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Supplementary Information

Silver-Catalyzed Regioselective Deuteration of (Hetero)Arenes and α-Deuteration of 2-Alkyl Azaarenes

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Table of Contents

1. General and Materials

General. All reactions dealing with air- or moisture-sensitive compounds were carried out in a flame-dried, sealed Schlenk reaction tube under an atmosphere of nitrogen. Flash silica gel column chromatography was performed on silica gel 60N (spherical and neutral, 140–325 mesh) as described by Still. NMR spectra were measured on a Bruker AV-500 spectrometer or a Bruker AV-400 spectrometer and reported in parts per million. ^{1}H NMR spectra were recorded at 500 or 400 MHz in $CDCl_3$ or DMSO-d_6 were referenced internally to tetramethylsilane as a standard, and ^{13}C NMR spectra were recorded at 126 or 100 MHz and referenced to the solvent resonance.

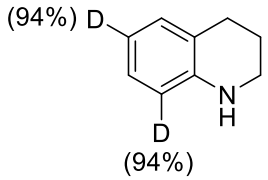
Materials. Unless otherwise noted, materials were purchased from Tokyo Chemical Industry Co., Aldrich Inc., Alfa Aesar, Adamas, and other commercial suppliers and used as received. Solvents were dried over sodium (for THF and ether) by refluxing for overnight and freshly distilled prior to use.

Determination of Deuterium Content: The amount of incorporated deuterium in a sample was quantified by the decrease of ^{1}H NMR integral intensities at the specified positions compared to the starting material. Integral intensities were calibrated against hydrogen signals that do not undergo H/D-exchange.

2. General Procedure for Silver-Catalyzed Regioselective Deuteration of (Hetero)Arenes Using D_2O as Deuterium Source

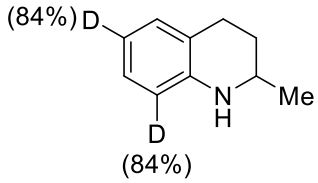
A dried Schlenk tube were placed aromatic compounds **1** or azaarenes **3** (0.5 mmol), AgOTf (3 mg, 0.025 mmol), D_2O (20 equiv) and $CDCl_3$ (1.0 mL). The reaction mixture was heated at 90 ^{o}C for 18 h. The mixture was then cooled to room temperature, diluted with 5 mL of ethyl acetate, filtered through a celite pad, and washed with 5 mL of ethyl acetate. The combined organic extracts were concentrated under vacuum to give deuterated products. The deuterium incorporation was determined by ^{1}H NMR.

3. Characterization of Synthesized Deuterated Products



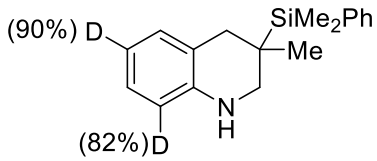
1,2,3,4-Tetrahydroquinoline-6,8-d_2 (2a)

Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.95-6.94 (m, 2H), 6.60 (t, J = 7.6 Hz, **0.06H**), 6.47 (d, J = 8.0 Hz, **0.06H**), 3.52 (brs, 1H), 3.26 (t, J = 5.6 Hz, 2H), 2.74 (t, J = 6.4 Hz, 2H), 1.96-1.90 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 144.4, 129.3, 126.5, 126.4, 121.6, 117.1, 117.0, 116.8, 116.7, 114.3, 114.1, 114.0, 113.8, 41.8, 26.8, 22.0. Deuterium incorporation expected at δ 6.60 and 6.47. The level of deuterium incorporation was determined as 94% for δ 6.60 and 94% for δ 6.47 (^{1}H NMR).



2-Methyl-1,2,3,4-tetrahydroquinoline-6,8-d_2 (2b)

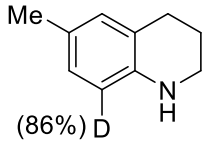
Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.95 (m, 2H), 6.61 (t, J = 6.0 Hz, **0.16H**), 6.48 (d, J = 7.0 Hz, **0.16H**), 4.17 (brs, 1H), 3.39-3.36 (m, 1H), 2.82-2.72 (m, 2H), 1.93-1.90 (m, 1H), 1.59-1.57 (m, 1H), 1.19 (d, J = 5.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 144.0, 143.9, 129.2, 129.1, 126.6, 126.5, 126.4, 121.4, 117.44, 117.35, 117.2, 117.0, 114.4, 114.2, 114.1, 113.9, 47.2, 29.9, 26.4, 22.3. Deuterium incorporation expected at δ 6.61 and 6.48. The level of deuterium incorporation was determined as 84% for δ 6.61 and 84% for δ 6.48 (^{1}H NMR).



3-(Dimethyl(phenyl)silyl)-3-methyl-1,2,3,4-tetrahydroquinoline-6,8-d_2 (2c)

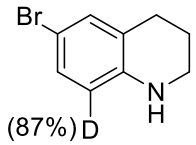
Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.53-7.52 (m, 2H), 7.38-7.34 (m, 3H), 6.95-6.91 (m, 2H), 6.60 (t, J = 6.0 Hz, **0.10H**), 6.45 (d, J = 6.0 Hz, **0.18H**), 3.98 (brs, 1H), 3.20 (d, J = 9.5 Hz, 1H), 2.92-2.87 (m, 2H), 2.32 (d, J = 13.5 Hz, 1H),

0.952 (s, 3H), 0.32-0.31 (m, 6H); ^{13}C NMR (126 MHz, $CDCl_3$): δ =143.44, 143.37, 136.5, 134.4, 133.0, 132.96, 130.0, 129.9, 129.6, 129.1, 127.9, 127.6, 126.4, 126.3, 120.4, 117.4, 114.1, 48.5, 34.9, 19.3, -6.1, -6.2. Deuterium incorporation expected at δ 6.60 and 6.45. The level of deuterium incorporation was determined as 90% for δ 6.60 and 82% for δ 6.45 (^{1}H NMR).



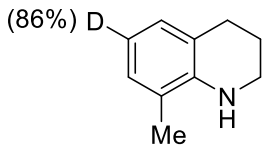
6-Methyl-1,2,3,4-tetrahydroquinoline-8-d (2d)

Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.78 (m, 2H), 6.44 (t, J = 7.0 Hz, **0.14H**), 4.35 (brs, 1H), 3.24 (t, J = 4.5 Hz, 2H), 2.70 (t, J = 5.5 Hz, 2H), 2.20, (s, 3H), 1.93-1.89 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ =141.1, 141.0, 130.0, 127.3, 127.23, 127.21, 127.20, 122.3, 1151.1, 115.0, 114.8, 114.7, 42.1, 26.7, 26.6, 22.1, 20.4. Deuterium incorporation expected at δ 6.44. The level of deuterium incorporation was determined as 86% (^{1}H NMR).



6-Bromo-1,2,3,4-tetrahydroquinoline-8-d (2e)

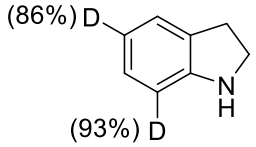
Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.04-7.02 (m, 2H), 6.34 (d, J = 7.0 Hz, **0.13H**), 4.16 (brs, 1H), 3.25 (t, J = 4.5 Hz, 2H), 2.69 (t, J = 5.5 Hz, 2H), 1.91-1.87 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 143.2, 143.1, 131.8, 129.3, 129.2, 123.6, 115.8, 115.7, 115.5, 115.3, 108.6, 41.7, 26.7, 21.5. Deuterium incorporation expected at δ 6.34. The level of deuterium incorporation was determined as 87% (^{1}H NMR).



8-Methyl-1,2,3,4-tetrahydroquinoline-6-d (2f)

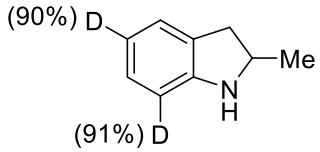
Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.87-6.84 (m, 2H), 6.56 (d, J = 6.5 Hz, **0.14H**), 3.77 (brs, 1H), 3.36 (t, J = 4.5 Hz, 2H), 2.77 (t, J = 5.0 Hz, 2H), 2.08 (s,

3H), 1.96-1.92 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 142.3, 127.8, 127.7, 127.3, 127.2, 121.4, 121.1, 116.7, 116.6, 116.4, 116.2, 42.3, 27.2, 22.0, 17.6. Deuterium incorporation expected at δ 6.56. The level of deuterium incorporation was determined as 86% (^{1}H NMR).



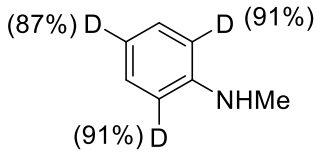
Indoline-5,7-d_2 (2g)

Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.11 (s, 1H), 7.01 (s, 1H), 6.69 (t, *J* = 7.6 Hz, **0.14H**), 6.64 (d, *J* = 8.0 Hz, **0.07H**), 3.49 (t, *J* = 8.0 Hz, 2H), 2.99 (t, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 151.2, 129.4, 127.0, 126.9, 124.6, 124.5, 118.8, 118.7, 118.5, 118.4, 109.6, 109.5, 109.3, 109.2, 47.2, 29.7. Deuterium incorporation expected at δ 6.69 and 6.64. The level of deuterium incorporation was determined as 86% for δ 6.69 and 93% for δ 6.64 (^{1}H NMR).



2-Methylindoline-5,7-d_2 (2h)

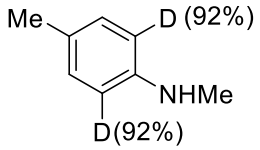
Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.06 (s, 1H), 7.00 (s, 1H), 6.69 (t, *J* = 6.0 Hz, **0.10H**), 6.61 (d, *J* = 6.0 Hz, **0.09H**), 4.16 (brs, 1H), 3.98-3.95 (m, 1H), 3.13-3.09 (m, 1H), 2.63-2.59 (m, 1H), 1.26 (d, *J* = 5.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 150.0, 129.1, 127.2, 127.1, 127.0, 124.7, 124.6, 119.0, 118.9, 118.8, 118.6, 109.6, 109.5, 109.4, 109.2, 55.2, 37.6, 21.9. Deuterium incorporation expected at δ 6.69 and 6.61. The level of deuterium incorporation was determined as 90% for δ 6.69 and 91% for δ 6.64 (^{1}H NMR).



***N*-methylbenzen-2,4,6-d_3-amine (2i)**

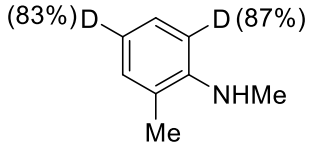
Yellowish liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.19 (s, 1H), 6.70 (t, *J* = 7.2 Hz, **0.13H**), 6.60 (d, *J* = 8.4 Hz, **0.17H**), 2.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ =

149.0, 129.0, 128.9, 117.3, 117.2, 117.1, 116.9, 112.5, 112.4, 112.2, 112.1, 30.7. Deuterium incorporation expected at δ 6.70 and 6.60. The level of deuterium incorporation was determined as 87% for δ 6.70 and 91% (1-0.17/2 = 0.915) for δ 6.60 (^{1}H NMR).



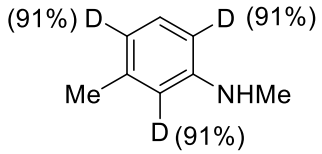
***N*,*4*-dimethylbenzen-2,6-d$_2$-amine (2j)**

Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.99 (s, 2H), 6.53 (d, J = 7.0 Hz, **0.15H**), 2.78 (s, 1H), 2.24 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 146.8, 129.6, 129.5, 126.5, 112.7, 112.6, 112.4, 112.2, 31.0, 20.3. Deuterium incorporation expected at δ 6.53. The level of deuterium incorporation was determined as 92% (1-0.15/2 = 0.925) for δ 6.60 (^{1}H NMR).



***N*,*2*-dimethylbenzen-4,6-d$_2$-amine (2k)**

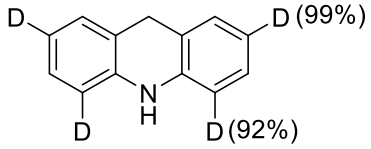
Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.15 (s, 1H), 7.05 (s, 1H), 6.67 (t, J = 6.0 Hz, **0.17H**), 6.62 (d, J = 6.5 Hz, **0.13H**), 3.84 (brs, 1H), 2.88 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 146.7, 129.9, 129.8, 127.0, 126.9, 117.2, 116.9, 109.5, 109.4, 109.2, 109.1, 30.9, 17.3. Deuterium incorporation expected at δ 6.67 and 6.62. The level of deuterium incorporation was determined as 83% for δ 6.69 and 87% for δ 6.62 (^{1}H NMR).



***N*,*3*-dimethylbenzen-2,4,6-d$_3$-amine (2l)**

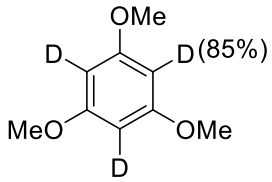
Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.07 (s, 1H), 6.53 (d, J = 6.0 Hz, **0.09H**), 6.42 (d, J = 6.5 Hz, **0.18H**), 2.79 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 149.2, 149.1, 138.8, 138.7, 128.9, 128.8, 118.3, 118.1, 118.0, 117.8, 113.3, 113.1, 112.9, 112.8, 109.7, 109.6, 109.4, 109.3, 30.7, 21.5, 21.4. Deuterium

incorporation expected at δ 6.53 and 6.42. The level of deuterium incorporation was determined as 91% for δ 6.53 and the average deuterium incorporation of C2 and C6 was determined as 91% (1-0.18/2 = 0.91) for δ 6.42 (^{1}H NMR).



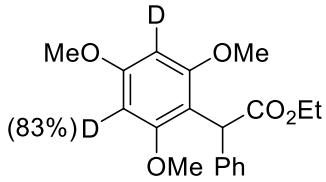
9,10-Dihydroacridine-2,4,5,7-d_4 (2m)

Yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.10-7.08 (m, 4H), 6.83 (t, J = 7.6 Hz, **1.01H**), 6.65 (d, J = 8.0 Hz, **0.15H**), 5.94 (brs, 1H), 4.05 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ =140.1, 128.6, 128.5, 126.8, 120.6, 120.0, 113.4, 113.3, 113.1, 113.0, 31.4. Deuterium incorporation expected at δ 6.83 and 6.65. The level of deuterium incorporation was determined as 99% (1-0.01/2 = 0.995) for δ 6.83 and 92% (1-0.15/2 = 0.925) for δ 6.65 (^{1}H NMR).



1,3,5-Trimethoxybenzene-2,4,6-d_3 (2n)

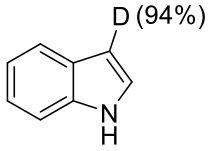
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.08 (s, 0.45H), 3.75 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 161.42, 161.38, 92.9, 92.7, 92.6, 92.4, 55.2. Deuterium incorporation expected at δ 6.08. The level of deuterium incorporation was determined as 85% (1-0.45/3 = 0.85) for δ 6.08 (^{1}H NMR).



Ethyl 2-phenyl-2-(2,4,6-trimethoxyphenyl-3,5-d_2)acetate (2o)

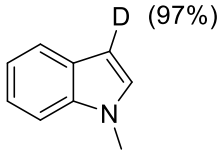
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.31 (d, J = 6.5 Hz, 2H), 7.26-7.23 (m, 2H), 7.16 (t, J = 6.0 Hz, 1H), 6.14 (s, **0.34H**), 5.29 (s, 1H), 4.22-4.19 (m, 1H), 4.15-4.12 (m, 1H), 3.78-3.76 (m, 9H), 1.18 (t, J = 6.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 173.6, 160.3, 160.2, 158.10, 158.06, 139.0, 129.2, 127.8, 126.4, 109.5,

90.8, 90.5, 67.9, 60.6, 55.6, 55.2, 45.8, 30.2, 29.6, 25.5, 14.2. Deuterium incorporation expected at δ 6.14. The level of deuterium incorporation was determined as 83% (1-0.34/2 = 0.83) (^{1}H NMR).



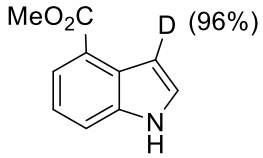
1*H*-Indole-3-d (4a)

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.63 (d, J = 8.0 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.20-7.16 (m, 1H), 7.13-7.10 (m, 2H), 6.53 (d, J = 2.8 Hz, **0.06H**); ^{13}C NMR (100 MHz, $CDCl_3$): δ =135.6, 127.7, 123.9, 121.9, 120.7, 120.6, 119.7, 111.0, 102.39, 102.36, 102.2, 102.0. Deuterium incorporation expected at δ 6.53. The level of deuterium incorporation was determined as 94% for (^{1}H NMR).



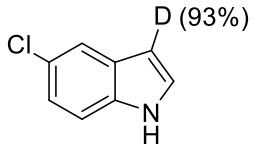
1-Methyl-1*H*-indole-3-d (4b)

Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.61 (d, J = 7.0 Hz, 1H), 7.28 (d, J = 7.0 Hz, 1H), 7.19 (t, J = 7.0 Hz, 1H), 7.08 (t, J = 6.0 Hz, 1H), 7.00 (s, 1H), 6.46 (d, J = 2.5 Hz, **0.03H**), 3.72 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 136.6, 128.7, 128.6, 128.3, 121.4, 120.8, 120.75, 119.2 ,109.1, 100.8, 100.75, 100.6, 100.4, 32.7. Deuterium incorporation expected at δ 6.46. The level of deuterium incorporation was determined as 97% (^{1}H NMR).



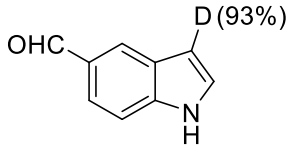
Methyl 1*H*-indole-4-carboxylate-3-d (4c)

Yellowish liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.92 (dd, J = 7.6, 1.2 Hz, 1H), 7.53 (dd, J = 8.0, 1.2 Hz, 1H), 7.28 (m, 1H), 7.12-7.18 (m, **1.04H**), 3.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 168.5, 136.6, 136.5, 127.2, 126.3, 123.3, 121.2, 120.9, 116.2, 116.1, 103.4, 103.36, 103.2, 103.0, 51.7. Deuterium incorporation expected at δ 7.12-7.18. The level of deuterium incorporation was determined as 96% (^{1}H NMR).



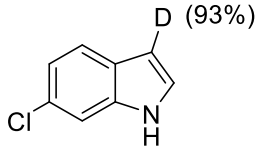
5-Chloro-1*H*-indole-3-d (4d)

Yellowish solid; ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.58 (d, J = 2.0 Hz, 1H), 7.43-7.41 (m, 2H), 7.07 (dd, J = 8.0, 2.0 Hz, 1H), 6.42 (d, J = 2.8 Hz, **0.07H**); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 134.4, 134.3, 128.82, 128.78, 127.03, 126.96, 126.87, 123.5, 120.9, 119.2, 112.93, 112.88, 100.9, 100.7, 100.5. Deuterium incorporation expected at δ 6.42. The level of deuterium incorporation was determined as 93% (^{1}H NMR).



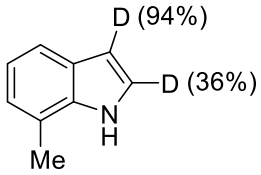
1*H*-Indole-3-d-5-carbaldehyde (4e)

Yellowish solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ = 11.61 (brs, 1H), 9.96 (s, 1H), 8.18 (s, 1H), 7.63 (d, J = 2.0 Hz, 1H), 7.56-7.51 (m, 2H), 6.66 (s, **0.07H**); ^{13}C NMR (126 MHz, DMSO-d_6): δ = 192.6, 139.4, 128.9, 127.6, 127.4, 125.9, 120.8, 112.2, 112.1, 103.2, 103.0. Deuterium incorporation expected at δ 6.66. The level of deuterium incorporation was determined as 93% (^{1}H NMR).



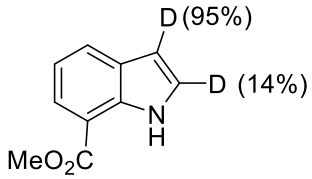
6-Chloro-1*H*-indole-3-d (4f)

Yellowish solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ = 11.22 (brs, 0.26H), 7.53 (d, J = 6.0 Hz, 1H), 7.45 (s, 1H), 7.38 (s, 1H), 7.00 (d, J = 7.0 Hz, 1H), 6.45 (s, **0.07H**); ^{13}C NMR (126 MHz, DMSO-d_6): δ = 136.4, 136.2, 126.41, 126.39, 126.3, 125.7, 121.4, 119.2, 111.1, 111.0, 101.3, 101.1, 100.9. Deuterium incorporation expected at δ 6.45. The level of deuterium incorporation was determined as 93% (^{1}H NMR).



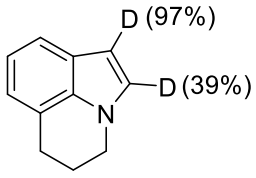
7-Methyl-1*H*-indole-2,3-d$_2$ (4g)

Yellowish liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.48 (d, J = 8.0 Hz, 1H), 7.09 (s, **0.64H**), 7.05-7.02 (m, 1H), 6.97 (d, J = 6.8 Hz, 1H), 6.50 (d, J = 2.8 Hz, **0.06H**), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 135.2, 127.2, 123.6, 122.3, 120.1, 119.9, 119.8, 118.4, 102.9, 102.8, 102.6, 102.4, 16.6. Deuterium incorporation expected at δ 7.09 and 6.50. The level of deuterium incorporation was determined as 36% for δ 7.09 and 94% for δ 6.50 (^{1}H NMR).



Methyl 1*H*-indole-7-carboxylate-3-d (4h)

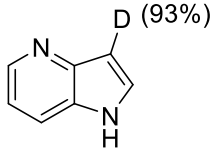
Yellowish liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.90-7.84 (m, 2H), 7.29 (s, **0.86H**), 7.12 (t, J = 7.6 Hz, 1H), 6.58 (d, J = 3.2 Hz, **0.05H**), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.9, 135.4, 128.9, 126.4, 125.1, 125.0, 124.9, 124.2, 119.0, 112.4, 102.41, 102.37, 102.2, 102.0, 51.8. Deuterium incorporation expected at δ 7.29 and 6.58. The level of deuterium incorporation was determined as 14% for δ 7.29 and 95% for δ 6.58 (^{1}H NMR).



5,6-Dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1-d (4i)

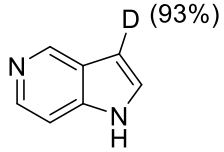
Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.44-7.42 (m, 1H), 7.02-6.97 (m, **1.61H**), 6.88 (dd, J = 8.5, 1.0 Hz, 0.81H), 6.43 (d, J = 2.5 Hz, **0.03H**), 4.07 (t, J = 7.0 Hz, 2H), 2.94 (t, J = 7.5 Hz, 2H), 2.21-2.15 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 134.1, 125.8, 125.7, 121.6, 119.6, 118.2, 100.30, 100.27, 100.1, 99.9, 44.1, 24.7, 22.9. Deuterium incorporation expected at δ 7.02-6.97 and 6.43. The level of

deuterium incorporation was determined as 39% for δ 7.02-6.97 and 97% for δ 6.43 (^{1}H NMR).



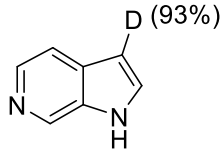
1*H*-Pyrrolo[3,2-*b*]pyridine-3-d (4j)

Yellowish solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 11.10 (brs, 1H), 8.46-8.45 (m, 1H), 7.76 (d, *J* = 7.0 Hz, 1H), 7.54 (s, 1H), 7.10 (dd, *J* = 7.0, 4.0 Hz, 1H), 6.69 (d, *J* = 2.5 Hz, **0.07H**); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 145.7, 142.2, 129.3, 129.1, 128.9, 119.5, 116.5, 101.8, 101.6, 101.4. Deuterium incorporation expected at δ 6.69. The level of deuterium incorporation was determined as 93% (^{1}H NMR).



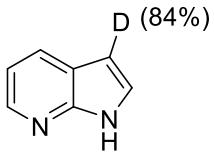
1*H*-Pyrrolo[3,2-*c*]pyridine-3-d (4k)

Yellowish solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 11.99 (brs, 1H), 8.96 (s, 1H), 8.24 (d, *J* = 5.0 Hz, 1H), 7.42 (d, *J* = 5.0 Hz, 1H), 7.37 (s, 1H), 6.66 (d, *J* = 2.5 Hz, **0.07H**); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 142.0, 142.3, 138.5, 126.9, 125.1, 107.5, 101.3, 101.1, 100.9. Deuterium incorporation expected at δ 6.66. The level of deuterium incorporation was determined as 93% (^{1}H NMR).



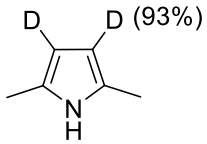
1*H*-Pyrrolo[2,3-*c*]pyridine-3-d (4l)

Yellowish solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 11.76 (brs, 1H), 8.85 (s, 1H), 8.18 (d, *J* = 5.0 Hz, 1H), 7.58 (d, *J* = 4.5 Hz, 1H), 7.48 (s, 1H), 6.55 (d, *J* = 2.5 Hz, **0.07H**); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 136.4, 133.5, 133.33, 133.26, 130.1, 130.0, 115.5, 101.4, 101.2, 100.0. Deuterium incorporation expected at δ 6.55. The level of deuterium incorporation was determined as 93% (^{1}H NMR).



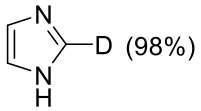
1*H*-Pyrrolo[2,3-*b*]pyridine-3-d (4m)

Yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 12.19 (brs, 1H), 8.31 (dd, J = 7.2, 0.8 Hz, 1H), 7.94 (dd, J = 5.2, 0.8 Hz, 1H), 7.38 (s, 1H), 7.05 (dd, J = 5.2, 3.2 Hz, 1H), 6.47 (d, J = 2.4 Hz, **0.16H**); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 148.7, 141.9, 129.2, 129.1, 125.5, 120.73, 120.65, 115.5, 100.3, 100.1, 100.0. Deuterium incorporation expected at δ 6.47. The level of deuterium incorporation was determined as 93% (^{1}H NMR).



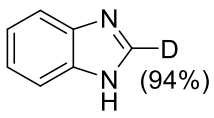
2,5-Dimethyl-1*H*-pyrrole-3,4-d_2 (4n)

Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 5.73 (s, **0.14H**), 4.92 (s, 2H), 2.22 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 125.8, 105.6, 105.5, 105.4, 105.2, 18.9, 12.9, 12.8. Deuterium incorporation expected at δ 5.73. The level of deuterium incorporation was determined as 93% (^{1}H NMR).



1*H*-Imidazole-2-d (4o)

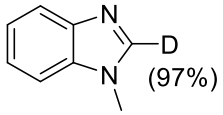
White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 12.23 (brs, 1H), 7.75 (s, **0.02H**), 7.11 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 135.3, 135.0, 134.8, 121.8. Deuterium incorporation expected at δ 7.75. The level of deuterium incorporation was determined as 98% (^{1}H NMR).



1*H*-Benzo[*d*]imidazole-2-d (4p)

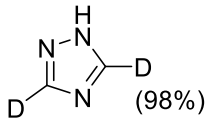
White solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ = 12.09 (brs, 0.29H), 8.24 (s, **0.06H**), 7.59 (dd, J = 7.5, 4.0 Hz, 2H), 7.18 (dd, J = 7.5, 4.0 Hz, 2H); ^{13}C NMR (126 MHz,

DMSO-d_6): δ = 142.0, 141.8, 141.6, 138.1, 121.8, 115.4. Deuterium incorporation expected at δ 8.24. The level of deuterium incorporation was determined as 94% (^{1}H NMR).



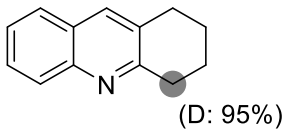
1-Methyl-1*H*-benzo[*d*]imidazole-2-d (4q)

Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.81 (s, **0.03H**), 7.78 (d, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.31-7.25 (m, 2H), 3.77 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 143.6, 143.5, 143.4, 143.1, 134.4, 123.0, 122.1, 120.1, 109.4, 31.0. Deuterium incorporation expected at δ 7.81. The level of deuterium incorporation was determined as 97% (^{1}H NMR).



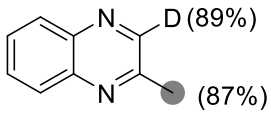
1*H*-1,2,4-Triazole-3,5-d_2 (4r)

White solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ = 14.09 (brs, 1H), 8.29 (s, **0.02H**); ^{13}C NMR (126 MHz, DMSO-d_6): δ = 149.3 (m), 143.8 (m). Deuterium incorporation expected at δ 8.29. The level of deuterium incorporation was determined as 98% (^{1}H NMR).



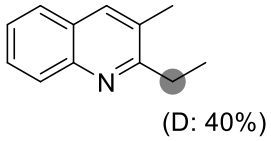
1,2,3,4-Tetrahydroacridine-4,4-d_2 (6a)

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.98 (d, *J* = 7.0 Hz, 1H), 7.79 (m, 1H), 7.67 (d, *J* = 5.6 Hz, 1H), 7.59 (td, *J* = 5.6, 0.8 Hz, 1H), 7.44-7.41 (m, 1H), 3.09 (t, *J* = 4.4 Hz, **0.10H**), 2.93 (t, *J* = 4.0 Hz, 2H), 1.95 (t, *J* = 4.0 Hz, 2H), 1.89-1.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.0, 145.9, 135.4, 131.0, 128.7, 127.7, 126.8, 125.6, 32.9, 32.8, 32.7, 32.5, 32.4, 32.3, 32.2, 29.0, 22.8, 22.7, 22.6. Deuterium incorporation expected at δ 3.09. The level of deuterium incorporation was determined as 95% (1-0.10/2 = 0.95) (^{1}H NMR).



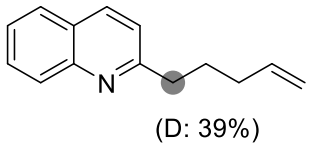
2-(Methyl-d_3)quinoxaline-3-d (6b)

White solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.74 (s, **0.11H**), 8.06 (dd, *J* = 5.6, 0.8 Hz, 1H), 8.01 (dd, *J* = 5.6, 0.8 Hz, 1H), 7.75-7.68 (m, 2H), 2.76-2.73 (m, **0.38H**); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 153.6, 153.5, 145.9, 141.95, 141.92, 140.8, 129.9, 128.8, 128.5, 22.1, 22.0, 21.9, 21.7, 21.6, 21.5. Deuterium incorporation expected at δ 8.74 and 2.76-2.73. The level of deuterium incorporation was determined as 89% for δ 8.74 and 87% for δ 2.76-2.73 and (1-0.38/3 = 0.87) (^{1}H NMR).



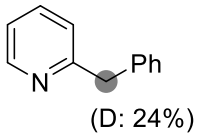
2-(Ethyl-1-d)-3-methylquinoline (6c)

Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.04 (d, *J* = 7.0 Hz, 1H), 7.82 (s, 1H), 7.69-7.68 (m, 1H), 7.62-7.59 (m, 1H), 7.45-7.42 (m, 1H), 3.03-2.98 (m, **1.2 H**), 2.47 (s, 3H), 1.38-1.35 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 163.3, 146.3, 136.1, 129.4, 128.4, 128.3, 127.3, 126.7, 125.7, 29.7, 29.5, 29.4, 29.2, 19.01, 19.00, 12.81, 12.74, 12.67. Deuterium incorporation expected at δ 3.03-2.98. The level of deuterium incorporation was determined as 40% [(2-1.2)/2 = 0.40)] (^{1}H NMR).



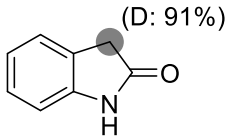
2-(Pent-4-en-1-yl-1-d)quinoline (6d)

Yellowish liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.08-8.05 (m, 2H), 7.95 (d, *J* = 6.5 Hz, 1H), 7.68-7.66 (m, 1H), 7.45 (t, *J* = 6.5 Hz, 1H), 7.27 (d, *J* = 7.0 Hz, 1H), 5.87-5.82 (m, 1H), 5.05-4.97 (m, 2H), 2.31-2.96 (m, **1.22H**), 2.18-2.14 (m, 2H), 1.95-1.89 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 162.56, 162.55, 147.5, 138.1, 136.5, 129.5, 128.5, 127.4, 126.7, 125.7, 121.3, 114.9, 38.6, 38.4, 38.2, 38.1, 33.4, 33.33, 33.31, 29.0, 28.94, 28.87. Deuterium incorporation expected at δ 2.31-2.96. The level of deuterium incorporation was determined as 39% [(2-1.22)/2 = 0.39)] (^{1}H NMR).



2-(Phenylmethyl-d)pyridine (6e)

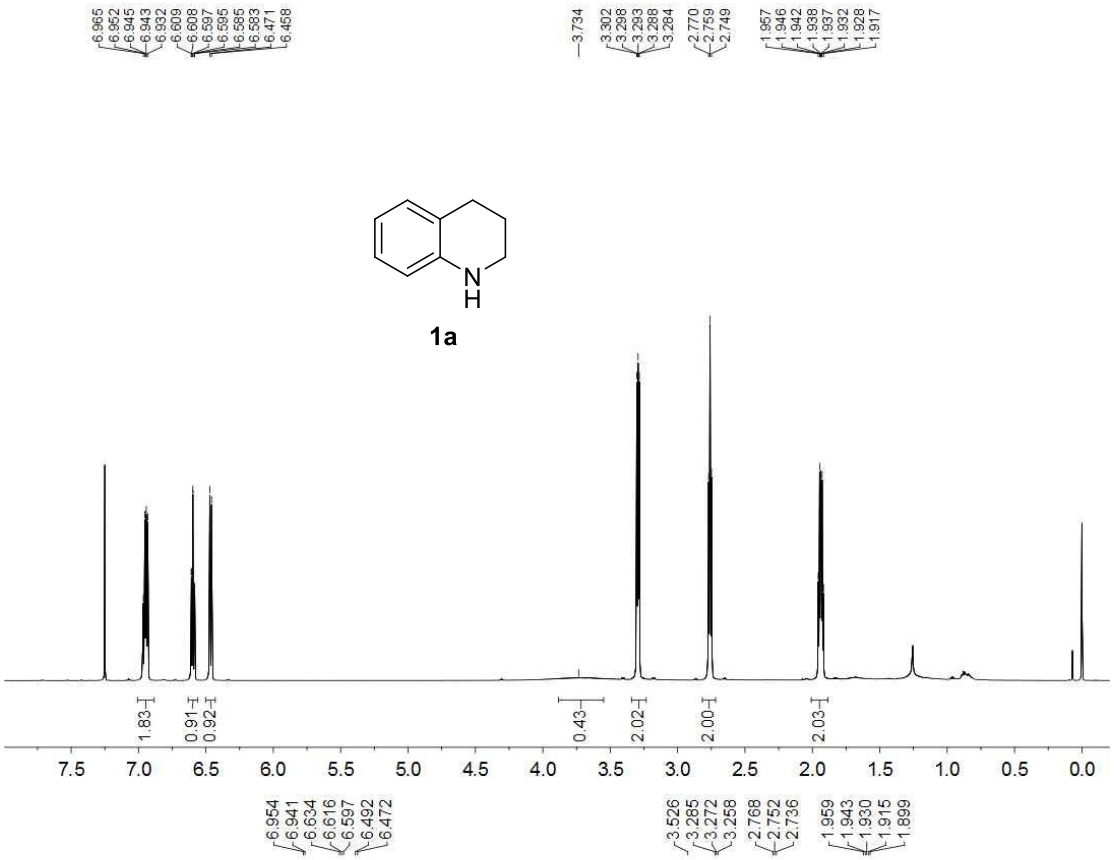
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.52 (d, *J* = 7.2 Hz, 1H), 7.56 (td, *J* = 5.2, 1.2 Hz, 1H), 7.29-7.27 (m, 2H), 7.25-7.19 (m, 3H), 7.12-7.10 (m, 2H), 4.14-4.13 (m, **1.52H**); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 160.74, 160.72, 149.4, 139.12, 139.09, 136.8, 128.99, 128.98, 128.5, 126.4, 123.3, 121.3, 44.6, 44.4, 44.3, 44.1. Deuterium incorporation expected at δ 4.14-4.13. The level of deuterium incorporation was determined as 24% [(2-1.52)/2 = 0.24)] (^{1}H NMR).

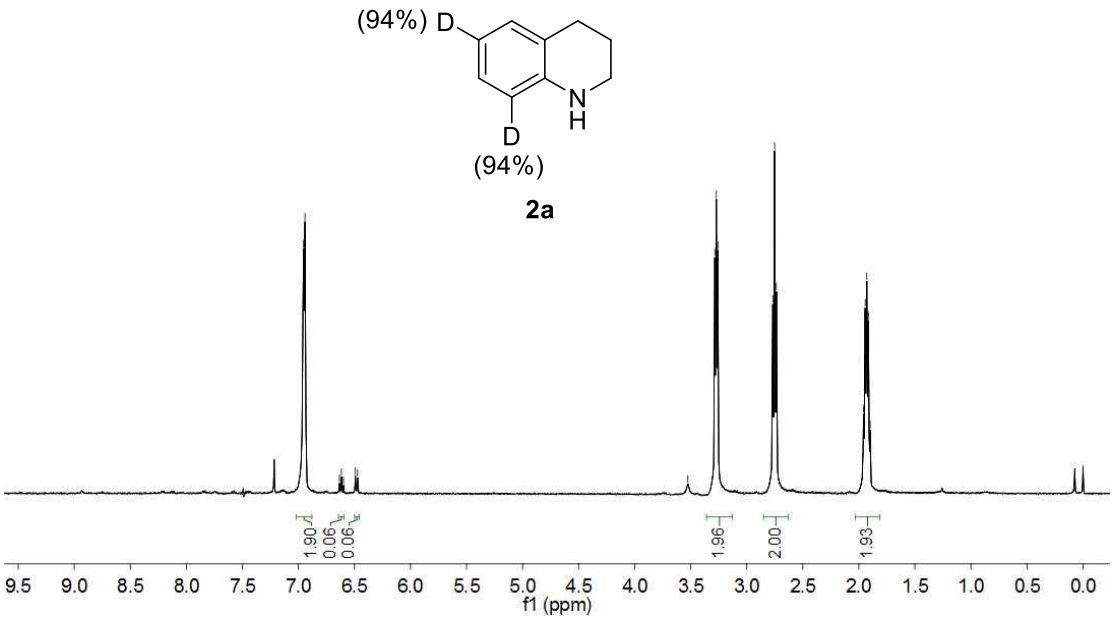


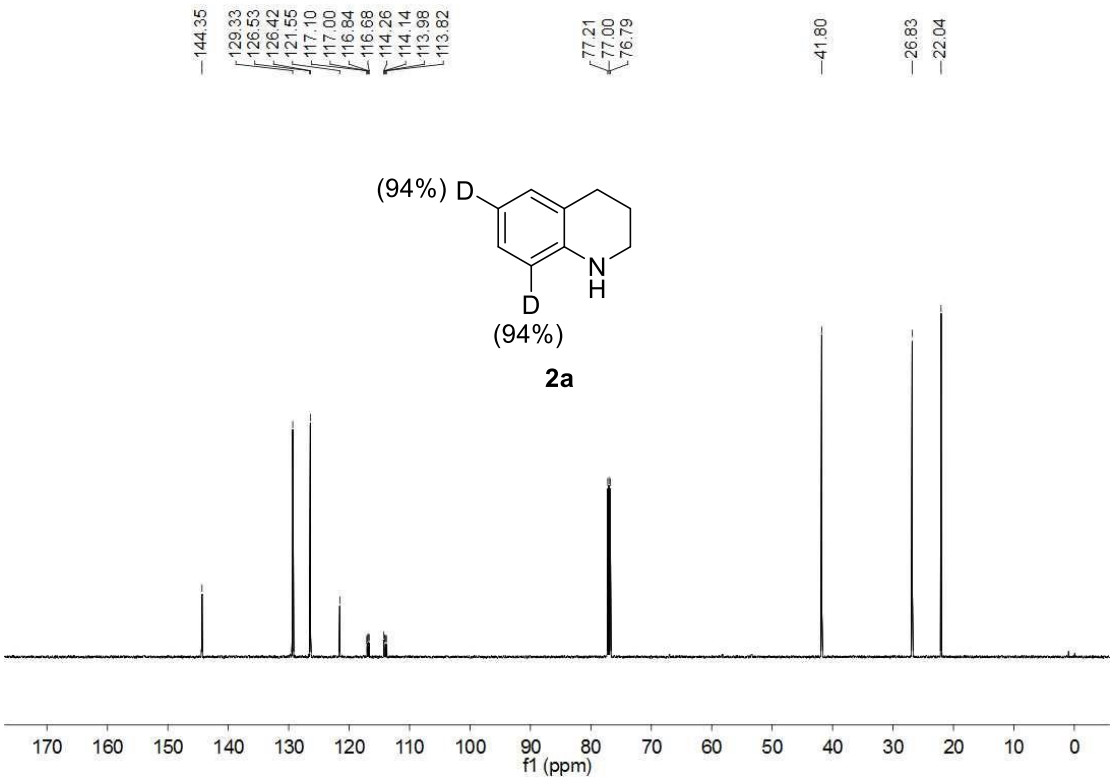
Indolin-2-one-3,3-d_2 (6f)

Yellowish solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.76 (brs, 1H), 7.20-7.19 (m, 2H), 6.98 (t, *J* = 6.5 Hz, 1H), 6.90 (d, *J* = 7.0 Hz, 1H), 3.50 (s, **0.17H**); ^{13}C NMR (126 MHz, $CDCl_3$): δ = 178.5, 178.4, 142.8, 142.74, 142.65, 127.8, 125.2, 125.1, 124.42, 124.40, 122.2, 109.9, 109.8, 36.1, 36.0, 35.8, 35.7, 35.6. Deuterium incorporation expected at δ 3.50. The level of deuterium incorporation was determined as 91% [(2-0.17)/2 = 0.915)] (^{1}H NMR).

4. ^{1}H, and ^{13}C NMR Spectra



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126.42
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117.00
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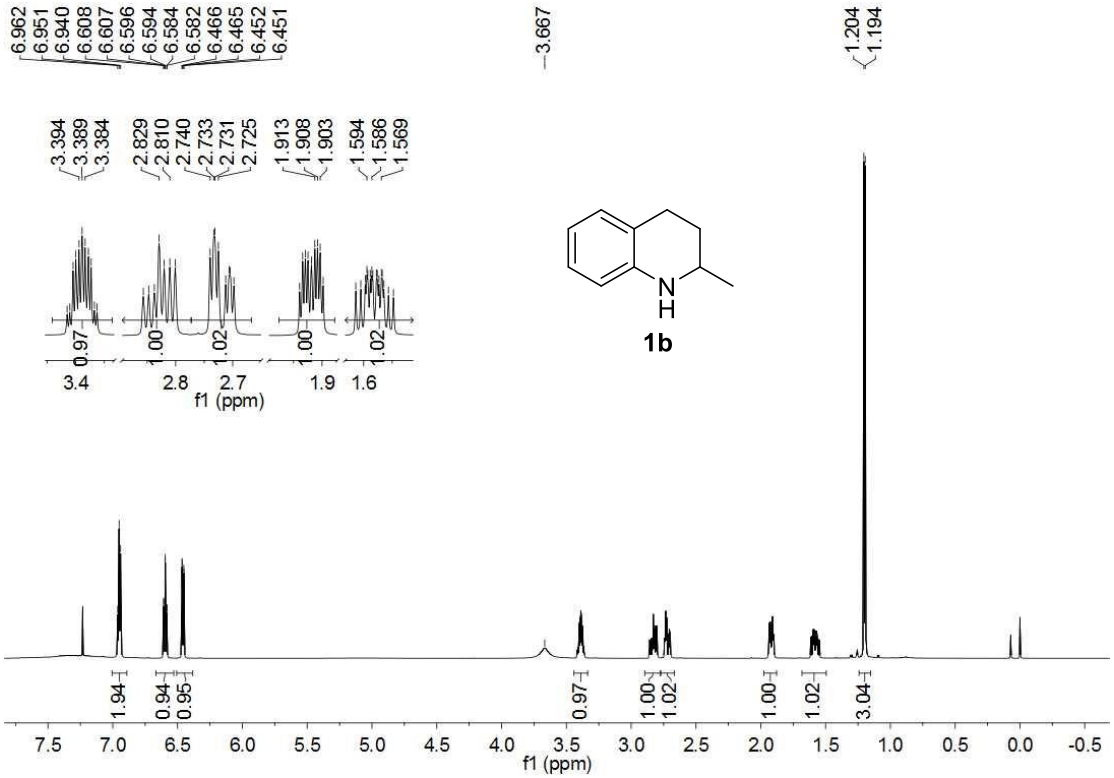
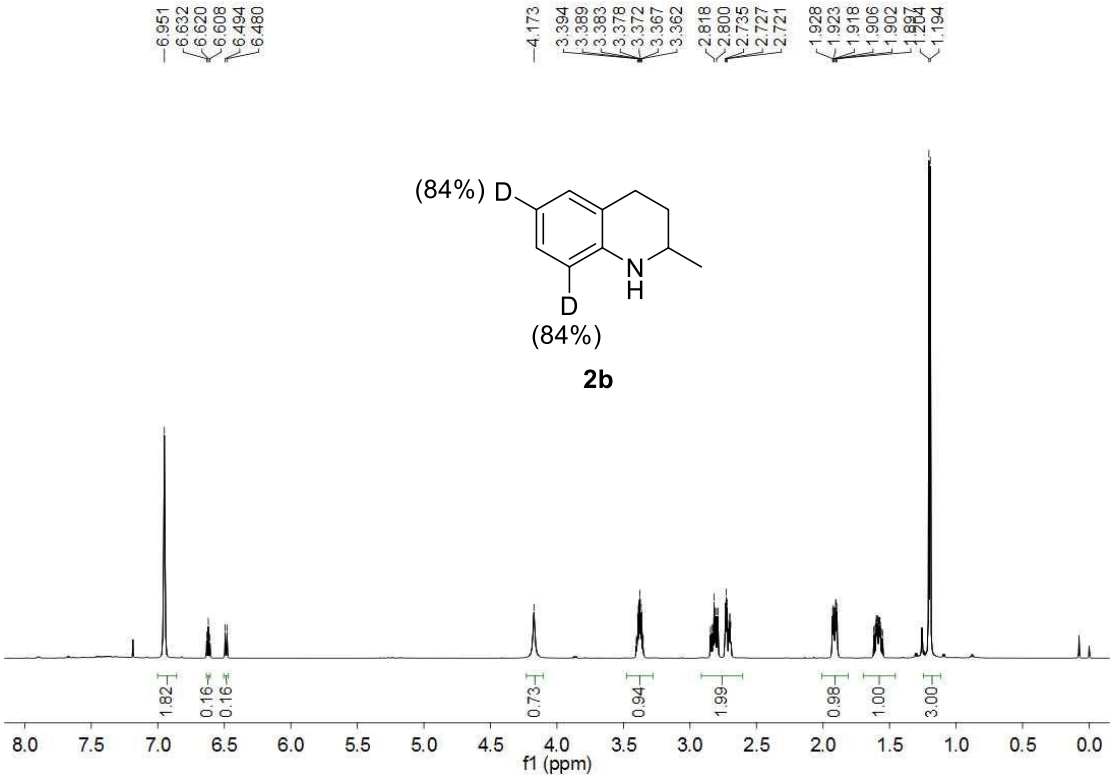
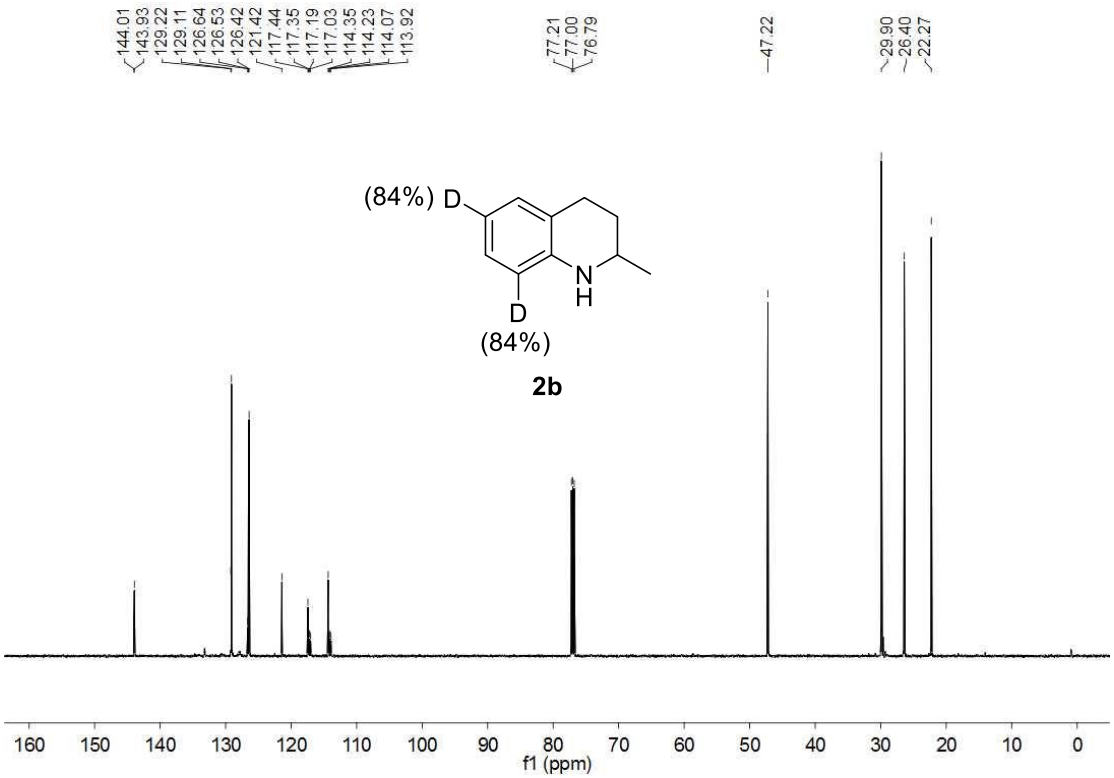
114.14
113.98
113.82
77.21
77.00
76.79
41.80
26.83
22.04
(94%) D
N
H
D
(94%)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

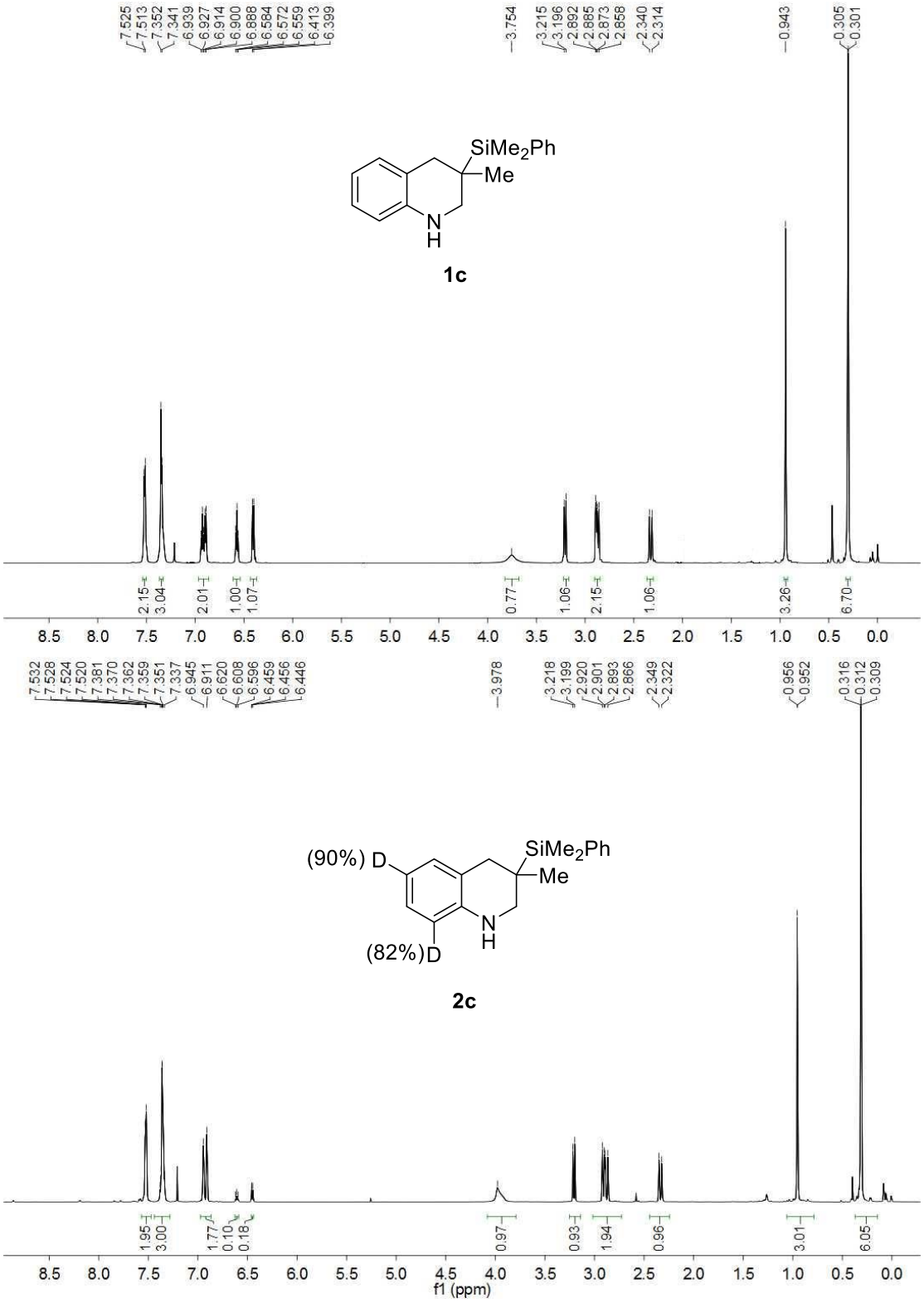
2a

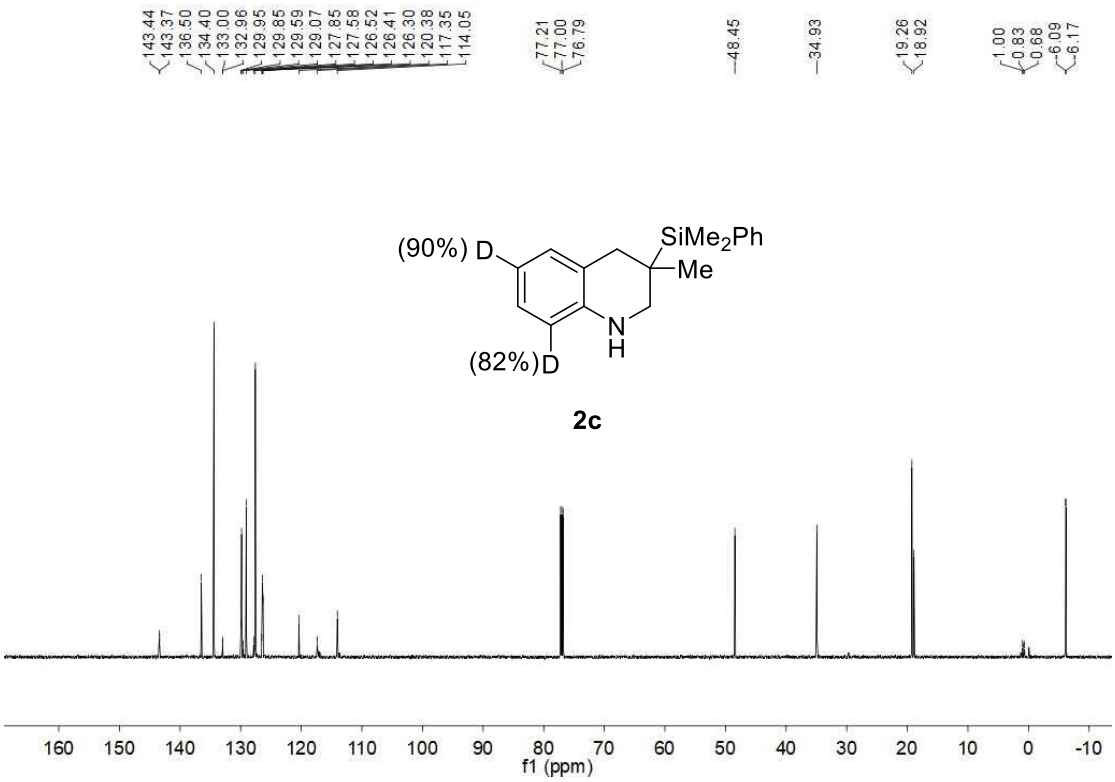

6.962
6.951
6.940
6.608
6.607
6.596
6.594
6.584
6.582
6.466
6.465
6.452
6.451
3.667
1.204
1.194
3.394
3.389
3.384
2.829
2.810
2.740
2.733
2.731
2.725
1.913
1.908
1.903
1.594
1.586
1.569
0.97
1.00
1.02
1.00
1.02
3.4
2.8
2.7
1.9
1.6
f1 (ppm)
1b
1.94
0.94
0.95
0.97
1.00
1.02
1.00
1.02
3.04
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

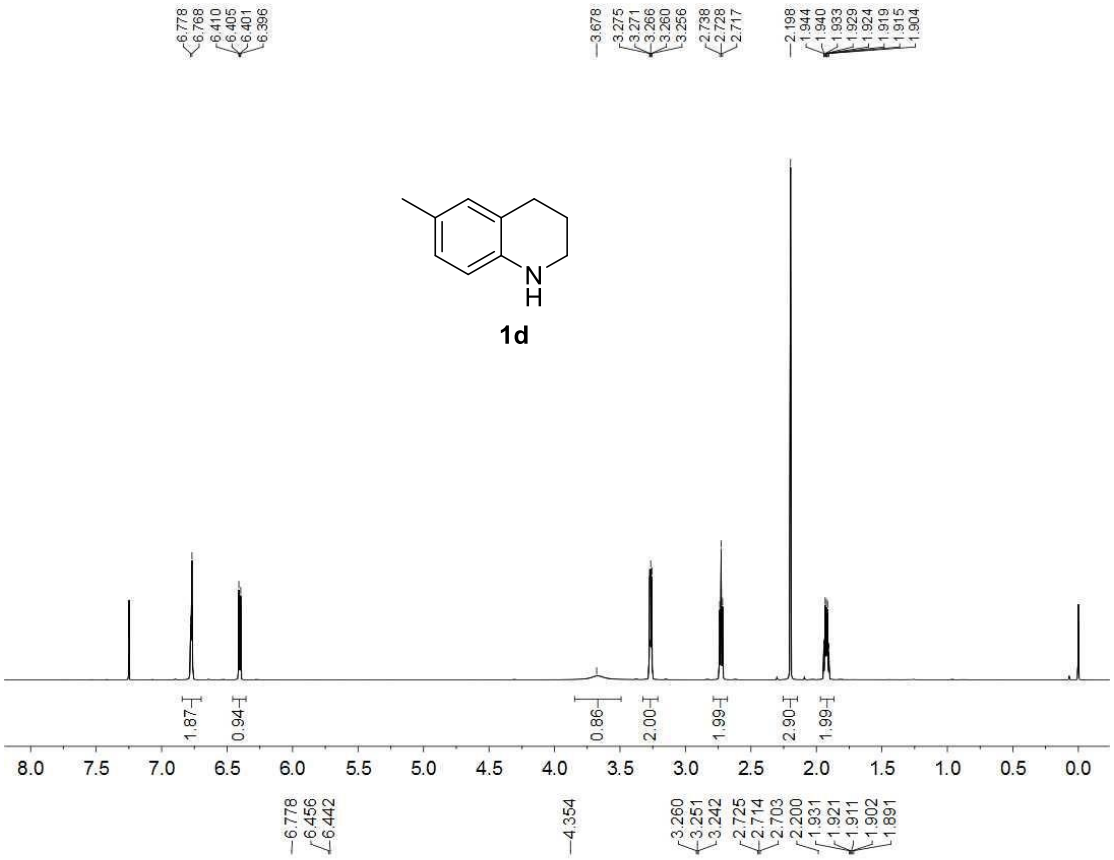

6.951
6.632
6.620
6.608
6.494
6.480
4.173
3.394
3.389
3.383
3.378
3.372
3.367
3.362
2.818
2.800
2.735
2.727
2.721
1.928
1.923
1.918
1.906
1.902
1.204
1.194
(84%) D
D
(84%)
2b
1.82
0.16
0.16
0.73
0.94
1.99
0.98
1.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

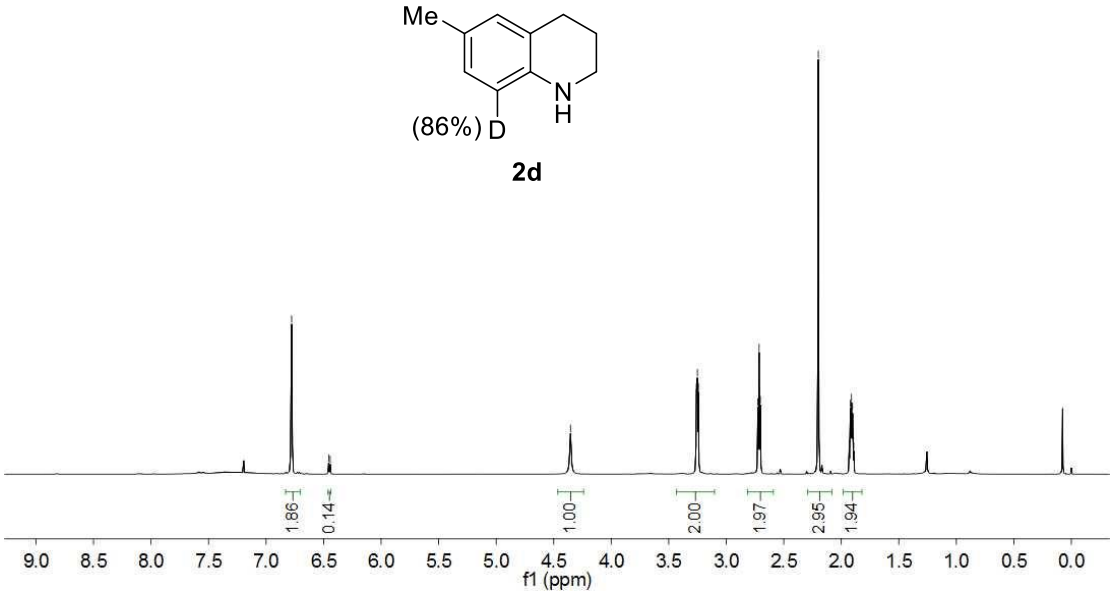

144.01
143.93
129.22
129.11
126.64
126.53
126.42
121.42
117.44
117.35
117.19
117.03
114.35
114.23
114.07
113.92
77.21
77.00
76.79
47.22
29.90
26.40
22.27
(84%) D
N
H
D
(84%)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

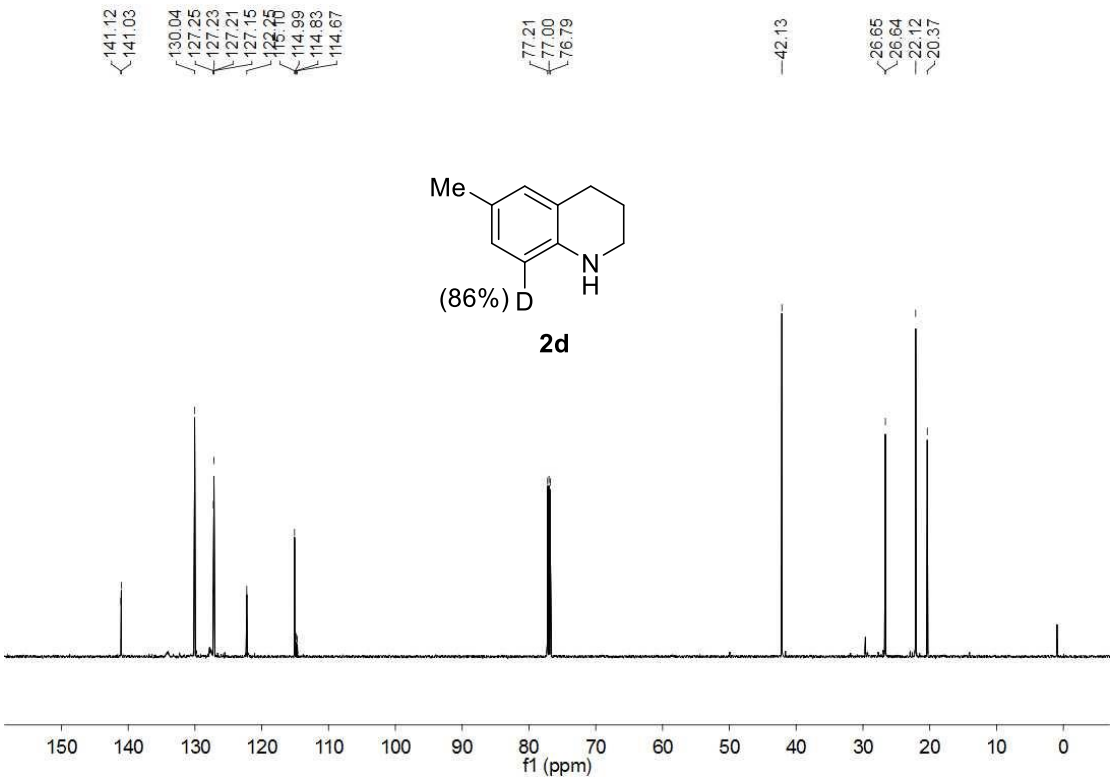
2b


7.525
7.513
7.352
7.341
6.939
6.927
6.914
6.900
6.888
6.584
6.572
6.559
6.413
6.399
3.754
3.215
3.196
2.892
2.885
2.873
2.858
2.340
2.314
0.943
0.305
0.301
SiMe2Ph
Me
N
H
1c
2.15
3.04
2.01
1.00
1.07
0.77
1.06
2.15
1.06
3.26
6.70
7.532
7.528
7.524
7.520
7.381
7.370
7.362
7.359
7.351
7.337
6.945
6.911
6.620
6.608
6.596
6.459
6.456
6.446
3.978
3.218
3.199
2.920
2.901
2.893
2.866
2.349
2.322
0.956
0.952
0.316
0.312
0.309
(90%) D
SiMe2Ph
Me
N
H
(82%)D
2c
1.95
3.00
1.77
0.10
0.18
0.97
0.93
1.94
0.96
3.01
6.05
f1 (ppm)

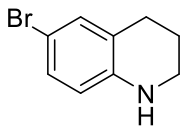

143.44
143.37
136.50
134.40
133.00
132.96
129.95
129.85
129.59
129.07
127.85
127.58
126.52
126.41
126.30
120.38
117.35
114.05
77.21
77.00
76.79
48.45
34.93
19.26
18.92
1.00
0.83
0.68
6.09
6.17
(90%) D
SiMe2Ph
Me
N
H
(82%)D
2c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


6.778
6.768
6.410
6.405
6.401
6.396
3.678
3.275
3.271
3.266
3.260
3.256
2.738
2.728
2.717
2.198
1.944
1.940
1.933
1.929
1.924
1.919
1.915
1.904
N
H
1d
1.87
0.94
0.86
2.00
1.99
2.90
1.99
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
6.778
6.456
6.442
4.354
3.260
3.251
3.242
2.725
2.714
2.703
2.200
1.931
1.921
1.911
1.902
1.891

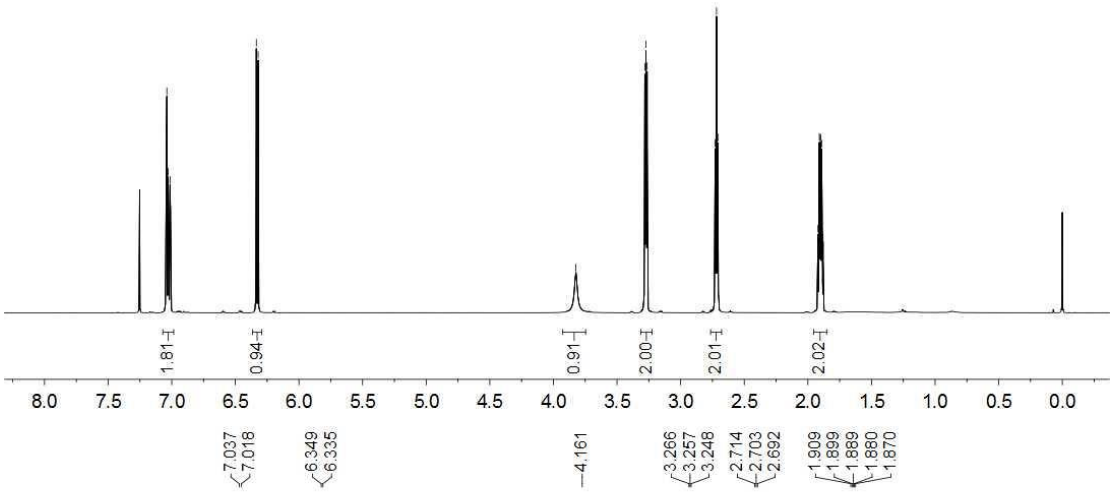

Me
N
H
(86%) D
2d
1.86
0.14
1.00
2.00
1.97
2.95
1.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

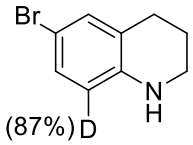

141.12
141.03
130.04
127.25
127.23
127.21
127.15
114.99
114.83
114.67
77.21
77.00
76.79
42.13
26.65
26.64
22.12
20.37
Me
N
H
(86%) D
2d
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.042
7.040
7.038
7.027
7.023
7.013
7.009
6.335
6.321
3.823
3.282
3.277
3.273
3.268
3.263
2.729
2.718
2.707
1.921
1.916
1.910
1.906
1.902
1.900
1.895
1.891
1.885
1.881

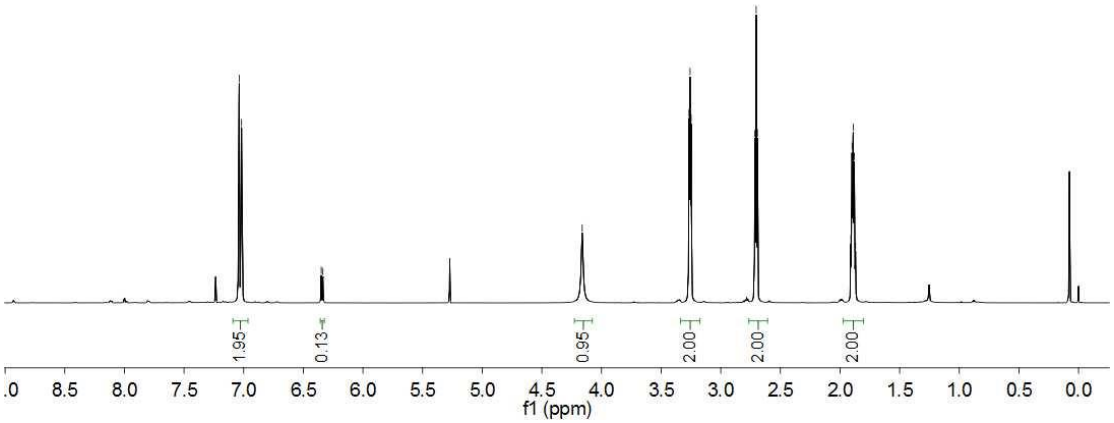

Br
N
H

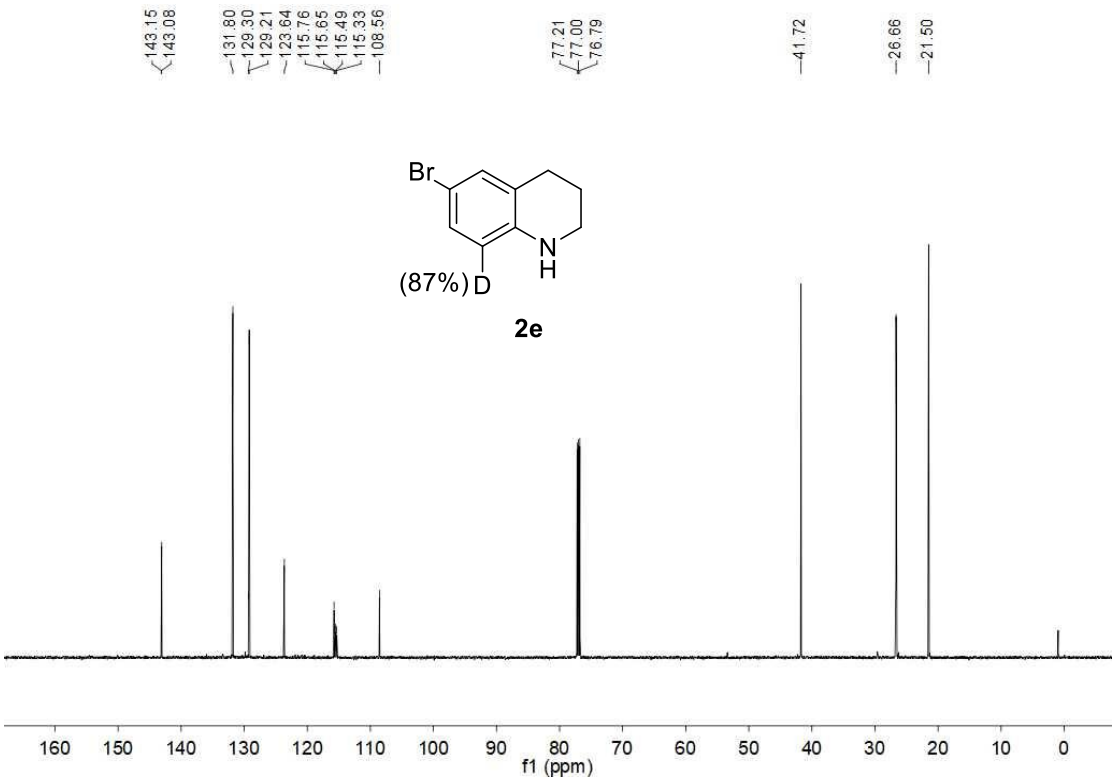
1e


1.81
0.94
0.91
2.00
2.01
2.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
7.037
7.018
6.349
6.335
4.161
3.266
3.257
3.248
2.714
2.703
2.692
1.909
1.899
1.889
1.880
1.870

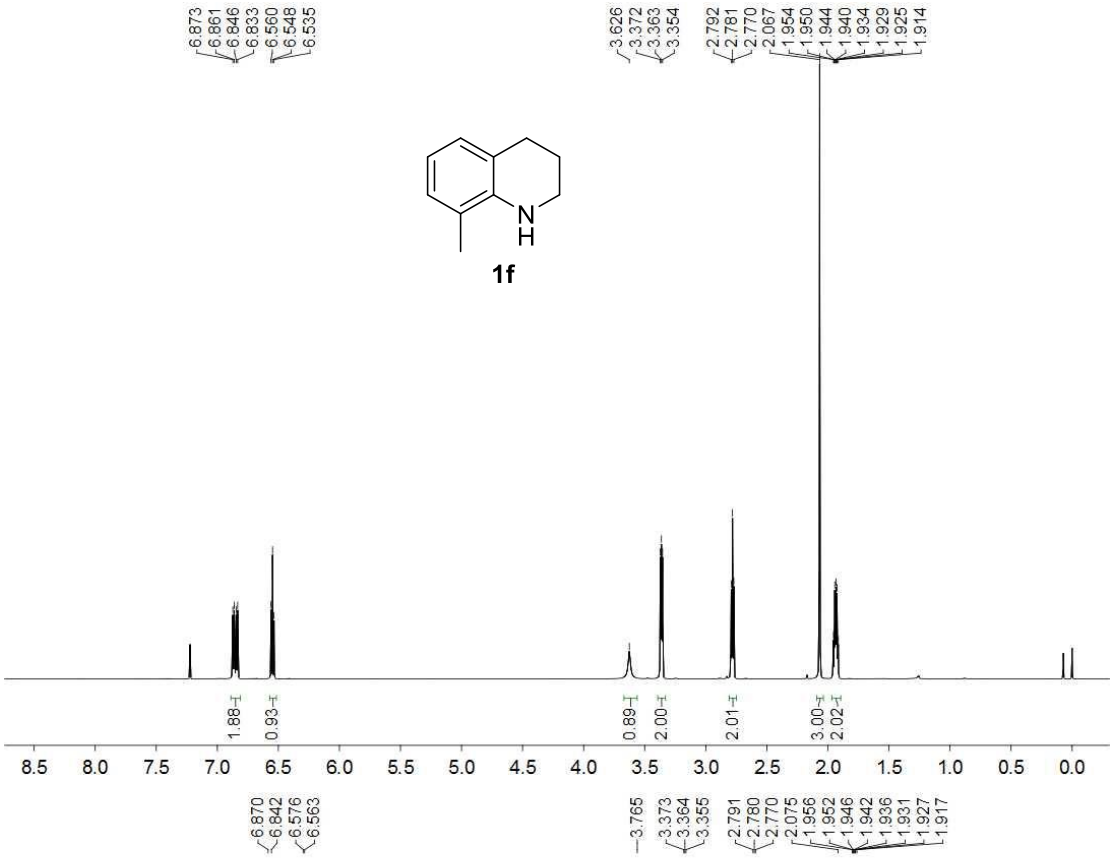

Br
N
H
(87%) D

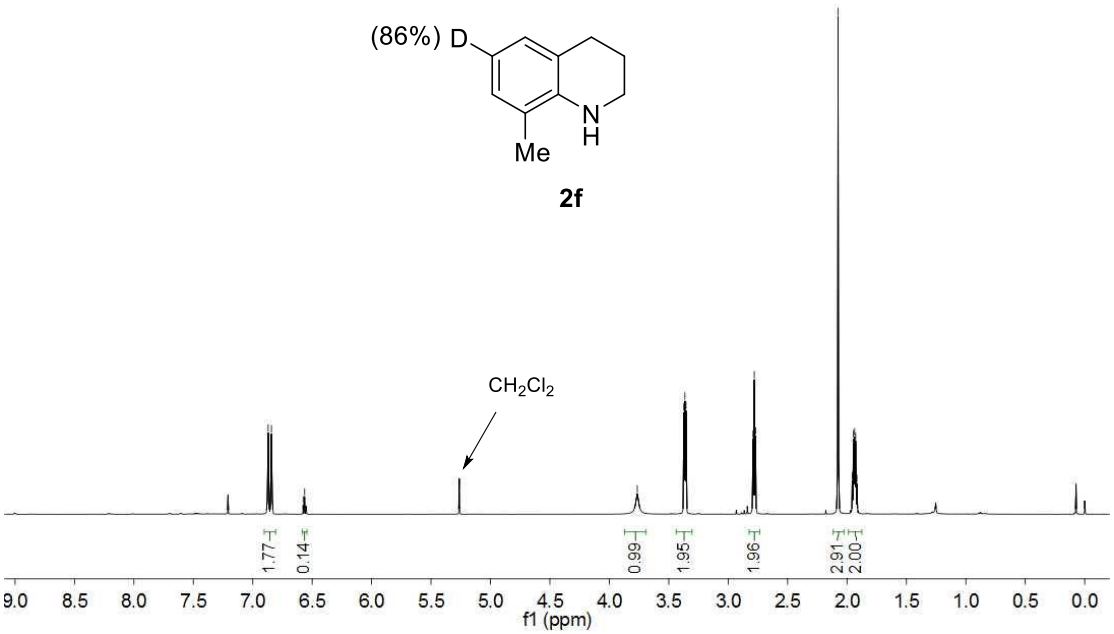
2e

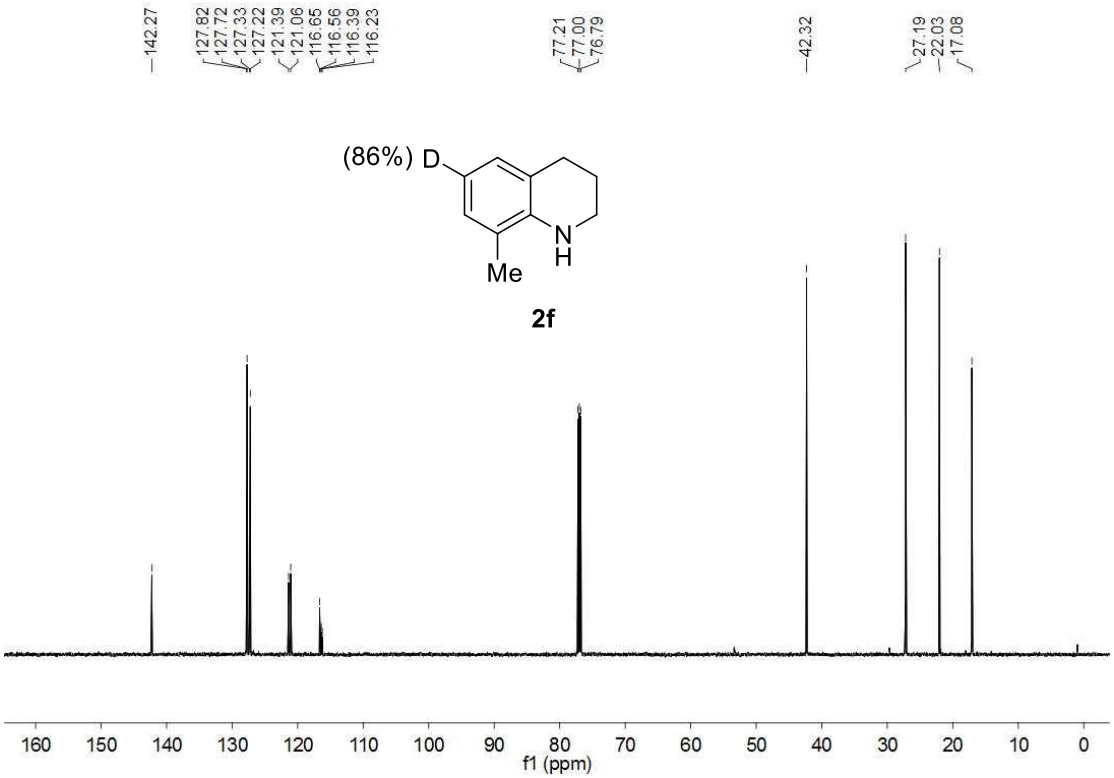

1.95
0.13
0.95
2.00
2.00
2.00
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

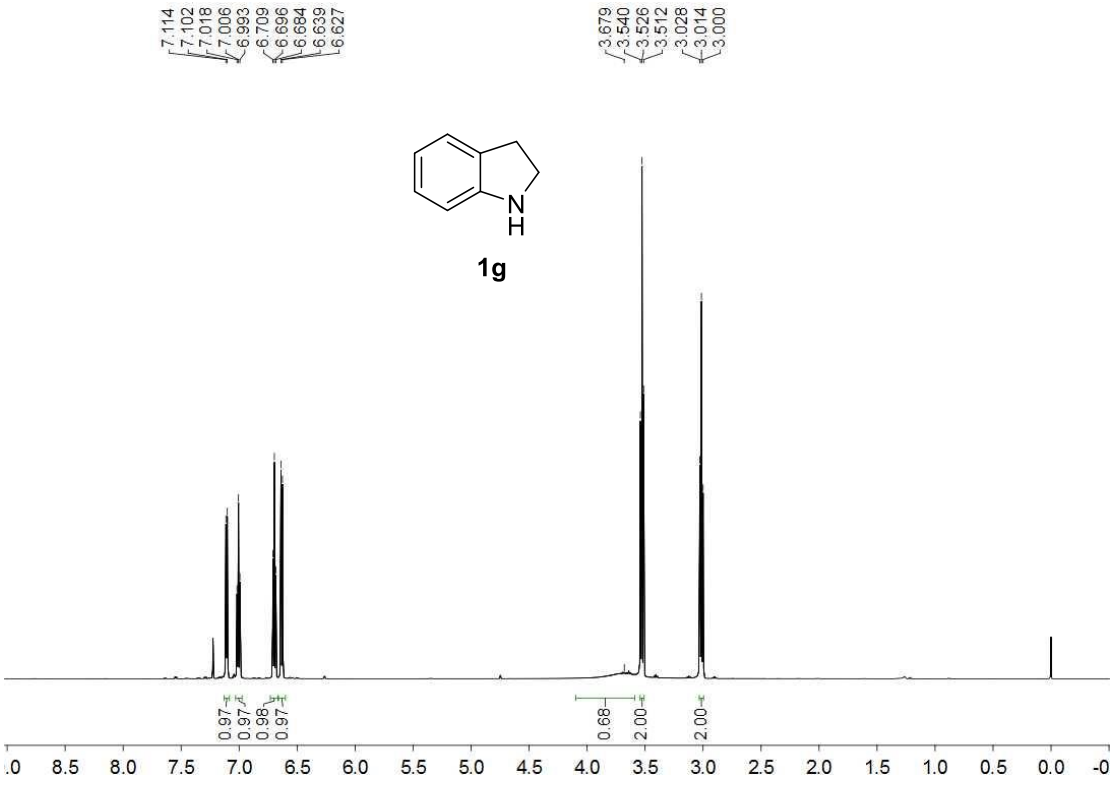

143.15
143.08
131.80
129.30
129.21
123.64
115.76
115.65
115.49
115.33
108.56
77.21
77.00
76.79
41.72
26.66
21.50
Br
N
H
(87%) D
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

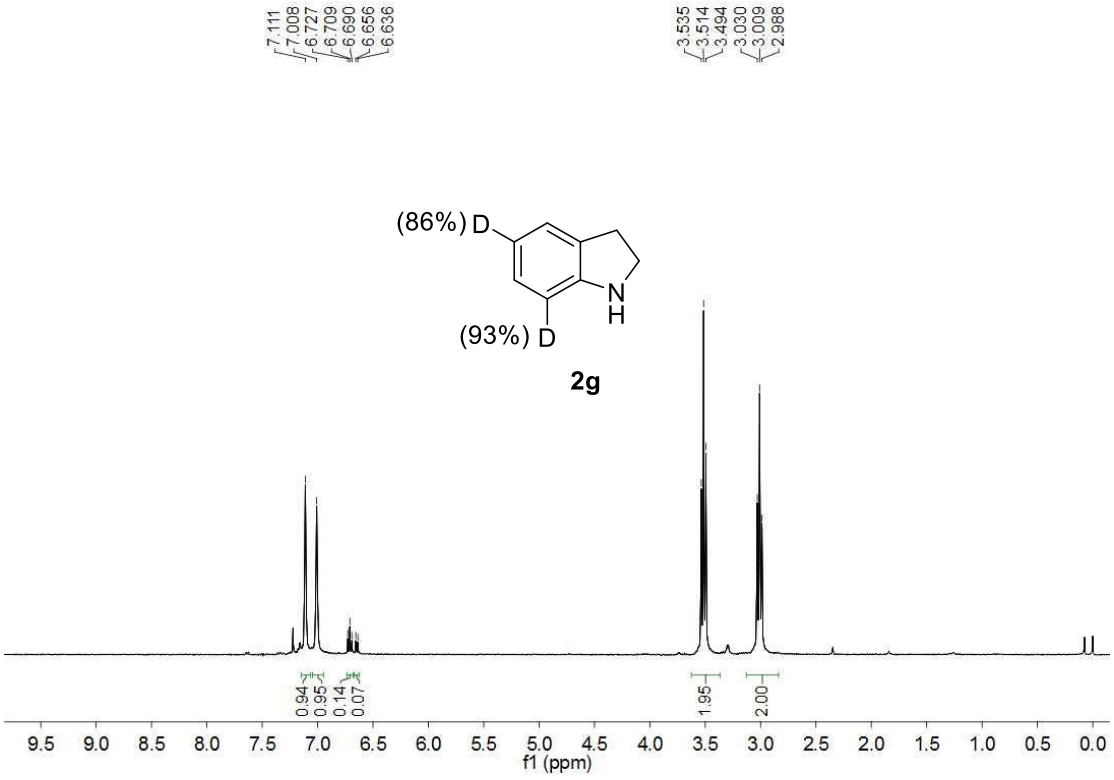
2e

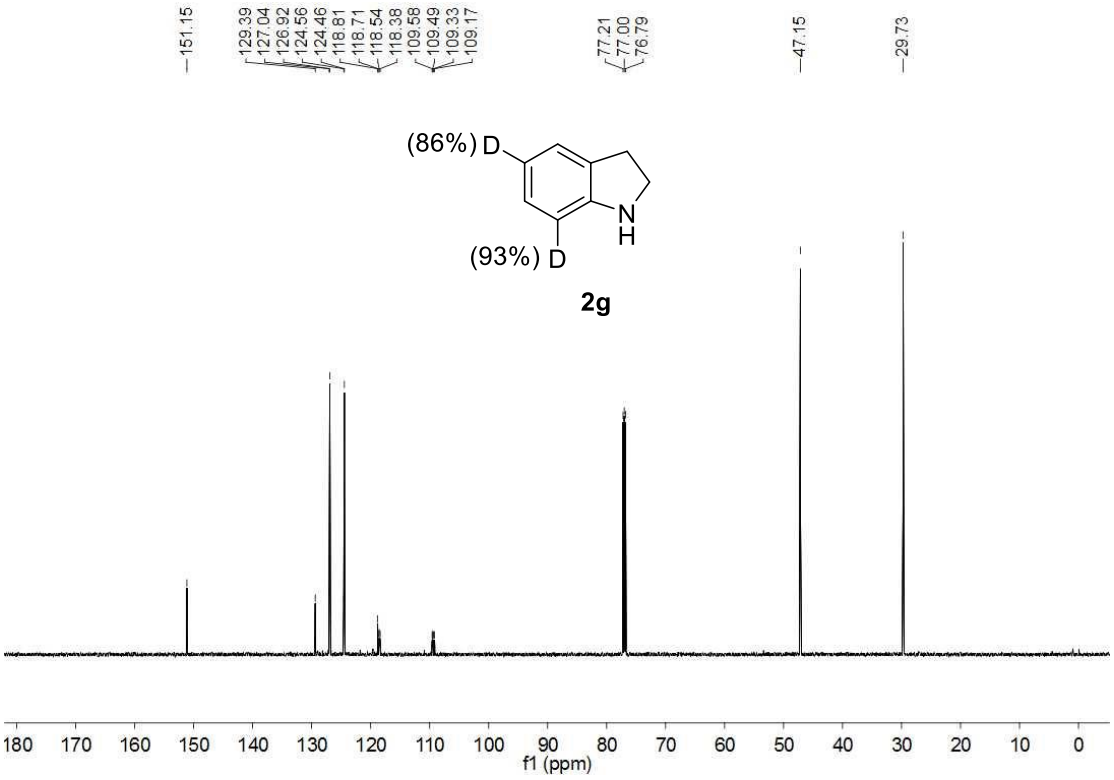

6.873
6.861
6.846
6.833
6.560
6.548
6.535
3.626
3.372
3.363
3.354
2.792
2.781
2.770
2.067
1.954
1.950
1.944
1.940
1.934
1.929
1.925
1.914
N
H
1f
1.88
0.93
0.89
2.00
2.01
3.00
2.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
6.870
6.842
6.576
6.563
3.765
3.373
3.364
3.355
2.791
2.780
2.770
2.075
1.956
1.952
1.946
1.942
1.936
1.931
1.927
1.917

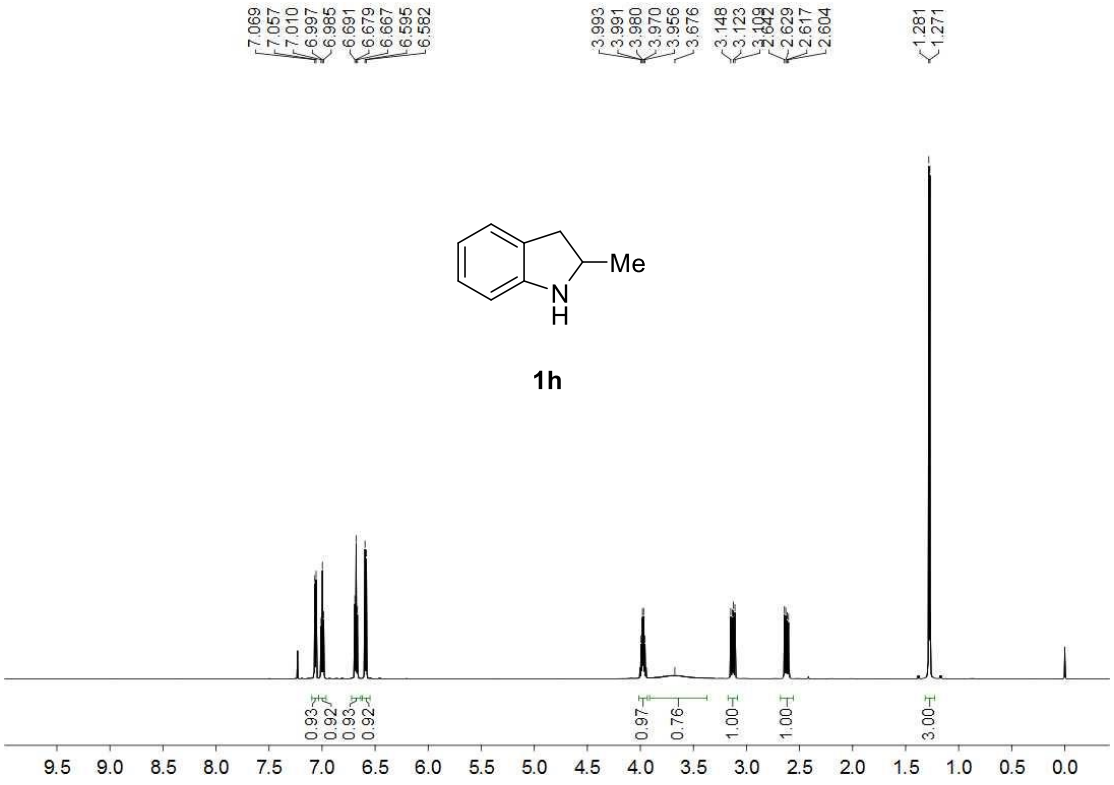

(86%) D
N
H
Me
2f
CH2Cl2
1.77
0.14
0.99
1.95
1.96
2.91
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

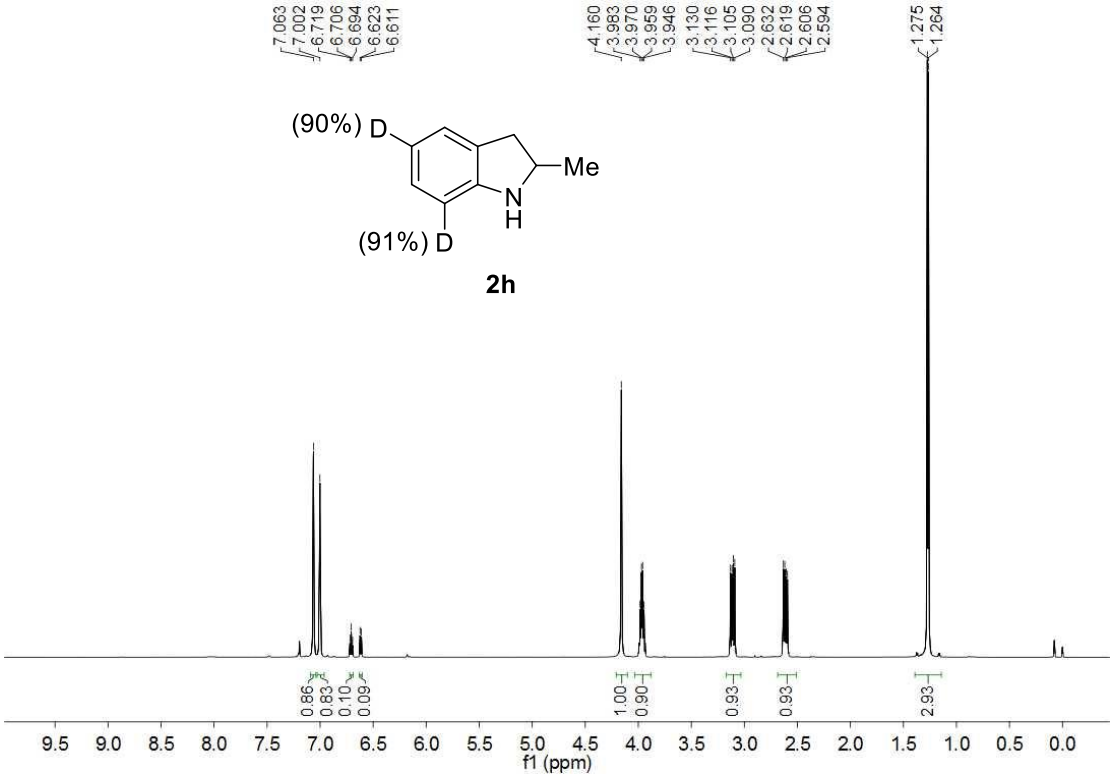

142.27
127.82
127.72
127.33
127.22
121.39
121.06
116.65
116.56
116.39
116.23
77.21
77.00
76.79
42.32
27.19
22.03
17.08
(86%) D
N
H
Me
2f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

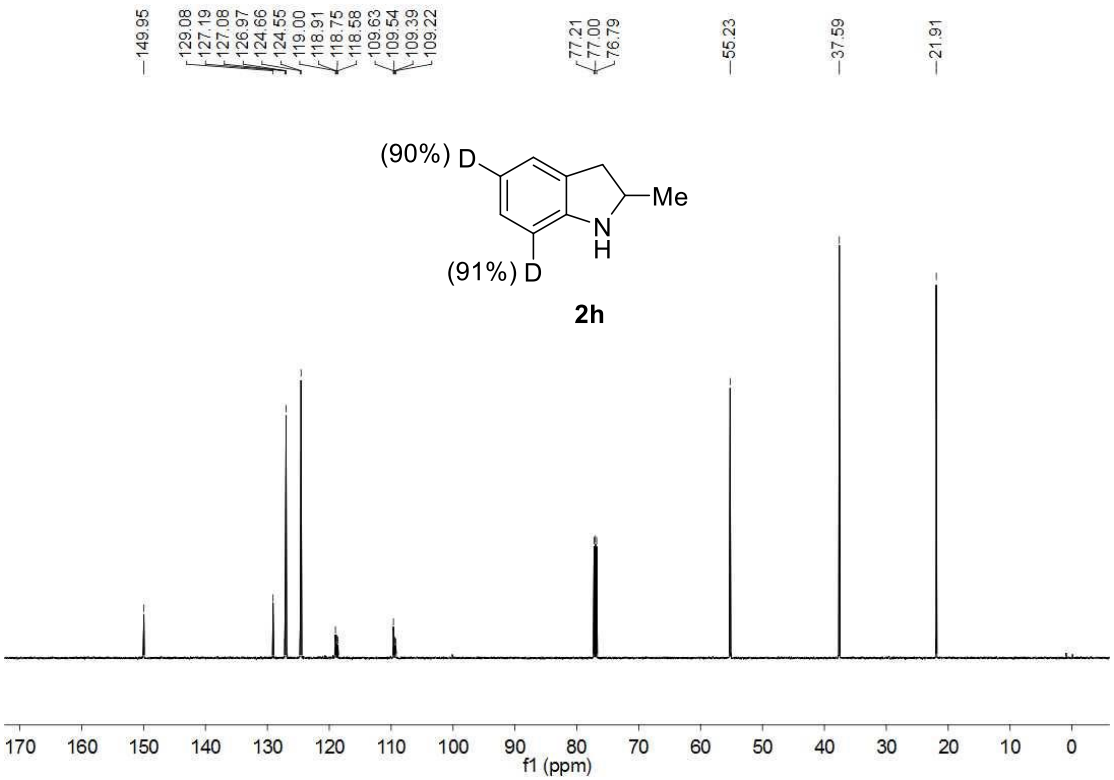

7.114
7.102
7.018
7.006
6.993
6.709
6.696
6.684
6.639
6.627
3.679
3.540
3.526
3.512
3.028
3.014
3.000
N
H
1g
0.97
0.97
0.98
0.97
0.68
2.00
2.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0

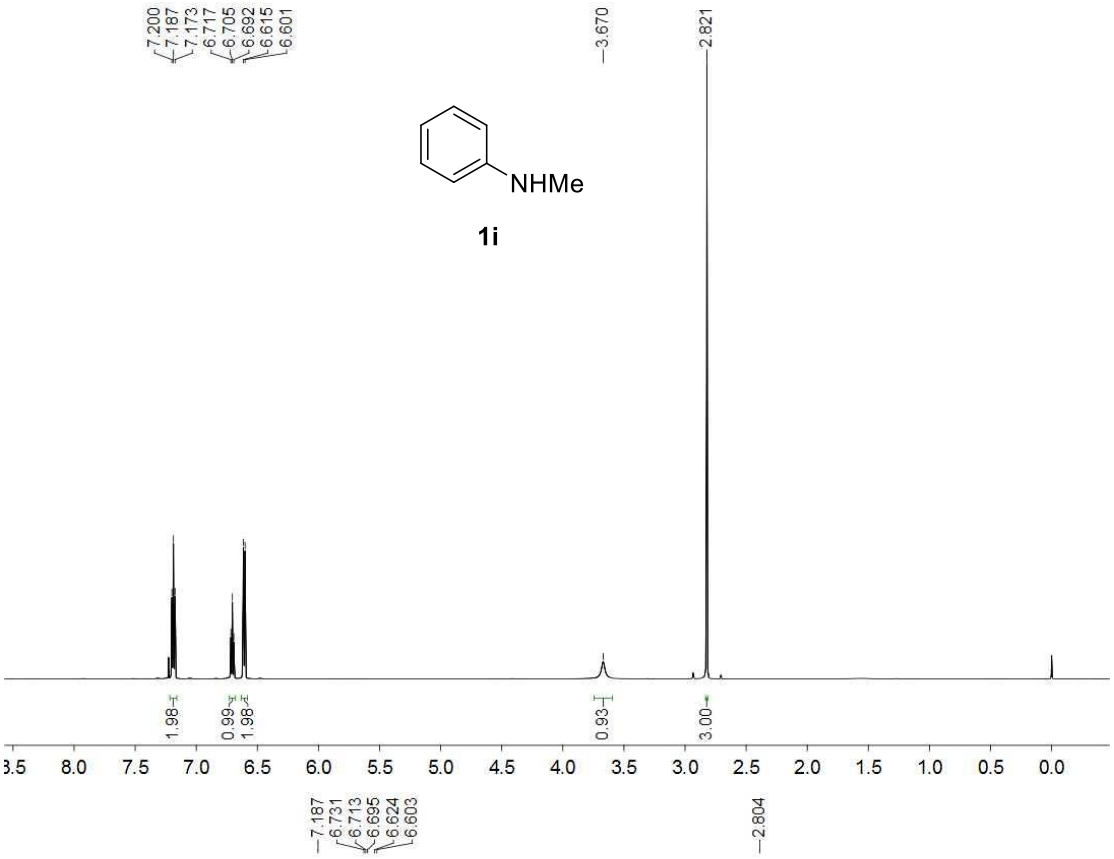

7.111
7.008
6.727
6.709
6.690
6.656
6.636
3.535
3.514
3.494
3.030
3.009
2.988
(86%) D
(93%) D
N
H
2g
0.94
0.95
0.14
0.07
1.95
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

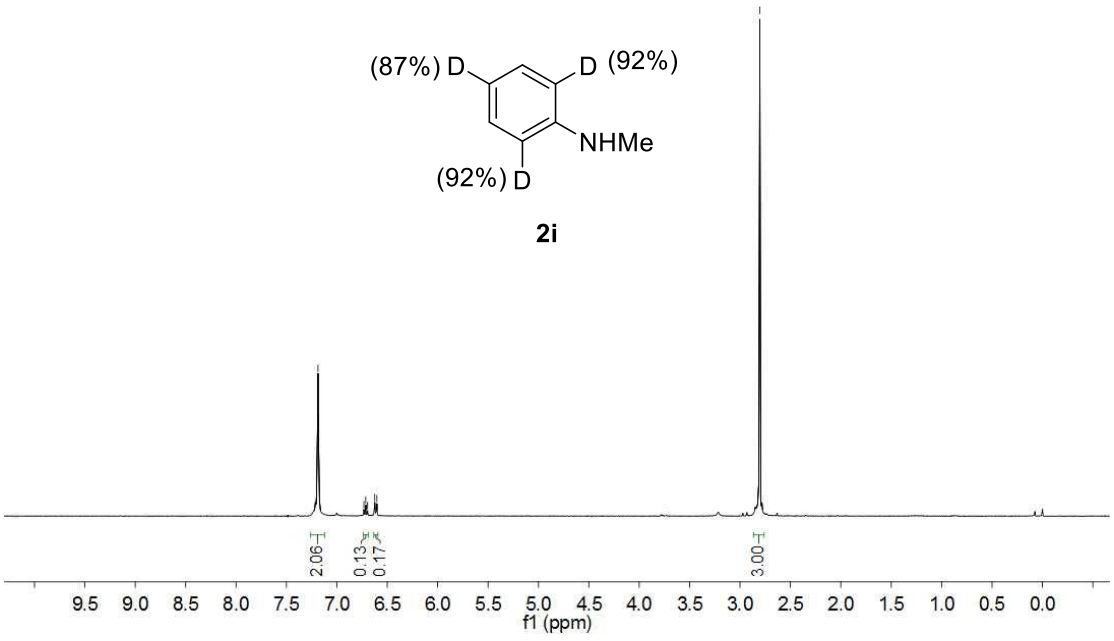

151.15
129.39
127.04
126.92
124.56
124.46
118.81
118.71
118.54
118.38
109.58
109.49
109.33
109.17
77.21
77.00
76.79
47.15
29.73
(86%) D
(93%) D
N
H
2g
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

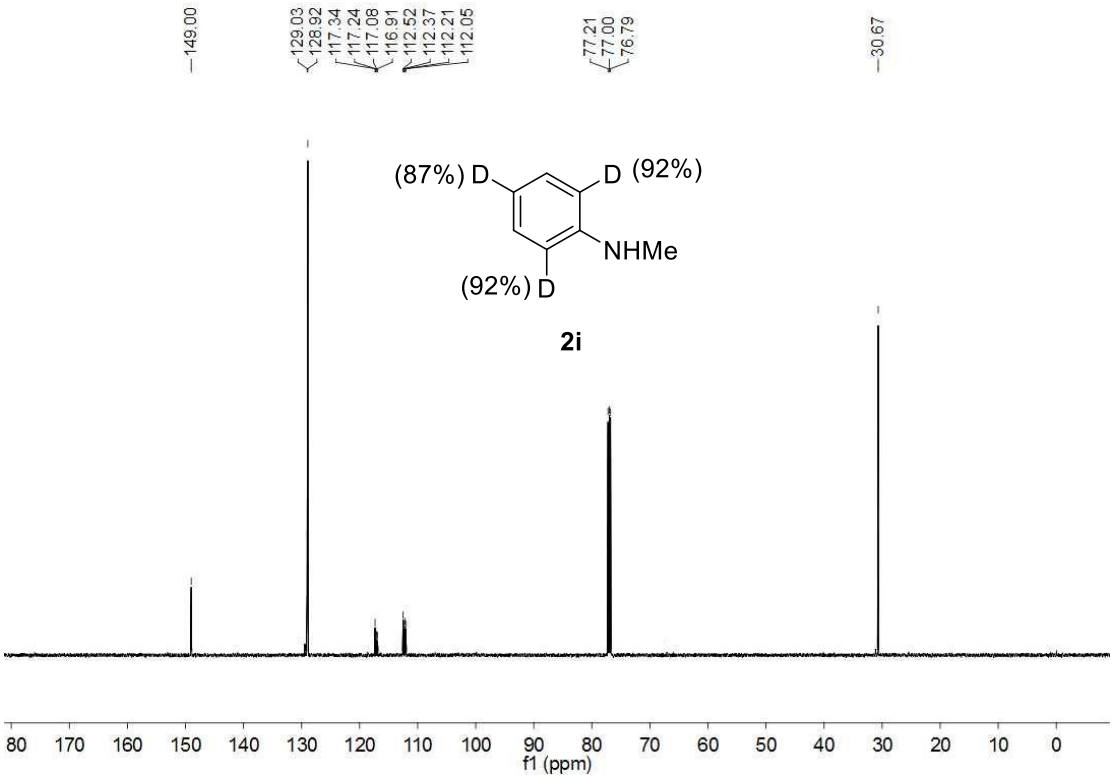

7.069
7.057
7.010
6.997
6.985
6.691
6.679
6.667
6.595
6.582
3.993
3.991
3.980
3.970
3.956
3.676
3.148
3.123
2.629
2.617
2.604
1.281
1.271
Me
N
H
1h
0.93
0.92
0.93
0.92
0.97
0.76
1.00
1.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

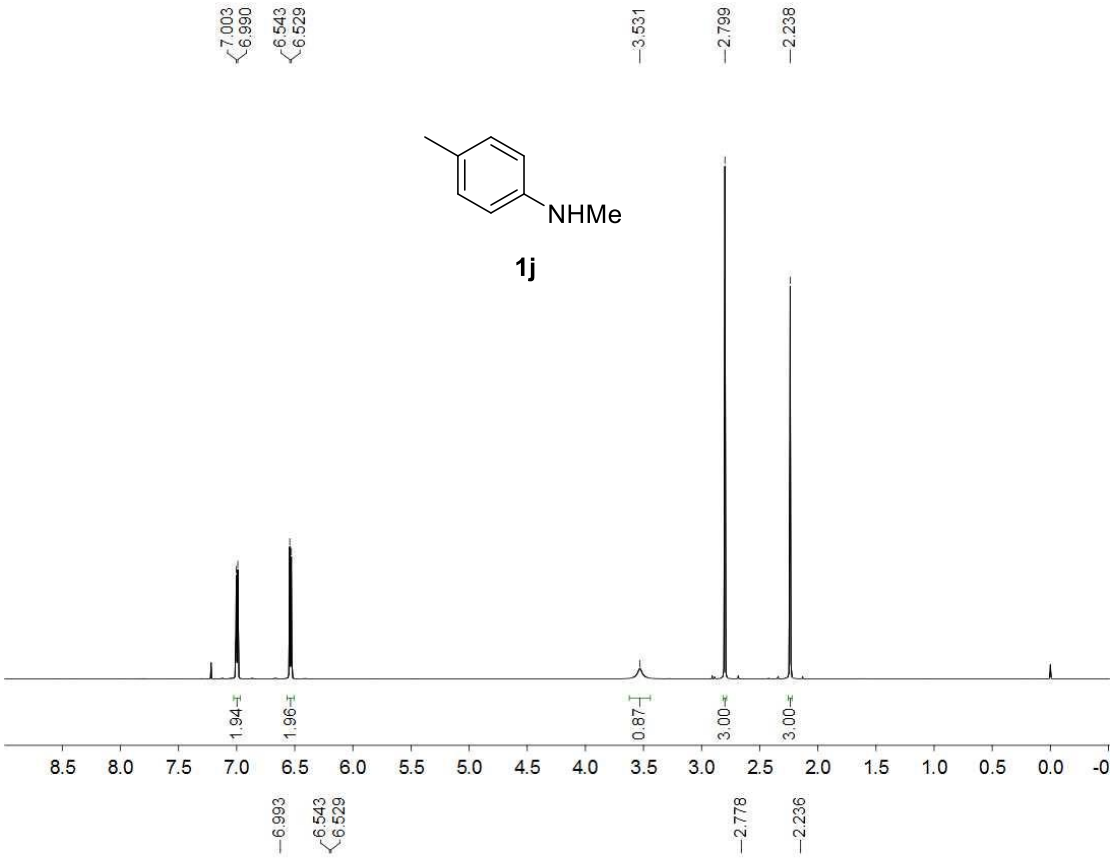

7.063
7.002
6.719
6.706
6.694
6.623
6.611
4.160
3.983
3.970
3.959
3.946
3.130
3.116
3.105
3.090
2.632
2.619
2.606
2.594
1.275
1.264
(90%) D
Me
N
H
(91%) D
2h
0.86
0.83
0.10
0.09
1.00
0.90
0.93
0.93
2.93
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

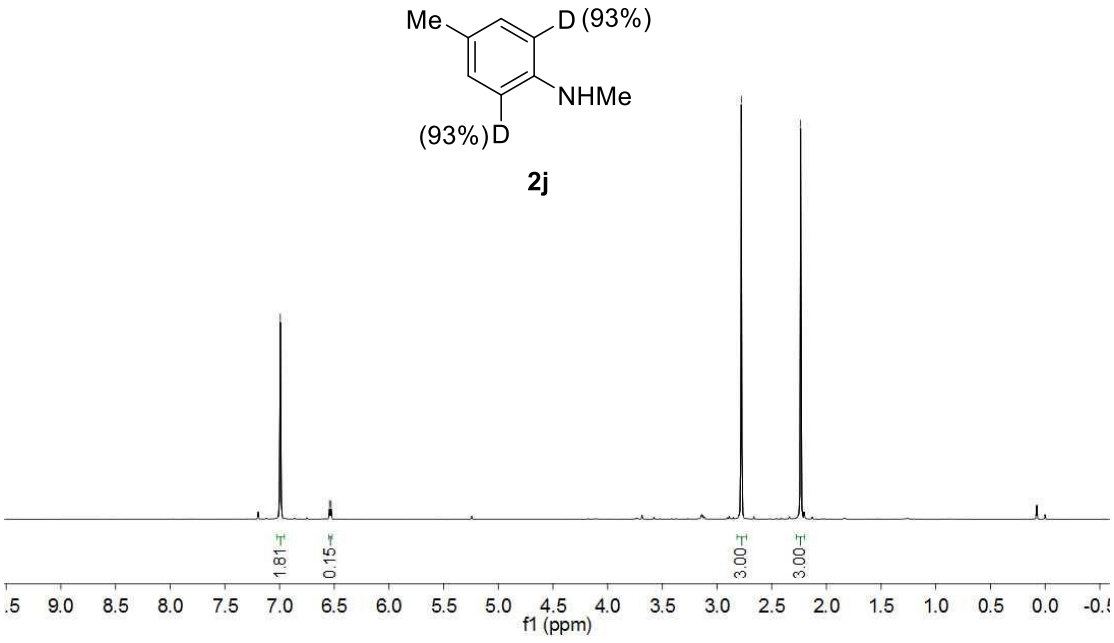

149.95
129.08
127.19
127.08
126.97
124.66
124.55
119.00
118.91
118.75
118.58
109.63
109.54
109.39
109.22
77.21
77.00
76.79
55.23
37.59
21.91
(90%) D
Me
N
H
(91%) D
2h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

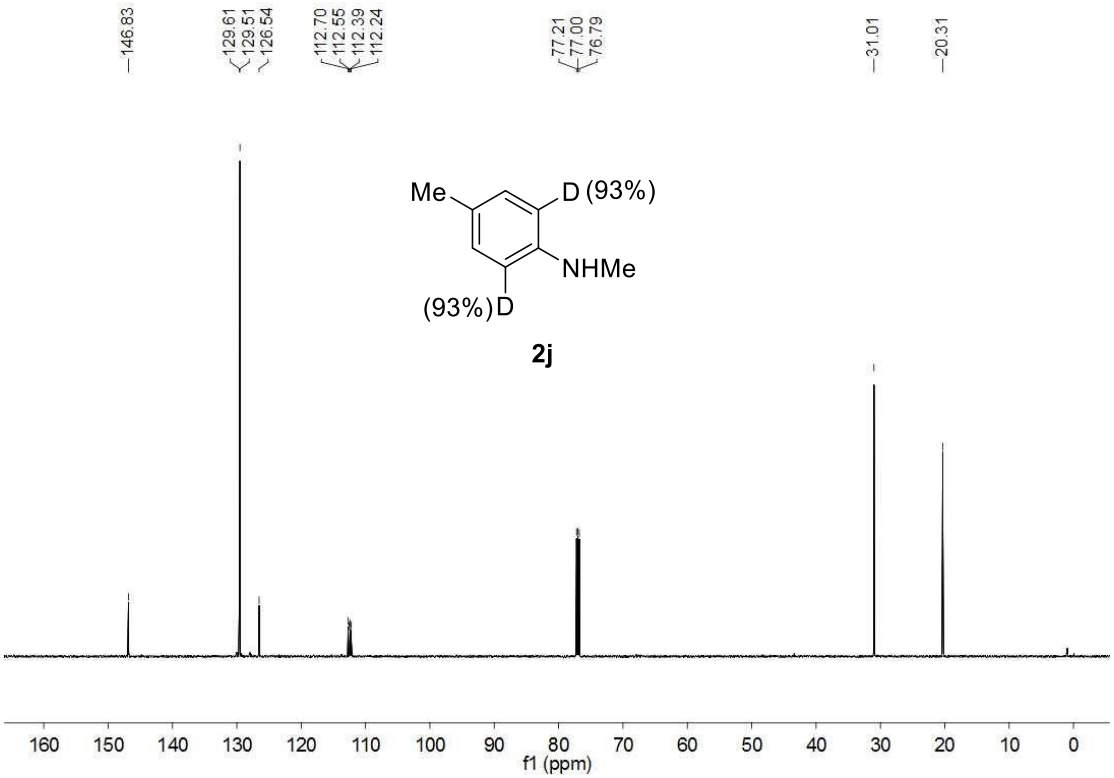

7.200
7.187
7.173
6.717
6.705
6.692
6.615
6.601
3.670
2.821
NHMe
1i
1.98
0.99
1.98
0.93
3.00
7.187
6.731
6.713
6.695
6.624
6.603
2.804


(87%) D
D (92%)
NHMe
(92%) D
2i
2.06
0.13
0.17
3.00
f1 (ppm)

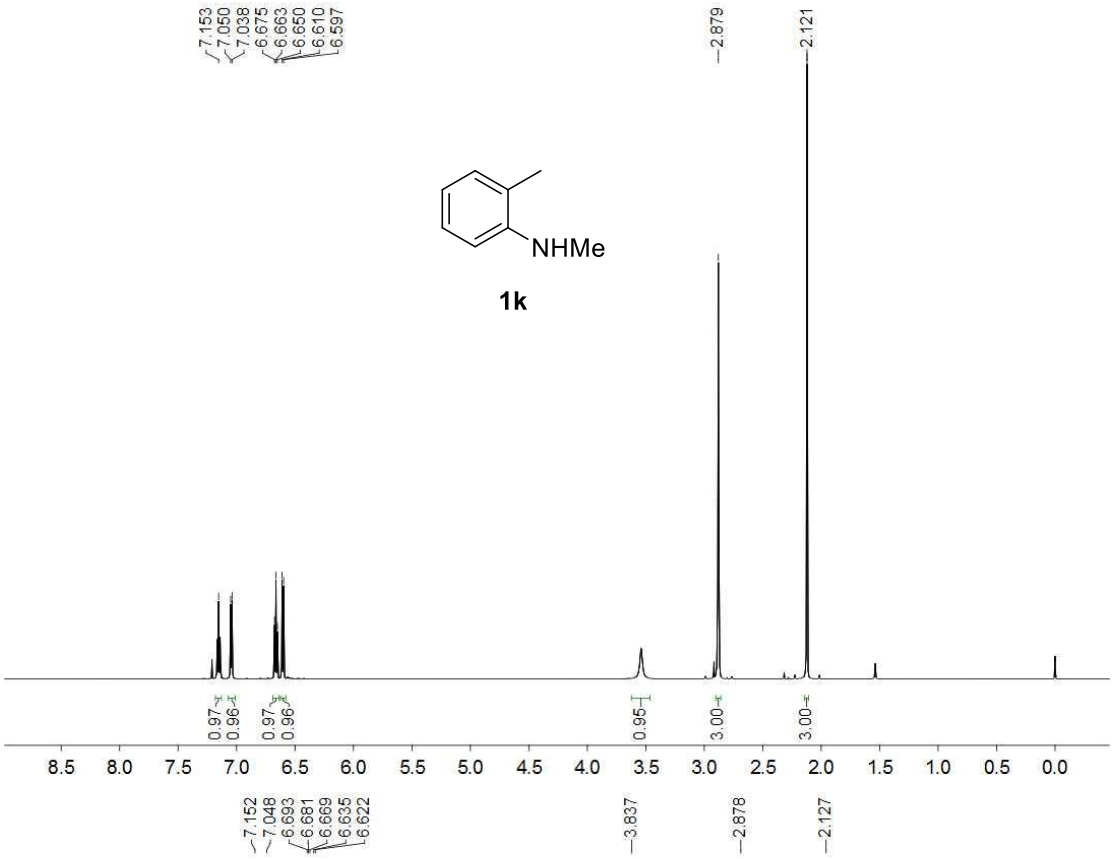

149.00
129.03
128.92
117.34
117.24
117.08
116.91
112.52
112.37
112.21
112.05
77.21
77.00
76.79
30.67
(87%) D
D (92%)
NHMe
(92%) D
2i
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

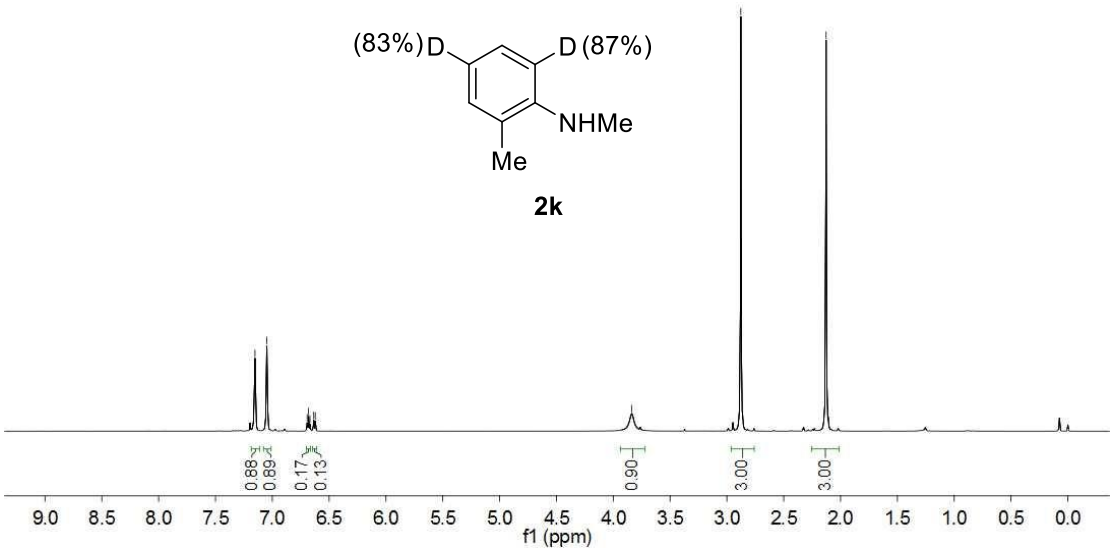

7.003
6.990
6.543
6.529
3.531
2.799
2.238
NHMe
1j
1.94
1.96
0.87
3.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
6.993
6.543
6.529
2.778
2.236

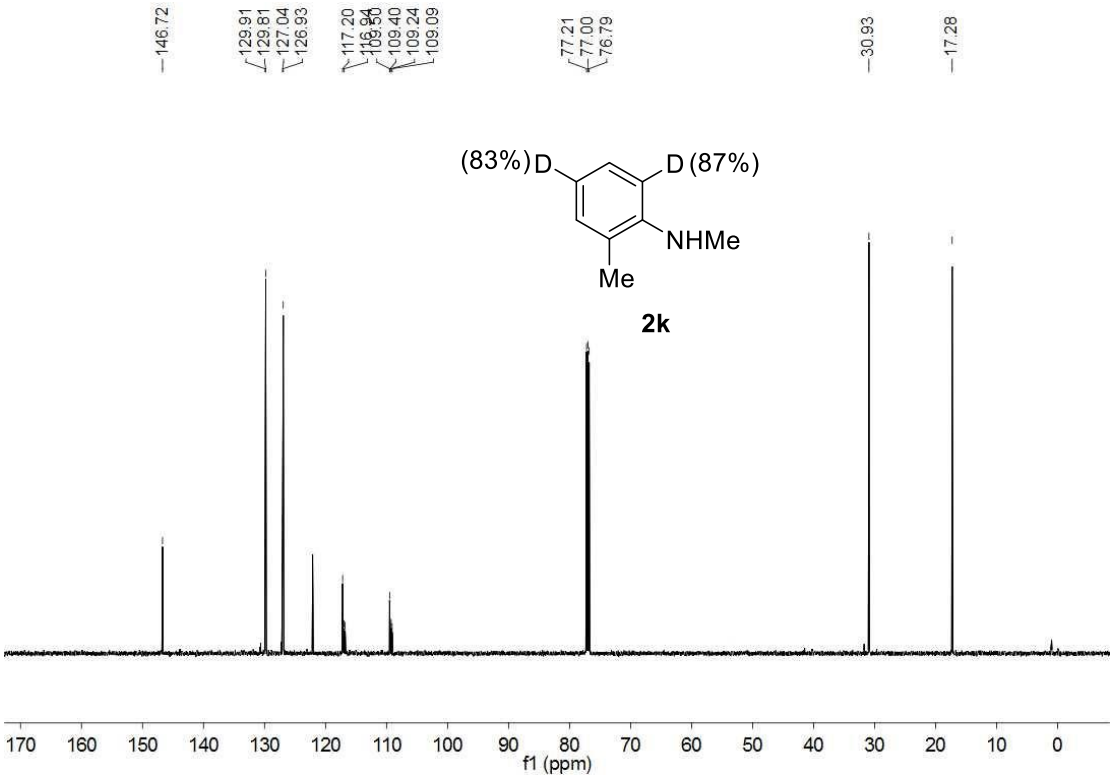

Me
D (93%)
NHMe
(93%) D
2j
1.81
0.15
3.00
3.00
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

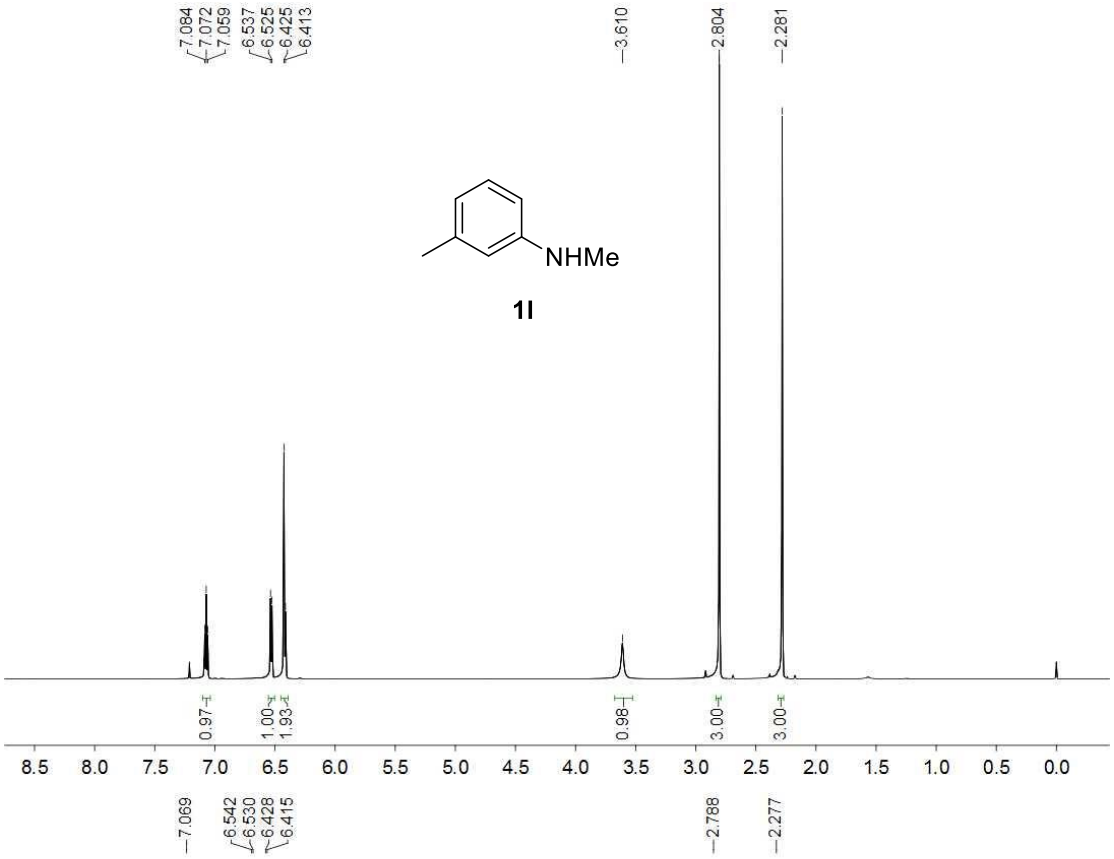

146.83
129.61
129.51
126.54
112.70
112.55
112.39
112.24
77.21
77.00
76.79
31.01
20.31
Me
D (93%)
NHMe
(93%) D
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

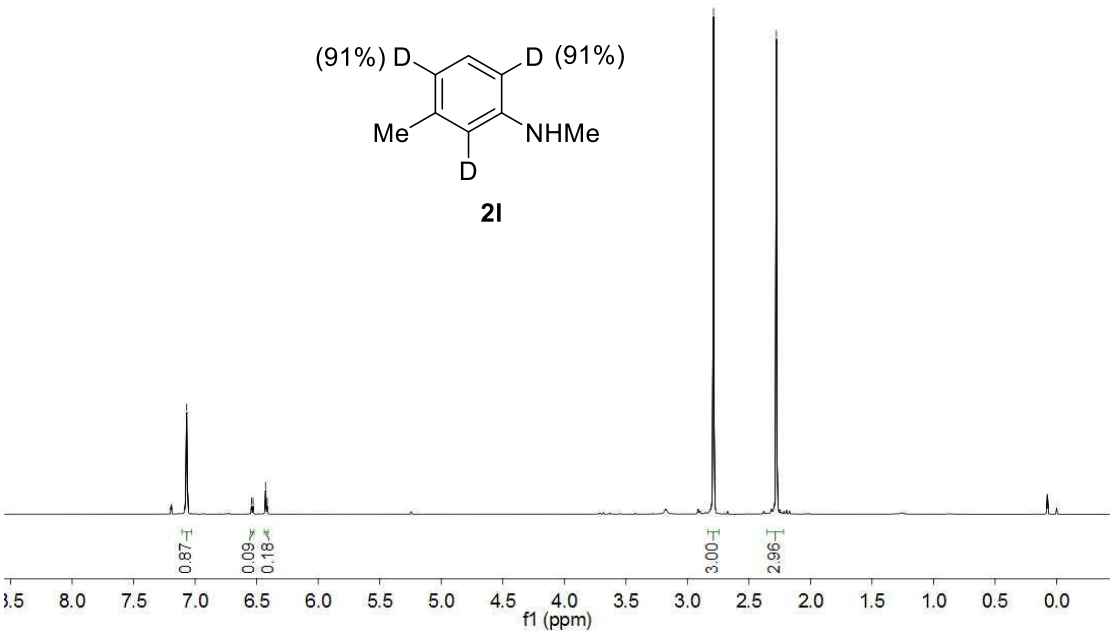
2j

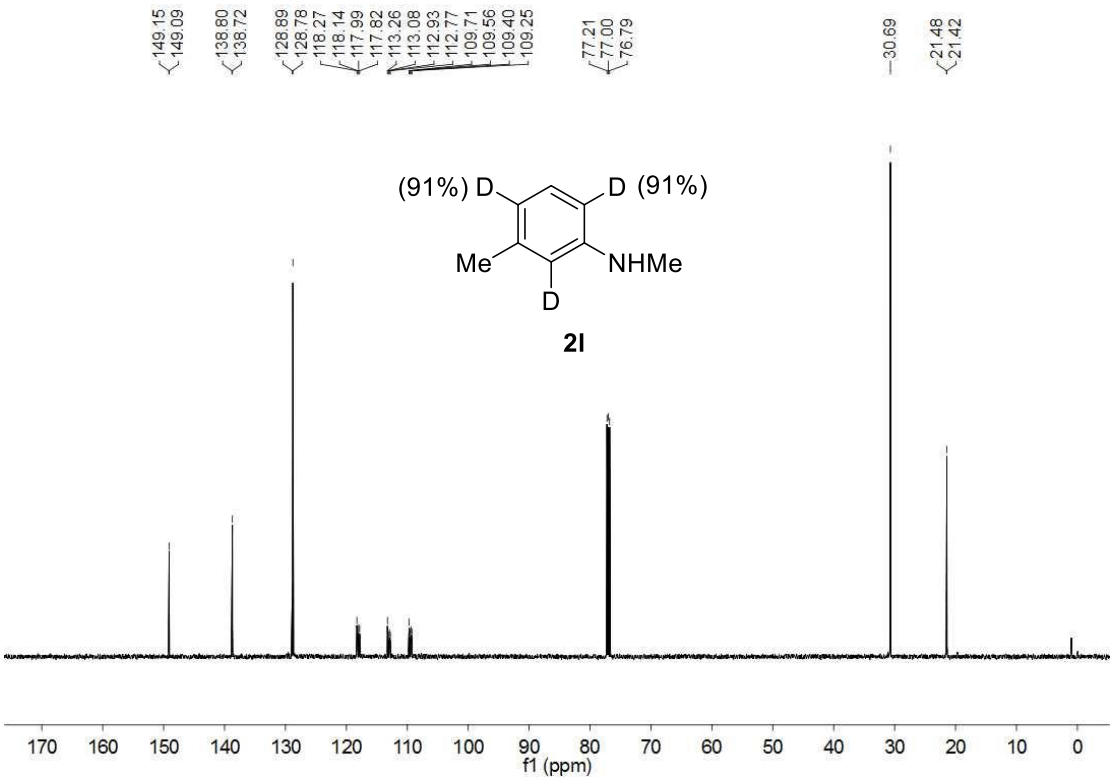

7.153
7.050
7.038
6.675
6.663
6.650
6.610
6.597
2.879
2.121
NHMe
1k
0.97
0.96
0.97
0.96
0.95
3.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
7.152
7.048
6.693
6.681
6.669
6.635
6.622
3.837
2.878
2.127

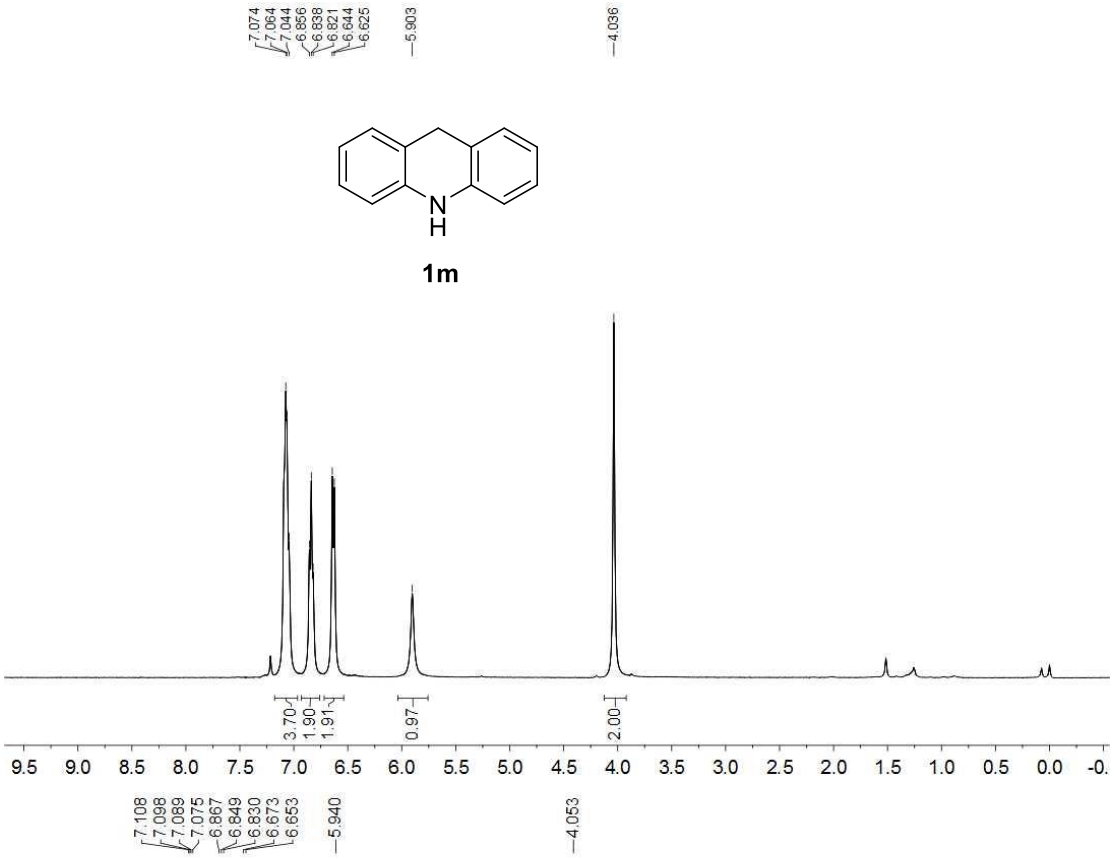

(83%)D
D (87%)
NHMe
Me
2k
0.88
0.89
0.17
0.13
0.90
3.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


146.72
129.91
129.81
127.04
126.93
117.20
116.94
109.40
109.24
109.09
77.21
77.00
76.79
30.93
17.28
(83%)D
D(87%)
NHMe
Me
2k
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

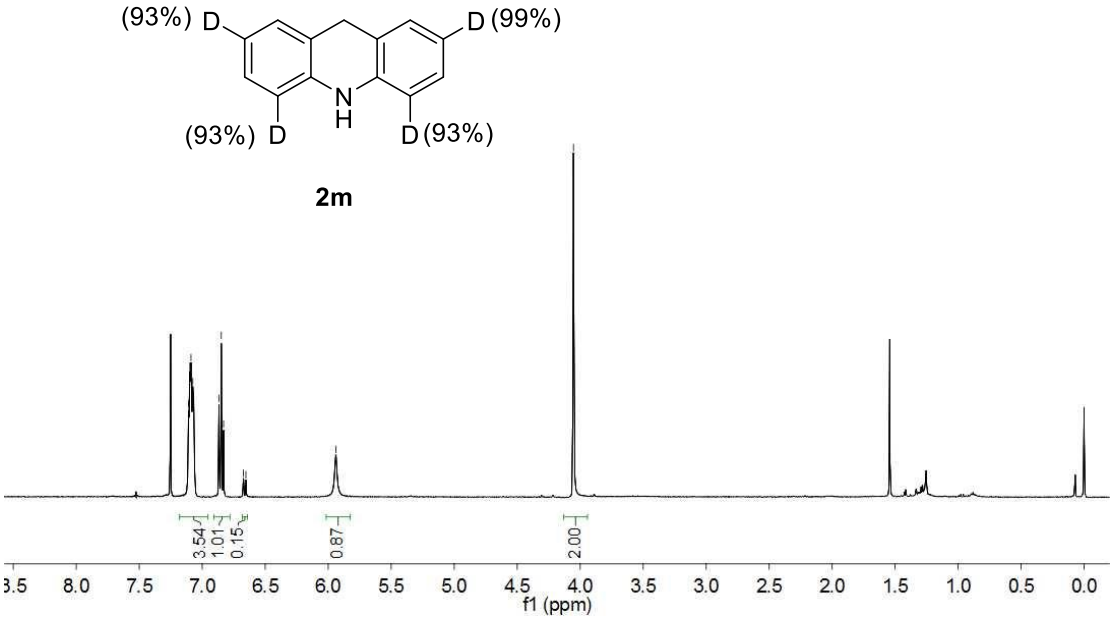

7.084
7.072
7.059
6.537
6.525
6.425
6.413
3.610
2.804
2.281
NHMe
1l
0.97
1.00
1.93
0.98
3.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


7.069
6.542
6.530
6.428
6.415
2.788
2.277
(91%) D
D (91%)
Me
NHMe
D
2l
0.87
0.09
0.18
3.00
2.96
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

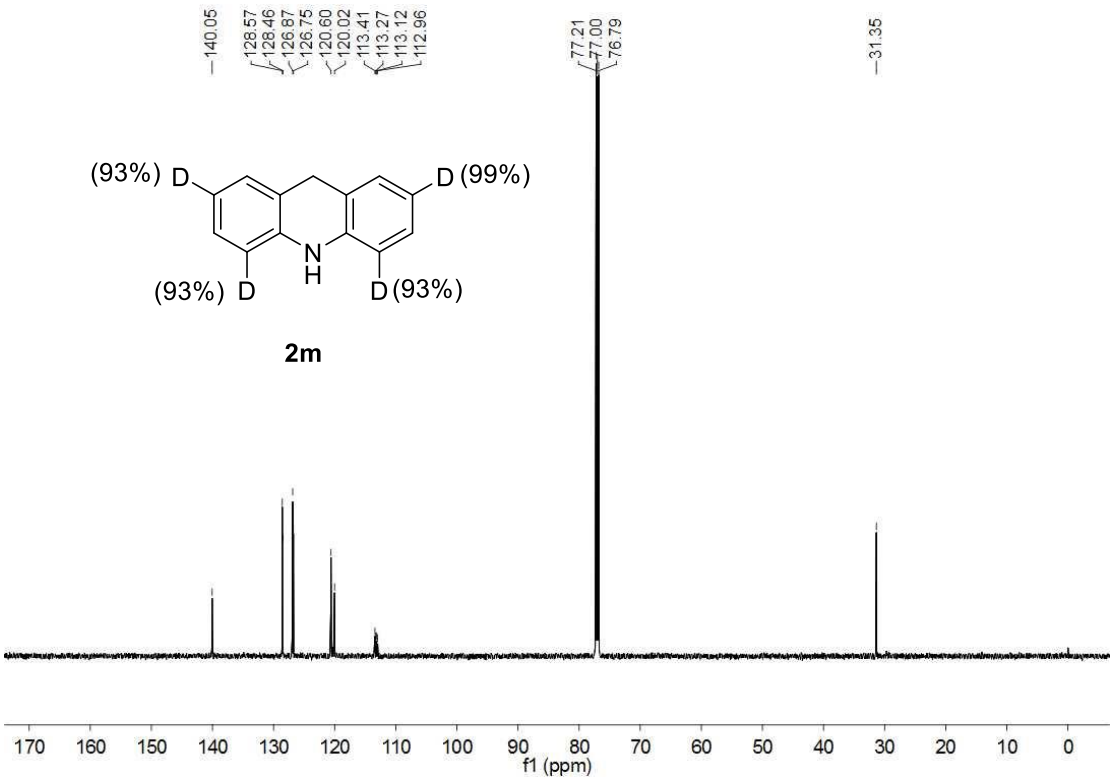

149.15
149.09
138.80
138.72
128.89
128.78
118.27
118.14
117.99
117.82
113.26
113.08
112.93
112.77
109.71
109.56
109.40
109.25
77.21
77.00
76.79
30.69
21.48
21.42
(91%) D
D (91%)
Me
NHMe
D
2l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

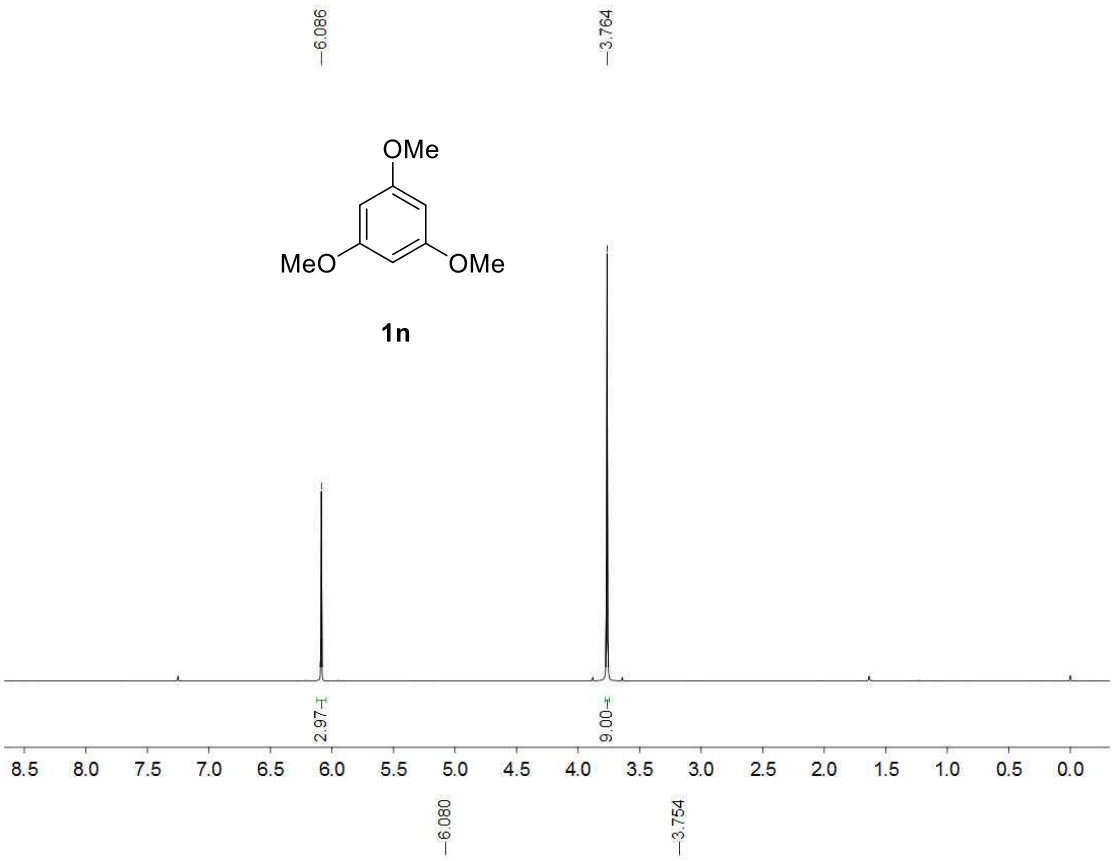

7.074
7.064
7.044
6.856
6.838
6.821
6.644
6.625
5.903
4.036
N
H
3.70
1.90
1.91
0.97
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
7.108
7.098
7.089
7.075
6.867
6.849
6.830
6.673
6.653
5.940
4.053

1m

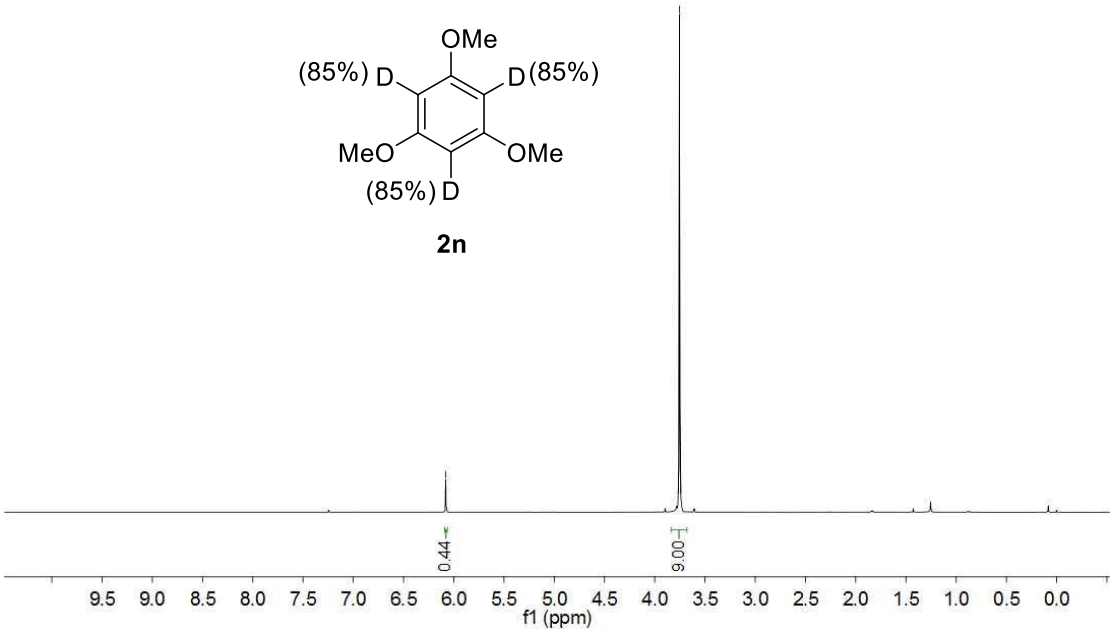

(93%) D
D (99%)
N
H
(93%) D
D (93%)
3.54
1.01
0.15
0.87
2.00
3.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

2m

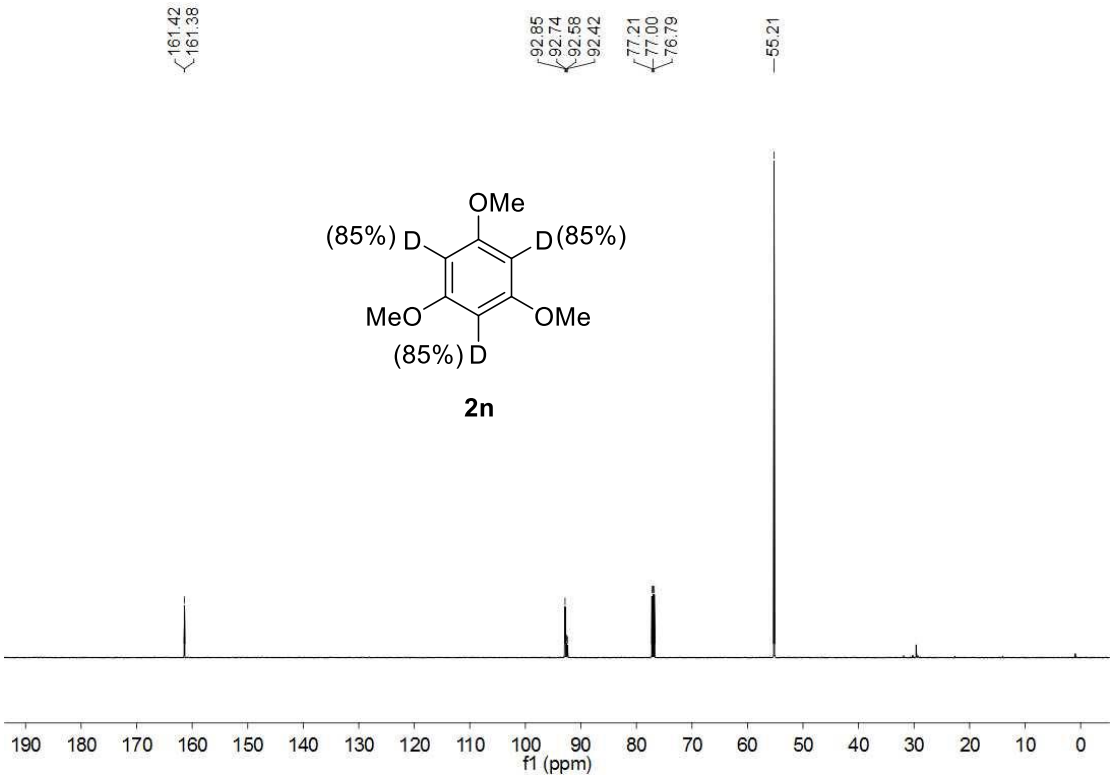

140.05
128.57
128.46
126.87
126.75
120.60
120.02
113.41
113.27
113.12
112.96
77.21
77.00
76.79
31.35
(93%) D
D (99%)
N
H
(93%) D
D (93%)
2m
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

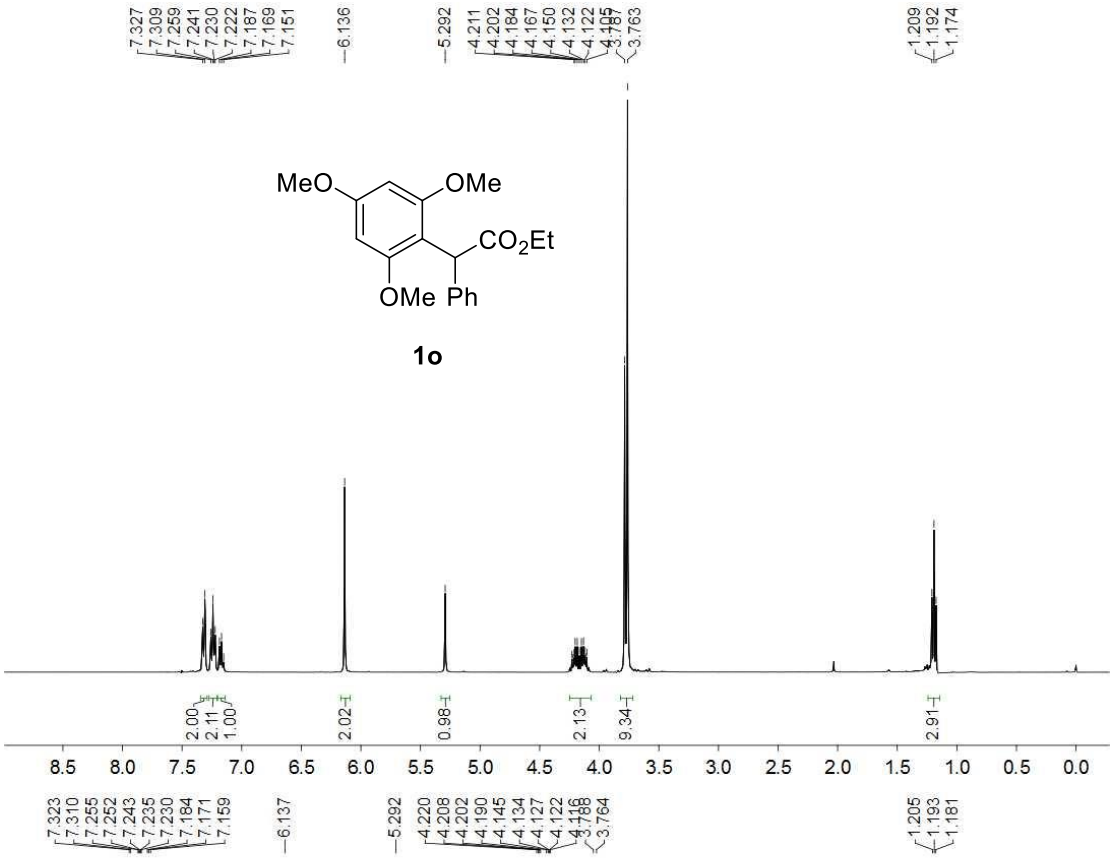

6.086
3.764
OMe
MeO
OMe
2.97
9.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

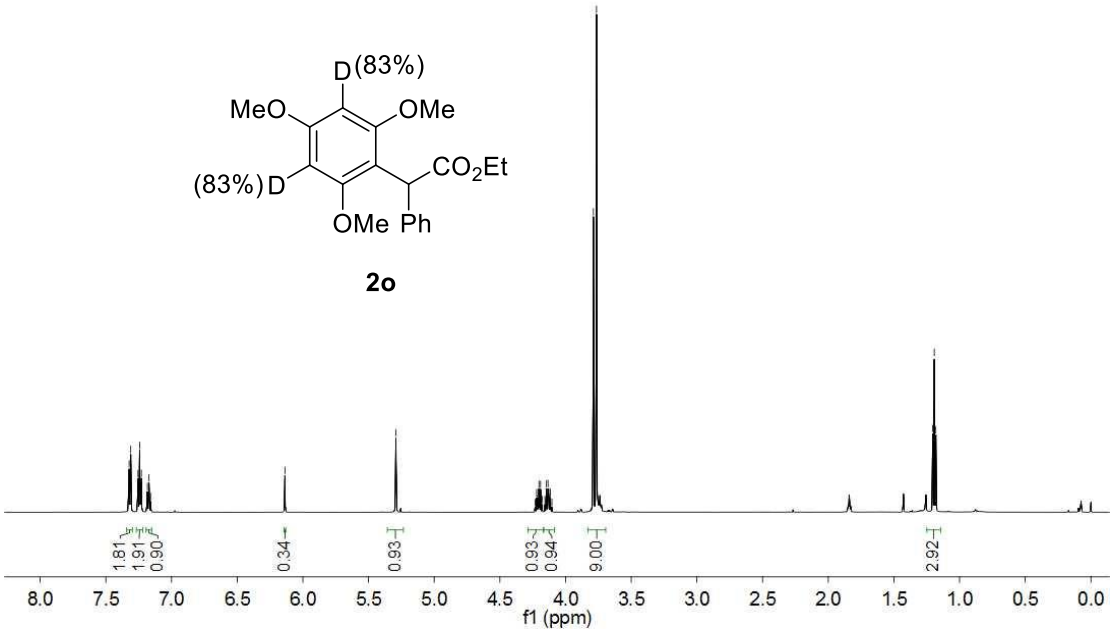
1n

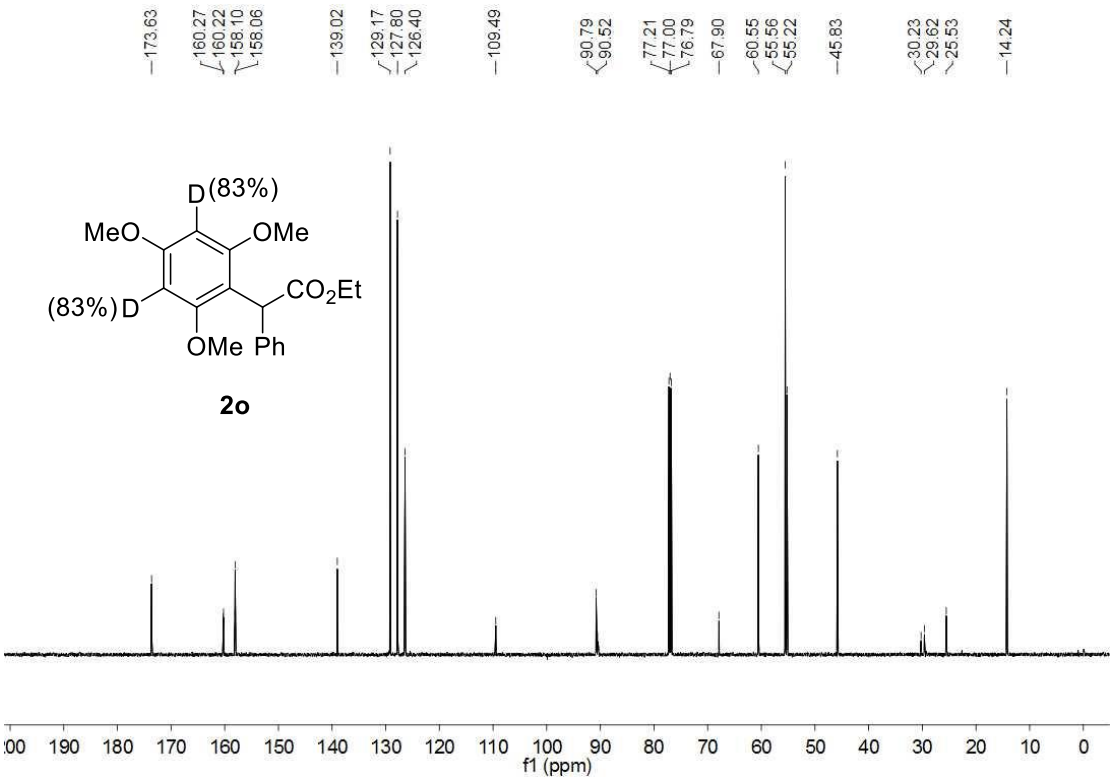

6.080
3.754
OMe
(85%) D
D (85%)
MeO
OMe
(85%) D
0.44
9.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

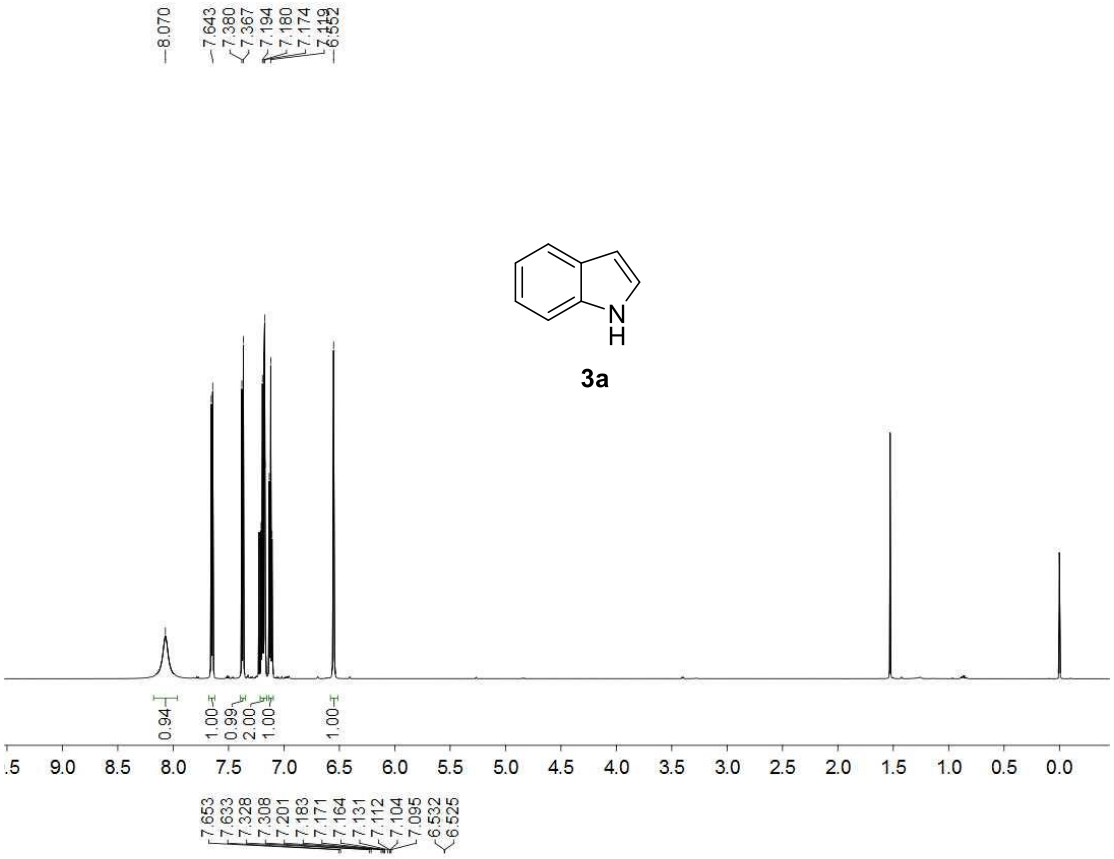
2n

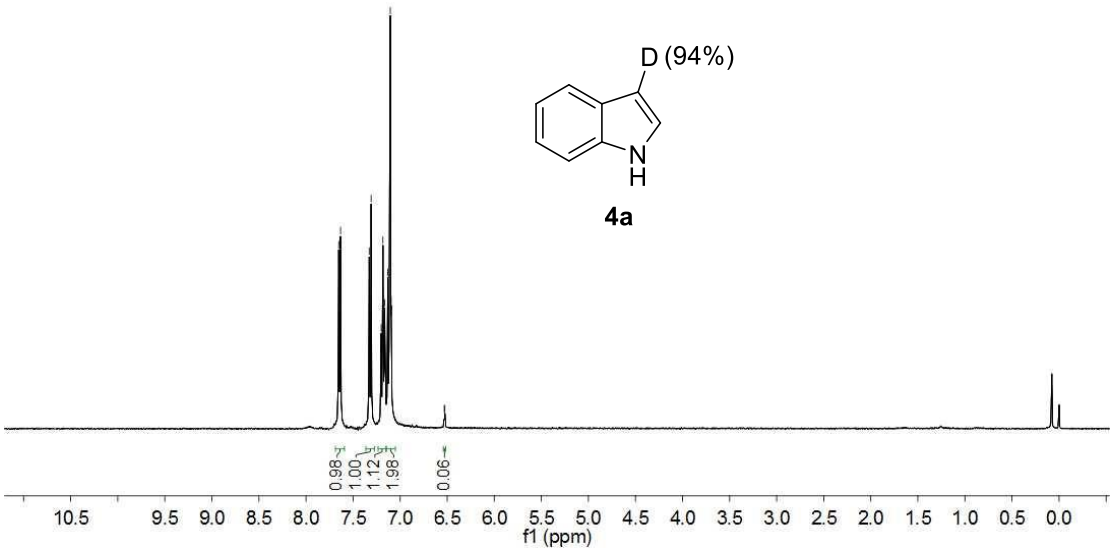

161.42
161.38
92.85
92.74
92.58
92.42
77.21
77.00
76.79
55.21
OMe
(85%) D
D (85%)
MeO
OMe
(85%) D
2n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

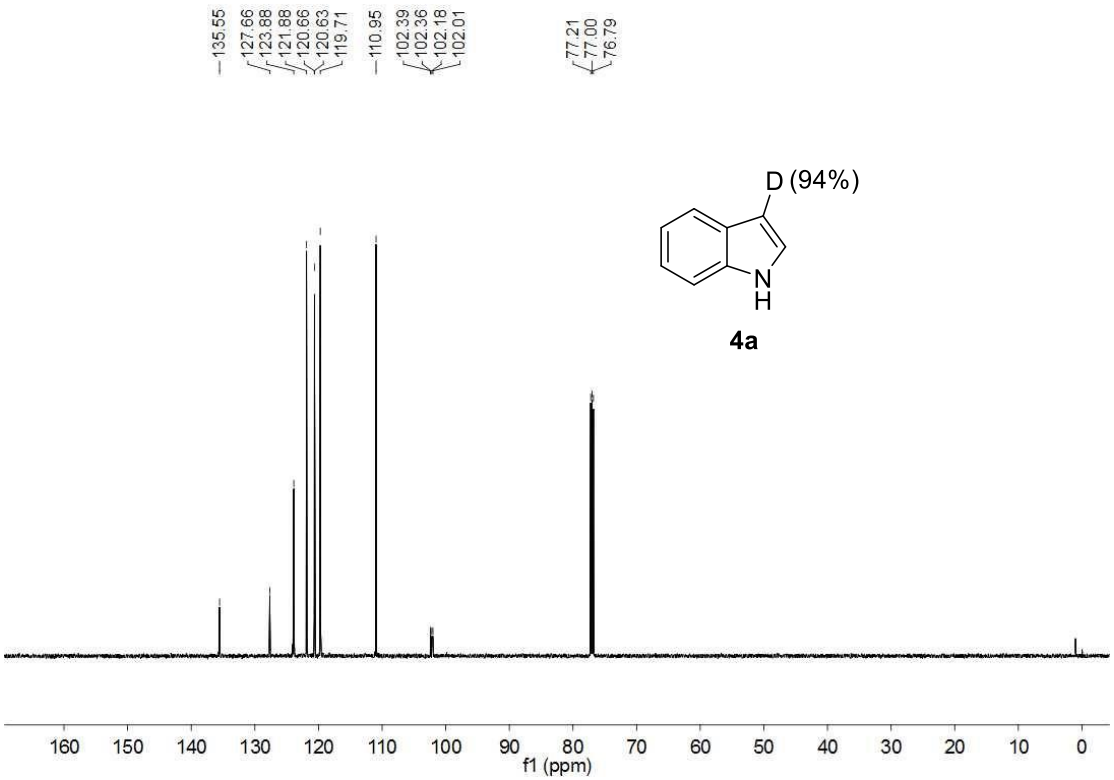

MeO
OMe
CO2Et
OMe Ph
1o


D(83%)
MeO
OMe
CO2Et
(83%)D
OMe Ph
2o
f1 (ppm)

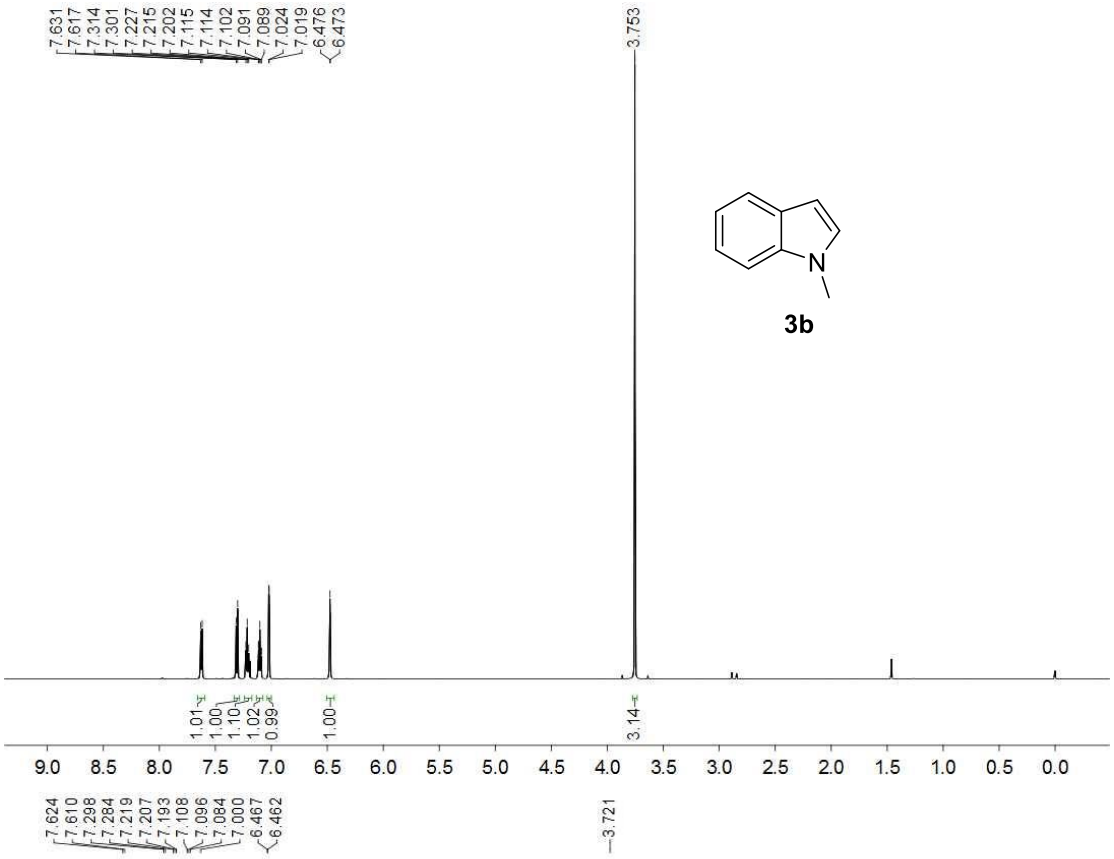

173.63
160.27
160.22
158.10
158.06
139.02
129.17
127.80
126.40
109.49
90.79
90.52
77.21
77.00
76.79
67.90
60.55
55.56
55.22
45.83
30.23
29.62
25.53
14.24
D(83%)
MeO
OMe
CO2Et
(83%)D
OMe Ph
2o
f1 (ppm)

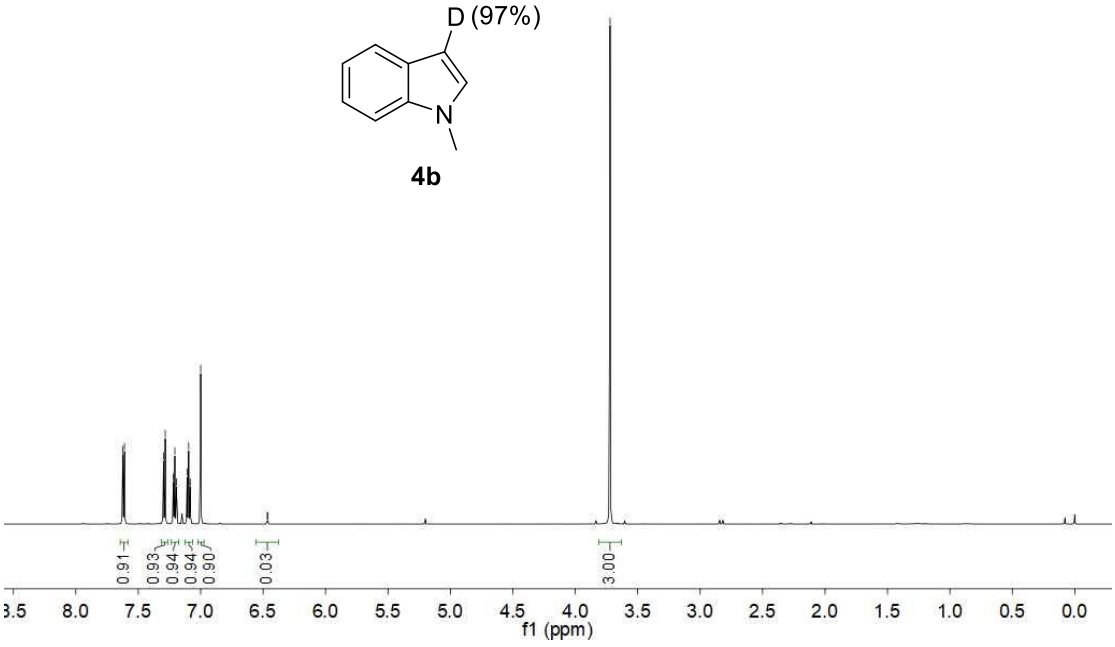

8.070
7.643
7.380
7.367
7.194
7.180
7.174
7.119
6.552
N
H
3a
0.94
1.00
0.99
2.00
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
7.653
7.633
7.328
7.308
7.201
7.183
7.171
7.164
7.131
7.112
7.104
7.095
6.532
6.525

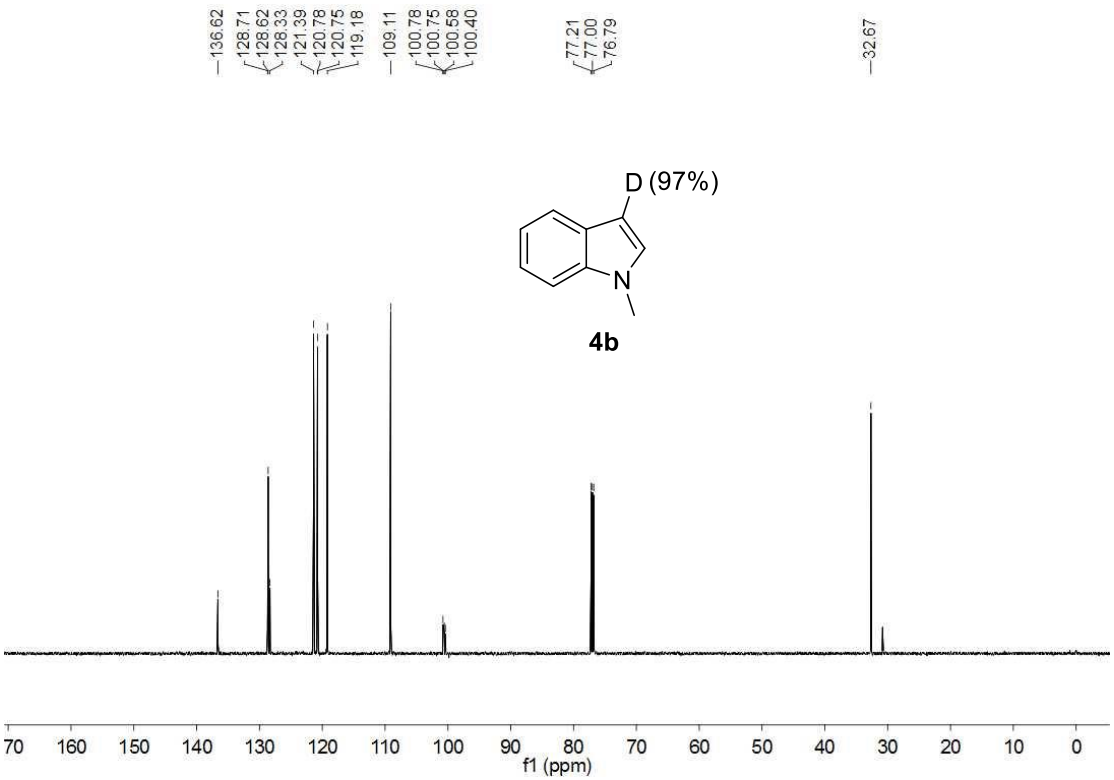

D (94%)
N
H
4a
0.98
1.00
1.12
1.98
0.06
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

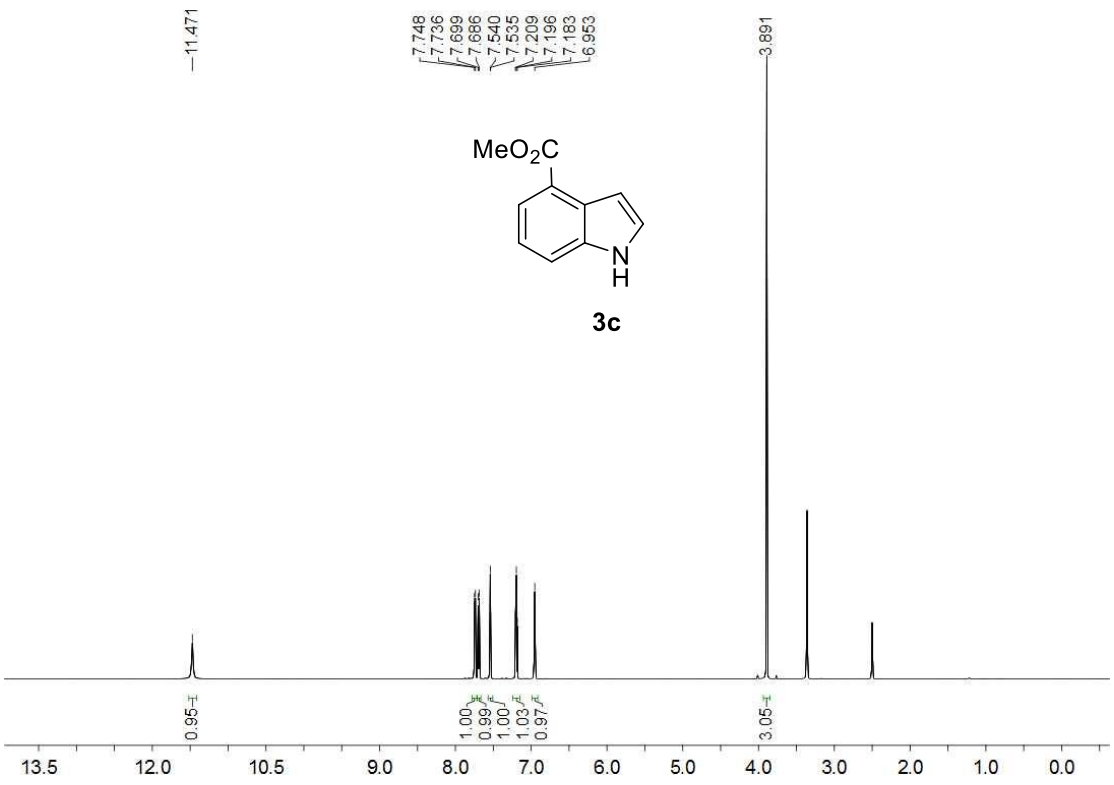

135.55
127.66
123.88
121.88
120.66
120.63
119.71
110.95
102.39
102.36
102.18
102.01
77.21
77.00
76.79
D (94%)
N
H
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

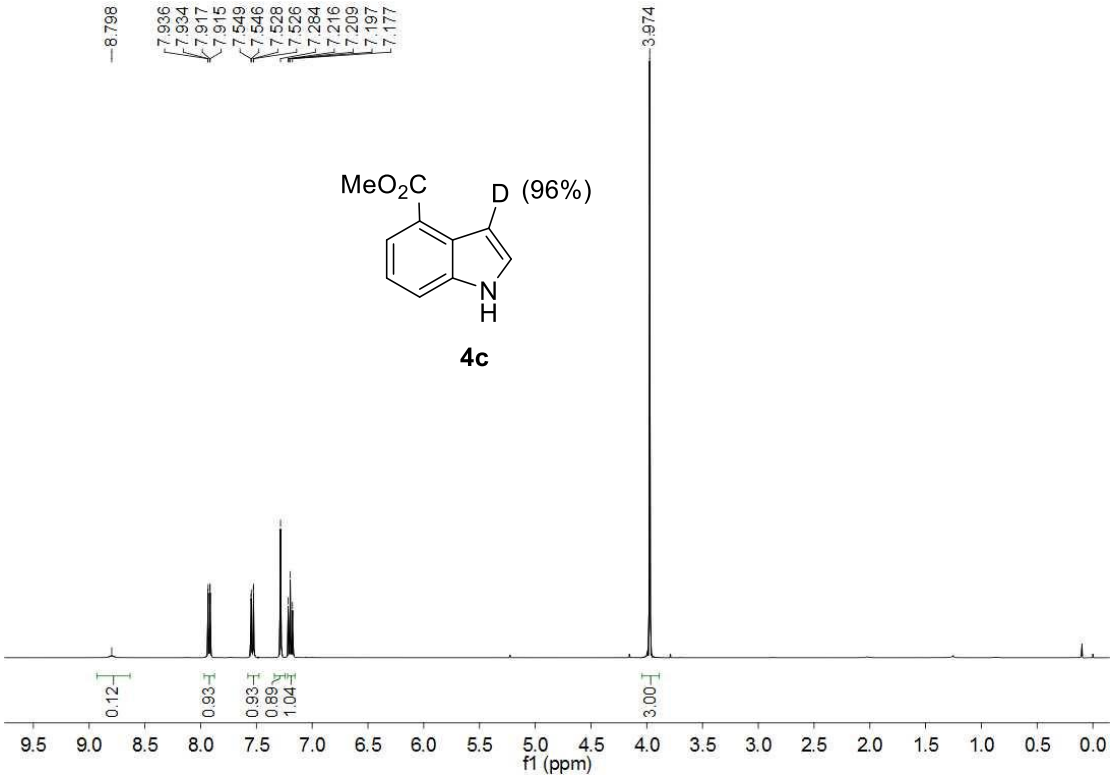
4a

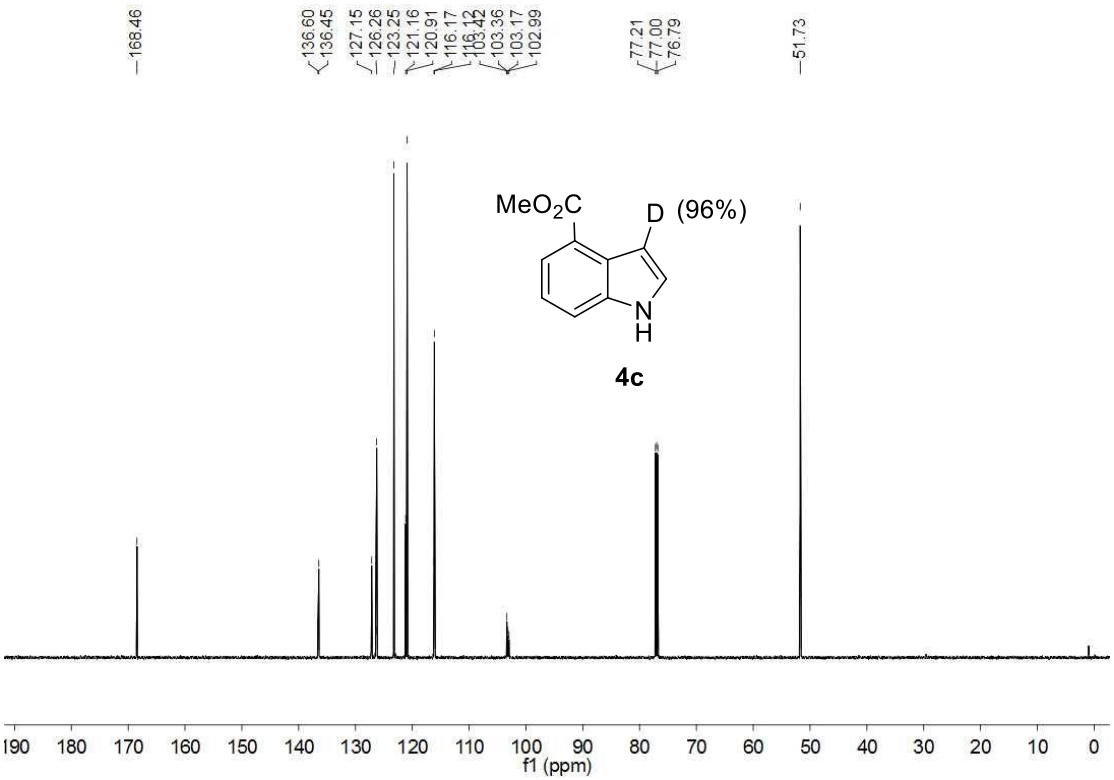

7.631
7.617
7.314
7.301
7.227
7.215
7.202
7.115
7.114
7.102
7.091
7.089
7.024
7.019
6.476
6.473
3.753
N
3b
1.01
1.00
1.10
1.02
0.99
1.00
3.14
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
7.624
7.610
7.298
7.284
7.219
7.207
7.193
7.108
7.096
7.084
7.000
6.467
6.462
3.721

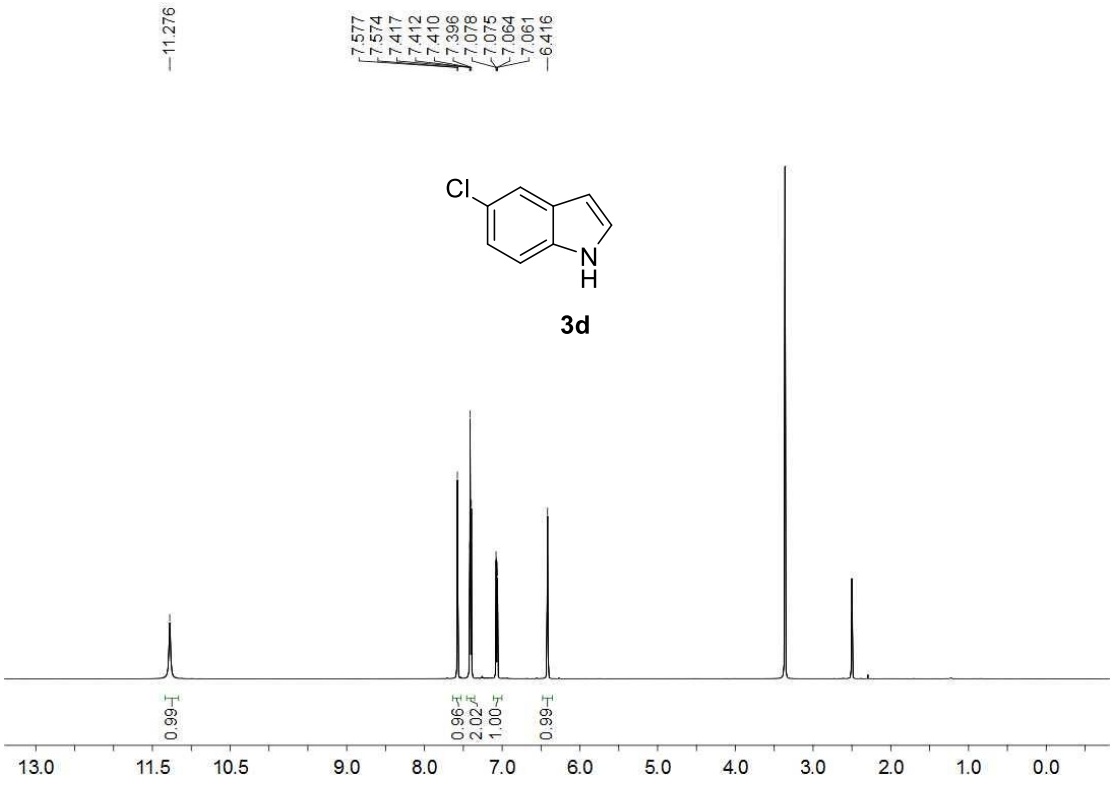

D (97%)
N
4b
0.91
0.93
0.94
0.94
0.90
0.03
3.00
3.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

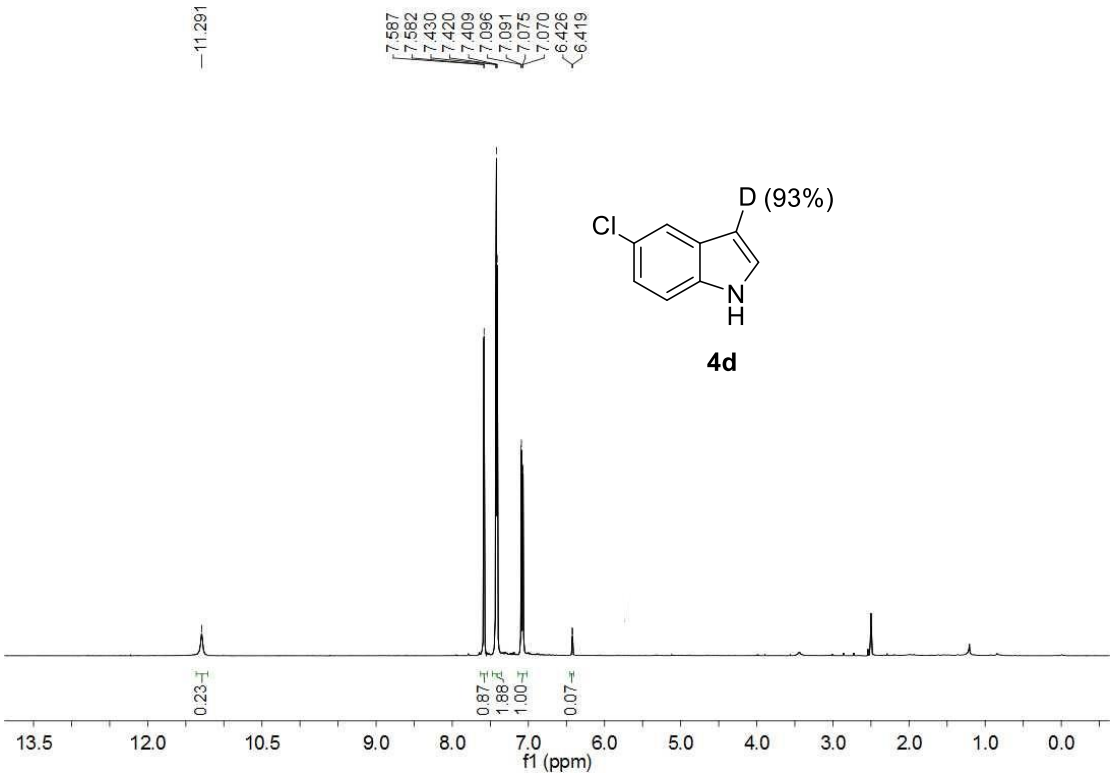

136.62
128.71
128.62
128.33
121.39
120.78
120.75
119.18
109.11
100.78
100.75
100.58
100.40
77.21
77.00
76.79
32.67
D (97%)
N
4b
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

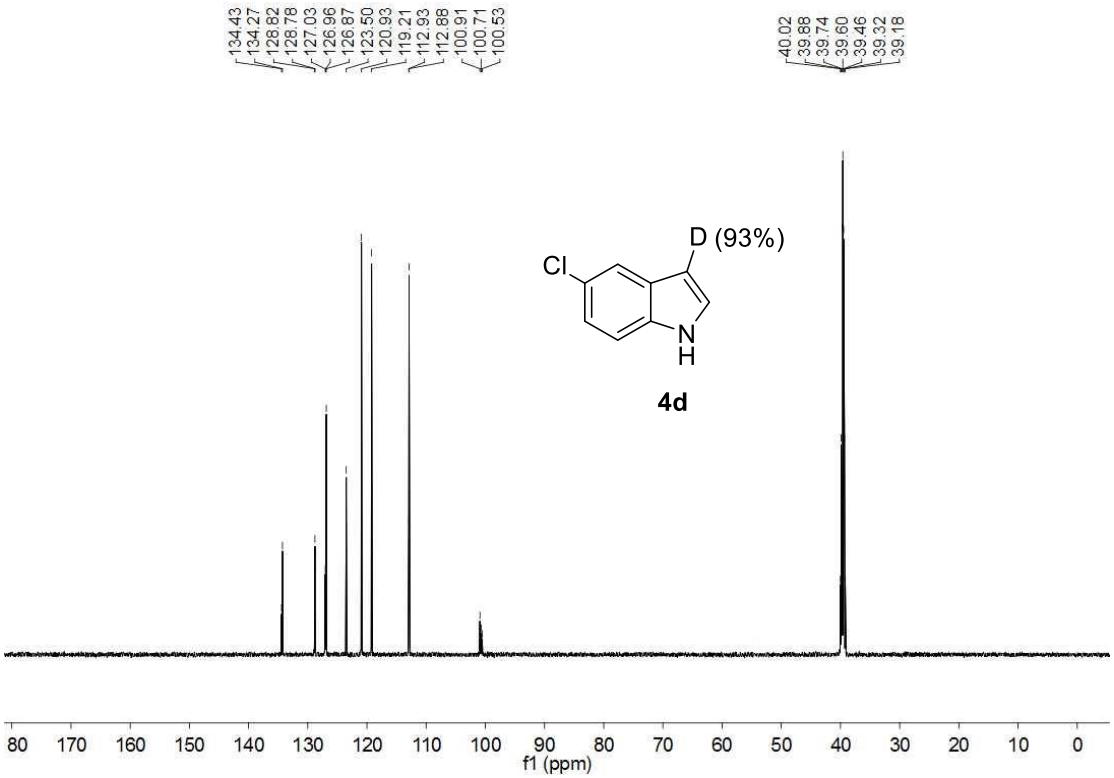

11.471
7.748
7.736
7.699
7.686
7.540
7.535
7.209
7.196
7.183
6.953
3.891
MeO2C
N
H
3c
0.95
1.00
0.99
1.00
1.03
0.97
3.05
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

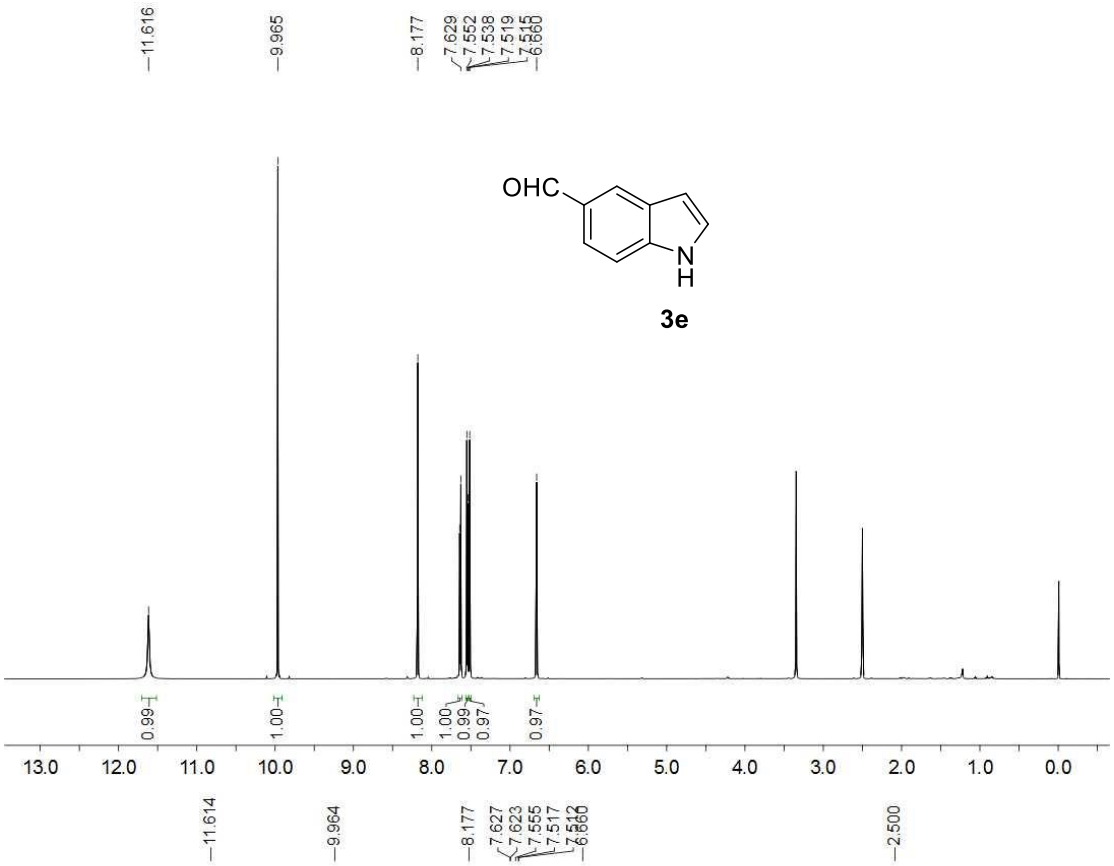

8.798
7.936
7.934
7.917
7.915
7.549
7.546
7.528
7.526
7.284
7.216
7.209
7.197
7.177
3.974
MeO2C
D (96%)
N
H
4c
0.12
0.93
0.93
0.89
1.04
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

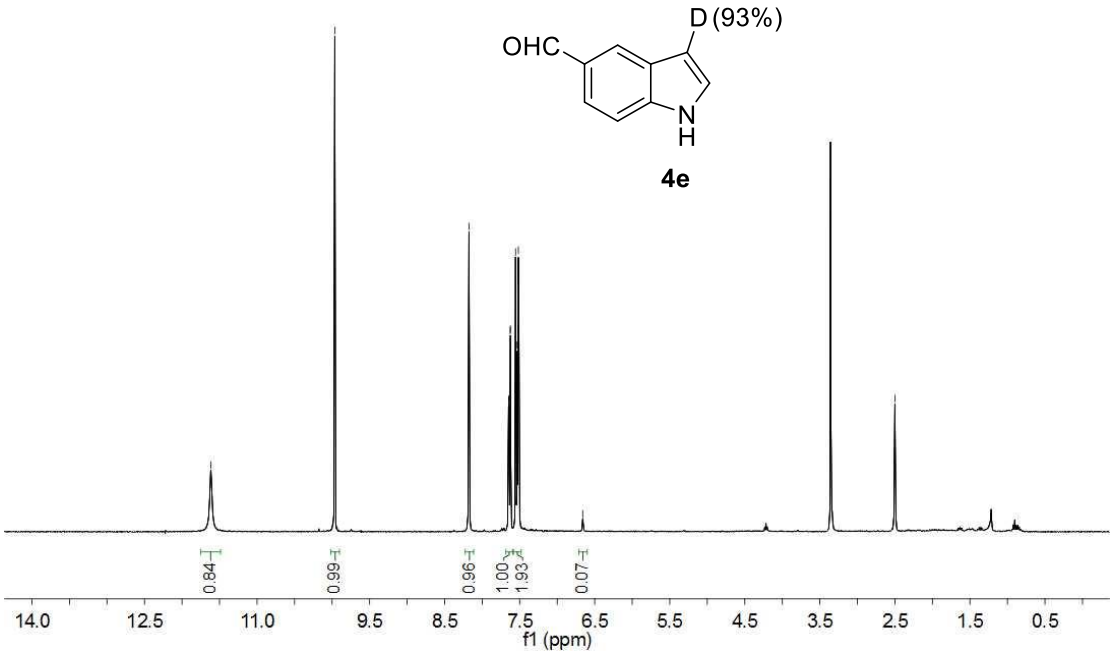

168.46
136.60
136.45
127.15
126.26
123.25
121.16
120.91
116.17
103.42
103.36
103.17
102.99
77.21
77.00
76.79
51.73
MeO2C
D (96%)
N
H
4c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

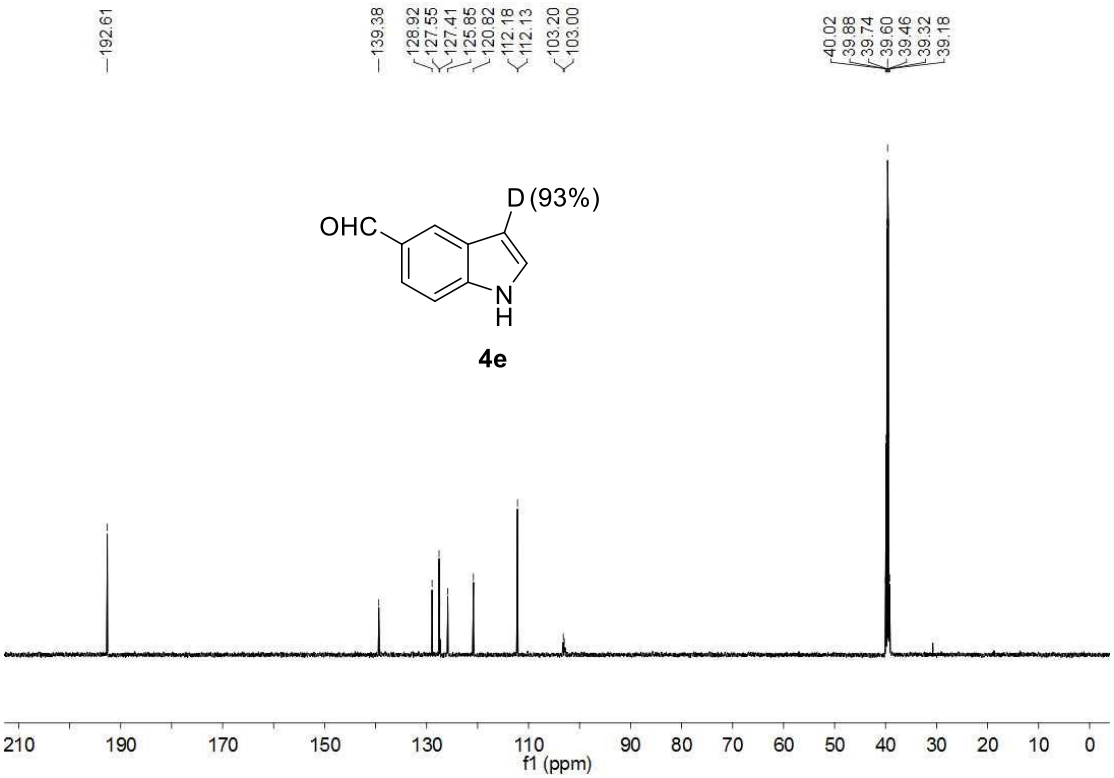

11.276
7.577
7.574
7.417
7.412
7.410
7.396
7.078
7.075
7.064
7.061
6.416
Cl
N
H
3d
0.99
0.96
2.02
1.00
0.99
13.0
11.5
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

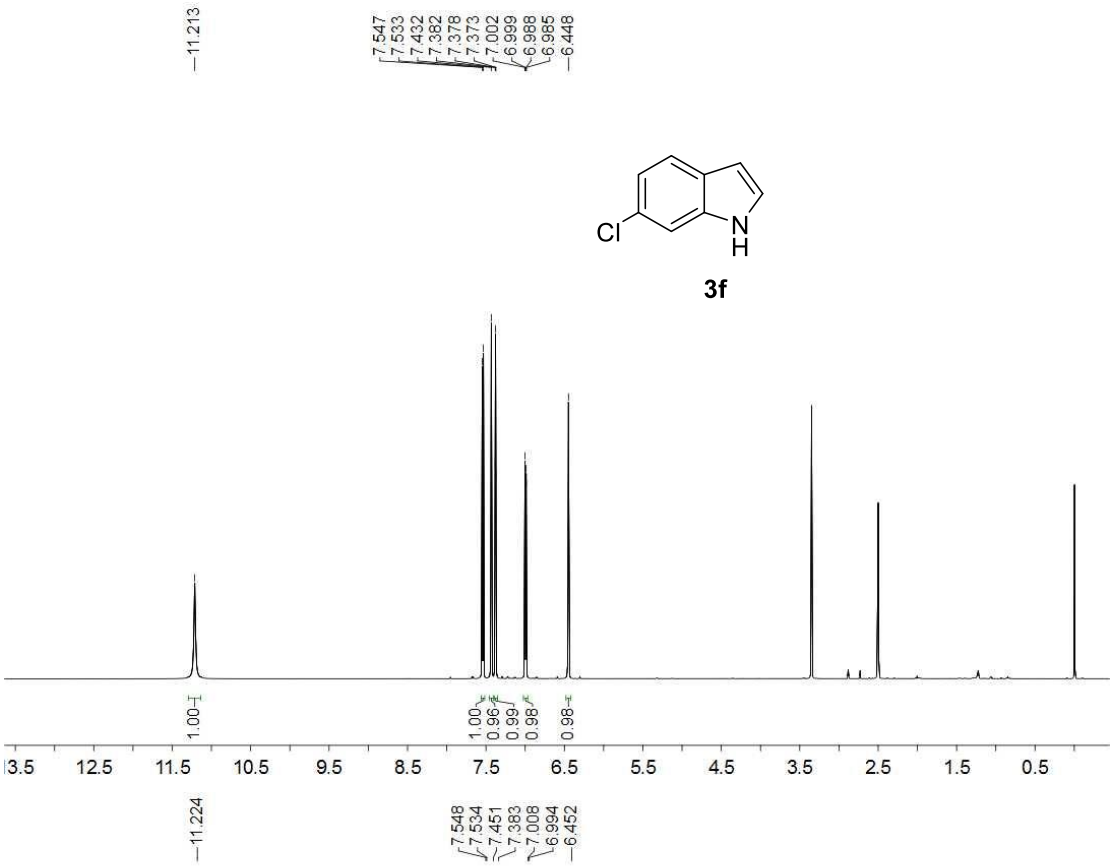

11.291
7.587
7.582
7.430
7.420
7.409
7.096
7.091
7.075
7.070
6.426
6.419
D (93%)
Cl
N
H
4d
0.23
0.87
1.88
1.00
0.07
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

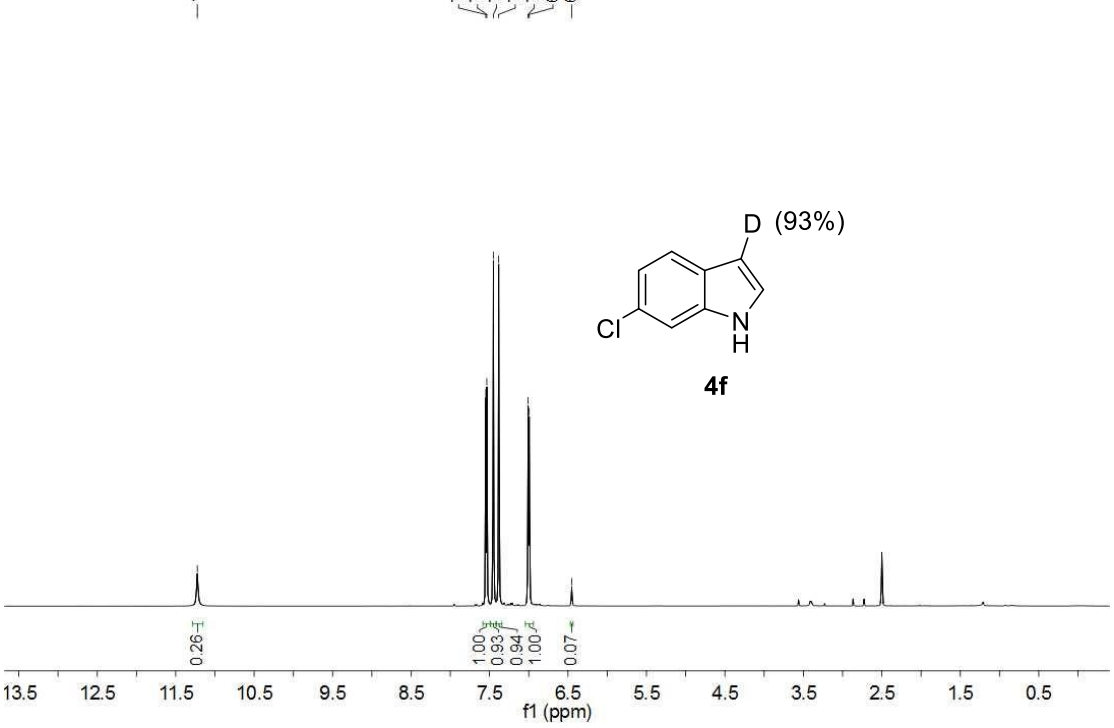

134.43
134.27
128.82
128.78
127.03
126.96
126.87
123.50
120.93
119.21
112.93
112.88
100.91
100.71
100.53
40.02
39.88
39.74
39.60
39.46
39.32
39.18
D (93%)
Cl
N
H
4d
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

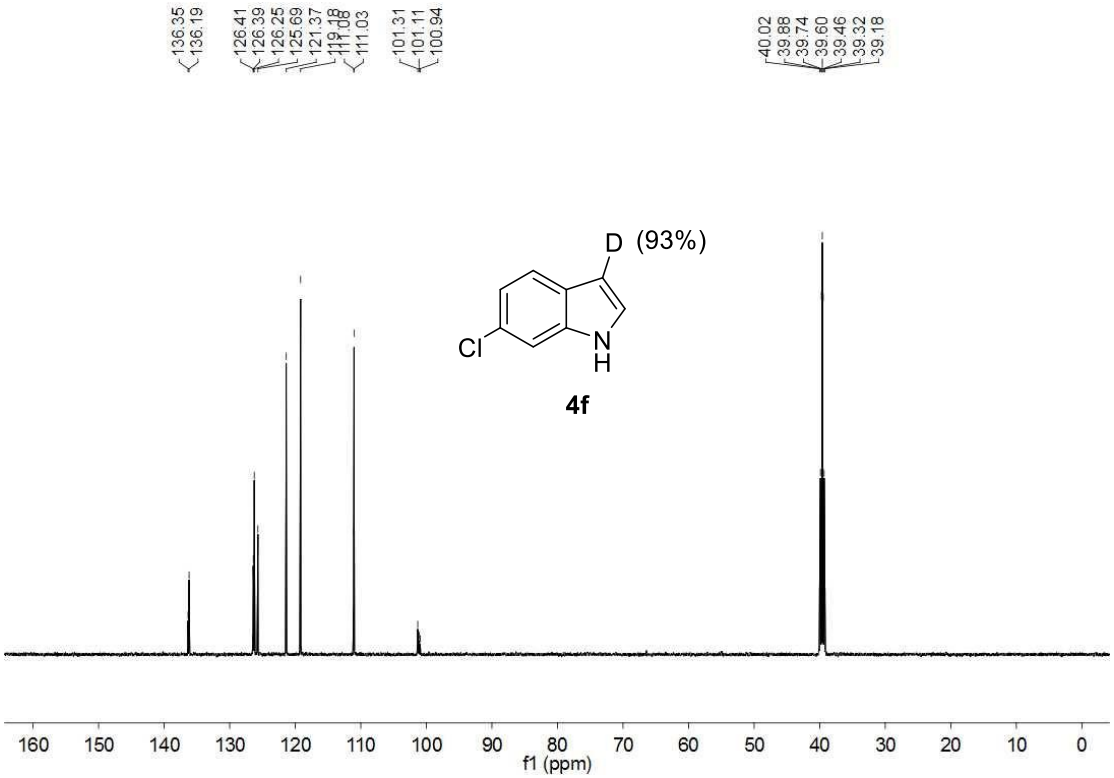

11.616
9.965
8.177
7.629
7.552
7.538
7.519
7.515
6.660
OHC
N
H
3e
0.99
1.00
1.00
1.00
0.99
0.97
0.97
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
11.614
9.964
8.177
7.627
7.623
7.555
7.517
2.500

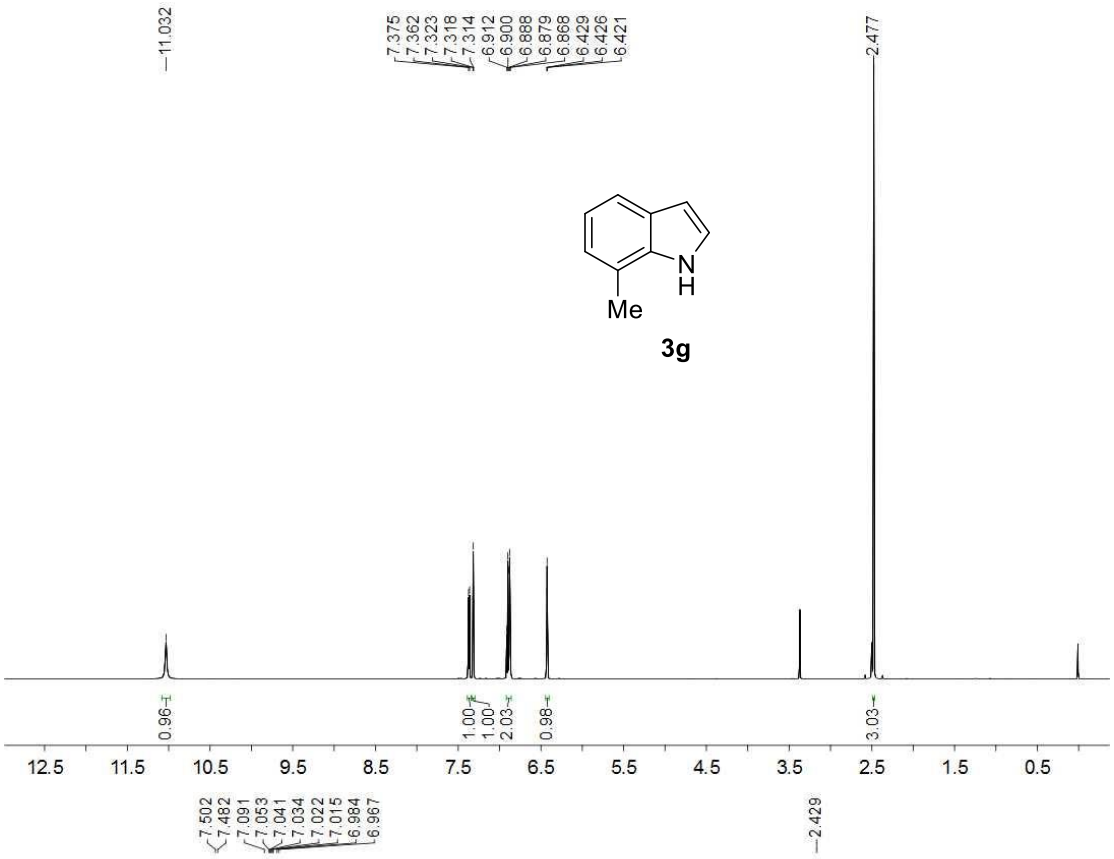

D (93%)
OHC
N
H
4e
0.84
0.99
0.96
1.00
1.93
0.07
14.0
12.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


192.61
139.38
128.92
127.55
127.41
125.85
120.82
112.18
112.13
103.20
103.00
40.02
39.88
39.74
39.60
39.46
39.32
39.18
D (93%)
OHC
N
H
4e
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

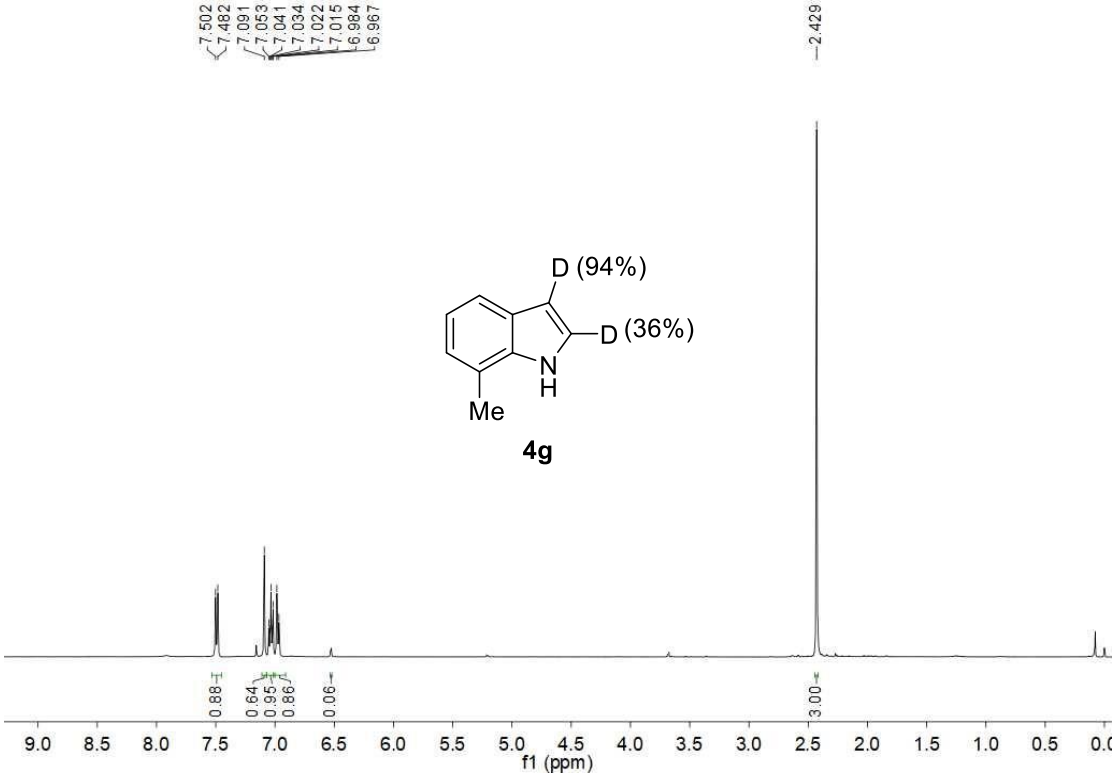

11.213
7.547
7.533
7.432
7.382
7.378
7.373
7.002
6.999
6.988
6.985
6.448
Cl
N
H
3f
1.00
1.00
0.96
0.99
0.98
0.98
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5


11.224
7.548
7.534
7.451
7.383
7.008
6.994
6.452
D (93%)
Cl
N
H
4f
0.26
1.00
0.93
0.94
1.00
0.07
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

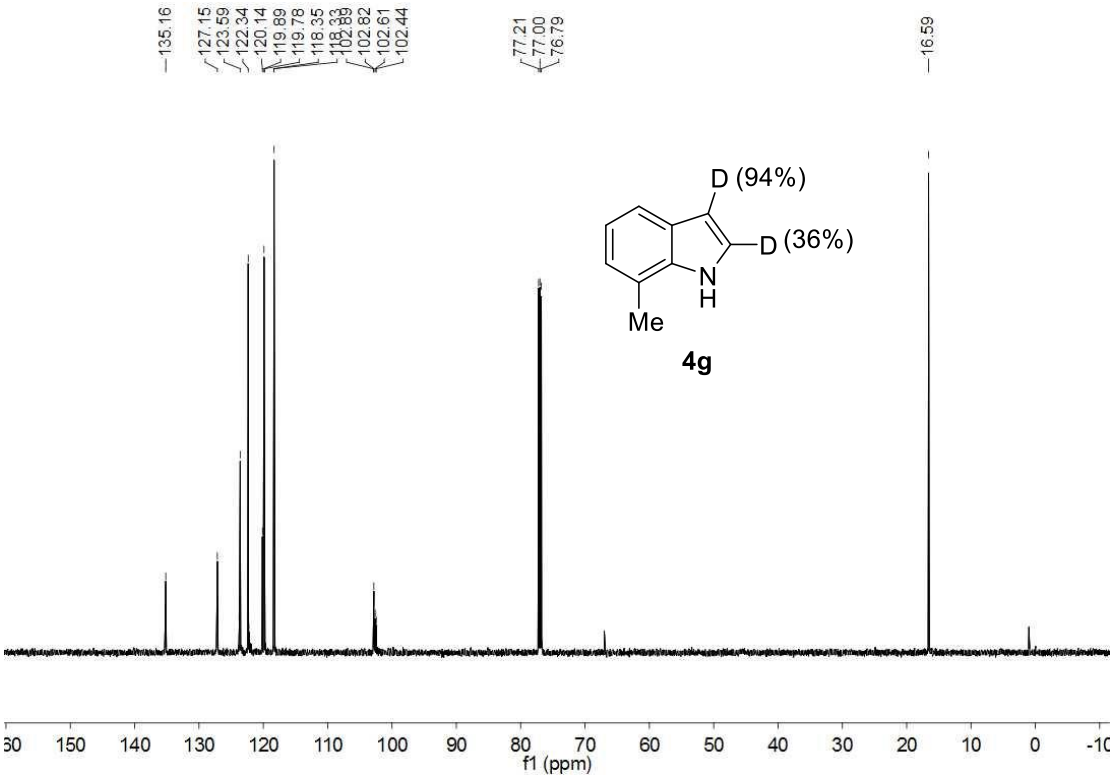

136.35
136.19
126.41
126.39
126.25
125.69
121.37
119.18
111.08
111.03
101.31
101.11
100.94
40.02
39.88
39.74
39.60
39.46
39.32
39.18
D (93%)
Cl
N
H
4f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

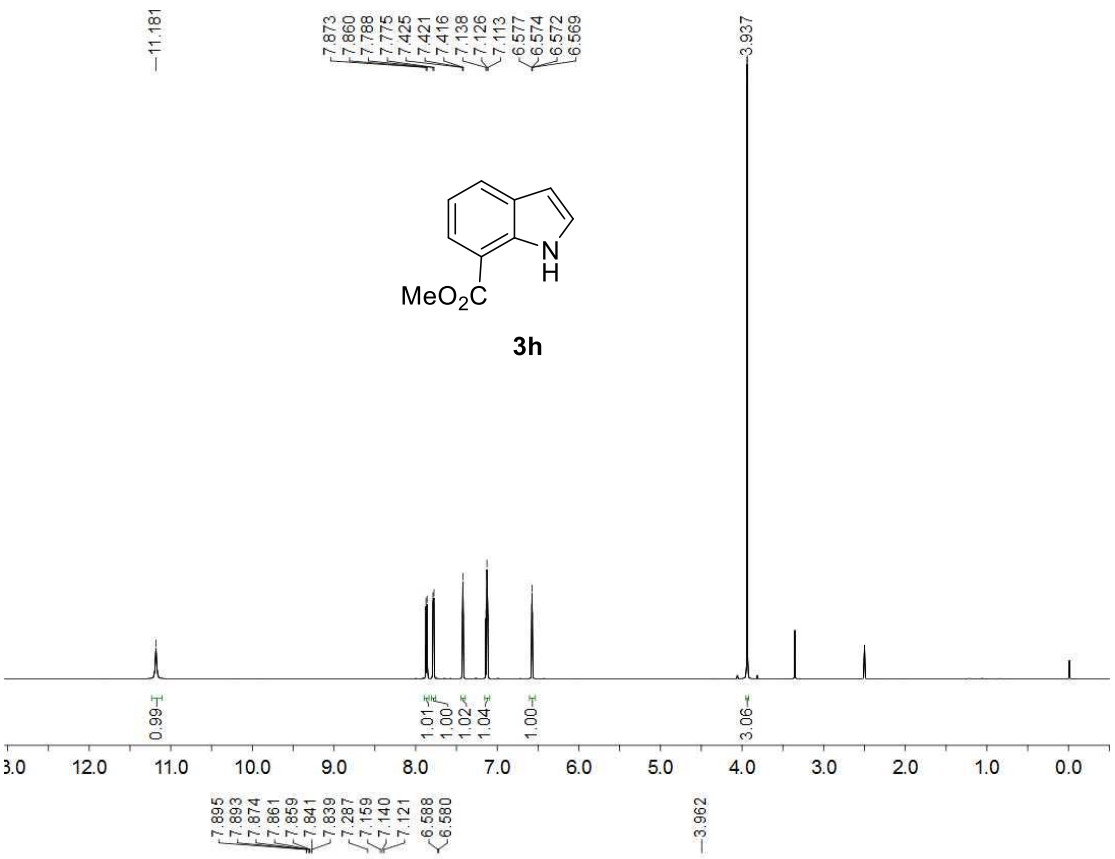

11.032
7.375
7.362
7.323
7.318
7.314
6.912
6.900
6.888
6.879
6.868
6.429
6.426
6.421
2.477
N
H
Me
0.96
1.00
1.00
2.03
0.98
3.03
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

3g

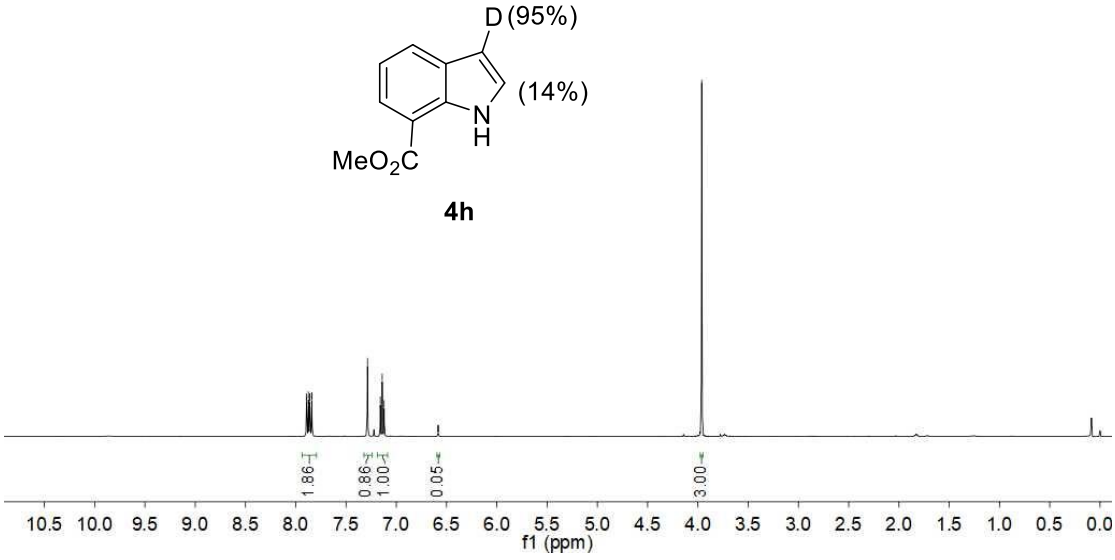

7.502
7.482
7.091
7.053
7.041
7.034
7.022
7.015
6.984
6.967
2.429
D (94%)
D (36%)
N
H
Me
0.88
0.64
0.95
0.86
0.06
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

4g

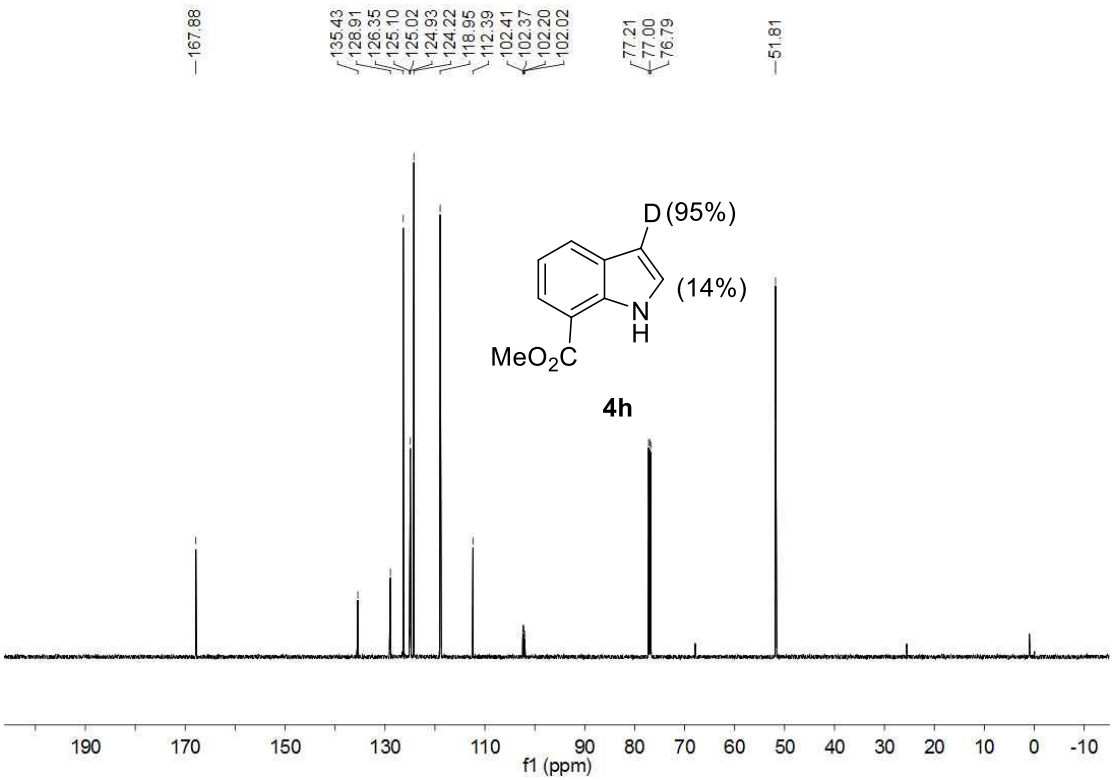

135.16
127.15
123.59
122.34
120.14
119.89
119.78
118.35
118.33
102.89
102.82
102.61
102.44
77.21
77.00
76.79
16.59
D (94%)
D (36%)
N
H
Me
4g
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

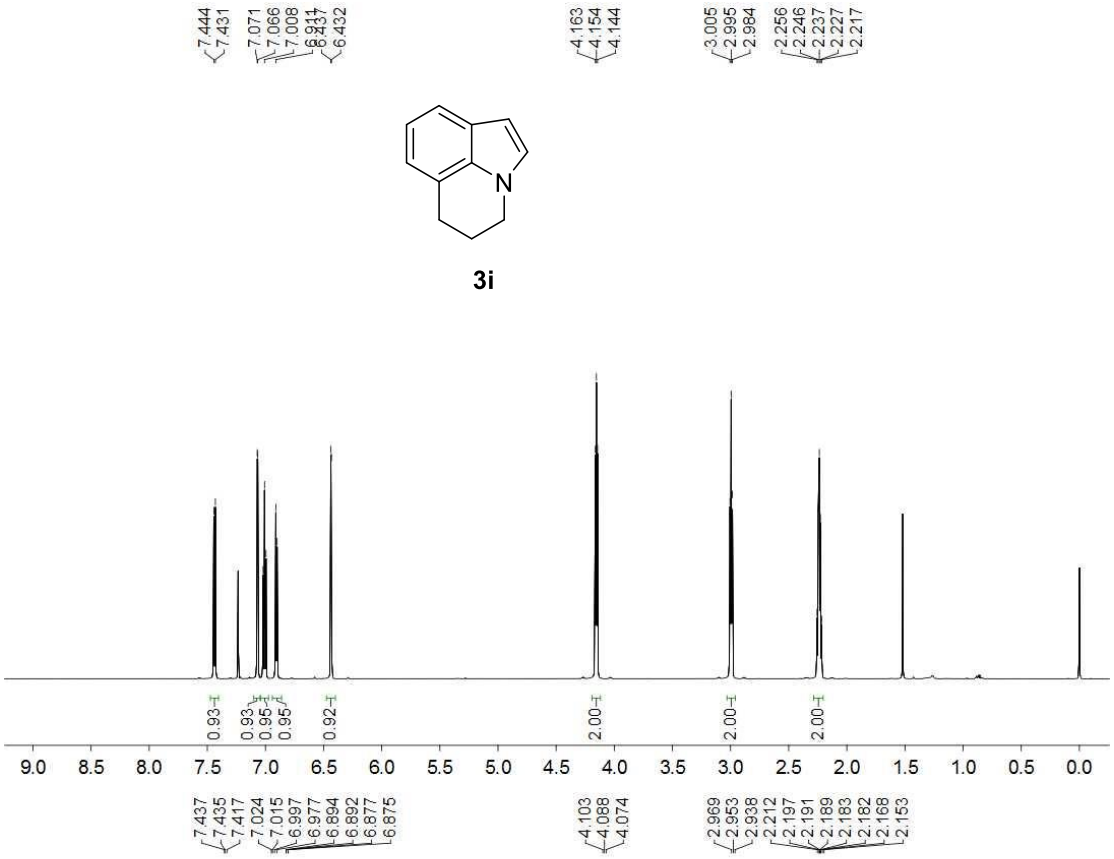

11.181
7.873
7.860
7.788
7.775
7.425
7.421
7.416
7.138
7.126
7.113
6.577
6.574
6.572
6.569
3.937
N
H
MeO2C
0.99
1.01
1.00
1.02
1.04
1.00
3.06
7.895
7.893
7.874
7.861
7.859
7.841
7.839
7.287
7.159
7.140
7.121
6.588
6.580
3.962

3h

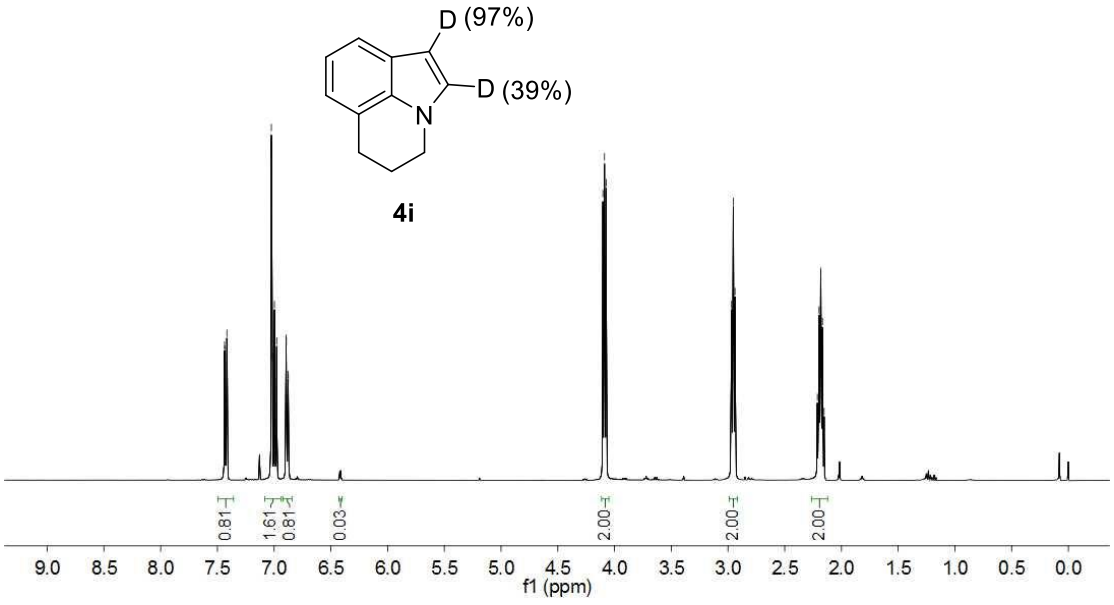

D (95%)
(14%)
N
H
MeO2C
1.86
0.86
1.00
0.05
3.00
f1 (ppm)

4h

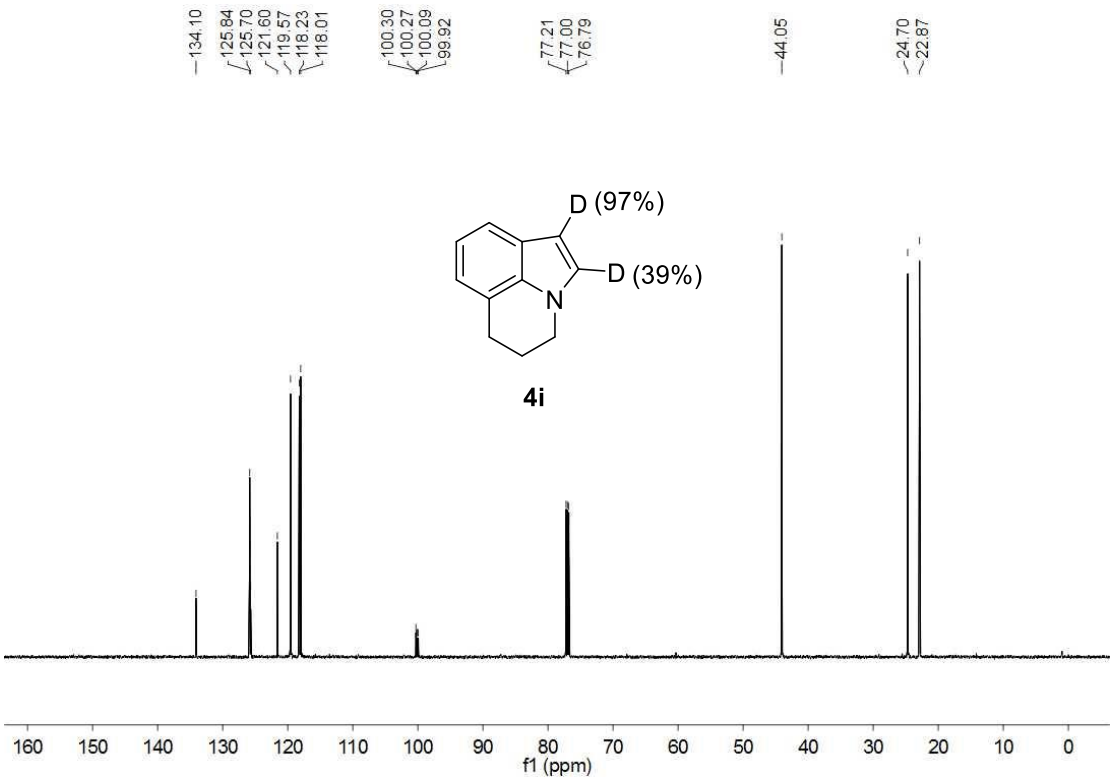

167.88
135.43
128.91
126.35
125.10
125.02
124.93
124.22
118.95
112.39
102.41
102.37
102.20
102.02
77.21
77.00
76.79
51.81
D (95%)
(14%)
N
H
MeO2C
4h
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

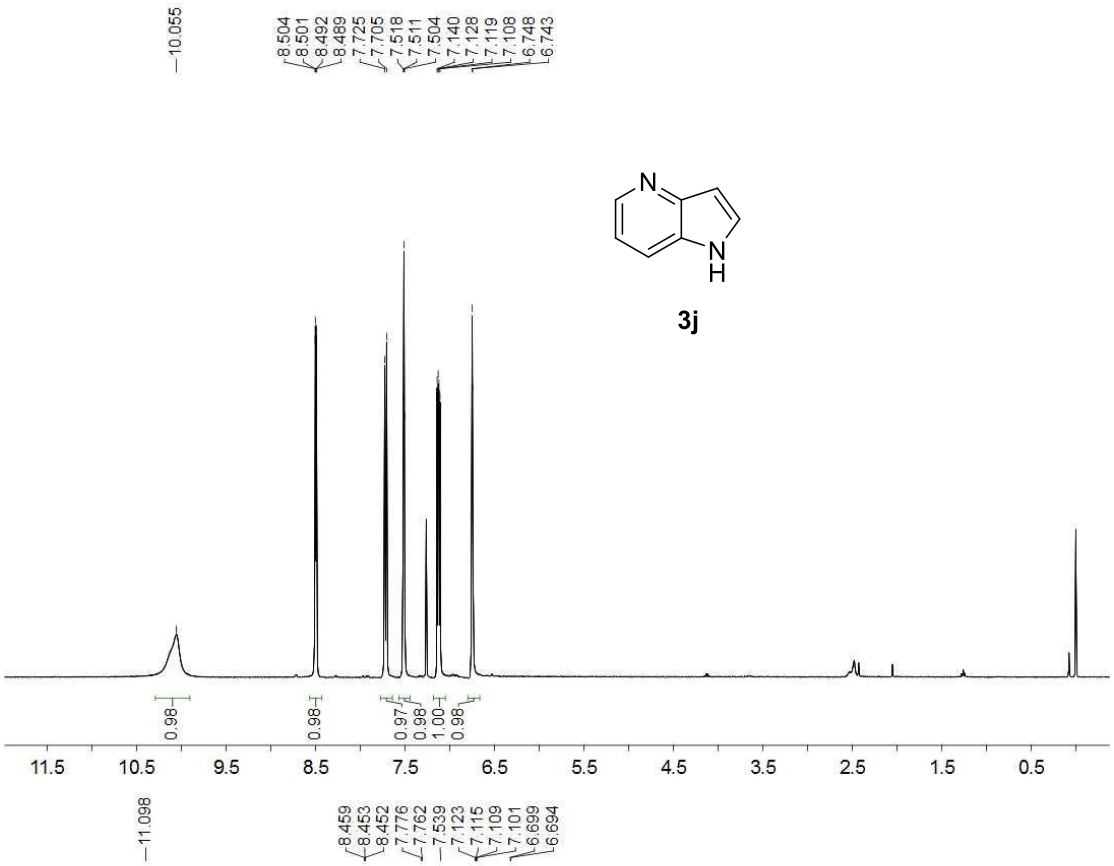

7.444
7.431
7.071
7.066
7.008
6.937
6.432
4.163
4.154
4.144
3.005
2.995
2.984
2.256
2.246
2.237
2.227
2.217
N
0.93
0.93
0.95
0.95
0.92
2.00
2.00
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
7.437
7.435
7.417
7.024
7.015
6.997
6.977
6.894
6.892
6.877
6.875
4.103
4.088
4.074
2.969
2.953
2.938
2.212
2.197
2.191
2.189
2.183
2.182
2.168
2.153

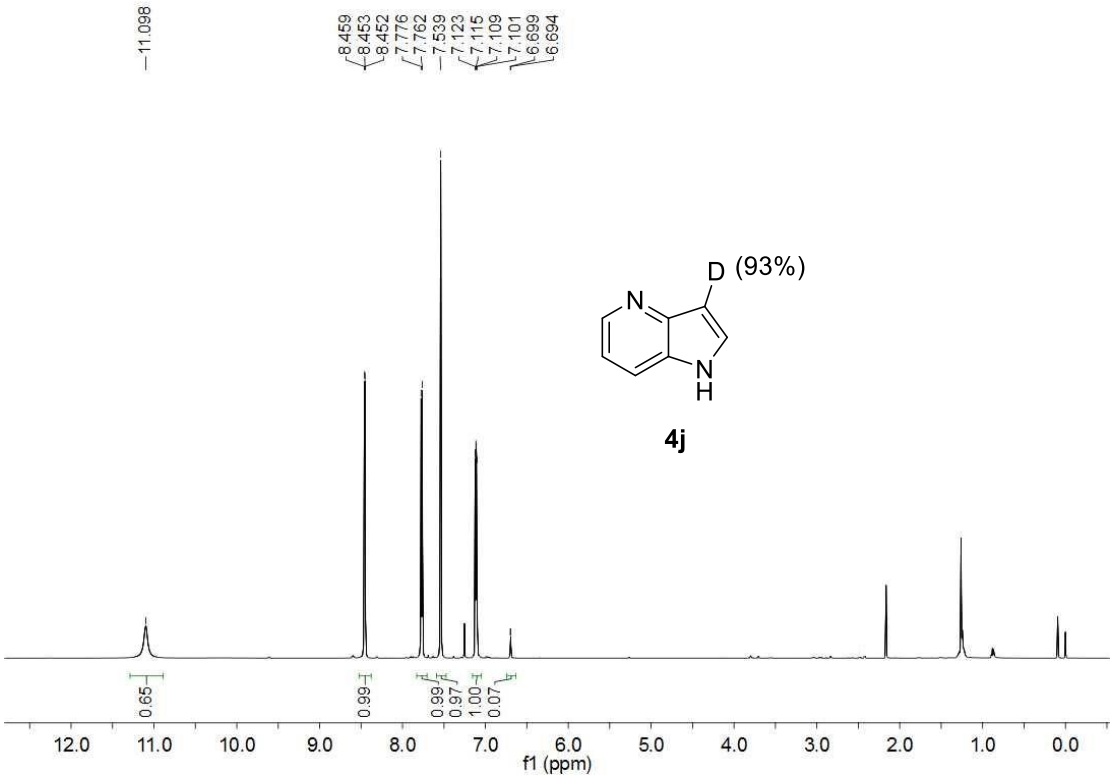
3i

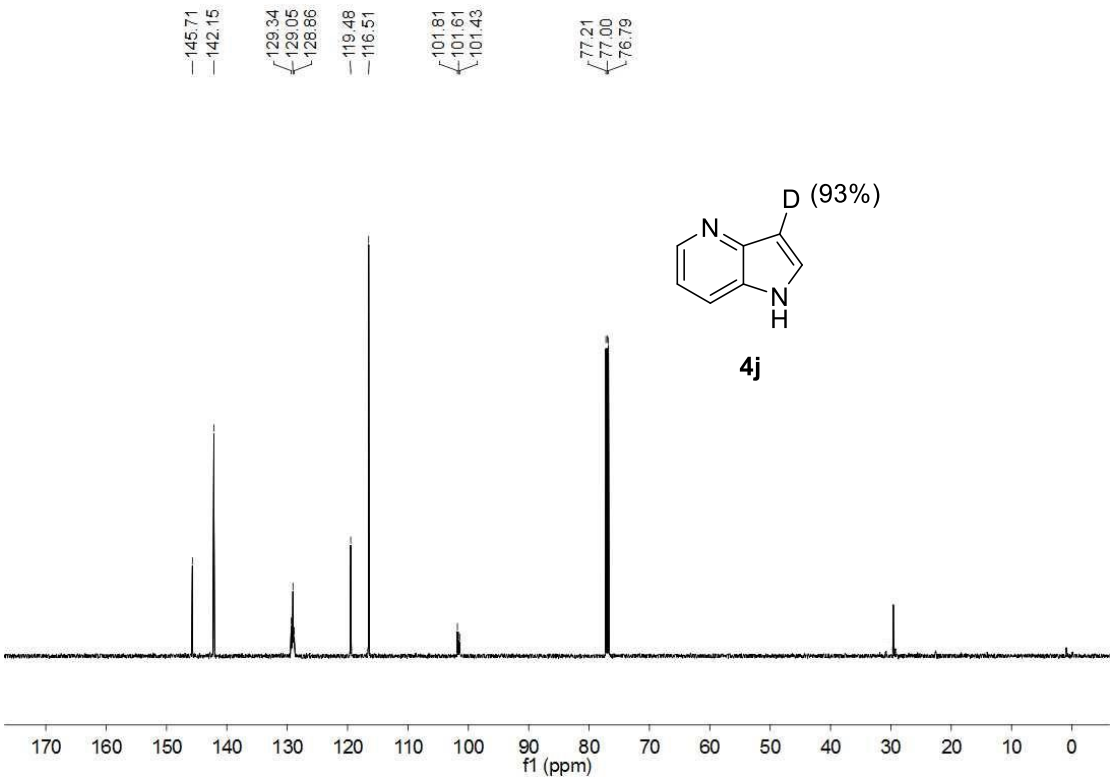

D (97%)
D (39%)
N
0.81
1.61
0.81
0.03
2.00
2.00
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

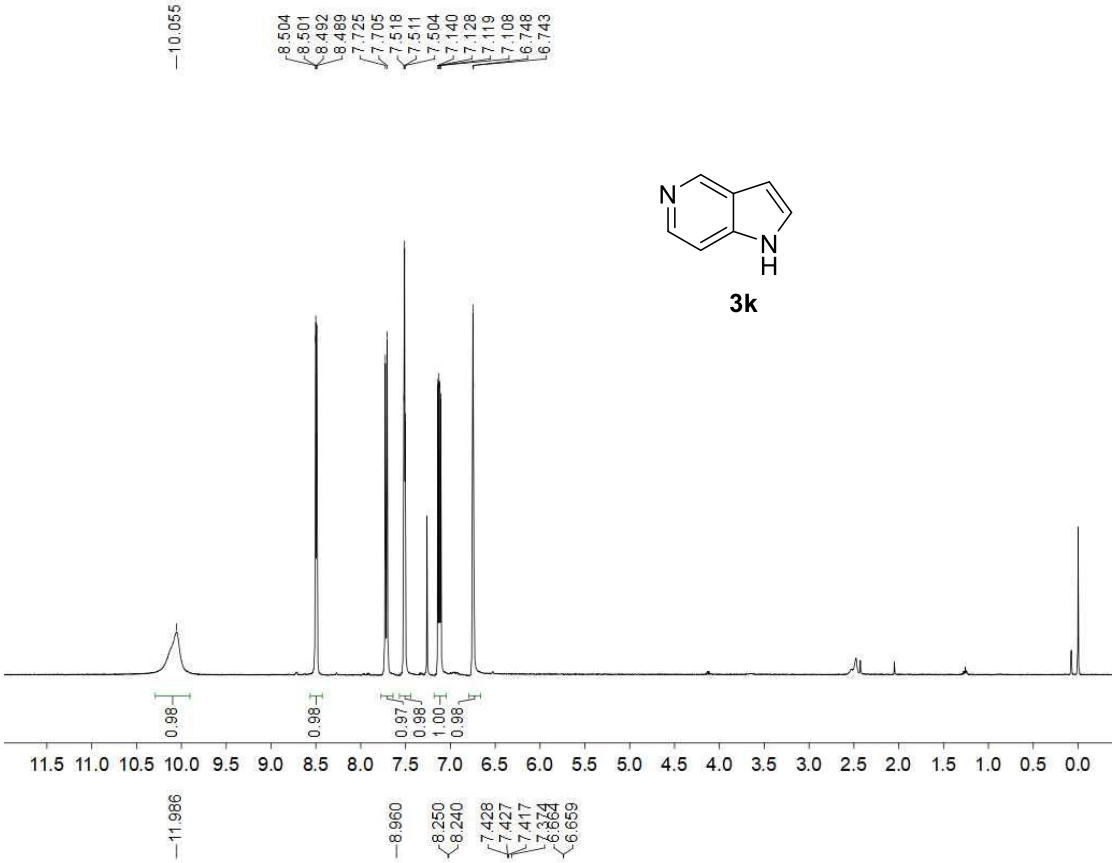
4i

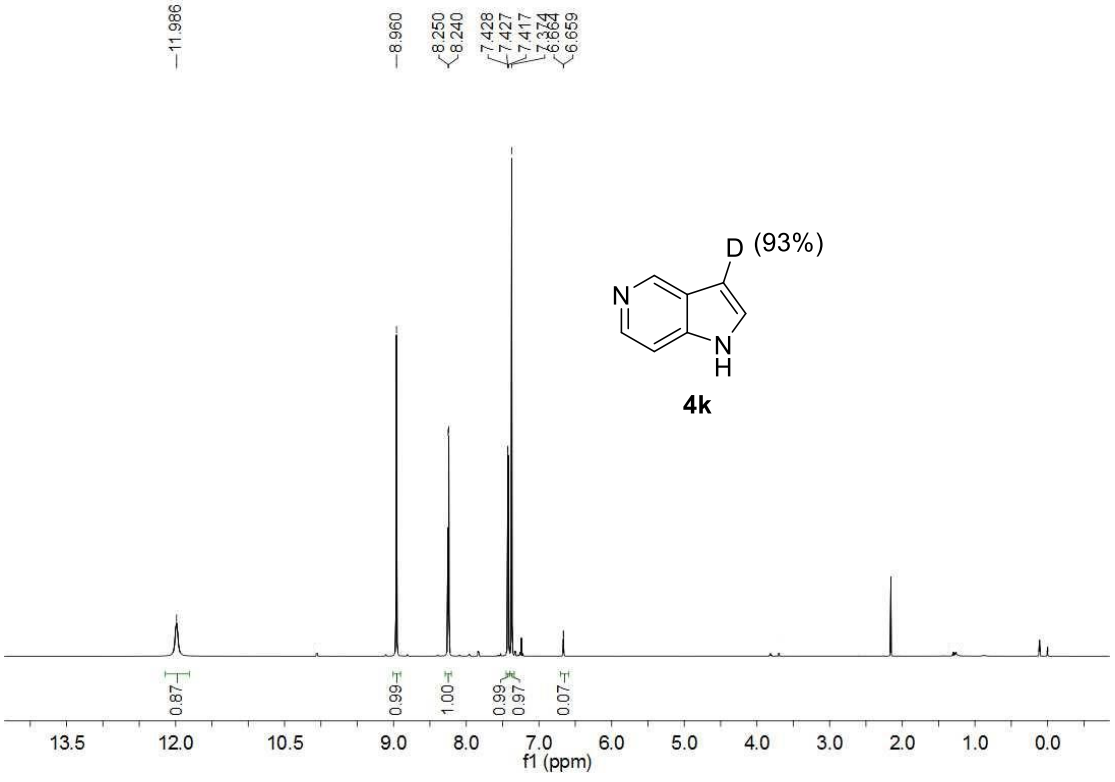

134.10
125.84
125.70
121.60
119.57
118.23
118.01
100.30
100.27
100.09
99.92
77.21
77.00
76.79
44.05
24.70
22.87
D (97%)
D (39%)
N
4i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

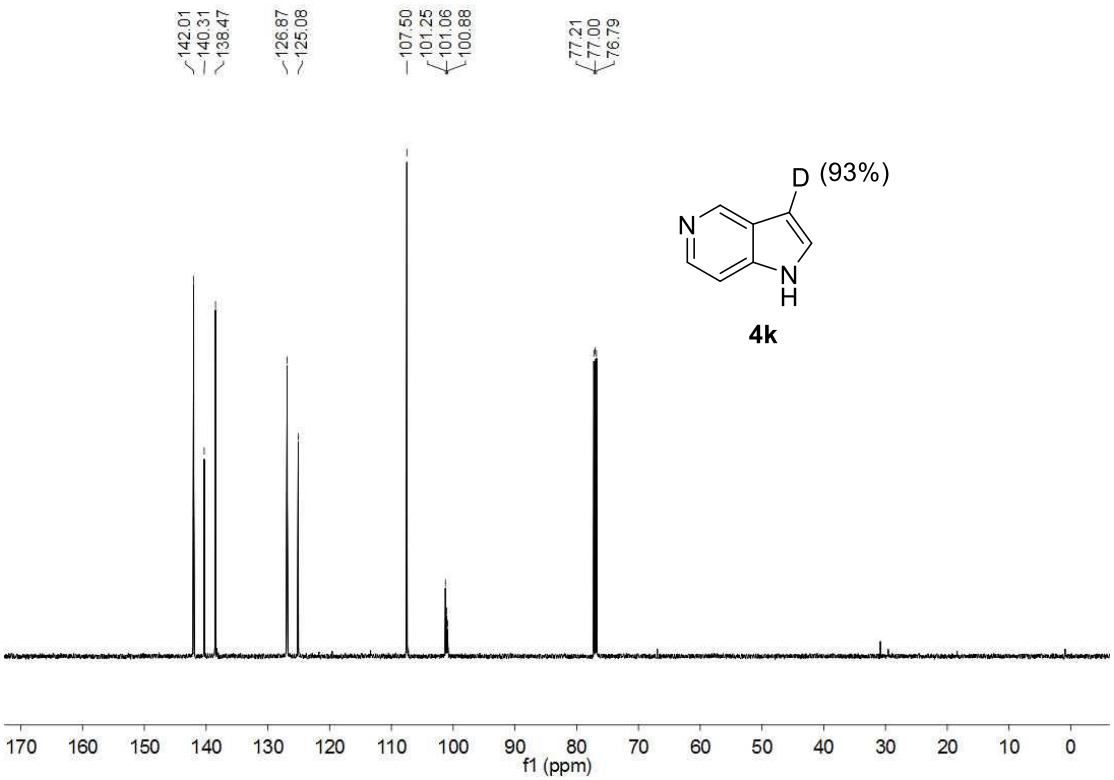

10.055
8.504
8.501
8.492
8.489
7.725
7.705
7.518
7.511
7.504
7.140
7.128
7.119
7.108
6.748
6.743
N
N
H
3j
0.98
0.98
0.97
0.98
1.00
0.98
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

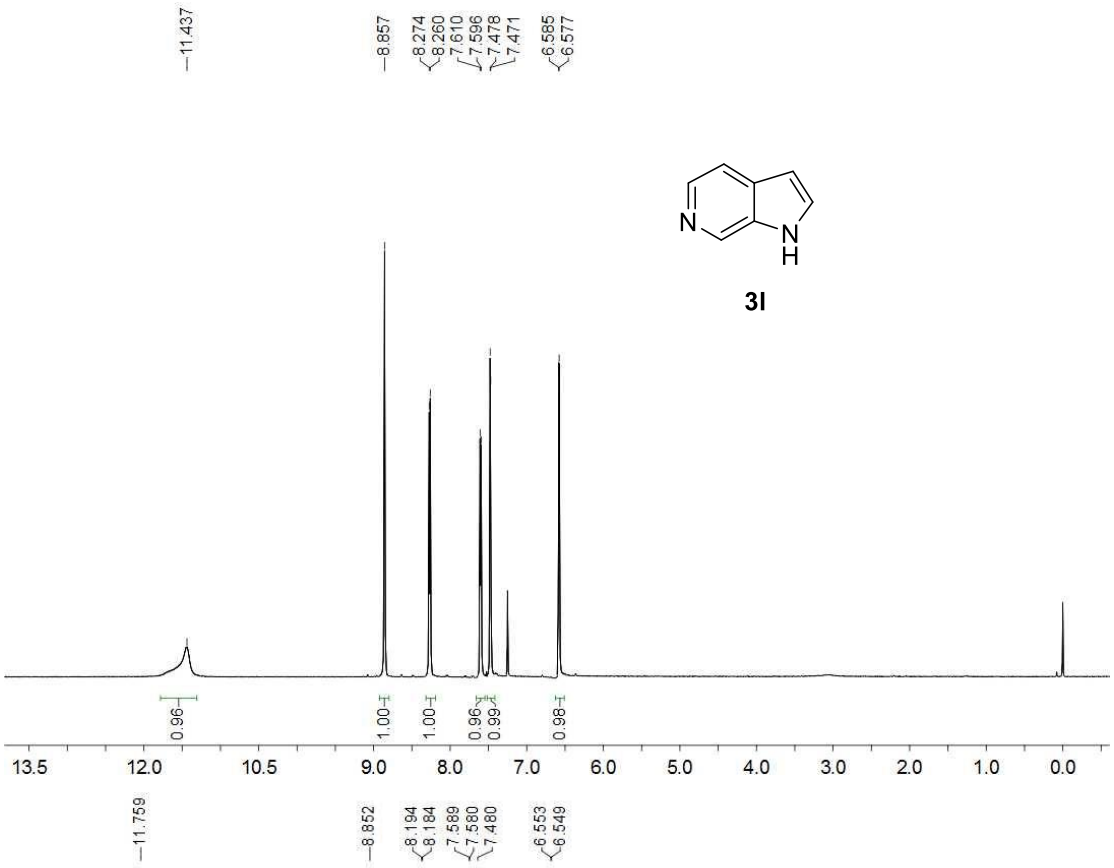

11.098
8.459
8.453
8.452
7.776
7.762
7.539
7.123
7.115
7.109
7.101
6.699
6.694
D (93%)
N
N
H
4j
0.65
0.99
0.99
0.97
1.00
0.07
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


145.71
142.15
129.34
129.05
128.86
119.48
116.51
101.81
101.61
101.43
77.21
77.00
76.79
D (93%)
N
N
H
4j
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

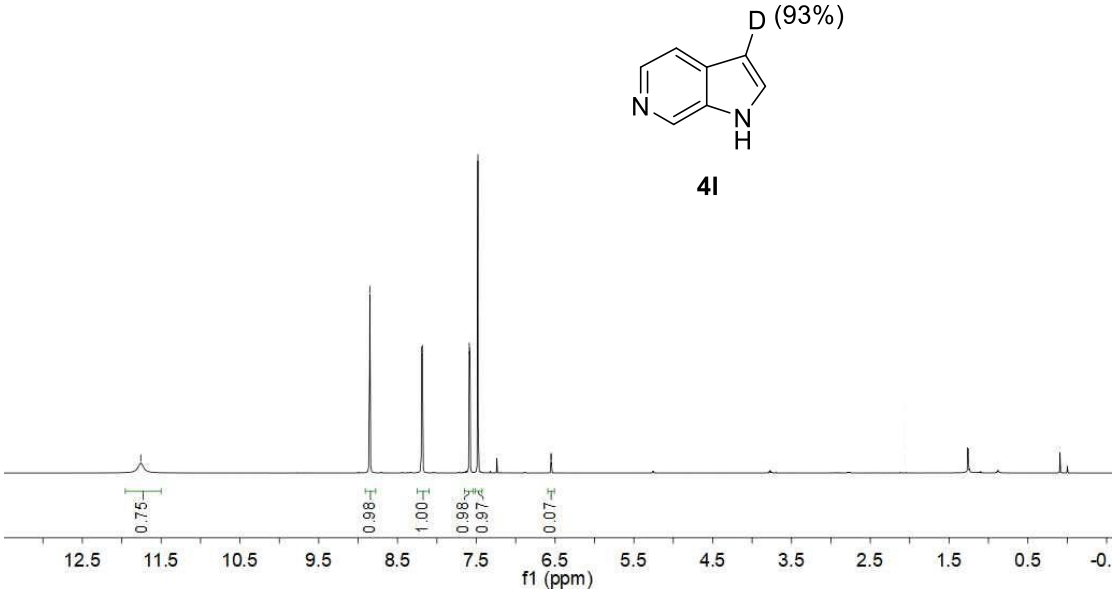

10.055
8.504
8.501
8.492
8.489
7.725
7.705
7.518
7.511
7.504
7.140
7.128
7.119
7.108
6.748
6.743
N
N
H
3k
0.98
0.98
0.97
0.98
1.00
0.98
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


11.986
8.960
8.250
8.240
7.428
7.427
7.417
7.374
6.664
6.659
D (93%)
N
N
H
4k
0.87
0.99
1.00
0.99
0.97
0.07
13.5 12.0 10.5 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

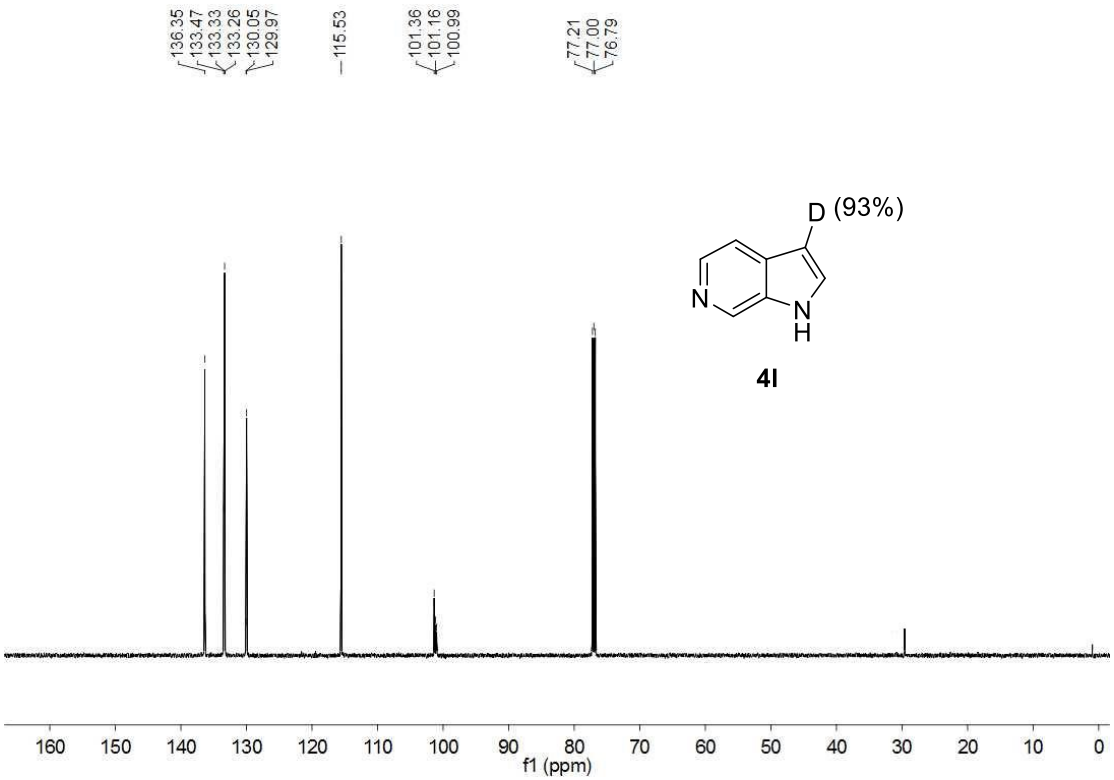

142.01
140.31
138.47
126.87
125.08
107.50
101.25
101.06
100.88
77.21
77.00
76.79
D (93%)
N
N
H
4k
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

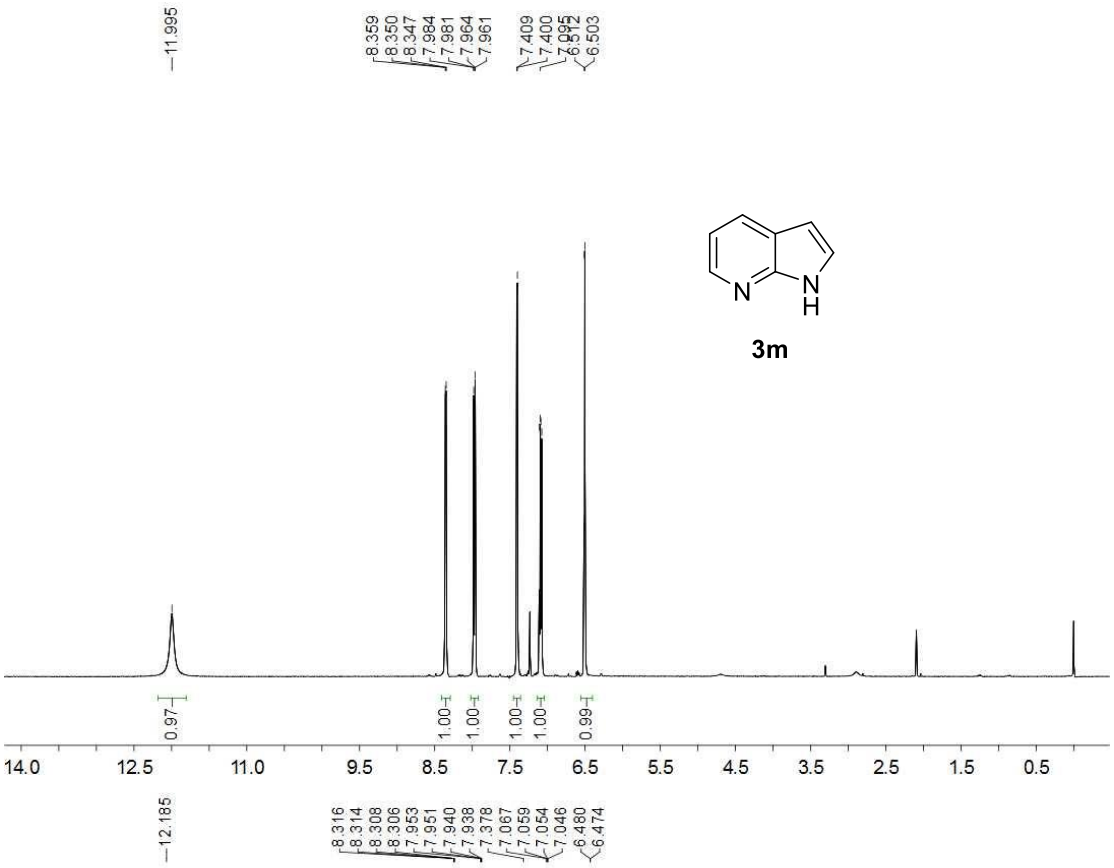

11.437
8.857
8.274
8.260
7.610
7.596
7.478
7.471
6.585
6.577
0.96
1.00
1.00
0.96
0.99
0.98
13.5
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
11.759
8.852
8.194
8.184
7.589
7.580
7.480
6.553
6.549

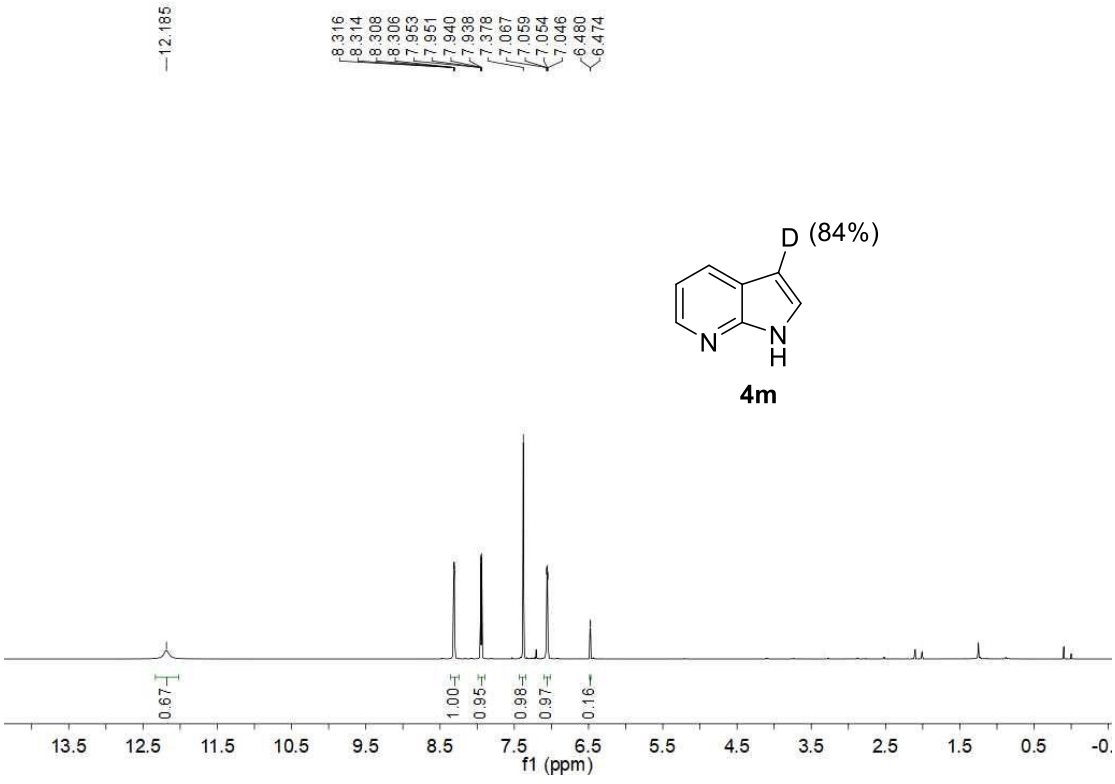
3l

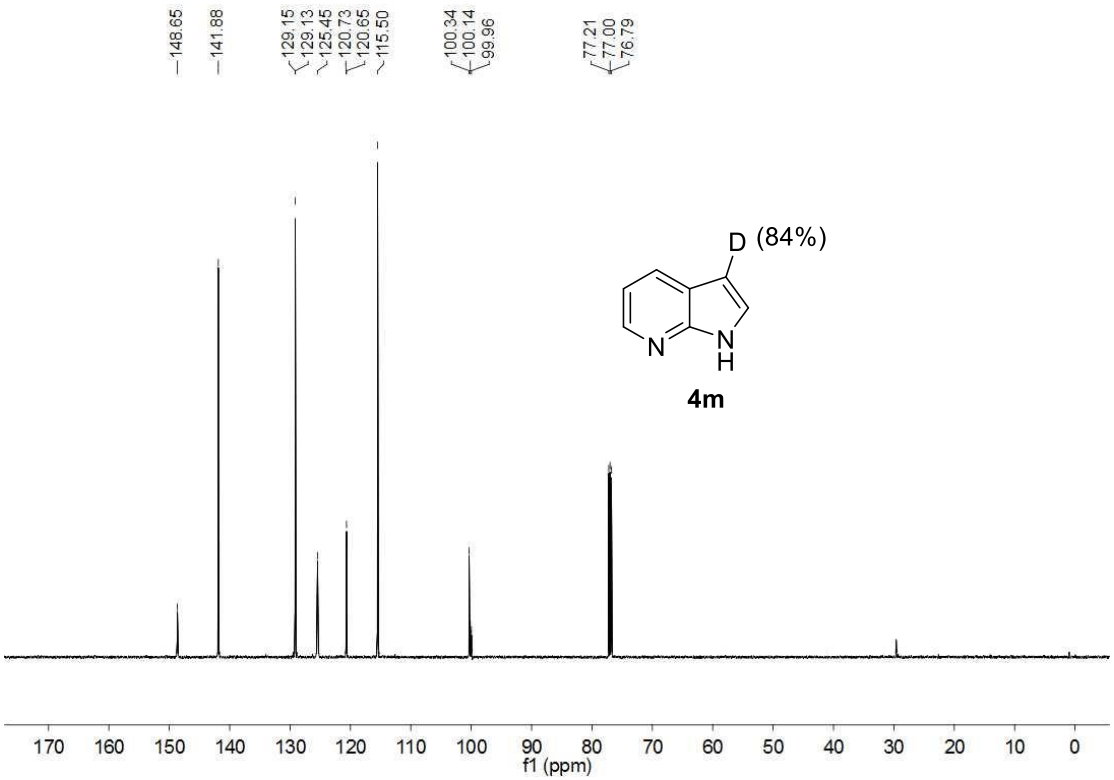

0.75
0.98
1.00
0.98
0.97
0.07
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

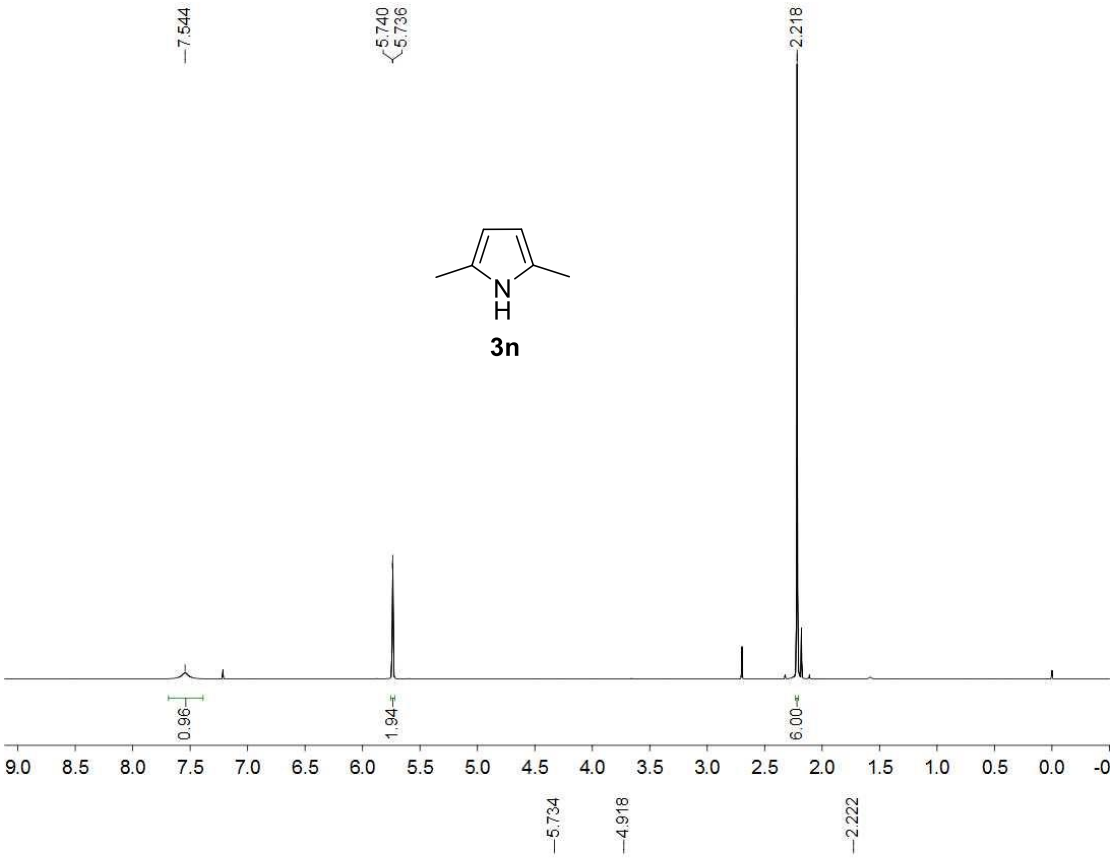
4l

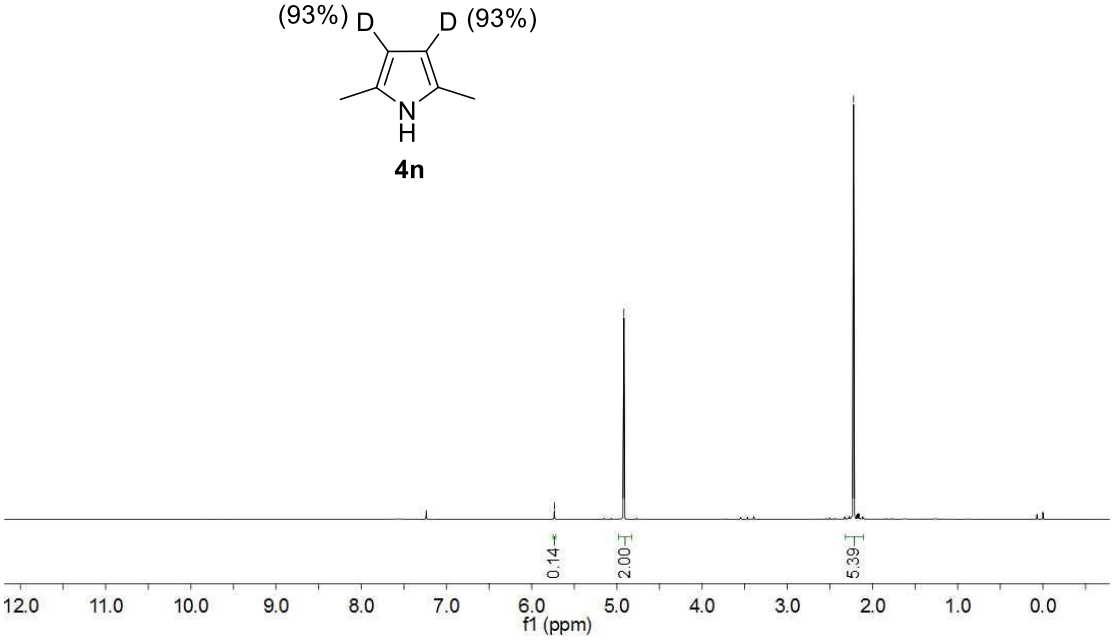

136.35
133.47
133.33
133.26
130.05
129.97
115.53
101.36
101.16
100.99
77.21
77.00
76.79
D (93%)
N
N
H
4l
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

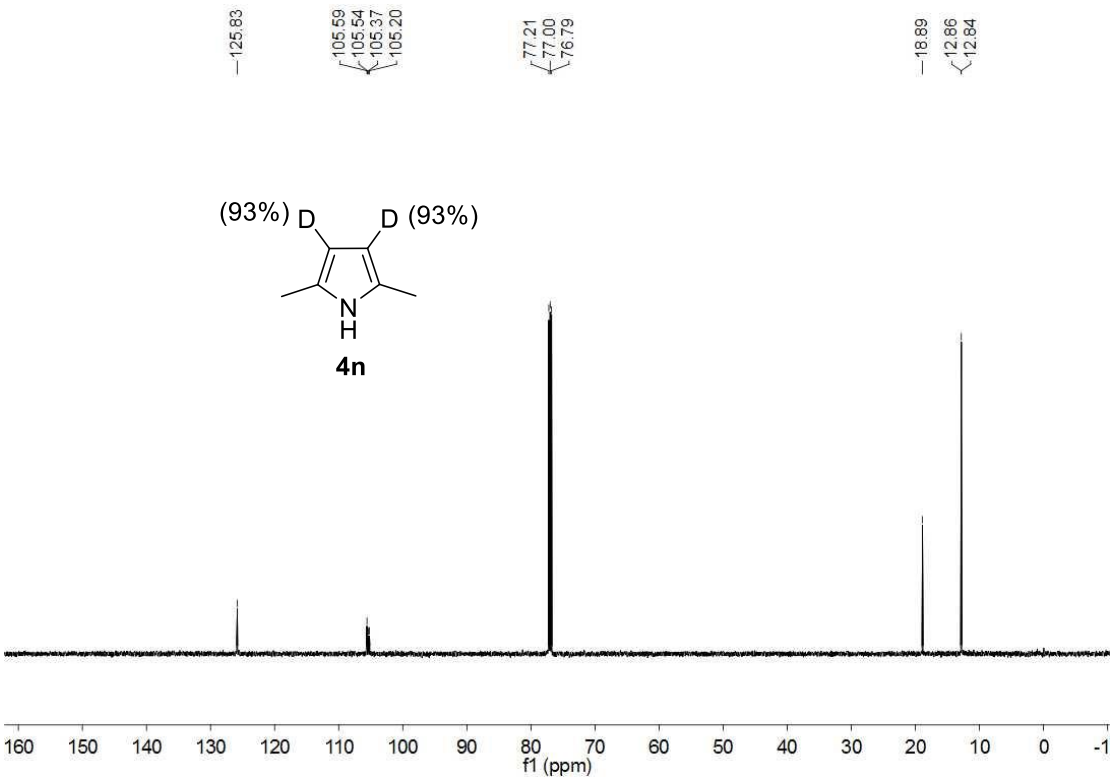

11.995
8.359
8.350
8.347
7.984
7.981
7.964
7.961
7.409
7.400
6.503
3m
0.97
1.00
1.00
1.00
0.99
14.0
12.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

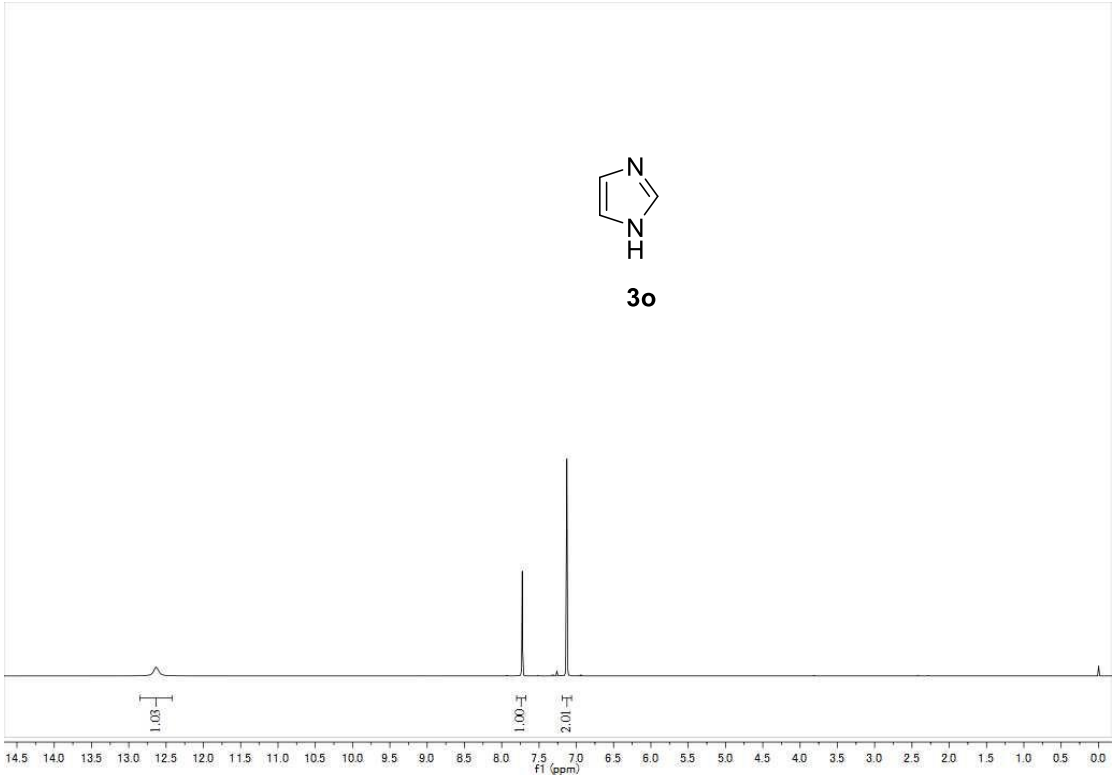

12.185
8.316
8.314
8.308
8.306
7.953
7.951
7.940
7.938
7.378
7.067
7.059
7.054
7.046
6.480
6.474
D (84%)
4m
0.67
1.00
0.95
0.98
0.97
0.16
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

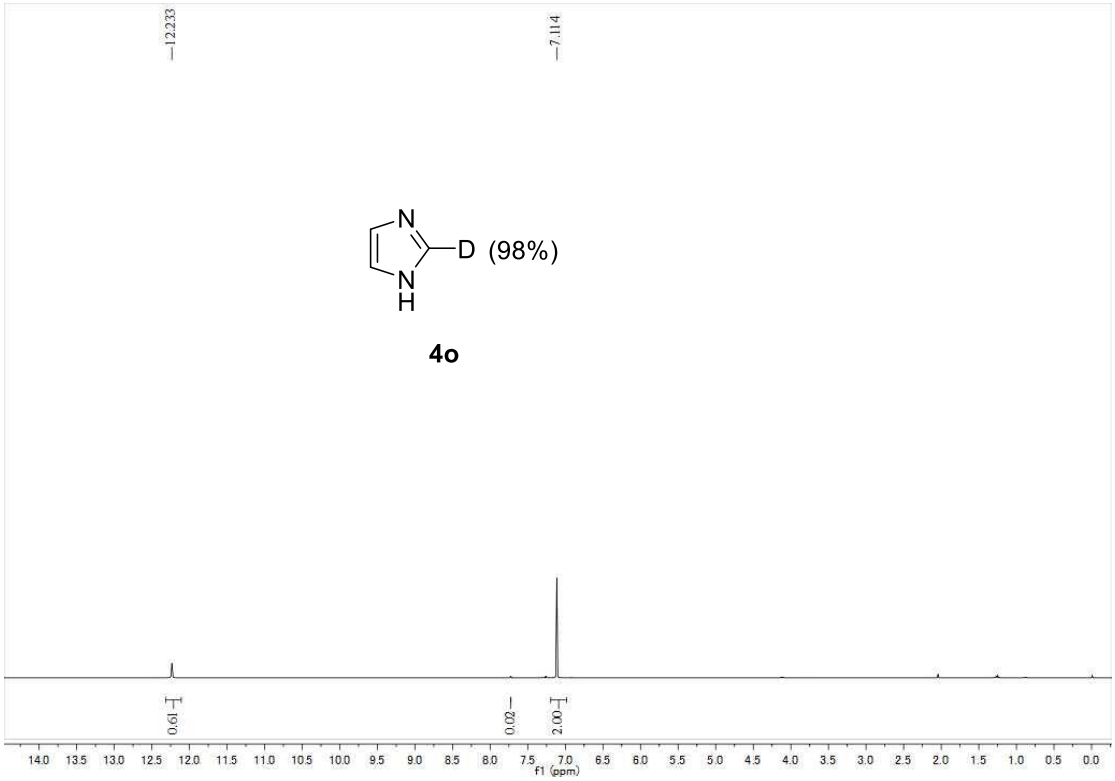

148.65
141.88
129.15
129.13
125.45
120.73
120.65
115.50
100.34
100.14
99.96
77.21
77.00
76.79
D (84%)
N
N
H
4m
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

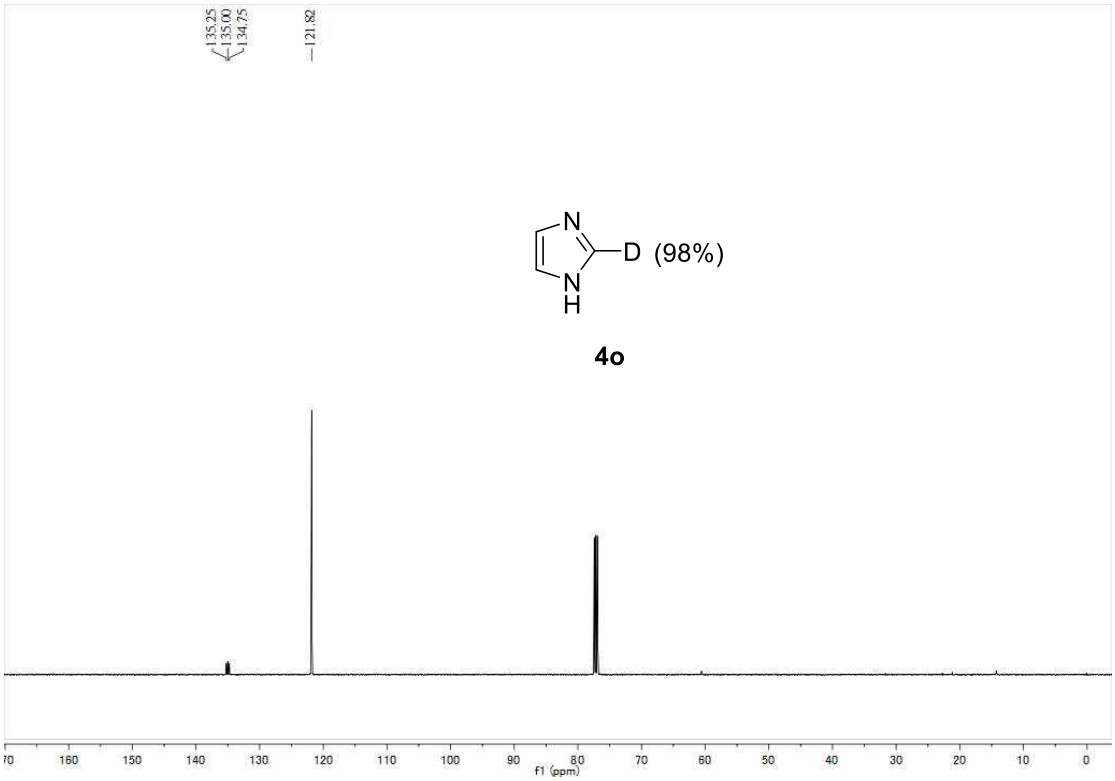

7.544
5.740
5.736
2.218
3n
0.96
1.94
6.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
5.734
4.918
2.222

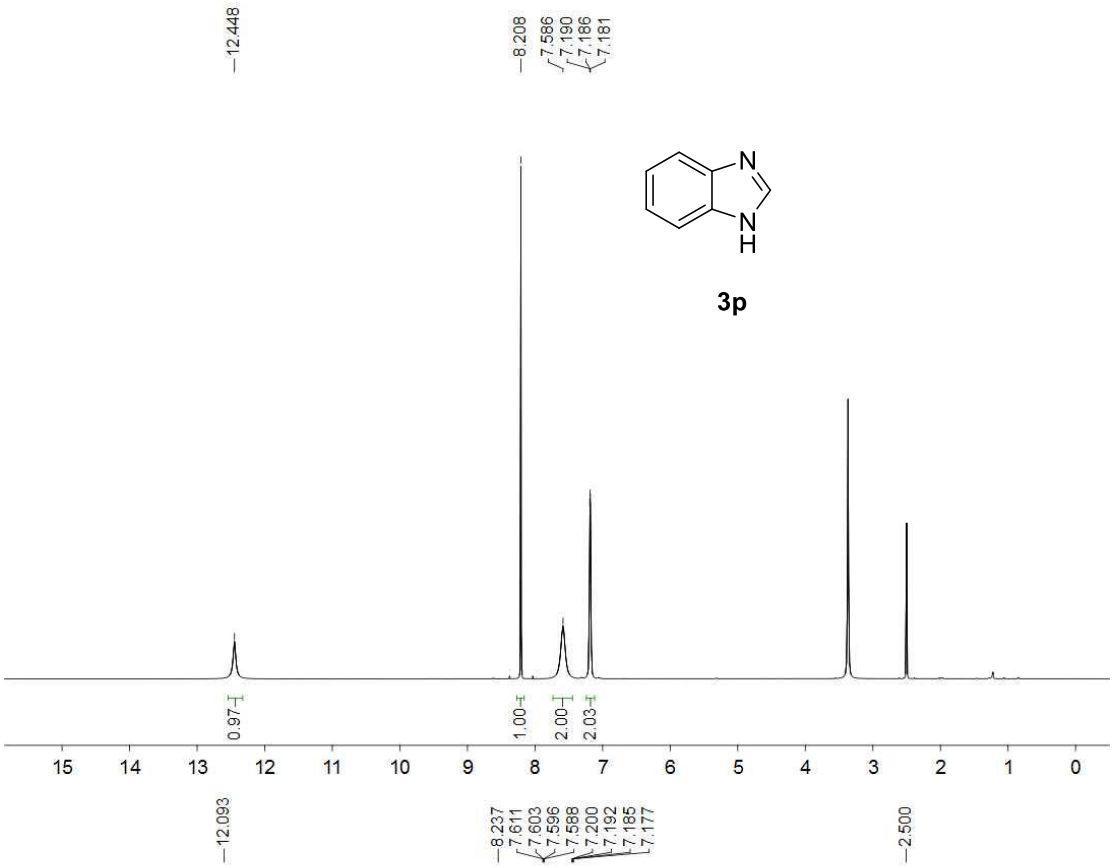

(93%) D
D (93%)
4n
0.14
2.00
5.39
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

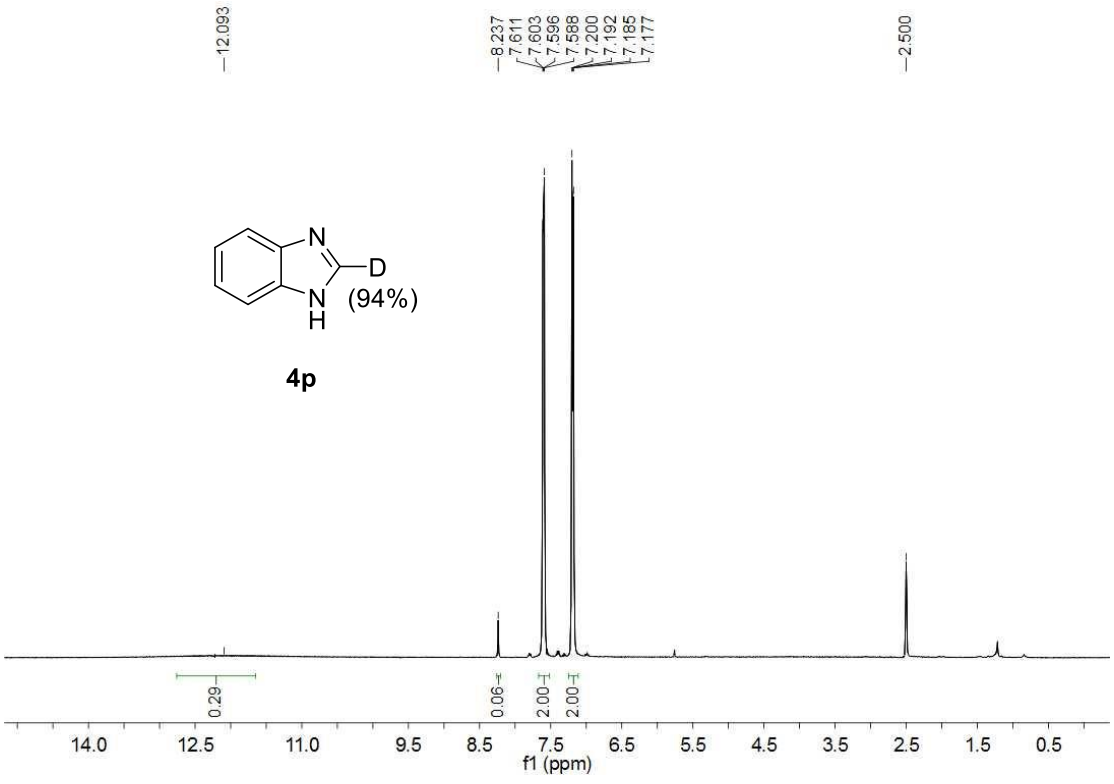

125.83
105.59
105.54
105.37
105.20
77.21
77.00
76.79
18.89
12.86
12.84
(93%) D
D (93%)
N
H
4n
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

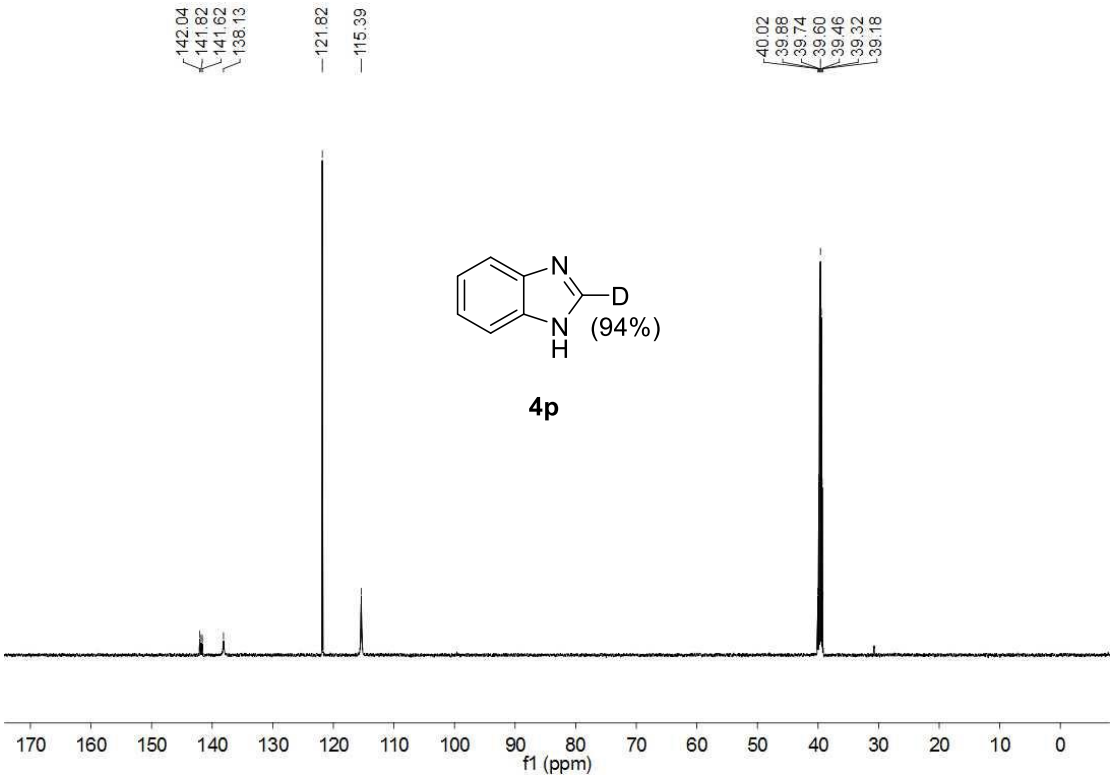

N
N
H
3o
1.03
1.00
2.01
14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
12.233
7.114

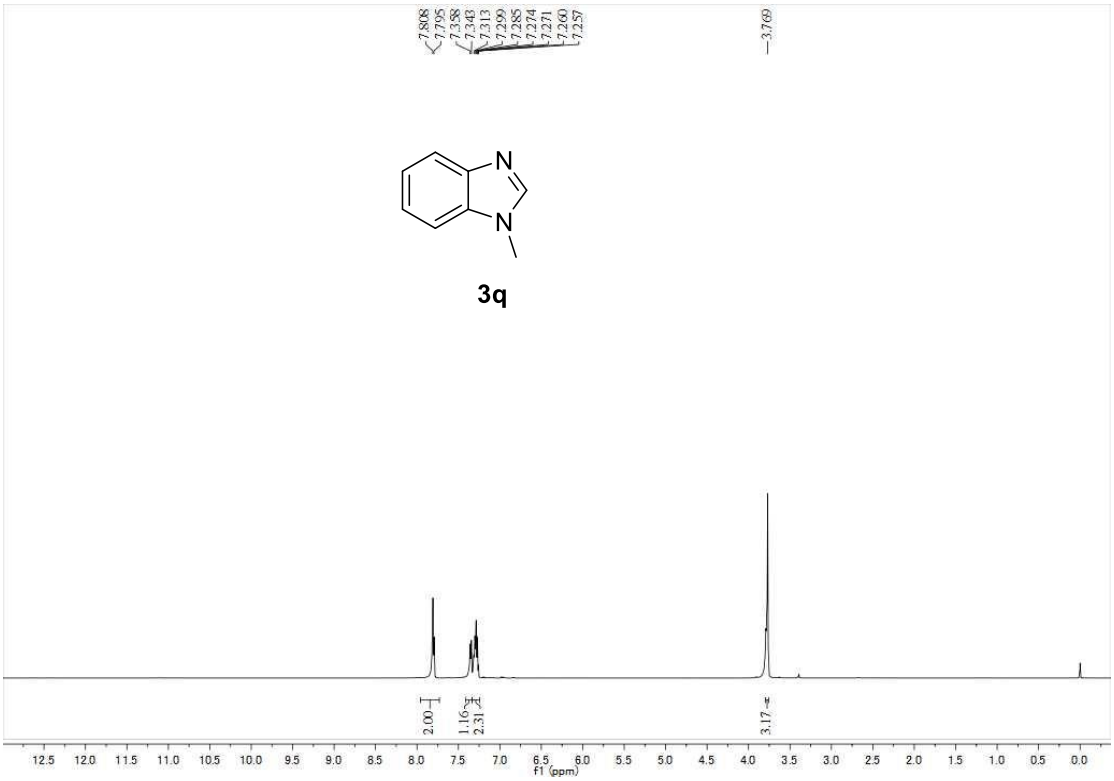

N
D (98%)
N
H
4o
0.61
0.02
2.00
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


135.25
135.00
134.75
121.82
N
D (98%)
N
H
4o
f1 (ppm)

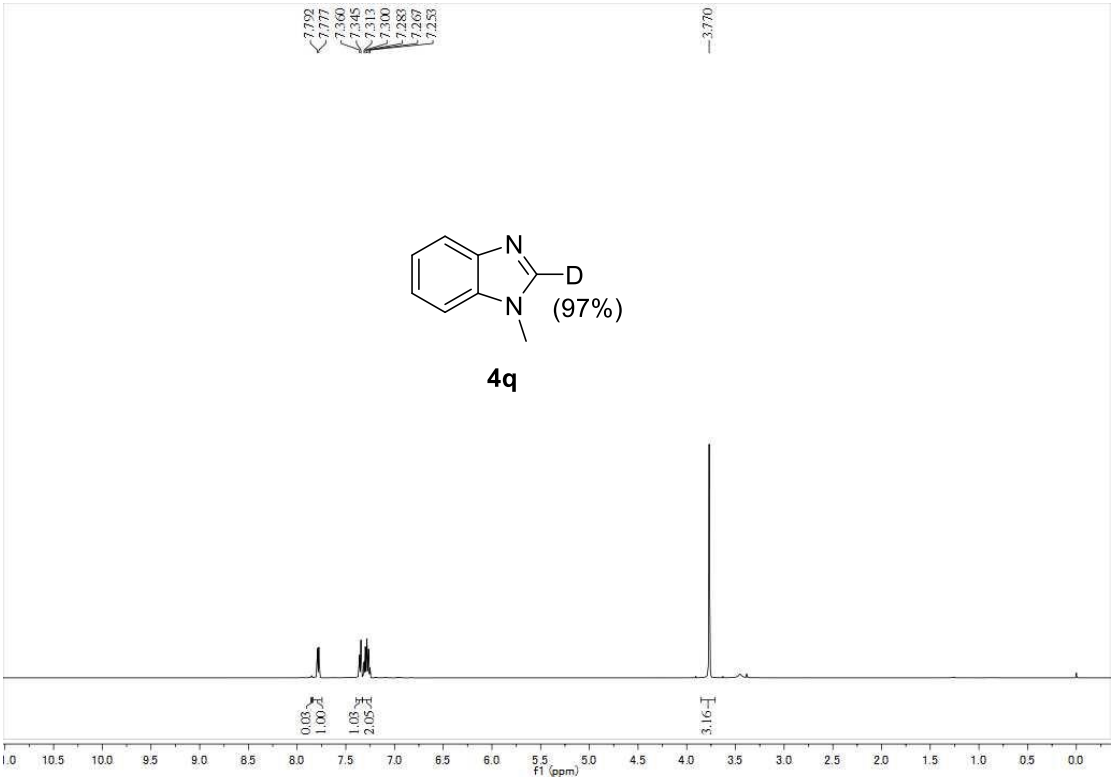

12.448
8.208
7.586
7.190
7.186
7.181
N
N
H
3p
0.97
1.00
2.00
2.03
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0


12.093
8.237
7.611
7.603
7.596
7.588
7.200
7.192
7.185
7.177
2.500
N
D
N
H
(94%)
4p
0.29
0.06
2.00
2.00
14.0 12.5 11.0 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)

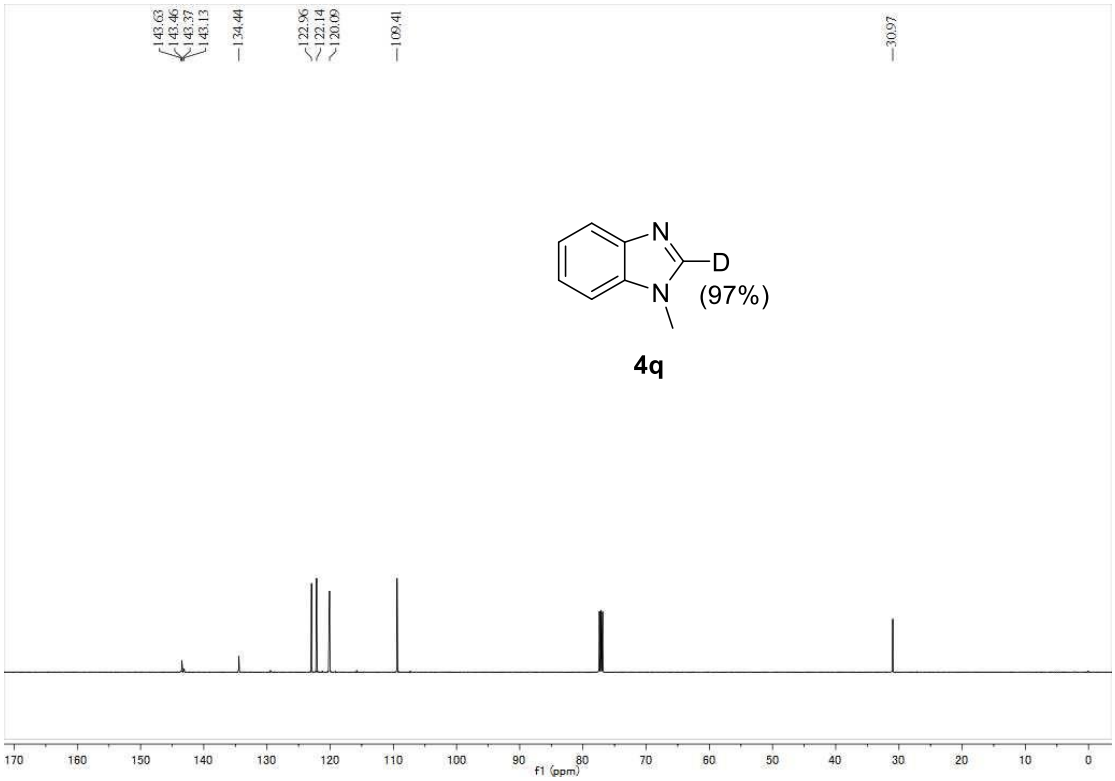

142.04
141.82
141.62
138.13
121.82
115.39
40.02
39.88
39.74
39.60
39.46
39.32
39.18
N
D
N
H
(94%)
4p
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.808
7.795
7.358
7.343
7.313
7.299
7.285
7.274
7.271
7.260
7.257
3.769
N
N
2.00
1.16
2.31
3.17
f1 (ppm)

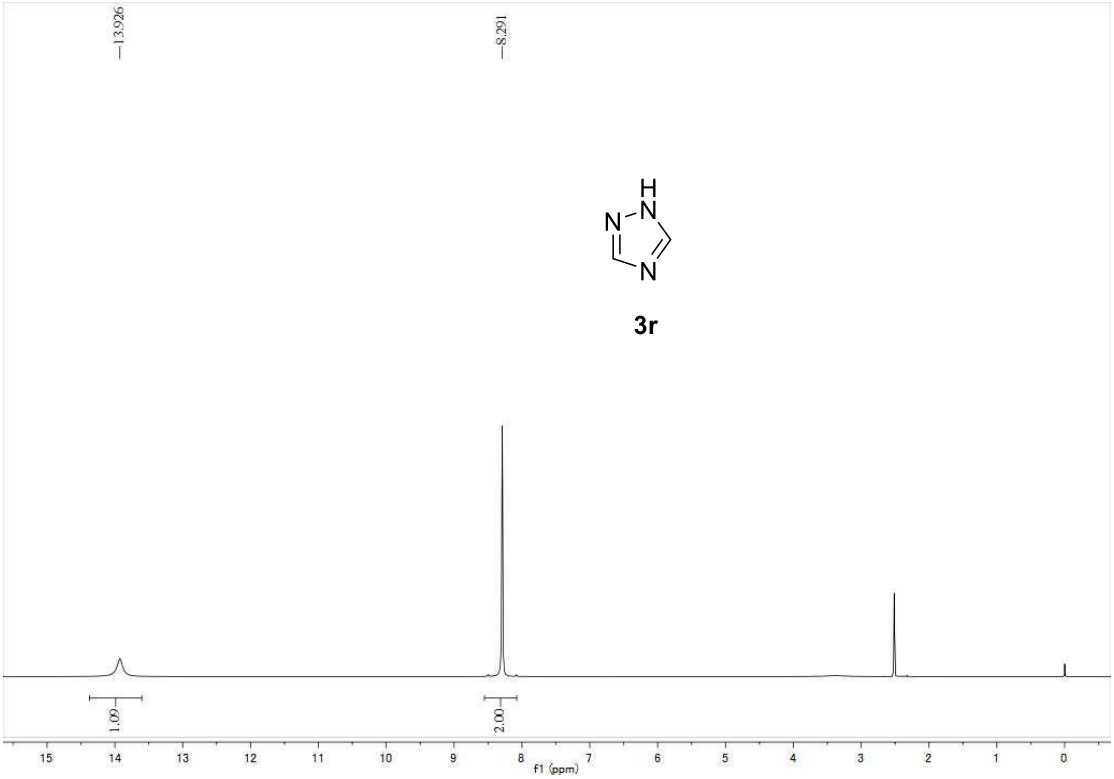
3q


7.792
7.777
7.360
7.345
7.313
7.300
7.283
7.267
7.253
3.770
N
D
N
(97%)
0.03
1.00
1.03
2.05
3.16
f1 (ppm)

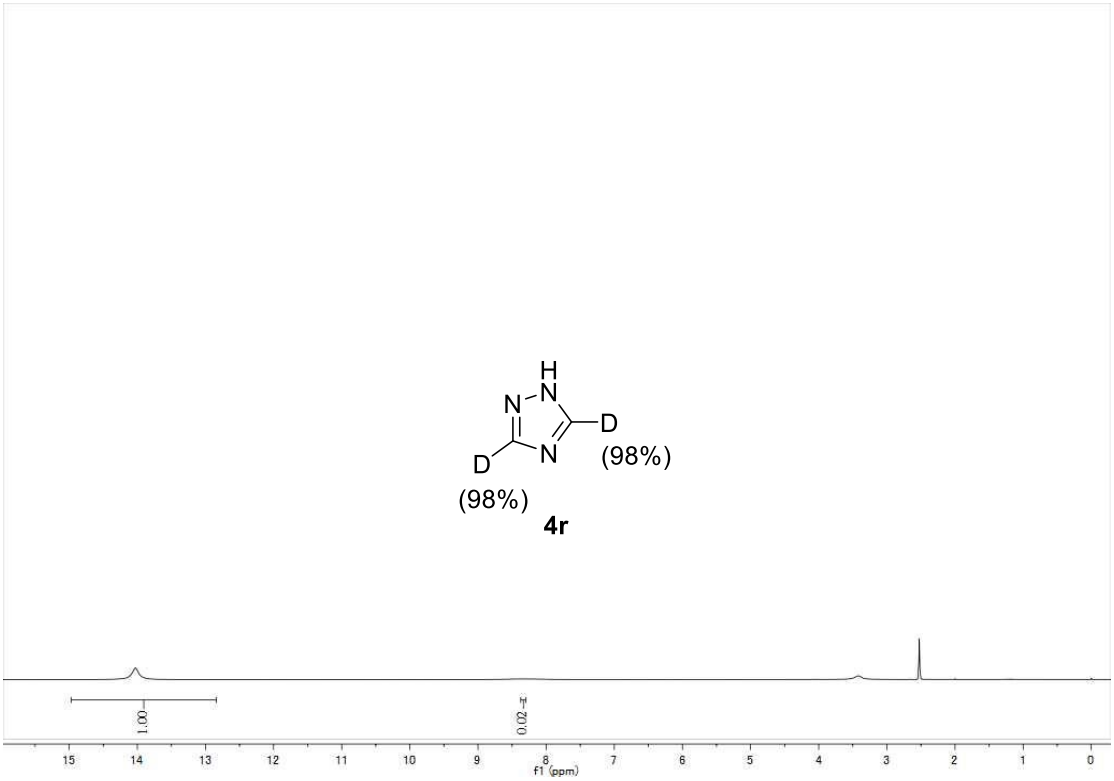
4q


143.63
143.46
143.37
143.13
134.44
122.96
122.14
120.09
109.41
30.97
N
D
N
(97%)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4q



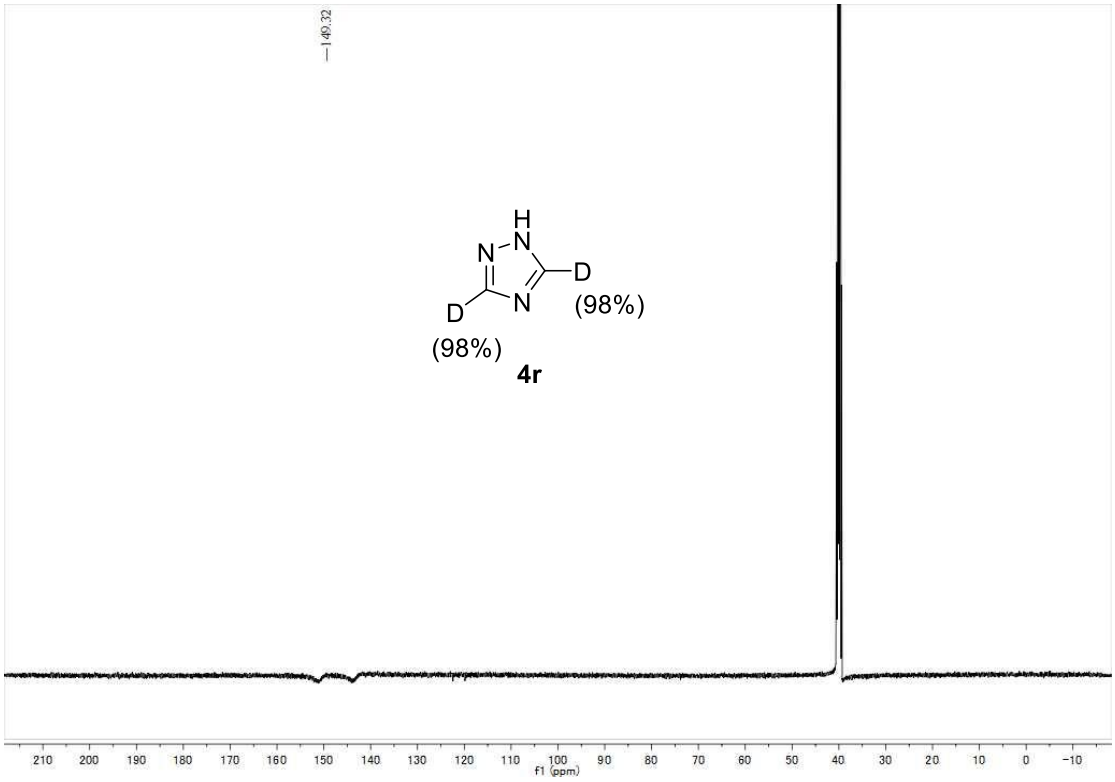
3r



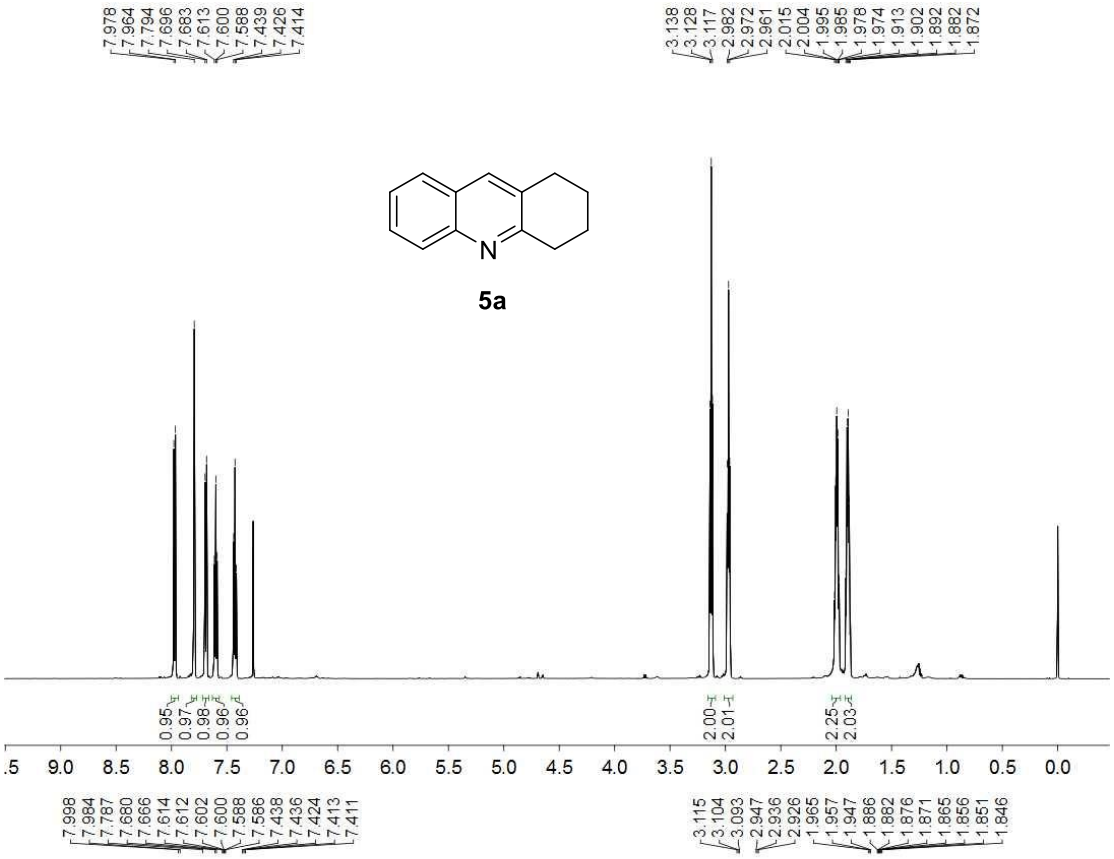
(98%)

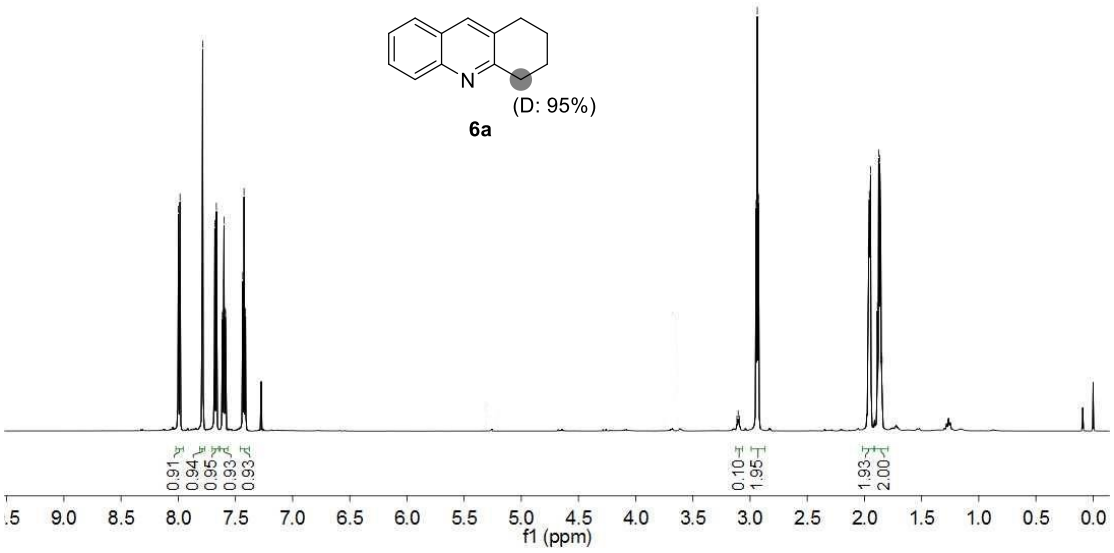
(98%)

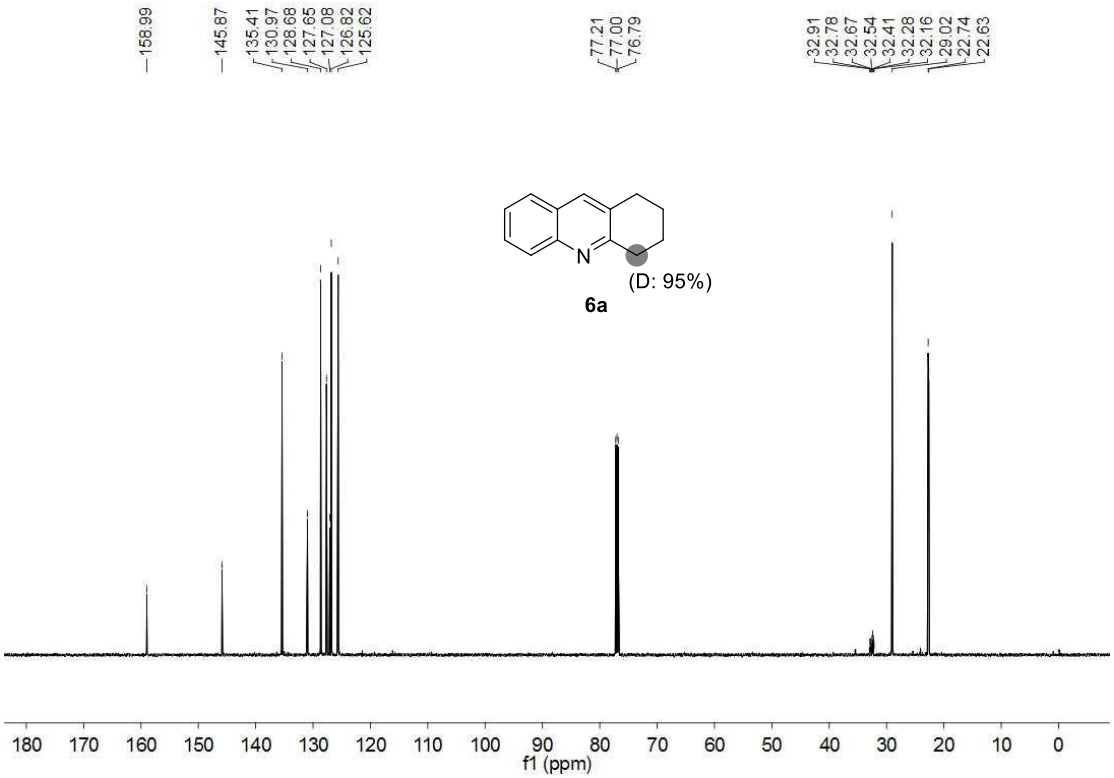
4r

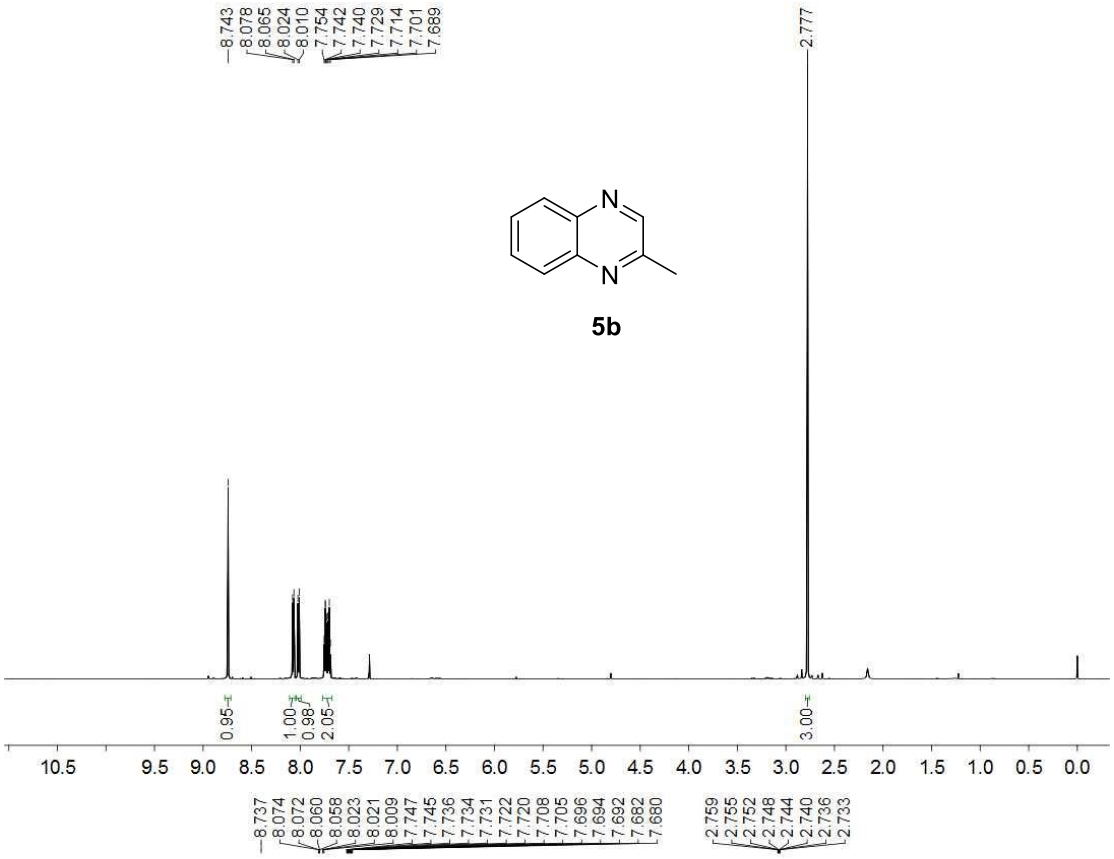

149.32
H
N
N
D
(98%)
D
(98%)
4r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

4r

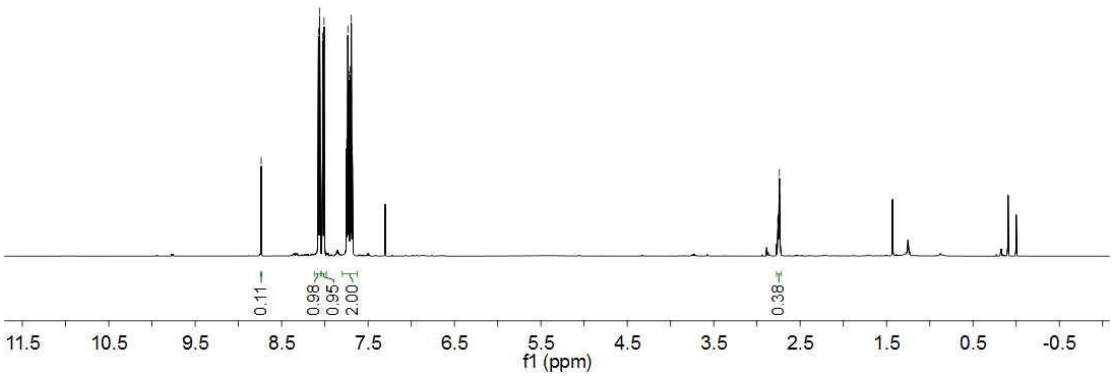

7.978
7.964
7.794
7.696
7.683
7.613
7.600
7.588
7.439
7.426
7.414
3.138
3.128
3.117
2.982
2.972
2.961
2.015
2.004
1.995
1.985
1.978
1.974
1.913
1.902
1.892
1.882
1.872
N
5a
0.95
0.97
0.98
0.96
0.96
2.00
2.01
2.25
2.03
7.998
7.984
7.787
7.680
7.666
7.614
7.612
7.602
7.600
7.588
7.586
7.438
7.436
7.424
7.413
7.411
3.115
3.104
3.093
2.947
2.936
2.926
1.965
1.957
1.947
1.886
1.882
1.876
1.871
1.865
1.856
1.851
1.846


N
(D: 95%)
6a
0.91
0.94
0.95
0.93
0.93
0.10
1.95
1.93
2.00
f1 (ppm)


158.99
145.87
135.41
130.97
128.68
127.65
127.08
126.82
125.62
77.21
77.00
76.79
32.91
32.78
32.67
32.54
32.41
32.28
32.16
29.02
22.74
22.63
N
(D: 95%)
6a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.743
8.078
8.065
8.024
8.010
7.754
7.742
7.740
7.729
7.714
7.701
7.689
2.777
0.95
1.00
0.98
2.05
3.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
8.737
8.074
8.072
8.060
8.058
8.023
8.021
8.009
7.747
7.745
7.736
7.734
7.731
7.722
7.720
7.708
7.705
7.696
7.694
7.692
7.682
7.680
2.759
2.755
2.752
2.748
2.744
2.740
2.736
2.733

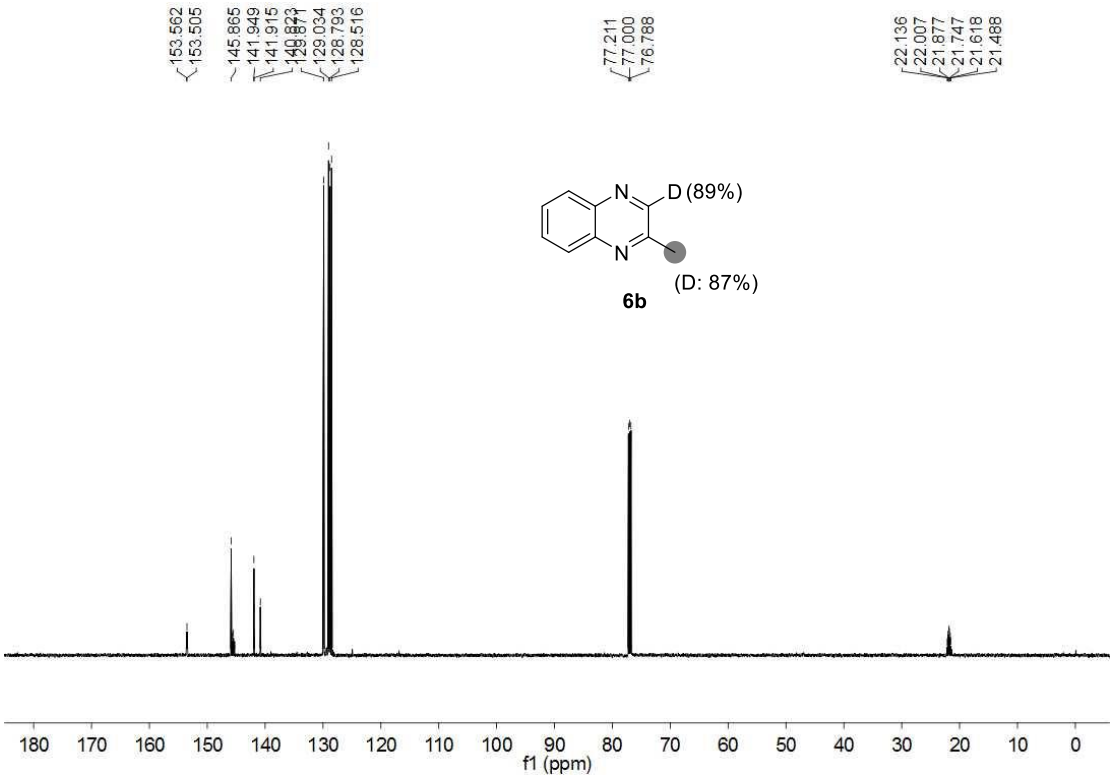
5b

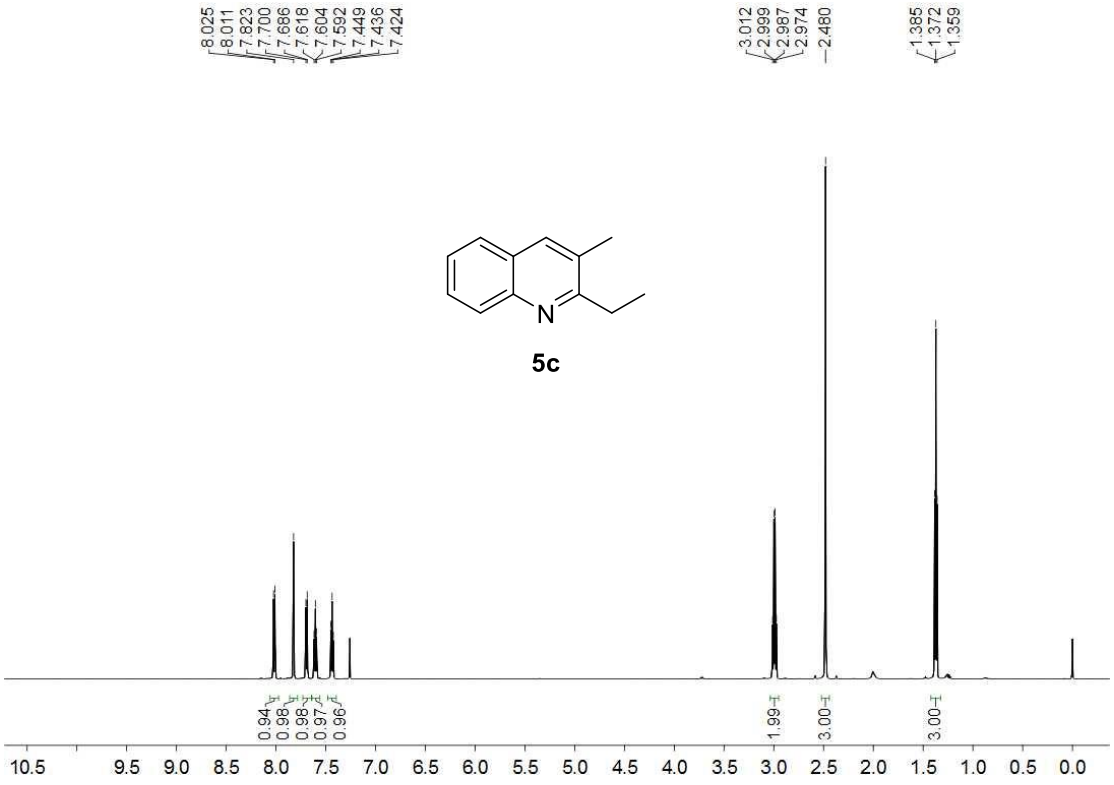

0.11
0.98
0.95
2.00
0.38
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)

D (89%)

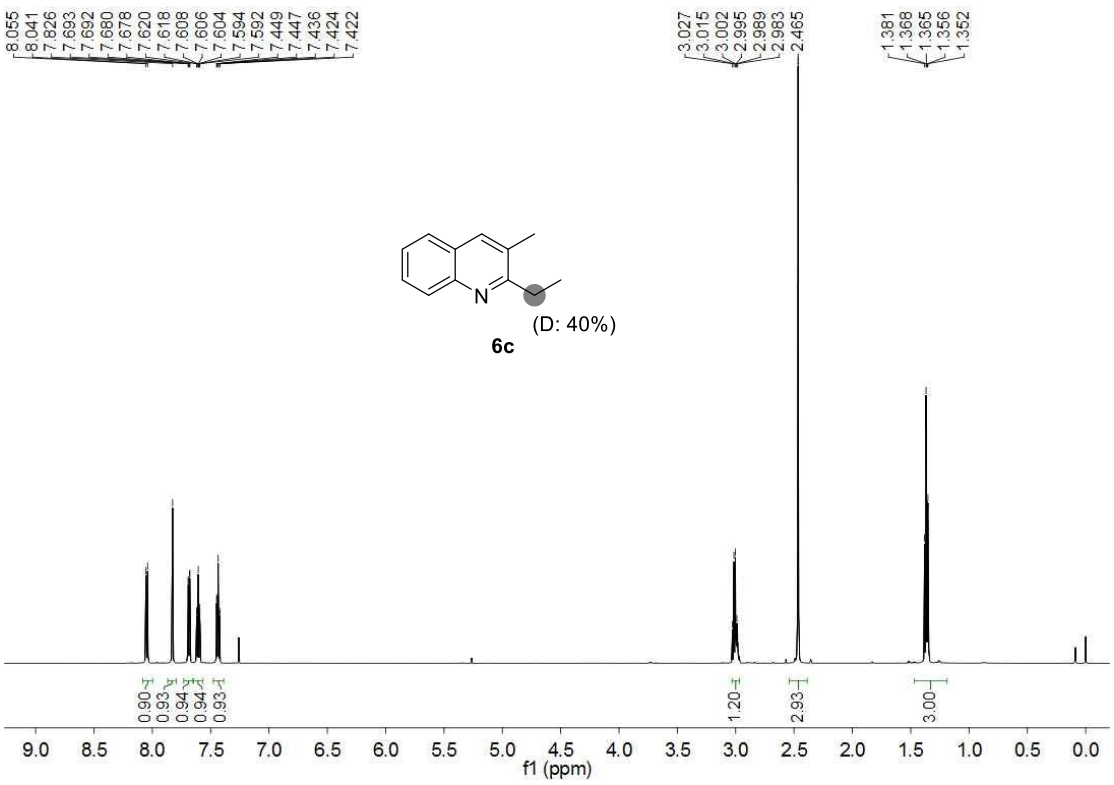
(D: 87%)

6b


153.562
153.505
145.865
141.949
141.915
129.034
128.793
128.516
77.211
77.000
76.788
22.136
22.007
21.877
21.747
21.618
21.488
N
D (89%)
N
(D: 87%)
6b
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

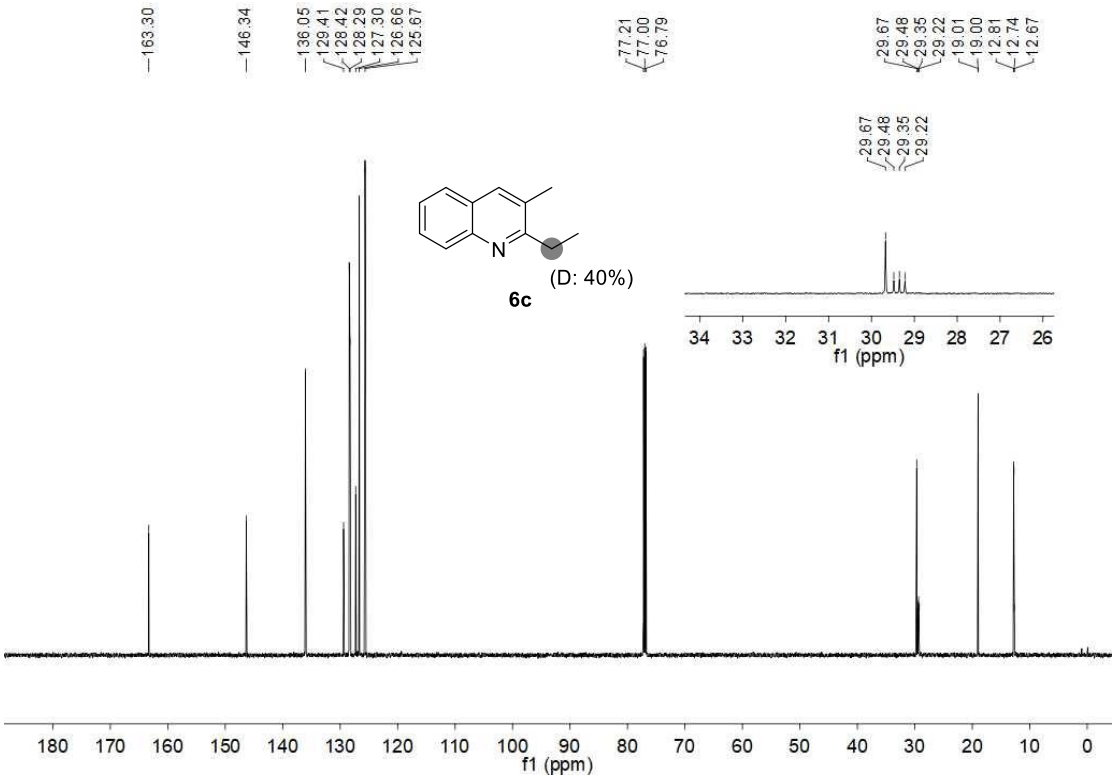

8.025
8.011
7.823
7.700
7.686
7.618
7.604
7.592
7.449
7.436
7.424
3.012
2.999
2.987
2.974
2.480
1.385
1.372
1.359
0.94
0.98
0.98
0.97
0.96
1.99
3.00
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

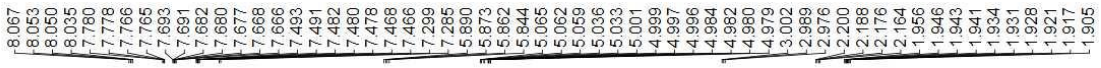
5c

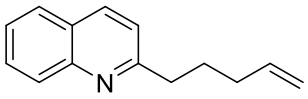

8.055
8.041
7.826
7.693
7.692
7.680
7.678
7.620
7.618
7.608
7.606
7.604
7.594
7.592
7.449
7.447
7.436
7.424
7.422
3.027
3.015
3.002
2.995
2.989
2.983
2.465
1.381
1.368
1.365
1.356
1.352
0.90
0.93
0.94
0.94
0.93
1.20
2.93
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

(D: 40%)

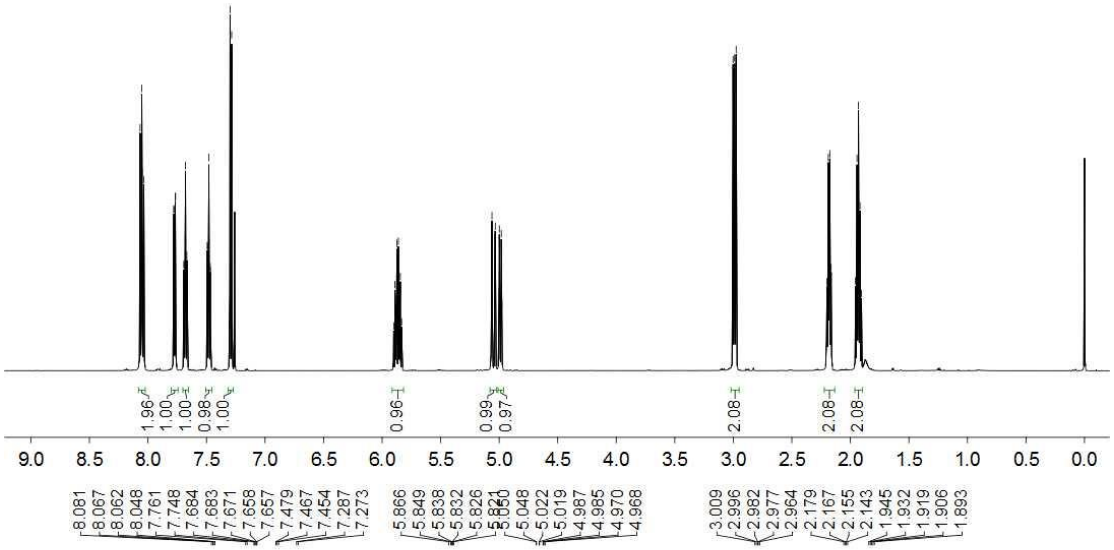
6c

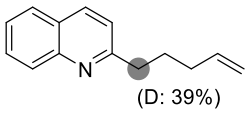

163.30
146.34
136.05
129.41
128.42
128.29
127.30
126.66
125.67
77.21
77.00
76.79
29.67
29.48
29.35
29.22
19.01
19.00
12.81
12.74
12.67
(D: 40%)
6c
f1 (ppm)
f1 (ppm)





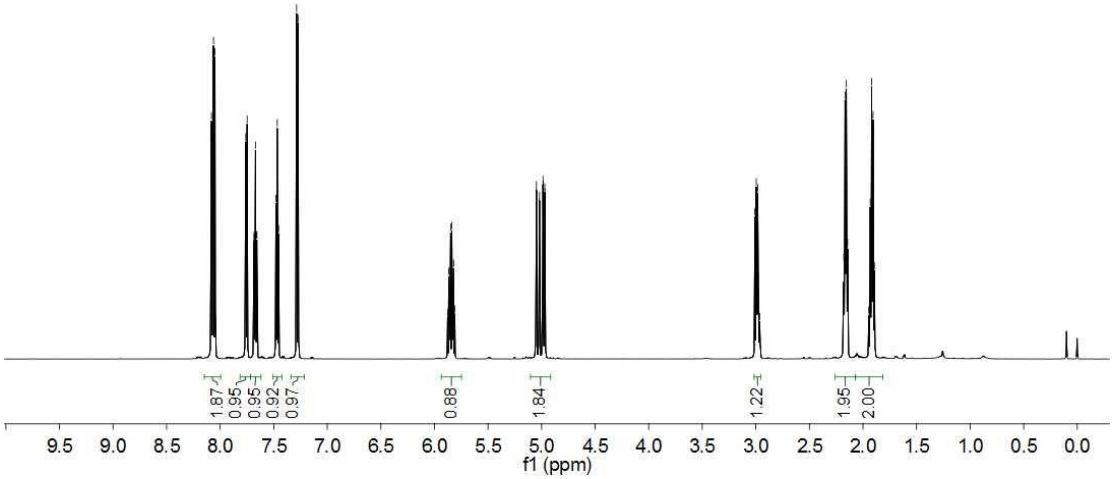
5d

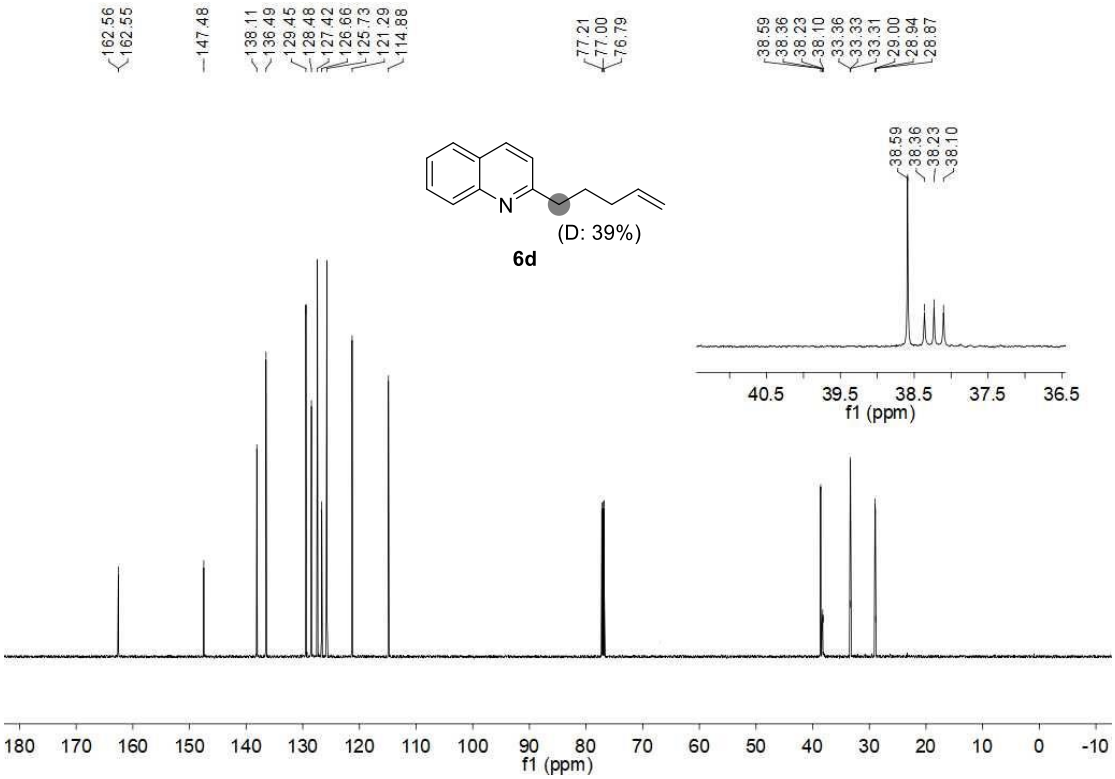


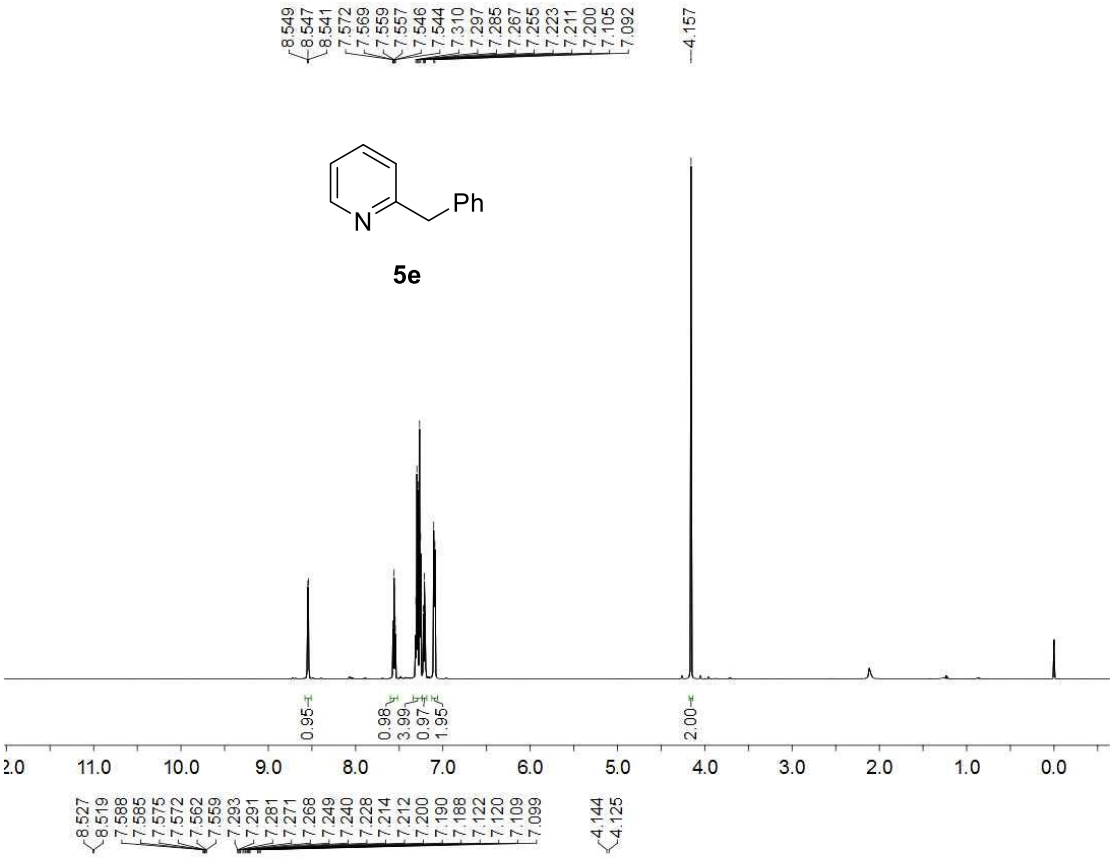


(D: 39%)

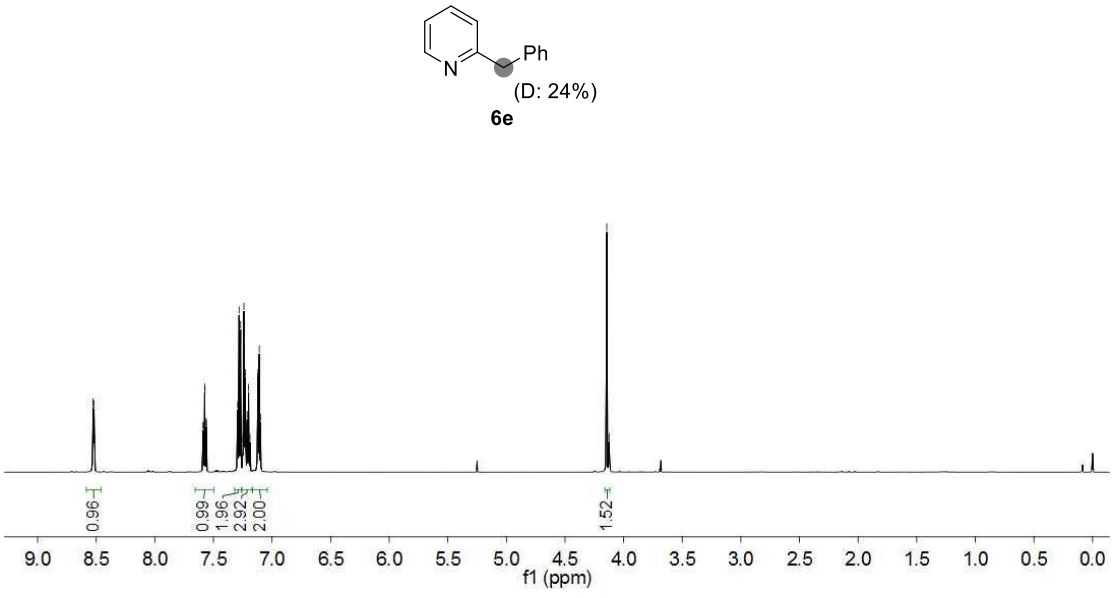
6d



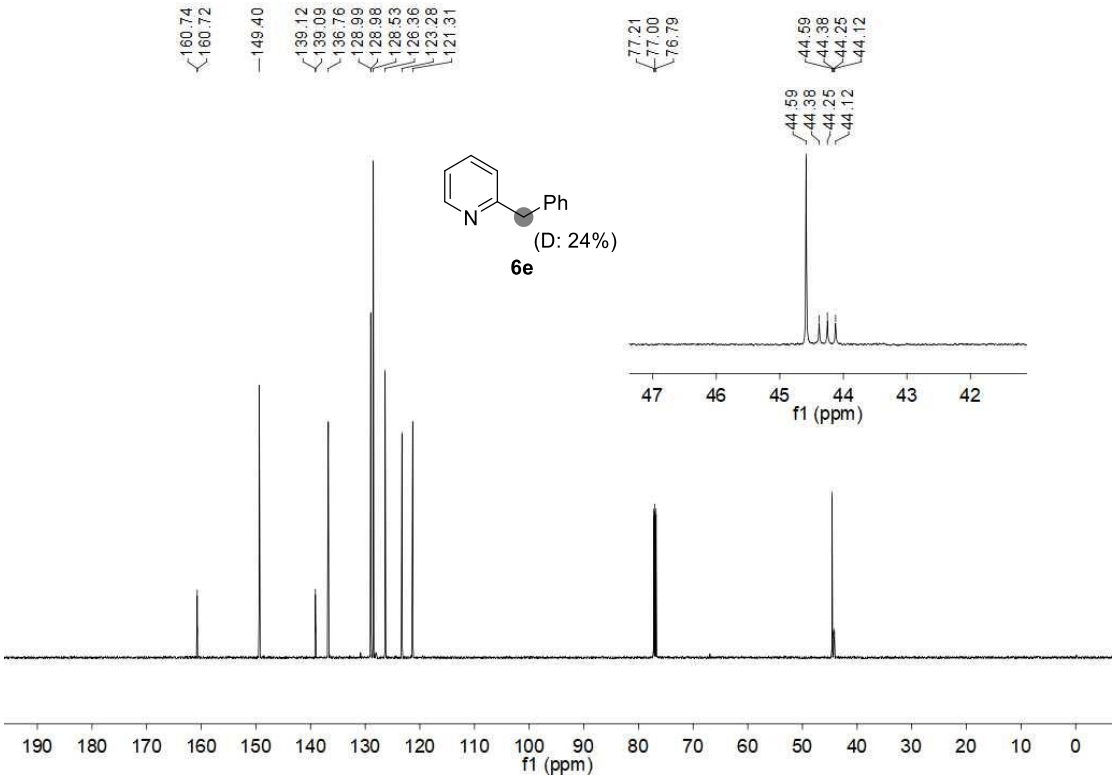

162.56
162.55
147.48
138.11
136.49
129.45
128.48
127.42
126.66
125.73
121.29
114.88
77.21
77.00
76.79
38.59
38.36
38.23
38.10
33.36
33.33
33.31
29.00
28.94
28.87
N
(D: 39%)
6d
f1 (ppm)
f1 (ppm)

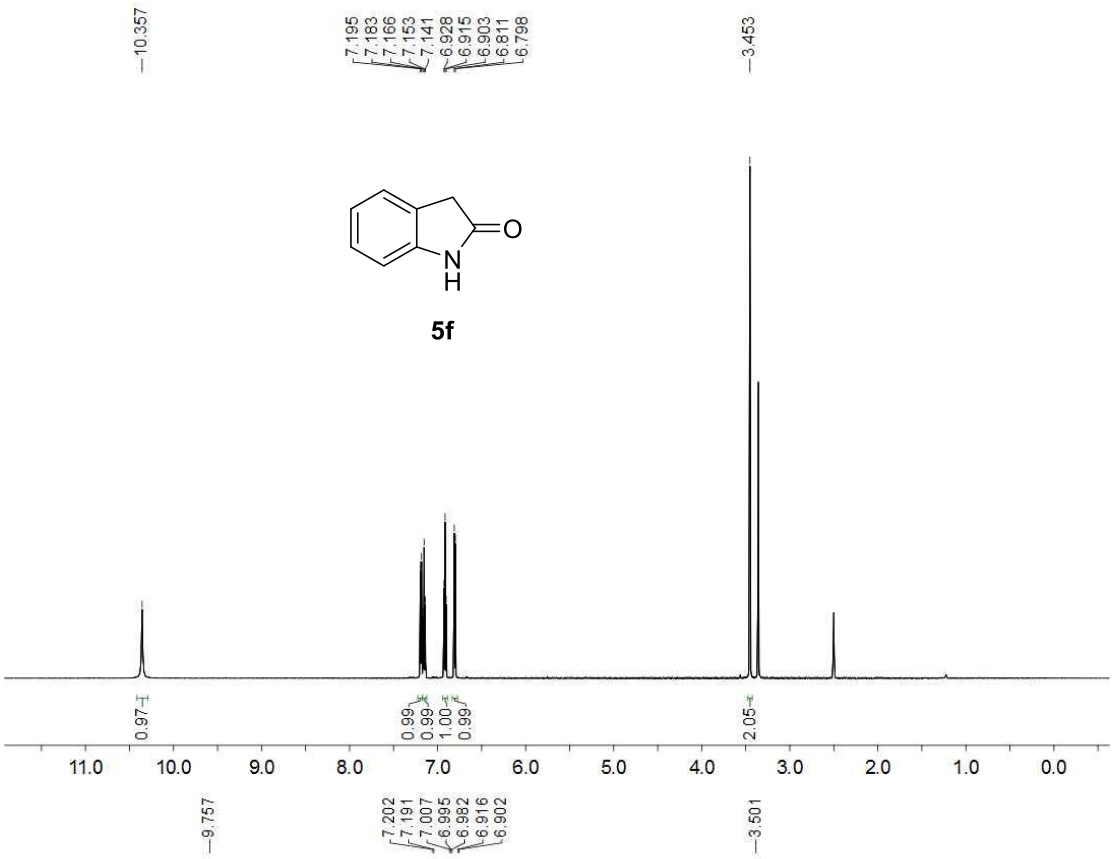

8.549
8.547
8.541
7.572
7.569
7.559
7.557
7.546
7.544
7.310
7.297
7.285
7.267
7.255
7.223
7.211
7.200
7.105
7.092
4.157
N
Ph
0.95
0.98
3.99
0.97
1.95
2.00
2.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
8.527
8.519
7.588
7.585
7.575
7.572
7.562
7.559
7.293
7.291
7.281
7.271
7.268
7.249
7.240
7.228
7.214
7.212
7.200
7.190
7.188
7.122
7.120
7.109
7.099
4.144
4.125

5e


N
Ph
(D: 24%)
0.96
0.99
1.96
2.92
2.00
1.52
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

6e

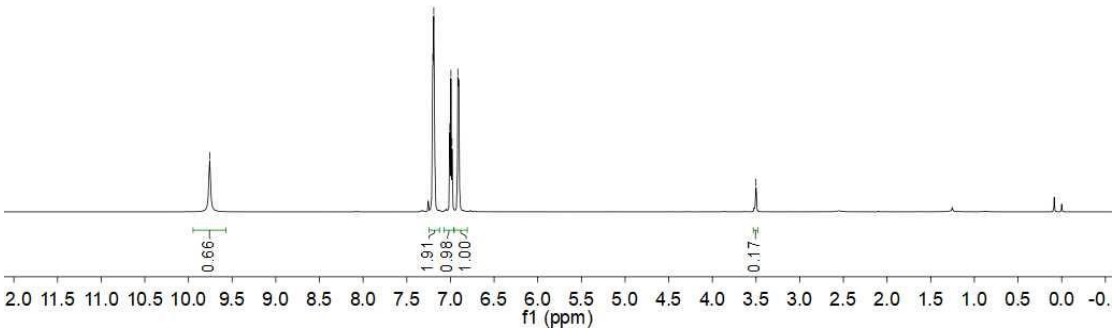

160.74
160.72
149.40
139.12
139.09
136.76
128.99
128.98
128.53
126.36
123.28
121.31
77.21
77.00
76.79
44.59
44.38
44.25
44.12
Ph
(D: 24%)
6e
f1 (ppm)
f1 (ppm)

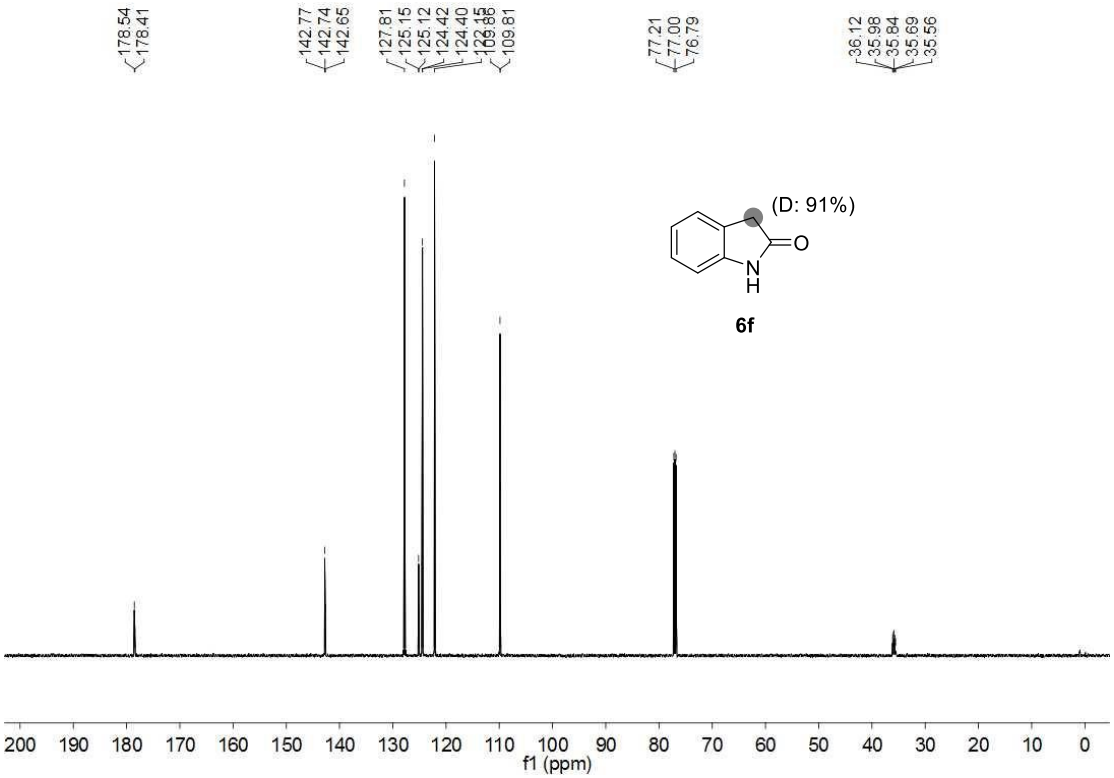

10.357
7.195
7.183
7.166
7.153
7.141
6.928
6.915
6.903
6.811
6.798
3.453
0.97
0.99
0.99
1.00
0.99
2.05
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
9.757
7.202
7.191
7.007
6.995
6.982
6.916
6.902
3.501

5f

(D: 91%)

6f


0.66
1.91
0.98
1.00
0.17
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


178.54
178.41
142.77
142.74
142.65
127.81
125.15
125.12
124.42
124.40
109.81
77.21
77.00
76.79
36.12
35.98
35.84
35.69
35.56
(D: 91%)
O
N
H
6f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)