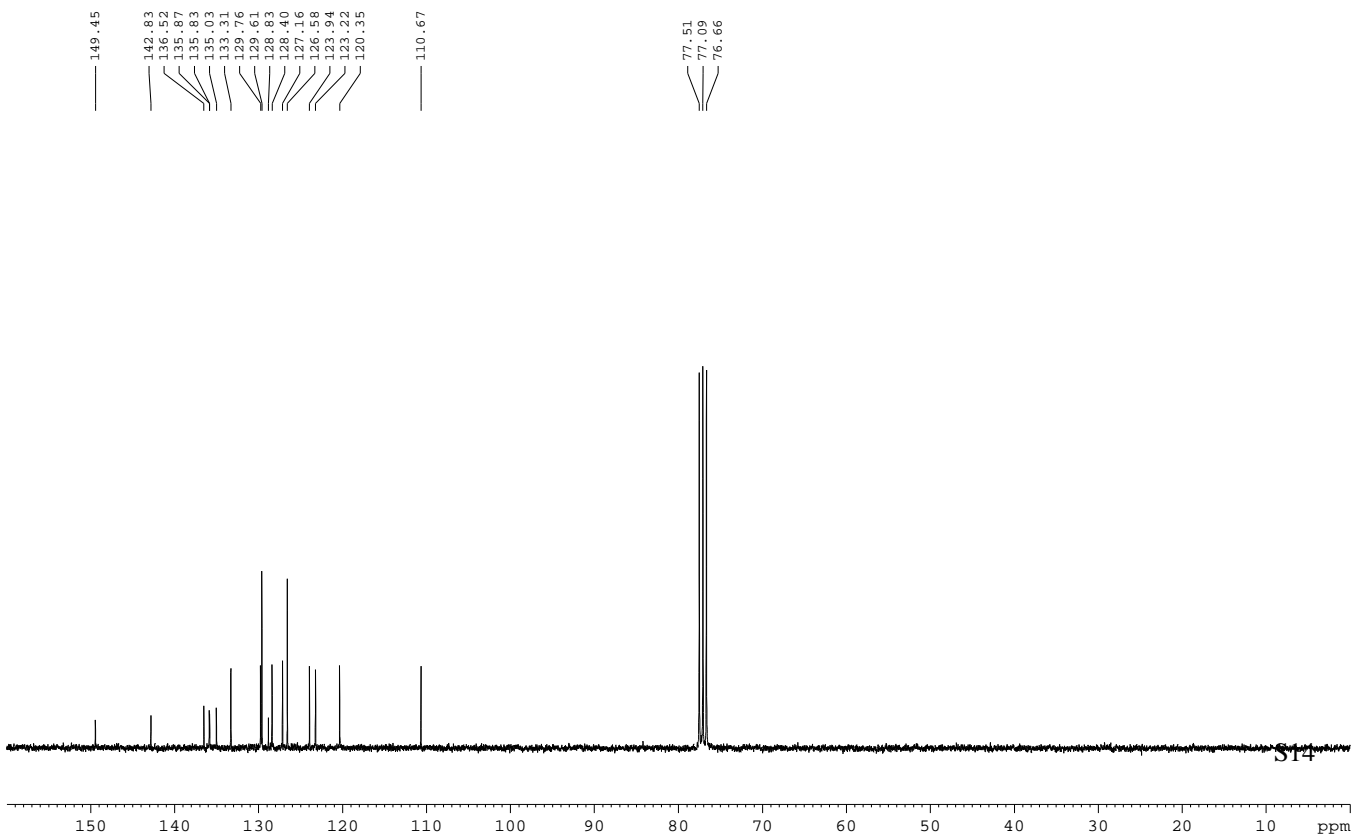


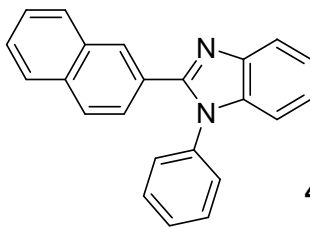
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1D proton NMR spectrum



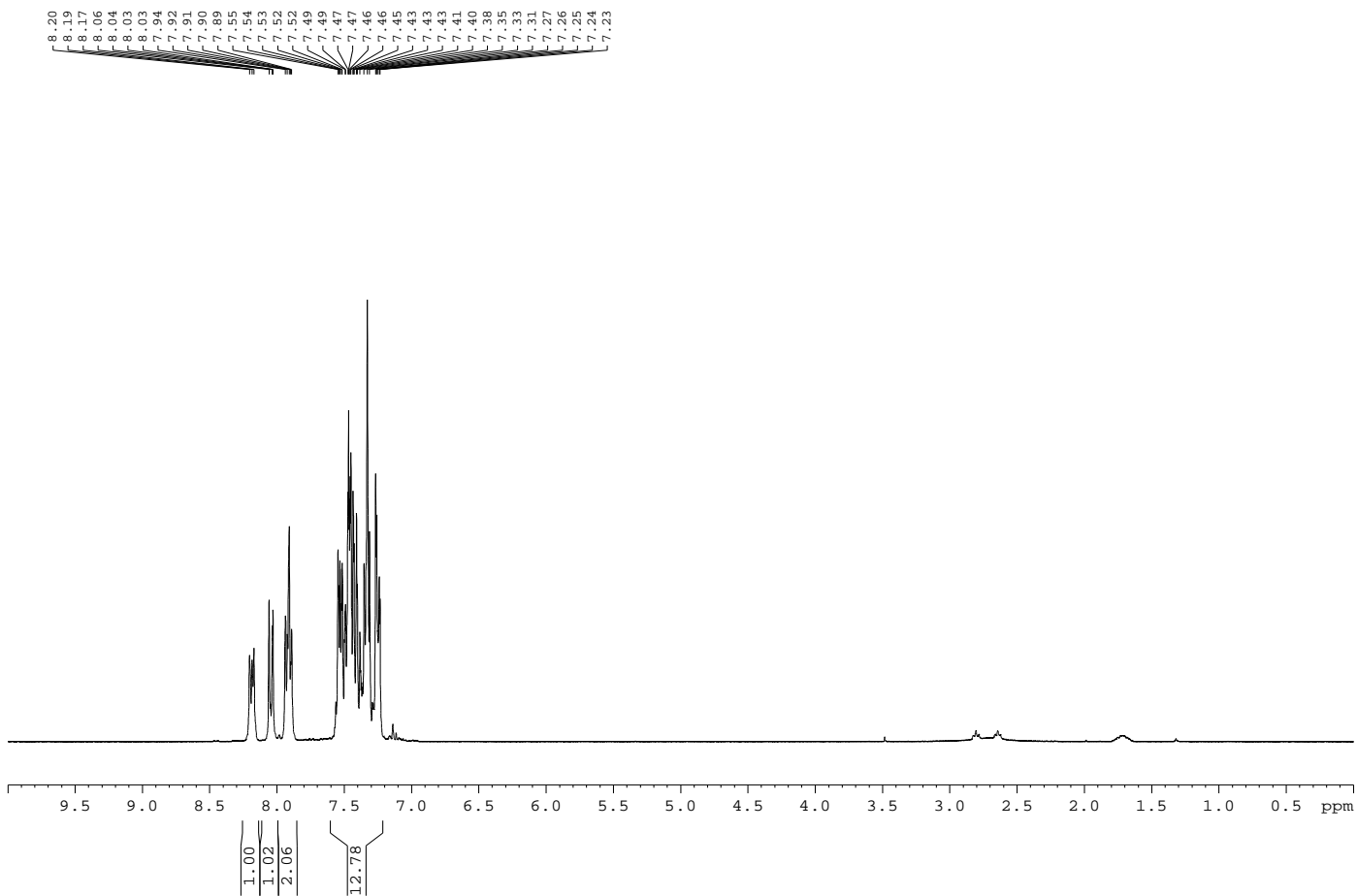
Proton-decoupled carbon NMR spectrum



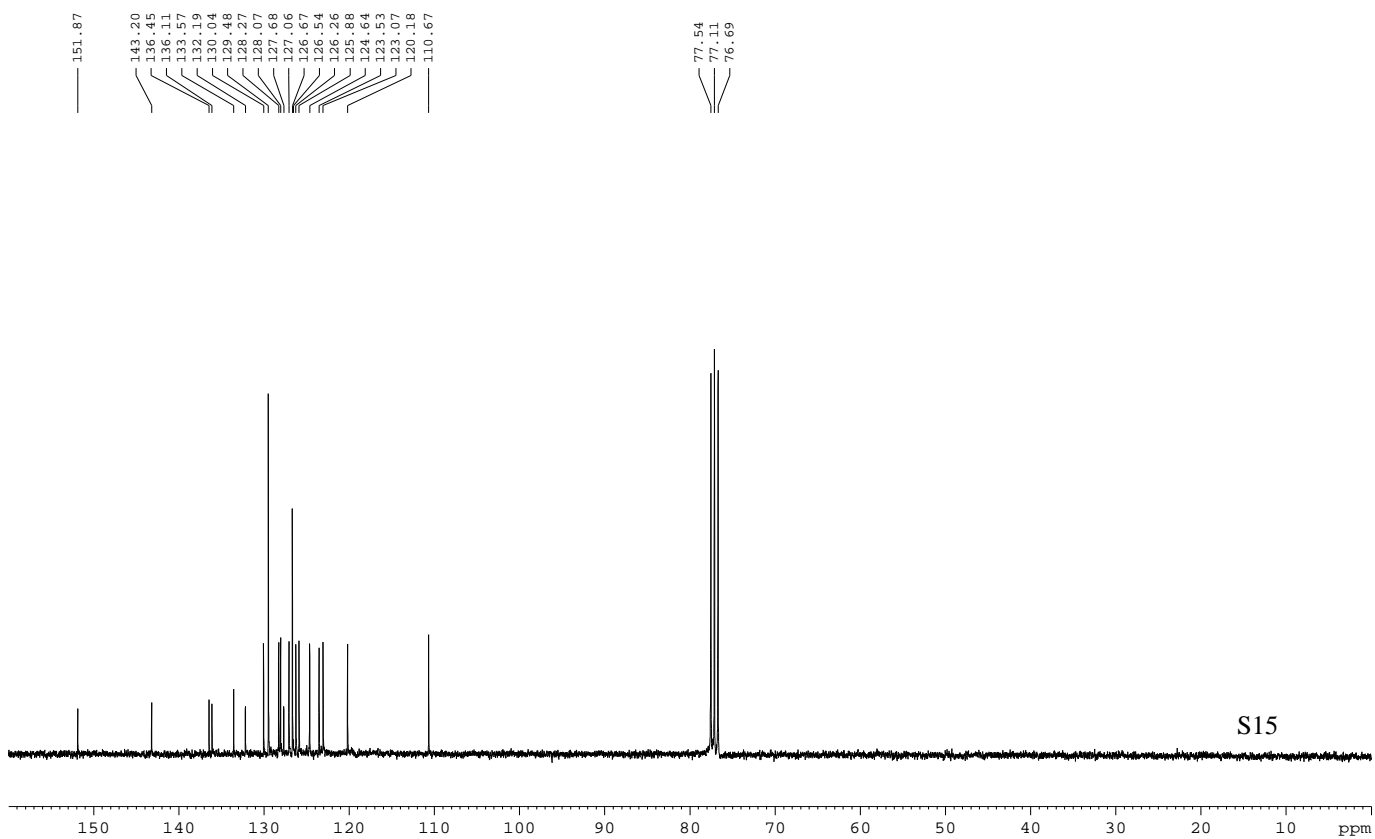


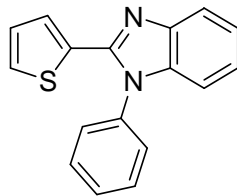
4j

1D proton NMR spectrum



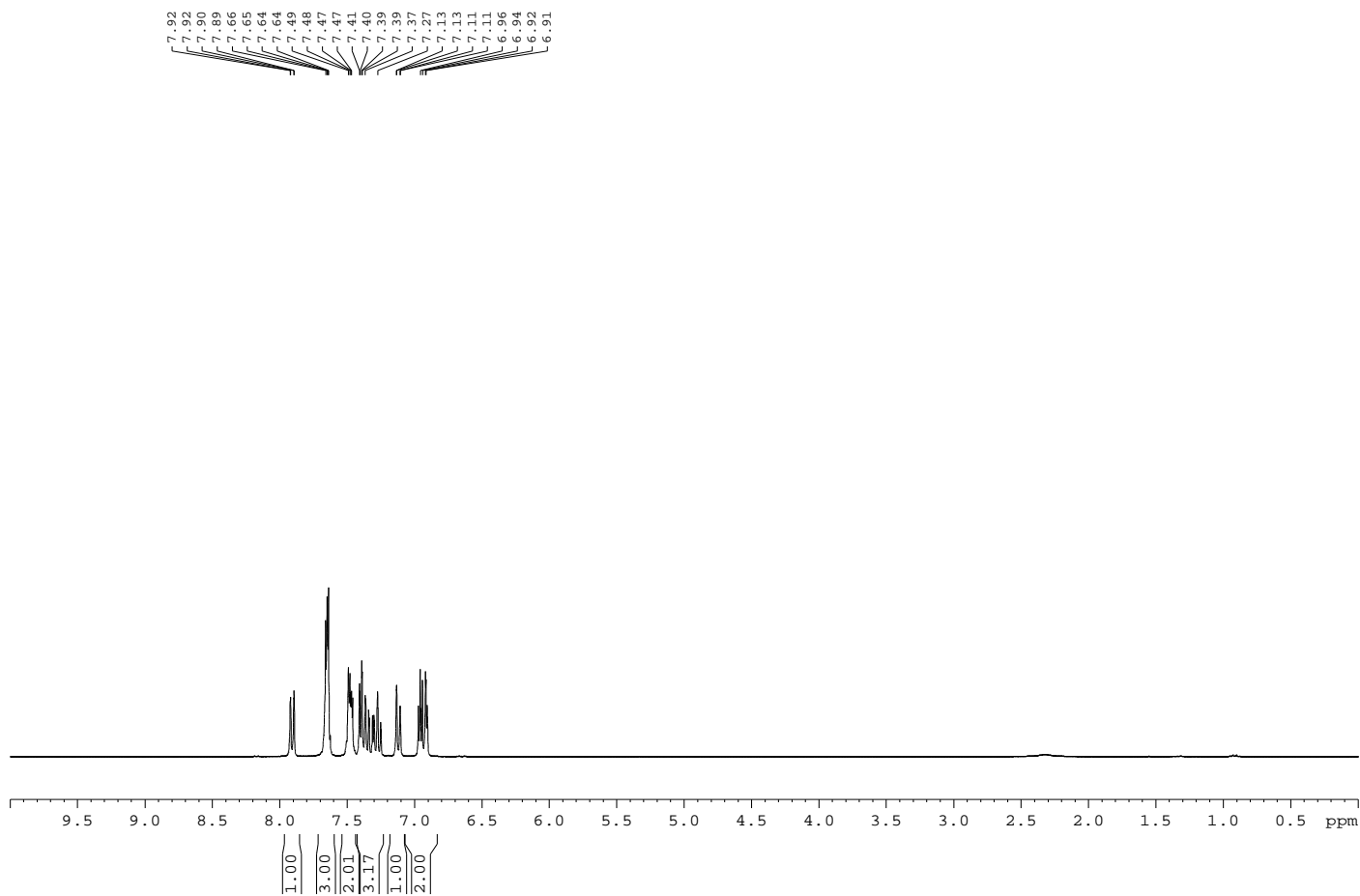
Proton-decoupled carbon NMR spectrum



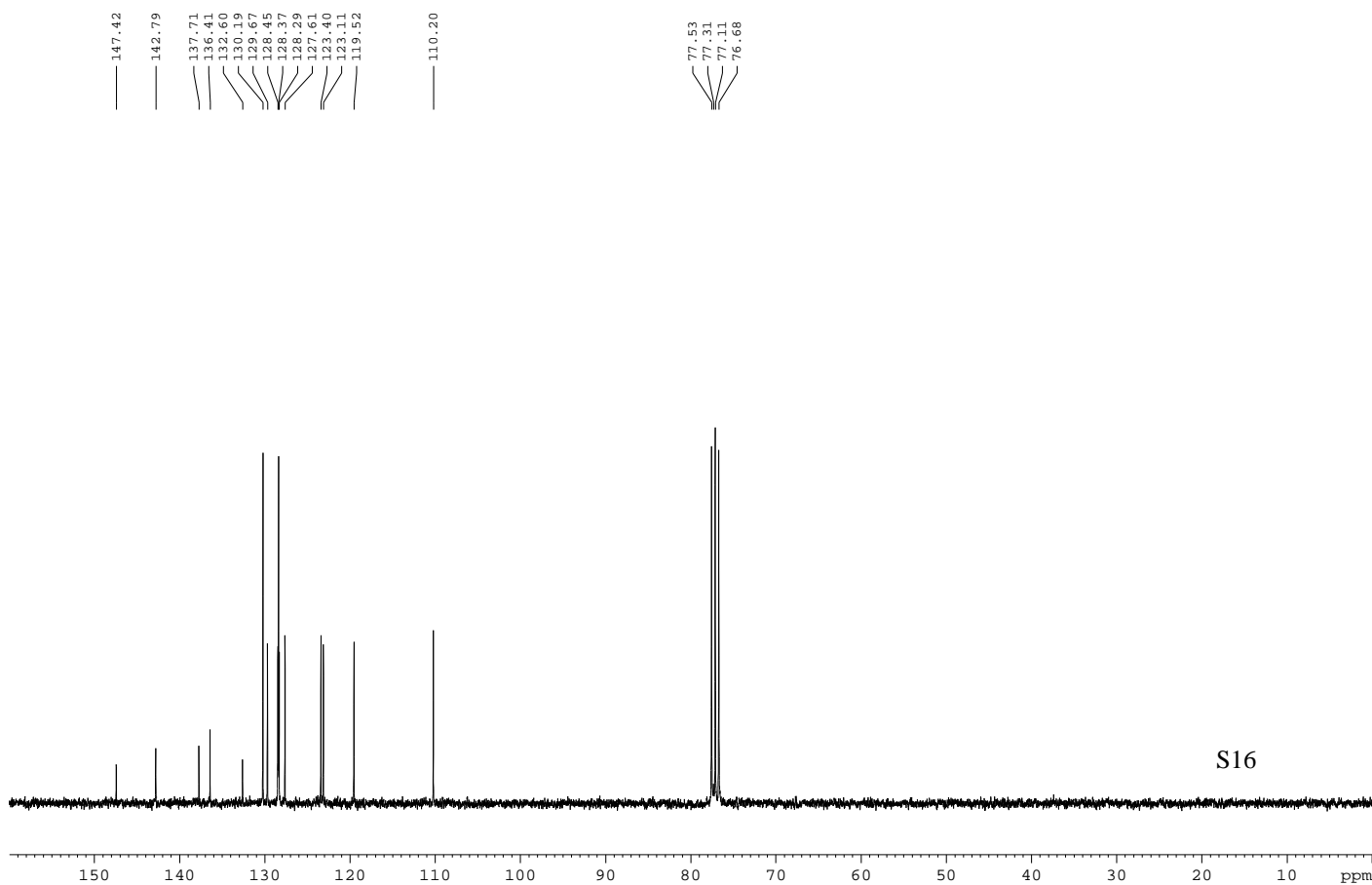


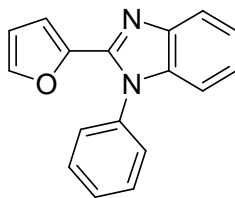
4k

1D proton NMR spectrum



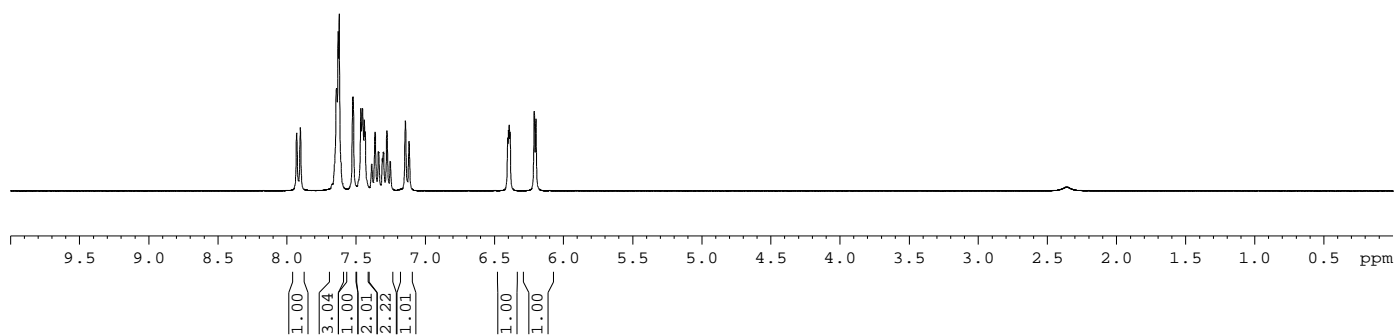
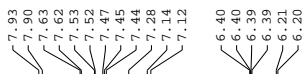
Proton-decoupled carbon NMR spectrum



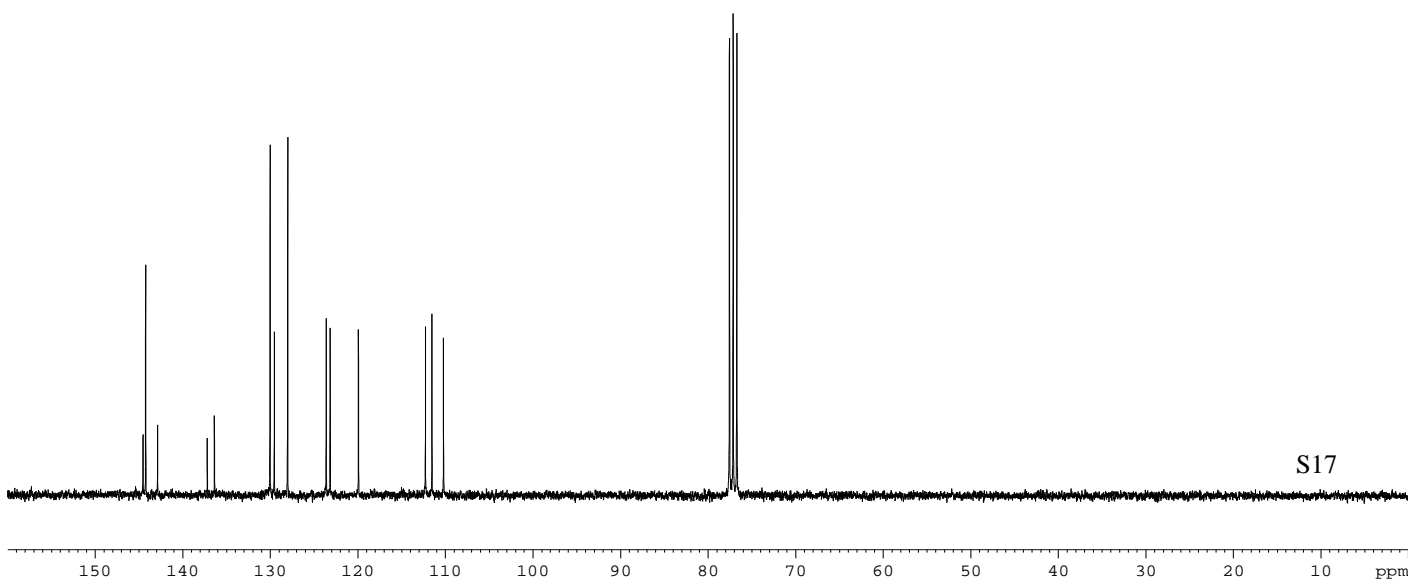
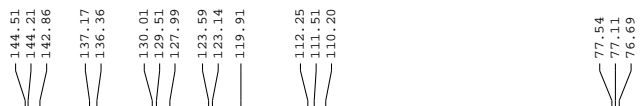


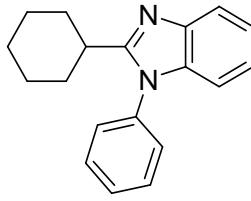
4I

1D proton NMR spectrum



Proton-decoupled carbon NMR spectrum



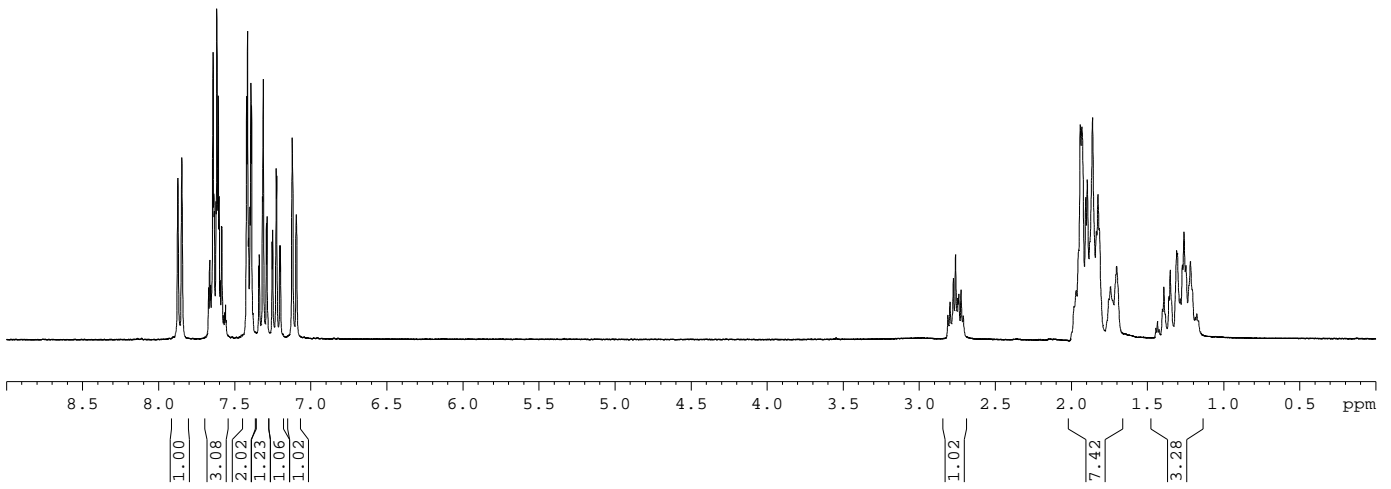


1D proton NMR spectrum

4m

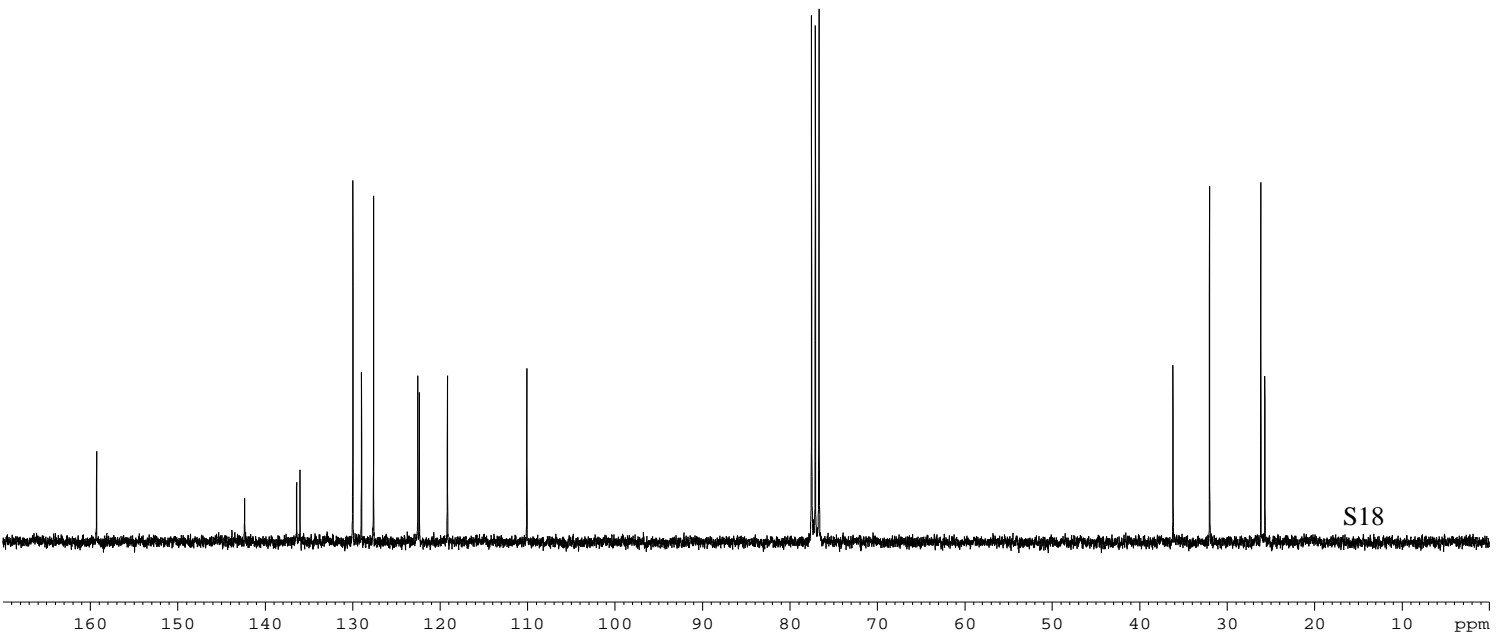
7.87
7.85
7.64
7.62
7.61
7.42
7.36
7.39
7.31
7.23
7.12
7.09

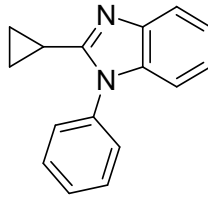
2.78
2.76
2.75
2.74
2.73
1.97
1.94
1.93
1.91
1.90
1.86
1.84
1.83
1.82
1.74
1.70
1.39
1.36
1.35
1.31
1.27
1.26
1.25
1.22



Proton-decoupled carbon NMR spectrum

159.28
142.34
136.39
136.01
129.96
128.99
127.60
122.53
122.36
119.15
110.07
77.51
77.09
76.66
36.21
32.02
26.16
25.70



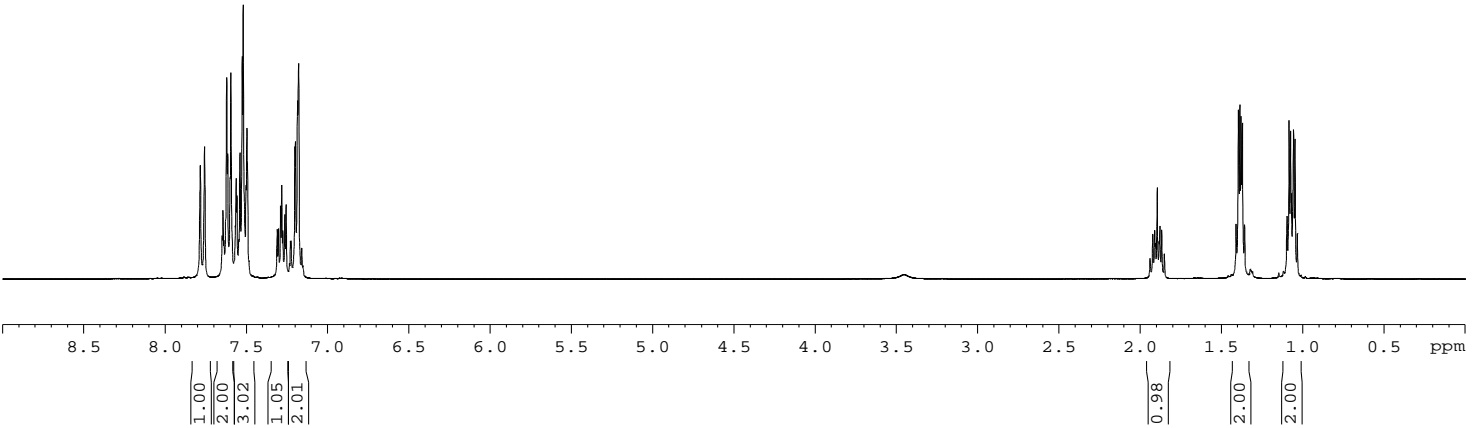


4n

1D proton NMR spectrum

7.78
7.76
7.62
7.61
7.54
7.52
7.50
7.29
7.28
7.26
7.25
7.20
7.18
7.18

1.90
1.40
1.39
1.38
1.37
1.10
1.08
1.07
1.06

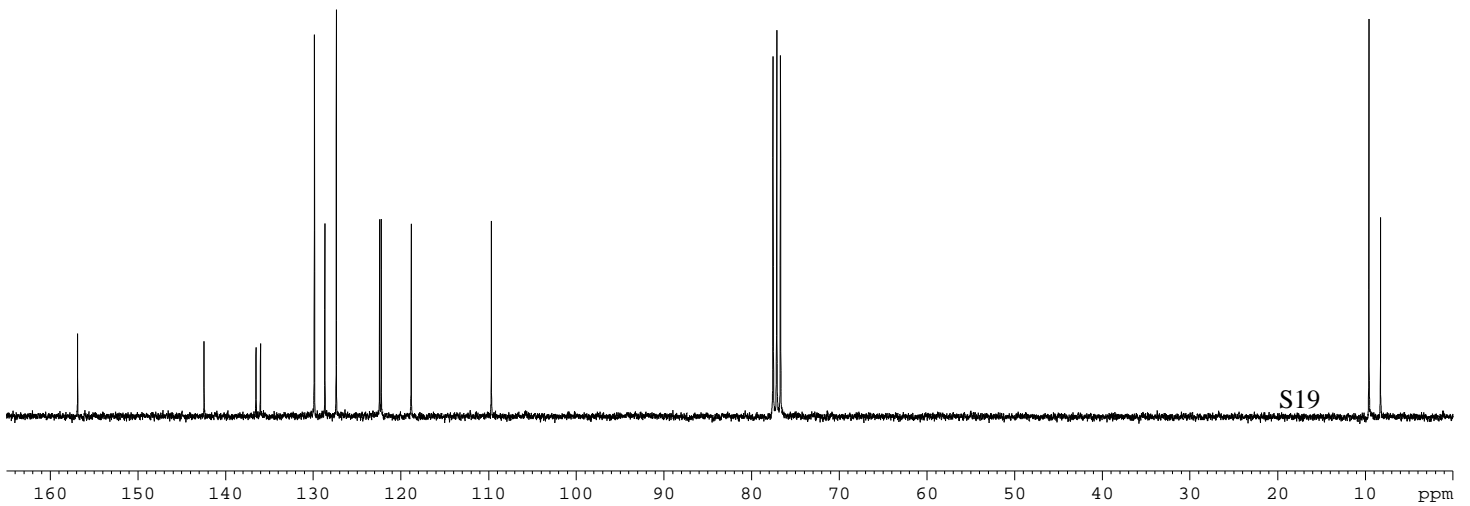


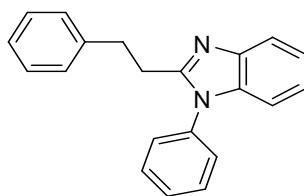
Proton-decoupled carbon NMR spectrum

156.88
142.45
136.52
136.02
129.86
128.66
127.37
122.43
122.23
118.82
109.68

77.55
77.12
76.70

9.61
8.29



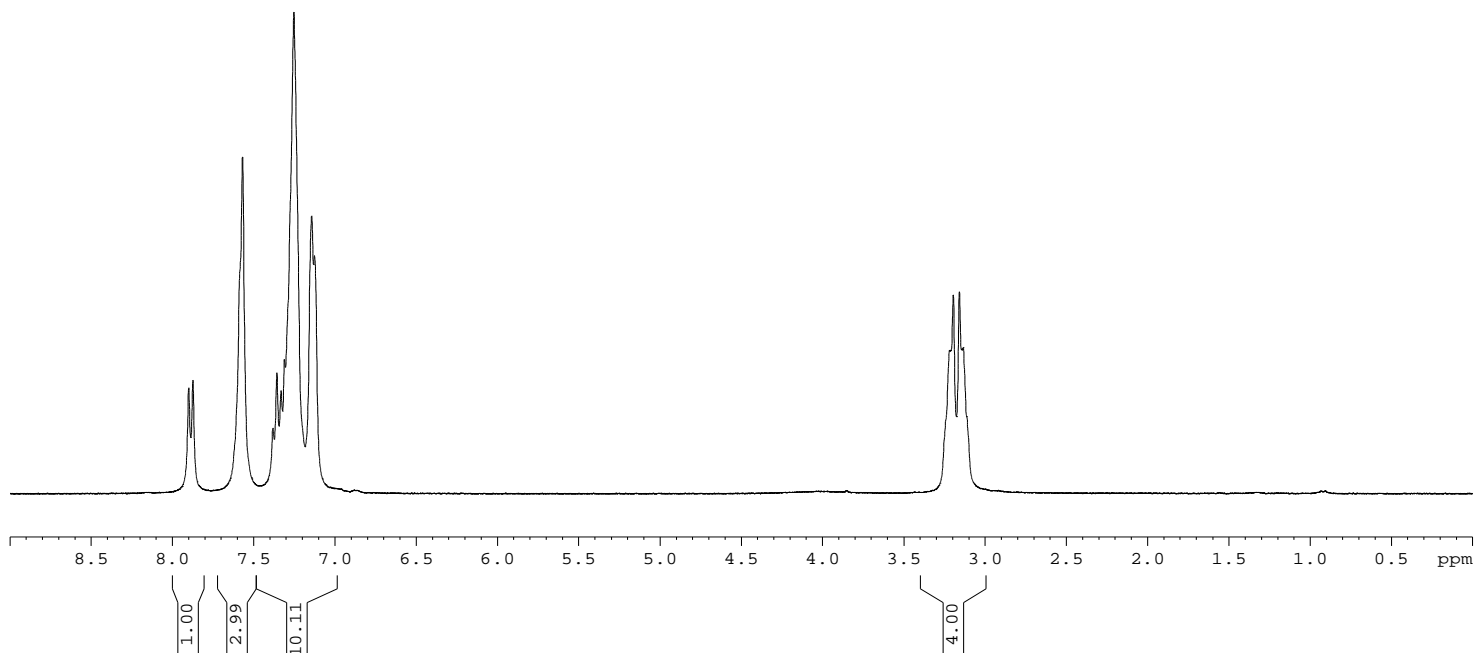


4o

1D proton NMR spectrum

7.90
7.87
7.57
7.36
7.33
7.31
7.25
7.14
7.13

3.20
3.16
3.13

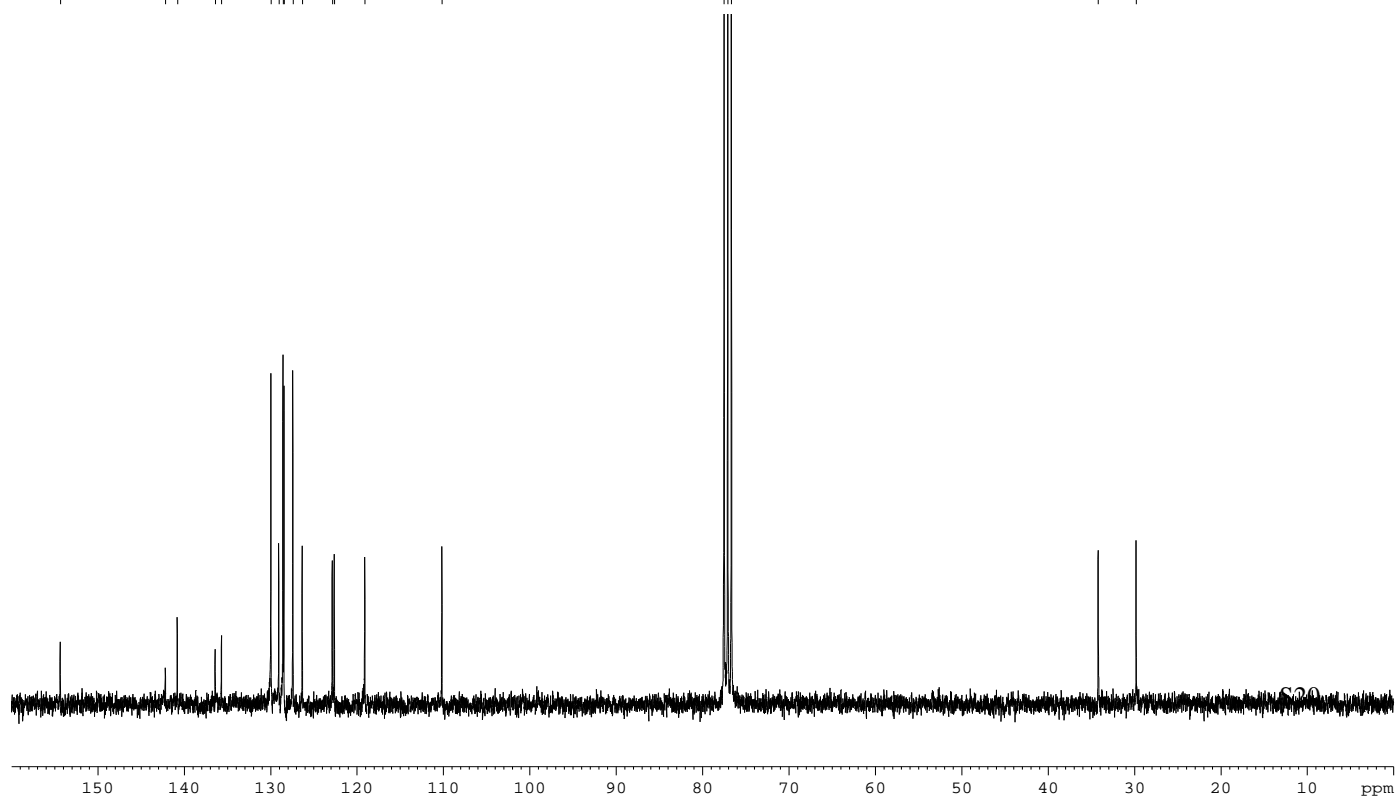


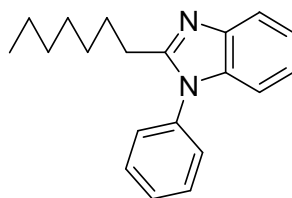
Proton-decoupled carbon NMR spectrum

154.32
142.16
140.78
136.40
135.68
129.95
129.03
128.55
128.43
127.41
126.32
122.65
119.08
110.16

77.51
77.09
76.66

34.21
29.82





4p

1D proton NMR spectrum

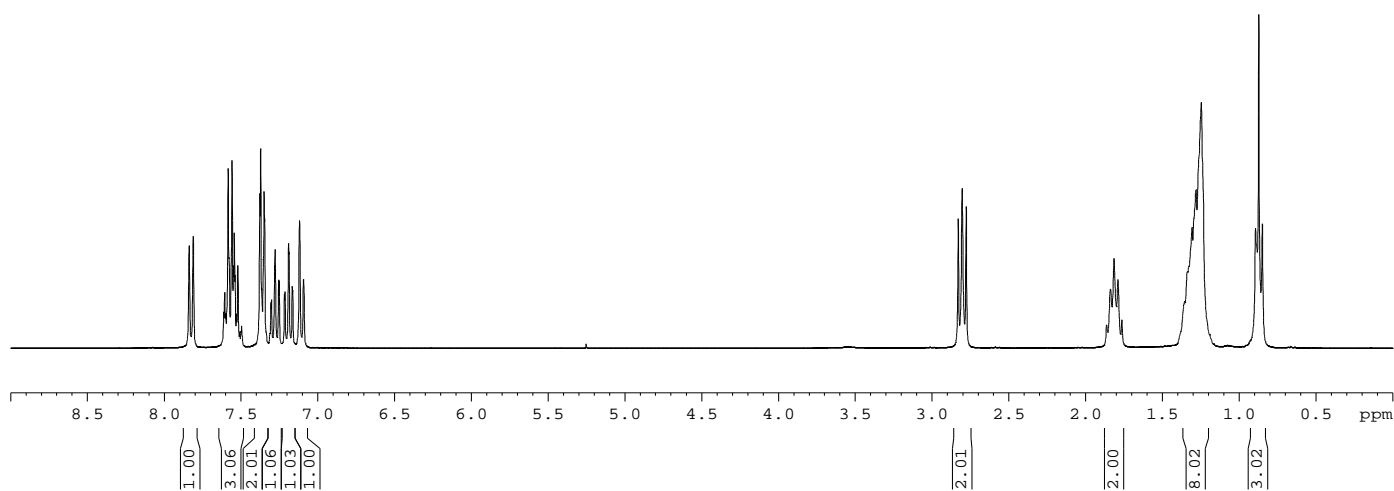
7.84
7.81
7.58
7.56
7.37
7.35
7.31
7.28
7.26
7.22
7.19
7.17
7.12
7.09

2.83
2.80
2.78

1.86
1.84
1.82
1.79
1.76

1.31
1.28
1.25

0.89
0.87
0.85



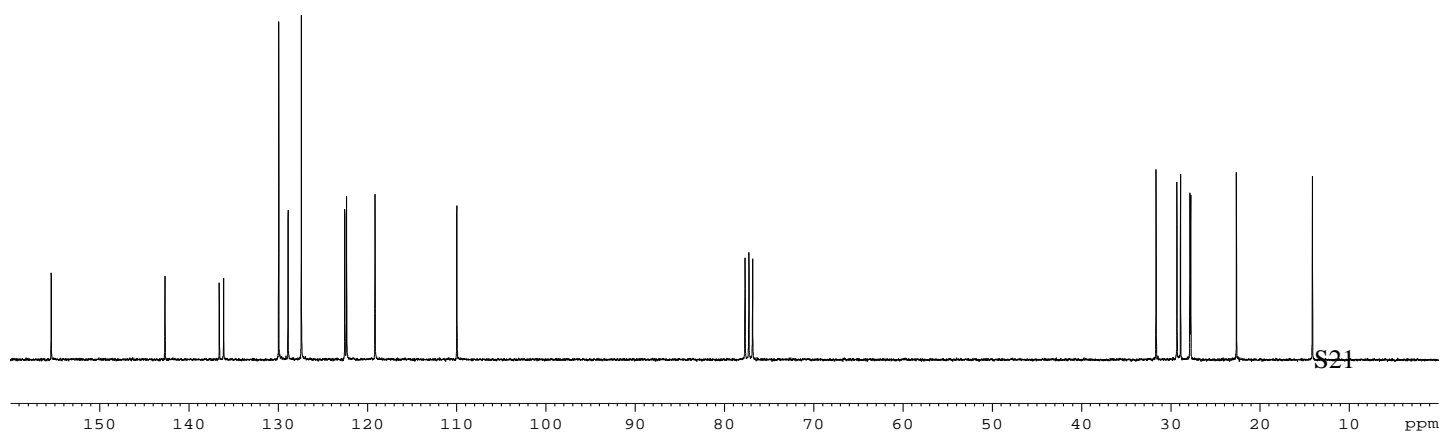
Proton-decoupled carbon NMR spectrum

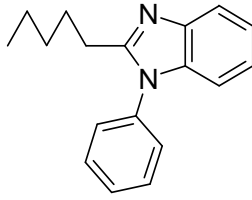
155.39
142.65
136.55
136.08
129.91
128.96
127.37
122.50
122.29
119.11
109.94

77.68
77.25
76.83

31.63
29.29
28.88
27.84
27.75
22.61

14.11





1D proton NMR spectrum

4q

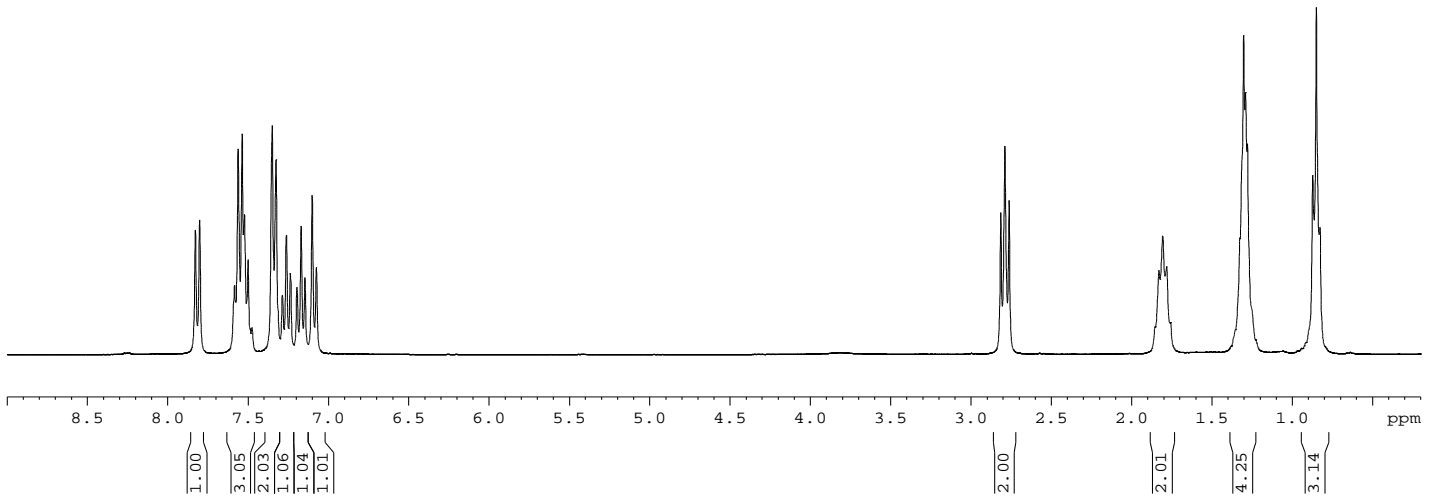
7.83
7.80
7.56
7.54
7.52
7.35
7.33
7.29
7.26
7.24
7.20
7.17
7.15
7.10
7.07

2.81
2.79
2.76

1.83
1.81
1.78

1.30
1.29
1.28

0.87
0.85
0.83

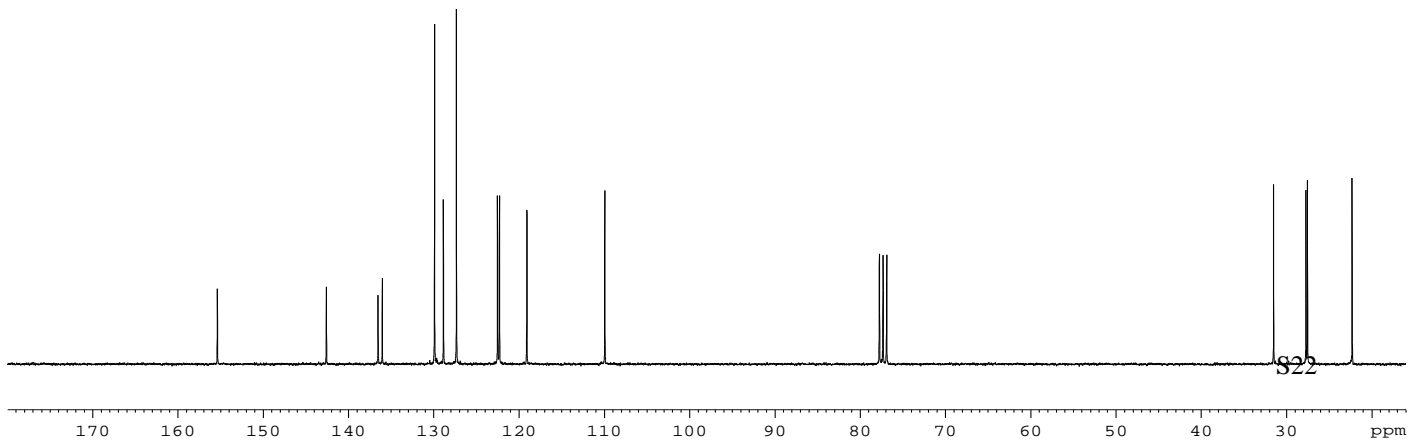


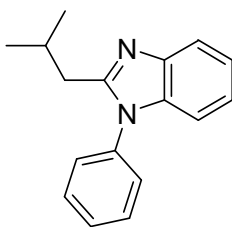
Proton-decoupled carbon NMR spectrum

155.36
142.60
136.54
136.04
129.91
128.86
127.34
122.52
122.29
119.09
109.94

77.73
77.31
76.88

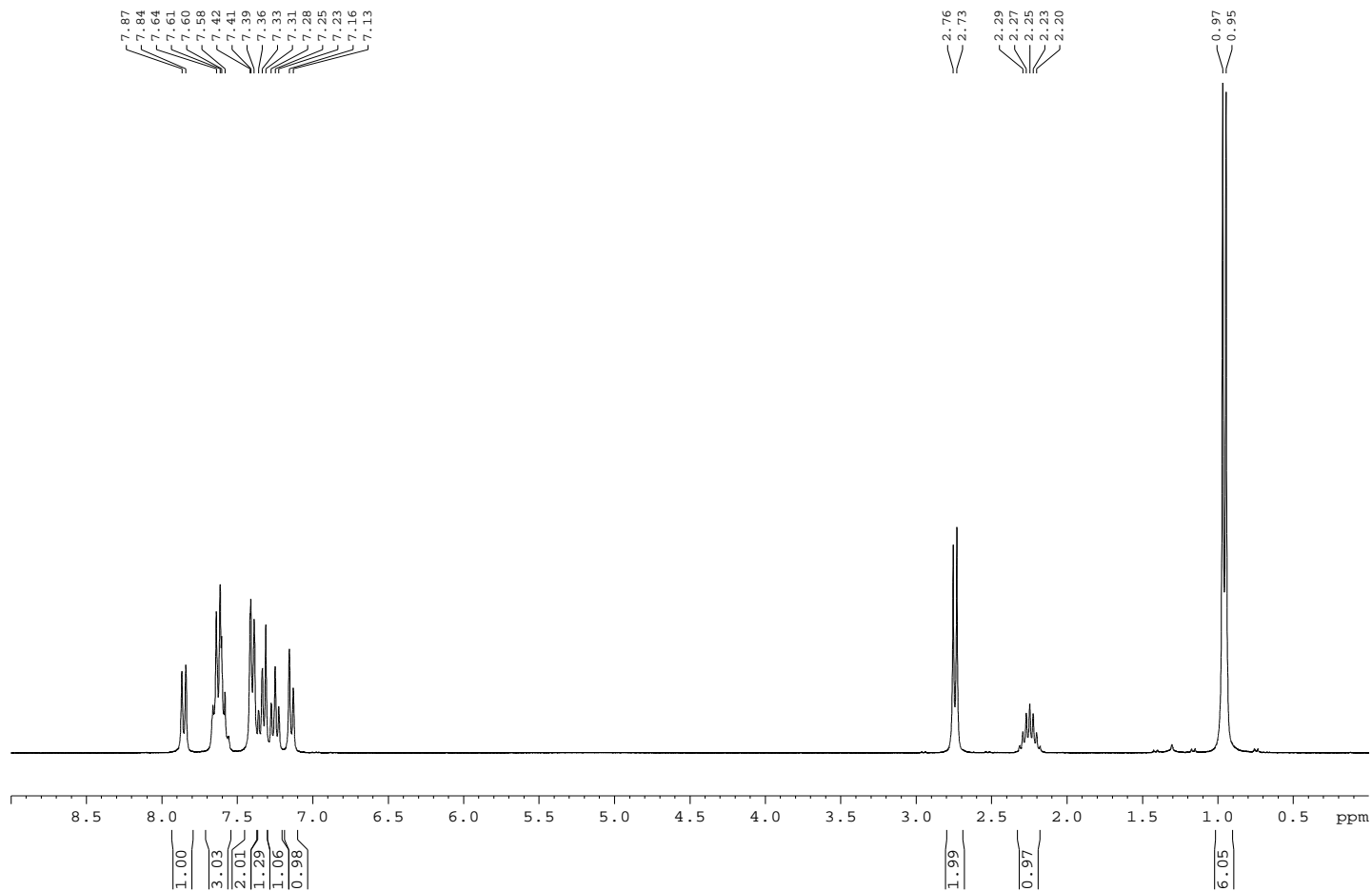
31.50
27.70
27.51
22.29



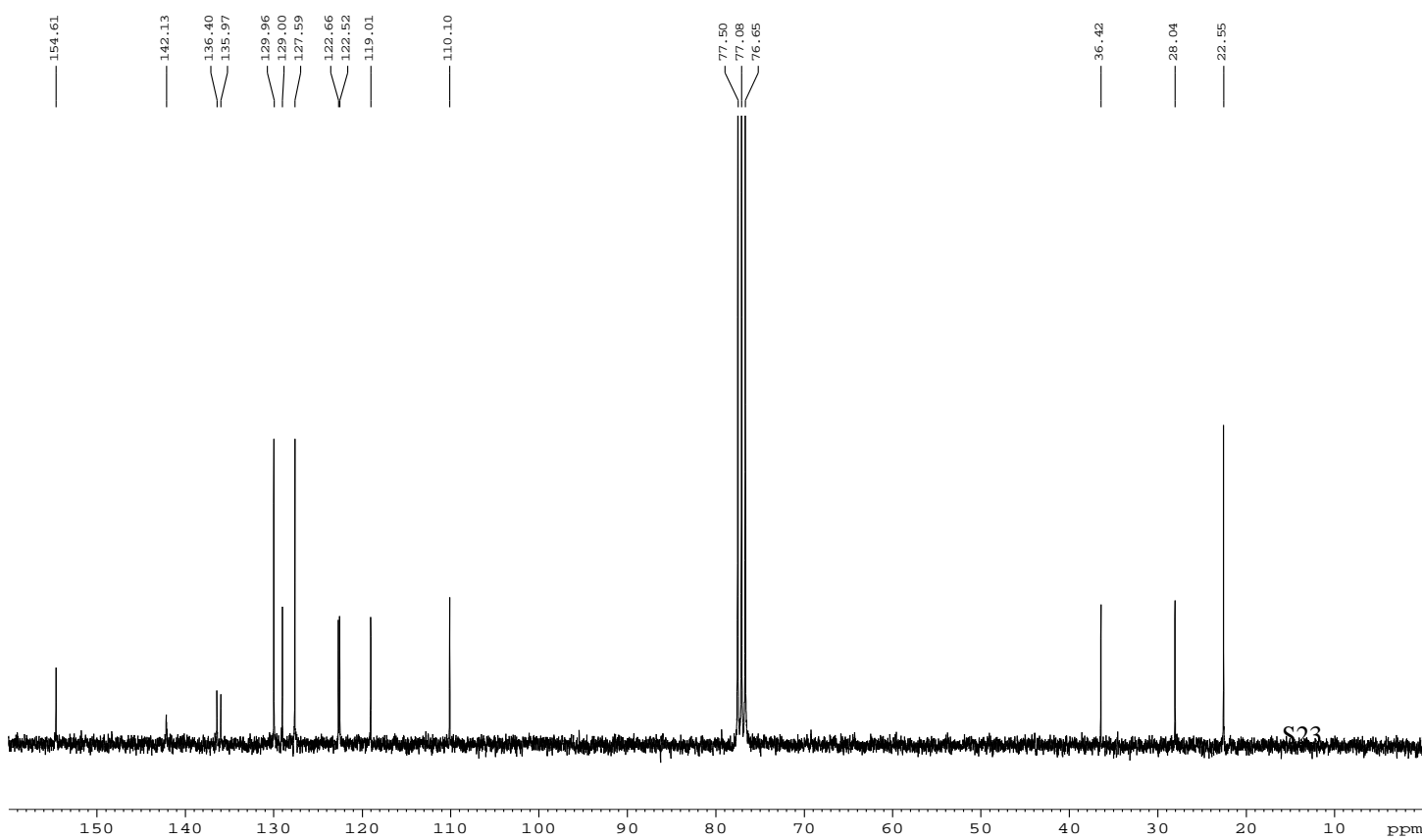


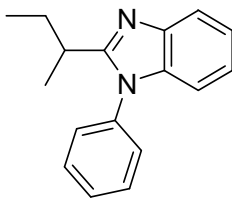
4r

1D proton NMR spectrum



Proton-decoupled carbon NMR spectrum



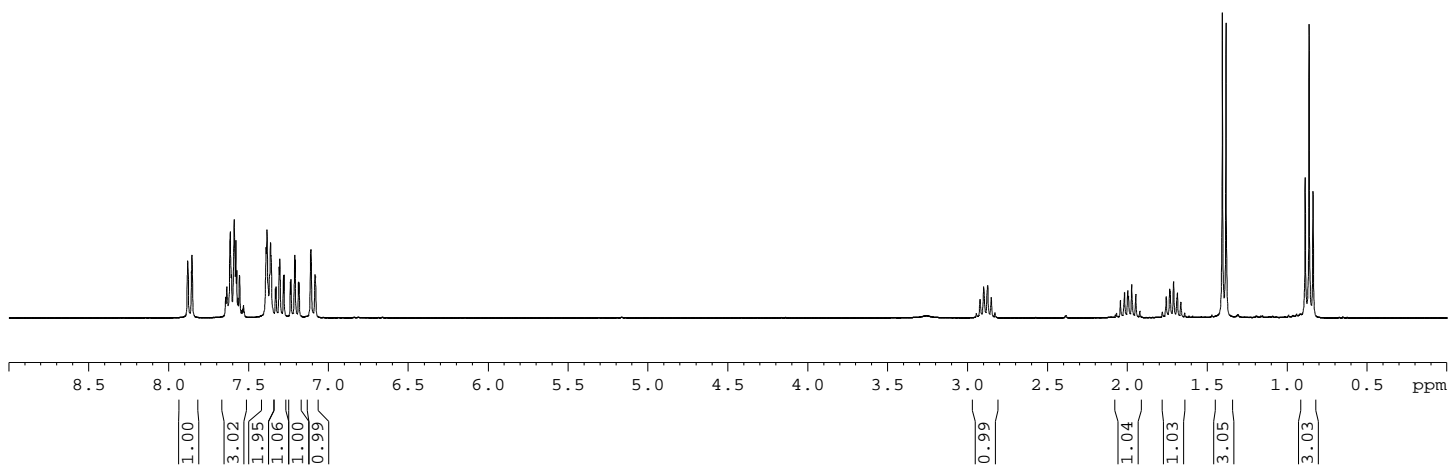


4s

1D proton NMR spectrum

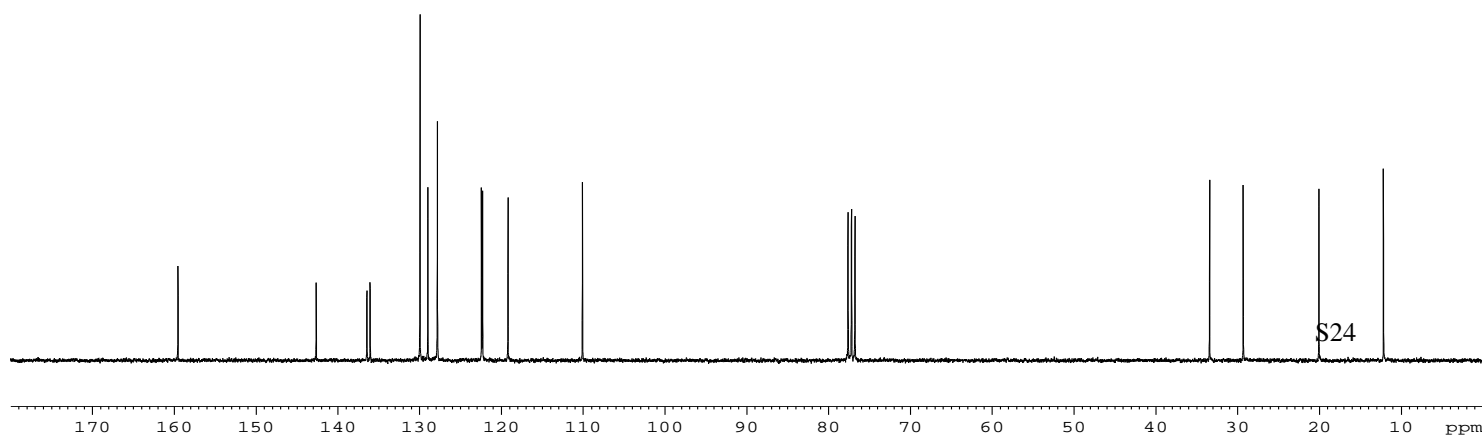
7.88
7.85
7.61
7.59
7.58
7.38
7.36
7.33
7.33
7.31
7.30
7.28
7.28
7.24
7.23
7.21
7.21
7.19
7.18
7.11
7.11
7.11
7.08
7.08

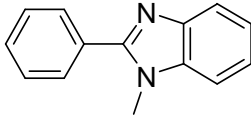
2.92
2.90
2.87
2.85
2.04
2.02
2.00
1.99
1.97
1.95
1.76
1.74
1.73
1.71
1.69
1.67
1.41
1.38
0.89
0.86
0.84



Proton-decoupled carbon NMR spectrum

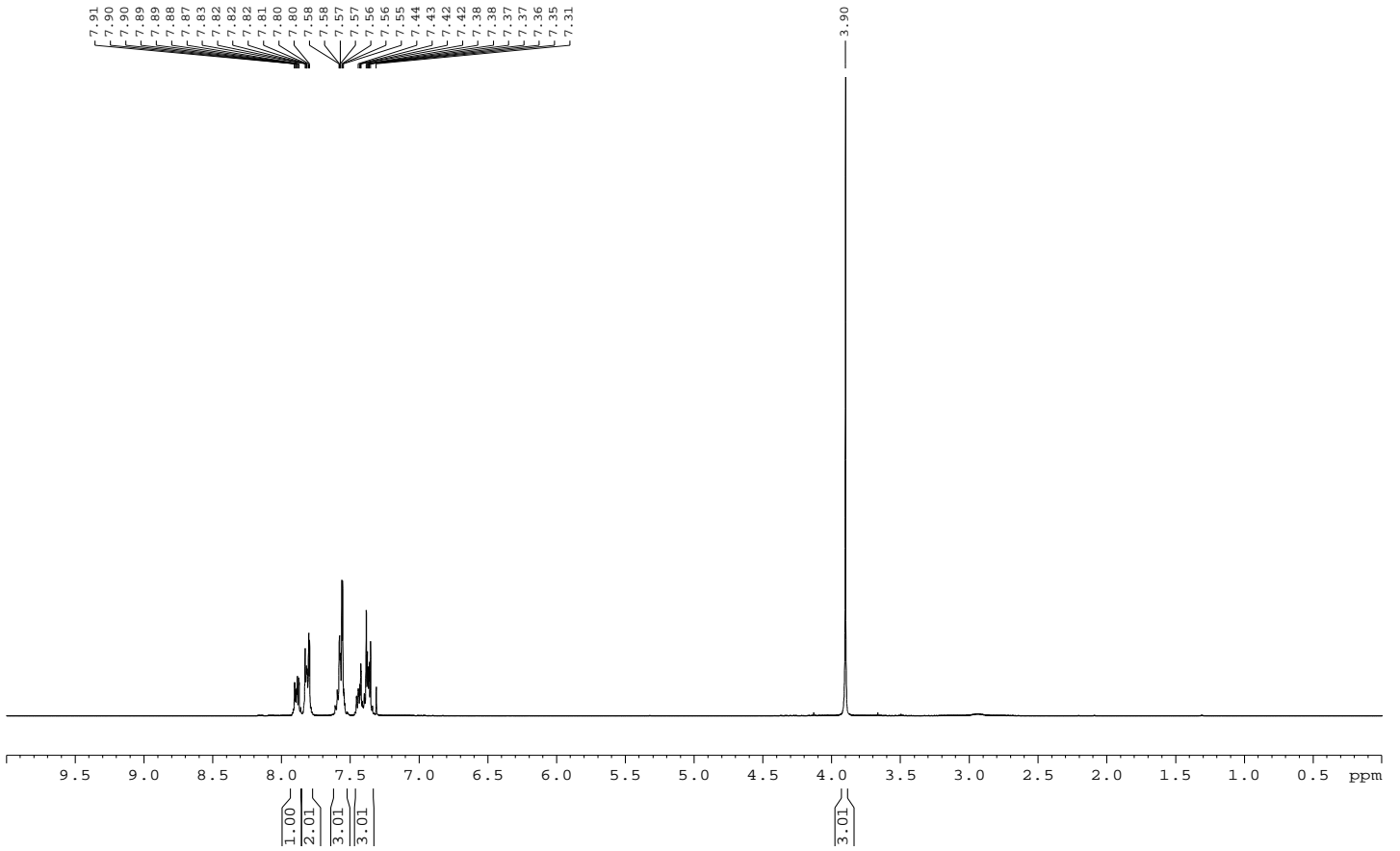
159.52
142.65
136.43
136.04
129.95
128.99
127.82
122.43
122.30
119.19
110.08
77.61
77.19
76.77
33.41
29.30
20.04
12.14



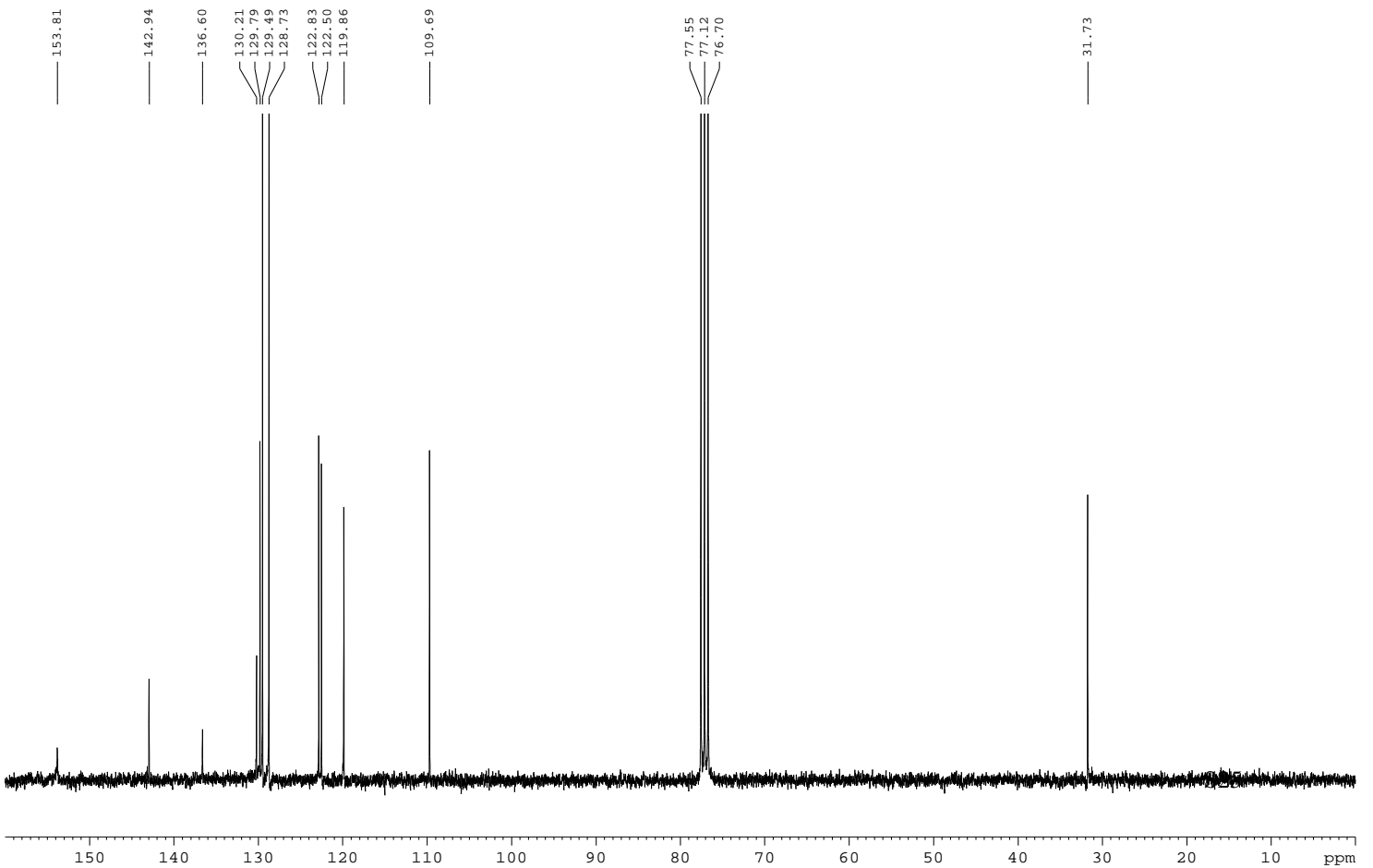


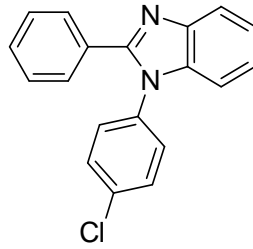
1D proton NMR spectrum

4t



Proton-decoupled carbon NMR spectrum

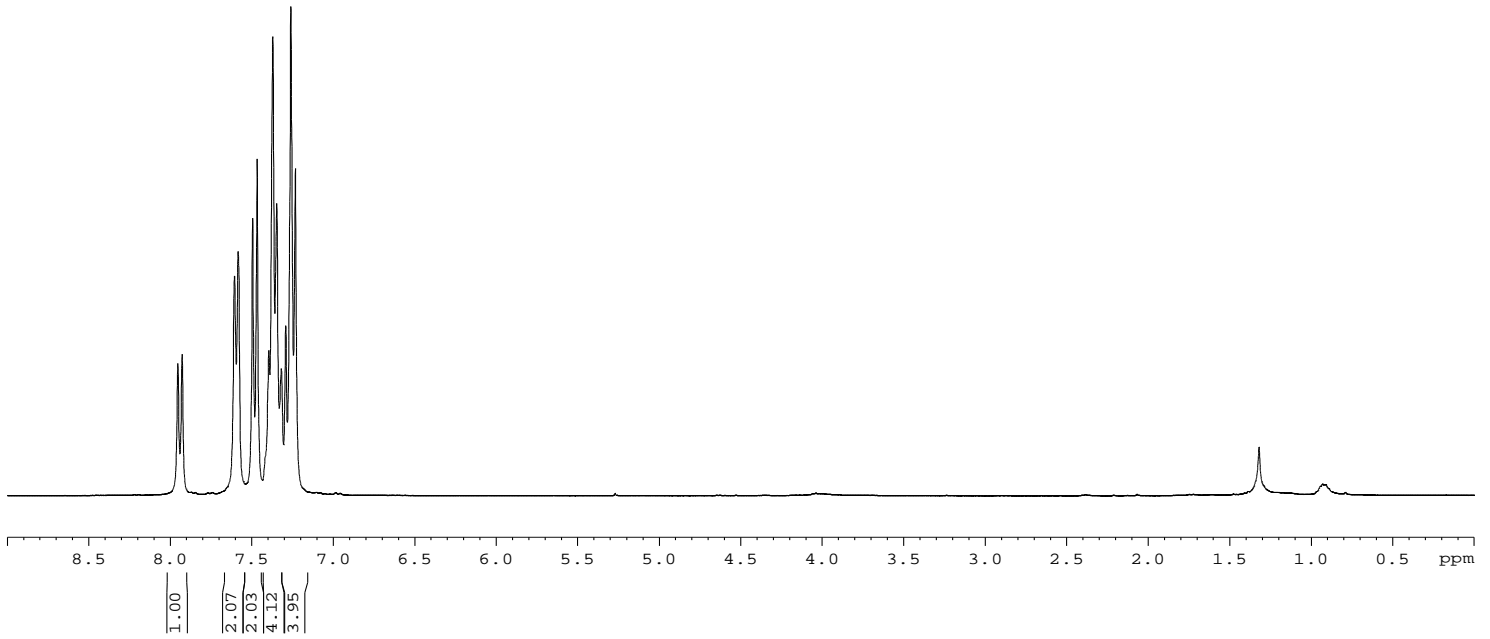




4u

1D proton NMR spectrum

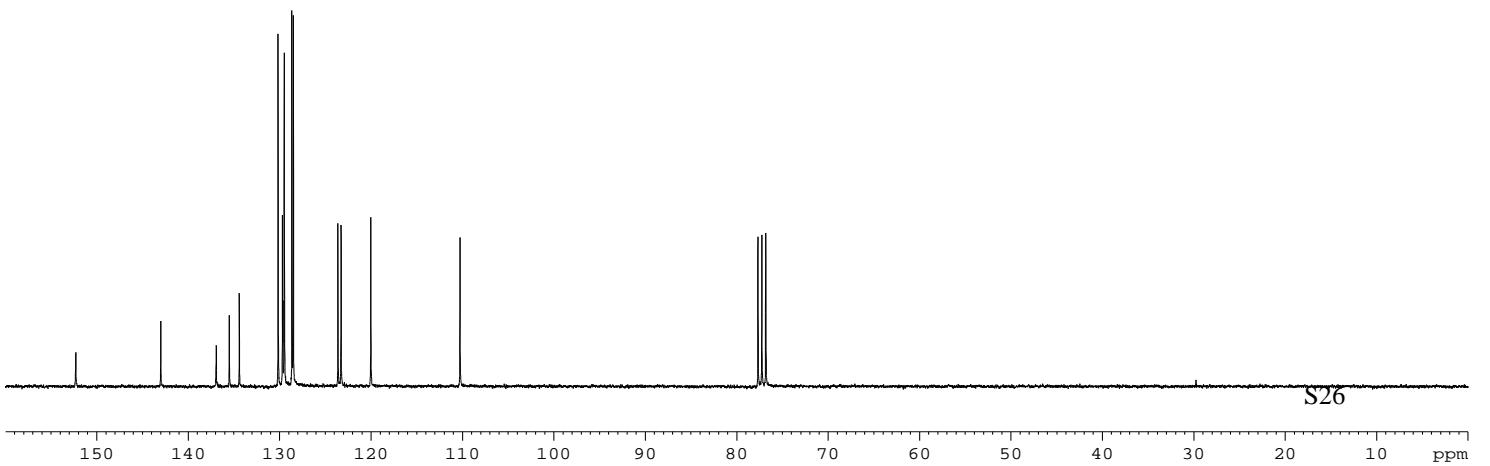
7.95
7.93
7.61
7.58
7.50
7.47
7.40
7.37
7.35
7.32
7.29
7.26
7.23

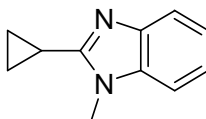


Proton-decoupled carbon NMR spectrum

152.26
143.00
136.95
135.51
134.41
130.17
129.70
129.64
129.49
128.66
128.51
123.63
123.29
120.03
110.27

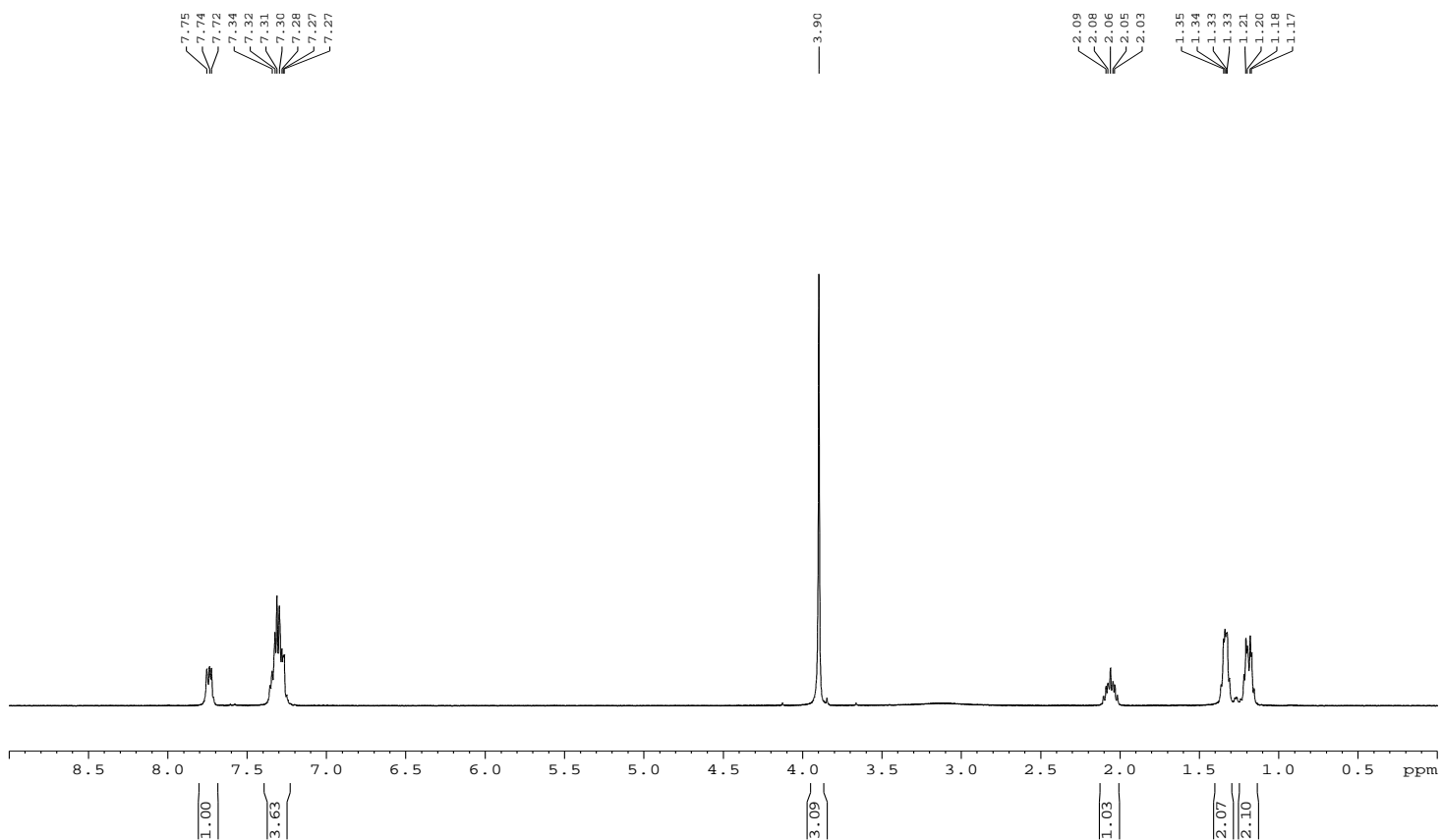
77.68
77.26
76.83



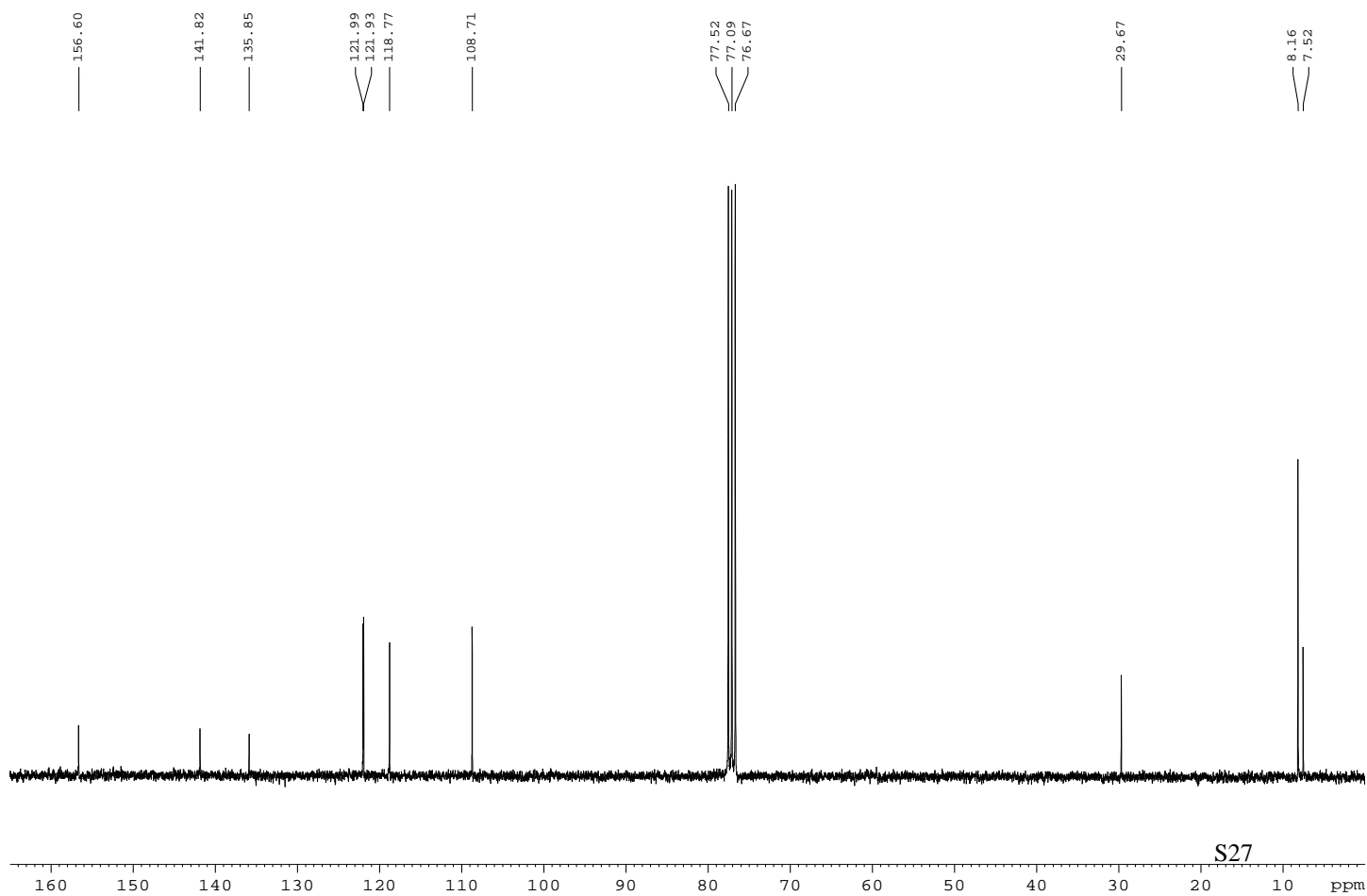


4v

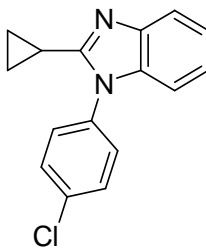
1D proton NMR spectrum



Proton-decoupled carbon NMR spectrum



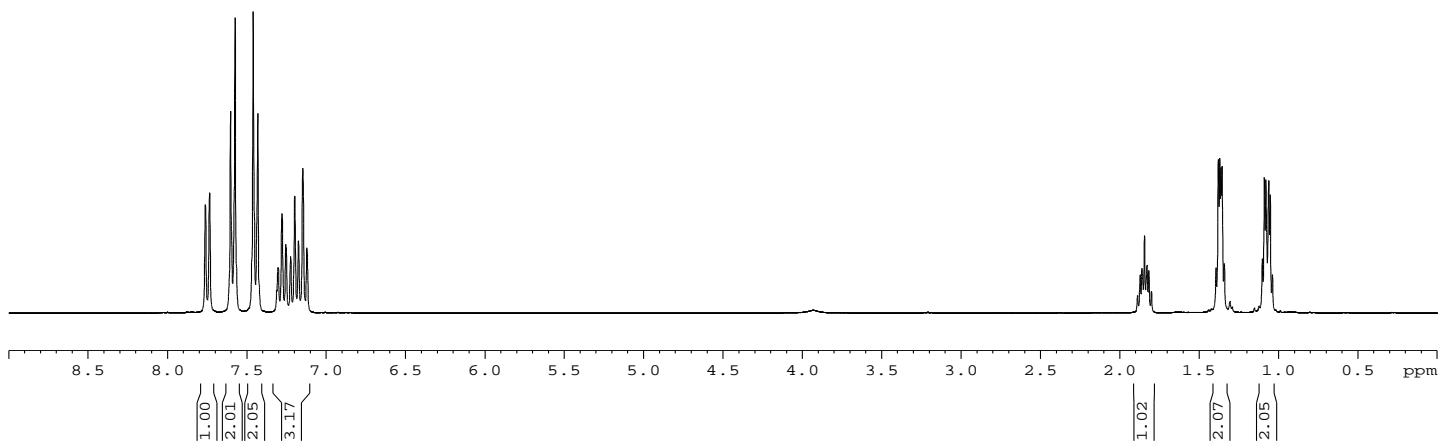
1D proton NMR spectrum



4w

7.76
7.73
7.70
7.67
7.66
7.63
7.60
7.58
7.55
7.52
7.50
7.47
7.45
7.42
7.39
7.36
7.35
7.32
7.29
7.26
7.23
7.20
7.17
7.15
7.12

1.87
1.86
1.84
1.83
1.82
1.39
1.38
1.37
1.36
1.36
1.34
1.10
1.09
1.08
1.06
1.05
1.04



Proton-decoupled carbon NMR spectrum

156.65
142.45
136.30
134.55
134.52
130.14
128.63
122.65
122.46
118.96
109.45

77.64
77.22
76.79

9.65
8.26

