Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Ortho-amino group functionalized 2,2'-bipyridine based Ru(II) complex catalysed alkylation of secondary alcohols, nitriles and amines using alcohols

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Text S1: X-ray crystallographic studies: Single-crystal X-ray data of all the complexes were collected at 100 K by using a Bruker SMART APEX II CCD diffractometer and Bruker D8 Quest single crystal diffractometer with graphite monochromated $Mo_{K\alpha}$ radiation (λ =0.71073 Å). The frames were indexed, integrated and scaled using SMART and SAINT software package[1] and the data were corrected for absorption using the SADABS program.[2] The structures were solved and refined using WINGX and SHELX programs.[3] The crystallographic figures have been generated using Diamond 3 software 10 (30% probability thermal ellipsoids).[4] The CCDC number of complex **1a**, **1b** and **1c** are CCDC 1568230, CCDC 1568231 and CCDC 1568232 respectively.

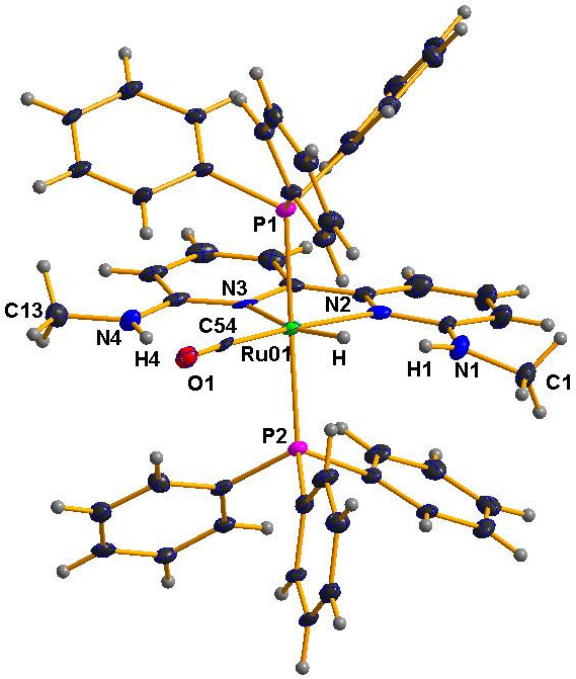


Figure S1: Solid state structure of complex **1a** (30% thermal ellipsoids; counter chloride anion and solvent molecules are omitted for clarity).

Table S1. Crystallographic data and refinement parameters for complex **1a**.

Identification code	Complex1a
Empirical formula	$C_{51}H_{51}N_4O_2Cl_5P_2Ru$
Formula weight	1092.21
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	12.074(3)
b/Å	22.964(6)
c/Å	17.711(5)
α/°	90
β/°	93.931(5)
γ/°	90
Volume/Å^3	4899(2)

Z	4
ρ_{calc}g/cm^3	1.481
μ/mm^{-1}	0.703
F(000)	2240.0
Crystal size/mm^3	0.02 × 0.02 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.908 to 51
Index ranges	-13 ≤ h ≤ 14, -27 ≤ k ≤ 27, -19 ≤ l ≤ 21
Reflections collected	25925
Independent reflections	9075 [R_{int} = 0.1006, R_{sigma} = 0.1286]
Data/restraints/parameters	9075/0/595
Goodness-of-fit on F^2	1.137
Final R indexes [I>=2σ (I)]	R_1 = 0.0865, wR_2 = 0.1957
Final R indexes [all data]	R_1 = 0.1545, wR_2 = 0.2339
Largest diff. peak/hole / e Å^{-3}	1.95/-1.60

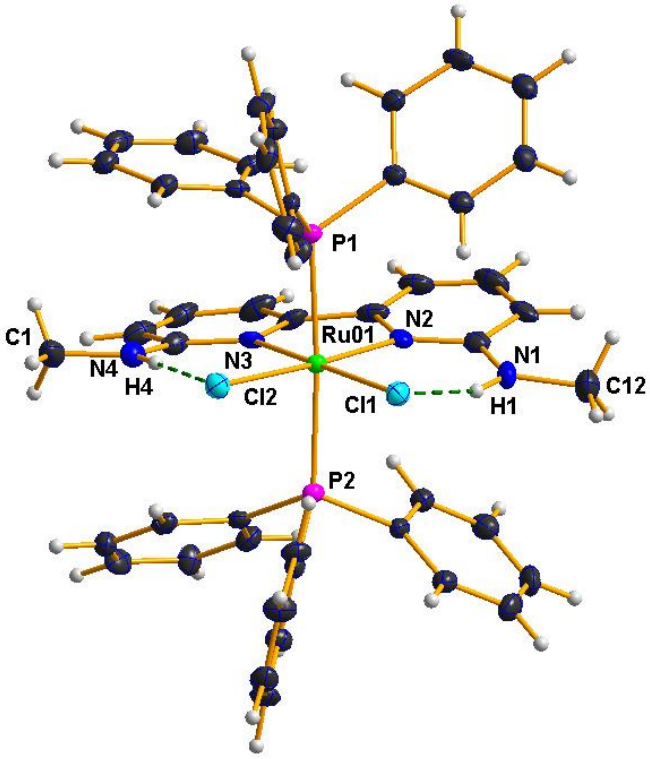


Figure S2: Solid state structure of complex **1b** (30% thermal ellipsoids).

Table S2. Crystallographic data and refinement parameters for complex **1b**.

Identification code	Complex1b
Empirical formula	$C_{48}H_{44}N_4RuCl_2P_2$
Formula weight	910.78

Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.679(3)
b/Å	19.168(6)
c/Å	21.719(7)
α/°	90
β/°	91.489(6)
γ/°	90
Volume/$Å^3$	4028(2)
Z	4
$\rho_{calc}g/cm^3$	1.502
μ/mm^{-1}	0.643
F(000)	1872.0
Crystal size/mm^3	0.02 × 0.02 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.834 to 50.224
Index ranges	$-9 \leq h \leq 11$, $-21 \leq k \leq 22$, $-25 \leq l \leq 24$
Reflections collected	21149
Independent reflections	7149 [R_{int} = 0.0955, R_{sigma} = 0.1141]
Data/restraints/parameters	7149/0/516
Goodness-of-fit on F^2	0.952
Final R indexes [I>=2σ (I)]	R_1 = 0.0606, wR_2 = 0.1423
Final R indexes [all data]	R_1 = 0.1188, wR_2 = 0.1855
Largest diff. peak/hole / e $Å^{-3}$	1.03/-1.09

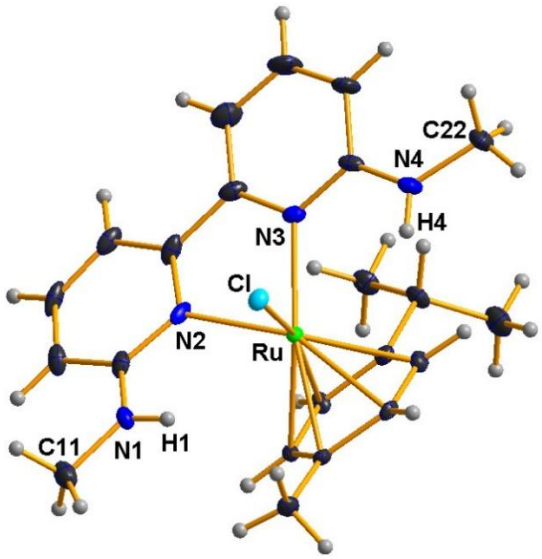
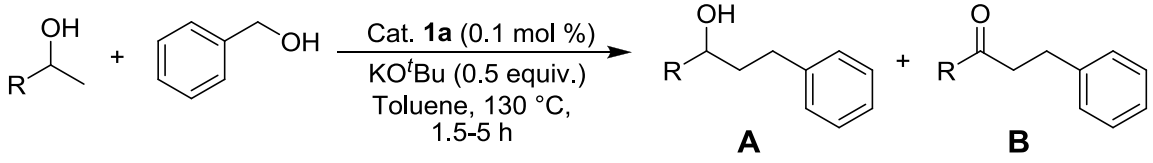


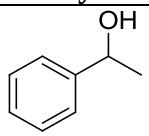
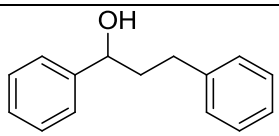
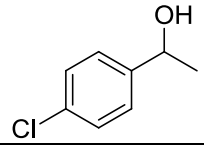
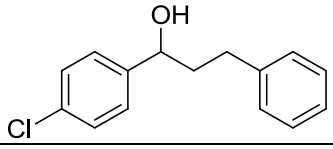
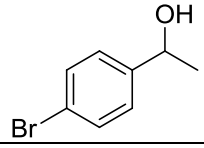
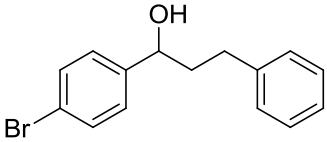
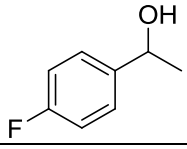
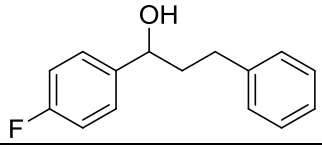
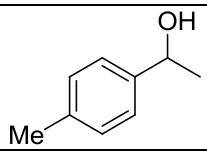
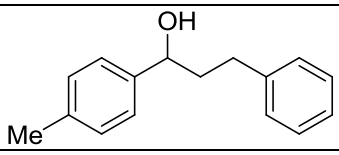
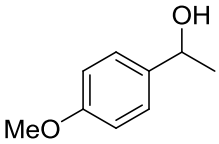
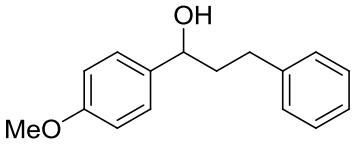
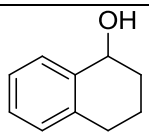
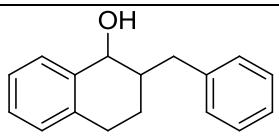
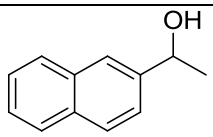
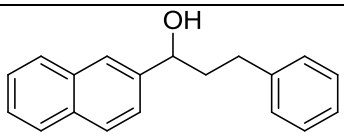
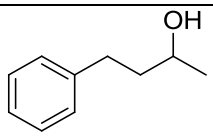
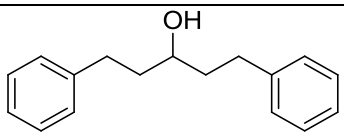
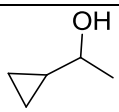
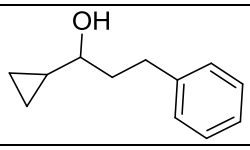
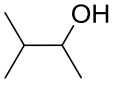
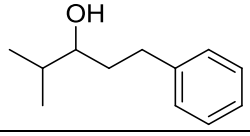
Figure S3: Solid state structure of complex **1c** (30% thermal ellipsoids; counter PF_6 anion is omitted for clarity).

Table S3. Crystallographic data and refinement parameters for complex **1c**.

Identification code	Complex1c
Empirical formula	$C_{22}H_{28}N_4F_6PClRu$
Formula weight	629.97
Temperature/K	100.0
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	24.447(6)
b/Å	12.950(3)
c/Å	7.9000(19)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2501.0(10)
Z	4
ρ_{calc}g/cm^3	1.673
μ/mm^{-1}	0.861
F(000)	1272.0
Crystal size/mm^3	0.02 × 0.02 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.308 to 50.048
Index ranges	$-28 \le h \le 29$, $-15 \le k \le 10$, $-9 \le l \le 9$
Reflections collected	12684
Independent reflections	4256 [R_{int} = 0.0446, R_{sigma} = 0.0481]
Data/restraints/parameters	4256/1/321
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0357, wR_2 = 0.0819
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.0865
Largest diff. peak/hole / e Å^{-3}	0.88/-0.35
Flack parameter	-0.01(3)

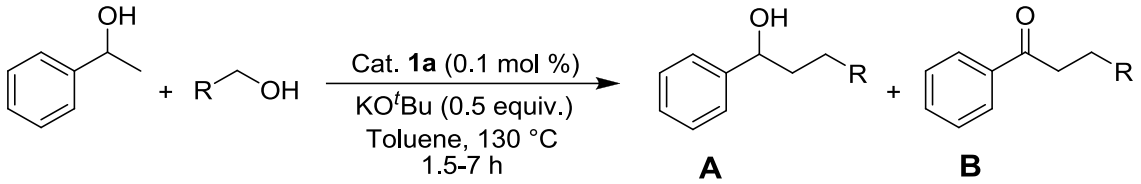
Table S4: β-Alkylation of different secondary alcohols with benzyl alcohol.[a]



Entry	Secondary alcohol	Product	Conv. (%)[b]	A/B ratio[b]
1			100	92:8
2			100	88:12
3			99	91:9
4			93	93:7
5			100	87:13
6			100	81:19
7			80	85:15
8[c]			95	93:7
9			54	99:1
10[d,e]			100	99:1
11[d,e]			97	93:7

[a] Reaction condition: Cat. **1a** (0.1 mol %), secondary alcohol (1.1 mmol), benzyl alcohol (1.1 mmol) and KO^{t}Bu (0.55 mmol) in 2 mL toluene at 130 °C for 1.5 h; closed argon condition in Schlenk tube. [b] Determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. [c] 2 h heating. [d] 5 h heating. [e] 2.2 mmol secondary alcohol and 1.1 mmol benzyl alcohol were used.

Table S5: β-Alkylation of 1-phenylethanol with different primary alcohols.[a]



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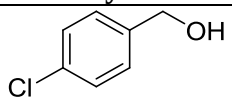
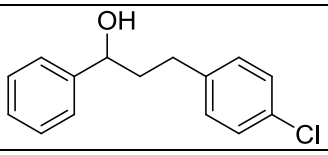
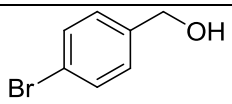
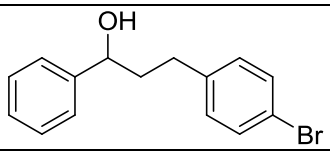
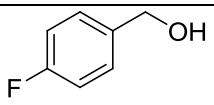
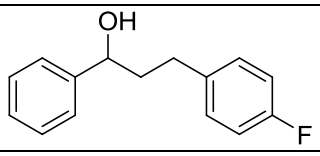
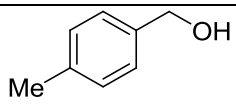
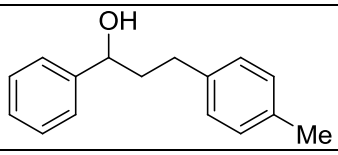
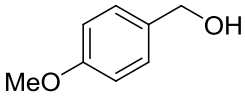
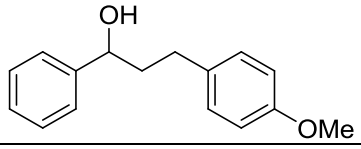
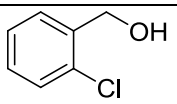
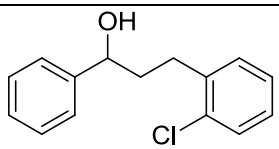
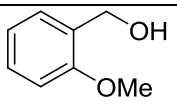
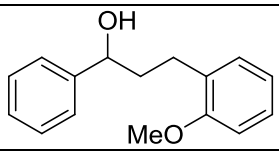
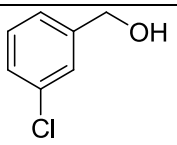
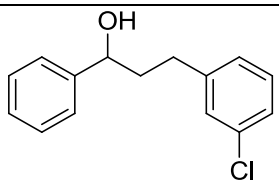
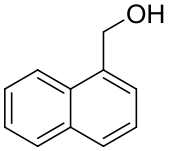
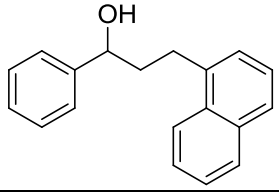
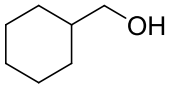
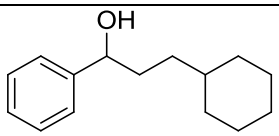
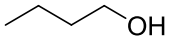
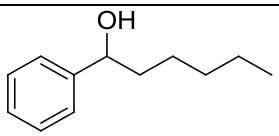
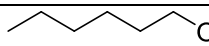
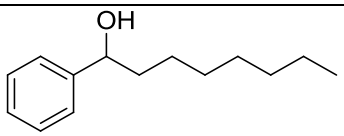
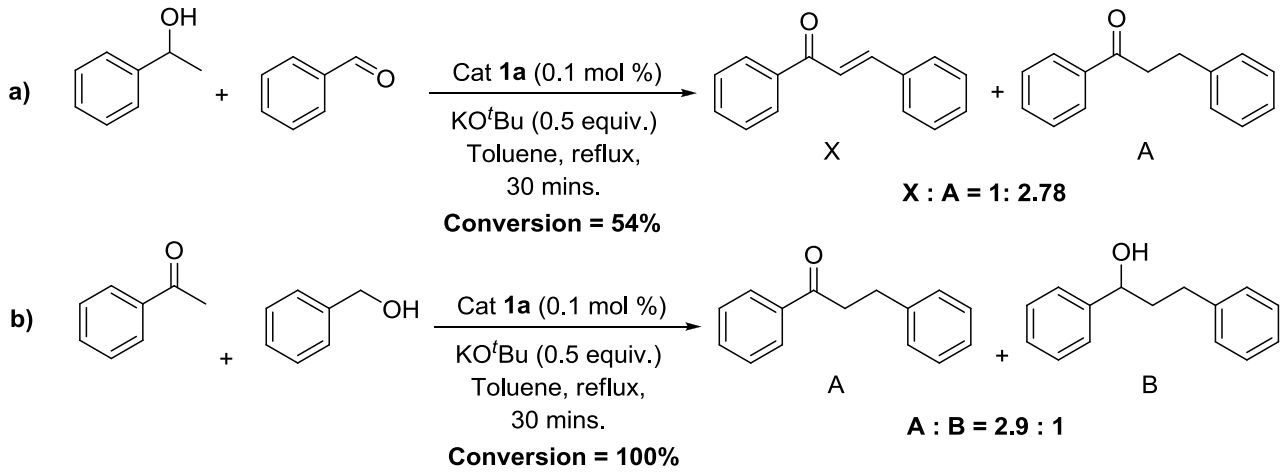
1			97	91:9
2			98	90:10
3			100	89:11
4			100	90:10
5			100	88:12
6			99	84:16
7			96	90:10
8			97	92:8
9[c]			100	79:21

10[d]			100	94:6
11[c]			90	98:2
12[c]			83	92:8

[a] Reaction condition: Cat. **1a** (0.1 mol %), 1-phenylethanol (1.1 mmol), primary alcohol (1.1 mmol) and KO^{t}Bu (0.55 mmol) in 2 mL toluene at 130 °C for 1.5 h; closed argon condition in Schlenk tube. [b] Determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. [c] 5 h heating. [d] 7 h heating.

Text S2: Procedure for the control experiments of β-alkylation secondary alcohol: Under argon condition, a mixture of cat. **1a** (0.1 mol %), KO^{t}Bu (0.55 mmol), 1-phenylethanol (1.1 mmol) and benzaldehyde (1.1 mmol) was added with 2 mL toluene and refluxed at 130 °C (oil



bath temperature) for 30 min (reaction a). After it was cooled to room temperature, the crude reaction mixture was analysed by GC check the conversion of 1-phenylethanol and further evaporating the solvent, the resulting mixture was submitted for ^{1}H NMR to calculate the product selectivity.

In the similar way, reaction b also was performed with cat. **1a** (0.1 mol %), KO^{t}Bu (0.55 mmol), acetophenone (1.1 mmol), and benzyl alcohol (1.1 mmol) in 2 mL toluene at 130 °C (oil bath temperature) for 30 min under closed argon condition.

Text S3: Procedure for time dependence product distribution of β-alkylation of secondary alcohol: To check the conversion and product selectivity of β-alkylation of secondary alcohol at different time interval, six identical reactions were performed following standard reaction condition in six Schlenk tubes using 1-phenylethanol and benzyl alcohol as model substrates only varying the reaction time (15 min, 30 min, 45 min, 60 min, 75 min and 90 min). After the reaction,

the conversion and product selectivity were determined by ^{1}H NMR and the data was plotted in % Mol vs. time (min) (figure S4).

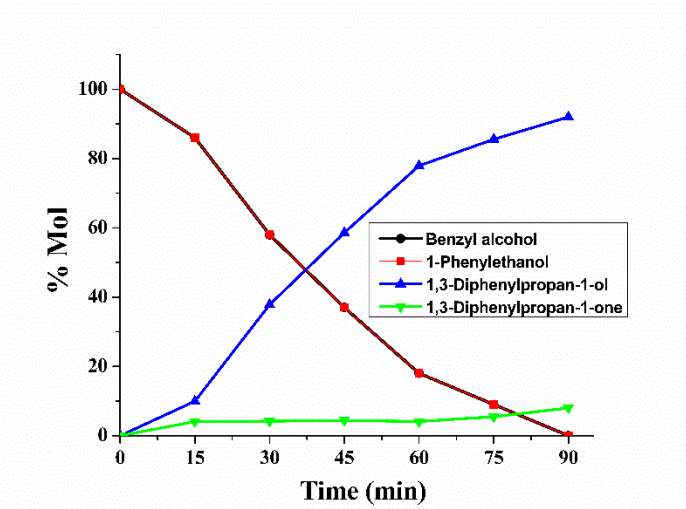
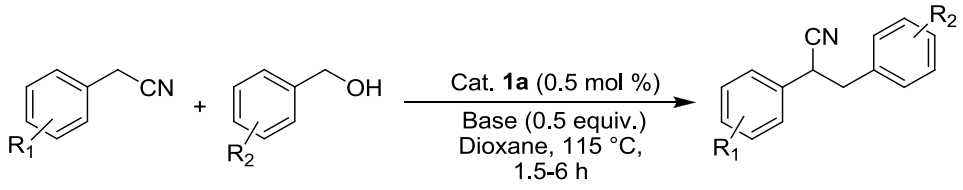


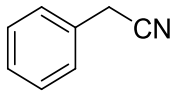
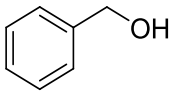
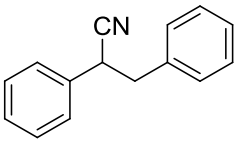
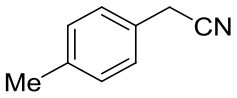
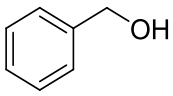
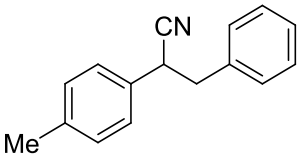
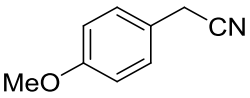
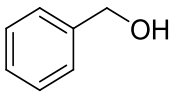
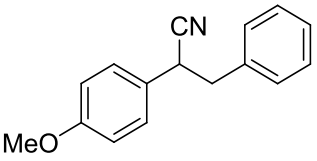
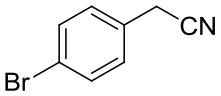
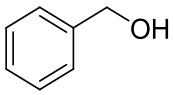
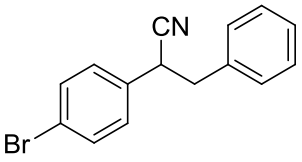
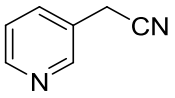
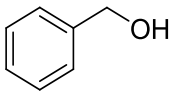
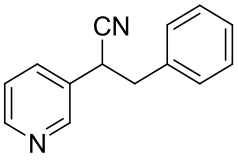
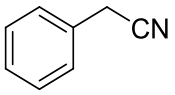
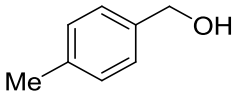
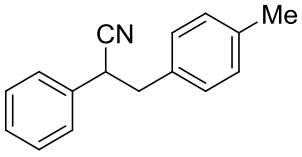
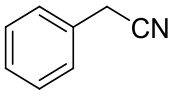
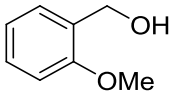
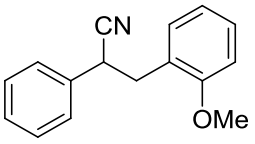
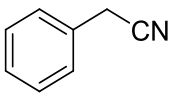
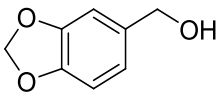
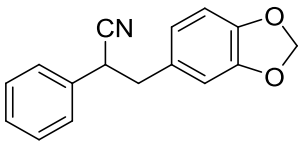
Figure S4. Time dependence product distribution of β-alkylation of 1-phenylethanol with benzyl alcohol using cat. **1a**.

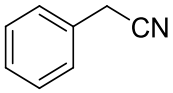
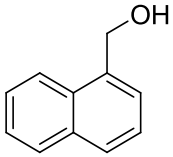
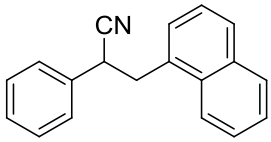
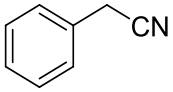
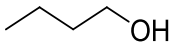
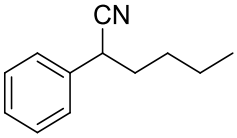
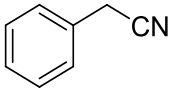
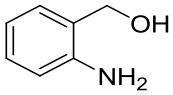
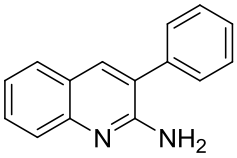
Text S4: TON Calculation in β-alkylation of secondary alcohols: 32 µL solution of cat. **1a** (4.4 × 10^{-4} mol % cat. **1a**) was taken from stock solution (1.5 mg cat. **1a** in 1.5 mL acetonitrile) and added in a Schlenk flask. After evaporating acetonitrile under reduced pressure, 1-phenylethanol (8.05 mmol), benzyl alcohol (8.05 mmol), KO^{t}Bu (4.025 mmol) and 15 mL toluene were taken into the flask, equipped with a magnetic stir bar. Then the flask was heated at 130 °C (oil bath temperature) for 30 hour. Based on the GC analysis conversion of 1-phenylethanol was 43.5%.

Text S5: Hg^0 poisoning experiment: To investigate the homogeneous nature of the catalyst in reaction condition, Hg^0 poisoning test was performed. Following the general procedure for β-alkylation of secondary alcohols, two identical reactions were performed in parallel using 1-phenylethanol and benzyl alcohol as substrates where one acted as the control reaction. Under argon condition, a mixture of cat. **1a** (0.1 mol %), KO^{t}Bu (0.55 mmol), 1-phenylethanol (1.1 mmol) and benzyl alcohol (1.1 mmol) was added in two different Schlenk tube with 2 mL toluene and refluxed at 130 °C (oil bath temperature) for 10 min. After 10 min, the two reaction mixtures were cooled down to room temperature under argon flow and a drop of Hg^0 was added in one tube, re-sealed and refluxed again at 130 °C (oil bath temperature) for another 80 min (the control Schlenk tube was also treated identically, without adding of Hg^0). After the reaction, the conversion of 1-phenylethanol was monitored by GC. The conversion of 1-phenylethanol without and with Hg^0 were 100% and 96% respectively.

Table S6: Substrate scope of α-alkylation of arylacetonitrles with primary alcohols.[a]

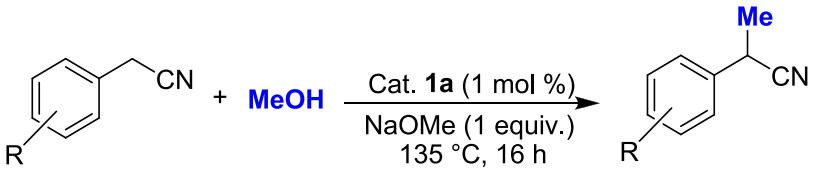


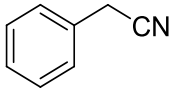
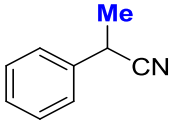
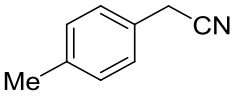
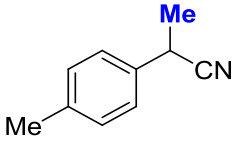
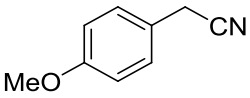
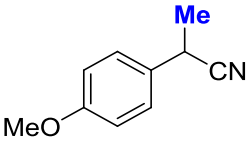
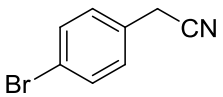
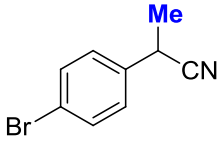
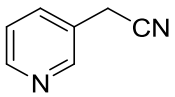
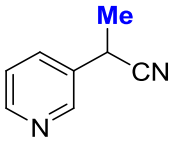
Entry	Nitrile	Alcohol	Product	Time (h)	Yield (%)[b]
1				2	99
2				1.5	>99
3				2	>99
4				1.5	98
5[c]				3	98
6				3	99
7				3	99
8				2	98

9				2	98
10				5	97
11[c,d,e]				6	88

[a] Reaction conditions: Cat. **1a** (0.5 mol %), arylacetonitrile (0.5 mmol), alcohol (2.5 mmol) and KOH (0.25 mmol) refluxed in 2 mL dioxane at 115 °C in necessary time; closed argon condition in Schlenk tube. [b] Determined by GC using mesitylene as an internal standard. [c] 1 mol % cat. **1a**. [d] Heated at 130 °C. [e] 1 equiv. KOH.

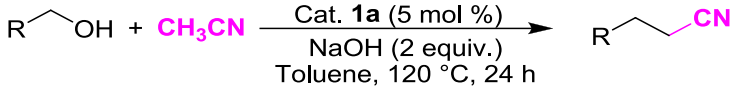
Table S7: Substrate scope for the α-methylation of arylacetonitrles using methanol.[a]

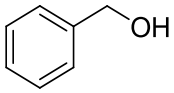
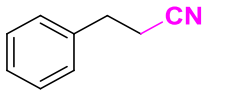
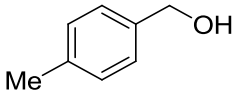
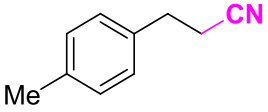
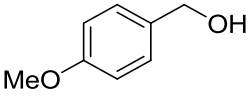
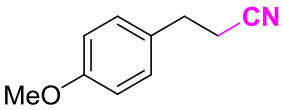
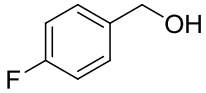
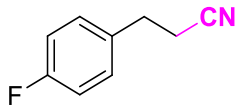
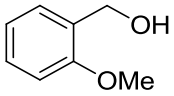
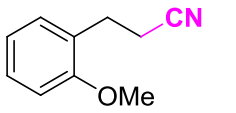
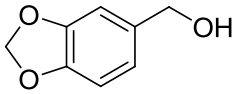
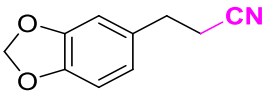
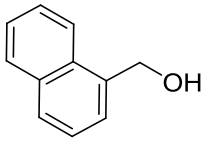
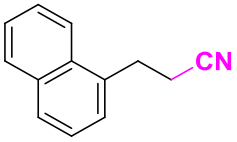
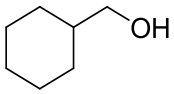
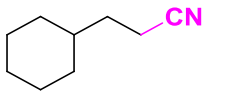
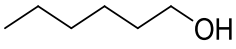
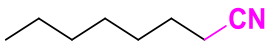


Entry	Nitrile	Product	Yield (%)[b]
1			92
2			88
3			76
4			68
5			81

[a] Reaction conditions: Cat. **1a** (1 mol %), arylacetonitrile (0.6 mmol) and NaOMe (0.6 mmol) in MeOH (1.0 mL) at 135 °C for 16 h; closed argon condition in pressure tube. [b] Determined by GC using mesitylene as an internal standard.

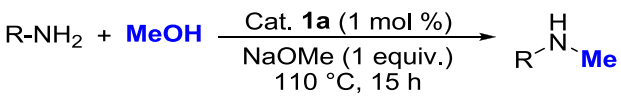
Table S8: Monoalkylation of acetonitrile using different alcohols.[a]

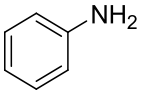
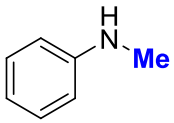
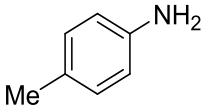
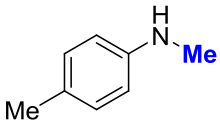
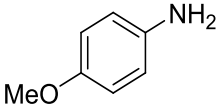
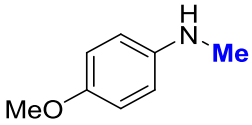
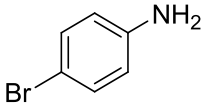
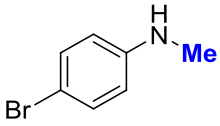
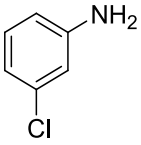
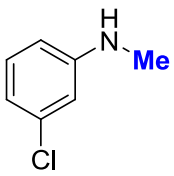
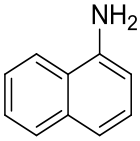
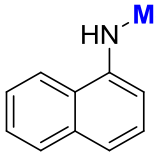
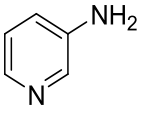
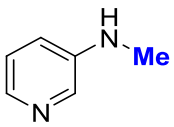
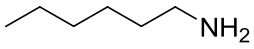
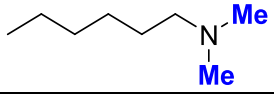


Entry	Substrate	Product	Yield (%)[b]
1			94
2			81
3			85
4			77
5			69
6			87
7			83
8			72
9			64

[a] Reaction conditions: Cat. **1a** (5 mol %), alcohol (0.5 mmol), NaOH (1.0 mmol) and CH_3CN (62.5 mmol) heated in 1 mL toluene at 120 °C for 24 h; closed argon condition in Schlenk tube. [b] Determined by GC using mesitylene as an internal standard.

Table S9: N-methylation of amines using methanol.[a]



Entry	Substrate	Product	Yield (%)[b]
1			86[c] 99
2			99
3			98
4			98
5			100
6[d]			80
7			95
8[d]			60

[a]Reaction conditions: Cat. **1a** (1 mol %), amine (0.8 mmol), NaOMe (0.8 mmol) in methanol (1.0 mL) refluxed at 110 °C for 15 h; closed argon condition in pressure tube. [b]Determined by GC using mesitylene as an internal standard. [c] 12 h. [d] 24 h.

Text S6: NMR Characterization Data of Isolated Products:

β-Alkylated alcohols

Secondary alcohol variation products: 1,3-diphenylpropan-1-ol (2a)[5]: Colourless oil (203 mg, 87% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.36-7.34 (m, 4H), 7.31-7.25 (m, 3H), 7.21-7.17 (m, 3H), 4.68 (dd, $J_{H,H}$ = 8.0, 5.6 Hz, 1H), 2.79-2.63 (m, 2H), 2.15-2.04 (m, 2H), 1.91 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.66, 141.88, 128.63, 128.55, 128.50, 127.75, 126.04, 125.98, 73.98, 40.56, 32.16.

1-(4-Chlorophenyl)-3-phenylpropan-1-ol (2b)[5]**:** Colourless oil (228 mg, 84% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.33-7.25 (m, 6H), 7.21-7.17 (m, 3H), 4.65 (dd, $J_{H,H}$ = 7.6, 5.2 Hz, 1H), 2.77-2.62 (m, 2H), 2.14-1.94 (m, 2H), 1.85 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 143.13, 141.60, 133.35, 128.75, 128.57, 128.53, 127.42, 126.09, 73.26, 40.60, 32.03.

1-(4-Bromophenyl)-3-phenylpropan-1-ol (2c)[6]: Colourless oil (272 mg, 85% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.48-7.46 (m, 2H), 7.31-7.28 (m, 2H), 7.22-7.17 (m, 5H), 4.62 (dd, $J_{H,H}$ = 8.0, 5.6 Hz, 1H), 2.76-2.61 (m, 2H), 2.20 (bs, 1H), 2.13-1.93 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 143.58, 141.53, 131.63, 128.53, 128.49, 127.75, 126.05, 121.39, 73.19, 40.49, 31.95.

1-(4-Fluorophenyl)-3-phenylpropan-1-ol (2d)[5]: Light yellow oil (203 mg, 80% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.32-7.25 (m, 4H), 7.20-7.17 (m, 3H), 7.05-7.01 (m, 2H), 4.66 (t, $J_{H,H}$ = 6.5 Hz, 1H), 2.75-2.62 (m, 2H), 2.14-1.96 (m, 3H).^{13}C NMR (125 MHz, $CDCl_3$): δ = 163.29, 161.34, 141.68, 140.41, 140.39, 128.54, 128.52, 127.70, 127.64, 126.04, 115.49, 115.32, 73.30, 40.65, 32.10.

1-(4-Methylphenyl)-3-phenylpropan-1-ol (2e)[5]**:** Colourless oil (204 mg, 82% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.30-7.16 (m, 9H), 4.65 (dd, $J_{H,H}$ = 7.6, 5.6 Hz, 1H), 2.78-2.62 (m, 2H), 2.35 (s, 3H), 2.18-1.97 (m, 2H), 1.82 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 141.97, 141.69, 137.45, 129.31, 128.56, 128.49, 126.02, 125.94, 73.85, 40.47, 32.21, 21.24.

1-(4-Methoxyphenyl)-3-phenylpropan-1-ol (2f)[7]: Pale yellow oil (203 mg, 76% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.29-7.16 (m, 7H), 6.90-6.87 (m, 2H), 4.63 (dd, $J_{H,H}$ = 7.6, 6.0 Hz, 1H), 3.81 (s, 3H), 2.76-2.60 (m, 2H), 2.18-1.97 (m, 2H), 1.79 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.24, 141.95, 136.81, 128.57, 128.50, 127.34, 125.96, 114.01, 73.63, 55.43, 40.47, 32.26.

2-Benzyl-1,2,3,4-tetrahydronaphthalen-1-ol (2g)[7]: White solid (157 mg, 60% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.52-7.49 (m, 1H), 7.32-7.29 (m, 2H), 7.24-7.19 (m, 5H), 7.10-7.08 (m, 1H), 4.50 (d, $J_{H,H}$ = 8.0 Hz, 1H), 3.07 (dd, $J_{H,H}$ = 12, 4 Hz, 1H), 2.77-2.74 (m, 2H), 2.51 (dd, $J_{H,H}$ = 12, 4 Hz, 1H), 2.10-1.94 (m, 2H), 1.70 (bs, 1H), 1.55-1.45 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 140.48, 138.69, 136.93, 130.50, 129.41, 128.86, 128.49, 127.57, 126.42, 126.15, 73.14, 44.13, 38.49, 27.75, 24.66.

1-(Naphthalen-2-yl)-3-phenylpropan-1-ol (2h)[7]: White solid (237 mg, 82% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85-7.82 (m, 3H), 7.79 (s, 1H), 7.50-7.46 (m, 3H), 7.30-727 (m, 2H), 7.21-7.17 (m, 3H), 4.86 (dd, $J_{H,H}$ = 7.6, 5.6 Hz, 1H), 2.82-2.66 (m, 2H), 2.27-2.12 (m, 2H), 1.89 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 142.00, 141.86, 133.40, 133.14, 128.59, 128.54, 128.52, 128.05, 127.82, 126.31, 126.01, 124.81, 124.17, 74.11, 40.45, 32.18.

1,5-Diphenylpentan-3-ol (2i)[5]: White solid (132 mg, 50% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.30-7.19 (m, 10H), 3.67 (m, 1H), 2.80-2.65 (m, 4H), 1.87-1.75 (m, 4H), 1.54 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 142.17, 128.58, 128.54, 126.00, 71.00, 39.37, 32.20.

1-cyclopropyl-3-phenylpropan-1-ol (2j)[8]: Colourless oil (178 mg, 92% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.32-7.18 (m, 5H), 2.94-2.71 (m, 3H), 2.14 (bs, 1H), 1.98-1.92 (m, 2H),

1.0-0.91 (m, 1H), 0.58-0.47 (m, 2H), 0.32-0.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 142.28, 128.43, 128.38, 125.70, 75.96, 38.75, 32.03, 17.93, 2.70, 2.60.

4-Methyl-1-phenylpentan-3-ol (2k)[9]: Colourless oil (168 mg, 86% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.30-7.27 (m, 2H), 7.22-7.16 (m, 3H), 3.40 (sept, $J_{H,H}$ = 3.6 Hz, 1H), 2.88-2.81 (m, 1H), 2.69-2.61 (m, 1H), 1.84-1.64 (m, 3H), 0.92 (dd, $J_{H,H}$ = 6.8, 1.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 142.47, 128.56, 128.51, 125.91, 76.26, 36.08, 33.80, 32.60, 18.90, 17.29.

Primary alcohol variation products: 3-(4-Chlorophenyl)-1-phenylpropan-1-ol (3a)[10]: White solid (222 mg, 82% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38-7.22 (m, 7H), 7.13-7.09 (m, 2H) 4.66 (t, $J_{H,H}$ = 5.9 Hz, 1H), 2.75-2.60 (m, 2H), 2.14-1.94 (m, 2H), 1.83 (d, $J_{H,H}$ = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.51, 140.33, 131.66, 129.92, 128.70, 128.58, 127.88, 126.00, 73.83, 40.43, 31.50.

3-(4-Bromophenyl)-1-phenylpropan-1-ol (3b)[11]: Colourless oil (266 mg, 83% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.40-7.25 (m, 7H), 7.05 (d, $J_{H,H}$ = 8.0 Hz, 2H), 4.65 (dd, $J_{H,H}$ = 8.0, 5.5 Hz, 1H), 2.72-2.59 (m, 2H), 2.13-1.96 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.49, 140.85, 131.52, 130.32, 128.67, 127.85, 125.99, 119.67, 73.78, 40.32, 31.53.

3-(4-Fluorophenyl)-1-phenylpropan-1-ol (3c)[12]: Colourless oil (208 mg, 82% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37-7.26 (m, 5H), 7.15-7.11 (m, 2H), 6.97-6.93 (m, 2H) 4.66 (t, $J_{H,H}$ = 6.4 Hz, 1H), 2.75-2.60 (m, 2H), 2.14-1.94 (m, 2H), 1.87 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.58, 160.16, 144.58, 137.48, 129.89, 129.82, 128.67, 127.83, 126.01, 115.31, 115.10, 73.86, 40.68, 31.33.

3-(4-Methylphenyl)-1-phenylpropan-1-ol (3d)[13]: White solid (214 mg, 86% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.35-7.33 (m, 4H), 7.31-7.26 (m, 1H), 7.08 (s, 4H), 4.68 (dd, $J_{H,H}$ = 7.6, 5.2 Hz, 1H), 2.74-2.59 (m, 2H), 2.31 (s, 3H), 2.16-1.96 (m, 2H), 1.75 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.70, 138.75, 135.39, 129.18, 128.60, 128.42, 127.71, 126.04, 73.98, 40.65, 31.69, 21.11.

3-(4-Methoxyphenyl)-1-phenylpropan-1-ol (3e)[13]: White solid (218 mg, 82% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.34-7.25 (m, 5H), 7.10 (d, $J_{H,H}$ = 8.4 Hz, 2H), 6.82 (d, $J_{H,H}$ = 8.4 Hz, 2H), 4.66 (dd, $J_{H,H}$ = 7.6, 5.2 Hz, 1H), 3.77 (s, 3H), 2.71-2.57 (m, 2H), , 2.14-1.94 (m, 2H), 1.76 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.83, 144.72, 133.95, 129.40, 128.57, 127.66, 126.02, 113.89, 73.88, 55.32, 40.77, 31.20.

3-(2-Chlorophenyl)-1-phenylpropan-1-ol (3f)[14]: Colourless dense oil (211 mg, 78% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37-7.11 (m, 9H), 4.72 (dd, $J_{H,H}$ = 7.8, 5.3 Hz, 1H), 2.93-2.87 (m, 1H), 2.80-2.74 (m, 1H), 2.13-2.02 (m, 2H), 1.94 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.50, 139.53, 134.06, 130.55, 129.63, 128.6,6 127.82, 127.52, 126.92, 126.03, 74.12, 38.84, 30.19.

3-(2-Methoxyphenyl)-1-phenylpropan-1-ol (3g)[15]: Pale yellow oil (213 mg, 80% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37-7.32 (m, 4H), 7.28-7.25 (m, 1H), 7.22-7.14 (m, 2H), 6.92-6.85 (m, 2H), 4.63 (dd, $J_{H,H}$ = 8.4, 4.8 Hz, 1H), 3.83 (s, 3H), 2.78-2.74 (m, 2H), 2.29 (bs, 1H),

2.12-1.95 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.45, 144.73, 130.17, 130.08, 128.45, 127.45, 127.31, 126.00, 120.78, 110.40, 73.63, 55.42, 39.47, 26.53.

3-(3-Chlorophenyl)-1-phenylpropan-1-ol (3h)[16]: Colourless dense liquid (222 mg, 82% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38-7.27 (m, 5H), 7.22-7.14 (m, 3H), 7.07-7.05 (m, 1H), 4.67 (dd, $J_{H,H}$ = 8, 5.6 Hz, 1H), 2.77-2.61 (m, 2H), 2.16-1.95 (m, 2H), 1.83 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.49, 143.99, 134.25, 129.74, 128.71, 127.90, 126.77, 126.18, 126.00, 73.84, 40.30, 31.85.

3-(Naphthalen-1-yl)-1-phenylpropan-1-ol (3i)[7]: Pale yellow oil (216 mg, 75% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.00-7.98 (m, 1H), 7.86-7.85 (m, 1H), 7.72 (d, $J_{H,H}$ = 8.0 Hz, 1H), 7.51-7.46 (m, 2H), 7.42-7.34 (m, 6H), 7.32-7.28 (m, 1H), 4.81-4.78 (m, 1H), 3.28-3.22 (m, 1H), 3.14-3.08 (m, 1H), 2.30-2.13 (m, 2H), 2.04 (d, $J_{H,H}$ = 3.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 144.65, 138.13, 134.04, 131.97, 128.88, 128.65, 127.80, 126.80, 126.07, 125.91, 125.66, 125.57, 123.90, 74.30, 39.95, 29.23.

3-Cyclohexyl-1-phenylpropan-1-ol (3j)[15]: Colourless dense liquid (211 mg, 88% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.36-7.29 (m, 4H), 7.28-7.26 (m, 1H), 4.62 (t, $J_{H,H}$ = 6.8 Hz, 1H), 1.82-1.74 (m, 2H), 1.55 (bs, 1H), 1.36-1.09 (m, 10H), 0.89-0.81 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.09, 128.57, 127.62, 126.05, 75.21, 37.79, 36.61, 33.62, 33.50, 33.42, 26.79, 26.50.

1-Phenylhexan-1-ol (3k)[5]: Colourless oil (160 mg, 82% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.37-7.33 (m, 4H), 7.30-7.27 (m, 1H), 4.64 (dd, $J_{H,H}$ = 5.4, 5.4 Hz, 1H), 2.18 (bs, 1H), 1.80-1.68 (m, 2H), 1.46-1.30 (m, 6H), 0.90 (t, $J_{H,H}$ = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 145.08, 128.46, 127.49, 126.00, 74.72, 39.15, 31.82, 25.59, 22.66, 14.11

1-Phenyloctan-1-ol (3l)[16]: Colourless oil (163 mg, 72% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.36-7.31 (m, 4H), 7.30-7.26 (m, 1H) 4.63 (dd, $J_{H,H}$ = 7.2, 6.0 Hz, 1H), 2.04 (bs, 1H), 1.78-1.66 (m, 2H), 1.32-1.22 (m, 10H), 0.88 (t, $J_{H,H}$ = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.10, 128.49, 127.52, 126.01, 74.76, 39.22, 31.92, 29.61, 29.48, 29.32, 25.92, 22.74, 14.17

<u>α-Alkylation of arylacetonitriles</u>: 2,3-Diphenylpropanenitrile (4a)[17]: Colourless solid (98 mg, 94% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38-7.35 (m, 8H), 7.15-7.13 (m, 2H), 4.0 (dd, $J_{H,H}$ = 8.3, 6.5 Hz, 1H), 3.22-3.10 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 136.36, 135.29, 129.32, 129.12, 128.31, 127.59, 127.49, 120.49, 42.30, 39.91; GC-MS: $[M^+]$ = 207.1

3-Phenyl-2-p-tolylpropanenitrile (4b)[18]: Colourless solid (105 mg, 95% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.31-7.11 (m, 10H), 3.95 (dd, $J_{H,H}$ = 8.4, 6.6 Hz, 1H), 3.19-3.07 (m, 2H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 138.10, 136.50, 132.30, 129.75, 129.29, 128.69, 127.41, 120.63, 42.33, 39.55, 29.79, 21.18; GC-MS: $[M^+]$ = 221.1

2-(4-Methoxyphenyl)-3-phenylpropanenitrile (4c)[18]: Colourless solid (111 mg, 94% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.29-7.25 (m, 3H), 7.17-7.11(m, 4H), 6.86 (d, $J_{H,H}$ = 8.8 Hz, 2H), 3.94 (dd, $J_{H,H}$ = 8.2, 6.6 Hz, 1H), 3.80 (s, 3H), 3.19-3.06 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.48, 136.47, 129.34, 128.72, 128.69, 127.41, 127.28, 120.74, 114.43, 55.42, 42.36, 39.06; GC-MS: $[M^+]$ = 237.1

2-(4-Bromophenyl)-3-phenylpropanenitrile (4d)[19]: Pale Yellow Solid (130 mg, 91% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.48-7.45 (m, 2H), 7.31-7.25 (m, 3H), 7.11-7.08 (m, 4H), 3.96 (dd, $J_{H,H}$ = 7.7, 6.9 Hz, 1H), 3.20-3.07 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 135.82, 134.19, 132.23, 129.23, 128.79, 127.63, 122.40, 119.95, 42.04, 39.31, 29.79; GC-MS: [M^+] = 285.0

3-Phenyl-2-(pyridin-3-yl)propanenitrile (4e)[17]: Colourless solid (94 mg, 90% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.58 (d, $J_{H,H}$ = 2.7 Hz, 1H), 8.46 (s, 1H), 7.58 (d, $J_{H,H}$ = 6.4 Hz, 1H), 7.31-7.25 (m, 2H), 7.10 (m, 2H), 4.05 (t, $J_{H,H}$ = 5.8 Hz, 1H), 3.25-3.12 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 149.65, 148.83, 135.37, 131.17, 129.33, 128.90, 127.82, 123.84, 119.46, 41.89, 37.35, 29.78; GC-MS: [M^+] = 208.1

2-Phenyl-3-p-tolylpropanenitrile (4f)[20]: Colourless liquid (104 mg, 94% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38-7.32 (m, 3H), 7.28-7.25 (m, 2H), 7.10 (d, $J_{H,H}$ = 7.9 Hz, 2H), 7.03 (d, $J_{H,H}$ = 8.0 Hz, 2H), 3.97 (dd, $J_{H,H}$ = 8.3, 7.7 Hz, 1H), 3.17-3.06 (m, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 137.10, 135.42, 133.32, 129.40, 129.17, 129.09, 128.25, 127.58, 120.56, 41.93, 40.06, 21.20; GC-MS: [M^+] = 221.1

3-(2-Methoxyphenyl)-2-phenylpropanenitrile (4g)[21]: Colourless liquid (107 mg, 90% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37-7.23 (m, 6H), 7.07 (dd, $J_{H,H}$ = 7.7, 1.7 Hz, 1H), 6.89-6.85 (m, 2H), 4.16 (dd, $J_{H,H}$ = 9.0, 6.4 Hz, 1H), 3.84 (s, 3H), 3.21-3.09 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.49, 136.12, 131.26, 128.97, 128.93, 128.04, 127.45, 124.99, 120.92, 120.69, 110.37, 55.37, 37.86, 37.73; GC-MS: [M^+] = 237.1

3-(Benzo[*d*][1,3]dioxol-5-yl)-2-phenylpropanenitrile (4h)[22]: Colourless liquid (114 mg, 91% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.38-7.24 (m, 5H), 6.71 (d, $J_{H,H}$ = 7.9 Hz, 1H), 6.58 (m, 2H), 5.93 (s, 2H), 3.94 (dd, $J_{H,H}$ = 8.2, 6.6 Hz, 1H), 3.12-3.01 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 147.82, 146.96, 135.19, 130.01, 129.13, 128.32, 127.55, 122.58, 120.42, 109.56, 108.45, 101.15, 42.06, 40.15; GC-MS: [M^+] = 250.8

3-(Naphthalen-1-yl)-2-phenylpropanenitrile (4i)[23]:White solid (118 mg, 92% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.94-7.88 (m, 2H), 7.79 (d, $J_{H,H}$ = 8.2 Hz, 1H), 7.57-7.49 (m, 2H), 7.41-7.29 (m, 7H), 4.16 (dd, $J_{H,H}$ = 8.6, 6.7 Hz, 1H), 3.67-3.57 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 135.69, 134.04, 132.28, 131.36, 129.35, 129.22, 128.42, 128.39, 128.22, 127.44, 126.64, 125.88, 125.57, 122.67, 120.56, 39.70, 38.91, 29.79; GC-MS: [M^+] = 257.1

2-Phenylhexanenitrile (4j)[22]: Colourless liquid (78 mg, 90% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.39-7.28 (m, 5H), 3.76 (dd, $J_{H,H}$ = 8.5, 6.4 Hz, 1H), 1.97-1.87 (m, 2H), 1.54-1.31 (m, 4H), 0.91 (t, $J_{H,H}$ = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 136.10, 129.03, 127.97, 127.23, 120.93, 37.38, 35.62, 29.12, 22.08, 13.75; GC-MS: [M^+] = 173.1

3-Phenylquinolin-2-amine (4k)[24]: Off-white solid (90 mg, 82% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.78 (s, 1H), 7.69 (d, $J_{H,H}$ = 8.4 Hz, 1H), 7.64 (dd, $J_{H,H}$ = 8.0, 1.2 Hz, 1H), 7.58-7.54 (m, 1H), 7.53-7.48 (m, 4H), 7.43 (tt, $J_{H,H}$ = 7.0, 1.7 Hz, 1H), 7.28-7.25 (m, 1H), 5.01 (bs, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 155.26, 147.21, 137.66, 137.35, 129.76, 125.25, 129.00, 128.33, 127.60, 125.67, 125.12, 124.30, 122.89; ESI-MS: *m/z* 221.1077 ([M+H]$^+$, predicted: 221.1079).

α-Methylation of aryl acetonitrile: 2-Phenylpropanenitrile (5a)[22]**:** Colourless liquid (69 mg, 88% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.40-7.30 (m, 5H), 3.89 (q, $J_{H,H}$ = 7.2 Hz, 1H), 1.64 (d, $J_{H,H}$ = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 137.20, 129.28, 128.18, 126.83, 121.71, 31.39, 21.61; GC-MS: [M^+] = 131.1

2-*P*-tolylpropanenitrile (5b)[22]**:** Colourless liquid (72 mg, 83% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.26-7.18 (m, 4H), 3.86 (q, $J_{H,H}$ = 7.0 Hz, 1H), 2.35 (s, 3H), 1.62 (d, $J_{H,H}$ = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 137.96, 134.19, 129.89, 126.69, 121.90, 30.98, 21.62, 21.16; GC-MS: [M^+] = 145.1

2-(4-Methoxyphenyl)propanenitrile (5c)[22]**:** Colourless liquid (70 mg, 72% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.26 (d, $J_{H,H}$ = 9.0 Hz, 2H), 6.90 (d, $J_{H,H}$ = 9.0 Hz, 2H), 3.85 (q, $J_{H,H}$ = 7.5 Hz, 1H), 3.80 (s, 3H), 1.60 (d, $J_{H,H}$ = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 159.37, 129.17, 127.94, 121.99, 114.56, 55.45, 30.55, 21.63; GC-MS: [M^+] = 161.1

2-(4-Bromophenyl)propanenitrile (5d)[22]**:** Colourless liquid (81 mg, 64% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.51(d, $J_{H,H}$ = 8.5 Hz, 2H), 7.26-7.22 (m, 2H), 3.86 (q, $J_{H,H}$ = 7.5 Hz, 1H), 1.62 (d, $J_{H,H}$ = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 136.17, 132.43, 128.55, 122.23, 121.15, 30.93, 21.45; GC-MS: [M^+] = 209.0

2-(Pyridin-3-yl)propanenitrile (5e)[25]**:** Colourless liquid (60 mg, 76% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.60-8.59 (m, 1H), 7.74 (dt, $J_{H,H}$ = 8.0, 1.5 Hz, 1H), 7.35 (q, $J_{H,H}$ = 8.0 Hz, 1H), 3.95 (q, $J_{H,H}$ = 7.0 Hz, 1H), 1.67 (d, $J_{H,H}$ = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 149.69, 148.34, 134.43, 133.00, 124.06, 120.65, 29.15, 21.37; GC-MS: [M^+] = 132.0

Monoalkylation of acetonitrile: 3-Phenylpropanenitrile (6a)[26]: Yellow oil (59 mg, 90% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.36-7.22 (m, 5H), 2.95 (t, $J_{H,H}$ = 7.44 Hz, 2H), 2.60 (t, $J_{H,H}$ = 7.44 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 138.18, 128.97, 128.39, 127.33, 119.30, 31.64, 19.45. GC-MS: [M^+] =131.1

3-*P*-tolylpropanenitrile (6b)[26]**:** Colourless oil (55 mg, 76% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.15-7.09 (m, 4H), 2.91 (t, $J_{H,H}$ = 7.44 Hz, 2H), 2.58 (t, $J_{H,H}$ = 7.44 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 141.44, 136.96, 135.08, 129.61, 128.21, 119.32, 31.26, 21.14, 19.60. GC-MS: [M^+] =145.0

3-(4-Methoxyphenyl)propanenitrile (6c)[26]**:** Yellow oil (64 mg, 80% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.14 (d, $J_{H,H}$ = 8.60 Hz, 2H), 6.86 (d, $J_{H,H}$ = 8.64 Hz, 2H), 3.78 (s, 3H), 2.89 (t, $J_{H,H}$ = 7.40 Hz, 2H), 2.57 (t, $J_{H,H}$ = 7.44 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.82, 130.20, 129.41, 119.34, 114.32, 55.37, 30.85, 19.80. GC-MS: [M^+] =161.1

3-(4-Fluorophenyl)propanenitrile (6d)[26]: Colourless oil (52 mg, 70% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.21-7.17 (m, 2H), 7.04-7.00 (m, 2H), 2.92 (t, $J_{H,H}$ = 7.36 Hz, 2H), 2.59 (t, $J_{H,H}$ = 7.48 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 163.33, 160.88, 133.78, 129.99, 129.91, 119.00, 115.96, 115.75, 30.87, 19.68. GC-MS: [M^+] =149.0

3-(2-Methoxyphenyl)propanenitrile (6e)[26]: Yellow oil (51 mg, 64% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.27-7.22 (m, 1H), 7.16 (dd, $J_{H,H}$ = 7.34, 1.36 Hz 1H), 6.93-6.85 (m, 2H),

3.83 (s, 3H), 2.95 (t, $J_{H,H}$ = 7.44 Hz, 2H), 2.61 (t, $J_{H,H}$ = 7.44 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 157.35, 130.29, 128.72, 126.38, 120.74, 119.77, 110.41, 56.26, 27.14, 17.54. GC-MS: [M^+] =161.0

3-(Benzo[*d*][1,3]dioxol-5-yl)propanenitrile (6f)[27]**:** Colourless oil (72 mg, 82% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.77-6.66 (m, 3H), 5.94 (s, 2H), 2.86 (t, $J_{H,H}$ = 7.32 Hz, 2H), 2.56 (t, $J_{H,H}$ = 7.40 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 148.01, 146.81, 131.80, 121.46, 119.16, 108.71, 108.63, 101.16, 31.41, 19.81. GC-MS: [M^+] =175.2

3-(Naphthalen1-yl)propanenitrile (6g)[28]**:** Yellow oil (71 mg, 78% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.93-7.87 (m, 2H), 7.79 (d, $J_{H,H}$ = 7.96 Hz, 1H), 7.58-7.49 (m, 2H), 7.45-7.38 (m, 2H), 3.44 (t, $J_{H,H}$ = 7.64 Hz, 2H), 2.76 (t, $J_{H,H}$ = 7.68 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 134.03, 133.93, 129.28, 128.24, 126.66, 125.99, 125.70, 122.68, 119.97, 28.93, 18.60. GC-MS: [M^+] =136.1

3-Cyclohexylpropanenitrile (6h)[29]**:** Yellow oil (45 mg, 66% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.33 (t, $J_{H,H}$ = 7.40 Hz, 2H), 1.72-1.64 (m, 5H), 1.56-1.52 (m, 2H), 1.39-1.34 (m, 1H), 1.28-1.13 (m, 3H), 0.93-0.87 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ =120.14, 36.69, 32.66, 32.61, 26.40, 26.04, 14.74. GC-MS: [M^+] =136.1

Octanenitrile (6i)[30]**:** Yellow oil (37 mg, 60% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.32 (t, $J_{H,H}$ = 7.20 Hz, 2H), 1.64 (q, $J_{H,H}$ = 7.44 Hz, 1H), 1.46-1.39 (m, 2H), 1.34-1.24 (m, 8H), 0.87 (t, $J_{H,H}$ = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 119.97, 31.56, 29.73, 28.70, 28.51, 25.44, 22.60, 17.21, 14.11. GC-MS: [M^+] =124.1

<u>N-methylation of amines</u>: N-methylaniline (7a): Yellow oil (81 mg, 95% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.20 (t, $J_{H,H}$ = 7.4 Hz, 2H), 6.72 (t, $J_{H,H}$ = 7.3 Hz, 1H), 6.62 (t, $J_{H,H}$ = 7.6 Hz, 2H), 3.46 (bs, 1H), 2.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 149.37, 129.32, 117.40, 112.56, 30.87. GC-MS: [M^+] = 107.0

N,4-dimethylaniline (7b)[31]**:** Yellow oil (91 mg, 94% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.96 (d, $J_{H,H}$ = 8.25 Hz, 2H), 6.52 (d, $J_{H,H}$ = 8.4 Hz, 2H), 2.92 (bs, 1H), 2.76 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 147.16, 129.68, 126.73, 112.88, 31.14, 20.30. GC-MS: [M^+] = 121.0

4-Methoxy-N-methylaniline (7c)[31]**:** Yellow oil (103 mg, 94% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.79 (d, $J_{H,H}$ = 8.9 Hz, 2H), 6.59 (d, $J_{H,H}$ = 8.9 Hz, 2H), 3.75 (s, 3H), 2.81 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 152.36, 143.70, 115.09, 113.91, 56.02, 31.85. GC-MS: [M^+] = 137.0

4-Bromo-N-methylaniline (7d)[32]**:** Yellow oil (137 mg, 92% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.26-7.24 (m, 2H), 6.48-6.46 (m, 2H), 3.72 (bs, 1H), 2.80 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 148.41, 131.99, 114.06, 108.92, 30.83. GC-MS: [M^+] = 184.9

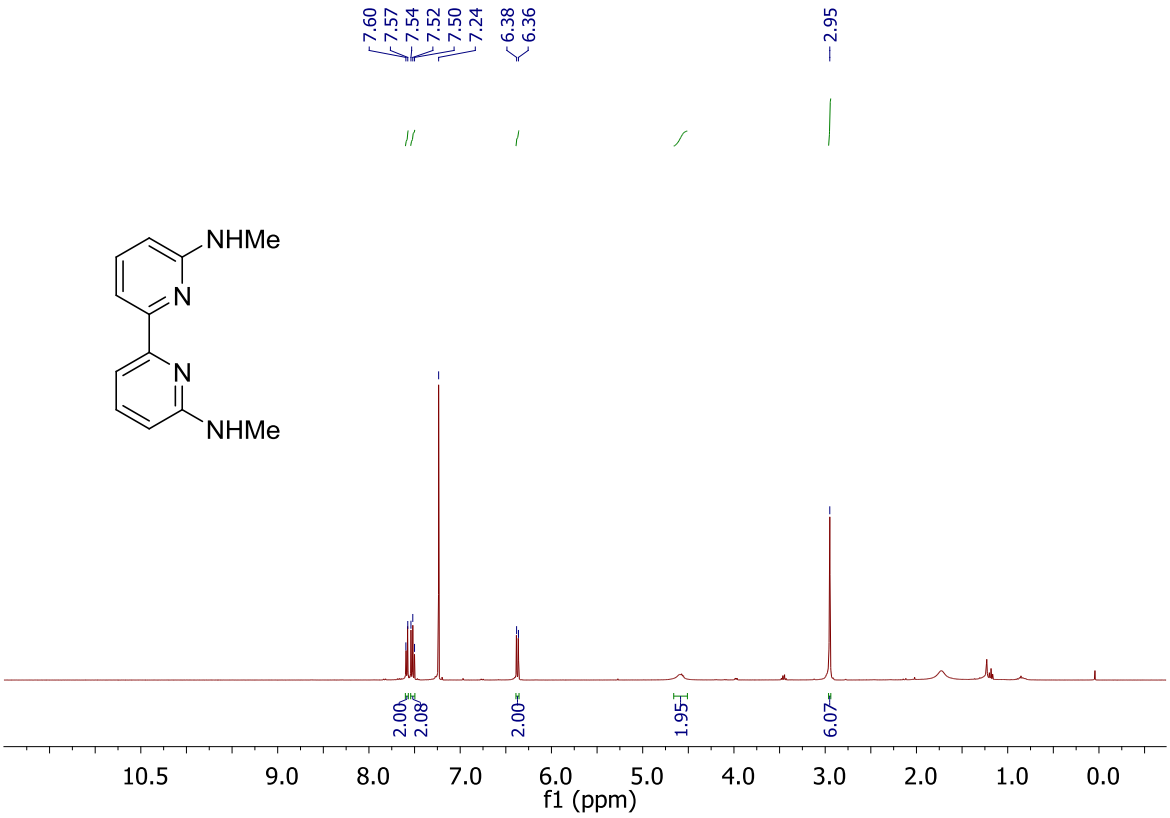
3-Chloro-N-methylaniline (7e)[33]**:** Yellow oil (105 mg, 93% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.01 (t, $J_{H,H}$ = 7.9 Hz, 1H), 6.59 (d, $J_{H,H}$ = 8.0 Hz, 1H), 6.51 (t, $J_{H,H}$ = 1.9 Hz, 1H),

6.42 (dd, $J_{H,H}$ = 8.0, 1.8 Hz, 1H), 2.73 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 150.55, 134.94, 130.08, 116.92, 111.94, 110.87, 30.34. GC-MS: [M^+] = 141.0

N-methylnaphthalen-1-amine (7f)[34]**:** Colourless oil (91 mg, 72% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.83 (d, $J_{H,H}$ = 8.1 Hz, 1H), 7.79 (d, $J_{H,H}$ = 8.2 Hz, 1H), 7.50-7.40 (m, 3H), 7.29 (d, $J_{H,H}$ = 8.0 Hz, 1H), 6.63 (d, $J_{H,H}$ = 7.5 Hz, 1H), 4.38 (bs, 1H), 3.03 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 144.61, 134.34, 128.75, 126.78, 125.81, 124.78, 123.57, 119.91, 117.43, 103.92, 31.12. GC-MS: [M^+] = 157.0

N-methylpyridin-3-amine (7g)[35]: Pale yellow oil (78 mg, 90% isolated yield); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.96 (d, $J_{H,H}$ = 2.8 Hz, 1H), 7.89 (dd, $J_{H,H}$ = 4.6 , 1.0 Hz, 1H), 7.07 (q, $J_{H,H}$ = 4.5 Hz, 1H), 6.85 (dq, $J_{H,H}$ = 8.0, 1.0 Hz, 1H), 2.81 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 145.35, 138.33, 135.49, 123.90, 118.35, 30.30. GC-MS: [M^+] = 108.0

N,N-dimethylhexan-1-amine (7h)[36]: Pale yellow oil (57 mg, 55% isolated yield); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.21-2.17 (m, 8H), 1.44-1.40 (m, 2H), 1.27-1.23 (m, 6H), 0.85 (t, $J_{H,H}$ = 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 60.10, 45.62, 31.97, 27.87, 27.32, 22.74, 14.17. GC-MS: [M^+] = 129.1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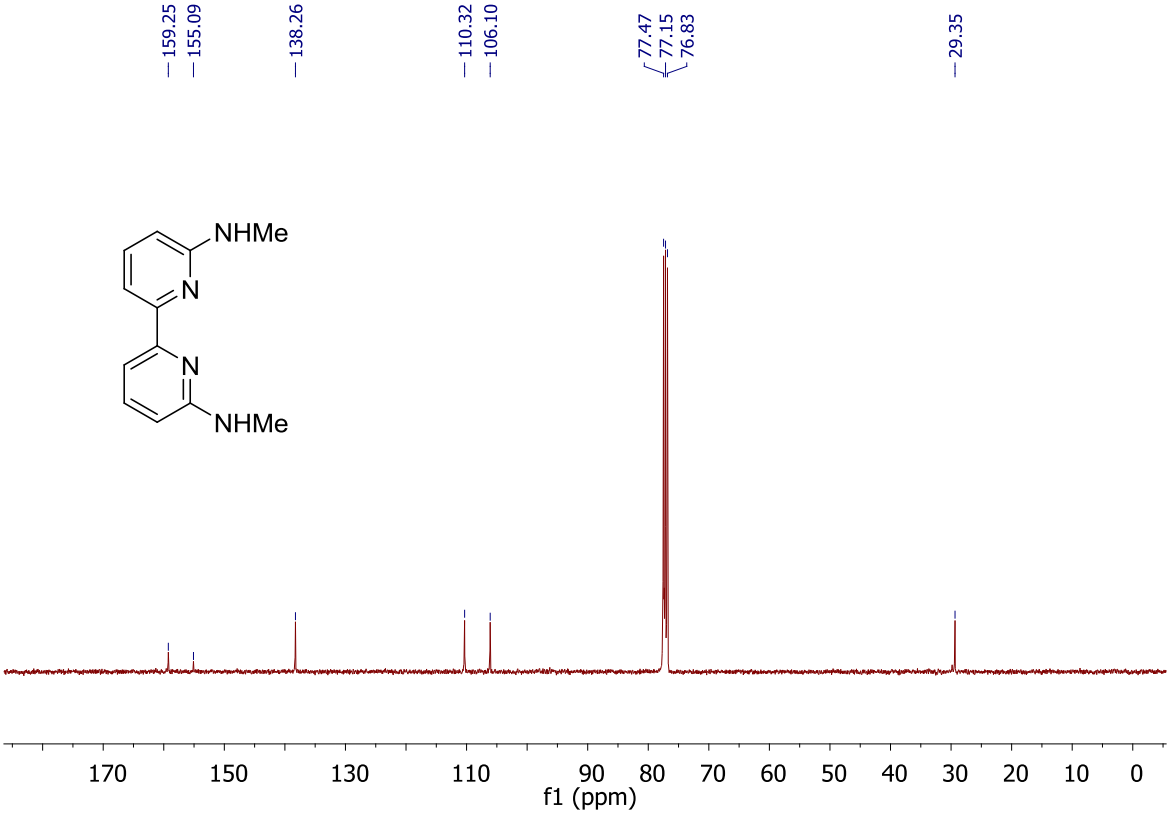
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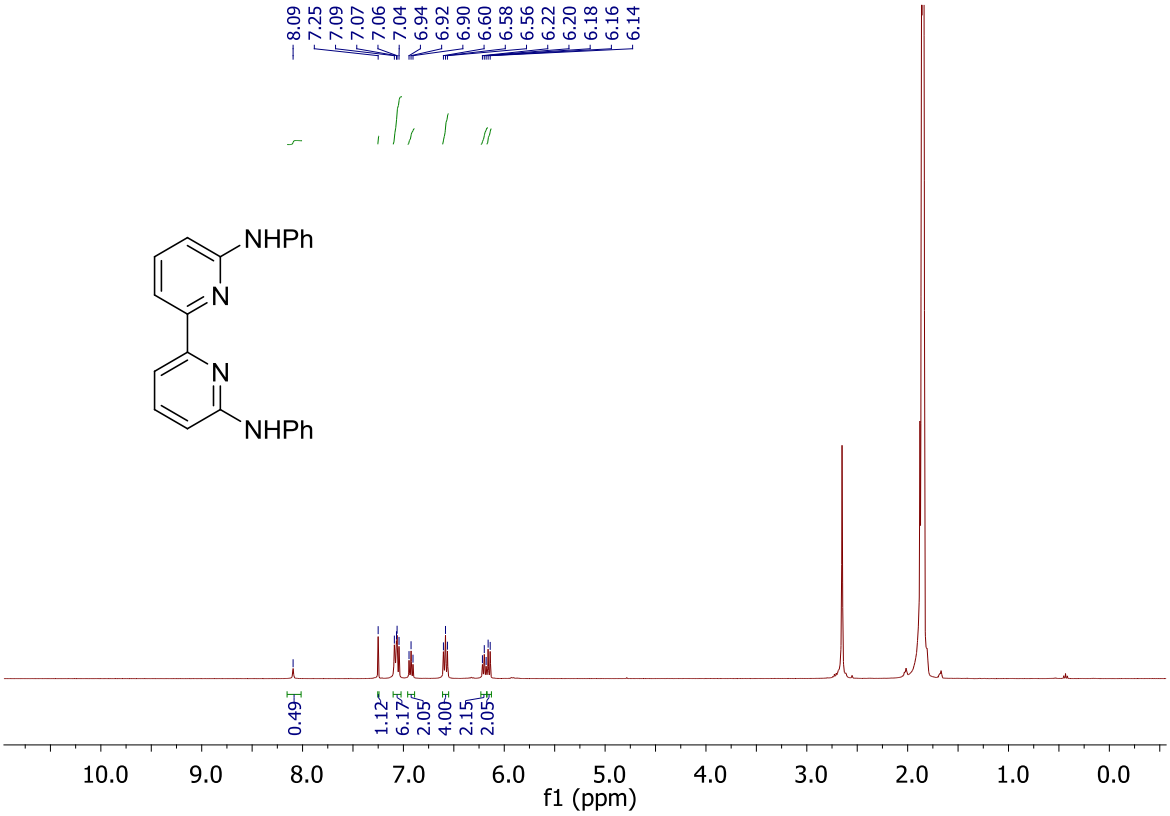
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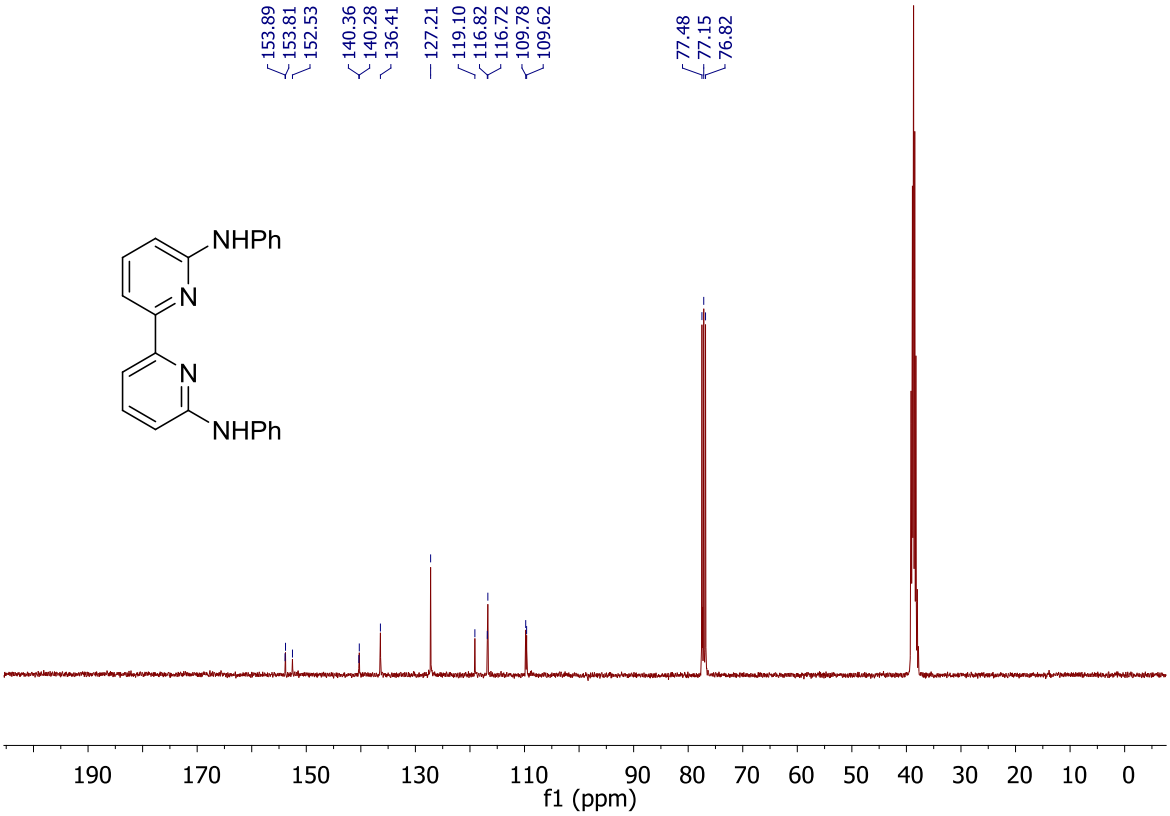
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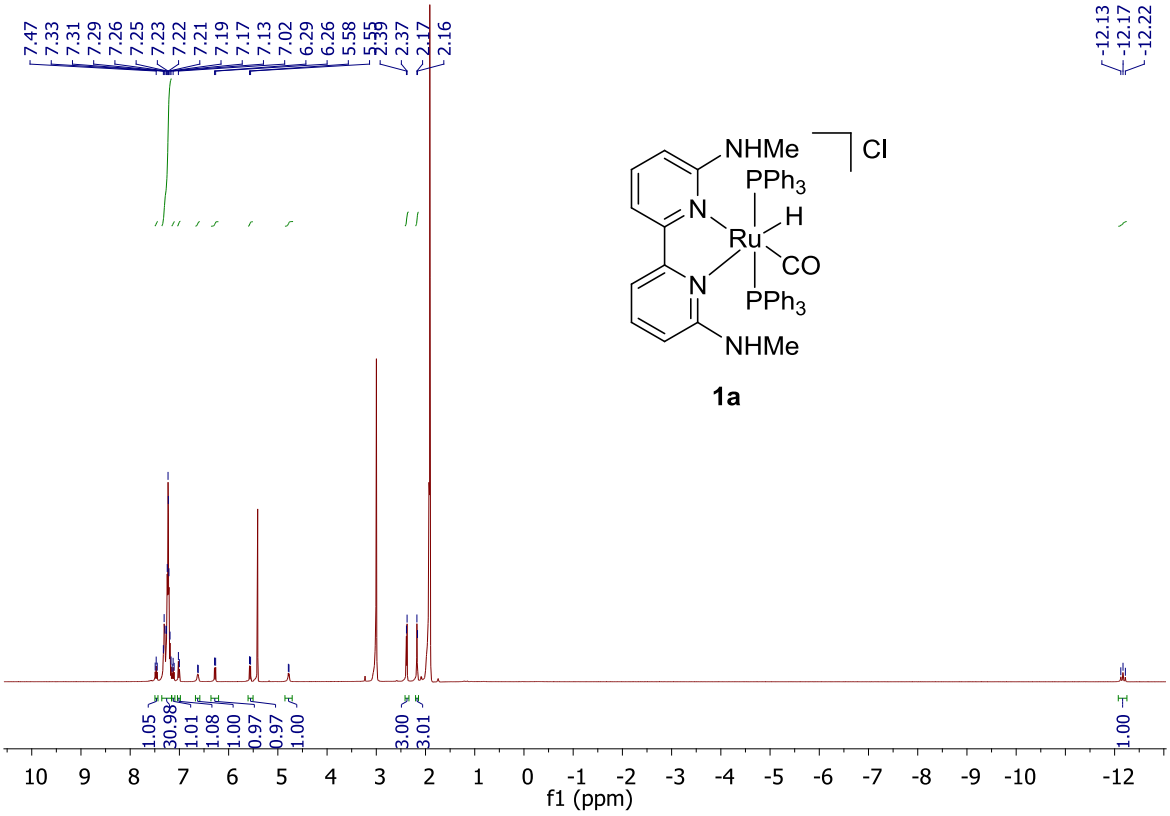
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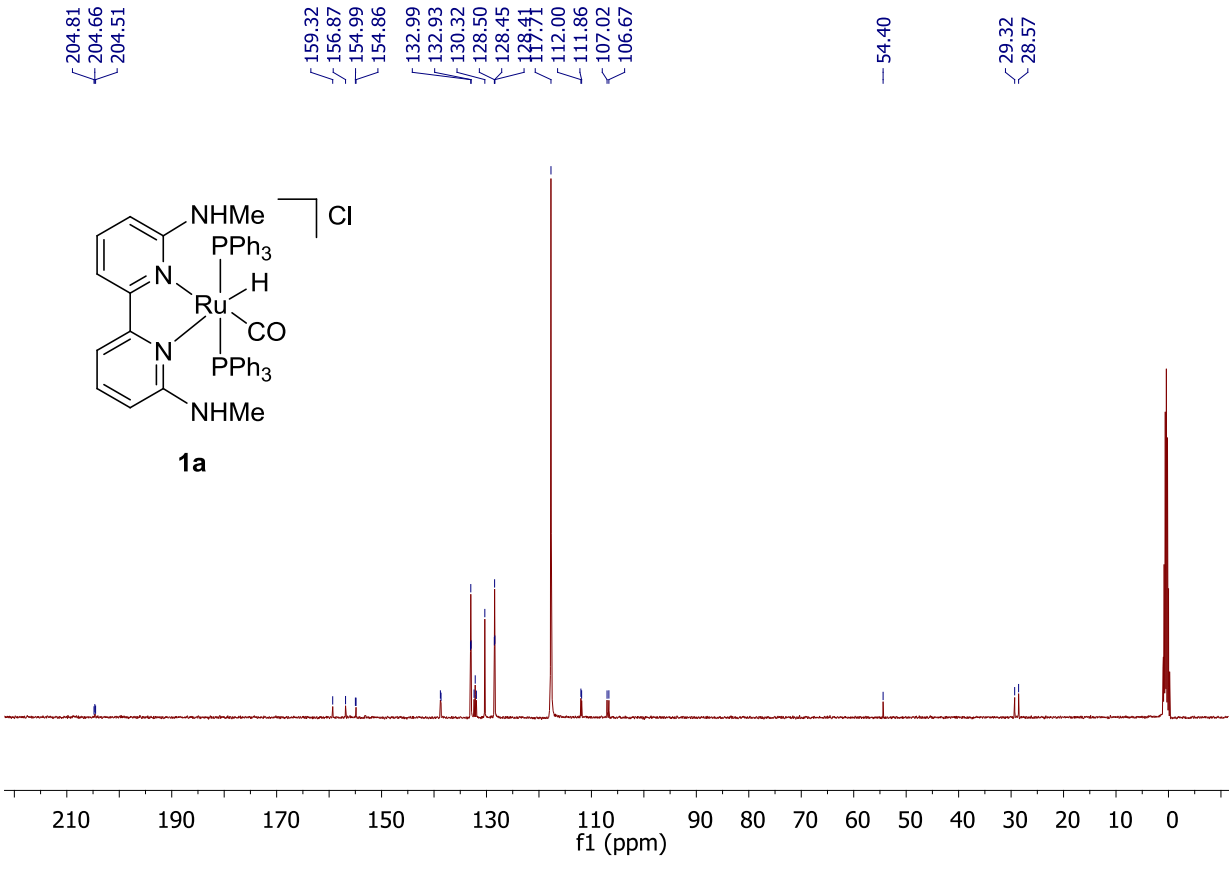
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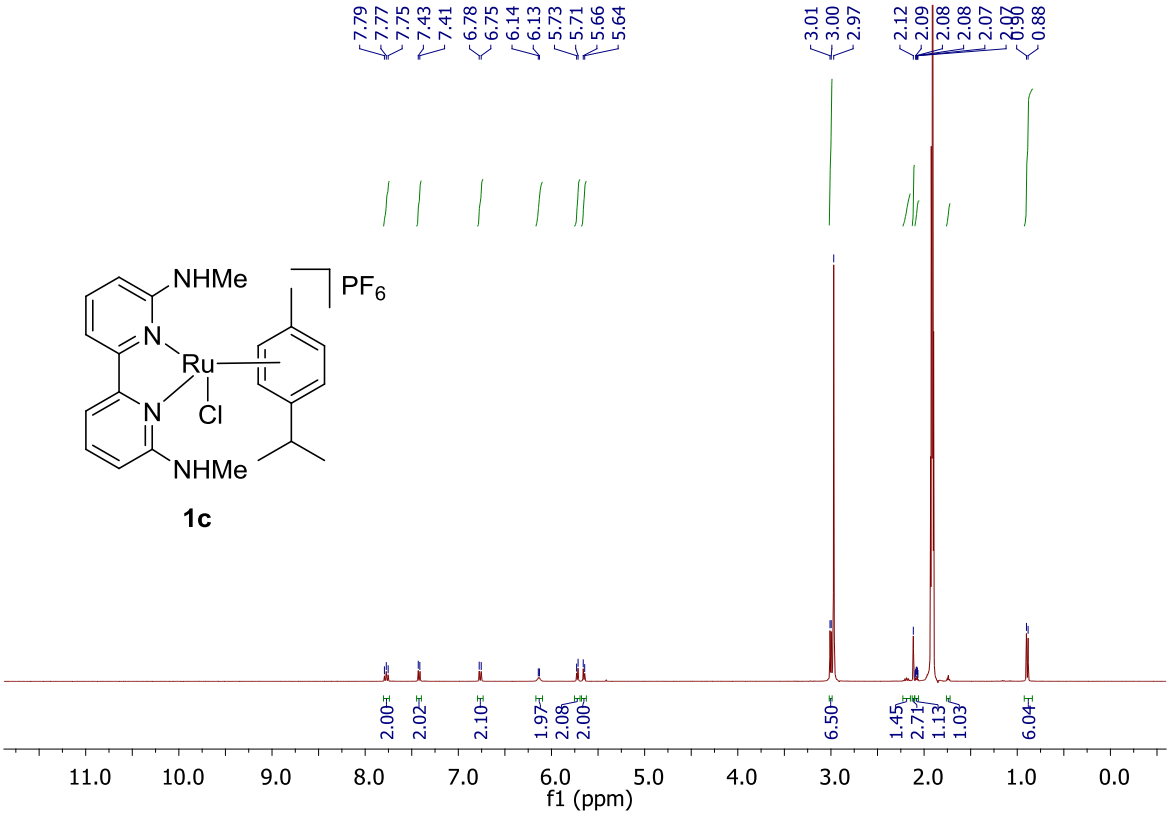
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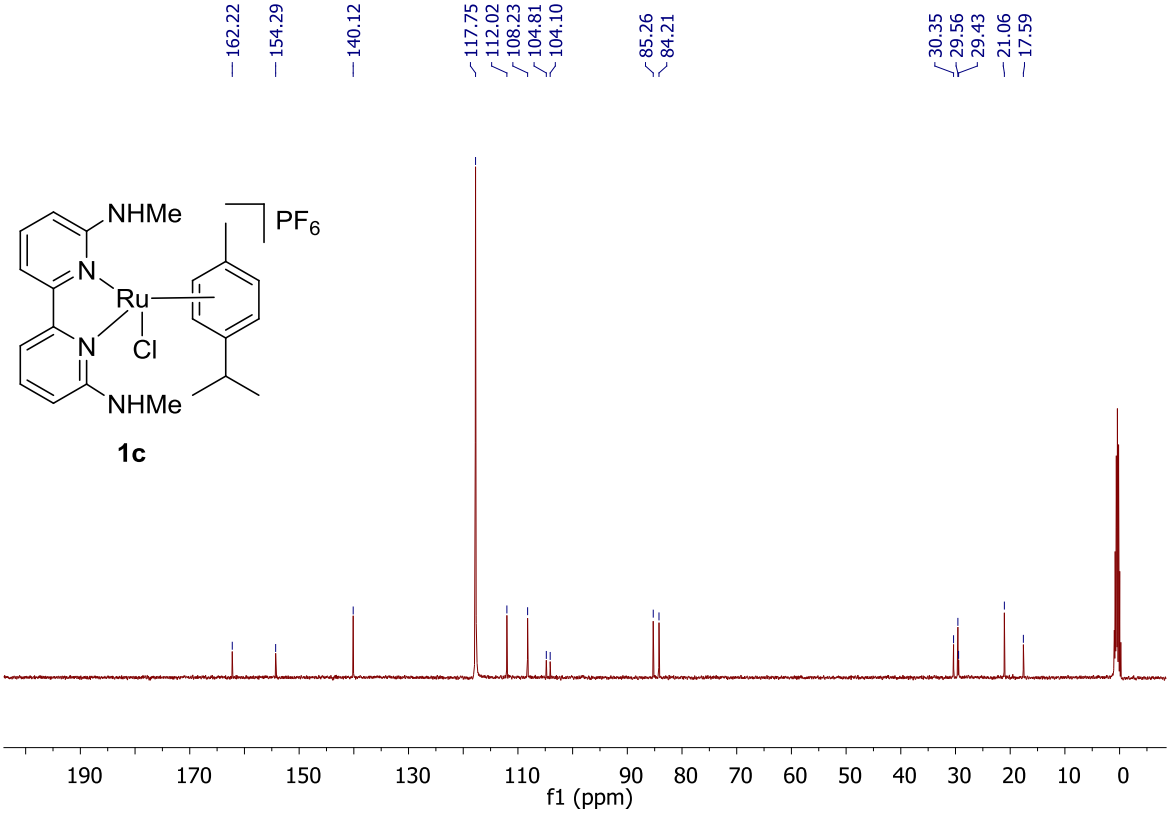
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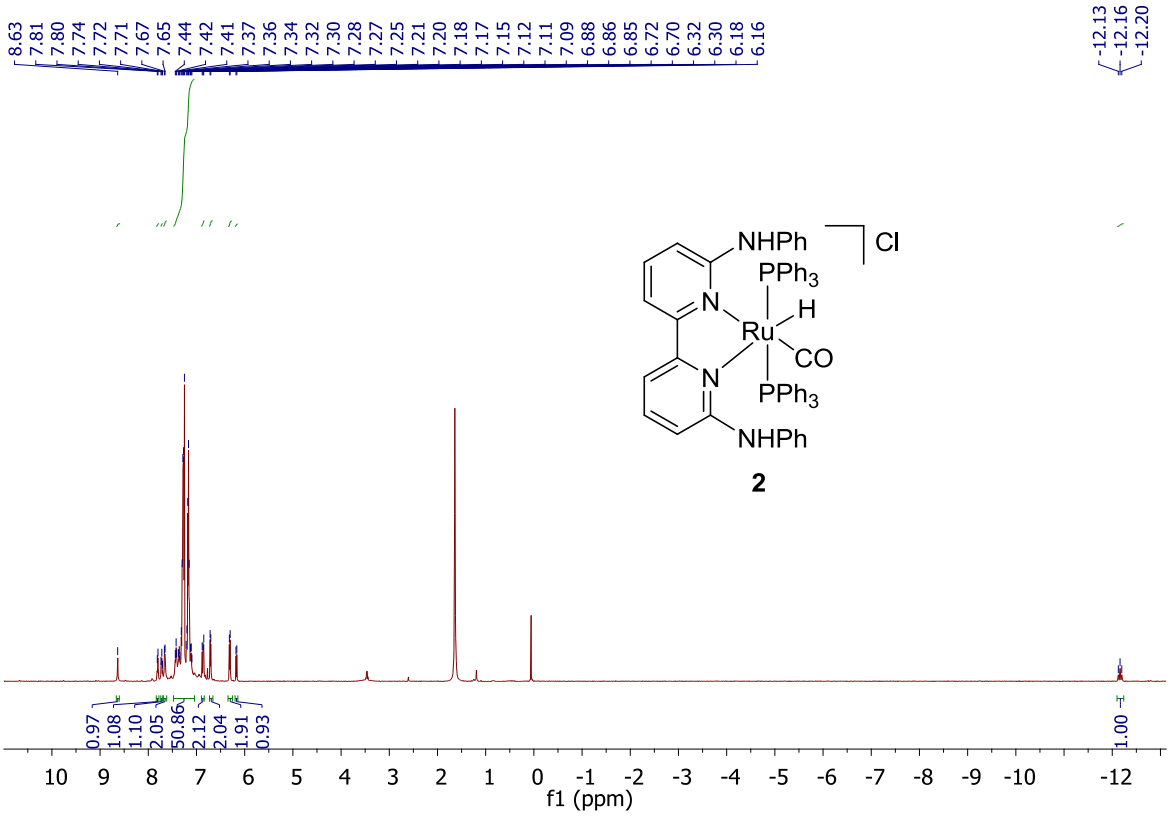
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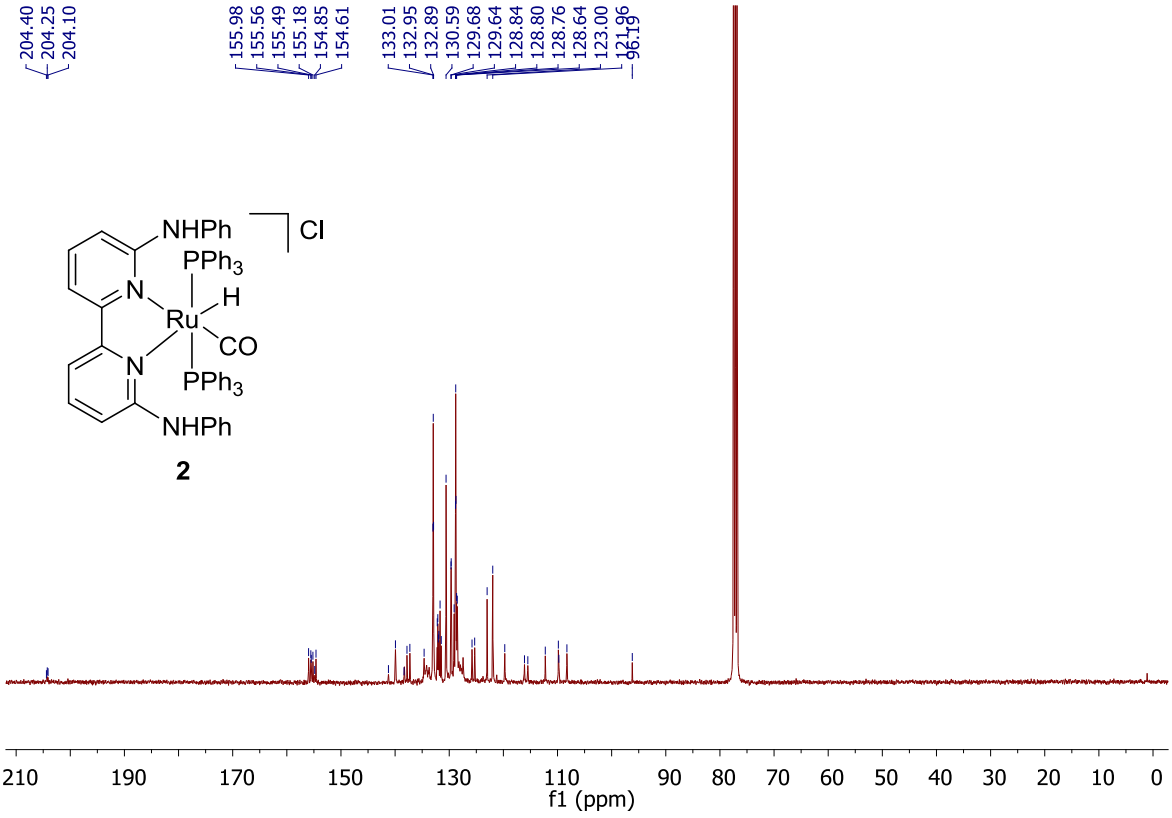
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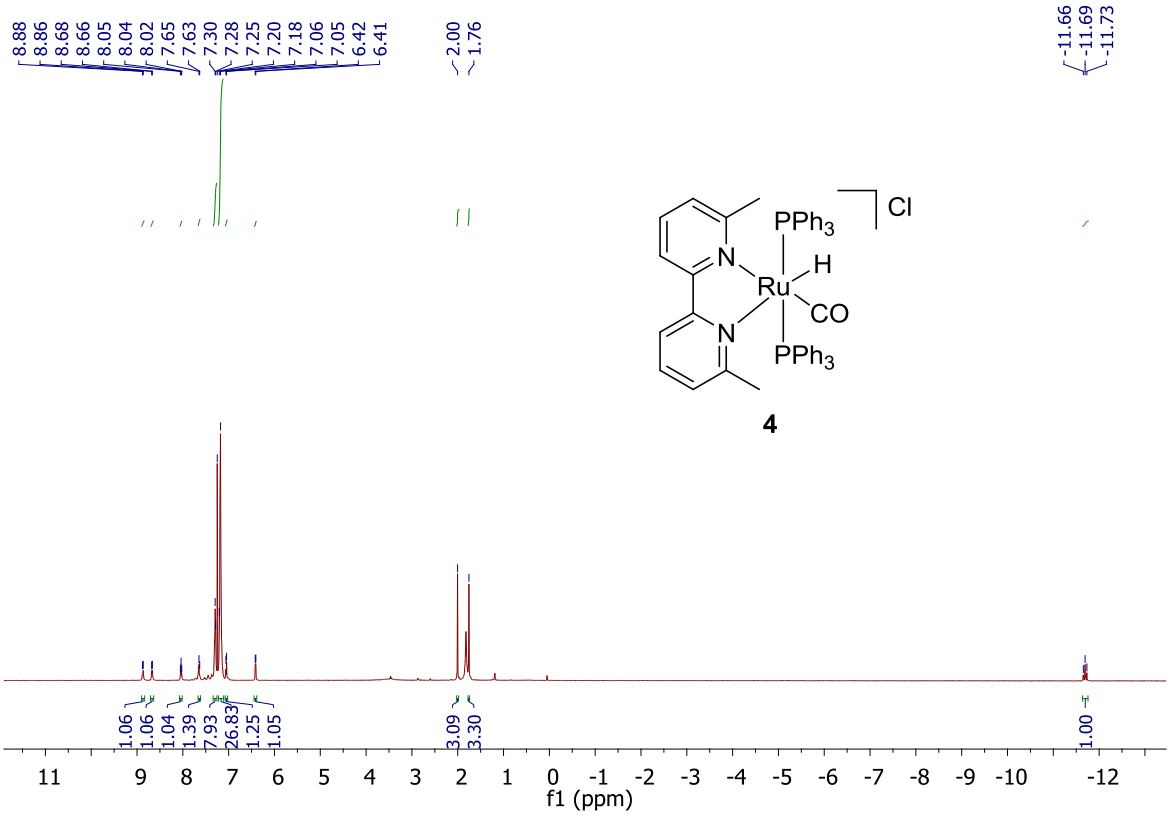
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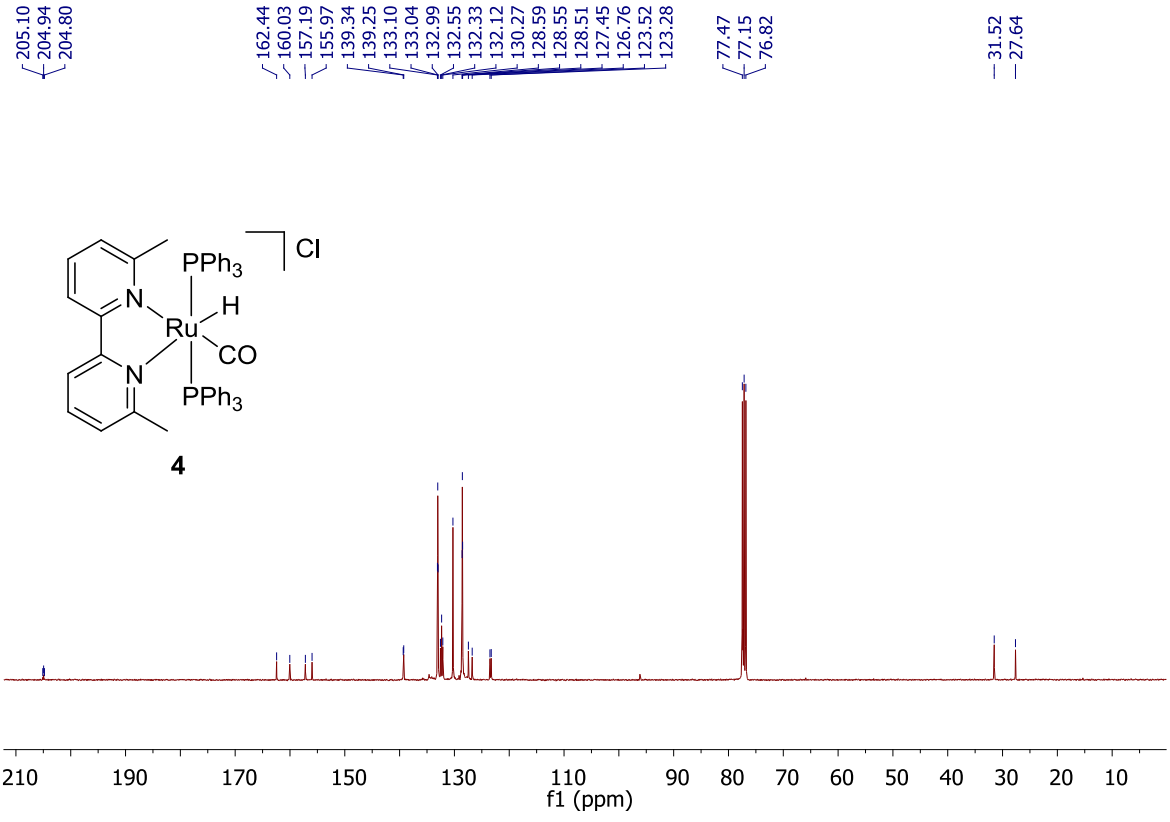
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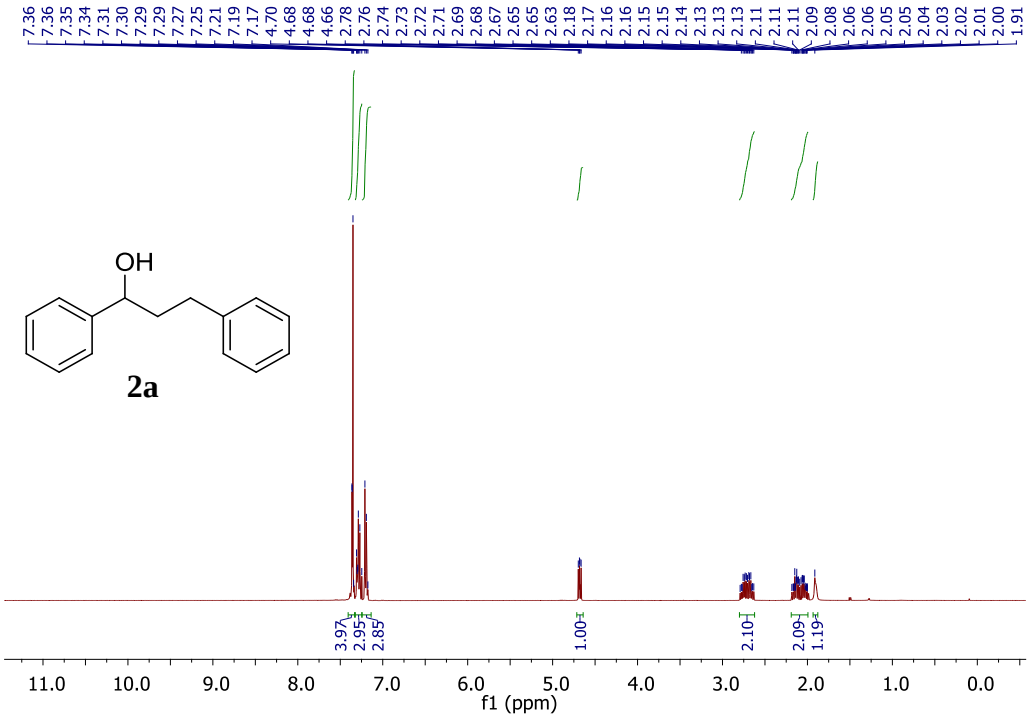
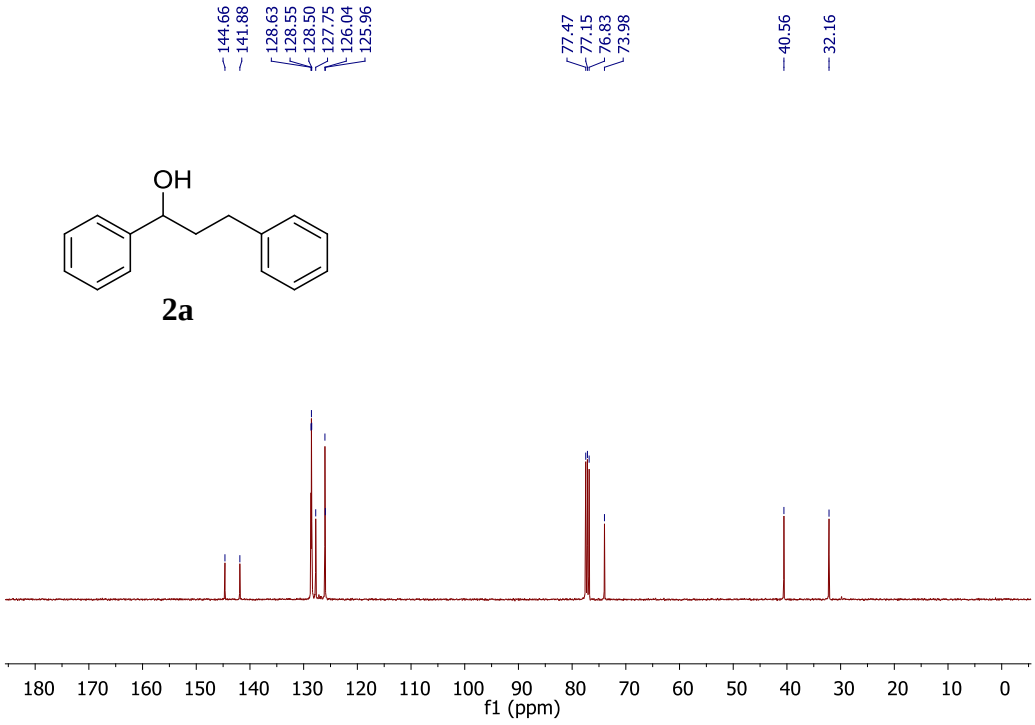
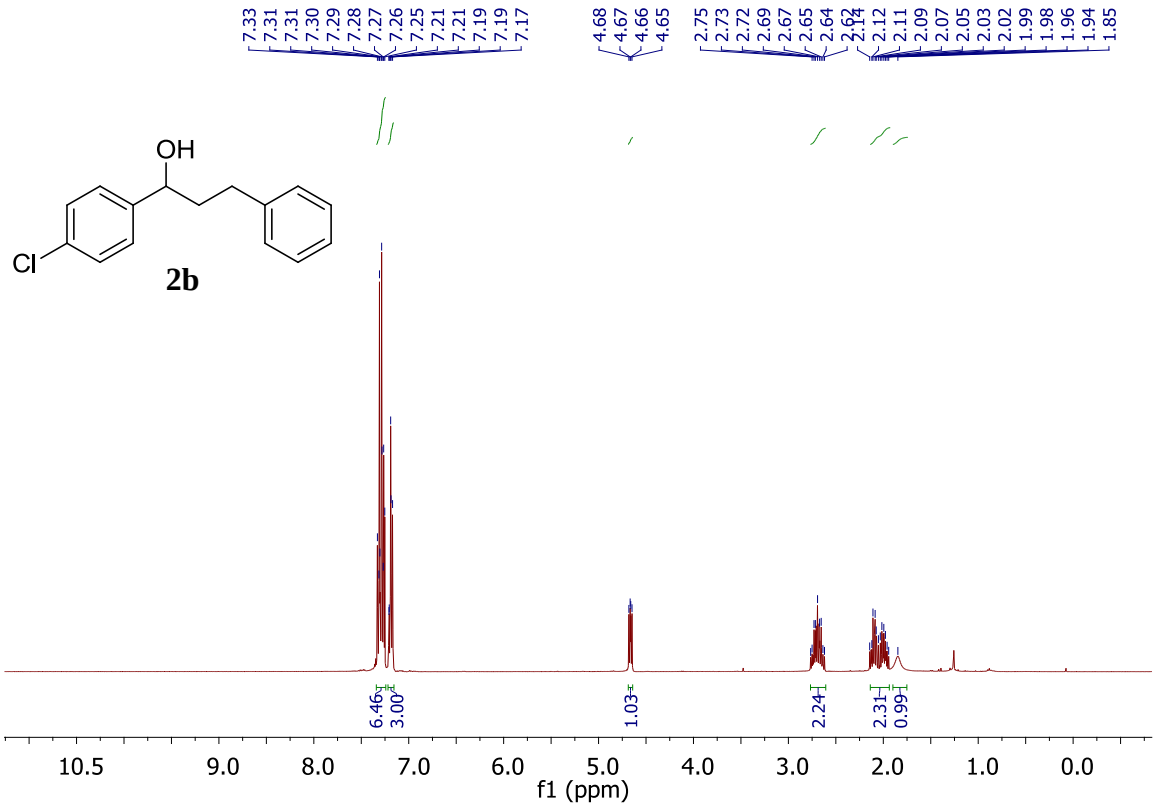
^{1}H and ^{13}C NMR Spectra of isolated products: ^{1}H and ^{13}C NMR of all the isolated compounds are given below.



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1.96
1.94
1.85
OH
Cl
2b
6.46
3.00
1.03
2.24
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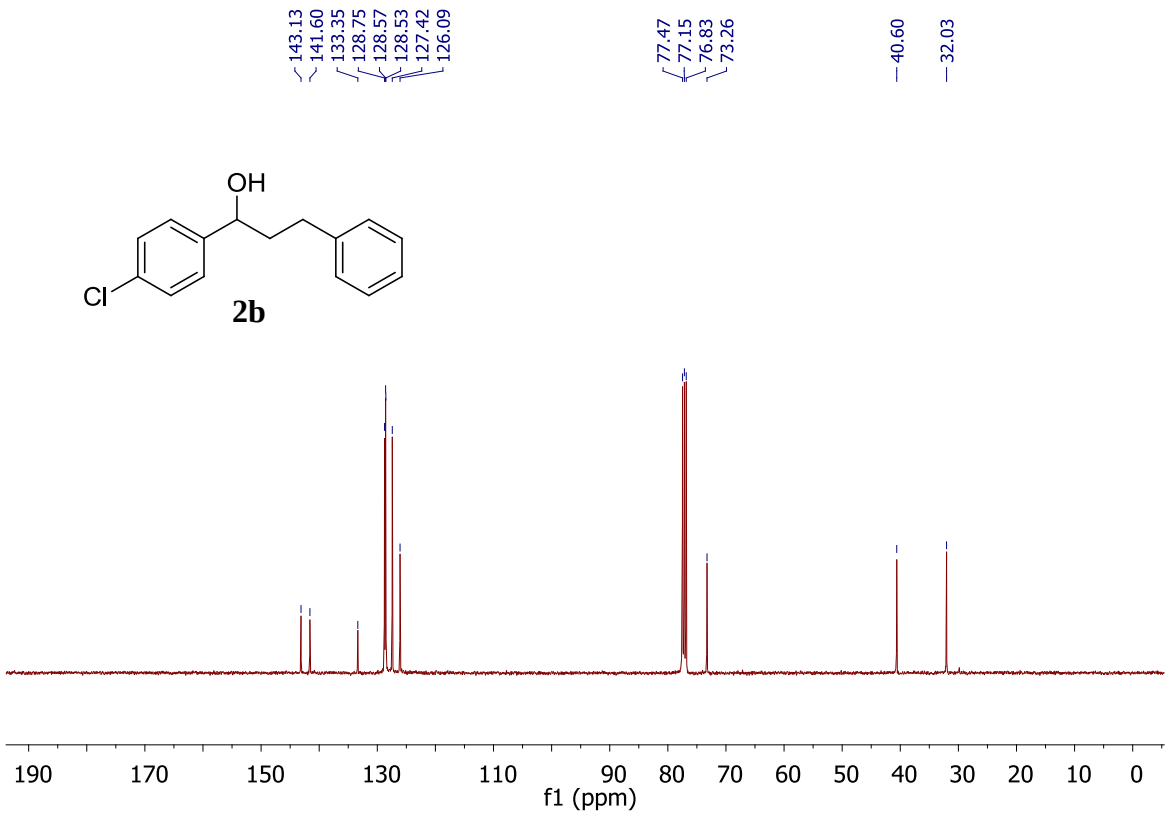
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32.03
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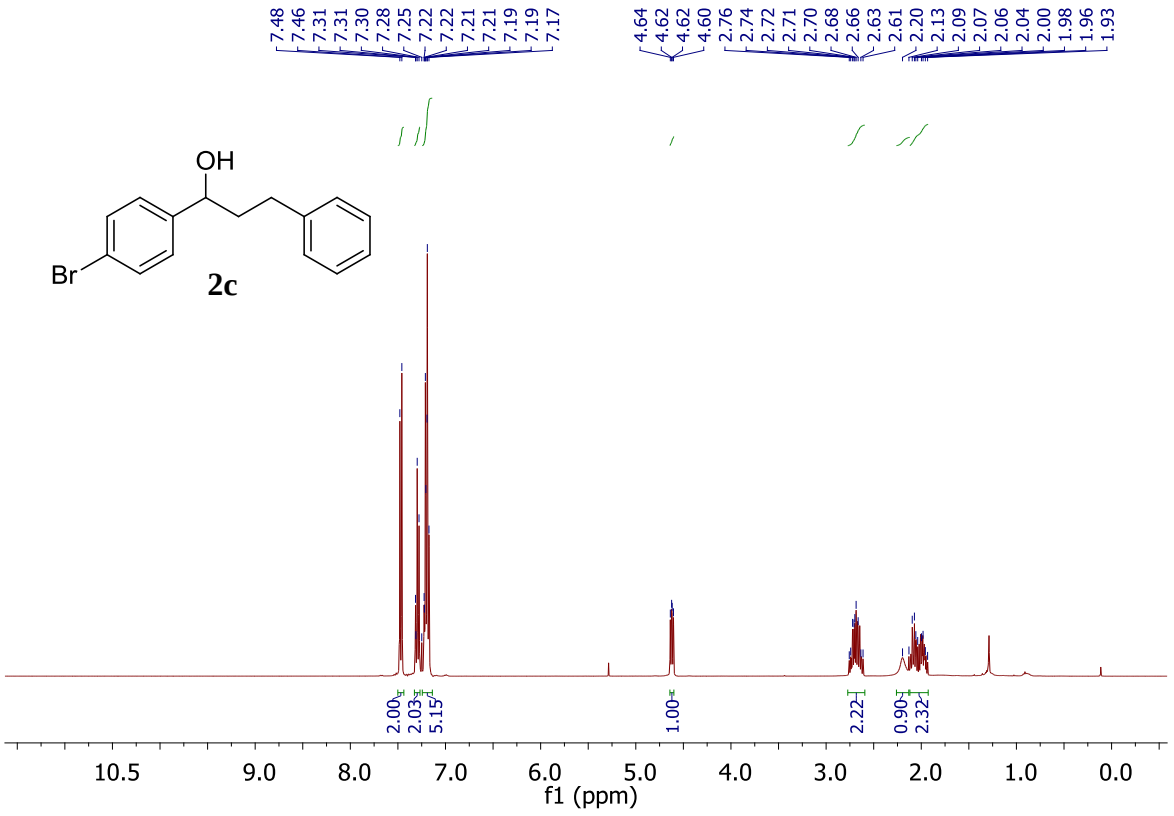
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7.19
7.17
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4.62
4.62
4.60
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2.74
2.72
2.71
2.70
2.68
2.66
2.63
2.61
2.20
2.13
2.09
2.07
2.06
2.04
2.00
1.98
1.96
1.93
OH
Br
2c
2.00
2.03
5.15
1.00
2.22
0.90
2.32
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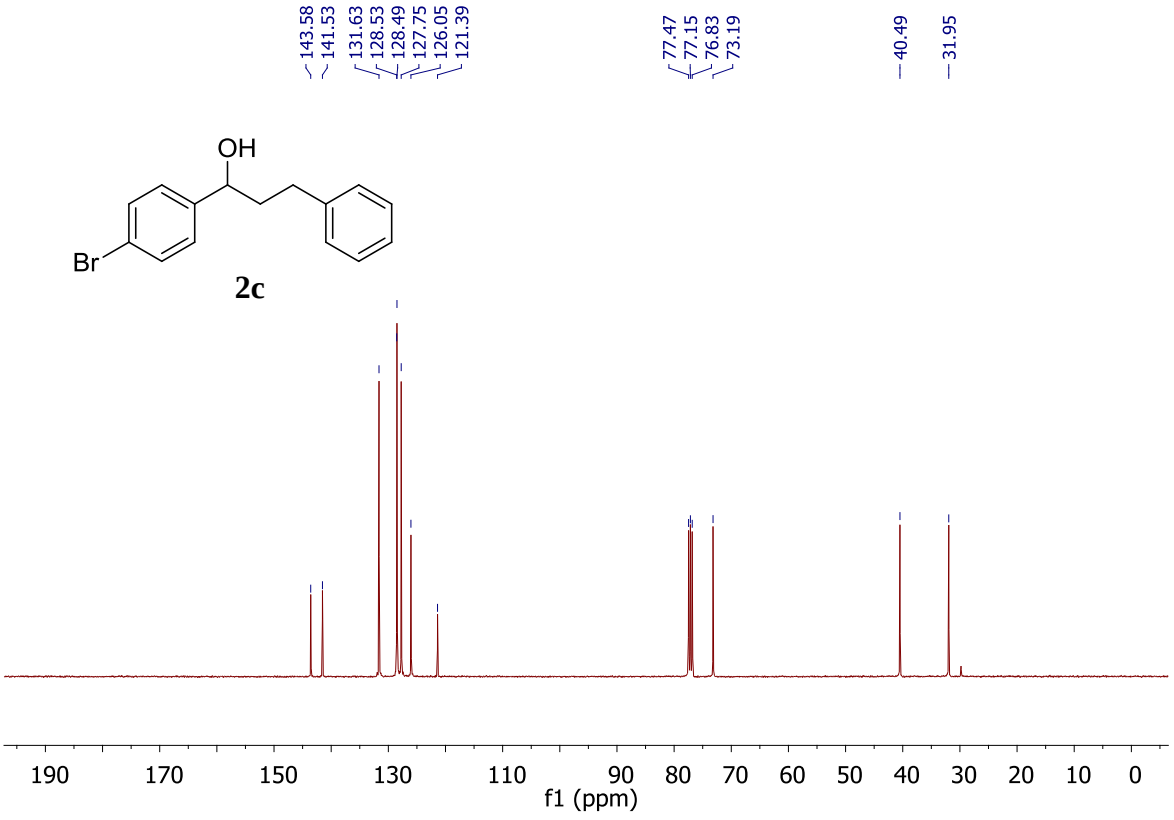
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31.95
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90
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50
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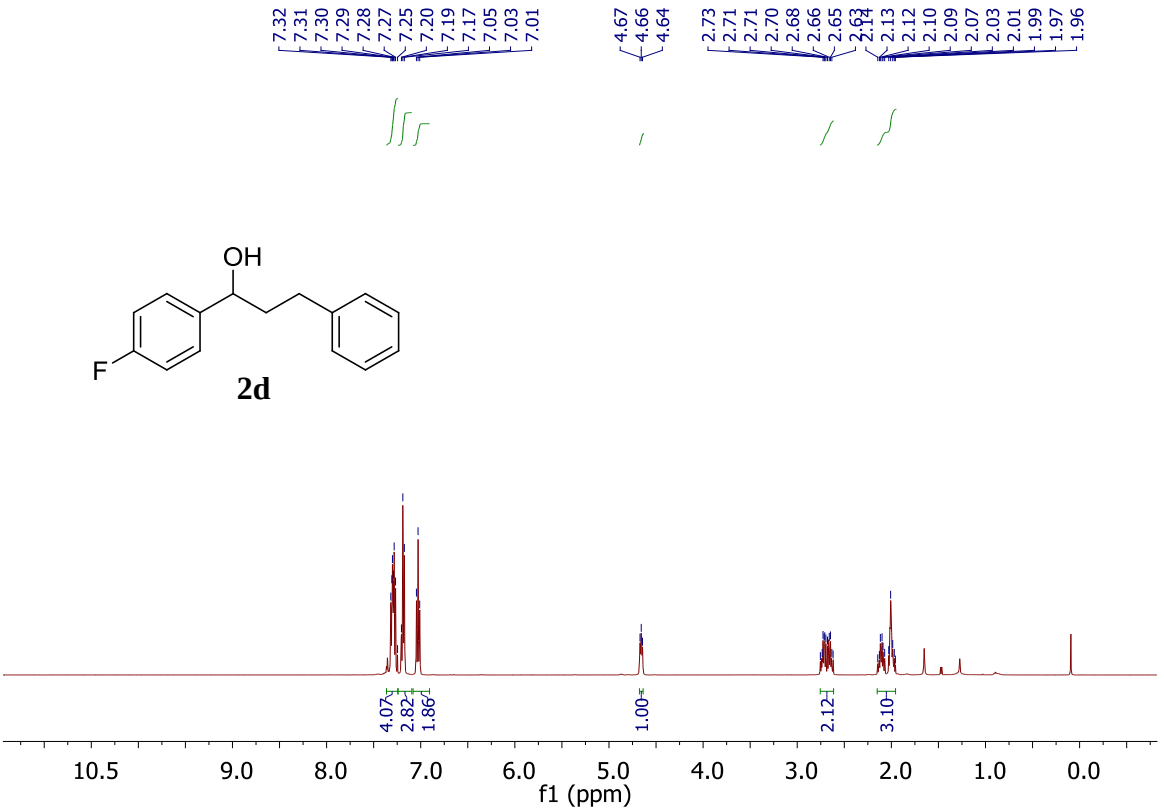
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7.03
7.01
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4.66
4.64
2.73
2.71
2.71
2.70
2.68
2.66
2.65
2.63
2.14
2.13
2.12
2.10
2.09
2.07
2.03
2.01
1.99
1.97
1.96
OH
F
2d
4.07
2.82
1.86
1.00
2.12
3.10
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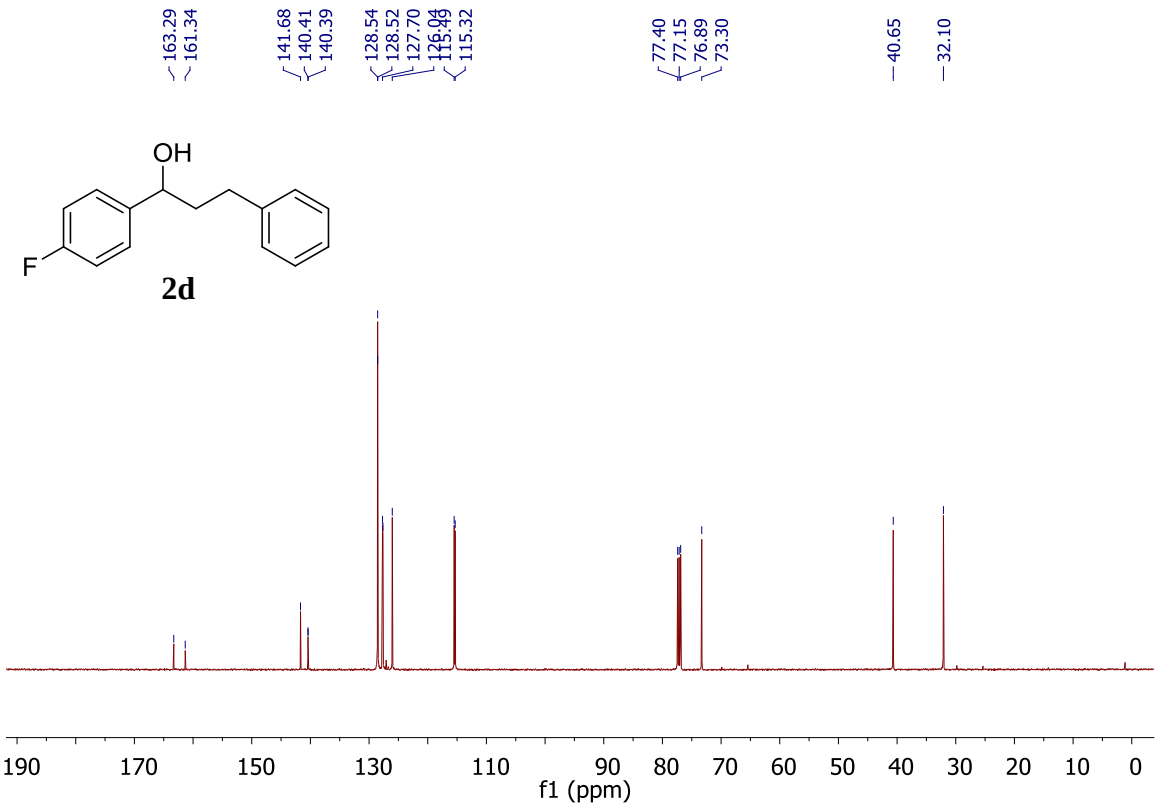
f1 (ppm)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115.32
77.40
77.15
76.89
73.30
40.65
32.10
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170
150
130
110
90
80
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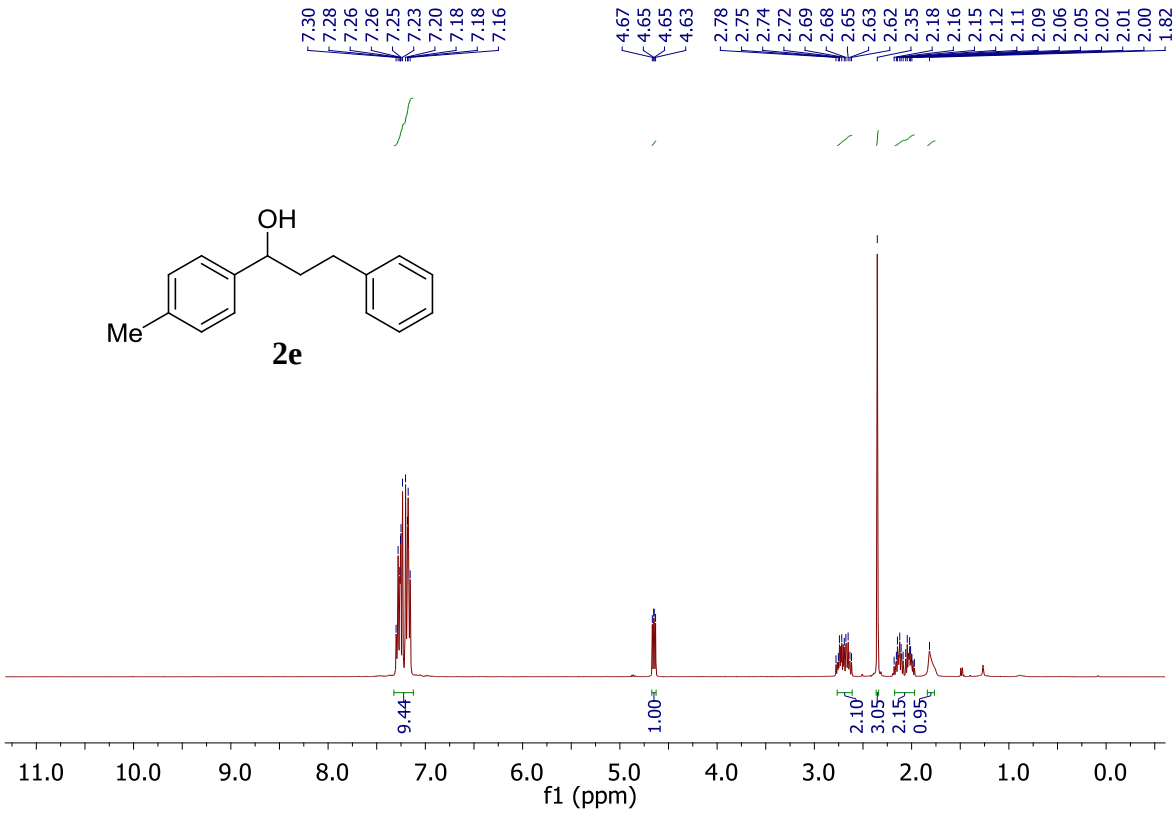
f1 (ppm)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4.63
2.78
2.75
2.74
2.72
2.69
2.68
2.65
2.63
2.62
2.35
2.18
2.16
2.15
2.12
2.11
2.09
2.06
2.05
2.02
2.01
2.00
1.82
OH
Me
2e
9.44
1.00
2.10
3.05
2.15
0.95
11.0
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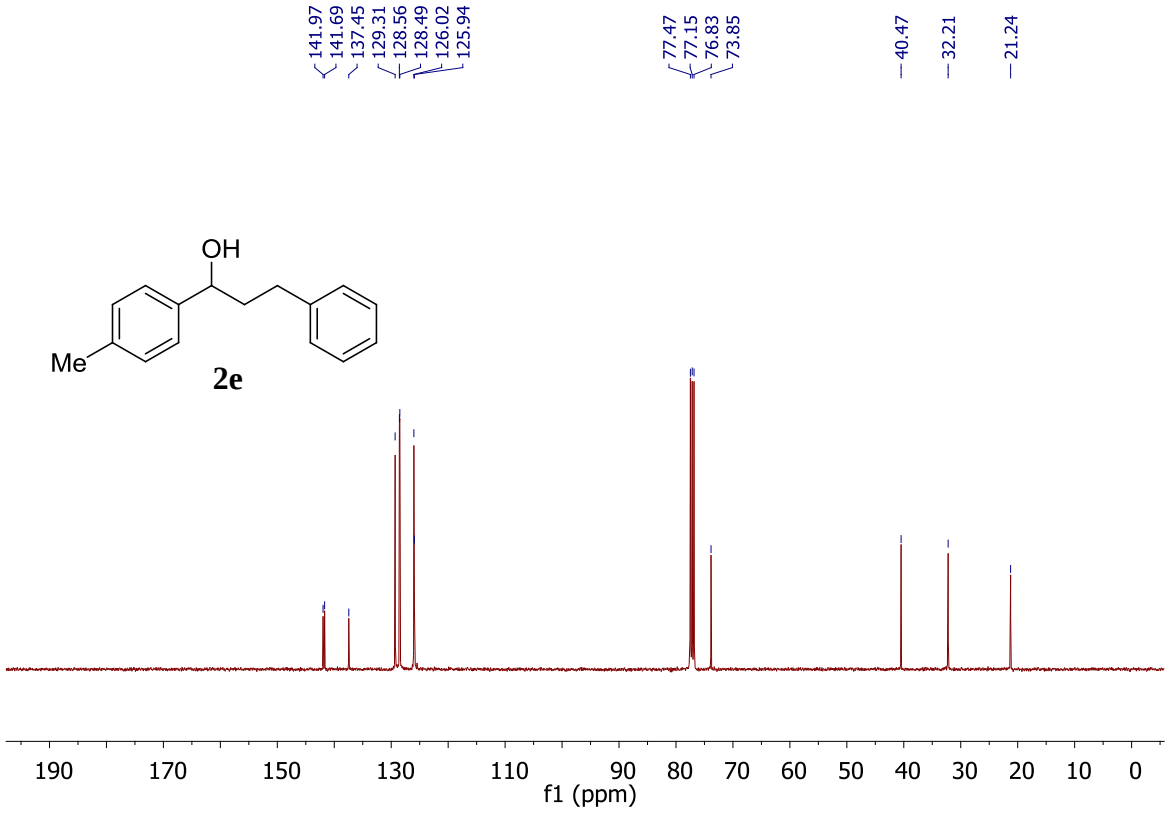
0.0
f1 (ppm)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128.49
126.02
125.94
77.47
77.15
76.83
73.85
40.47
32.21
21.24
OH
Me
2e
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170
150
130
110
90
80
70
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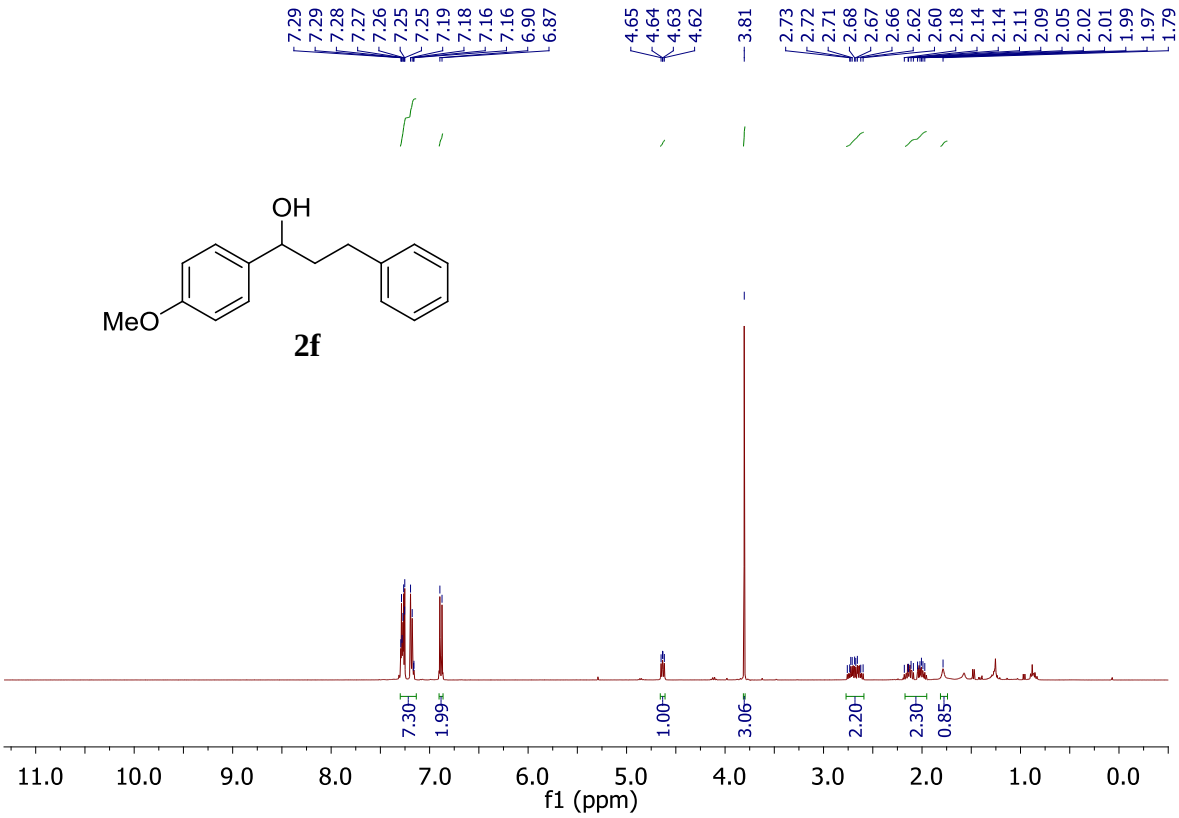
50
40
30
20
10
0
f1 (ppm)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7.25
7.25
7.19
7.18
7.16
7.16
6.90
6.87
4.65
4.64
4.63
4.62
3.81
2.73
2.72
2.71
2.68
2.67
2.66
2.62
2.60
2.18
2.14
2.14
2.11
2.09
2.05
2.02
2.01
1.99
1.97
1.79
OH
MeO
2f
7.30
1.99
1.00
3.06
2.20
2.30
0.85
11.0
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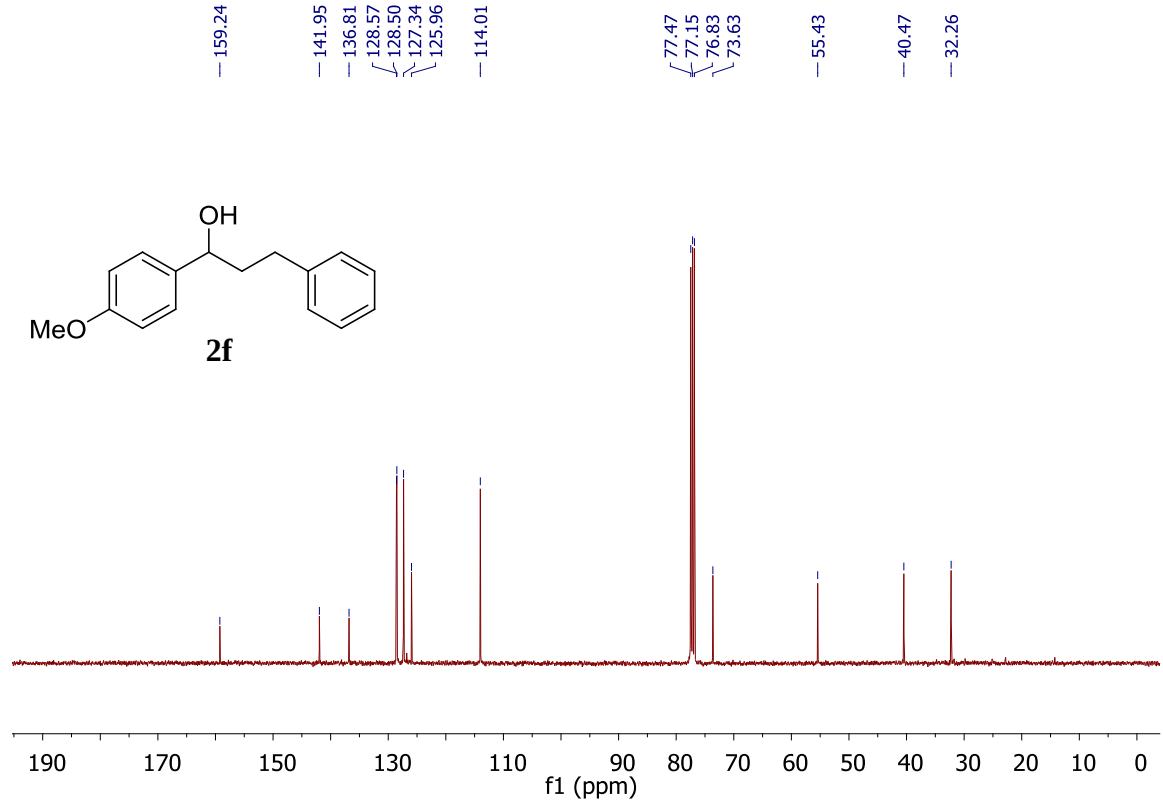
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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127.34
125.96
114.01
77.47
77.15
76.83
73.63
55.43
40.47
32.26
OH
MeO
2f
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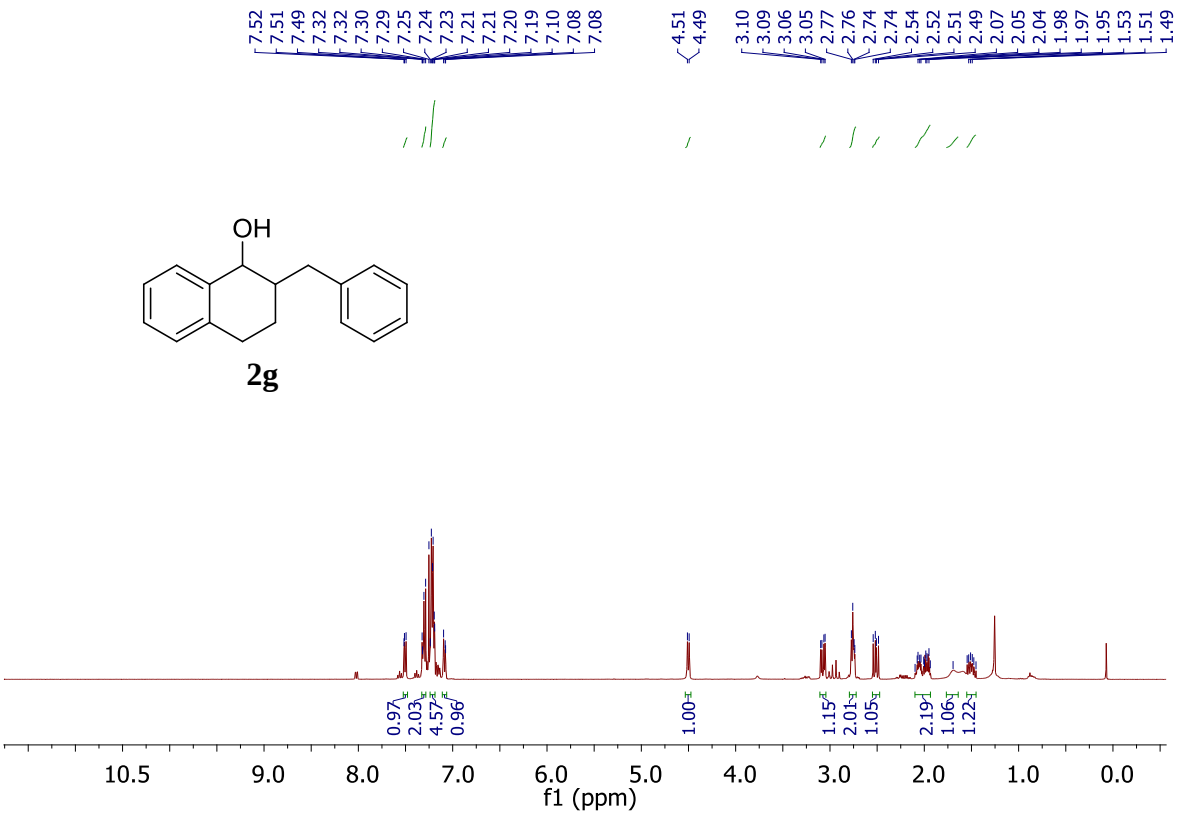
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.51
7.49
7.32
7.32
7.30
7.29
7.25
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7.23
7.21
7.21
7.20
7.19
7.10
7.08
7.08
4.51
4.49
3.10
3.09
3.06
3.05
2.77
2.76
2.74
2.74
2.54
2.52
2.51
2.49
2.07
2.05
2.04
1.98
1.97
1.95
1.53
1.51
1.49
OH
2g
0.97
2.03
4.57
0.96
1.00
1.15
2.01
1.05
2.19
1.06
1.22
10.5
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7.0
6.0
5.0
4.0
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2.0
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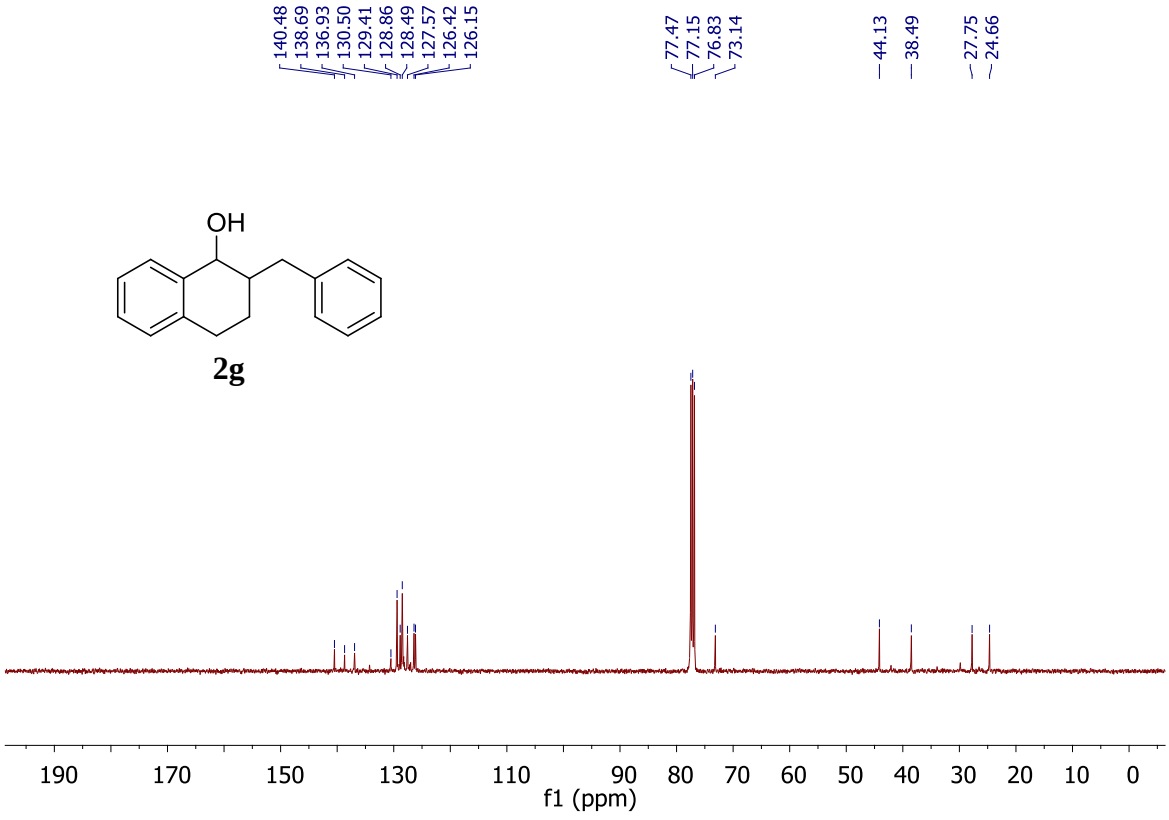
0.0
f1 (ppm)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128.49
127.57
126.42
126.15
77.47
77.15
76.83
73.14
44.13
38.49
27.75
24.66
OH
2g
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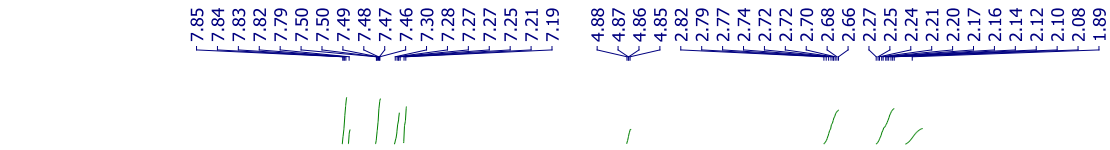
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.49
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7.47
7.46
7.30
7.28
7.27
7.27
7.25
7.21
7.19
4.88
4.87
4.86
4.85
2.82
2.79
2.77
2.74
2.72
2.72
2.70
2.68
2.66
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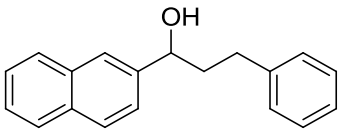
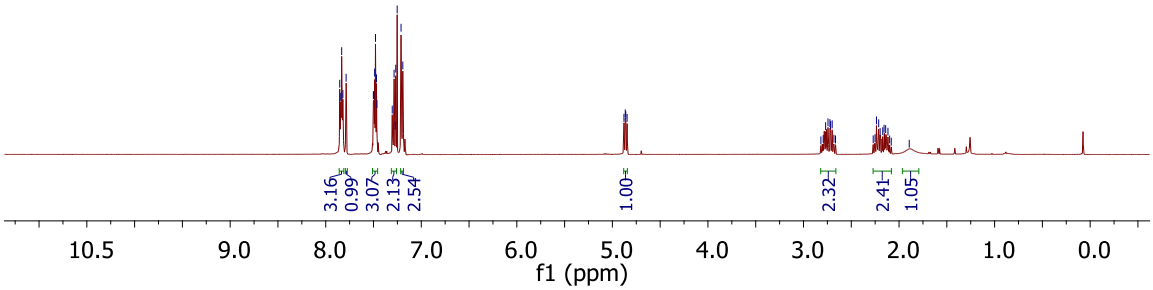
2.10
2.08
1.89


OH

2h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2.41
1.05
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


142.00
141.86
133.40
133.14
128.59
128.54
128.52
128.05
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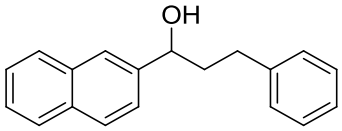
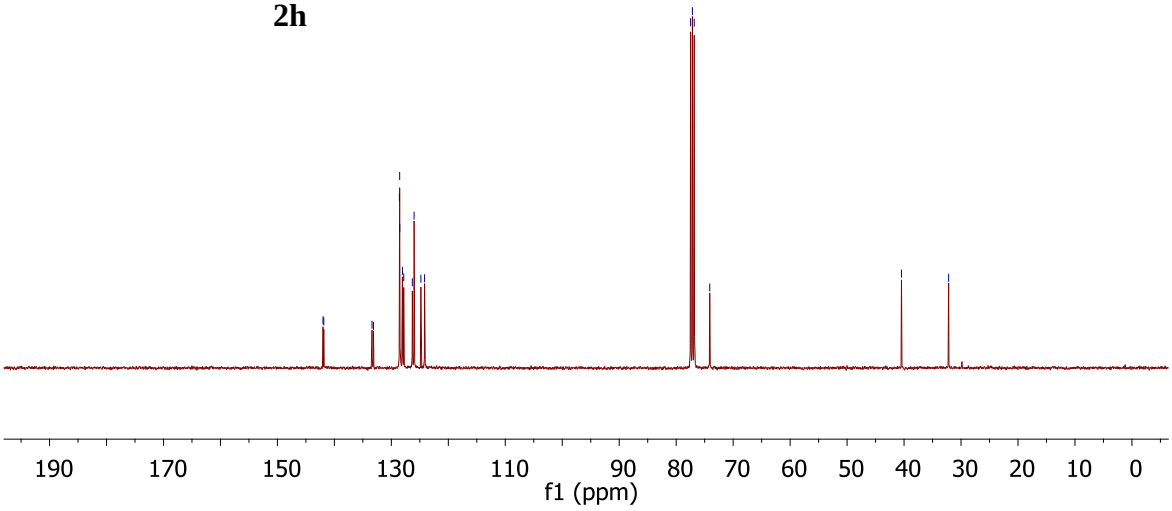
126.31
126.01
124.81
124.17
77.47
77.15
76.83
74.11
40.45
32.18


OH

2h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170
150
130
110
90
80
70
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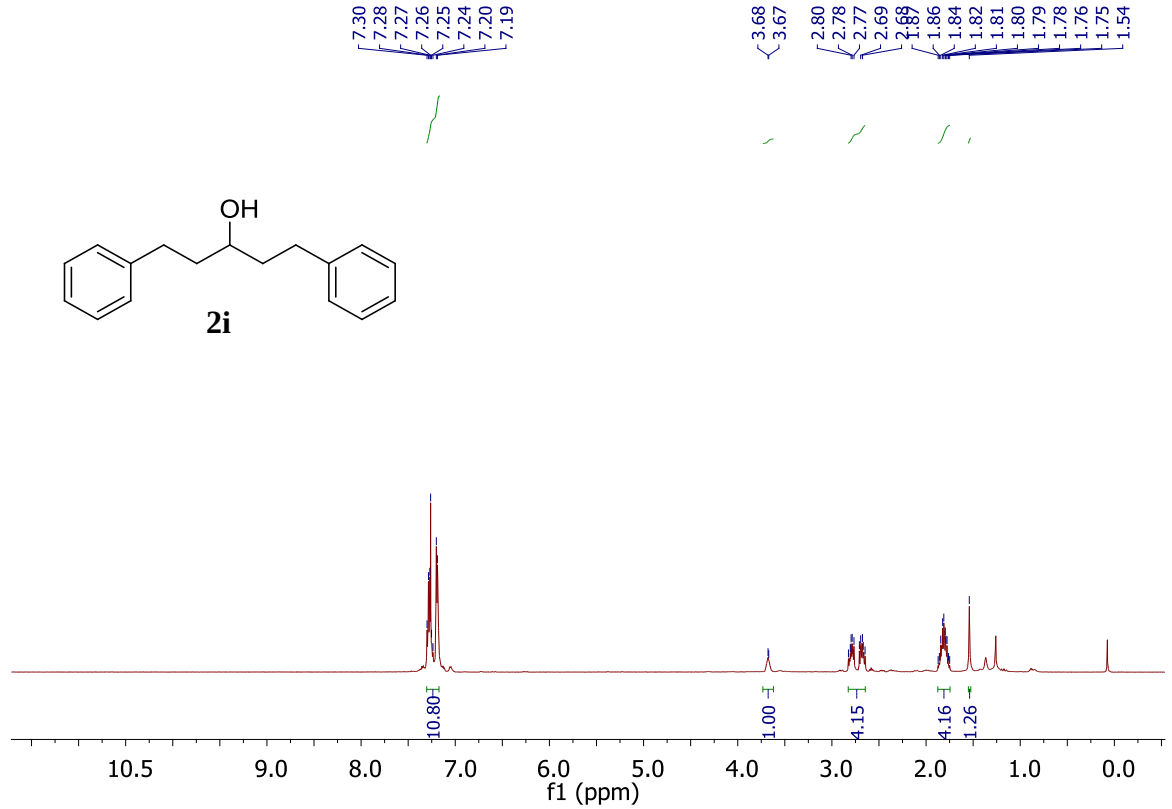
50
40
30
20
10
0
f1 (ppm)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7.24
7.20
7.19
3.68
3.67
2.80
2.78
2.77
2.69
1.86
1.84
1.82
1.81
1.80
1.79
1.78
1.76
1.75
1.54
OH
2i
10.80
1.00
4.15
4.16
1.26
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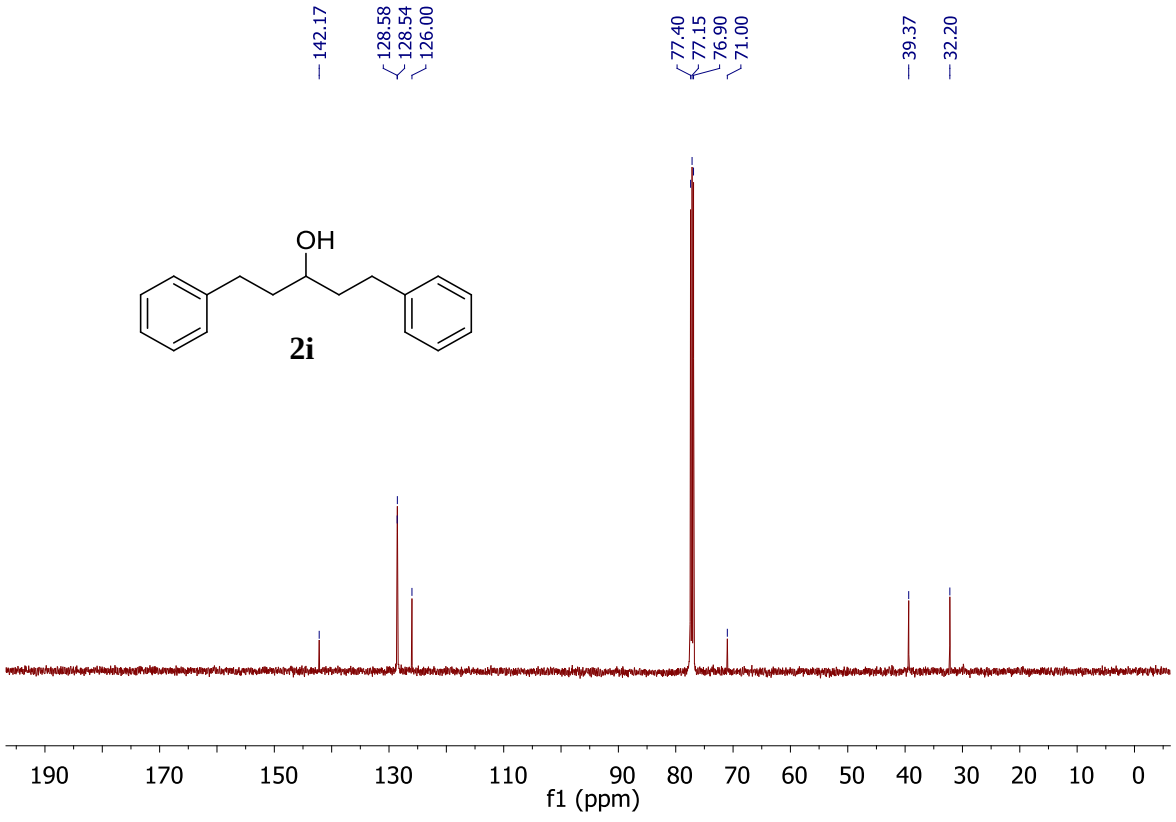
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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77.15
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71.00
39.37
32.20
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2i
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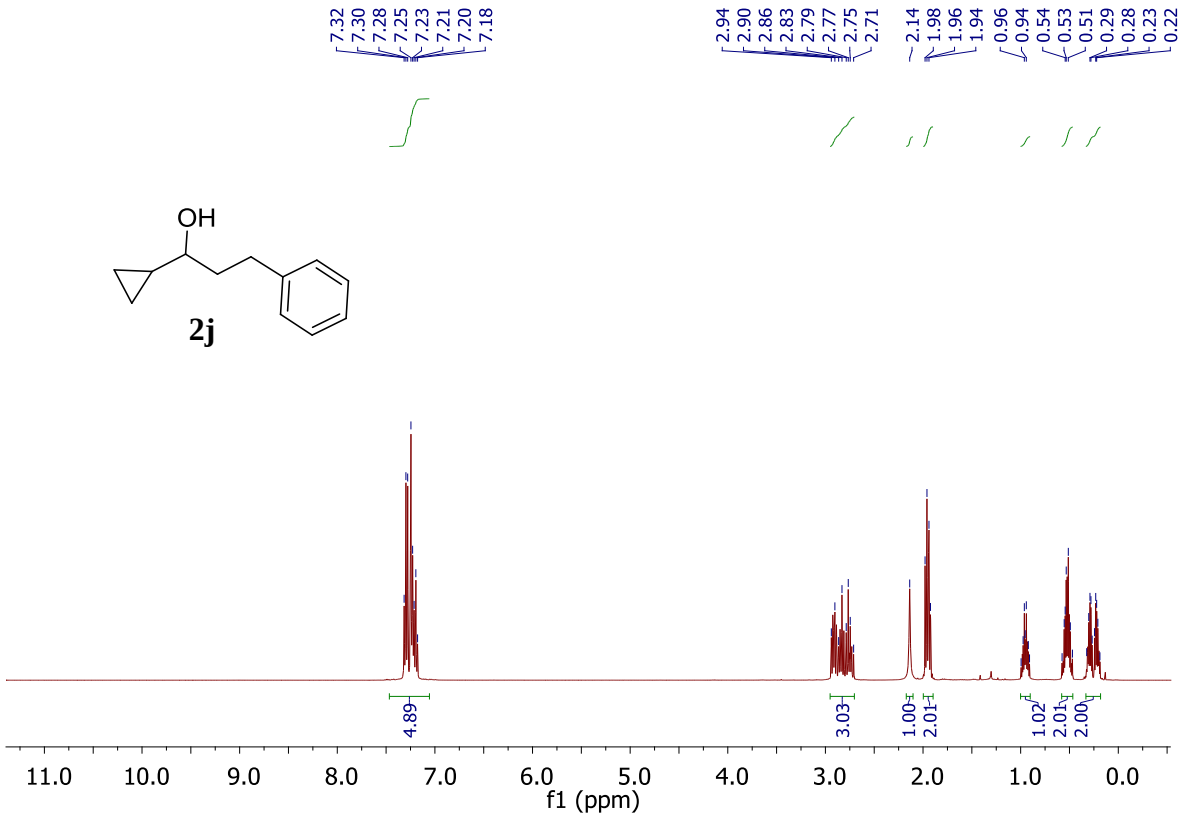
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.20
7.18
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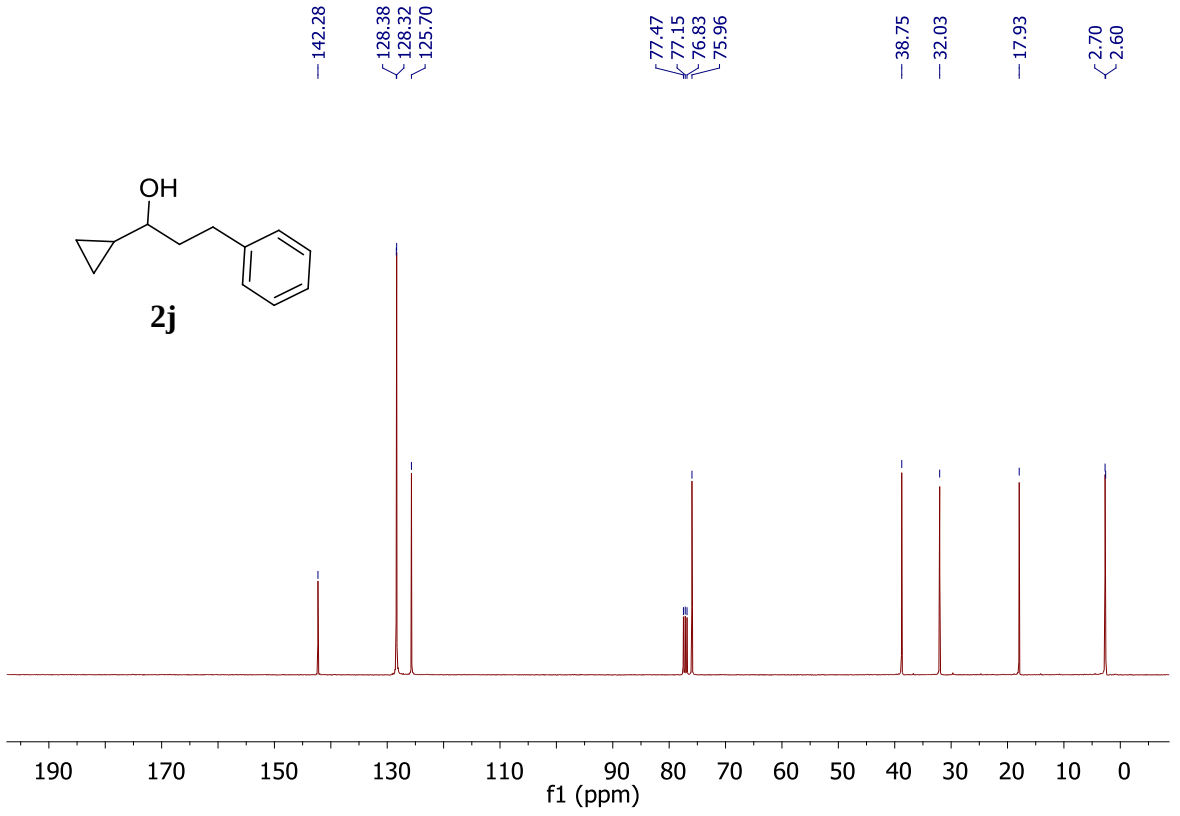
2.90
2.86
2.83
2.79
2.77
2.75
2.71
2.14
1.98
1.96
1.94
0.96
0.94
0.54
0.53
0.51
0.29
0.28
0.23
0.22
OH
2j
4.89
3.03
1.00
2.01
1.02
2.01
2.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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125.70
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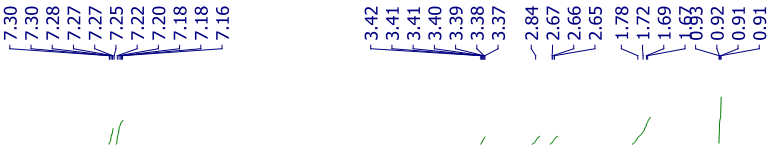
77.15
76.83
75.96
38.75
32.03
17.93
2.70
2.60
OH
2j
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.25
7.22
7.20
7.18
7.18
7.16
3.42
3.41
3.41
3.40
3.39
3.38
3.37
2.84
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2.65
1.78
1.72
1.69
1.63
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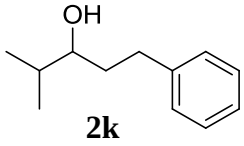
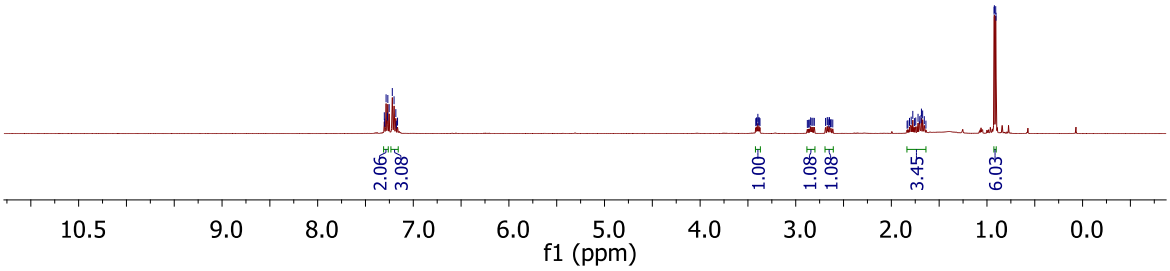
0.92
0.91
0.91


OH

2k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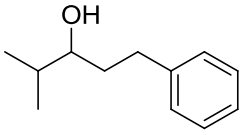
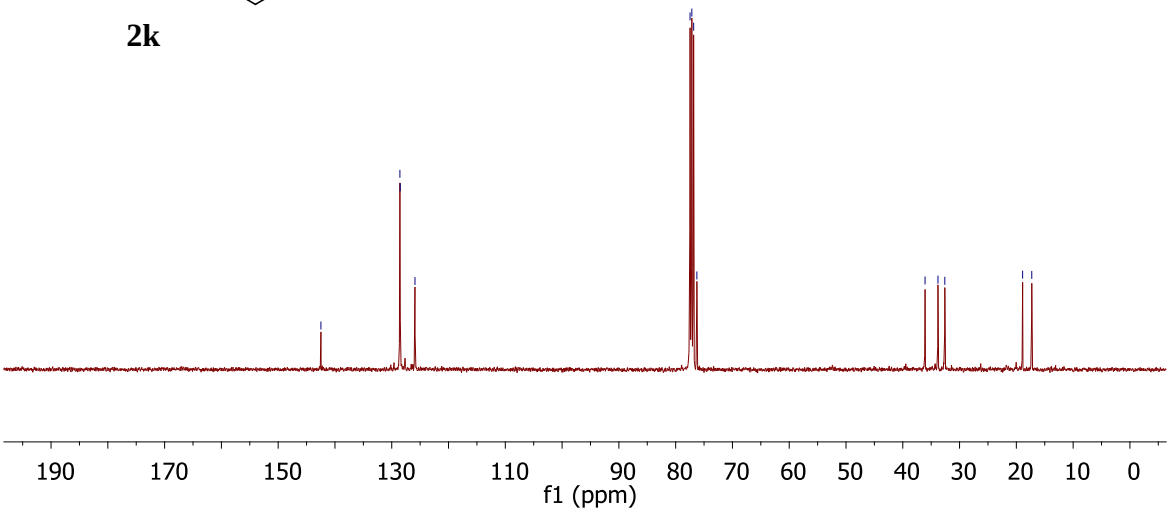
3.08
1.00
1.08
1.08
3.45
6.03
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


142.47
128.56
128.51
125.91
77.47
77.15
76.83
76.26
36.08
33.80
32.60
18.90
17.29


OH

2k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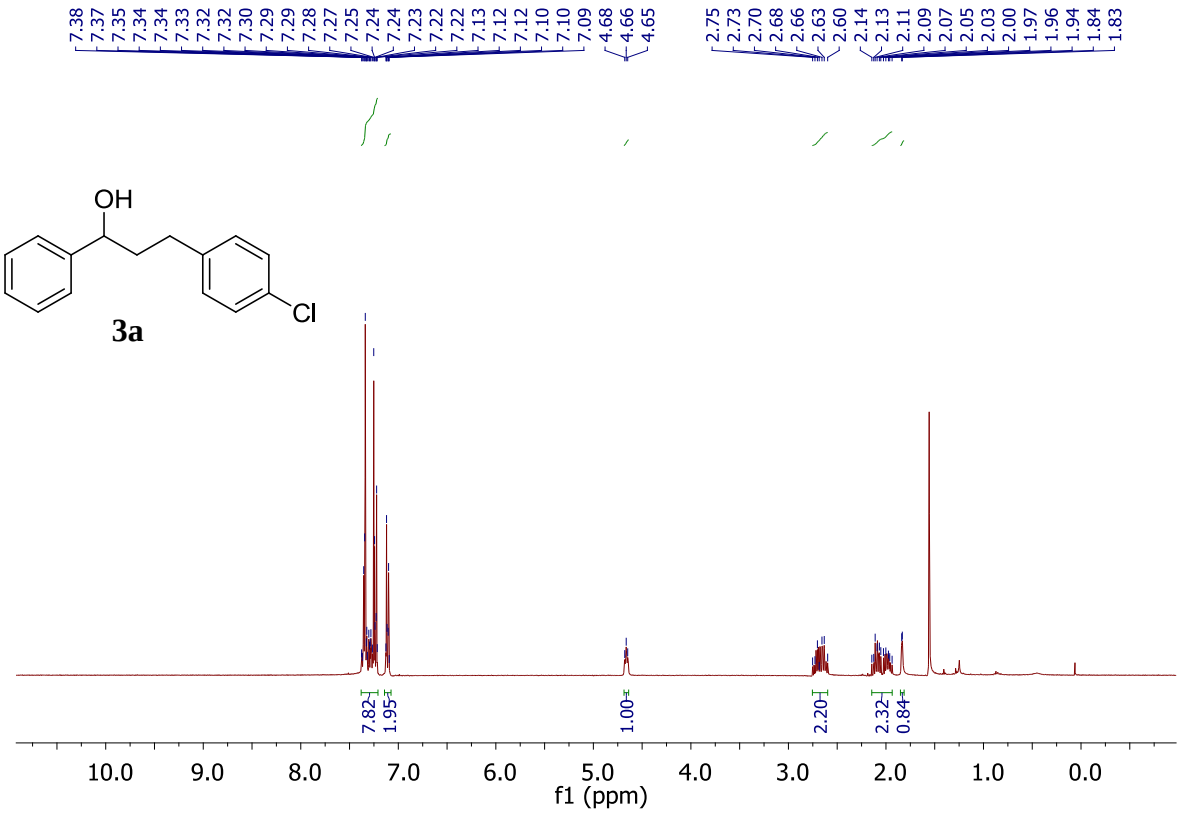
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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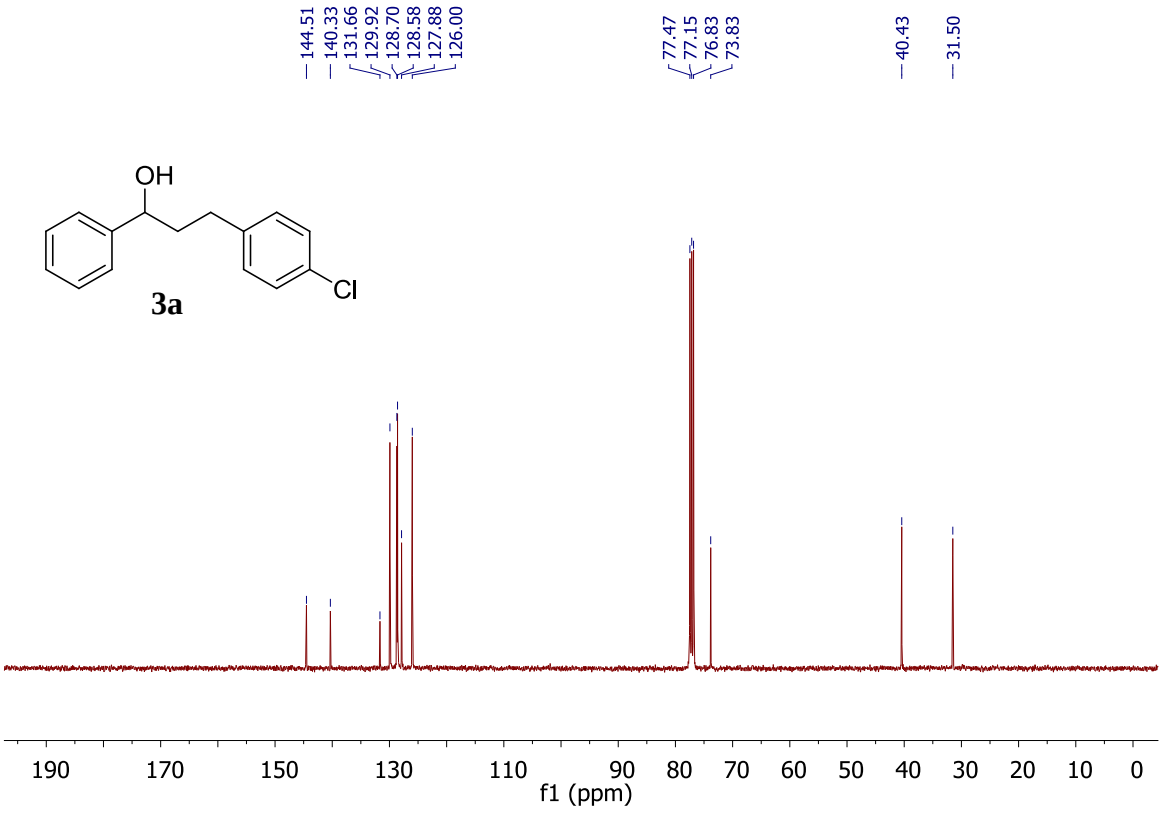
7.27
7.25
7.24
7.24
7.23
7.22
7.22
7.13
7.12
7.12
7.10
7.10
7.09
4.68
4.66
4.65
2.75
2.73
2.70
2.68
2.66
2.63
2.60
2.14
2.13
2.11
2.09
2.07
2.05
2.03
2.00
1.97
1.96
1.94
1.84
1.83
OH
Cl
3a
7.82
1.95
1.00
2.20
2.32
0.84
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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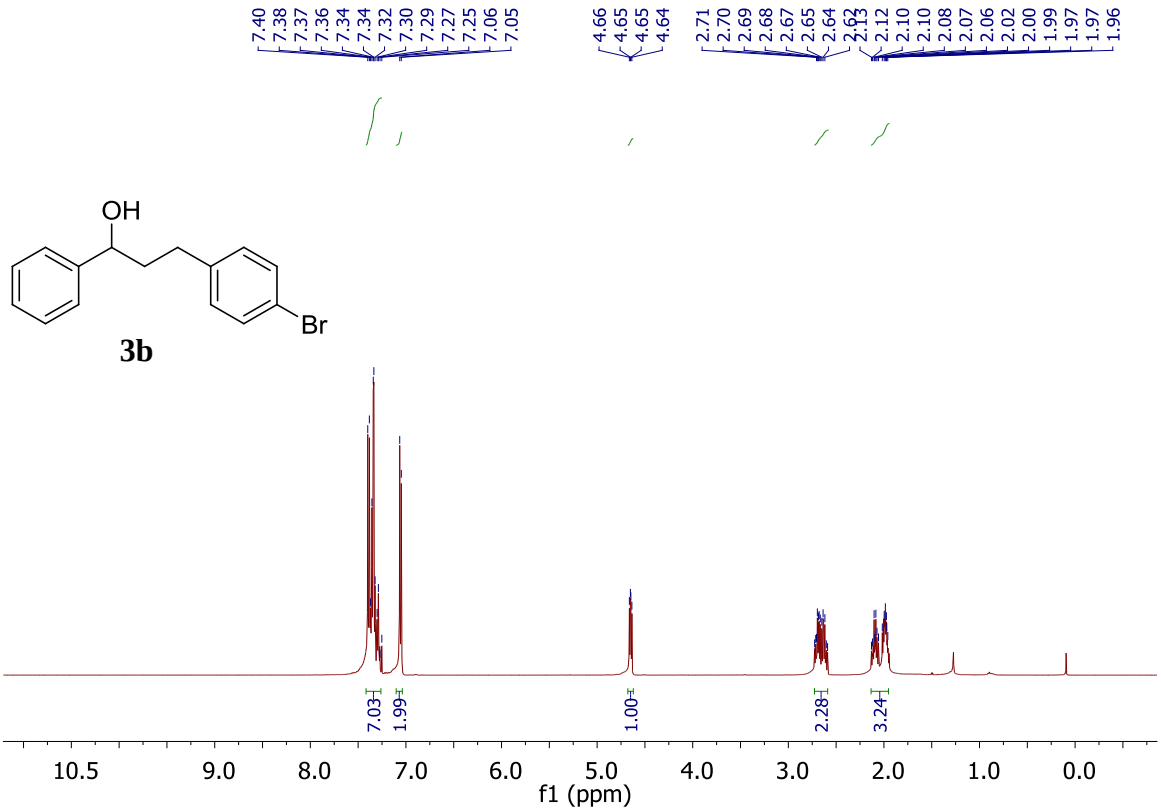
127.88
126.00
77.47
77.15
76.83
73.83
40.43
31.50
OH
Cl
3a
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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4.65
4.64
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2.69
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2.64
2.62
2.13
2.12
2.10
2.10
2.08
2.07
2.06
2.02
2.00
1.99
1.97
1.97
1.96
OH
Br
3b
7.03
1.99
1.00
2.28
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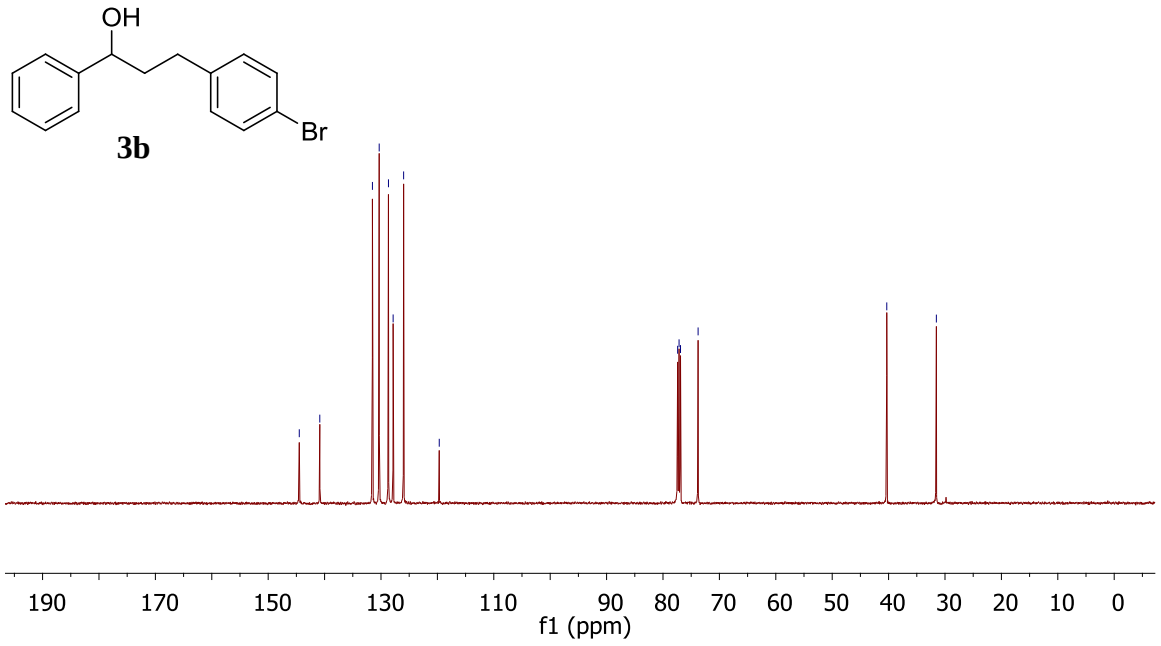
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40.32
31.53
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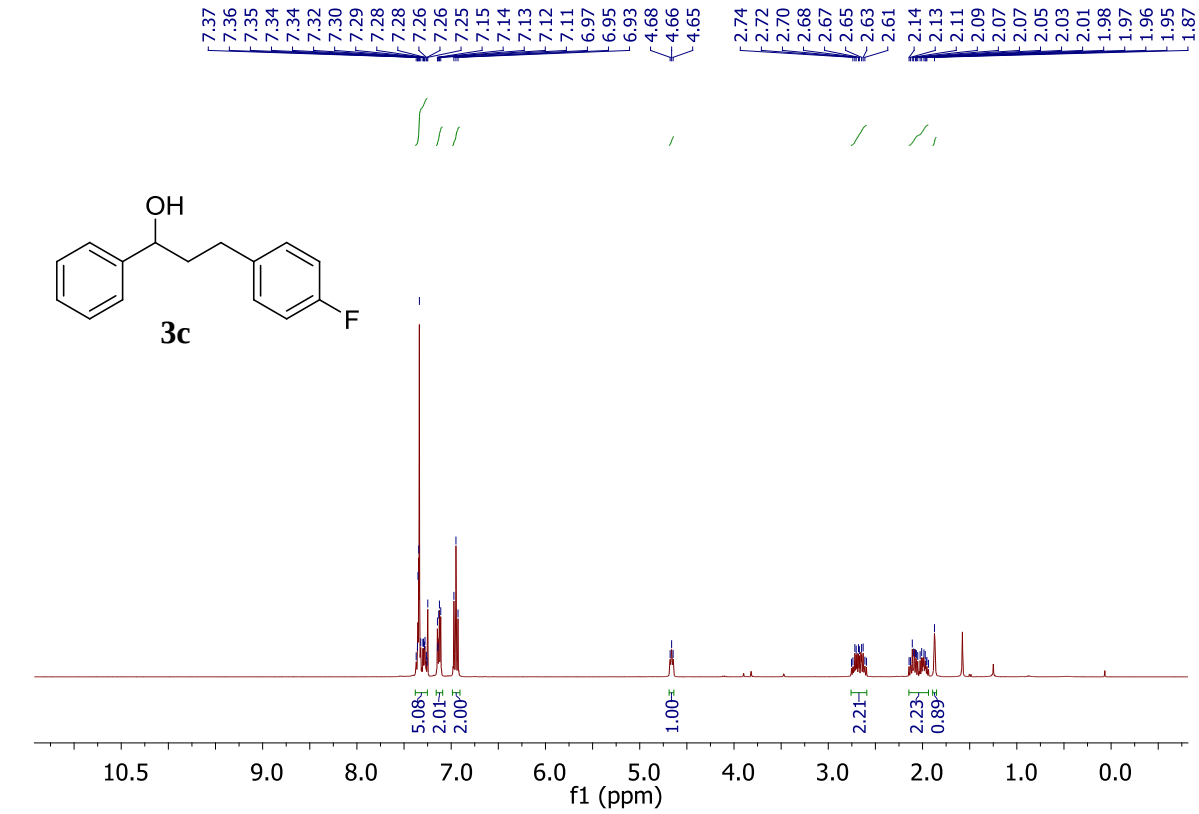
f1 (ppm)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2.11
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2.07
2.07
2.05
2.03
2.01
1.98
1.97
1.96
1.95
1.87
OH
F
3c
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2.01
2.00
1.00
2.21
2.23
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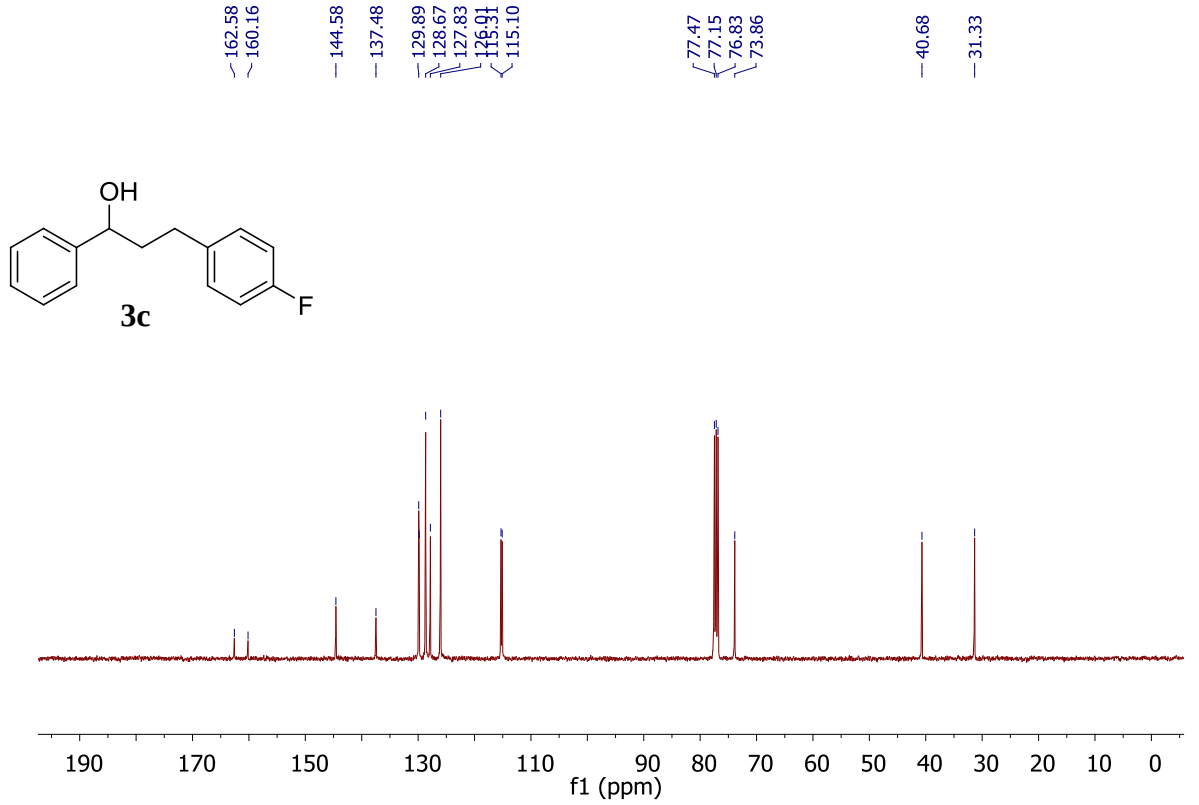
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76.83
73.86
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31.33
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150
130
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90
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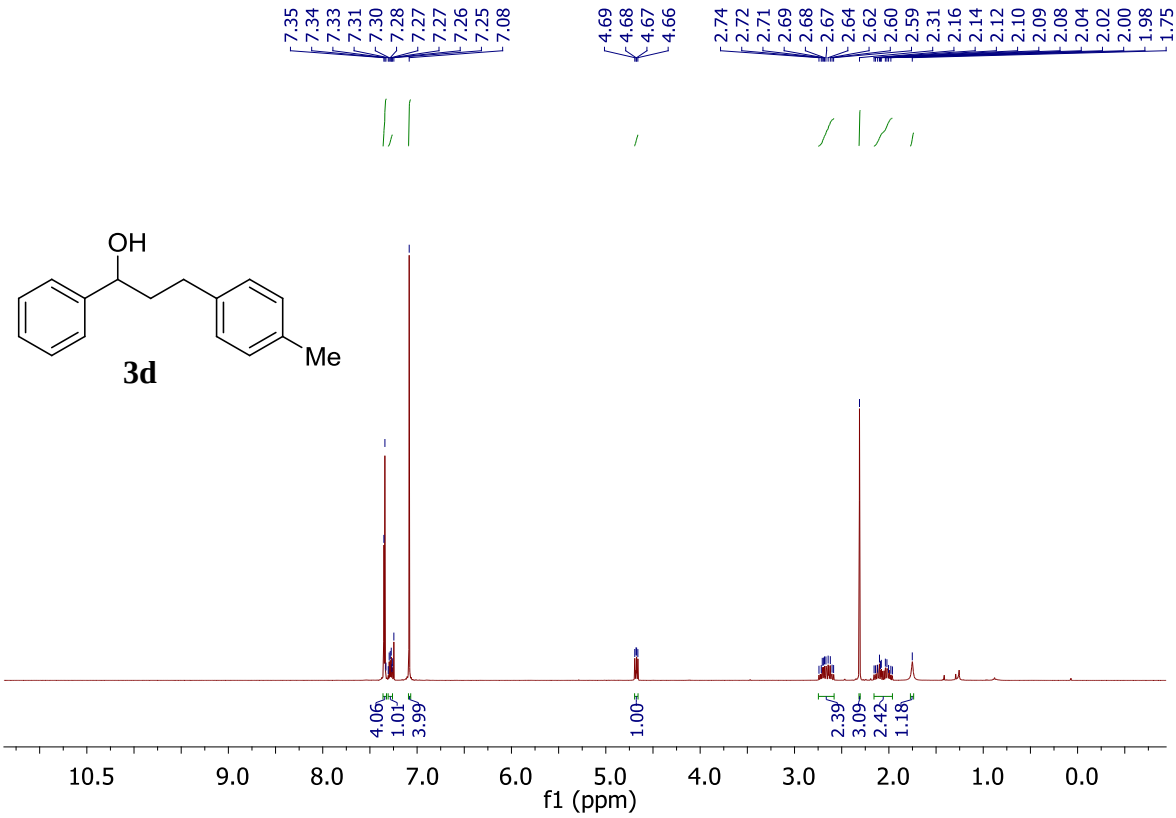
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4.66
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2.68
2.67
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2.62
2.60
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2.31
2.16
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2.12
2.10
2.09
2.08
2.04
2.02
2.00
1.98
1.75
OH
Me
3d
4.06
1.01
3.99
1.00
2.39
3.09
2.42
1.18
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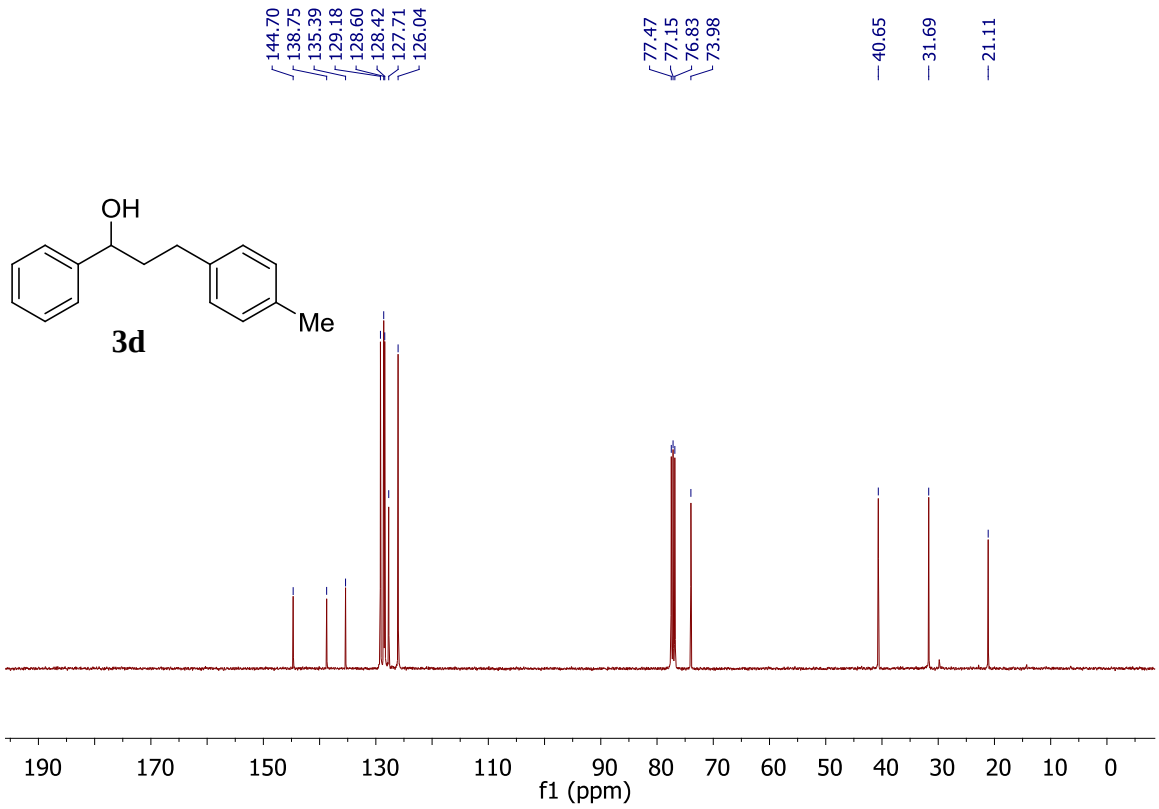
f1 (ppm)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31.69
21.11
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150
130
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90
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50
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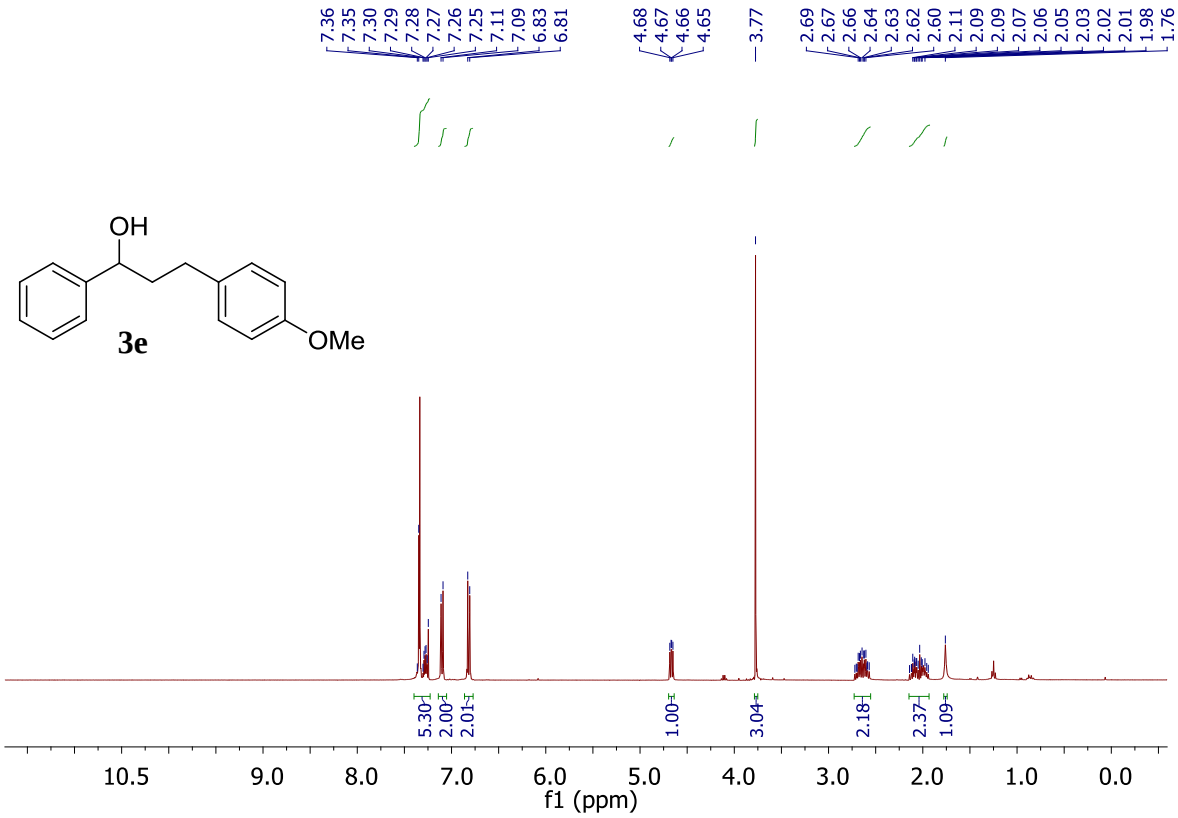
f1 (ppm)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4.66
4.65
3.77
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2.62
2.60
2.11
2.09
2.09
2.07
2.06
2.05
2.03
2.02
2.01
1.98
1.76
OH
OMe
3e
5.30
2.00
2.01
1.00
3.04
2.18
2.37
1.09
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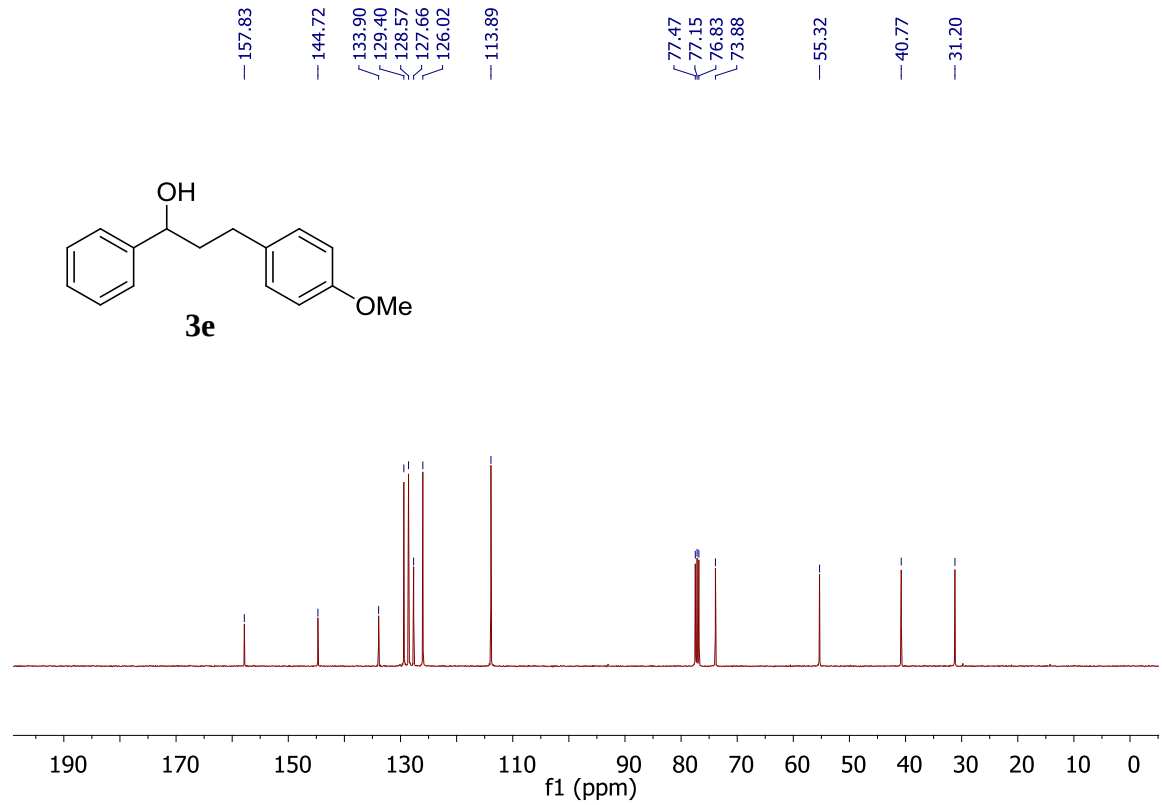
f1 (ppm)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113.89
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77.15
76.83
73.88
55.32
40.77
31.20
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3e
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110
90
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70
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50
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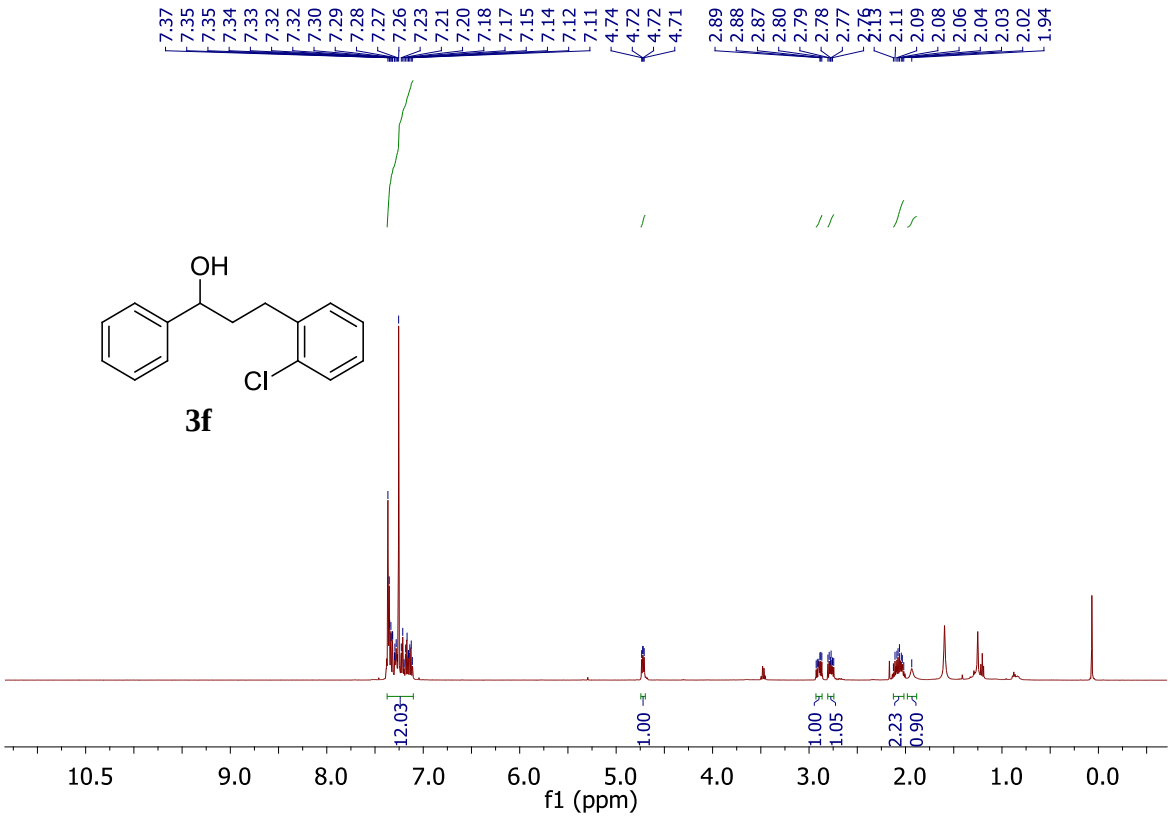
10
0
f1 (ppm)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7.17
7.15
7.14
7.12
7.11
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4.72
4.71
2.89
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2.76
2.13
2.11
2.09
2.08
2.06
2.04
2.03
2.02
1.94
OH
Cl
12.03
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1.00
1.05
2.23
0.90
10.5
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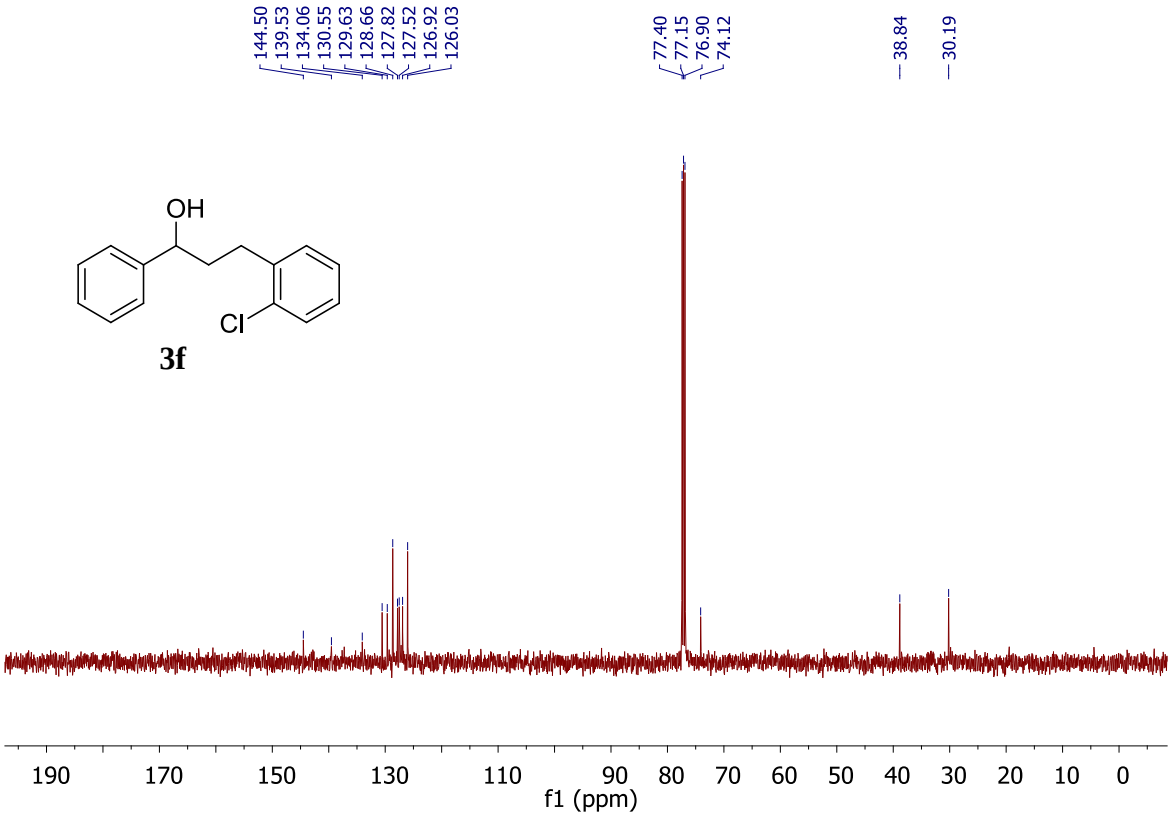
f1 (ppm)

3f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74.12
38.84
30.19
OH
Cl
190
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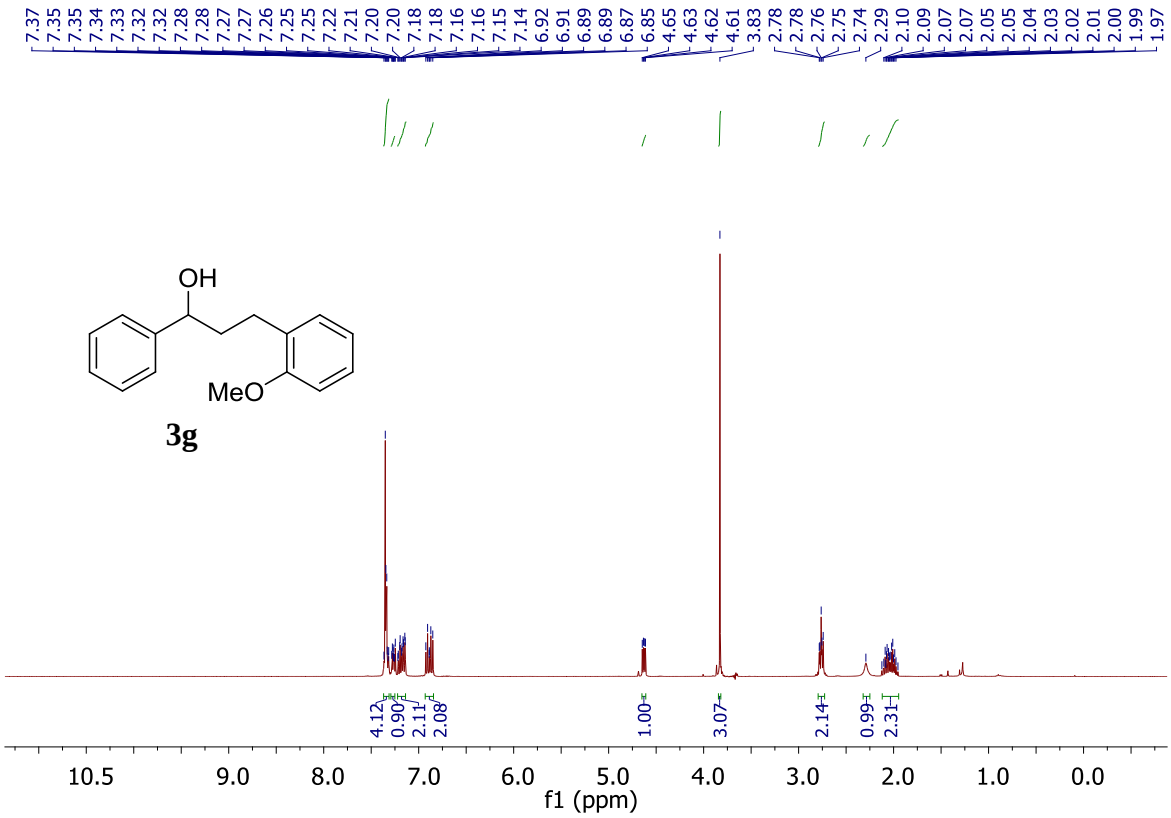
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3f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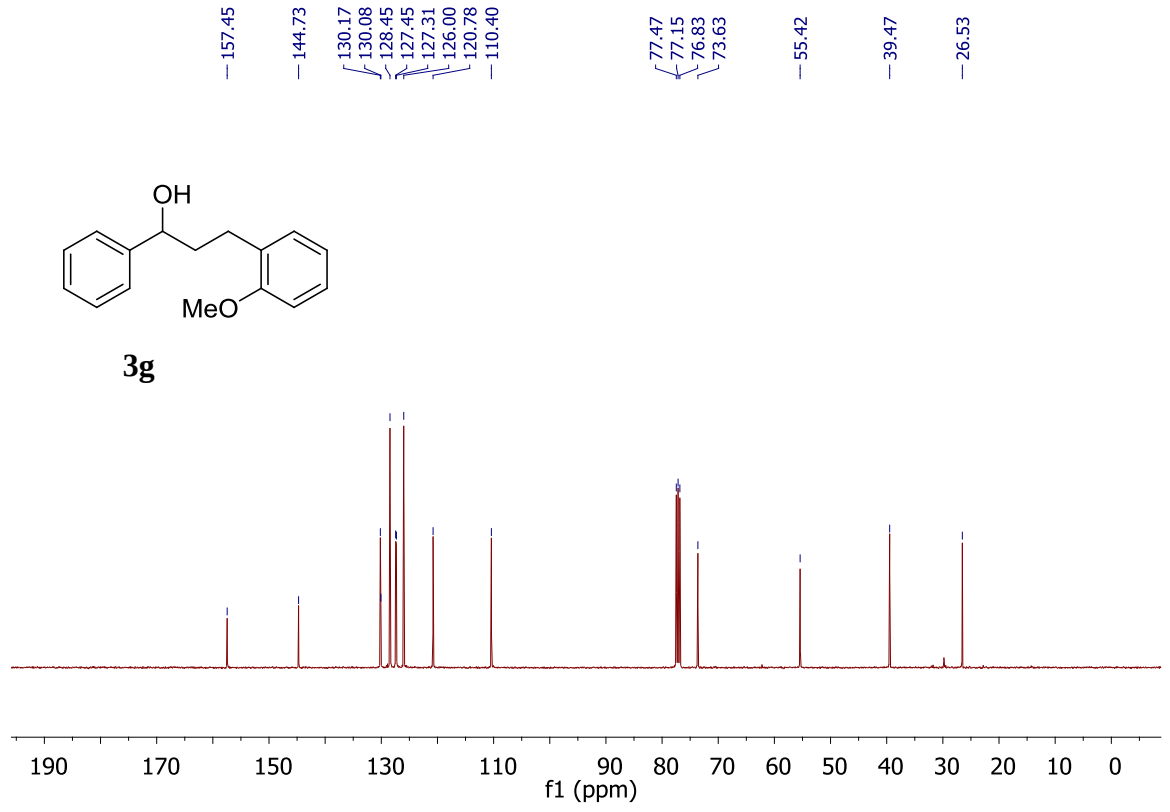
OH
MeO
3g
4.12 0.90 2.11 2.08 1.00 3.07 2.14 0.99 2.31
10.5 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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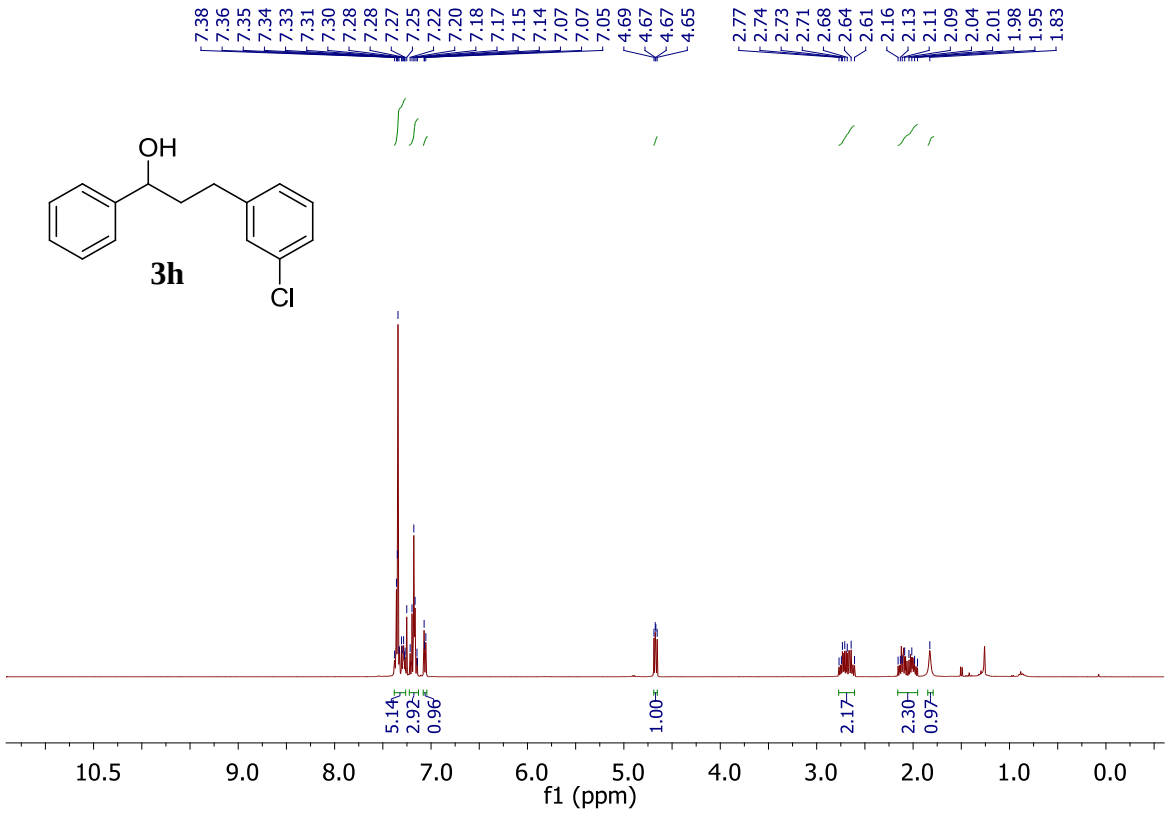
OH
MeO
3g
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.07
7.07
7.05
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2.13
2.11
2.09
2.04
2.01
1.98
1.95
1.83
OH
3h
Cl
5.14
2.92
0.96
1.00
2.17
2.30
0.97
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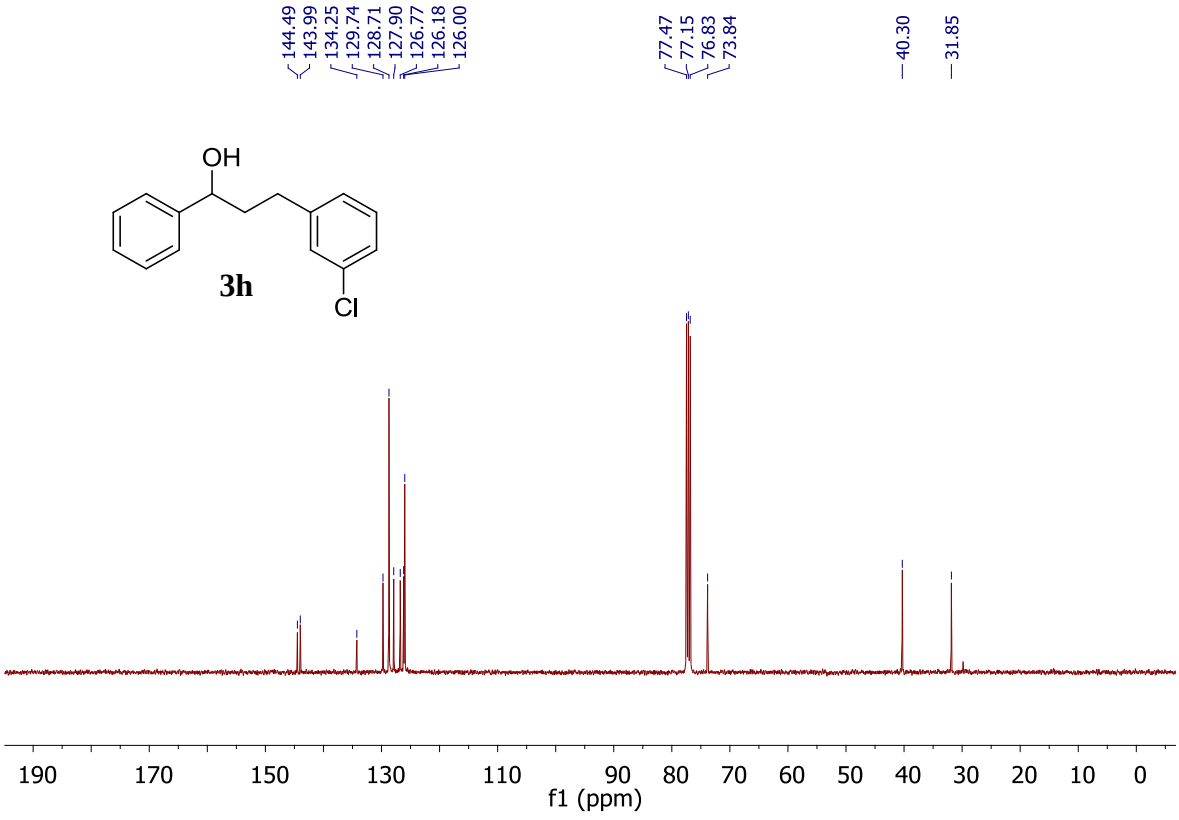
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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126.00
77.47
77.15
76.83
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40.30
31.85
OH
3h
Cl
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170
150
130
110
90
80
70
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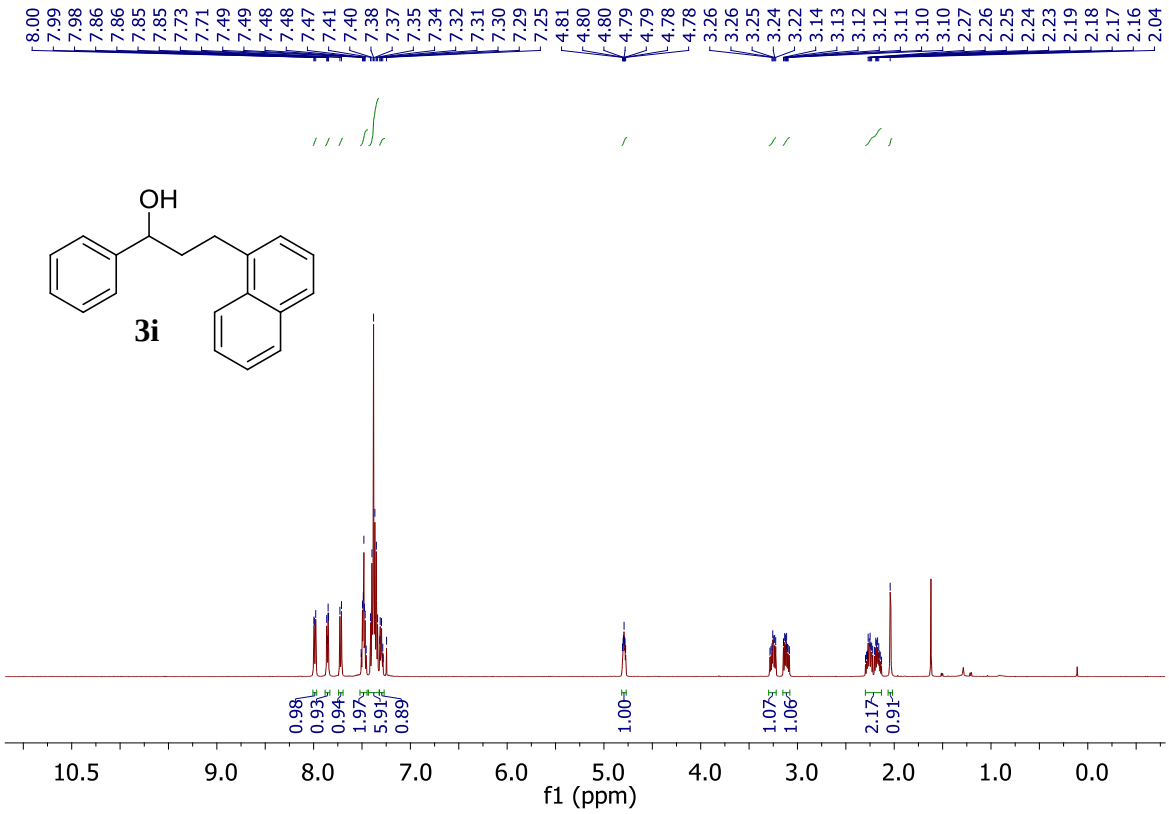
50
40
30
20
10
0
f1 (ppm)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7.41
7.40
7.38
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7.34
7.32
7.31
7.30
7.29
7.25
4.81
4.80
4.80
4.79
4.79
4.78
4.78
3.26
3.26
3.25
3.24
3.22
3.14
3.13
3.12
3.12
3.11
3.10
3.10
2.27
2.26
2.25
2.24
2.23
2.19
2.18
2.17
2.16
2.04
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3i
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0.93
0.94
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5.91
0.89
1.00
1.07
1.06
2.17
0.91
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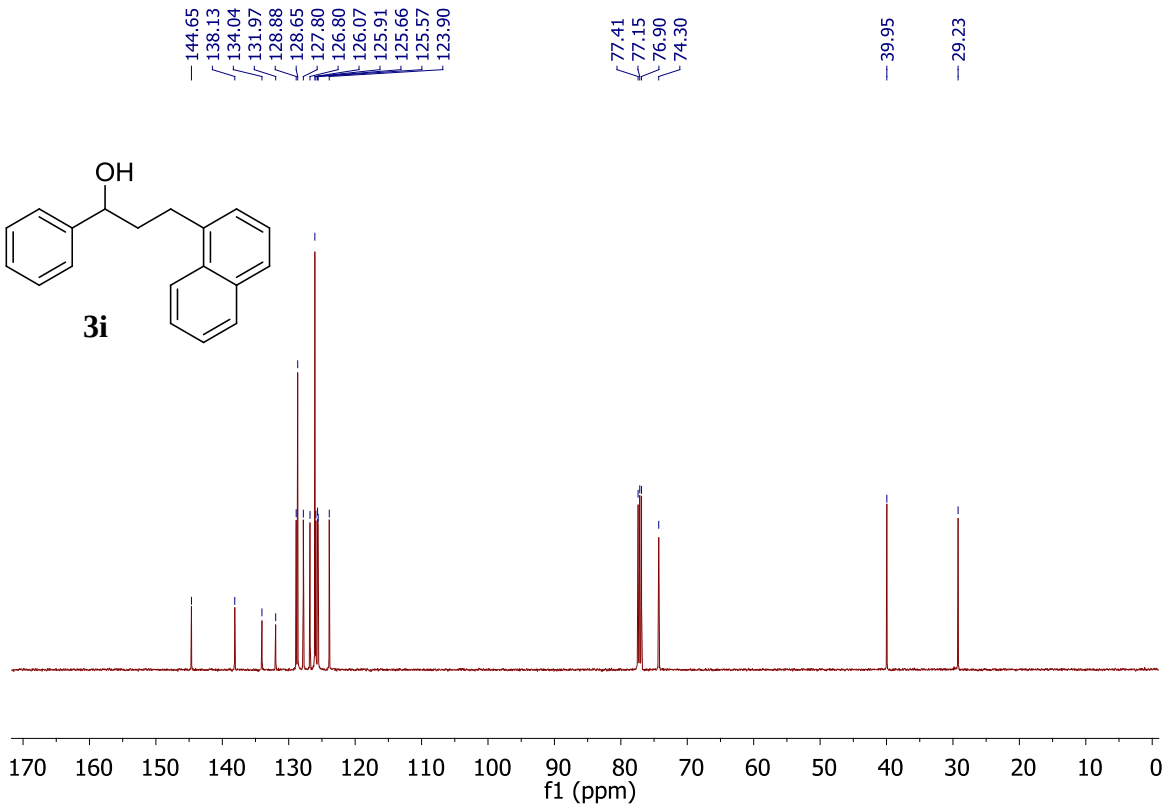
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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125.66
125.57
123.90
77.41
77.15
76.90
74.30
39.95
29.23
OH
3i
170
160
150
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130
120
110
100
90
80
70
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50
40
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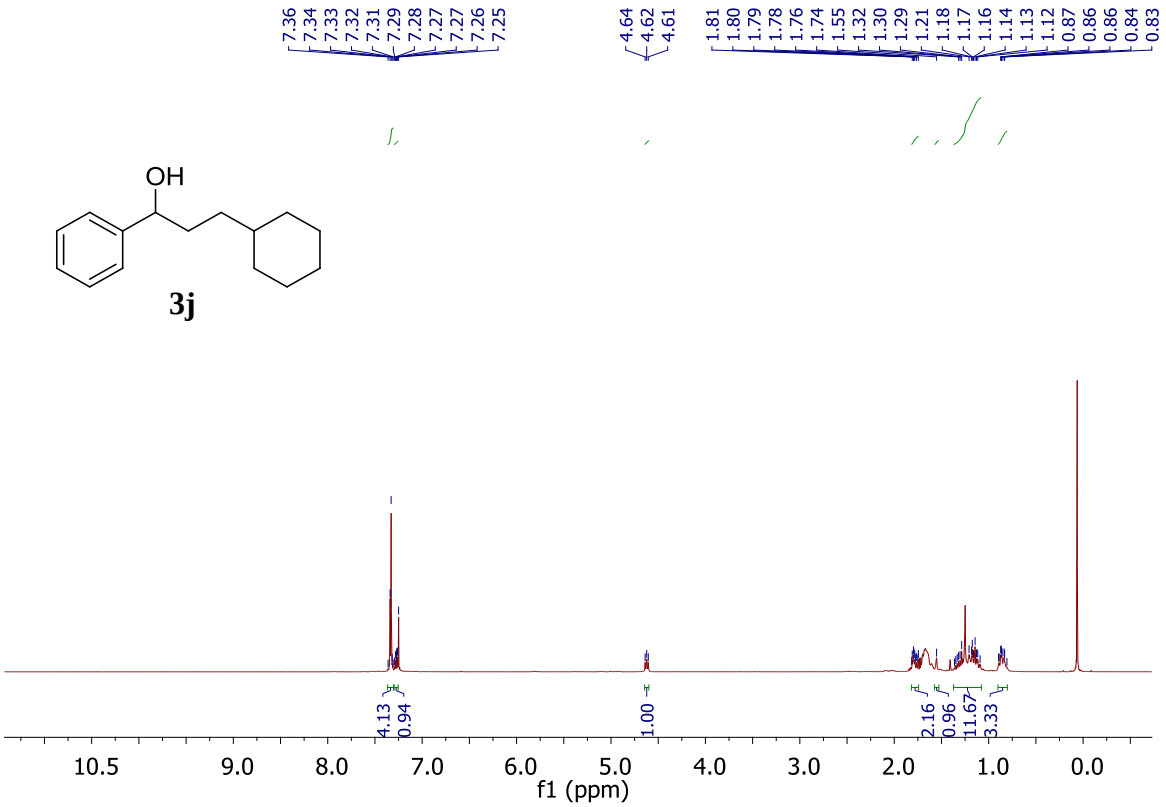
10
0
f1 (ppm)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4.61
1.81
1.80
1.79
1.78
1.76
1.74
1.55
1.32
1.30
1.29
1.21
1.18
1.17
1.16
1.14
1.13
1.12
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0.86
0.86
0.84
0.83
OH
3j
4.13
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1.00
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0.96
11.67
3.33
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6.0
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4.0
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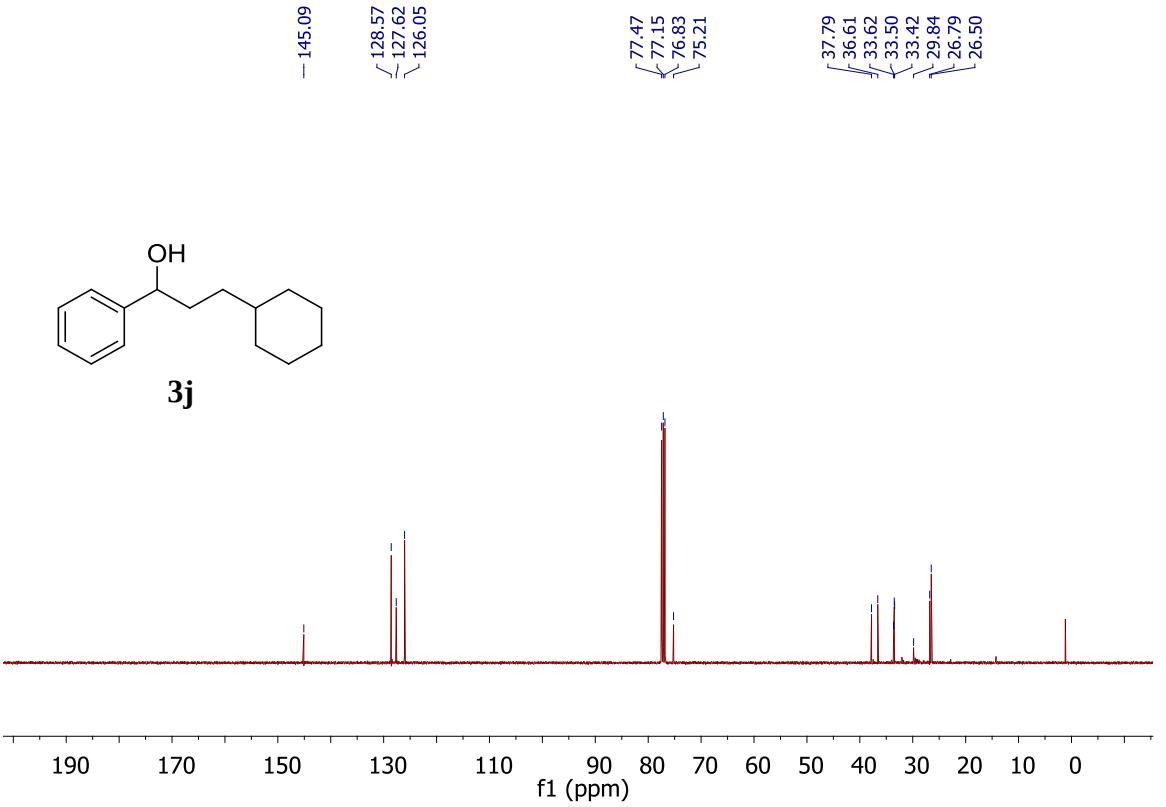
2.0
1.0
0.0
f1 (ppm)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75.21
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36.61
33.62
33.50
33.42
29.84
26.79
26.50
OH
3j
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170
150
130
110
90
80
70
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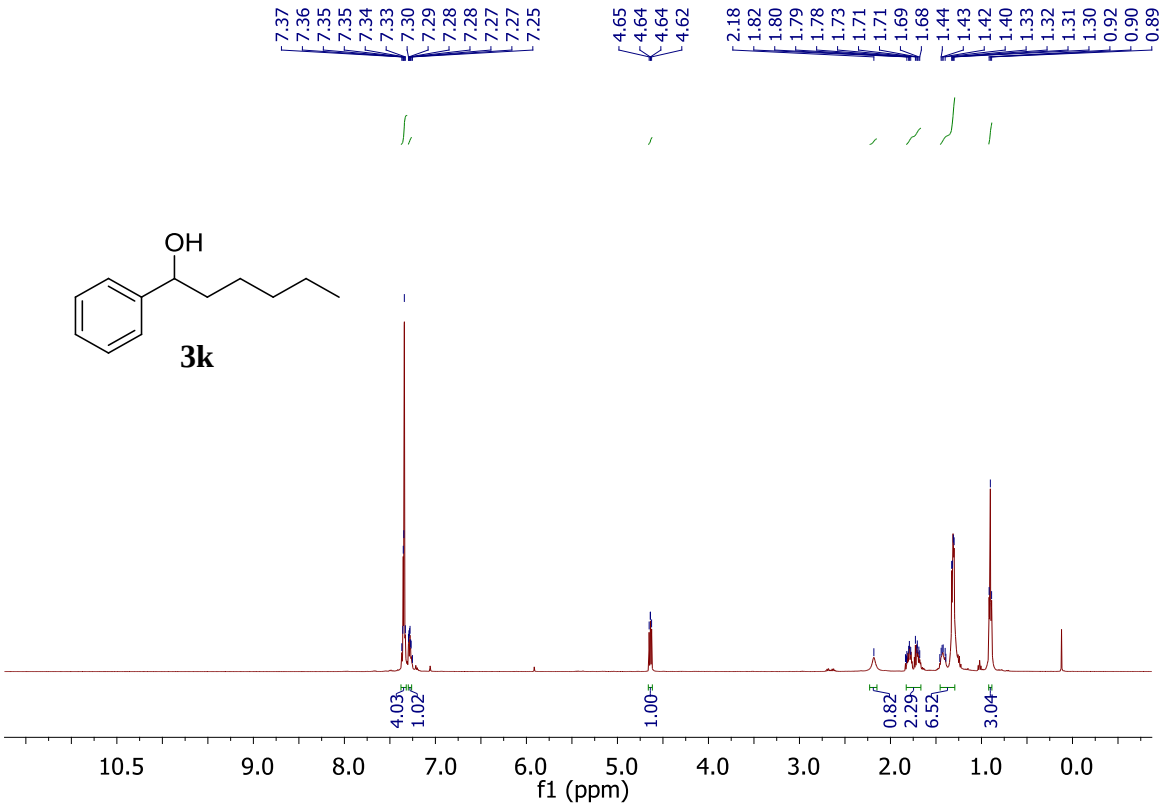
50
40
30
20
10
0
f1 (ppm)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4.64
4.64
4.62
2.18
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1.80
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1.78
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1.43
1.42
1.40
1.33
1.32
1.31
1.30
0.92
0.90
0.89
OH
3k
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1.02
1.00
0.82
2.29
6.52
3.04
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7.0
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4.0
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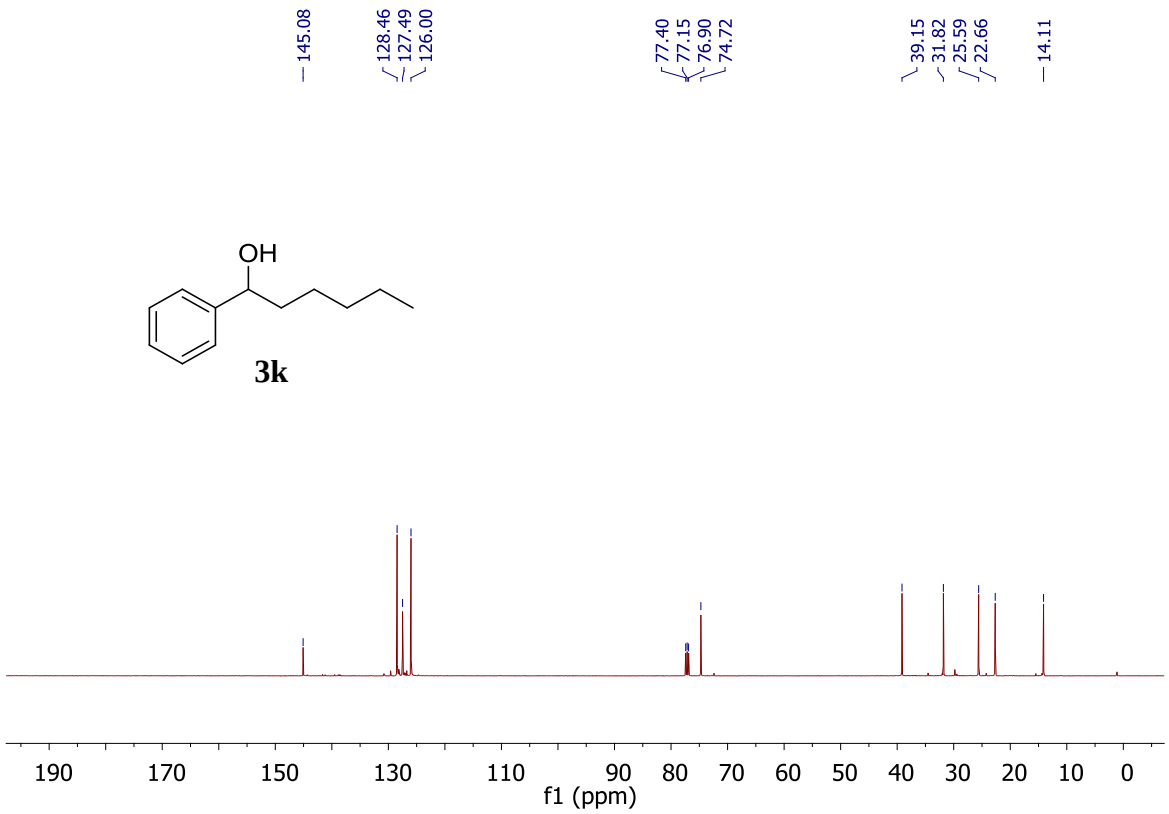
2.0
1.0
0.0
f1 (ppm)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77.15
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74.72
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31.82
25.59
22.66
14.11
OH
3k
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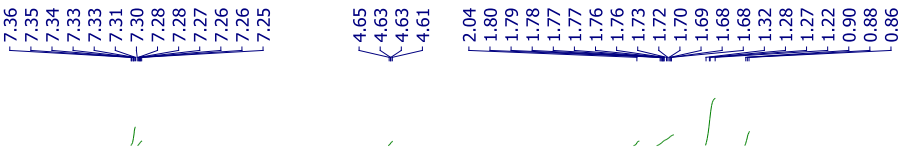
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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4.65
4.63
4.63
4.61
2.04
1.80
1.79
1.78
1.77
1.77
1.76
1.76
1.73
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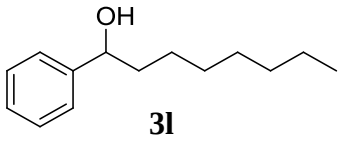
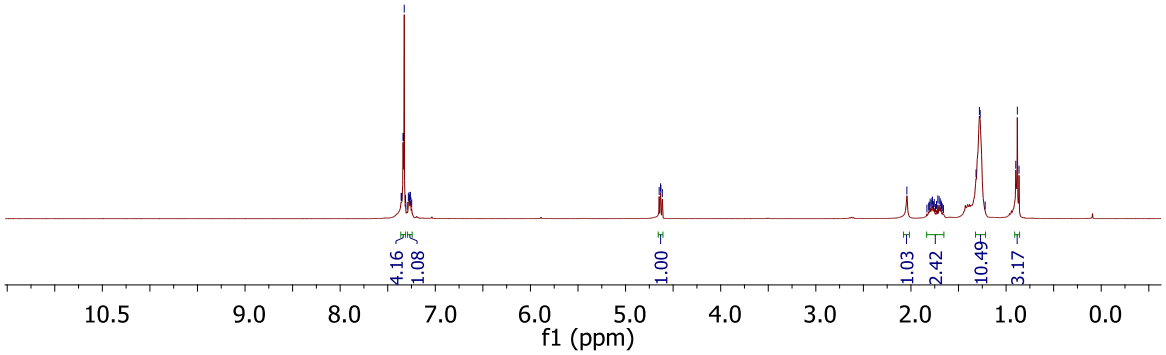
0.88
0.86


OH

3l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1.00
1.03
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9.0
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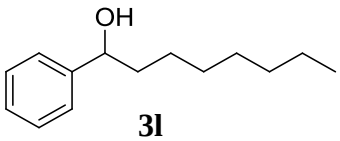
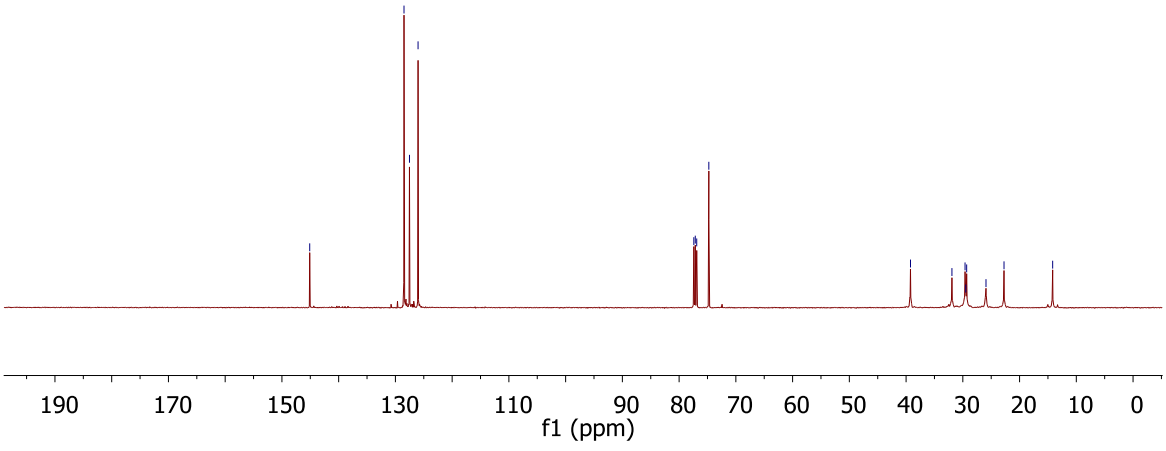
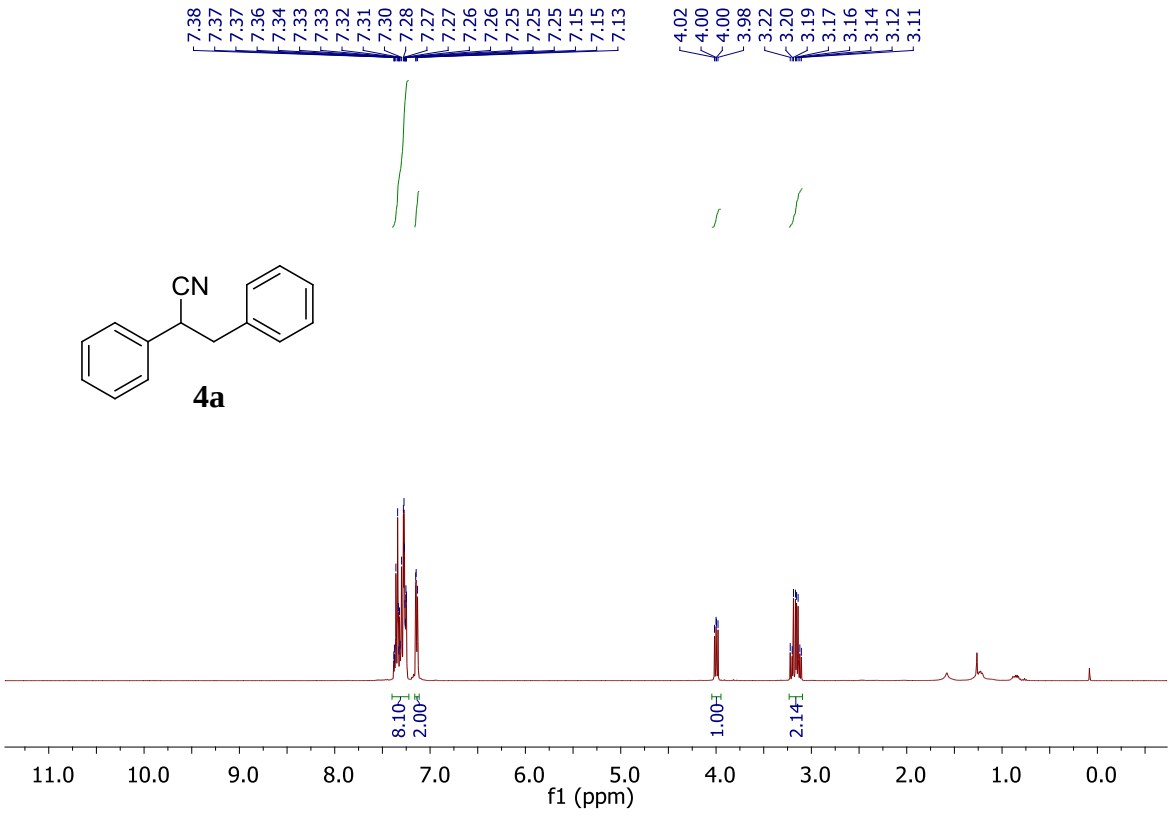
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


145.10
128.49
127.52
126.01
77.41
77.15
76.90
74.76
39.22
31.92
29.61
29.48
29.32
25.92
22.74
14.17


OH

3l


190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.26
7.25
7.25
7.25
7.15
7.15
7.13
4.02
4.00
4.00
3.98
3.22
3.20
3.19
3.17
3.16
3.14
3.12
3.11
CN
8.10
2.00
1.00
2.14
11.0
10.0
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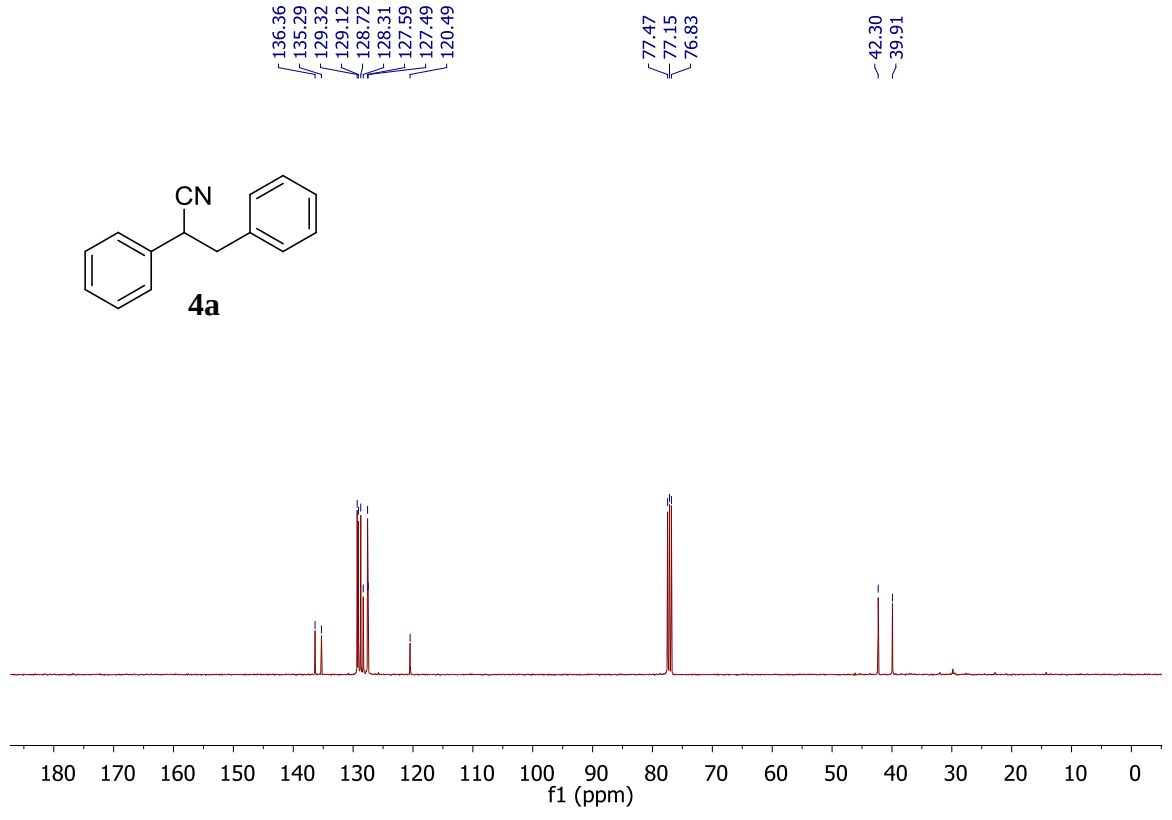
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

4a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77.47
77.15
76.83
42.30
39.91
CN
180
170
160
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120
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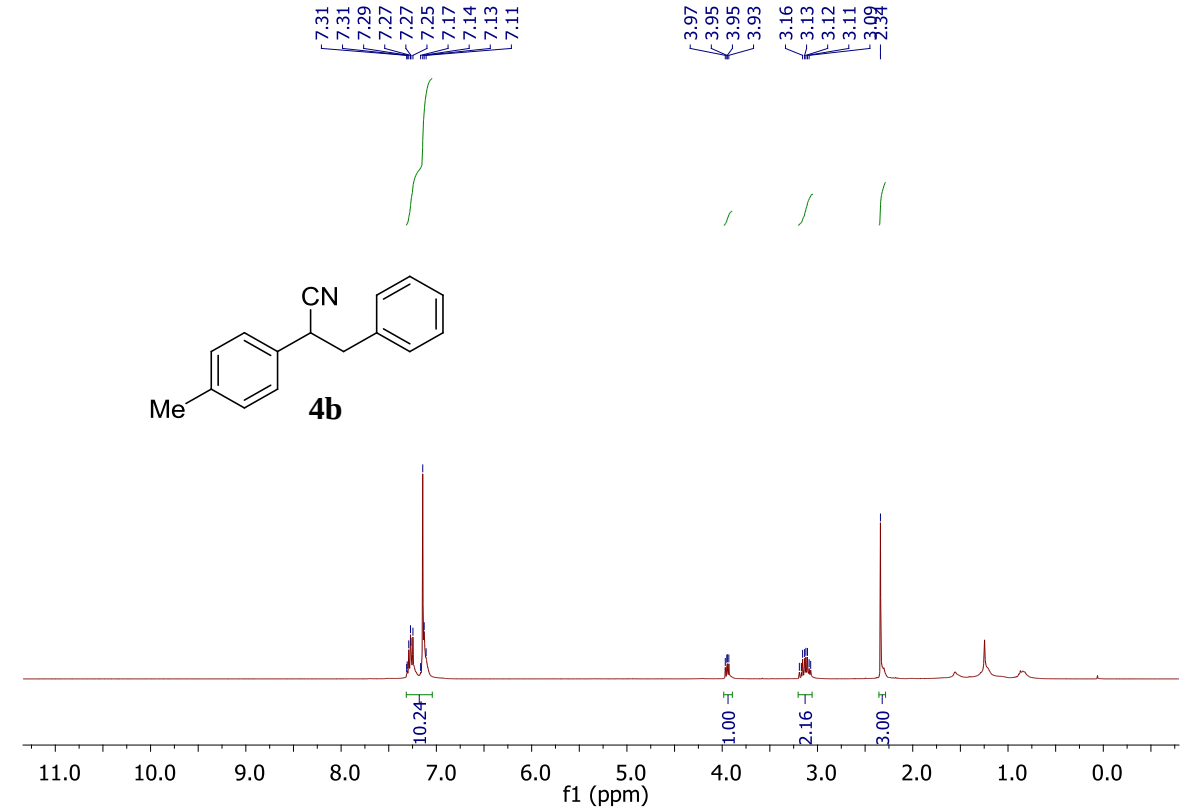
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4a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3.95
3.93
3.16
3.13
3.12
3.11
3.09
2.34
CN
Me
4b
10.24
1.00
2.16
3.00
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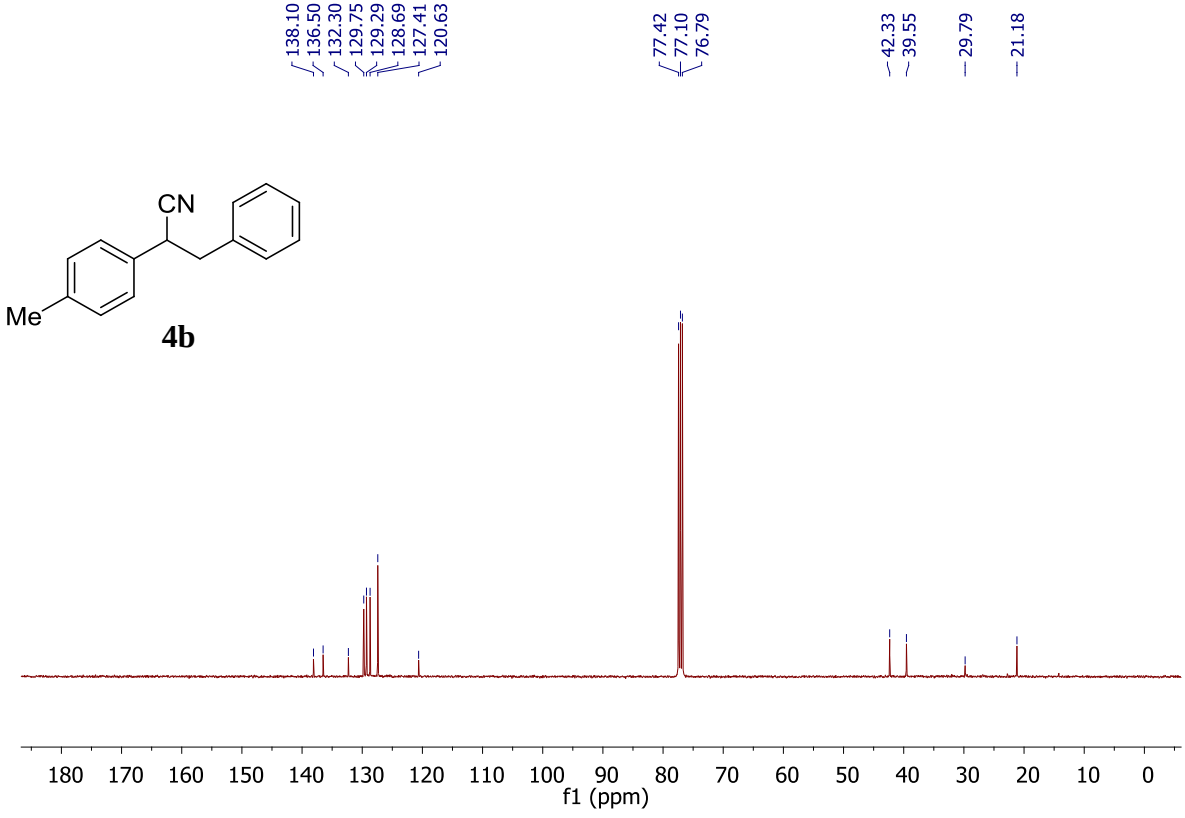
f1 (ppm)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42.33
39.55
29.79
21.18
CN
Me
4b
180
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110
100
90
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70
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50
40
30
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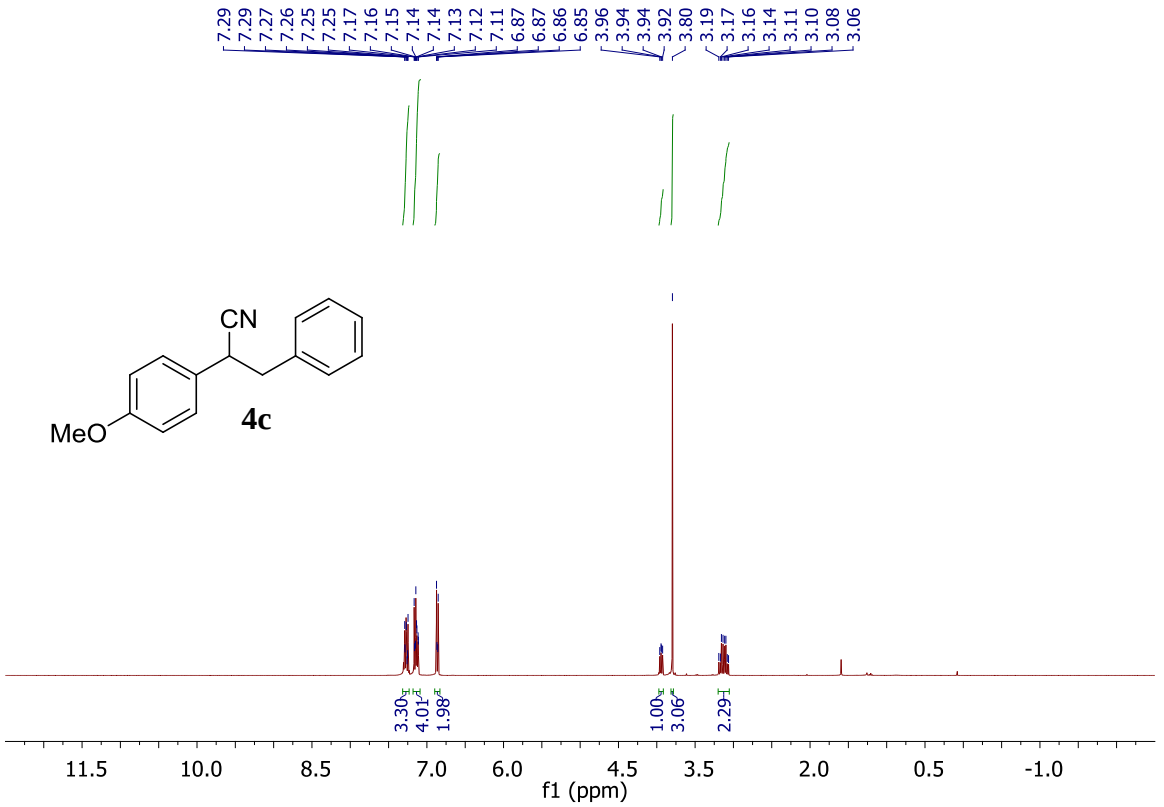
10
0
f1 (ppm)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7.13
7.12
7.11
6.87
6.87
6.86
6.85
3.96
3.94
3.94
3.92
3.80
3.19
3.17
3.16
3.14
3.11
3.10
3.08
3.06
CN
MeO
4c
3.30
4.01
1.98
1.00
3.06
2.29
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8.5
7.0
6.0
4.5
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2.0
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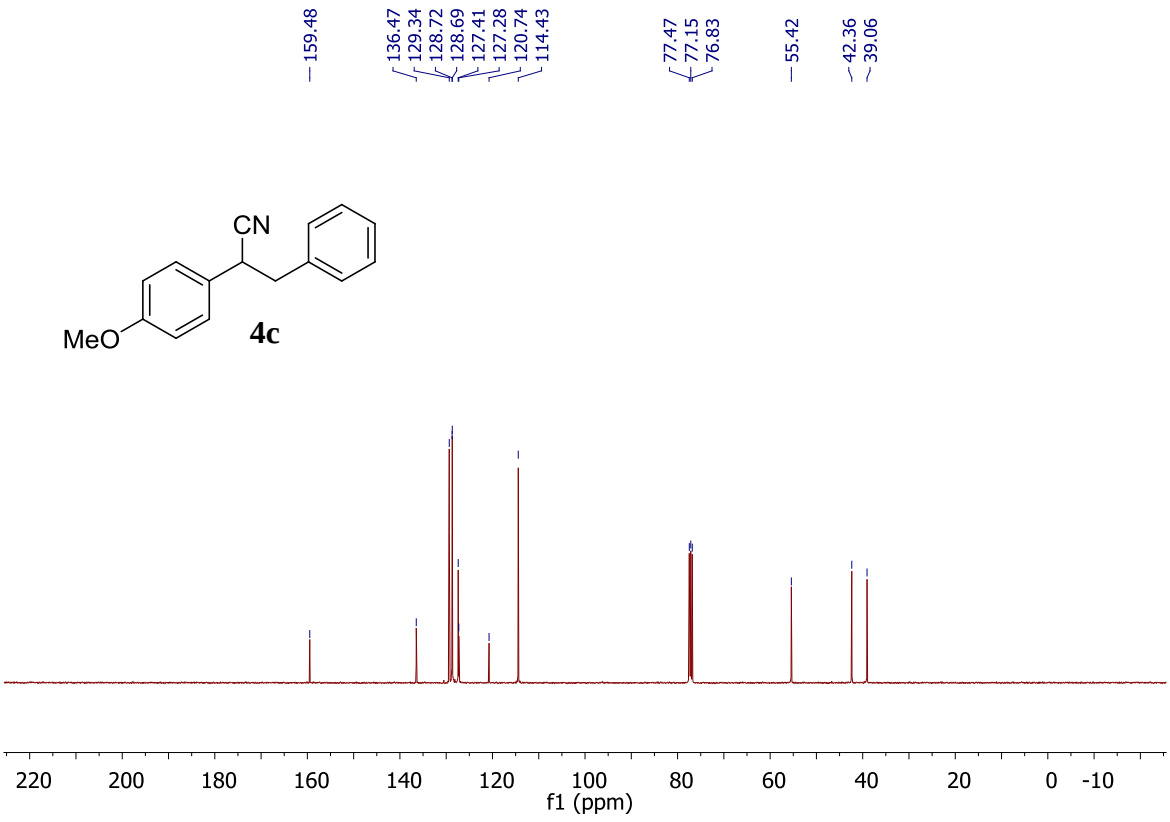
f1 (ppm)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77.47
77.15
76.83
55.42
42.36
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120
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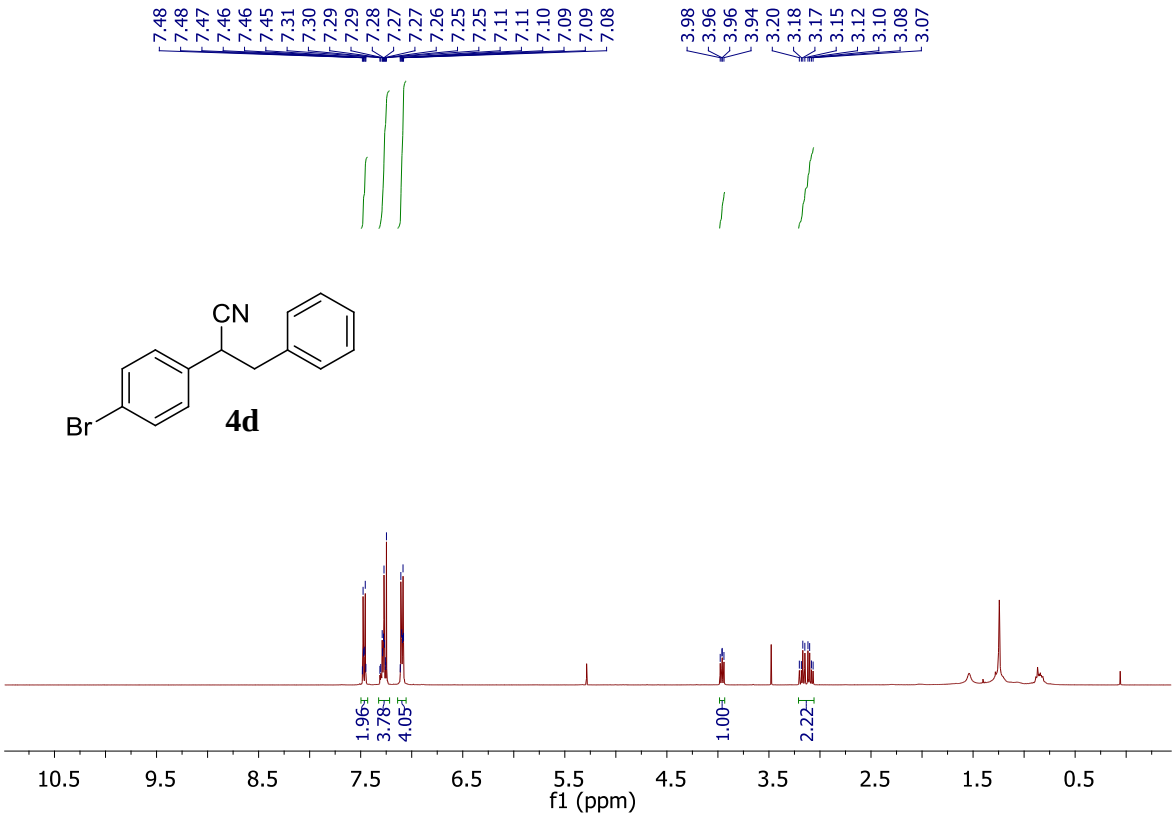
f1 (ppm)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7.28
7.27
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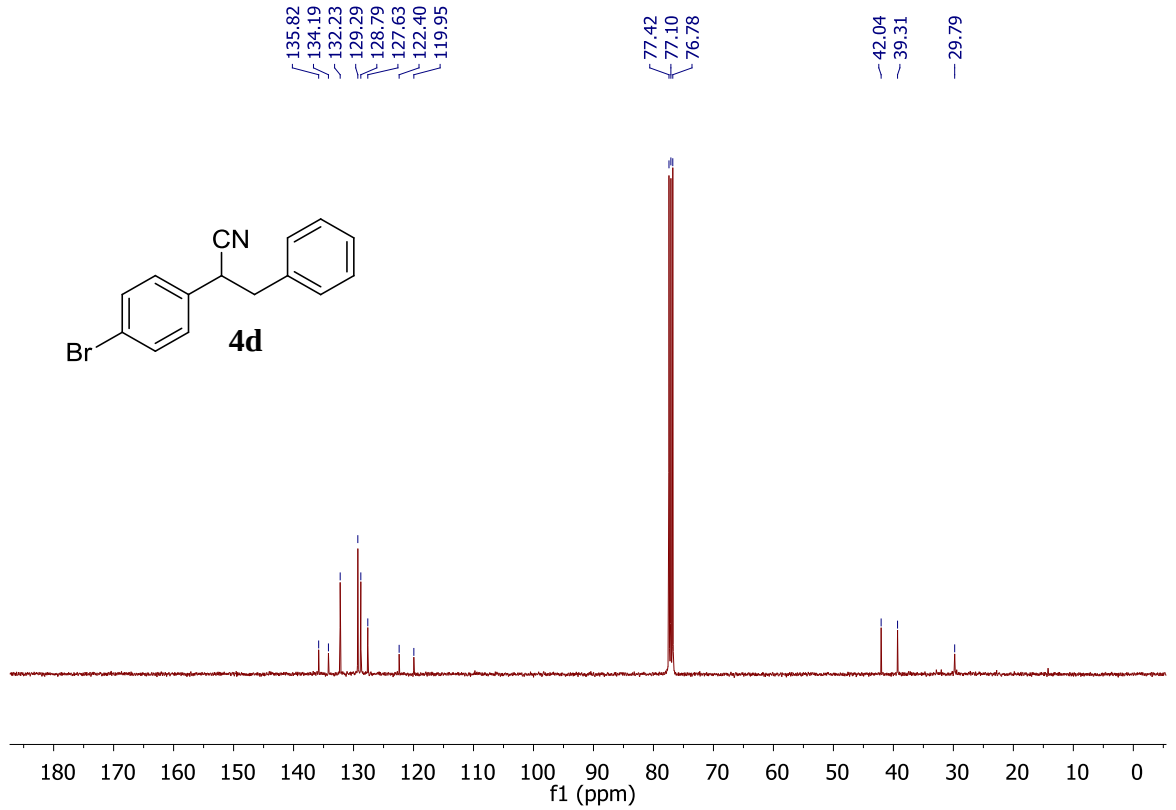
7.26
7.25
7.25
7.11
7.11
7.10
7.09
7.09
7.08
3.98
3.96
3.96
3.94
3.20
3.18
3.17
3.15
3.12
3.10
3.08
3.07
CN
Br
4d
1.96
3.78
4.05
1.00
2.22
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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77.42
77.10
76.78
42.04
39.31
29.79
CN
Br
4d
180
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160
150
140
130
120
110
100
90
80
70
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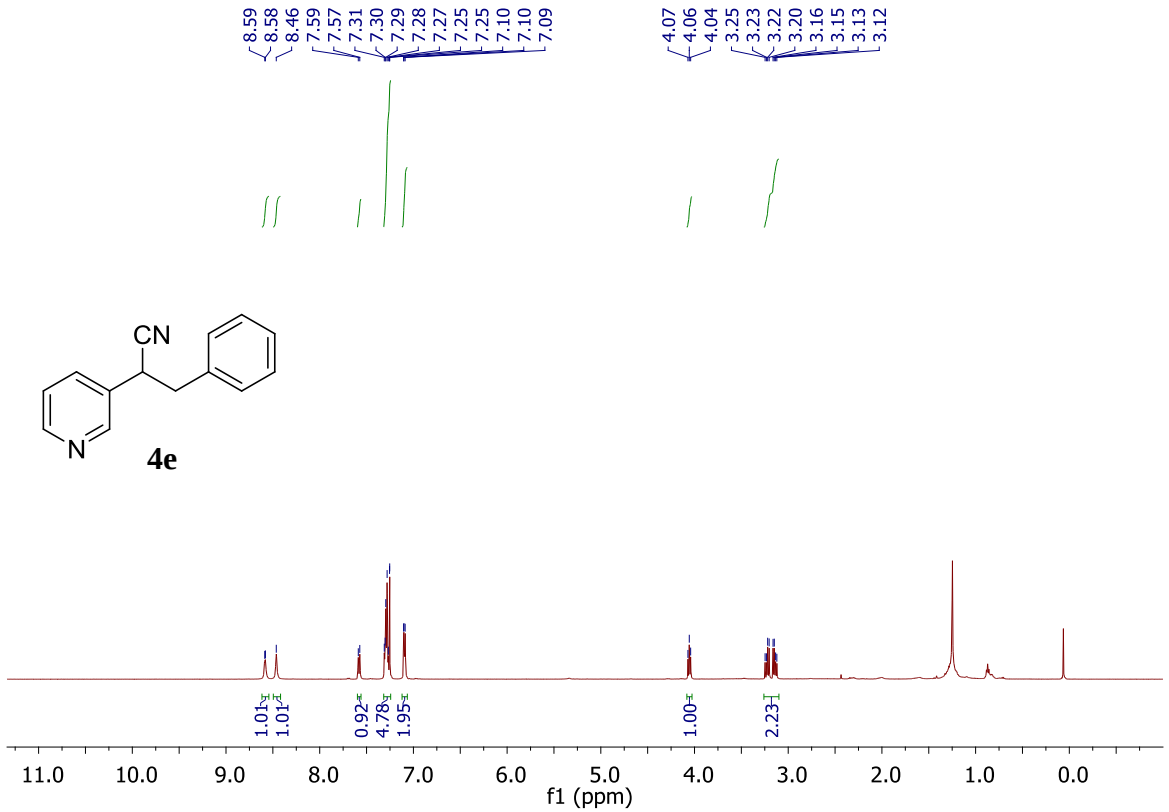
50
40
30
20
10
0
f1 (ppm)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7.25
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7.10
7.10
7.09
4.07
4.06
4.04
3.25
3.23
3.22
3.20
3.16
3.15
3.13
3.12
CN
N
4e
1.01
1.01
0.92
4.78
1.95
1.00
2.23
11.0
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9.0
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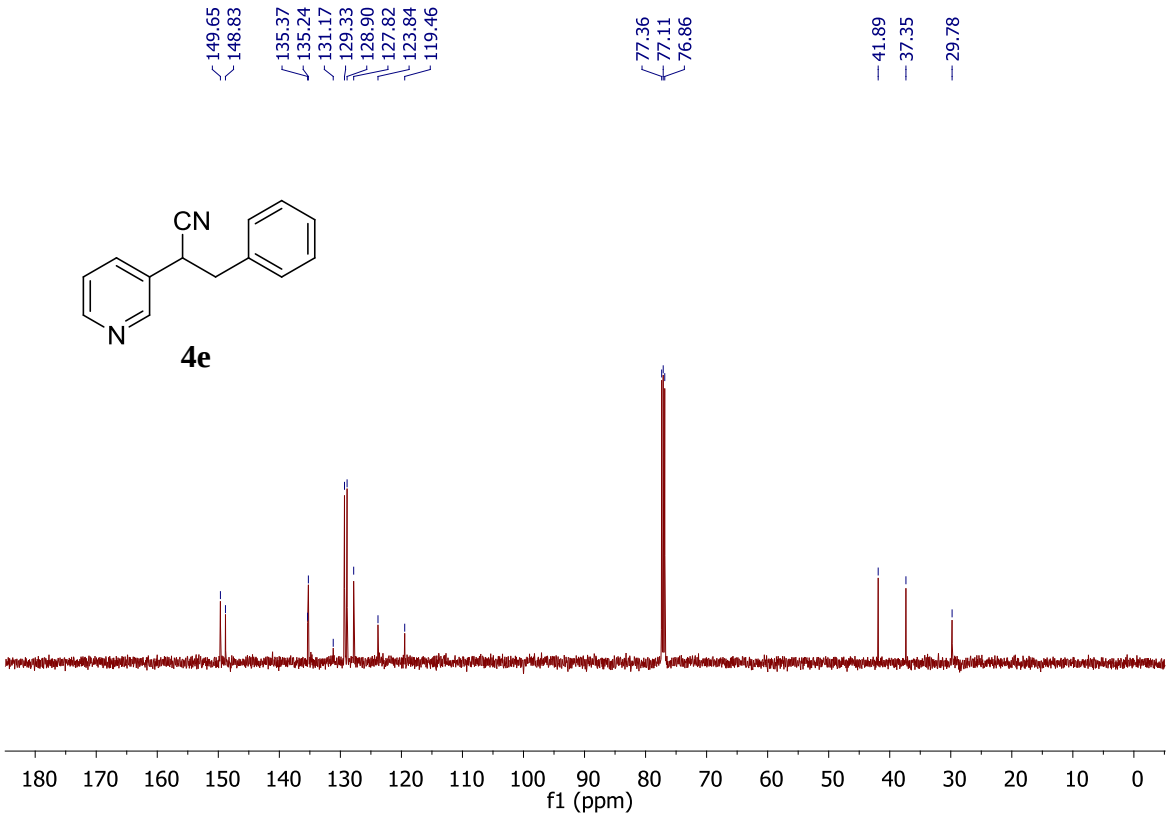
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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148.83
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129.33
128.90
127.82
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119.46
77.36
77.11
76.86
41.89
37.35
29.78
CN
N
4e
180
170
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130
120
110
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90
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70
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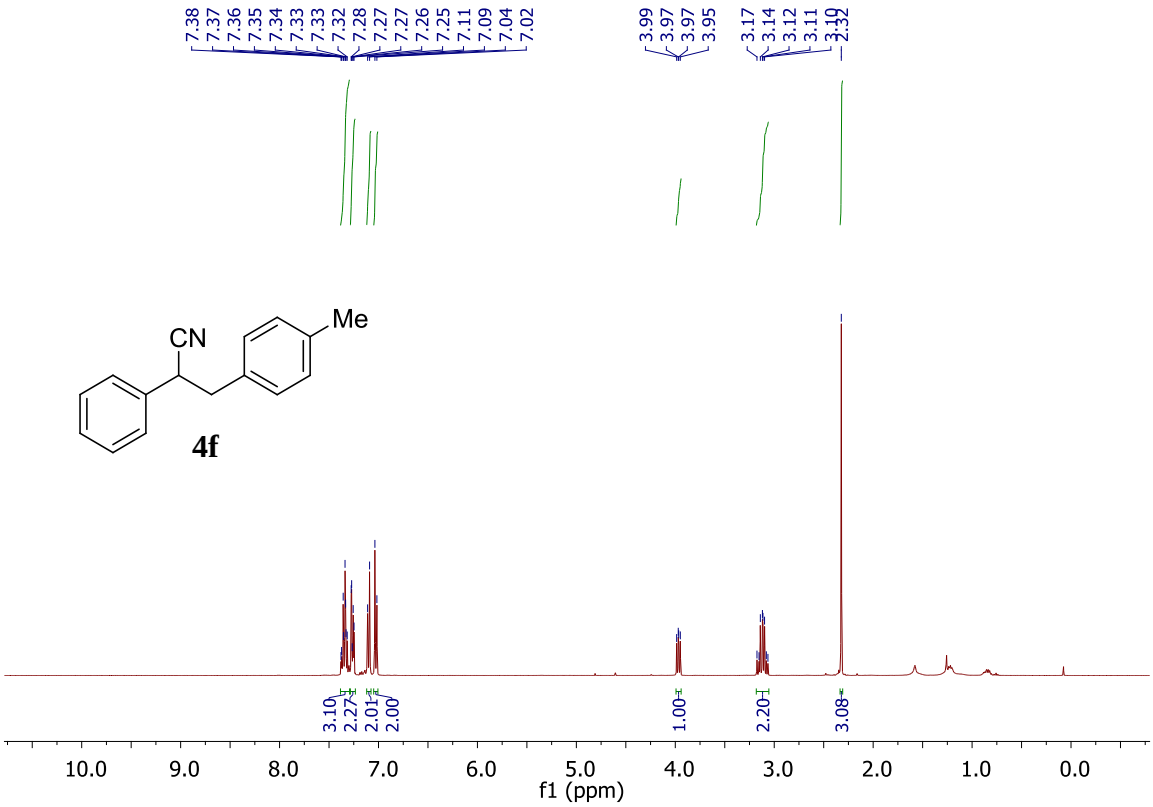
10
0
f1 (ppm)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7.09
7.04
7.02
3.99
3.97
3.97
3.95
3.17
3.14
3.12
3.11
3.10
2.32
CN
Me
4f
3.10
2.27
2.01
2.00
1.00
2.20
3.08
10.0
9.0
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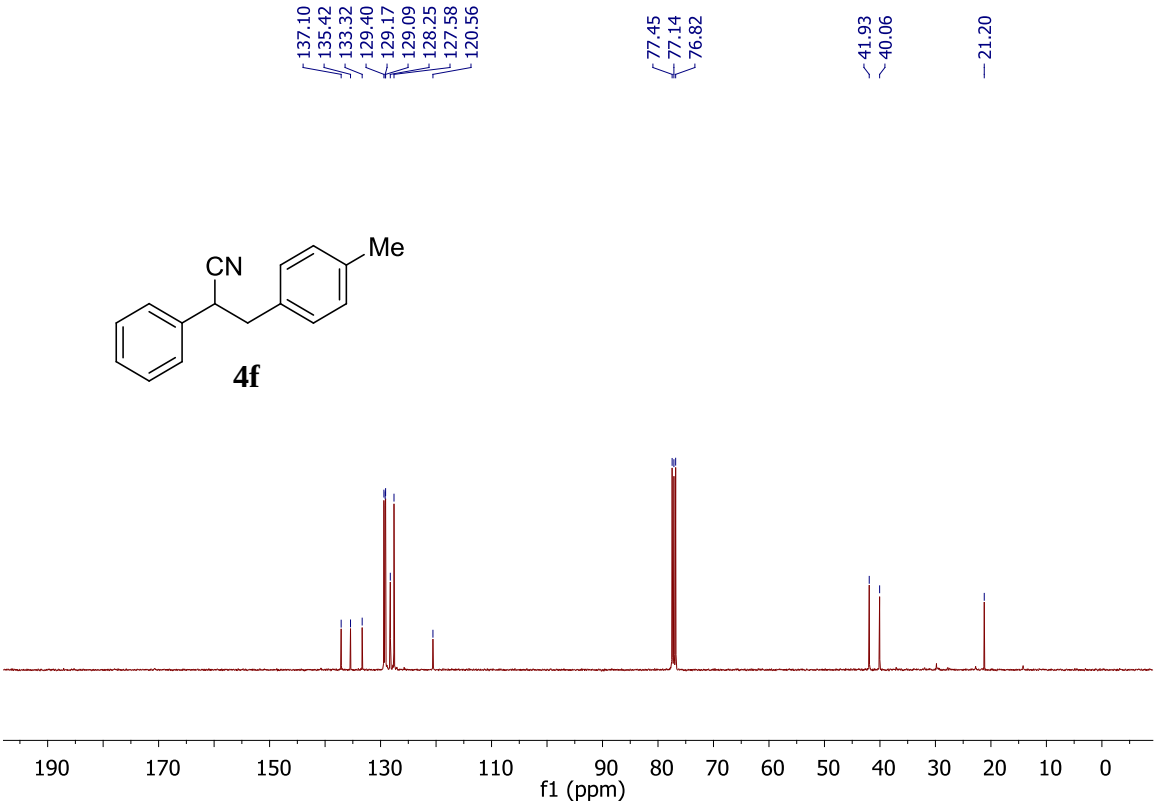
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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133.32
129.40
129.17
129.09
128.25
127.58
120.56
77.45
77.14
76.82
41.93
40.06
21.20
CN
Me
4f
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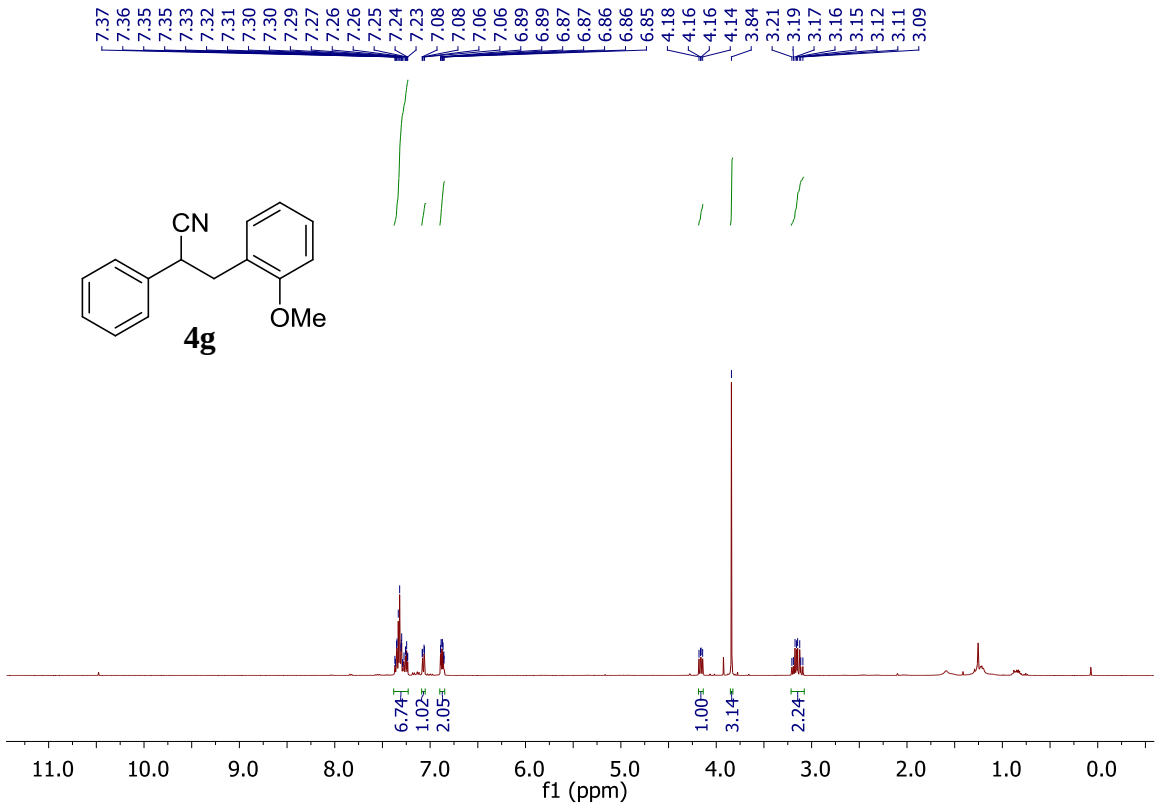
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.26
7.25
7.24
7.23
7.08
7.08
7.06
7.06
6.89
6.89
6.87
6.87
6.86
6.86
6.85
4.18
4.16
4.16
4.14
3.84
3.21
3.19
3.17
3.16
3.15
3.12
3.11
3.09
CN
OMe
6.74
1.02
2.05
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3.14
2.24
11.0
10.0
9.0
8.0
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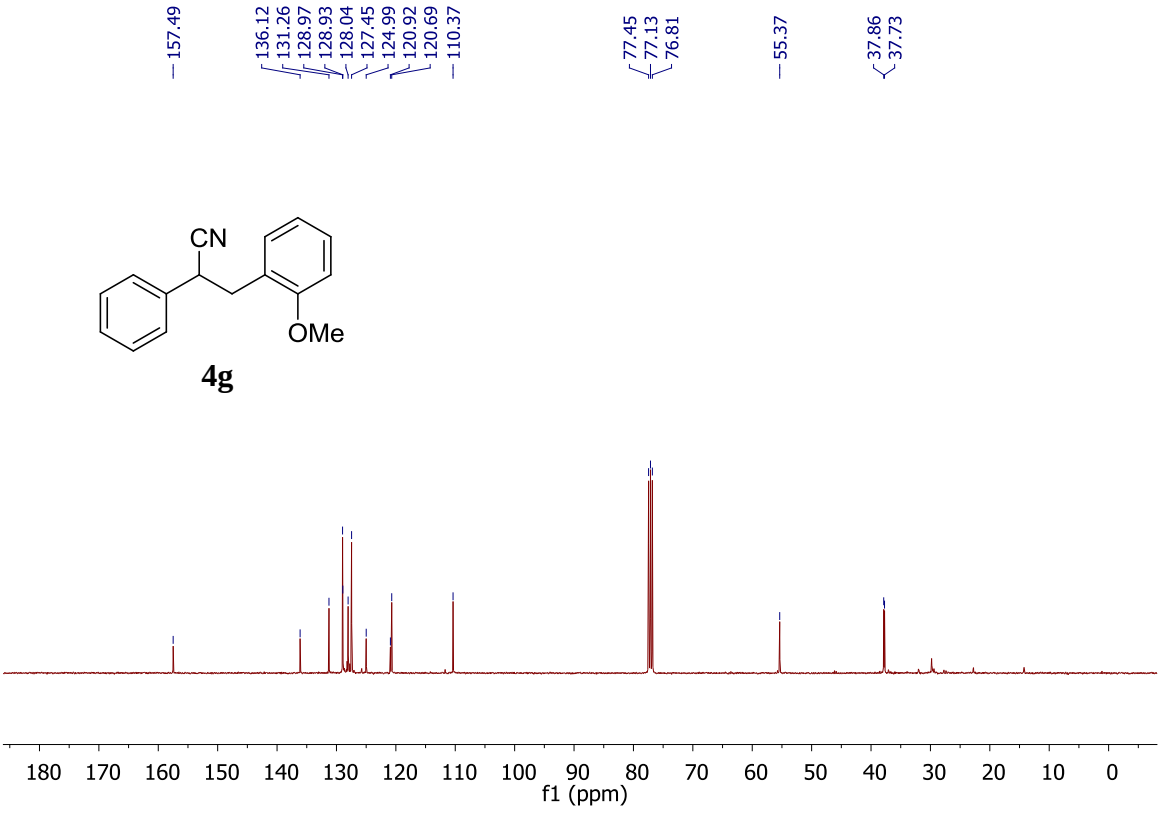
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

4g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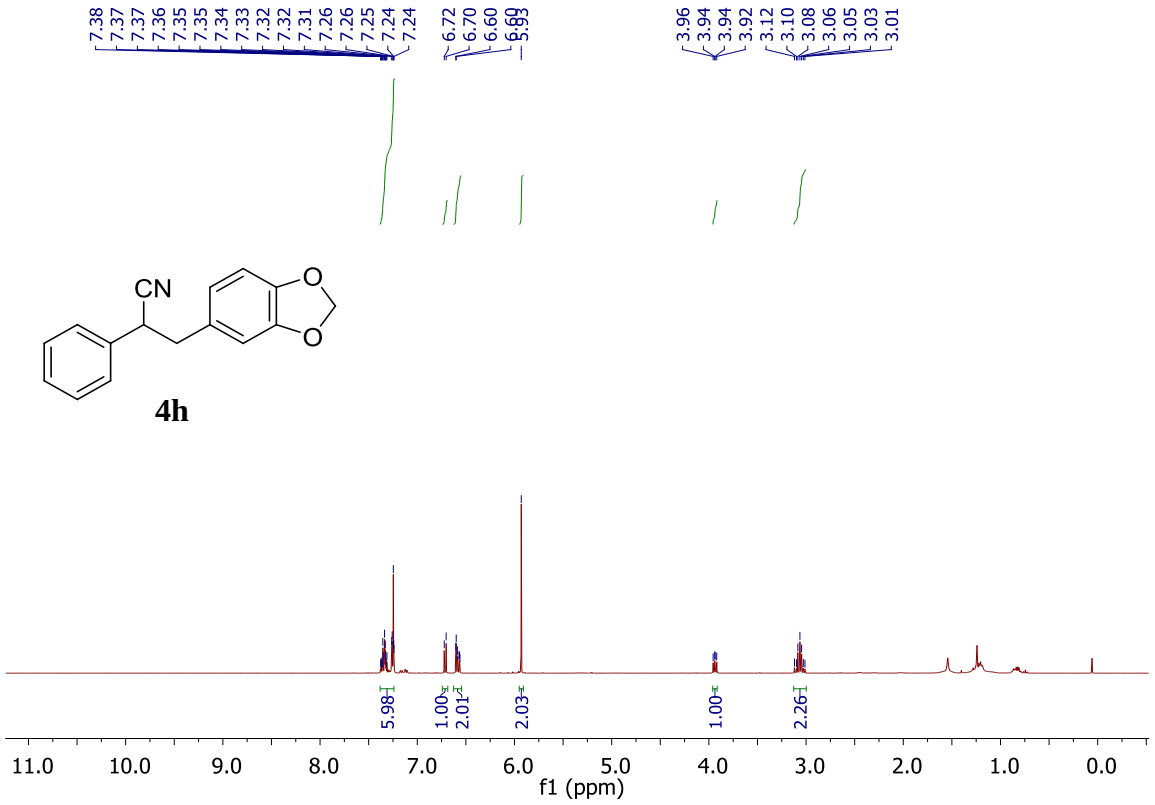
131.26
128.97
128.93
128.04
127.45
124.99
120.92
120.69
110.37
77.45
77.13
76.81
55.37
37.86
37.73
CN
OMe
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4g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7.37
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7.33
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7.32
7.31
7.26
7.26
7.25
7.24
7.24
6.72
6.70
6.60
3.96
3.94
3.94
3.92
3.12
3.10
3.08
3.06
3.05
3.03
3.01
CN
O
O
4h
5.98
1.00
2.01
2.03
1.00
2.26
11.0
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9.0
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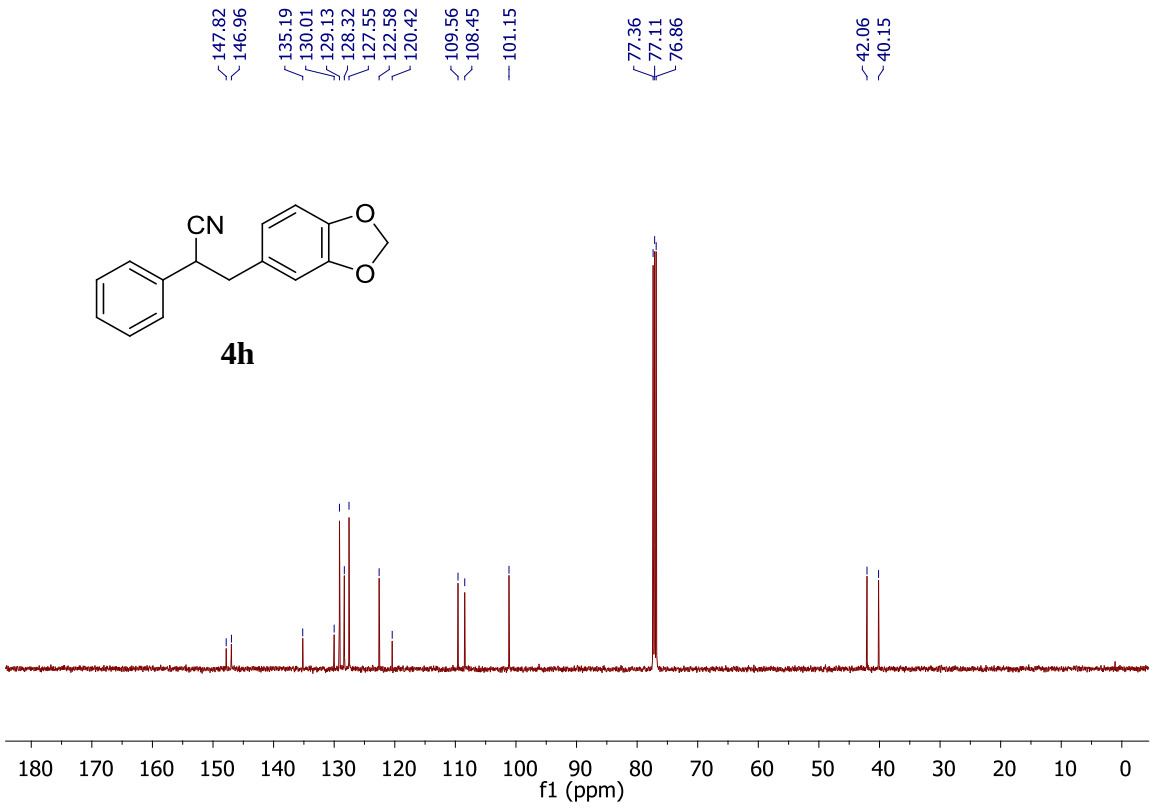
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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146.96
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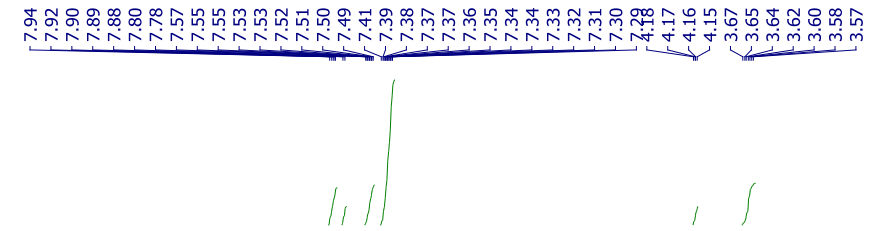
129.13
128.32
127.55
122.58
120.42
109.56
108.45
101.15
77.36
77.11
76.86
42.06
40.15
CN
O
O
4h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.89
7.88
7.80
7.78
7.57
7.55
7.55
7.53
7.53
7.52
7.51
7.50
7.49
7.41
7.39
7.38
7.37
7.37
7.36
7.35
7.34
7.34
7.33
7.32
7.31
7.30
4.18
4.17
4.16
4.15
3.67
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3.64
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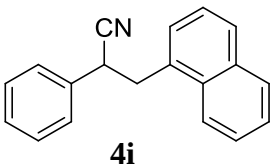
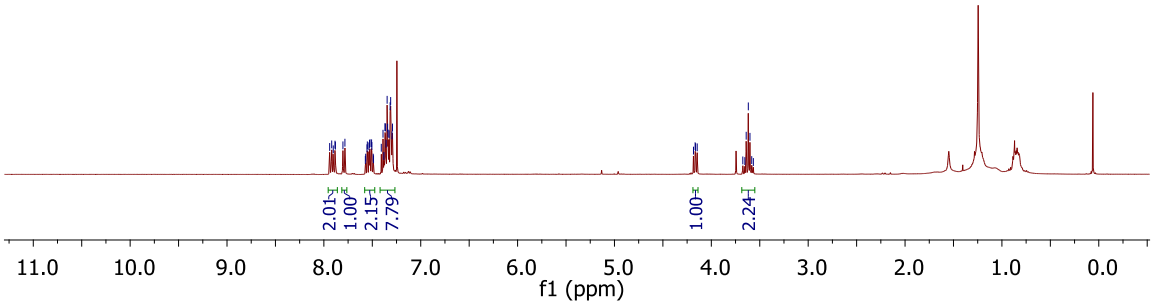
3.60
3.58
3.57


CN

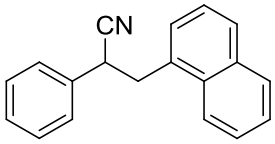
4i


2.01
1.00
2.15
7.79
1.00
2.24
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


135.69
134.04
132.28
131.36
129.35
129.22
128.42
128.39
128.22
127.44
126.64
125.88
125.57
122.67
120.56

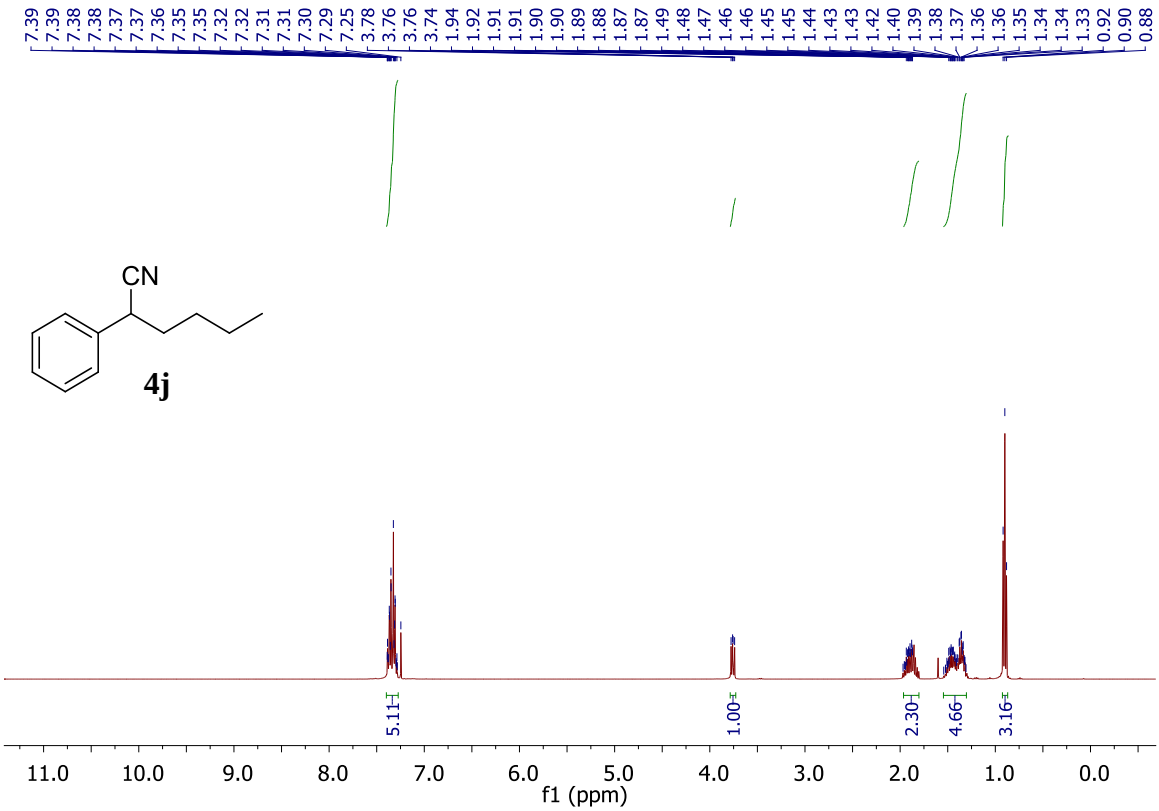

77.42
77.10
76.78

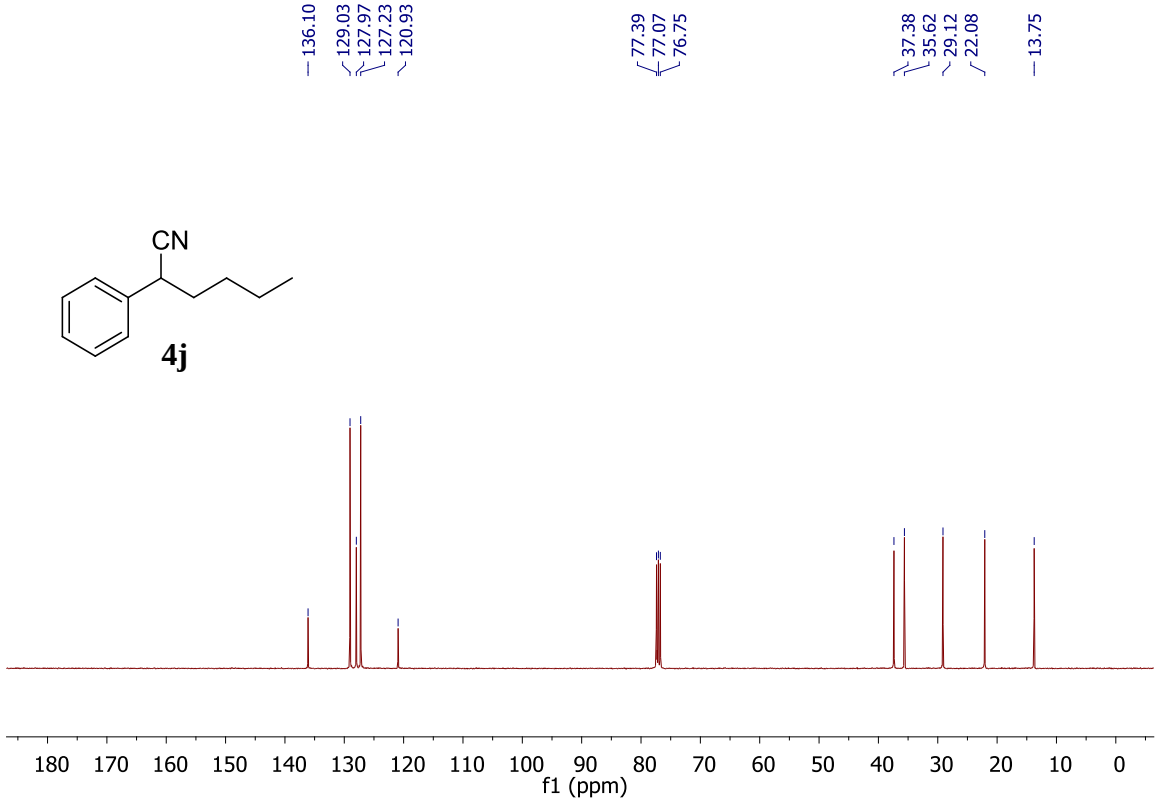

39.70
38.91
29.79


CN

4i

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.35 7.35 7.32 7.32 7.31 7.31 7.30 7.29 7.25 3.78 3.76 3.76 3.74 1.94 1.92 1.91 1.91 1.90 1.90 1.89 1.88 1.87 1.87 1.49 1.48 1.47 1.46 1.46 1.45 1.45 1.44 1.43 1.43 1.42 1.40 1.39 1.38 1.37 1.36 1.36 1.35 1.34 1.34 1.33 0.92 0.90 0.88
CN
4j
5.11
1.00
2.30
4.66
3.16
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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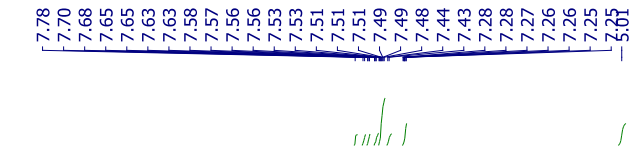
129.03
127.97
127.23
120.93
77.39
77.07
76.75
37.38
35.62
29.12
22.08
13.75
CN
4j
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.78
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7.58
7.57
7.56
7.56
7.53
7.53
7.51
7.51
7.51
7.49
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7.27
7.26
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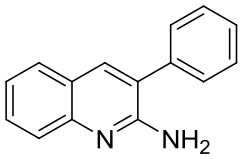
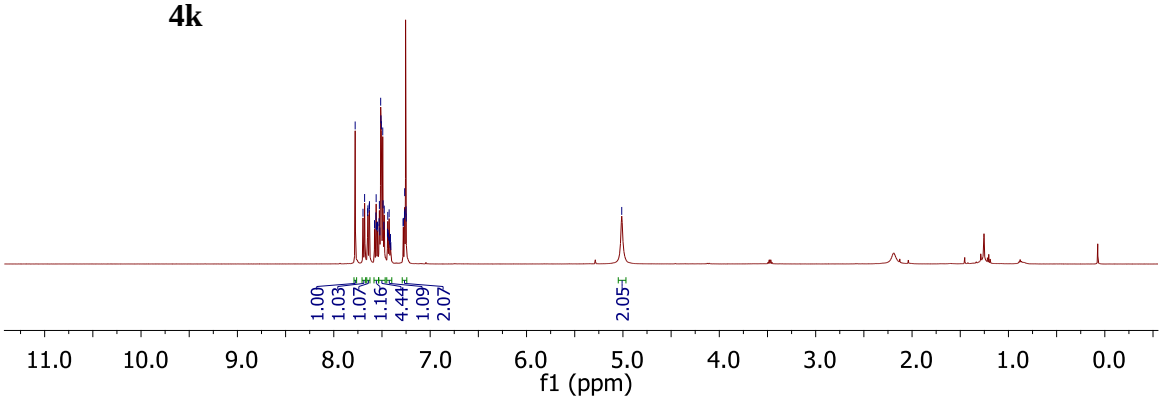
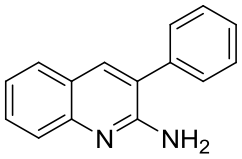
7.25
7.25
5.01


N
NH2

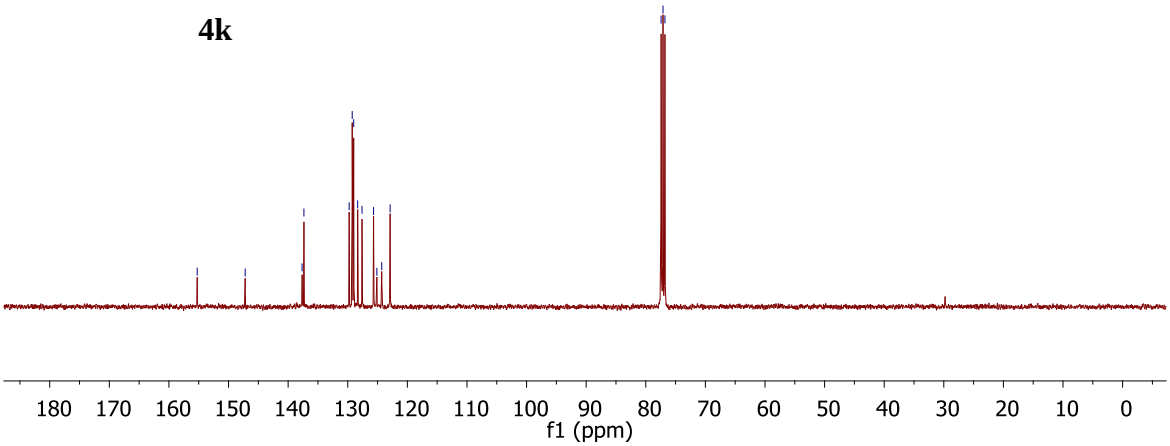
4k


1.00
1.03
1.07
1.16
4.44
1.09
2.07
2.05
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


155.26
147.21
137.66
137.35
129.76
129.25
129.00
128.33
127.60
125.67
125.12
124.30
122.89
77.43
77.11
76.79


N
NH2

4k


180
170
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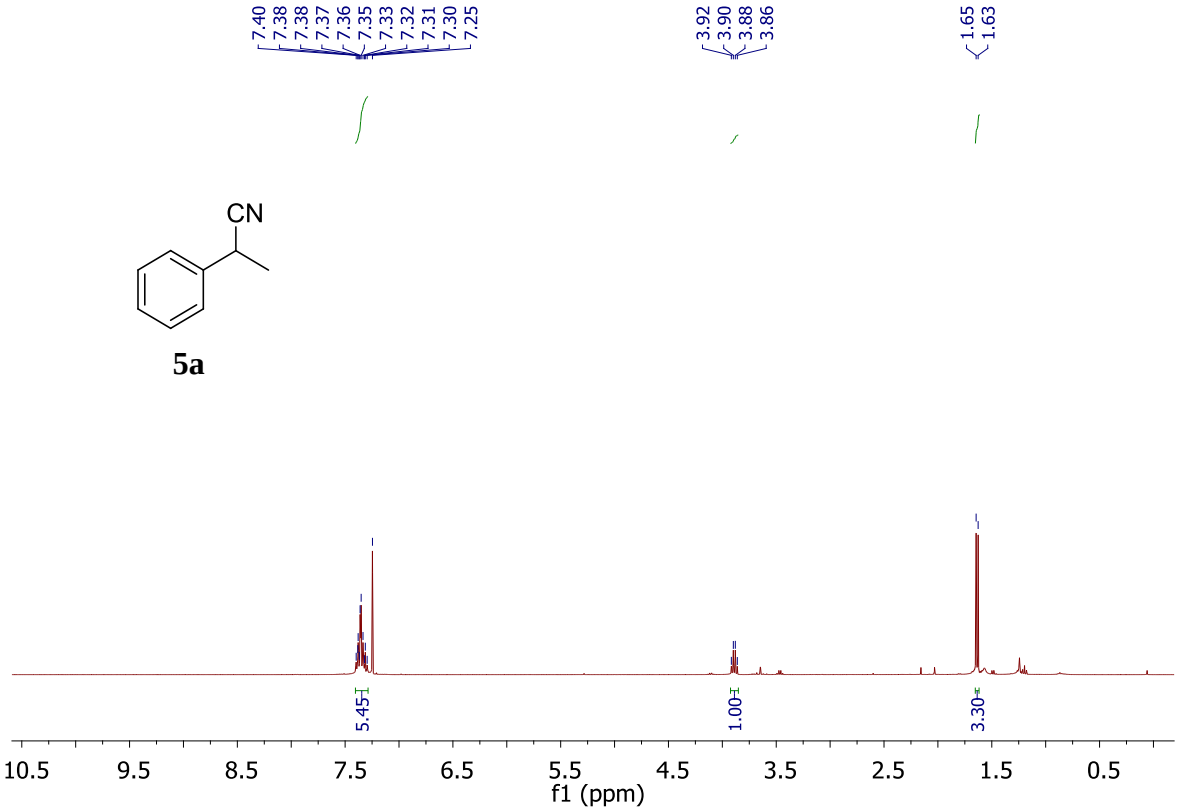
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.38
7.38
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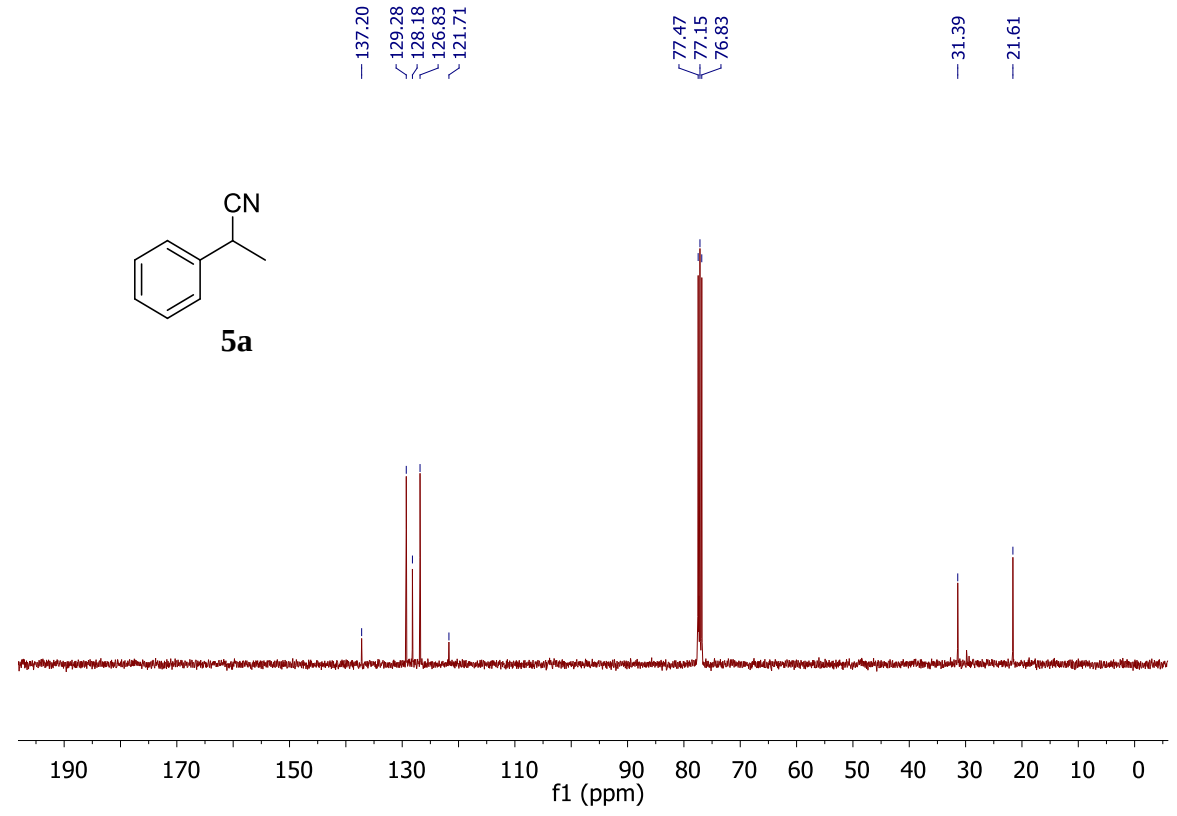
7.35
7.33
7.32
7.31
7.30
7.25
3.92
3.90
3.88
3.86
1.65
1.63
CN
5a
5.45
1.00
3.30
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


137.20
129.28
128.18
126.83
121.71
77.47
77.15
76.83
31.39
21.61
CN
5a
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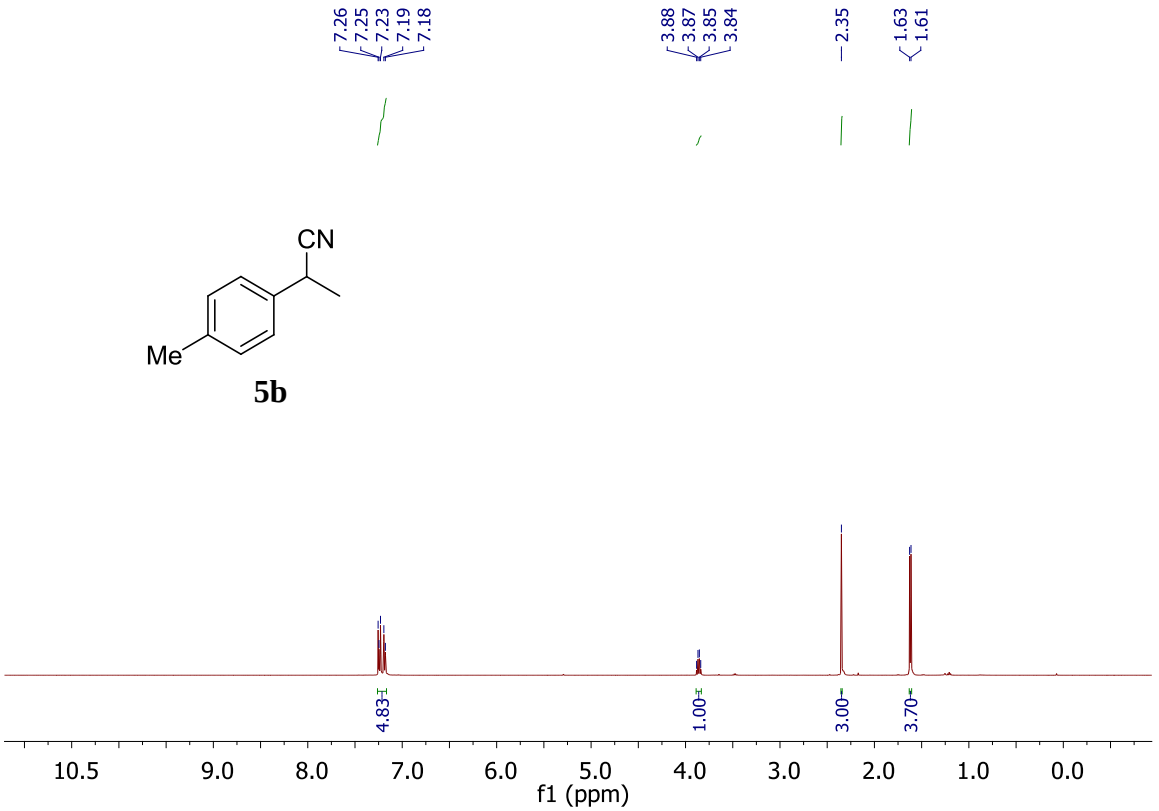
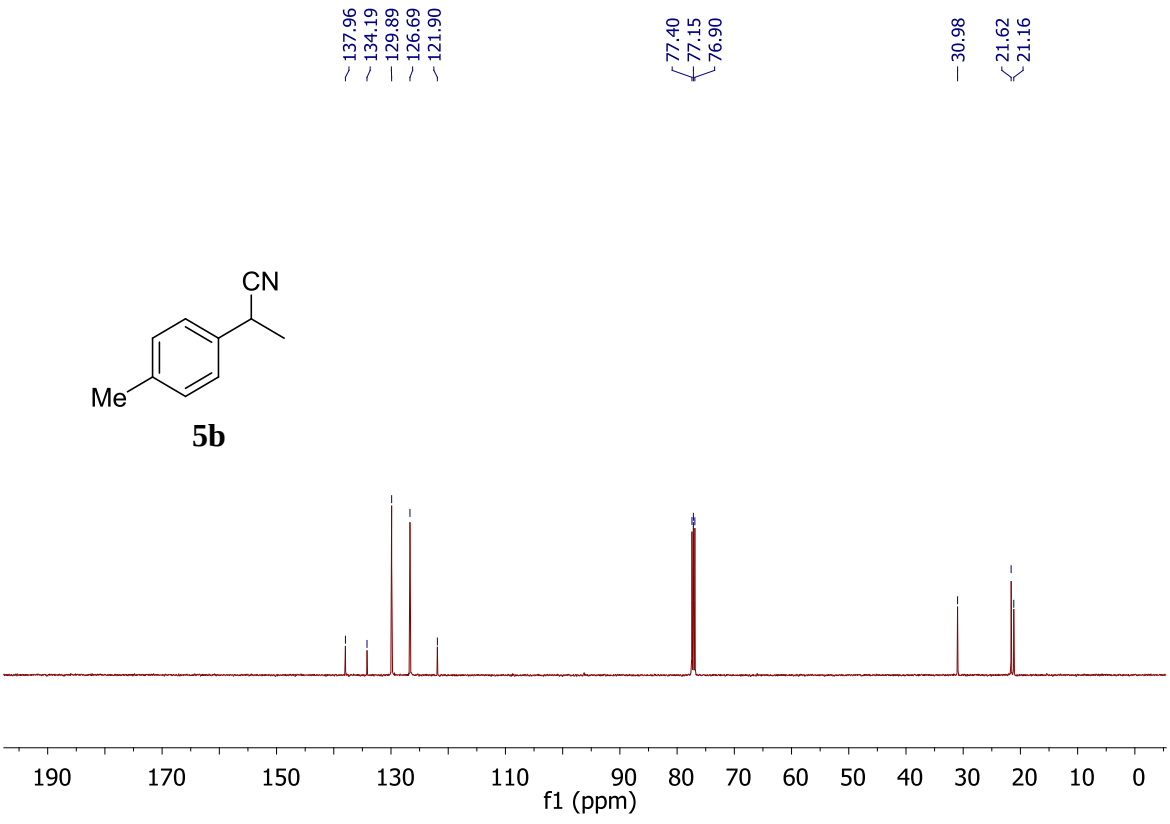
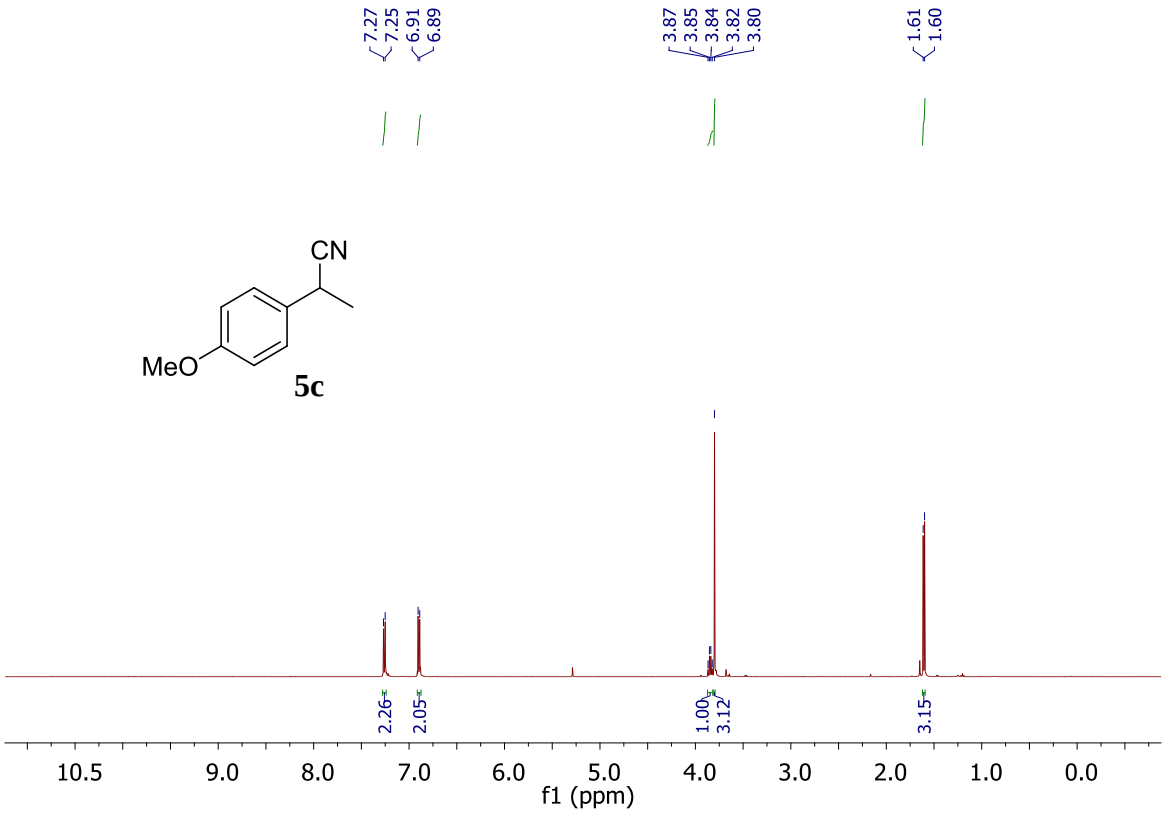
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.26
7.25
7.23
7.19
7.18
3.88
3.87
3.85
3.84
2.35
1.63
1.61
CN
Me
4.83
1.00
3.00
3.70
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

5b


137.96
134.19
129.89
126.69
121.90
77.40
77.15
76.90
30.98
21.62
21.16
CN
Me
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5b


7.27
7.25
6.91
6.89
3.87
3.85
3.84
3.82
3.80
1.61
1.60
CN
MeO
2.26
2.05
1.00
3.12
3.15
10.5
9.0
8.0
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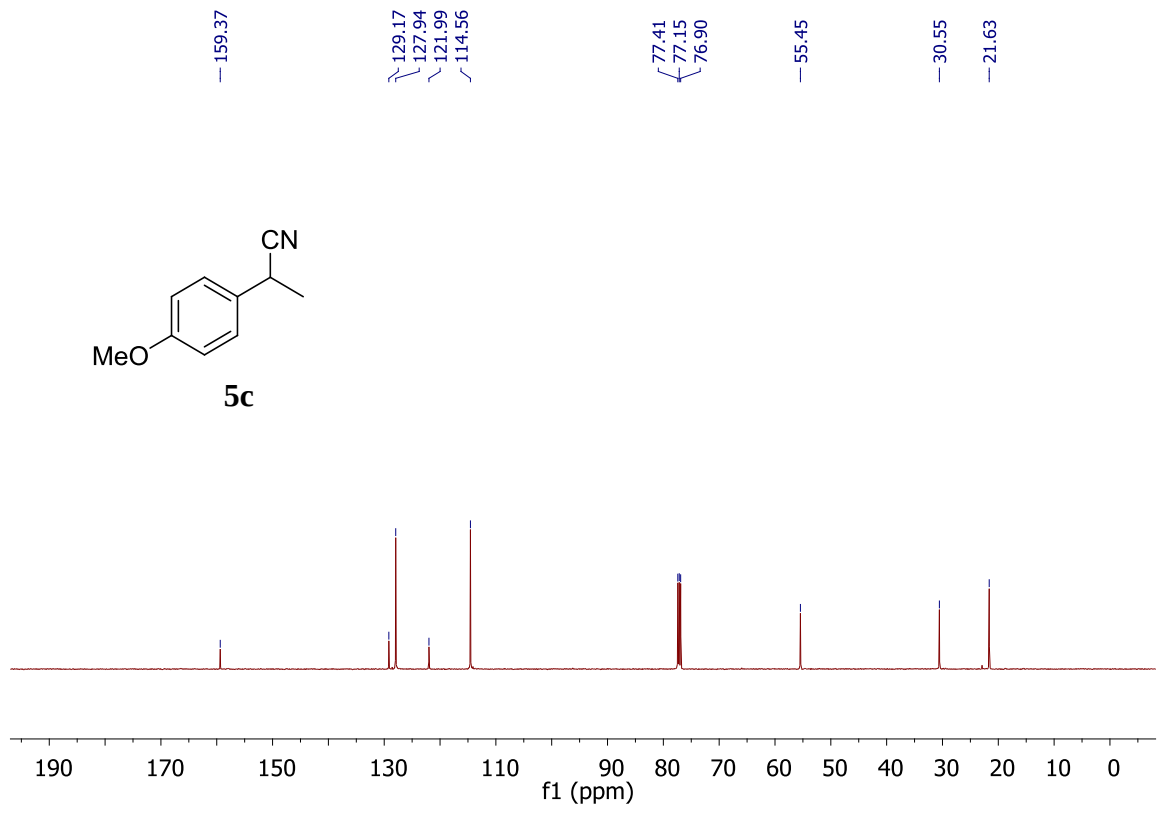
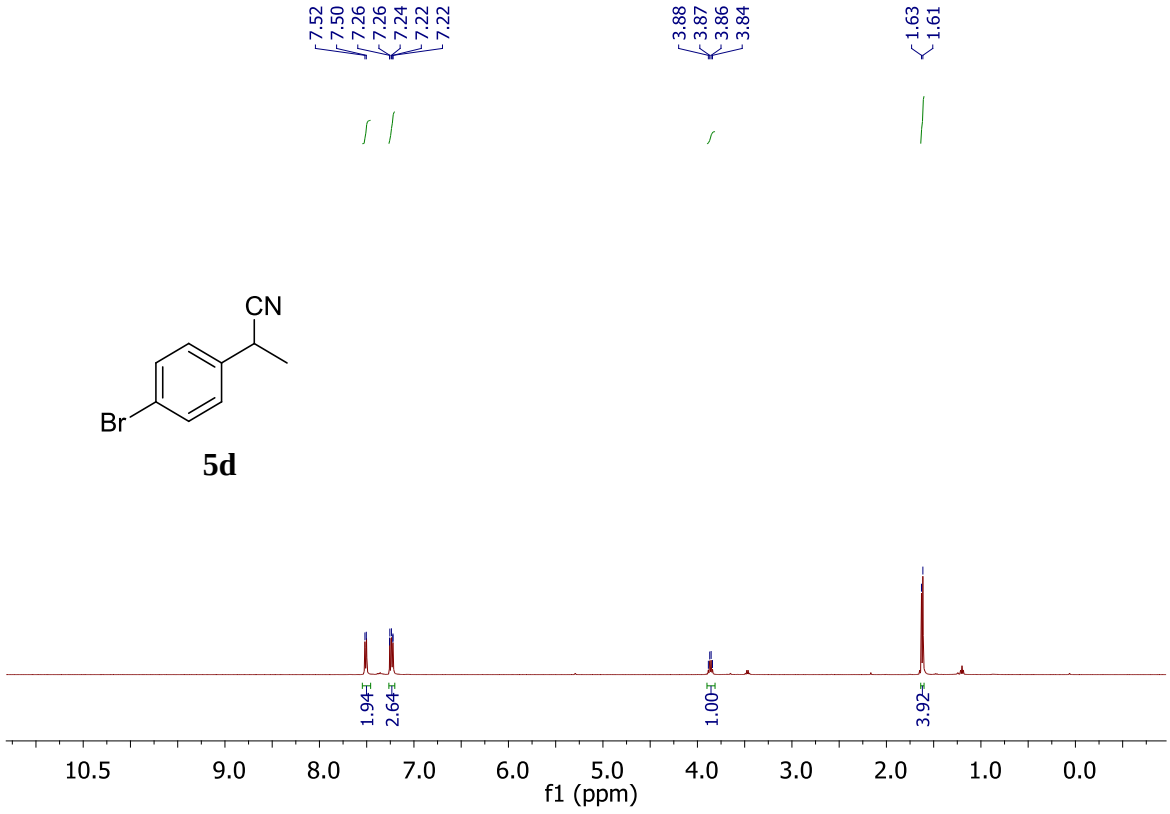
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

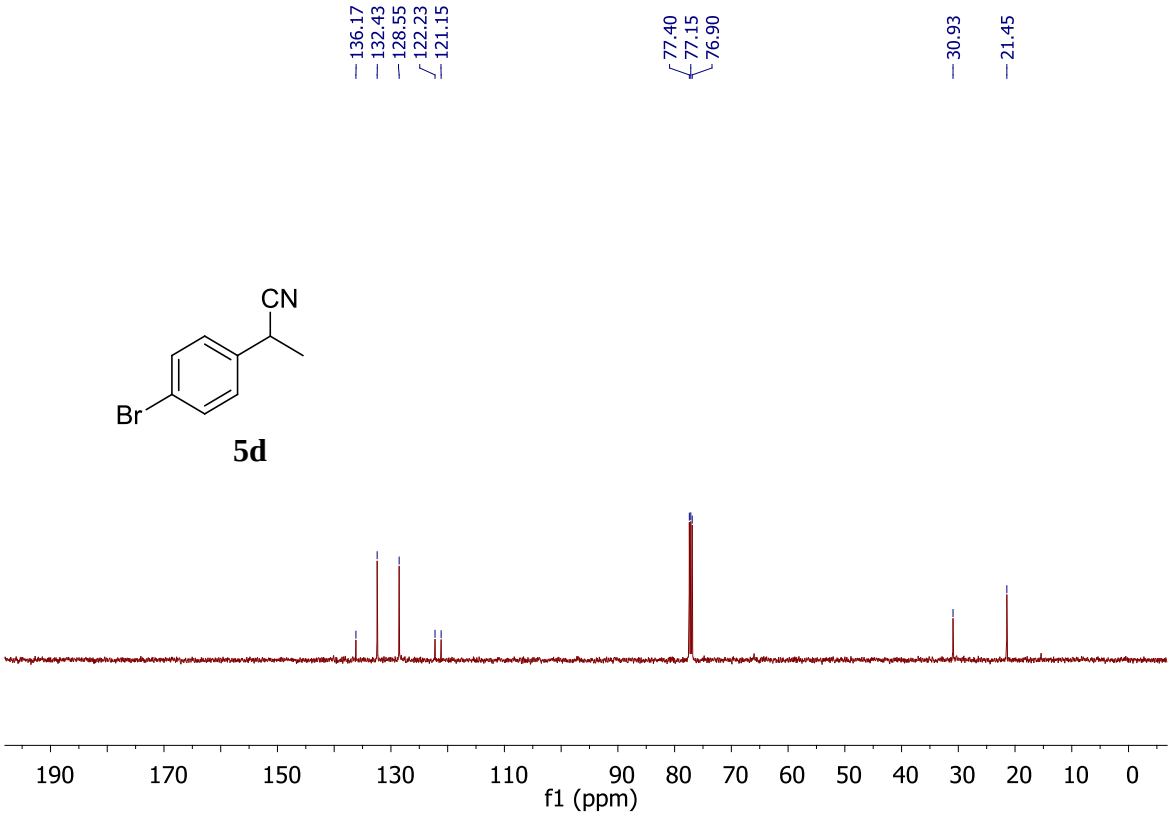
5c


159.37
129.17
127.94
121.99
114.56
77.41
77.15
76.90
55.45
30.55
21.63
CN
MeO
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

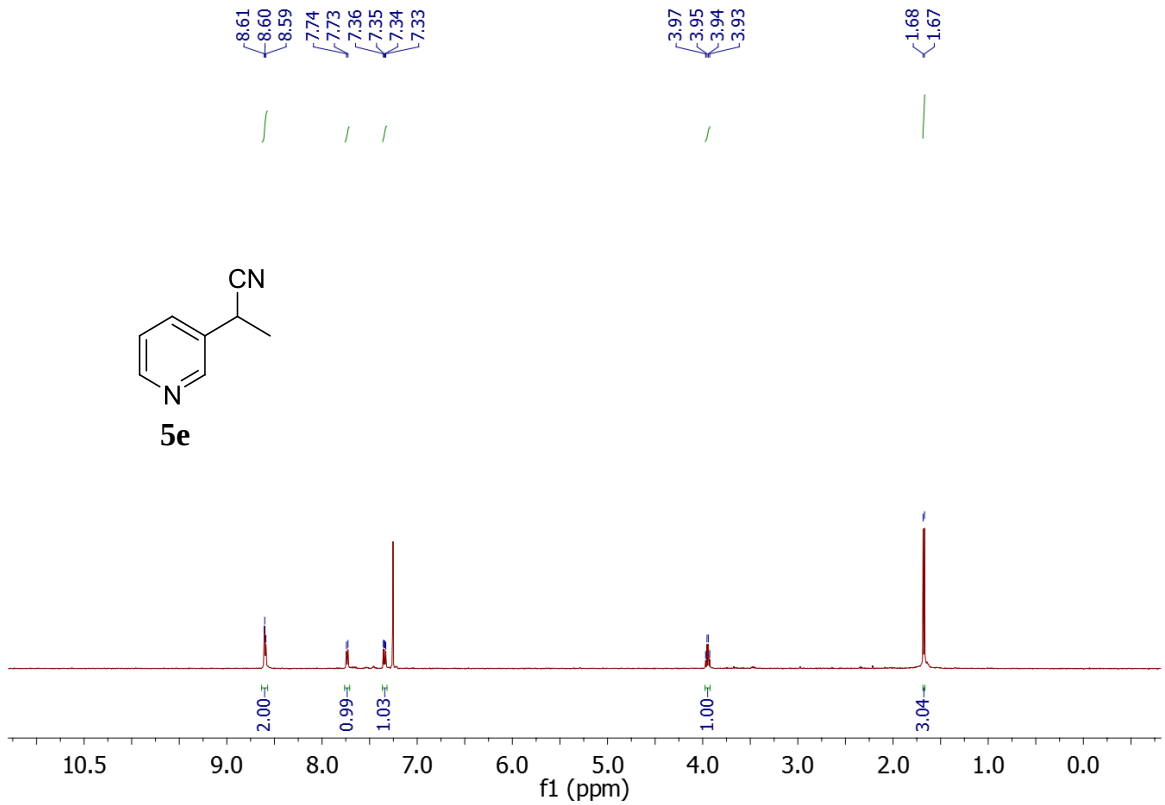
5c


7.52
7.50
7.26
7.26
7.24
7.22
7.22
3.88
3.87
3.86
3.84
1.63
1.61
CN
Br
1.94
2.64
1.00
3.92
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

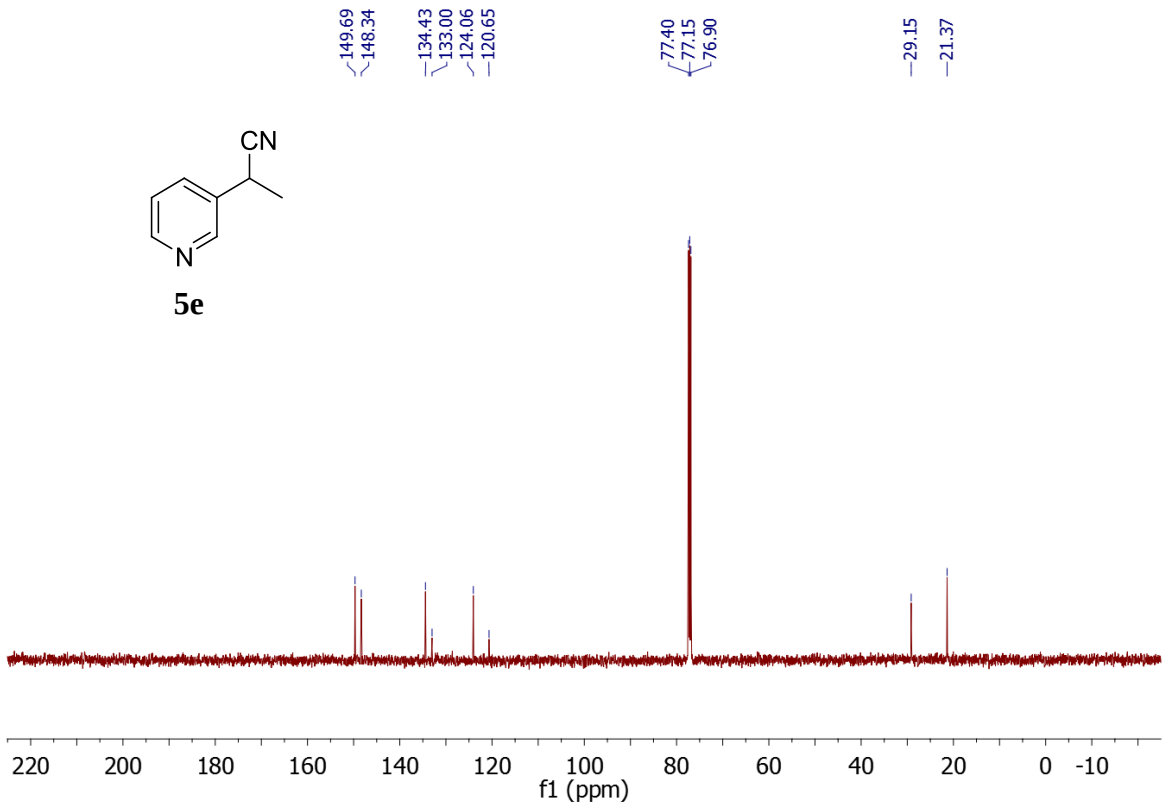
5d


136.17
132.43
128.55
122.23
121.15
77.40
77.15
76.90
30.93
21.45
CN
Br
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

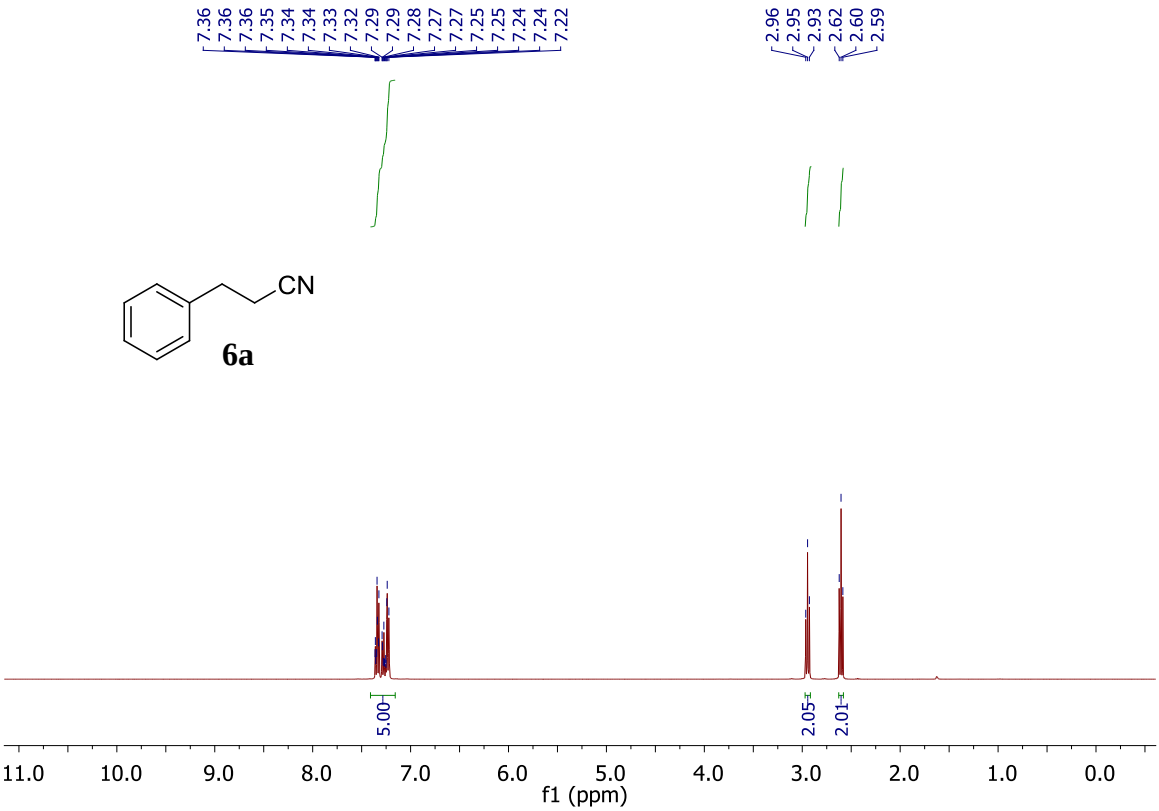
5d

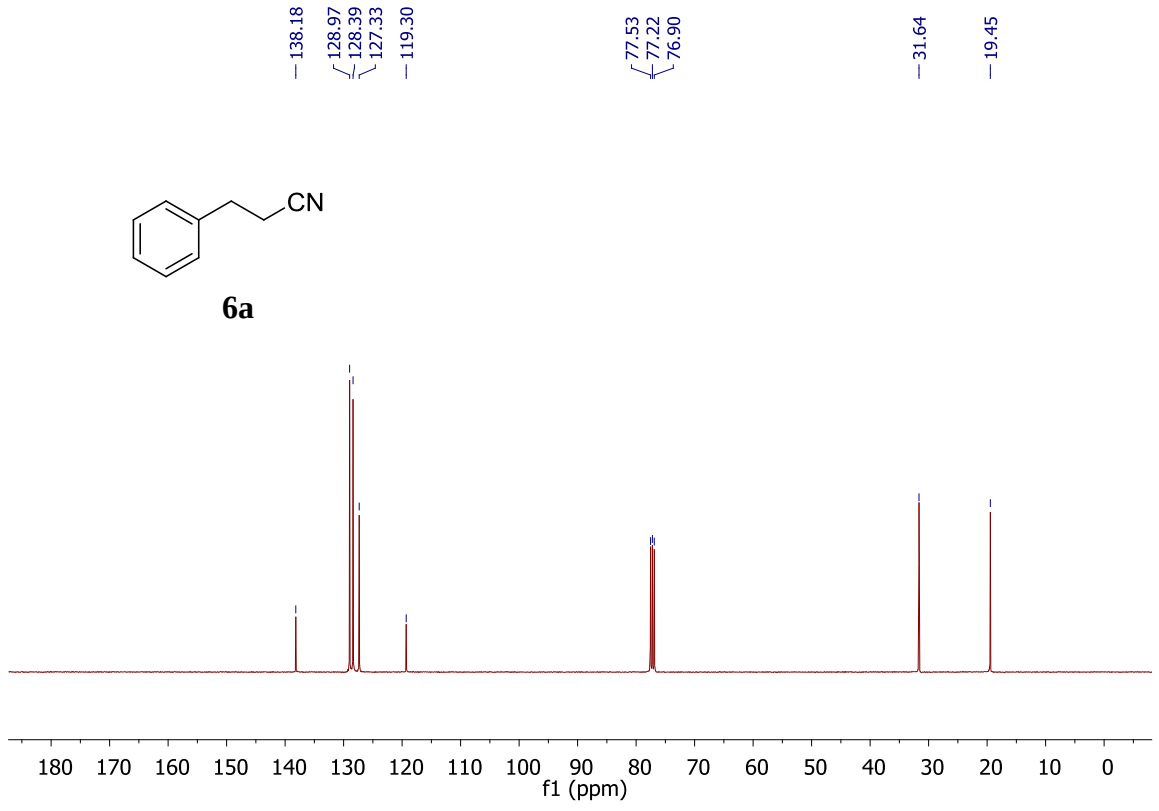

8.61
8.60
8.59
7.74
7.73
7.36
7.35
7.34
7.33
3.97
3.95
3.94
3.93
1.68
1.67
CN
N
2.00
0.99
1.03
1.00
3.04
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

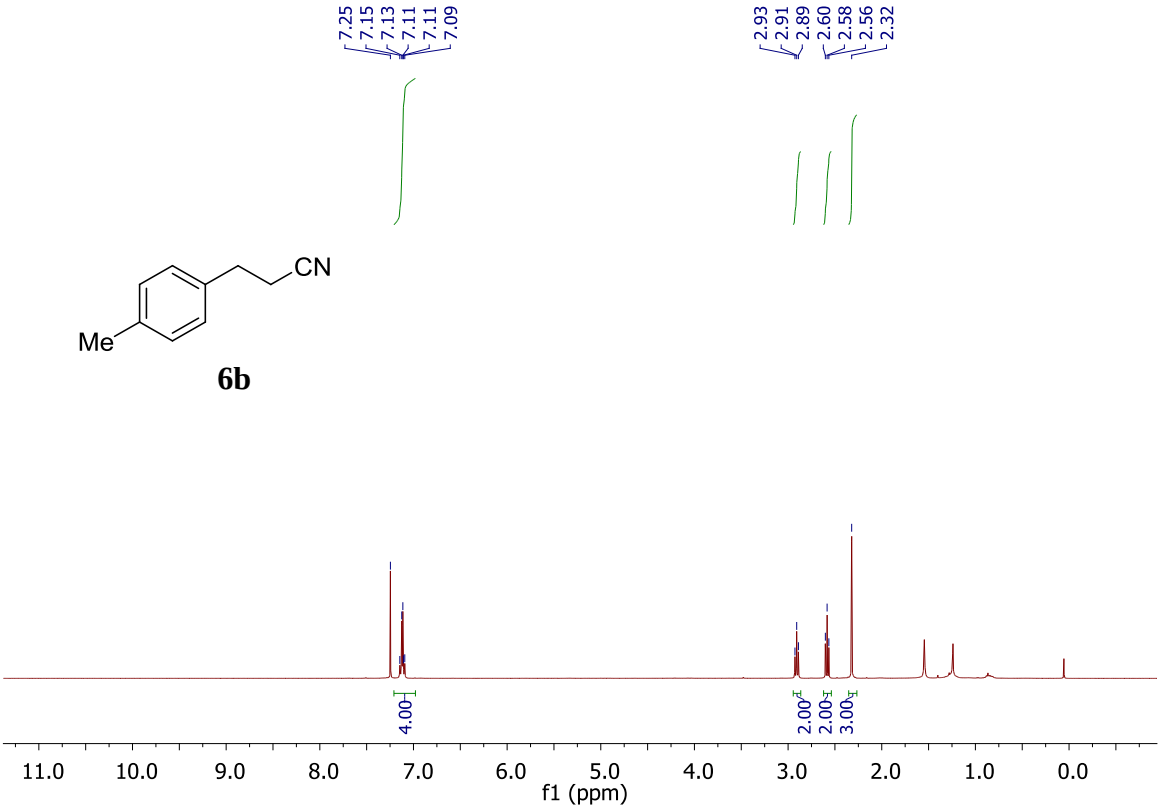
5e


149.69
148.34
134.43
133.00
124.06
120.65
77.40
77.15
76.90
29.15
21.37
CN
N
220
200
180
160
140
120
100
80
60
40
20
0
-10
f1 (ppm)

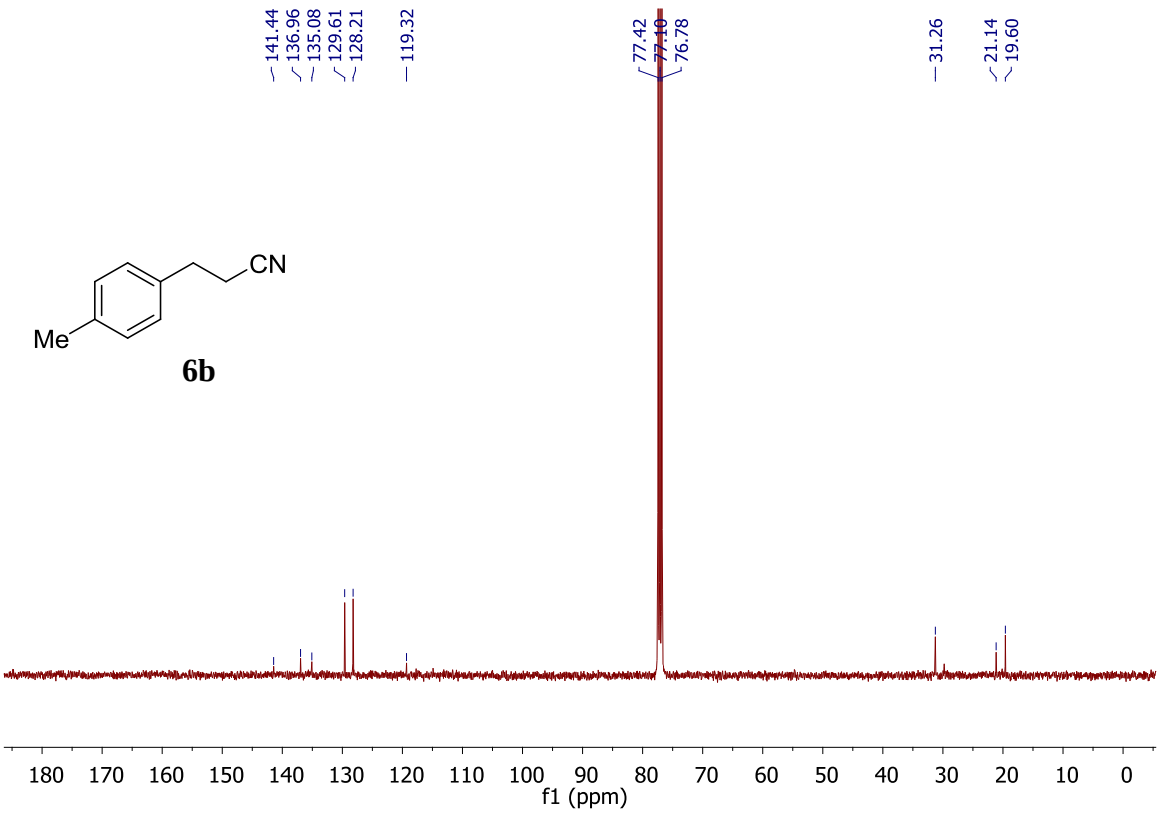
5e


7.36
7.36
7.36
7.35
7.34
7.34
7.33
7.32
7.29
7.29
7.28
7.27
7.27
7.25
7.25
7.24
7.24
7.22
2.96
2.95
2.93
2.62
2.60
2.59
CN
6a
5.00
2.05
2.01
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

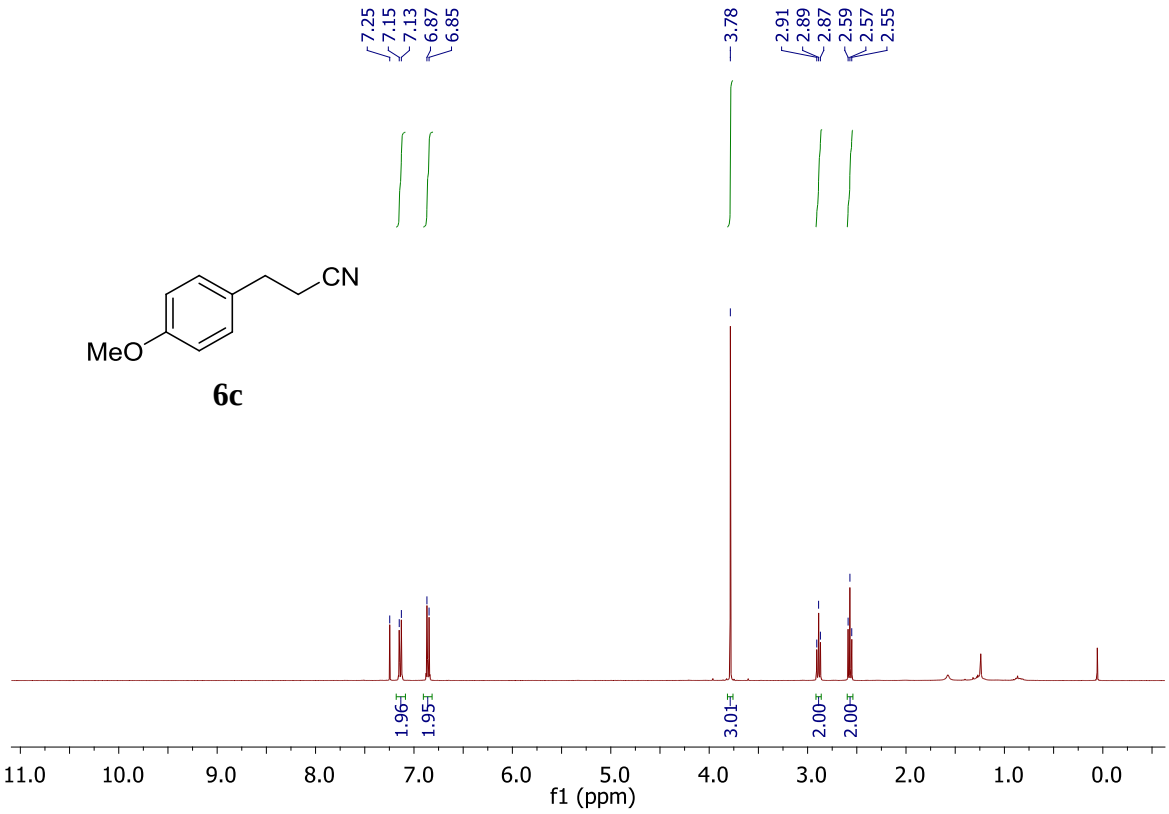

138.18
128.97
128.39
127.33
119.30
77.53
77.22
76.90
31.64
19.45
CN
6a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.25
7.15
7.13
7.11
7.11
7.09
2.93
2.91
2.89
2.60
2.58
2.56
2.32
CN
Me
4.00
2.00
2.00
3.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

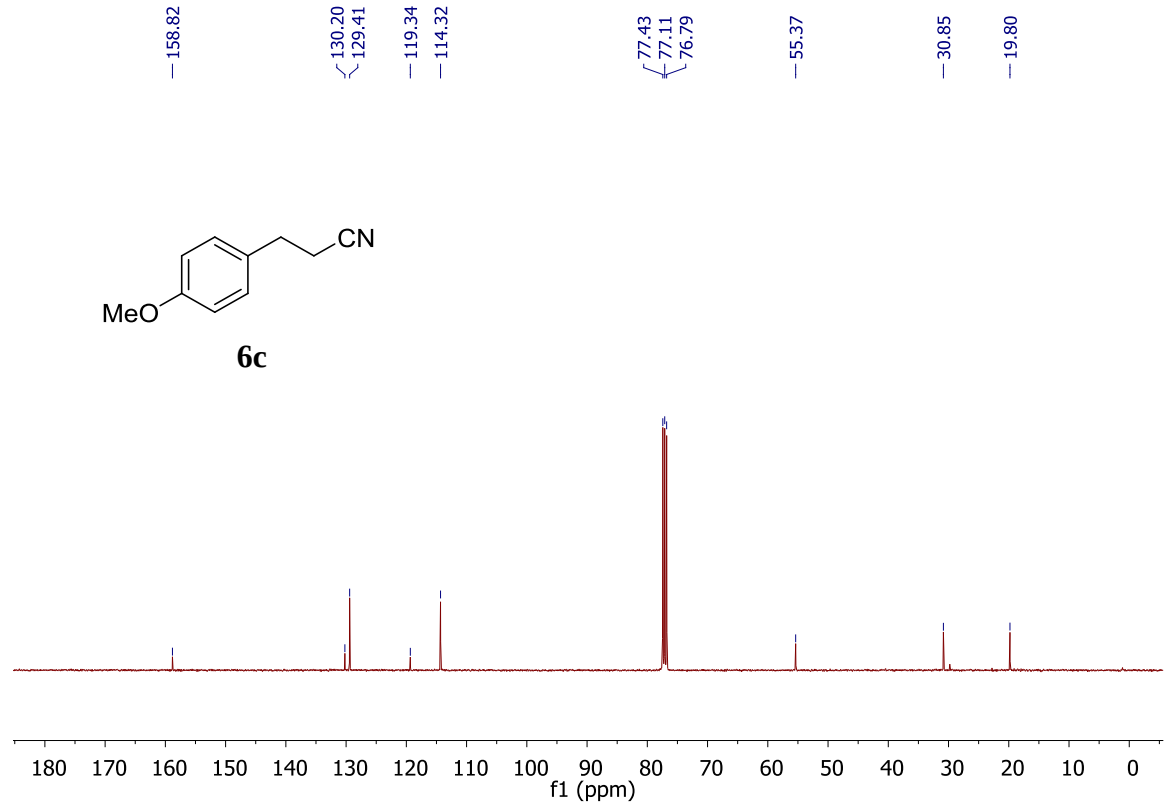
6b


141.44
136.96
135.08
129.61
128.21
119.32
77.42
77.10
76.78
31.26
21.14
19.60
CN
Me
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

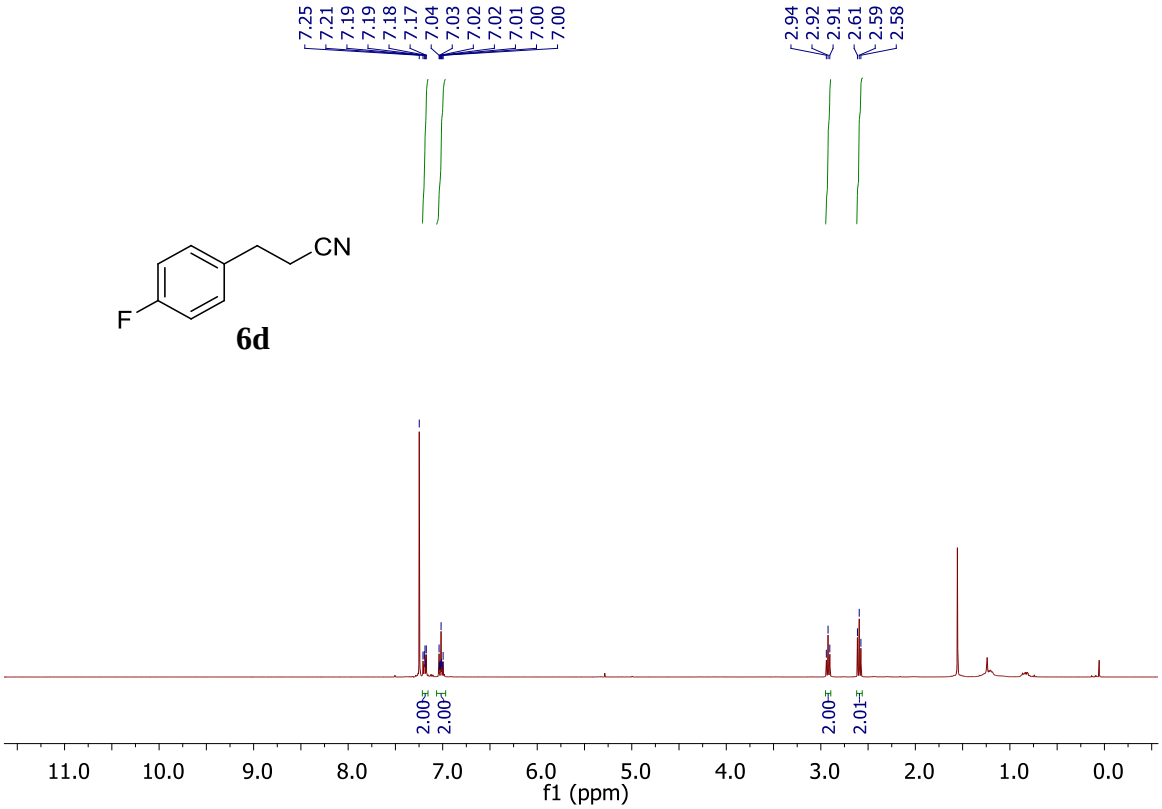
6b

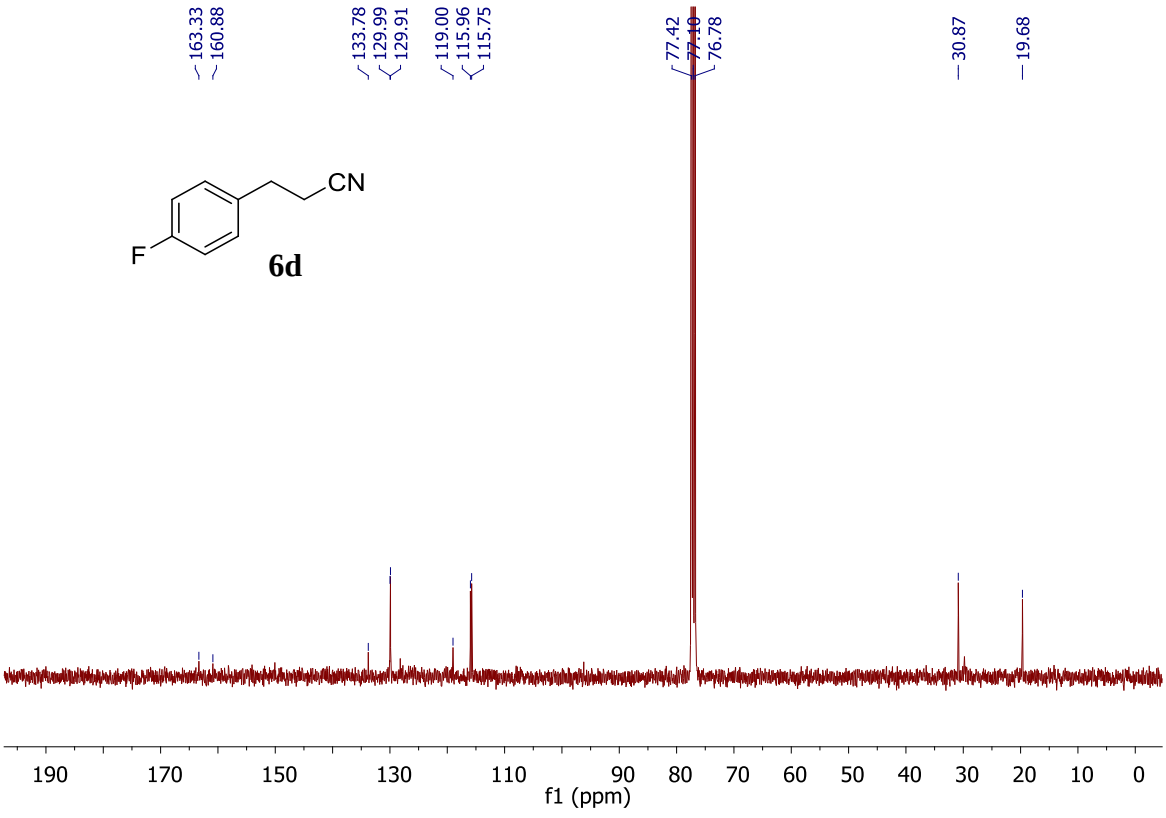

7.25
7.15
7.13
6.87
6.85
3.78
2.91
2.89
2.87
2.59
2.57
2.55
CN
MeO
1.96
1.95
3.01
2.00
2.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

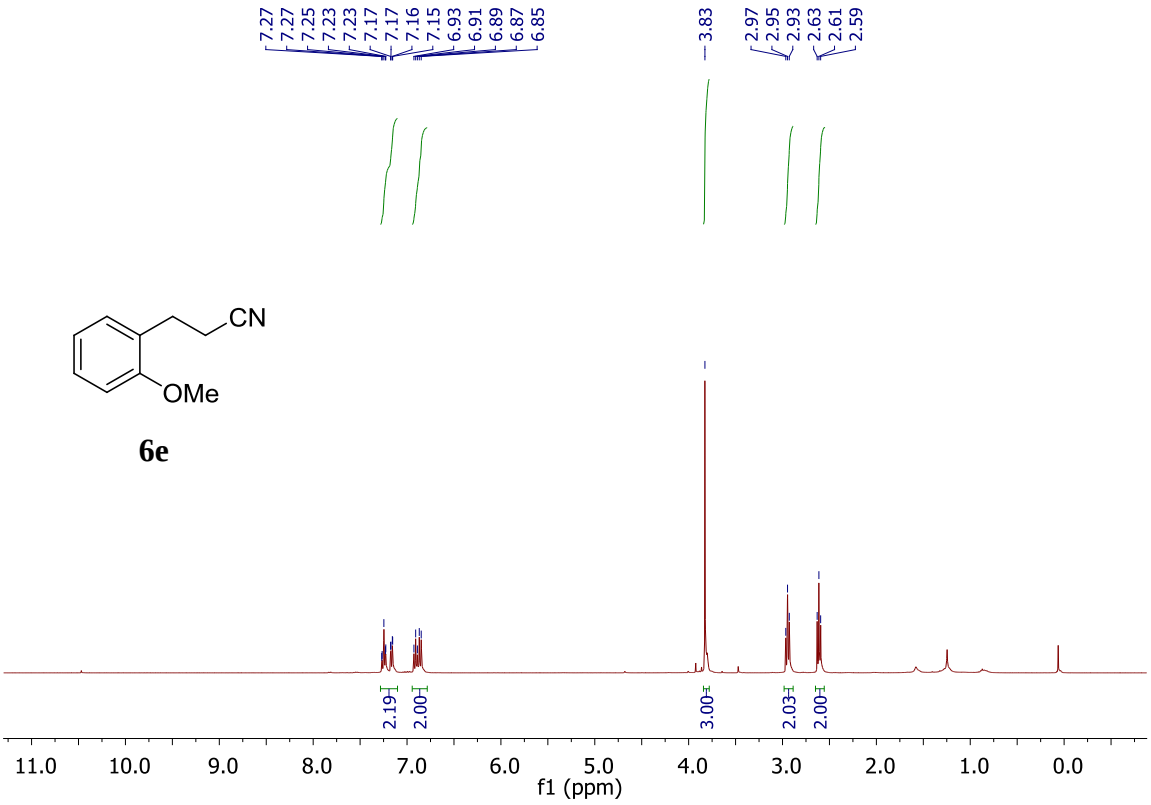
6c


158.82
130.20
129.41
119.34
114.32
77.43
77.11
76.79
55.37
30.85
19.80
CN
MeO
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

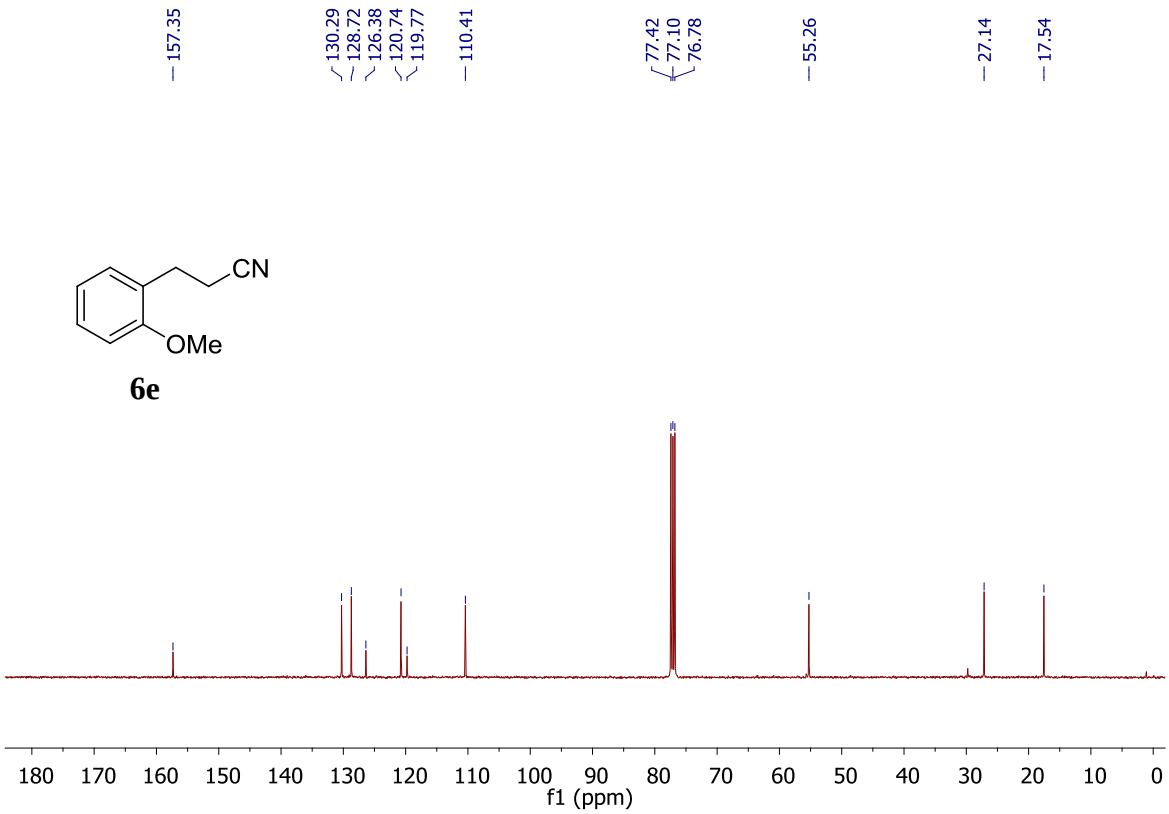
6c


7.25
7.21
7.19
7.19
7.18
7.17
7.04
7.03
7.02
7.02
7.01
7.00
7.00
2.94
2.92
2.91
2.61
2.59
2.58
CN
F
6d
2.00
2.00
2.00
2.01
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

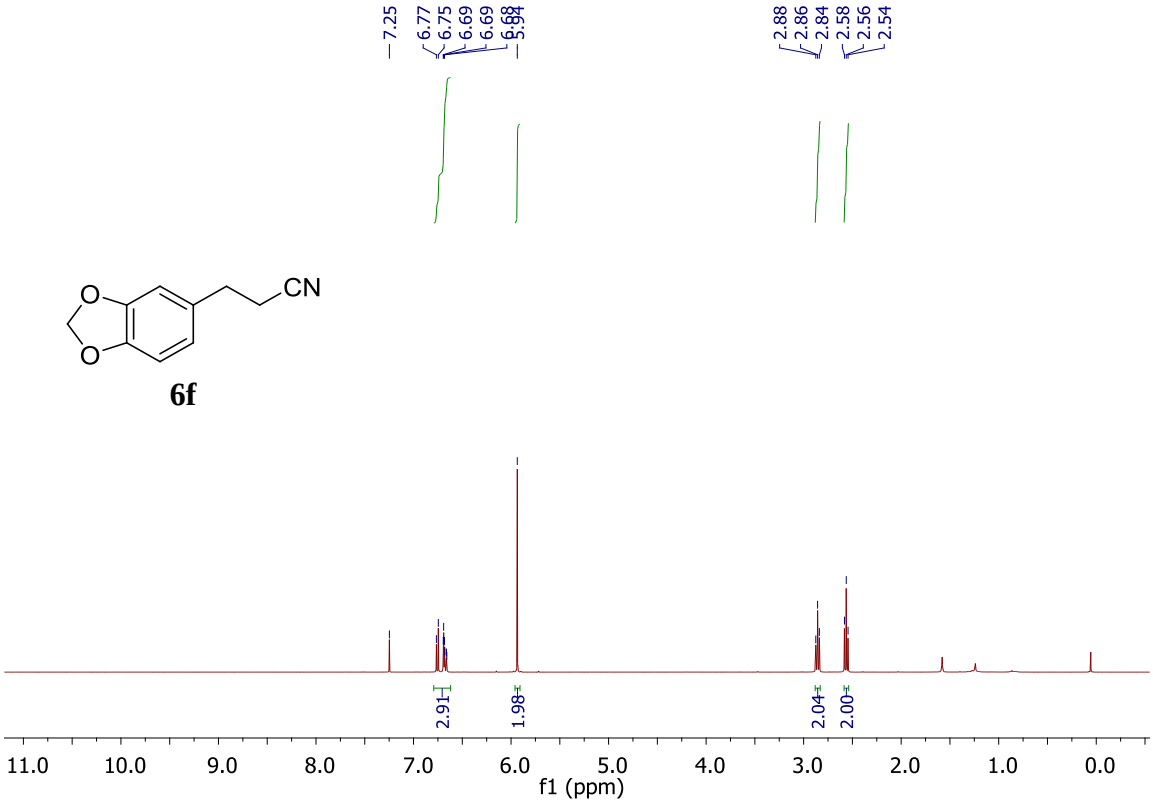

163.33
160.88
133.78
129.99
129.91
119.00
115.96
115.75
77.42
77.10
76.78
30.87
19.68
CN
F
6d
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.27
7.27
7.25
7.23
7.23
7.17
7.17
7.16
7.15
6.93
6.91
6.89
6.87
6.85
3.83
2.97
2.95
2.93
2.63
2.61
2.59
CN
OMe
2.19
2.00
3.00
2.03
2.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

6e


157.35
130.29
128.72
126.38
120.74
119.77
110.41
77.42
77.10
76.78
55.26
27.14
17.54
CN
OMe
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

6e


7.25
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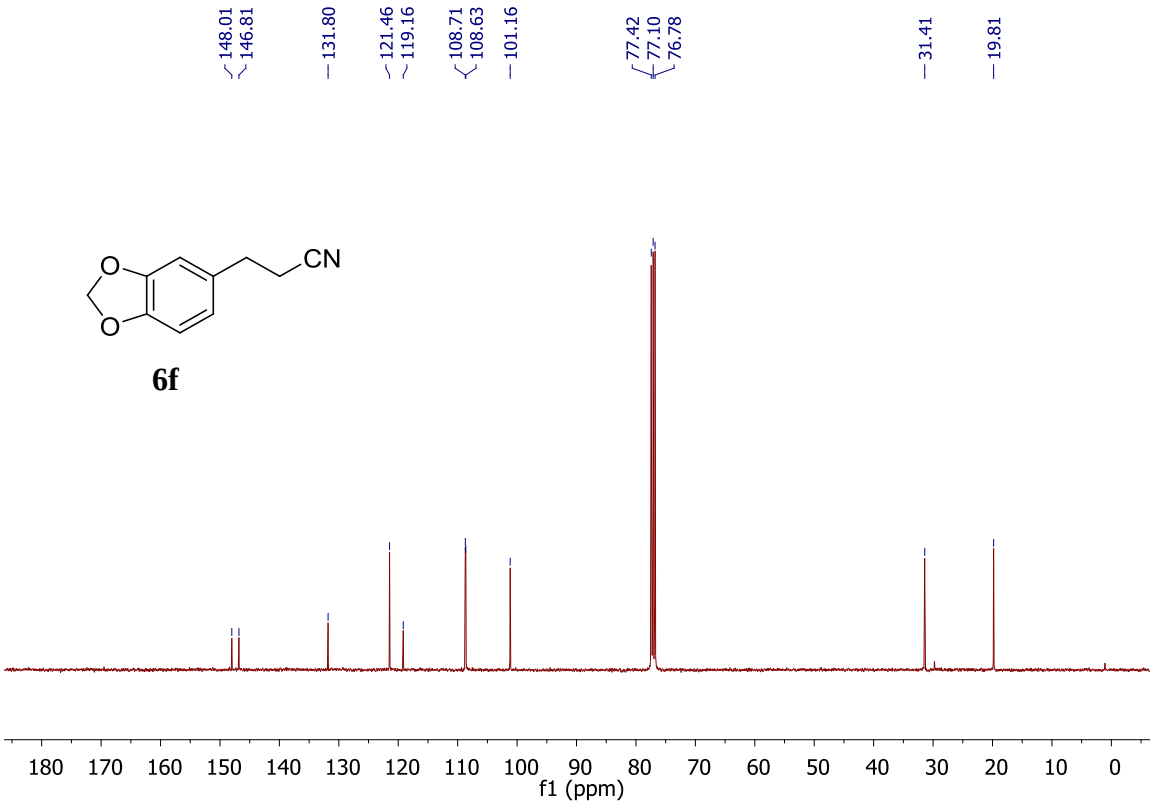
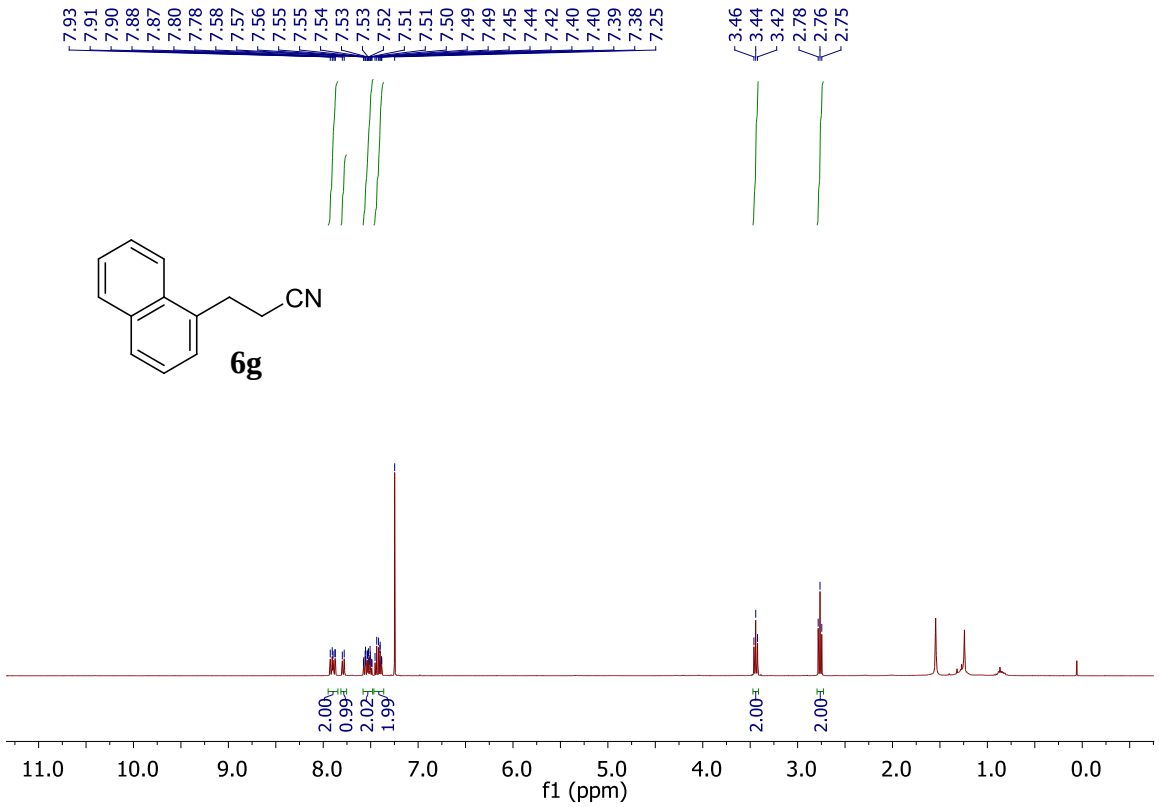
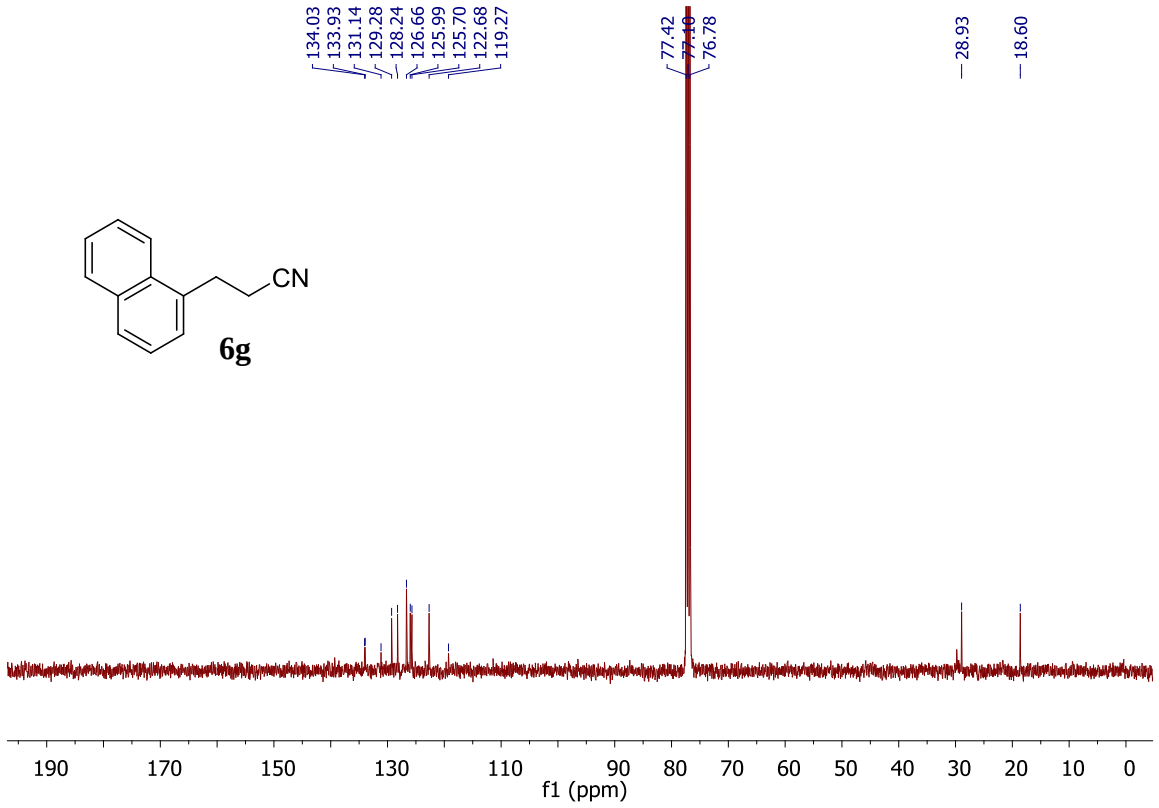
6.75
6.69
6.69
6.68
5.94
2.88
2.86
2.84
2.58
2.56
2.54
CN
O
O
2.91
1.98
2.04
2.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

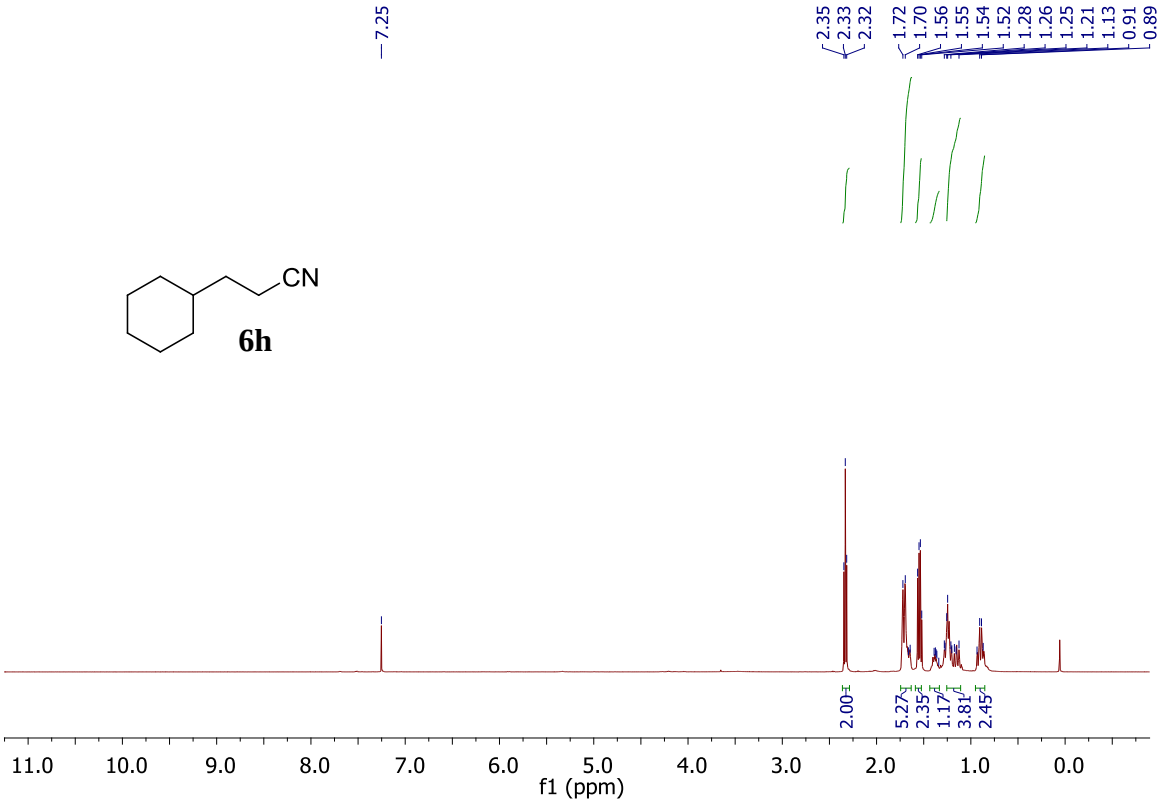
6f

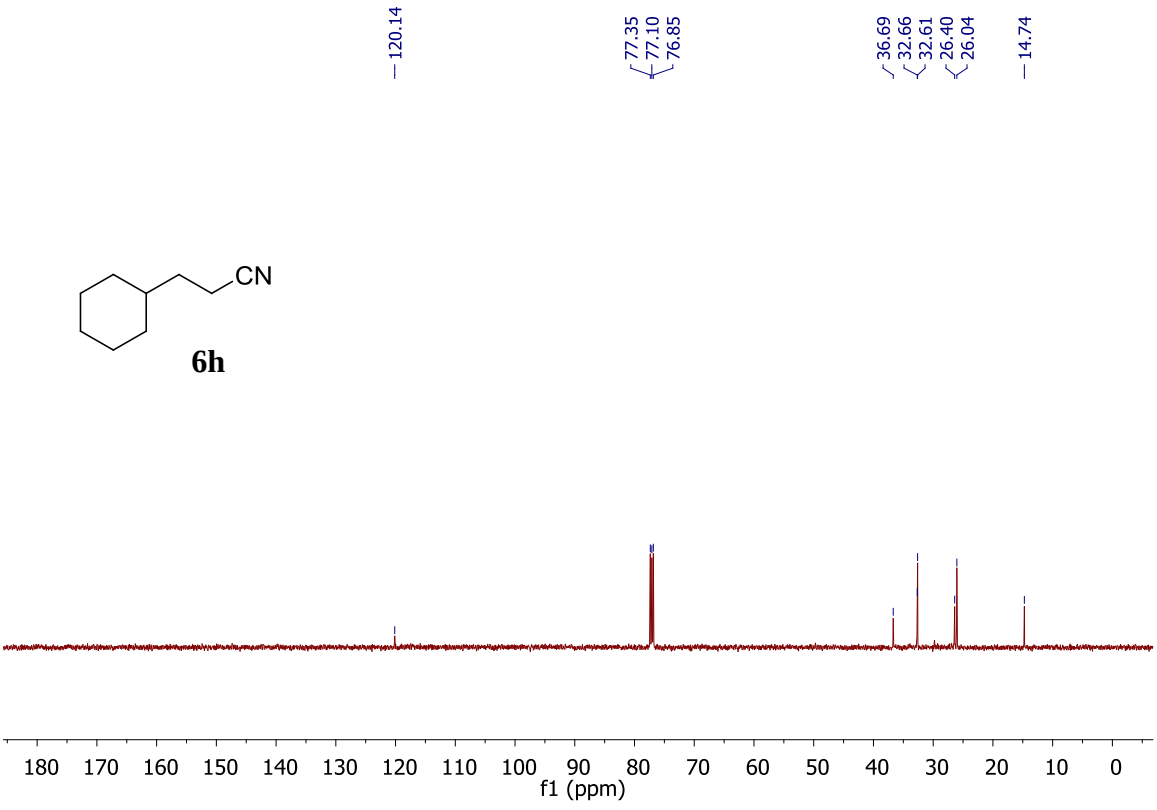

148.01
146.81
131.80
121.46
119.16
108.71
108.63
101.16
77.42
77.10
76.78
31.41
19.81
CN
O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

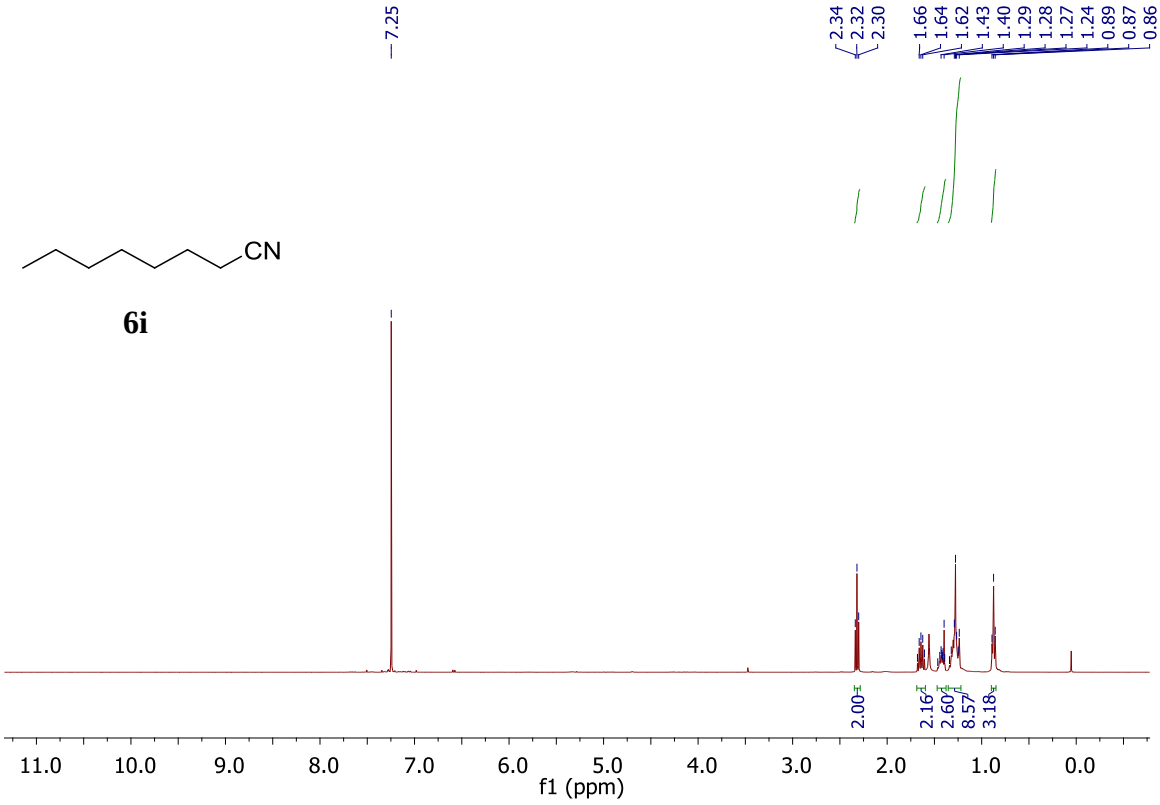
6f

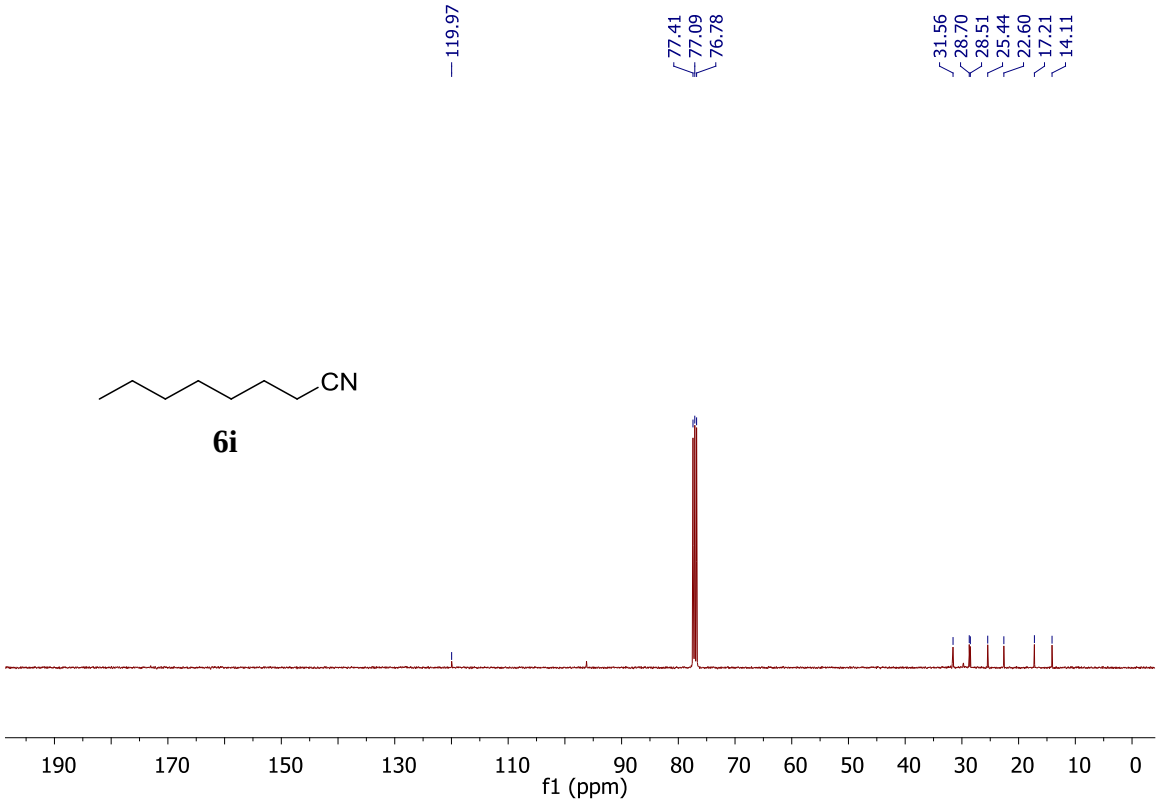

7.93
7.91
7.90
7.88
7.87
7.80
7.78
7.58
7.57
7.56
7.55
7.55
7.54
7.53
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.45
7.44
7.42
7.40
7.40
7.39
7.38
7.25
3.46
3.44
3.42
2.78
2.76
2.75
CN
6g
2.00
0.99
2.02
1.99
2.00
2.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

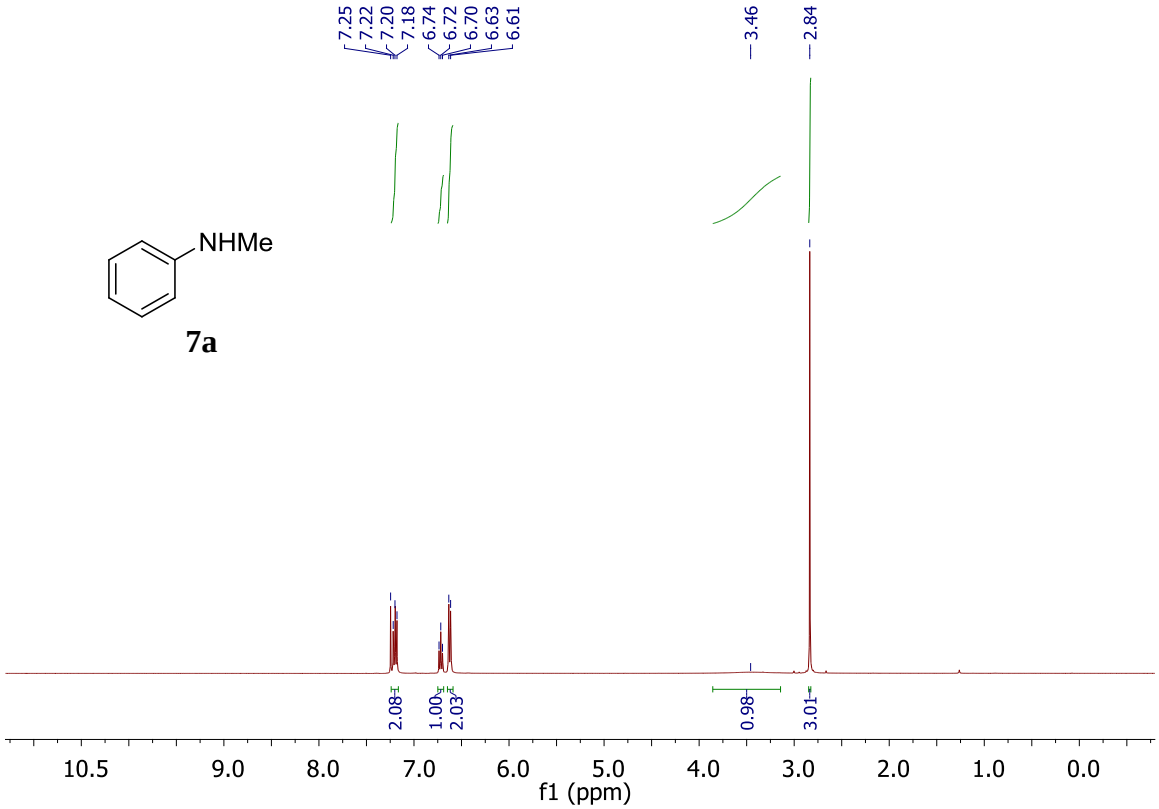

134.03
133.93
131.14
129.28
128.24
126.66
125.99
125.70
122.68
119.27
77.42
77.10
76.78
28.93
18.60
CN
6g
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.25
2.35
2.33
2.32
1.72
1.70
1.56
1.55
1.54
1.52
1.28
1.26
1.25
1.21
1.13
0.91
0.89
CN
6h
2.00
5.27
2.35
1.17
3.81
2.45
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

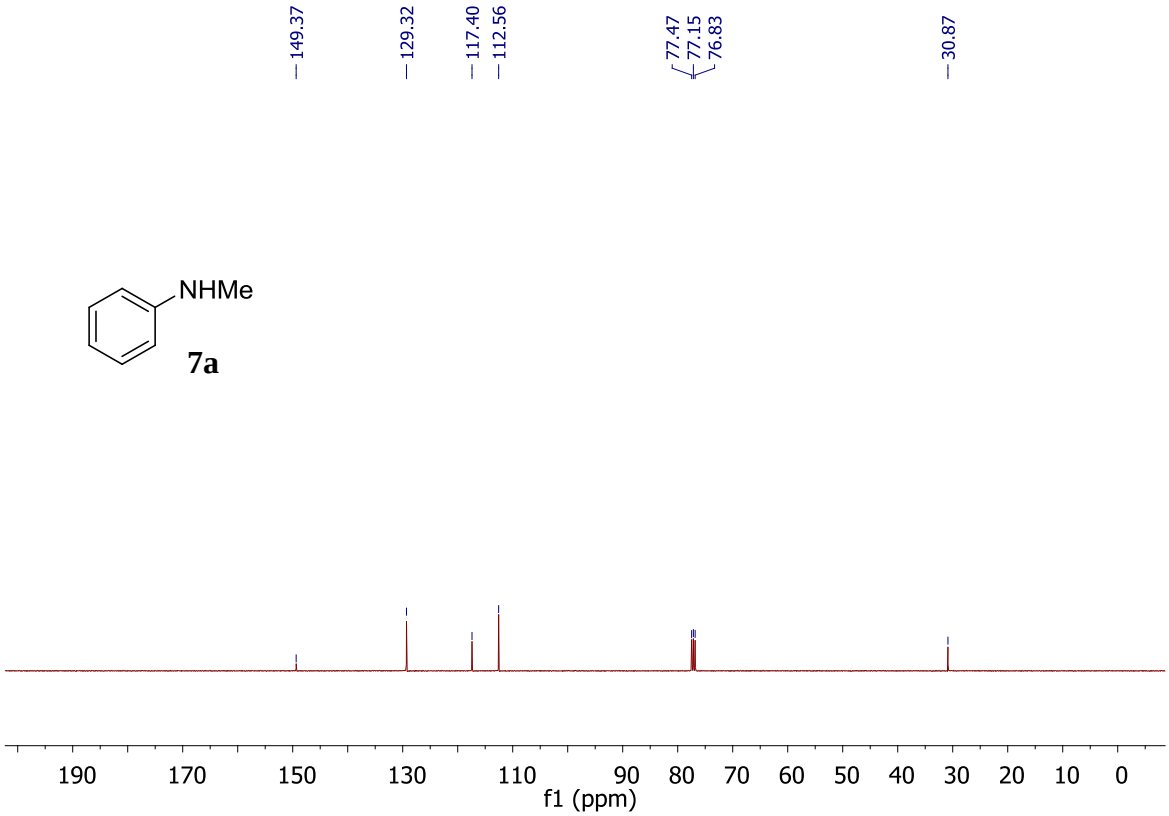

120.14
77.35
77.10
76.85
36.69
32.66
32.61
26.40
26.04
14.74
CN
6h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.25
2.34
2.32
2.30
1.66
1.64
1.62
1.43
1.40
1.29
1.28
1.27
1.24
0.89
0.87
0.86
CN
6i
2.00
2.16
2.60
8.57
3.18
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

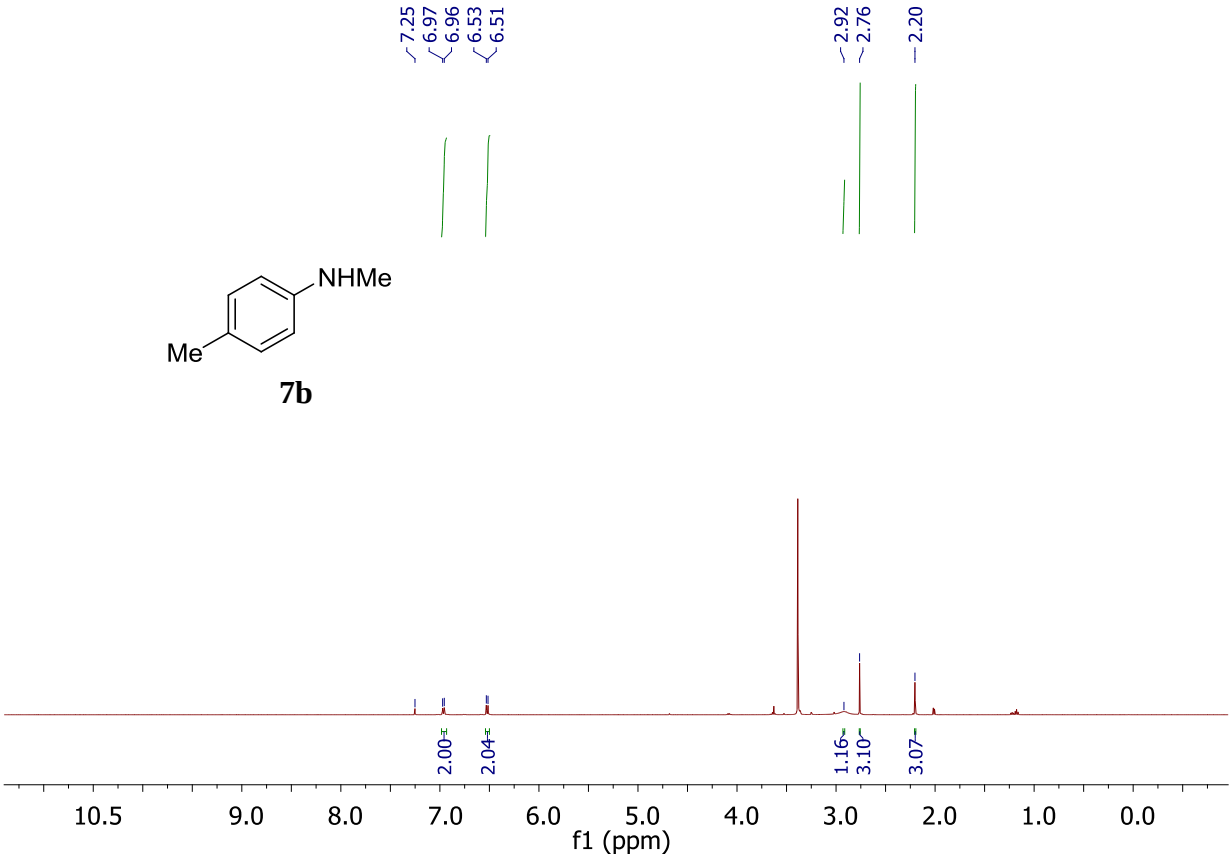

119.97
77.41
77.09
76.78
31.56
28.70
28.51
25.44
22.60
17.21
14.11
CN
6i
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.25
7.22
7.20
7.18
6.74
6.72
6.70
6.63
6.61
3.46
2.84
NHMe
2.08
1.00
2.03
0.98
3.01
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

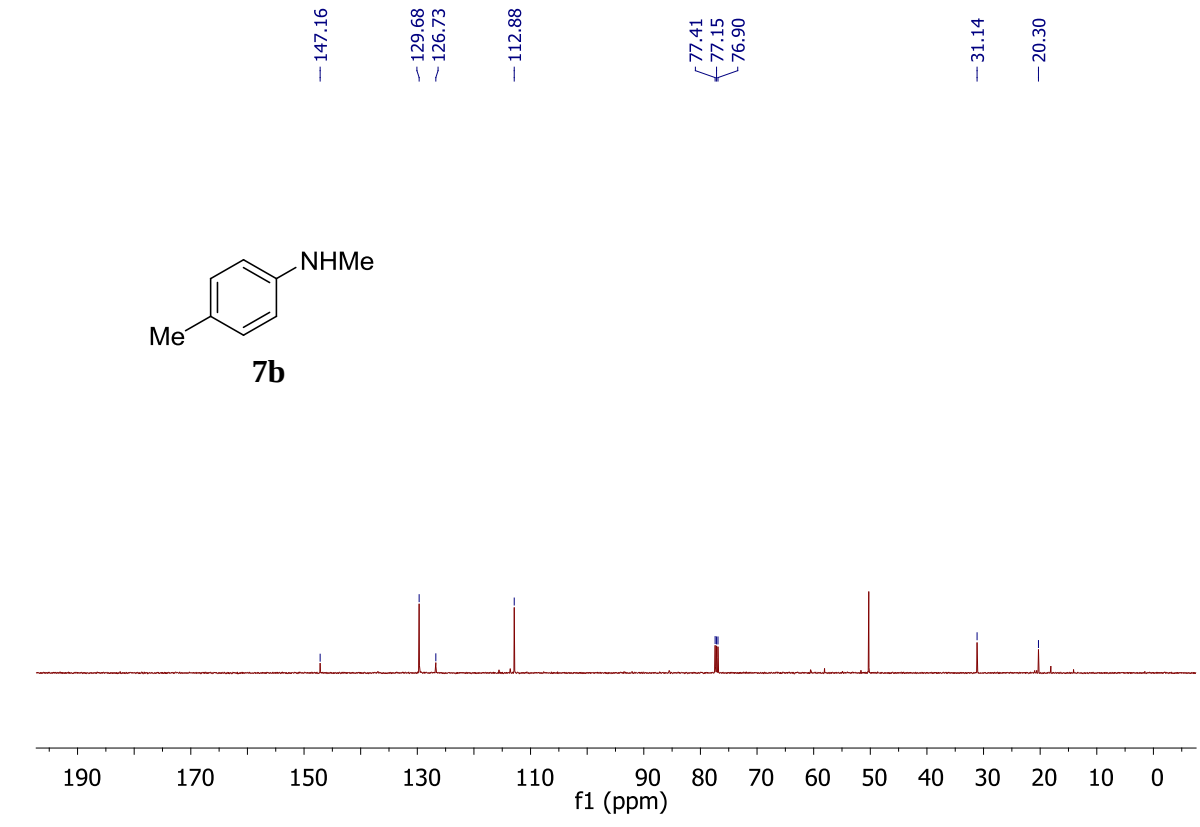
7a


149.37
129.32
117.40
112.56
77.47
77.15
76.83
30.87
NHMe
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

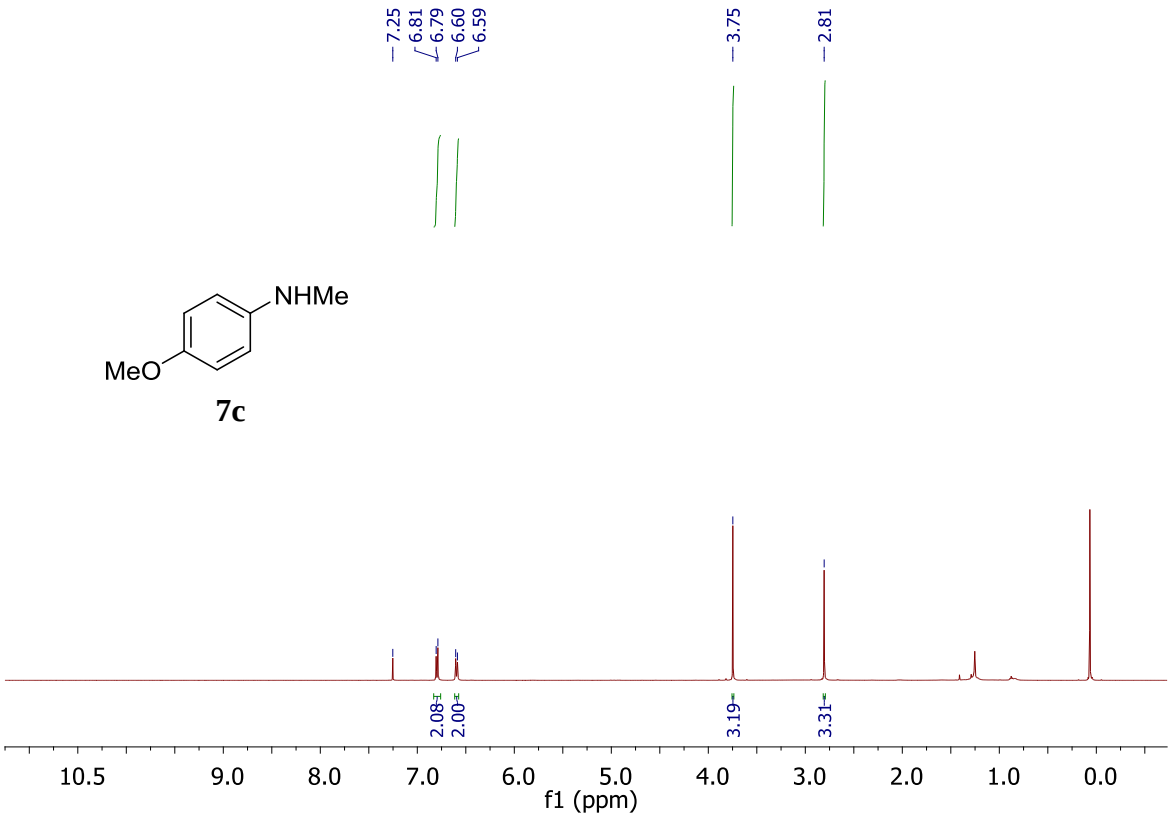
7a


7.25
6.97
6.96
6.53
6.51
2.92
2.76
2.20
NHMe
Me
2.00
2.04
1.16
3.10
3.07
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

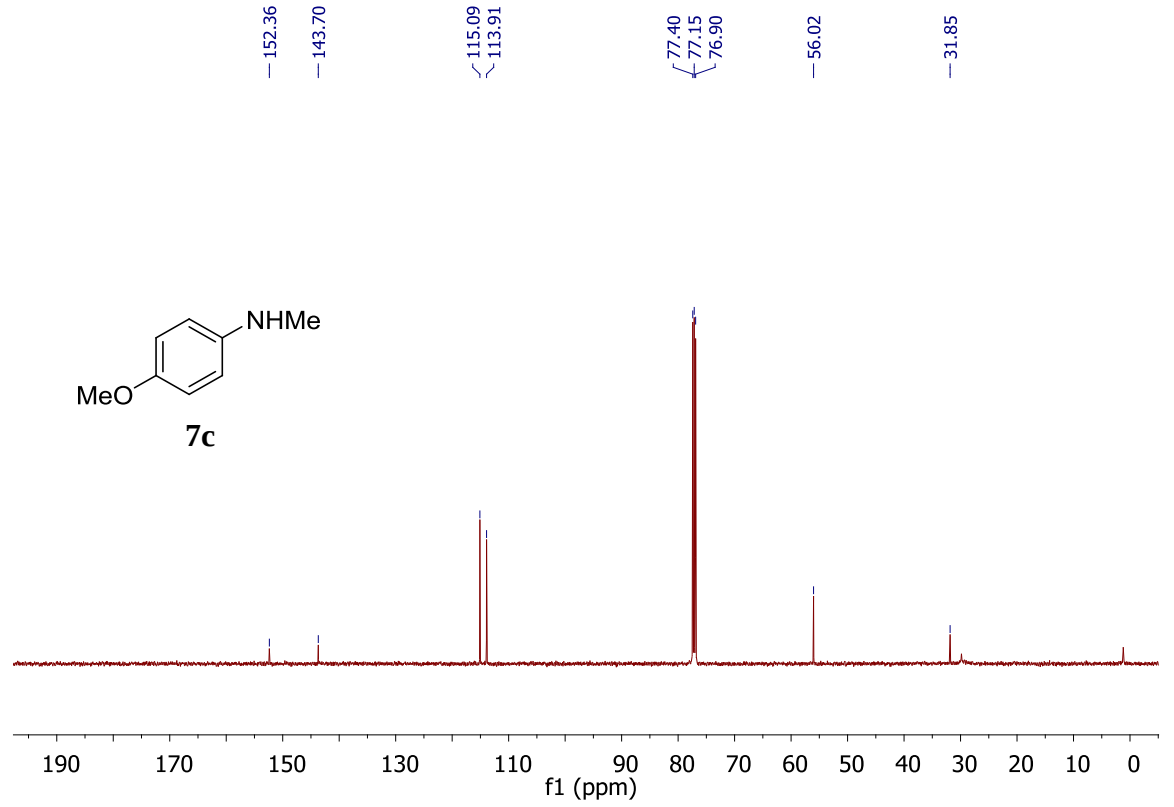
7b


147.16
129.68
126.73
112.88
77.41
77.15
76.90
31.14
20.30
NHMe
Me
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

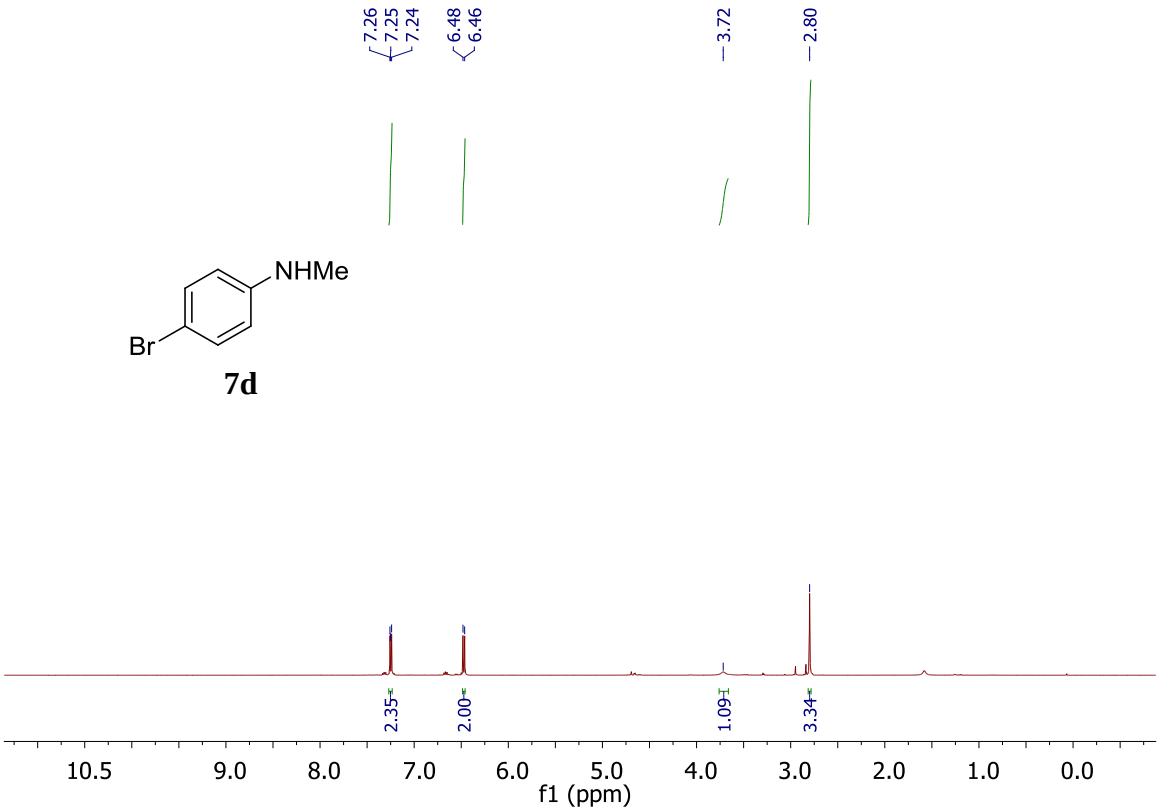
7b


7.25
6.81
6.79
6.60
6.59
3.75
2.81
NHMe
MeO
2.08
2.00
3.19
3.31
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

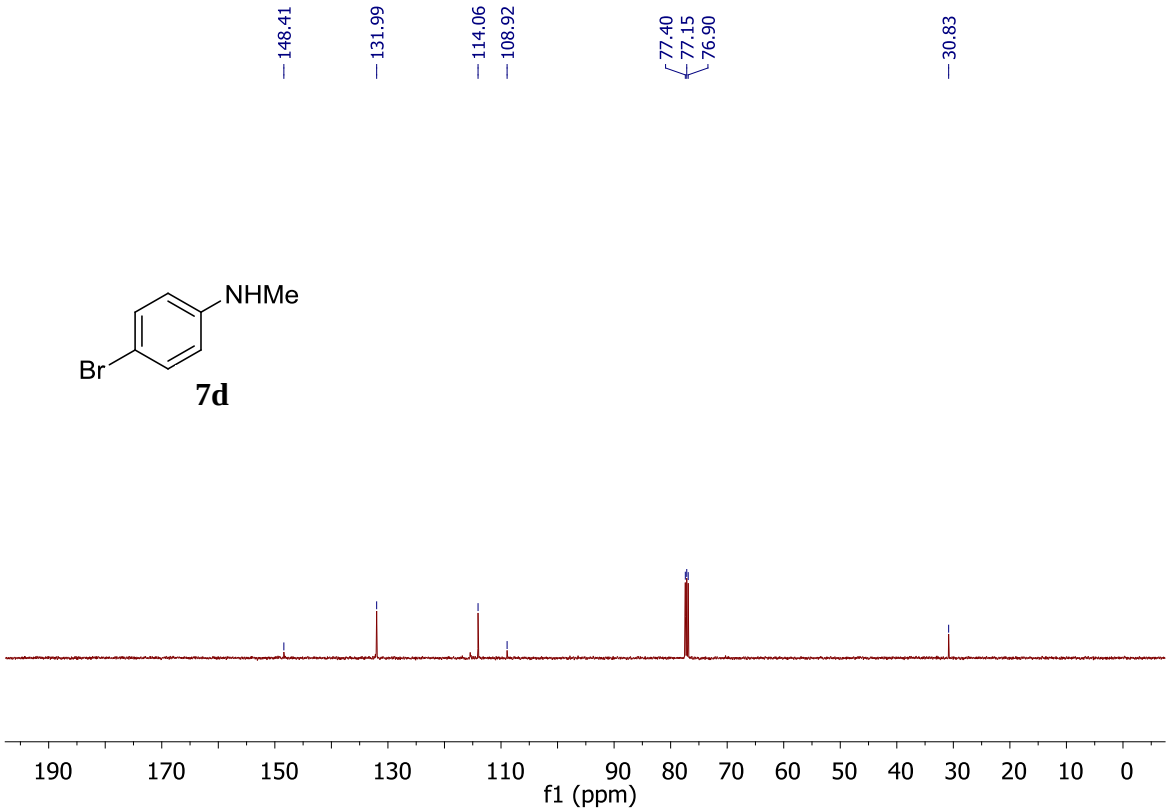
7c


152.36
143.70
115.09
113.91
77.40
77.15
76.90
56.02
31.85
NHMe
MeO
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

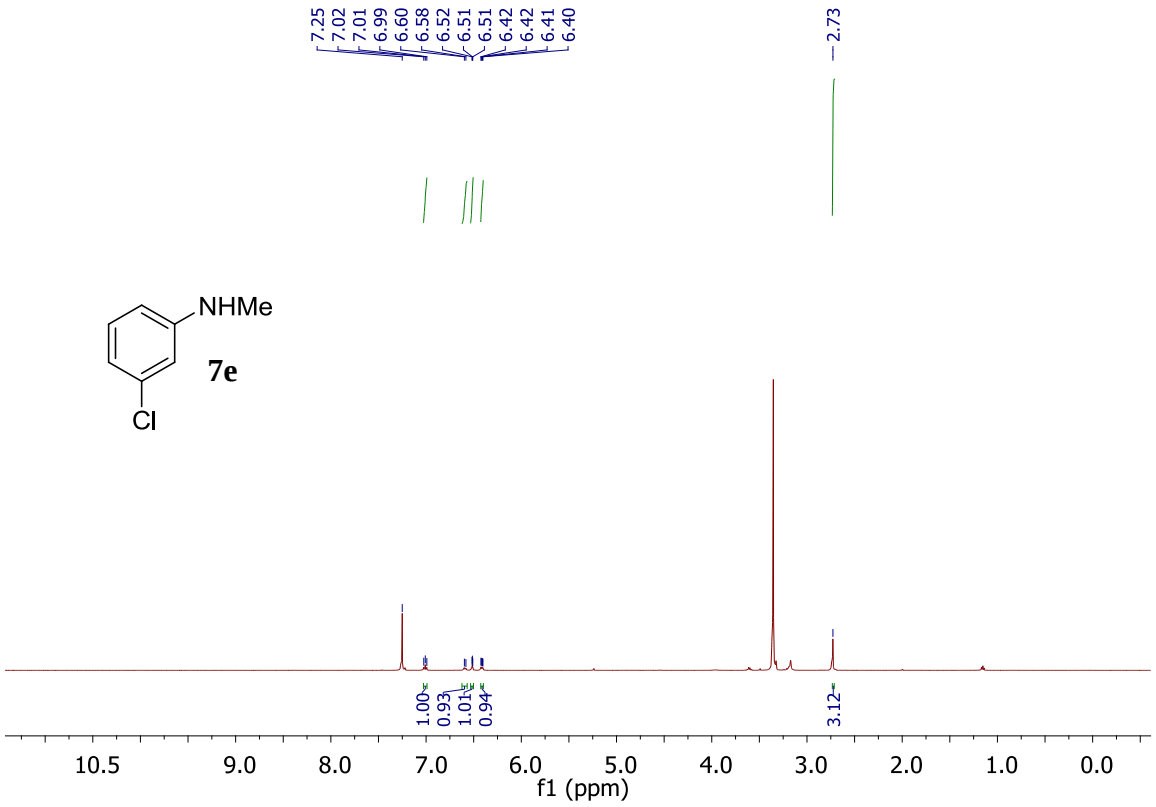
7c

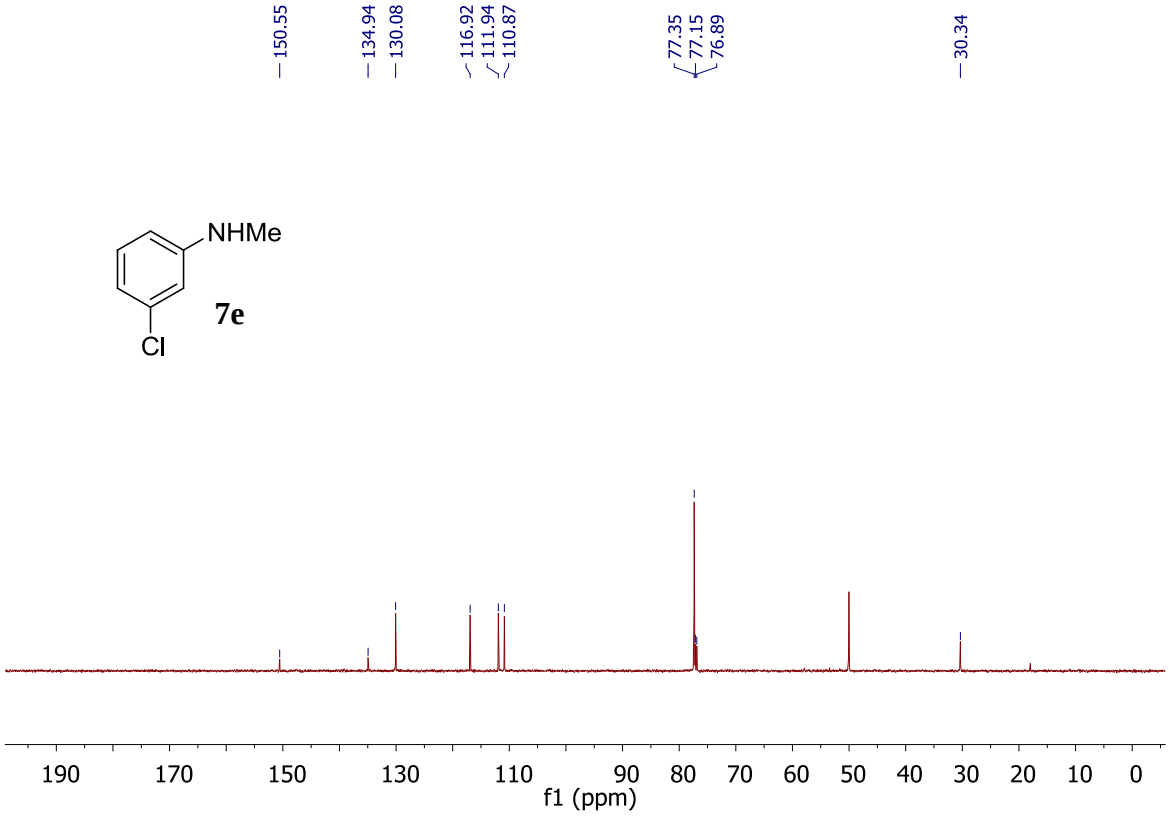

7.26
7.25
7.24
6.48
6.46
3.72
2.80
NHMe
Br
2.35
2.00
1.09
3.34
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

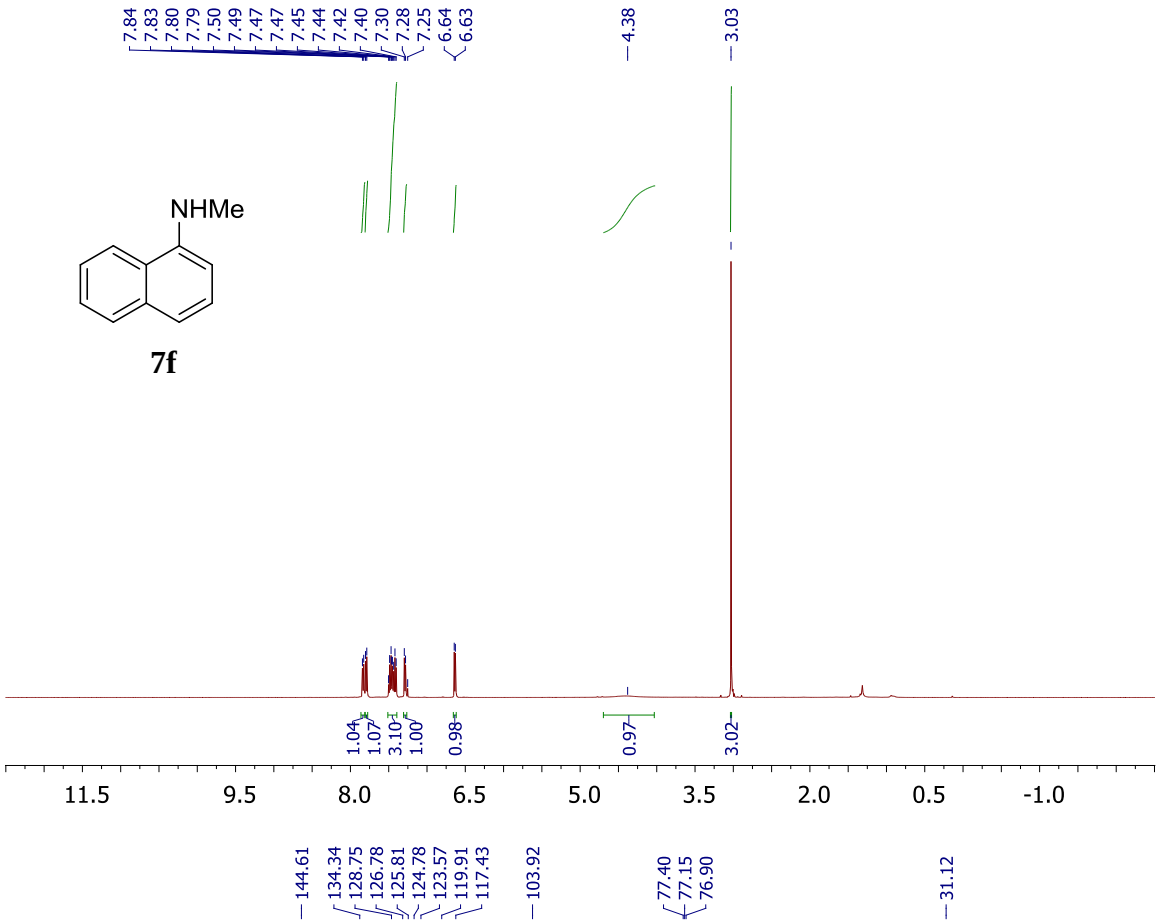
7d


148.41
131.99
114.06
108.92
77.40
77.15
76.90
30.83
NHMe
Br
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

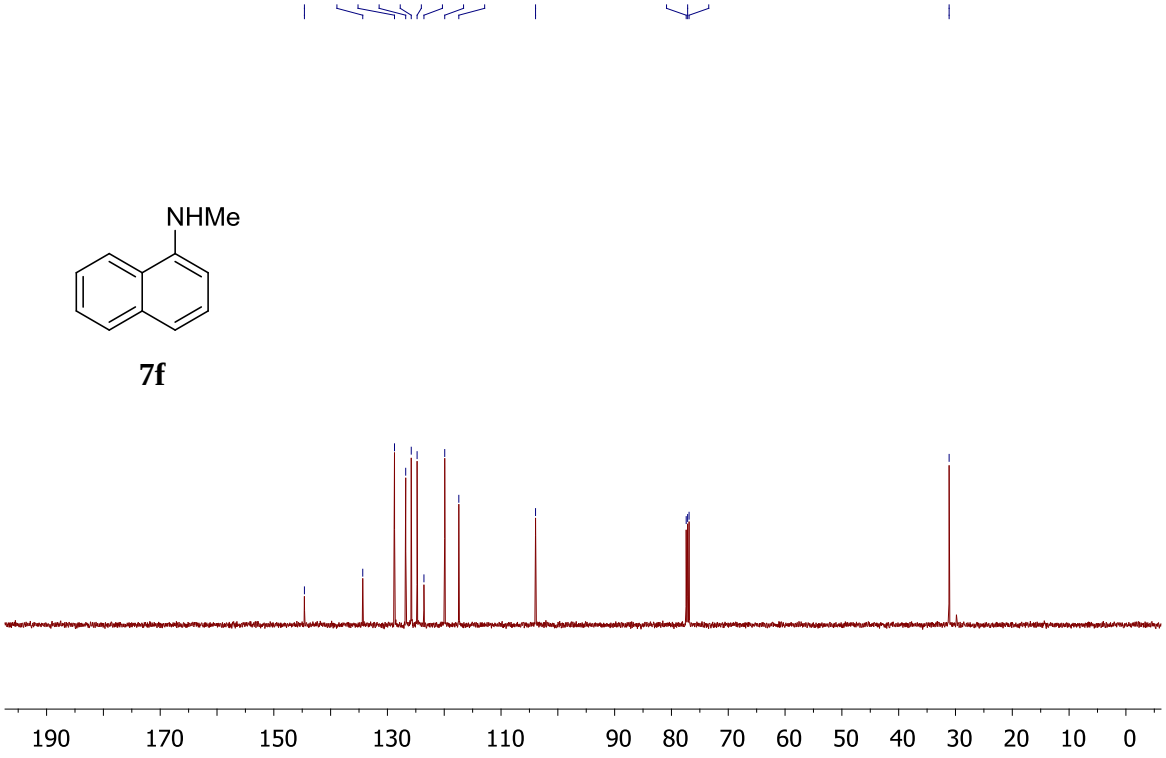
7d


7.25
7.02
7.01
6.99
6.60
6.58
6.52
6.51
6.51
6.42
6.42
6.41
6.40
2.73
NHMe
Cl
7e
1.00
0.93
1.01
0.94
3.12
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

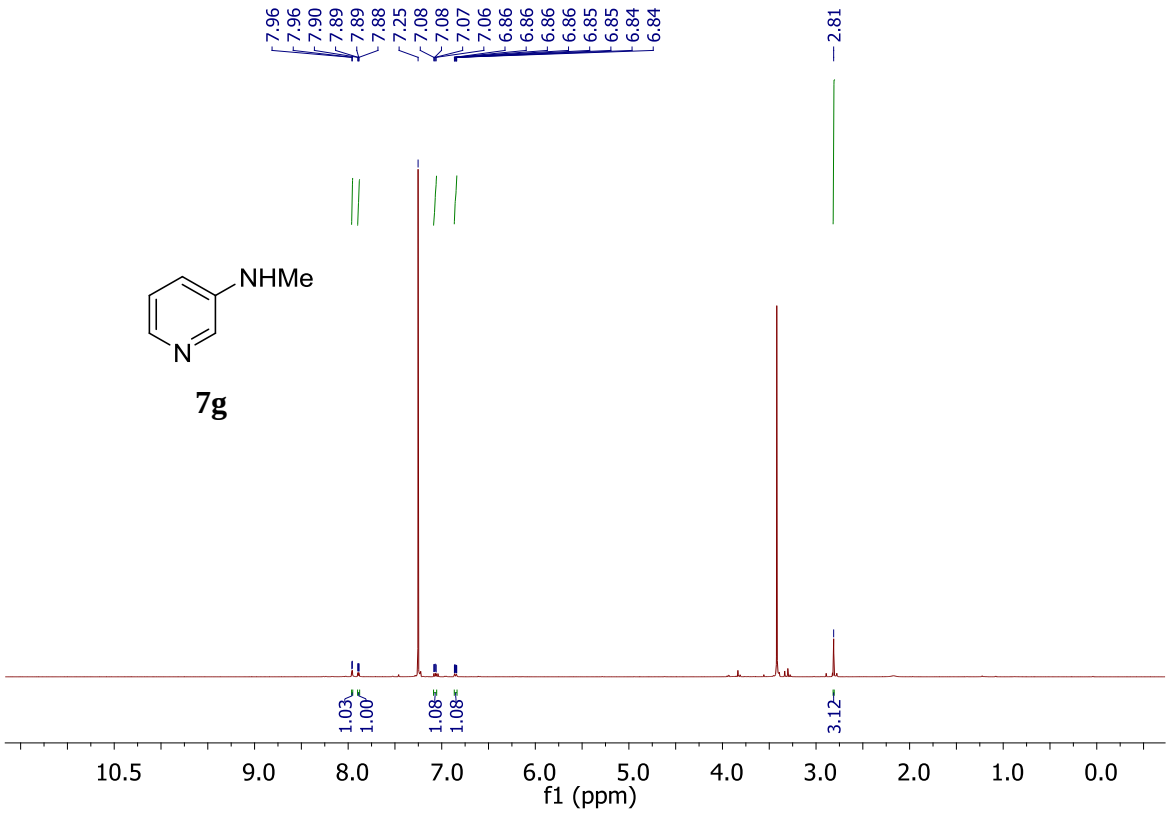

150.55
134.94
130.08
116.92
111.94
110.87
77.35
77.15
76.89
30.34
NHMe
Cl
7e
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.84
7.83
7.80
7.79
7.50
7.49
7.47
7.47
7.45
7.44
7.42
7.40
7.30
7.28
7.25
6.64
6.63
4.38
3.03
NHMe
1.04
1.07
3.10
1.00
0.98
0.97
3.02
11.5
9.5
8.0
6.5
5.0
3.5
2.0
0.5
-1.0

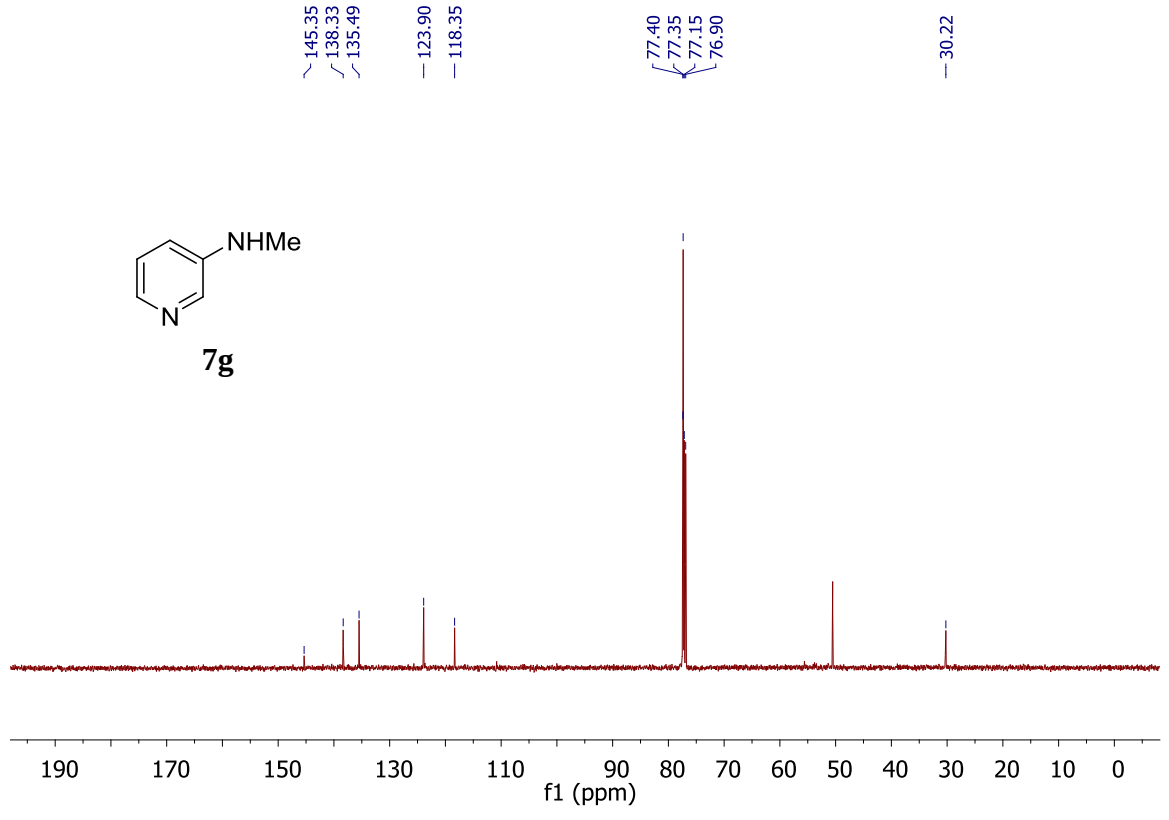
7f


144.61
134.34
128.75
126.78
125.81
124.78
123.57
119.91
117.43
103.92
77.40
77.15
76.90
31.12
NHMe
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

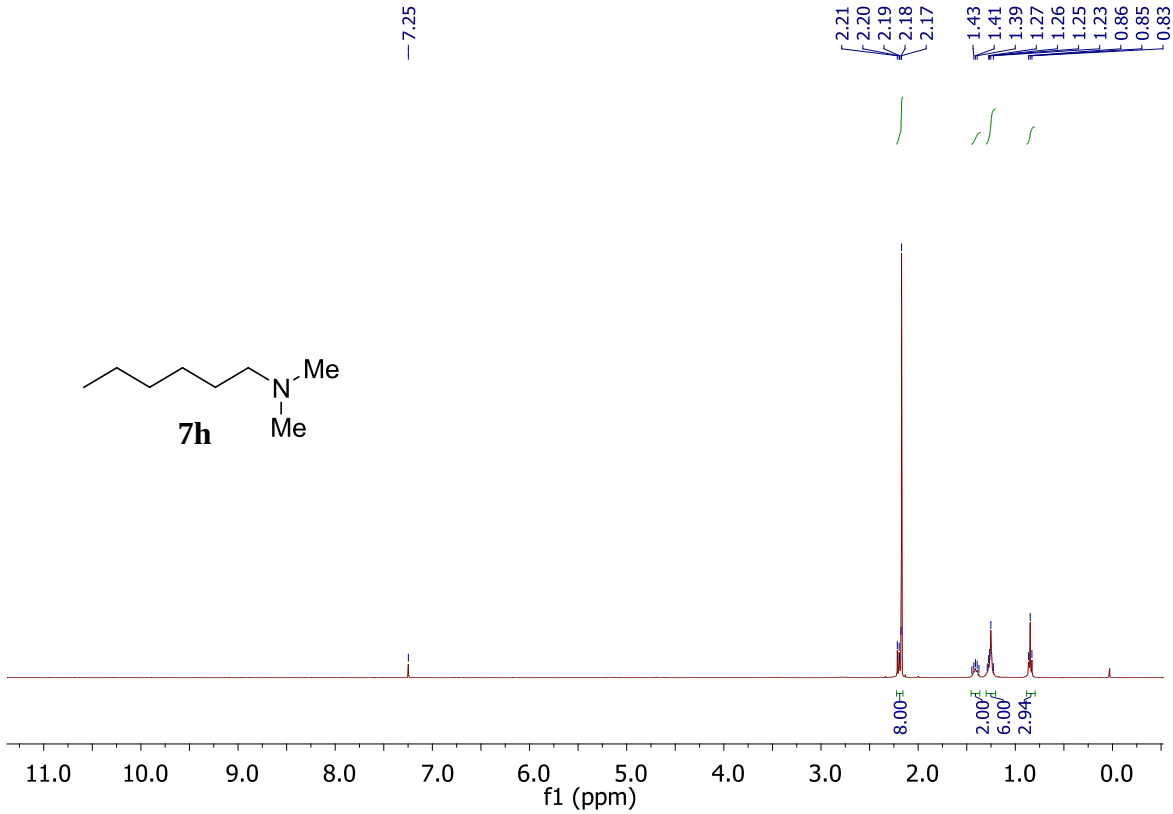
7f


7.96
7.96
7.90
7.89
7.89
7.88
7.25
7.08
7.08
7.07
7.06
6.86
6.86
6.86
6.86
6.85
6.85
6.84
6.84
2.81
NHMe
N
1.03
1.00
1.08
1.08
3.12
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

7g

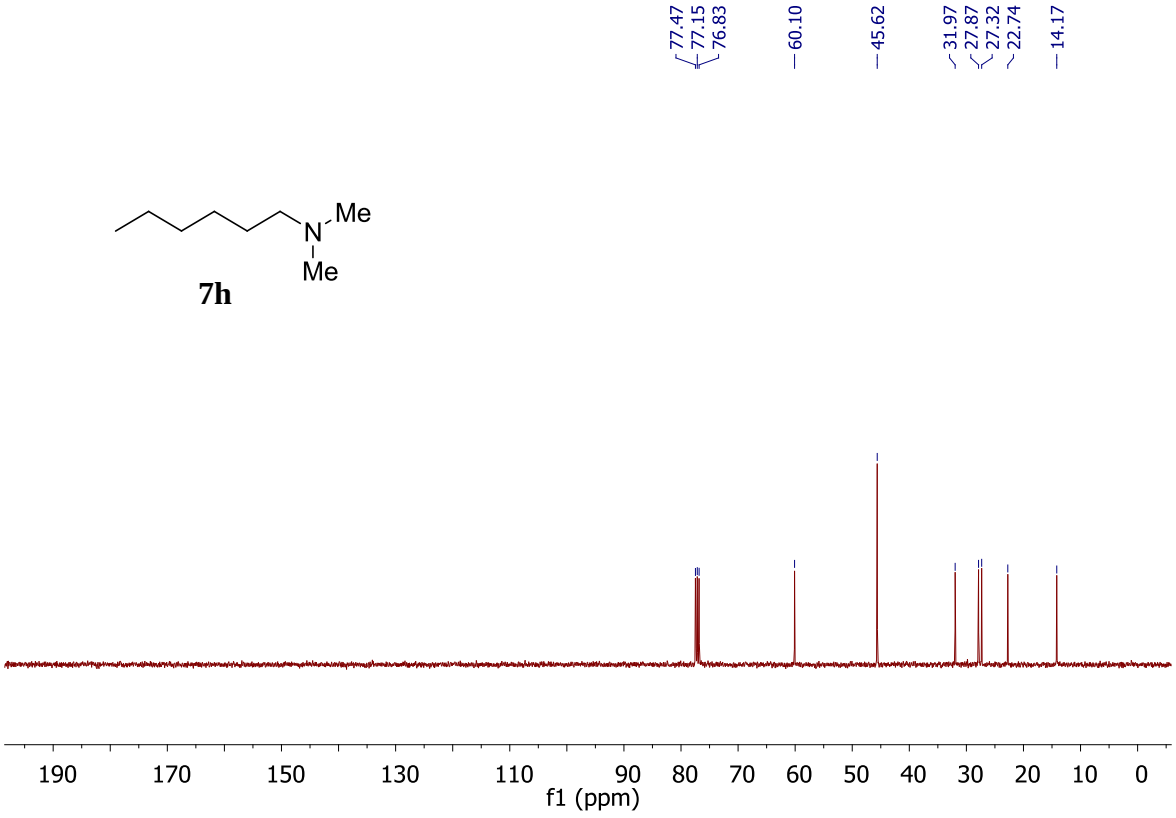

145.35
138.33
135.49
123.90
118.35
77.40
77.35
77.15
76.90
30.22
NHMe
N
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

7g


7.25
2.21
2.20
2.19
2.18
2.17
1.43
1.41
1.39
1.27
1.26
1.25
1.23
0.86
0.85
0.83
8.00
2.00
6.00
2.94
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

N
Me
Me

7h


77.47
77.15
76.83
60.10
45.62
31.97
27.87
27.32
22.74
14.17
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

N
Me
Me

7h

References:

1. SAINT+ Software for CCD Difractometers, Bruker AXS, Madison, WI, **2000**.
2. G. M. Sheldrick; SADABS Program for Correction of Area Detector Data, University of Gottingen, Gottingen, Germany, **1999**.
3. (a) SHELXTL Package v. 6.10, Bruker AXS, Madison, WI, **2000**. (b) G. M. Sheldrick,; SHELXS-86 and SHELXL-97, University of Gottingen, Gottingen, Germany, **1997**.
4. K. Bradenburg; Diamond, version 3.1e; Crystal Impact GbR: Bonn, Germany, **2005**.
5. J. Yang, X. Liu, D.-L. Meng, H.-Y. Chen, Z.-H. Zong, T.-T. Feng and K. Sun, *Adv. Synth. Catal.*, 2012, **354**, 328-334.
6. X. Gong, H. Zhang and X. Li, *Tetrahedron Lett.*, 2011, **52**, 5596-5600.
7. C. S. Cho, B. T. Kim, H.-S. Kim, T.-J. Kim and S. C. Shim, *Organometallics*, 2003, **22**, 3608-3610.
8. J. R. Frost, C. B. Cheong, W. M. Akhtar, D. F. J. Caputo, N. G. Stevenson and T. J. Donohoe, *J. Am. Chem. Soc.*, 2015, **137**, 15664-15667.
9. Z.-L. Shen, Y.-L. Yeo and T.-P. Loh, *J. Org. Chem.*, 2008, **73**, 3922-3924.
10. K.-i. Fujita, C. Asai, T. Yamaguchi, F. Hanasaka and R. Yamaguchi, *Org. Lett.*, 2005, **7**, 4017-4019.
11. J. M. Khurana and Kiran, *J. Chem. Res.*, 2006, **2006**, 374-375.
12. H. W. Cheung, T. Y. Lee, H. Y. Lui, C. H. Yeung and C. P. Lau, *Adv. Synth. Catal.*, 2008, **350**, 2975-2983.
13. O. Kose and S. Saito, *Org. Biomol. Chem.*, 2010, **8**, 896-900.
14. Q. Xu, J. Chen and Q. Liu, *Adv. Synth. Catal.*, 2013, **355**, 697-704.
15. R. Martínez, D. J. Ramón and M. Yus, *Tetrahedron*, 2006, **62**, 8982-8987.
16. A. F. Trindade, P. M. P. Gois, L. F. Veiros, V. André, M. T. Duarte, C. A. M. Afonso, S. Caddick and F. G. N. Cloke, *J. Org. Chem.*, 2008, **73**, 4076-4086.
17. C. Löfberg, R. Grigg, M. A. Whittaker, A. Keep and A. Derrick, *J. Org. Chem.*, 2006, **71**, 8023-8027.
18. M. Wieteck, Y. Tokimizu, M. Rudolph, F. Rominger, H. Ohno, N. Fujii and A. S. K. Hashmi, *Chem. Eur. J.*, 2014, **20**, 16331-16336.
19. B. W. H. Turnbull and P. A. Evans, *J. Am. Chem. Soc.*, 2015, **137**, 6156-6159.
20. M. D. Bhor, M. J. Bhanushali, N. S. Nandurkar and B. M. Bhanage, *Catal. Commun.*, 2007, **8**, 2064-2068.
21. H. W. Cheung, J. Li, W. Zheng, Z. Zhou, Y. H. Chiu, Z. Lin and C. P. Lau, *Dalton Trans.*, 2010, **39**, 265-274.
22. S. Thiyagarajan and C. Gunanathan, *ACS Catal.*, 2017, **7**, 5483-5490.
23. J. Xiao, J. Yang, T. Chen and L.-B. Han, *Adv. Synth. Catal.*, 2016, **358**, 816-819.
24. W. Lv, B. Xiong, H. Jiang and M. Zhang, *Adv. Synth. Catal.*, 2017, **359**, 1202-1207.
25. A. Falk, A. Cavalieri, G. S. Nichol, D. Vogt and H.-G. Schmalz, *Adv. Synth. Catal.*, 2015, **357**, 3317-3320.
26. B. Anxionnat, D. Gomez Pardo, G. Ricci and J. Cossy, *Org. Lett.*, 2011, **13**, 4084-4087.
27. G. Blay, L. Cardona, B. García, L. Lahoz and J. Pedro, *Tetrahedron*, 1996, **52**, 8611-8618.
28. N. Z. Yagafarov, D. L. Usanov, A. P. Moskovets, N. D. Kagramanov, V. I. Maleev and D. Chusov, *ChemCatChem*, 2015, **7**, 2590-2593.
28. T. Kuwahara, T. Fukuyama and I. Ryu, *Chem. Lett.*, 2013, **42**, 1163-1165.
30. T. Sawaguchi and Y. Obora, *Chem. Lett.*, 2011, **40**, 1055-1057.
31. L. M. Broomfield, Y. Wu, E. Martin and A. Shafir, *Adv. Synth. Catal.*, 2015, **357**, 3538-3548.
32. S. Elangovan, J. Neumann, J.-B. Sortais, K. Junge, C. Darcel and M. Beller, *Nat. Commun.*, 2016, **7**, 12641.
33. F. Li, J. Xie, H. Shan, C. Sun and L. Chen, *RSC Adv.*, 2012, **2**, 8645-8652.
34. M. P. Paudyal, A. M. Adebesin, S. R. Burt, D. H. Ess, Z. Ma, L. Kürti and J. R. Falck, *Science*, 2016, **353**, 1144-1147.
35. B. P. Fors, D. A. Watson, M. R. Biscoe and S. L. Buchwald, *J. Am. Chem. Soc.*, 2008, **130**, 13552-13554.
36. C. Guyon, E. Da Silva, R. Lafon, E. Metay and M. Lemaire, *RSC Adv.*, 2015, **5**, 2292-2298.