Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Manganese Catalyzed *N*-Alkylation of Amines with Alcohols: Ligand Enabled Selectivity

Vinod G Landge, Akash Mondal, Vinit Kumar, Avanashiappn Nandakumar, and Ekambaram Balaraman*

Organic Chemistry Division, Dr. Homi Bhabha Road, CSIR-National Chemical Laboratory (CSIR-NCL), Pune - 411008, India.

Contents

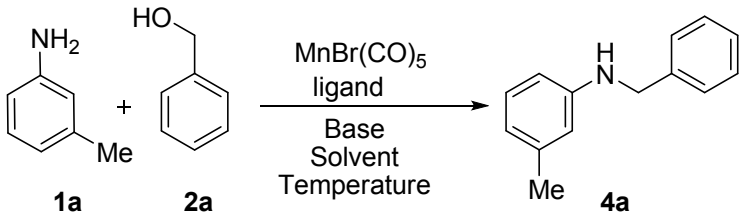
1. General Information

All catalytic experiments were carried out using standard Schlenk techniques. All solvents were reagent grade or better. Deuterated solvents were used as received. Toluene was refluxed over sodium/benzophenoneand followed by distilled under argon atmosphere and stored over sodium. Metal complexes and other chemicals used in catalysis reactions were used without additional purification. Thin layer chromatography (TLC) was performed using silica gel precoated glass plates, which were visualized with visualized with UV light at 254 nm or under iodine. Column chromatography was performed with SiO_2 (SilicycleSiliaflash F60 (230-400 mesh). ^1H NMR (400 or 500 MHz), $^{13}C\{^1H\}$ NMR (100 MHz) spectra were recorded on the NMR spectrometer. Deuterated chloroform was used as the solvent, and chemical shift values (δ) are reported in parts per million relative to the residual signals of this solvent [δ 7.26 for ^1H (chloroform-d), δ 77.2 for 13C$\{^1H\}$ (chloroform-d). Abbreviations used in the NMR follow-up experiments: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. GC analysis was carried out using a HP-5 column (30 m, 0.25 mm, 0.25μ). Mass spectra were obtained on a GCMS-QP 5000 instruments with ionization voltages of 70 eV. High resolution mass spectra (HRMS) were obtained by fast atom bombardment (FAB) using a double focusing magnetic sector mass spectrometer and electron impact (EI) ionization technique (magnetic sector-electric sector double focusing mass analyzer). HPLC analysis was performed on Agilent Technologies 1260 Infinity with UV detector.

2. Experimental Section

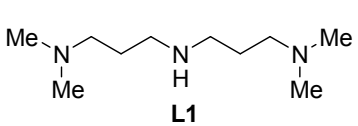
2.1 Reaction Optimization

Table S1: Screening of ligands[a]

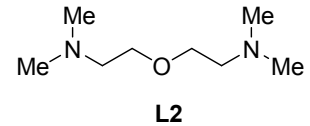


1a **2a** **4a**

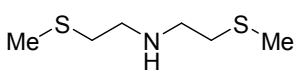
Entry	Ligand	Yield (%)[b]
1	2,2'-Bipyridine	50
2	2,2′-Bipyridine-4,4′-dicarboxylic acid	40
3	1,10-Phenanthroline	10
4	1,1′-Binaphthyl-2,2′-diamine	40
5	**L_1**	**92**
6	L2	70
7	L_3	74
8	L_4	80
9	L_5	91



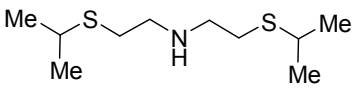
L1



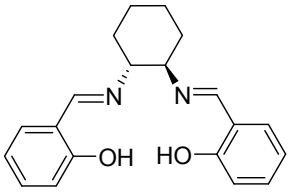
L2



L3



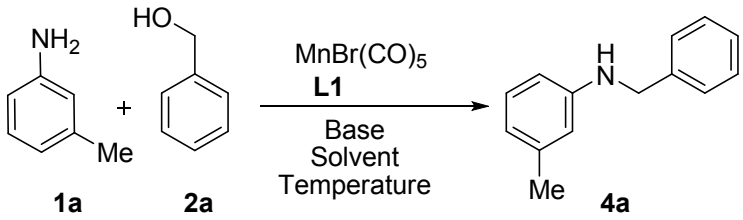
L4



L5

[a]Reaction conditions: aniline **1a** (0.5 mmol), alcohol **2a** (0.55 mmol), Mn catalyst (5 mol%), Ligand (5 mol%), KO*t*Bu (0.55 mmol), 1 mL toluene, 140 °C (oil-bath temperature), 18 h. [b] Yield determined by GC using dibromobutane as an internal standard. **L1** = N^1-(3-(dimethylamino)propyl)-N^3,N^3-dimethylpropane-1,3-diamine; **L2** = 2,2'-oxybis(*N*,*N*-dimethylethanamine); **L3** = bis(2-(methylthio)ethyl)amine; **L4** = bis(2 (isopropylthio)ethyl)amine.

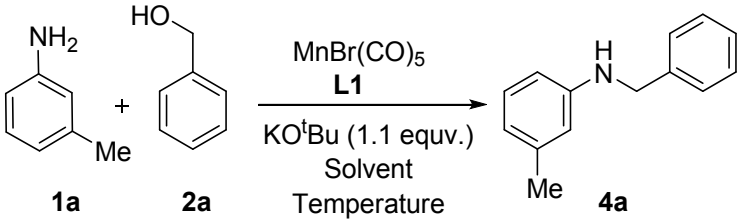
Table S2: Screening of base[a]



Entry	Base	Yield (%)[b]
1	LiO^{t}Bu	51
2	NaO^{t}Bu	60
	KO^{t}Bu	**75**
3	NaO^{i}Pr	39
4	KOH	40
5	K_2CO_3	NR
6	CsOAc	trace
7	NaOAc	trace
8	KO^{t}Bu (50 mol%)	45
9	KO^{t}Bu (25 mol%)	23

[a]Reaction conditions: aniline **1a** (0.5 mmol), alcohol **2a** (0.55 mmol), $MnBr(CO)_5$ (5 mol%), **L1** (5 mol%), base (0.55 mmol), 1 mL solvent, 140 °C (oil-bath temperature), 18 h. [b] Yield determined by GC using dibromobutane as an internal standard. NR = No reaction.

Table S3: Screening of solvent[a]

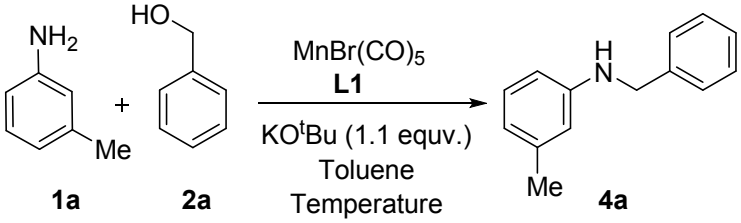


1a 2a 4a

Entry	Solvent	Yield (%)[b]
1	Xylene	53
2	Mesitylene	45
3	**Toluene**	**85**
4	THF	32
5	MeCN	NR
6	n-Octane	44
7	1,4 Dioxane	75
8	1,4 Dioxane + Toluene	77

[a]Reaction conditions: aniline **1a** (0.5 mmol), alcohol **2a** (0.55 mmol), $MnBr(CO)_5$ (5 mol%), **L1** (5 mol%), KO*t*Bu (0.55 mmol), 1 mL solvent, 140 °C (oil-bath temperature), 18 h. [b] Yield determined by GC using dibromobutane as an internal standard. NR = No reaction.

Table S4: Screening of temperature[a]



1a 2a 4a

Entry	Temperature	Yield (%)[b]
1	50	NR
2	80	38
3	100	55
4	120	63
5	**140**	**92**

[a]Reaction conditions: aniline **1a** (0.5 mmol), alcohol **2a** (0.55 mmol), $MnBr(CO)_5$ (5 mol%), Ligand (5 mol%), KO*t*Bu (0.55 mmol), 1 mL toluene, temperature (oil-bath temperature), 18 h. [b] Yield determined by GC using dibromobutane as an internal standard. NR = No reaction.

2.2 General Procedure for the Manganese-Catalyzed *N*-Alkylation of anilines

To an oven-dried 10 mL screw-capped vial, $MnBr(CO)_5$ (0.025 mmol, 5 mol%), ligand **L1** or **L5** (0.025 mmol, 5mol%), alcohol **2** (0.55 mmol, 1.1 equivalent), amine **1** (0.5 mmol), KO*t*Bu (0.55 mmol, 1.1 equivalent), toluene (1 mL) were added under a gentle stream of argon. The reaction mixture was kept for stirring at 140 ^oC for 18 h. Then, the reaction mixture was diluted with water (4 mL) and extracted with dichloromethane (3 x 5 mL). The resultant organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography (230-400 mesh size) using petroleum-ether/ethyl acetate as an eluting system.

3. Mechanistic studies

2.2.1. Identification of Mn-Complex:

To an oven-dried 10 mL screw-capped vial, $MnBr(CO)_5$ (0.01 mmol), ligand **L1** (0.01 mmol, 5mol%), KO*t*Bu (0.01 mmol), toluene (2 mL) were added under a gentle stream of argon. The reaction mixture was kept for stirring at 140 ^oC for 2 h. Then, the reaction mixture was passed through celite and submitted for HRMS.

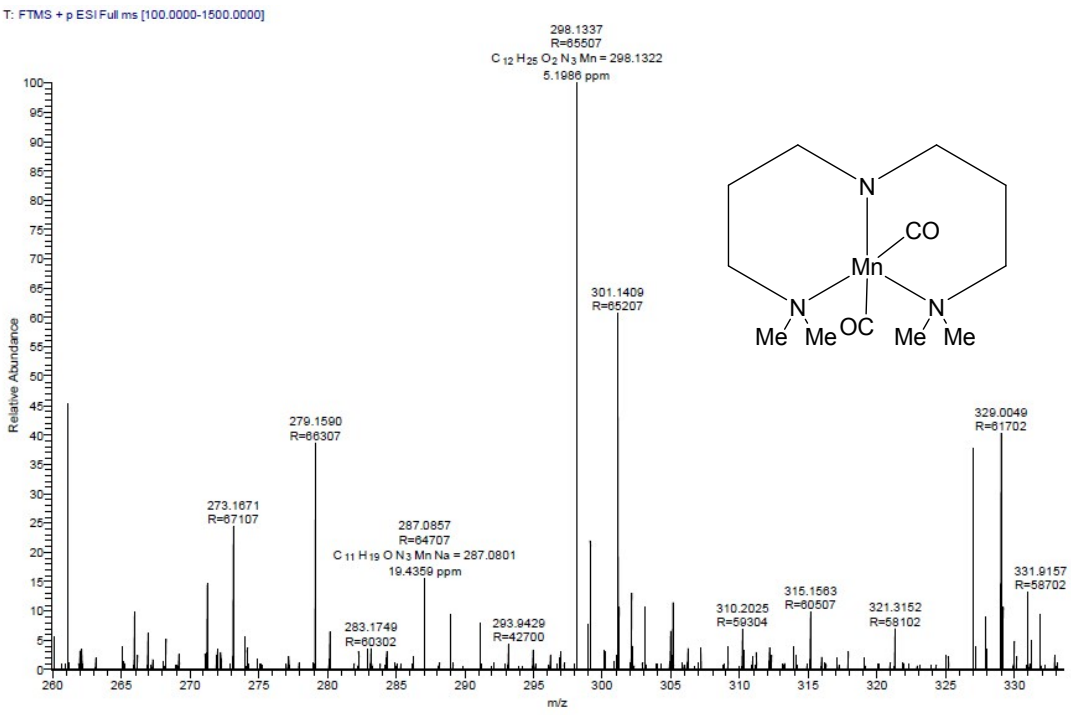
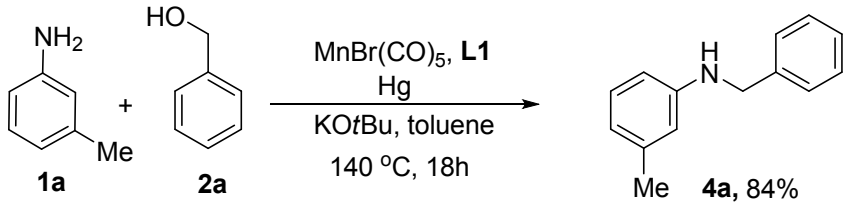


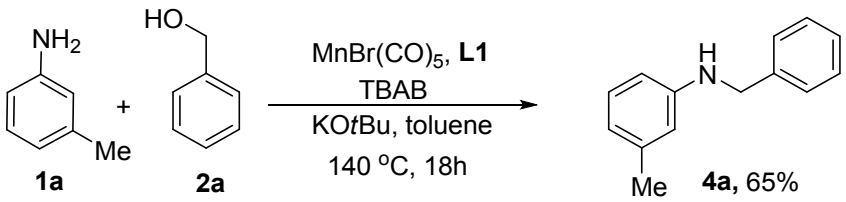
Figure S1. HRMS of Mn:L1 complex.

2.2.2 Homogeneous nature of Mn-catalysis

a) To an oven-dried 10 mL screw-capped vial, $MnBr(CO)_5$ (0.025 mmol, 5 mol%), ligand **L1** (0.025 mmol, 5mol%), mercury (300 equivalent with respect to catalyst), benzyl alcohol **2a** (0.55 mmol, 1.1 equivalent), *m*-toludine **1a** (0.5 mmol), KO*t*Bu (0.55 mmol, 1.1 equivalent), toluene (1 mL) were added under a gentle stream of argon. The reaction mixture was kept for stirring at 140 ^oC for 18 h. Then, the reaction mixture was diluted with water (4 mL) and extracted with dichloromethane (3 x 5 mL). The resultant organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography (230-400 mesh size) using petroleum-ether/ethyl acetate as an eluting system.

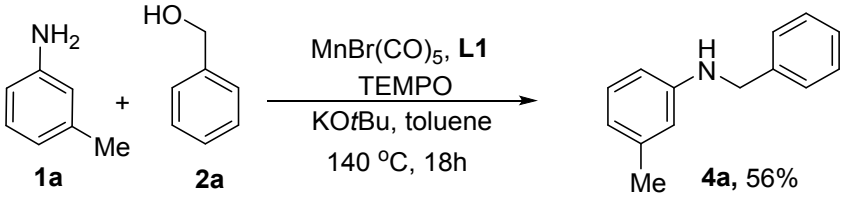


b) To an oven-dried 10 mL screw-capped vial, $MnBr(CO)_5$ (0.025 mmol, 5 mol%), ligand **L1** (0.025 mmol, 5mol%), *tetra*-butyl ammonium bromide (0.025 mmol, 5 mol%), benzyl alcohol **2a** (0.55 mmol, 1.1 equivalent), *m*-toludine **1a** (0.5 mmol), KO*t*Bu (0.55 mmol, 1.1 equivalent), toluene (1 mL) were added under a gentle stream of argon. The reaction mixture was kept for stirring at 140 ^oC for 18 h. Then, the reaction mixture was diluted with water (4 mL) and extracted with dichloromethane (3 x 5 mL). The resultant organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography (230-400 mesh size) using petroleum-ether/ethyl acetate as an eluting system.



1a **2a** **4a,** 65%

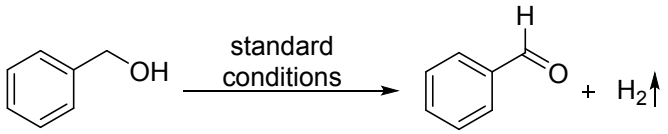
c) To an oven-dried 10 mL screw-capped vial, $MnBr(CO)_5$ (0.025 mmol, 5 mol%), ligand **L1** (0.025 mmol, 5mol%), TEMPO (1 equivalent), benzyl alcohol **2a** (0.55 mmol, 1.1 equivalent), *m*-toludine **1a** (0.5 mmol), KO*t*Bu (0.55 mmol, 1.1 equivalent), toluene (1 mL) were added under a gentle stream of argon. The reaction mixture was kept for stirring at 140 ^oC for 18 h. Then, the reaction mixture was diluted with water (4 mL) and extracted with dichloromethane (3 x 5 mL). The resultant organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude mixture was purified by silica gel column chromatography (230-400 mesh size) using petroleum-ether/ethyl acetate as an eluting system.



1a **2a** **4a,** 56%

2.2.3 Qualitative analysis of hydrogen gas and aldehyde intermediate

To an oven-dried 10 mL screw-capped vial, $MnBr(CO)_5$ (0.025 mmol, 5 mol%), ligand **L1** (0.025 mmol, 5 mol%), benzyl alcohol **2a** (0.50 mmol), KO*t*Bu (0.55 mmol), and toluene (1 mL) were added under a gentle stream of argon. The reaction mixture was kept for stirring at 140 °C for 12 h. GC analysis showed the formation of dihydrogen gas (TCD detector).



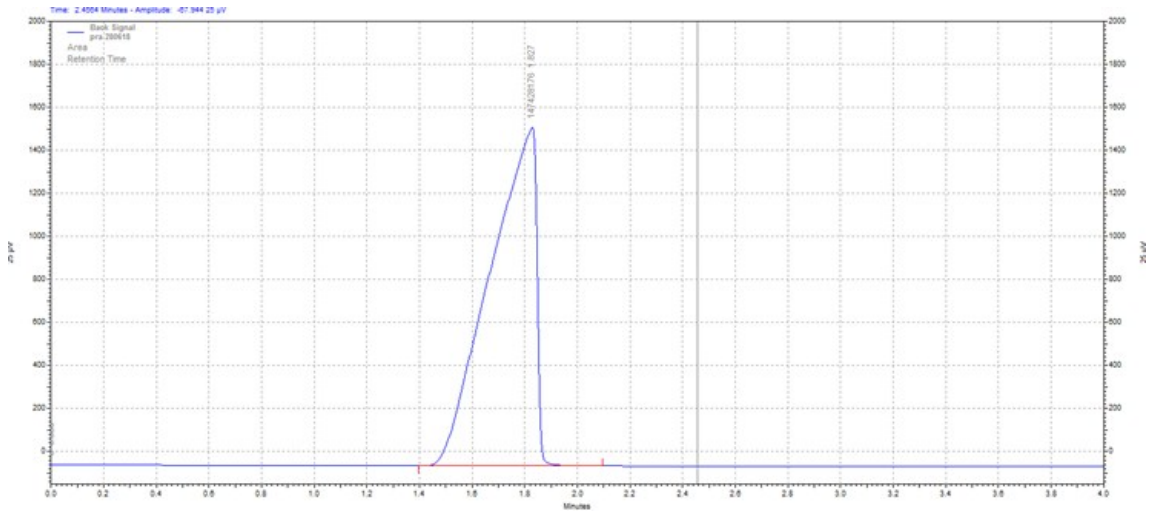


Figure S2. Hydrogen gas detection (GC Analysis)

2.2.4 Reaction kinetics

To an oven-dried 10 mL screw-capped vial, seven parallel reaction carried out using $MnBr(CO)_5$ (0.025 mmol, 5 mol%), ligand **L1** or **L5** (0.025 mmol, 5mol%), benzyl alcohol **2a** (0.55 mmol, 1.1 equivalent), *m*-toludine**1a** (0.5 mmol), KO*t*Bu (0.55 mmol, 1.1 equivalent), n-decane (0.25mmol) as internal standard and toluene (2 mL) were added under a gentle stream of argon. The mixture was stirred at 140 °C (oil-bath temperature). At regular time intervals, the reaction vessel was cooled to 28 °C and 15 µL of the sample was diluted with 0.5 mL of CH_2Cl_2, and subjected to GC analysis. The concentration of the product **4a** obtained in each sample was determined with respect to the internal standard *n*-decane.

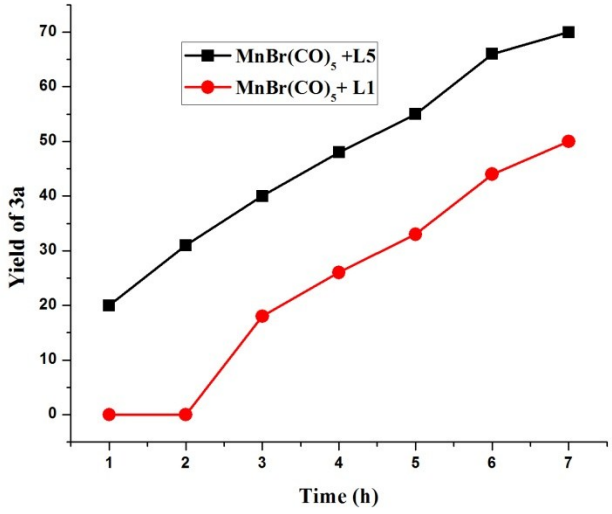
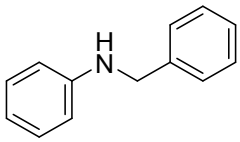


Figure S3. Reaction profile for the manganese-catalyzed formation of **4a** by using **L1** and **L5** ligand.

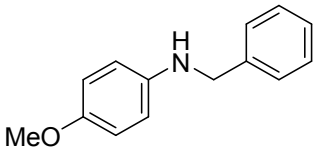
4. Characterization Data

N-benzylaniline (**3a**)[1]



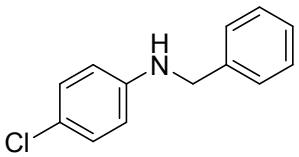
73 mg, 80% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. The spectral data is consistent with the literature compound. ^{11}H NMR (200 MHz, *CHLOROFORM-d*) δ = 7.54 - 7.23 (m, 5H), 7.21 - 7.01 (m, 2H), 6.53 - 6.25 (m, 3H), 4.33 (s, 2 H), 4.19 (brs, 1H). ^{13}C NMR (50 MHz, *CHLOROFORM-d*) δ = 148.12, 139.41, 129.23, 128.60, 127.48, 127.19, 117.53, 112.81, 48.29.

N-benzyl-4-methoxyaniline (**3b**)



71 mg, 67% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.45 - 7.31 (m, 4H), 7.29 (s, 1H), 6.85 - 6.71 (m, 2H), 6.67 - 6.53 (m, 2H), 4.30 (s, 2H), 3.76 (s, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 152.2, 142.4, 139.7, 128.6, 127.5, 127.1, 114.9, 114.1, 55.8, 49.2. HRMS (EI): *m/z* Calcd for [M-H] $C_{14}H_{14}NO$: 212.1070; Found: 212.1072.

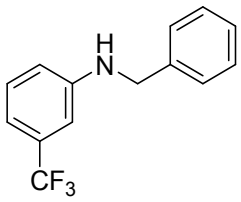
N-benzyl-4-chloroaniline (**3c**)



70 mg, 65% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.45 - 7.37 (m, 4H), 7.37 - 7.30 (m, 1H), 7.20 - 7.11 (m, *J* = 8.5 Hz, 2H), 6.63 - 6.54 (m, *J* = 8.5 Hz, 2H), 4.34 (s, 2H), 4.10 (brs, 1H). ^{13}C NMR (126 MHz,

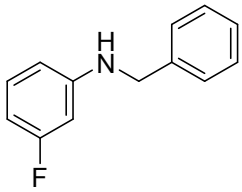
CHLOROFORM-d) δ = 146.6, 138.9, 129.0, 128.7, 127.4, 127.3, 122.0, 113.9, 48.3. HRMS (EI): *m/z* Calcd for [M+H] $C_{13}H_{13}NCl$: 218.0731; Found: 218.0730.

N-benzyl-3-(trifluoromethyl)aniline (**3d**)



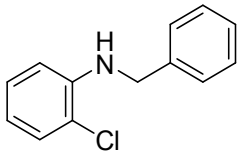
102 mg, 81% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.39 (brs, 4H), 7.33 (brs, 1H), 6.98 (brs, 1H), 6.87 (brs, 1H), 6.78 (brs, 1H), 4.37 (brs, 2H), 4.24 (brs, 1H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 148.2, 138.5, 131.5 (q, J_{C-F} = 31.5 Hz), 129.6, 128.7, 127.5, 123.3 (q, J_{C-F} = 272 Hz), 115.7, 113.9 (q, J_{C-F} = 3.81 Hz), 109.0 (q, J_{C-F} = 3.81 Hz), 48.1. HRMS (EI): *m/z* Calcd for [M+H] $C_{14}H_{13}NF_3$: 252.0995; Found: 252.0993.

N-benzyl-3-fluoroaniline (**3e**)



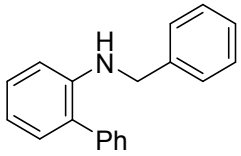
60 mg, 60% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz*, CHLOROFORM-d)* δ = 7.38 (brs, 4H), 7.32 (brs, 1H), 7.17 - 7.04 (m, 1H), 6.42 (brs, 2H), 6.34 (d, *J* = 11.0 Hz, 1H), 4.33 (brs, 2H), 4.19 (brs, 1H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 164.1 (q, J_{C-F} = 240 Hz), 149.9, 149.8, 138.8, 130.3, 130.2, 128.7, 127.4, 127.4, 108.7, 103.9 (q, J_{C-F} = 22 Hz), 99.5 (q, J_{C-F} = 25.7 Hz), 48.2. HRMS (EI): *m/z* Calcd for [M+H] $C_{13}H_{13}NF$: 202.1027; Found: 202.1025.

N-benzyl-2-chloroaniline (**3f**)



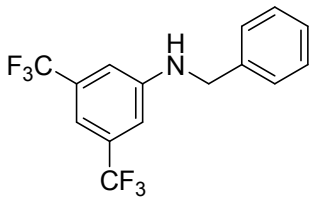
70 mg, 65% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.45 - 7.39 (m, 3H), 7.38 - 7.29 (m, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.76 - 6.57 (m, 2H), 4.79 (brs, 1H), 4.45 (s, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 143.8, 138.7, 129.1, 128.7, 127.8, 127.3, 127.2, 119.1, 117.4, 111.5, 47.8. HRMS (EI): *m/z* Calcd for [M+H] $C_{13}H_{13}NCl$: 218.0731; Found: 218.0730.

N-benzylbiphenyl-2-amine (**3g**)



101 mg, 78% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.57 - 7.45 (m, 4H), 7.45 - 7.32 (m, 5H), 7.29 (d, *J* = 3.1 Hz, 1H), 7.24 (s, 1H), 7.16 (d, *J* = 7.2 Hz, 1H), 6.83 (s, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 4.53 (brs, 1H), 4.38 (s, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 144.8, 139.4, 130.2, 129.4, 128.9, 128.7, 128.6, 127.2, 127.1, 117.3, 110.9, 48.2. HRMS (EI): *m/z* Calcd for [M+H] $C_{19}H_{18}N$: 260.1434; Found: 260.1433.

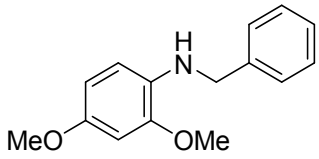
N-benzyl-3,5-bis(trifluoromethyl)aniline (**3h**)



151 mg, 95% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.47 - 7.30 (m, 5H), 7.20 (s, 1H), 7.00 (s, 2H), 4.47 (brs, 1H), 4.39 (d, *J* = 5.0 Hz, 2H). ^{13}C NMR (126MHz, *CHLOROFORM-d*) δ = 148.6, 137.6, 132.4 (q, J_{C-F} =

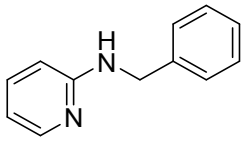
33.9 Hz), 128.9, 127.9, 127.5, 124.5(q, J_{C-F} = 273 Hz), 112.0, 110.5, 110.4, 110.4, 48.0. HRMS (EI): *m/z* Calcd for [M+H] $C_{15}H_{12}NF_6$: 320.0868; Found: 320.0863.

N-benzyl-2,4-dimethoxyaniline (**3i**)[2]



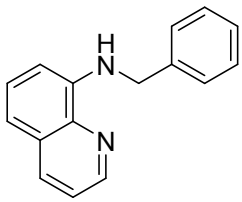
55 mg, 45% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.41 - 7.35 (m, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.28 - 7.23 (m, 1H), 6.51 (d, *J* = 8.4 Hz, 1H), 6.46 (d, *J* = 2.3 Hz, 1H), 6.36 (dd, *J* = 2.5, 8.6 Hz, 1H), 4.30 (s, 3H), 3.86 - 3.80 (m, 3H), 3.74 (s, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 152.1, 147.9, 139.8, 128.5, 127.6, 127.1, 110.5, 103.7, 99.2, 55.8, 55.5, 48.9.

N-benzylpyridin-2-amine (**3j**)



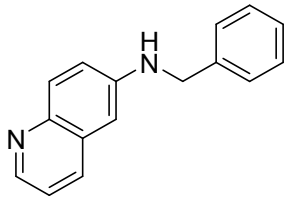
78 mg, 85% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d)*δ = 8.09 (brs, 1H), 7.49 - 7.31 (m, 6H), 6.58 (brs, 1H), 6.36 (d, *J* = 7.3 Hz, 1H), 5.02 (brs, 1H), 4.50 (brs, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 158.6, 148.2, 139.2, 137.4, 128.6, 127.4, 127.2, 113.1, 106.7,46.3. HRMS (EI): *m/z* Calcd for [M+H] $C_{12}H_{13}N_2$: 185.1073; Found: 185.1072.

N-benzylquinolin-8-amine (**3k**)



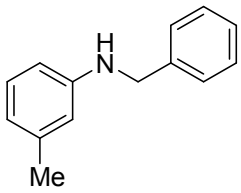
84 mg, 72% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 8.77 (d, *J* = 3.1 Hz, 1H), 8.10 (d, *J* = 7.3 Hz, 1H), 7.49 (d, *J* = 7.3 Hz, 2H), 7.45 - 7.35 (m, 4H), 7.35 - 7.30 (m, 1H), 7.10 (d, *J* = 8.5 Hz, 1H), 6.77 - 6.56 (m, 2H), 4.61 (d, *J* = 5.5 Hz, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 146.9, 144.5, 139.2, 138.2, 136.0, 128.6, 127.7, 127.4, 127.1, 121.4, 114.1, 105.1, 47.6. HRMS (EI): *m/z* Calcd for [M+H] $C_{16}H_{15}N_2$: 235.1230; Found: 235.1229.

N-benzylquinolin-6-amine (**3l**)



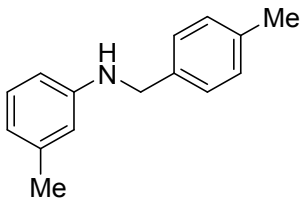
87 mg, 75% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 8.64 (s, 1H), 7.91 (s, 2H), 7.40 (s, 2H), 7.43 (s, 2H), 7.34 (brs, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 6.74 (brs, 1H), 4.46 (brs, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 146.2, 145.9, 143.2, 138.6, 133.8, 130.2, 130.0, 128.7, 127.5, 127.4, 121.3, 121.3, 103.2, 48.2. HRMS (EI): *m/z* Calcd for [M+H] $C_{16}H_{15}N_2$: 235.1230; Found: 235.1229.

N-benzyl-3-methylaniline (**4a**)



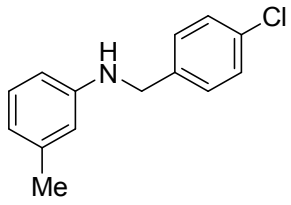
91 mg, 92% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (200 MHz, *CHLOROFORM-d*) δ = 7.54 - 7.29 (m, 5H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.61 (d, *J* = 7.3 Hz, 1H), 6.56 - 6.43 (m, 2H), 4.37 (s, 2H), 4.01 (brs, 1H), 2.34 (s, 3H). ^{13}C NMR (50 MHz, *CHLOROFORM-d*) δ = 148.2, 139.5, 139.0, 129.1, 128.6, 127.5, 127.1, 118.5, 113.6, 109.9, 48.3, 21.6. HRMS (EI): *m/z* Calcd for [M+H] $C_{14}H_{16}N$: 198.1277; Found: 198.1278.

3-methyl-*N*-(4-methylbenzyl)aniline (**4b**)



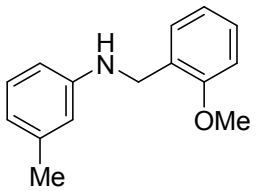
71 mg, 67% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.34 - 7.26 (m, 2H), 7.19 (d, *J* = 7.6 Hz, 2H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.58 (d, *J* = 7.6 Hz, 1H), 6.53 - 6.44 (m, 2H), 4.30 (s, 2H), 2.38 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 148.3, 139.0, 136.8, 136.4, 129.3, 129.1, 127.5, 118.4, 113.6, 109.9, 48.1, 21.6, 21.1. HRMS (EI): *m/z* Calcd for [M+H] $C_{15}H_{18}N$: 212.1434; Found: 212.1433.

***N*-(4-chlorobenzyl)-3-methylaniline (4c)**[1]



39 mg, 45% isolated yield. ^{1}H NMR (200 MHz, *CHLOROFORM-d*) δ 7.31 (m, 4H), 7.07 (t, *J* = 8Hz, 1H), 6.57 (d, *J* = 7Hz, 1H), 6.49 - 6.36 (m, 2H), 4.31 (s, 2H), 4.01 (s, br, 1H), 2.28 (s, 3H). ^{13}C NMR (50 MHz, *CHLOROFORM-d*) δ 147.88, 139.10, 138.10, 132.83, 129.17, 128.69, 118.77, 113.68, 109.98, 47.64, 21.60.

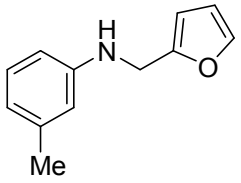
N-(2-methoxybenzyl)-3-methylaniline **(4d)**



88 mg, 78% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d)* δ = 7.38 (d, *J* = 7.2 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.12 (t, *J* = 7.6

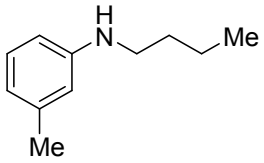
Hz, 1H), 7.01 - 6.90 (m, 2H), 6.59 (d, *J* = 7.6 Hz, 1H), 6.58 - 6.50 (m, 2H), 4.39 (s, 2H), 3.92 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 157.3, 148.4, 138.8, 129.0, 128.8, 128.2, 127.4, 120.5, 118.2, 113.8, 110.1, 110.1, 55.2, 43.4, 21.6. HRMS (EI): *m/z* Calcd for [M+H] $C_{15}H_{18}NO$: 228.1383; Found: 228.1382.

N-(furan-2-ylmethyl)-3-methylaniline **(4e)**



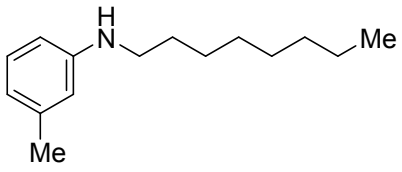
69 mg, 74% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.38 (dd, *J* = 0.6, 1.8 Hz, 1H), 7.12 - 7.05 (m, 1H), 6.58 (d, *J* = 7.0 Hz, 1H), 6.55 - 6.47 (m, 2H), 6.33 (dd, *J* = 2.0, 3.2 Hz, 1H), 6.24 (dd, *J* = 0.6, 3.4 Hz, 1H), 4.32 (s, 2H), 3.98 (brs 1H), 2.29 (s, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 152.8, 147.6, 141.9, 139.0, 129.1, 119.0, 114.0, 110.3, 110.2, 106.9, 41.5, 21.6. HRMS (EI): *m/z* Calcd for [M+H] $C_{12}H_{14}NO$: 188.1070; Found: 188.1068.

N-butyl-3-methylaniline **(4f)**



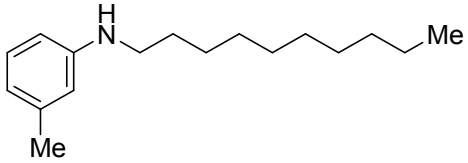
27 mg, 33% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.14 - 6.98 (m, 1H), 6.53 (d, *J* = 7.2 Hz, 1H), 6.49 - 6.35 (m, 2H), 3.12 (t, *J* = 7.1 Hz, 2H), 2.29 (s, 3H), 1.66 - 1.55 (m, 2H), 1.53 - 1.38 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 148.5, 139.0, 129.1, 118.1, 113.5, 109.9, 43.7, 31.7, 21.6, 20.3, 13.9. HRMS (EI): *m/z* Calcd for [M+H] $C_{11}H_{18}N$: 164.1434; Found: 164.1432.

3-methyl-*N*-octylaniline **(4g)**



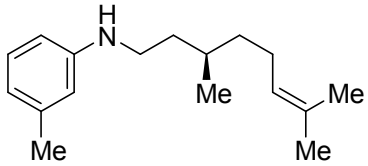
46 mg, 42% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.08 (t, *J* = 7.4 Hz, 1H), 6.54 (d, *J* = 7.2 Hz, 1H), 6.49 - 6.38 (m, 2H), 3.11 (t, *J* = 7.2 Hz, 2H), 2.30 (s, 3H), 1.66 - 1.57 (m, 2H), 1.44 - 1.35 (m, 3H), 1.35 - 1.26 (m, 7H), 1.01 - 0.84 (m, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 148.4, 139.0, 129.1, 118.2, 113.6, 110.0, 31.8, 29.5, 29.4, 29.3, 27.2, 22.6, 21.6, 14.1. HRMS (EI): *m/z* Calcd for [M+H] $C_{15}H_{26}N$: 220.2060; Found: 220.2060.

N-decyl-3-methylaniline **(4h)**



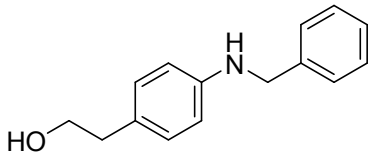
71 mg, 58% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (200 MHz, *CHLOROFORM-d*) δ = 7.05 (d, *J* = 8.5 Hz, 1H), 6.52 (d, *J* = 7.3 Hz, 1H), 6.47 - 6.36 (m, 2H), 3.10 (t, *J* = 7.0 Hz, 2H), 2.29 (s, 3H), 1.60 (d, *J* = 6.6 Hz, 3H), 1.28 (brs, 13H), 0.96 - 0.84 (m, 4H). ^{13}C NMR (50 MHz, *CHLOROFORM-d*) δ = 139.0, 129.1, 118.0, 113.5, 109.9, 44.0, 31.9, 29.6, 29.4, 29.3, 27.2, 22.7, 21.6, 14.1. HRMS (EI): *m/z* Calcd for [M+H] $C_{17}H_{30}N$: 248.2373; Found: 248.2375.

(*R*)-*N*-(3,7-dimethyloct-6-enyl)-3-methylaniline **(4i)**



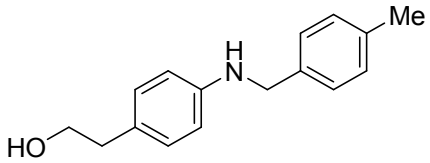
92 mg, 75% isolated yield. R_f = 0.32 (hexane/EtOAc = 90/1). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.11 (t, *J* = 7.8 Hz, 1H), 6.56 (d, *J* = 7.6 Hz, 1H), 6.50 - 6.40 (m, 2H), 5.16 (t, *J* = 7.1 Hz, 1H), 3.25 - 3.06 (m, 2H), 2.33 (s, 3H), 2.15 - 1.93 (m, 2H), 1.79 - 1.70 (m, 4H), 1.70 - 1.57 (m, 5H), 1.52 - 1.35 (m, 2H), 1.34 - 1.21 (m, 1H), 1.04 - 0.94 (m, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 148.6, 138.9, 131.2, 129.0, 124.6, 118.0, 113.4, 109.8, 41.9, 37.1, 36.7, 30.4, 25.7, 25.4, 21.6, 19.6, 17.6. HRMS (EI): *m/z* Calcd for [M+H] $C_{17}H_8N$: 246.2216; Found: 246.2216.

2-(4-(benzylamino)phenyl)ethanol (**6a**)



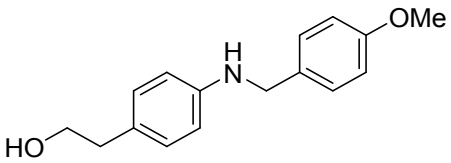
91 mg, yellow liquid, 80% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.46 - 7.23 (m, 5H), 7.09 - 7.01 (m, *J* = 8.0 Hz, 2H), 6.68 - 6.56 (m, *J* = 8.4 Hz, 2H), 4.34 (s, 2H), 4.02 (brs, 1H), 3.80 (t, *J* = 6.5 Hz, 2H), 2.78 (t, *J* = 6.7 Hz, 2H), 1.69 (brs, 1H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 146.7, 139.4, 129.8, 128.6, 127.4, 127.1, 127.0, 113.0, 63.8, 48.4, 38.2. HRMS (EI): *m/z* Calcd for [M+H] $C_{15}H_{18}NO$: 228.1383; Found: 228.1381.

2-(4-(4-methylbenzylamino)phenyl)ethanol (**6b**)



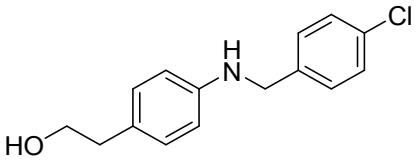
94 mg, yellow liquid, 78% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). Yellow liquid. ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.29 (s, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.08 - 6.85 (m, *J* = 8.4 Hz, 2H), 6.71 - 6.48 (m, *J* = 8.0 Hz, 2H), 4.29 (s, 2H), 3.81 (t, *J* = 6.5 Hz, 2H), 2.77 (t, *J* = 6.5 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 146.9, 136.8, 136.3, 129.8, 129.7, 127.5, 126.9, 113.1, 63.9, 48.2, 38.3, 21.1. HRMS (EI): *m/z* Calcd for [M+H] $C_{16}H_{20}NO$: 242.1539; Found: 242.1533.

2-(4-(4-methoxybenzylamino)phenyl)ethanol (**6c**)



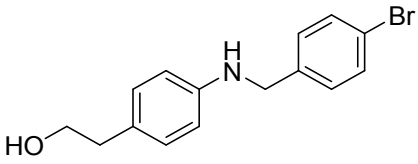
92 mg, yellow liquid, 72% isolated yield. R_f = 0.32 (hexane/EtOAc = 60/40). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.41 - 7.18 (m, *J* = 8.4 Hz, 2H), 7.10 - 6.97 (m, *J* = 8.0 Hz, 2H), 6.97 - 6.75 (m, *J* = 8.8 Hz, 2H), 6.66 - 6.54 (m, *J* = 8.4 Hz, 2H), 4.25 (s, 2H), 3.88 - 3.64 (m, 5H), 2.77 (t, *J* = 6.5 Hz, 2H), 1.61 (brs, 1H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 158.9, 146.9, 131.4, 129.8, 128.8, 127.0, 114.0, 113.1, 63.9, 55.3, 48.0, 38.3. HRMS (EI): *m/z* Calcd for [M+H] $C_{16}H_{20}NO_2$: 258.1489; Found: 258.1486.

2-(4-(4-chlorobenzylamino)phenyl)ethanol (**6d**)



110 mg, 85% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (400 MHz, *CHLOROFORM-d*) δ = 7.31 (s, 4H), 7.12 - 6.97 (m, *J* = 8.2 Hz, 2H), 6.66 - 6.45 (m, *J* = 8.7 Hz, 2H), 4.30 (s, 2H), 3.80 (t, *J* = 6.4 Hz, 2H), 2.76 (t, *J* = 6.6 Hz, 2H). ^{13}C NMR (50 MHz, *CHLOROFORM-d*) δ = 146.4, 138.0, 132.9, 129.9, 128.7, 128.7, 127.4, 113.2, 63.9, 47.8, 38.2. HRMS (EI): *m/z* Calcd for [M+H] $C_{15}H_{17}NOCl$: 262.0993; Found: 262.0991.

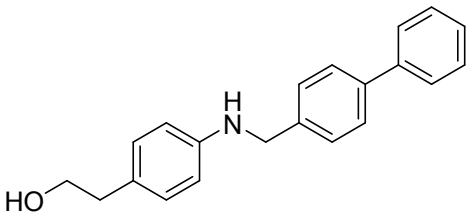
2-(4-(4-bromobenzylamino)phenyl)ethanol (**6e**)



96 mg, yellow liquid, 63% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.47 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.14 - 6.98 (m, *J* = 8.4 Hz, 2H), 6.65 - 6.50 (m, *J* = 8.4 Hz, 2H), 4.29 (s, 2H), 3.80 (t, *J* = 6.5 Hz, 2H), 2.76 (t, *J*

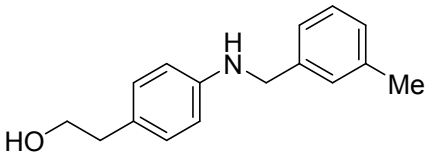
= 6.5 Hz, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 146.7, 138.8, 131.9, 130.1, 129.3, 127.6, 121.2, 113.4, 64.1, 48.0, 38.5. HRMS (EI): *m/z* Calcd for [M+H] $C_{15}H_{17}NOBr$: 306.0488; Found: 306.0490.

2-(4-(biphenyl-4-ylmethylamino)phenyl)ethanol (**6f**)



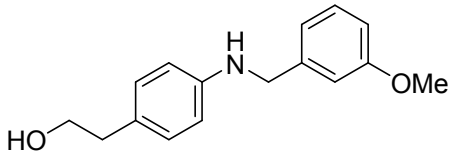
113 mg, yellow solid, 75% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.67 - 7.52 (m, 4H), 7.49 - 7.39 (m, 4H), 7.39 - 7.31 (m, 1H), 7.12 - 6.98 (m, *J* = 8.0 Hz, 2H), 6.75 - 6.53 (m, *J* = 8.4 Hz, 2H), 4.38 (s, 2H), 3.81 (t, *J* = 6.5 Hz, 2H), 2.78 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 146.8, 140.8, 140.2, 138.5, 129.9, 128.8, 127.9, 127.4, 127.2, 127.1, 127.0, 113.2, 63.9, 48.2, 38.3. HRMS (EI): *m/z* Calcd for [M+H] $C_{21}H_{22}NO$: 304.1696; Found: 304.1693.

2-(4-(3-methylbenzylamino)phenyl)ethanol (**6g**)



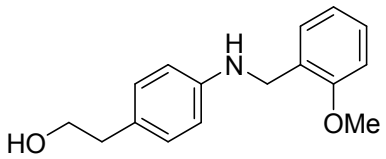
87 mg, yellow liquid, 72% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.34 (d, *J* = 7.2 Hz, 1H), 7.25 - 7.14 (m, 3H), 7.11 - 7.02 (m, *J* = 8.4 Hz, 2H), 6.66 - 6.58 (m, *J* = 8.4 Hz, 2H), 4.27 (s, 2H), 3.81 (t, *J* = 6.5 Hz, 3H), 2.78 (t, *J*= 6.5 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 147.0, 137.0, 136.3, 130.4, 129.9, 128.2, 127.4, 126.9, 126.1, 113.0, 63.9, 46.5, 38.3, 18.9. HRMS (EI): *m/z* Calcd for [M+H] $C_{16}H_{20}NO$: 242.1545; Found: 242.1540.

2-(4-(3-methoxybenzylamino)phenyl)ethanol (**6h**)



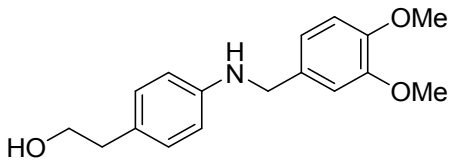
87 mg, yellow liquid, 68% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.32 - 7.25 (m, 1H), 7.11 - 7.02 (m, *J* = 8.4 Hz, 2H), 7.02 - 6.91 (m, 2H), 6.84 (dd, *J* = 2.1, 8.2 Hz, 1H), 6.68 - 6.59 (m, *J* = 8.4 Hz, 2H), 4.32 (s, 2H), 3.87 - 3.78 (m, 5H), 2.78 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 159.9, 146.8, 141.2, 129.8, 129.6, 127.1, 119.7, 113.1, 113.0, 112.6, 63.9, 55.2, 48.4, 38.2. HRMS (EI): *m/z* Calcd for [M+H] $C_{16}H_{20}O_2$: 258.1489; Found: 258.1486.

2-(4-(2-methoxybenzylamino)phenyl)ethanol (**6i**)



80 mg, white solid, 63% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.33 (d, *J* = 7.2 Hz, 1H), 7.30 - 7.27 (m, 1H), 7.10 - 6.99 (m, *J* = 8.4 Hz, 2H), 6.92 (t, *J* = 7.4 Hz, 2H), 6.75 - 6.60 (m, *J* = 8.4 Hz, 2H), 4.34 (s, 2H), 3.89 (s, 3H), 3.81 (t, *J* = 6.5 Hz, 2H), 2.78 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 157.4, 147.0, 129.8, 128.9, 128.3, 127.3, 126.8, 120.5, 113.4, 110.2, 63.9, 55.3, 43.6, 38.3. HRMS (EI): *m/z* Calcd for [M+H] $C_{16}H_{20}NO_2$: 258.1489; Found: 258.1486.

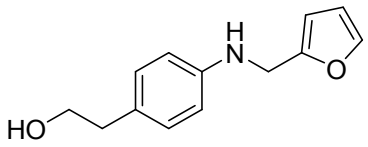
2-(4-(3,4-dimethoxybenzylamino)phenyl)ethanol (**6j**)



109 mg, white solid, 76% isolated yield. R_f = 0.32 (hexane/EtOAc = 60/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.05 (d, *J* = 8.4 Hz, 2H), 6.92 (brs, 2H), 6.85 (s, 1H), 6.63 (d, *J* = 8.4 Hz,

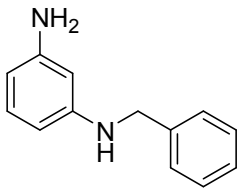
2H), 4.25 (s, 2H), 3.88 (d, *J* = 2.3 Hz, 6H), 3.80 (t, *J* = 6.7 Hz, 3H), 2.77 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 149.1, 146.8, 131.9, 129.8, 127.1, 119.7, 113.2, 113.1, 111.1, 110.8, 63.9, 55.9, 55.8, 48.4, 38.2. HRMS (EI): *m/z* Calcd for [M+H] $C_{17}H_{22}NO_3$: 288.1594; Found: 288.1592

2-(4-(furan-2-ylmethylamino)phenyl)ethanol (**6k**)



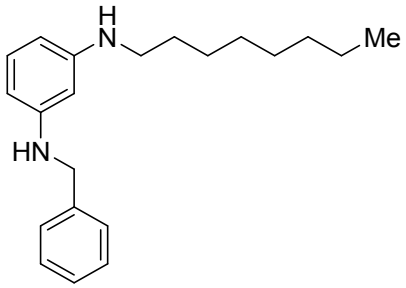
68 mg, yellow liquid, 63% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.38 (s, 1H), 7.12 - 6.98 (m, *J* = 8.0 Hz, 2H), 6.69 - 6.60 (m, *J* = 8.4 Hz, 2H), 6.35 - 6.30 (m, 1H), 6.24 (d, *J* = 2.7 Hz, 1H), 4.31 (s, 2H), 3.80 (t, *J* = 6.7 Hz, 2H), 2.77 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 152.7, 146.3, 141.9, 129.8, 127.5, 113.4, 110.3, 106.9, 63.9, 41.6, 38.2. HRMS (EI): *m/z* Calcd for [M+H] $C_{13}H_{16}NO_2$: 218.1176; Found: 218.1174.

N^1-benzylbenzene-1,3-diamine (**7b**)



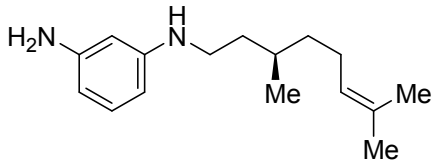
64 mg, yellow liquid, 65% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.49 - 7.34 (m, 4H), 7.34 - 7.27 (m, 1H), 7.00 (t, *J* = 7.8 Hz, 1H), 6.17 - 6.09 (m, 2H), 6.01 (t, *J* = 1.9 Hz, 1H), 4.33 (s, 2H), 3.51 (brs, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 149.3, 147.5, 139.6, 130.1, 128.6, 127.5, 127.1, 105.1, 104.0, 99.5, 48.3. HRMS (EI): *m/z* Calcd for [M+H] $C_{13}H_{15}N_2$: 199.1230; Found: 199.1227.

N^1-benzyl-N^3-octylbenzene-1,2-diamine (**7c**)



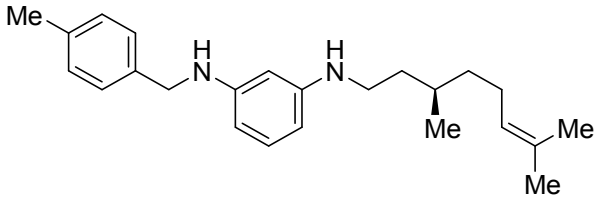
93 mg, yellow liquid, 60% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (500 MHz, *CHLOROFORM-d*) δ = 7.42 - 7.32 (m, 4H), 7.29 - 7.24 (m, 1H), 6.98 (t, *J* = 8.0 Hz, 1H), 6.07 - 5.99 (m, 2H), 5.91 (s, 1H), 4.33 - 4.25 (m, 2H), 3.10 - 3.00 (m, 2H), 1.62 - 1.54 (m, 2H), 1.39 - 1.26 (m, 12H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, *CHLOROFORM-d*) δ = 149.6, 149.4, 139.7, 130.0, 128.6, 127.5, 127.1, 103.1, 102.7, 97.2, 48.4, 44.1, 31.8, 29.6, 29.4, 29.2, 27.2, 22.6, 14.1. HRMS (EI): *m/z* Calcd for [M+H] $C_{21}H_{31}N_2$: 311.2482; Found: 311.2480.

(*R*)-N^1-(3,7-dimethyloct-6-enyl)benzene-1,3-diamine (**7d**)



95 mg, yellow liquid, 78% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (400 MHz, *CHLOROFORM-d)* δ = 6.97 (t, *J* = 8.0 Hz, 1 H), 6.08 (dd, *J* = 2.3, 7.6 Hz, 2 H), 5.97 (t, *J* = 1.9 Hz, 1 H), 5.19 - 5.06 (m, 1 H), 3.35 (brs, 2 H), 3.16 - 3.03 (m, 3 H), 2.10 - 1.94 (m, 2 H), 1.75 - 1.68 (m, 3 H), 1.66 - 1.54 (m, 5 H), 1.48 - 1.36 (m, 2 H), 1.27 - 1.18 (m, 1 H), 0.99 - 0.92 (m, 3 H). ^{13}C NMR (101MHz, *CHLOROFORM-d*) δ = 149.7, 147.4, 131.3, 130.0, 124.6, 104.7, 104.0, 99.3, 77.3, 76.7, 41.9, 37.0, 36.7, 30.4, 25.7, 25.4, 19.5, 17.6. HRMS (EI): *m/z* Calcd for [M+H] $C_{16}H_{27}N_2$: 247.2169; Found: 247.2167.

(*R*)-N^1-(3,7-dimethyloct-6-enyl)-N^3-(4-methylbenzyl)benzene-1,3-diamine (**7e**)



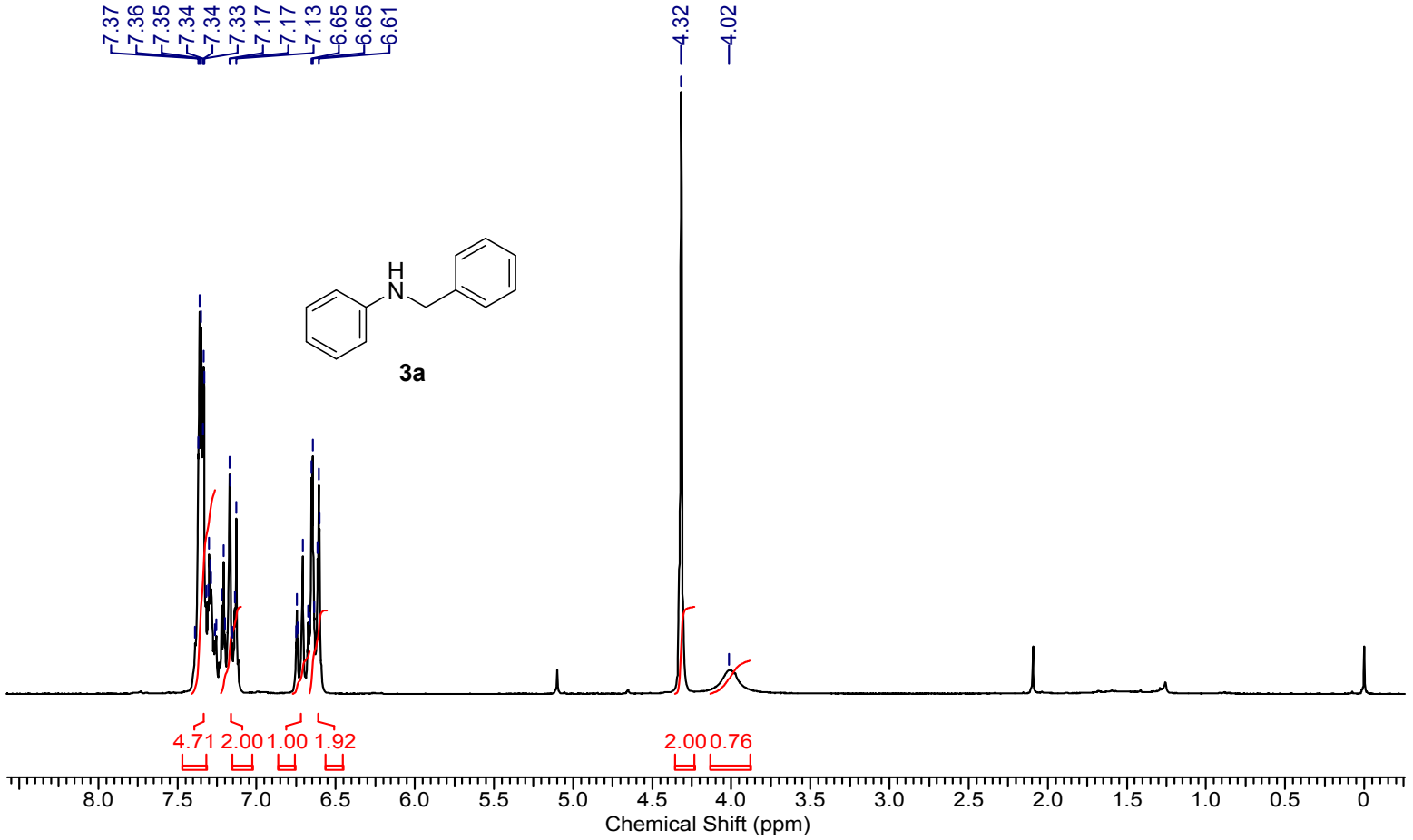
113 mg, yellow liquid, 65% isolated yield. R_f = 0.32 (hexane/EtOAc = 70/30). ^{1}H NMR (400 MHz, *CHLOROFORM-d*) δ = 7.35 - 7.28 (m, *J* = 7.6 Hz, 2 H), 7.24 - 7.13 (m, *J* = 7.6 Hz, 2 H), 7.03 (dt, *J* = 1.5, 8.0 Hz, 1 H), 6.12 - 6.03 (m, 2 H), 5.95 (s, 1 H), 5.21 - 5.05 (m, 1 H), 4.30 (s, 2 H), 3.69 (brs, 2 H), 3.20 - 3.01 (m, 2 H), 2.39 (s, 3 H), 2.12 - 1.99 (m, 2 H), 1.75 (s, 3 H), 1.72 - 1.58 (m, 5 H), 1.50 - 1.40 (m, 2 H), 1.30 - 1.18 (m, 1 H), 0.98 (dd, *J* = 1.9, 6.5 Hz, 4 H). ^{13}C NMR (101 MHz, *CHLOROFORM-d*) δ = 149.5, 149.4, 136.6, 136.6, 131.2, 129.9, 129.2, 127.5, 124.7, 103.0, 102.7, 97.1, 77.3, 76.7, 48.1, 42.0, 37.0, 36.6, 30.4, 25.7, 25.4, 21.0, 19.5, 17.6. HRMS (EI): *m/z* Calcd for [M+H] $C_{24}H_{35}N_2$: 351.2795; Found: 351.2793.

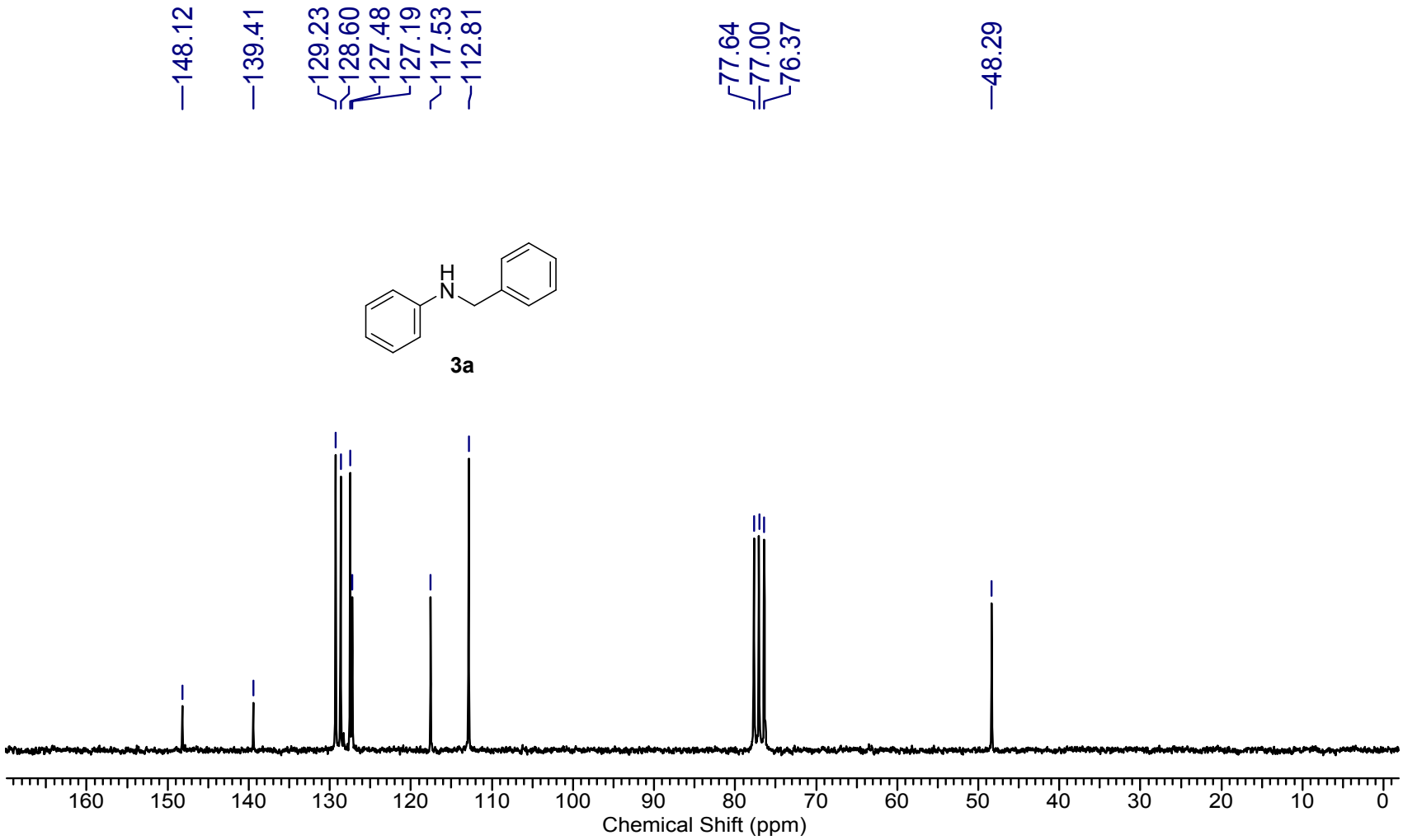
5. References

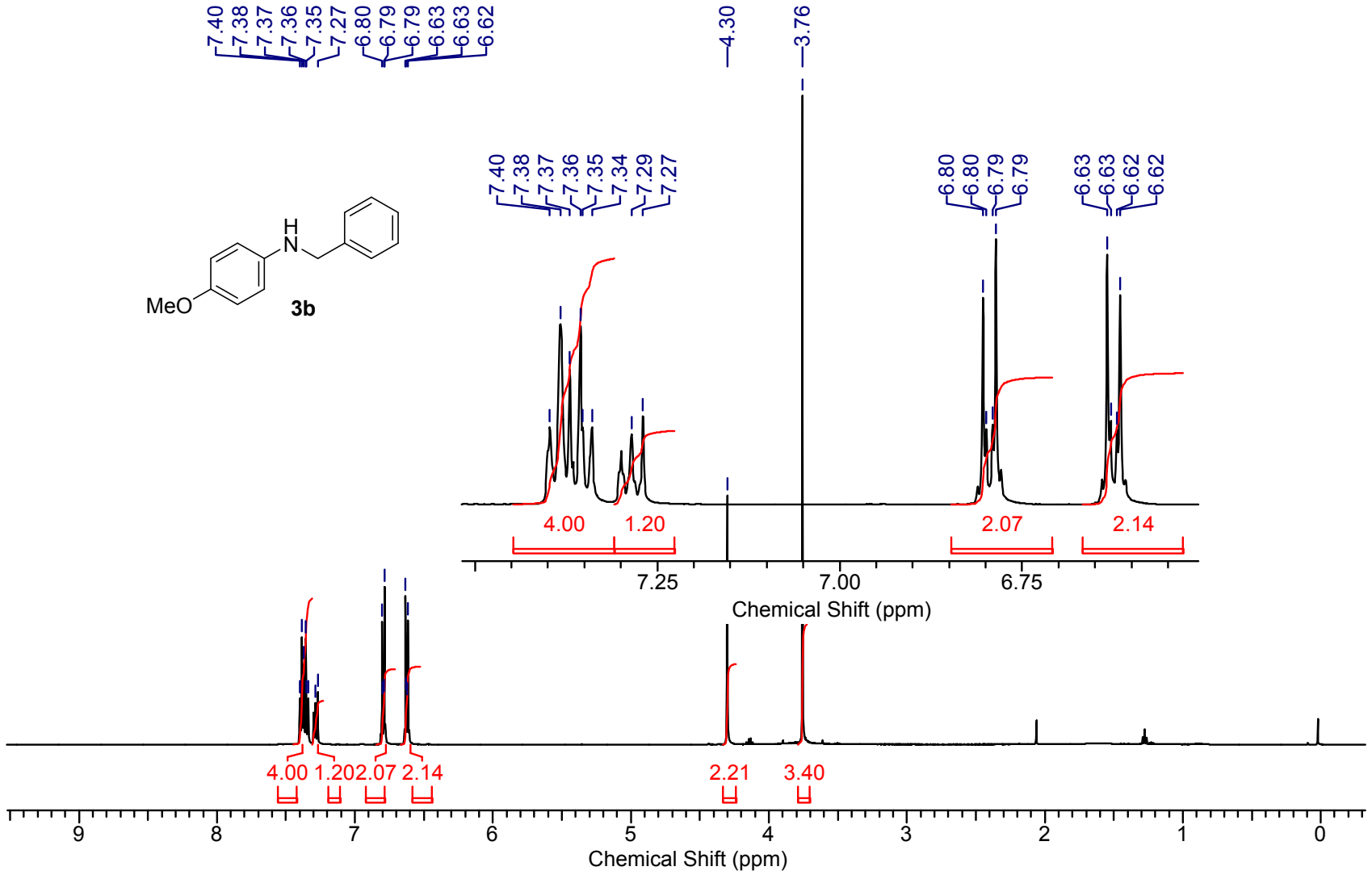
1) S. Rosler, M. Ertl, T. Irrgang and R. Kempe, *Angew. Chem. Int. Ed*. 2015, **54**, 15046.

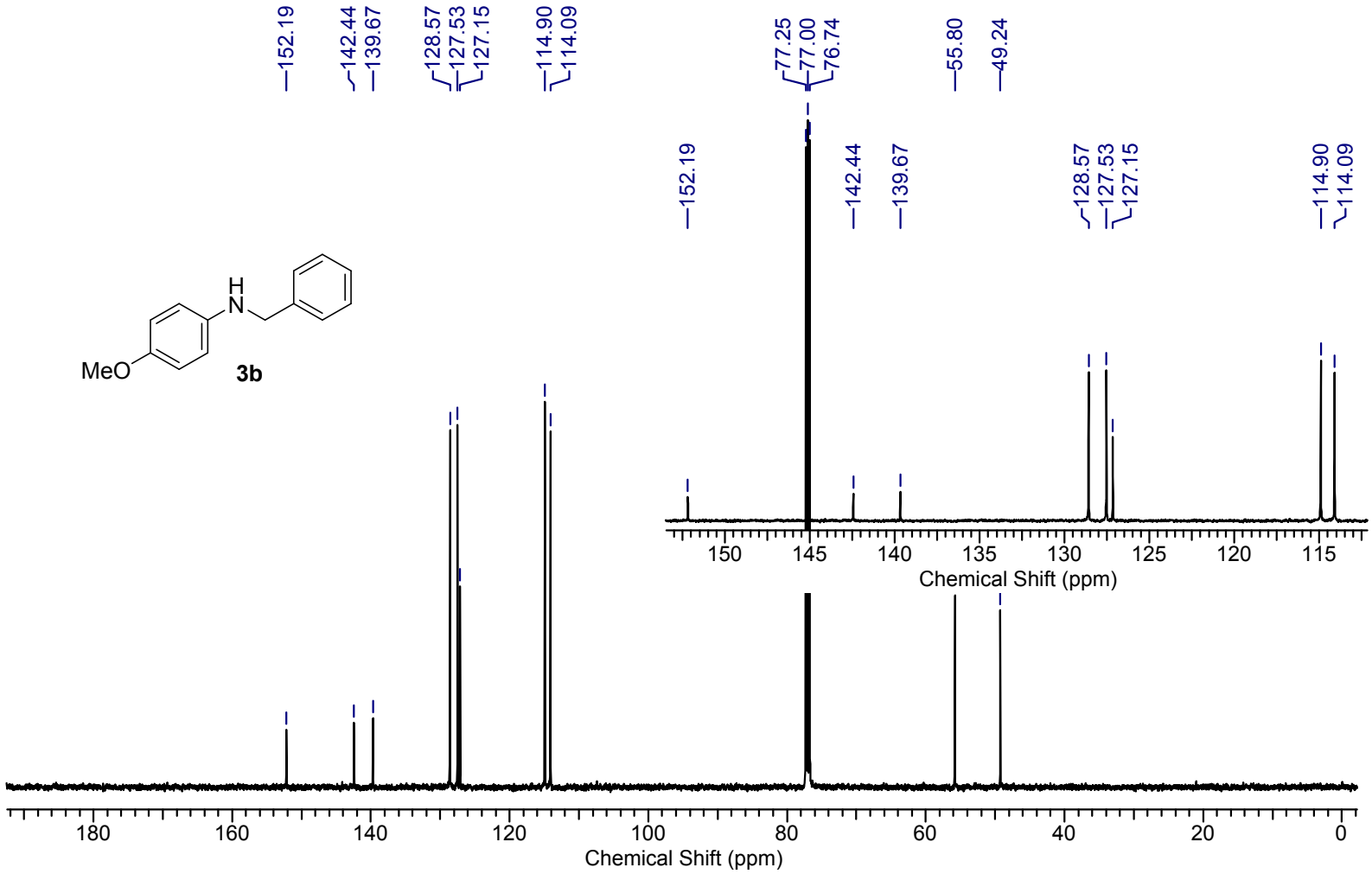
2) W. Zhou, M. Fan, J. Yin, Y. Jiang and D. Ma, *J. Am. Chem. Soc.* 2015, **137**, 11942.

6. Spectral data




148.12
139.41
129.23
128.60
127.48
127.19
117.53
112.81
77.64
77.00
76.37
48.29
H
N
3a
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


7.40
7.38
7.37
7.36
7.35
7.27
6.80
6.79
6.79
6.63
6.63
6.62
4.30
3.76
MeO
H
N
3b
7.40
7.38
7.37
7.36
7.35
7.34
7.29
7.27
6.80
6.80
6.79
6.79
6.63
6.63
6.62
6.62
4.00
1.20
2.07
2.14
7.25
7.00
6.75
Chemical Shift (ppm)
4.00
1.20
2.07
2.14
2.21
3.40
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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127.15
114.90
114.09
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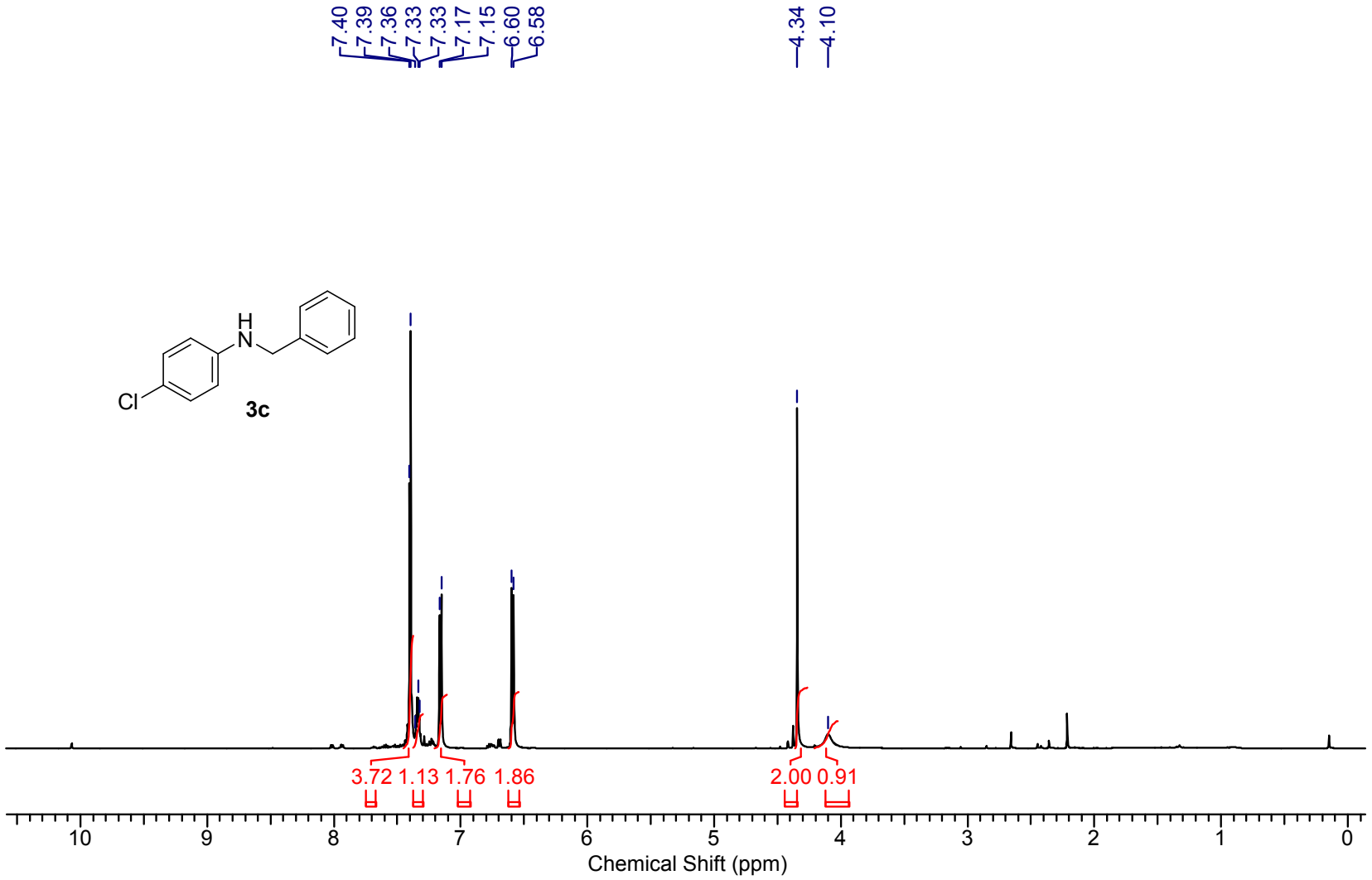
77.00
76.74
55.80
49.24
MeO
H
N
3b
Chemical Shift (ppm)
Chemical Shift (ppm)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7.36
7.33
7.33
7.17
7.15
6.60
6.58
4.34
4.10
H
N
Cl
3c
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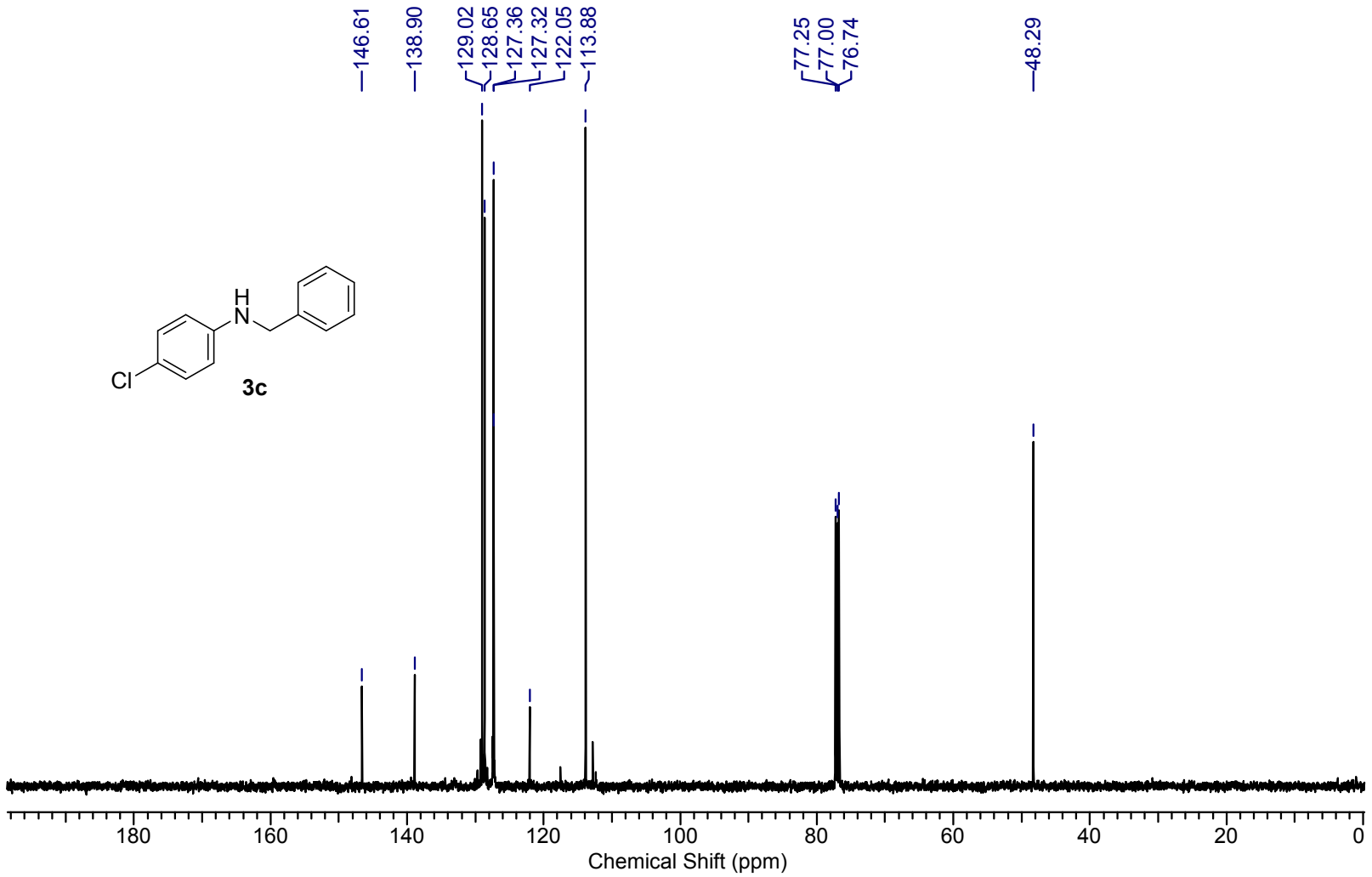
2.00 0.91
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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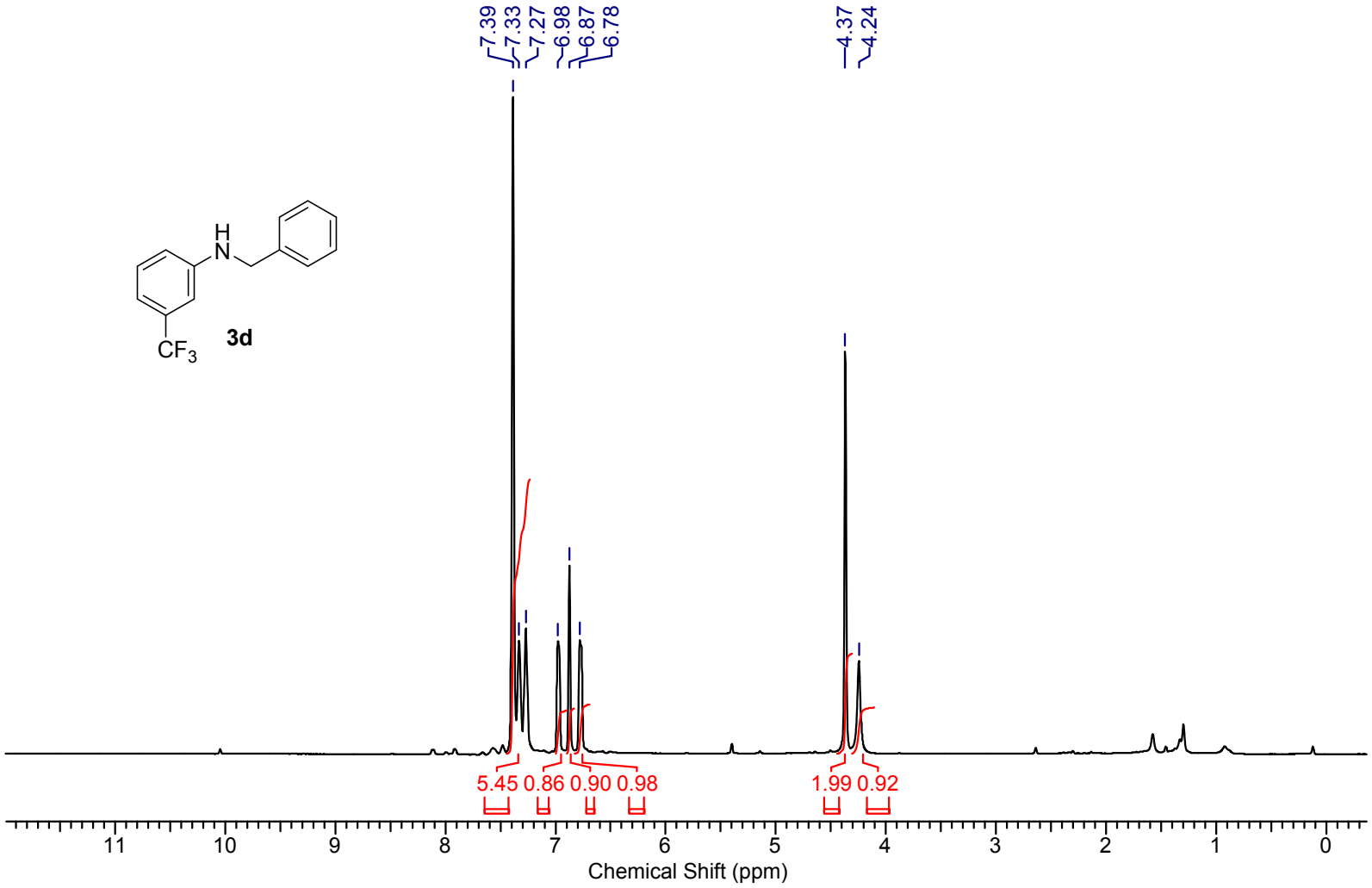
128.65
127.36
127.32
122.05
113.88
77.25
77.00
76.74
48.29
H
N
Cl
3c
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)


7.39
7.33
7.27
6.98
6.87
6.78
4.37
4.24
H
N
CF3
3d
5.45 0.86 0.90 0.98
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11
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7
6
5
4
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2
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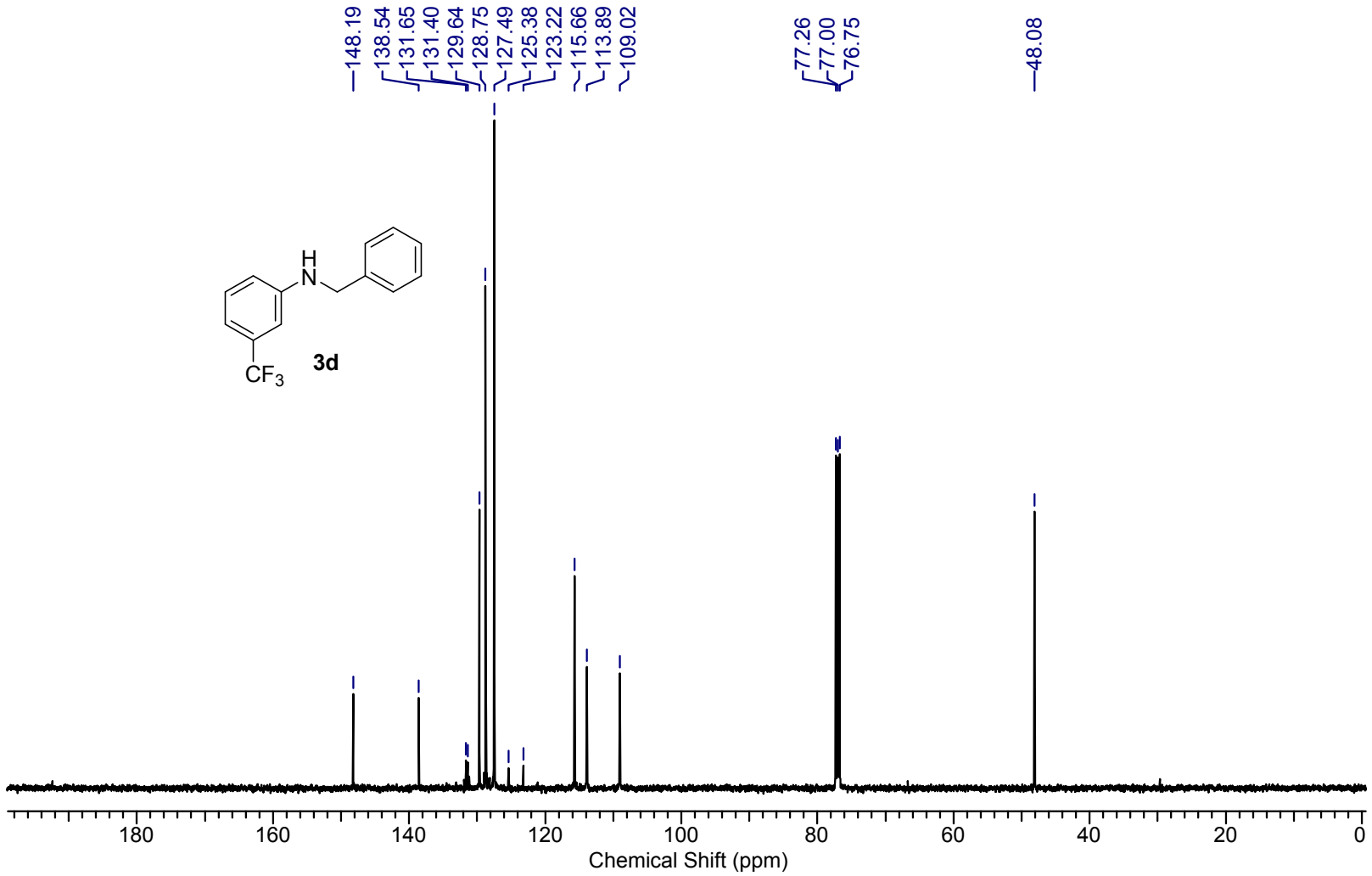
0
Chemical Shift (ppm)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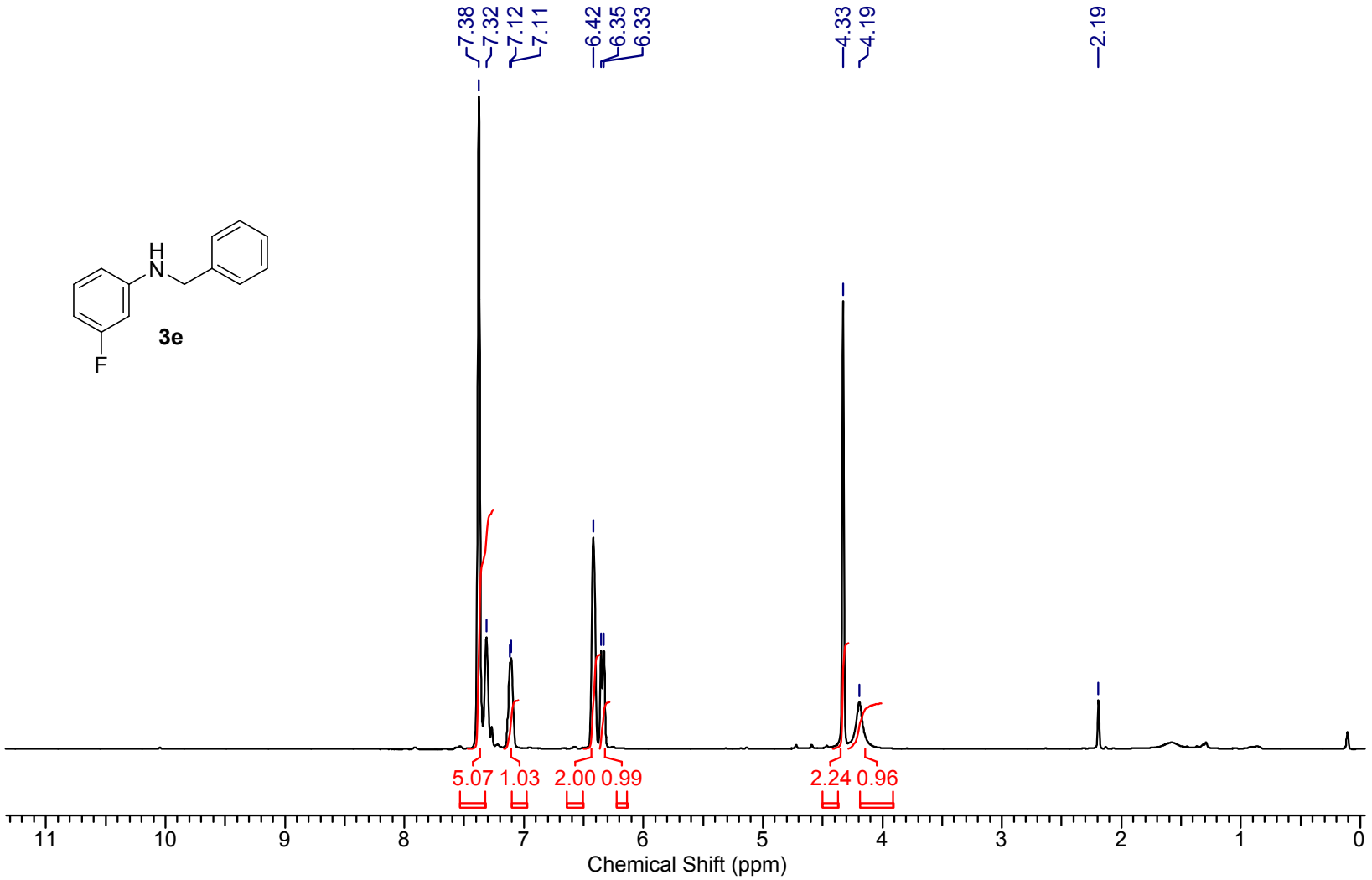
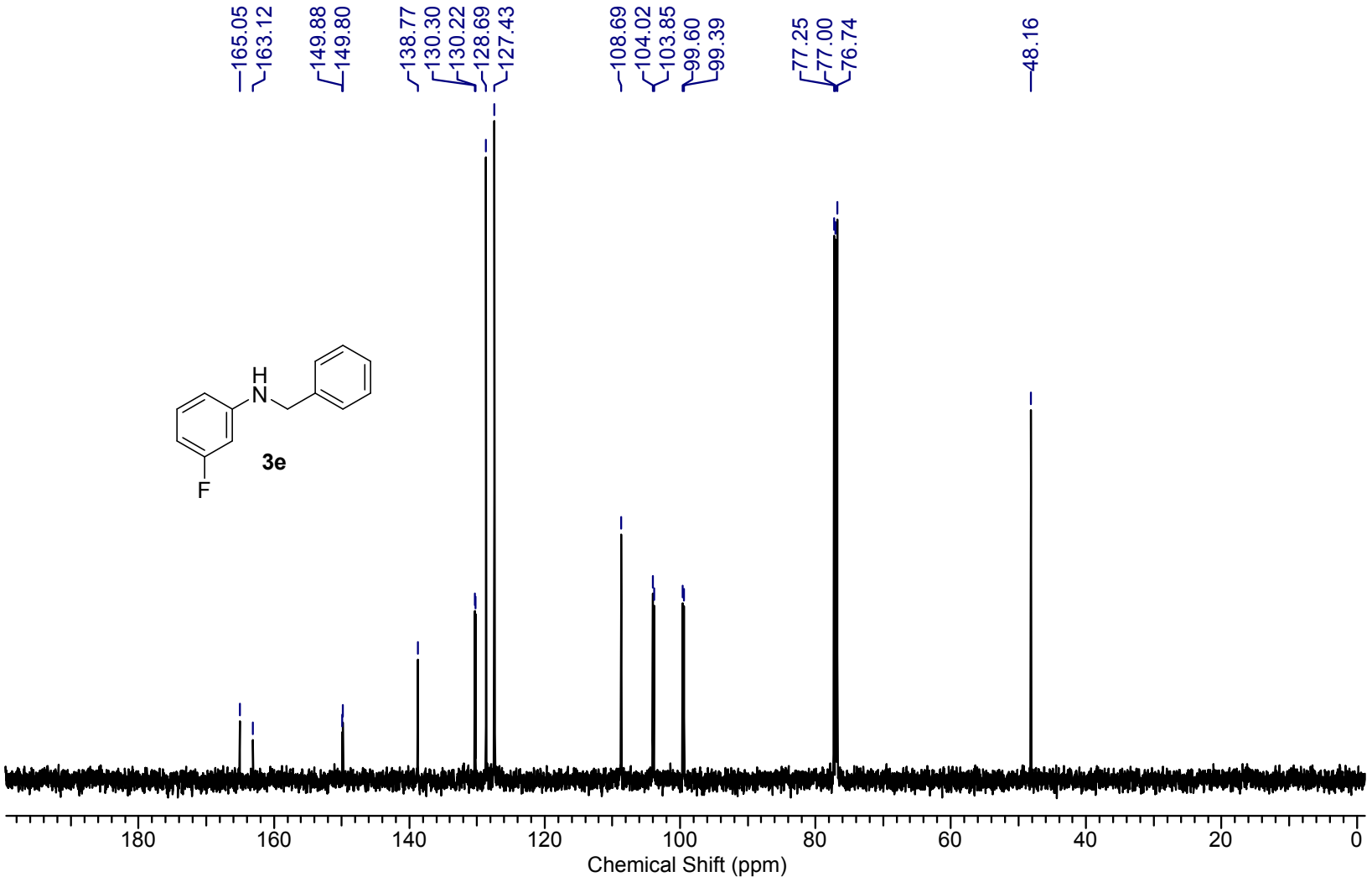
131.65
131.40
129.64
128.75
127.49
125.38
123.22
115.66
113.89
109.02
77.26
77.00
76.75
48.08
H
N
CF3
3d
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)


7.38
7.32
7.12
7.11
6.42
6.35
6.33
4.33
4.19
2.19
H
N
F
3e
5.07 1.03 2.00 0.99
2.24 0.96
11 10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)


165.05
163.12
149.88
149.80
138.77
130.30
130.22
128.69
127.43
108.69
104.02
103.85
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99.39
77.25
77.00
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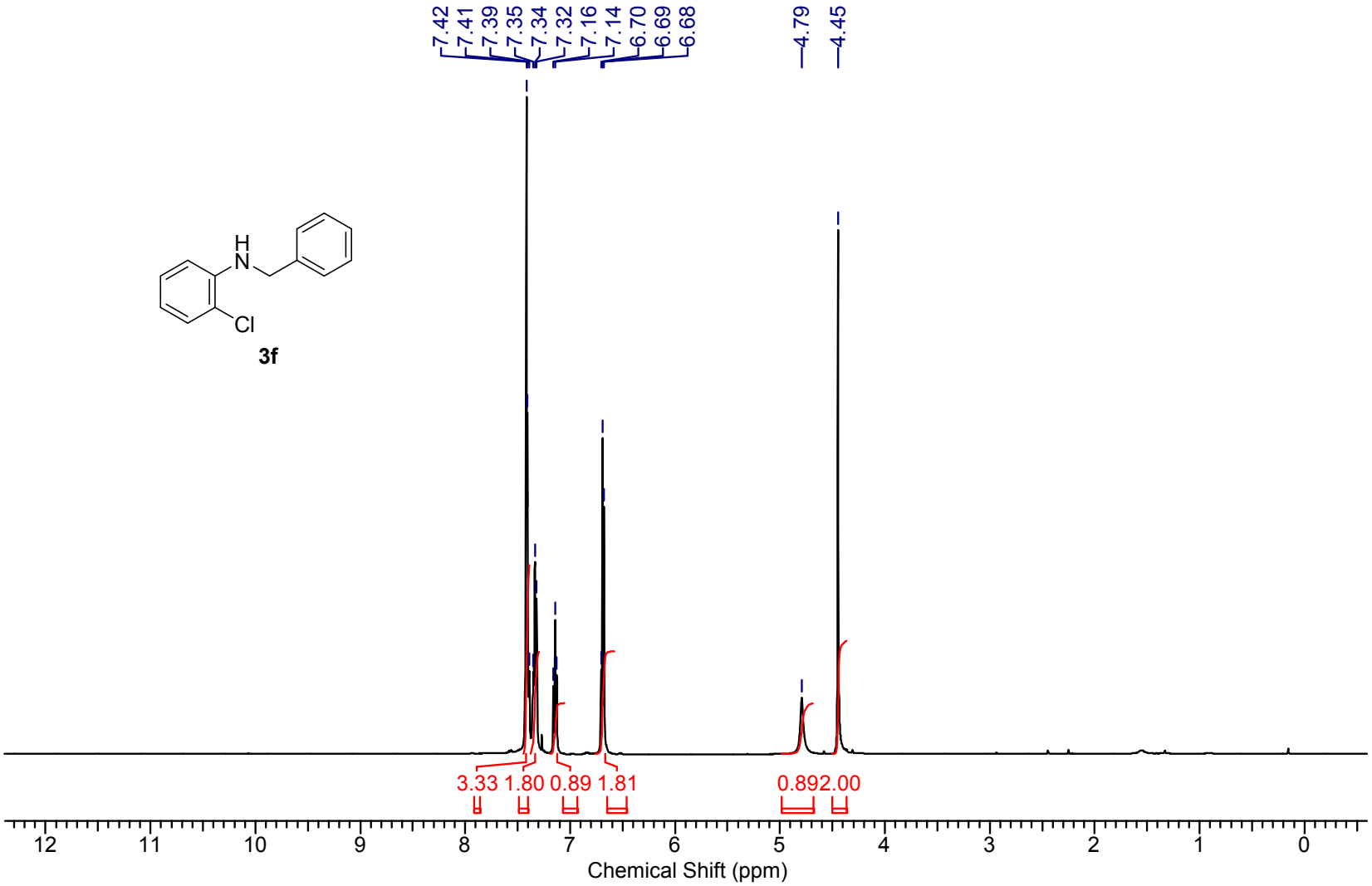
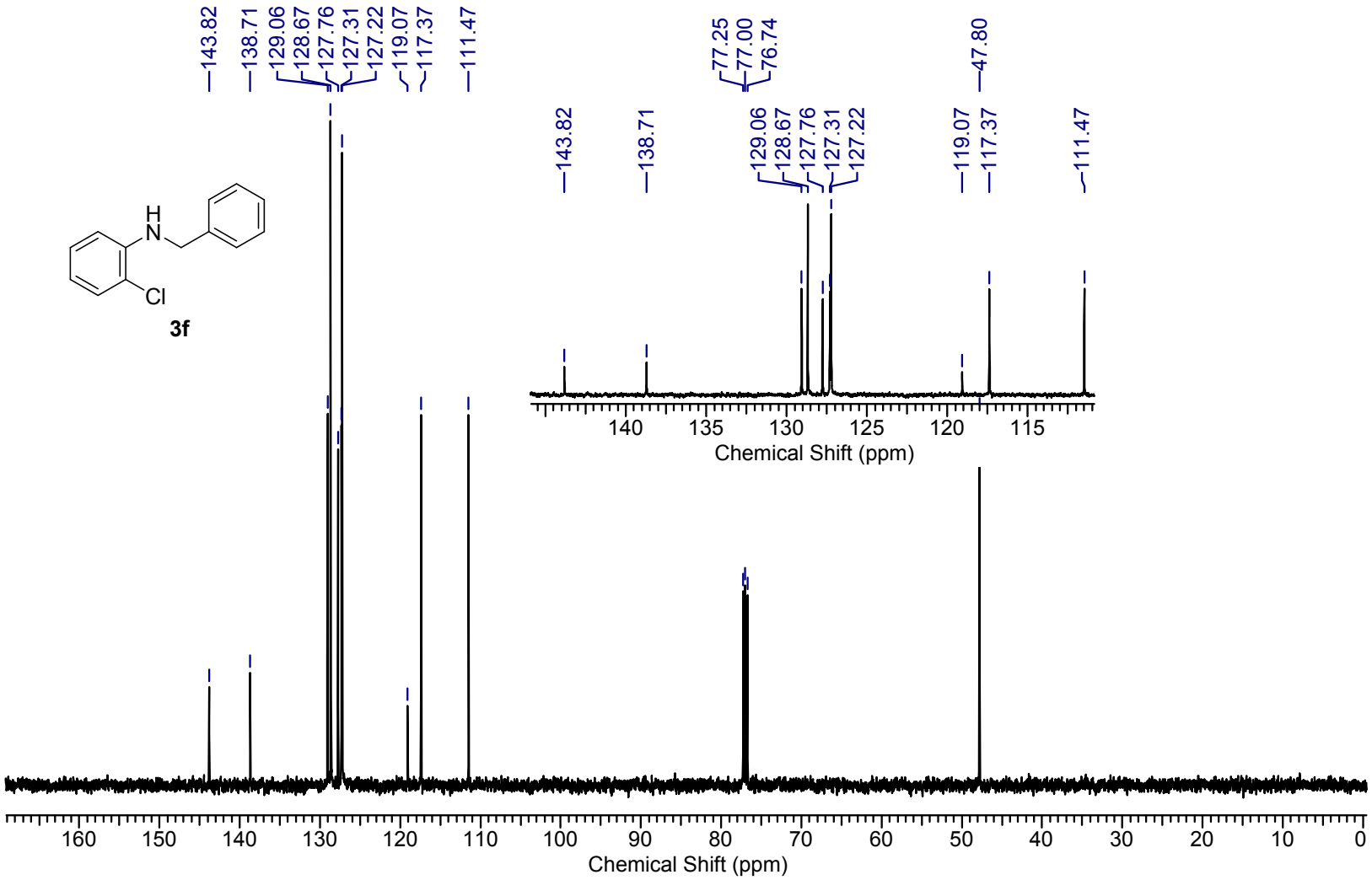
N
F
3e
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)


7.42
7.41
7.39
7.35
7.34
7.32
7.16
7.14
6.70
6.69
6.68
4.79
4.45
H
N
Cl
3f
3.33 1.80 0.89 1.81
0.89 2.00
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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111.47
77.25
77.00
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47.80
H
N
Cl
3f
160
150
140
130
120
110
100
90
80
70
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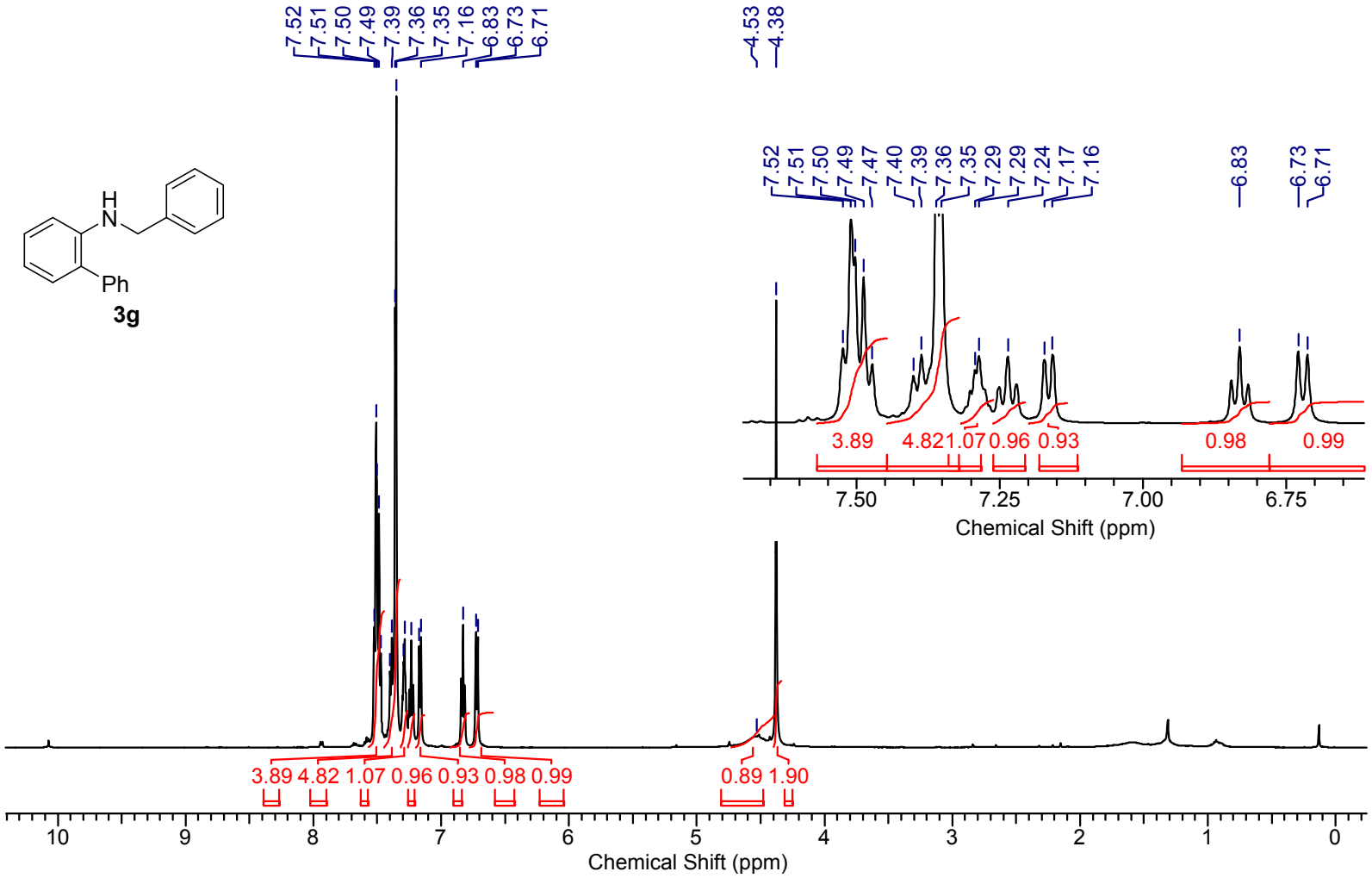
40
30
20
10
0
Chemical Shift (ppm)
140
135
130
125
120
115
Chemical Shift (ppm)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6.73
6.71
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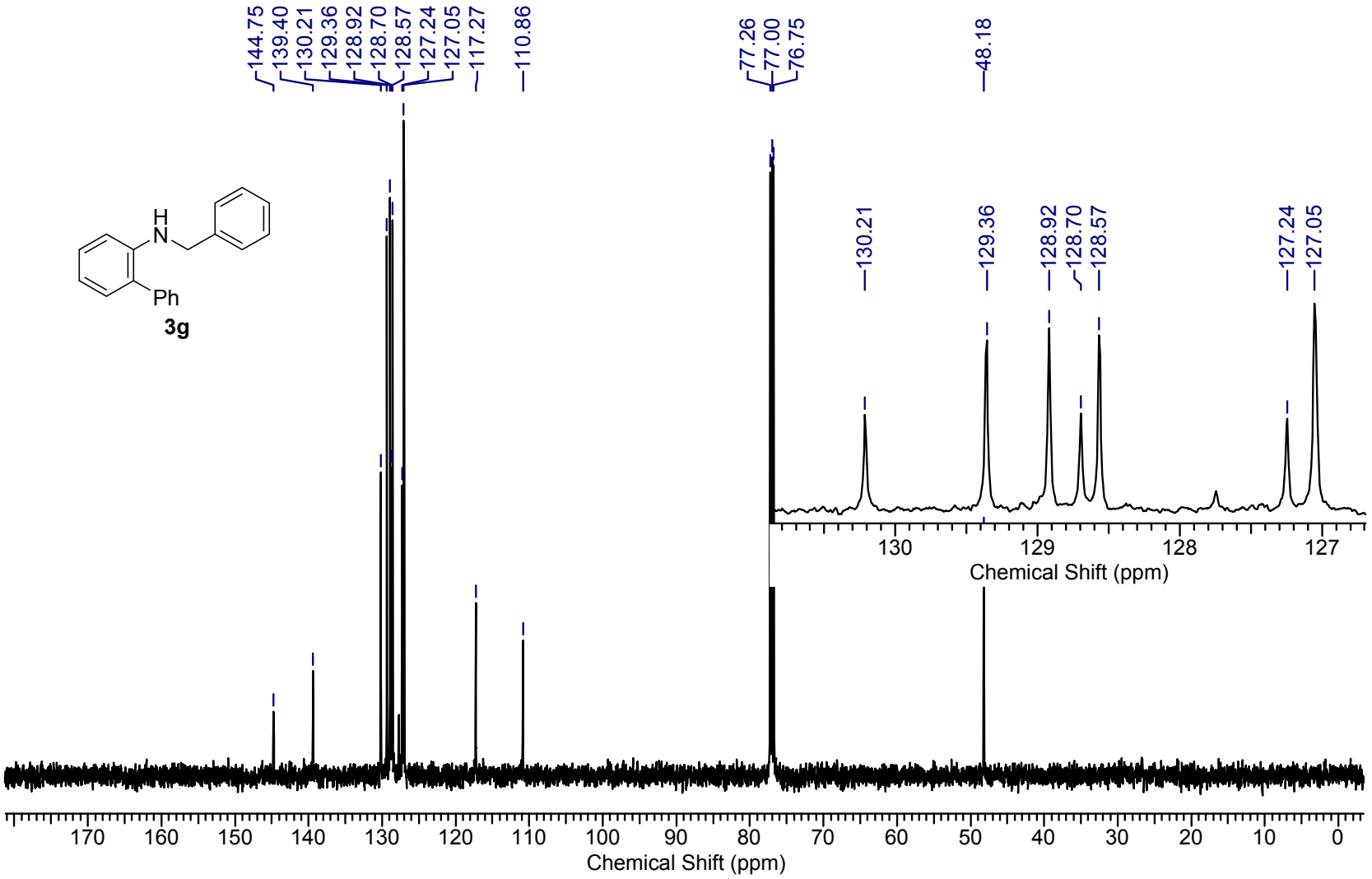
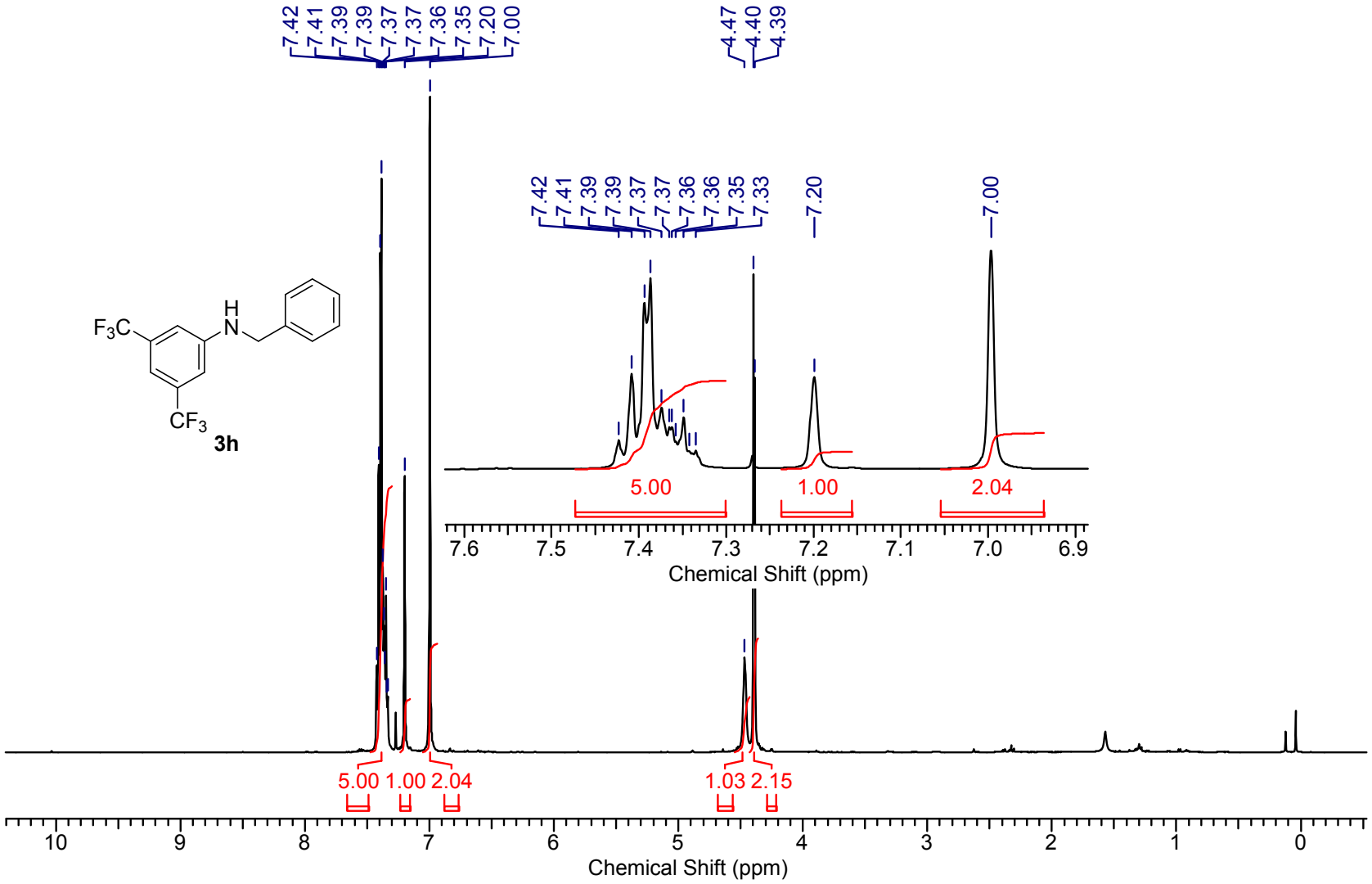
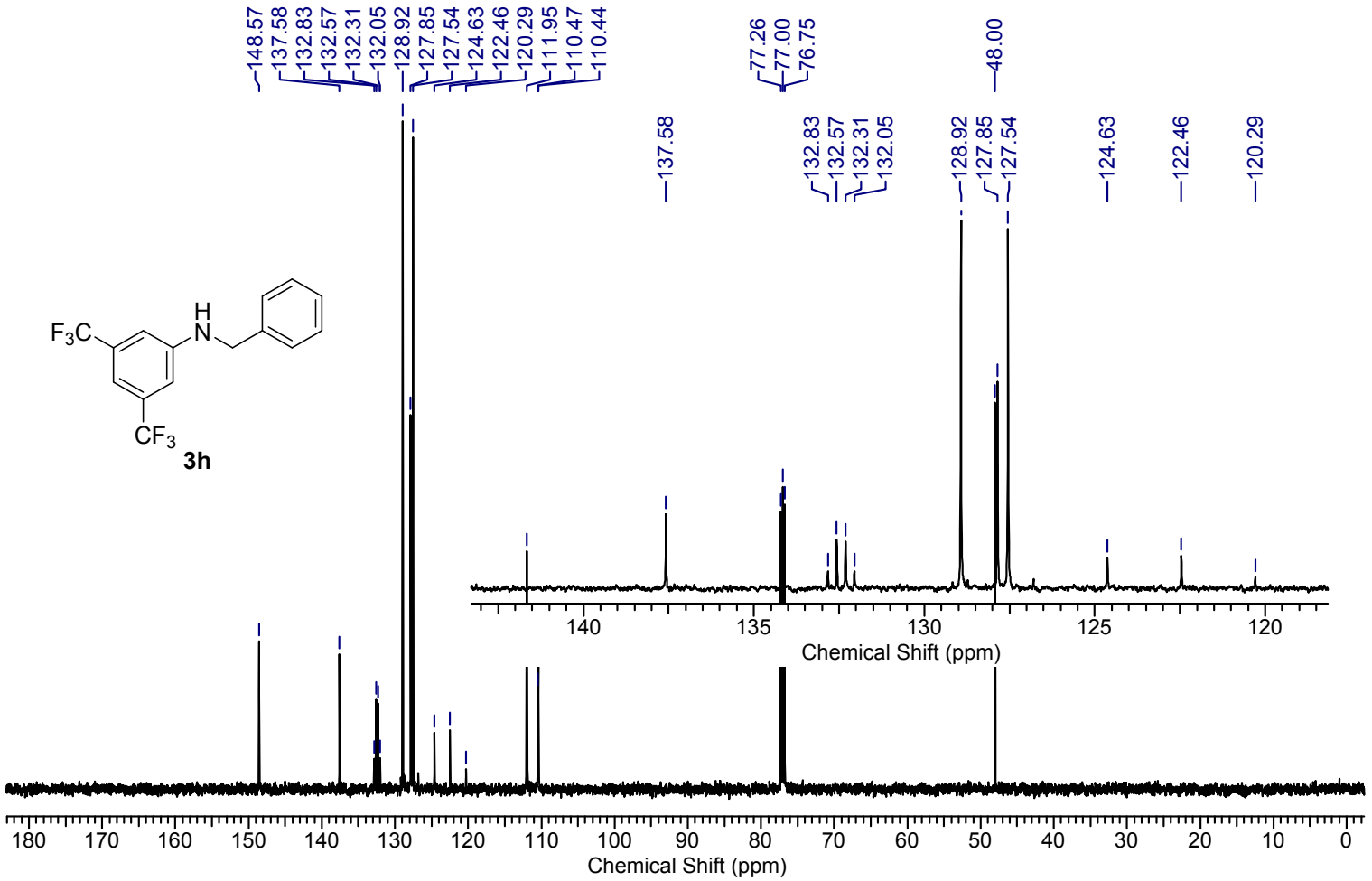
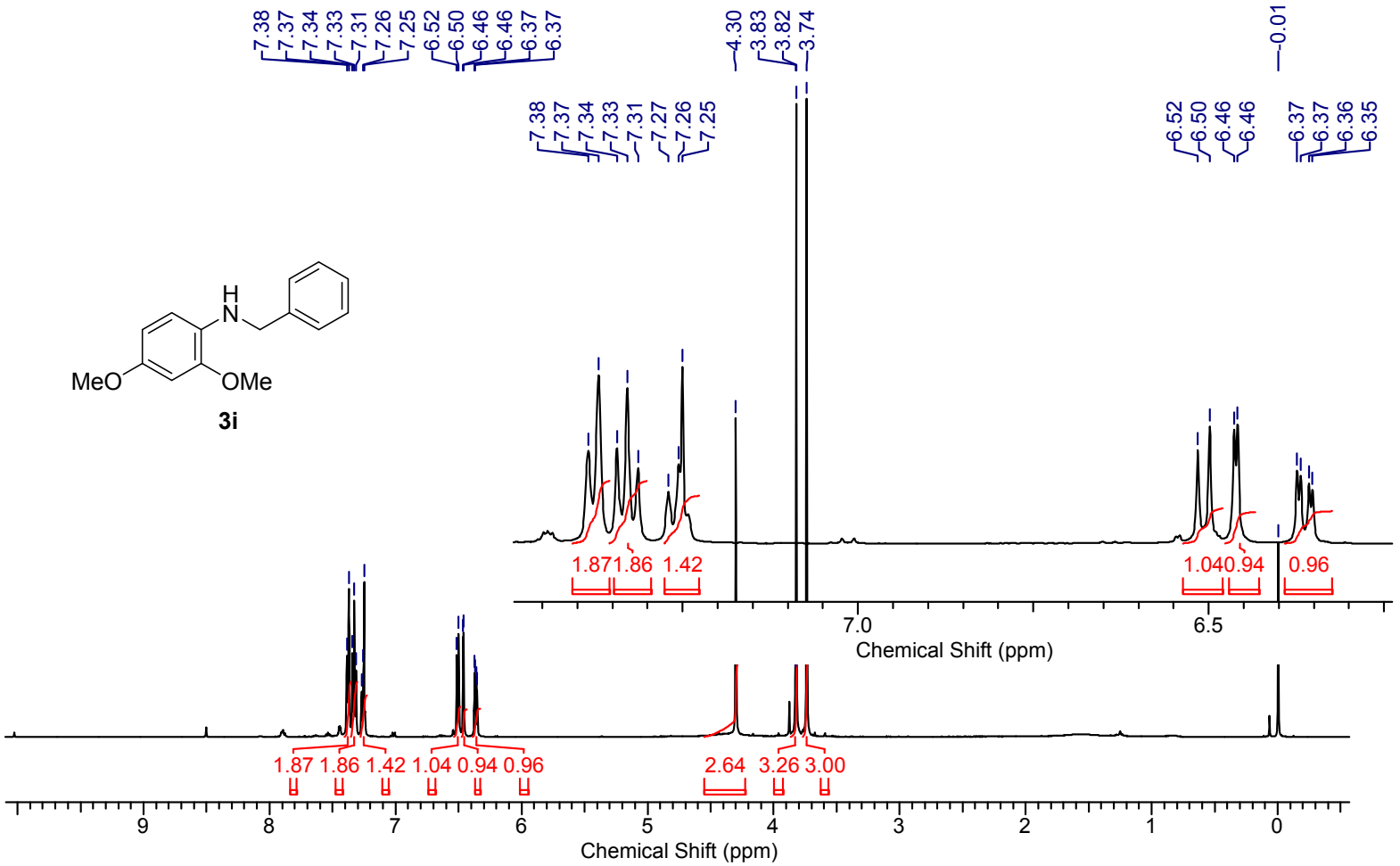
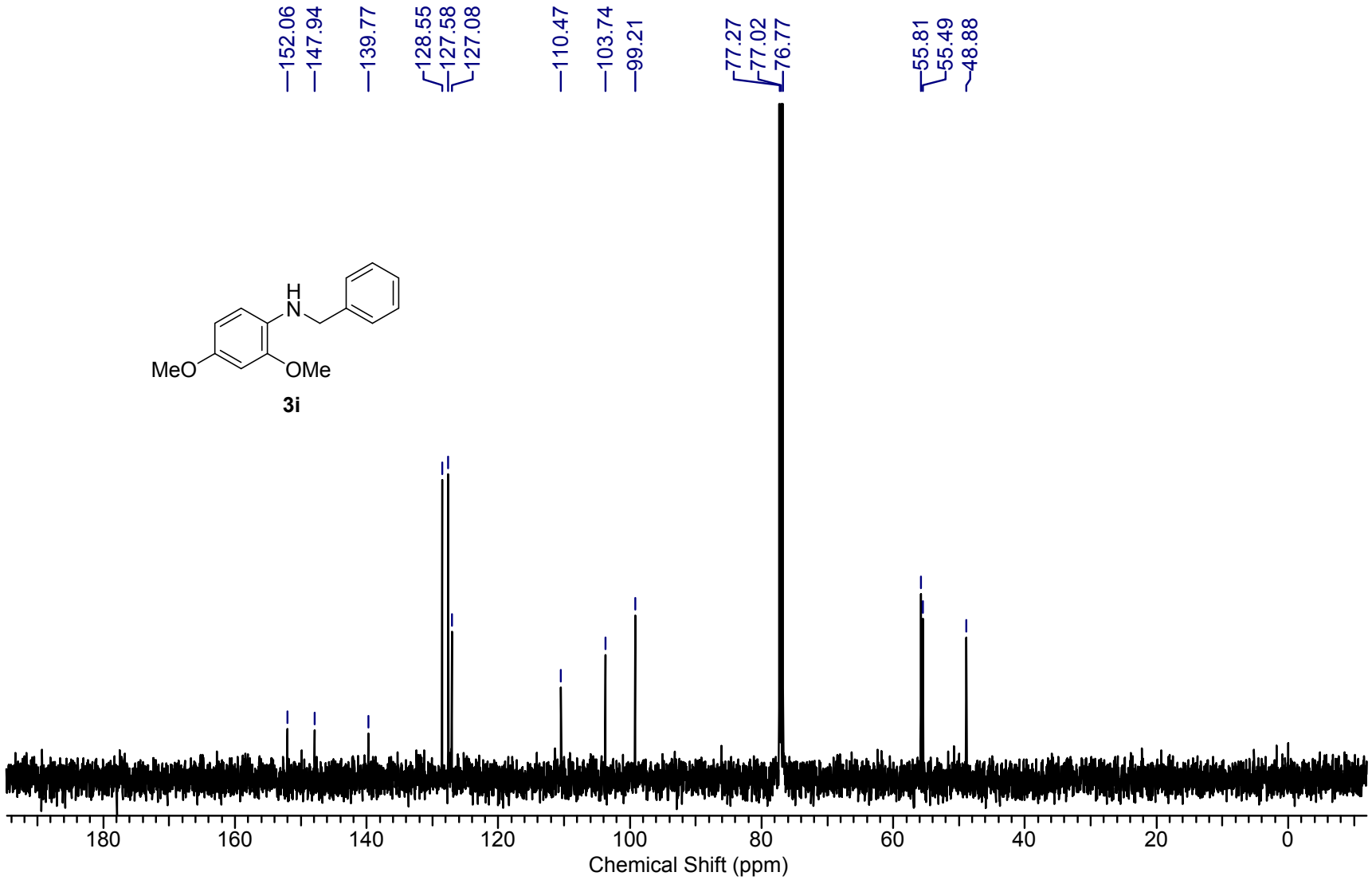
4.38
H
N
Ph
3g
3.89 4.82 1.07 0.96 0.93 0.98 0.99
0.89 1.90
Chemical Shift (ppm)
7.52
7.51
7.50
7.49
7.47
7.40
7.39
7.36
7.35
7.29
7.29
7.24
7.17
7.16
6.83
6.73
6.71
3.89 4.82 1.07 0.96 0.93 0.98 0.99
Chemical Shift (ppm)

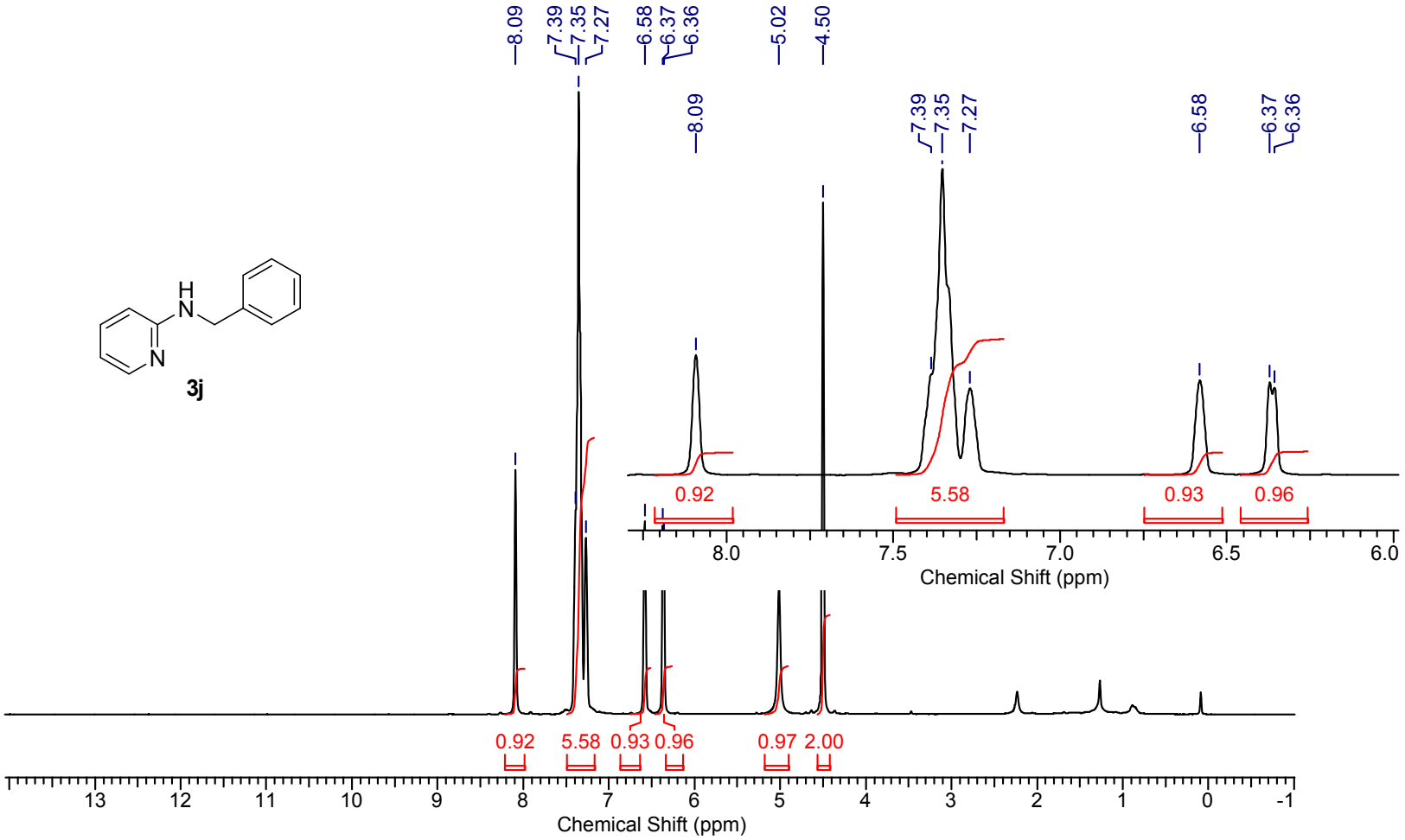

144.75
139.40
130.21
129.36
128.92
128.70
128.57
127.24
127.05
117.27
110.86
77.26
77.00
76.75
48.18
H
N
Ph
3g
130.21
129.36
128.92
128.70
128.57
127.24
127.05
130
129
128
127
Chemical Shift (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

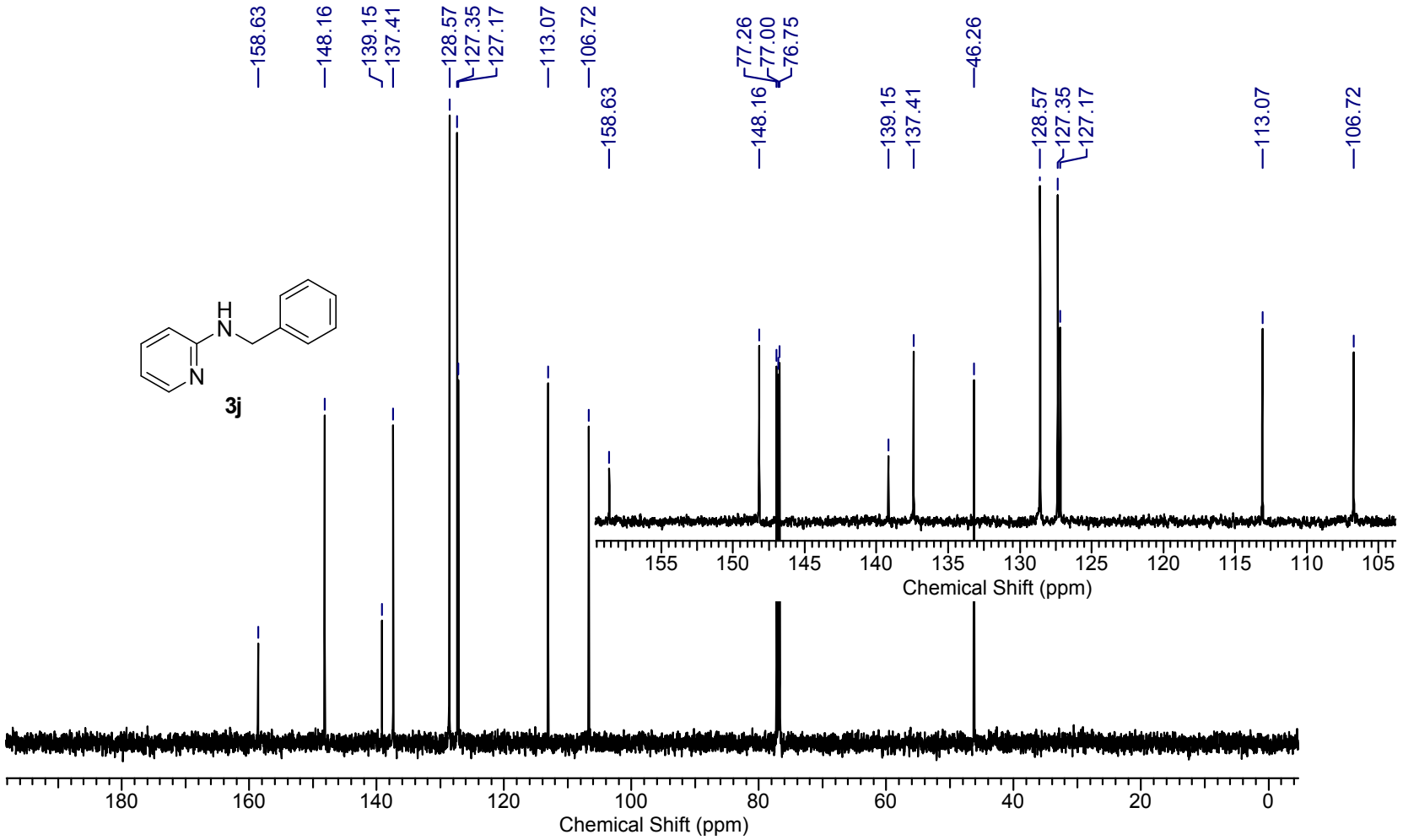

7.42
7.41
7.39
7.39
7.37
7.37
7.36
7.35
7.20
7.00
4.47
4.40
4.39
F3C
CF3
H
N
3h
5.00
1.00
2.04
1.03
2.15
Chemical Shift (ppm)

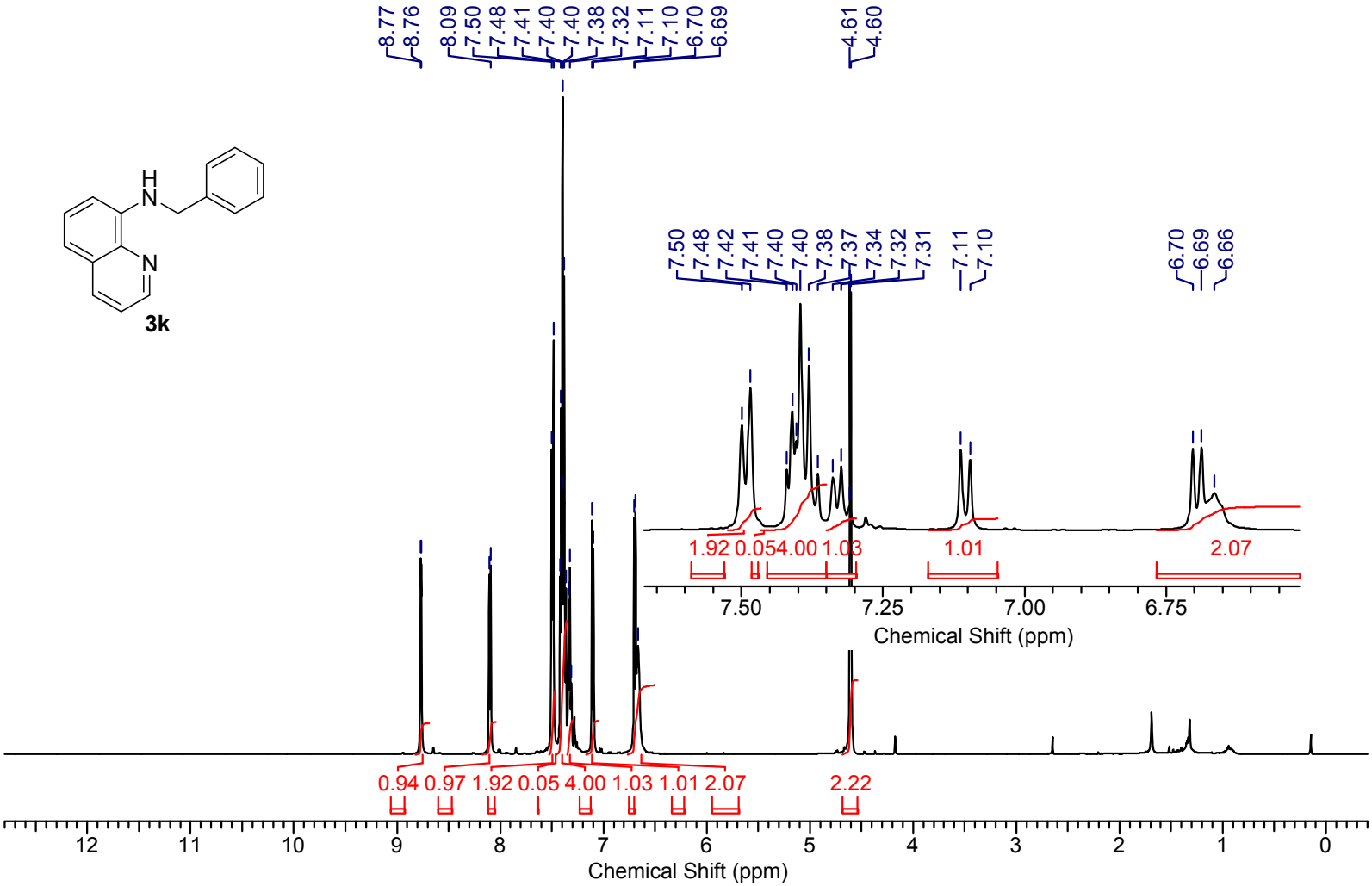

148.57
137.58
132.83
132.57
132.31
132.05
128.92
127.85
127.54
124.63
122.46
120.29
111.95
110.47
110.44
77.26
77.00
76.75
48.00
F3C
H
N
CF3
3h
Chemical Shift (ppm)
Chemical Shift (ppm)

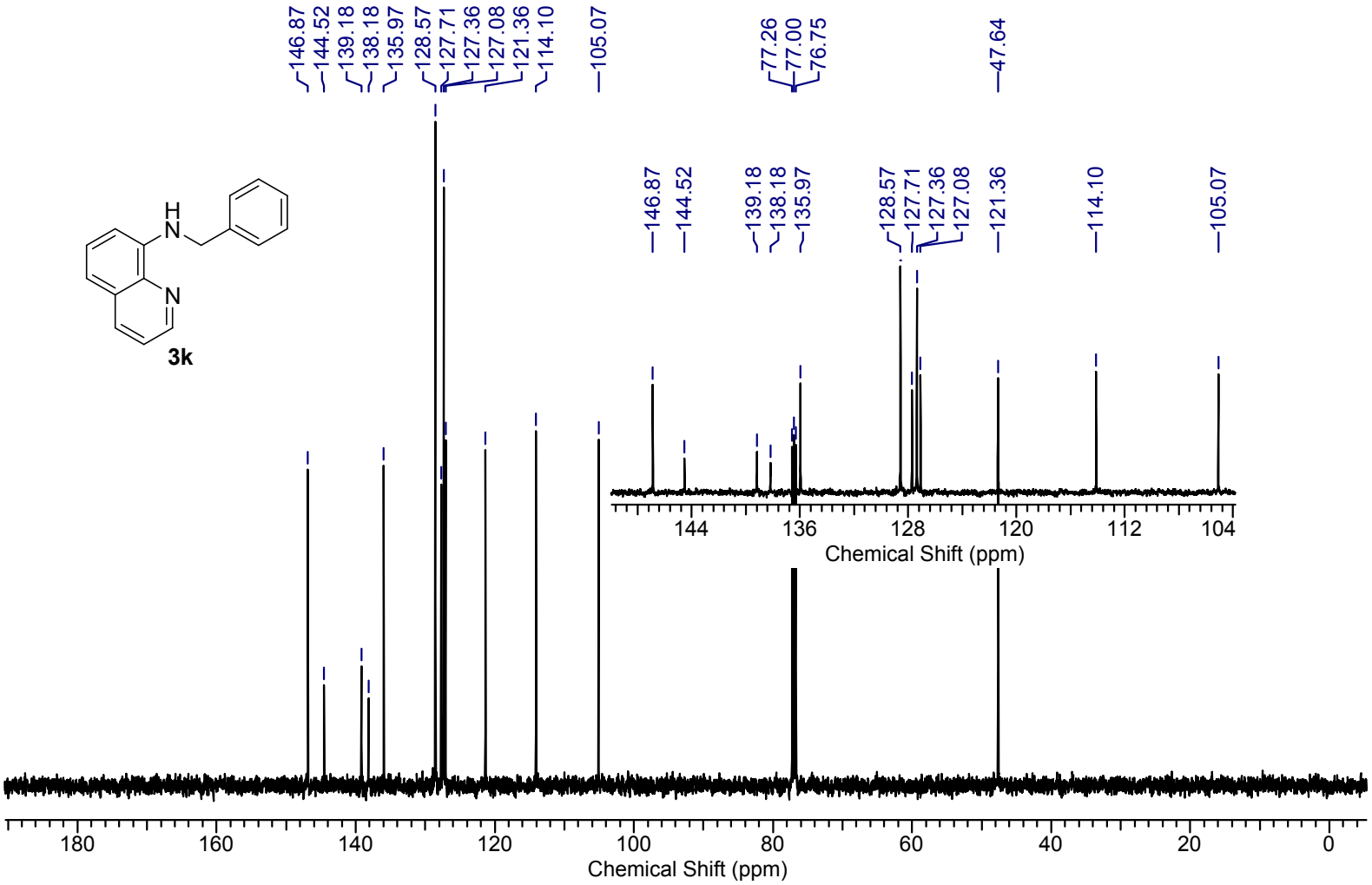

7.38
7.37
7.34
7.33
7.31
7.26
7.25
6.52
6.50
6.46
6.46
6.37
6.37
4.30
3.83
3.82
3.74
0.01
MeO
OMe
3i
1.87 1.86 1.42 1.04 0.94 0.96 2.64 3.26 3.00
Chemical Shift (ppm)

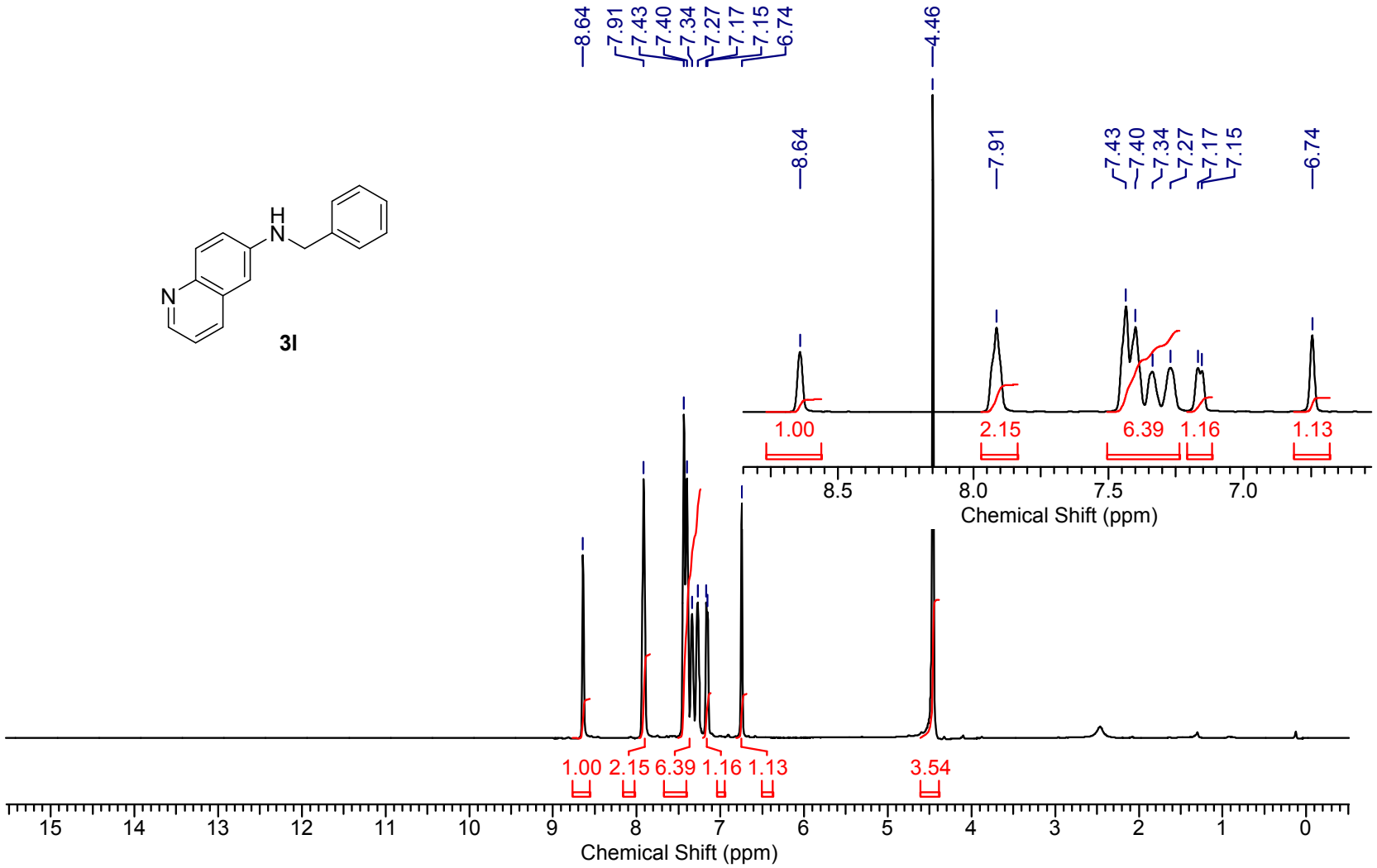

152.06
147.94
139.77
128.55
127.58
127.08
110.47
103.74
99.21
77.27
77.02
76.77
55.81
55.49
48.88
H
N
MeO
OMe
3i
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

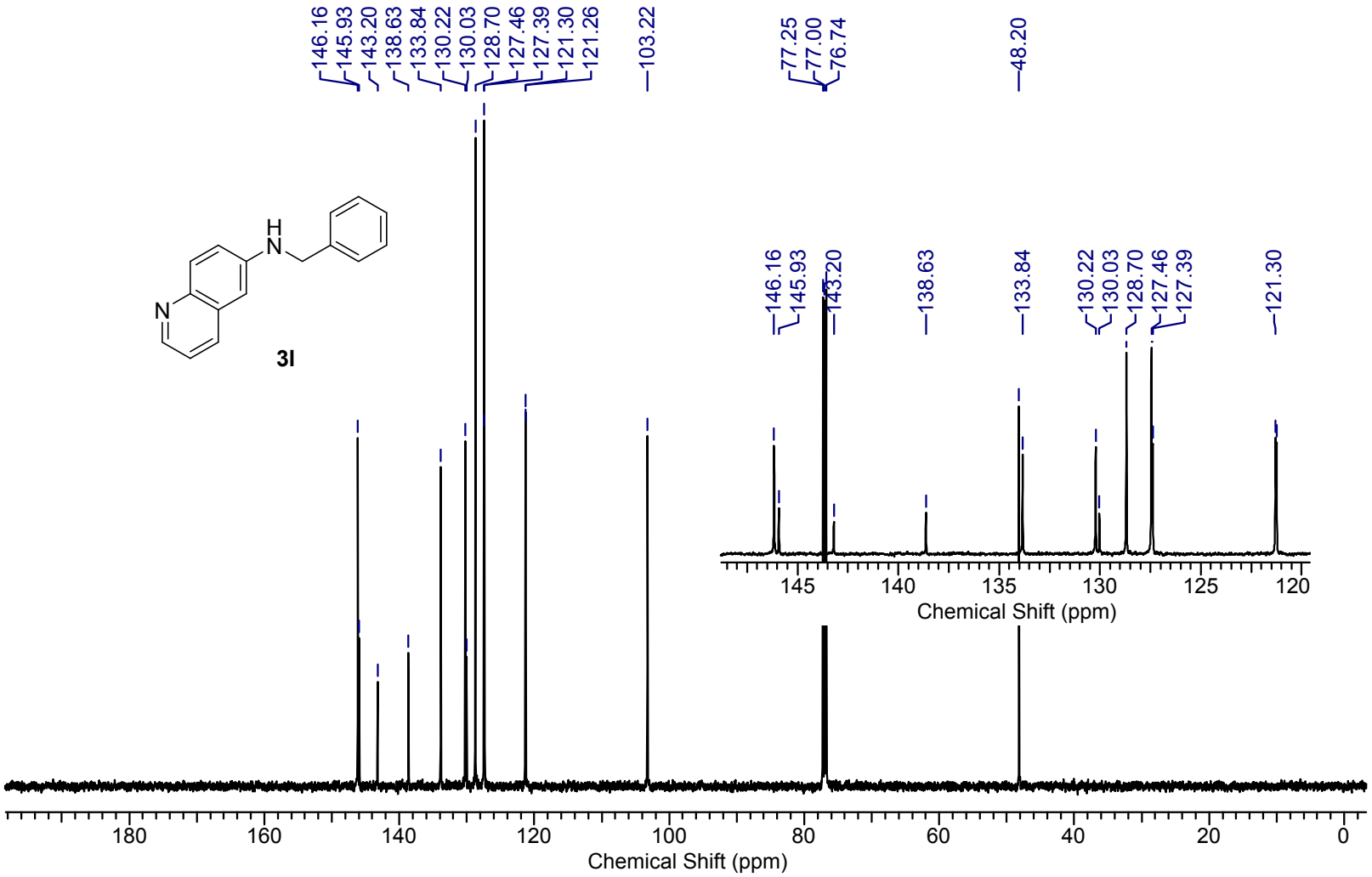

8.09
7.39
7.35
7.27
6.58
6.37
6.36
5.02
4.50
3j
0.92
5.58
0.93
0.96
0.97
2.00
Chemical Shift (ppm)

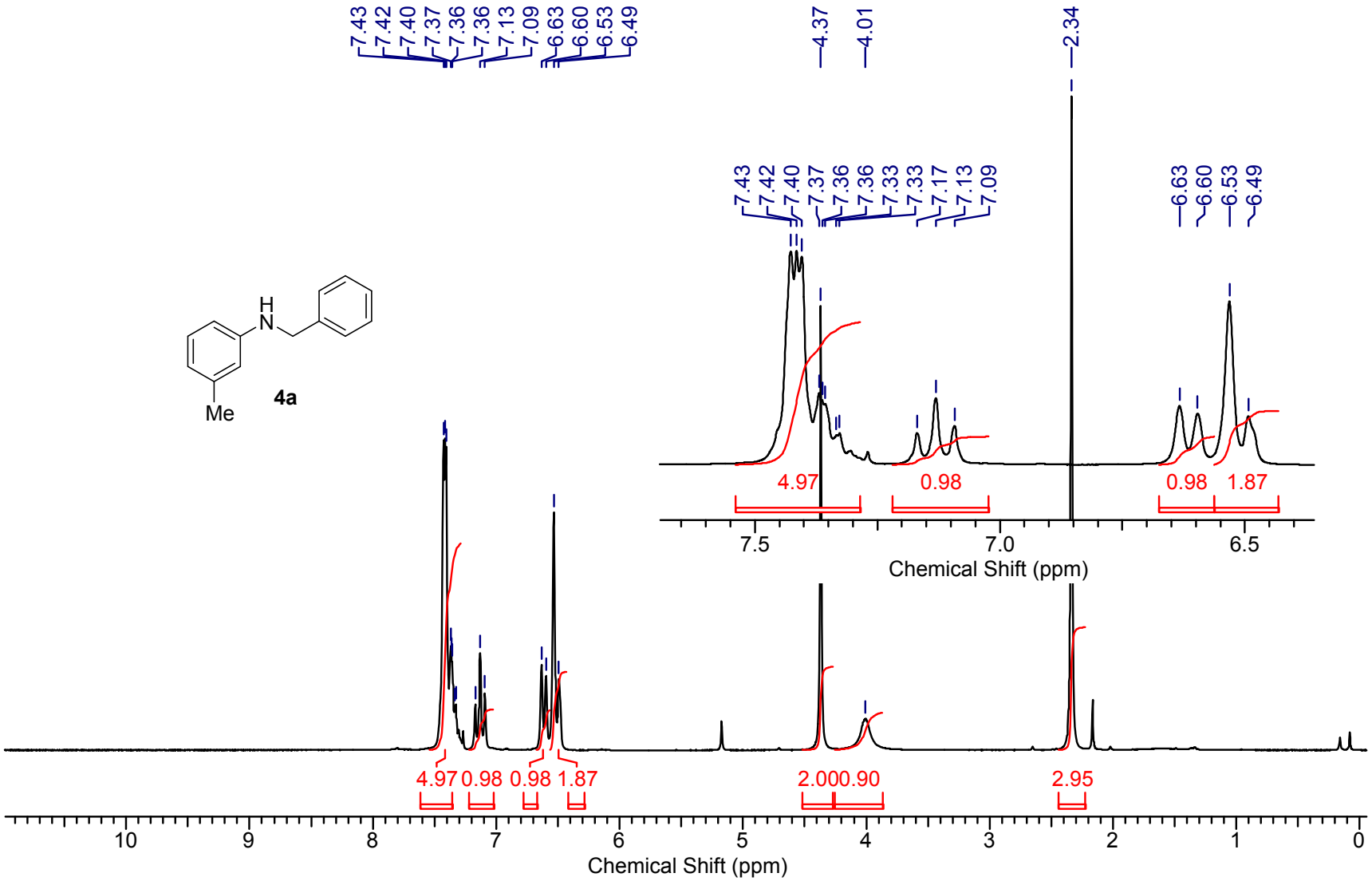

158.63
148.16
139.15
137.41
128.57
127.35
127.17
113.07
106.72
77.26
77.00
76.75
46.26
3j
Chemical Shift (ppm)
Chemical Shift (ppm)

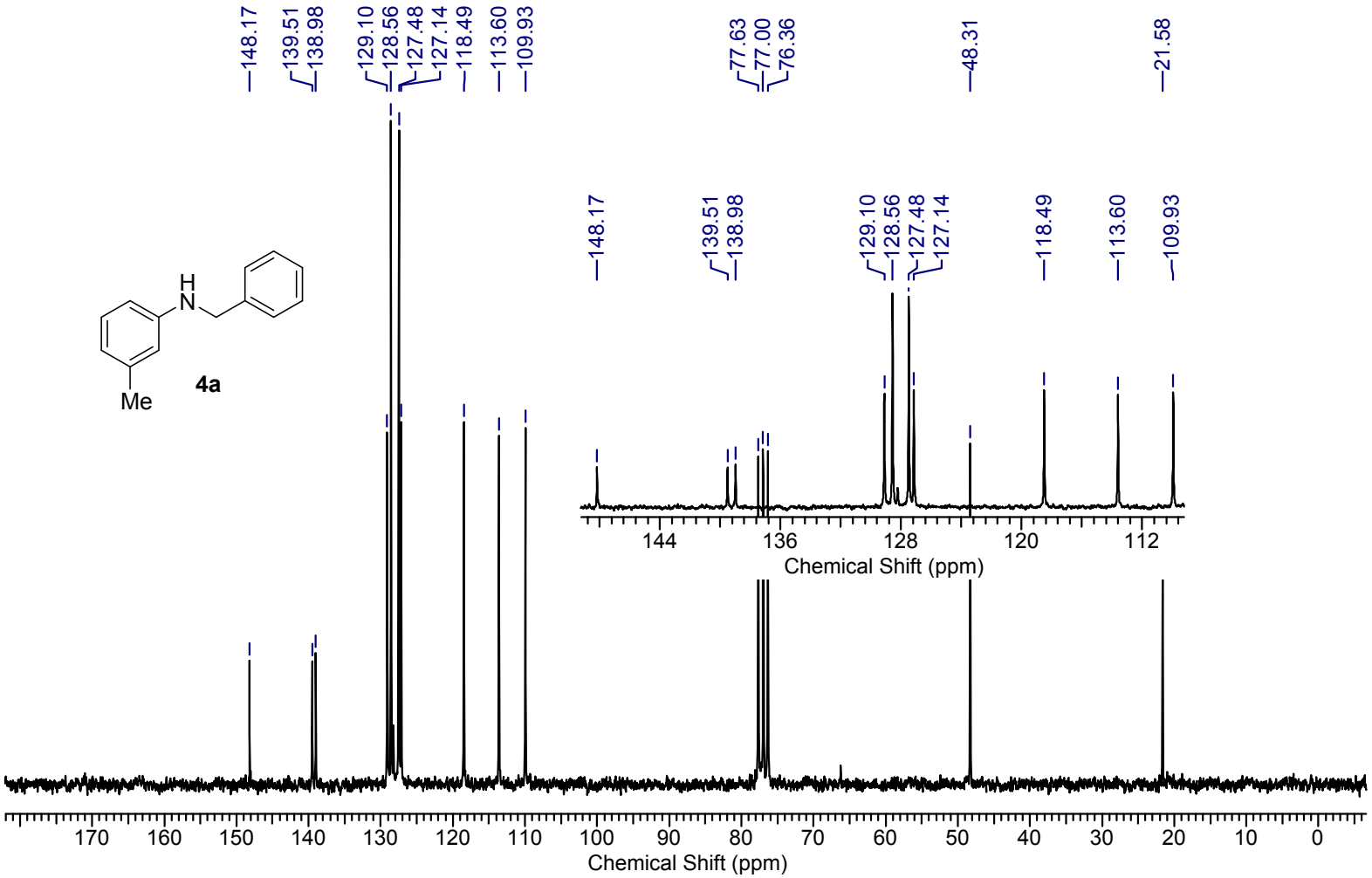

8.77
8.76
8.09
7.50
7.48
7.41
7.40
7.40
7.38
7.32
7.11
7.10
6.70
6.69
4.61
4.60
H
N
N
3k
7.50
7.48
7.42
7.41
7.40
7.40
7.38
7.37
7.34
7.32
7.31
7.11
7.10
6.70
6.69
6.66
1.92 0.05 4.00 1.03
1.01
2.07
7.50
7.25
7.00
6.75
Chemical Shift (ppm)
0.94 0.97 1.92 0.05 4.00 1.03 1.01 2.07
2.22
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

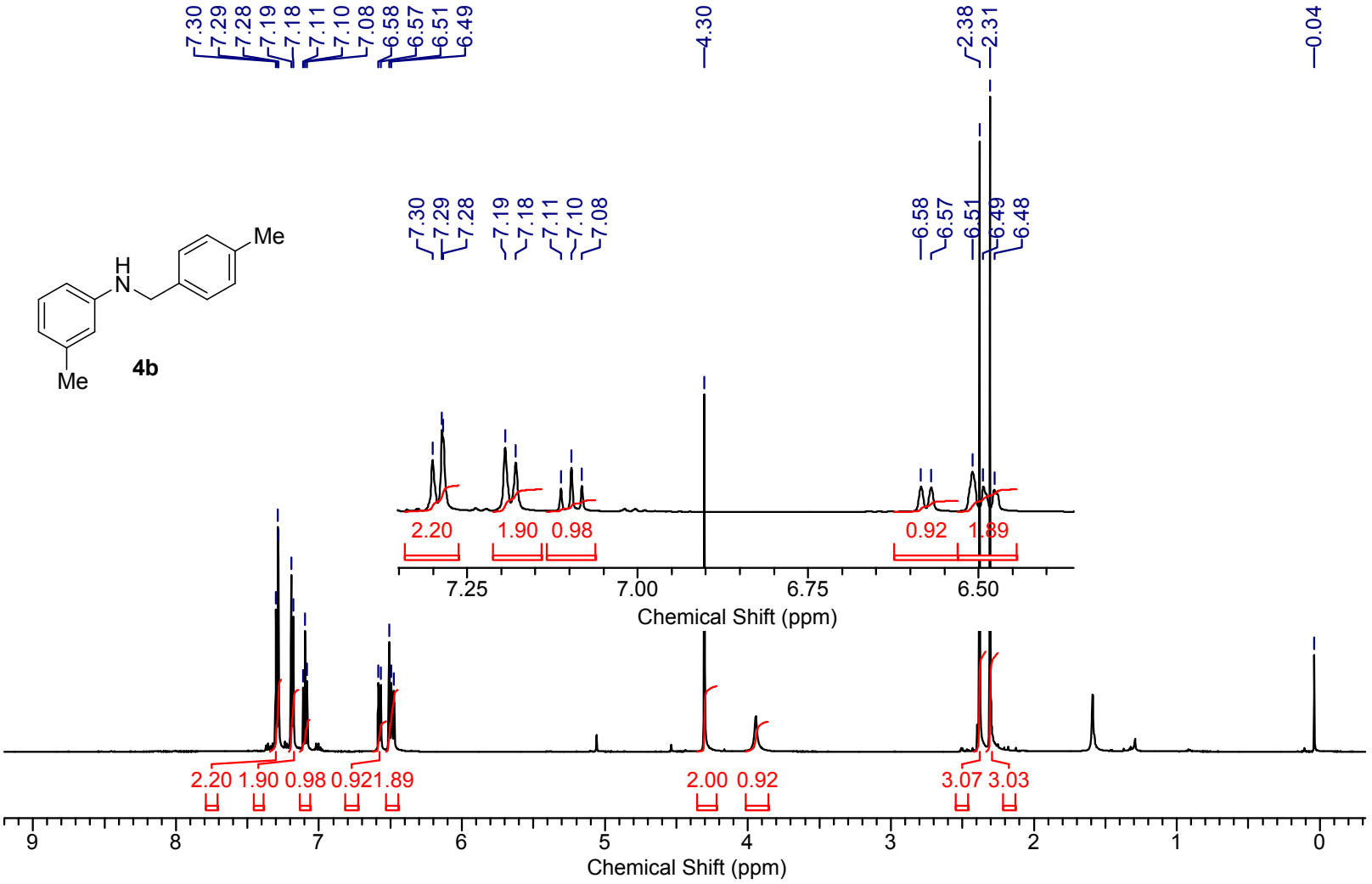

146.87
144.52
139.18
138.18
135.97
128.57
127.71
127.36
127.08
121.36
114.10
105.07
77.26
77.00
76.75
47.64
H
N
N
3k
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
144
136
128
120
112
104
Chemical Shift (ppm)

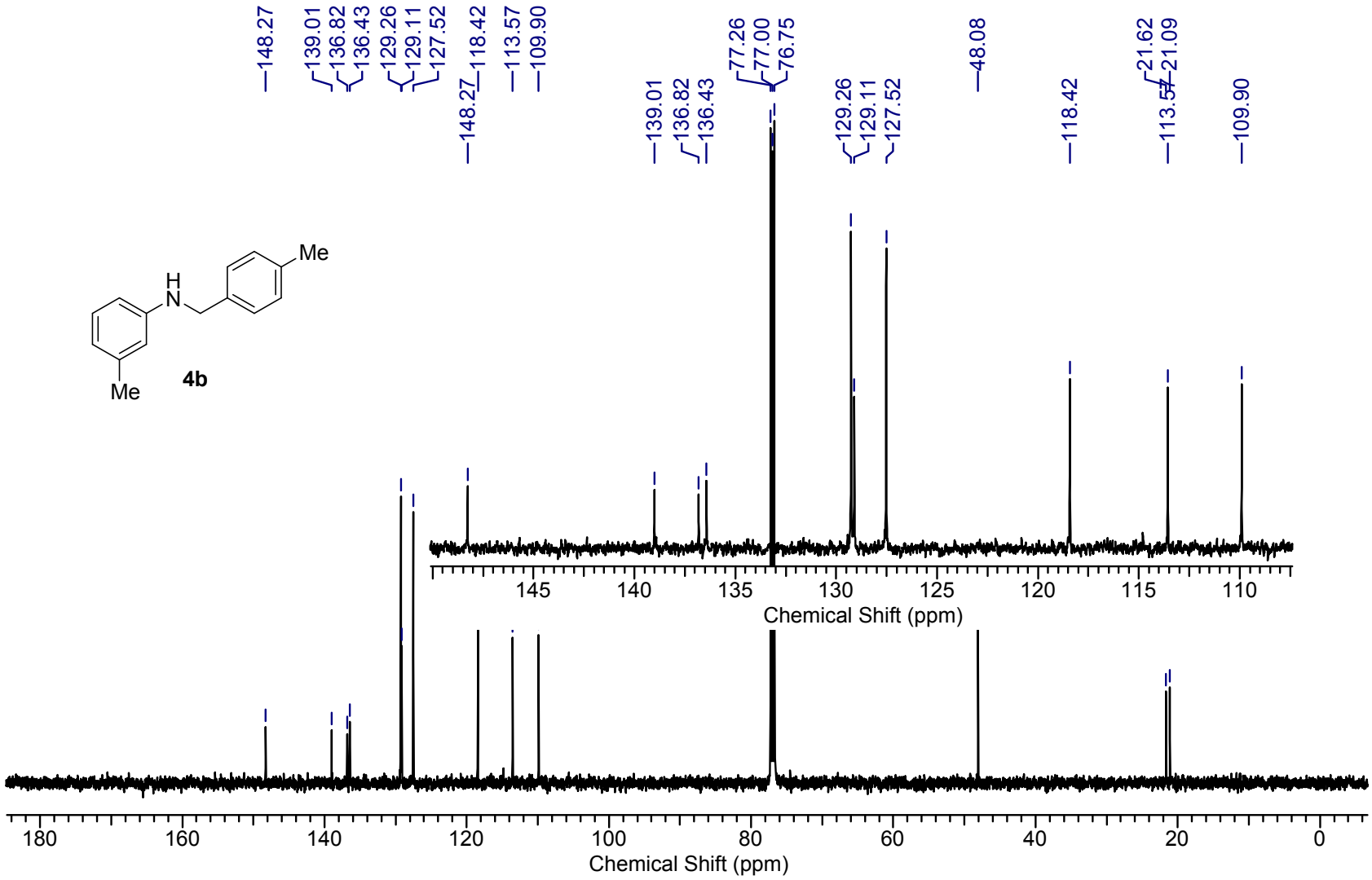

8.64
7.91
7.43
7.40
7.34
7.27
7.17
7.15
6.74
4.46
1.00
2.15
6.39
1.16
1.13
3.54
Chemical Shift (ppm)
3l

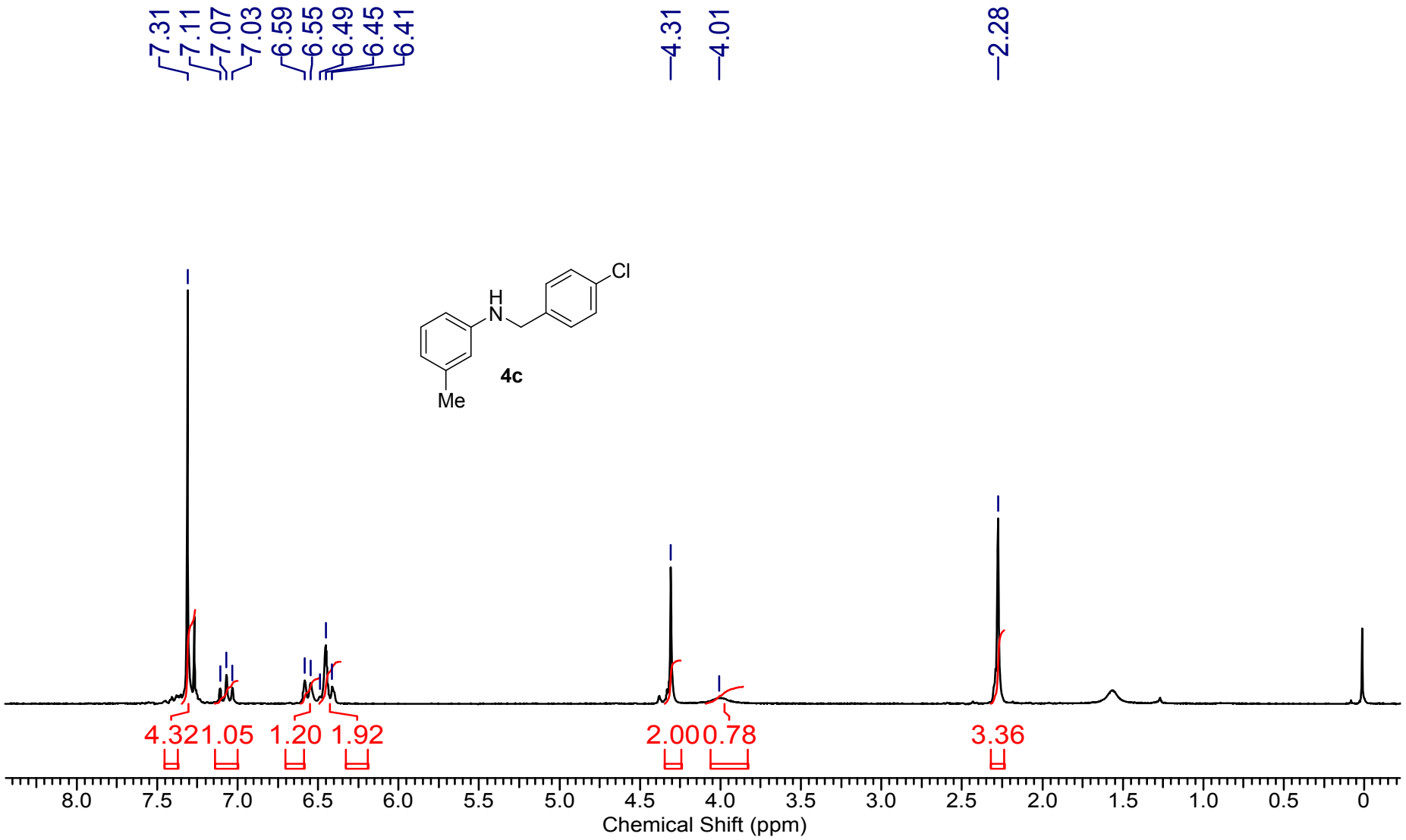

146.16
145.93
143.20
138.63
133.84
130.22
130.03
128.70
127.46
127.39
121.30
121.26
103.22
77.25
77.00
76.74
48.20
H
N
N
3l
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
145
140
135
130
125
120
Chemical Shift (ppm)

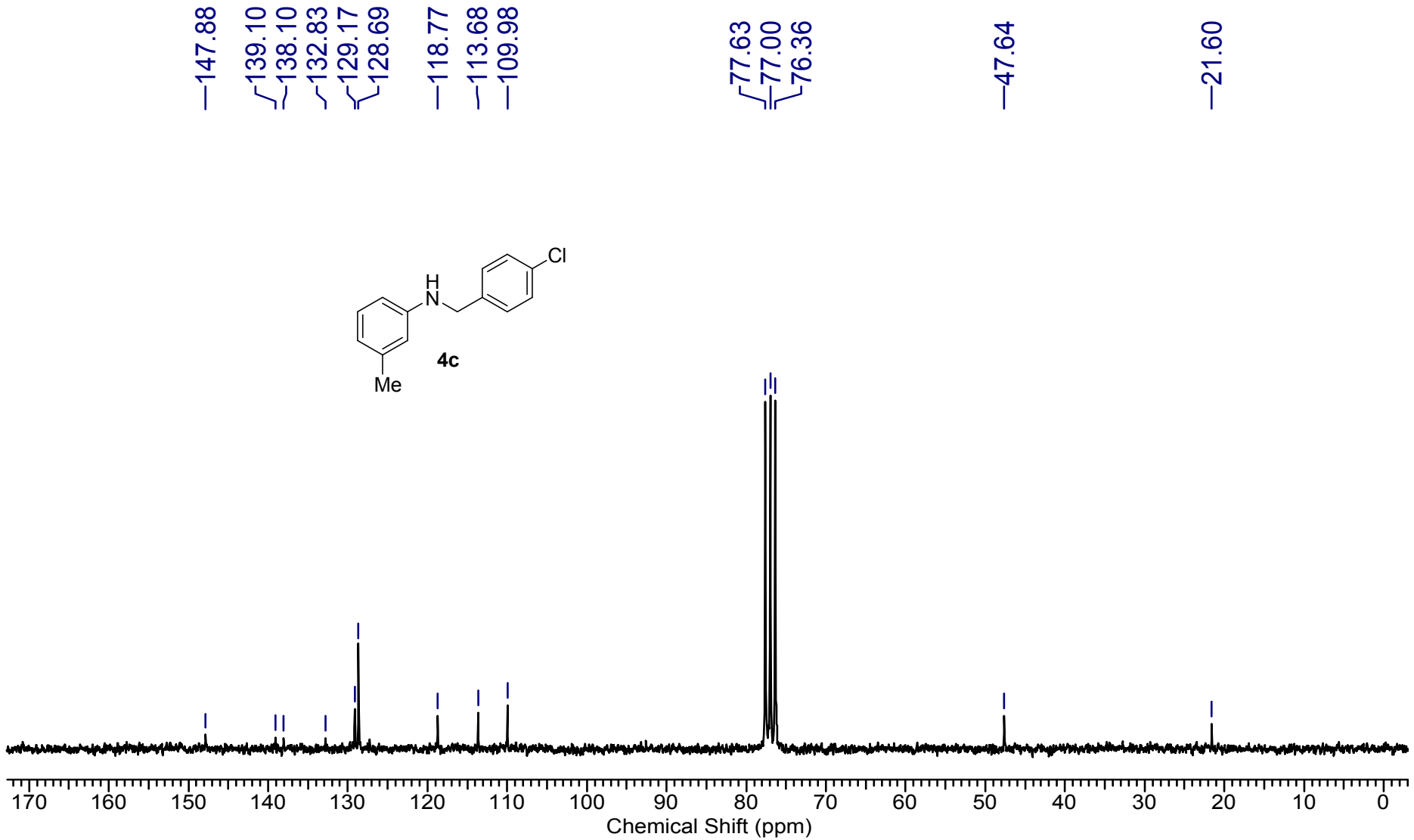

7.43
7.42
7.40
7.37
7.36
7.36
7.13
7.09
6.63
6.60
6.53
6.49
4.37
4.01
2.34
H
N
Me
4a
4.97
0.98
0.98
1.87
2.00
0.90
2.95
Chemical Shift (ppm)
7.5
7.0
6.5
10
9
8
7
6
5
4
3
2
1
0

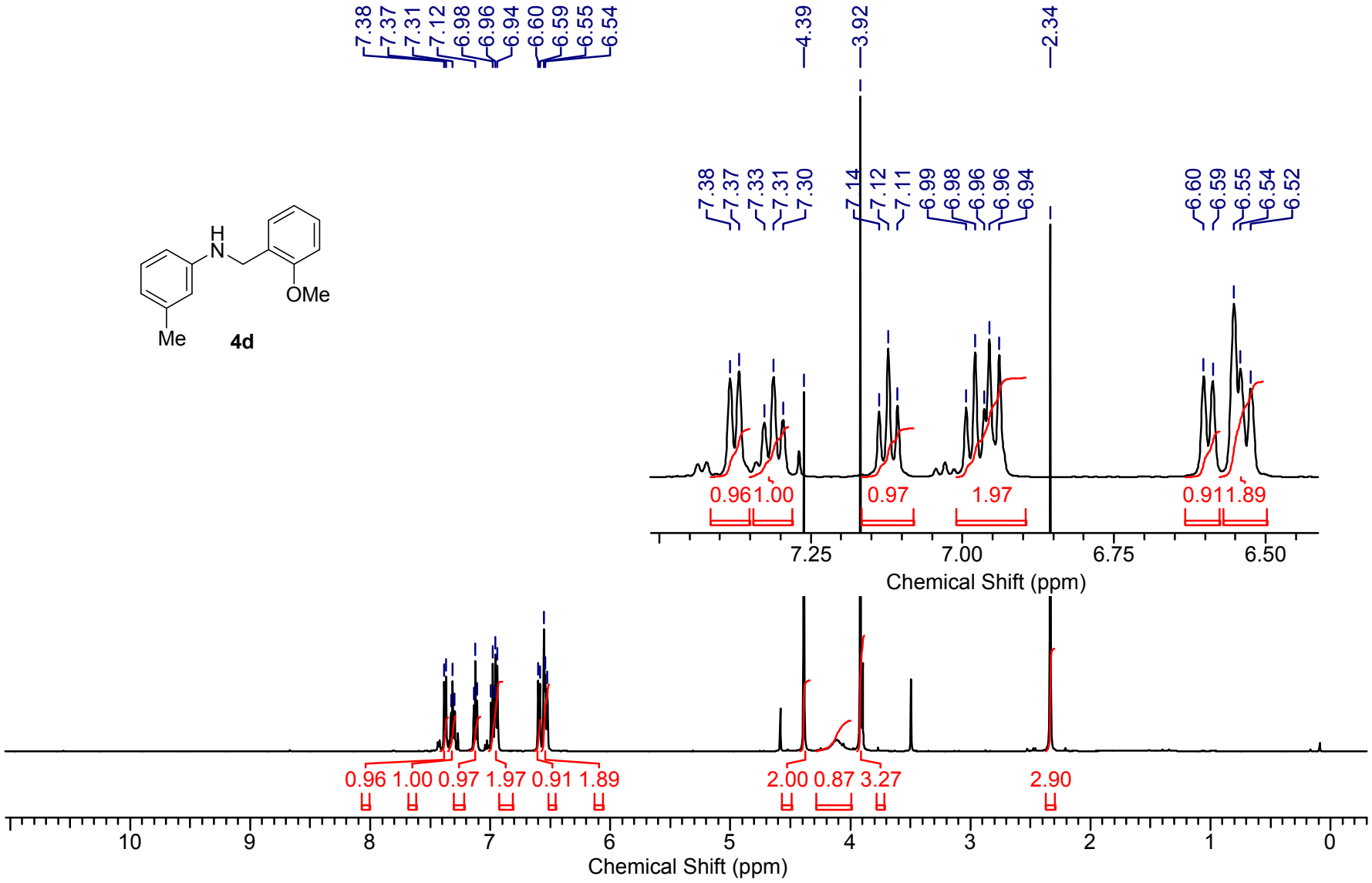

148.17
139.51
138.98
129.10
128.56
127.48
127.14
118.49
113.60
109.93
77.63
77.00
76.36
48.31
21.58
H
N
Me
4a
Chemical Shift (ppm)
Chemical Shift (ppm)

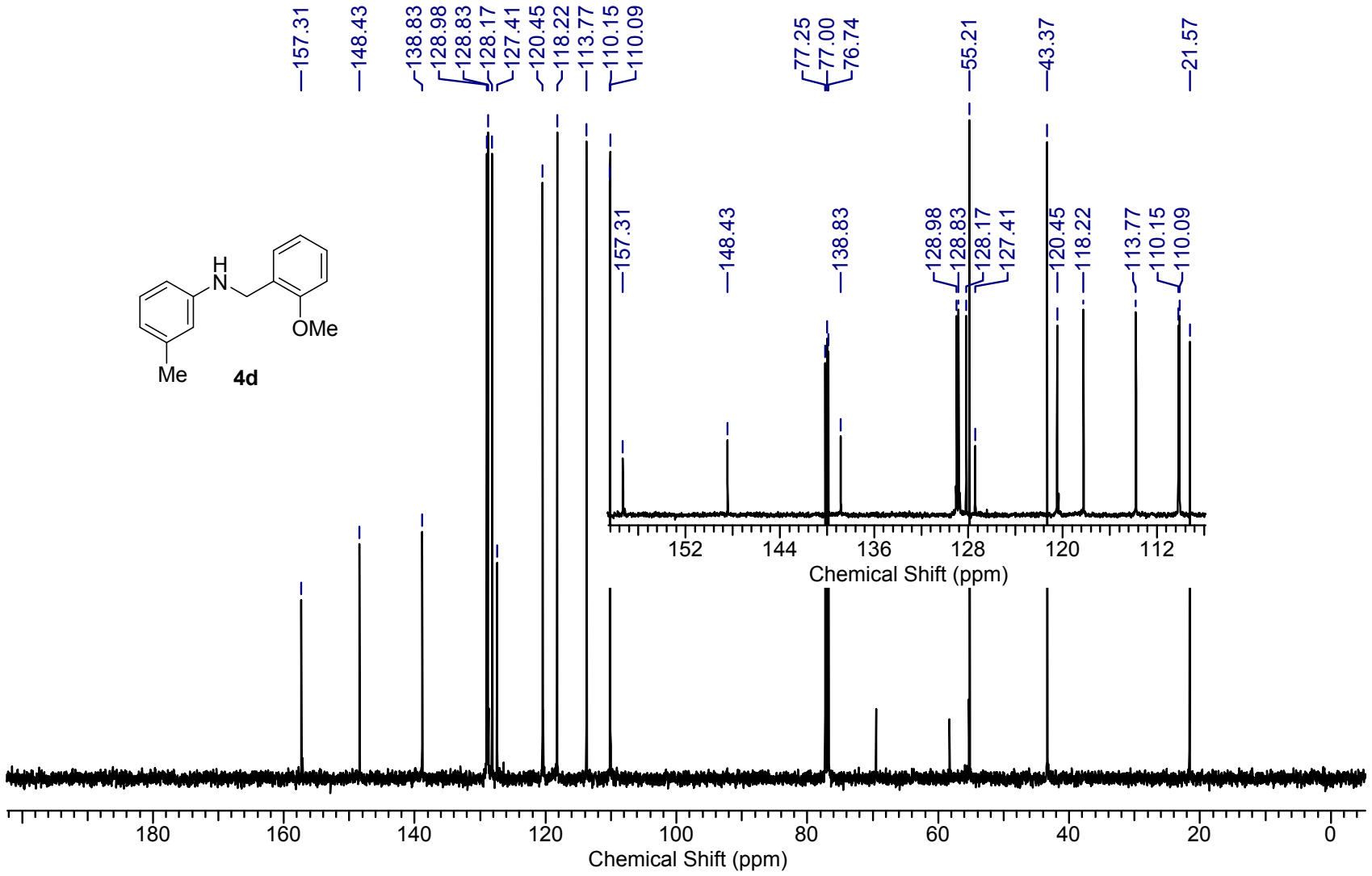

7.30
7.29
7.28
7.19
7.18
7.11
7.10
7.08
6.58
6.57
6.51
6.49
4.30
2.38
2.31
0.04
Me
H
N
Me
4b
6.48
2.20 1.90 0.98 0.92 1.89
2.00 0.92
3.07 3.03
Chemical Shift (ppm)
2.20 1.90 0.98
0.92 1.89
7.25
7.00
6.75
6.50
Chemical Shift (ppm)

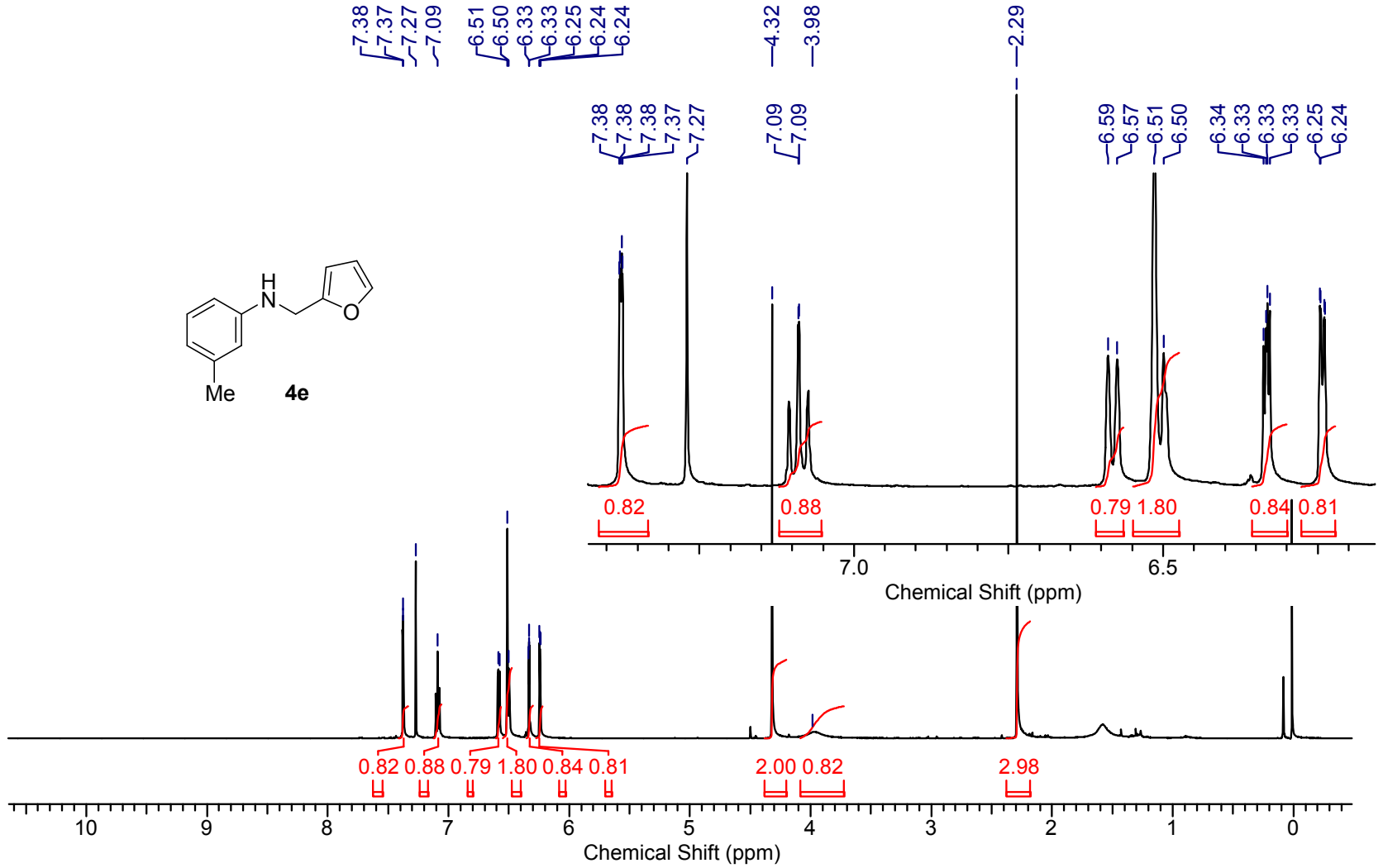

148.27
139.01
136.82
136.43
129.26
129.11
127.52
118.42
113.57
109.90
77.26
77.00
76.75
48.08
21.62
21.09
Me
H
N
Me
4b
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
145
140
135
130
125
120
115
110
Chemical Shift (ppm)

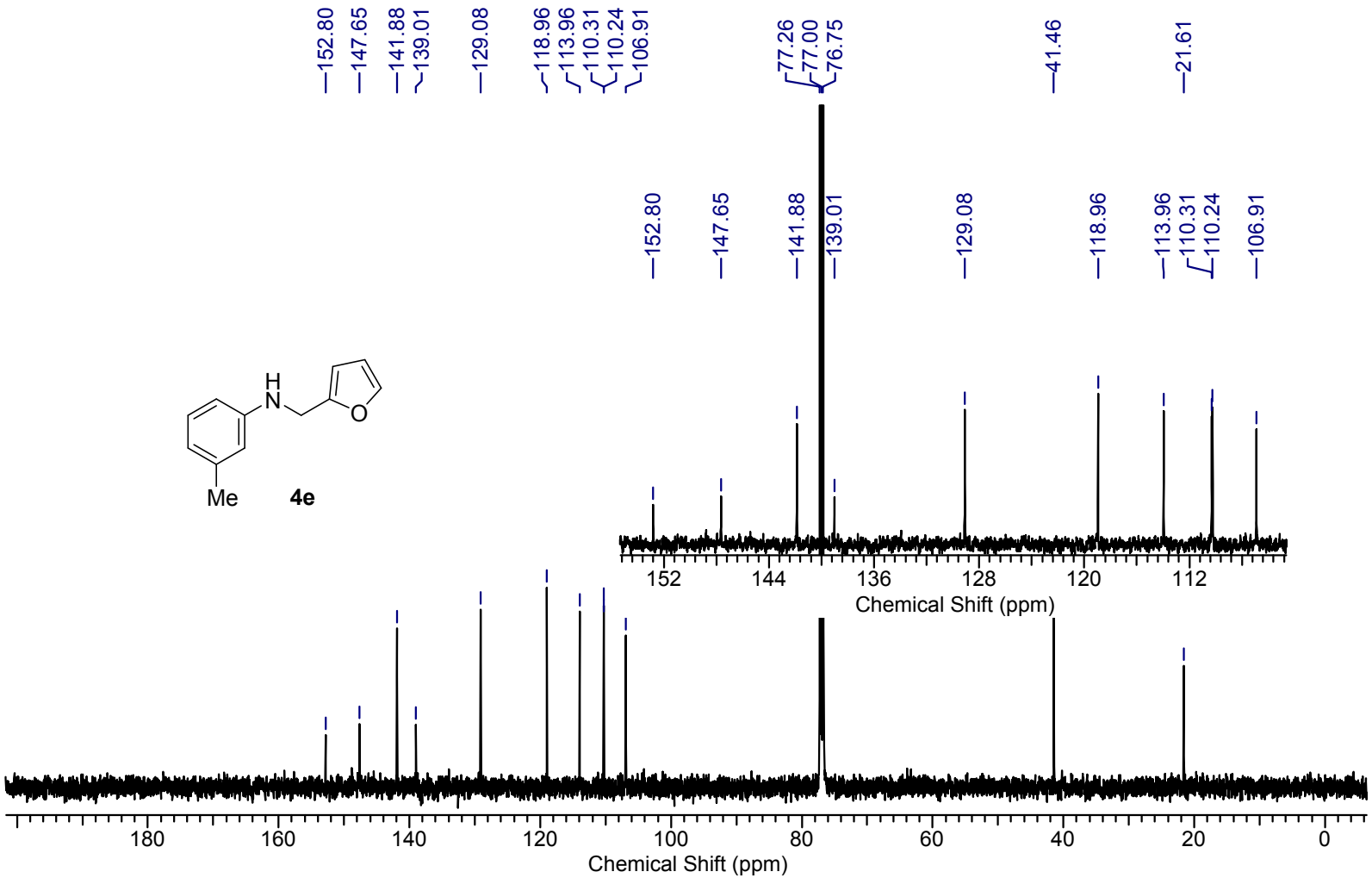

7.31
7.11
7.07
7.03
6.59
6.55
6.49
6.45
6.41
4.31
4.01
2.28
Cl
H
N
Me
4c
4.32
1.05
1.20
1.92
2.00
0.78
3.36
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

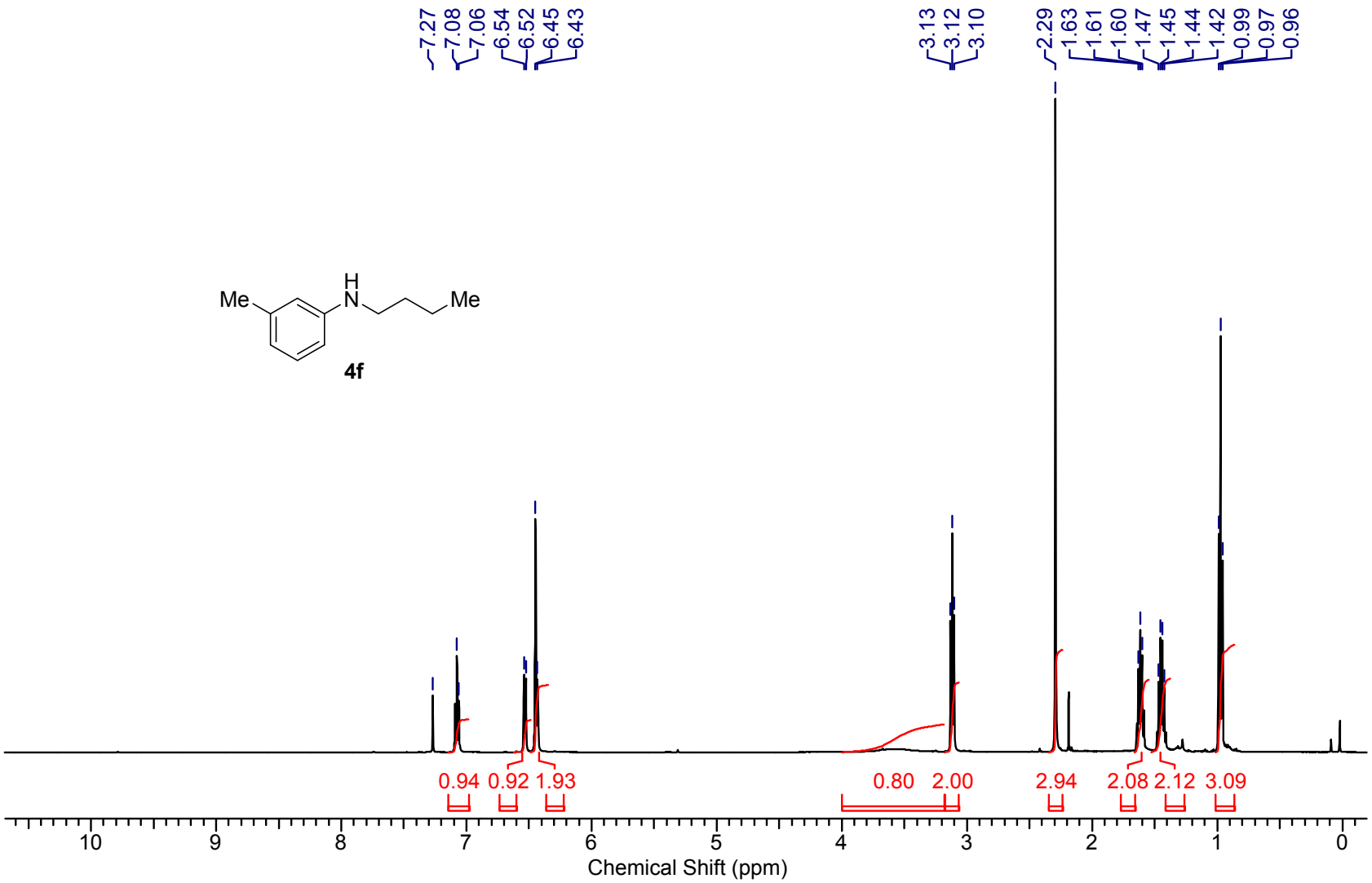

147.88
139.10
138.10
132.83
129.17
128.69
118.77
113.68
109.98
77.63
77.00
76.36
47.64
21.60
Cl
H
N
Me
4c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

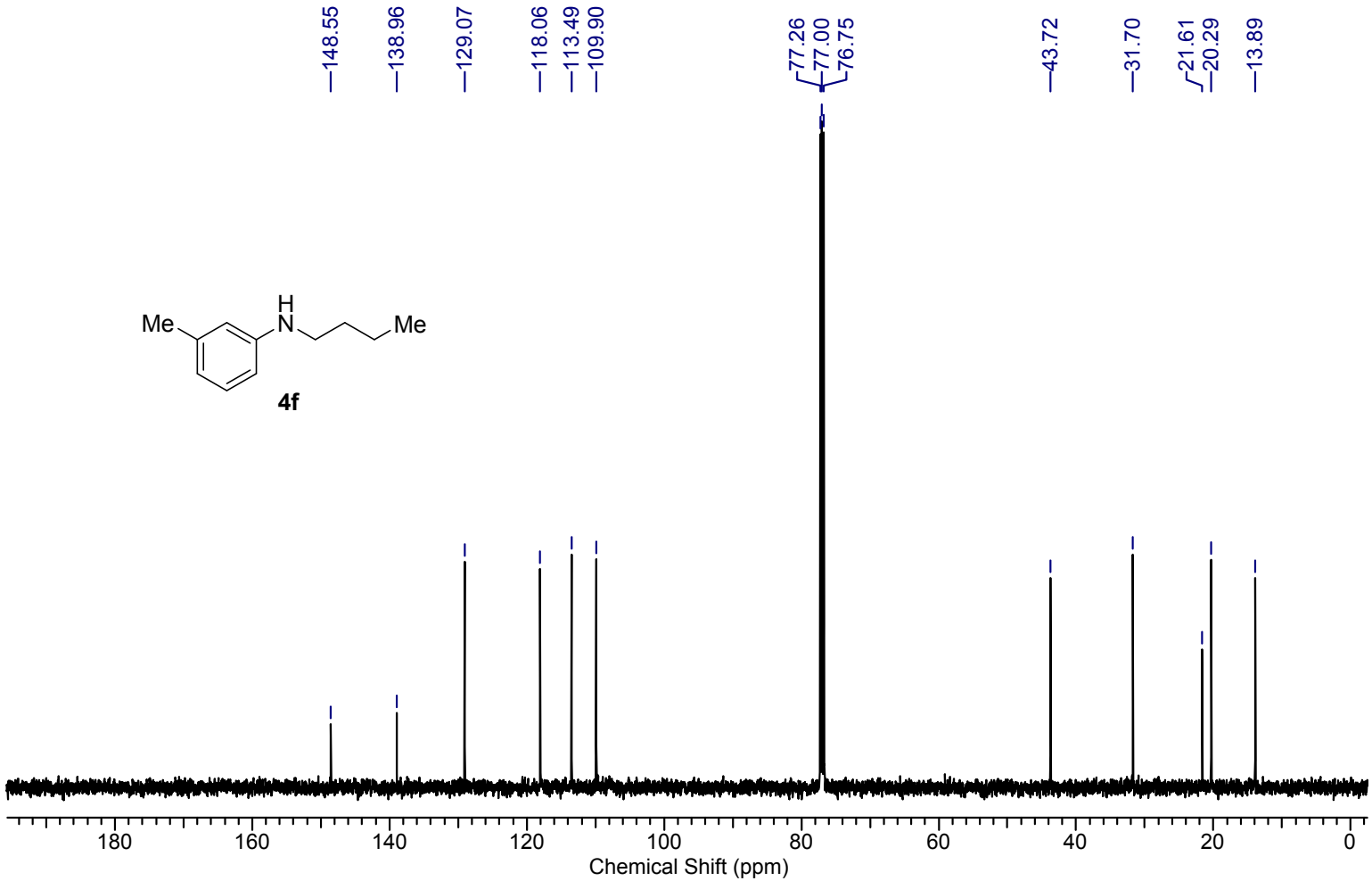

7.38
7.37
7.31
7.12
6.98
6.96
6.94
6.60
6.59
6.55
6.54
4.39
3.92
2.34
H
N
OMe
Me
4d
7.38
7.37
7.33
7.31
7.30
7.14
7.12
7.11
6.99
6.98
6.96
6.96
6.94
6.60
6.59
6.55
6.54
6.52
0.96 1.00
0.97
1.97
0.91 1.89
7.25
7.00
6.75
6.50
Chemical Shift (ppm)
0.96 1.00 0.97 1.97 0.91 1.89
2.00 0.87 3.27
2.90
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


157.31
148.43
138.83
128.98
128.83
128.17
127.41
120.45
118.22
113.77
110.15
110.09
77.25
77.00
76.74
55.21
43.37
21.57
H
N
OMe
Me
4d
Chemical Shift (ppm)
Chemical Shift (ppm)


7.38
7.37
7.27
7.09
6.51
6.50
6.33
6.33
6.25
6.24
6.24
4.32
3.98
2.29
H
N
O
Me
4e
0.82 0.88 0.79 1.80 0.84 0.81
2.00 0.82
2.98
Chemical Shift (ppm)
0.82
0.88
0.79 1.80
0.84 0.81
Chemical Shift (ppm)


152.80
147.65
141.88
139.01
129.08
118.96
113.96
110.31
110.24
106.91
77.26
77.00
76.75
41.46
21.61
H
N
O
Me
4e
Chemical Shift (ppm)
Chemical Shift (ppm)


7.27
7.08
7.06
6.54
6.52
6.45
6.43
3.13
3.12
3.10
2.29
1.63
1.61
1.60
1.47
1.45
1.44
1.42
0.99
0.97
0.96
Me
H
N
Me
4f
0.94
0.92
1.93
0.80
2.00
2.94
2.08
2.12
3.09
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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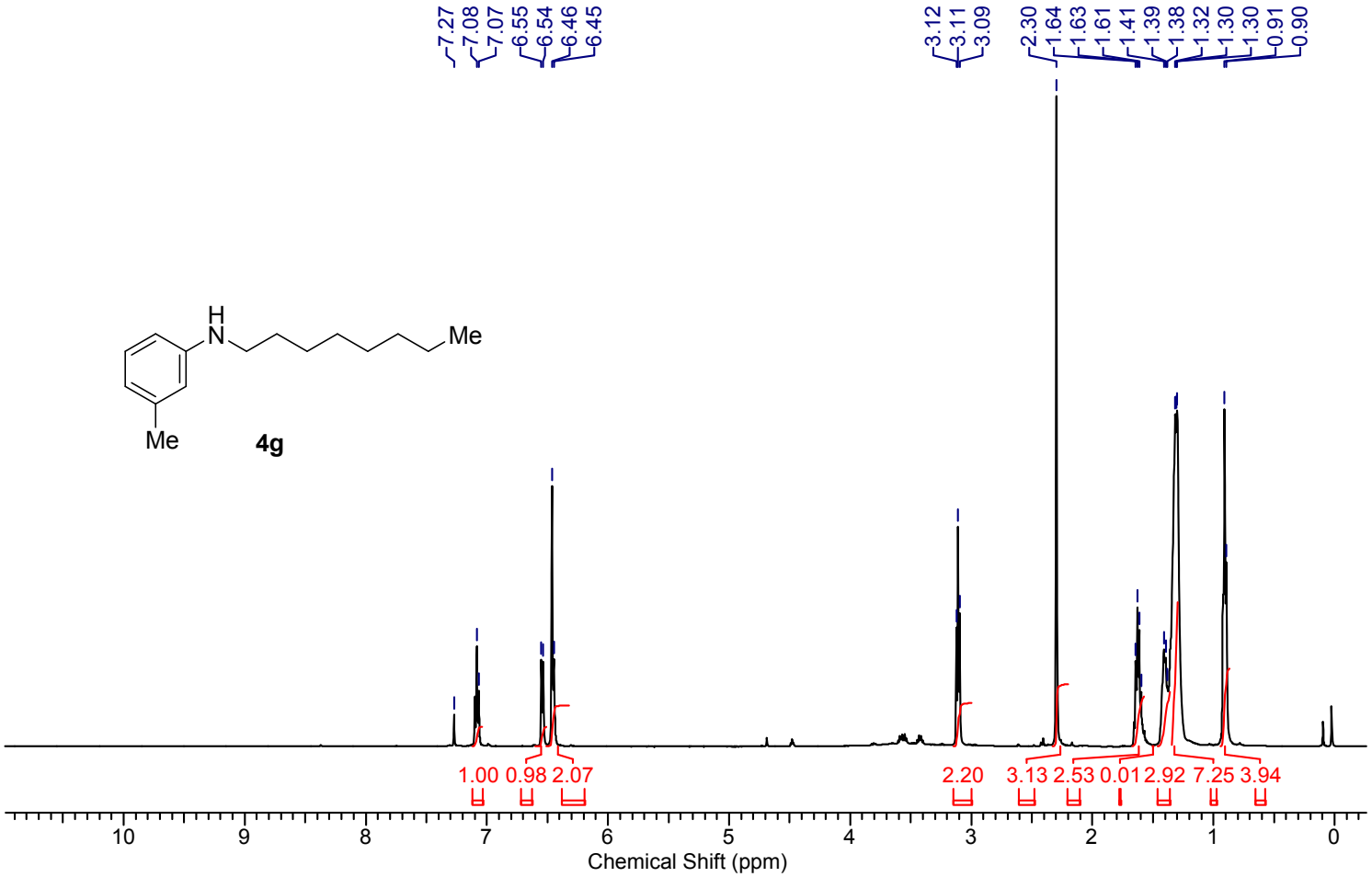
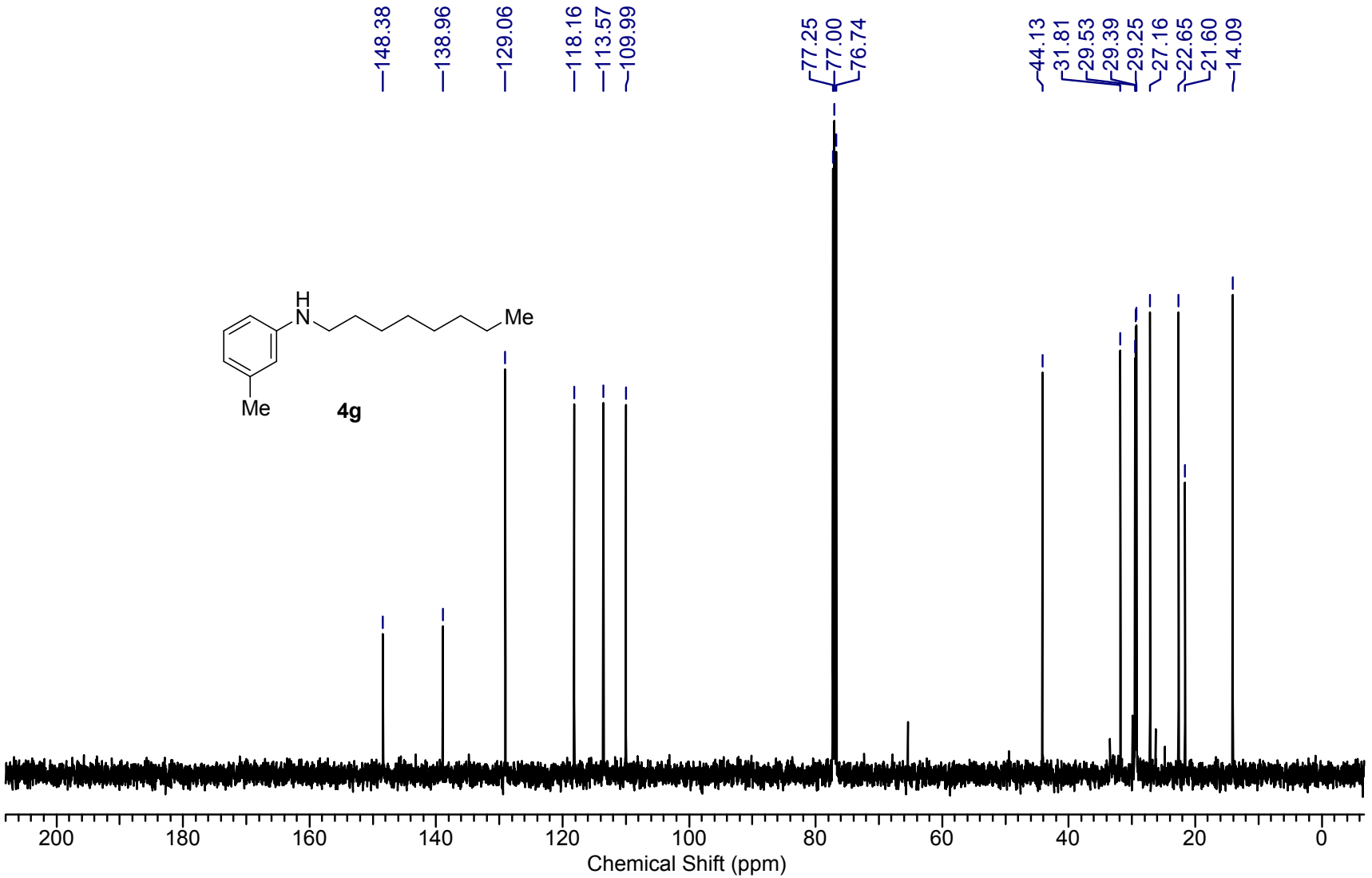
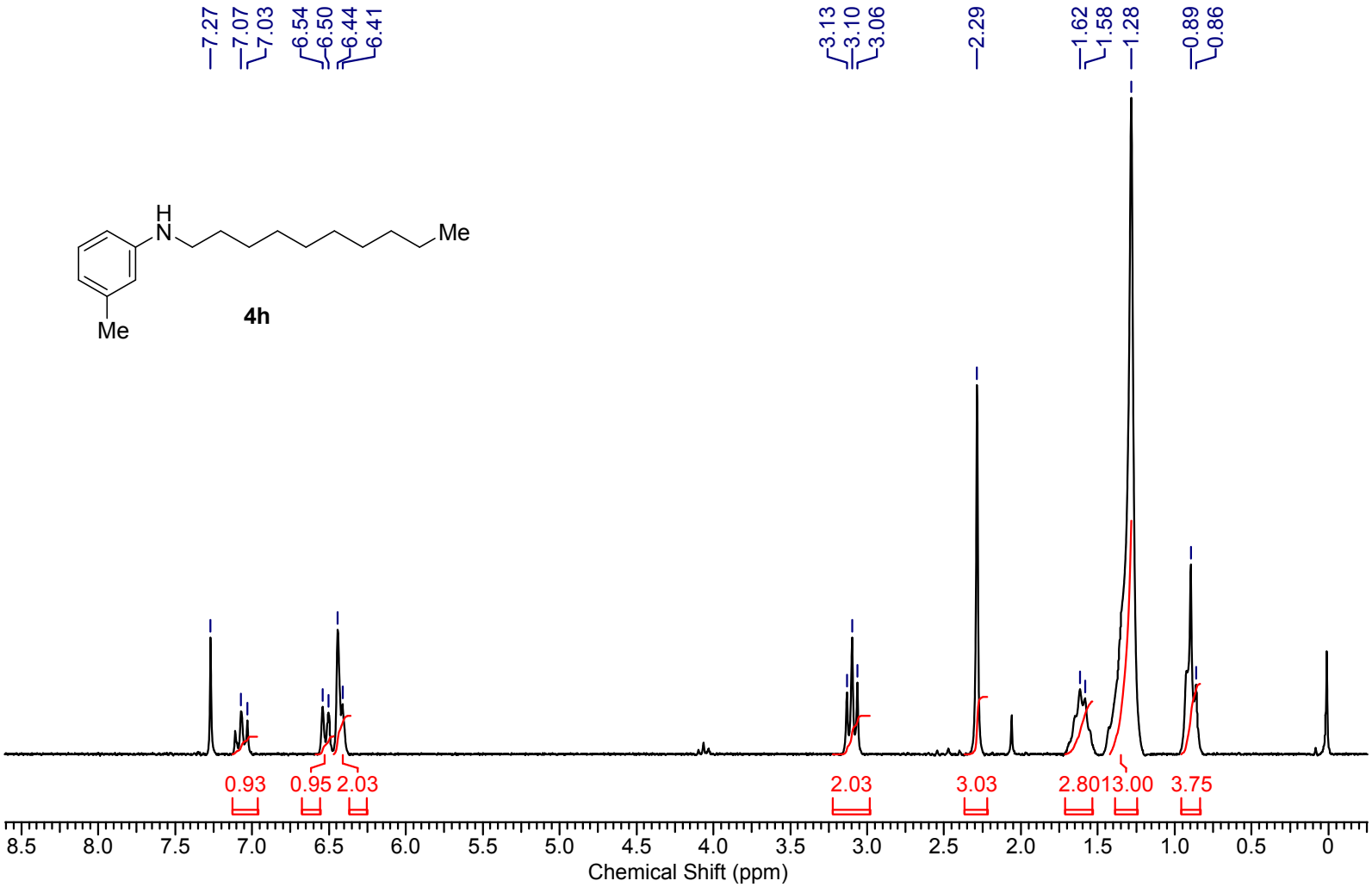
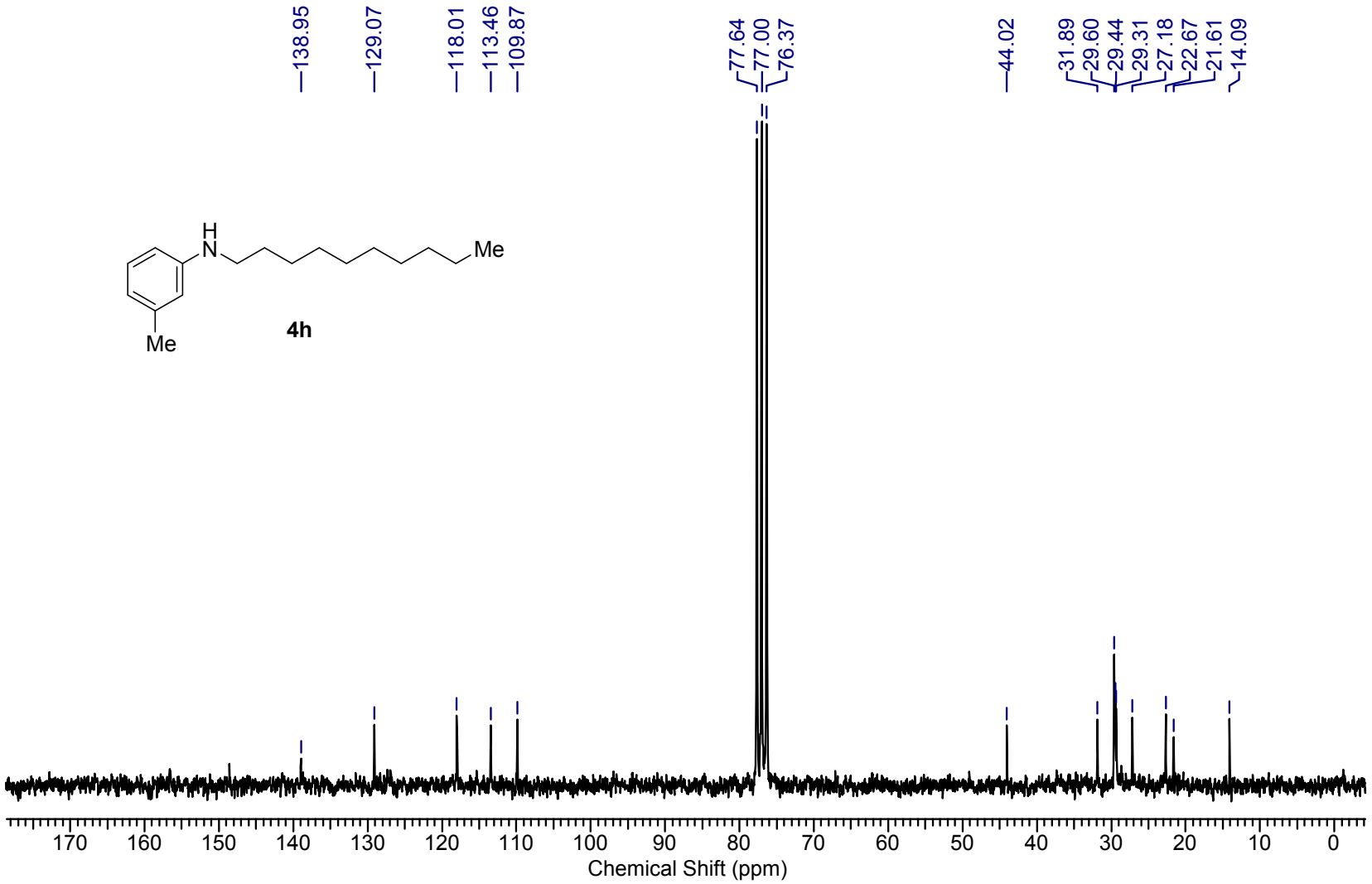
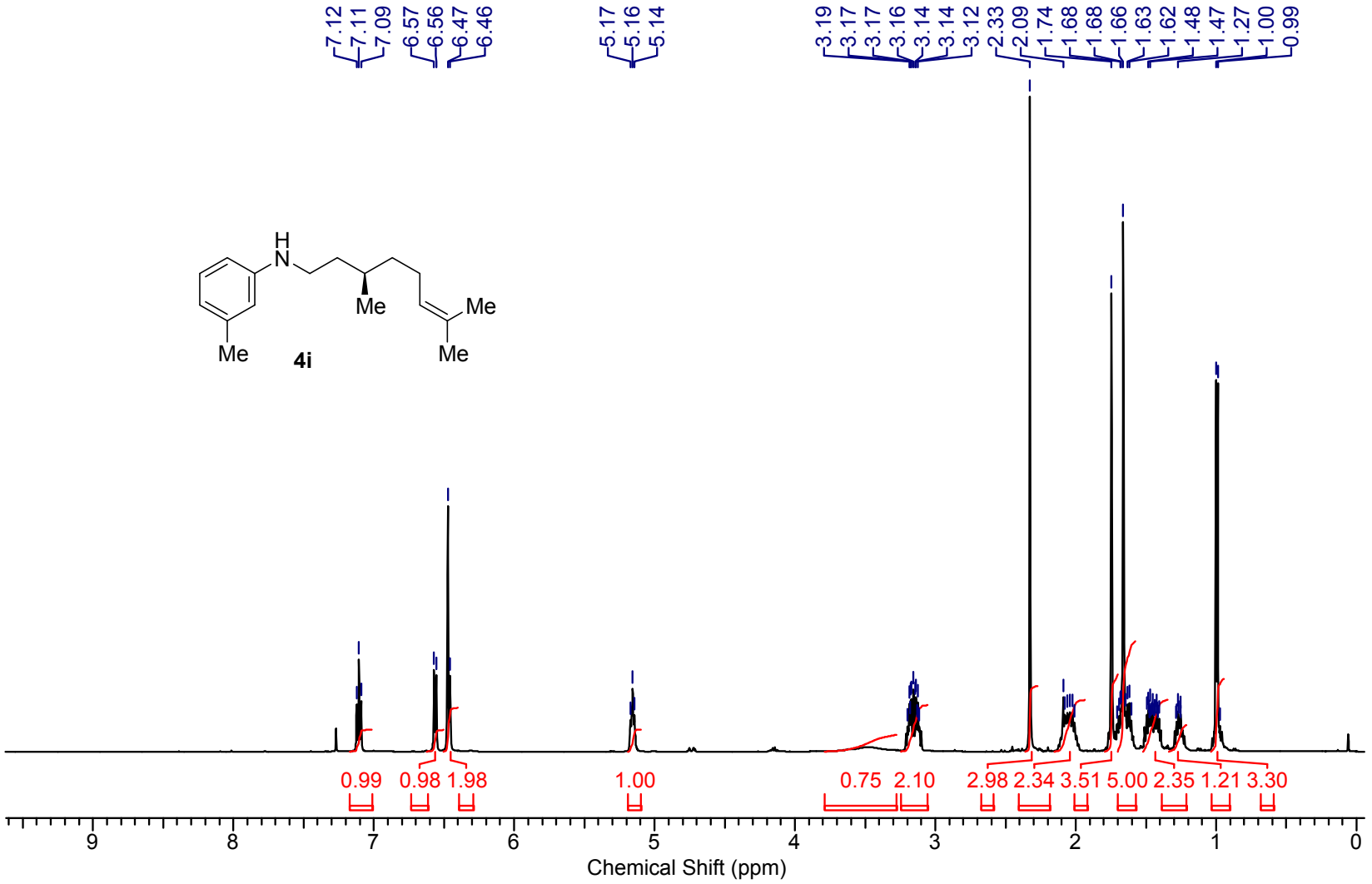
138.96
129.07
118.06
113.49
109.90
77.26
77.00
76.75
43.72
31.70
21.61
20.29
13.89
Me
H
N
Me
4f
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

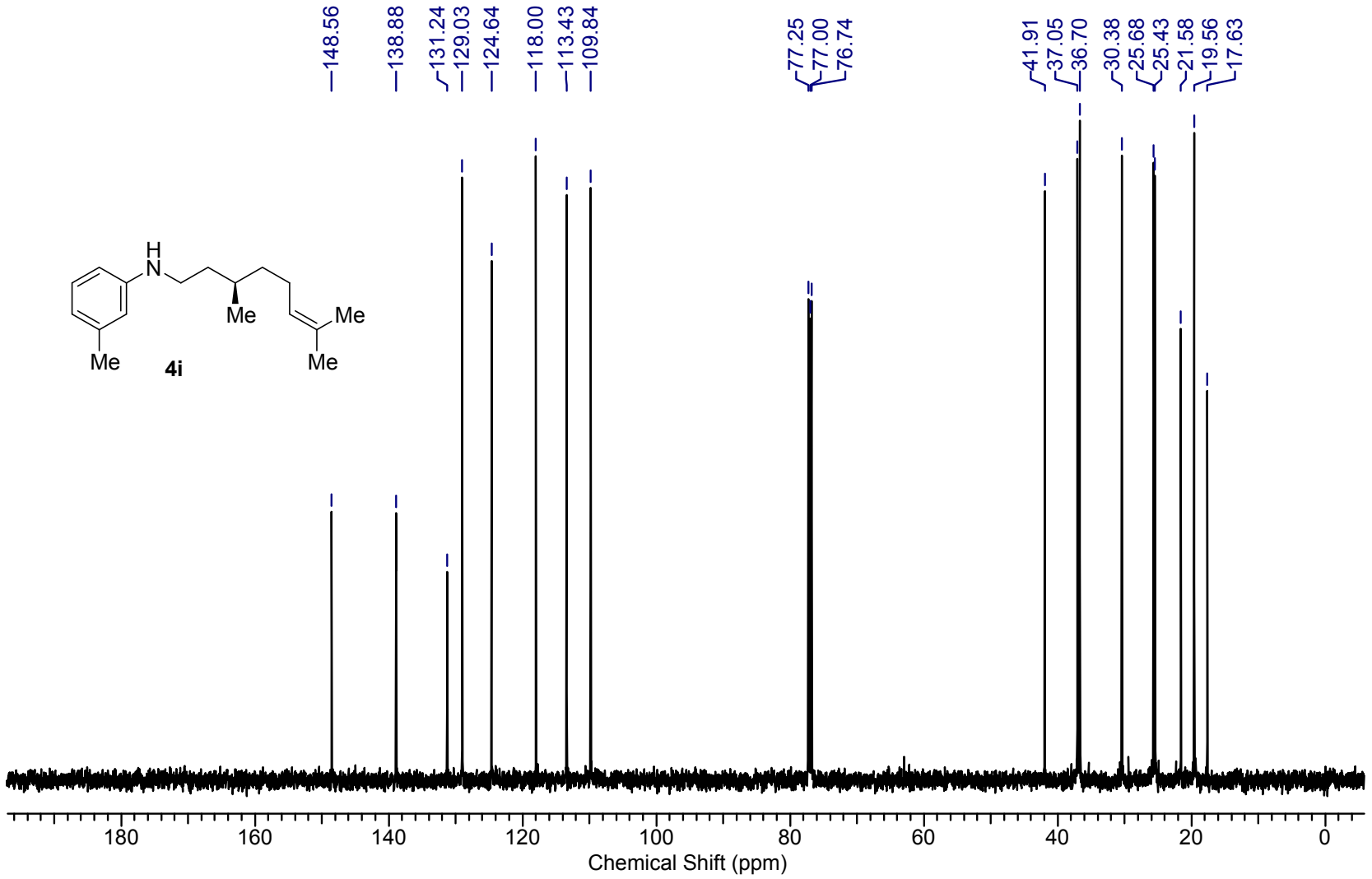

7.27
7.08
7.07
6.55
6.54
6.46
6.45
3.12
3.11
3.09
2.30
1.64
1.63
1.61
1.41
1.39
1.38
1.32
1.30
1.30
0.91
0.90
H
N
Me
Me
4g
1.00 0.98 2.07
2.20 3.13 2.53 0.01 2.92 7.25 3.94
10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)

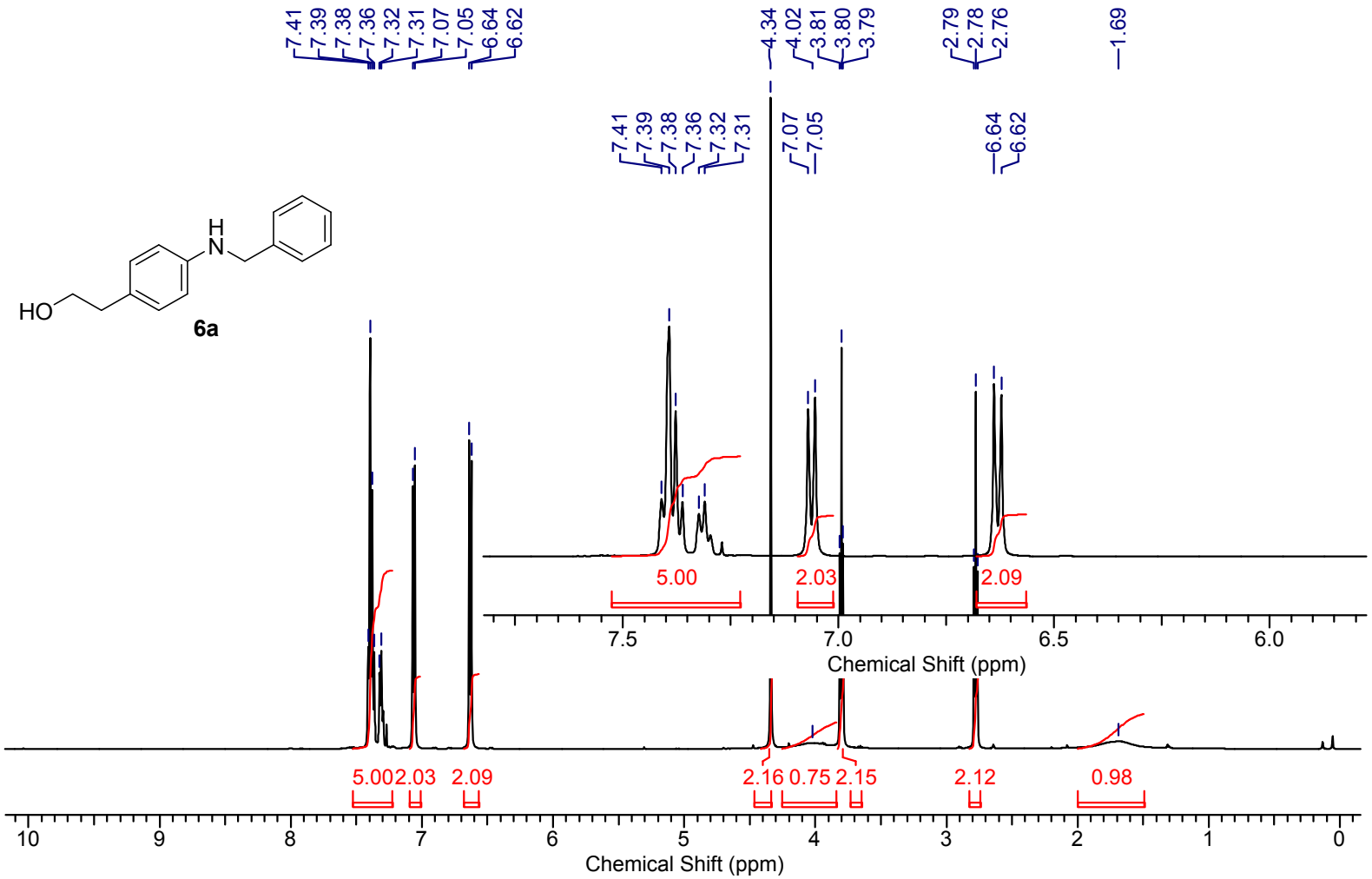

148.38
138.96
129.06
118.16
113.57
109.99
77.25
77.00
76.74
44.13
31.81
29.53
29.39
29.25
27.16
22.65
21.60
14.09
H
N
Me
Me
4g
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

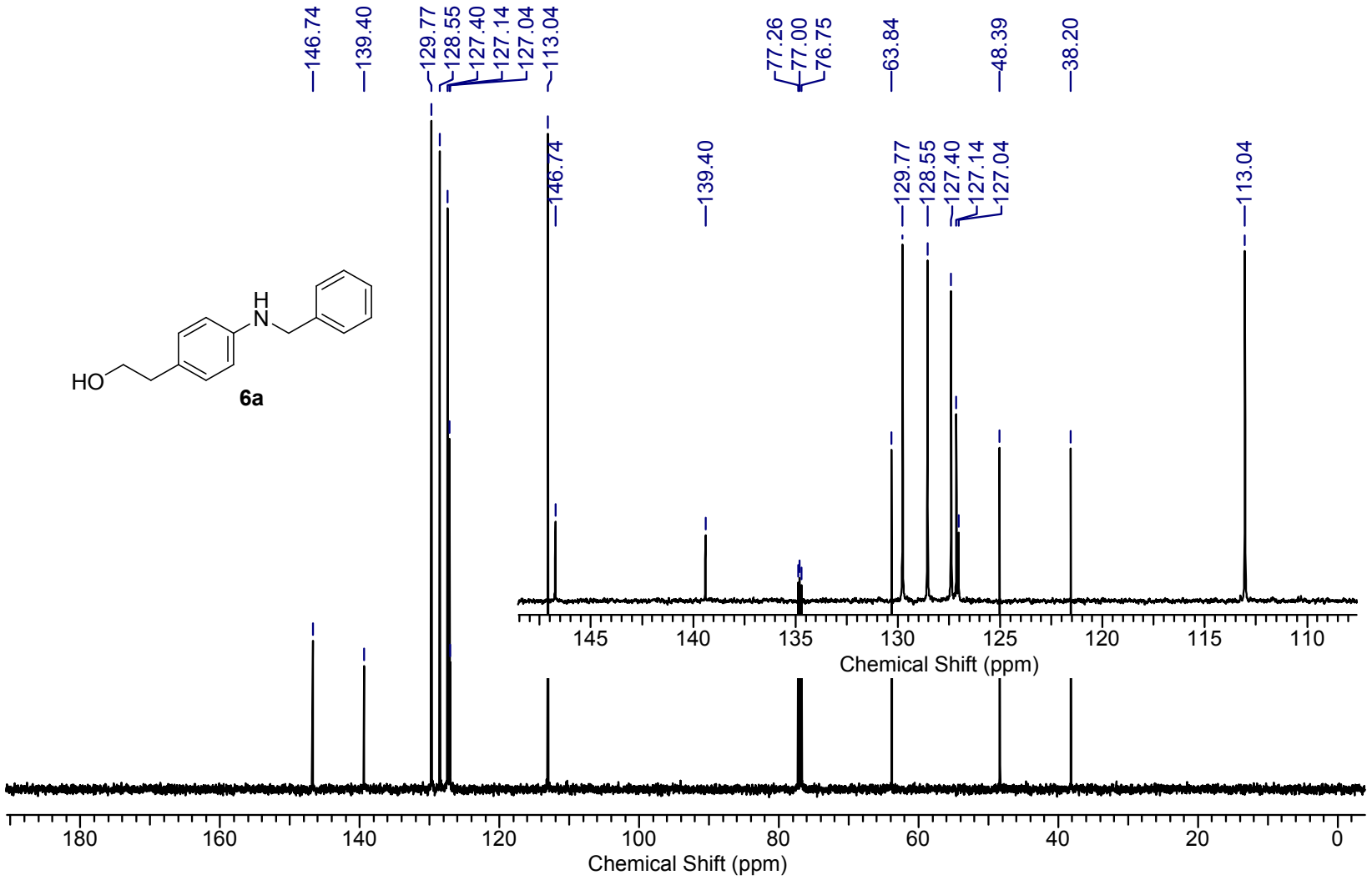

7.27
7.07
7.03
6.54
6.50
6.44
6.41
3.13
3.10
3.06
2.29
1.62
1.58
1.28
0.89
0.86
H
N
Me
Me
4h
0.93
0.95
2.03
2.03
3.03
2.80
13.00
3.75
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

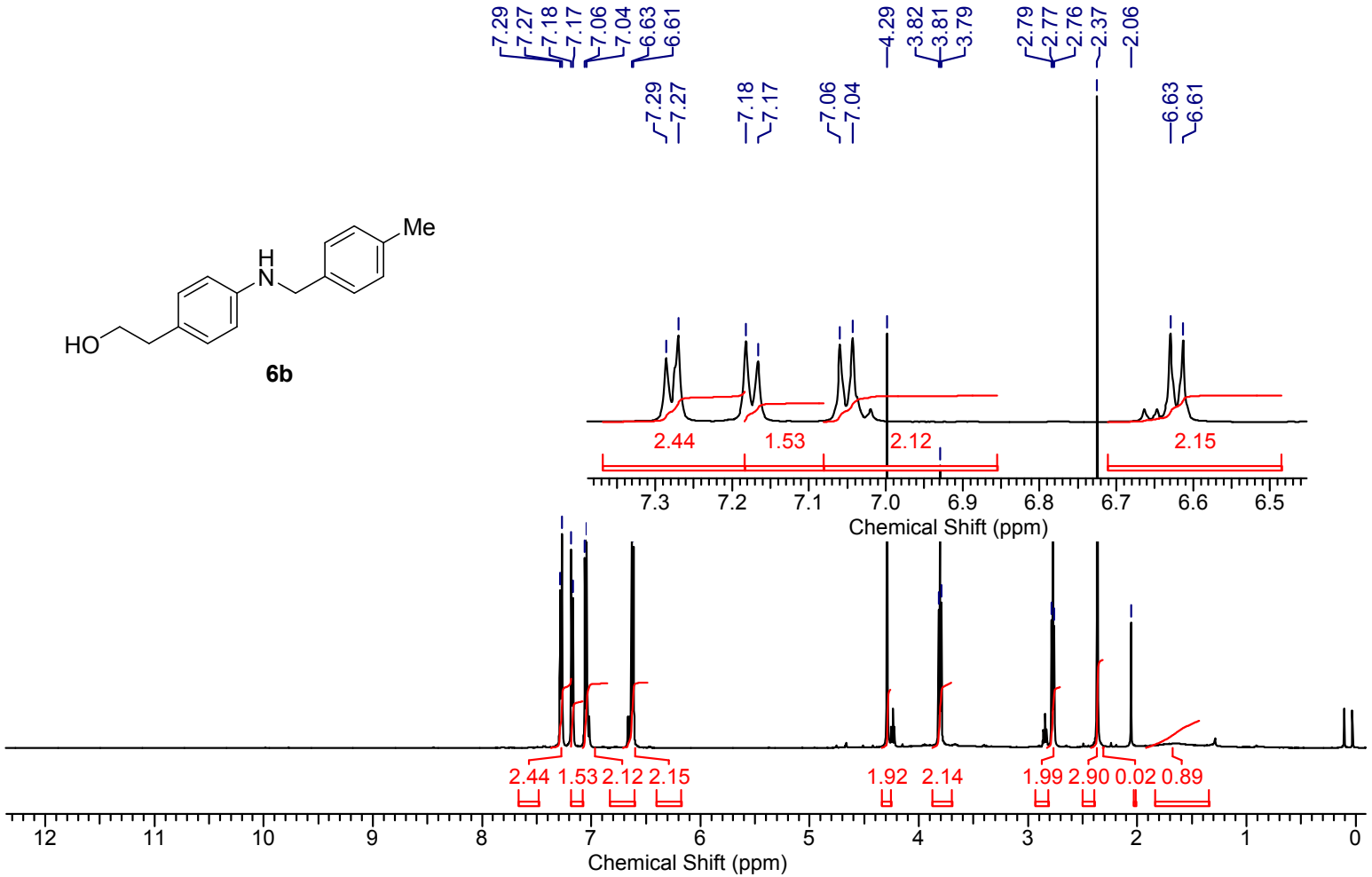

138.95
129.07
118.01
113.46
109.87
77.64
77.00
76.37
44.02
31.89
29.60
29.44
29.31
27.18
22.67
21.61
14.09
H
N
Me
Me
4h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

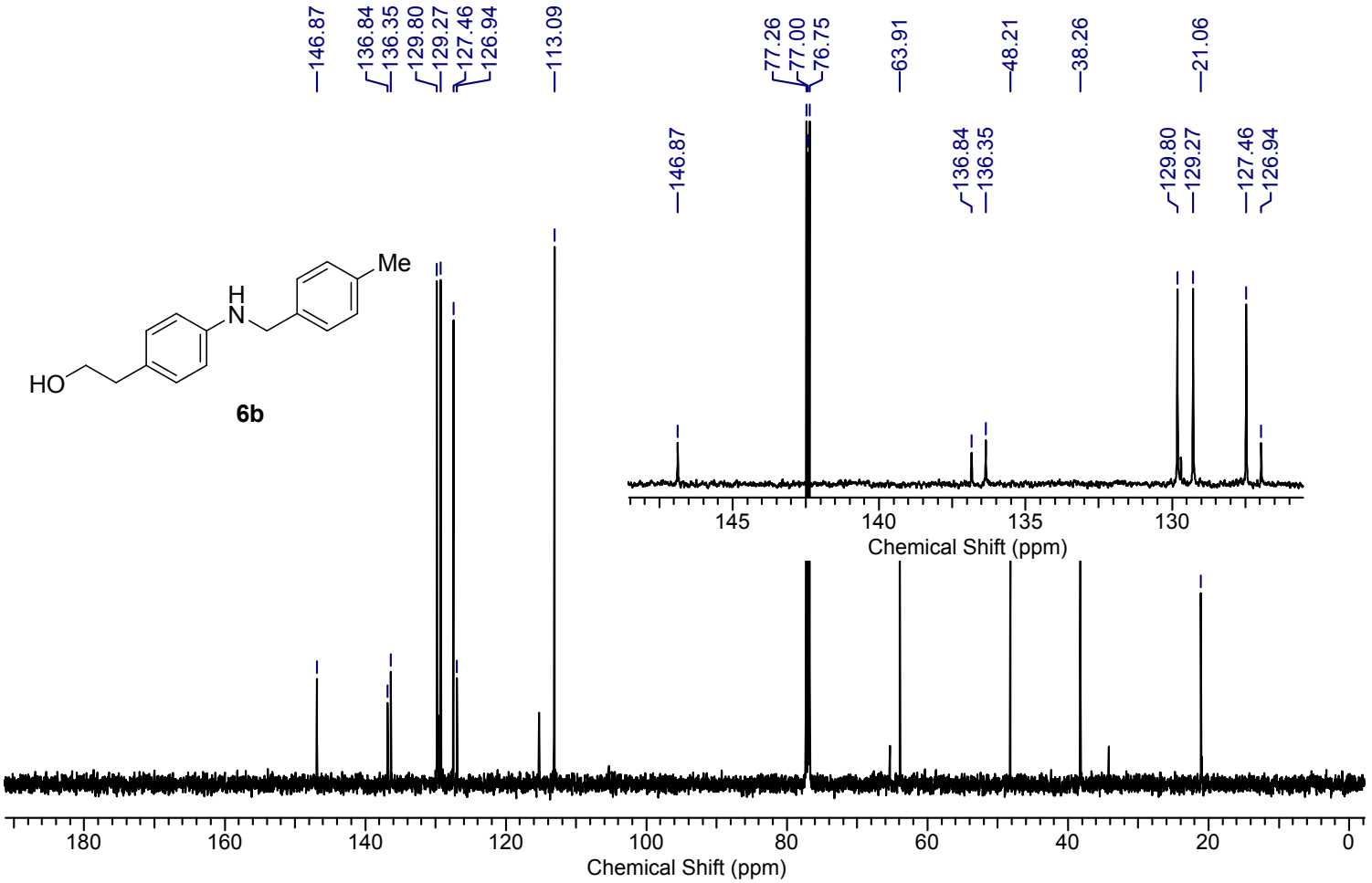

7.12
7.11
7.09
6.57
6.56
6.47
6.46
5.17
5.16
5.14
3.19
3.17
3.17
3.16
3.14
3.14
3.12
2.33
2.09
1.74
1.68
1.68
1.66
1.63
1.62
1.48
1.47
1.27
1.00
0.99
H
N
Me
Me
Me
Me
4i
0.99
0.98
1.98
1.00
0.75
2.10
2.98
2.34
3.51
5.00
2.35
1.21
3.30
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

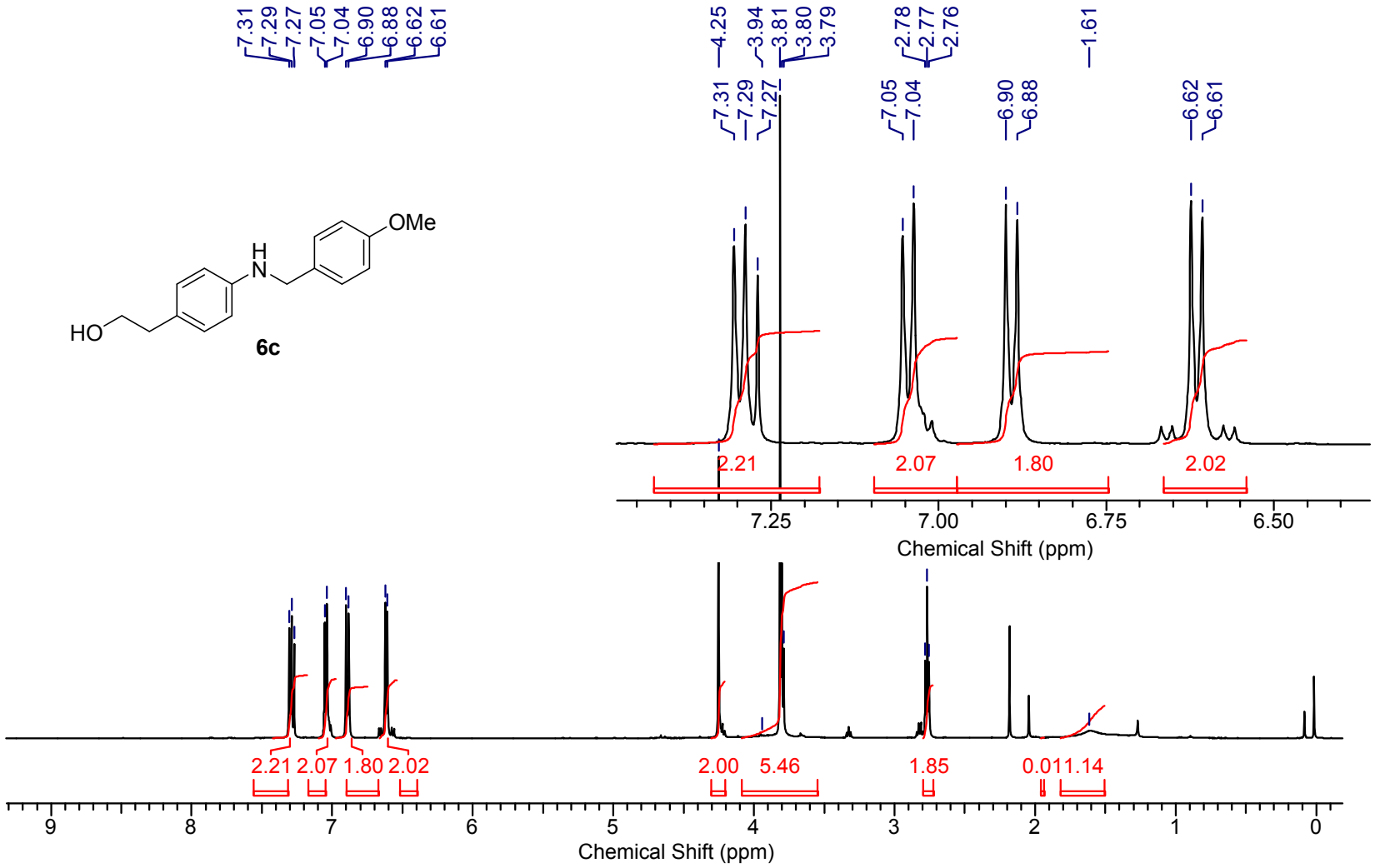

148.56
138.88
131.24
129.03
124.64
118.00
113.43
109.84
77.25
77.00
76.74
41.91
37.05
36.70
30.38
25.68
25.43
21.58
19.56
17.63
H
N
Me
Me
Me
Me
4i
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

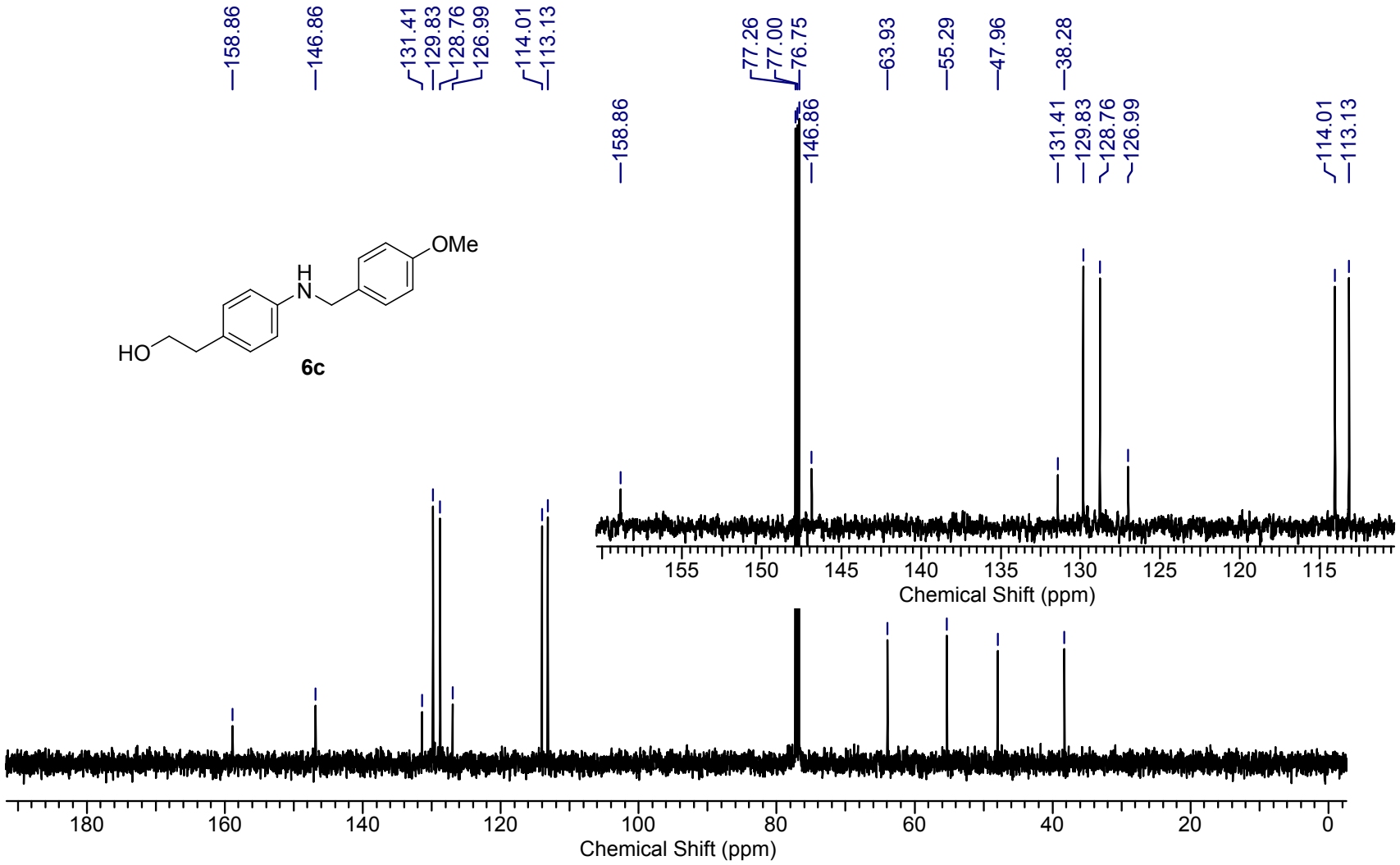

7.41
7.39
7.38
7.36
7.32
7.31
7.07
7.05
6.64
6.62
4.34
4.02
3.81
3.80
3.79
2.79
2.78
2.76
1.69
HO
H
N
6a
5.00
2.03
2.09
7.5
7.0
6.5
6.0
Chemical Shift (ppm)
5.00
2.03
2.09
2.16
0.75
2.15
2.12
0.98
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

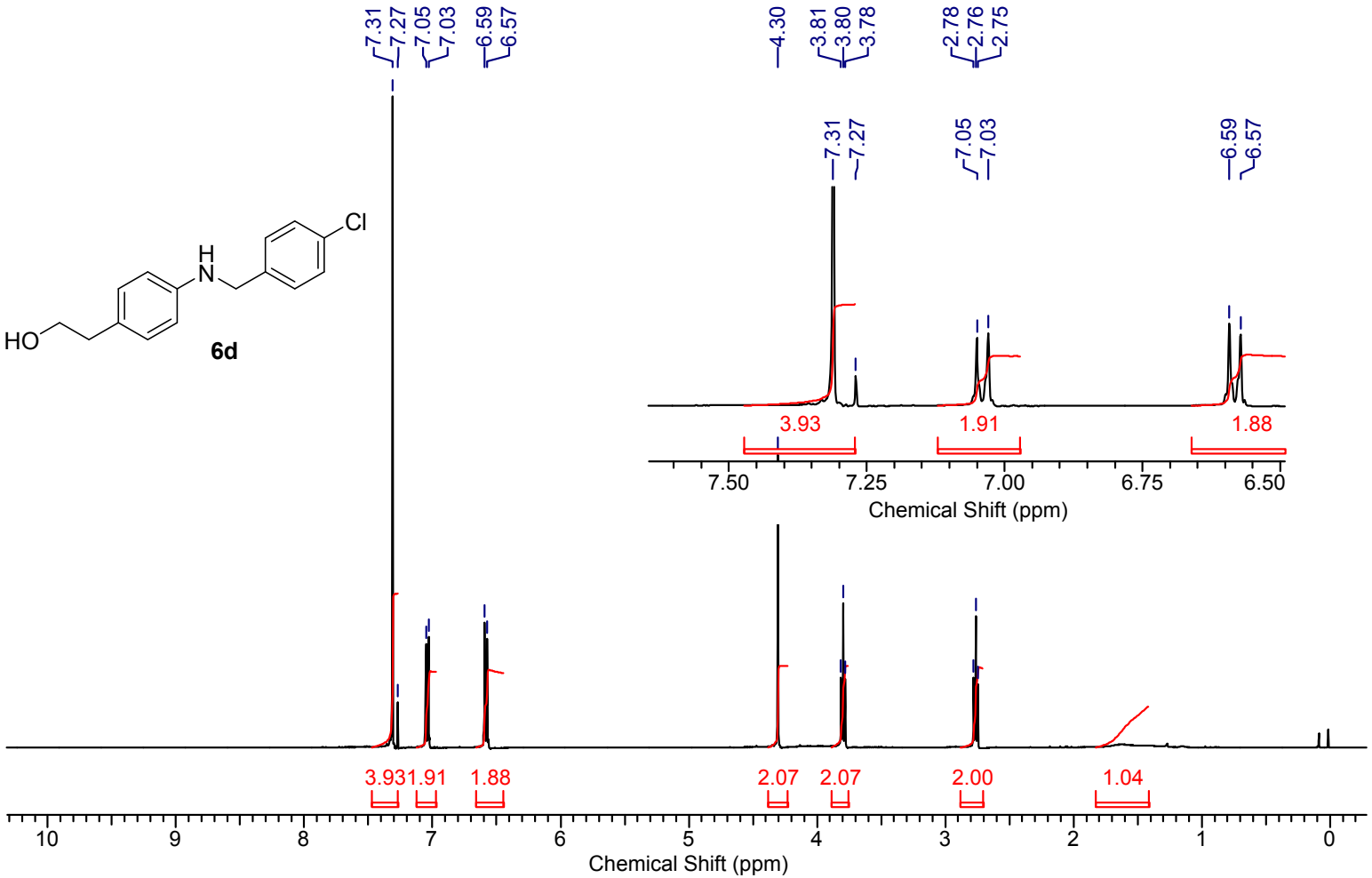

146.74
139.40
129.77
128.55
127.40
127.14
127.04
113.04
77.26
77.00
76.75
63.84
48.39
38.20
HO
H
N
6a
Chemical Shift (ppm)
Chemical Shift (ppm)

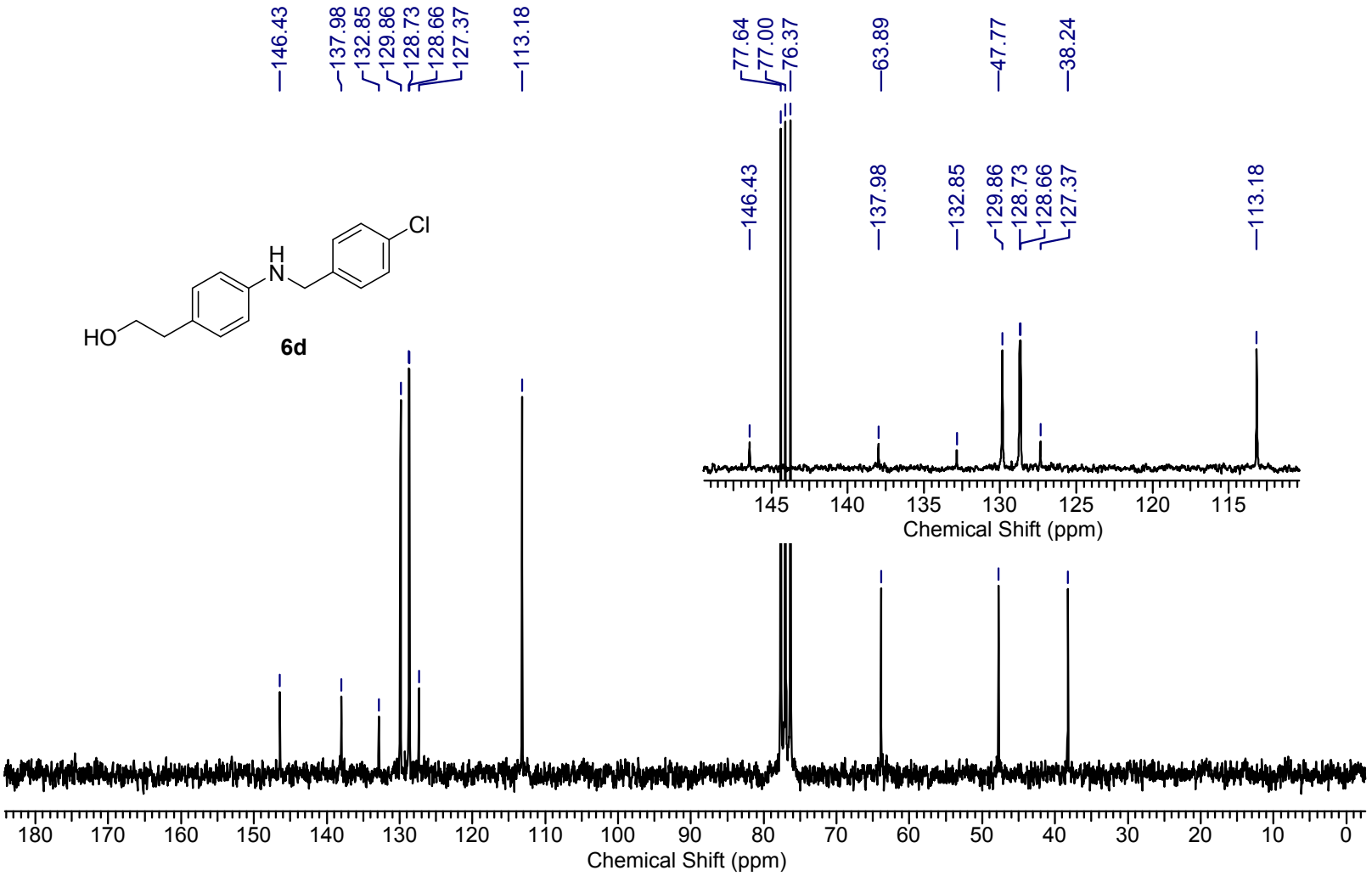

7.29
7.27
7.18
7.17
7.06
7.04
6.63
6.61
4.29
3.82
3.81
3.79
2.79
2.77
2.76
2.37
2.06
Me
H
N
HO
6b
2.44
1.53
2.12
2.15
Chemical Shift (ppm)
1.92
2.14
1.99
2.90
0.02
0.89

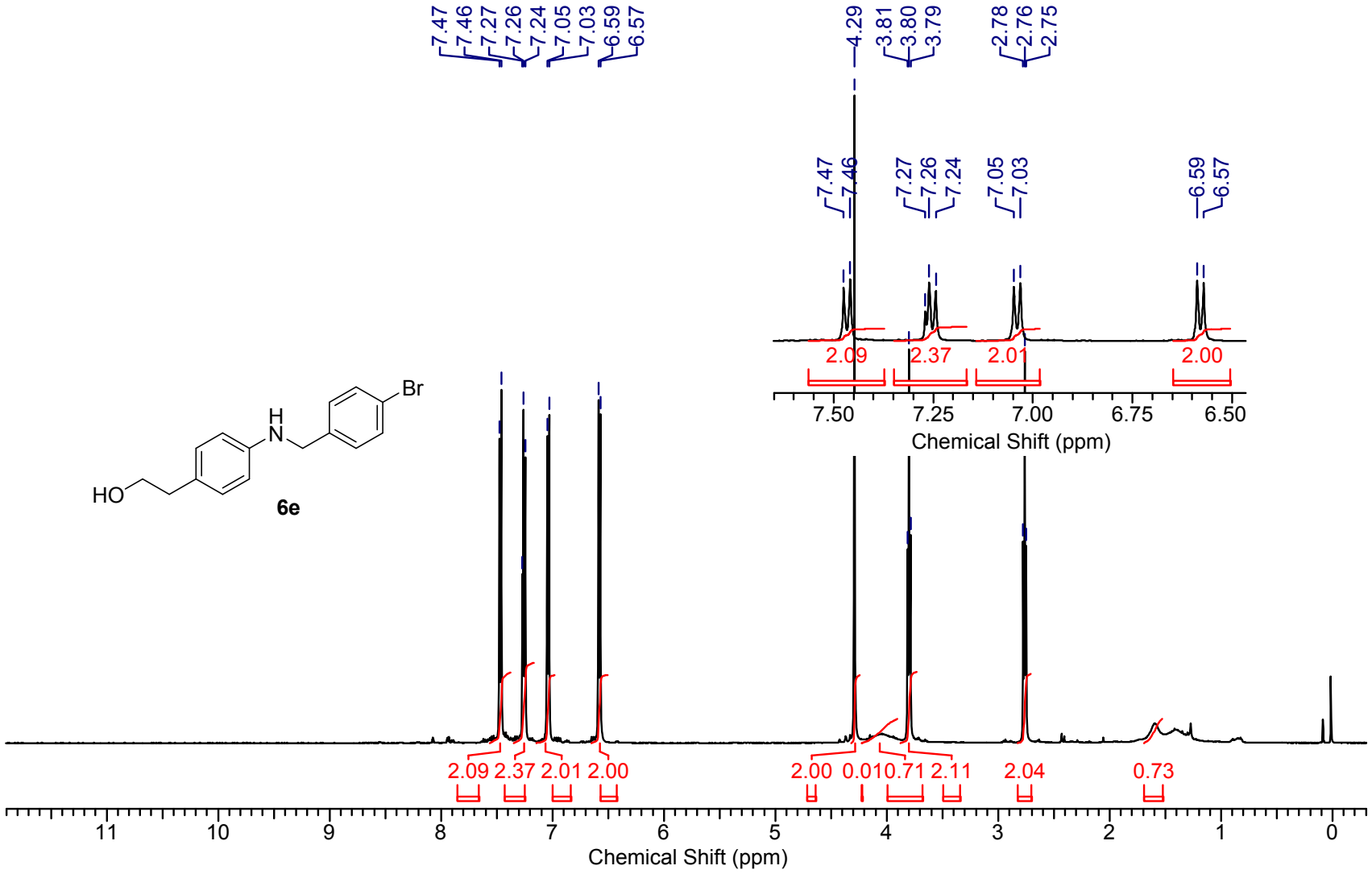

146.87
136.84
136.35
129.80
129.27
127.46
126.94
113.09
77.26
77.00
76.75
63.91
48.21
38.26
21.06
Me
H
N
HO
6b
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
145
140
135
130
Chemical Shift (ppm)

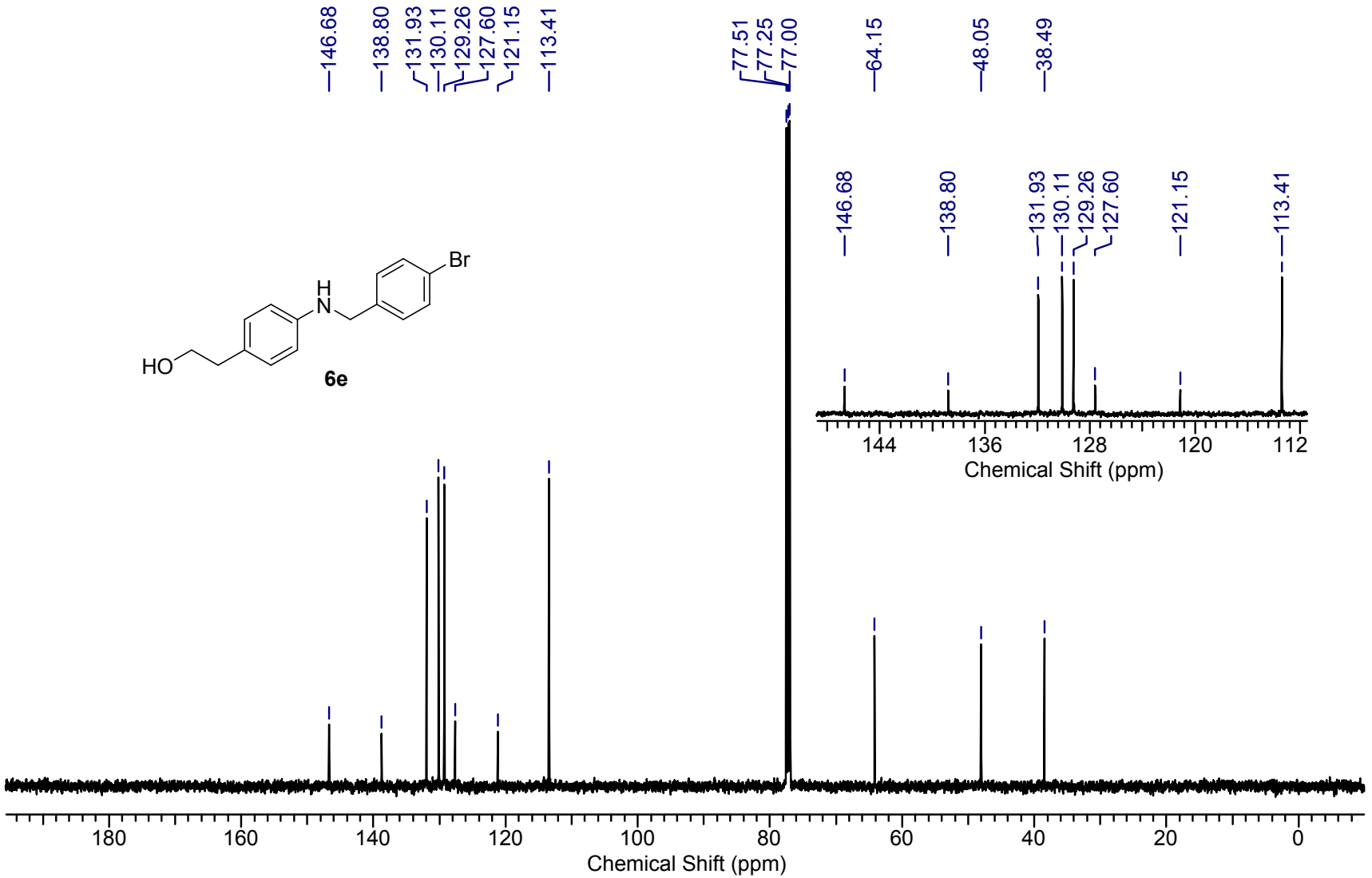

7.31
7.29
7.27
7.05
7.04
6.90
6.88
6.62
6.61
4.25
3.94
3.81
3.80
3.79
2.78
2.77
2.76
1.61
OMe
H
N
HO
6c
2.21
2.07
1.80
2.02
7.25
7.00
6.75
6.50
Chemical Shift (ppm)
2.21 2.07 1.80 2.02
2.00 5.46
1.85
0.01 1.14
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

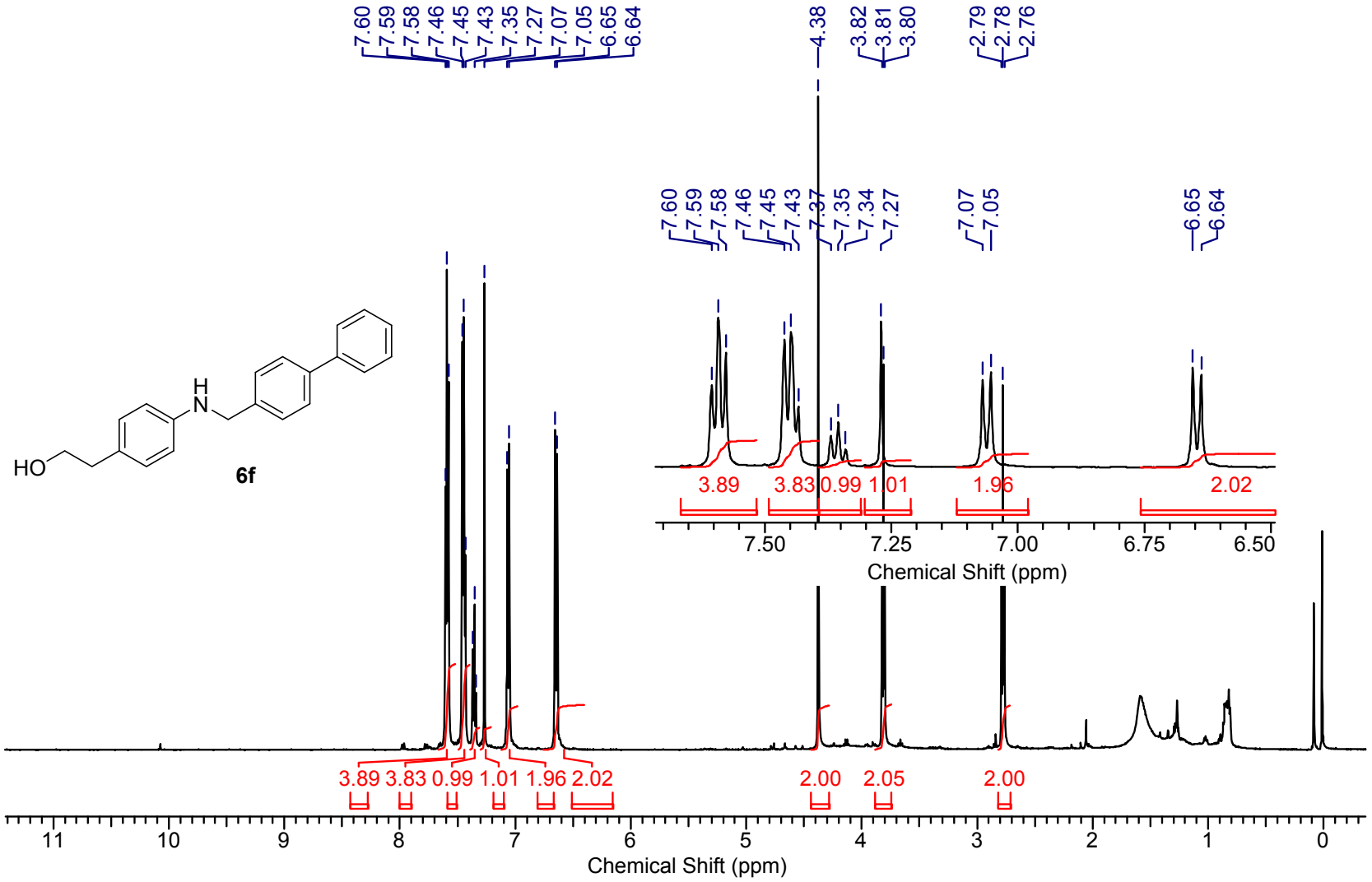

158.86
146.86
131.41
129.83
128.76
126.99
114.01
113.13
77.26
77.00
76.75
63.93
55.29
47.96
38.28
OMe
H
N
HO
6c
Chemical Shift (ppm)
Chemical Shift (ppm)

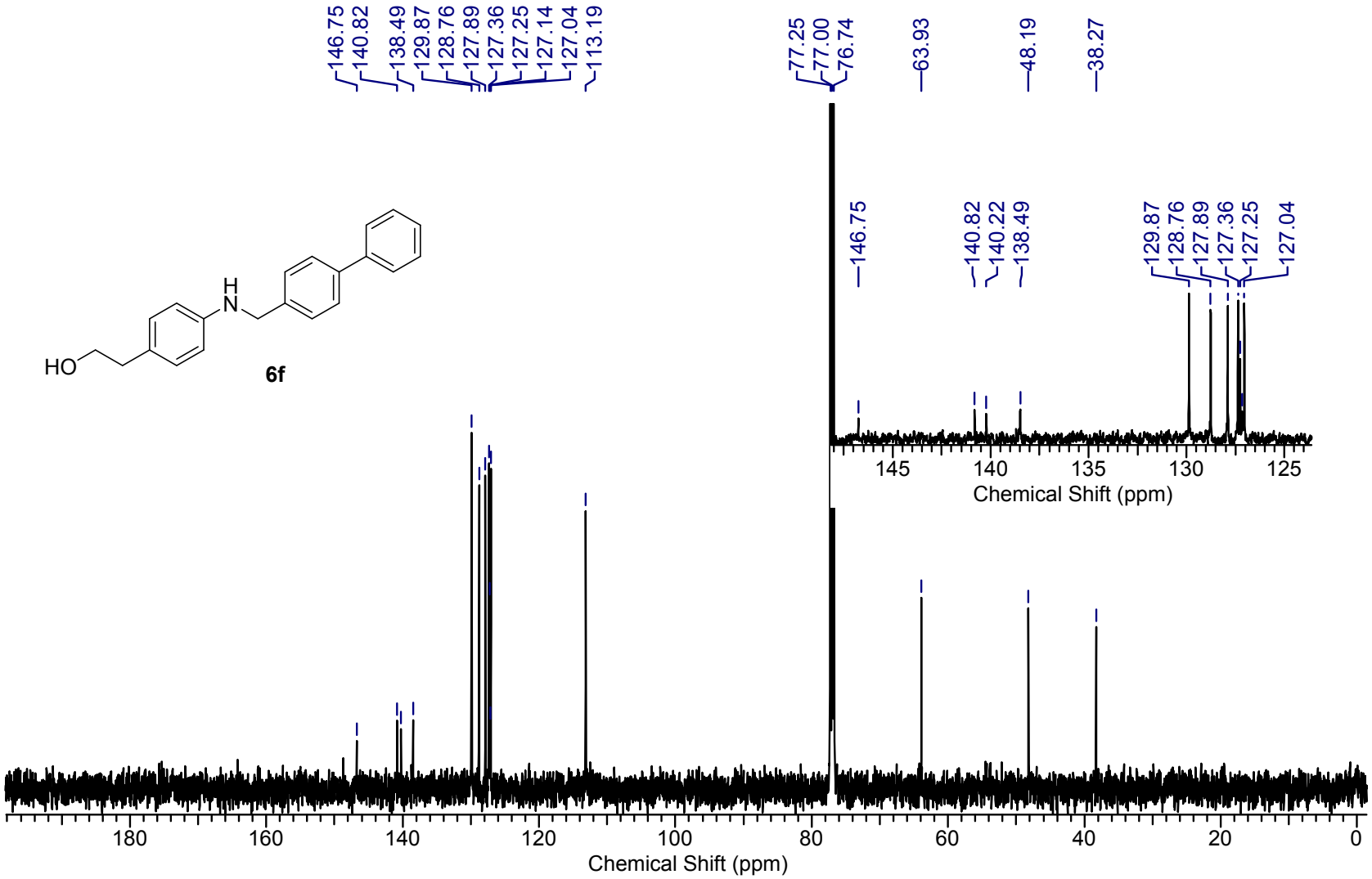

7.31
7.27
7.05
7.03
6.59
6.57
4.30
3.81
3.80
3.78
2.78
2.76
2.75
Cl
H
N
HO
6d
3.93
1.91
1.88
7.50
7.25
7.00
6.75
6.50
Chemical Shift (ppm)
3.93
1.91
1.88
2.07
2.07
2.00
1.04
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

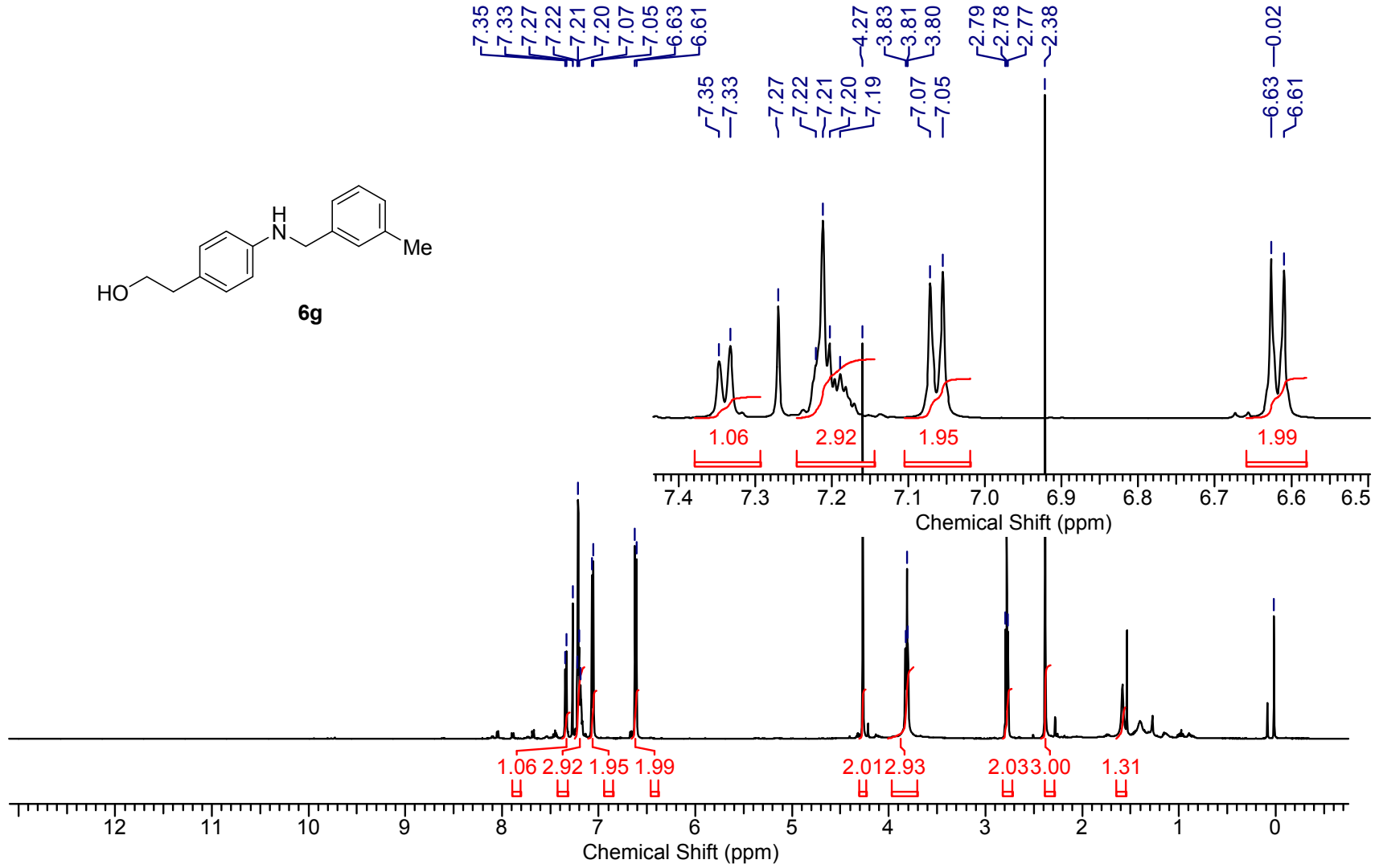

146.43
137.98
132.85
129.86
128.73
128.66
127.37
113.18
77.64
77.00
76.37
63.89
47.77
38.24
Cl
H
N
HO
6d
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)
145 140 135 130 125 120 115
Chemical Shift (ppm)

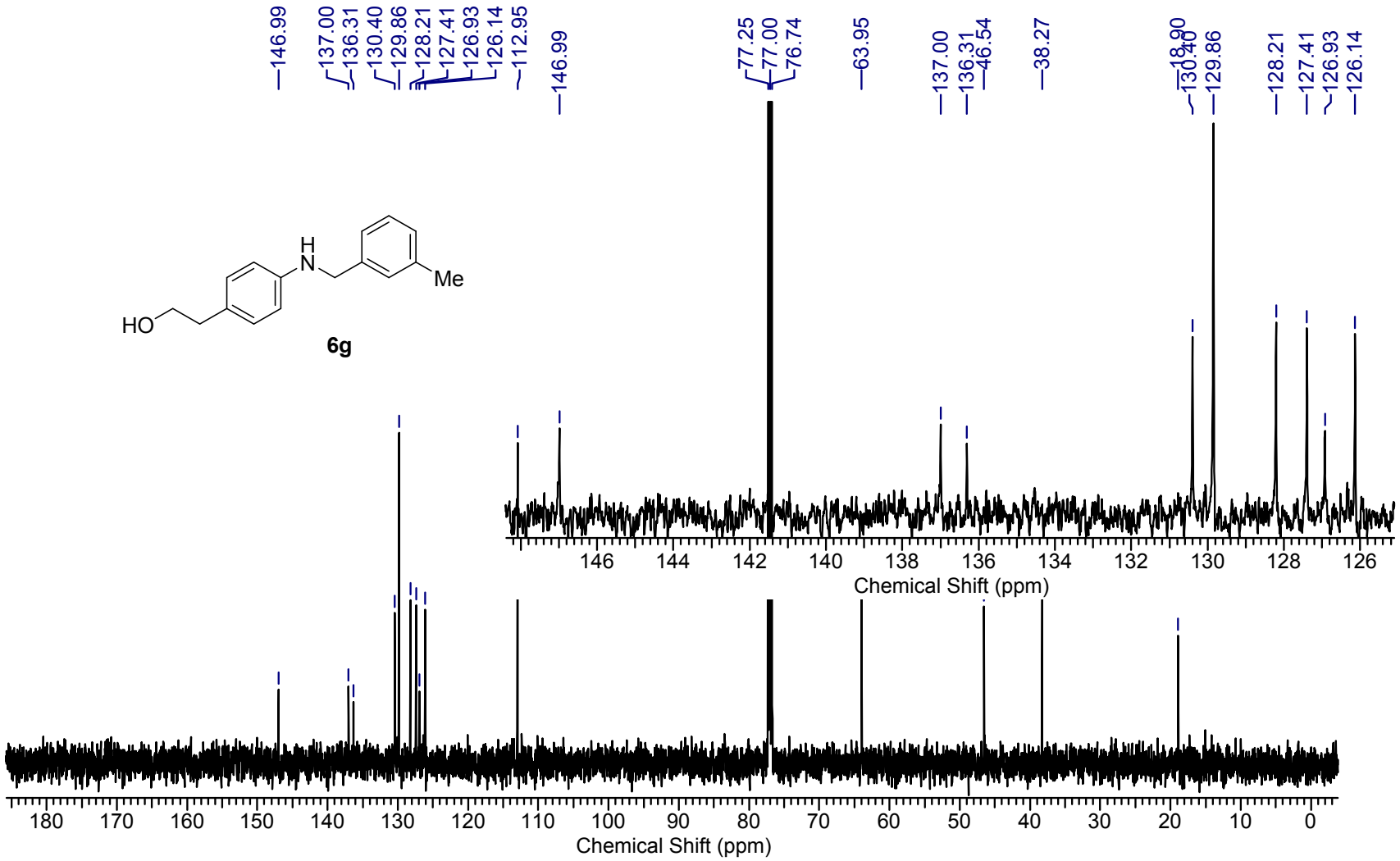

7.47
7.46
7.27
7.26
7.24
7.05
7.03
6.59
6.57
4.29
3.81
3.80
3.79
2.78
2.76
2.75
2.09
2.37
2.01
2.00
7.50
7.25
7.00
6.75
6.50
Chemical Shift (ppm)
Br
H
N
HO
6e
2.09 2.37 2.01 2.00
2.00 0.01 0.71 2.11
2.04
0.73
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

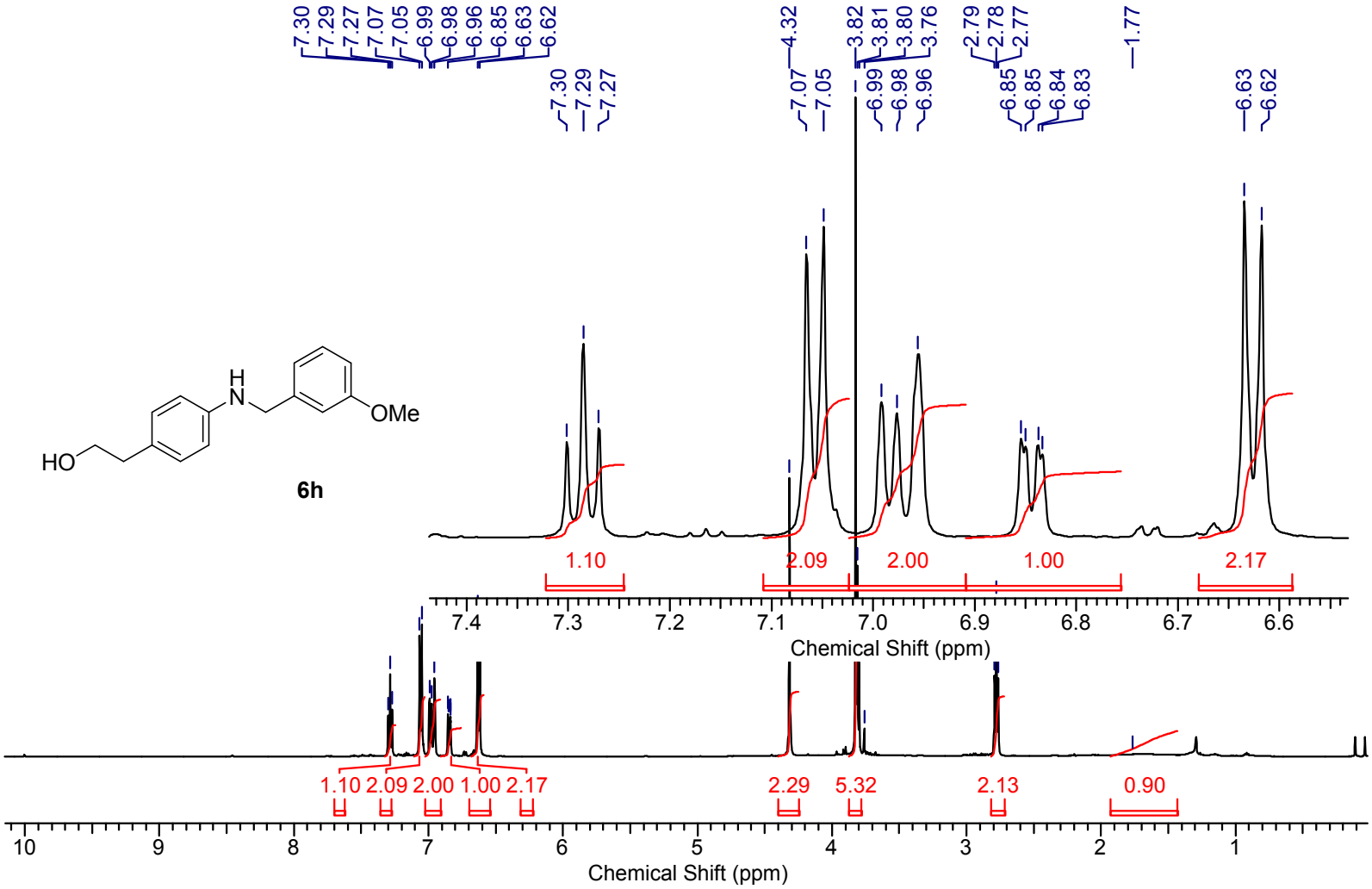

146.68
138.80
131.93
130.11
129.26
127.60
121.15
113.41
77.51
77.25
77.00
64.15
48.05
38.49
Br
H
N
HO
6e
Chemical Shift (ppm)
Chemical Shift (ppm)

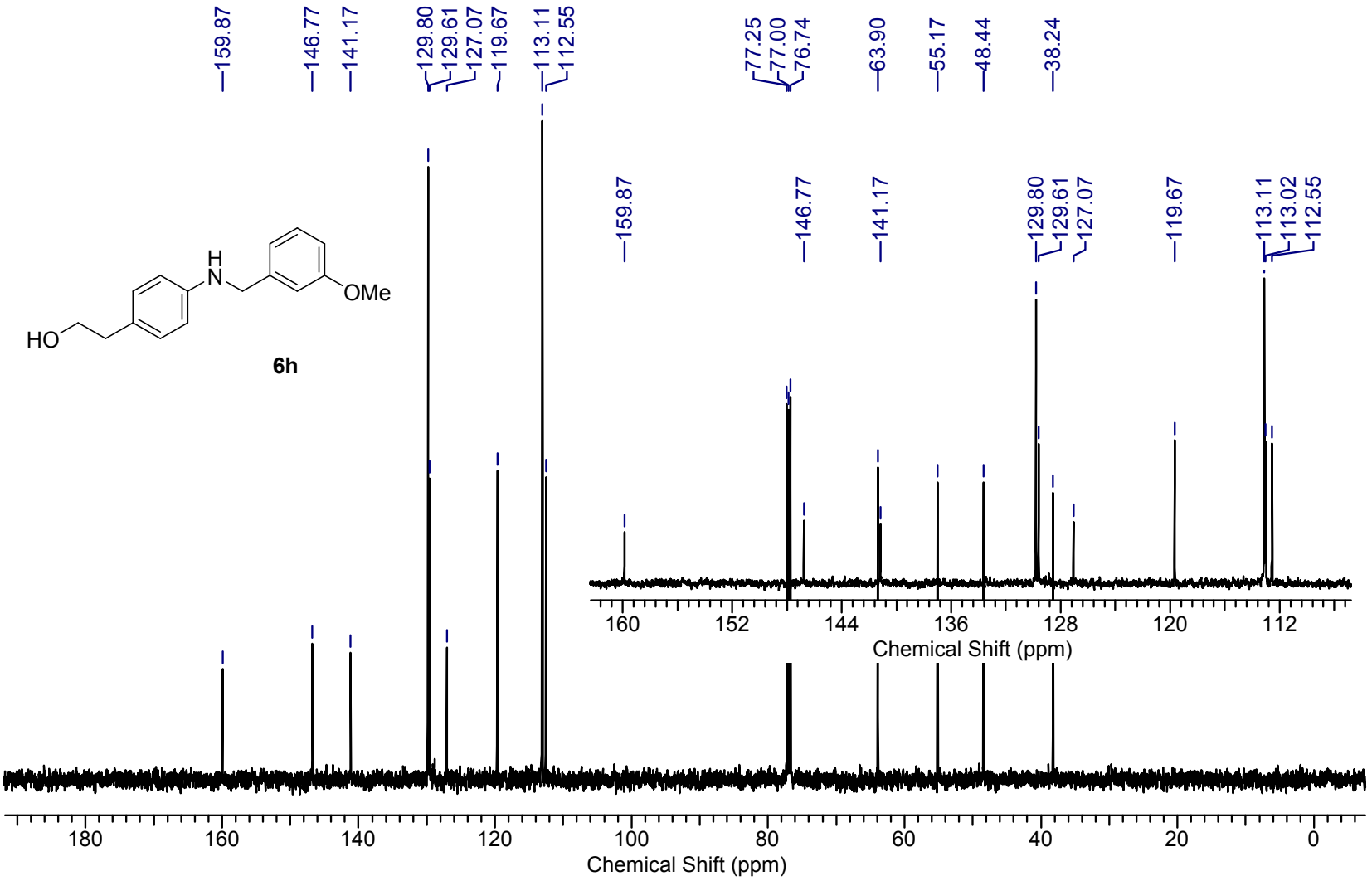

7.60
7.59
7.58
7.46
7.45
7.43
7.35
7.27
7.07
7.05
6.65
6.64
4.38
3.82
3.81
3.80
2.79
2.78
2.76
HO
H
N
6f
3.89 3.83 0.99 1.01 1.96 2.02
2.00 2.05 2.00
Chemical Shift (ppm)
7.37
7.34
3.89 3.83 0.99 1.01 1.96 2.02
7.50 7.25 7.00 6.75 6.50
Chemical Shift (ppm)

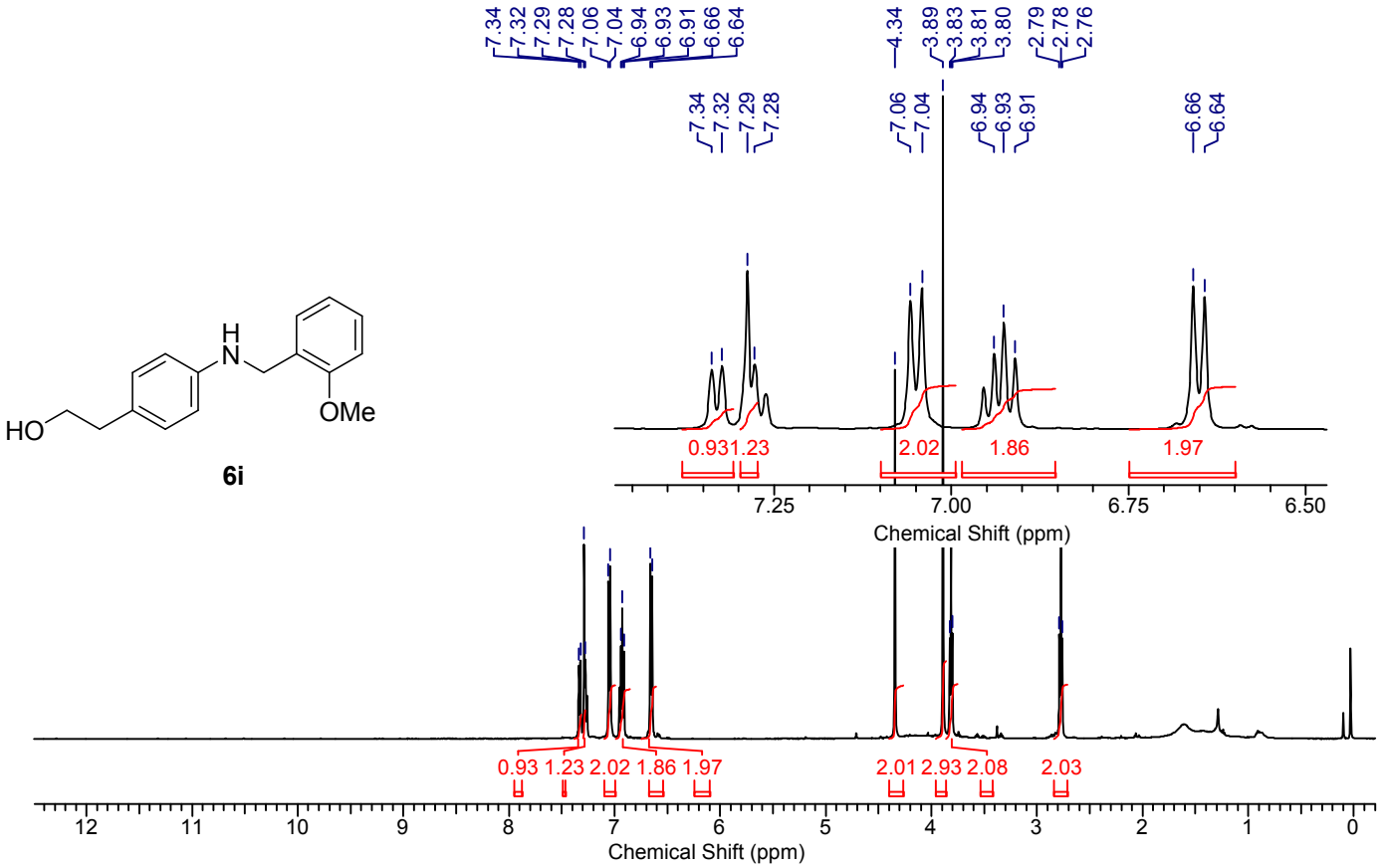

146.75
140.82
138.49
129.87
128.76
127.89
127.36
127.25
127.14
127.04
113.19
77.25
77.00
76.74
63.93
48.19
38.27
HO
H
N
6f
Chemical Shift (ppm)
Chemical Shift (ppm)

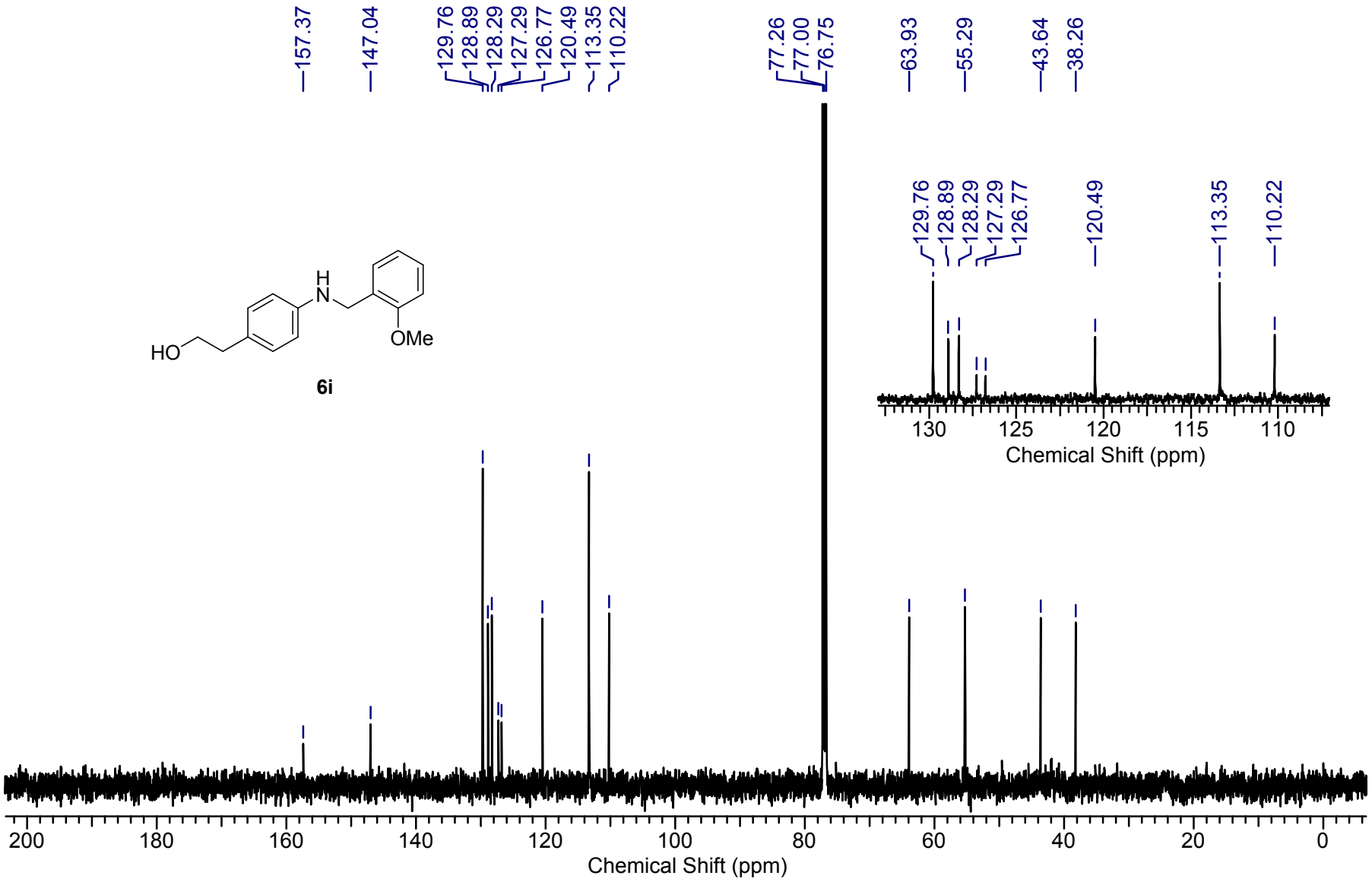

7.35
7.33
7.27
7.22
7.21
7.20
7.07
7.05
6.63
6.61
4.27
3.83
3.81
3.80
2.79
2.78
2.77
2.38
0.02
HO
H
N
Me
6g
1.06
2.92
1.95
1.99
Chemical Shift (ppm)
1.06 2.92 1.95 1.99
2.01 2.93
2.03 3.00
1.31
Chemical Shift (ppm)

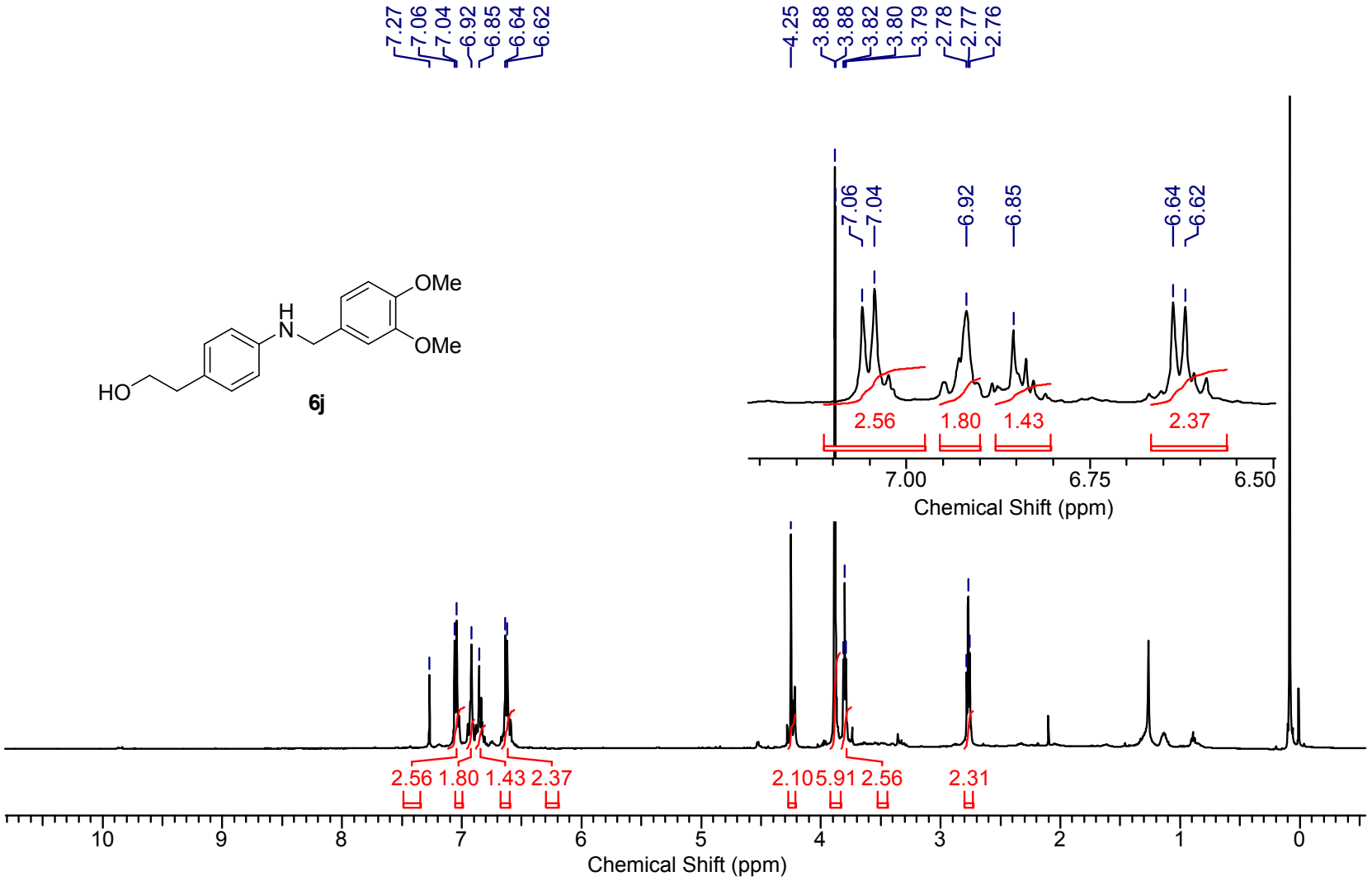

146.99
137.00
136.31
130.40
129.86
128.21
127.41
126.93
126.14
112.95
146.99
77.25
77.00
76.74
63.95
137.00
136.31
46.54
38.27
18.90
130.40
129.86
128.21
127.41
126.93
126.14
H
N
Me
HO
6g
Chemical Shift (ppm)
Chemical Shift (ppm)

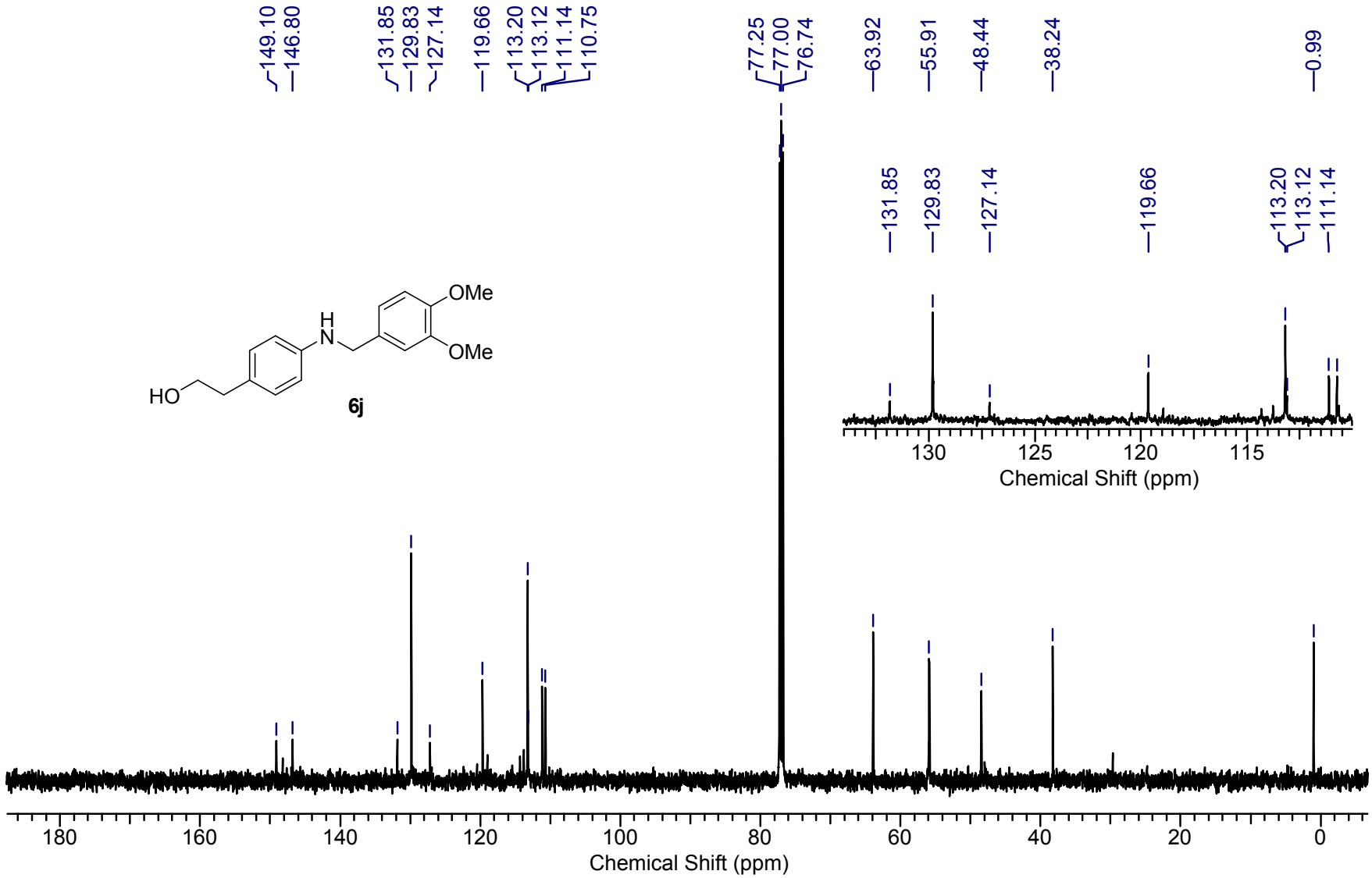

7.30
7.29
7.27
7.07
7.05
6.99
6.98
6.96
6.85
6.63
6.62
4.32
3.82
3.81
3.80
3.76
2.79
2.78
2.77
1.77
HO
N
H
OMe
6h
1.10
2.09
2.00
1.00
2.17
Chemical Shift (ppm)
2.29
5.32
2.13
0.90

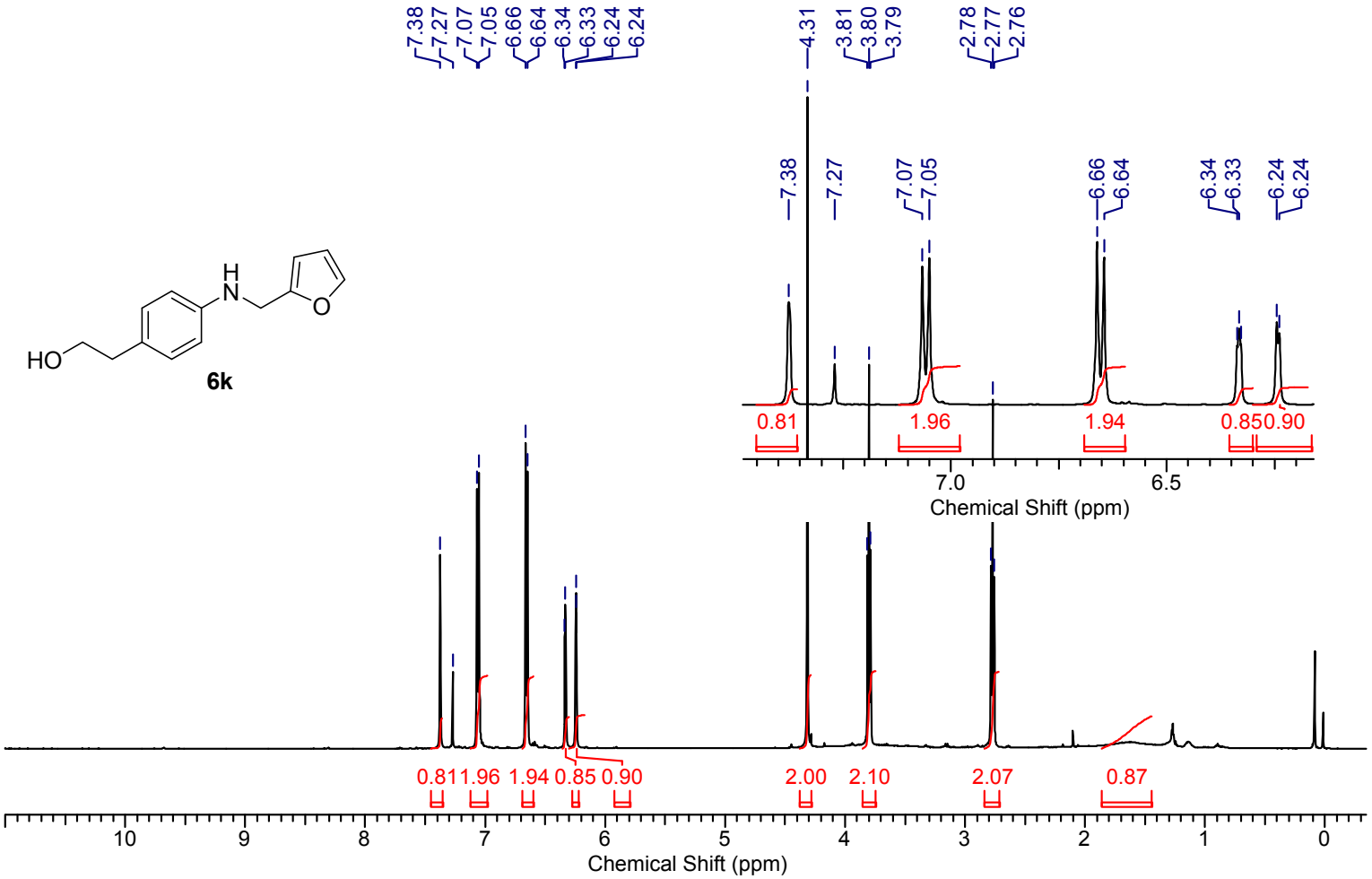

159.87
146.77
141.17
129.80
129.61
127.07
119.67
113.11
112.55
77.25
77.00
76.74
63.90
55.17
48.44
38.24
HO
N
H
OMe
6h
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
160
152
144
136
128
120
112
Chemical Shift (ppm)

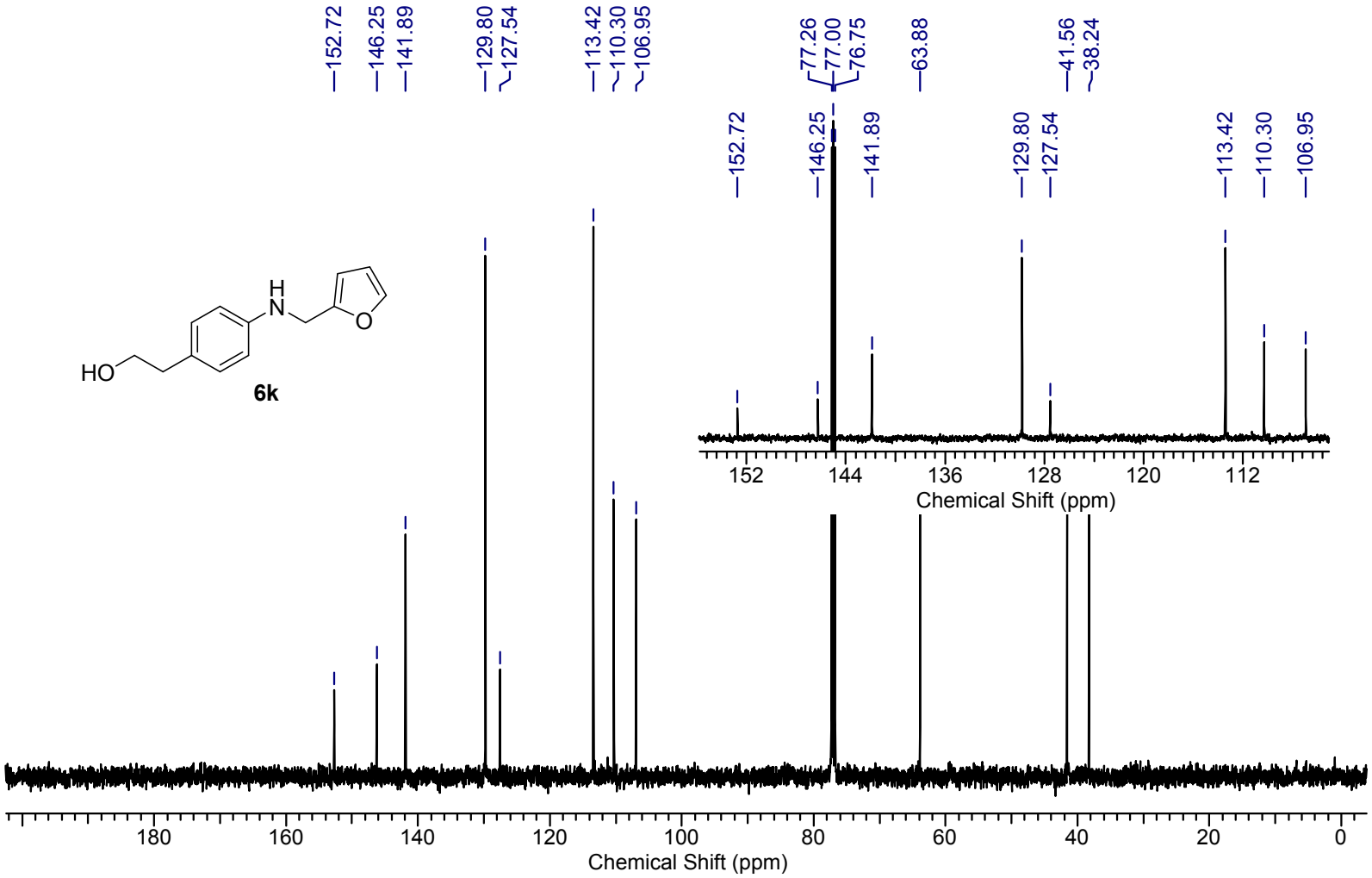

7.34
7.32
7.29
7.28
7.06
7.04
6.94
6.93
6.91
6.66
6.64
4.34
3.89
3.83
3.81
3.80
2.79
2.78
2.76
HO
H
N
OMe
6i
0.93 1.23
2.02
1.86
1.97
7.25
7.00
6.75
6.50
Chemical Shift (ppm)
0.93 1.23 2.02 1.86 1.97
2.01 2.93 2.08
2.03
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

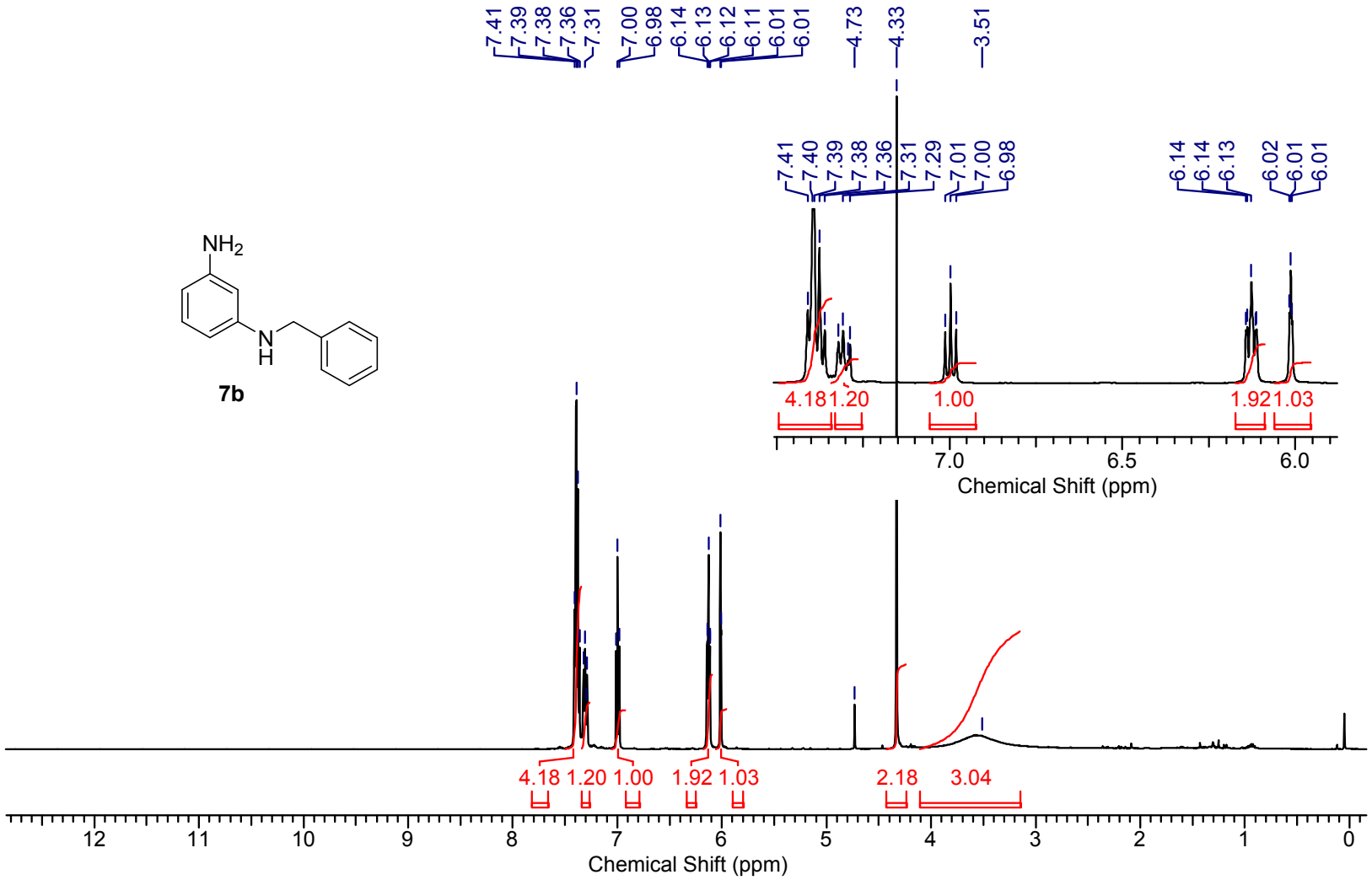

157.37
147.04
129.76
128.89
128.29
127.29
126.77
120.49
113.35
110.22
77.26
77.00
76.75
63.93
55.29
43.64
38.26
HO
H
N
OMe
6i
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
130
125
120
115
110
Chemical Shift (ppm)

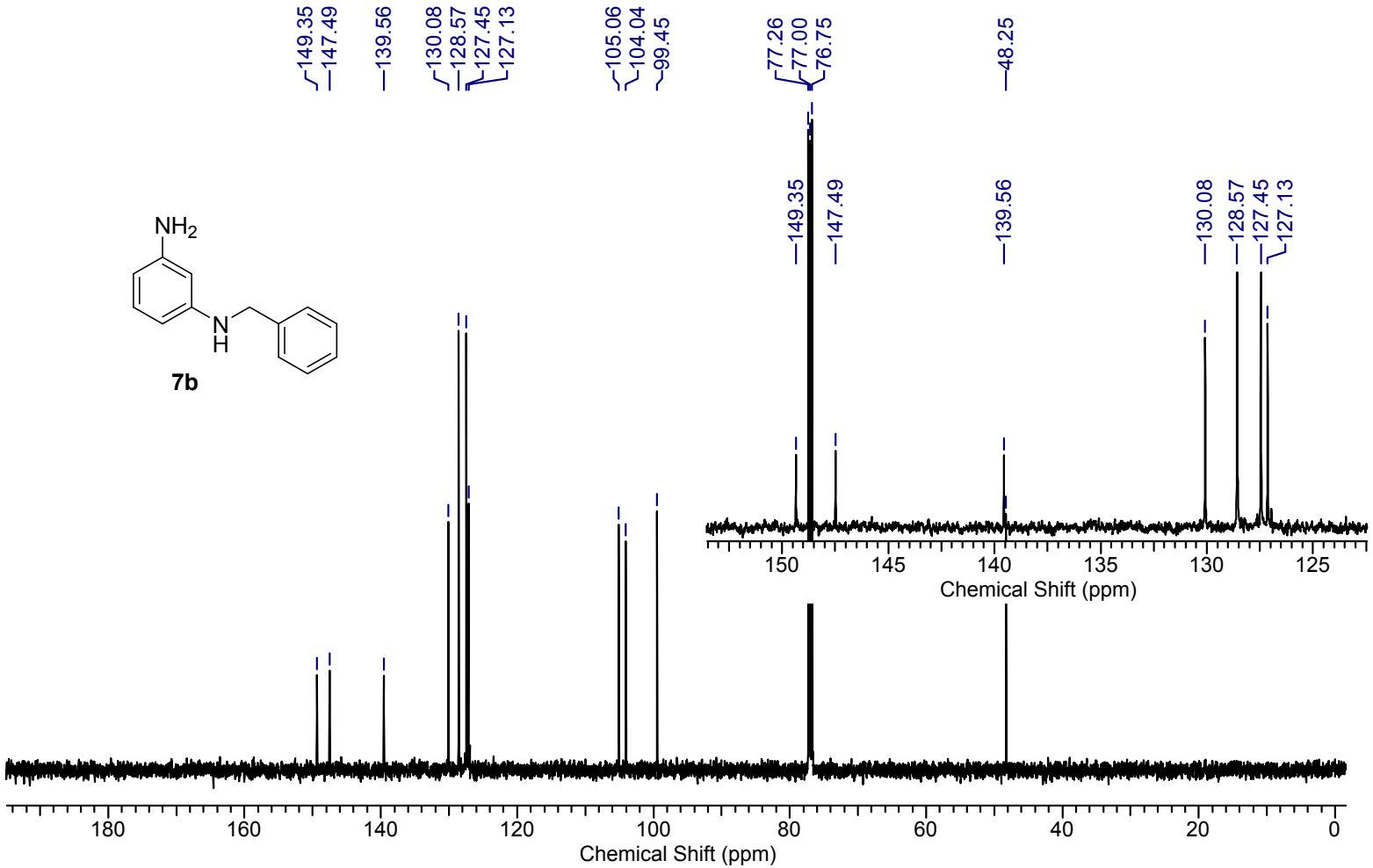

7.27
7.06
7.04
6.92
6.85
6.64
6.62
4.25
3.88
3.88
3.82
3.80
3.79
2.78
2.77
2.76
OMe
OMe
H
N
HO
6j
2.56
1.80
1.43
2.37
7.00
6.75
6.50
Chemical Shift (ppm)
2.56 1.80 1.43 2.37
2.10 5.91 2.56
2.31
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

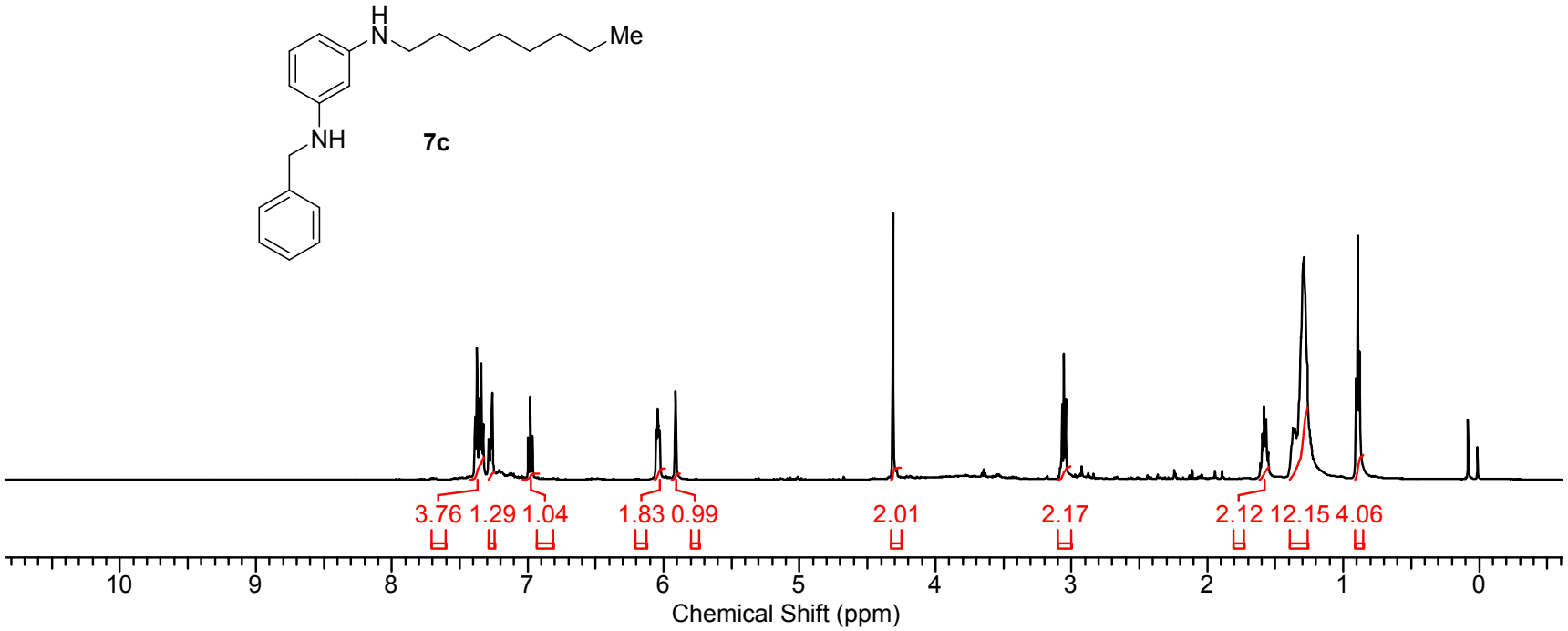

149.10
146.80
131.85
129.83
127.14
119.66
113.20
113.12
111.14
110.75
77.25
77.00
76.74
63.92
55.91
48.44
38.24
0.99
OMe
OMe
H
N
HO
6j
131.85
129.83
127.14
119.66
113.20
113.12
111.14
130
125
120
115
Chemical Shift (ppm)
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

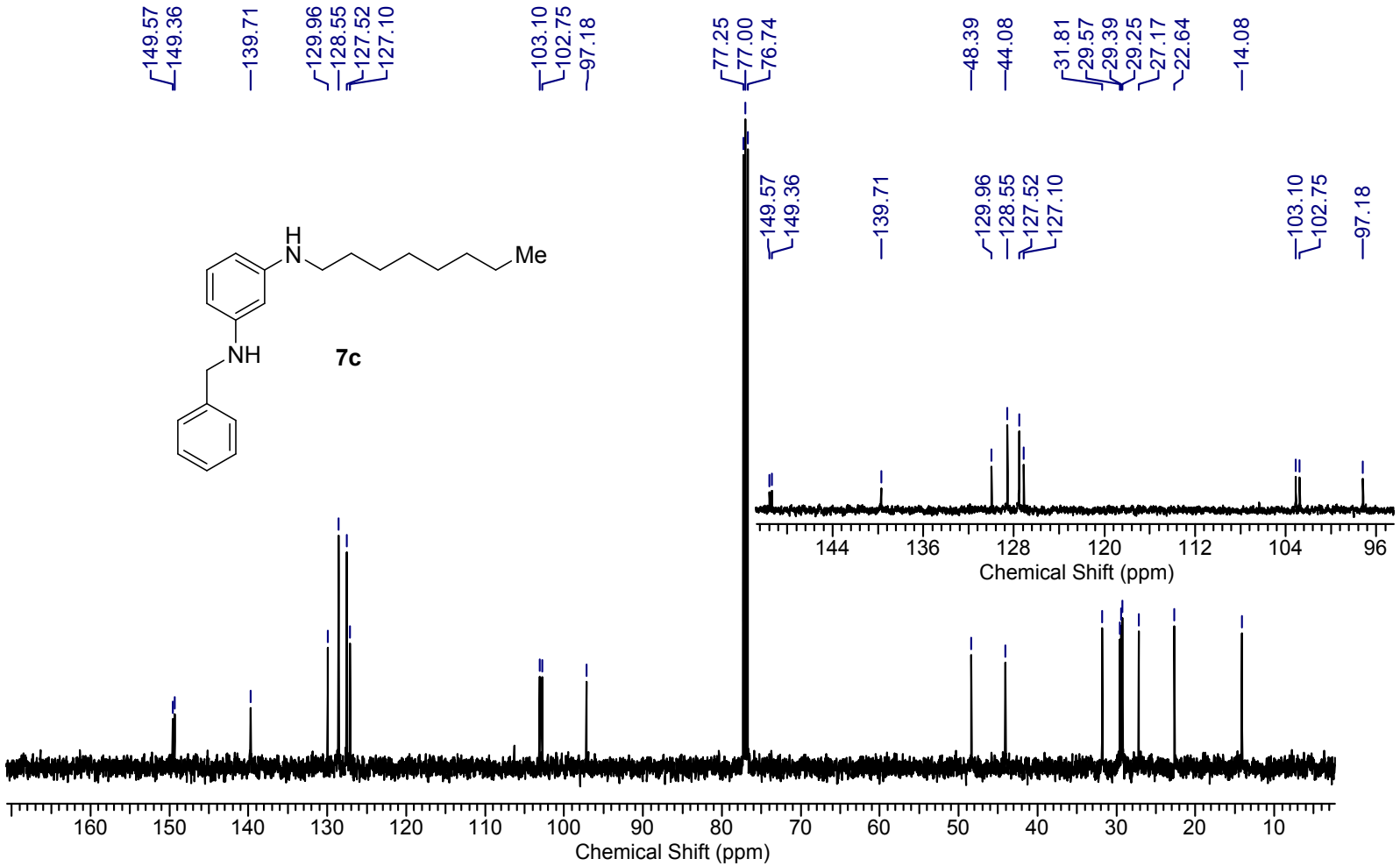

7.38
7.27
7.07
7.05
6.66
6.64
6.34
6.33
6.24
6.24
4.31
3.81
3.80
3.79
2.78
2.77
2.76
HO
H
N
O
6k
0.81
1.96
1.94
0.85
0.90
2.00
2.10
2.07
0.87
Chemical Shift (ppm)

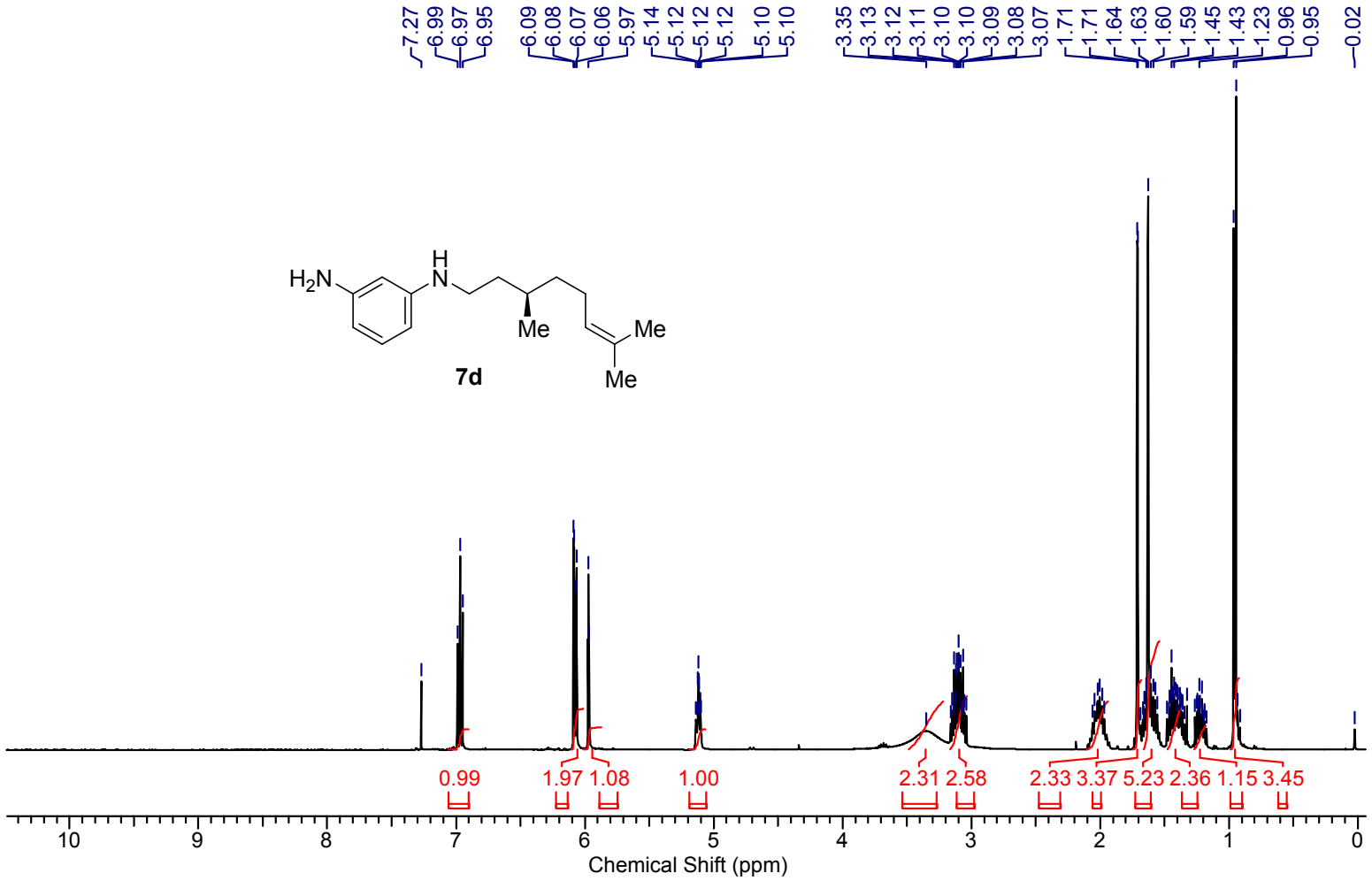

152.72
146.25
141.89
129.80
127.54
113.42
110.30
106.95
77.26
77.00
76.75
63.88
41.56
38.24
HO
H
N
O
6k
Chemical Shift (ppm)
Chemical Shift (ppm)

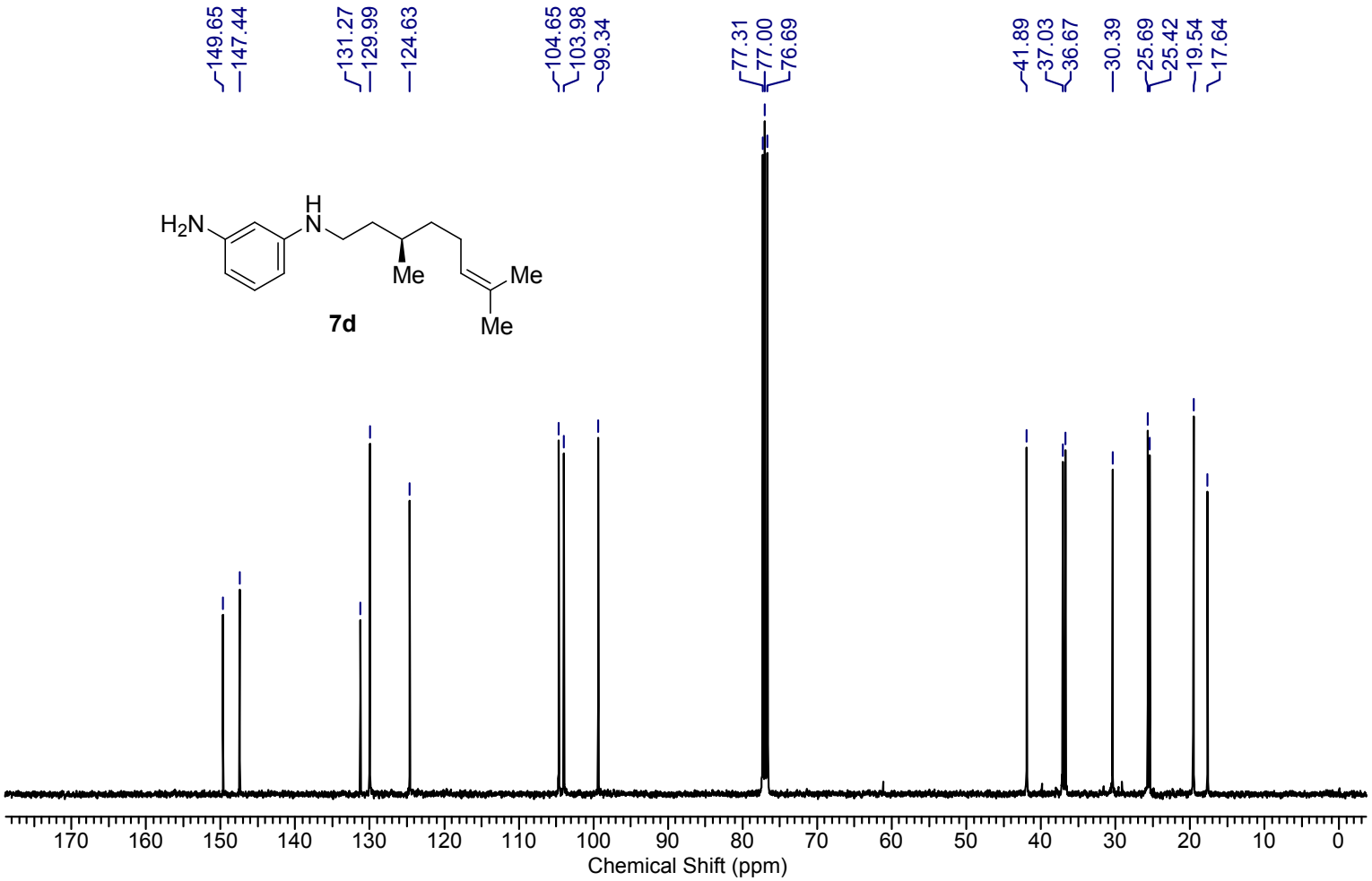

7.41
7.39
7.38
7.36
7.31
7.00
6.98
6.14
6.13
6.12
6.11
6.01
6.01
4.73
4.33
3.51
NH2
N
H
7b
4.18 1.20 1.00 1.92 1.03 2.18 3.04
Chemical Shift (ppm)
7.41
7.40
7.39
7.38
7.36
7.31
7.29
7.01
7.00
6.98
6.14
6.14
6.13
6.02
6.01
6.01
4.18 1.20 1.00 1.92 1.03
Chemical Shift (ppm)

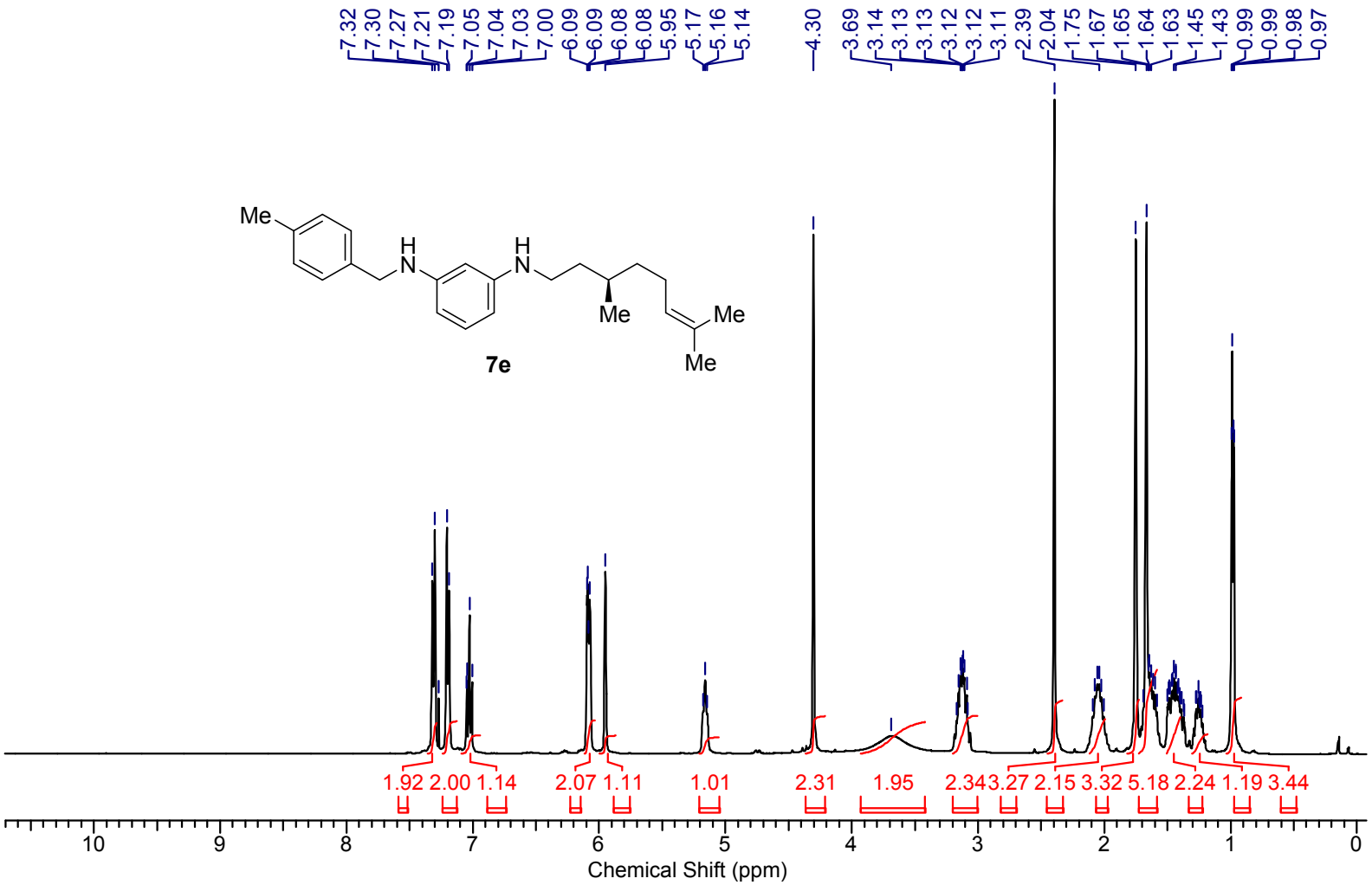

149.35
147.49
139.56
130.08
128.57
127.45
127.13
105.06
104.04
99.45
77.26
77.00
76.75
48.25
NH2
N
H
7b
Chemical Shift (ppm)
Chemical Shift (ppm)

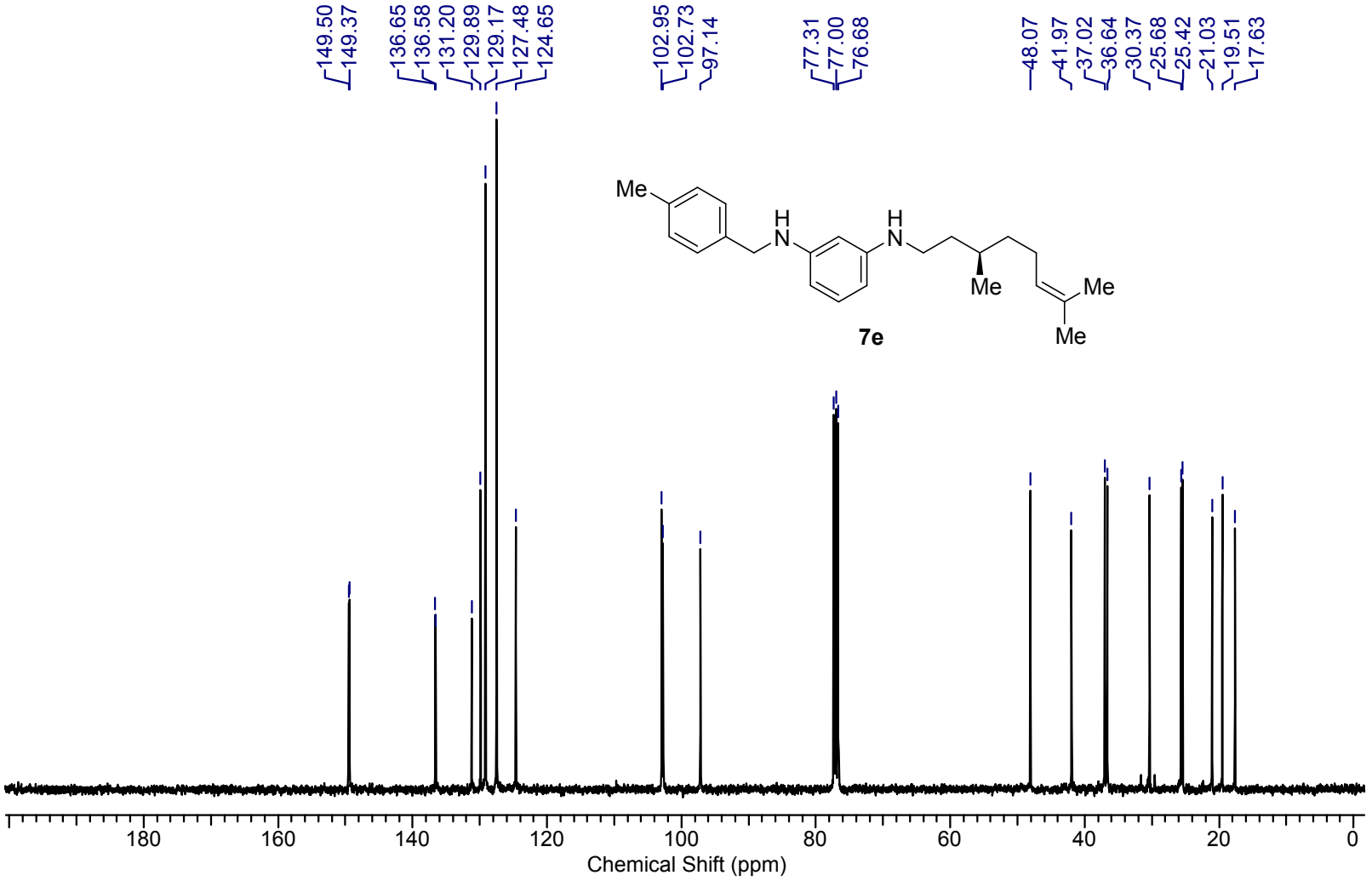

H
N
Me
NH
7c
3.76 1.29 1.04 1.83 0.99 2.01 2.17 2.12 12.15 4.06
10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)


149.57
149.36
139.71
129.96
128.55
127.52
127.10
103.10
102.75
97.18
77.25
77.00
76.74
48.39
44.08
31.81
29.57
29.39
29.25
27.17
22.64
14.08
H
N
Me
NH
7c
Chemical Shift (ppm)
Chemical Shift (ppm)


7.27
6.99
6.97
6.95
6.09
6.08
6.07
6.06
5.97
5.14
5.12
5.12
5.12
5.10
5.10
3.35
3.13
3.12
3.11
3.10
3.10
3.09
3.08
3.07
1.71
1.71
1.64
1.63
1.60
1.59
1.45
1.43
1.23
0.96
0.95
0.02
H2N
H
N
Me
Me
Me
7d
0.99
1.97
1.08
1.00
2.31
2.58
2.33
3.37
5.23
2.36
1.15
3.45
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


149.65
147.44
131.27
129.99
124.63
104.65
103.98
99.34
77.31
77.00
76.69
41.89
37.03
36.67
30.39
25.69
25.42
19.54
17.64
H2N
H
N
Me
Me
Me
7d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)


7.32
7.30
7.27
7.21
7.19
7.05
7.04
7.03
7.00
6.09
6.09
6.08
6.08
5.95
5.17
5.16
5.14
4.30
3.69
3.14
3.13
3.13
3.12
3.12
3.11
2.39
2.04
1.75
1.67
1.65
1.64
1.63
1.45
1.43
0.99
0.99
0.98
0.97
Me
H
N
H
N
Me
Me
Me
7e
1.92 2.00 1.14 2.07 1.11 1.01 2.31 1.95 2.34 3.27 2.15 3.32 5.18 2.24 1.19 3.44
10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)


149.50
149.37
136.65
136.58
131.20
129.89
129.17
127.48
124.65
102.95
102.73
97.14
77.31
77.00
76.68
48.07
41.97
37.02
36.64
30.37
25.68
25.42
21.03
19.51
17.63
Me
H
N
H
N
Me
Me
Me
7e
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)