Supporting Information

Photoinduced radical alkylation of aldehydes with potassium alkyltrifluoroborates

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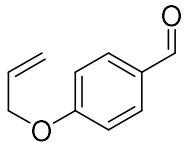
General Methods

Precoated silica gel plates F-254 were used for thin-layer analytical chromatography visualizing with UV and/or acidic aq. $KMnO_4$ solution. High resolution mass spectra (HRMS) were measured using electrospray ionization (ESI) and time-of-flight (TOF) mass analyzer. The measurements were done in a positive ion mode (interface capillary voltage – 4500 V) or in a negative ion mode (3200 V); mass range from m/z 50 to m/z 3000. For irradiation, a strip of light emitting diodes smd 3528, 50 cm (3528-120LED-1M, 12 V, IP 33; 60W 400 nm) was used. Reactions were performed in a glass tube (outer diameter 12 mm, inner diameter 9 mm). The reaction tube was placed in a glass jacket cooled with water (water temperature *ca*. 20 °C), and the system was wrapped by a strip of LEDs. The distance between the reaction vessel and diodes was about 1 cm. [1]

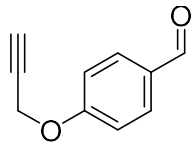
Starting materials

All reactions were performed under air atmosphere unless otherwise noted. Acetonitrile, ethyl acetate, 1,2-dichloroethane, toluene and dichloromethane were distilled from CaH_2. Commercial reagents and solvents were purchased in ABCR, TCI, BLDPharm, Angene Chemicals and were used without further purification unless otherwise stated.

Following compounds were prepared according to literature procedures:



SI-1 [2]



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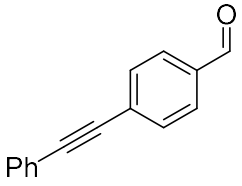

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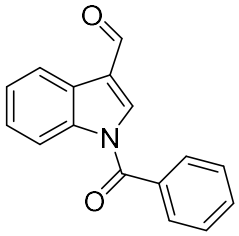

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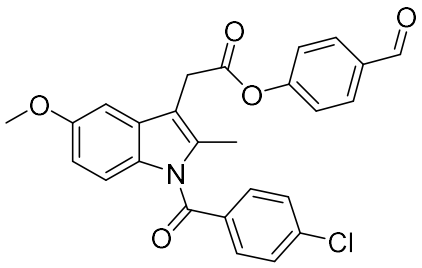
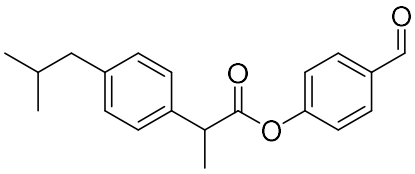


SI-5 [6]



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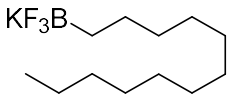

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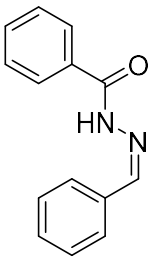
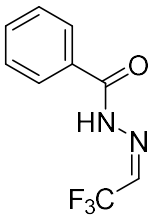


SI-8 [9]



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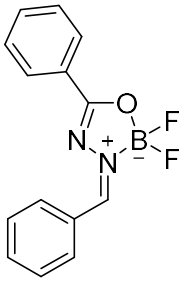
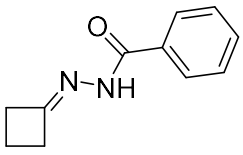
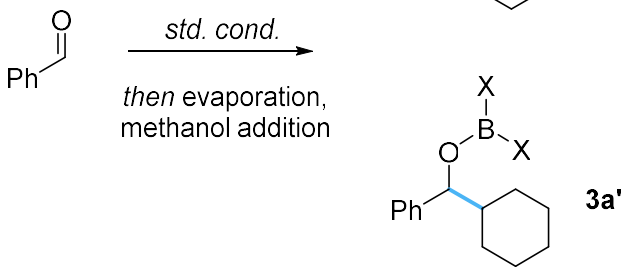


SI-10 [11]



SI-11 [12]

Optimization of work-up conditions



additives	time, h	3a/3a'
none	0	55/45
sat. aq. LiOH	18	14/86
sat. aq. $NaHCO_3$	18	55/45
25% aq. NH_4OH	18	55/45
sat. NH_3 in methanol	18	55/45
sat. aq. KF	18	60/40
sat. aq. KOH	2	97/3
sat. aq. KHF_2	0.5	100/0 (98)
aq. $FeCl_3$ (5 mol.%) imidazole (4 equiv) mannitol (1 equiv)	18	100/0 (92)

Table S1. Hydrolysis studies. [a] Relative amount of **3a** and **3a′** by ^{1}H NMR (**3a**+**3a′**=100) was determined by ^{1}H NMR. [b] ^{1}H NMR yields of **3a** in parenthesis (determined by using CH_2Br_2 as an internal standard).

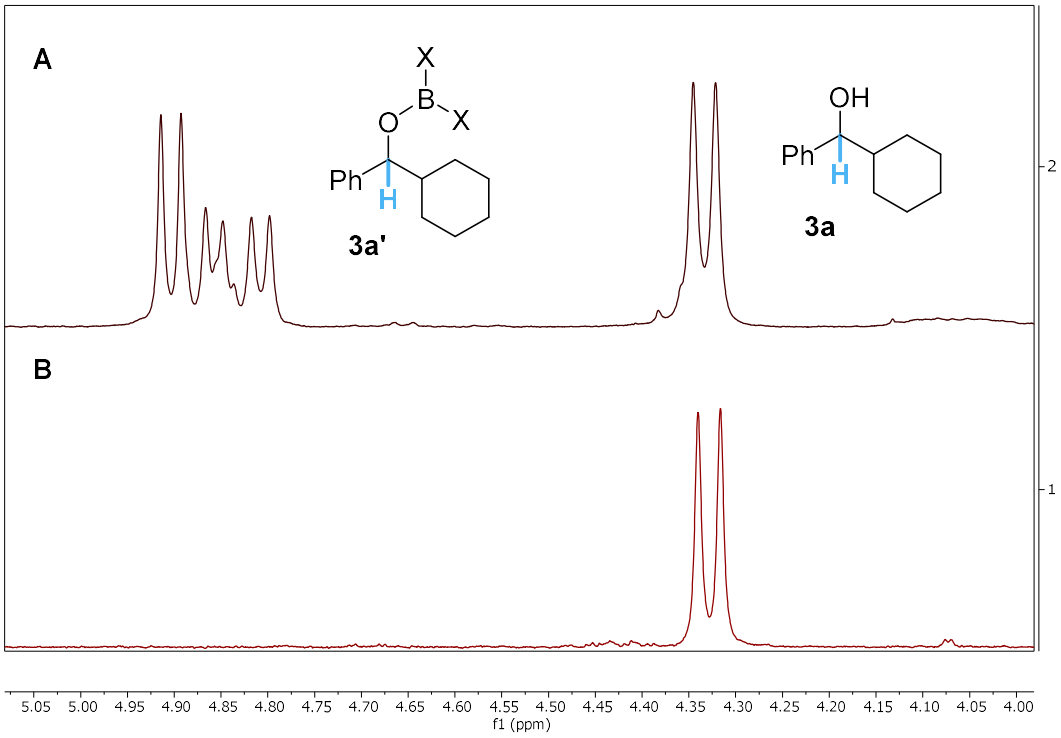
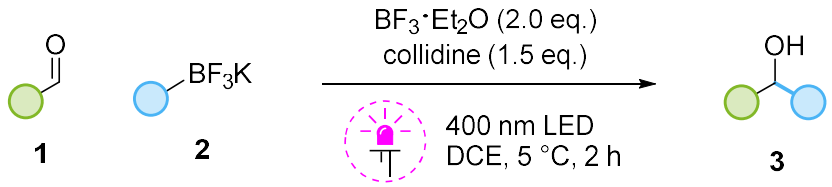


Figure S1. A. ^{1}H NMR spectrum of reaction mixture before workup. B. ^{1}H NMR spectrum of crude after KHF_2 workup.

Synthesis of alcohols 3a-o, 3r-u, 3w-ai (General procedure I)



A tube equipped with an argon outlet (*Note 1*) and a stirring bar was charged with solid potassium alkyltrifluoroborate **2** (2.0 equiv, 1.0 mmol) followed by dry 1,2-dichloroethane (2 mL), aldehyde **1** (1.0 equiv, 0.5 mmol) and 2,4,6-collidine (1.5 equiv, 0.75 mmol, 99 μL) under inert atmosphere. Then, the reaction mixture was cooled to 5 °C and boron trifluoride etherate (2.0 equiv, 1.0 mmol, 123 μL) was added with microsyringe in one portion. The mixture was irradiated by 400 nm LEDs at 5 °C (60W LEDs for 2 hours for **3a-o**, **3r-u**, **3w-z**; 5W LEDs for 18 hours for **3aa-ai**). The solvent was evaporated under reduced pressure, the residue was dissolved in methanol (2 mL)

For compounds **3a-3e, 3g, 3h, 3k-o, 3t, 3z, 3aa-3ai**, aqueous saturated solution of KHF_2 (0.5 mL) was added to the resulting methanol solution with cooling at room temperature water bath (*Note 2*). The mixture was stirred for 30 minutes at room temperature, diluted with water (5 mL), and extracted with diethyl ether (3×5 mL) (*Note 3*). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

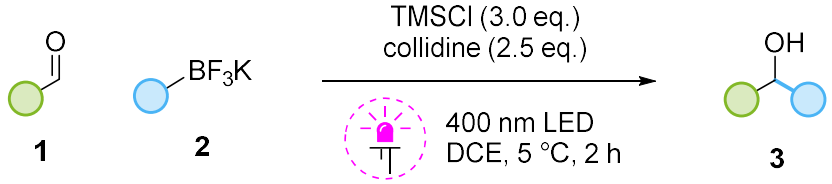
For compounds **3f, 3i, 3j, 3r, 3s, 3u-y**, aqueous solution of $FeCl_3$ (5 mol%, 0.025 mmol, 4 mg in 0.5 mL) was added to the resulting methanol solution followed by addition of solid imidazole (4.0 equiv, 2.0 mmol, 136 mg) and mannitol (1.0 equiv, 0.5 mmol, 91 mg). The resulting light brown cloudy suspension was stirred overnight at room temperature, diluted with water (5 mL), and extracted with diethyl ether (3×5 mL) (*Note 3*). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

Note 1: The reaction can be set up under air without noticeable yield loss due to the excess of trifluoroborate. However, the heavy byproduct alcohol stemming from the oxidation of trifluoroborate may sometimes interfere isolation.

Note 2: Under the standard reaction conditions, the resulting alcohol **3** was partially bound in mixed boronic esters, which were surprisingly resistant to hydrolysis. The conditions for its complete quenching were found after some optimizations and literature search (see Table S1).

Note 3: Sticky white precipitate formed in some cases meddled phase separation. It can be conveniently removed by placing the reaction tube on a centrifuge (2000 rpm, 1 min).

Synthesis of alcohols 3p, 3q, 3v (General procedure II)

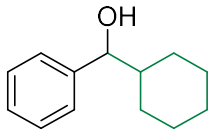


A tube equipped with an argon outlet (*Note 1*) and a stirring bar was charged with dry 1,2-dichloroethane (2 mL), aldehyde **1** (1.0 equiv, 0.5 mmol) and 2,4,6-collidine (2.5 equiv, 1.25 mmol, 165 µL) under inert atmosphere. Then, trimethylsilyl chloride (3.0 equiv, 1.5 mmol, 190 µL) was added and the reaction was stirred for 30 min at room temperature. The reaction mixture was cooled to 5 °C and solid potassium alkyltrifluoroborate **2** (2.0 equiv, 1 mmol) was added in one portion. The mixture was irradiated by 60W 400 nm LEDs for 2 hours at 5 °C. For the work-up, aqueous saturated solution of KHF_2 (0.5 mL) was added to the reaction mixture with cooling at room temperature water bath (*Note 2*). The mixture was stirred for 30 minutes at room temperature, diluted with water (5 mL), and extracted with diethyl ether (3×5 mL). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

Note 1: The reaction can be set up under air without noticeable yield loss due to the excess of trifluoroborate. However, the heavy byproduct alcohol stemming from borate oxidation may sometimes interfere isolation.

Note 2: Under the standard reaction conditions, the resulting alcohol **3** was partially bound in mixed boronic esters, which were surprisingly resistant to hydrolysis. The conditions for its complete quenching were found after some optimizations and literature search (see Table SI-1).

Cyclohexyl(phenyl)methanol (3a). [13]



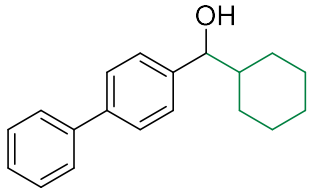
Yield 90 mg (95%). Colorless oil.

Chromatography: EtOAc/PE, 1/5. R_f 0.33.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.39 – 7.20 (m, 5H), 4.36 (dd, *J* = 7.2, 2.3 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.87 (d, *J* = 2.3 Hz, 1H), 1.83 – 1.53 (m, 4H), 1.44 – 0.85 (m, 6H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 143.6, 128.1, 127.4, 126.6, 79.3, 44.9, 29.3, 28.8, 26.4, 26.1, 26.0.

[1,1'-Biphenyl]-4-yl(cyclohexyl)methanol (3b). [14]



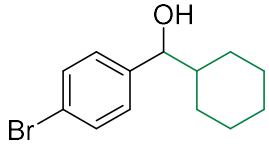
Yield 129 mg (97%). Colorless crystals. Mp 107-109 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.28.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.67 – 7.55 (m, 4H), 7.52 – 7.43 (m, 2H), 7.42 – 7.33 (m, 3H), 4.42 (d, *J* = 7.1 Hz, 1H), 2.14 (s, 1H), 2.09 – 2.01 (m, 1H), 1.86 – 1.59 (m, 4H), 1.55 – 1.41 (m, 1H), 1.36 – 0.91 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-d) δ 142.6, 140.8, 140.2, 128.7, 127.1, 127.0, 127.0, 126.8, 79.0, 44.9, 29.2, 28.8, 26.4, 26.1, 26.0.

(4-Bromophenyl)(cyclohexyl)methanol (3c). [15]



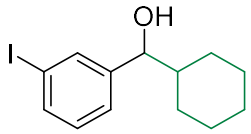
Yield 131 mg (97%). Colorless crystals. Mp 70-72 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.30.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 4.31 (d, *J* = 6.9 Hz, 1H), 2.06 (s, 1H), 1.95 – 1.86 (m, 1H), 1.81 – 1.47 (m, 4H), 1.42 – 1.33 (m, 1H), 1.29 – 0.78 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 142.5, 131.2, 128.3, 121.0, 78.6, 44.9, 29.1, 28.6, 26.3, 26.0, 25.9.

Cyclohexyl(3-iodophenyl)methanol (3d).



Yield 142 mg (90%). Colorless oil.

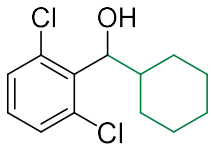
Chromatography: EtOAc/PE, 1/5. R_f 0.31.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.63 (t, *J* = 1.5 Hz, 1H), 7.58 (dt, *J* = 7.7, 1.5 Hz, 1H), 7.21 (dt, *J* = 7.7, 1.5 Hz, 1H), 7.05 (t, *J* = 7.7 Hz, 1H), 4.25 (d, *J* = 6.9 Hz, 1H), 2.28 (s, 1H), 1.95 – 1.83 (m, 1H), 1.80 – 1.48 (m, 4H), 1.44 – 1.30 (m, 1H), 1.28 – 0.72 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 145.9, 136.3, 135.5, 129.9, 125.8, 94.2, 78.4, 44.8, 29.1, 28.4, 26.3, 25.9, 25.86.

HRMS (ESI): calcd for $C_{13}H_{21}INO$ (M+NH_4) 334.0662, found 334.0663, calcd for $C_{13}H_{17}IONa$ (M+Na) 339.0216, found 339.0218.

Cyclohexyl(2,6-dichlorophenyl)methanol (3e).



Yield 92 mg (71%). Colorless crystals. Mp 96-98 °C ($CDCl_3$).

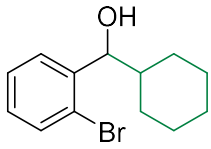
Chromatography: EtOAc/PE, 1/10. R_f 0.23.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.30 (d, *J* = 8.5 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.13 (dd, *J* = 8.5, 7.6 Hz, 1H), 5.09 (t, *J* = 10.0 Hz, 1H), 2.79 (d, *J* = 10.2 Hz, 1H), 2.37 – 2.10 (m, 2H), 1.89 – 1.80 (m, 1H), 1.74 – 1.59 (m, 2H), 1.40 – 0.93 (m, 6H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 137.4, 134.8, 129.7, 128.7, 76.7, 42.4, 30.4, 29.0, 26.3, 26.0, 25.8.

HRMS (ESI): calcd for $C_{13}H_{16}{}^{35}Cl^{35}ClONa$ (M+Na) 281.0470, found 281.0468, calcd for $C_{13}H_{16}{}^{35}Cl^{37}ClONa$ (M+Na) 283.0441, found 283.0439, calcd for $C_{13}H_{16}{}^{37}Cl^{37}ClONa$ (M+Na) 285.0412, found 285.0429.

(2-Bromophenyl)(cyclohexyl)methanol (3f).



Yield 109 mg (81%). Colorless crystals. Mp 97-99 °C ($CHCl_3$).

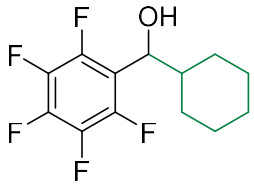
Chromatography: EtOAc/PE, 1/5. R_f 0.40.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.51 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.46 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.31 (td, *J* = 7.7, 1.3 Hz, 1H), 7.10 (td, *J* = 7.8, 1.8 Hz, 1H), 4.85 (dd, *J* = 6.3, 3.0 Hz, 1H), 2.19 (d, *J* = 3.0 Hz, 1H), 1.93 – 1.59 (m, 5H), 1.43 (d, *J* = 2.5 Hz, 1H), 1.33 – 0.93 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 142.6, 132.5, 128.5, 128.4, 127.3, 122.7, 76.95, 43.9, 29.5, 27.5, 26.3, 26.3, 26.0.

HRMS (ESI): calcd for $C_{13}H_{17}{}^{79}BrONa$ (M+Na) 291.0355, found 291.0359, calcd for $C_{13}H_{17}{}^{81}BrONa$ (M+Na) 293.0335, found 293.0347.

Cyclohexyl(perfluorophenyl)methanol (3g). [16]



Yield 92 mg (66%). Colorless crystals. Mp 75-77 °C ($CHCl_3$).

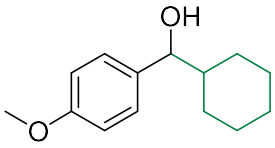
Chromatography: EtOAc/PE, 1/5. R_f 0.42.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 4.69 (t, *J* = 8.5 Hz, 1H), 2.23 (d, *J* = 8.5 Hz, 1H), 2.20 – 2.11 (m, 1H), 1.91 – 1.56 (m, 4H), 1.39 – 0.79 (m, 6H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 144.7 (dm, *J* = 245.2 Hz), 140.3 (dm, *J* = 253.6 Hz), 137.5 (dm, *J* = 253.1 Hz), 116.5 (tm, *J* = 15.7 Hz), 71.4, 43.4, 29.7, 28.9, 26.1, 25.6, 25.5.

^{19}F NMR (282 MHz, Chloroform-*d*) δ -142.9 (dd, *J* = 22.6, 8.5 Hz, 2F), -155.5 (tt, *J* = 20.7, 1.3 Hz, 1F), -161.9 – -162.2 (m, 2F).

Cyclohexyl(4-methoxyphenyl)methanol (3h). [17]



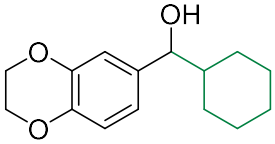
Yield 96 mg (87%). Colorless crystals. Mp 87-89 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.27.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.20 (d, *J* = 8.2 Hz, 2H), 6.86 (d, *J* = 8.2 Hz, 2H), 4.27 (d, *J* = 7.4 Hz, 1H), 3.79 (s, 3H), 2.09 – 1.89 (m, 2H), 1.84 – 1.49 (m, 4H), 1.45 – 0.77 (m, 6H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 158.8, 135.8, 127.7, 113.5, 78.9, 55.2, 44.88, 29.2, 29.0, 26.4, 26.0, 25.9.

Cyclohexyl(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)methanol (3i).



Yield 104 mg (84%). Colorless oil.

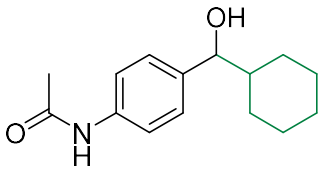
Chromatography: EtOAc/PE, 1/5. R_f 0.15.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 6.80 (d, *J* = 8.2 Hz, 1H), 6.79 (d, *J* = 2.0 Hz, 1H), 6.74 (dd, *J* = 8.2, 2.0 Hz, 1H), 4.22 (s, 4H), 4.21 (d, *J* = 7.4 Hz, 1H), 1.99 (s, 1H), 2.04 – 1.91 (m, 1H), 1.86 – 1.45 (m, 4H), 1.42 – 1.30 (m, 1H), 1.30 – 0.79 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 143.1, 142.7, 137.1, 119.6, 116.8, 115.4, 78.8, 64.3, 64.3, 44.8, 29.2, 29.0, 26.4, 26.0, 25.9.

HRMS (ESI): calcd for $C_{15}H_{20}O_3Na$ (M+Na) 271.1305, found 271.1308, calcd for $C_{15}H_{20}OK$ (M+K) 287.1044, found 287.1031.

***N*-(4-[cyclohexyl{hydroxy}methyl]phenyl)acetamide (3j).**



Prepared according to General procedure I, with the addition of saturated aqueous $NaHSO_3$ (1 mL) solution on the extraction step to get rid of unreacted aldehyde.

Yield 51 mg (41%). Colorless crystals. Mp 174-176 °C ($CHCl_3$).

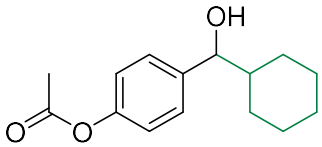
Chromatography: MeOH/CH_2Cl_2, 1/20. R_f 0.23.

^{1}H NMR (300 MHz, Methanol-d_4) δ 7.50 (d, J = 8.1 Hz, 2H), 7.22 (d, J = 8.1 Hz, 2H), 4.25 (d, J = 7.3 Hz, 1H), 3.31 (s, 1H), 2.11 (s, 3H), 2.06 – 1.95 (m, 1H), 1.81 – 1.47 (m, 4H), 1.39 – 0.82 (m, 6H).

^{13}C{^{1}H} NMR (76 MHz, Methanol-d_4) δ 171.5, 141.1, 138.7, 128.2, 120.8, 79.7, 46.3, 30.4, 30.3, 27.6, 27.2, 27.2, 23.8.

HRMS (ESI): calcd for $C_{15}H_{22}NO_2$ (M+H) 248.1645, found 248.1643, calcd for $C_{15}H_{21}NO_2Na$ (M+Na) 270.1465, found 270.1461, calcd for $C_{15}H_{21}NO_2K$ 286.1204, found 286.1195.

4-(Cyclohexyl[hydroxy]methyl)phenyl acetate (3k). [18]



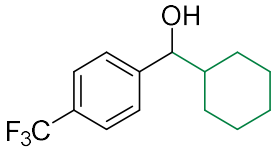
Yield 103 mg (83%). Colorless crystals. Mp 56-58 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.15.

^{1}H NMR (300 MHz, Chloroform-d) δ 7.29 (d, J = 8.5 Hz, 2H), 7.05 (d, J = 8.5 Hz, 2H), 4.34 (d, J = 7.1 Hz, 1H), 2.29 (s, 3H), 2.28 (s, 1H), 2.03 – 1.88 (m, 1H), 1.84 – 1.51 (m, 4H), 1.47 – 1.34 (m, 1H), 1.32 – 0.85 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-d) δ 169.5, 149.7, 141.1, 127.5, 121.0, 78.6, 44.8, 29.1, 28.6, 26.3, 26.0, 25.9, 21.0.

Cyclohexyl(4-[trifluoromethyl]phenyl)methanol (3l). [19]



Yield 115 mg (89%). Colorless crystals. Mp 73-75 °C ($CHCl_3$).

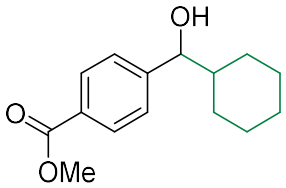
Chromatography: EtOAc/PE, 1/10. R_f 0.16.

^{1}H NMR (300 MHz, Chloroform-d) δ 7.58 (d, J = 8.1 Hz, 2H), 7.39 (d, J = 8.1 Hz, 2H), 4.42 (dd, J = 6.8, 2.8 Hz, 1H), 2.24 (d, J = 2.8 Hz, 1H), 1.95 – 1.83 (m, 1H), 1.81 – 1.51 (m, 4H), 1.46 – 1.33 (m, 1H), 1.29 – 0.80 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-d) δ 147.5 (q, J = 1.4 Hz), 129.5 (q, J = 32.2 Hz), 126.9, 125.0 (q, J = 3.8 Hz), 124.2 (q, J = 271.9 Hz), 78.6, 45.0, 29.2, 28.4, 26.3, 26.0, 25.9.

^{19}F NMR (282 MHz, Chloroform-d) δ -62.4.

Methyl 4-(cyclohexyl[hydroxy]methyl)benzoate(3m). [18]



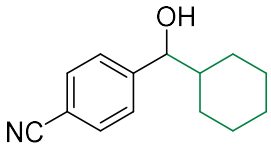
Yield 114 mg (92%). Colorless crystals. Mp 94-96 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.17.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.3 Hz, 2H), 4.38 (d, *J* = 6.6 Hz, 1H), 3.85 (s, 3H), 2.62 (s, 1H), 1.92 – 1.78 (m, 1H), 1.79 – 1.48 (m, 4H), 1.42 – 1.28 (m, 1H), 1.25 – 0.79 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 167.0, 148.9, 129.3, 128.8, 126.5, 78.5, 51.9, 44.9, 29.1, 28.3, 26.2, 25.9, 25.9.

4-(Cyclohexyl[hydroxy]methyl)benzonitrile (3n). [19]



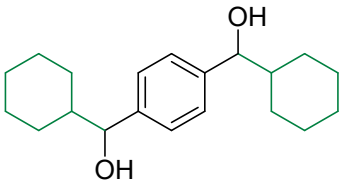
Yield 93 mg (86%). Colorless crystals. Mp 55-57 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.10.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.3 Hz, 2H), 4.42 (d, *J* = 6.4 Hz, 1H), 2.50 (s, 1H), 1.88 – 1.46 (m, 5H), 1.44 – 1.30 (m, 1H), 1.25 – 0.84 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 149.0, 131.8, 127.2, 118.8, 110.6, 78.1, 44.9, 29.1, 28.0, 26.1, 25.9, 25.8.

1,4-Phenylenebis(cyclohexylmethanol) (3o).



Yield 132 mg (87%). Colorless crystals. Mp 130-132 °C ($CHCl_3$).

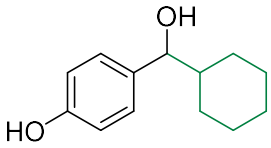
Chromatography: EtOAc/PE, 1/5. R_f 0.29.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.34 – 7.15 (m, 4H), 4.32 (d, *J* = 7.2 Hz, 2H), 2.11 – 1.91 (m, 4H), 1.86 – 1.49 (m, 8H), 1.40 – 0.74 (m, 12H).

$^{13}C\{^{1}H\}$ NMR (76 MHz, Chloroform-*d*) δ 142.7, 126.4, 79.1, 79.1, 44.9, 29.3, 28.8, 26.4, 26.0, 26.0.

HRMS (ESI): calcd for $C_{20}H_{34}O_2N$ (M+NH_4) 320.2584, found 320.2582, calcd for $C_{20}H_{30}O_2Na$ (M+Na) 325.2138, found 325.2141, calcd for $C_{20}H_{30}O_2K$ (M+K) 341.1877, found 341.1869.

4-(Cyclohexyl[hydroxy]methyl)phenol (3p).



Yield 83 mg (80%). Colorless crystals. Mp 120-122 °C ($CDCl_3$).

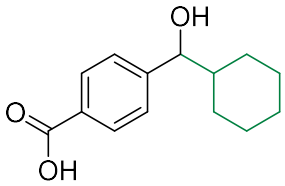
Chromatography: EtOAc/PE, 1/2. R_f 0.28.

^{1}H NMR (300 MHz, DMSO-d_6) δ 9.16 (s, 1H), 7.04 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 8.4 Hz, 2H), 4.84 (d, *J* = 4.2 Hz, 1H), 4.10 (dd, *J* = 6.8, 4.2 Hz, 1H), 1.99 – 1.81 (m, 1H), 1.78 – 1.51 (m, 3H), 1.46 – 1.24 (m, 2H), 1.23 – 0.76 (m, 5H).

$^{13}C\{^{1}H\}$ NMR (76 MHz, DMSO-d_6) δ 156.0, 135.3, 127.6, 114.4, 76.9, 45.0, 29.0, 28.6, 26.2, 25.8, 25.7.

HRMS (ESI): calcd for $C_{13}H_{18}O_2Na$ (M+Na) 229.1199, found 229.1208.

4-(Cyclohexyl[hydroxy]methyl)benzoic acid (3q).



Yield 104 mg (89%). Colorless crystals. Mp 168-170 °C (Methanol).

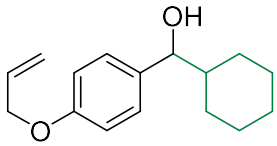
Chromatography: EtOAc/PE, 1/1. R_f 0.20.

^{1}H NMR (300 MHz, Methanol-d_4) δ 8.00 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.3 Hz, 2H), 4.40 (d, *J* = 6.9 Hz, 1H), 2.09 – 1.51 (m, 5H), 1.49 – 0.86 (m, 7H).

$^{13}C\{^{1}H\}$ NMR (76 MHz, Methanol-d_4) δ 169.9, 150.9, 130.6, 130.5, 127.8, 79.5, 46.3, 30.5, 29.9, 27.6, 27.2, 27.2.

HRMS (ESI): calcd for $C_{14}H_{18}O_3Na$ (M+Na) 257.1148, found 257.1146.

(4-[Allyloxy]phenyl)(cyclohexyl)methanol (3r).



Yield 78 mg (63%). Colorless oil.

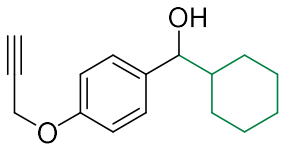
Chromatography: EtOAc/PE, 1/5. R_f 0.31.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.19 (d, *J* = 8.6 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.06 (ddt, *J* = 17.3, 10.5, 5.3 Hz, 1H), 5.41 (dq, *J* = 17.3, 1.5 Hz, 1H), 5.28 (dq, *J* = 10.5, 1.5 Hz, 1H), 4.52 (dt, *J* = 5.3, 1.5 Hz, 2H), 4.27 (d, *J* = 7.4 Hz, 1H), 2.08 – 1.92 (m, 2H), 1.86 – 1.70 (m, 1H), 1.72 – 1.48 (m, 3H), 1.42 – 1.26 (m, 1H), 1.29 – 0.74 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 157.9, 136.0, 133.3, 127.7, 117.5, 114.3, 78.9, 68.7, 44.9, 29.2, 29.0, 26.4, 26.0, 25.9.

HRMS (ESI): calcd for $C_{16}H_{22}O_2Na$ (M+Na) 269.1512, found 269.1507.

Cyclohexyl(4-[prop-2-yn-1-yloxy]phenyl)methanol (3s).



Yield 86 mg (70%). Colorless oil.

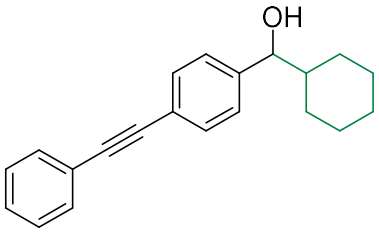
Chromatography: EtOAc/PE, 1/5. R_f 0.21.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.21 (d, *J* = 8.7 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H), 4.67 (d, *J* = 2.4 Hz, 2H), 4.29 (d, *J* = 7.3 Hz, 1H), 2.52 (t, *J* = 2.4 Hz, 1H), 2.05 – 1.89 (m, 2H), 1.82 – 1.49 (m, 4H), 1.41 – 0.77 (m, 6H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 156.8, 136.7, 127.7, 114.5, 78.8, 78.6, 75.5, 55.8, 44.9, 29.2, 29.0, 26.4, 26.0, 25.9.

HRMS (ESI): calcd for $C_{16}H_{20}O_2Na$ (M+Na) 267.1356, found 267.1364, calcd for $C_{16}H_{20}O_2K$ (M+K) 283.1095, found 283.1084.

Cyclohexyl(4-[phenylethynyl]phenyl)methanol (3t).



Yield 123 mg (85%). Colorless crystals. Mp 95-97 °C ($CHCl_3$).

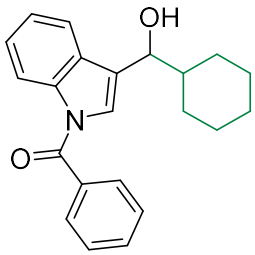
Chromatography: EtOAc/PE, 1/5. R_f 0.32.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.63 – 7.50 (m, 4H), 7.42 – 7.34 (m, 3H), 7.30 (d, *J* = 8.0 Hz, 2H), 4.39 (d, *J* = 6.9 Hz, 1H), 2.17 (s, 1H), 2.02 – 1.91 (m, 1H), 1.86 – 1.56 (m, 4H), 1.52 – 1.38 (m, 1H), 1.35 – 0.89 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 143.8, 131.5, 131.3, 128.3, 128.1, 126.6, 123.2, 122.10, 89.3, 89.2, 78.9, 44.9, 29.1, 28.6, 26.3, 26.0, 25.9.

HRMS (ESI): calcd for $C_{21}H_{26}ON$ (M+NH_4) 308.2009, found 308.2010, calcd for $C_{21}H_{22}ONa$ (M+Na) 313.1563, found 313.1564, calcd for $C_{21}H_{22}OK$ (M+K) 329.1302, found 329.1299.

(3-[Cyclohexyl{hydroxy}methyl]-1H-indol-1-yl)(phenyl)methanone (3u).



Yield 43 mg (26%). Dark yellow oil.

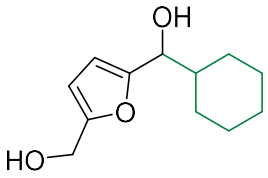
Chromatography: EtOAc/PE, 1/3. R_f 0.26.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.39 (d, *J* = 8.2 Hz, 1H), 7.77 – 7.65 (m, 3H), 7.65 – 7.46 (m, 3H), 7.45 – 7.28 (m, 2H), 7.22 (s, 1H), 4.65 (d, *J* = 7.0 Hz, 1H), 2.08 – 1.40 (m, 7H), 1.34 – 0.89 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 168.5, 136.7, 134.6, 131.9, 129.2, 129.1, 128.6, 125.1, 124.6, 124.4, 123.8, 120.2, 116.6, 73.0, 43.7, 29.6, 28.7, 26.3, 26.1, 25.9.

HRMS (ESI): calcd for $C_{22}H_{23}NO_2Na$ (M+Na) 356.1621, found 356.1609, calcd for $C_{22}H_{23}NO_2K$ (M+K) 372.1360, found 372.1356.

Cyclohexyl(5-[hydroxymethyl]furan-2-yl)methanol (3v).



Yield 54 mg (51%). Colorless crystals. Mp 93-95 °C ($CHCl_3$).

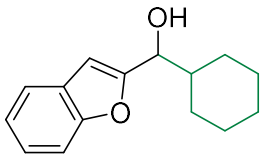
Chromatography: EtOAc/PE, 1/1. R_f 0.37.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 6.17 (d, *J* = 3.1 Hz, 1H), 6.10 (d, *J* = 3.1 Hz, 1H), 4.49 (s, 2H), 4.28 (d, *J* = 7.6 Hz, 1H), 3.03 (s, 1H), 2.79 (s, 1H), 2.10 – 1.86 (m, 1H), 1.83 – 1.54 (m, 4H), 1.50 – 1.36 (m, 1H), 1.34 – 0.80 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 156.0, 153.2, 108.2, 107.3, 72.6, 57.3, 42.6, 29.1, 28.8, 26.3, 25.9, 25.8.

HRMS (ESI): calcd for $C_{12}H_{22}O_3N$ (M+NH_4) 228.1594, found 228.1602, calcd for $C_{12}H_{18}O_3Na$ (M+Na) 233.1148, found 233.1151, calcd for $C_{12}H_{18}O_3K$ (M+K) 249.0888, found 249.0894.

Benzofuran-2-yl(cyclohexyl)methanol (3w). [20]



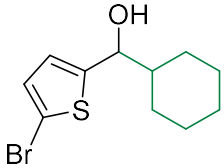
Yield 81 mg (70%). Yellow oil.

Chromatography: EtOAc/PE, 1/5. R_f 0.27.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.59 – 7.54 (m, 1H), 7.53 – 7.45 (m, 1H), 7.35 – 7.19 (m, 2H), 6.62 (s, 1H), 4.55 (dd, *J* = 6.9, 5.0 Hz, 1H), 2.34 (d, *J* = 5.2 Hz, 1H), 2.09 – 1.65 (m, 5H), 1.62 – 1.51 (m, 1H), 1.40 – 1.01 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 158.7, 154.6, 128.1, 123.9, 122.7, 120.8, 111.2, 103.3, 73.1, 42.7, 29.1, 28.4, 26.3, 25.9, 25.8.

(5-Bromothiophen-2-yl)(cyclohexyl)methanol (3x).



Yield 107 mg (78%). Yellow oil.

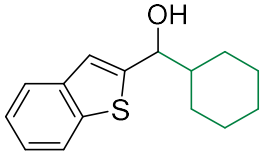
Chromatography: EtOAc/PE, 1/10. R_f 0.20.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 6.88 (d, *J* = 3.7 Hz, 1H), 6.65 (dd, *J* = 3.7, 0.8 Hz, 1H), 4.50 (dd, *J* = 7.2, 2.7 Hz, 1H), 2.35 (d, *J* = 2.7 Hz, 1H), 2.09 – 1.86 (m, 1H), 1.83 – 1.45 (m, 5H), 1.37 – 0.81 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 149.3, 129.1, 124.5, 111.1, 75.3, 45.3, 29.1, 28.7, 26.2, 25.87, 25.8.

HRMS (ESI): calcd for $C_{11}H_{15}{}^{79}BrOSNa$ (M+Na) 296.9919, found 296.9907, calcd for $C_{11}H_{15}{}^{81}BrOSNa$ (M+Na) 298.9899, found 298.9893.

Benzo[b]thiophen-2-yl(cyclohexyl)methanol (3y). [21]



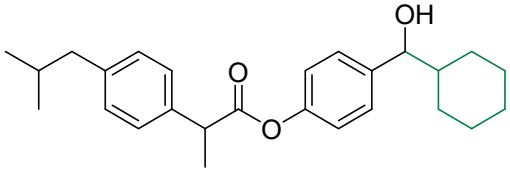
Yield 91 mg (74%). Colorless crystals. Mp 87-89 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.25.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 7.0 Hz, 1H), 7.72 (dd, *J* = 7.0, 1.9 Hz, 1H), 7.41 – 7.25 (m, 2H), 7.14 (s, 1H), 4.68 (dd, *J* = 7.2, 3.5 Hz, 1H), 2.39 (d, *J* = 3.5 Hz, 1H), 2.11 – 1.99 (m, 1H), 1.85 – 1.63 (m, 4H), 1.61 – 1.50 (m, 1H), 1.36 – 0.96 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 148.3, 139.3, 139.3, 124.1, 124.0, 123.3, 122.4, 120.8, 75.6, 45.1, 29.2, 28.6, 26.3, 25.9, 25.8.

4-(Cyclohexyl[hydroxy]methyl)phenyl 2-(4-isobutylphenyl)propanoate (3z).



Yield 85 mg (43%). Colorless crystals. Mp 71-73 °C ($CHCl_3$).

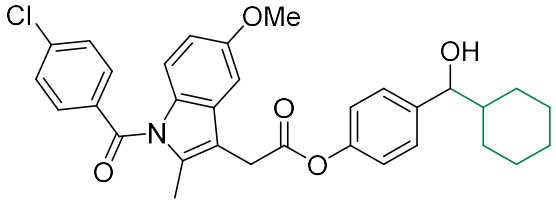
Chromatography: EtOAc/PE, 1/5. R_f 0.23.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.34 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 7.00 (d, *J* = 8.5 Hz, 2H), 4.36 (d, *J* = 7.1 Hz, 1H), 3.97 (q, *J* = 7.1 Hz, 1H), 2.52 (d, *J* = 7.1 Hz, 2H), 2.20 – 1.49 (m, 6H), 1.64 (d, *J* = 7.1 Hz, 3H), 1.46 – 0.81 (m, 7H), 0.96 (d, *J* = 6.6 Hz, 6H).

$^{13}C\{^{1}H\}$ NMR (76 MHz, Chloroform-*d*) δ 173.2, 149.9, 141.0, 140.7, 137.2, 129.4, 127.4, 127.1, 121.0, 78.6, 45.2, 45.0, 44.9, 30.1, 29.1, 28.7, 26.3, 26.0, 25.9, 22.3, 18.4.

HRMS (ESI): calcd for $C_{26}H_{38}O_3N$ (M+NH_4) 412.2846, found 412.2841, calcd for $C_{26}H_{34}O_3Na$ (M+Na) 417.2400, found 417.2395, calcd for $C_{26}H_{34}O_3K$ (M+K) 433.2140, found 433.2133.

4-(Cyclohexyl[hydroxy]methyl)phenyl 2-(1-[4-chlorobenzoyl]-5-methoxy-2-methyl-1*H*-indol-3-yl)acetate (3aa).



Yield 126 mg (46%). Colorless crystals. Mp 156-158 °C ($CHCl_3$).

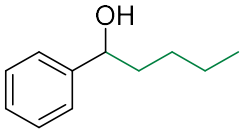
.Chromatography: EtOAc/PE, 1/2. R_f 0.34.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 8.5 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.06 (d, *J* = 2.5 Hz, 1H), 7.03 (d, *J* = 8.5 Hz, 2H), 6.89 (d, *J* = 9.0 Hz, 1H), 6.69 (dd, *J* = 9.0, 2.5 Hz, 1H), 4.36 (d, *J* = 7.0 Hz, 1H), 3.90 (s, 2H), 3.84 (s, 3H), 2.45 (s, 3H), 2.02 – 1.88 (m, 1H), 1.83 – 1.49 (m, 5H), 1.45 – 1.30 (m, 1H), 1.31 – 0.79 (m, 5H).

$^{13}C\{^{1}H\}$ NMR (76 MHz, Chloroform-*d*) δ 169.3, 168.3, 156.1, 149.8, 141.3, 139.3, 136.2, 133.8, 131.2, 130.8, 130.5, 129.1, 127.6, 121.0, 115.0, 112.0, 111.8, 101.2, 78.7, 55.7, 44.96, 30.6, 29.2, 28.6, 26.3, 26.0, 25.9, 13.4.

HRMS (ESI): calcd for $C_{32}H_{33}{}^{35}ClNO_5$ (M+H) 546.2042, found 546.2040, calcd for $C_{32}H_{36}{}^{35}ClN_2O_5$ (M+NH_4) 563.2307, found 563.2306, calcd for $C_{32}H_{32}{}^{35}ClNO_5Na$ (M+Na) 568.1861, found 568.1866, calcd for $C_{32}H_{32}{}^{35}ClNO_5K$ (M+K) 584.1601, found 584.1609.

1-Phenylpentan-1-ol (3ab). [22]



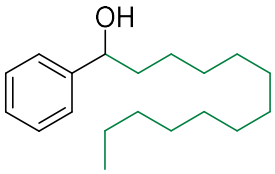
Yield 43 mg (52%). Colorless oil.

Chromatography: EtOAc/PE, 1/5. R_f 0.19.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.45 – 7.23 (m, 5H), 4.67 (dd, *J* = 7.4, 5.9 Hz, 1H), 2.02 (s, 1H), 1.89 – 1.64 (m, 2H), 1.51 – 1.19 (m, 4H), 0.92 (t, *J* = 7.0 Hz, 3H).

$^{13}C\{^{1}H\}$ NMR (76 MHz, Chloroform-*d*) δ 144.9, 128.4, 127.4, 125.9, 74.6, 38.8, 27.9, 22.6, 14.0.

1-Phenyltridecan-1-ol (3ac). [23]



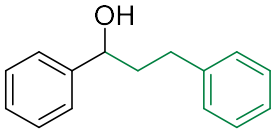
Yield 68 mg (49%). Colorless oil.

Chromatography: EtOAc/PE, 1/10. R_f 0.2.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.50 – 7.22 (m, 5H), 4.68 (dd, *J* = 7.5, 5.8 Hz, 1H), 1.96 (s, 1H), 1.89 – 1.66 (m, 2H), 1.52 – 1.15 (m, 20H), 0.92 (t, *J* = 6.7 Hz, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 144.9, 128.4, 127.4, 125.9, 74.7, 39.1, 31.9, 29.64, 29.62, 29.57, 29.53, 29.51, 29.3, 25.8, 22.7, 14.1.

1,3-Diphenylpropan-1-ol (3ad). [24]



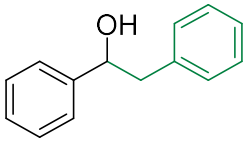
Yield 56 mg (53%). Colorless oil.

Chromatography: EtOAc/PE, 1/10. R_f 0.08.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.45 – 7.30 (m, 7H), 7.29 – 7.20 (m, 3H), 4.72 (dd, *J* = 7.8, 5.4 Hz, 1H), 2.88 – 2.63 (m, 2H), 2.28 – 1.98 (m, 3H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 144.5, 141.7, 128.5, 128.4, 128.3, 127.6, 125.9, 125.8, 73.8, 40.4, 32.0.

1,2-Diphenylethan-1-ol (3ae). [25]



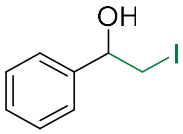
Yield 66 mg (67%). Colorless crystals. Mp 61-63 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.24.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.46 – 7.19 (m, 10H), 4.93 (ddd, *J* = 7.9, 5.3, 2.2 Hz, 1H),3.10 (dd, *J* = 13.6, 5.3 Hz, 1H), 3.04 (dd, *J* = 13.6, 7.9 Hz, 1H), 2.14 (d, *J* = 2.2 Hz, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 143.76, 137.99, 129.46, 128.41, 128.32, 127.52, 126.52, 125.85, 75.25, 45.99.

2-Iodo-1-phenylethan-1-ol (3af). [26]



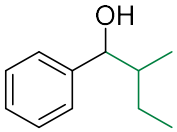
Yield 63 mg (51%). Colorless oil.

Chromatography: EtOAc/PE, 1/5. R_f 0.32.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.45 – 7.27 (m, 5H), 4.84 (dd, *J* = 8.8, 3.7 Hz, 1H), 3.50 (dd, *J* = 10.3, 3.7 Hz, 1H), 3.41 (dd, *J* = 10.3, 8.8 Hz, 1H), 2.49 (s, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 141.1, 128.7, 128.4, 125.7, 74.0, 15.3.

2-Methyl-1-phenylbutan-1-ol [dr = 2/3] (3ag). [27,28]



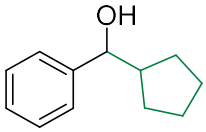
Yield 41 mg (50%). Colorless oil.

Chromatography: EtOAc/PE, 1/10. R_f 0.15.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.45 – 7.25 (m, 5H), [4.78 (d, *J* = 8.1 Hz) + 4.76 (d, *J* = 8.3 Hz) 1H], 1.88 (s, 1H), 1.83 – 1.66 (m, 2H), 1.61 – 1.46 (m, 1H), 1.04 – 0.93 (m, 6H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 145.2, 128.4, 127.5, 125.8, 72.8, 48.3, 24.8, 23.1, 22.2.

Cyclopentyl(phenyl)methanol (3ah). [29]



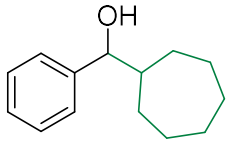
Yield 44 mg (50%). Colorless oil.

Chromatography: EtOAc/PE, 1/10. R_f 0.13.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.46 – 7.23 (m, 5H), 4.42 (d, *J* = 8.4 Hz, 1H), 2.35 – 2.17 (m, 1H), 2.10 (s, 1H), 2.00 – 1.85 (m, 1H), 1.79 – 1.47 (m, 5H), 1.47 – 1.34 (m, 1H), 1.30 – 1.07 (m, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 144.4, 128.3, 127.5, 126.5, 79.1, 47.6, 29.5, 29.4, 25.5, 25.3.

Cycloheptyl(phenyl)methanol (3ai). [30]



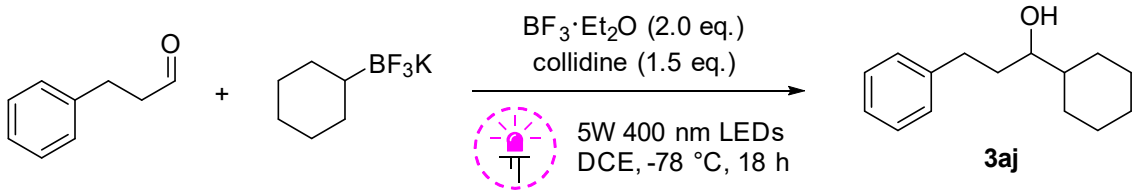
Yield 53 mg (52%). Colorless oil.

Chromatography: EtOAc/PE, 1/10. R_f 0.18.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.45 – 7.23 (m, 5H), 4.48 (d, *J* = 6.5 Hz, 1H), 2.09 – 1.80 (m, 3H), 1.80 – 1.30 (m, 10H), 1.28 – 1.12 (m, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 143.8, 128.1, 127.2, 126.6, 79.1, 46.2, 31.0, 29.2, 28.4, 28.3, 26.7, 26.5.

1-Cyclohexyl-3-phenylpropan-1-ol (3aj). [15]



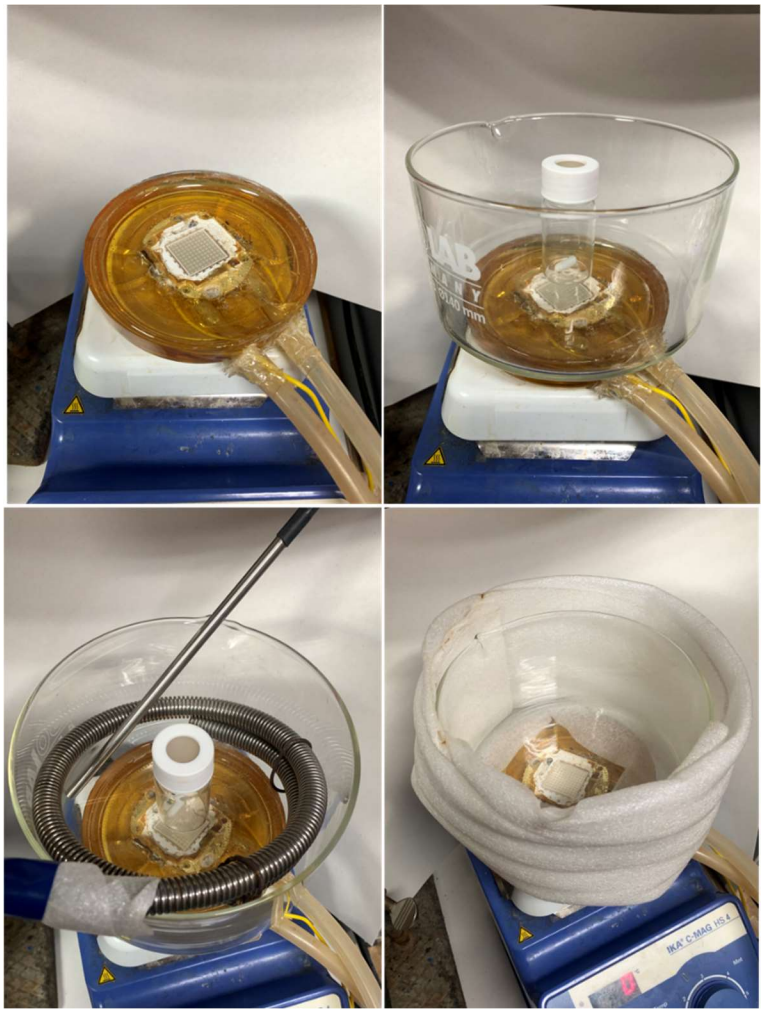


Figure S2. Low temperature photoreaction setup. The reaction at -78 °C was performed using the immersion cooler Huber TC100E. LED-chip was cooled to 20 °C via separate water line.

A 10 ml screw-cap tube equipped with argon/vacuum outlet, magnetic stirring bar and rubber septum was charged with solid potassium cyclohexyltrifluoroborate **2a** (2.0 equiv, 1.0 mmol, 190 mg), then evacuated and refilled with argon 3 times. Then, dry 1,2-dichloroethane (2 mL) was added and the reaction mixture was cooled to -78 °C using Huber TC100E thermostat. Hydrocinnamic aldehyde (1.0 equiv, 0.5 mmol, 67 mg) and boron trifluoride etherate (2.0 equiv,

1.0 mmol, 123 μL) were added successively, and the cloudy mixture was stirred for 18 hours at -78 °C under 5W 400 nm LED irradiation. For the workup, methanol (2 mL) and aqueous saturated solution of KHF_2 (0.5 mL) were added to reaction vial at -78 °C (*Note 1*). The mixture was warmed up and stirred for 30 min at room temperature. Then, the mixture was diluted with additional 5 mL of water containing a small amount of aqueous solution of hydroxylamine (100μL, 50% aq). The product was extracted by diethyl ether (3×5 mL), the combined organic phases were dried over Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

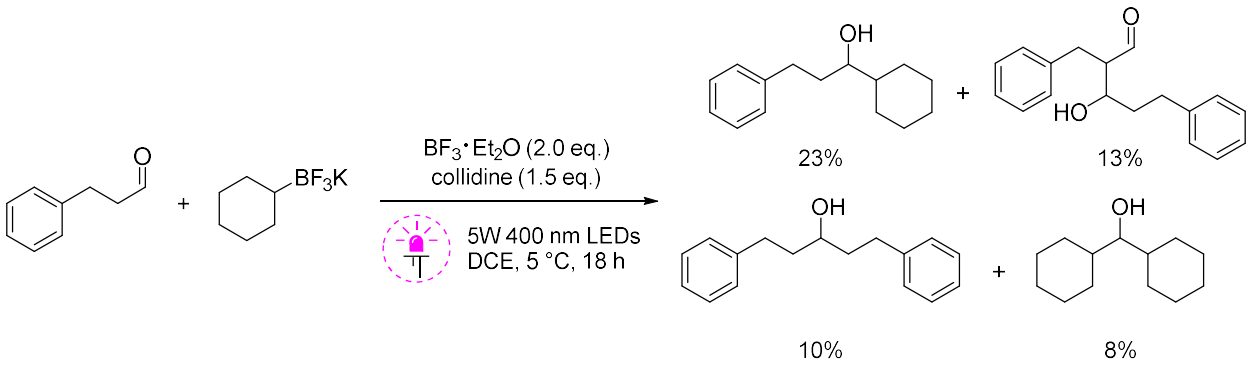
Yield 39 mg (58%). Colorless crystals. Mp 85-87 °C ($CHCl_3$).

Chromatography: EtOAc/PE, 1/5. R_f 0.30.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.46 – 7.09 (m, 5H), 3.49 – 3.36 (m, 1H), 2.88 (ddd, *J* = 13.7, 10.0, 5.5 Hz, 1H), 2.68 (ddd, *J* = 13.7, 9.8, 6.7 Hz, 1H), 1.95 – 1.62 (m, 7H), 1.43 (s, 1H), 1.41 – 0.95 (m, 6H).

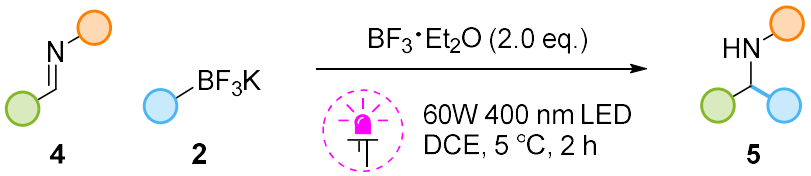
^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 142.4, 128.4, 128.3, 125.7, 75.6, 43.8, 35.9, 32.4, 29.2, 27.8, 26.5, 26.3, 26.2.

Note 1: Following the General procedure I, the same reaction was initially conducted at 5 °C and a mixture of products was obtained. The crude material was subjected to column chromatography (EtOAc/PE, 1/5) and 4 overlapping fractions were collected. Solvent was evaporated and each fraction was analyzed by ^{1}H NMR and GS-MS. Yields of byproducts were calculated from ^{1}H NMR data and fraction weights.



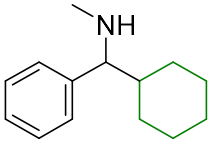
Scheme S1. Aliphatic aldehyde reaction at 5 °C.

Radical alkylation of azomethines (General procedure III)



A tube equipped with an argon outlet and a stirring bar was charged with solid potassium cyclohexyltrifluoroborate **2a** (2.0 equiv, 1.0 mmol, 190 mg) and azomethine **4** (1.0 equiv, 0.5 mmol), followed by dry 1,2-dichloroethane (2 mL) under inert atmosphere. The reaction mixture was cooled to 5 °C and boron trifluoride etherate (2.0 equiv, 1.0 mmol, 123 μL) was added with microsyringe in one portion. The mixture was irradiated by 60W 400 nm LEDs for 2 hours at 5 °C. Then, the solvent was evaporated under reduced pressure and the residue was dissolved in methanol (2 mL). Aqueous saturated solution of KF (0.5 mL) was added to the reaction mixture with cooling at room temperature water bath. The mixture was stirred for 30 minutes at room temperature. The reaction was diluted with water (5 mL), extracted with diethyl ether (3×5 mL), the combined organic phases were filtered through Na_2SO_4, concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel.

1-Cyclohexyl-*N*-methyl-1-phenylmethanamine (5a). [31]



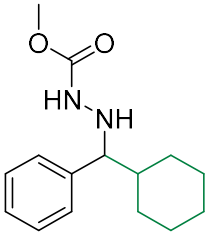
Yield 65 mg (64%). Yellow oil.

Chromatography: EtOAc/PE, 1/5 (1% Et_3N). R_f 0.14.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.39 – 7.20 (m, 5H), 3.24 (d, *J* = 7.1 Hz, 1H), 2.24 (s, 3H), 2.04 – 1.89 (m, 1H), 1.84 – 1.72 (m, 1H), 1.70 – 1.36 (m, 5H), 1.34 – 0.78 (m, 5H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 142.5, 128.0, 128.0, 126.7, 71.1, 44.0, 34.7, 30.3, 29.8, 26.5, 26.3, 26.3.

Methyl 2-(cyclohexyl[phenyl]methyl)hydrazine-1-carboxylate (5b).



Yield 45 mg (34%). Yellow oil.

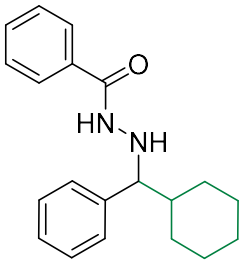
Chromatography: EtOAc/PE, 1/2 (1% Et_3N). R_f 0.30.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.38 – 7.23 (m, 5H), 5.97 (s, 1H), 4.41 (s, 1H), 3.82 (s, 1H), 3.67 (s, 3H), 2.02 – 1.89 (m, 1H), 1.84 – 1.73 (m, 1H), 1.72 – 1.53 (m, 3H), 1.51 – 1.39 (m, 1H), 1.37 – 1.00 (m, 5H), 0.96 – 0.77 (m, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 157.6, 140.8, 128.4, 128.1, 127.2, 69.9, 52.3, 42.0, 30.0, 29.2, 26.4, 26.1, 26.1.

HRMS (ESI): calcd for $C_{15}H_{23}N_2O_2$ (M+H) 263.1754, found 263.1755, calcd for $C_{15}H_{22}N_2O_2Na$ (M+Na) 285.1573, found 285.1577.

***N′*-(Cyclohexyl[phenyl]methyl)benzohydrazide (5c).** [11]



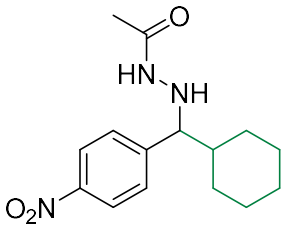
Yield 130 mg (84%). Colorless crystals. Mp 139-141 °C (CH_2Cl_2).

Chromatography: EtOAc/PE, 1/5 (1% Et_3N). R_f 0.24.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.56 – 7.49 (m, 2H), 7.49 – 7.40 (m, 1H), 7.39 – 7.27 (m, 7H), 5.40 (s, 1H), 3.85 (d, J = 7.5 Hz, 1H), 2.11 – 1.98 (m, 1H), 1.87 – 1.56 (m, 4H), 1.51 – 1.40 (m, 1H), 1.38 – 1.04 (m, 4H), 0.99 – 0.80 (m, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 166.9, 140.9, 132.9, 131.5, 128.4, 128.1, 127.2, 126.7, 70.3, 42.2, 29.9, 29.2, 26.3, 26.0.

***N′*-(Cyclohexyl[4-nitrophenyl]methyl)acetohydrazide (5d).**



Yield 86 mg (59%). Yellow oil.

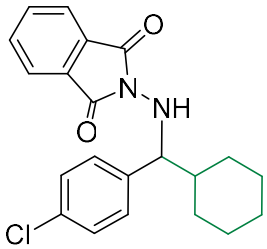
Chromatography: isopropanol/CH_2Cl_2, 1/10 (1% Et_3N). R_f 0.43.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 8.7 Hz, 2H), 7.45 (d, *J* = 8.7 Hz, 2H), 6.98 (d, *J* = 5.3 Hz, 1H), 5.07 (d, *J* = 5.3 Hz, 1H), 3.89 (d, *J* = 6.8 Hz, 1H), 1.95 – 1.85 (m, 1H), 1.81 (s, 3H), 1.79 – 1.70 (m, 1H), 1.70 – 1.54 (m, 3H), 1.49 – 1.34 (m, 1H), 1.33 – 0.96 (m, 4H), 0.90 – 0.72 (m, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 169.6, 149.1, 147.1, 129.2, 123.2, 69.6, 42.2, 29.8, 28.9, 26.1, 26.0, 25.9, 21.0.

HRMS (ESI): calcd for $C_{15}H_{22}N_3O_3$ (M+H) 292.1656, found 292.1668, calcd for $C_{15}H_{21}N_3O_3Na$ (M+Na) 314.1475, found 314.1480.

2-([{4-Chlorophenyl}(cyclohexyl)methyl]amino)isoindoline-1,3-dione (5e).



Yield 92 mg (50%). Colorless crystals. Mp 108-110 °C ($CDCl_3$).

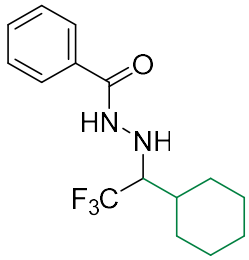
Chromatography: EtOAc/PE, 1/2 (1% Et_3N). R_f 0.46.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.77 – 7.69 (m, 2H), 7.72 – 7.61 (m, 2H), 7.30 (d, *J* = 8.6 Hz, 2H), 7.21 (d, *J* = 8.5 Hz, 2H), 4.84 (s, 1H), 4.24 (d, *J* = 6.5 Hz, 1H), 2.12 – 1.97 (m, 1H), 1.89 – 1.57 (m, 4H), 1.58 – 1.46 (m, 1H), 1.37 – 1.03 (m, 4H), 0.95 – 0.76 (m, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 166.7, 137.4, 134.0, 133.3, 130.0, 129.9, 128.0, 123.2, 68.2, 42.1, 30.1, 29.0, 26.2, 25.9, 25.9.

HRMS (ESI): calcd for $C_{21}H_{22}{}^{35}ClN_2O_2$ (M+H) 369.1364, found 369.1350, calcd for $C_{21}H_{21}{}^{35}ClN_2O_2Na$ (M+Na) 391.1184, found 391.1178, calcd for $C_{21}H_{21}{}^{35}ClN_2O_2K$ (M+K) 407.0923, found 407.0913.

***N′*-(1-Cyclohexyl-2,2,2-trifluoroethyl)benzohydrazide (5f).**



Yield 122 mg (81%). Colorless crystals. Mp 95-97 °C (CH_2Cl_2).

Chromatography: EtOAc/PE, 1/5 (1% Et_3N). R_f 0.38.

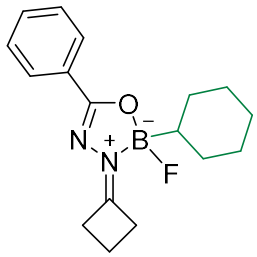
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.03 (d, *J* = 6.5 Hz, 1H), 7.72 (d, *J* = 7.0 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 2H), 5.01 (d, *J* = 6.4 Hz, 1H), 3.16 (dq, *J* = 8.1, 4.3 Hz, 1H), 1.99 (d, *J* = 7.3 Hz, 1H), 1.90 – 1.73 (m, 4H), 1.72 – 1.62 (m, 1H), 1.59 – 1.43 (m, 1H), 1.37 – 1.11 (m, 4H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 167.3, 132.2, 132.0, 128.6, 126.9, 126.6 (q, *J* = 283.1 Hz), 66.9 (q, *J* = 25.3 Hz), 37.1, 30.0, 28.2, 26.3, 26.2, 25.9.

^{19}F NMR (282 MHz, Chloroform-*d*) δ -70.69 (d, *J* = 8.0 Hz).

HRMS (ESI): calcd for $C_{15}H_{20}F_3N_2O$ (M+H) 301.1522, found 301.1531, calcd for $C_{15}H_{19}F_3N_2ONa$ (M+Na) 323.1342, found 323.1351.

3-Cyclobutylidene-2-cyclohexyl-2-fluoro-5-phenyl-2,3-dihydro-1,3λ^4,4,2λ^4-oxadiazaborole (5g).



Yield 96 mg (64%). Light yellow crystals. Mp 114-116 °C (ethanol/water 1:1).

Chromatography: EtOAc/PE, 1/5 (1% Et_3N). R_f 0.28.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.13 – 8.04 (m, 2H), 7.58 – 7.49 (m, 1H), 7.48 – 7.39 (m, 2H), 3.48 – 3.21 (m, 4H), 2.35 – 2.21 (m, 2H), 1.94 – 1.54 (m, 4H), 1.44 – 1.31 (m, 1H), 1.30 – 1.08 (m, 4H), 1.03 – 0.80 (m, 1H), 0.78 – 0.59 (m, 1H).

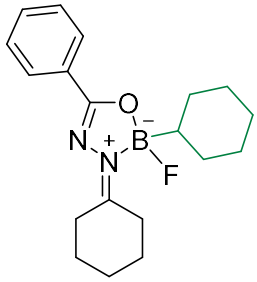
^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 173.8, 171.2, 132.4, 128.5, 128.4, 127.8, 34.3, 33.1, 27.9, 27.9, 27.8, 27.7, 27.5, 27.1, 14.8.

^{19}F NMR (282 MHz, Chloroform-*d*) δ -161.7 – -162.8 (br).

^{11}B NMR (96 MHz, Chloroform-*d*) δ 17.8 – 4.1 (br).

HRMS (ESI): calcd for $C_{17}H_{23}BFN_2O$ (M+H) 301.1885, found 301.1879, calcd for $C_{17}H_{22}BFN_2ONa$ (M+Na) 323.1704, found 323.1697.

2-Cyclohexyl-3-cyclohexylidene-2-fluoro-5-phenyl-2,3-dihydro-1,3λ^{4},4,2λ^{4}-oxadiazaborole (5h).



Yield 74 mg (45%). Light yellow crystals. Mp 120-120 °C (CH_2Cl_2).

Chromatography: EtOAc/PE, 1/5 (1% Et_3N). R_f 0.43.

^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.14 – 8.05 (m, 2H), 7.58 – 7.49 (m, 1H), 7.49 – 7.40 (m, 2H), 3.12 – 2.89 (m, 2H), 2.87 – 2.67 (m, 2H), 2.01 – 1.50 (m, 10H), 1.38 – 1.05 (m, 5H), 0.96 – 0.78 (m, 1H), 0.76 – 0.61 (m, 1H).

^{13}C{^{1}H} NMR (76 MHz, Chloroform-*d*) δ 174.3, 170.0, 132.2, 128.4, 128.3, 128.1, 32.1, 30.9, 27.9, 27.8, 27.75, 27.73, 27.5, 27.1, 26.8, 25.1.

^{19}F NMR (282 MHz, Chloroform-*d*) δ -160.7 – -162.2 (br).

^{11}B NMR (96 MHz, Chloroform-*d*) δ 19.2 – 6.2 (br).

HRMS (ESI): calcd for $C_{19}H_{27}BFN_2O$ (M+H) 329.2198, found 329.2203, calcd for $C_{19}H_{26}BFN_2ONa$ (M+Na) 351.2018, found 351.2018, calcd for $C_{19}H_{26}BFN_2OK$ (M+K) 367.1757, found 367.1750.

Unsuccessful substrates

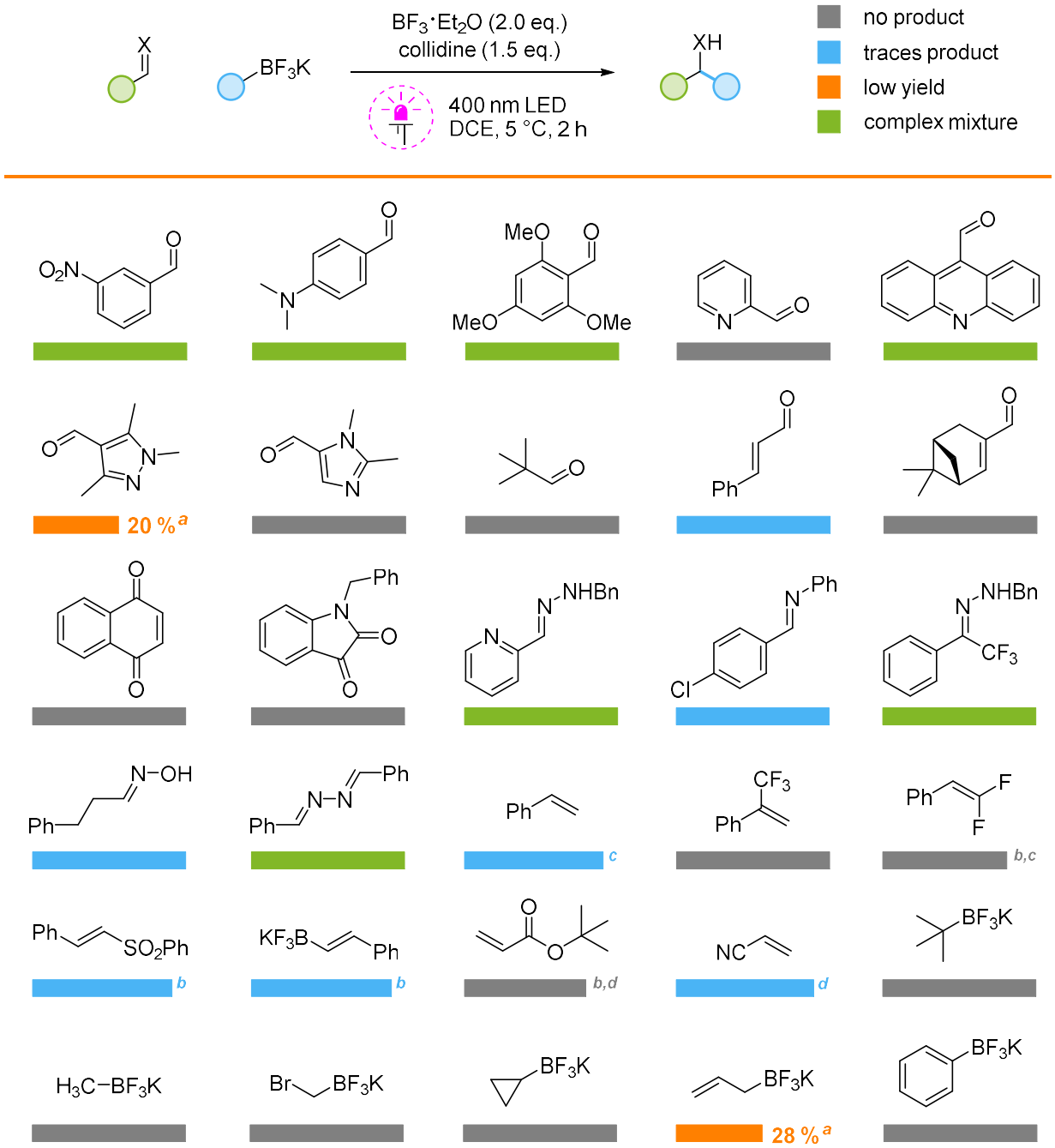
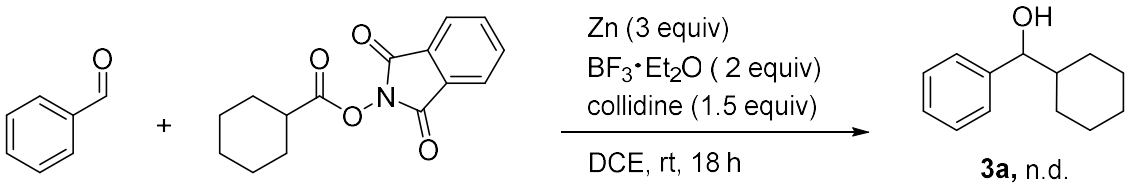


Table S2. Unsuccessful substrates according the reaction mixture analysis (by GS-MS or ^{1}H NMR). [a] ^{1}H NMR yield using CH_2Br_2 as an internal standard. [b] The reaction was conducted without collidine. [c] The reaction was conducted on air. [d] The reaction was conducted with addition of γ-terpinene (1 equiv.)

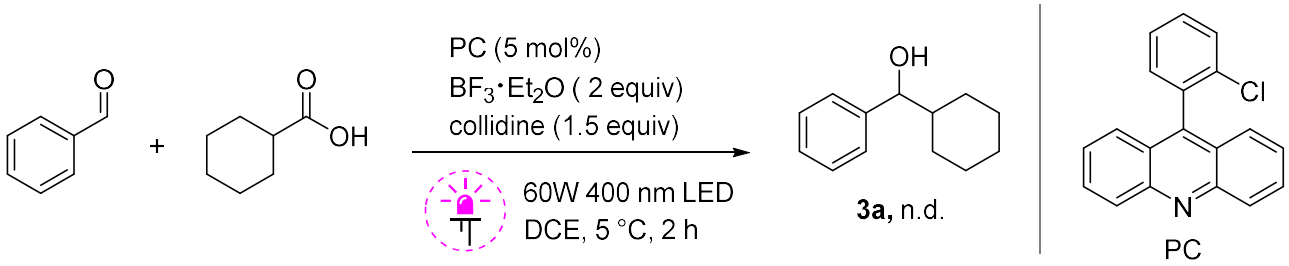
Additional experiments

The reaction with *N*-(cyclohexanecarbonyloxy)phtalimide



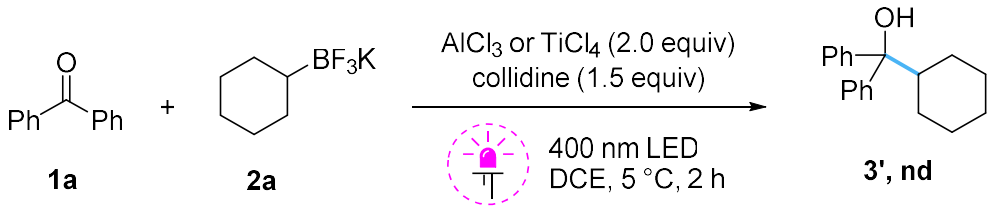
A tube equipped with an argon outlet and a stirring bar was charged with solid N-(cyclohexanecarbonyloxy)phtalimide (2.0 equiv, 1.0 mmol, 273 mg) and zinc dust (3.0 equiv, 1.5 mmol, 98 mg) followed by dry 1,2-dichloroethane (2 mL), benzaldehyde (1.0 equiv, 0.5 mmol, 53 mg) and 2,4,6-collidine (1.5 equiv, 0.75 mmol, 99 µL) under inert atmosphere. Then, the reaction mixture was cooled to 5 °C and boron trifluoride etherate (2.0 equiv, 1.0 mmol, 123 µL) was added by microsyringe in one portion. The mixture was stirred at room temperature for 18 h. The solvent was evaporated under reduced pressure, the residue was dissolved in methanol (2 mL), aqueous saturated solution of KHF_2 (0.5 mL) was added to the methanol solution with cooling by room temperature water bath. The mixture was stirred for 30 minutes at room temperature, diluted with water (5 mL), and extracted with diethyl ether (3×5 mL). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure and dissolved in 2 mL of $CDCl_3$. ^1H NMR analysis with CH_2Br_2 as an internal standard along with GC-MS data revealed no product formation.

The reaction with cyclohexanecarboxylic acid



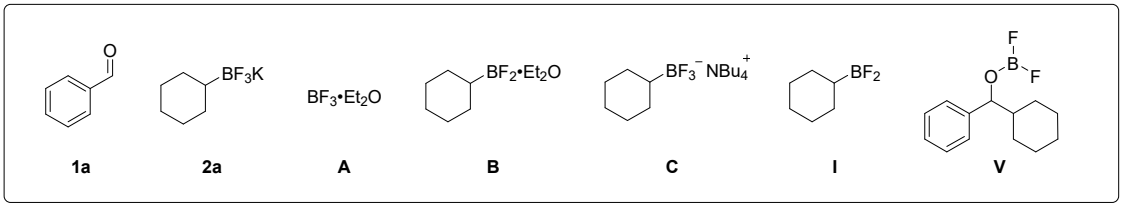
A tube equipped with an argon outlet and a stirring bar was charged with solid cyclohexylcarboxilyc acid (2.0 equiv, 1.0 mmol, 128 mg) and 9-(o-chlorphenyl)acridine (5 mol %, 0.025 mmol, 7 mg) followed by dry 1,2-dichloroethane (2 mL), benzaldehyde (1.0 equiv, 0.5 mmol, 53 mg) and 2,4,6-collidine (1.5 equiv, 0.75 mmol, 99 µL) under inert atmosphere. Then, the reaction mixture was cooled to 5 °C and boron trifluoride etherate (2.0 equiv, 1.0 mmol, 123

μL) was added with micro syringe in one portion. The mixture was irradiated by 400 nm LEDs at 5 °C (60W LEDs for 2 hours). The solvent was evaporated under reduced pressure, the residue was dissolved in methanol (2 mL), aqueous saturated solution of KHF_2 (0.5 mL) was added to the resulting methanol solution with with cooling by room temperature water bath. The mixture was stirred for 30 minutes at room temperature, diluted with water (5 mL), and extracted with diethyl ether (3×5 mL). The combined organic layers were filtered through Na_2SO_4, concentrated under reduced pressure and dissolved in 2 mL of $CDCl_3$. ^1H NMR analysis with CH_2Br_2 as an internal standard along with GC-MS data revealed no product formation.



Scheme S2. The reactions were conducted according to GP1 with KHF_2 workup. No product **3'** was detected by ^1H NMR and GC-MS analysis of reaction mixtures.

NMR Studies



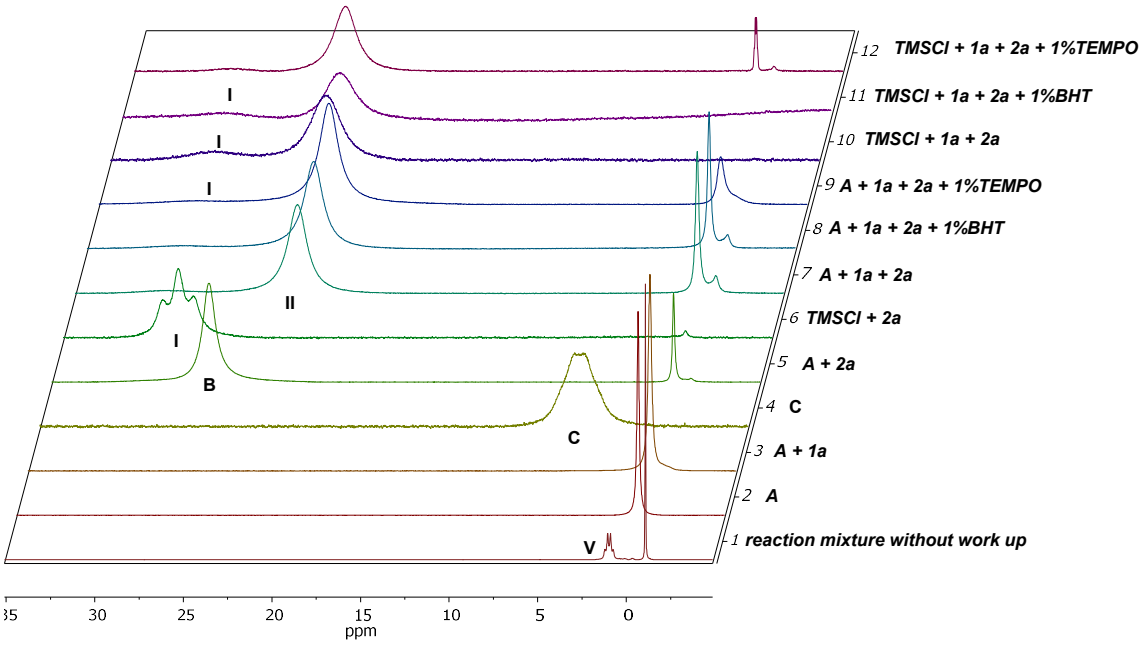


Figure S3. ^{11}B NMR monitoring.

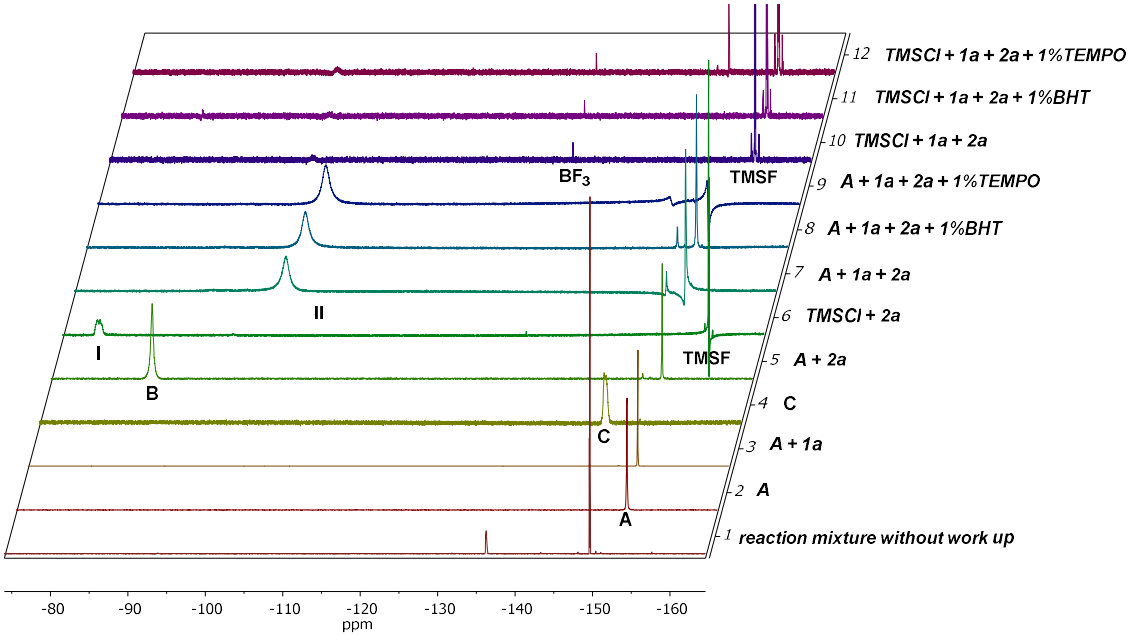


Figure S4. ^{19}F NMR monitoring.

For the NMR study, solid reagents were added to the NMR tube, and then it was degassed and refilled with argon. After that, in the flow of argon, dry DCE was added to the NMR-tube, and then liquid reagents were added with microsyringes. Boron trifluoride etherate and trimethylsilyl chloride were added last for the corresponding samples. The reagents were mixed in 1:1 ratio (0.2 mmol of each reagent). A sample for the study of spectrum **C** was prepared by the reaction of **2a** (20 mg) with TBABr (20 mg) under air in 2 mL of DCE for 20 min and a sample of this mixture was used for analysis.

The NMR study showed the formation of cyclohexyldifluoroborane (**I**) in a mixture with TMSCl. The NMR spectra of **I** were in accordance with the literature data [32] and ^{11}B spectrum showed a triplet signal of **I**: ^{11}B NMR (96 MHz) δ 28.63 (t, J = 85.9 Hz) (Fig. S3 plot **TMSCl + 2a**). In the case of the mixture of **2a** and **A**, the peaks of the alkyldifluoroborane adduct shifted to the upper field in both ^{11}B and ^{19}F spectra, which may be interpreted as a formation of tetracoordinated boron species **B**. Mixtures including benzaldehyde had a similar number of main peaks in boron spectra in both systems with BF_3 and TMSCl.

UV-Vis studies

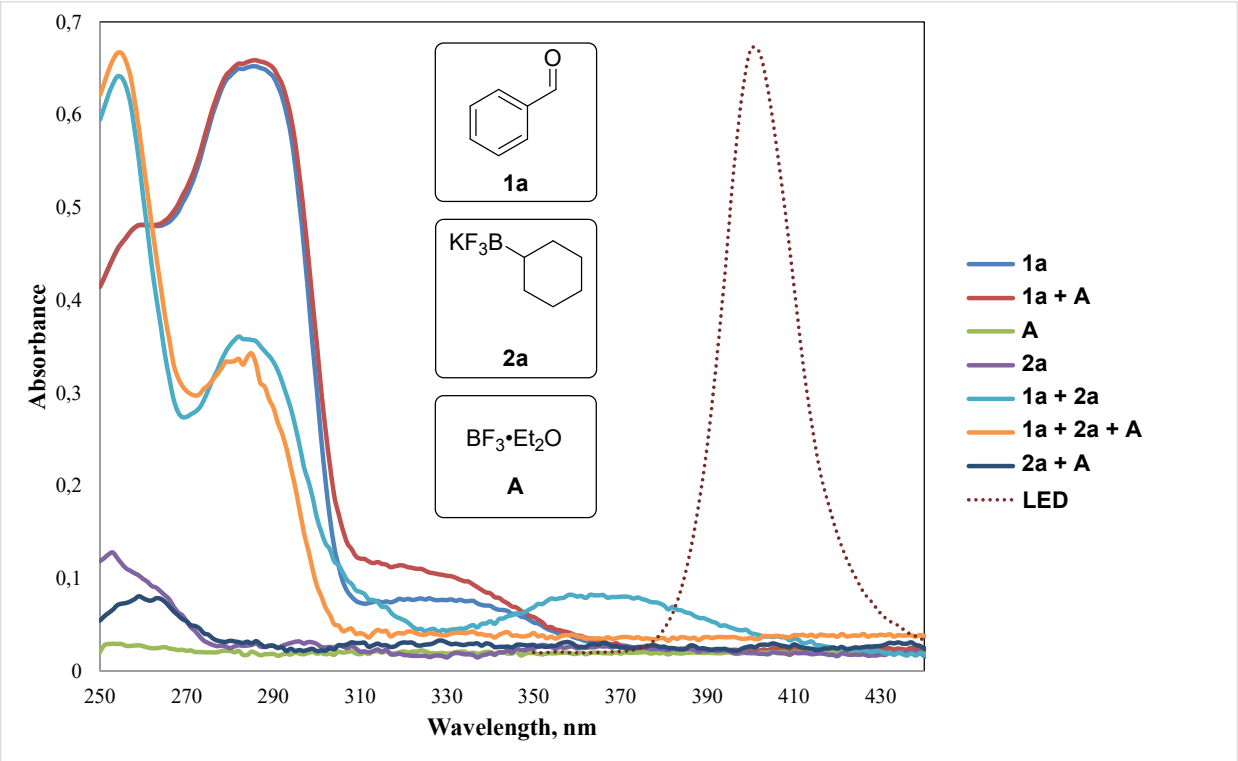
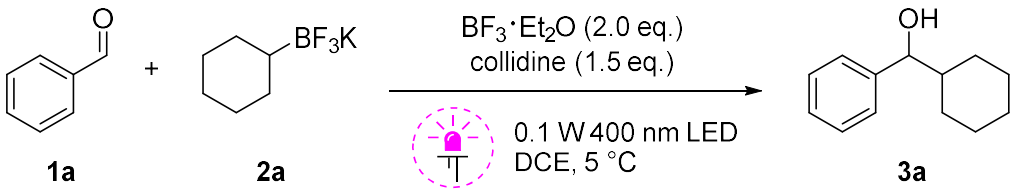


Figure S5. UV-vis spectra of reaction components mixtures in DCE. Components were mixed in 1:1 ratio. The concentration was 1×10^{-4} M.

Light on/off experiments



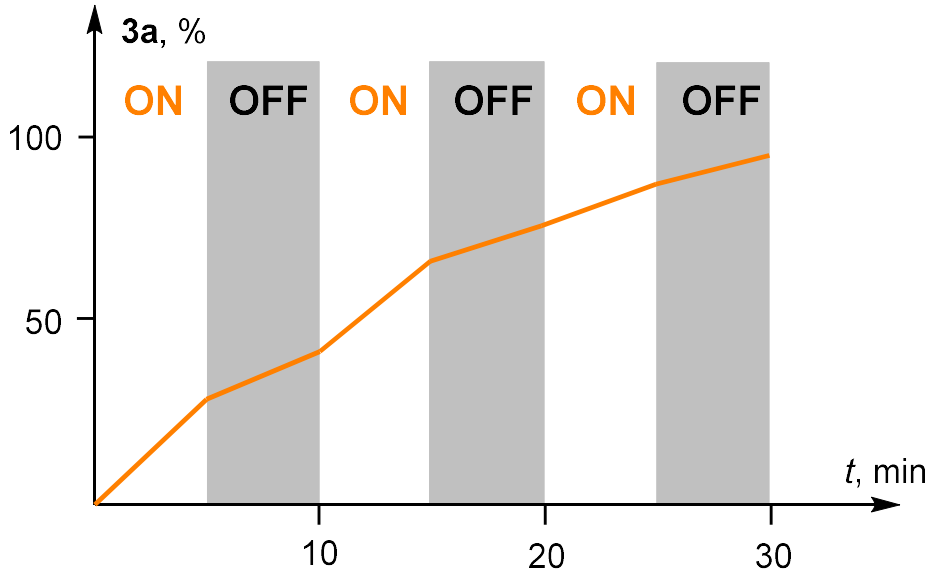


Figure S6. The reaction was conducted under conditions of GP I except 0.1 W 400 nm diode was used. The yields were determined by GC-FID with 1,3,5-triisopropyl benzene as internal standard. The same reaction in the dark gave 13% yield in 2 h.

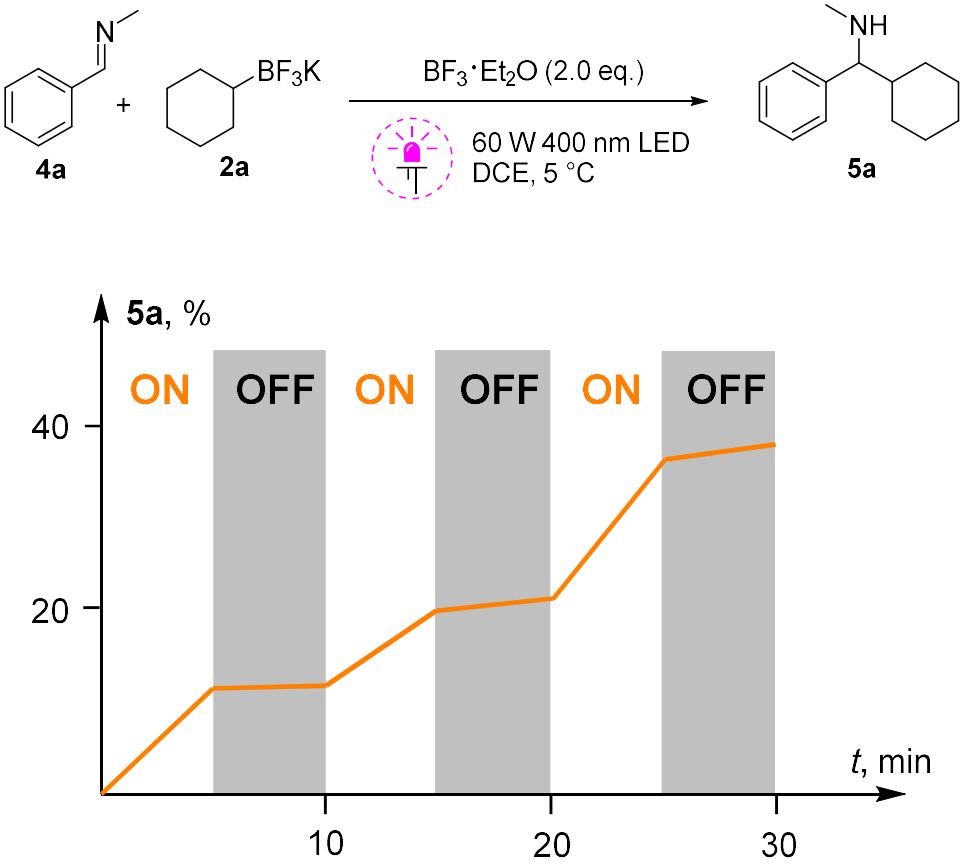


Figure S7. The reaction was conducted under conditions of GP III. The yields were determined by GC-FID with 1,3,5-triisopropyl benzene as internal standard. The same reaction in the dark gave no product in 2 h.

X-ray crystallographic data and refinement details

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program. [33] The structure was solved by direct methods using SHELXT [34] and refined on F^2 using SHELXL-2018 [35] in the OLEX2 program. [36] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. Locations of H1 and H3 hydrogen atoms of compounds **5g,h** were found from the electron density-difference map; these hydrogen atoms were refined with individual isotropic displacement parameters. All other hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters.

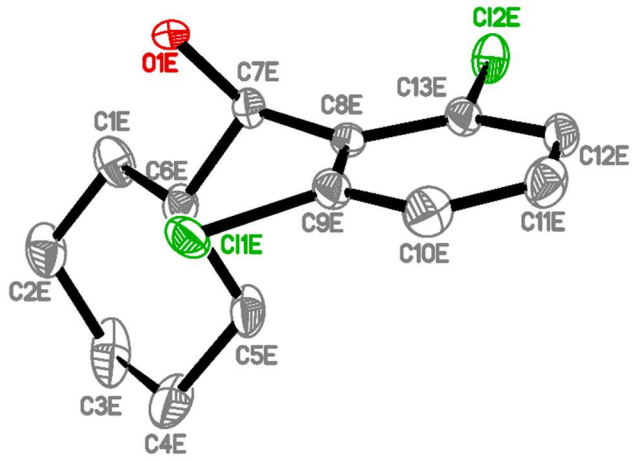


Figure S8. X-ray structure of compound **3e**. Anisotropic displacement parameters are drawn at the 50% probability.

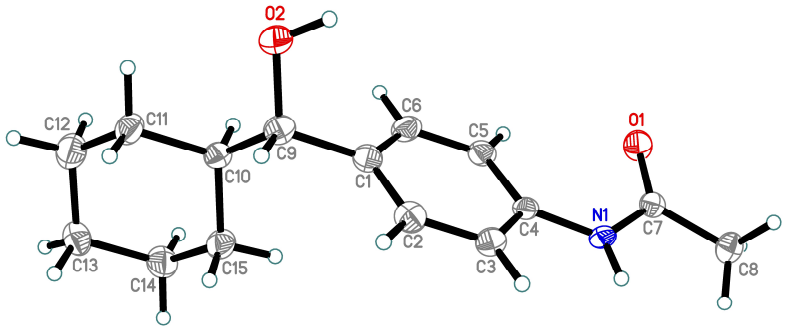


Figure S9. X-ray structure of compound **3j**. Anisotropic displacement parameters are drawn at the 50% probability.

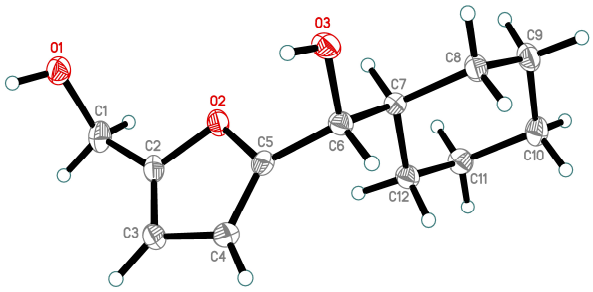


Figure S10. X-ray structure of compound **3v**. Anisotropic displacement parameters are drawn at the 50% probability.

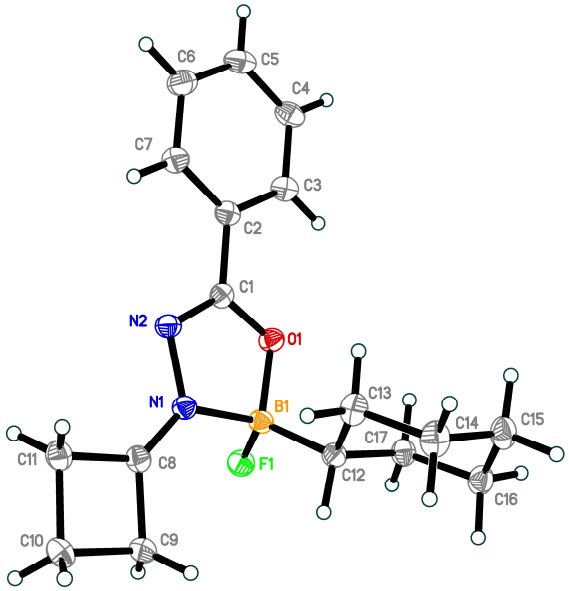


Figure S11. X-ray structure of compound **5g**. Anisotropic displacement parameters are drawn at the 50% probability.

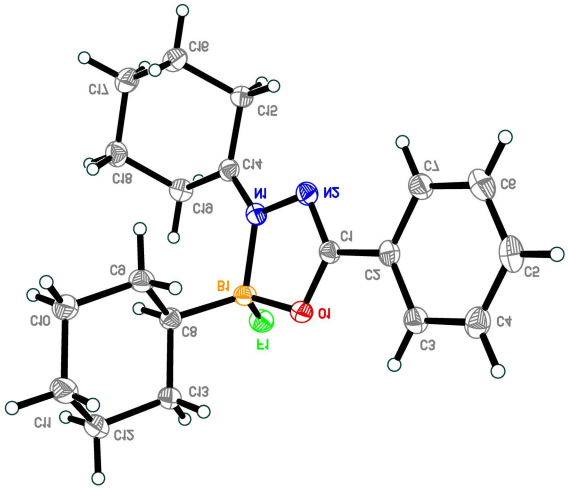


Figure S12. X-ray structure of compound **5h**. Anisotropic displacement parameters are drawn at the 50% probability.

Table S3. Crystal data and structure refinement for **3e**.

CCDC number	2336546	
Empirical formula	$C_{13}H_{16}Cl_2O$	
Formula weight	259.16	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 18.89737(7) Å	a= 90°
	b = 12.24079(6) Å	b= 94.0661(4)°
	c = 22.05573(9) Å	g = 90°
Volume	5089.06(4) $Å^3$	
Z	16	
Density (calculated)	1.353 g/cm^3	
Absorption coefficient	4.390 mm^{-1}	
F(000)	2176	
Crystal size	0.33 x 0.19 x 0.18 mm^3	
Theta range for data collection	2.344 to 80.618°	
Index ranges	$-17 \leq h \leq 23$, $-15 \leq k \leq 15$, $-28 \leq l \leq 28$	
Reflections collected	71168	
Independent reflections	11049 [R(int) = 0.0278]	
Observed reflections	10520	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.70827	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11049 / 22 / 653	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.1018	
R indices (all data)	R1 = 0.0397, wR2 = 0.1028	
Largest diff. peak and hole	0.668 and -0.538 $e.Å^{-3}$	

Table S4. Crystal data and structure refinement for **3j**.

CCDC number	2336547	
Empirical formula	$C_{15}H_{21}NO_2$	
Formula weight	247.33	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 12.0689(2) Å	a= 90°
	b = 11.9115(2) Å	b= 102.217(2)°
	c = 9.37870(10) Å	g = 90°
Volume	1317.74(4) Å^3	
Z	4	
Density (calculated)	1.247 g/cm^3	
Absorption coefficient	0.651 mm^{-1}	
F(000)	536	
Crystal size	0.316 x 0.147 x 0.041 mm^3	
Theta range for data collection	3.747 to 80.810°	
Index ranges	$-15 \le h \le 15$, $-15 \le k \le 15$, $-12 \le l \le 9$	
Reflections collected	5581	
Independent reflections	5581	
Observed reflections	5413	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.96463	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5581 / 0 / 173	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0554, wR2 = 0.1507	
R indices (all data)	R1 = 0.0566, wR2 = 0.1518	
Largest diff. peak and hole	0.703 and -0.267 e.Å^{-3}	

Table S5. Crystal data and structure refinement for **3v**.

CCDC number	2336548	
Empirical formula	$C_{12}H_{18}O_3$	
Formula weight	210.26	
Temperature	100.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	a = 9.13130(10) Å	a= 90°
	b = 13.6328(2) Å	b= 90°
	c = 9.04630(10) Å	g = 90°
Volume	1126.13(2) $Å^3$	
Z	4	
Density (calculated)	1.240 g/cm^3	
Absorption coefficient	0.711 mm^{-1}	
F(000)	456	
Crystal size	0.33 x 0.22 x 0.2 mm^3	
Theta range for data collection	3.242 to 81.093°	
Index ranges	$-11 \leq h \leq 11$, $-17 \leq k \leq 17$, $-11 \leq l \leq 11$	
Reflections collected	14533	
Independent reflections	2367 [R(int) = 0.0303]	
Observed reflections	2350	
Completeness to theta = 67.684°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.78599	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2367 / 1 / 138	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0728	
R indices (all data)	R1 = 0.0288, wR2 = 0.0729	
Absolute structure parameter	0.5	
Largest diff. peak and hole	0.197 and -0.165 $e.Å^{-3}$	

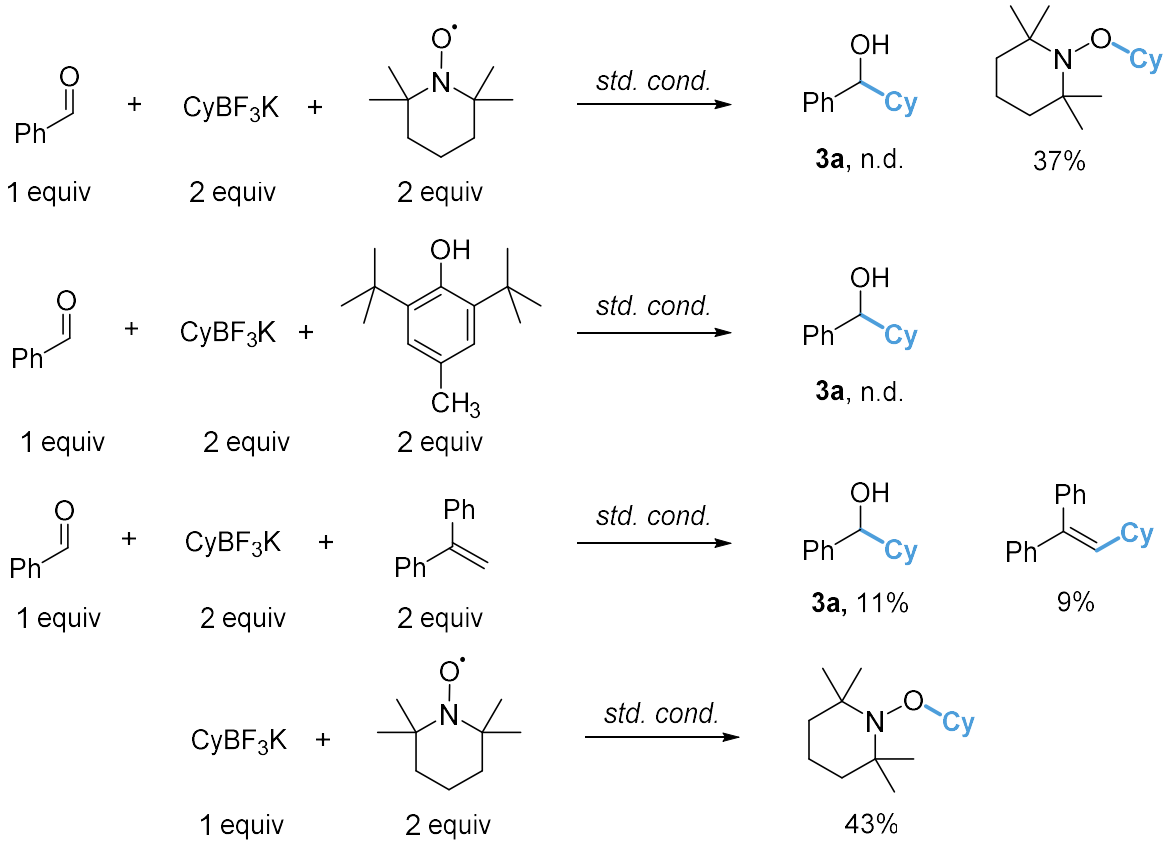
Table S6. Crystal data and structure refinement for **5g**.

CCDC number	2336549	
Empirical formula	$C_{17}H_{22}BFN_2O$	
Formula weight	300.17	
Temperature	100.0(3) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 14.16710(10) Å	a= 90°
	b = 10.20320(10) Å	b= 90°
	c = 22.0229(2) Å	g = 90°
Volume	3183.41(5) $Å^3$	
Z	8	
Density (calculated)	1.253 Mg/m^3	
Absorption coefficient	0.687 mm^{-1}	
F(000)	1280	
Crystal size	0.5 x 0.3 x 0.2 mm^3	
Theta range for data collection	4.015 to 77.583°	
Index ranges	$-15 \leq h \leq 17$, $-11 \leq k \leq 12$, $-27 \leq l \leq 27$	
Reflections collected	21992	
Independent reflections	3379 [R(int) = 0.0237]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.85786	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3379 / 0 / 199	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0882	
R indices (all data)	R1 = 0.0360, wR2 = 0.0894	
Largest diff. peak and hole	0.276 and -0.180 $e.Å^{-3}$	

Table S7. Crystal data and structure refinement for **5h**.

CCDC number	2336550	
Empirical formula	$C_{19}H_{26}BFN_2O$	
Formula weight	328.23	
Temperature	99.9(3) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.52990(10) Å	a= 101.2000(10)°
	b = 11.13290(10) Å	b= 94.3790(10)°
	c = 18.1267(2) Å	g = 105.7310(10)°
Volume	1798.84(3) $Å^3$	
Z	4	
Density (calculated)	1.212 Mg/m^3	
Absorption coefficient	0.648 mm^{-1}	
F(000)	704	
Crystal size	0.5 x 0.3 x 0.2 mm^3	
Theta range for data collection	2.508 to 77.888°	
Index ranges	$-9 \le h \le 11$, $-14 \le k \le 14$, $-22 \le l \le 22$	
Reflections collected	47208	
Independent reflections	7592 [R(int) = 0.0423]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.60533	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7592 / 0 / 433	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0376, wR2 = 0.0962	
R indices (all data)	R1 = 0.0390, wR2 = 0.0973	
Largest diff. peak and hole	0.391 and -0.240 $e.Å^{-3}$	

Radical trapping experiments



Scheme S3.

EPR study

A Schlenk tube equipped with a stirring bar was charged with solid potassium cyclohexyltrifluoroborate **2a** (2.0 equiv, 0.6 mmol, 114 mg) and *N*-benzylidene-*tert*-butylamine *N*-oxide (1.5 equiv, 0.45 mmol). Then, the flask was evacuated and filled with argon. Dry 1,2-dichloroethane (2 mL) and benzaldehyde **1** (1.0 equiv, 0.3 mmol, 31 µL) were added under argon atmosphere. Then, boron trifluoride etherate (2.0 equiv, 0.6 mmol, 74 µL) was added with microsyringe in one portion. After stirring for 5 minutes, the precipitate was allowed to settle. The solution was taken into a Young tube under argon, and the tube was irradiated by 60W 400 nm LEDs for 30 seconds, the EPR spectrum was immediately recorded at 298 K on EPR spectrometer SPINSCAN X (ADANI).

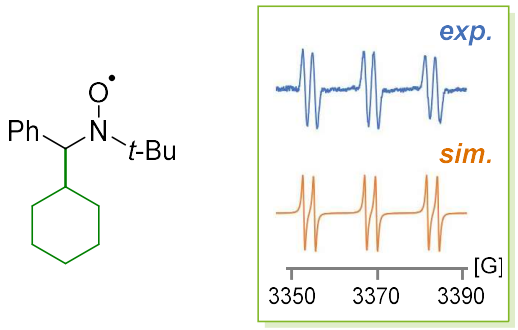


Figure S13. The X-band EPR spectrum of trapped cyclohexyl radical and corresponding simulated spectrum based on hyperfine coupling constants of A_N = 14.5 G, A_H = 2.8 G (g-factor = 2.0065).

Experiment parameters:

Center-Field: 3365 G

Width: 60 G

Points: 3000

Modulation Amplitude: 100 µT

Modulation Frequency: 9.458138 GHz

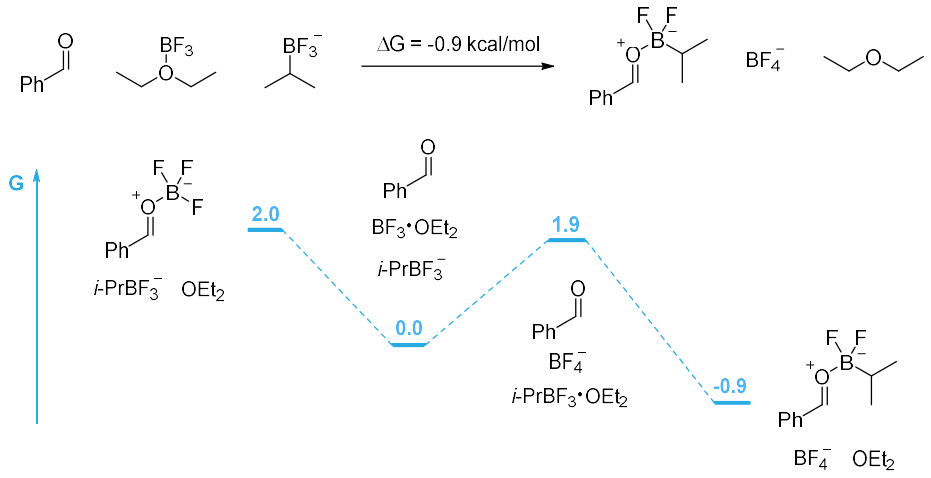
Microwave Power: 1.0 mW

Time constant: 0.015 s

Number of scans: 1

DFT calculations

All calculations were carried out using the Gaussian16 package [37]. Geometries of stationary points were optimized using the (U)ωB97XD functional with the def2SVP basis set. Stationary points were verified by vibrational analysis (no imaginary frequencies for intermediates and single imaginary frequency for the transition states). Key transition states were subjected to IRC calculations in forward and reverse directions. Solvation effects were evaluated using the PCM model (dichloromethane as solvent). Structures are given in the xyz format with energies in Hartrees.



Scheme S4. DFT calculations of equilibrium between starting reagents.

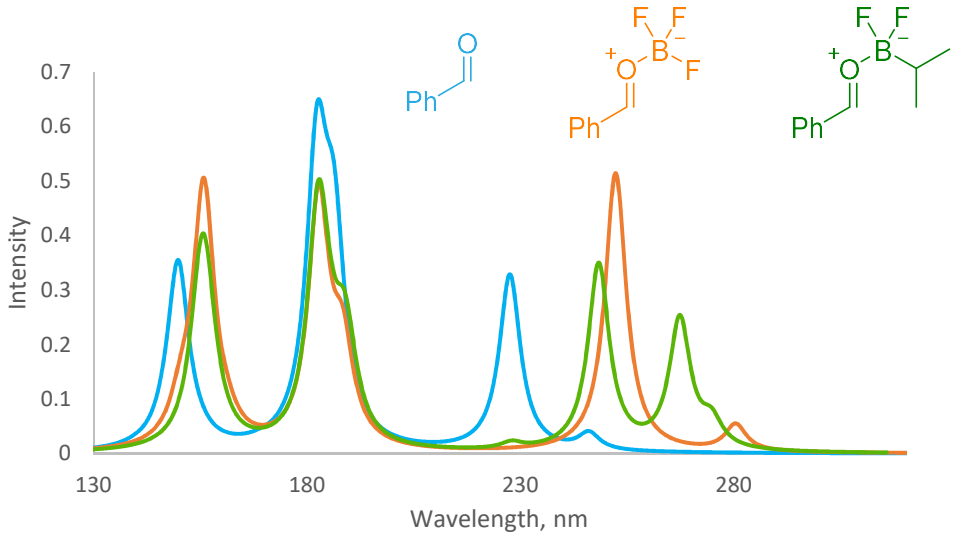
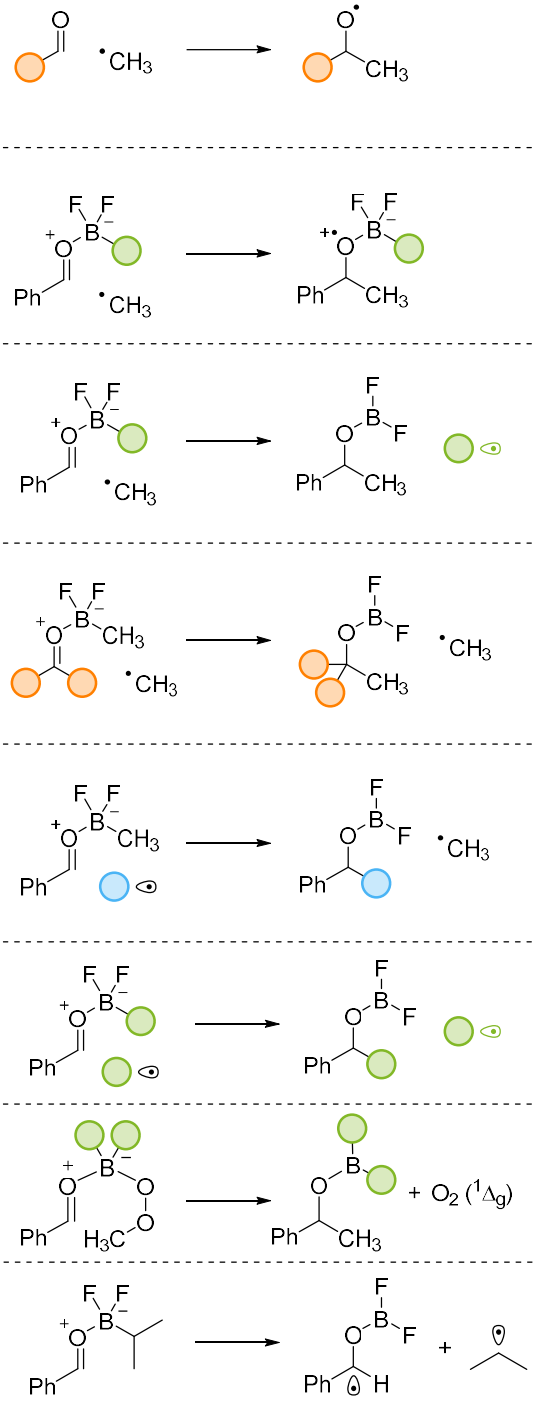


Figure S13. Calculated TD-DFT spectra of benzaldehyde and its complexes (first 15 excitations).



	Ph	CH_3
$\Delta G^{\ddagger}$	17.4	17.9
ΔG	4.0	1.8
$d_{C\text{-}C}$, Å	2.12	2.14

	BF_3	BF_2Ph
$\Delta G^{\ddagger}$	9.8	10.7
ΔG	6.0	-4.8
$d_{C\text{-}C}$, Å	2.28	2.25

	Me	Et	*i*-Pr	*t*-Bu	Me (BMe_3)
$\Delta G^{\ddagger}$	11.0	11.2	10.4	11.3	13.2
ΔG	-23.7	-28.5	-33.2	-35.9	-32.8
$d_{C\text{-}C}$, Å	2.23	2.24	2.25	2.26	2.21

	Ph, H	Me, H	Ph, Me	Me, Me
$\Delta G^{\ddagger}$	11.0	11.2	16.0	15.4
ΔG	-23.7	-26.4	-18.4	-20.5
$d_{C\text{-}C}$, Å	2.23	2.30	2.12	2.15

	Me	Et	*i*-Pr	*t*-Bu
$\Delta G^{\ddagger}$	11.0	7.6	8.1	11.1
ΔG	-23.7	-21.0	-18.0	-14.4
$d_{C\text{-}C}$, Å	2.23	2.36	1.70	1.72

	Me	Et	*i*-Pr	*t*-Bu
ΔG	-23.7	-25.9	-27.5	-26.6

	Cl	F
ΔG	41.5	42.0

ΔH = 82.9

Scheme S5. Summary of DFT calculations.

Energies and Cartesian coordinates

Benzaldehyde

SCF Energy = -345.209705960
Zero-point correction = 0.111079
Thermal correction to Energy = 0.117322
Thermal correction to Enthalpy = 0.118266
Thermal correction to Gibbs Free Energy = 0.080568
Sum of electronic and zero-point Energies = -345.098627
Sum of electronic and thermal Energies = -345.092384
Sum of electronic and thermal Enthalpies = -345.091440
Sum of electronic and thermal Free Energies = -345.129138

C	0.533583000	0.212937000	-0.000088000
C	-0.357806000	1.291552000	-0.000029000
C	0.044546000	-1.100606000	-0.000051000
C	-1.732170000	1.061080000	0.000057000
C	-1.326760000	-1.329542000	0.000035000
C	-2.214030000	-0.248500000	0.000090000
H	0.029477000	2.314394000	-0.000057000
H	0.757241000	-1.928151000	-0.000097000
H	-2.428878000	1.901578000	0.000099000
H	-1.711437000	-2.351419000	0.000060000
H	-3.291000000	-0.430745000	0.000158000
C	1.993958000	0.466470000	-0.000204000
O	2.839663000	-0.396621000	0.000107000
H	2.279362000	1.546973000	0.000121000

Acetaldehyde

SCF Energy = -153.669658122
Zero-point correction = 0.055808
Thermal correction to Energy = 0.059697
Thermal correction to Enthalpy = 0.060641
Thermal correction to Gibbs Free Energy = 0.030865
Sum of electronic and zero-point Energies = -153.613850
Sum of electronic and thermal Energies = -153.609962
Sum of electronic and thermal Enthalpies = -153.609017
Sum of electronic and thermal Free Energies = -153.638793

O	-1.203386000	0.383832000	0.000000000
C	0.000000000	0.458071000	0.000000000
C	0.930404000	-0.715701000	0.000000000
H	1.585878000	-0.661623000	0.883465000
H	0.369794000	-1.659260000	0.000000000
H	1.585878000	-0.661623000	-0.883465000
H	0.503116000	1.457630000	0.000000000

Benzaldehyde/BF_3 complex

SCF Energy = -669.464765423
Zero-point correction = 0.126299
Thermal correction to Energy = 0.136647
Thermal correction to Enthalpy = 0.137591
Thermal correction to Gibbs Free Energy = 0.088567
Sum of electronic and zero-point Energies = -669.338467
Sum of electronic and thermal Energies = -669.328118
Sum of electronic and thermal Enthalpies = -669.327174
Sum of electronic and thermal Free Energies = -669.376198

C	-1.166775000	-0.216645000	0.000039000
C	-2.080751000	-1.284953000	0.000006000
C	-1.624914000	1.114840000	0.000040000
C	-3.445649000	-1.023089000	-0.000028000
C	-2.988211000	1.366780000	0.000003000
C	-3.893902000	0.299195000	-0.000030000
H	-1.714985000	-2.314448000	0.000002000
H	-0.901254000	1.931683000	0.000071000
H	-4.162009000	-1.845809000	-0.000056000
H	-3.355230000	2.394238000	0.000001000
H	-4.966577000	0.504168000	-0.000064000
C	0.242799000	-0.518166000	0.000062000
O	1.114107000	0.365008000	0.000023000
H	0.563139000	-1.572852000	0.000129000
B	2.689209000	0.044432000	-0.000022000
F	3.150485000	0.625473000	-1.147269000
F	2.801151000	-1.326508000	0.000839000
F	3.150856000	0.626926000	1.146352000

Benzaldehyde/BF_2Ph complex

SCF Energy = -801.076628660
Zero-point correction = 0.215053
Thermal correction to Energy = 0.229475
Thermal correction to Enthalpy = 0.230419
Thermal correction to Gibbs Free Energy = 0.170999
Sum of electronic and zero-point Energies = -800.861576
Sum of electronic and thermal Energies = -800.847154
Sum of electronic and thermal Enthalpies = -800.846210
Sum of electronic and thermal Free Energies = -800.905630

C	2.371047000	0.121857000	-0.148846000
C	3.342311000	0.117017000	-1.163753000
C	2.635267000	-0.484733000	1.092952000
C	4.572432000	-0.490376000	-0.937999000
C	3.864423000	-1.089520000	1.310003000
C	4.829196000	-1.090736000	0.295863000
H	3.127468000	0.590442000	-2.124690000
H	1.868505000	-0.472696000	1.869422000
H	5.332123000	-0.497808000	-1.720971000
H	4.079469000	-1.563580000	2.268985000
H	5.795424000	-1.568147000	0.472391000
C	1.100228000	0.760818000	-0.409241000
O	0.197520000	0.818223000	0.434170000
H	0.928048000	1.215894000	-1.399395000
B	-1.281745000	1.475768000	0.119798000
F	-1.084133000	2.193794000	-1.049334000
F	-1.475075000	2.291708000	1.209642000
C	-2.268430000	0.222986000	-0.008837000
C	-2.395791000	-0.474350000	-1.219664000
C	-3.014372000	-0.230865000	1.088211000
C	-3.233660000	-1.583954000	-1.333922000
C	-3.856536000	-1.339160000	0.984383000
C	-3.966768000	-2.019695000	-0.228761000
H	-1.832818000	-0.139627000	-2.096249000
H	-2.938427000	0.297188000	2.042782000
H	-3.318784000	-2.110336000	-2.287948000
H	-4.430592000	-1.673472000	1.852250000
H	-4.625060000	-2.887733000	-0.314029000

Benzaldehyde/BF_2Me complex

SCF Energy = -609.540793930
Zero-point correction = 0.160040
Thermal correction to Energy = 0.171520
Thermal correction to Enthalpy = 0.172464
Thermal correction to Gibbs Free Energy = 0.121459
Sum of electronic and zero-point Energies = -609.380754

Sum of electronic and thermal Energies = -609.369274
Sum of electronic and thermal Enthalpies = -609.368330
Sum of electronic and thermal Free Energies = -609.419335

C	-1.190783000	0.213539000	-0.003098000
C	-2.104869000	1.276791000	0.076092000
C	-1.648228000	-1.115014000	-0.069053000
C	-3.470255000	1.013301000	0.089681000
C	-3.011730000	-1.370046000	-0.054720000
C	-3.918719000	-0.306990000	0.024434000
H	-1.739648000	2.305434000	0.125877000
H	-0.923518000	-1.928728000	-0.130611000
H	-4.186457000	1.834066000	0.150864000
H	-3.377158000	-2.396978000	-0.105369000
H	-4.991057000	-0.513568000	0.035051000
C	0.225428000	0.515924000	-0.015859000
O	1.094351000	-0.358949000	-0.085742000
H	0.541337000	1.571624000	0.038735000
B	2.721143000	-0.016624000	-0.052731000
F	2.767363000	1.364680000	-0.206947000
F	3.167399000	-0.659191000	-1.190070000
C	3.243753000	-0.579775000	1.342723000
H	2.770943000	-0.067788000	2.195826000
H	3.052410000	-1.659369000	1.445498000
H	4.332165000	-0.425772000	1.425655000

Benzaldehyde/BF_2Et complex

SCF Energy = -648.814159729
Zero-point correction = 0.188926
Thermal correction to Energy = 0.201723
Thermal correction to Enthalpy = 0.202667
Thermal correction to Gibbs Free Energy = 0.148235
Sum of electronic and zero-point Energies = -648.625233
Sum of electronic and thermal Energies = -648.612437
Sum of electronic and thermal Enthalpies = -648.611492
Sum of electronic and thermal Free Energies = -648.665925

C	-1.407955000	0.074589000	-0.230189000
C	-2.300952000	0.999579000	-0.795346000
C	-1.881305000	-0.952130000	0.606895000
C	-3.661336000	0.898224000	-0.525602000
C	-3.239604000	-1.046160000	0.872133000
C	-4.125631000	-0.122339000	0.305959000
H	-1.923537000	1.793585000	-1.444021000
H	-1.172602000	-1.661395000	1.037839000
H	-4.361363000	1.612658000	-0.961277000
H	-3.617250000	-1.838334000	1.520592000
H	-5.194063000	-0.201090000	0.517946000
C	0.003418000	0.203144000	-0.524993000
O	0.852434000	-0.572644000	-0.072750000
H	0.336309000	1.027224000	-1.178888000
B	2.474480000	-0.366140000	-0.323222000
F	2.530496000	0.549045000	-1.370277000
F	2.866868000	-1.623741000	-0.734616000
C	3.063585000	0.141598000	1.072138000
H	2.876515000	-0.621422000	1.847445000
H	4.161917000	0.187523000	0.958454000
C	2.539468000	1.501902000	1.532943000
H	1.451416000	1.479015000	1.713442000
H	2.727304000	2.279570000	0.775811000
H	3.009079000	1.836347000	2.471179000

Benzaldehyde/BF_2*i*-Pr complex

SCF Energy = -688.088691911
Zero-point correction = 0.217272
Thermal correction to Energy = 0.231399
Thermal correction to Enthalpy = 0.232343
Thermal correction to Gibbs Free Energy = 0.174951
Sum of electronic and zero-point Energies = -687.871420
Sum of electronic and thermal Energies = -687.857293
Sum of electronic and thermal Enthalpies = -687.856349
Sum of electronic and thermal Free Energies = -687.913741

C	1.785399000	0.042694000	-0.233028000
C	2.697288000	0.872706000	-0.905703000
C	2.227577000	-0.826616000	0.780964000
C	4.045289000	0.833334000	-0.567013000
C	3.573785000	-0.859780000	1.113463000
C	4.478610000	-0.031264000	0.439640000
H	2.344071000	1.544676000	-1.691399000
H	1.504934000	-1.463990000	1.293339000
H	4.759758000	1.474604000	-1.085222000
H	3.927459000	-1.530327000	1.898252000
H	5.537467000	-0.061795000	0.705300000
C	0.388527000	0.103685000	-0.604878000
O	-0.476519000	-0.594882000	-0.064226000
H	0.080490000	0.802011000	-1.401542000
B	-2.076956000	-0.467349000	-0.421838000
F	-2.424897000	-1.782632000	-0.664924000
F	-2.100073000	0.282959000	-1.595271000
C	-2.763508000	0.222844000	0.852611000
H	-2.543936000	-0.415600000	1.728617000
C	-4.285699000	0.257104000	0.665595000
C	-2.216093000	1.624829000	1.134171000
H	-1.135463000	1.615019000	1.350970000
H	-2.375066000	2.292103000	0.270717000
H	-2.713041000	2.089413000	2.002027000
H	-4.561215000	0.875278000	-0.205255000
H	-4.794471000	0.684685000	1.545823000
H	-4.696368000	-0.750438000	0.498194000

Benzaldehyde/BF_2*t*-Bu complex

SCF Energy = -727.365263738
Zero-point correction = 0.244664
Thermal correction to Energy = 0.260177
Thermal correction to Enthalpy = 0.261122
Thermal correction to Gibbs Free Energy = 0.200674
Sum of electronic and zero-point Energies = -727.120600
Sum of electronic and thermal Energies = -727.105086
Sum of electronic and thermal Enthalpies = -727.104142
Sum of electronic and thermal Free Energies = -727.164590

C	-1.976087000	-0.293940000	-0.055826000
C	-2.928432000	-1.166078000	0.496901000
C	-2.357463000	0.982055000	-0.509832000
C	-4.256110000	-0.764794000	0.594784000
C	-3.683610000	1.375384000	-0.407694000
C	-4.628944000	0.502412000	0.143224000
H	-2.622923000	-2.154894000	0.847154000
H	-1.604212000	1.647026000	-0.935922000
H	-5.001733000	-1.436635000	1.022471000
H	-3.990042000	2.362981000	-0.756094000
H	-5.671770000	0.817324000	0.220845000
C	-0.600761000	-0.733695000	-0.142329000
O	0.294828000	-0.027351000	-0.619441000
H	-0.337631000	-1.736410000	0.234955000
B	1.873990000	-0.469542000	-0.616961000
F	2.247254000	-0.227001000	-1.925570000

F	1.838994000	-1.836623000	-0.351375000
C	2.601806000	0.427936000	0.507689000
C	4.088196000	0.032455000	0.515463000
C	2.002880000	0.156609000	1.894728000
H	0.948714000	0.475214000	1.958394000
H	2.047533000	-0.913527000	2.152691000
H	2.550306000	0.710139000	2.677441000
H	4.219704000	-1.032797000	0.763361000
H	4.650144000	0.621594000	1.261534000
H	4.554269000	0.207407000	-0.467206000
C	2.475346000	1.921182000	0.175890000
H	2.904213000	2.150613000	-0.812145000
H	1.422208000	2.245189000	0.165074000
H	3.005478000	2.538734000	0.922304000

Benzaldehyde/B(Me)$_3$ complex

SCF Energy = -489.686244984
Zero-point correction = 0.227773
Thermal correction to Energy = 0.241169
Thermal correction to Enthalpy = 0.242114
Thermal correction to Gibbs Free Energy = 0.187501
Sum of electronic and zero-point Energies = -489.458472
Sum of electronic and thermal Energies = -489.445076
Sum of electronic and thermal Enthalpies = -489.444131
Sum of electronic and thermal Free Energies = -489.498744

C	1.238415000	0.237002000	-0.002286000
C	2.170490000	1.285486000	-0.000560000
C	1.674117000	-1.098867000	-0.002173000
C	3.532566000	1.000523000	0.001657000
C	3.034173000	-1.376778000	-0.000414000
C	3.960272000	-0.327941000	0.001621000
H	1.823372000	2.321818000	-0.000725000
H	0.935040000	-1.902021000	-0.003681000
H	4.262044000	1.812046000	0.003354000
H	3.381078000	-2.411535000	-0.000625000
H	5.029255000	-0.551584000	0.003125000
C	-0.181952000	0.559672000	-0.004048000
O	-1.058560000	-0.300232000	-0.001747000
H	-0.465797000	1.627402000	-0.007342000
B	-2.742551000	-0.037902000	0.000639000
C	-3.198432000	-0.822391000	-1.338361000
H	-4.298268000	-0.780976000	-1.430171000
H	-2.784025000	-0.378303000	-2.260642000
H	-2.918302000	-1.889996000	-1.325017000
C	-2.979787000	1.561772000	-0.041183000
H	-2.585388000	2.100824000	0.839360000
H	-2.580846000	2.053606000	-0.946965000
H	-4.068900000	1.741808000	-0.048350000
C	-3.183602000	-0.748548000	1.385291000
H	-2.756708000	-0.256710000	2.277177000
H	-4.282113000	-0.698303000	1.487938000
H	-2.906775000	-1.816292000	1.426079000

Acetaldehyde/BF_2Me complex

SCF Energy = -418.000206174
Zero-point correction = 0.105041
Thermal correction to Energy = 0.113897
Thermal correction to Enthalpy = 0.114841
Thermal correction to Gibbs Free Energy = 0.071469
Sum of electronic and zero-point Energies = -417.895165
Sum of electronic and thermal Energies = -417.886309
Sum of electronic and thermal Enthalpies = -417.885365
Sum of electronic and thermal Free Energies = -417.928737

C	1.517950000	-0.095560000	0.258574000
O	0.566907000	0.180107000	-0.466197000
H	1.313138000	-0.554359000	1.242174000
B	-1.035821000	-0.077761000	-0.008101000
F	-0.916109000	-0.849519000	1.137902000
F	-1.500999000	-0.822516000	-1.069180000
C	-1.647275000	1.378520000	0.181783000
H	-1.148524000	1.932621000	0.992616000
H	-1.570955000	1.977874000	-0.738679000
H	-2.715915000	1.302892000	0.441294000
C	2.913084000	0.164586000	-0.136253000
H	3.471416000	-0.783790000	-0.094969000
H	2.975551000	0.612345000	-1.134313000
H	3.370554000	0.823406000	0.618837000

Acetophenone/BF_2Me complex

SCF Energy = -648.824382061
Zero-point correction = 0.187420
Thermal correction to Energy = 0.200599
Thermal correction to Enthalpy = 0.201544
Thermal correction to Gibbs Free Energy = 0.146326
Sum of electronic and zero-point Energies = -648.636962
Sum of electronic and thermal Energies = -648.623783
Sum of electronic and thermal Enthalpies = -648.622838
Sum of electronic and thermal Free Energies = -648.678056

C	-1.263969000	-0.187061000	-0.044918000
C	-2.285578000	-1.145335000	0.057287000
C	-1.599796000	1.177500000	-0.100376000
C	-3.616844000	-0.743936000	0.105024000
C	-2.930327000	1.572619000	-0.062178000
C	-3.939379000	0.611860000	0.041546000
H	-2.051878000	-2.208930000	0.112038000
H	-0.801745000	1.916843000	-0.176203000
H	-4.406105000	-1.492550000	0.190497000
H	-3.185409000	2.632583000	-0.111303000
H	-4.985558000	0.923375000	0.073665000
C	0.160295000	-0.567779000	-0.071827000
O	0.992487000	0.356479000	-0.036891000
B	2.644809000	0.265999000	0.031692000
F	2.997223000	-0.405159000	-1.134286000
F	2.878655000	-0.527208000	1.146823000
C	3.128041000	1.779482000	0.131540000
H	2.814922000	2.364661000	-0.747635000
H	2.727930000	2.277028000	1.029131000
H	4.227865000	1.825538000	0.187548000
C	0.591753000	-1.995141000	-0.102457000
H	-0.158424000	-2.650522000	-0.554288000
H	1.542834000	-2.076275000	-0.639067000
H	0.763561000	-2.315519000	0.937613000

Acetone/BF_2Me complex

SCF Energy = -457.287971337
Zero-point correction = 0.132960
Thermal correction to Energy = 0.143152
Thermal correction to Enthalpy = 0.144096
Thermal correction to Gibbs Free Energy = 0.097723
Sum of electronic and zero-point Energies = -457.155012
Sum of electronic and thermal Energies = -457.144819
Sum of electronic and thermal Enthalpies = -457.143875
Sum of electronic and thermal Free Energies = -457.190248

C	1.386078000	0.158439000	-0.001058000

O	0.275612000	0.706880000	-0.001622000
B	-1.220294000	-0.028031000	-0.000264000
F	-1.190779000	-0.818944000	1.140614000
F	-1.196970000	-0.811205000	-1.146808000
C	-2.262112000	1.174116000	0.006174000
H	-2.145581000	1.809461000	0.898297000
H	-2.150244000	1.814742000	-0.882755000
H	-3.292713000	0.783393000	0.007721000
C	2.595811000	1.021882000	-0.000269000
H	3.202976000	0.784548000	-0.887749000
H	2.326071000	2.083350000	0.008066000
H	3.212501000	0.771898000	0.876976000
C	1.544439000	-1.322934000	0.001108000
H	1.001651000	-1.735101000	-0.861353000
H	2.597293000	-1.621966000	-0.022632000
H	1.049066000	-1.722882000	0.897745000

Benzaldehyde/$BF_2(O_2Me)$ complex

SCF Energy = -759.760804465
Zero-point correction = 0.170106
Thermal correction to Energy = 0.183362
Thermal correction to Enthalpy = 0.184306
Thermal correction to Gibbs Free Energy = 0.128643
Sum of electronic and zero-point Energies = -759.590698
Sum of electronic and thermal Energies = -759.577442
Sum of electronic and thermal Enthalpies = -759.576498
Sum of electronic and thermal Free Energies = -759.632161

C	0.024059000	-0.460552000	0.572368000
O	-0.807200000	-0.837327000	-0.270834000
H	-0.321917000	-0.235570000	1.593232000
B	-2.371752000	-0.663882000	0.010457000
F	-2.531216000	-0.884208000	1.360771000
F	-2.995350000	-1.581460000	-0.781543000
O	-2.680233000	0.662019000	-0.440799000
O	-1.902943000	1.577570000	0.317639000
C	-1.320504000	2.471212000	-0.596680000
H	-0.646620000	1.949790000	-1.297945000
H	-2.090031000	3.017461000	-1.165338000
H	-0.743652000	3.178340000	0.014986000
C	1.424430000	-0.310965000	0.260203000
C	2.299160000	0.103859000	1.278980000
C	1.908182000	-0.559542000	-1.038190000
C	3.651352000	0.266970000	1.001626000
C	3.258570000	-0.393750000	-1.306500000
C	4.125783000	0.017958000	-0.287693000
H	1.912373000	0.297079000	2.282297000
H	1.213968000	-0.878404000	-1.817563000
H	4.337428000	0.588419000	1.786529000
H	3.644932000	-0.583027000	-2.309182000
H	5.188197000	0.147102000	-0.505089000

Benzaldehyde/$BCl_2(O_2Me)$ complex

SCF Energy = -1480.35650581
Zero-point correction = 0.167096
Thermal correction to Energy = 0.181149
Thermal correction to Enthalpy = 0.182093
Thermal correction to Gibbs Free Energy = 0.124109
Sum of electronic and zero-point Energies = -1480.189410
Sum of electronic and thermal Energies = -1480.175357
Sum of electronic and thermal Enthalpies = -1480.174412
Sum of electronic and thermal Free Energies = -1480.232397

C	0.409842000	-0.041286000	0.639367000
O	-0.464643000	-0.646137000	-0.015928000
H	0.093664000	0.605426000	1.471950000
B	-1.962515000	-0.238186000	-0.001926000
O	-2.076671000	0.874028000	-0.886444000
O	-1.198450000	1.902938000	-0.442362000
C	-0.548996000	2.401026000	-1.586520000
H	0.060647000	1.623059000	-2.075851000
H	-1.273748000	2.810807000	-2.307293000
H	0.101020000	3.206510000	-1.219016000
C	1.809603000	-0.186687000	0.347809000
C	2.736312000	0.501617000	1.151937000
C	2.249779000	-0.985971000	-0.725888000
C	4.094988000	0.389473000	0.884800000
C	3.607379000	-1.091372000	-0.984619000
C	4.525026000	-0.404879000	-0.180214000
H	2.384526000	1.120318000	1.980601000
H	1.516792000	-1.510911000	-1.340704000
H	4.821159000	0.919267000	1.502764000
H	3.960752000	-1.706837000	-1.813184000
H	5.593308000	-0.491375000	-0.389821000
Cl	-2.897626000	-1.637332000	-0.723120000
Cl	-2.445375000	0.112421000	1.763004000

Transition state of the methyl radical addition to benzaldehyde

SCF Energy = -384.995819445
Zero-point correction = 0.145095
Thermal correction to Energy = 0.153487
Thermal correction to Enthalpy = 0.154431
Thermal correction to Gibbs Free Energy = 0.111125
Sum of electronic and zero-point Energies = -384.850724
Sum of electronic and thermal Energies = -384.842333
Sum of electronic and thermal Enthalpies = -384.841388
Sum of electronic and thermal Free Energies = -384.884694

C	-0.174628000	0.001355000	-0.305540000
C	0.595683000	1.151602000	-0.501644000
C	0.435173000	-1.172314000	0.149105000
C	1.964854000	1.131665000	-0.241361000
C	1.802501000	-1.192256000	0.411486000
C	2.568617000	-0.040118000	0.217634000
H	0.119080000	2.068090000	-0.862262000
H	-0.180201000	-2.064049000	0.286961000
H	2.563694000	2.031403000	-0.397850000
H	2.276744000	-2.109887000	0.766519000
H	3.641289000	-0.056790000	0.422954000
C	-1.645191000	0.012550000	-0.604515000
O	-2.316549000	-1.024047000	-0.660463000
H	-1.998572000	0.937317000	-1.119650000
C	-2.330576000	0.867324000	1.213293000
H	-1.984823000	0.106017000	1.915696000
H	-1.799411000	1.821992000	1.224010000
H	-3.404014000	0.899443000	1.016571000

Transition state of the methyl radical addition to acetaldehyde

SCF Energy = -193.455253024
Zero-point correction = 0.090274
Thermal correction to Energy = 0.096005
Thermal correction to Enthalpy = 0.096949
Thermal correction to Gibbs Free Energy = 0.061611
Sum of electronic and zero-point Energies = -193.364979
Sum of electronic and thermal Energies = -193.359248
Sum of electronic and thermal Enthalpies = -193.358304
Sum of electronic and thermal Free Energies = -193.393642

C	0.318990000	0.274520000	0.380911000
O	0.343574000	1.364198000	-0.198791000
H	0.026833000	0.230529000	1.458253000
C	-1.663154000	-0.398379000	-0.079163000
H	-1.565642000	-0.533474000	-1.158639000
H	-1.719714000	-1.303041000	0.531306000
H	-2.248355000	0.460661000	0.253799000
C	1.126964000	-0.908777000	-0.106540000
H	1.133152000	-0.943774000	-1.204877000
H	2.165073000	-0.767735000	0.237336000
H	0.763263000	-1.860936000	0.301906000

Transition state of the methyl radical addition to benzaldehyde/BF_3 complex

SCF Energy = -709.262425648
Zero-point correction = 0.159858
Thermal correction to Energy = 0.172611
Thermal correction to Enthalpy = 0.173555
Thermal correction to Gibbs Free Energy = 0.118544
Sum of electronic and zero-point Energies = -709.102568
Sum of electronic and thermal Energies = -709.089815
Sum of electronic and thermal Enthalpies = -709.088871
Sum of electronic and thermal Free Energies = -709.143882

C	1.208001000	0.066170000	-0.196544000
C	2.133326000	0.958917000	-0.761297000
C	1.654928000	-1.085554000	0.471981000
C	3.495200000	0.700199000	-0.659096000
C	3.017156000	-1.336343000	0.572345000
C	3.935214000	-0.444843000	0.008661000
H	1.780528000	1.852501000	-1.282059000
H	0.924637000	-1.772246000	0.903124000
H	4.216844000	1.389602000	-1.100258000
H	3.370344000	-2.229829000	1.089962000
H	5.005371000	-0.646331000	0.090179000
C	-0.216931000	0.342466000	-0.332238000
O	-1.072458000	-0.525637000	-0.008866000
H	-0.537170000	1.186857000	-0.961420000
B	-2.613415000	-0.284905000	-0.164002000
F	-2.773498000	0.885711000	-0.884782000
F	-3.088298000	-0.168296000	1.121379000
C	-0.424357000	1.821583000	1.386580000
H	-0.241031000	1.105751000	2.189841000
H	0.356530000	2.548404000	1.156248000
H	-1.459172000	2.078897000	1.154805000
F	-3.092132000	-1.386255000	-0.824578000

Transition state of the methyl radical addition to benzaldehyde/BF_2Ph complex

SCF Energy = -840.873038363
Zero-point correction = 0.248731
Thermal correction to Energy = 0.265479
Thermal correction to Enthalpy = 0.266423
Thermal correction to Gibbs Free Energy = 0.201159
Sum of electronic and zero-point Energies = -840.624307
Sum of electronic and thermal Energies = -840.607560
Sum of electronic and thermal Enthalpies = -840.606615
Sum of electronic and thermal Free Energies = -840.671879

C	2.219585000	-0.144099000	-0.125161000
C	3.123734000	-0.379951000	-1.172295000
C	2.466628000	-0.671137000	1.152112000
C	4.266740000	-1.137802000	-0.943080000
C	3.611722000	-1.425591000	1.375202000
C	4.510732000	-1.657557000	0.329945000
H	2.925618000	0.031309000	-2.165371000
H	1.751973000	-0.484578000	1.955446000
H	4.969559000	-1.325833000	-1.756453000
H	3.807753000	-1.838494000	2.366304000
H	5.409595000	-2.250989000	0.509924000
C	1.010620000	0.635536000	-0.388868000
O	0.093661000	0.705868000	0.470102000
H	0.782825000	0.916230000	-1.429174000
B	-1.332092000	1.357644000	0.159915000
F	-1.147382000	2.098552000	-1.010280000
F	-1.550258000	2.180559000	1.249614000
C	1.934914000	2.685994000	-0.234867000
H	2.175452000	2.649365000	0.829246000
H	2.759279000	2.617676000	-0.947201000
H	1.026597000	3.207535000	-0.540690000
C	-2.356854000	0.132270000	0.005109000
C	-2.487585000	-0.549943000	-1.214126000
C	-3.126688000	-0.316828000	1.087610000
C	-3.350097000	-1.638227000	-1.350505000
C	-3.993490000	-1.403943000	0.962524000
C	-4.106048000	-2.069147000	-0.258920000
H	-1.907561000	-0.219470000	-2.081290000
H	-3.049771000	0.198909000	2.048967000
H	-3.436394000	-2.151941000	-2.311439000
H	-4.585091000	-1.733744000	1.820420000
H	-4.783388000	-2.920595000	-0.361182000

Transition state of the methyl radical addition to benzaldehyde/BF_2Me complex

SCF Energy = -649.336814214
Zero-point correction = 0.193874
Thermal correction to Energy = 0.207608
Thermal correction to Enthalpy = 0.208552
Thermal correction to Gibbs Free Energy = 0.151693
Sum of electronic and zero-point Energies = -649.142940
Sum of electronic and thermal Energies = -649.129207
Sum of electronic and thermal Enthalpies = -649.128262
Sum of electronic and thermal Free Energies = -649.185121

C	1.218165000	0.054676000	-0.177105000
C	2.143914000	0.826075000	-0.895866000
C	1.661344000	-0.997280000	0.639133000
C	3.502773000	0.546022000	-0.799776000
C	3.020523000	-1.270736000	0.733048000
C	3.939947000	-0.499948000	0.015565000
H	1.794761000	1.644043000	-1.531304000
H	0.929928000	-1.591714000	1.189278000
H	4.224085000	1.142373000	-1.361084000
H	3.369349000	-2.088518000	1.366188000
H	5.007234000	-0.718018000	0.092234000
C	-0.211505000	0.347775000	-0.305420000
O	-1.070429000	-0.444137000	0.160726000
H	-0.530638000	1.090560000	-1.053641000
B	-2.646175000	-0.262094000	-0.097351000
F	-2.774294000	1.020687000	-0.651224000
F	-3.174671000	-0.281689000	1.187232000
C	-0.312018000	2.037224000	1.152376000
H	-0.105064000	1.458029000	2.054222000
H	0.469995000	2.704985000	0.785847000
H	-1.350776000	2.281816000	0.924944000
C	-3.098897000	-1.454225000	-1.059982000
H	-2.881522000	-2.440003000	-0.618884000

H	-4.184619000	-1.404455000	-1.244931000
H	-2.593216000	-1.404004000	-2.037826000

Transition state of the methyl radical addition to benzaldehyde/BF_2Et complex

SCF Energy = -688.609622091
Zero-point correction = 0.222685
Thermal correction to Energy = 0.237803
Thermal correction to Enthalpy = 0.238747
Thermal correction to Gibbs Free Energy = 0.178280
Sum of electronic and zero-point Energies = -688.386937
Sum of electronic and thermal Energies = -688.371819
Sum of electronic and thermal Enthalpies = -688.370875
Sum of electronic and thermal Free Energies = -688.431342

C	-1.440195000	-0.095281000	-0.166355000
C	-2.424262000	-0.622646000	-1.016052000
C	-1.783155000	0.863143000	0.799730000
C	-3.741943000	-0.192934000	-0.901255000
C	-3.101889000	1.286499000	0.911389000
C	-4.079862000	0.758885000	0.063026000
H	-2.151513000	-1.367965000	-1.767645000
H	-1.006833000	1.267445000	1.451623000
H	-4.508296000	-0.598561000	-1.563938000
H	-3.373255000	2.032145000	1.660836000
H	-5.115038000	1.094439000	0.154249000
C	-0.053087000	-0.540222000	-0.316829000
O	0.878212000	0.055430000	0.281900000
H	0.198295000	-1.193720000	-1.167506000
B	2.426422000	-0.243616000	-0.018912000
F	2.435682000	-1.492119000	-0.658889000
F	2.973922000	-0.348736000	1.253398000
C	-0.216090000	-2.436217000	0.868080000
H	-0.382704000	-1.976738000	1.844181000
H	-1.060036000	-2.938675000	0.391546000
H	0.793513000	-2.767377000	0.620267000
C	2.971457000	0.961783000	-0.921566000
H	4.031925000	0.751143000	-1.151183000
H	2.448496000	0.947594000	-1.894971000
C	2.845192000	2.344935000	-0.281995000
H	3.380180000	2.387951000	0.679971000
H	1.791408000	2.592800000	-0.076079000
H	3.252625000	3.144181000	-0.921613000

Transition state of the methyl radical addition to benzaldehyde/BF_2*i*-Pr complex

SCF Energy = -727.885660023
Zero-point correction = 0.250753
Thermal correction to Energy = 0.267234
Thermal correction to Enthalpy = 0.268178
Thermal correction to Gibbs Free Energy = 0.205109
Sum of electronic and zero-point Energies = -727.634907
Sum of electronic and thermal Energies = -727.618426
Sum of electronic and thermal Enthalpies = -727.617482
Sum of electronic and thermal Free Energies = -727.680551

C	1.596317000	0.097576000	-0.117627000
C	2.545608000	0.380068000	-1.111454000
C	1.959298000	-0.652378000	1.011730000
C	3.849115000	-0.085467000	-0.976743000
C	3.263927000	-1.112348000	1.141847000
C	4.207406000	-0.828714000	0.149861000
H	2.257004000	0.963033000	-1.989893000
H	1.209057000	-0.868302000	1.774343000
H	4.588409000	0.129174000	-1.750248000
H	3.551081000	-1.696607000	2.017900000
H	5.231583000	-1.192449000	0.256079000
C	0.222090000	0.571429000	-0.287932000
O	-0.692318000	0.171486000	0.476694000
H	-0.057733000	1.040817000	-1.244222000
B	-2.238798000	0.446160000	0.179529000
F	-2.248604000	1.503258000	-0.743513000
F	-2.728543000	0.873225000	1.406871000
C	0.530111000	2.680502000	0.440913000
H	0.754983000	2.435168000	1.480503000
H	1.351249000	3.022633000	-0.191865000
H	-0.483754000	2.999011000	0.193672000
C	-2.865483000	-0.925060000	-0.380908000
H	-3.932935000	-0.695091000	-0.565690000
C	-2.798328000	-2.059742000	0.644589000
C	-2.243177000	-1.344802000	-1.715318000
H	-2.306462000	-0.541438000	-2.465660000
H	-1.176310000	-1.604359000	-1.595043000
H	-2.738130000	-2.235311000	-2.137698000
H	-1.751018000	-2.321289000	0.872010000
H	-3.292119000	-2.975331000	0.277213000
H	-3.279360000	-1.777072000	1.593422000

Transition state of the methyl radical addition to benzaldehyde/BF_2*t*-Bu complex

SCF Energy = -767.161872108
Zero-point correction = 0.278736
Thermal correction to Energy = 0.296451
Thermal correction to Enthalpy = 0.297395
Thermal correction to Gibbs Free Energy = 0.232017
Sum of electronic and zero-point Energies = -766.883136
Sum of electronic and thermal Energies = -766.865421
Sum of electronic and thermal Enthalpies = -766.864477
Sum of electronic and thermal Free Energies = -766.929855

C	-1.898135000	0.076353000	0.139099000
C	-2.837817000	0.332781000	1.149168000
C	-2.260102000	-0.682057000	-0.985082000
C	-4.130493000	-0.167136000	1.035799000
C	-3.553948000	-1.176642000	-1.093626000
C	-4.487717000	-0.918943000	-0.085493000
H	-2.550314000	0.923227000	2.022903000
H	-1.517538000	-0.876910000	-1.760770000
H	-4.862230000	0.027437000	1.821687000
H	-3.840268000	-1.767576000	-1.965449000
H	-5.503520000	-1.309659000	-0.174935000
C	-0.535068000	0.587291000	0.285623000
O	0.374238000	0.215784000	-0.499201000
H	-0.248408000	1.061478000	1.237410000
B	1.912296000	0.551486000	-0.252924000
F	1.912356000	1.579618000	0.703045000
F	2.330191000	1.042496000	-1.484520000
C	-0.917080000	2.694605000	-0.428464000
H	-1.149880000	2.446777000	-1.465698000
H	-1.738316000	3.008170000	0.218777000
H	0.090869000	3.040486000	-0.193993000
C	2.638376000	-0.807227000	0.236642000
C	2.500385000	-1.902292000	-0.829667000
C	2.027246000	-1.298351000	1.556232000
H	2.088039000	-0.527678000	2.341380000
H	0.966315000	-1.576842000	1.438837000
H	2.553725000	-2.194481000	1.929324000

H	1.443640000	-2.158874000	-1.008057000
H	3.020296000	-2.826749000	-0.520966000
H	2.931684000	-1.582236000	-1.791288000
C	4.126760000	-0.493144000	0.456501000
H	4.263602000	0.284950000	1.224372000
H	4.677904000	-1.391173000	0.788219000
H	4.601645000	-0.134505000	-0.470639000

Transition state of the methyl radical addition to benzaldehyde/$B(Me)_3$ complex

SCF Energy = -529.480383318
Zero-point correction = 0.261823
Thermal correction to Energy = 0.277296
Thermal correction to Enthalpy = 0.278241
Thermal correction to Gibbs Free Energy = 0.219356
Sum of electronic and zero-point Energies = -529.218560
Sum of electronic and thermal Energies = -529.203087
Sum of electronic and thermal Enthalpies = -529.202143
Sum of electronic and thermal Free Energies = -529.261027

C	1.260182000	0.102727000	-0.166347000
C	2.205957000	0.926450000	-0.791253000
C	1.677186000	-1.039099000	0.531629000
C	3.559553000	0.610584000	-0.719402000
C	3.030777000	-1.349290000	0.603298000
C	3.971594000	-0.525417000	-0.020585000
H	1.878110000	1.814669000	-1.337528000
H	0.929667000	-1.674963000	1.009239000
H	4.295658000	1.250120000	-1.209872000
H	3.357613000	-2.238402000	1.145874000
H	5.033801000	-0.772327000	0.037347000
C	-0.172782000	0.435616000	-0.270846000
O	-1.042461000	-0.393981000	0.078956000
H	-0.456524000	1.261817000	-0.944968000
B	-2.668181000	-0.277629000	-0.170193000
C	-0.239355000	1.907127000	1.370369000
H	0.017106000	1.229778000	2.187141000
H	0.521382000	2.620608000	1.047783000
H	-1.286685000	2.195137000	1.266609000
C	-2.966364000	1.046735000	-1.060750000
H	-2.487794000	1.030886000	-2.057287000
H	-4.053726000	1.097829000	-1.243870000
H	-2.694278000	2.001657000	-0.575401000
C	-3.278358000	-0.219634000	1.334415000
H	-4.381341000	-0.243992000	1.282280000
H	-2.968325000	-1.082370000	1.949880000
H	-3.008619000	0.696253000	1.888904000
C	-3.000434000	-1.665057000	-0.945051000
H	-2.504575000	-1.735043000	-1.929698000
H	-2.711233000	-2.557645000	-0.362773000
H	-4.087379000	-1.738470000	-1.127219000

Transition state of the methyl radical addition to acetaldehyde/BF_2Me complex

SCF Energy = -457.796361044
Zero-point correction = 0.139092
Thermal correction to Energy = 0.150032
Thermal correction to Enthalpy = 0.150977
Thermal correction to Gibbs Free Energy = 0.102117
Sum of electronic and zero-point Energies = -457.657269
Sum of electronic and thermal Energies = -457.646329
Sum of electronic and thermal Enthalpies = -457.645384
Sum of electronic and thermal Free Energies = -457.694245

C	-1.190903000	-0.518415000	0.265813000
O	-0.186158000	-0.524390000	-0.477909000
H	-1.059574000	-0.217279000	1.317460000
B	1.248459000	0.073756000	-0.018613000
F	0.973196000	0.802888000	1.143718000
F	1.563674000	0.930539000	-1.062547000
C	-1.934478000	1.637926000	0.000438000
H	-2.065597000	1.598463000	-1.082697000
H	-2.824621000	1.611361000	0.632560000
H	-1.028466000	2.098185000	0.396714000
C	2.217287000	-1.178882000	0.185650000
H	2.309189000	-1.780173000	-0.732657000
H	3.228031000	-0.835266000	0.460759000
H	1.863072000	-1.843038000	0.990515000
C	-2.409956000	-1.265718000	-0.137866000
H	-2.552111000	-1.231968000	-1.225443000
H	-2.244836000	-2.316918000	0.155743000
H	-3.301649000	-0.907340000	0.388647000

Transition state of the methyl radical addition to acetophenone/BF_2Me complex

SCF Energy = -688.616735887
Zero-point correction = 0.222744
Thermal correction to Energy = 0.237461
Thermal correction to Enthalpy = 0.238406
Thermal correction to Gibbs Free Energy = 0.180796
Sum of electronic and zero-point Energies = -688.393992
Sum of electronic and thermal Energies = -688.379274
Sum of electronic and thermal Enthalpies = -688.378330
Sum of electronic and thermal Free Energies = -688.435940

C	-1.276808000	-0.116592000	-0.093711000
C	-2.306226000	-1.040967000	-0.328550000
C	-1.603837000	1.232002000	0.122450000
C	-3.633345000	-0.622015000	-0.352195000
C	-2.930442000	1.645624000	0.100604000
C	-3.948761000	0.719595000	-0.136044000
H	-2.082670000	-2.094681000	-0.498042000
H	-0.801889000	1.948663000	0.302273000
H	-4.425730000	-1.348600000	-0.540717000
H	-3.173470000	2.696825000	0.266786000
H	-4.990960000	1.045070000	-0.152735000
C	0.160810000	-0.521665000	-0.079166000
O	0.994847000	0.444236000	-0.031497000
B	2.579217000	0.384556000	-0.180035000
F	2.807580000	-0.040104000	-1.490681000
F	3.004703000	-0.611643000	0.719913000
C	0.172869000	-1.081433000	1.960926000
H	-0.136349000	-0.145874000	2.430418000
H	-0.543434000	-1.905036000	1.989230000
H	1.237596000	-1.319683000	1.987857000
C	3.111577000	1.851543000	0.162167000
H	2.848447000	2.150000000	1.189892000
H	4.209500000	1.895276000	0.073936000
H	2.692330000	2.605591000	-0.523447000
C	0.577264000	-1.843576000	-0.672849000
H	1.595246000	-2.096532000	-0.362006000
H	-0.103677000	-2.658710000	-0.409097000
H	0.571044000	-1.718350000	-1.767086000

Transition state of the methyl radical addition to acetone/BF_2Me complex

SCF Energy = -497.079424726

Zero-point correction = 0.167826
Thermal correction to Energy = 0.179757
Thermal correction to Enthalpy = 0.180701
Thermal correction to Gibbs Free Energy = 0.130461
Sum of electronic and zero-point Energies = -496.911599
Sum of electronic and thermal Energies = -496.899668
Sum of electronic and thermal Enthalpies = -496.898723
Sum of electronic and thermal Free Energies = -496.948964

C	1.161540000	-0.263127000	0.233432000
O	0.029704000	0.041036000	0.727136000
B	-1.396216000	-0.028013000	-0.000560000
F	-1.585301000	-1.382030000	-0.281955000
F	-1.237553000	0.688846000	-1.198937000
C	1.674981000	1.661260000	-0.575079000
H	1.671410000	2.252918000	0.342339000
H	2.645407000	1.439797000	-1.024818000
H	0.809607000	1.756240000	-1.232507000
C	-2.445862000	0.609798000	1.019894000
H	-2.203648000	1.660087000	1.249197000
H	-3.461144000	0.588516000	0.591075000
H	-2.475287000	0.056773000	1.972522000
C	1.268474000	-1.053828000	-1.042716000
H	0.574267000	-0.686692000	-1.805503000
H	2.297170000	-1.058849000	-1.420761000
H	0.978709000	-2.087419000	-0.793083000
C	2.284520000	-0.378924000	1.227387000
H	2.215401000	-1.391480000	1.659887000
H	3.270302000	-0.278884000	0.758478000
H	2.165019000	0.348357000	2.039401000

Transition state of the *e*thyl radical addition to benzaldehyde/BF_2Me complex

SCF Energy = -688.623963045
Zero-point correction = 0.222713
Thermal correction to Energy = 0.237788
Thermal correction to Enthalpy = 0.238732
Thermal correction to Gibbs Free Energy = 0.179072
Sum of electronic and zero-point Energies = -688.401251
Sum of electronic and thermal Energies = -688.386175
Sum of electronic and thermal Enthalpies = -688.385231
Sum of electronic and thermal Free Energies = -688.444891

C	-1.246588000	-0.316699000	0.258972000
C	-2.181995000	-0.179532000	1.296033000
C	-1.681430000	-0.547054000	-1.055450000
C	-3.541770000	-0.270859000	1.020055000
C	-3.042036000	-0.634330000	-1.325672000
C	-3.970475000	-0.495680000	-0.290108000
H	-1.837153000	-0.000384000	2.317597000
H	-0.942482000	-0.656698000	-1.851009000
H	-4.270890000	-0.167063000	1.825450000
H	-3.384746000	-0.812546000	-2.346534000
H	-5.038602000	-0.564793000	-0.506657000
C	0.178249000	-0.223666000	0.565964000
O	1.040357000	-0.503551000	-0.301393000
H	0.489298000	-0.135273000	1.617276000
B	2.615031000	-0.493598000	0.000750000
F	2.732979000	0.013851000	1.302891000
F	3.097022000	0.436972000	-0.917761000
C	0.311206000	2.137269000	0.580142000
H	-0.574623000	2.348690000	1.186032000
H	1.264450000	2.085677000	1.113158000
C	3.138370000	-1.990831000	-0.187677000
H	2.928826000	-2.370346000	-1.200438000
H	4.228843000	-2.038697000	-0.033127000
H	2.670024000	-2.679742000	0.533671000
C	0.311038000	2.469378000	-0.862021000
H	1.134009000	1.961426000	-1.384371000
H	-0.647111000	2.222533000	-1.343560000
H	0.464728000	3.558224000	-0.987690000

Transition state of the *iso*-propyl radical addition to benzaldehyde/BF_2Me complex

SCF Energy = -727.909143121
Zero-point correction = 0.253001
Thermal correction to Energy = 0.268477
Thermal correction to Enthalpy = 0.269422
Thermal correction to Gibbs Free Energy = 0.209765
Sum of electronic and zero-point Energies = -727.656142
Sum of electronic and thermal Energies = -727.640666
Sum of electronic and thermal Enthalpies = -727.639721
Sum of electronic and thermal Free Energies = -727.699378

C	1.177658000	-0.228703000	-0.173551000
C	2.091589000	-0.052840000	-1.217951000
C	1.603048000	-0.805149000	1.028308000
C	3.419705000	-0.445491000	-1.060981000
C	2.930470000	-1.194904000	1.183642000
C	3.841507000	-1.013129000	0.140962000
H	1.762117000	0.383971000	-2.163956000
H	0.885739000	-0.954266000	1.837453000
H	4.125879000	-0.310530000	-1.882575000
H	3.256672000	-1.645885000	2.122980000
H	4.882343000	-1.319257000	0.265236000
C	-0.247234000	0.194657000	-0.364504000
O	-1.124230000	-0.472167000	0.376292000
H	-0.552198000	0.275687000	-1.422905000
B	-2.604069000	-0.724372000	-0.097906000
F	-2.911543000	0.276592000	-1.023383000
F	-3.365533000	-0.585230000	1.051188000
C	-0.464550000	1.817152000	0.111050000
H	-1.529721000	1.948732000	-0.114907000
C	-0.191557000	1.985447000	1.589041000
H	0.862459000	1.791611000	1.836056000
H	-0.410211000	3.030574000	1.858758000
H	-0.830280000	1.334985000	2.200176000
C	0.381288000	2.698779000	-0.783281000
H	1.455664000	2.579922000	-0.584341000
H	0.189678000	2.520903000	-1.850499000
H	0.109119000	3.744100000	-0.566239000
C	-2.547175000	-2.207800000	-0.727396000
H	-1.873595000	-2.262320000	-1.596545000
H	-2.230089000	-2.963392000	0.006463000
H	-3.564202000	-2.466003000	-1.068242000

Transition state of the *tert*-butyl radical addition to benzaldehyde/BF_2Me complex

SCF Energy = -767.186316164
Zero-point correction = 0.280964
Thermal correction to Energy = 0.297749
Thermal correction to Enthalpy = 0.298693
Thermal correction to Gibbs Free Energy = 0.236554
Sum of electronic and zero-point Energies = -766.905352
Sum of electronic and thermal Energies = -766.888567
Sum of electronic and thermal Enthalpies = -766.887623
Sum of electronic and thermal Free Energies = -766.949762

C	1.243035000	-0.193742000	-0.154399000
C	2.130601000	-0.020865000	-1.220822000
C	1.699281000	-0.764607000	1.038063000
C	3.466201000	-0.398994000	-1.090842000
C	3.033962000	-1.140137000	1.166565000
C	3.921117000	-0.954101000	0.104590000
H	1.775365000	0.403204000	-2.163101000
H	1.000935000	-0.922211000	1.861696000
H	4.151517000	-0.263554000	-1.929932000
H	3.383429000	-1.585899000	2.100083000
H	4.967213000	-1.250124000	0.207254000
C	-0.200885000	0.196204000	-0.328341000
O	-1.035960000	-0.500780000	0.438925000
H	-0.513806000	0.227217000	-1.384977000
B	-2.317903000	-1.203072000	-0.114241000
F	-2.681284000	-0.582876000	-1.306372000
F	-3.288442000	-1.033446000	0.858558000
C	-0.456341000	1.830971000	0.151834000
C	0.383464000	2.677424000	-0.794097000
H	0.118761000	2.505891000	-1.847569000
H	0.173699000	3.734828000	-0.566246000
H	1.460410000	2.512406000	-0.660348000
C	-1.942208000	2.120642000	-0.022484000
H	-2.283080000	1.903268000	-1.042983000
H	-2.555138000	1.539976000	0.679175000
H	-2.108624000	3.190635000	0.176254000
C	-1.785703000	-2.723869000	-0.307389000
H	-0.965757000	-2.787330000	-1.038377000
H	-1.452335000	-3.174761000	0.638089000
H	-2.639190000	-3.307563000	-0.693392000
C	-0.019279000	1.986677000	1.599207000
H	-0.581272000	1.320004000	2.267177000
H	1.055977000	1.804179000	1.729684000
H	-0.222846000	3.024714000	1.906324000

Product of the methyl radical addition to benzaldehyde

SCF Energy = -385.020924385
Zero-point correction = 0.148751
Thermal correction to Energy = 0.156792
Thermal correction to Enthalpy = 0.157736
Thermal correction to Gibbs Free Energy = 0.114911
Sum of electronic and zero-point Energies = -384.872173
Sum of electronic and thermal Energies = -384.864133
Sum of electronic and thermal Enthalpies = -384.863188
Sum of electronic and thermal Free Energies = -384.906013

C	0.177271000	-0.073580000	-0.202561000
C	-0.625344000	-1.209212000	-0.346107000
C	-0.419883000	1.148615000	0.113764000
C	-2.006005000	-1.126808000	-0.168597000
C	-1.800855000	1.233240000	0.291461000
C	-2.597202000	0.096028000	0.152214000
H	-0.167036000	-2.169161000	-0.602689000
H	0.208225000	2.036696000	0.210686000
H	-2.623639000	-2.020207000	-0.285294000
H	-2.258508000	2.194260000	0.537524000
H	-3.678750000	0.162922000	0.289442000
C	1.687082000	-0.179115000	-0.362761000
O	2.307468000	0.983494000	-0.675096000
H	1.934339000	-0.947419000	-1.127914000
C	2.354133000	-0.677213000	0.953244000
H	2.155967000	0.038271000	1.762974000
H	1.917067000	-1.648757000	1.219023000
H	3.437413000	-0.786282000	0.813077000

Product of the methyl radical addition to acetaldehyde

SCF Energy = -193.485766127
Zero-point correction = 0.094346
Thermal correction to Energy = 0.099478
Thermal correction to Enthalpy = 0.100422
Thermal correction to Gibbs Free Energy = 0.066499
Sum of electronic and zero-point Energies = -193.391421
Sum of electronic and thermal Energies = -193.386288
Sum of electronic and thermal Enthalpies = -193.385344
Sum of electronic and thermal Free Energies = -193.419267

C	0.000097000	0.128132000	0.287375000
H	-0.000355000	0.270125000	1.399819000
O	-0.000443000	1.417859000	-0.145110000
C	-1.282212000	-0.625594000	-0.076765000
H	-2.165081000	-0.048609000	0.231616000
H	-1.329170000	-0.781914000	-1.165443000
H	-1.311466000	-1.609562000	0.412786000
C	1.282533000	-0.624988000	-0.076739000
H	1.312266000	-1.608940000	0.412853000
H	1.329485000	-0.781451000	-1.165408000
H	2.165351000	-0.047827000	0.231434000

Product of the methyl radical addition to benzaldehyde/BF_3 complex

SCF Energy = -609.581880641
Zero-point correction = 0.163359
Thermal correction to Energy = 0.174261
Thermal correction to Enthalpy = 0.175206
Thermal correction to Gibbs Free Energy = 0.124849
Sum of electronic and zero-point Energies = -609.418522
Sum of electronic and thermal Energies = -609.407619
Sum of electronic and thermal Enthalpies = -609.406675
Sum of electronic and thermal Free Energies = -609.457032

C	0.667404000	0.418876000	-0.063559000
C	1.619891000	0.486756000	-1.083989000
C	0.953841000	-0.322685000	1.087504000
C	2.842490000	-0.171874000	-0.956725000
C	2.173296000	-0.986890000	1.213120000
C	3.121657000	-0.911592000	0.192524000
H	1.401472000	1.057248000	-1.990984000
H	0.213896000	-0.384747000	1.888920000
H	3.577084000	-0.113269000	-1.762883000
H	2.384404000	-1.566275000	2.114698000
H	4.076443000	-1.432626000	0.291150000
C	-0.635916000	1.183628000	-0.189709000
O	-1.709895000	0.457043000	0.413027000
H	-0.858746000	1.321350000	-1.260394000
B	-2.232503000	-0.633461000	-0.157607000
F	-1.843934000	-1.084587000	-1.345326000
F	-3.190563000	-1.299826000	0.471477000
C	-0.572547000	2.543676000	0.485329000
H	-0.358449000	2.426753000	1.557895000
H	0.224596000	3.150486000	0.034377000
H	-1.529243000	3.072381000	0.368718000

Product of the methyl radical addition to benzaldehyde/BF_2Ph complex

SCF Energy = -840.904207917
Zero-point correction = 0.252720
Thermal correction to Energy = 0.268765

Thermal correction to Enthalpy = 0.269710
Thermal correction to Gibbs Free Energy = 0.207565
Sum of electronic and zero-point Energies = -840.651488
Sum of electronic and thermal Energies = -840.635443
Sum of electronic and thermal Enthalpies = -840.634498
Sum of electronic and thermal Free Energies = -840.696643

C	1.209051000	1.112004000	0.050318000
C	2.142467000	1.133855000	-0.988818000
C	1.475026000	0.351754000	1.192641000
C	3.321308000	0.394468000	-0.895624000
C	2.648866000	-0.393200000	1.283667000
C	3.574404000	-0.375938000	0.239031000
H	1.937962000	1.720568000	-1.888789000
H	0.742177000	0.322750000	2.001501000
H	4.039228000	0.411418000	-1.718589000
H	2.840538000	-0.995396000	2.174586000
H	4.491855000	-0.964378000	0.309088000
C	-0.074627000	1.910438000	-0.078660000
O	-1.144071000	1.258160000	0.582913000
H	-0.321085000	2.021335000	-1.146071000
B	-2.238838000	0.600904000	-0.137392000
F	-2.468475000	1.106650000	-1.398458000
F	-3.368825000	0.545653000	0.640751000
C	0.046829000	3.298338000	0.549002000
H	0.277342000	3.213708000	1.620754000
H	0.858158000	3.852450000	0.056681000
H	-0.890930000	3.857446000	0.424981000
C	-1.363410000	-0.827643000	-0.144844000
C	-0.573576000	-1.162882000	-1.259814000
C	-1.398059000	-1.669238000	0.981828000
C	0.035668000	-2.409325000	-1.311930000
C	-0.789179000	-2.916134000	0.921225000
C	-0.068637000	-3.282328000	-0.221701000
H	-0.475236000	-0.464722000	-2.093067000
H	-1.929870000	-1.352502000	1.881090000
H	0.608970000	-2.700756000	-2.194005000
H	-0.851929000	-3.598429000	1.771098000
H	0.438488000	-4.249030000	-0.254181000

Product of the methyl radical addition to benzaldehyde/BF_2Me complex

SCF Energy = -609.581880641
Zero-point correction = 0.163359
Thermal correction to Energy = 0.174261
Thermal correction to Enthalpy = 0.175206
Thermal correction to Gibbs Free Energy = 0.124849
Sum of electronic and zero-point Energies = -609.418522
Sum of electronic and thermal Energies = -609.407619
Sum of electronic and thermal Enthalpies = -609.406675
Sum of electronic and thermal Free Energies = -609.457032

C	0.667404000	0.418876000	-0.063559000
C	1.619891000	0.486756000	-1.083989000
C	0.953841000	-0.322685000	1.087504000
C	2.842490000	-0.171874000	-0.956725000
C	2.173296000	-0.986890000	1.213120000
C	3.121657000	-0.911592000	0.192524000
H	1.401472000	1.057248000	-1.990984000
H	0.213896000	-0.384747000	1.888920000
H	3.577084000	-0.113269000	-1.762883000
H	2.384404000	-1.566275000	2.114698000
H	4.076443000	-1.432626000	0.291150000
C	-0.635916000	1.183628000	-0.189709000
O	-1.709895000	0.457043000	0.413027000
H	-0.858746000	1.321350000	-1.260394000
B	-2.232503000	-0.633461000	-0.157607000
F	-1.843934000	-1.084587000	-1.345326000
F	-3.190563000	-1.299826000	0.471477000
C	-0.572547000	2.543676000	0.485329000
H	-0.358449000	2.426753000	1.557895000
H	0.224596000	3.150486000	0.034377000
H	-1.529243000	3.072381000	0.368718000

Product of the methyl radical addition to benzaldehyde/$B(Me)_3$ complex

SCF Energy = -489.741446534
Zero-point correction = 0.230852
Thermal correction to Energy = 0.243866
Thermal correction to Enthalpy = 0.244810
Thermal correction to Gibbs Free Energy = 0.190479
Sum of electronic and zero-point Energies = -489.510594
Sum of electronic and thermal Energies = -489.497581
Sum of electronic and thermal Enthalpies = -489.496637
Sum of electronic and thermal Free Energies = -489.550967

C	-0.928230000	-0.233685000	0.025956000
C	-1.880341000	-1.088037000	-0.540238000
C	-1.317431000	1.051828000	0.413445000
C	-3.199018000	-0.669433000	-0.712339000
C	-2.635726000	1.473692000	0.238495000
C	-3.580877000	0.615006000	-0.322890000
H	-1.585594000	-2.093716000	-0.854123000
H	-0.576429000	1.725674000	0.846918000
H	-3.930213000	-1.347196000	-1.158773000
H	-2.926103000	2.482141000	0.542446000
H	-4.612357000	0.946948000	-0.460624000
C	0.485606000	-0.732302000	0.256748000
O	1.379784000	0.365229000	0.256195000
H	0.738677000	-1.422285000	-0.565448000
B	2.639914000	0.341448000	-0.263197000
C	0.604453000	-1.480996000	1.580943000
H	0.366807000	-0.806417000	2.416991000
H	-0.093453000	-2.329891000	1.608144000
H	1.626713000	-1.864513000	1.716129000
C	3.480341000	1.671547000	-0.132961000
H	3.848806000	1.989469000	-1.123113000
H	2.922769000	2.502972000	0.322277000
H	4.382323000	1.479741000	0.474103000
C	3.224908000	-0.949983000	-0.973388000
H	4.290206000	-0.842057000	-1.222664000
H	3.105398000	-1.858804000	-0.361111000
H	2.682490000	-1.136954000	-1.917352000

Product of the methyl radical addition to acetaldehyde/BF_2Me complex

SCF Energy = -418.047284590
Zero-point correction = 0.109414
Thermal correction to Energy = 0.117319
Thermal correction to Enthalpy = 0.118263
Thermal correction to Gibbs Free Energy = 0.076479
Sum of electronic and zero-point Energies = -417.937871
Sum of electronic and thermal Energies = -417.929966
Sum of electronic and thermal Enthalpies = -417.929022
Sum of electronic and thermal Free Energies = -417.970806

C	-1.118781000	0.068465000	-0.252712000
O	0.072292000	-0.565038000	0.241106000

H	-0.905704000	0.469755000	-1.257340000
B	1.295527000	-0.102641000	-0.016603000
F	1.525190000	0.964716000	-0.778565000
F	2.351328000	-0.721806000	0.497499000
C	-2.189471000	-1.000260000	-0.357427000
H	-2.407134000	-1.424444000	0.634447000
H	-3.115789000	-0.570493000	-0.764204000
H	-1.861651000	-1.812738000	-1.021076000
C	-1.500608000	1.211753000	0.672633000
H	-1.679445000	0.836248000	1.691565000
H	-0.703708000	1.968605000	0.710668000
H	-2.418039000	1.700631000	0.314740000

Product of the methyl radical addition to acetophenone/BF_2Me complex

SCF Energy = -648.859716525
Zero-point correction = 0.191173
Thermal correction to Energy = 0.203241
Thermal correction to Enthalpy = 0.204185
Thermal correction to Gibbs Free Energy = 0.152368
Sum of electronic and zero-point Energies = -648.668543
Sum of electronic and thermal Energies = -648.656476
Sum of electronic and thermal Enthalpies = -648.655531
Sum of electronic and thermal Free Energies = -648.707349

C	-0.691368000	0.384362000	-0.105921000
C	-1.647139000	0.751759000	0.845255000
C	-1.008911000	-0.634906000	-1.013971000
C	-2.888398000	0.114724000	0.890854000
C	-2.244660000	-1.275399000	-0.966553000
C	-3.191550000	-0.901752000	-0.012173000
H	-1.434112000	1.540637000	1.567880000
H	-0.277513000	-0.934637000	-1.768299000
H	-3.620360000	0.415302000	1.643764000
H	-2.469691000	-2.070542000	-1.680790000
H	-4.161314000	-1.402456000	0.027089000
C	0.661146000	1.091942000	-0.219254000
O	1.678494000	0.119774000	-0.540925000
B	1.980636000	-0.948300000	0.201884000
F	1.391830000	-1.248519000	1.355427000
F	2.932010000	-1.772911000	-0.222232000
C	0.638004000	2.051280000	-1.409006000
H	0.411676000	1.507235000	-2.336659000
H	-0.132470000	2.820167000	-1.259064000
H	1.615876000	2.542771000	-1.517750000
C	1.079688000	1.831416000	1.050050000
H	0.432640000	2.700244000	1.230522000
H	1.040891000	1.177249000	1.931451000
H	2.107820000	2.199659000	0.925404000

Product of the methyl radical addition to acetone/BF_2Me complex

SCF Energy = -457.326182353
Zero-point correction = 0.137027
Thermal correction to Energy = 0.146162
Thermal correction to Enthalpy = 0.147106
Thermal correction to Gibbs Free Energy = 0.103220
Sum of electronic and zero-point Energies = -457.189155
Sum of electronic and thermal Energies = -457.180020
Sum of electronic and thermal Enthalpies = -457.179076
Sum of electronic and thermal Free Energies = -457.222963

C	-1.040951000	-0.043562000	0.000020000
O	0.242937000	-0.711637000	0.001175000
B	1.445684000	-0.141589000	0.000282000
F	1.660270000	1.174393000	-0.000297000
F	2.525590000	-0.917658000	0.000337000
C	-2.066883000	-1.171131000	0.001700000
H	-1.943861000	-1.799784000	0.895461000
H	-3.086589000	-0.760729000	-0.000152000
H	-1.942215000	-1.803774000	-0.889024000
C	-1.166584000	0.806026000	1.263040000
H	-1.015693000	0.184130000	2.157734000
H	-0.429337000	1.620719000	1.270035000
H	-2.170033000	1.251788000	1.318023000
C	-1.166159000	0.801626000	-1.265903000
H	-2.169201000	1.248160000	-1.322087000
H	-0.428168000	1.615645000	-1.275809000
H	-1.016095000	0.176524000	-2.158493000

Product of the ethyl radical addition to benzaldehyde/BF_2Me complex

SCF Energy = -648.858209411
Zero-point correction = 0.191890
Thermal correction to Energy = 0.204222
Thermal correction to Enthalpy = 0.205166
Thermal correction to Gibbs Free Energy = 0.151085
Sum of electronic and zero-point Energies = -648.666320
Sum of electronic and thermal Energies = -648.653987
Sum of electronic and thermal Enthalpies = -648.653043
Sum of electronic and thermal Free Energies = -648.707125

C	-0.801494000	0.298826000	0.084620000
C	-1.729235000	0.576180000	1.092827000
C	-1.234037000	-0.340264000	-1.081804000
C	-3.069620000	0.224808000	0.938307000
C	-2.573293000	-0.697385000	-1.235001000
C	-3.494881000	-0.414161000	-0.226701000
H	-1.398480000	1.068595000	2.011511000
H	-0.515068000	-0.564213000	-1.873068000
H	-3.783677000	0.444134000	1.735152000
H	-2.898927000	-1.199470000	-2.148777000
H	-4.543459000	-0.694989000	-0.346921000
C	0.639601000	0.738270000	0.241892000
O	1.521070000	-0.185311000	-0.399720000
H	0.883435000	0.771902000	1.317510000
B	1.840772000	-1.359954000	0.151970000
F	1.413641000	-1.734309000	1.353125000
F	2.626463000	-2.196876000	-0.511308000
C	0.891201000	2.116772000	-0.361344000
H	0.649028000	2.069708000	-1.436067000
H	0.168667000	2.812450000	0.093341000
C	2.314720000	2.616332000	-0.152350000
H	2.555273000	2.689489000	0.919916000
H	3.042881000	1.936125000	-0.617039000
H	2.449207000	3.612931000	-0.596675000

Product of the *iso*-propyl radical addition to benzaldehyde/BF_2Me complex

SCF Energy = -688.135344696
Zero-point correction = 0.219887
Thermal correction to Energy = 0.233571
Thermal correction to Enthalpy = 0.234515
Thermal correction to Gibbs Free Energy = 0.177703
Sum of electronic and zero-point Energies = -687.915458
Sum of electronic and thermal Energies = -687.901774
Sum of electronic and thermal Enthalpies = -687.900830

Sum of electronic and thermal Free Energies = -687.957641

C	-0.787624000	0.102215000	0.065702000
C	-1.652589000	0.111782000	1.162333000
C	-1.288165000	-0.248559000	-1.193508000
C	-3.000609000	-0.211715000	1.005174000
C	-2.632864000	-0.577249000	-1.351727000
C	-3.493488000	-0.556740000	-0.252583000
H	-1.267695000	0.374645000	2.151161000
H	-0.616353000	-0.270958000	-2.055064000
H	-3.666331000	-0.200288000	1.870929000
H	-3.012422000	-0.851279000	-2.338590000
H	-4.547534000	-0.814489000	-0.376899000
C	0.667427000	0.486895000	0.227494000
O	1.496130000	-0.478585000	-0.427068000
H	0.913597000	0.497501000	1.303743000
B	1.734975000	-1.681268000	0.103340000
F	1.281817000	-2.047729000	1.297756000
F	2.464403000	-2.557516000	-0.573790000
C	1.010572000	1.864291000	-0.356680000
H	0.800691000	1.809055000	-1.439695000
C	2.493770000	2.178323000	-0.165257000
H	2.743197000	2.238443000	0.907157000
H	3.130070000	1.408179000	-0.621758000
H	2.745784000	3.146371000	-0.623064000
C	0.131081000	2.954208000	0.253535000
H	-0.936119000	2.785786000	0.049860000
H	0.264676000	3.001389000	1.347132000
H	0.403486000	3.937159000	-0.157653000

Product of the *tert*-butyl radical addition to benzaldehyde/BF_2Me complex

SCF Energy = -727.412232413
Zero-point correction = 0.247992
Thermal correction to Energy = 0.262817
Thermal correction to Enthalpy = 0.263761
Thermal correction to Gibbs Free Energy = 0.205175
Sum of electronic and zero-point Energies = -727.164240
Sum of electronic and thermal Energies = -727.149416
Sum of electronic and thermal Enthalpies = -727.148471
Sum of electronic and thermal Free Energies = -727.207057

C	0.875545000	0.022332000	-0.143579000
C	1.791986000	0.296268000	-1.163831000
C	1.350687000	-0.473559000	1.075618000
C	3.157837000	0.099788000	-0.965604000
C	2.715799000	-0.676016000	1.274256000
C	3.624000000	-0.385554000	0.256148000
H	1.432235000	0.664655000	-2.127951000
H	0.644245000	-0.708815000	1.873996000
H	3.860030000	0.318107000	-1.773138000
H	3.071717000	-1.064300000	2.231112000
H	4.693173000	-0.545161000	0.411802000
C	-0.603436000	0.267704000	-0.366773000
O	-1.366083000	-0.718411000	0.329189000
H	-0.804517000	0.172402000	-1.447414000
B	-1.531463000	-1.955325000	-0.146646000
F	-1.051852000	-2.348361000	-1.321940000
F	-2.211548000	-2.840998000	0.568460000
C	-1.121549000	1.664791000	0.067446000
C	-2.614628000	1.744132000	-0.283376000
H	-2.777821000	1.581884000	-1.360955000
H	-3.195415000	0.991657000	0.268269000
H	-3.013136000	2.737799000	-0.028157000
C	-0.365614000	2.748896000	-0.709900000
H	0.703701000	2.767124000	-0.452718000
H	-0.453803000	2.600972000	-1.798309000
H	-0.785379000	3.737958000	-0.471979000
C	-0.934551000	1.881216000	1.573298000
H	-1.432686000	1.090333000	2.153033000
H	0.129792000	1.896695000	1.851643000
H	-1.372009000	2.846845000	1.869590000

Product of the benzaldehyde/$BCl_2(O_2Me)$ complex rearrangement

SCF Energy = -1330.17796611
Zero-point correction = 0.160147
Thermal correction to Energy = 0.171748
Thermal correction to Enthalpy = 0.172692
Thermal correction to Gibbs Free Energy = 0.119811
Sum of electronic and zero-point Energies = -1330.017819
Sum of electronic and thermal Energies = -1330.006218
Sum of electronic and thermal Enthalpies = -1330.005274
Sum of electronic and thermal Free Energies = -1330.058155

C	-1.225086000	0.438378000	0.153892000
C	-2.116929000	-0.111952000	1.077515000
C	-1.446486000	0.237232000	-1.212910000
C	-3.220388000	-0.846976000	0.644102000
C	-2.544657000	-0.503106000	-1.646840000
C	-3.435932000	-1.044870000	-0.719329000
H	-1.943889000	0.030109000	2.147662000
H	-0.749506000	0.657072000	-1.942297000
H	-3.909492000	-1.274018000	1.375957000
H	-2.706147000	-0.657923000	-2.715910000
H	-4.296114000	-1.625303000	-1.059942000
C	-0.057520000	1.276250000	0.632845000
O	1.119644000	0.970072000	-0.129233000
H	0.141407000	1.035299000	1.688973000
B	1.880730000	-0.107917000	0.024161000
C	-0.309876000	2.767216000	0.492603000
H	-0.496242000	3.028139000	-0.559415000
H	-1.191102000	3.051450000	1.083889000
H	0.557296000	3.338113000	0.853515000
Cl	3.252949000	-0.324666000	-1.072324000
Cl	1.592594000	-1.326920000	1.278757000

Synglet oxygen

SCF Energy = -150.093247741
Zero-point correction = 0.004013
Thermal correction to Energy = 0.006375
Thermal correction to Enthalpy = 0.007319
Thermal correction to Gibbs Free Energy = -0.014892
Sum of electronic and zero-point Energies = -150.089235
Sum of electronic and thermal Energies = -150.086873
Sum of electronic and thermal Enthalpies = -150.085929
Sum of electronic and thermal Free Energies = -150.108139

O	0.000000000	0.000000000	0.595397000
O	0.000000000	0.000000000	-0.595397000

Methyl radical

SCF Energy = -39.7929753480
Zero-point correction = 0.029506
Thermal correction to Energy = 0.032608
Thermal correction to Enthalpy = 0.033552
Thermal correction to Gibbs Free Energy = 0.009662
Sum of electronic and zero-point Energies = -39.763470

Sum of electronic and thermal Energies = -39.760367
Sum of electronic and thermal Enthalpies = -39.759423
Sum of electronic and thermal Free Energies = -39.783313

C	-0.000076000	-0.000029000	-0.000118000
H	0.463536000	0.987426000	0.000235000
H	0.624094000	-0.894670000	0.000235000
H	-1.087174000	-0.092580000	0.000235000

Ethyl radical

SCF Energy = -79.0727068688
Zero-point correction = 0.059203
Thermal correction to Energy = 0.063173
Thermal correction to Enthalpy = 0.064117
Thermal correction to Gibbs Free Energy = 0.035073
Sum of electronic and zero-point Energies = -79.013504
Sum of electronic and thermal Energies = -79.009534
Sum of electronic and thermal Enthalpies = -79.008590
Sum of electronic and thermal Free Energies = -79.037634

C	0.011918000	0.793445000	0.000000000
H	-0.071532000	1.352945000	0.935434000
H	-0.071532000	1.352945000	-0.935434000
C	0.011918000	-0.692318000	0.000000000
H	0.508888000	-1.104011000	0.892609000
H	0.508888000	-1.104011000	-0.892609000
H	-1.017726000	-1.104629000	0.000000000

iso-Propyl radical

SCF Energy = -118.353762184
Zero-point correction = 0.087983
Thermal correction to Energy = 0.093160
Thermal correction to Enthalpy = 0.094104
Thermal correction to Gibbs Free Energy = 0.060757
Sum of electronic and zero-point Energies = -118.265779
Sum of electronic and thermal Energies = -118.260602
Sum of electronic and thermal Enthalpies = -118.259658
Sum of electronic and thermal Free Energies = -118.293006

C	0.011931000	0.535518000	0.000000000
H	-0.238042000	1.601621000	0.000000000
C	0.011931000	-0.197377000	1.296577000
C	0.011931000	-0.197377000	-1.296577000
H	0.231708000	0.465017000	-2.146995000
H	0.750703000	-1.017900000	-1.298302000
H	-0.970771000	-0.670216000	-1.502561000
H	0.750703000	-1.017900000	1.298302000
H	-0.970771000	-0.670216000	1.502561000
H	0.231708000	0.465017000	2.146995000

tert-Butyl radical

SCF Energy = -157.635313765
Zero-point correction = 0.116610
Thermal correction to Energy = 0.122973
Thermal correction to Enthalpy = 0.123917
Thermal correction to Gibbs Free Energy = 0.087153
Sum of electronic and zero-point Energies = -157.518704
Sum of electronic and thermal Energies = -157.512341
Sum of electronic and thermal Enthalpies = -157.511397
Sum of electronic and thermal Free Energies = -157.548160

C	0.000000000	-0.000005000	-0.152649000
C	1.286351000	-0.741610000	0.014783000
C	-1.285455000	-0.743162000	0.014783000
H	-2.133253000	-0.201409000	-0.434923000
H	-1.239103000	-1.748148000	-0.435118000
H	-1.537540000	-0.889202000	1.086593000
H	1.241212000	-1.746652000	-0.435118000
H	1.538612000	-0.887346000	1.086593000
H	2.133494000	-0.198834000	-0.434923000
C	-0.000896000	1.484782000	0.014792000
H	-0.894467000	1.947156000	-0.434972000
H	-0.001072000	1.776175000	1.086586000
H	0.892115000	1.948234000	-0.434972000

Tetrafluoroborate anion

Energy = -424.163284284
Zero-point correction = 0.014509
Thermal correction to Energy = 0.018839
Thermal correction to Enthalpy = 0.019783
Thermal correction to Gibbs Free Energy = -0.010723
Sum of electronic and zero-point Energies = -424.148775
Sum of electronic and thermal Energies = -424.144445
Sum of electronic and thermal Enthalpies = -424.143501
Sum of electronic and thermal Free Energies = -424.174007

B	0.000000000	0.000000000	0.000000000
F	0.810590000	0.810590000	0.810590000
F	-0.810590000	-0.810590000	0.810590000
F	-0.810590000	0.810590000	-0.810590000
F	0.810590000	-0.810590000	-0.810590000

iso-Propyltrifluoroborate anion

Energy = -442.779752299
Zero-point correction = 0.105131
Thermal correction to Energy = 0.113194
Thermal correction to Enthalpy = 0.114138
Thermal correction to Gibbs Free Energy = 0.072773
Sum of electronic and zero-point Energies = -442.674621
Sum of electronic and thermal Energies = -442.666559
Sum of electronic and thermal Enthalpies = -442.665615
Sum of electronic and thermal Free Energies = -442.706980

B	0.103805000	-0.688872000	0.000000000
F	-0.264088000	-1.448798000	1.148881000
F	-0.264088000	-1.448798000	-1.148881000
F	1.526588000	-0.577259000	0.000000000
C	-0.609382000	0.774143000	0.000000000
H	-1.704264000	0.601002000	0.000000000
C	-0.264088000	1.569013000	-1.260914000
C	-0.264088000	1.569013000	1.260914000
H	-0.554793000	1.020595000	2.170824000
H	0.824026000	1.743194000	1.323015000
H	-0.756797000	2.558229000	1.292150000
H	0.824026000	1.743194000	-1.323015000
H	-0.756797000	2.558229000	-1.292150000
H	-0.554793000	1.020595000	-2.170824000

Boron trifluoride / diethyl ether complex

Energy = -557.681392814
Zero-point correction = 0.152978
Thermal correction to Energy = 0.163597
Thermal correction to Enthalpy = 0.164542
Thermal correction to Gibbs Free Energy = 0.116455
Sum of electronic and zero-point Energies = -557.528415
Sum of electronic and thermal Energies = -557.517795
Sum of electronic and thermal Enthalpies = -557.516851
Sum of electronic and thermal Free Energies = -557.564938

B	1.195916000	-0.156567000	-0.103353000
O	-0.252735000	-0.054984000	0.586094000

F	1.816827000	1.012983000	0.243550000
F	1.767620000	-1.273002000	0.447856000
F	0.974697000	-0.280466000	-1.451910000
H	-2.796929000	-0.539967000	-0.532070000
C	-0.870412000	1.238807000	0.804771000
C	-1.103157000	2.004777000	-0.478070000
H	-0.195757000	1.779481000	1.478855000
H	-1.807134000	1.038610000	1.341486000
H	-1.749432000	1.453637000	-1.173393000
H	-1.594045000	2.957039000	-0.231037000
H	-0.152646000	2.229478000	-0.978209000
C	-1.092056000	-1.233810000	0.630510000
C	-2.039705000	-1.336571000	-0.542238000
H	-1.621799000	-1.203283000	1.593073000
H	-0.384517000	-2.069336000	0.657592000
H	-1.488259000	-1.298804000	-1.491093000
H	-2.567505000	-2.299003000	-0.482505000

Difluoro(*iso*-propyl)boran / diethyl ether complex

Energy = -576.299767042
Zero-point correction = 0.244777
Thermal correction to Energy = 0.258820
Thermal correction to Enthalpy = 0.259765
Thermal correction to Gibbs Free Energy = 0.204967
Sum of electronic and zero-point Energies = -576.054991
Sum of electronic and thermal Energies = -576.040947
Sum of electronic and thermal Enthalpies = -576.040002
Sum of electronic and thermal Free Energies = -576.094800

B	0.521822000	0.049310000	0.662490000
O	-1.061305000	0.137787000	-0.003444000
F	0.523015000	1.116562000	1.544211000
F	0.475350000	-1.153167000	1.342642000
H	-1.931319000	-1.901306000	-1.548668000
C	-1.676683000	1.440701000	-0.136501000
C	-0.820981000	2.405986000	-0.919883000
H	-1.898355000	1.823685000	0.871169000
H	-2.625073000	1.273971000	-0.664749000
H	-0.543699000	1.984932000	-1.896512000
H	-1.410206000	3.317764000	-1.093117000
H	0.087122000	2.685347000	-0.372814000
C	-1.988817000	-0.913308000	0.373511000
C	-1.788869000	-2.138523000	-0.484749000
H	-2.998563000	-0.504985000	0.239391000
H	-1.845203000	-1.131219000	1.439207000
H	-0.786082000	-2.559624000	-0.342360000
H	-2.528129000	-2.900006000	-0.196877000
C	1.591513000	0.113504000	-0.528315000
H	1.546352000	1.116821000	-0.983013000
C	1.336641000	-0.912902000	-1.633441000
C	2.999109000	-0.054859000	0.062248000
H	3.210578000	0.703070000	0.832658000
H	3.114373000	-1.045497000	0.531984000
H	3.776534000	0.033462000	-0.714913000
H	1.370303000	-1.941230000	-1.236455000
H	2.096498000	-0.846563000	-2.429915000
H	0.349441000	-0.771623000	-2.098813000

Diethyl ether

Energy = -233.422367899
Zero-point correction = 0.137071
Thermal correction to Energy = 0.143862
Thermal correction to Enthalpy = 0.144807
Thermal correction to Gibbs Free Energy = 0.107571
Sum of electronic and zero-point Energies = -233.285297
Sum of electronic and thermal Energies = -233.278506
Sum of electronic and thermal Enthalpies = -233.277561
Sum of electronic and thermal Free Energies = -233.314797

O	0.000000000	0.000000000	0.255102000
H	-0.891543000	2.366096000	1.055112000
C	0.000000000	-1.174577000	-0.512281000
C	0.000000000	-2.373969000	0.410886000
H	0.888836000	-1.199216000	-1.175637000
H	-0.888836000	-1.199216000	-1.175637000
H	-0.891543000	-2.366096000	1.055112000
H	0.000000000	-3.306877000	-0.170988000
H	0.891543000	-2.366096000	1.055112000
C	0.000000000	1.174577000	-0.512281000
C	0.000000000	2.373969000	0.410886000
H	-0.888836000	1.199216000	-1.175637000
H	0.888836000	1.199216000	-1.175637000
H	0.891543000	2.366096000	1.055112000
H	0.000000000	3.306877000	-0.170988000

(Difluoroboryloxy)benzyl radical

Energy = -569.653829369
Zero-point correction = 0.121384
Thermal correction to Energy = 0.130884
Thermal correction to Enthalpy = 0.131829
Thermal correction to Gibbs Free Energy = 0.084333
Sum of electronic and zero-point Energies = -569.532445
Sum of electronic and thermal Energies = -569.522945
Sum of electronic and thermal Enthalpies = -569.522001
Sum of electronic and thermal Free Energies = -569.569496

C	-0.823371000	0.285831000	-0.000075000
C	-1.822997000	1.297664000	-0.000052000
C	-1.242549000	-1.072504000	0.000046000
C	-3.167637000	0.961532000	0.000003000
C	-2.593039000	-1.390352000	0.000104000
C	-3.565090000	-0.382360000	0.000061000
H	-1.520803000	2.348028000	-0.000086000
H	-0.489538000	-1.862143000	0.000092000
H	-3.921332000	1.752211000	-0.000012000
H	-2.898572000	-2.439251000	0.000171000
H	-4.625736000	-0.641423000	0.000093000
C	0.538062000	0.649816000	-0.000160000
O	1.487656000	-0.322790000	-0.000189000
H	0.880586000	1.686796000	-0.000283000
B	2.816330000	-0.090765000	0.000058000
F	3.639613000	-1.121673000	-0.000070000
F	3.321744000	1.132136000	0.000257000

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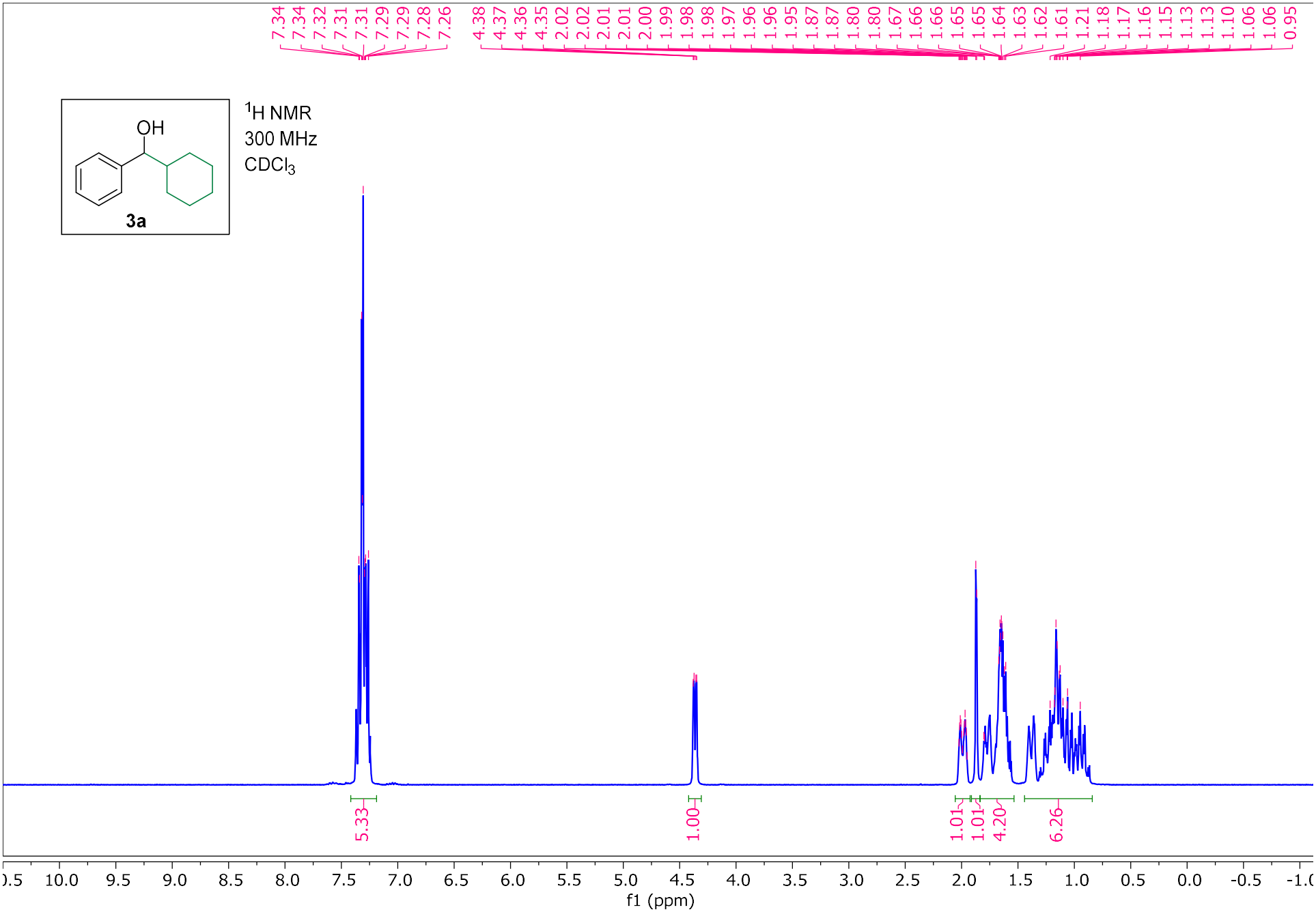
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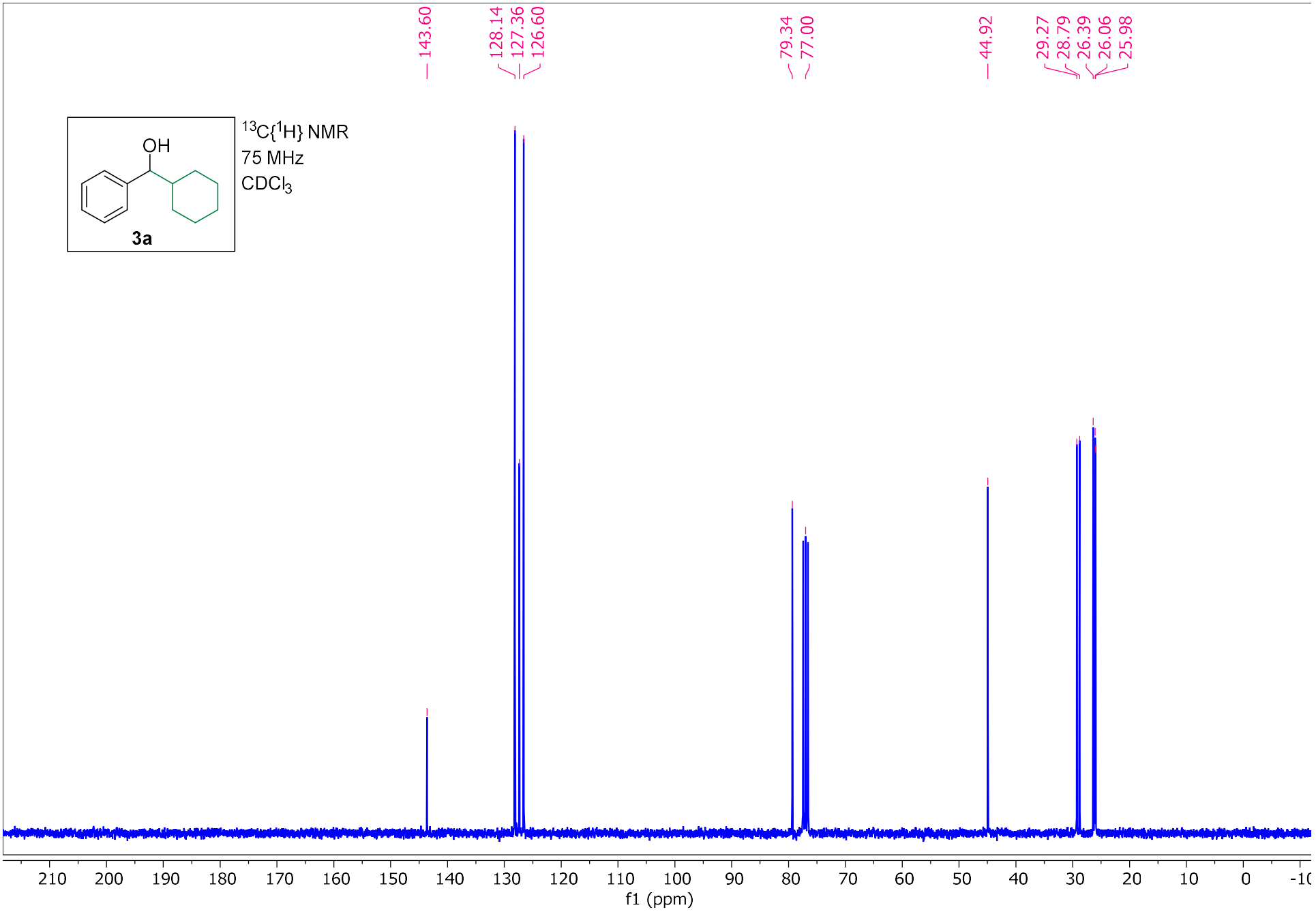
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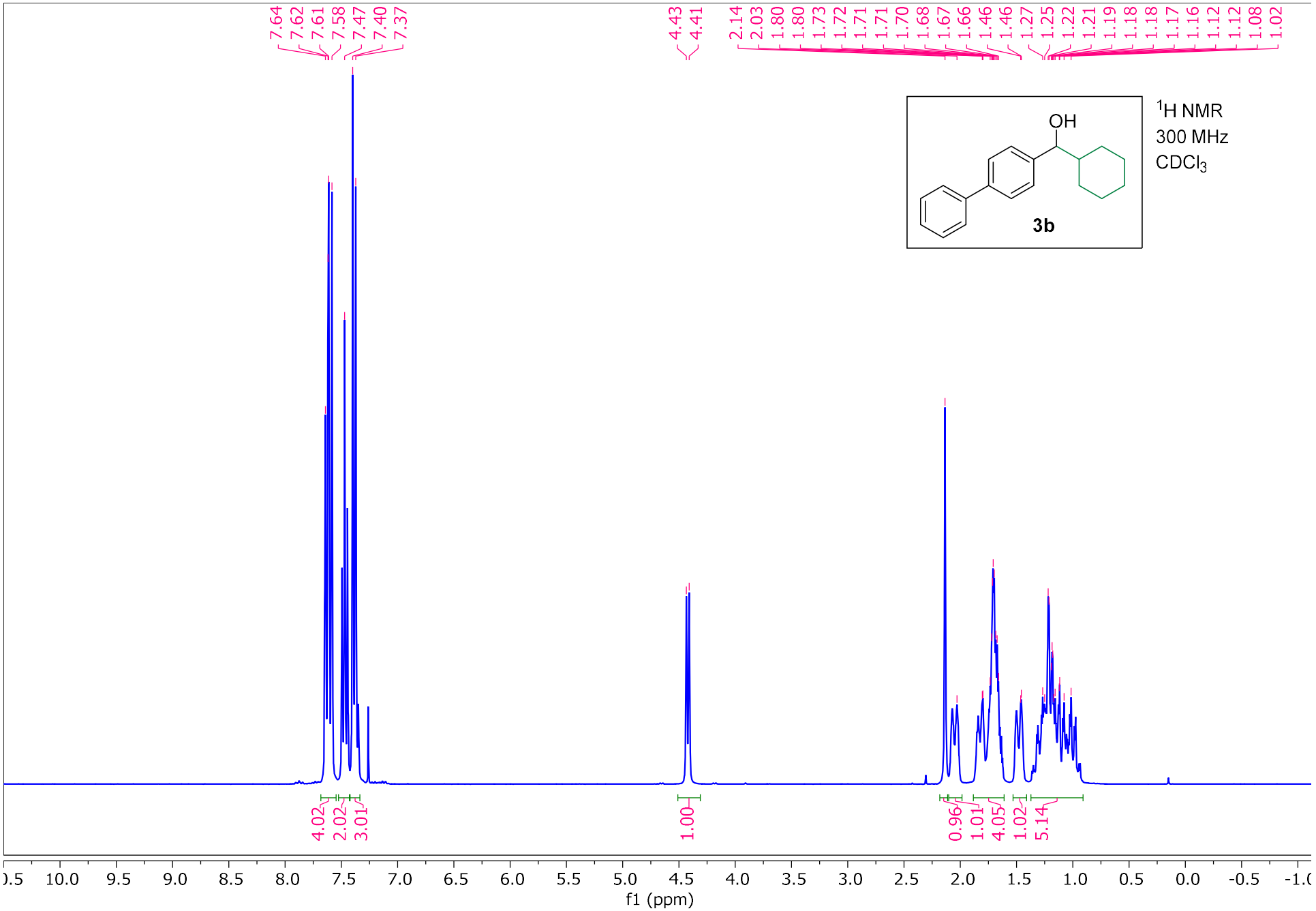
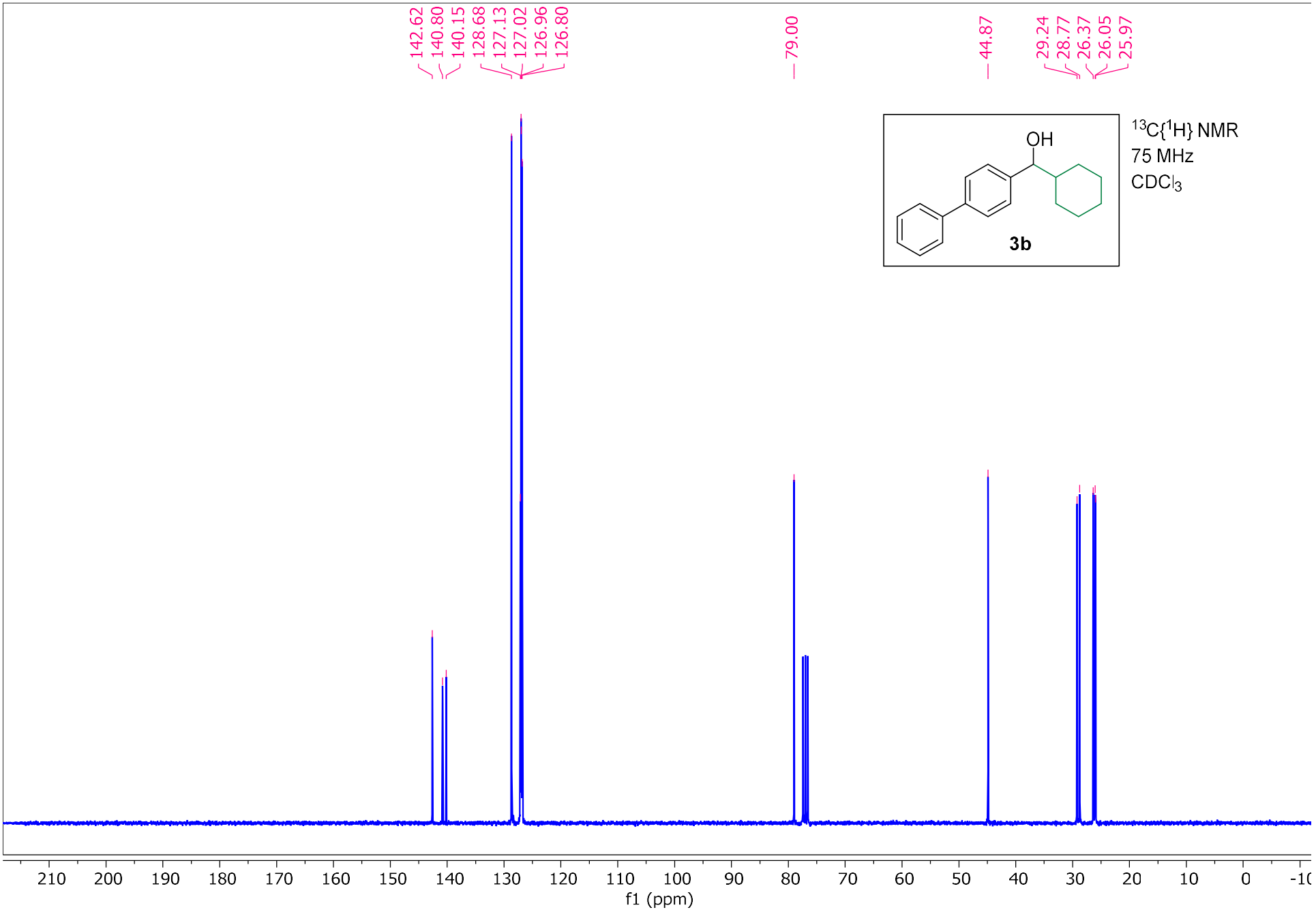
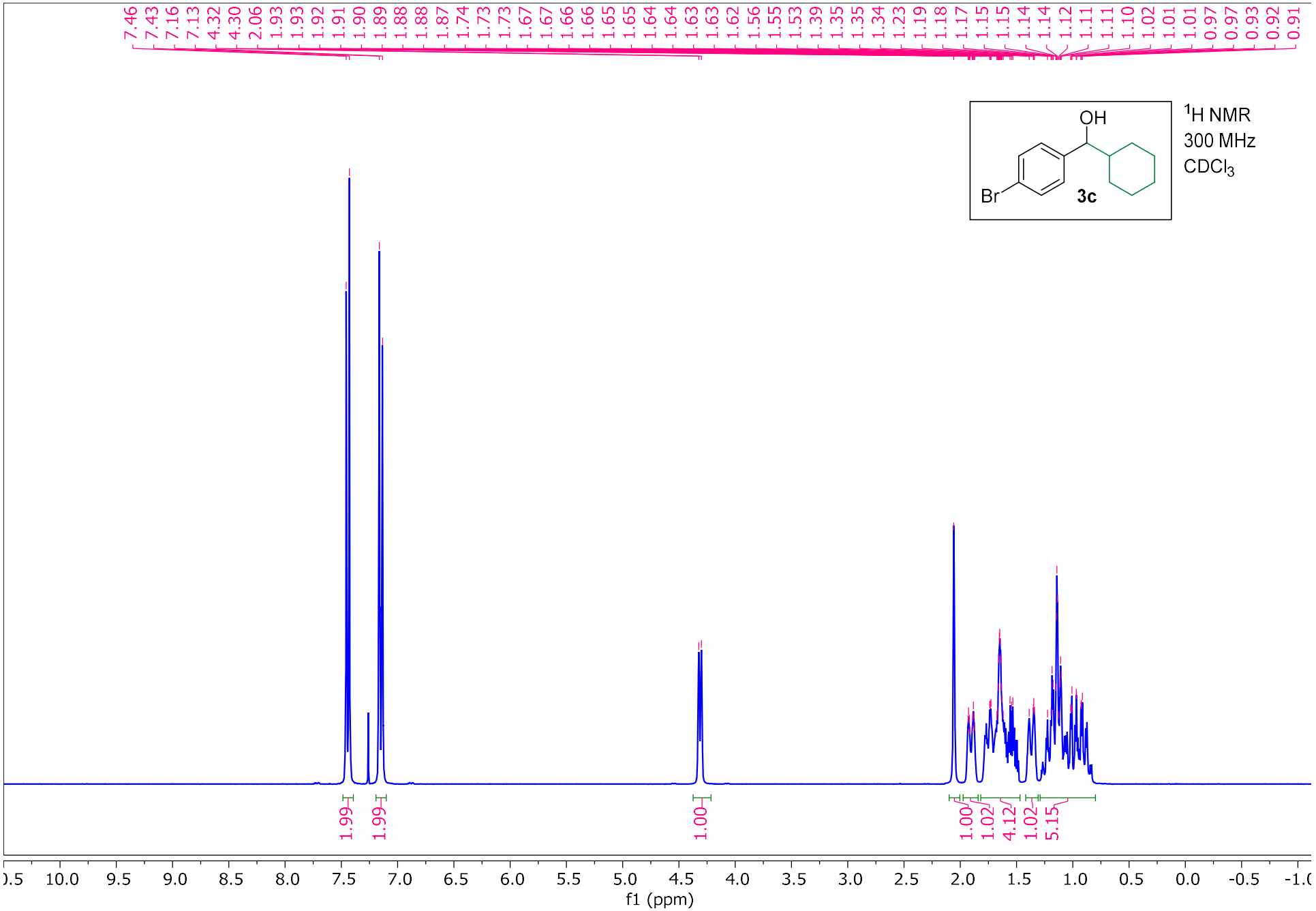
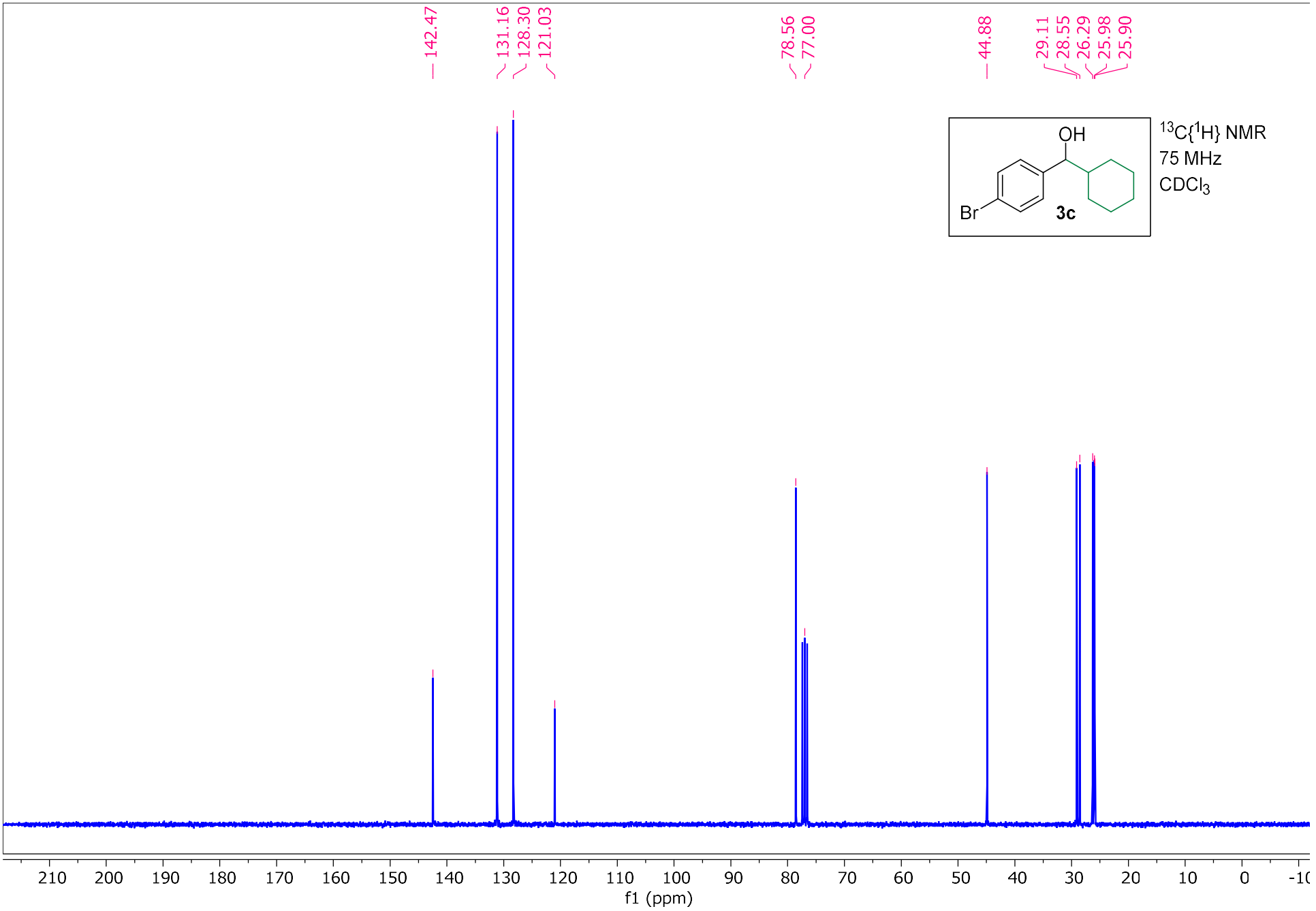
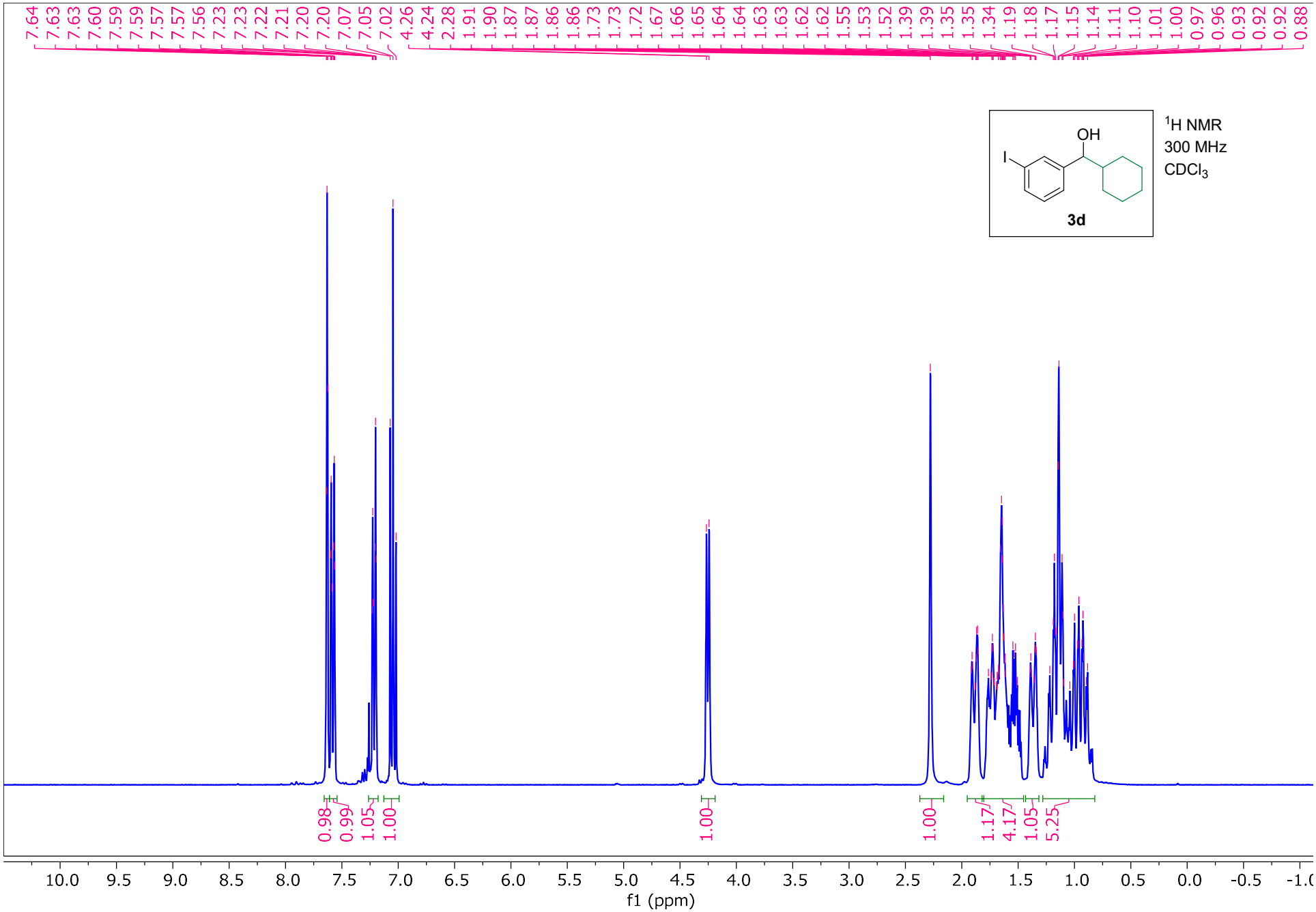
f1 (ppm)

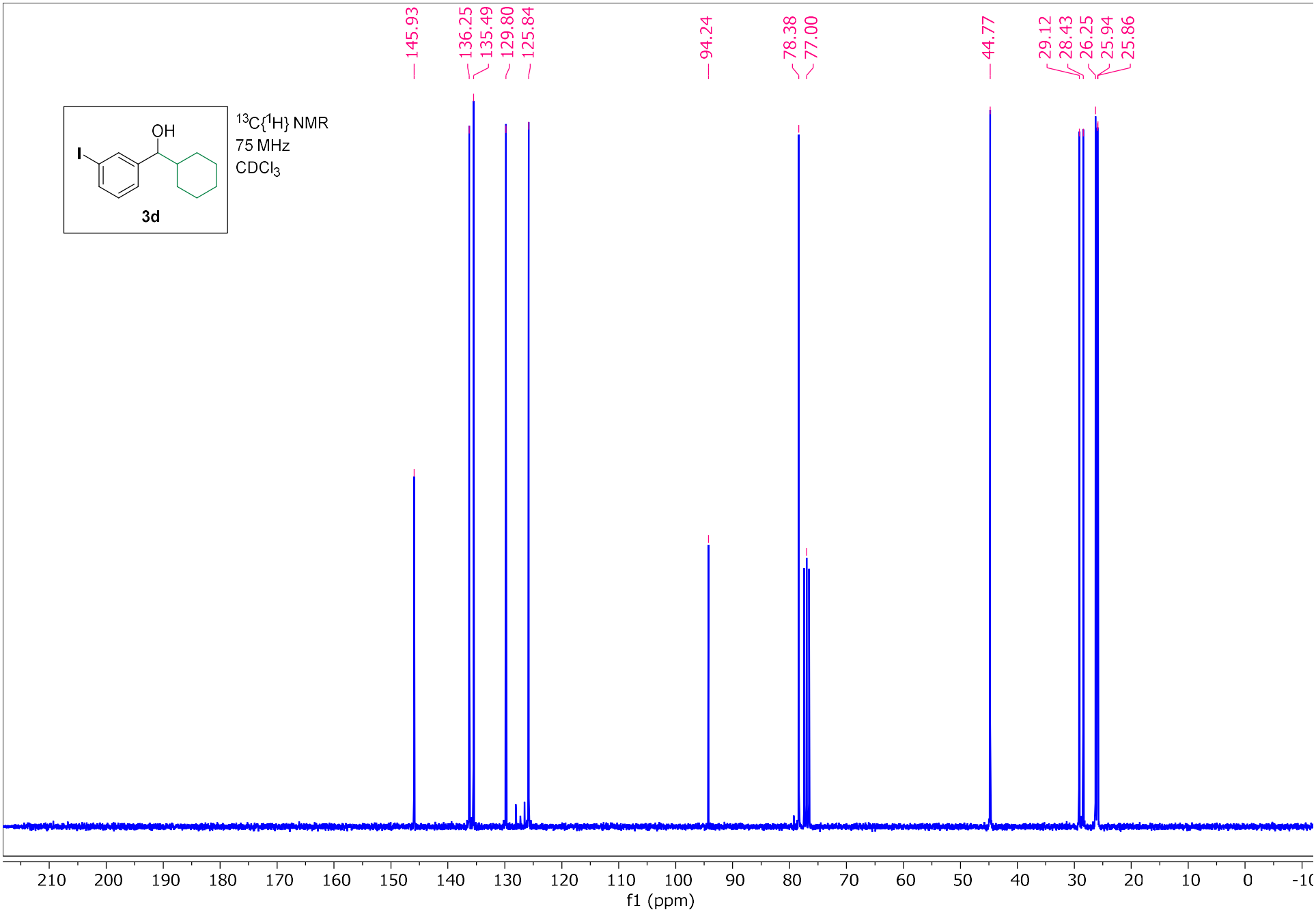

7.64
7.62
7.61
7.58
7.47
7.40
7.37
4.43
4.41
2.14
2.03
1.80
1.80
1.73
1.72
1.71
1.71
1.70
1.68
1.67
1.66
1.46
1.46
1.27
1.25
1.22
1.21
1.19
1.18
1.18
1.17
1.16
1.12
1.12
1.08
1.02
OH
3b
1H NMR
300 MHz
CDCl3
4.02
2.02
3.01
1.00
0.96
1.01
4.05
1.02
5.14
f1 (ppm)

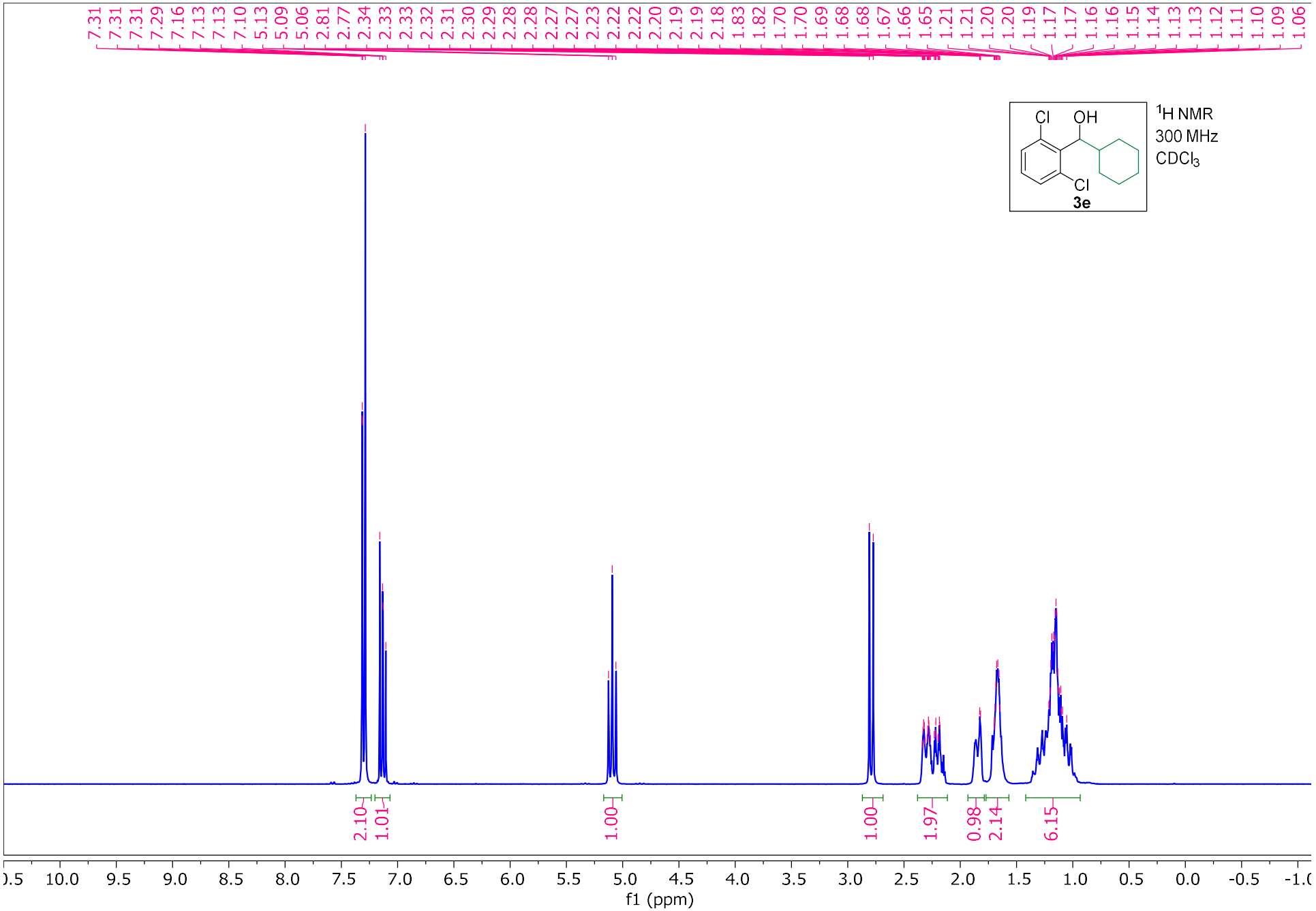

142.62
140.80
140.15
128.68
127.13
127.02
126.96
126.80
79.00
44.87
29.24
28.77
26.37
26.05
25.97
OH
3b
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

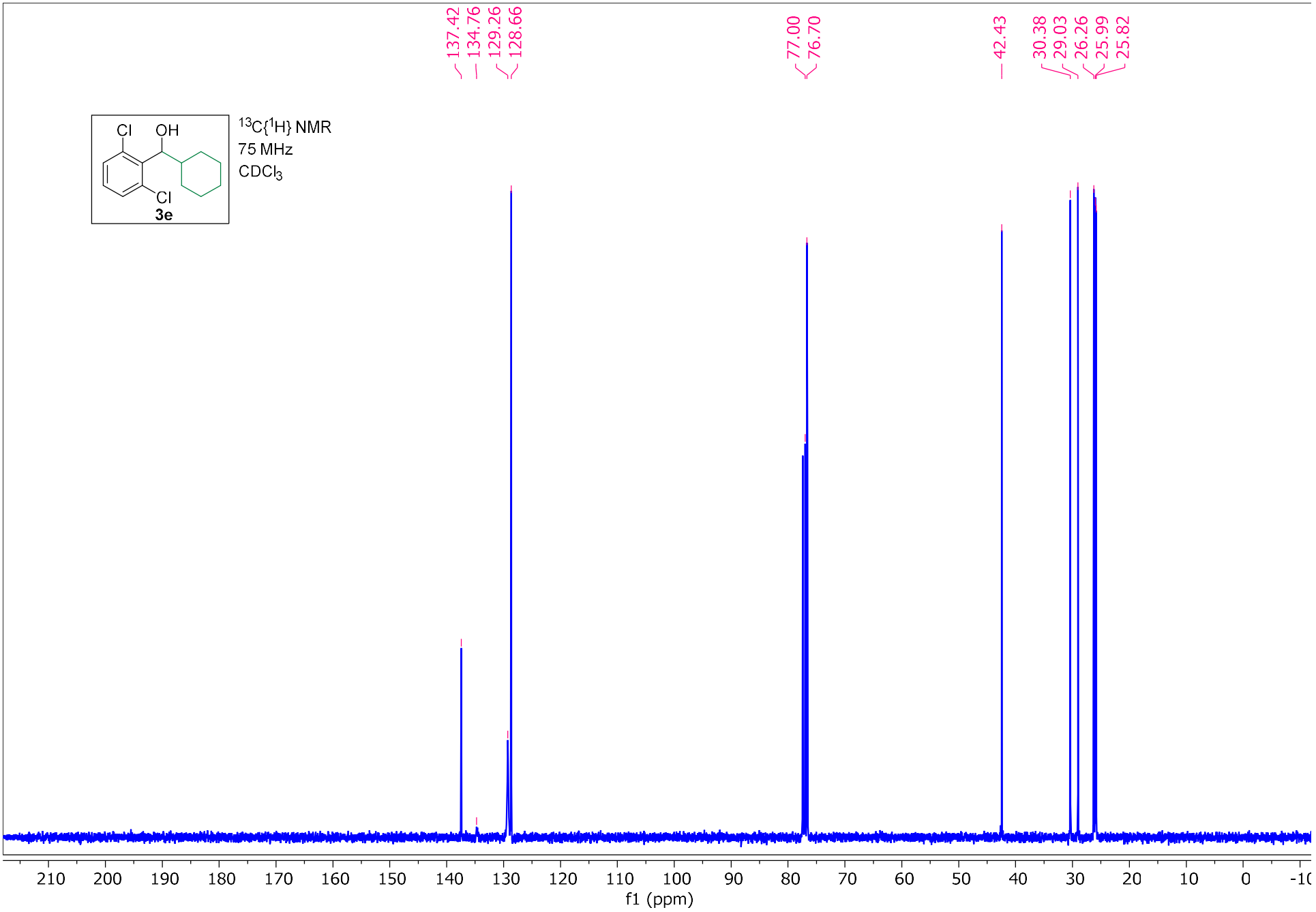

7.46 7.43 7.16 7.13 4.32 4.30 2.06 1.93 1.93 1.92 1.91 1.90 1.89 1.88 1.88 1.87 1.74 1.73 1.73 1.67 1.67 1.66 1.66 1.65 1.65 1.64 1.64 1.63 1.63 1.62 1.56 1.55 1.53 1.39 1.35 1.35 1.34 1.23 1.19 1.18 1.17 1.15 1.15 1.14 1.14 1.12 1.11 1.11 1.10 1.02 1.01 1.01 0.97 0.97 0.93 0.92 0.91
OH
Br
3c
1H NMR
300 MHz
CDCl3
1.99 1.99 1.00 1.00 1.02 4.12 1.02 5.15
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 -0.5
f1 (ppm)

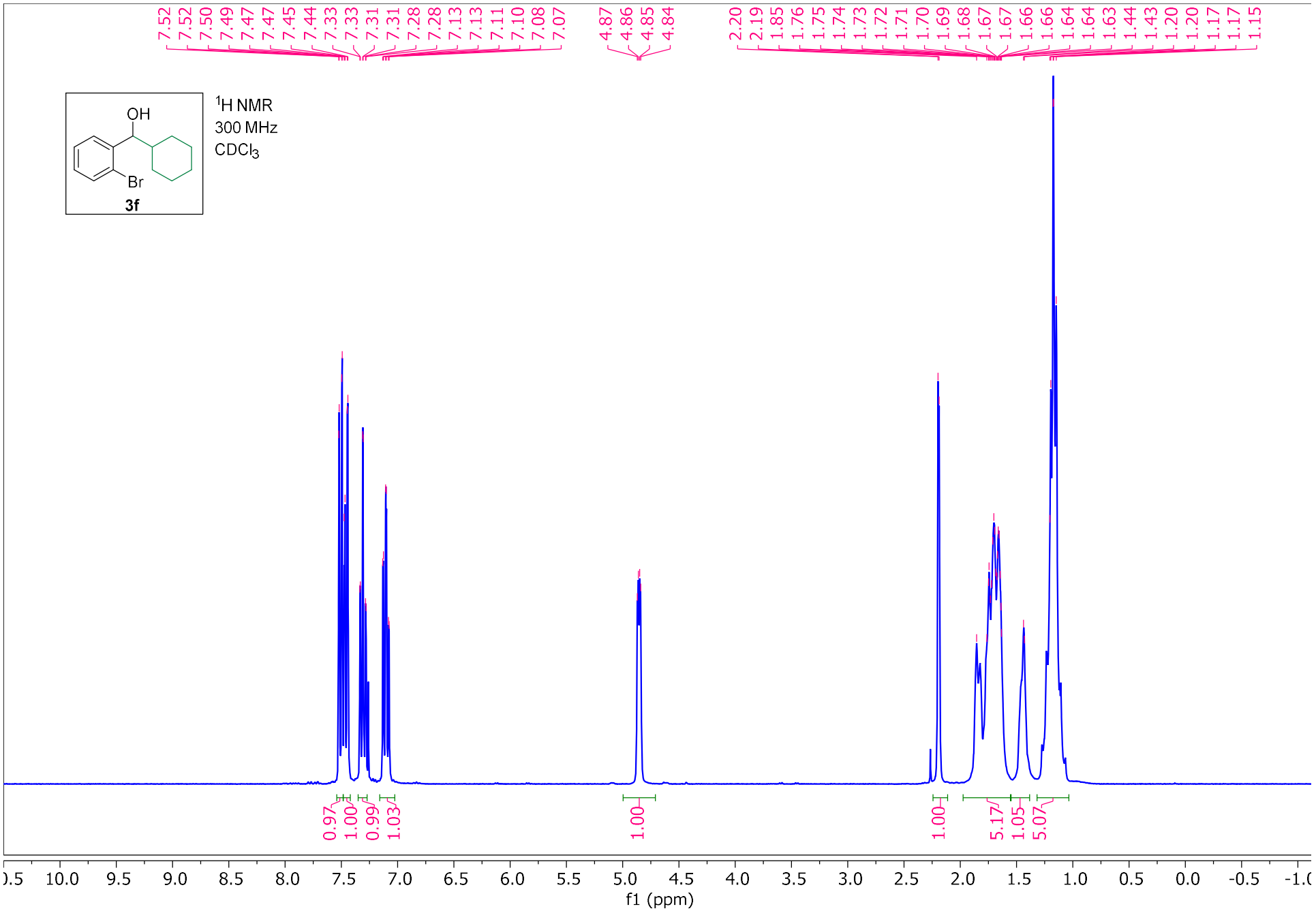

142.47
131.16
128.30
121.03
78.56
77.00
44.88
29.11
28.55
26.29
25.98
25.90
OH
Br
3c
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

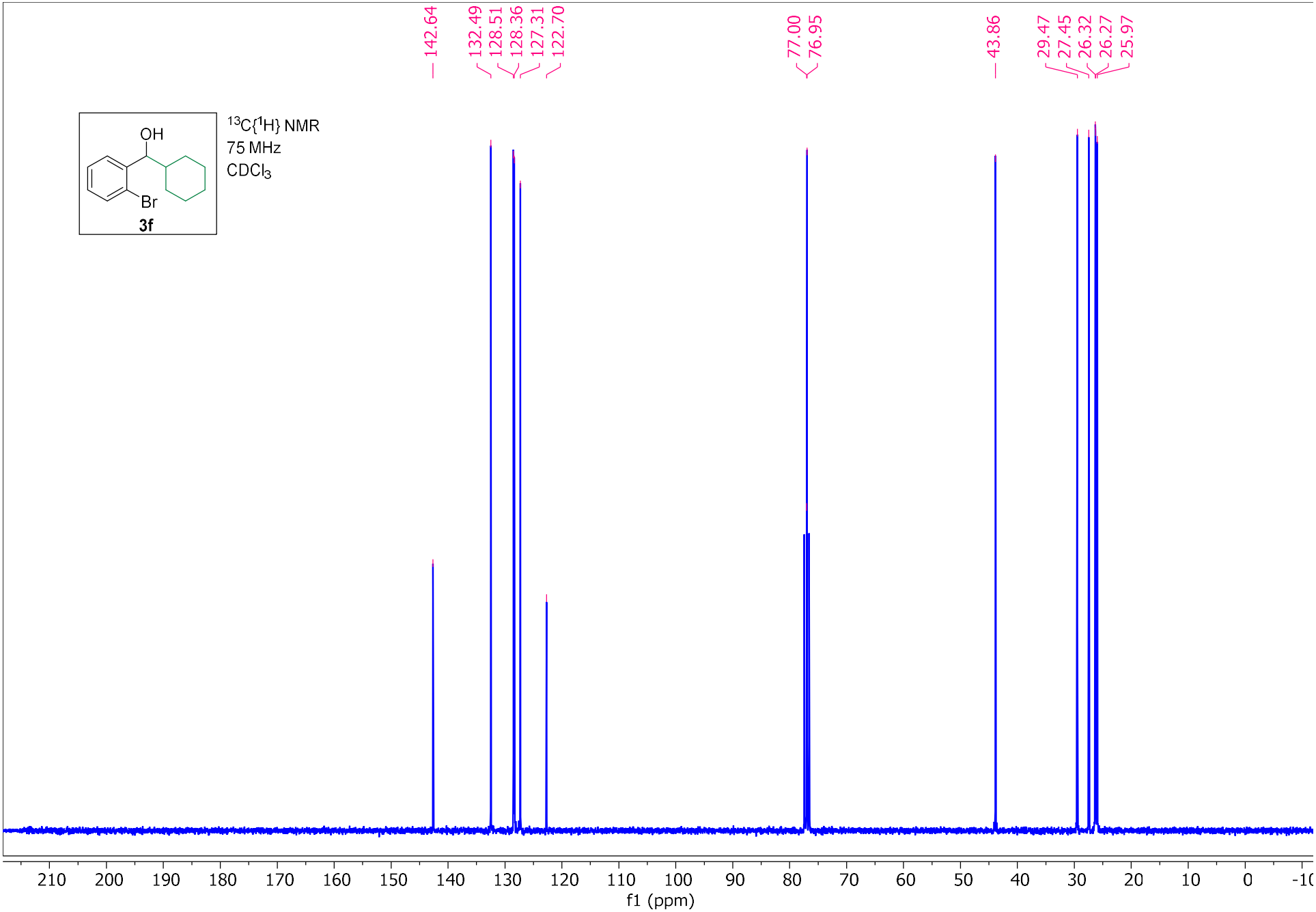

7.64 7.63 7.63 7.60 7.59 7.59 7.57 7.57 7.56 7.23 7.23 7.22 7.21 7.20 7.20 7.07 7.05 7.02 4.26 4.24 2.28 1.91 1.90 1.87 1.87 1.86 1.86 1.73 1.73 1.72 1.67 1.66 1.65 1.64 1.64 1.63 1.63 1.62 1.62 1.55 1.53 1.52 1.39 1.39 1.35 1.35 1.34 1.19 1.18 1.17 1.15 1.14 1.11 1.10 1.01 1.00 0.97 0.96 0.93 0.92 0.92 0.88
OH
I
3d
1H NMR
300 MHz
CDCl3
0.98 0.99 1.05 1.00 1.00 1.00 1.17 4.17 1.05 5.25
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 -0.5
f1 (ppm)

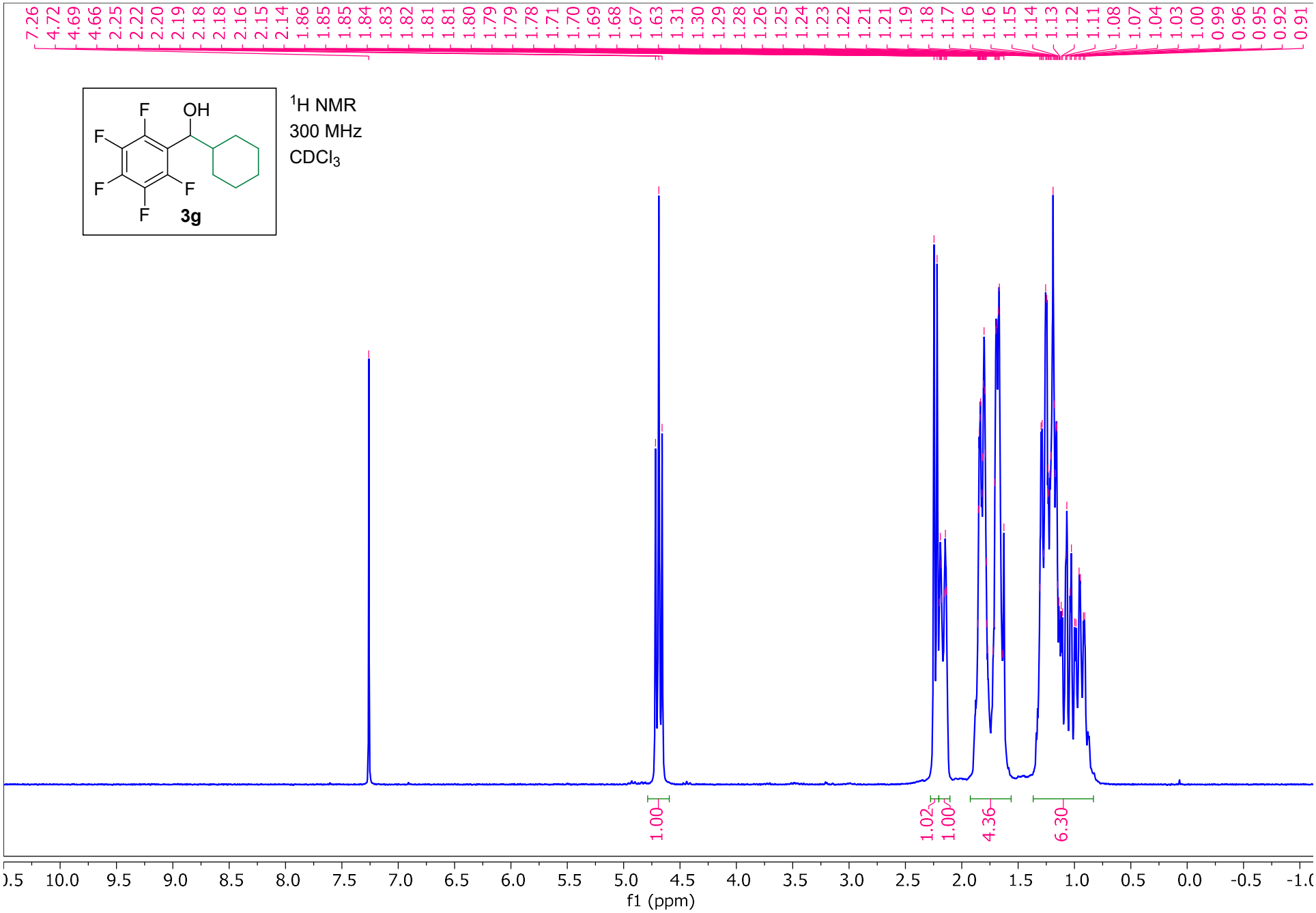

145.93
136.25
135.49
129.80
125.84
94.24
78.38
77.00
44.77
29.12
28.43
26.25
25.94
25.86
OH
I
3d
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

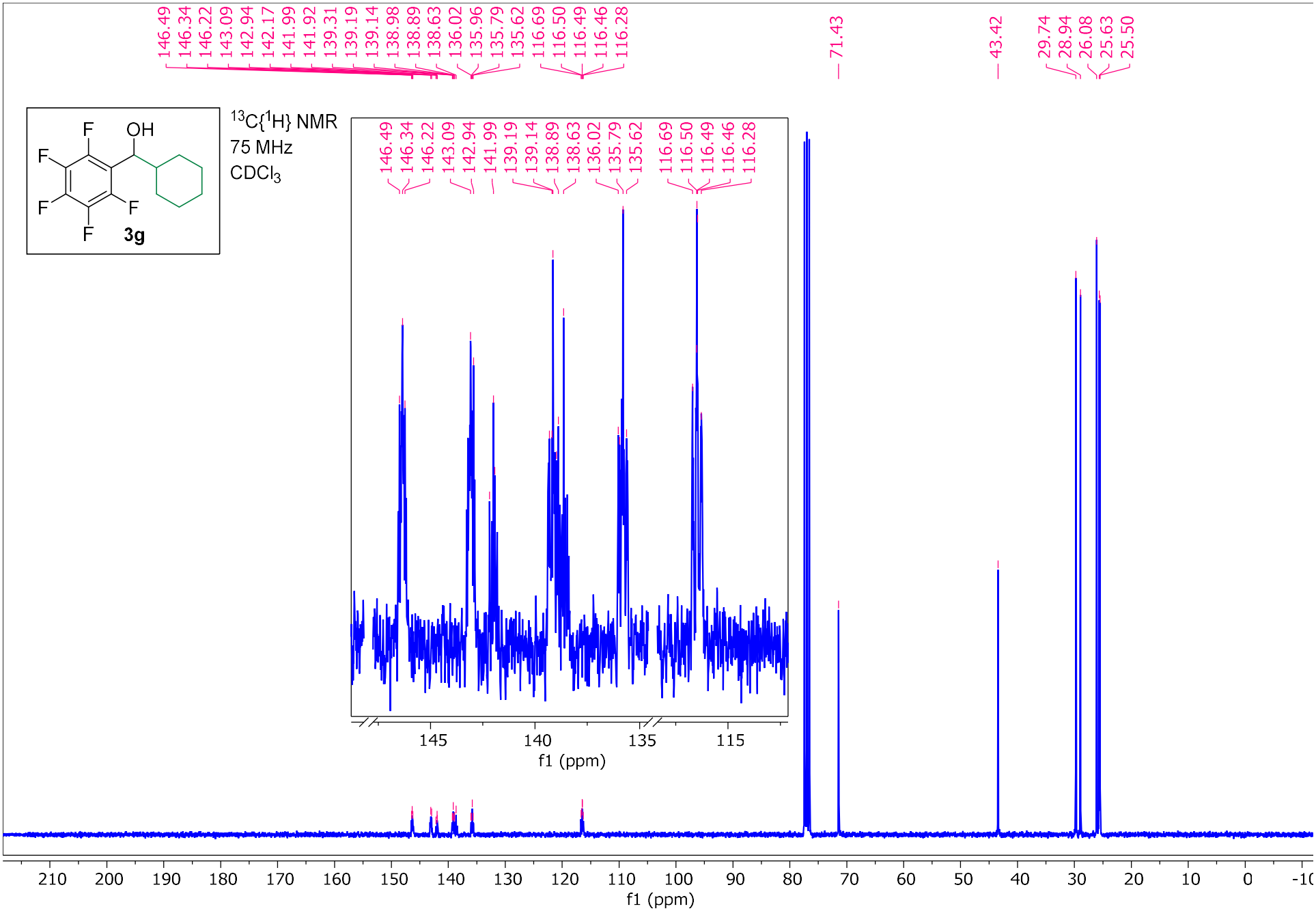

7.31 7.31 7.31 7.29 7.16 7.13 7.13 7.10 5.13 5.09 5.06 2.81 2.77 2.34 2.33 2.33 2.32 2.31 2.30 2.29 2.28 2.28 2.27 2.27 2.23 2.22 2.22 2.20 2.19 2.19 2.18 1.83 1.82 1.70 1.70 1.69 1.68 1.68 1.67 1.66 1.65 1.21 1.21 1.20 1.20 1.19 1.17 1.17 1.16 1.16 1.15 1.14 1.13 1.13 1.12 1.11 1.10 1.09 1.06
Cl
OH
Cl
3e
1H NMR
300 MHz
CDCl3
2.10
1.01
1.00
1.00
1.97
0.98
2.14
6.15
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 -0.5
f1 (ppm)

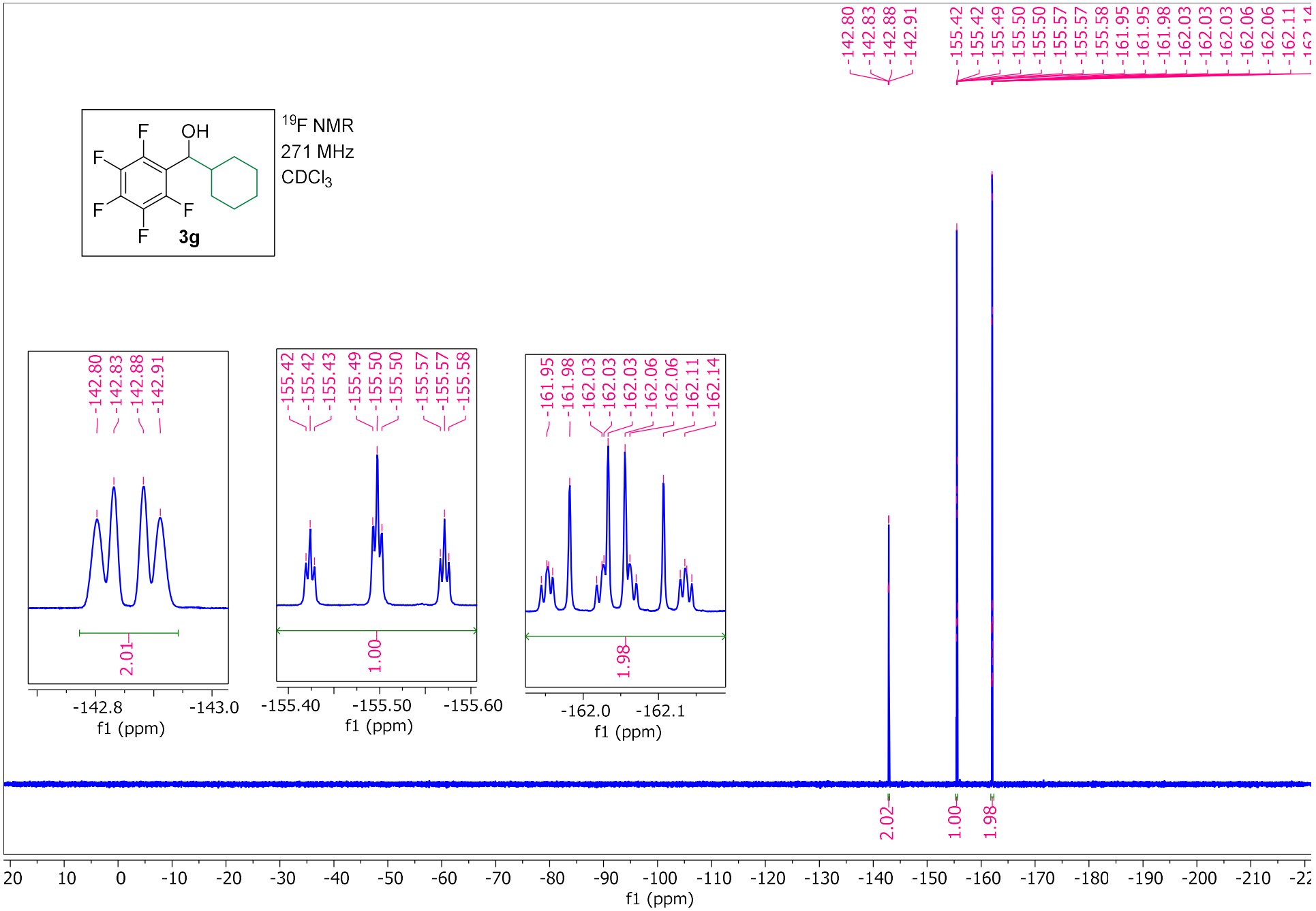

137.42
134.76
129.26
128.66
77.00
76.70
42.43
30.38
29.03
26.26
25.99
25.82
Cl
OH
Cl
3e
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

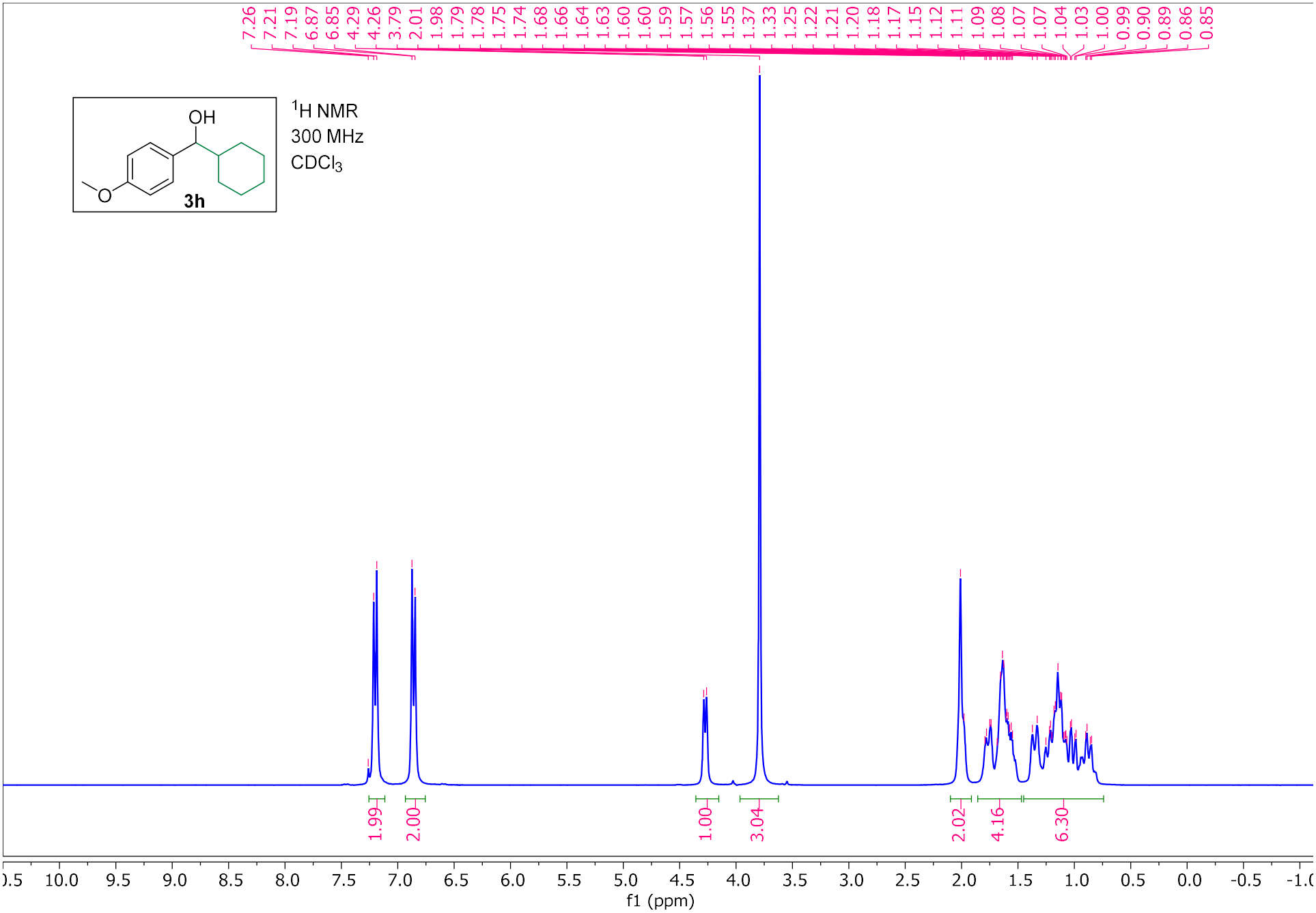

7.52 7.52 7.50 7.49 7.47 7.47 7.45 7.44 7.33 7.33 7.31 7.31 7.28 7.28 7.13 7.13 7.11 7.10 7.08 7.07
4.87 4.86 4.85 4.84
2.20 2.19 1.85 1.76 1.75 1.74 1.73 1.72 1.71 1.70 1.69 1.68 1.67 1.67 1.66 1.66 1.64 1.64 1.63 1.44 1.43 1.20 1.20 1.17 1.17 1.15
OH
Br
3f
1H NMR
300 MHz
CDCl3
0.97 1.00 0.99 1.03
1.00
1.00 5.17 1.05 5.07
f1 (ppm)

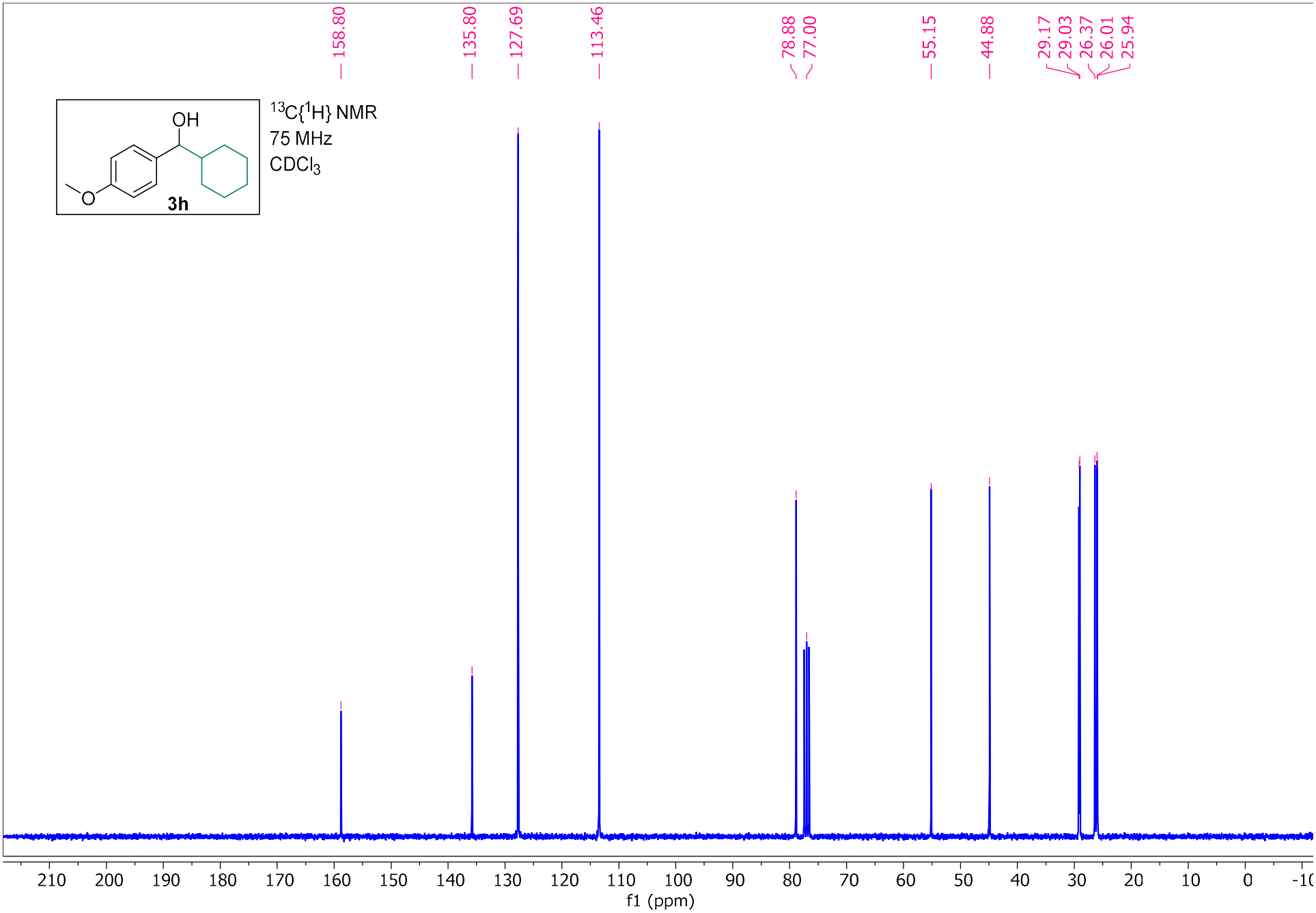

142.64
132.49
128.51
128.36
127.31
122.70
77.00
76.95
43.86
29.47
27.45
26.32
26.27
25.97
OH
Br
3f
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

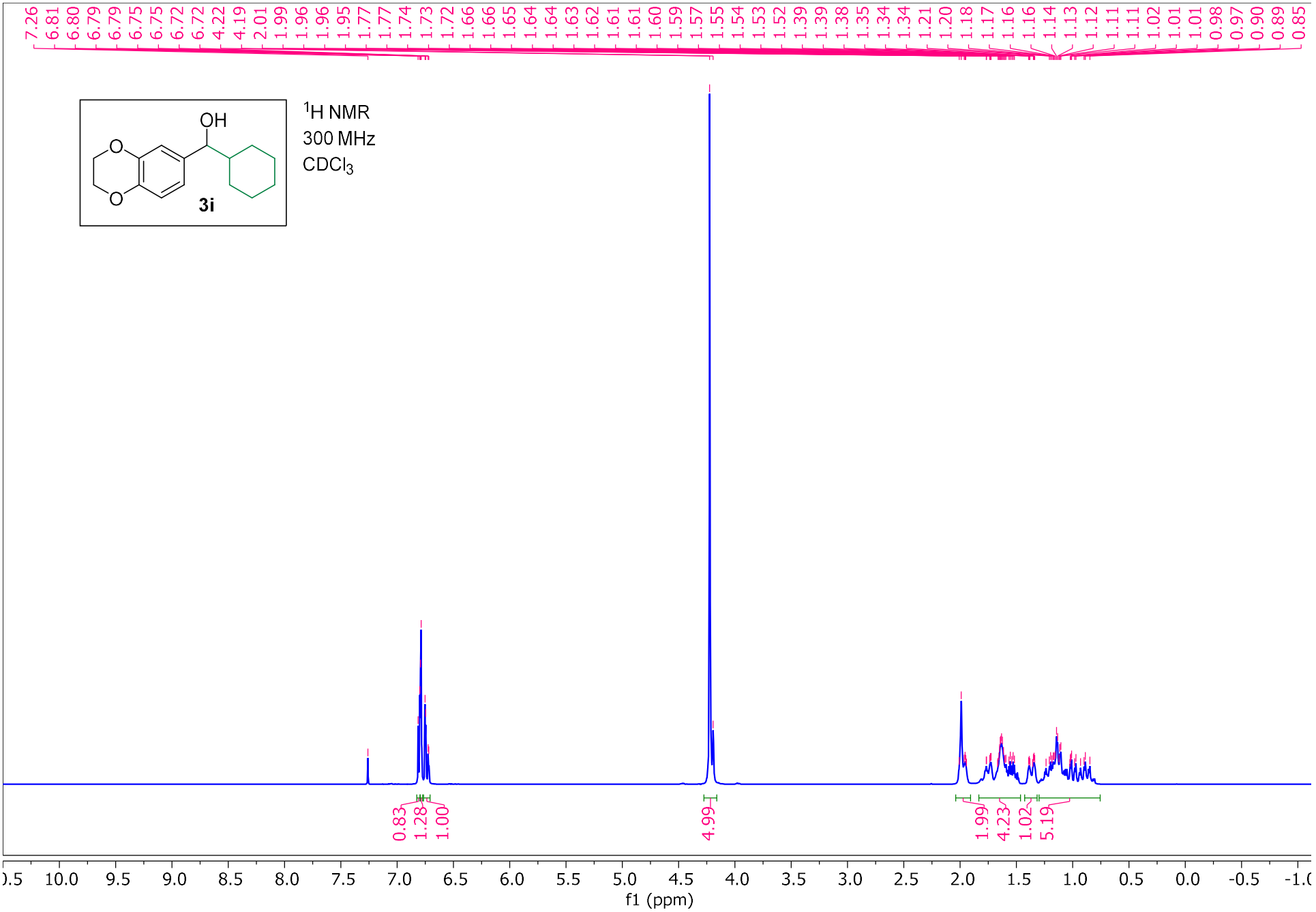

7.26 4.72 4.69 4.66 2.25 2.22 2.20 2.19 2.18 2.18 2.16 2.15 2.14 1.86 1.85 1.85 1.84 1.83 1.82 1.81 1.81 1.80 1.79 1.79 1.78 1.71 1.70 1.69 1.68 1.67 1.63 1.31 1.30 1.29 1.28 1.26 1.25 1.24 1.23 1.22 1.21 1.21 1.19 1.18 1.17 1.16 1.16 1.15 1.14 1.13 1.12 1.11 1.08 1.07 1.04 1.03 1.00 0.99 0.96 0.95 0.92 0.91
F
OH
F
F
F
F
3g
1H NMR
300 MHz
CDCl3
1.00
1.02
1.00
4.36
6.30
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 -0.5
f1 (ppm)

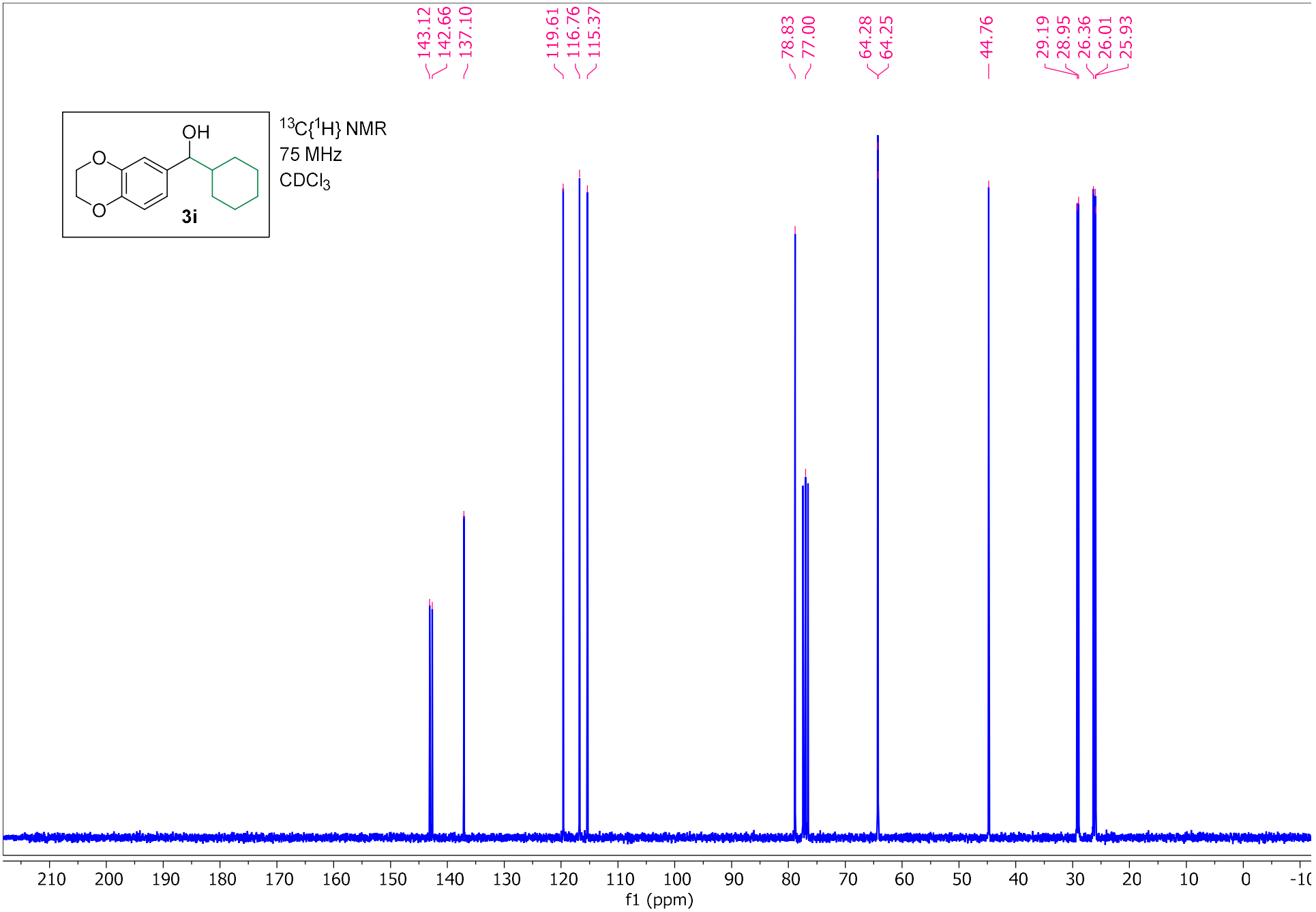

146.49
146.34
146.22
143.09
142.94
142.17
141.99
141.92
139.31
139.19
139.14
138.98
138.89
138.63
136.02
135.96
135.79
135.62
116.69
116.50
116.49
116.46
116.28
71.43
43.42
29.74
28.94
26.08
25.63
25.50
F
OH
F
F
F
F
3g
13C{1H} NMR
75 MHz
CDCl3
145
140
135
115
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

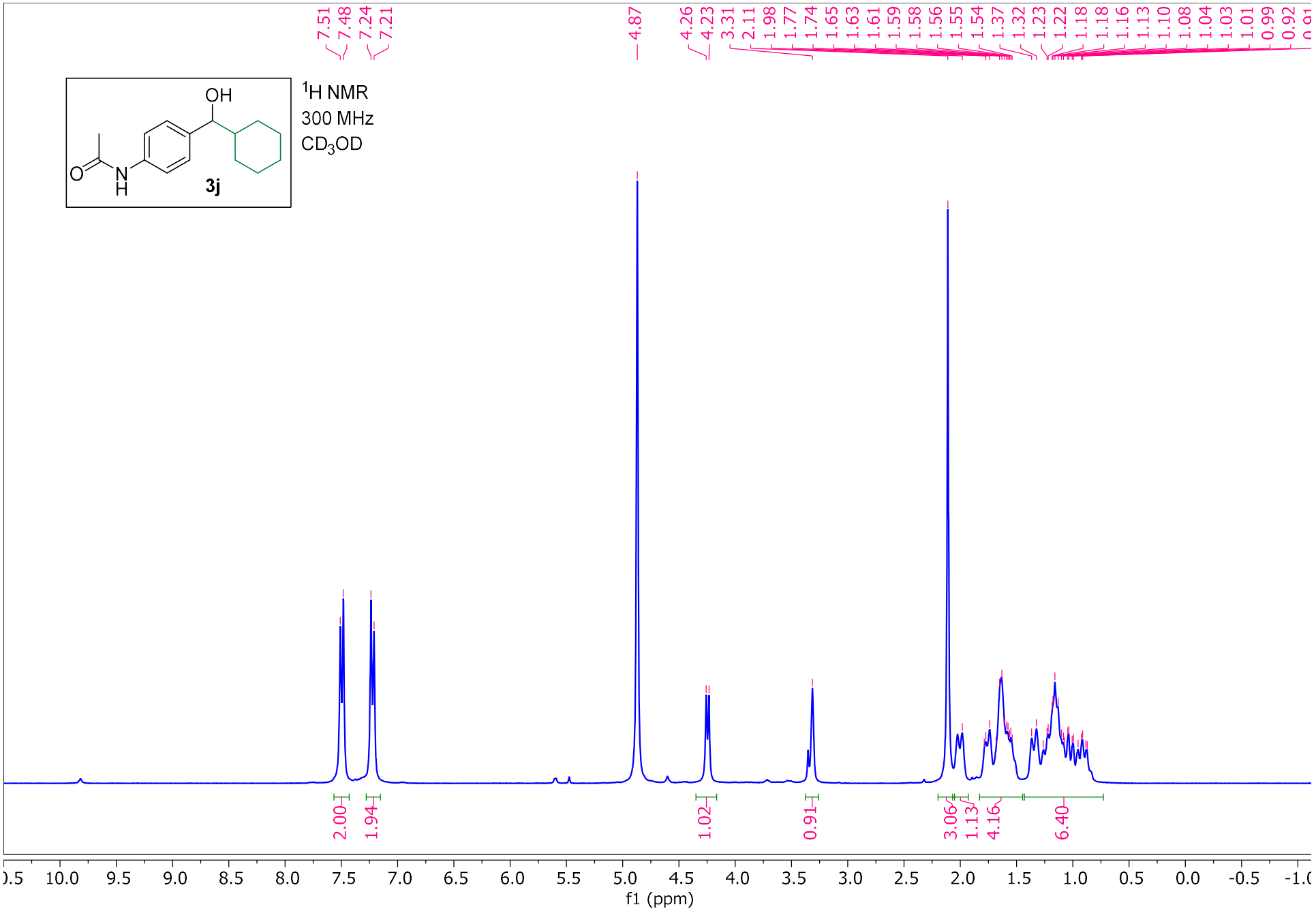

F
OH
F
F
F
F
3g
19F NMR
271 MHz
CDCl3
-142.80
-142.83
-142.88
-142.91
2.01
-142.8
-143.0
f1 (ppm)
-155.42
-155.42
-155.43
-155.49
-155.50
-155.50
-155.57
-155.57
-155.58
1.00
-155.40
-155.50
-155.60
f1 (ppm)
-161.95
-161.98
-162.03
-162.03
-162.03
-162.06
-162.06
-162.11
-162.14
1.98
-162.0
-162.1
f1 (ppm)
-142.80
-142.83
-142.88
-142.91
-155.42
-155.42
-155.49
-155.50
-155.50
-155.57
-155.57
-155.58
-161.95
-161.98
-162.03
-162.03
-162.03
-162.06
-162.06
-162.11
2.02
1.00
1.98
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

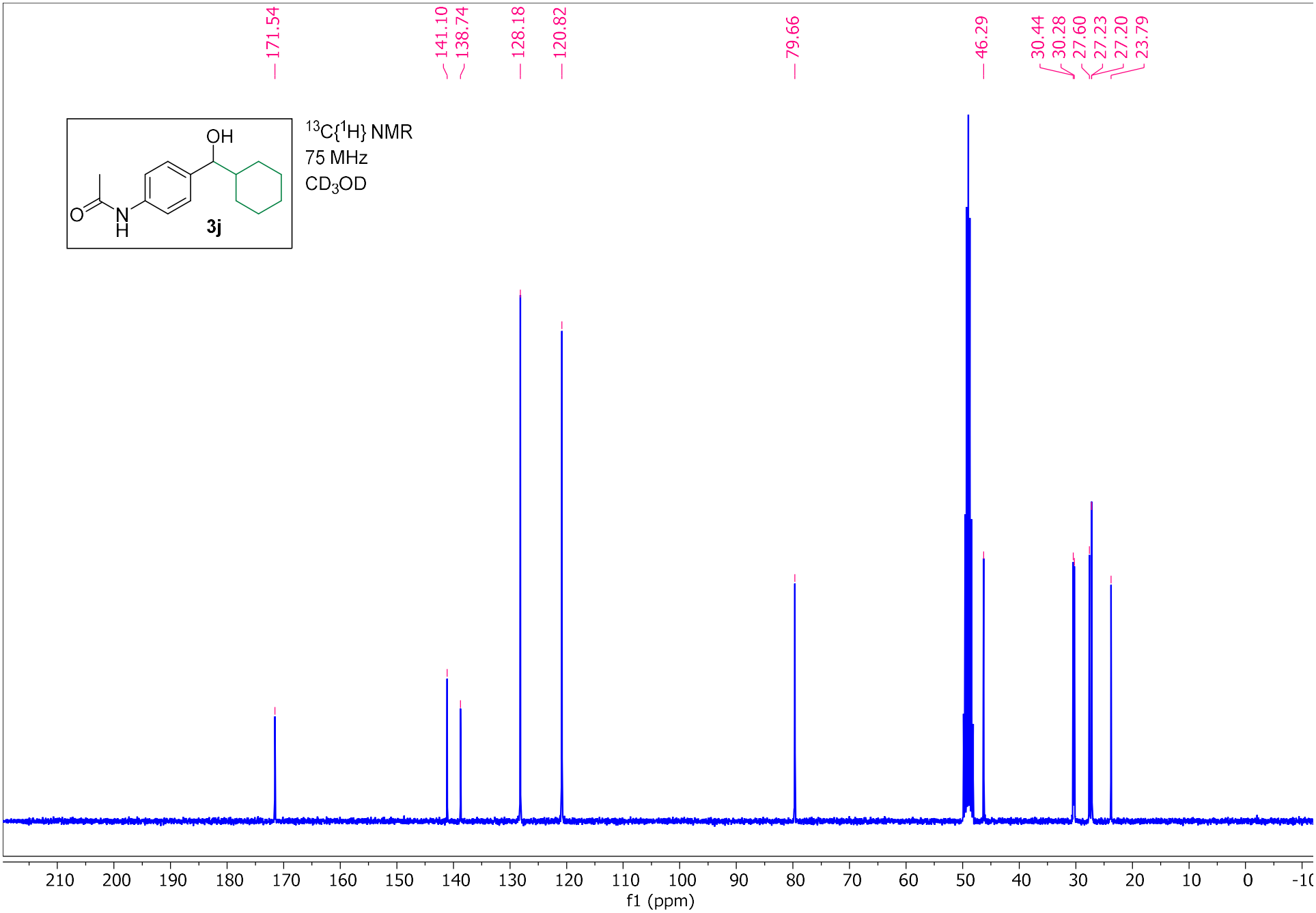

7.26 7.21 7.19 6.87 6.85 4.29 4.26 3.79 2.01 1.98 1.79 1.78 1.75 1.74 1.68 1.66 1.64 1.63 1.60 1.60 1.59 1.57 1.56 1.55 1.37 1.33 1.25 1.22 1.21 1.20 1.18 1.17 1.15 1.12 1.11 1.09 1.08 1.07 1.07 1.04 1.03 1.00 0.99 0.90 0.89 0.86 0.85
OH
O
3h
1H NMR
300 MHz
CDCl3
1.99 2.00 1.00 3.04 2.02 4.16 6.30
10.0 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 -0.5
f1 (ppm)

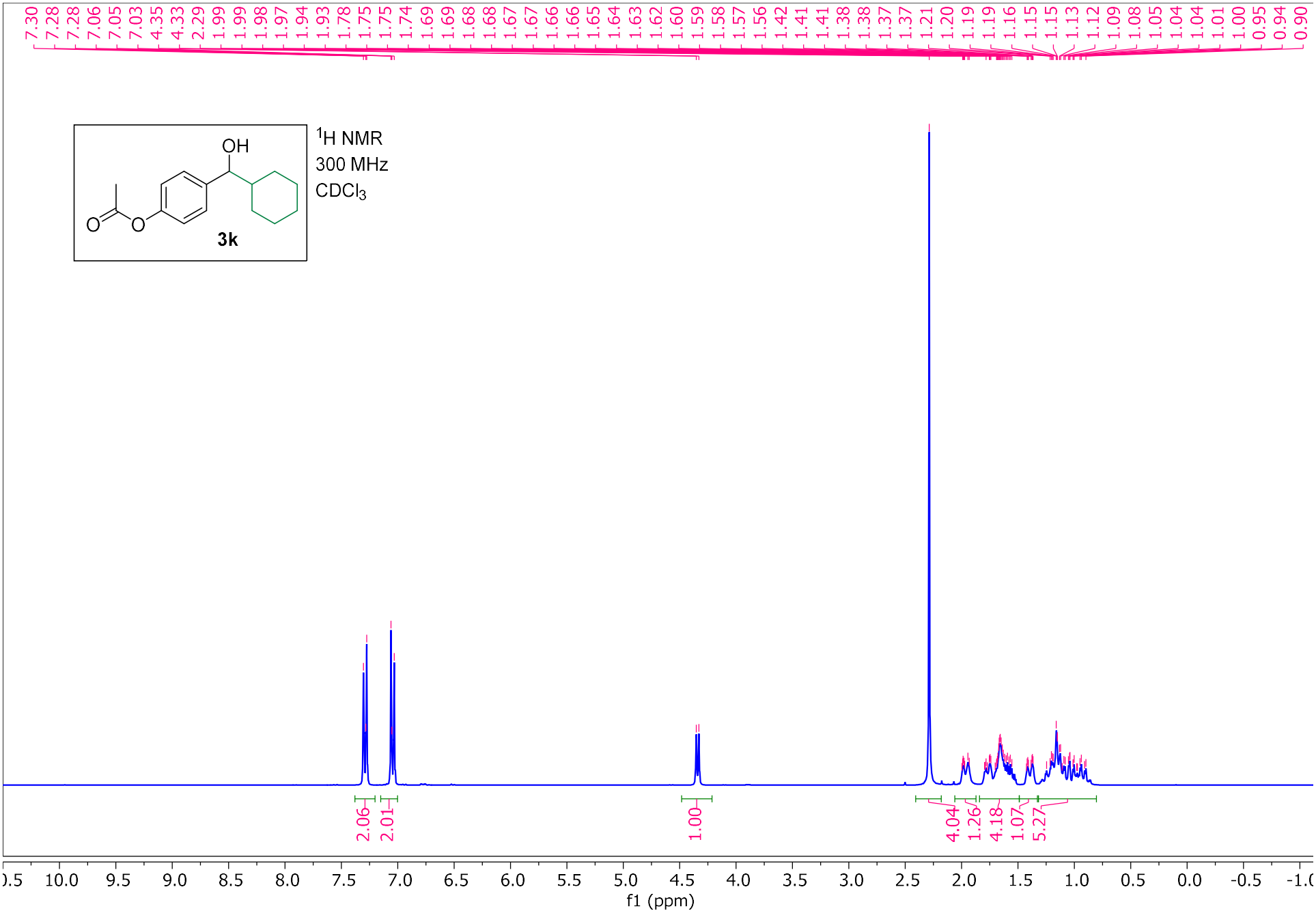

158.80
135.80
127.69
113.46
78.88
77.00
55.15
44.88
29.17
29.03
26.37
26.01
25.94
OH
O
3h
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

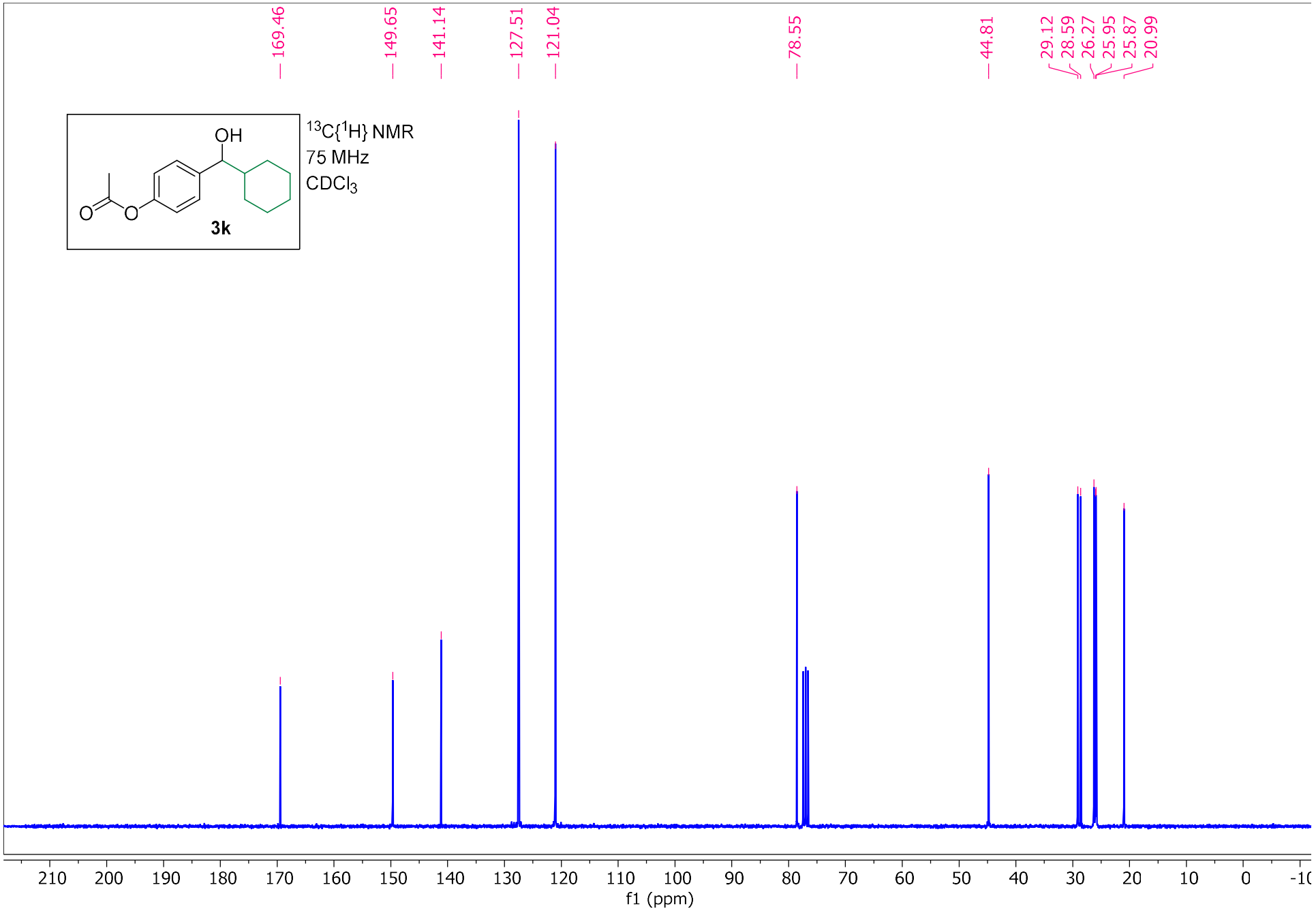

7.26 6.81 6.80 6.79 6.79 6.75 6.75 6.72 6.72 4.22 4.19 2.01 1.99 1.96 1.96 1.95 1.77 1.77 1.74 1.73 1.72 1.66 1.66 1.65 1.64 1.64 1.63 1.62 1.61 1.61 1.60 1.59 1.57 1.55 1.54 1.53 1.52 1.39 1.39 1.38 1.35 1.34 1.34 1.21 1.20 1.18 1.17 1.16 1.16 1.14 1.13 1.12 1.11 1.11 1.02 1.01 1.01 0.98 0.97 0.90 0.89 0.85
OH
O
O
3i
1H NMR
300 MHz
CDCl3
0.83
1.28
1.00
4.99
1.99
4.23
1.02
5.19
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 -0.5
f1 (ppm)

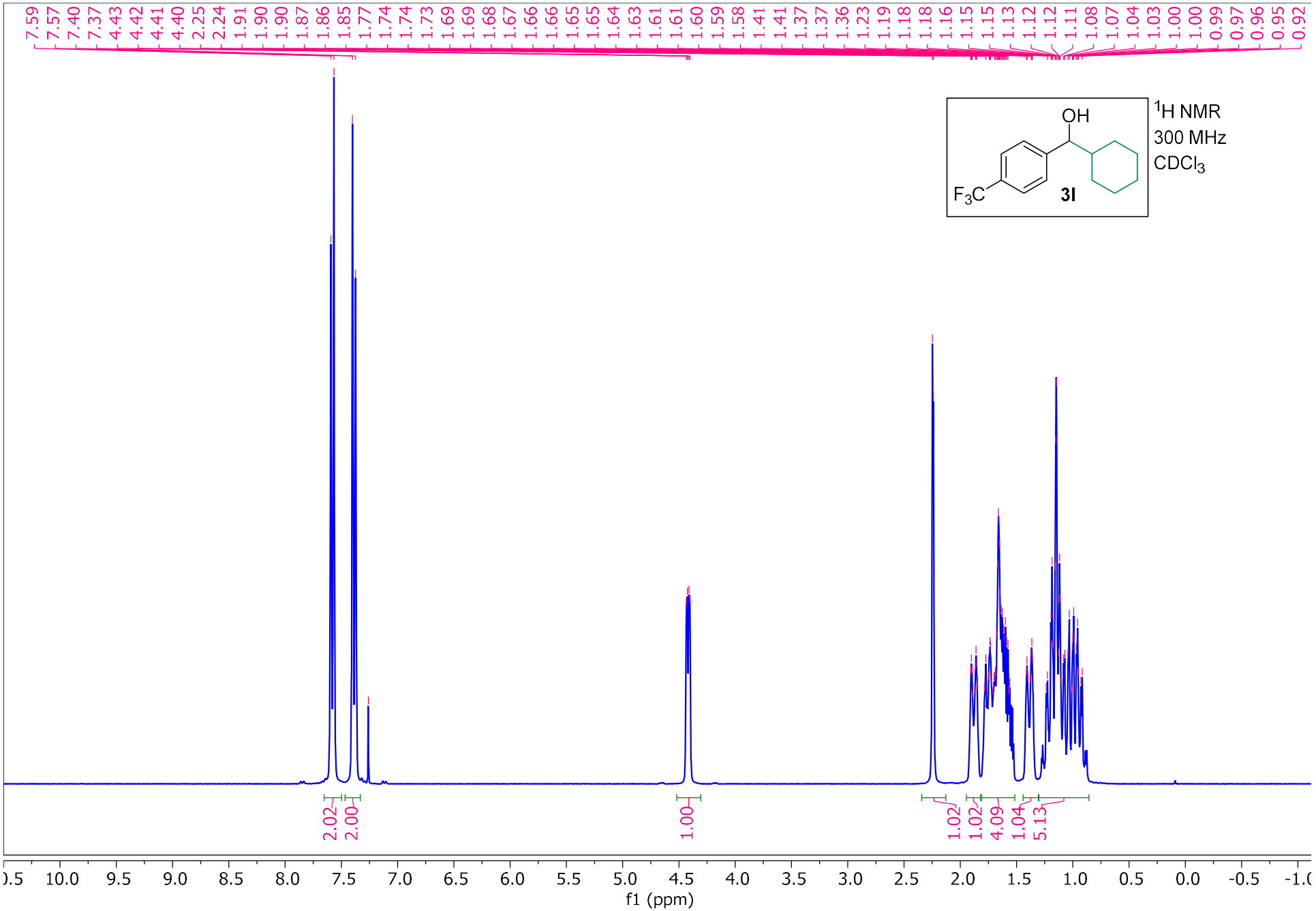

143.12
142.66
137.10
119.61
116.76
115.37
78.83
77.00
64.28
64.25
44.76
29.19
28.95
26.36
26.01
25.93
OH
O
O
3i
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

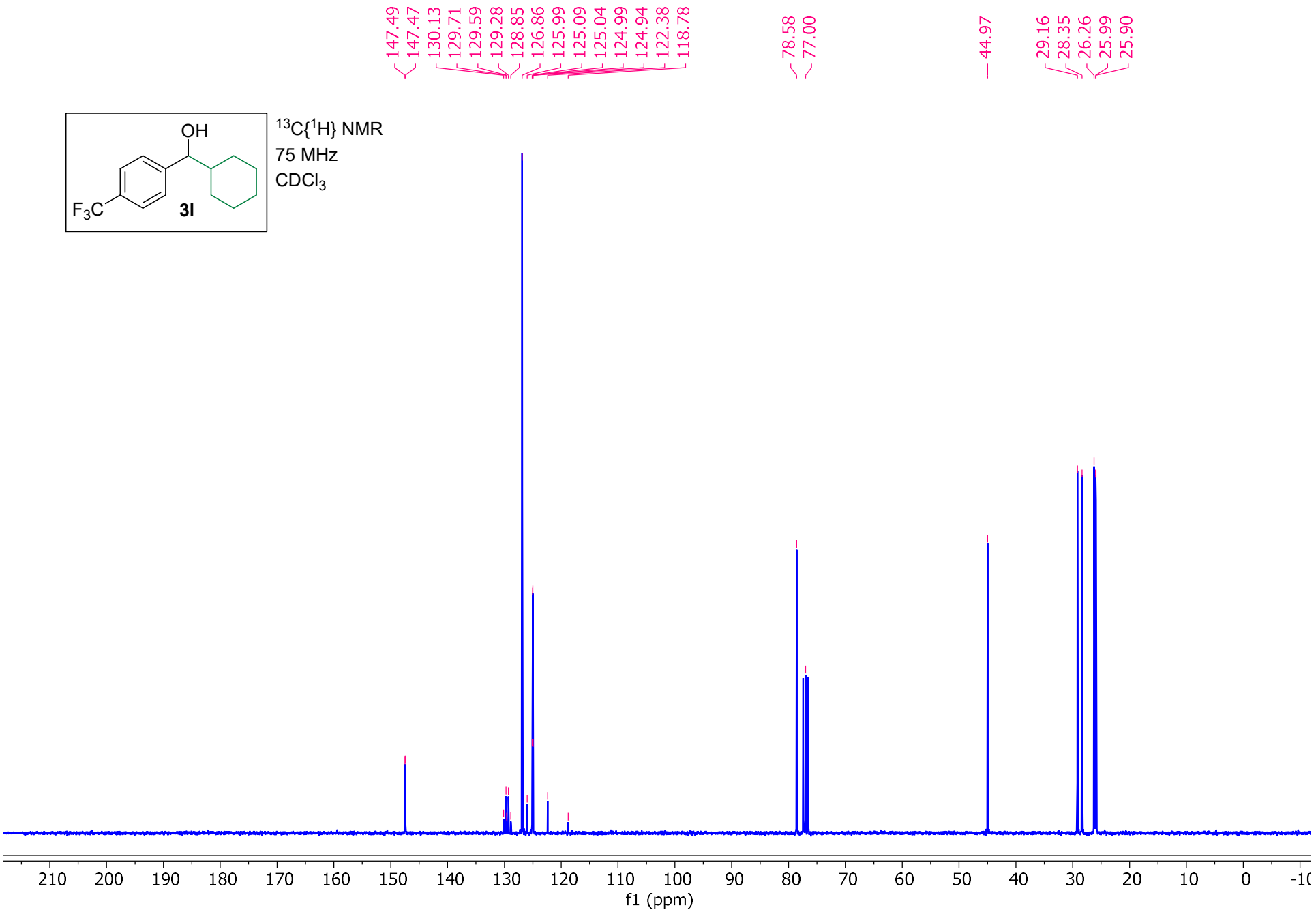

7.51
7.48
7.24
7.21
4.87
4.26
4.23
3.31
2.11
1.98
1.77
1.74
1.65
1.63
1.61
1.59
1.58
1.56
1.55
1.54
1.37
1.32
1.23
1.22
1.18
1.18
1.16
1.13
1.10
1.08
1.04
1.03
1.01
0.99
0.92
OH
O
N
H
3j
1H NMR
300 MHz
CD3OD
2.00
1.94
1.02
0.91
3.06
1.13
4.16
6.40
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

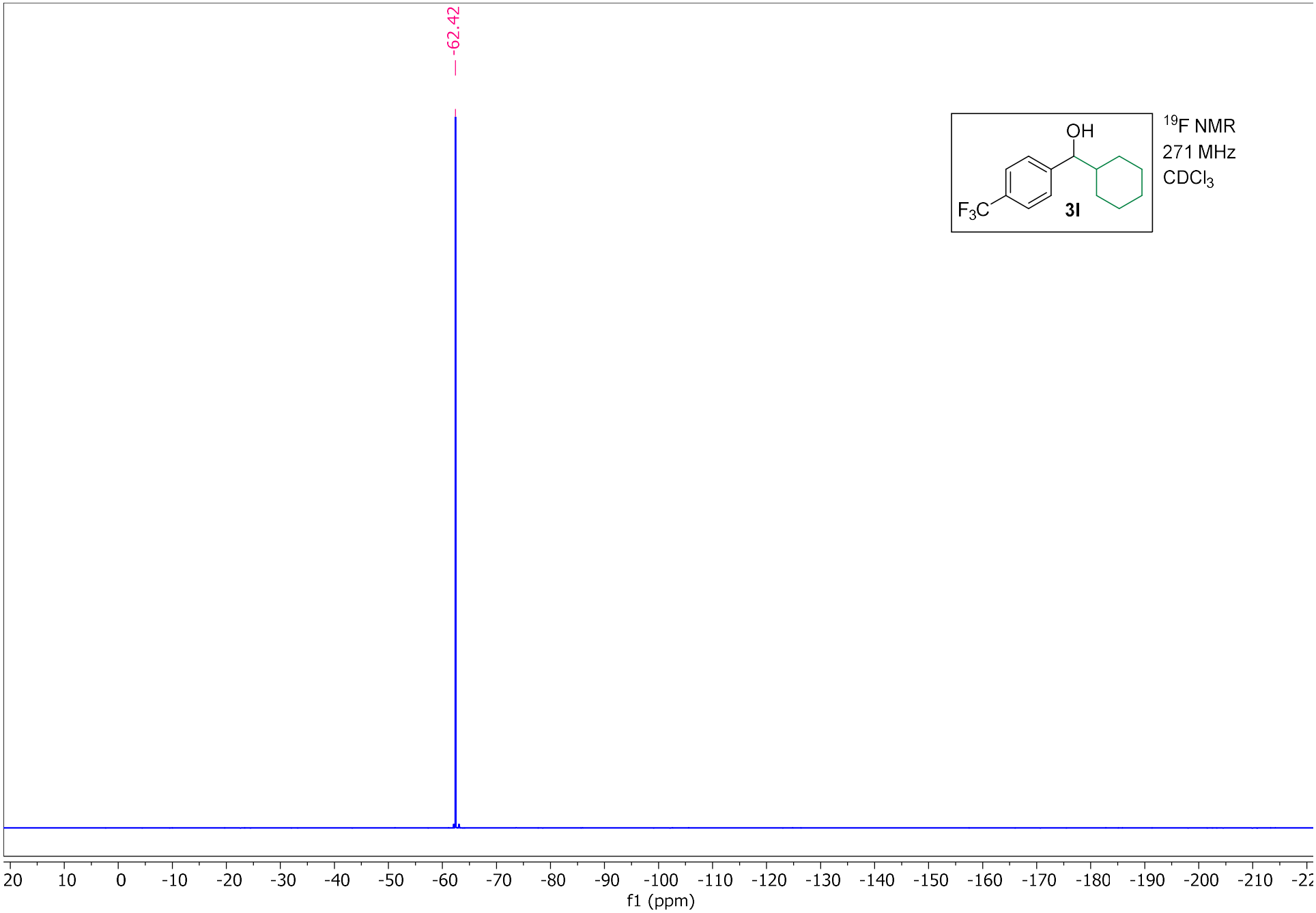

171.54
141.10
138.74
128.18
120.82
79.66
46.29
30.44
30.28
27.60
27.23
27.20
23.79
OH
O
N
H
3j
13C{1H} NMR
75 MHz
CD3OD
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

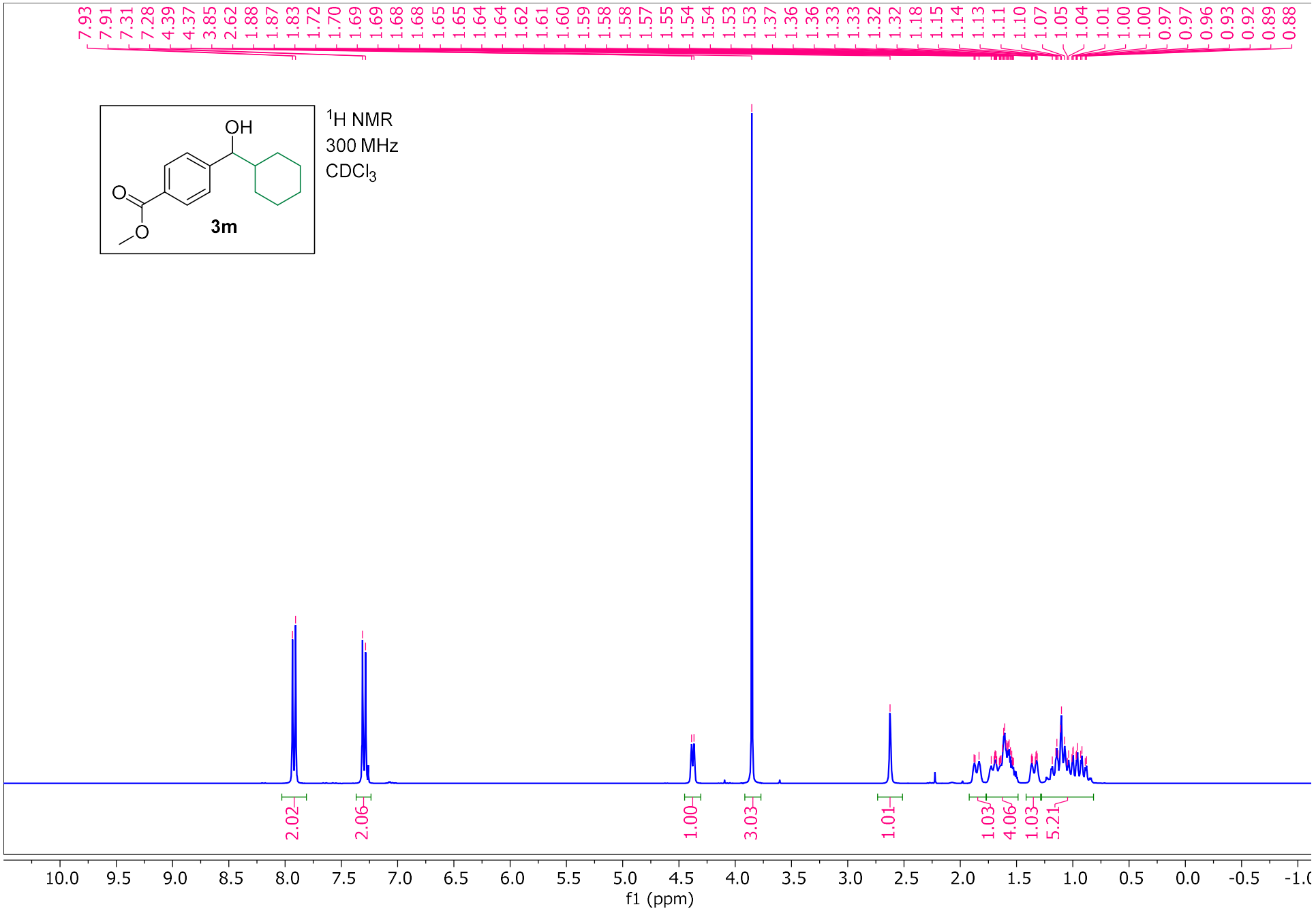

7.30 7.28 7.28 7.06 7.05 7.03 4.35 4.33 2.29 1.99 1.99 1.98 1.97 1.94 1.93 1.78 1.75 1.75 1.74 1.69 1.69 1.68 1.68 1.67 1.67 1.66 1.66 1.65 1.64 1.63 1.62 1.60 1.59 1.58 1.57 1.56 1.42 1.41 1.41 1.38 1.38 1.37 1.37 1.21 1.20 1.19 1.19 1.16 1.15 1.15 1.13 1.12 1.09 1.08 1.05 1.04 1.04 1.01 1.00 0.95 0.94 0.90
OH
O
O
3k
1H NMR
300 MHz
CDCl3
2.06
2.01
1.00
4.04
1.26
4.18
1.07
5.27
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 -0.5
f1 (ppm)

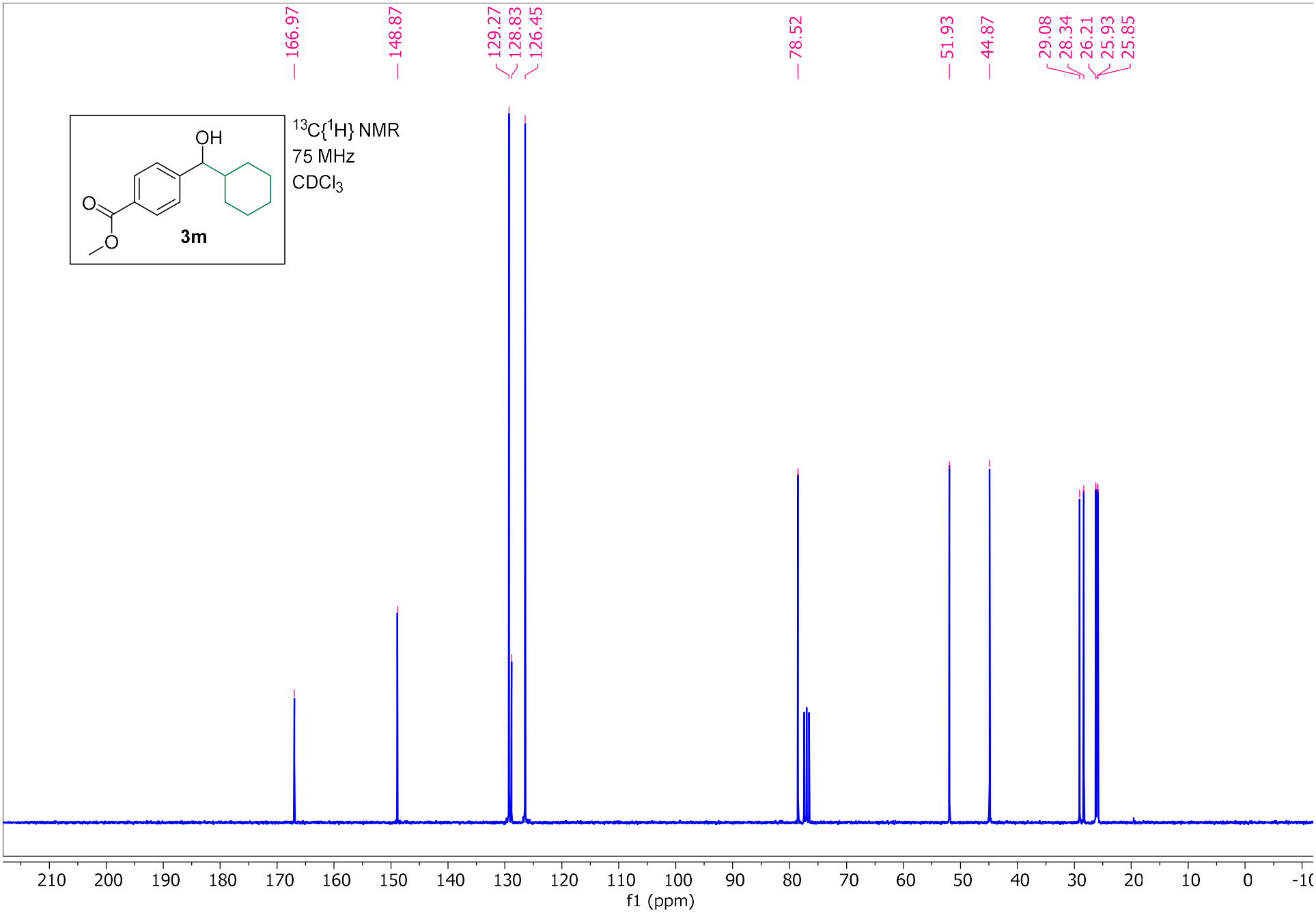

169.46
149.65
141.14
127.51
121.04
78.55
44.81
29.12
28.59
26.27
25.95
25.87
20.99
OH
O
O
3k
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

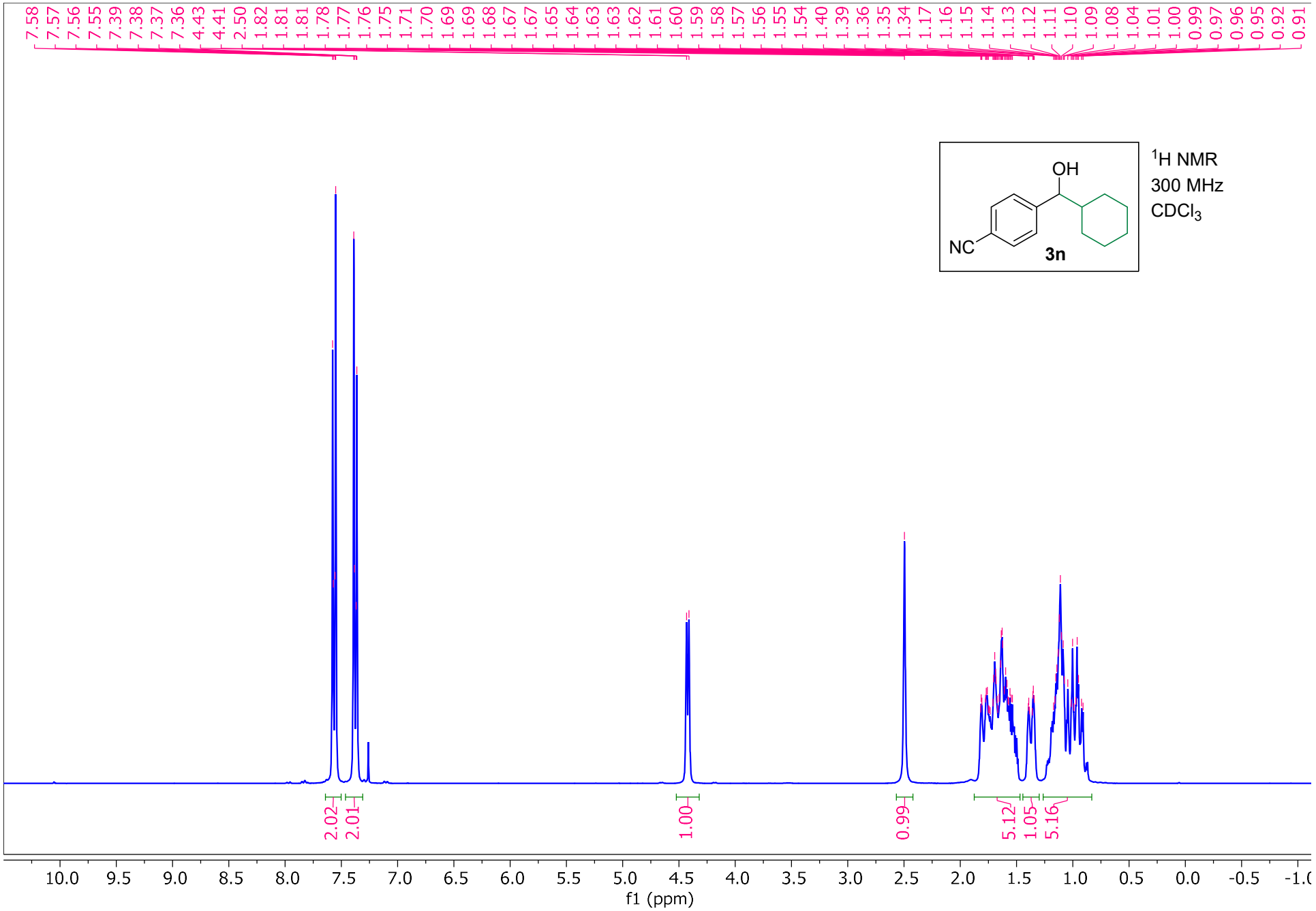

7.59 7.57 7.40 7.37 4.43 4.42 4.41 4.40 2.25 2.24 1.91 1.90 1.90 1.87 1.86 1.85 1.77 1.74 1.74 1.73 1.69 1.69 1.68 1.67 1.66 1.66 1.65 1.65 1.64 1.63 1.61 1.61 1.60 1.59 1.58 1.41 1.41 1.37 1.37 1.36 1.23 1.19 1.18 1.18 1.16 1.15 1.15 1.13 1.12 1.12 1.11 1.08 1.07 1.04 1.03 1.00 1.00 0.99 0.97 0.96 0.95 0.92
OH
F3C
3l
1H NMR
300 MHz
CDCl3
2.02 2.00 1.00 1.02 1.02 4.09 1.04 5.13
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 -0.5
f1 (ppm)

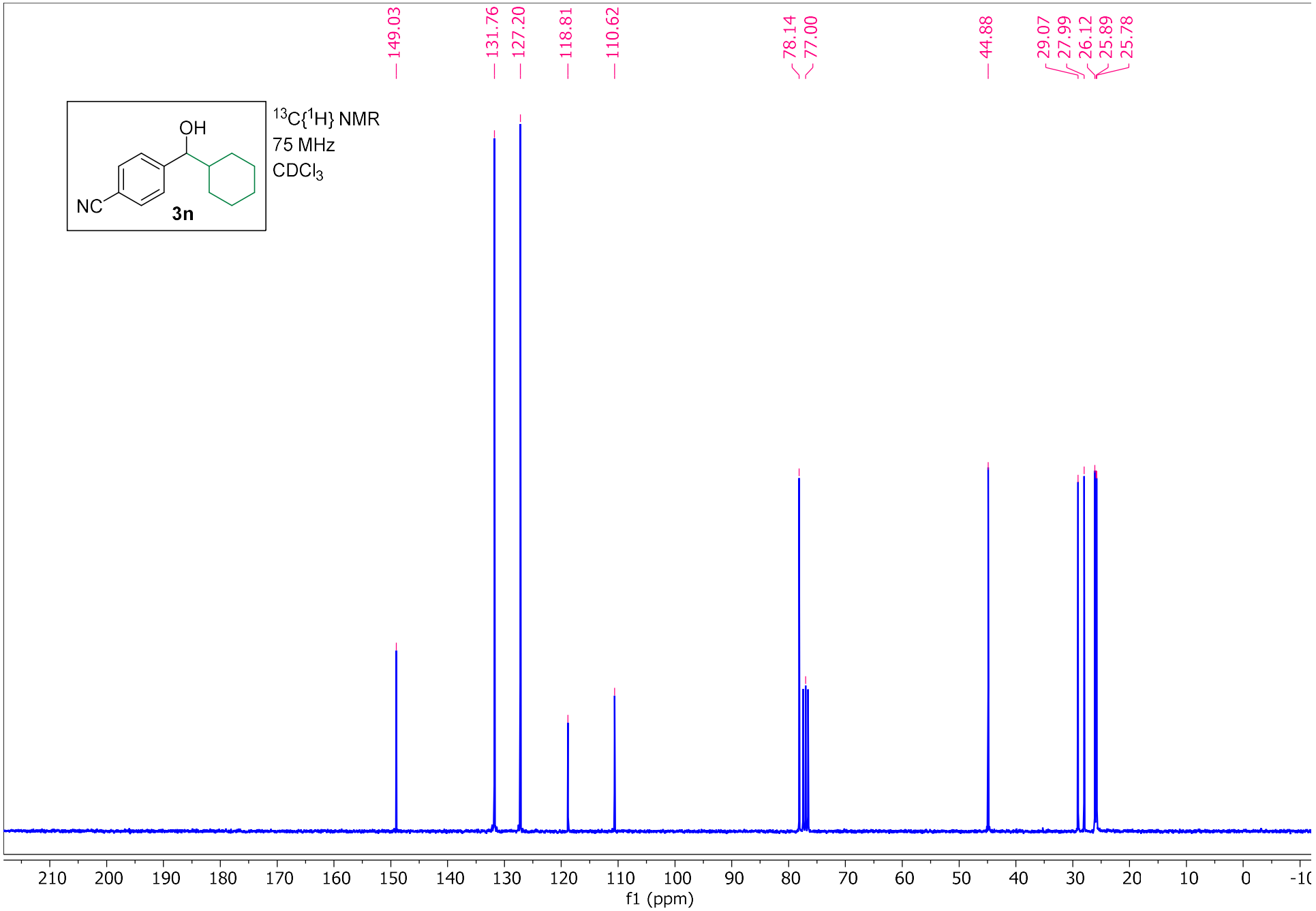

147.49
147.47
130.13
129.71
129.59
129.28
128.85
126.86
125.99
125.09
125.04
124.99
124.94
122.38
118.78
78.58
77.00
44.97
29.16
28.35
26.26
25.99
25.90
OH
F3C
3l
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

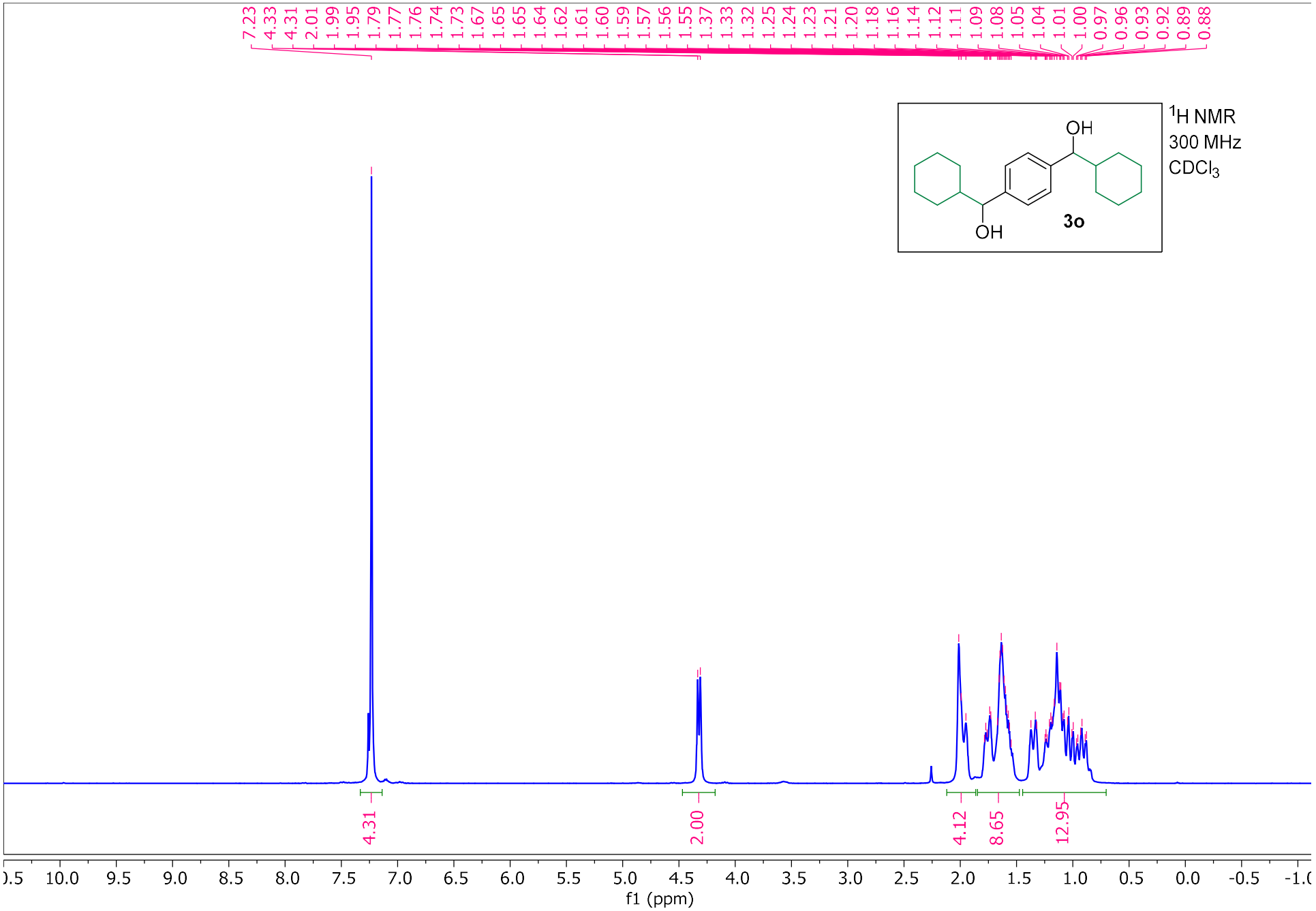

-62.42
OH
F3C
3l
19F NMR
271 MHz
CDCl3
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)

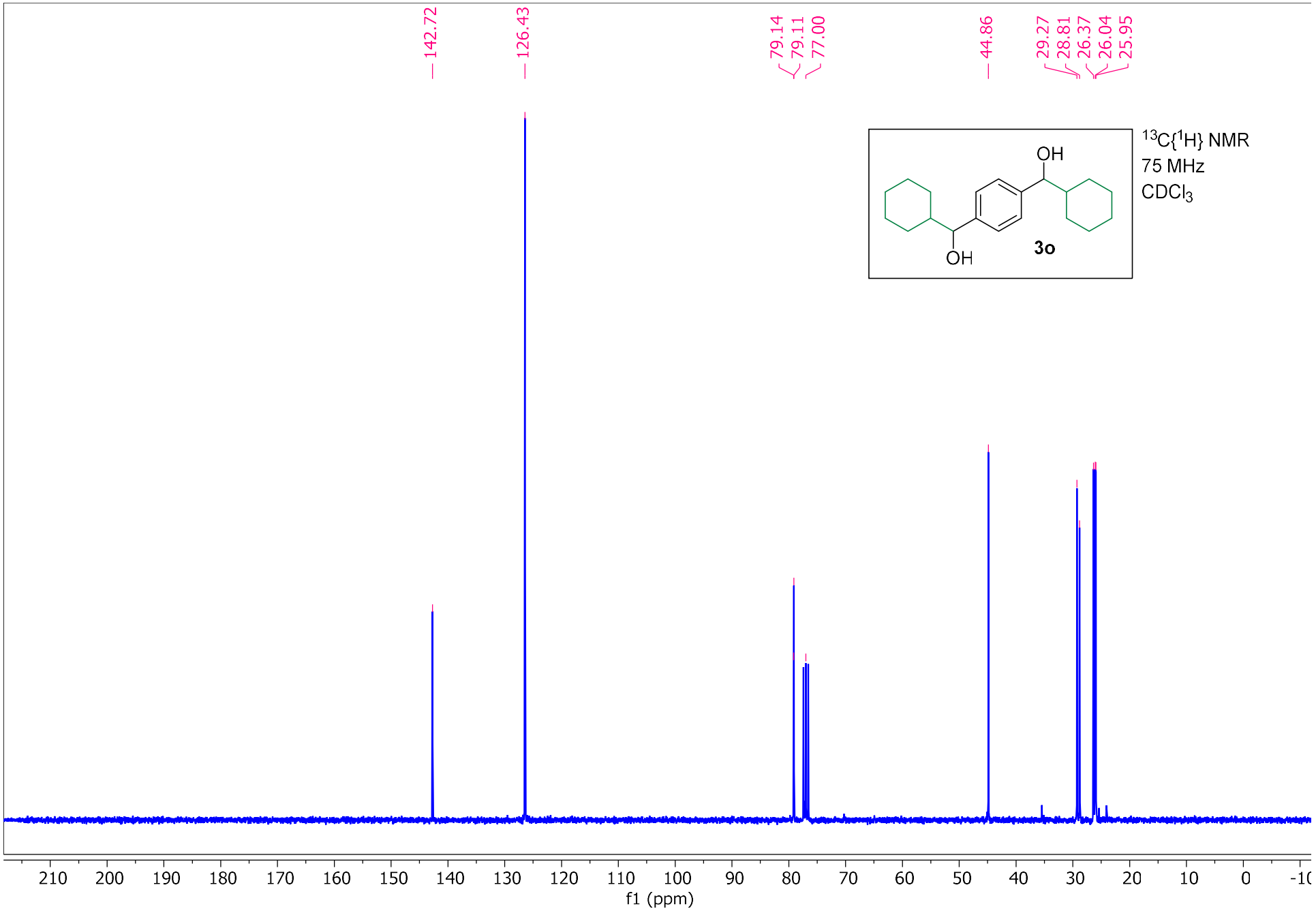

7.93 7.91 7.31 7.28 4.39 4.37 3.85 2.62 1.88 1.87 1.83 1.72 1.70 1.69 1.69 1.68 1.68 1.65 1.65 1.64 1.64 1.62 1.61 1.60 1.59 1.58 1.58 1.57 1.55 1.54 1.54 1.53 1.53 1.37 1.36 1.36 1.33 1.33 1.32 1.32 1.18 1.15 1.14 1.13 1.11 1.10 1.07 1.05 1.04 1.01 1.00 1.00 0.97 0.97 0.96 0.93 0.92 0.89 0.88
OH
O
O
3m
1H NMR
300 MHz
CDCl3
2.02
2.06
1.00
3.03
1.01
1.03
4.06
1.03
5.21
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 -0.5
f1 (ppm)

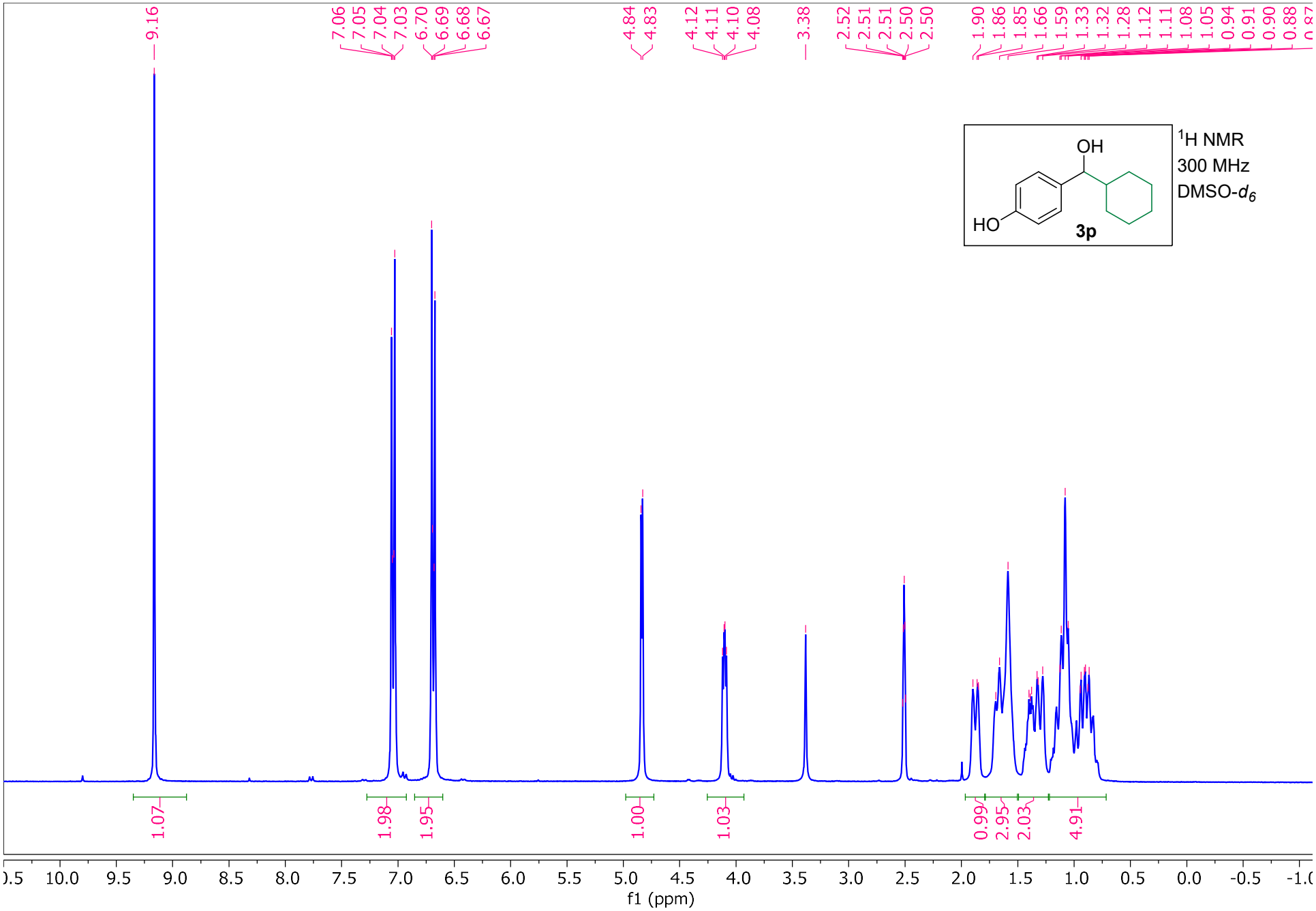

166.97
148.87
129.27
128.83
126.45
78.52
51.93
44.87
29.08
28.34
26.21
25.93
25.85
OH
O
O
3m
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

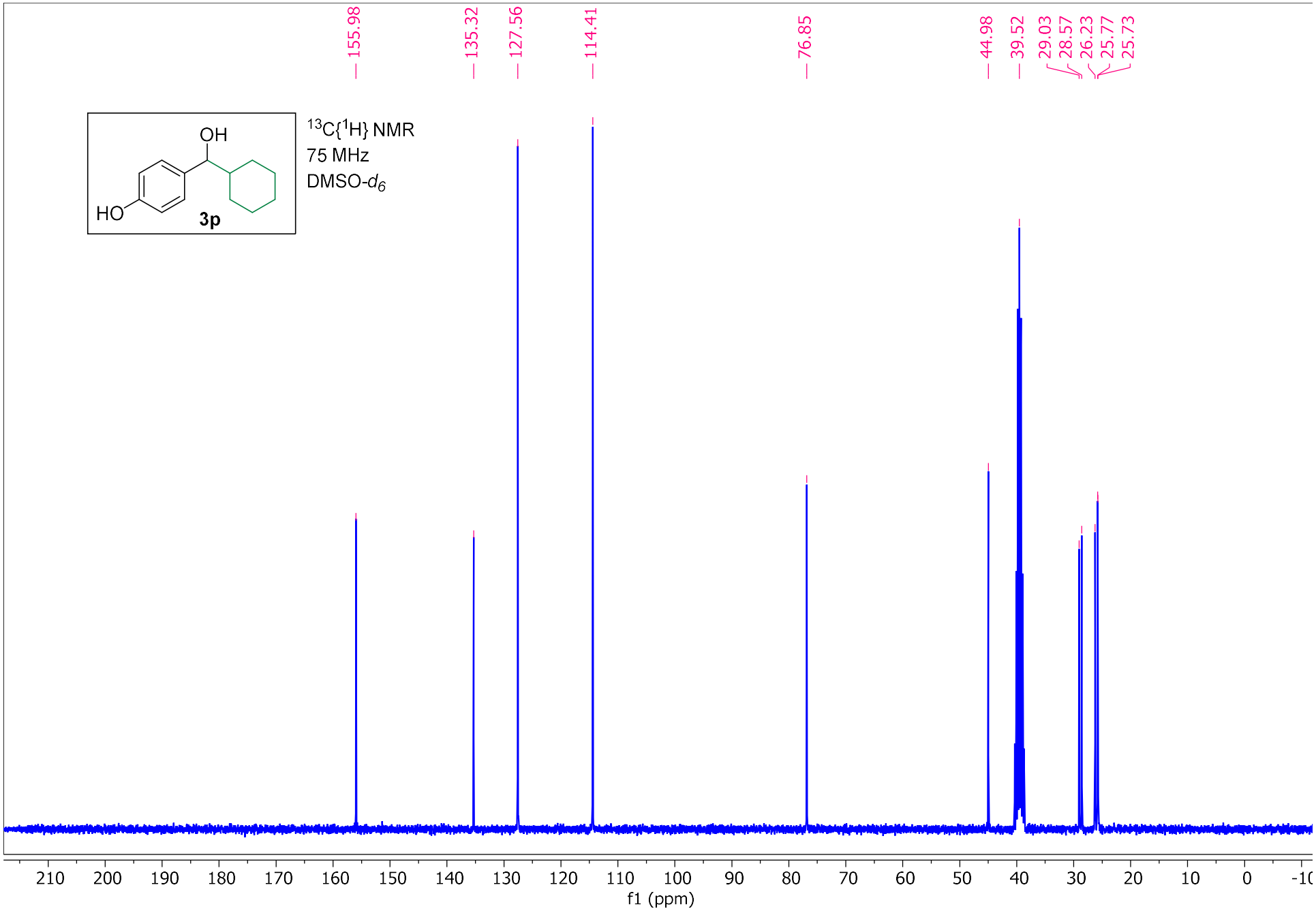

7.58 7.57 7.56 7.55 7.39 7.38 7.37 7.36 4.43 4.41 2.50 1.82 1.81 1.81 1.78 1.77 1.76 1.75 1.71 1.70 1.69 1.69 1.68 1.67 1.67 1.65 1.64 1.63 1.63 1.62 1.61 1.60 1.59 1.58 1.57 1.56 1.55 1.54 1.40 1.39 1.36 1.35 1.34 1.17 1.16 1.15 1.14 1.13 1.12 1.11 1.10 1.09 1.08 1.04 1.01 1.00 0.99 0.97 0.96 0.95 0.92 0.91
OH
NC
3n
1H NMR
300 MHz
CDCl3
2.02
2.01
1.00
0.99
5.12
1.05
5.16
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 -0.5
f1 (ppm)

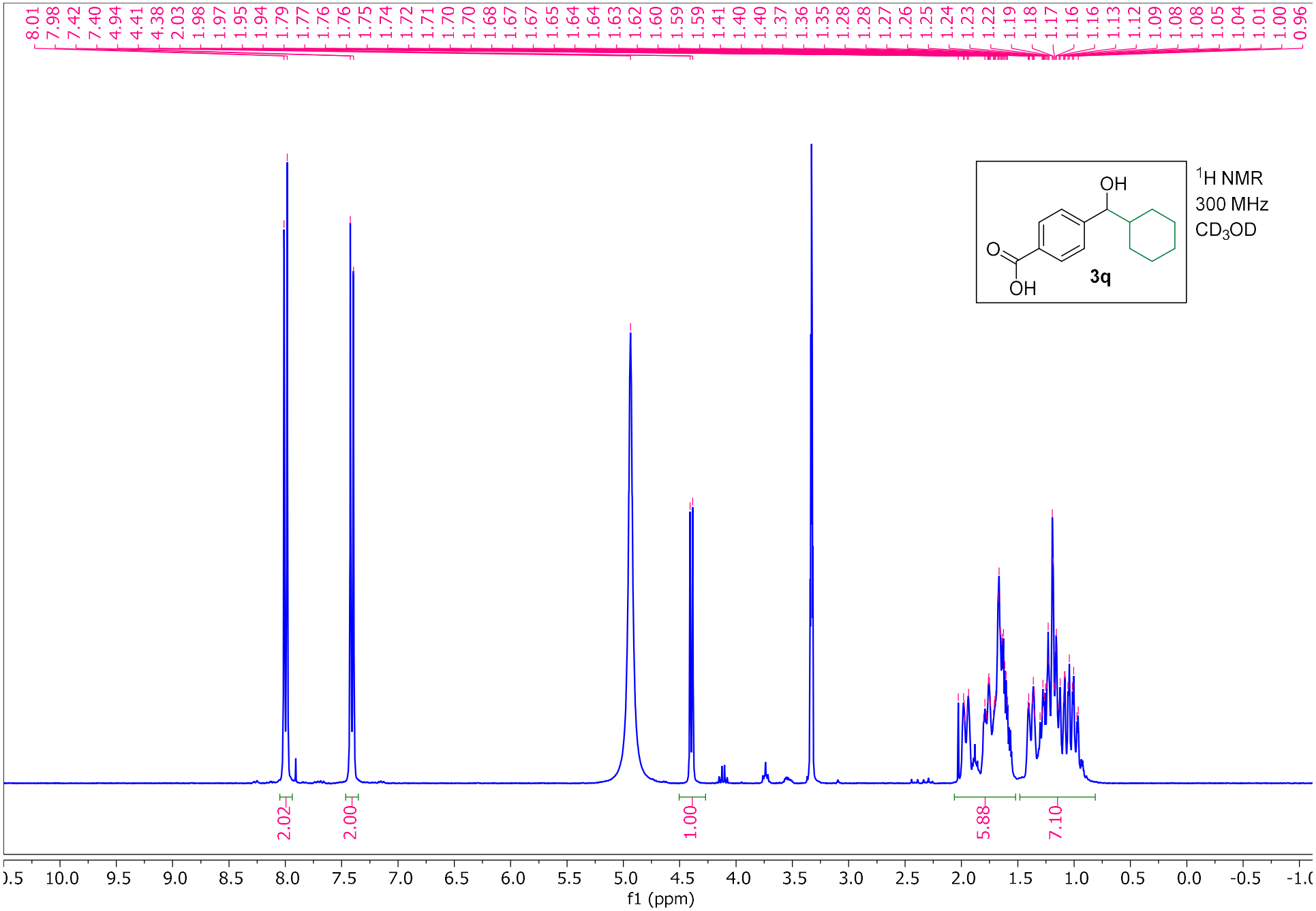

149.03
131.76
127.20
118.81
110.62
78.14
77.00
44.88
29.07
27.99
26.12
25.89
25.78
OH
NC
3n
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

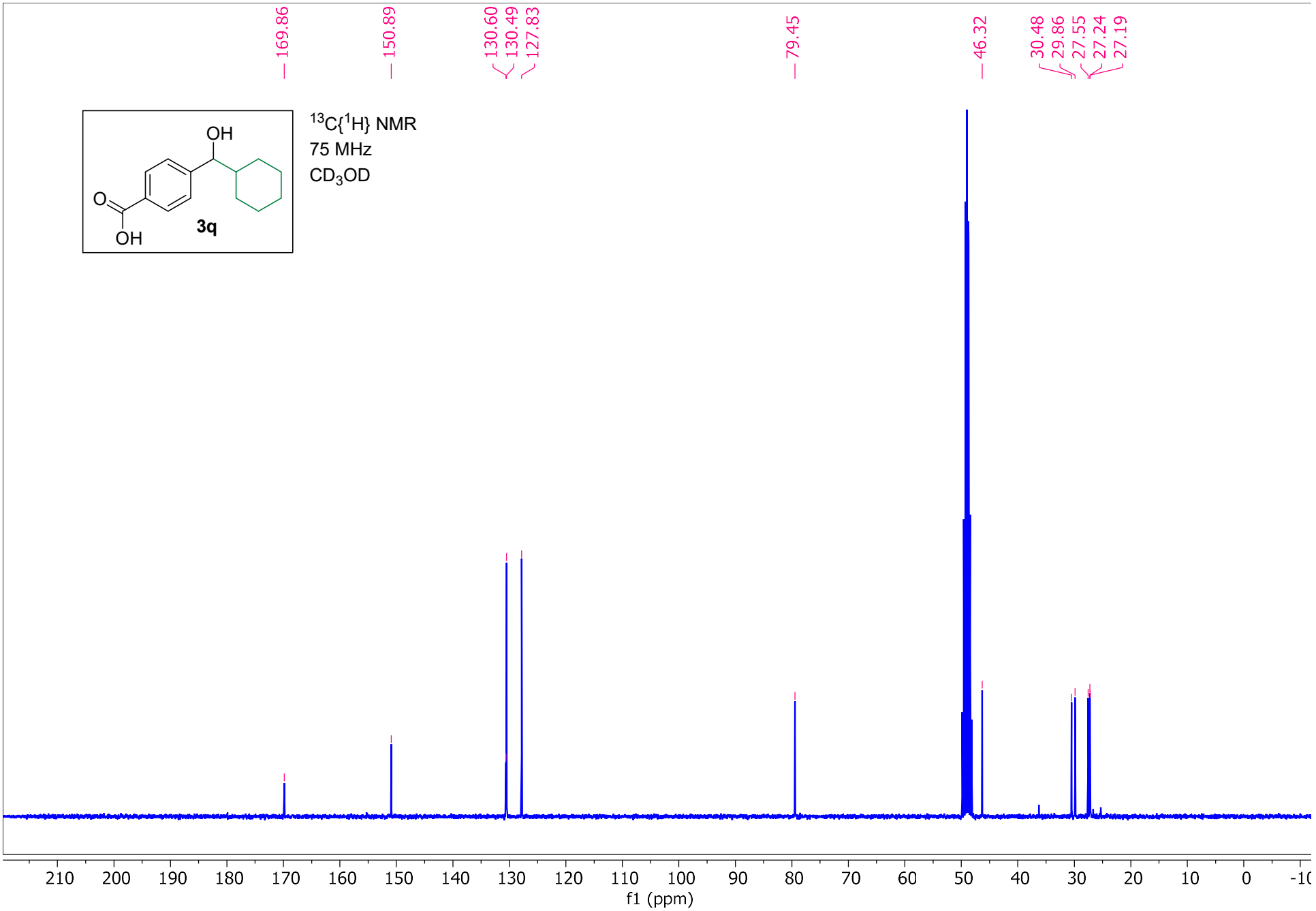

7.23 4.33 4.31 2.01 1.99 1.95 1.79 1.77 1.76 1.74 1.73 1.67 1.65 1.65 1.64 1.62 1.61 1.60 1.59 1.57 1.56 1.55 1.37 1.33 1.32 1.25 1.24 1.23 1.21 1.20 1.18 1.16 1.14 1.12 1.11 1.09 1.08 1.05 1.04 1.01 1.00 0.97 0.96 0.93 0.92 0.89 0.88
OH
OH
3o
1H NMR
300 MHz
CDCl3
4.31
2.00
4.12
8.65
12.95
10.0 9.5 9.0 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 -0.5
f1 (ppm)

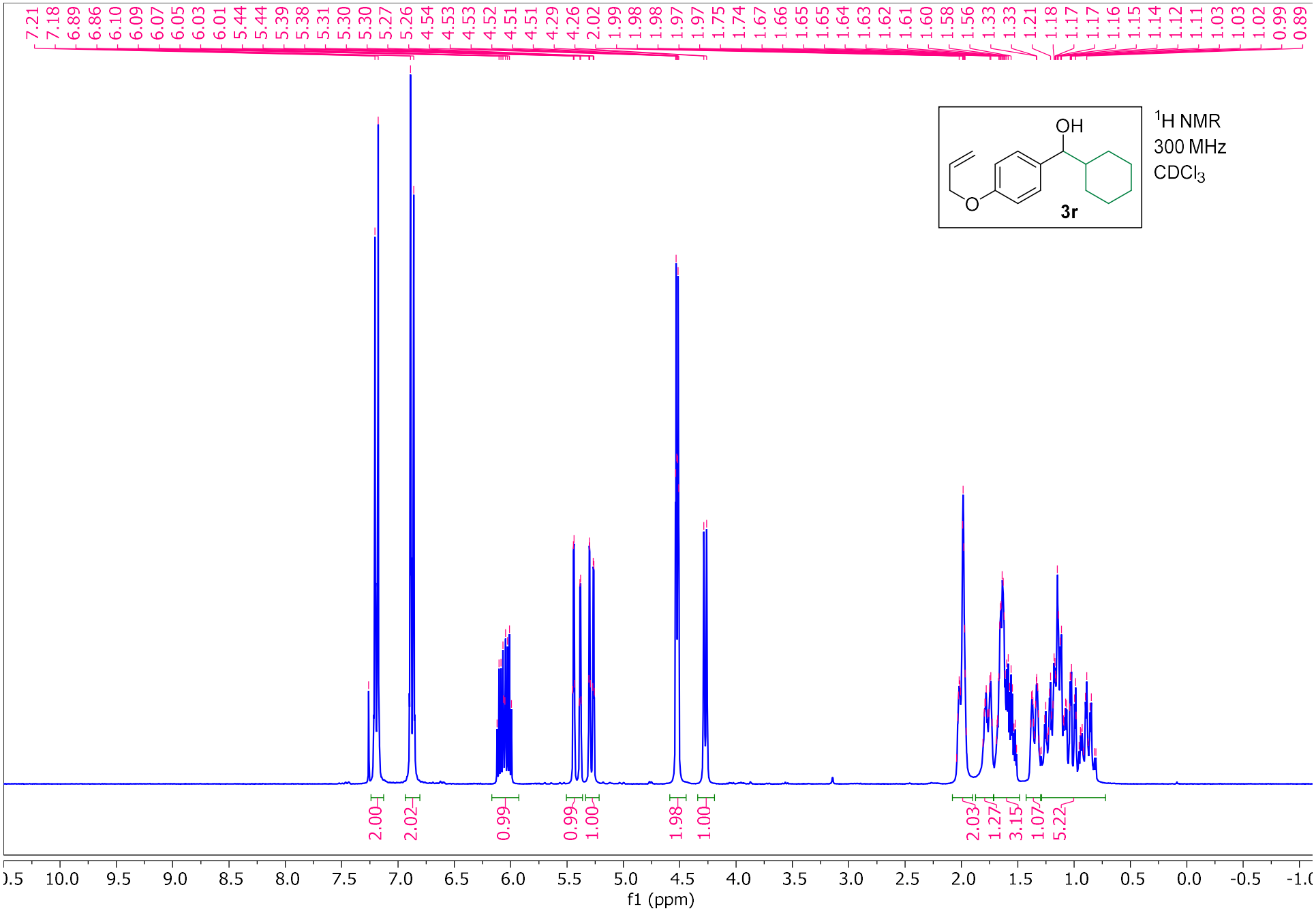

142.72
126.43
79.14
79.11
77.00
44.86
29.27
28.81
26.37
26.04
25.95
OH
OH
3o
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

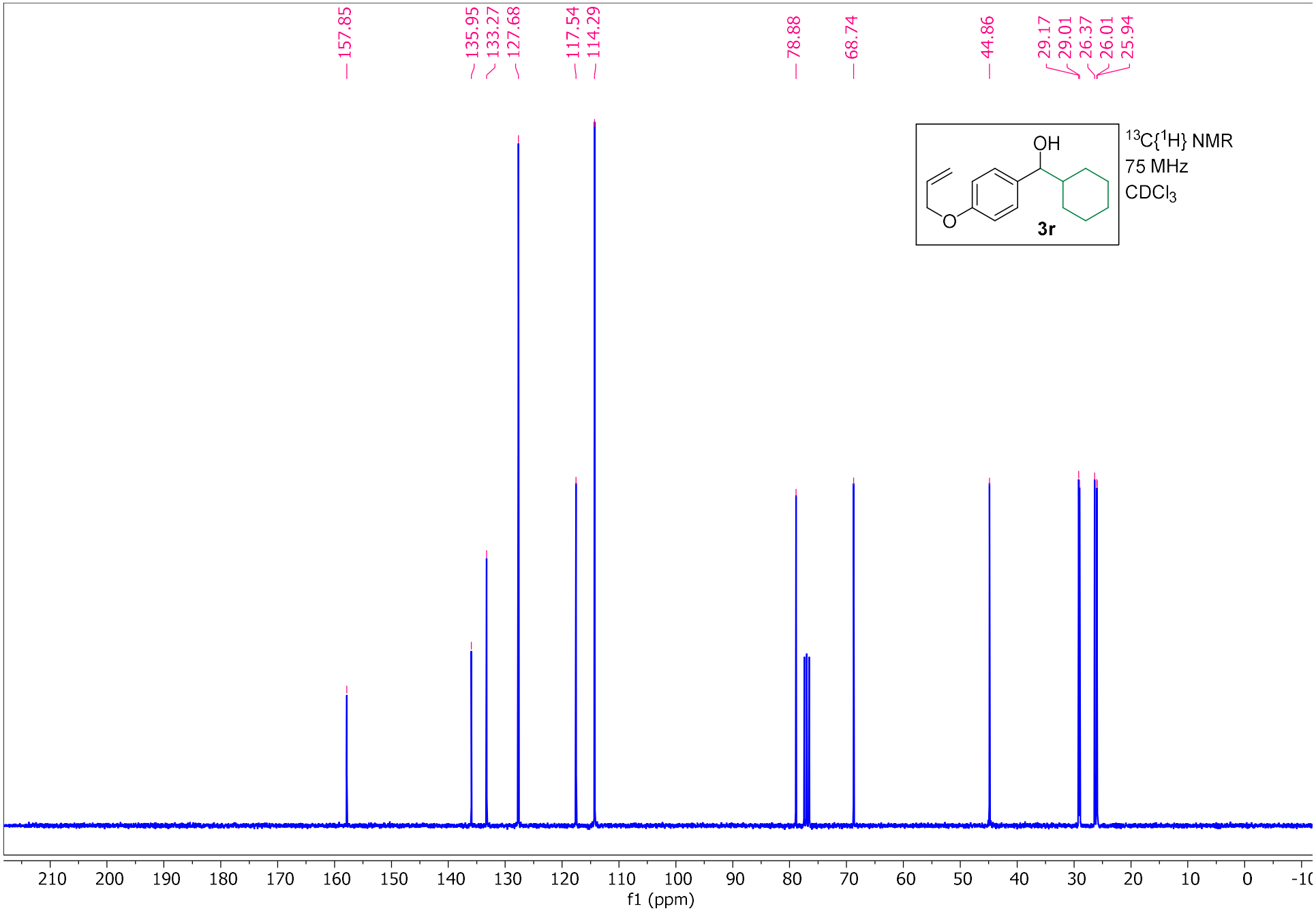

9.16
7.06
7.05
7.04
7.03
6.70
6.69
6.68
6.67
4.84
4.83
4.12
4.11
4.10
4.08
3.38
2.52
2.51
2.51
2.50
2.50
1.90
1.86
1.85
1.66
1.59
1.33
1.32
1.28
1.12
1.11
1.08
1.05
0.94
0.91
0.90
0.88
OH
HO
3p
1H NMR
300 MHz
DMSO-d6
1.07
1.98
1.95
1.00
1.03
0.99
2.95
2.03
4.91
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

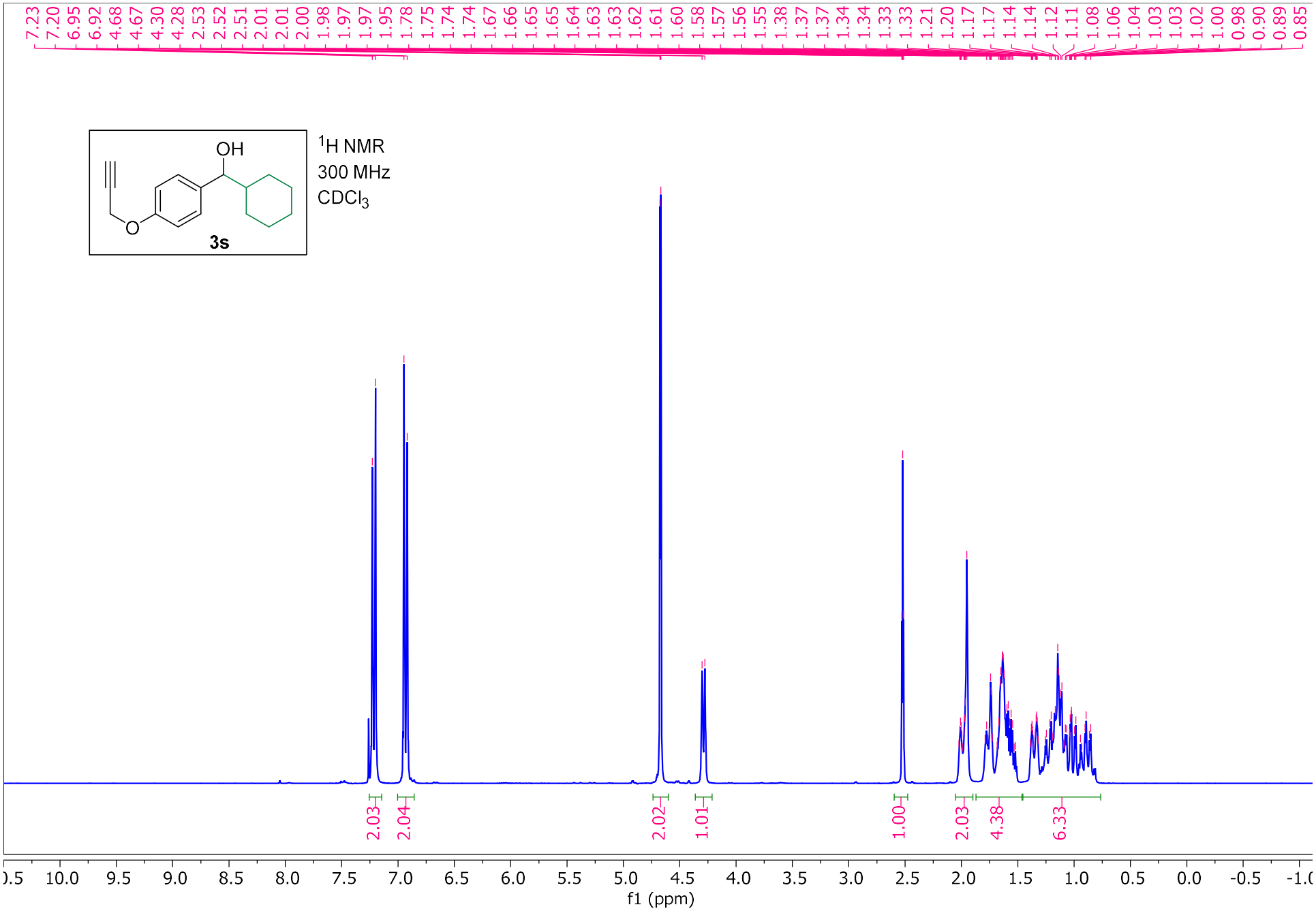

155.98
135.32
127.56
114.41
76.85
44.98
39.52
29.03
28.57
26.23
25.77
25.73
OH
HO
3p
$^{13}C\{^{1}H\}$ NMR
75 MHz
DMSO-d_6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

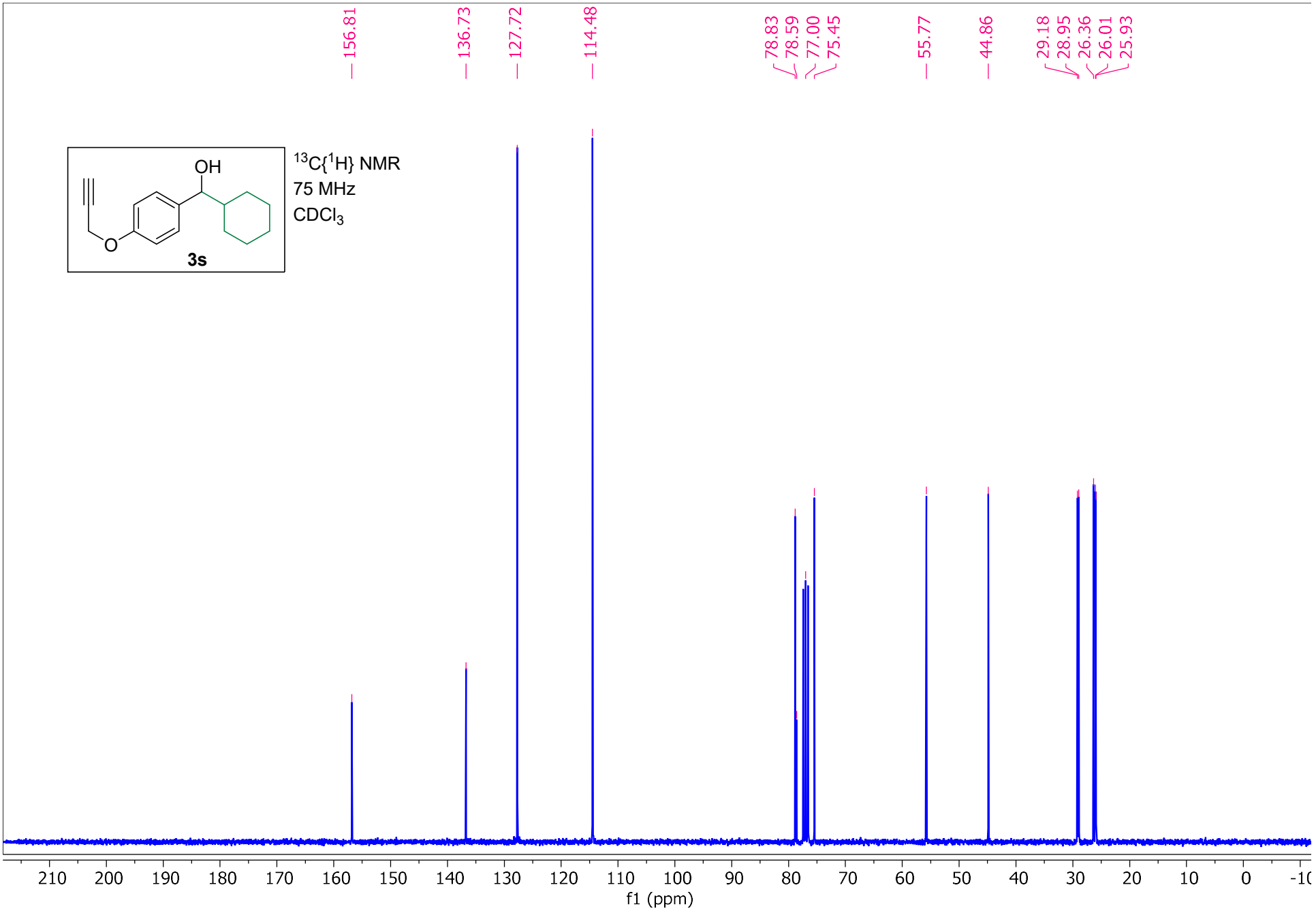

8.01 7.98 7.42 7.40 4.94 4.41 4.38 2.03 1.98 1.97 1.95 1.94 1.79 1.77 1.76 1.76 1.75 1.74 1.72 1.71 1.70 1.70 1.68 1.67 1.67 1.65 1.64 1.64 1.63 1.62 1.60 1.59 1.59 1.41 1.40 1.40 1.37 1.36 1.35 1.28 1.28 1.27 1.26 1.25 1.24 1.23 1.22 1.19 1.18 1.17 1.16 1.16 1.13 1.12 1.09 1.08 1.08 1.05 1.04 1.01 1.00 0.96
OH
O
OH
3q
1H NMR
300 MHz
CD3OD
2.02
2.00
1.00
5.88
7.10
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 -0.5
f1 (ppm)

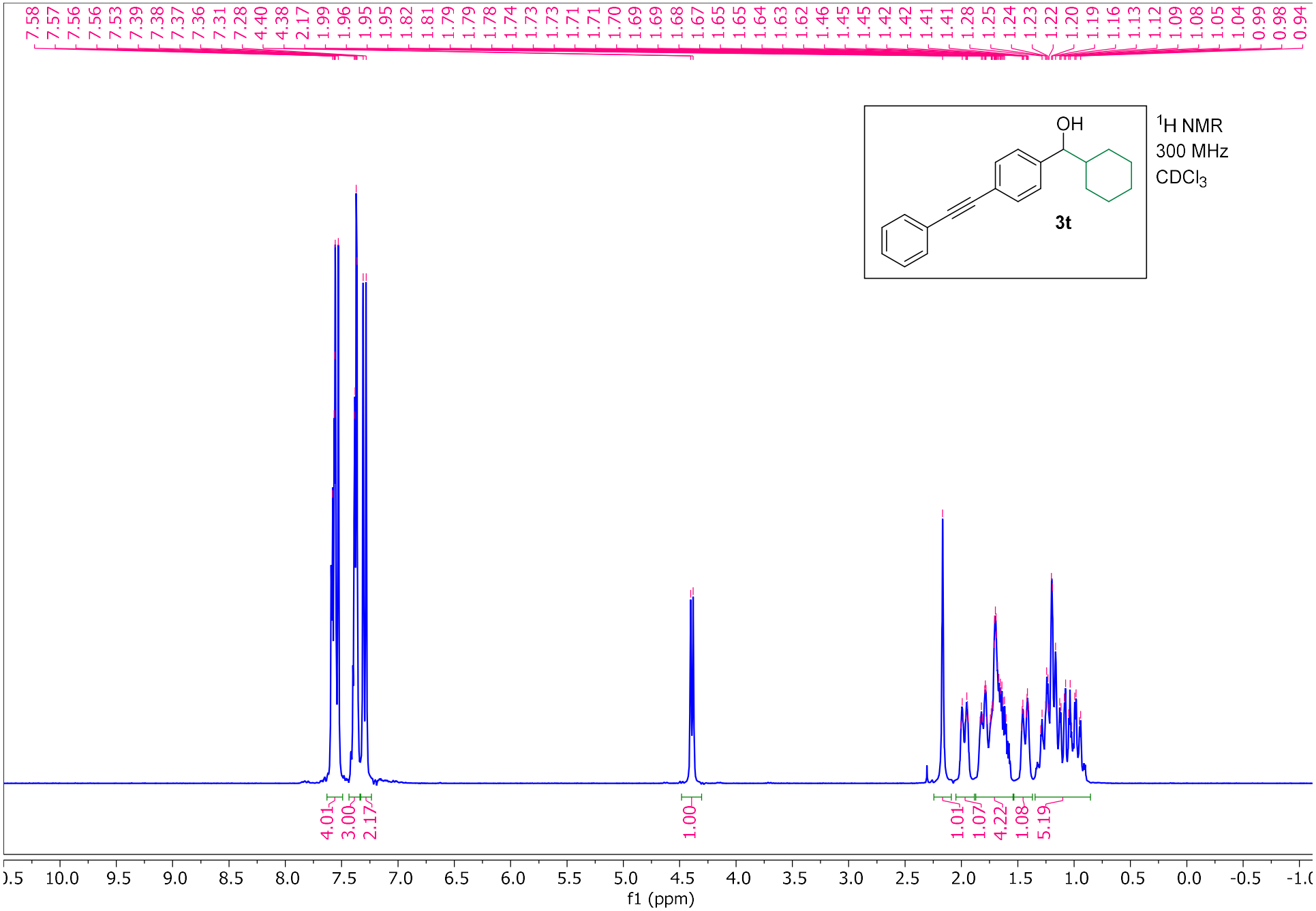

169.86
150.89
130.60
130.49
127.83
79.45
46.32
30.48
29.86
27.55
27.24
27.19
OH
O
OH
3q
$^{13}C\{^{1}H\}$ NMR
75 MHz
CD_3OD
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

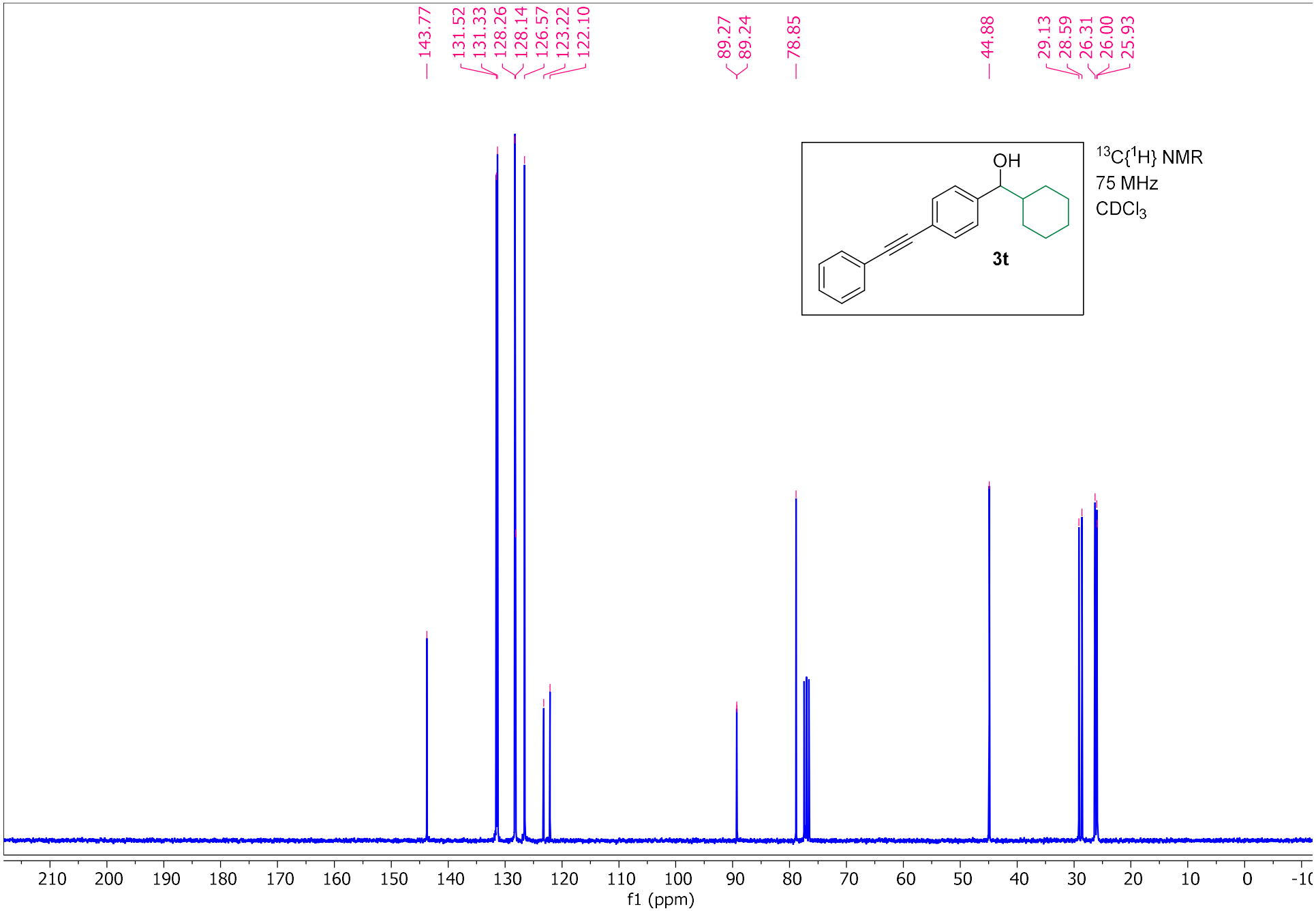

7.21 7.18 6.89 6.86 6.10 6.09 6.07 6.05 6.03 6.01 5.44 5.44 5.39 5.38 5.31 5.30 5.30 5.27 5.26 4.54 4.53 4.53 4.52 4.51 4.51 4.29 4.26 2.02 1.99 1.98 1.98 1.97 1.97 1.75 1.74 1.67 1.66 1.65 1.65 1.64 1.63 1.62 1.61 1.60 1.58 1.56 1.33 1.33 1.21 1.18 1.17 1.17 1.16 1.15 1.14 1.12 1.11 1.03 1.03 1.02 0.99 0.89
OH
O
3r
^{1}H NMR
300 MHz
$CDCl_3$
2.00 2.02 0.99 0.99 1.00 1.98 1.00 2.03 1.27 3.15 1.07 5.22
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 -0.5
f1 (ppm)

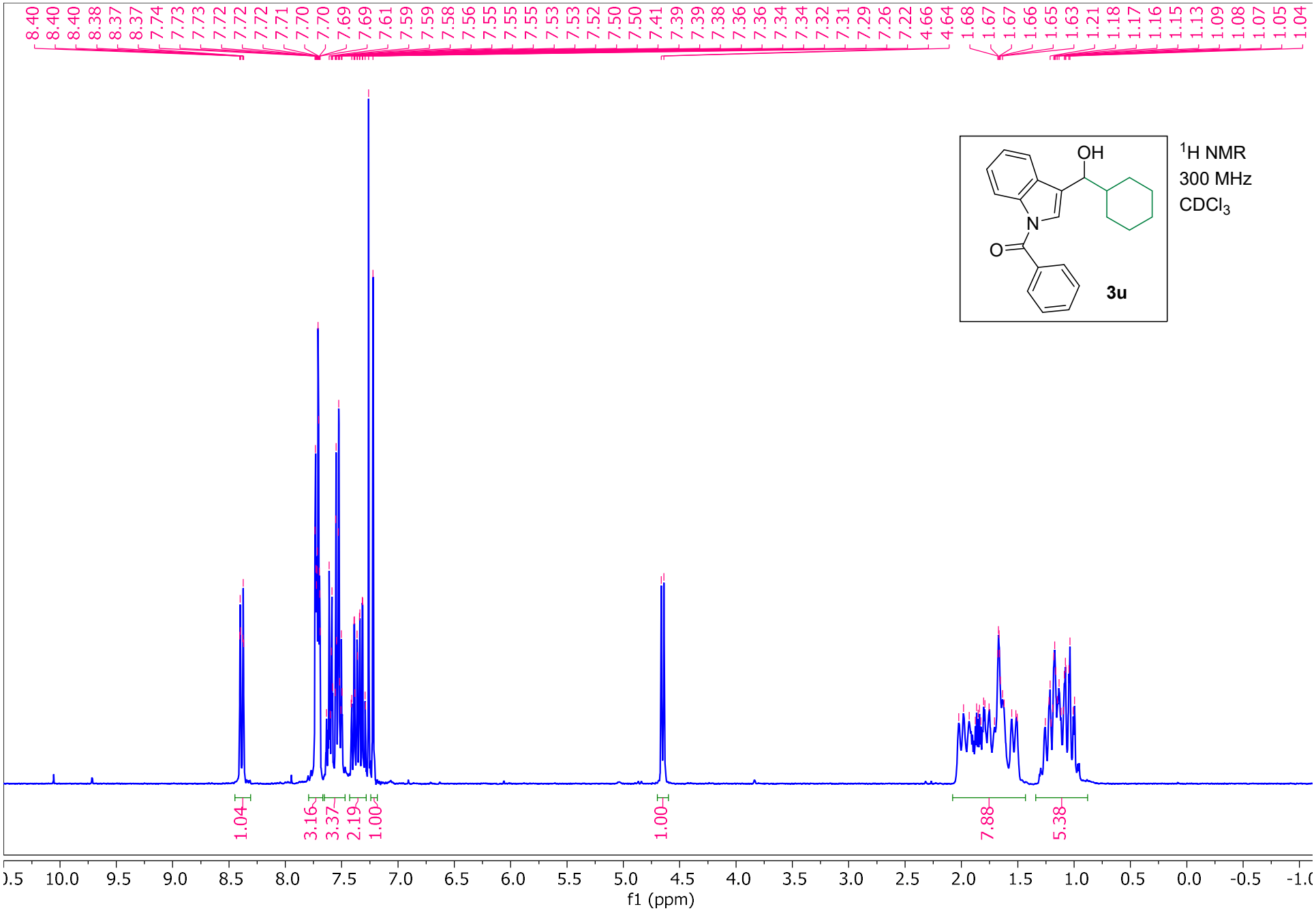

157.85
135.95
133.27
127.68
117.54
114.29
78.88
68.74
44.86
29.17
29.01
26.37
26.01
25.94
OH
O
3r
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

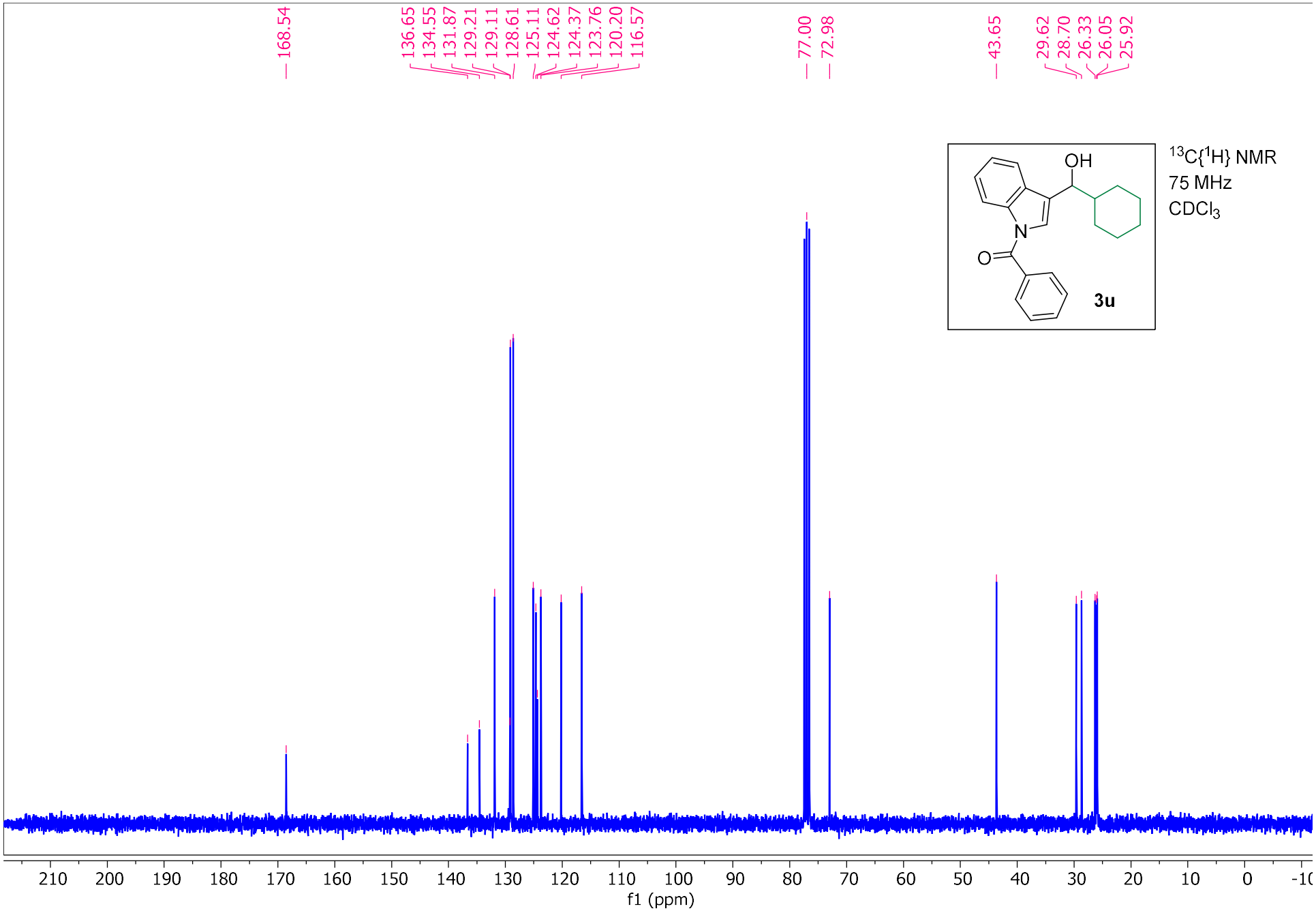

7.23 7.20 6.95 6.92 4.68 4.67 4.30 4.28 2.53 2.52 2.51 2.01 2.01 2.00 1.98 1.97 1.97 1.95 1.78 1.75 1.74 1.74 1.67 1.66 1.65 1.65 1.64 1.63 1.63 1.62 1.61 1.60 1.58 1.57 1.56 1.55 1.38 1.37 1.37 1.34 1.34 1.33 1.33 1.21 1.20 1.17 1.17 1.14 1.14 1.12 1.11 1.08 1.06 1.04 1.03 1.03 1.02 1.00 0.98 0.90 0.89 0.85
OH
O
3s
1H NMR
300 MHz
CDCl3
2.03
2.04
2.02
1.01
1.00
2.03
4.38
6.33
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 -0.5
f1 (ppm)

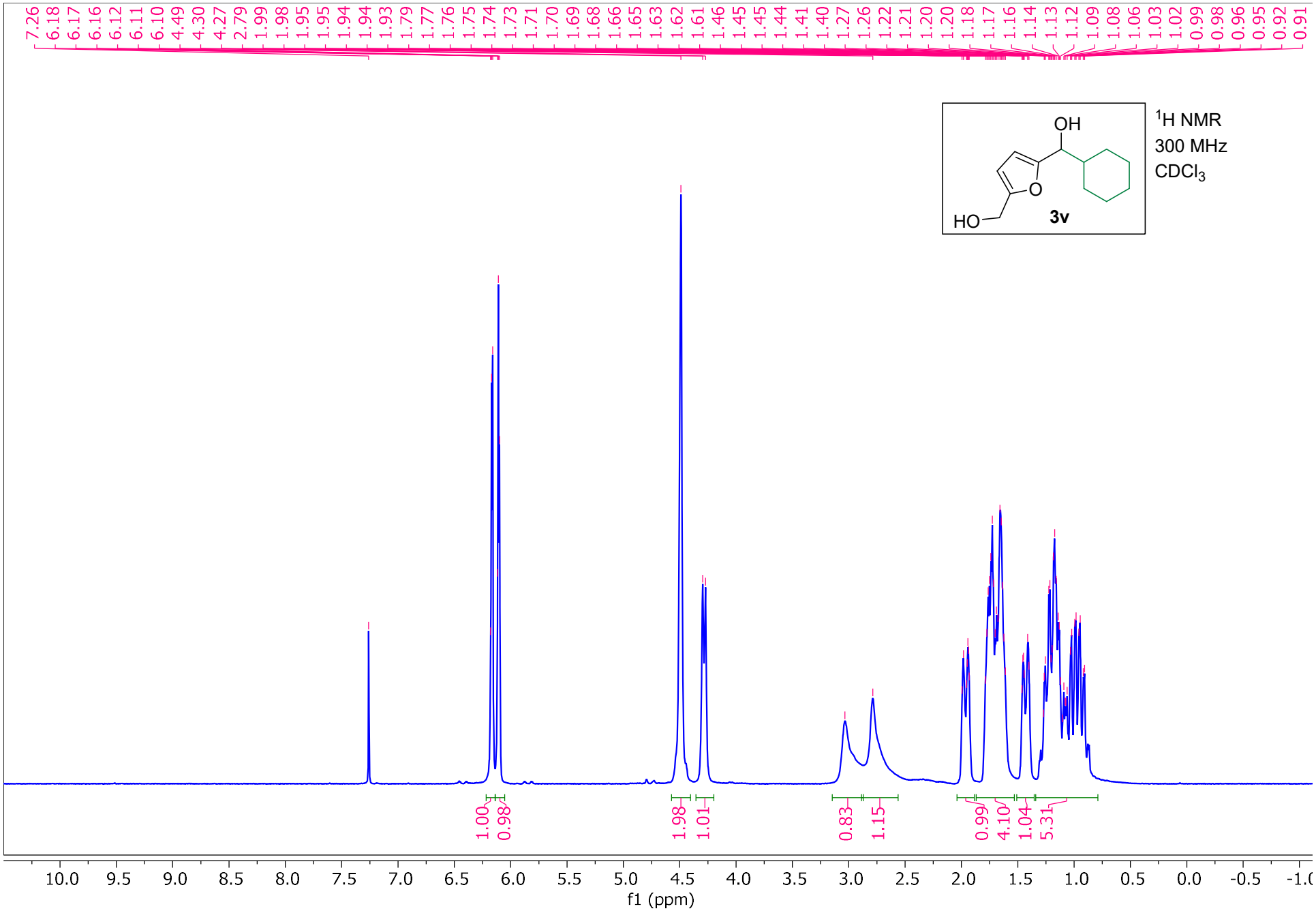

156.81
136.73
127.72
114.48
78.83
78.59
77.00
75.45
55.77
44.86
29.18
28.95
26.36
26.01
25.93
OH
O
3s
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

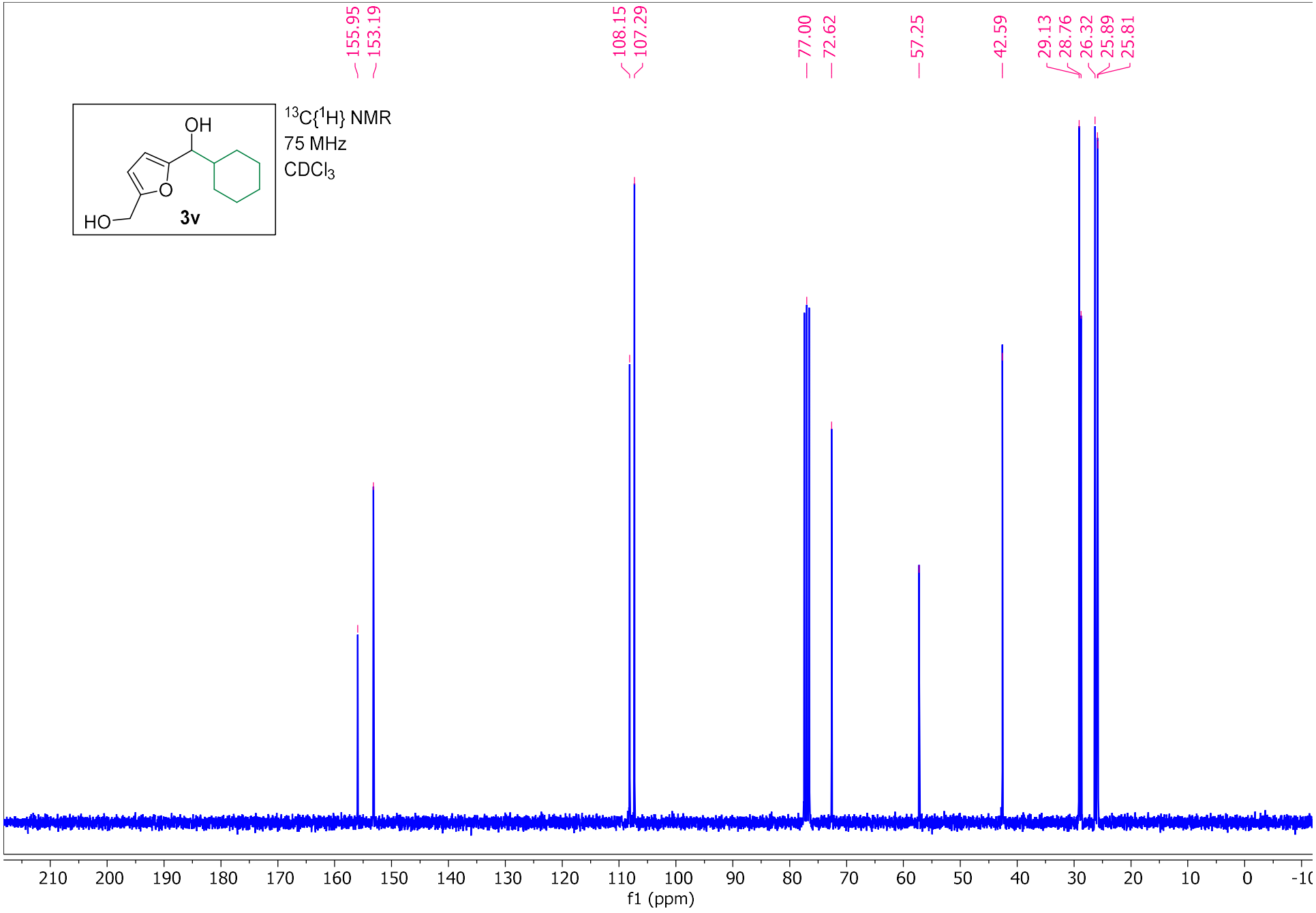

7.58 7.57 7.56 7.56 7.53 7.39 7.38 7.37 7.36 7.31 7.28 4.40 4.38 2.17 1.99 1.96 1.95 1.95 1.82 1.81 1.79 1.79 1.78 1.74 1.73 1.73 1.71 1.71 1.70 1.69 1.69 1.68 1.67 1.65 1.65 1.64 1.63 1.62 1.46 1.45 1.45 1.42 1.42 1.41 1.41 1.28 1.25 1.24 1.23 1.22 1.20 1.19 1.16 1.13 1.12 1.09 1.08 1.05 1.04 0.99 0.98 0.94
OH
3t
^{1}H NMR
300 MHz
$CDCl_3$
4.01 3.00 2.17 1.00 1.01 1.07 4.22 1.08 5.19
f1 (ppm)

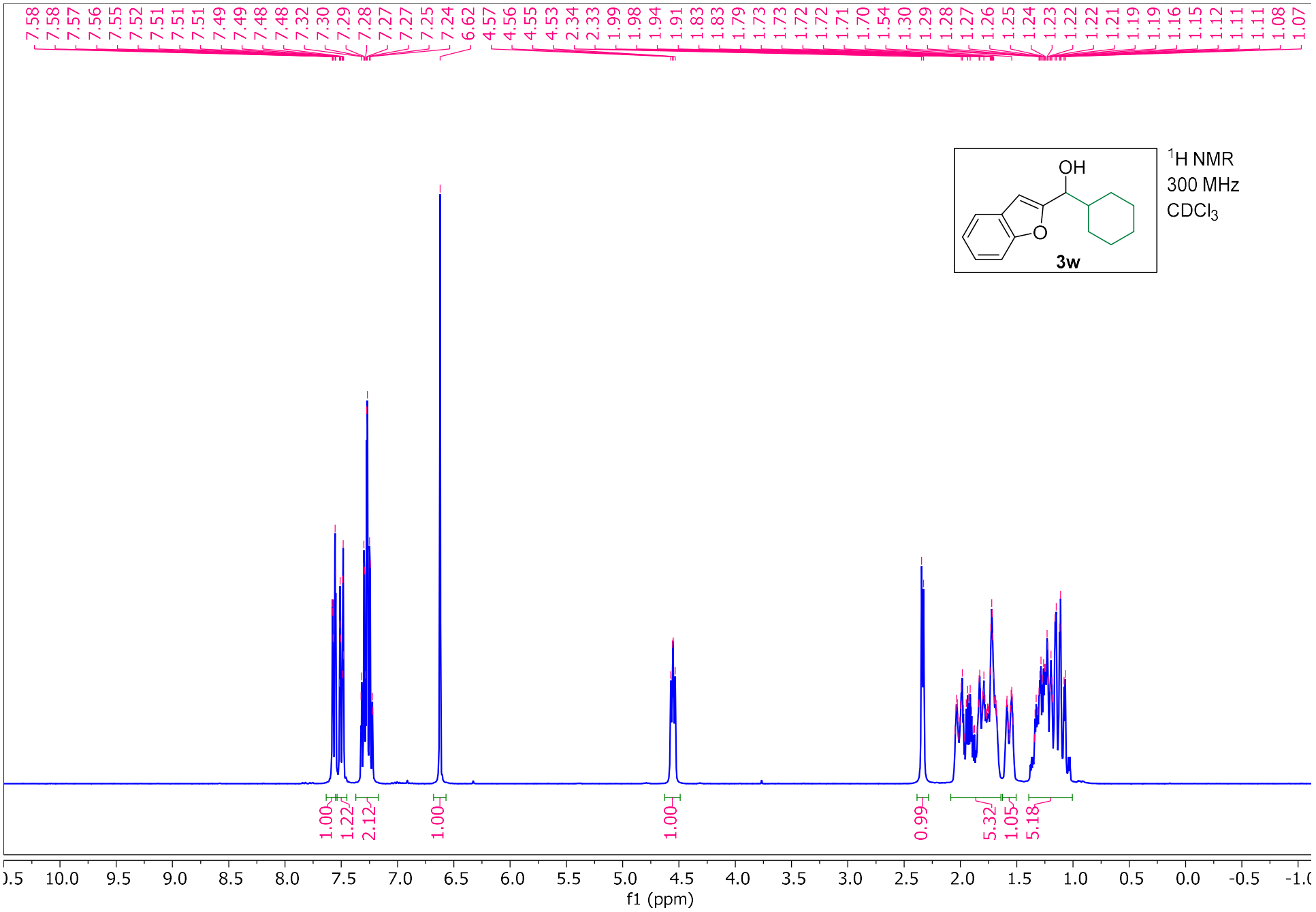

143.77
131.52
131.33
128.26
128.14
126.57
123.22
122.10
89.27
89.24
78.85
44.88
29.13
28.59
26.31
26.00
25.93
OH
3t
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

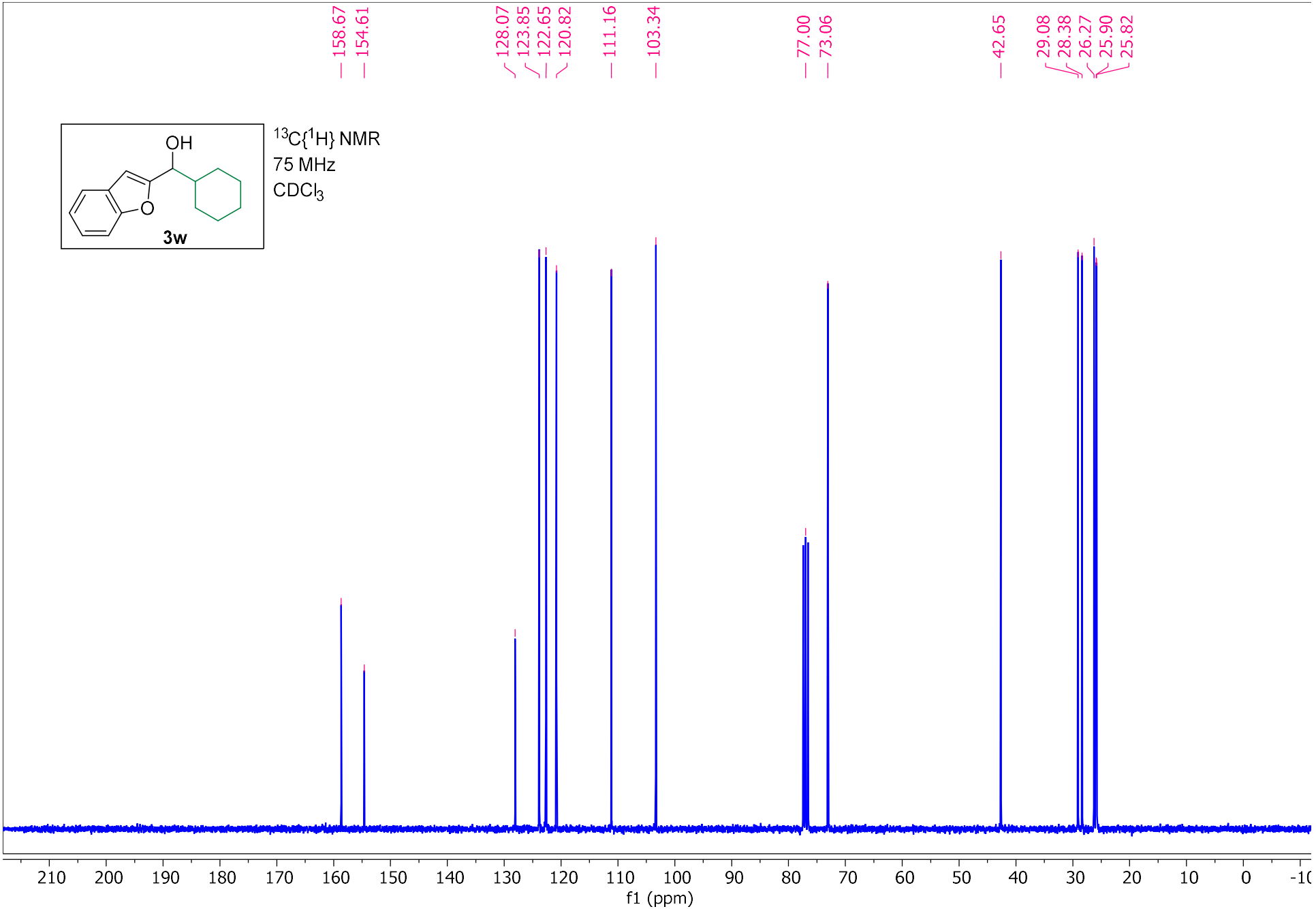

8.40 8.40 8.40 8.38 8.37 8.37 7.74 7.73 7.73 7.72 7.72 7.72 7.71 7.70 7.70 7.69 7.69 7.61 7.59 7.59 7.58 7.56 7.55 7.55 7.55 7.53 7.53 7.52 7.50 7.50 7.41 7.39 7.39 7.38 7.36 7.36 7.34 7.34 7.32 7.31 7.29 7.26 7.22 4.66 4.64 1.68 1.67 1.67 1.66 1.65 1.63 1.21 1.18 1.17 1.16 1.15 1.13 1.09 1.08 1.07 1.05 1.04
OH
N
O
3u
1H NMR
300 MHz
CDCl3
1.04
3.16
3.37
2.19
1.00
1.00
7.88
5.38
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 -0.5
f1 (ppm)

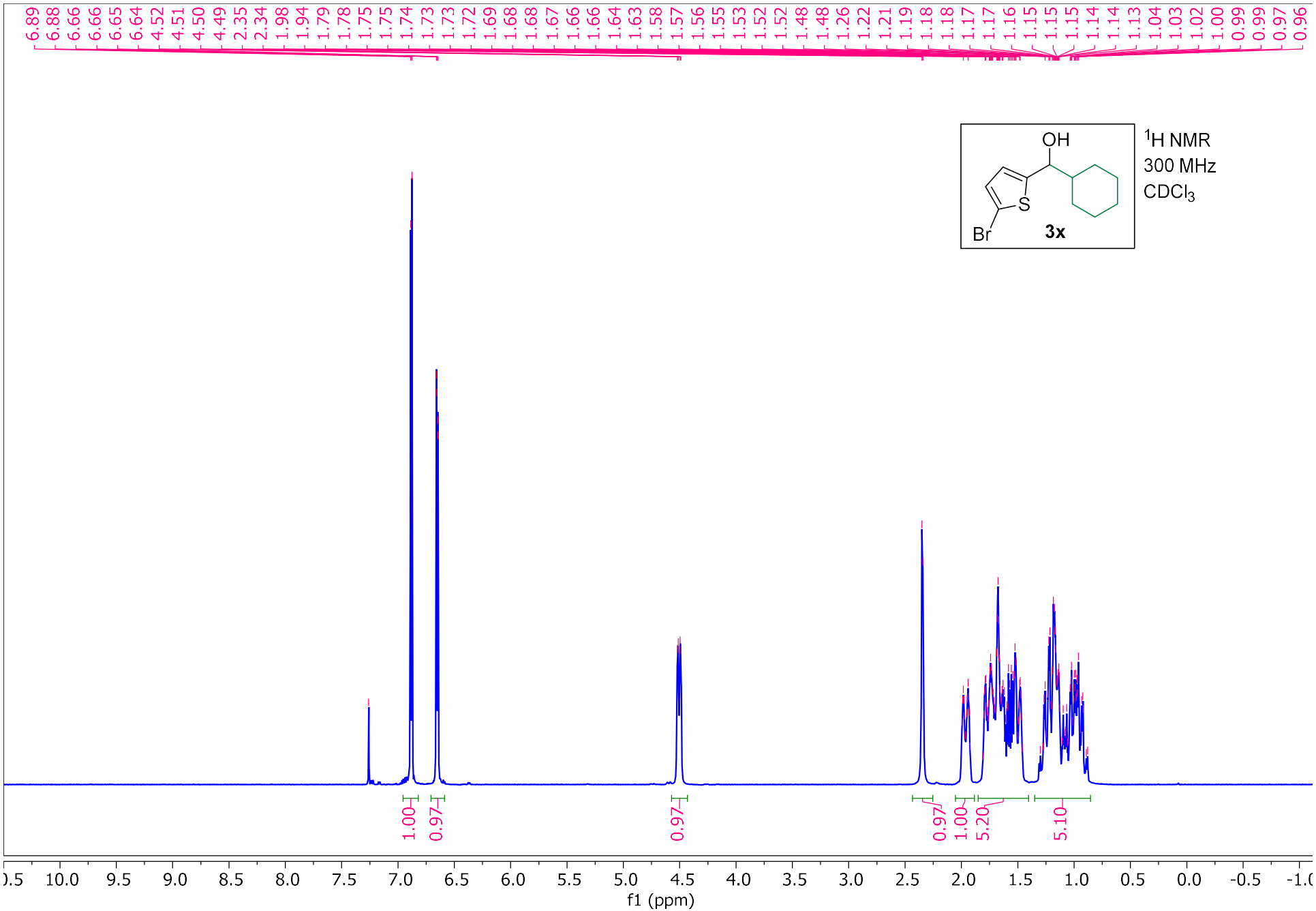

168.54
136.65
134.55
131.87
129.21
129.11
128.61
125.11
124.62
124.37
123.76
120.20
116.57
77.00
72.98
43.65
29.62
28.70
26.33
26.05
25.92
OH
N
O
3u
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

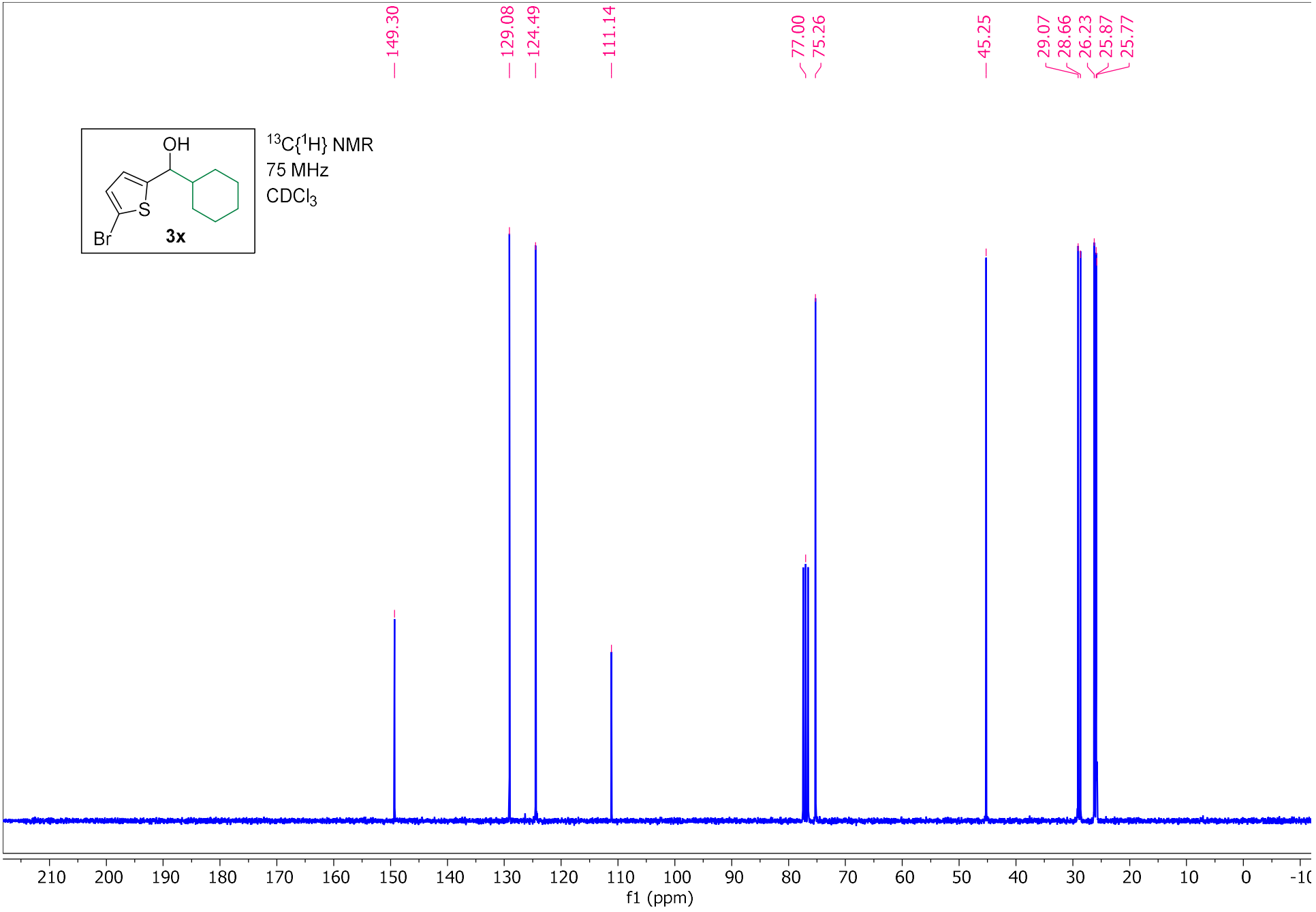

7.26 6.18 6.17 6.16 6.12 6.11 6.10 4.49 4.30 4.27 2.79 1.99 1.98 1.95 1.95 1.94 1.94 1.93 1.79 1.77 1.76 1.75 1.74 1.73 1.71 1.70 1.69 1.68 1.66 1.65 1.63 1.62 1.61 1.46 1.45 1.45 1.44 1.41 1.40 1.27 1.26 1.22 1.21 1.20 1.20 1.18 1.17 1.16 1.14 1.13 1.12 1.09 1.08 1.06 1.03 1.02 0.99 0.98 0.96 0.95 0.92 0.91
OH
O
HO
3v
1H NMR
300 MHz
CDCl3
1.00 0.98 1.98 1.01 0.83 1.15 0.99 4.10 1.04 5.31
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 -0.5
f1 (ppm)

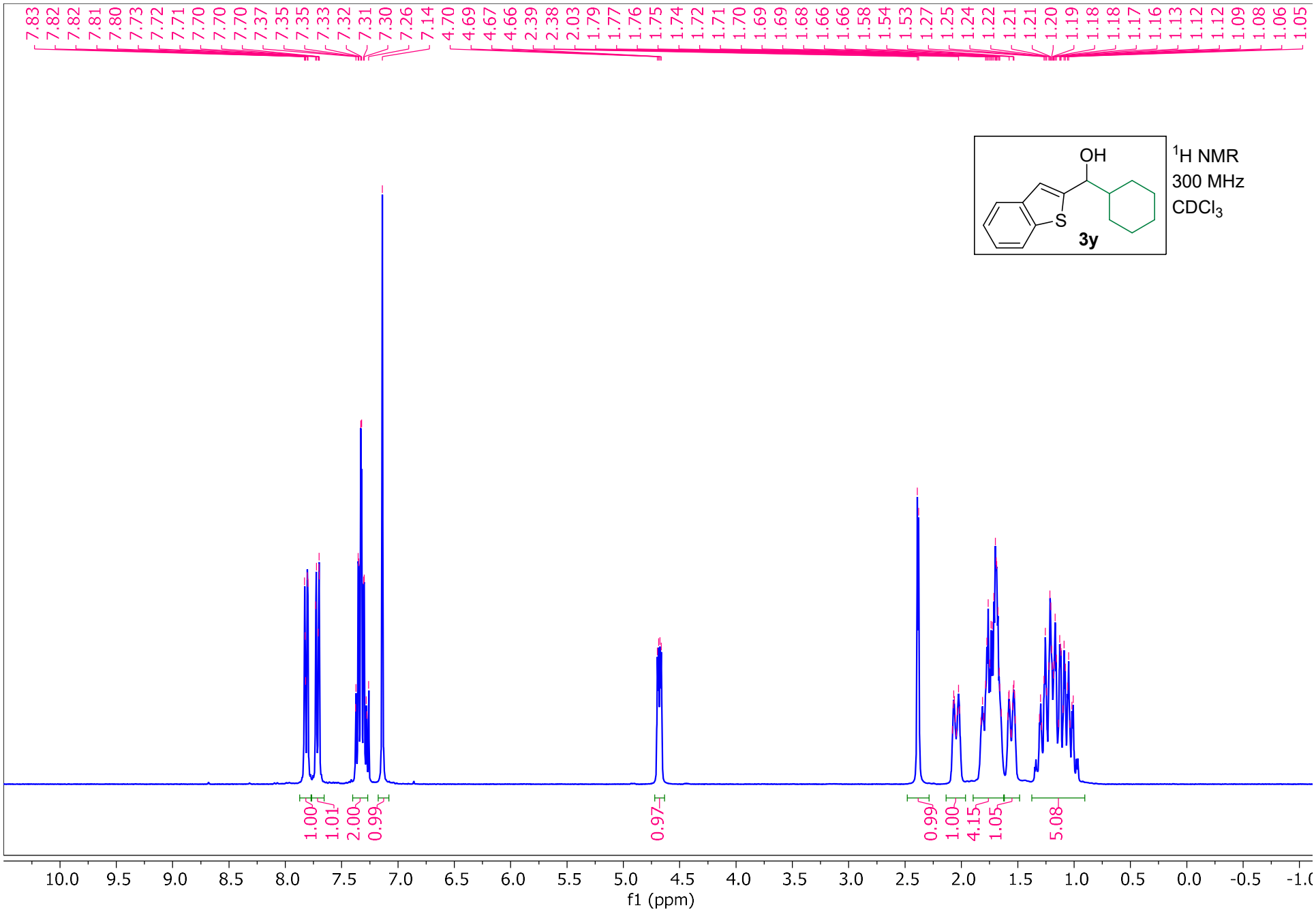

155.95
153.19
108.15
107.29
77.00
72.62
57.25
42.59
29.13
28.76
26.32
25.89
25.81
OH
O
HO
3v
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

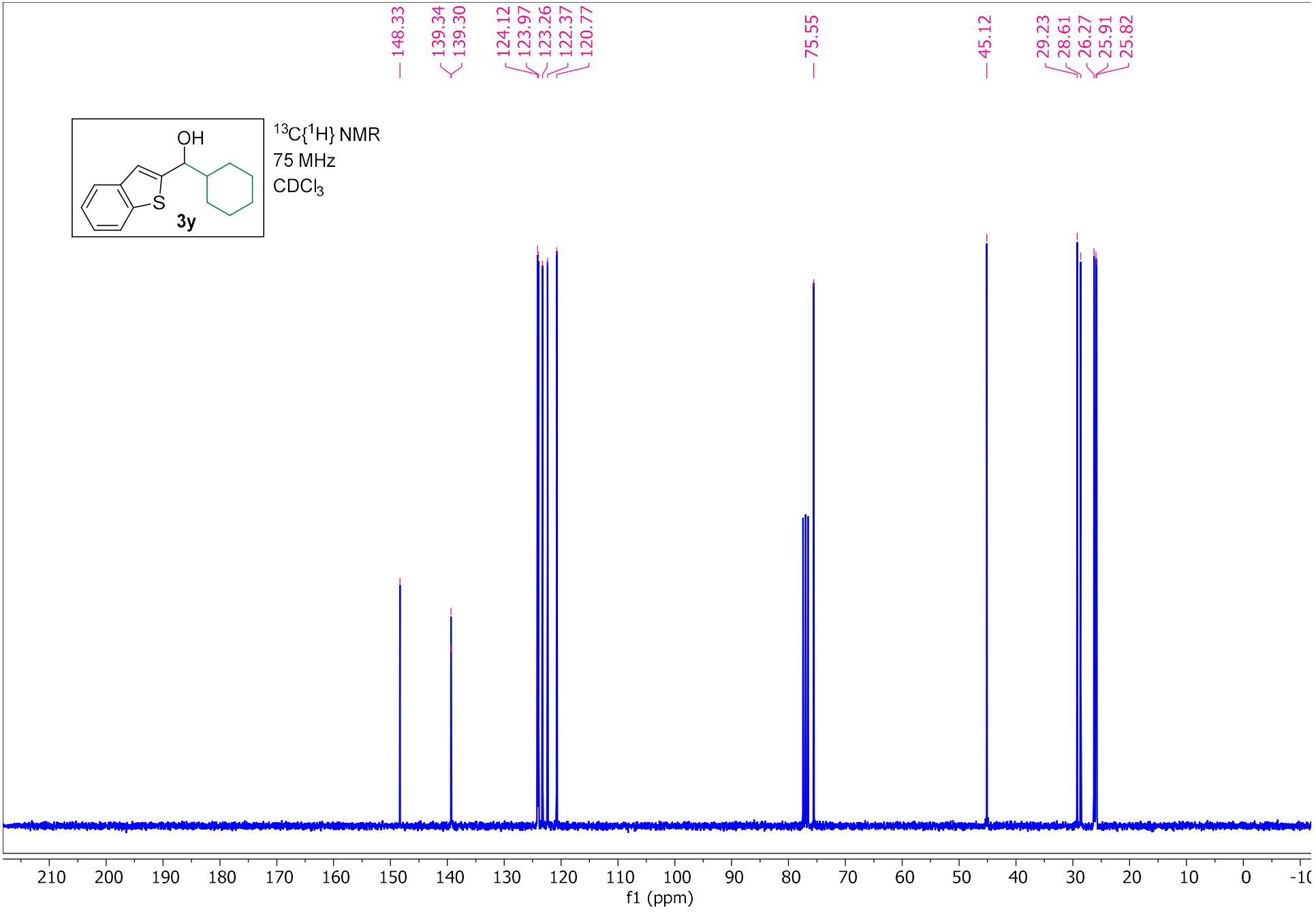

7.58 7.58 7.57 7.56 7.55 7.52 7.51 7.51 7.51 7.49 7.49 7.48 7.48 7.32 7.30 7.29 7.28 7.27 7.27 7.25 7.24 6.62 4.57 4.56 4.55 4.53 2.34 2.33 1.99 1.98 1.94 1.91 1.83 1.83 1.79 1.73 1.73 1.72 1.72 1.71 1.70 1.54 1.30 1.29 1.28 1.27 1.26 1.25 1.24 1.23 1.22 1.22 1.21 1.19 1.19 1.16 1.15 1.12 1.11 1.11 1.08 1.07
OH
O
3w
1H NMR
300 MHz
CDCl3
1.00 1.22 2.12 1.00 1.00 0.99 5.32 1.05 5.18
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 -0.5
f1 (ppm)

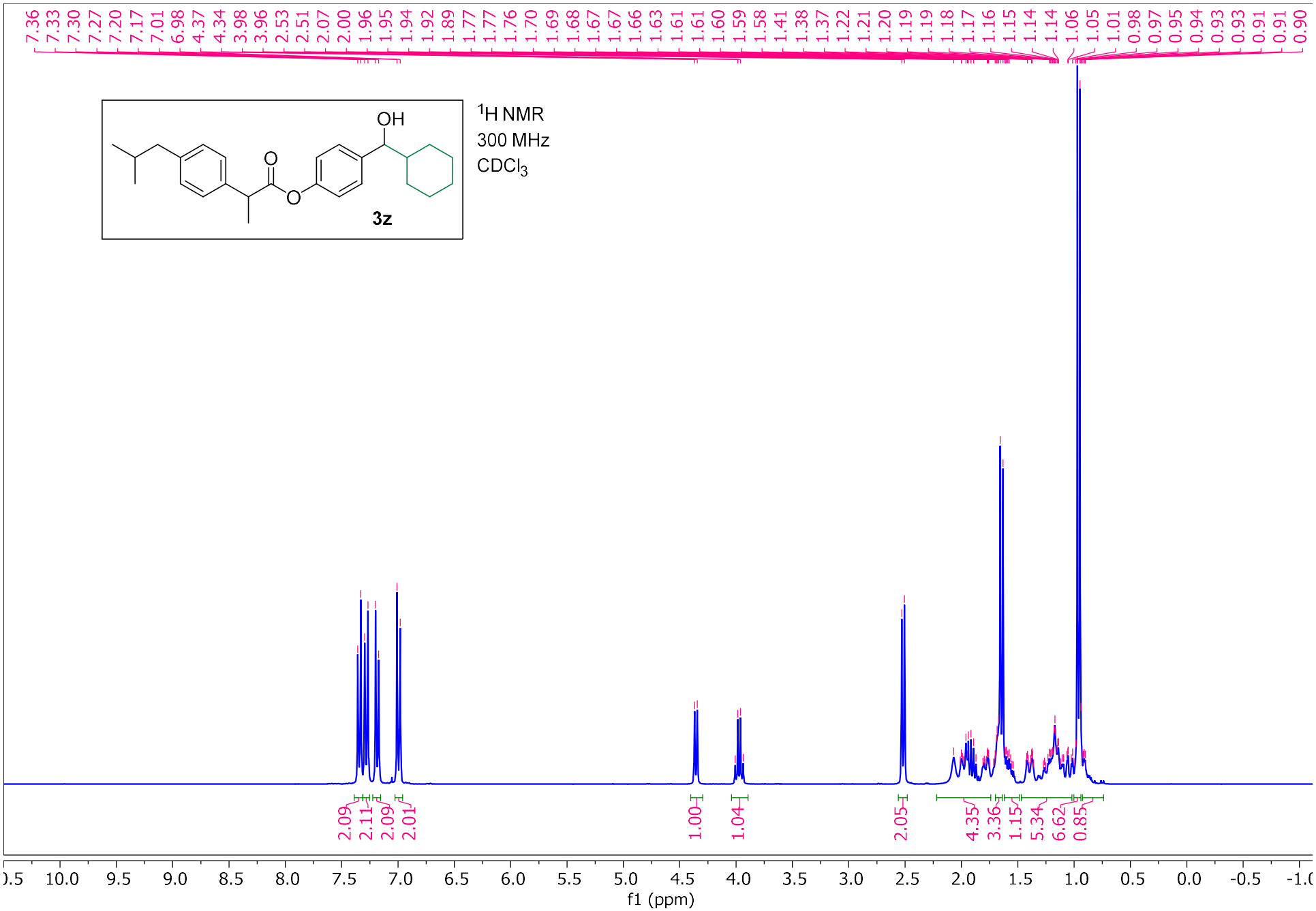

158.67
154.61
128.07
123.85
122.65
120.82
111.16
103.34
77.00
73.06
42.65
29.08
28.38
26.27
25.90
25.82
OH
O
3w
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

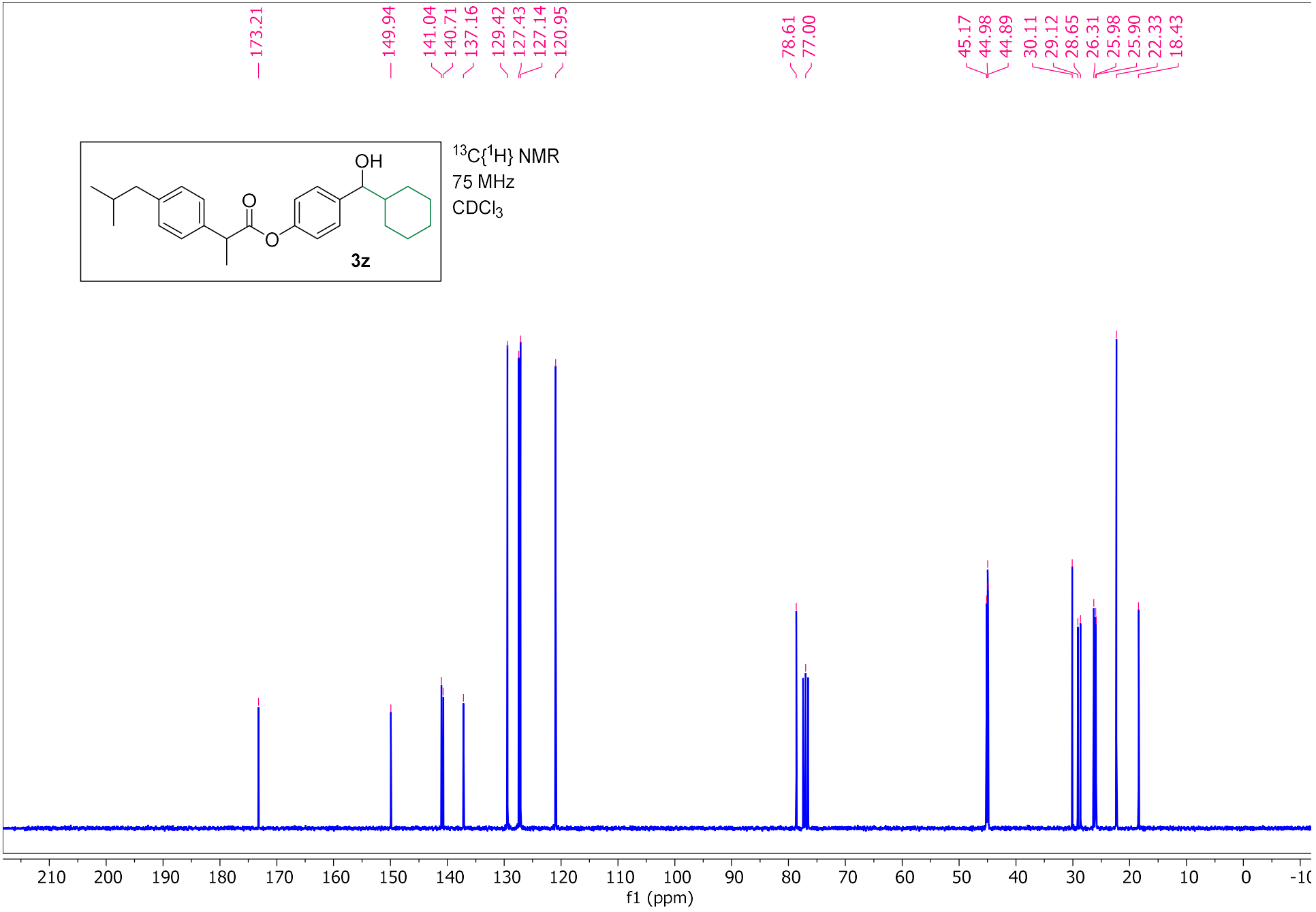

6.89 6.88 6.66 6.66 6.65 6.64 4.52 4.51 4.50 4.49 2.35 2.34 1.98 1.94 1.79 1.78 1.75 1.75 1.74 1.73 1.73 1.72 1.69 1.68 1.68 1.67 1.66 1.66 1.64 1.63 1.58 1.57 1.56 1.55 1.53 1.52 1.52 1.48 1.48 1.26 1.22 1.21 1.19 1.18 1.18 1.17 1.17 1.16 1.15 1.15 1.15 1.14 1.14 1.13 1.04 1.03 1.02 1.00 0.99 0.99 0.97 0.96
OH
S
Br
3x
1H NMR
300 MHz
CDCl3
1.00
0.97
0.97
0.97
1.00
5.20
5.10
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 -0.5
f1 (ppm)

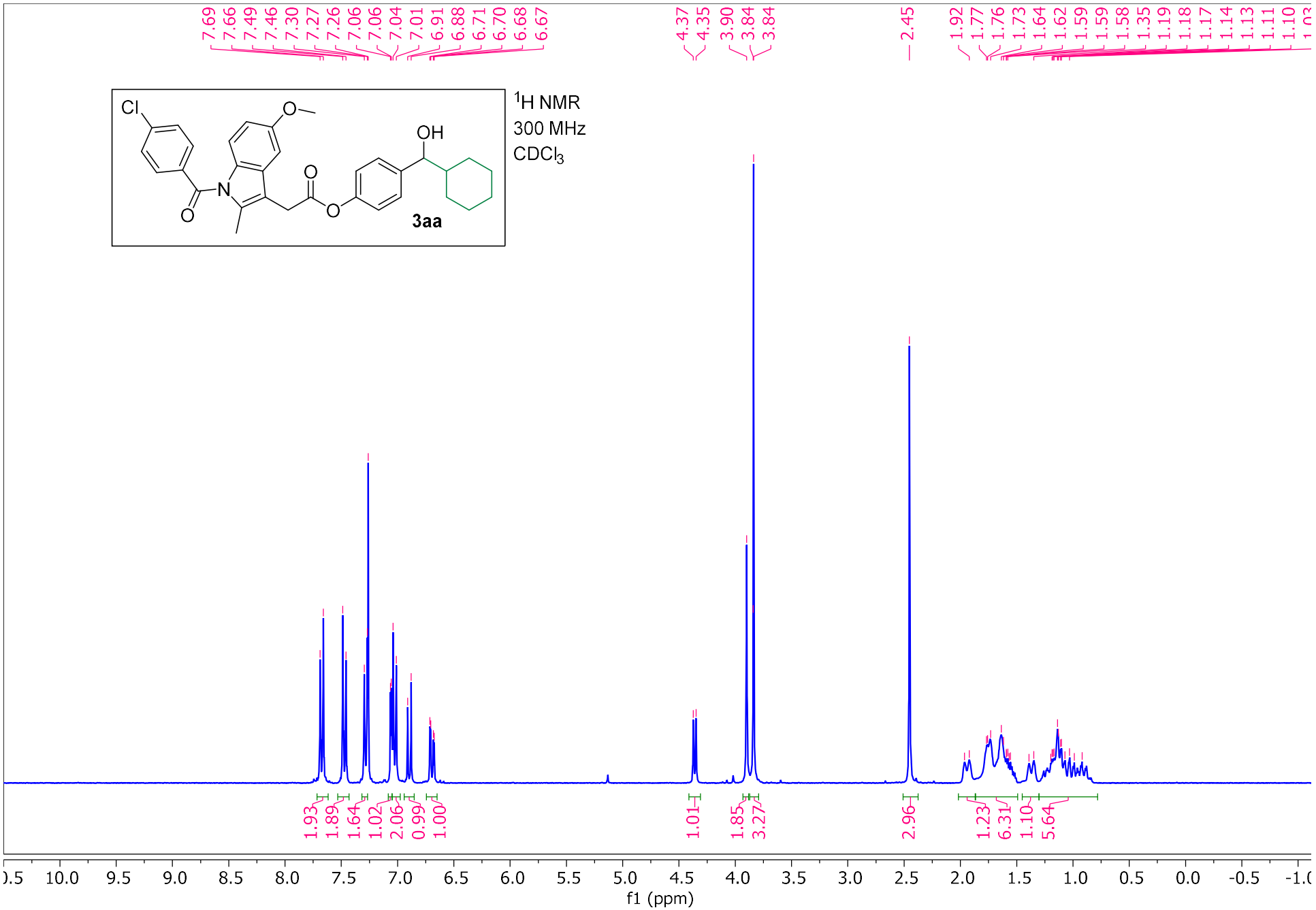

149.30
129.08
124.49
111.14
77.00
75.26
45.25
29.07
28.66
26.23
25.87
25.77
OH
S
Br
3x
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

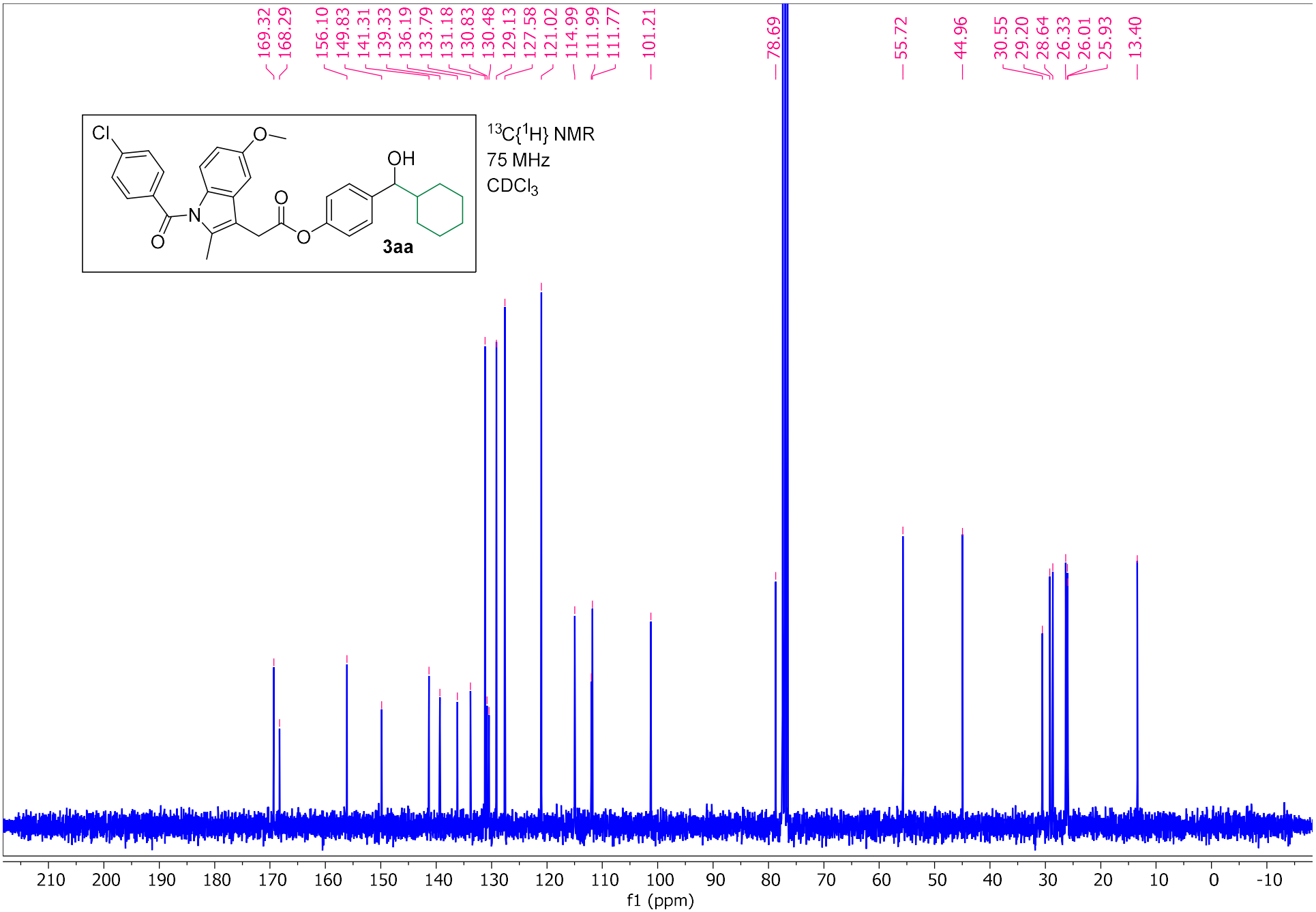

7.83 7.82 7.82 7.81 7.80 7.73 7.72 7.71 7.70 7.70 7.70 7.37 7.35 7.35 7.33 7.32 7.31 7.30 7.26 7.14
4.70 4.69 4.67 4.66 2.39 2.38 2.03 1.79 1.77 1.76 1.75 1.74 1.72 1.71 1.70 1.69 1.69 1.68 1.66 1.66 1.58 1.54 1.53 1.27 1.25 1.24 1.22 1.21 1.21 1.20 1.19 1.18 1.18 1.17 1.16 1.13 1.12 1.12 1.09 1.08 1.06 1.05
OH
S
3y
1H NMR
300 MHz
CDCl3
1.00 1.01 2.00 0.99 0.97 0.99 1.00 4.15 1.05 5.08
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 -0.5
f1 (ppm)

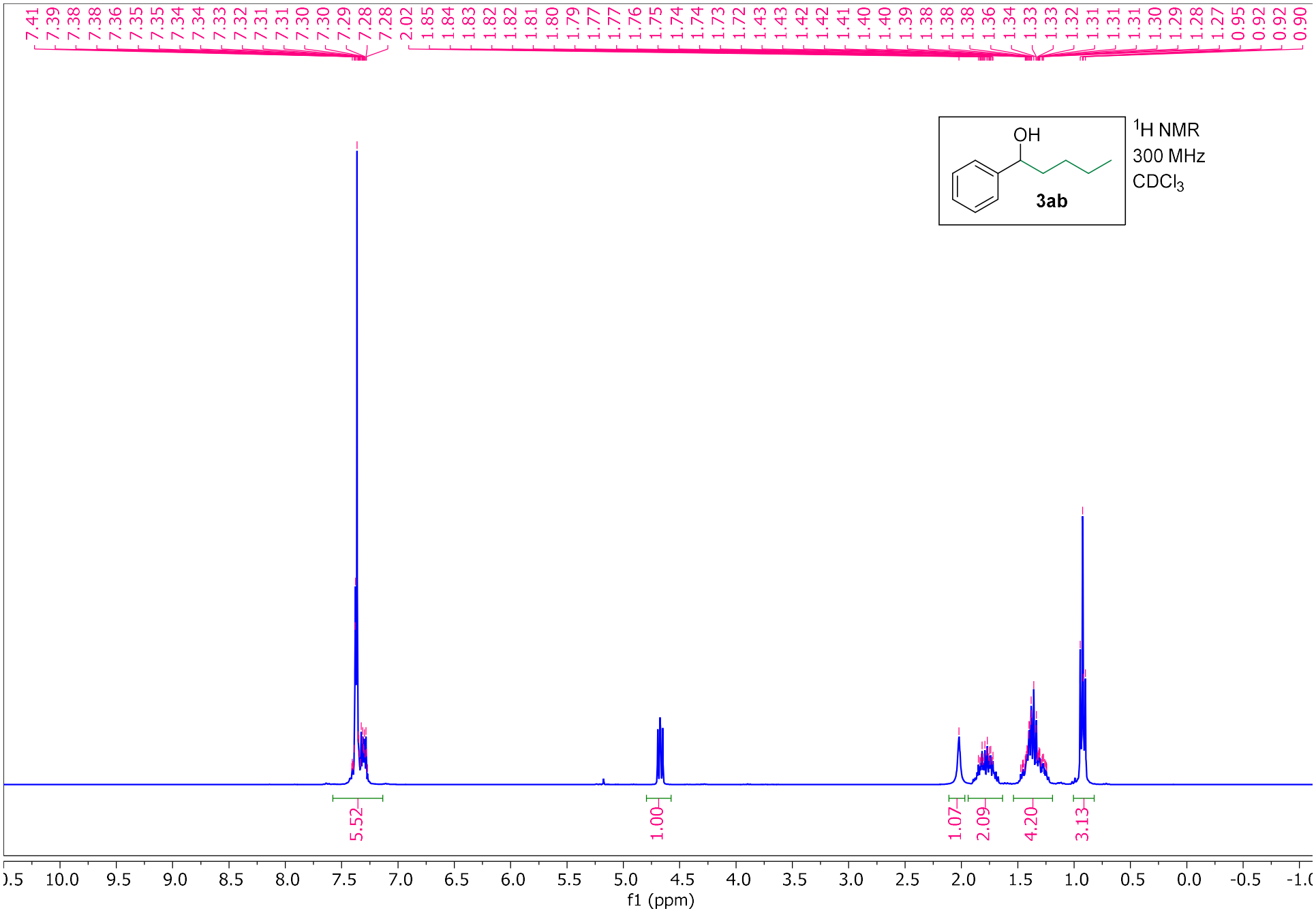

148.33
139.34
139.30
124.12
123.97
123.26
122.37
120.77
75.55
45.12
29.23
28.61
26.27
25.91
25.82
OH
S
3y
13C{1H} NMR
75 MHz
CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

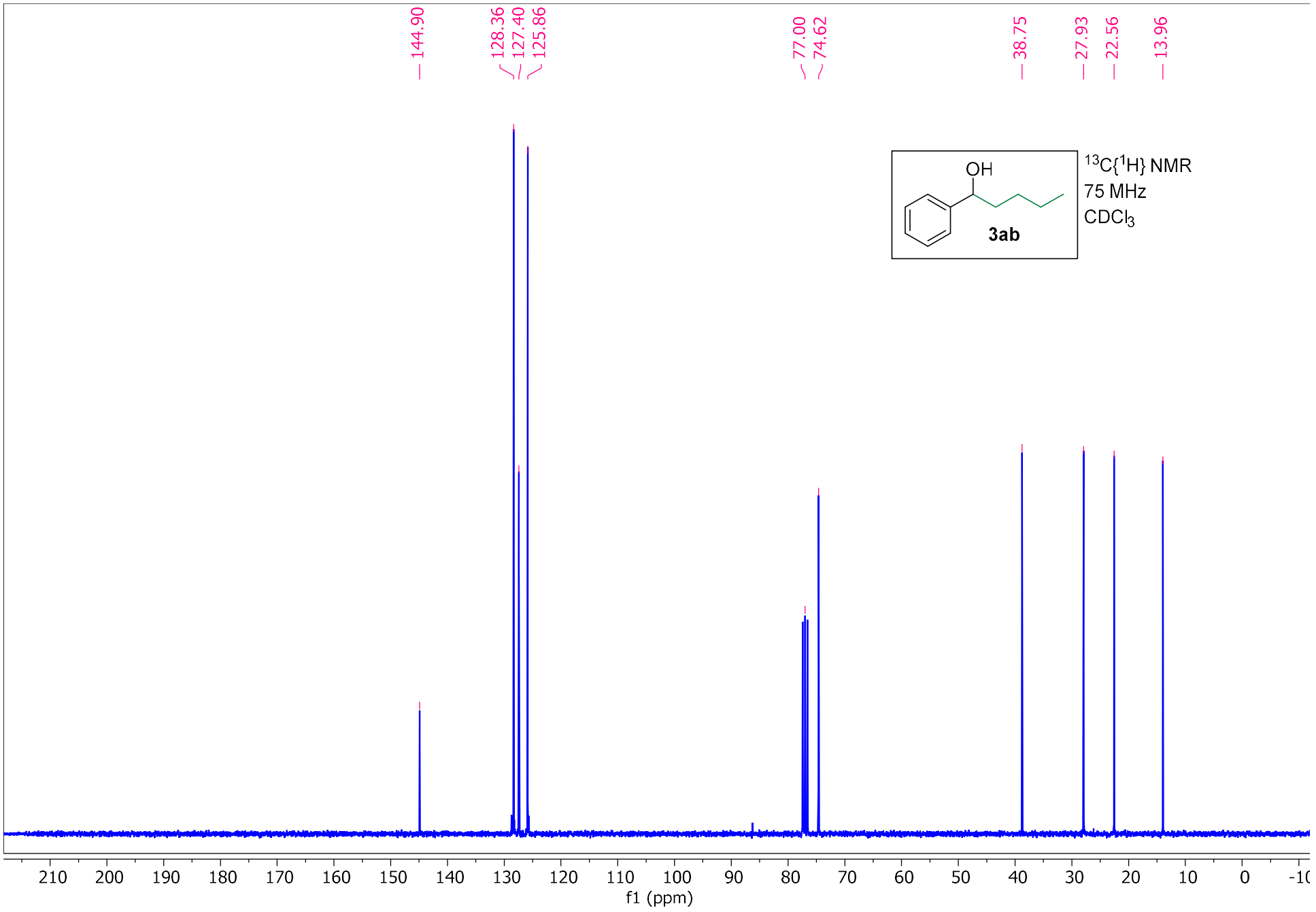

7.36 7.33 7.30 7.27 7.20 7.17 7.01 6.98 4.37 4.34 3.98 3.96 2.53 2.51 2.07 2.00 1.96 1.95 1.94 1.92 1.89 1.77 1.77 1.76 1.70 1.69 1.68 1.67 1.67 1.66 1.63 1.61 1.61 1.60 1.59 1.58 1.41 1.38 1.37 1.22 1.21 1.20 1.19 1.19 1.18 1.17 1.16 1.15 1.14 1.14 1.06 1.05 1.01 0.98 0.97 0.95 0.94 0.93 0.93 0.91 0.91 0.90
OH
O
O
3z
1H NMR
300 MHz
CDCl3
2.09 2.11 2.09 2.01 1.00 1.04 2.05 4.35 3.36 1.15 5.34 6.62 0.85
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 -0.5
f1 (ppm)

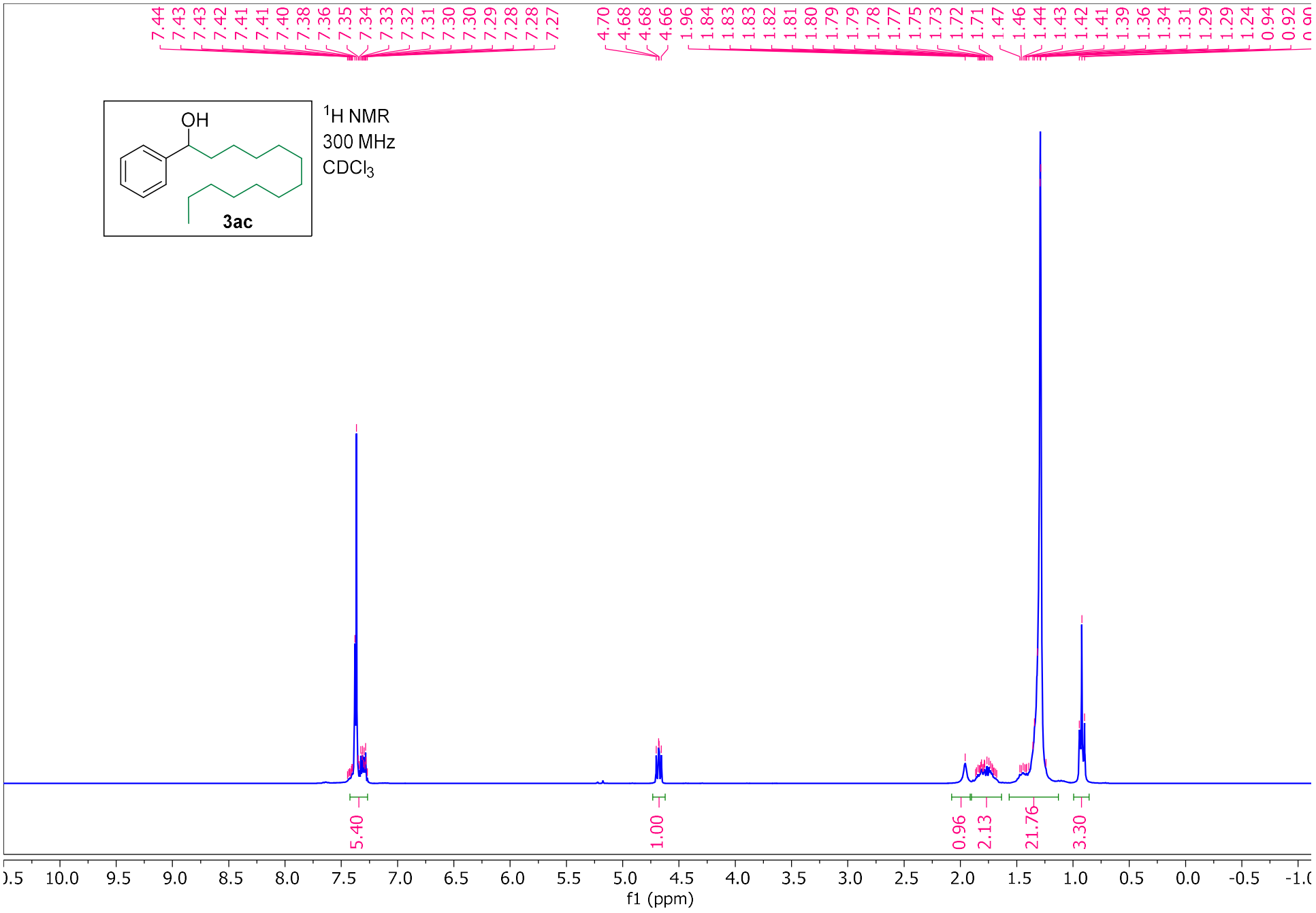

173.21
149.94
141.04
140.71
137.16
129.42
127.43
127.14
120.95
78.61
77.00
45.17
44.98
44.89
30.11
29.12
28.65
26.31
25.98
25.90
22.33
18.43
OH
O
O
3z
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

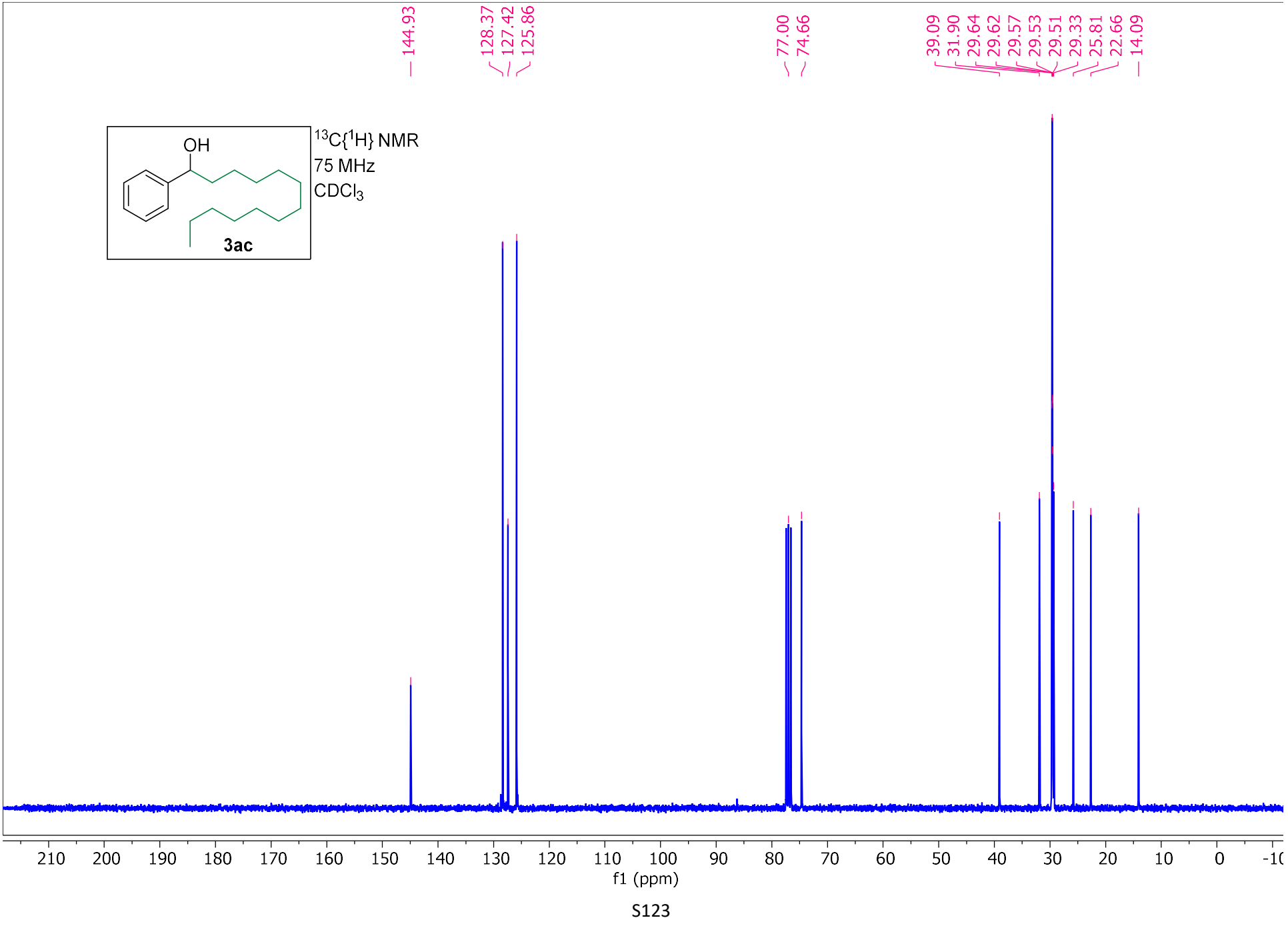

7.69
7.66
7.49
7.46
7.30
7.27
7.26
7.06
7.06
7.04
7.01
6.91
6.88
6.71
6.70
6.68
6.67
4.37
4.35
3.90
3.84
3.84
2.45
1.92
1.77
1.76
1.73
1.64
1.62
1.59
1.59
1.58
1.35
1.19
1.18
1.17
1.14
1.13
1.11
1.10
Cl
O
OH
N
O
O
O
3aa
1H NMR
300 MHz
CDCl3
1.93
1.89
1.64
1.02
2.06
0.99
1.00
1.01
1.85
3.27
2.96
1.23
6.31
1.10
5.64
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
-0.5
f1 (ppm)

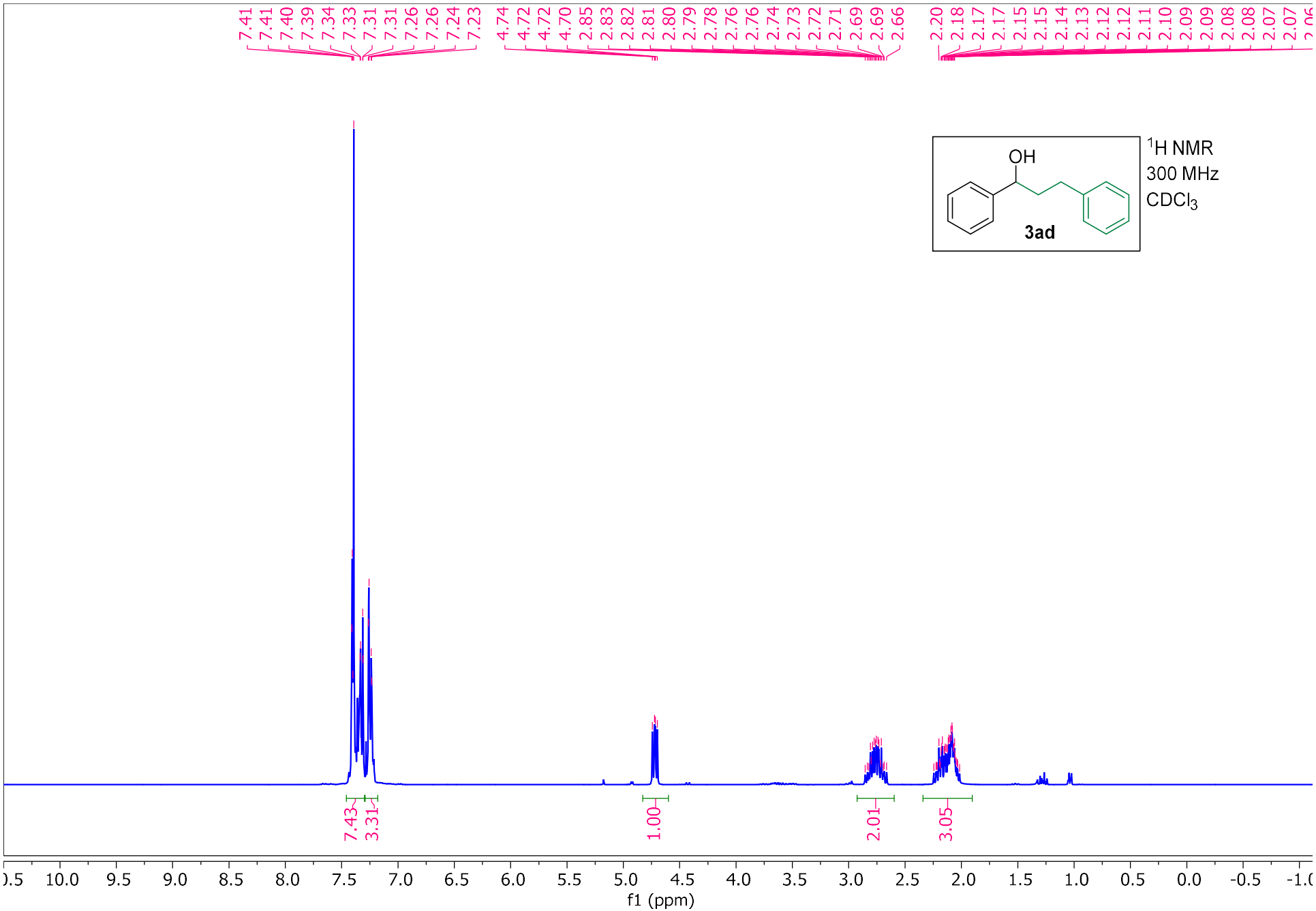

169.32
168.29
156.10
149.83
141.31
139.33
136.19
133.79
131.18
130.83
130.48
129.13
127.58
121.02
114.99
111.99
111.77
101.21
78.69
55.72
44.96
30.55
29.20
28.64
26.33
26.01
25.93
13.40
Cl
O
N
O
O
O
OH
3aa
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

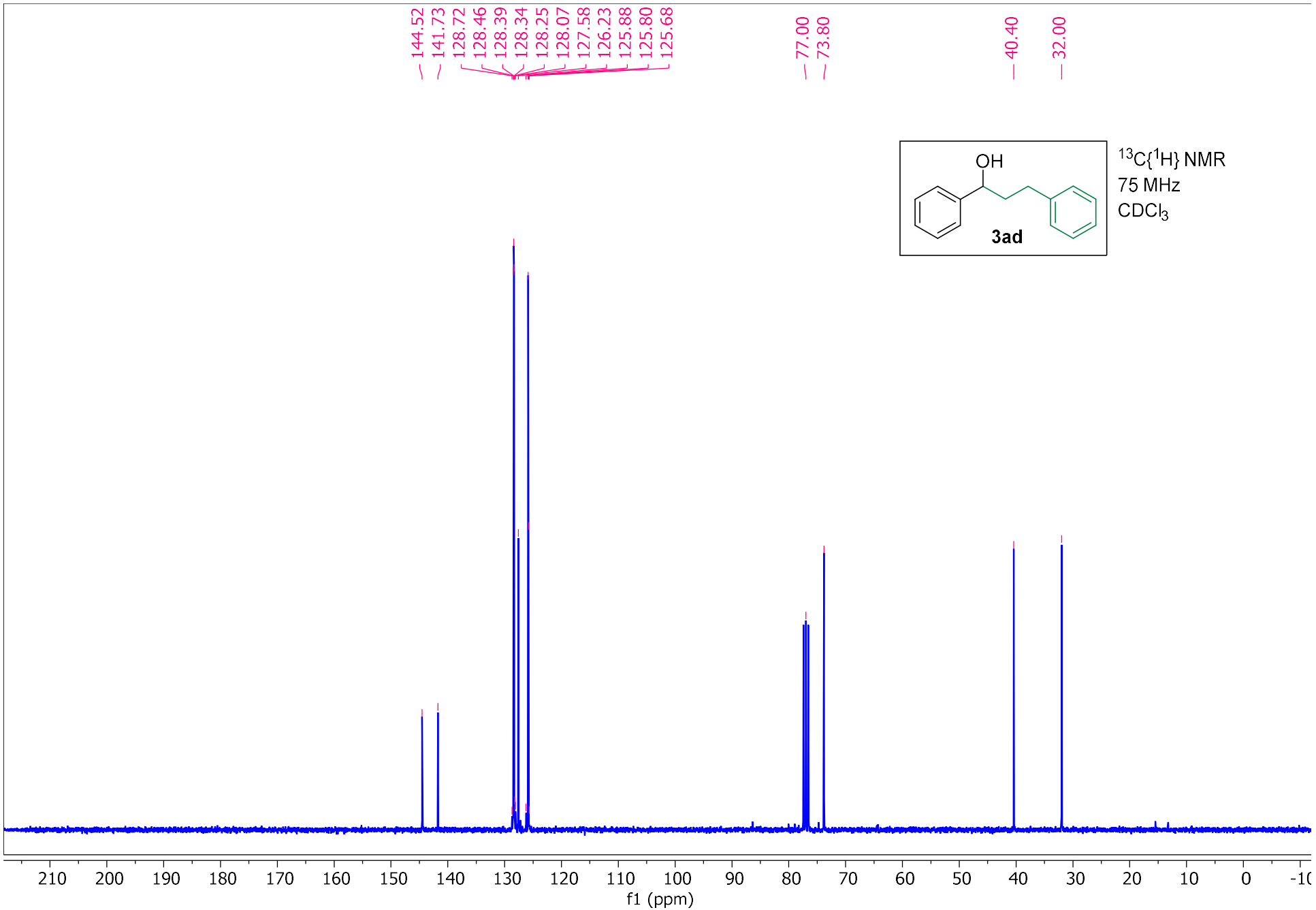

7.41 7.39 7.38 7.38 7.36 7.35 7.35 7.34 7.34 7.33 7.32 7.31 7.31 7.30 7.30 7.29 7.28 7.28
2.02 1.85 1.84 1.83 1.82 1.82 1.81 1.80 1.79 1.77 1.77 1.76 1.75 1.74 1.74 1.73 1.72 1.43 1.43 1.42 1.42 1.41 1.40 1.40 1.39 1.38 1.38 1.38 1.36 1.34 1.33 1.33 1.32 1.31 1.31 1.31 1.30 1.29 1.28 1.27 0.95 0.92 0.92 0.90
OH
3ab
^{1}H NMR
300 MHz
$CDCl_3$
5.52
1.00
1.07
2.09
4.20
3.13
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 -0.5
f1 (ppm)

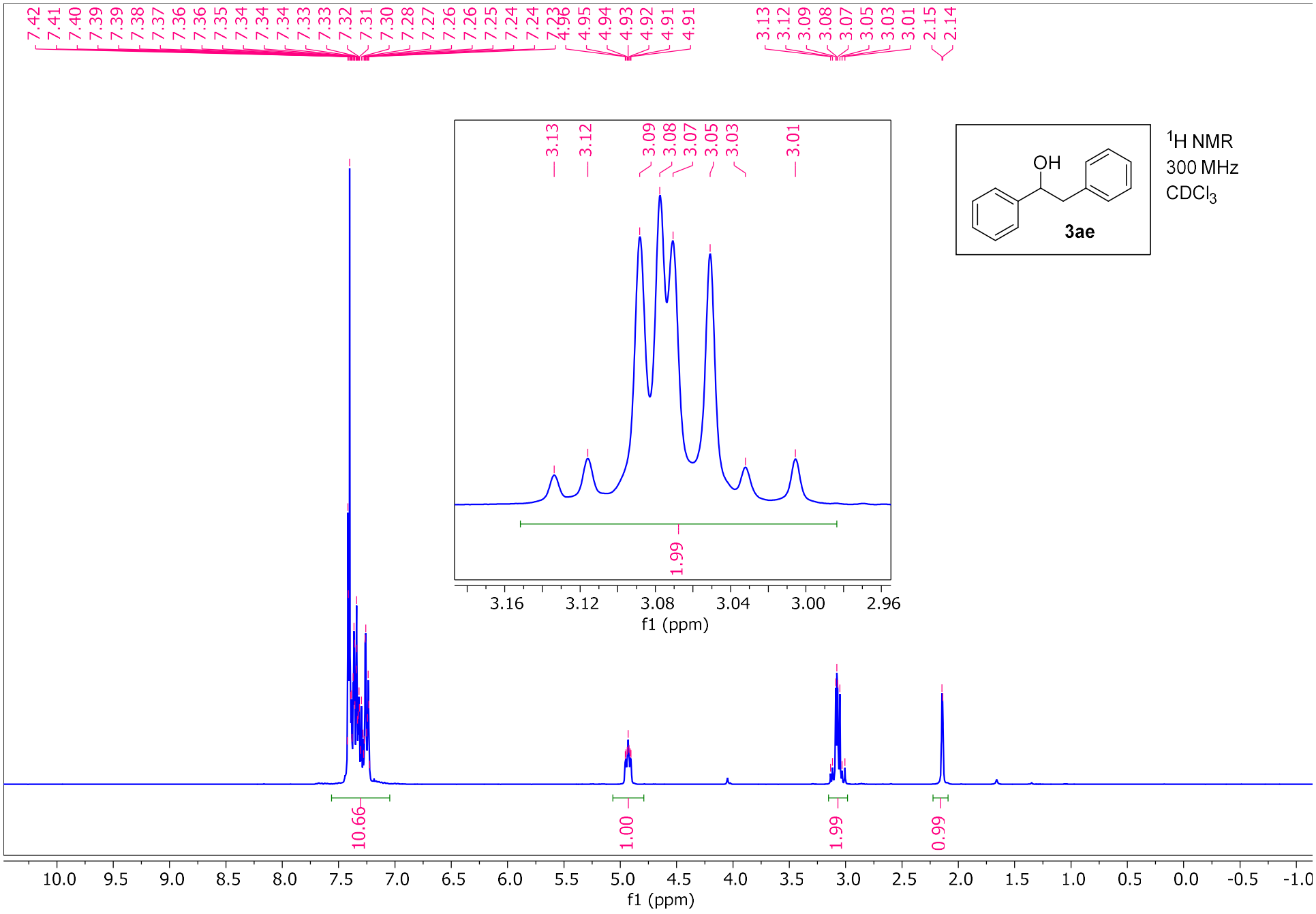

144.90
128.36
127.40
125.86
77.00
74.62
38.75
27.93
22.56
13.96
OH
3ab
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

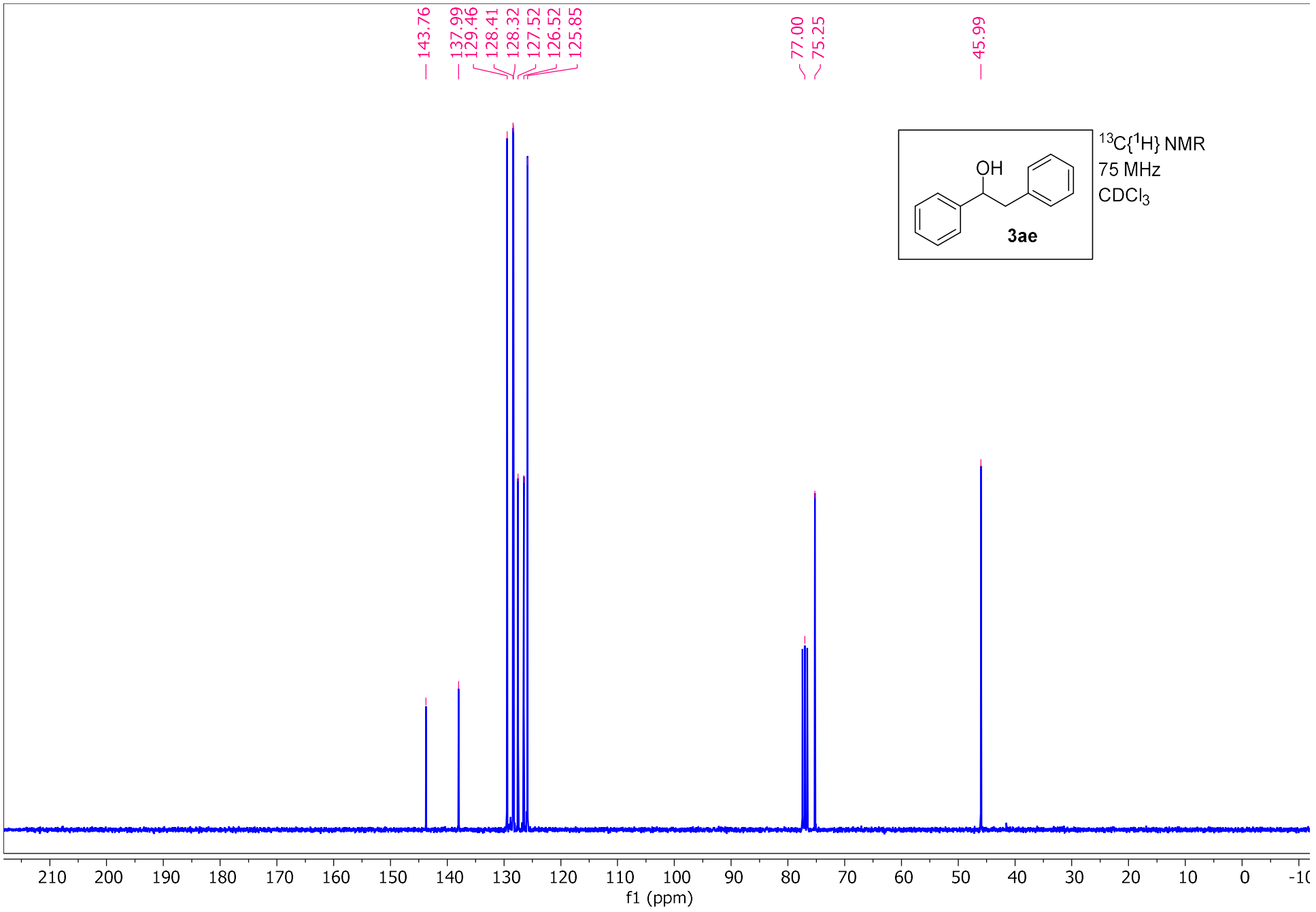

7.44 7.43 7.43 7.42 7.41 7.41 7.40 7.38 7.36 7.35 7.34 7.33 7.32 7.31 7.30 7.30 7.29 7.28 7.28 7.27
4.70 4.68 4.68 4.66 1.96 1.84 1.83 1.83 1.82 1.81 1.80 1.79 1.79 1.78 1.77 1.75 1.73 1.72 1.71 1.47 1.46 1.44 1.43 1.42 1.41 1.39 1.36 1.34 1.31 1.29 1.29 1.24 0.94 0.92
OH
3ac
1H NMR
300 MHz
CDCl3
5.40
1.00
0.96
2.13
21.76
3.30
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 -0.5
f1 (ppm)

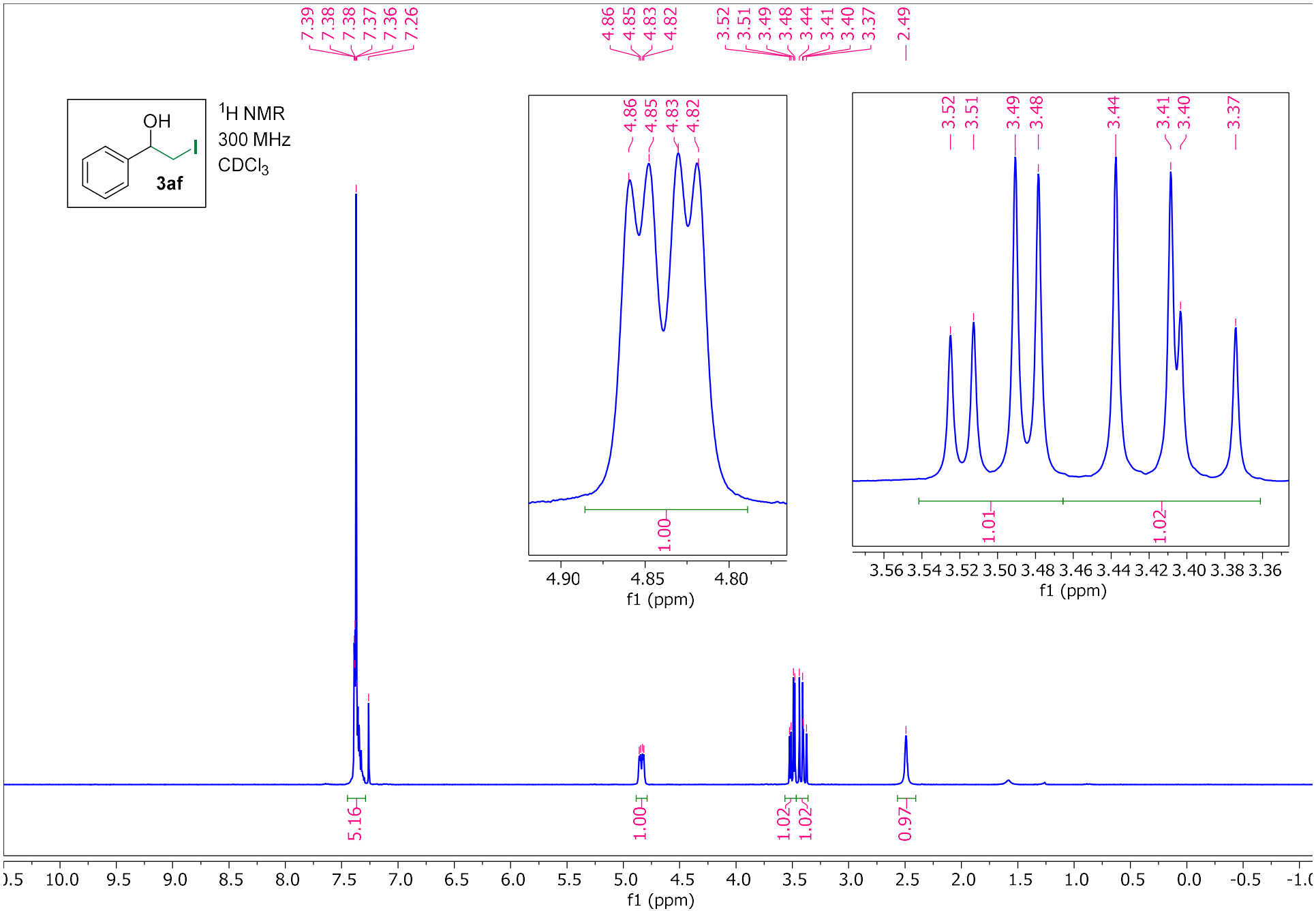

144.93
128.37
127.42
125.86
77.00
74.66
39.09
31.90
29.64
29.62
29.57
29.53
29.51
29.33
25.81
22.66
14.09
OH
3ac
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.41 7.41 7.40 7.39 7.34 7.33 7.31 7.31 7.26 7.26 7.24 7.23
4.74 4.72 4.72 4.70 2.85 2.83 2.82 2.81 2.80 2.79 2.78 2.76 2.76 2.74 2.73 2.72 2.71 2.69 2.69 2.66
2.20 2.18 2.17 2.17 2.15 2.15 2.14 2.13 2.12 2.12 2.11 2.10 2.09 2.09 2.08 2.08 2.07 2.07
OH
3ad
1H NMR
300 MHz
CDCl3
7.43
3.31
1.00
2.01
3.05
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 -0.5
f1 (ppm)


144.52
141.73
128.72
128.46
128.39
128.34
128.25
128.07
127.58
126.23
125.88
125.80
125.68
77.00
73.80
40.40
32.00
OH
3ad
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
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)


7.42 7.41 7.40 7.39 7.39 7.38 7.37 7.36 7.36 7.35 7.34 7.34 7.34 7.33 7.33 7.32 7.31 7.30 7.28 7.27 7.26 7.26 7.25 7.24 7.24 7.23 4.96 4.95 4.94 4.93 4.92 4.91 4.91
3.13 3.12 3.09 3.08 3.07 3.05 3.03 3.01 2.15 2.14
3.13 3.12 3.09 3.08 3.07 3.05 3.03 3.01
1.99
3.16 3.12 3.08 3.04 3.00 2.96
f1 (ppm)
OH
3ae
1H NMR
300 MHz
CDCl3
10.66 1.00 1.99 0.99
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 -0.5 -1.0
f1 (ppm)


143.76
137.99
129.46
128.41
128.32
127.52
126.52
125.85
77.00
75.25
45.99
OH
3ae
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
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)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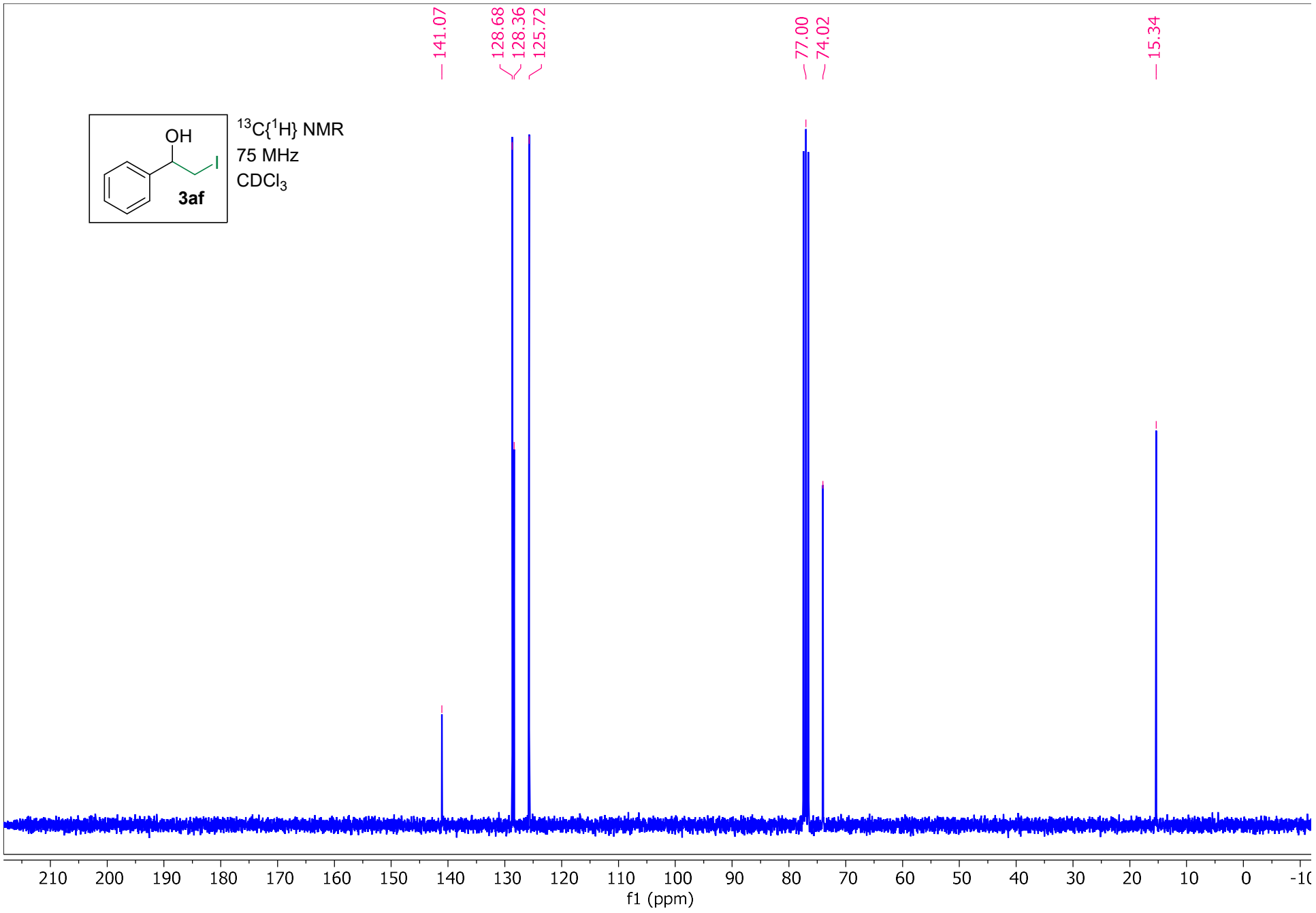
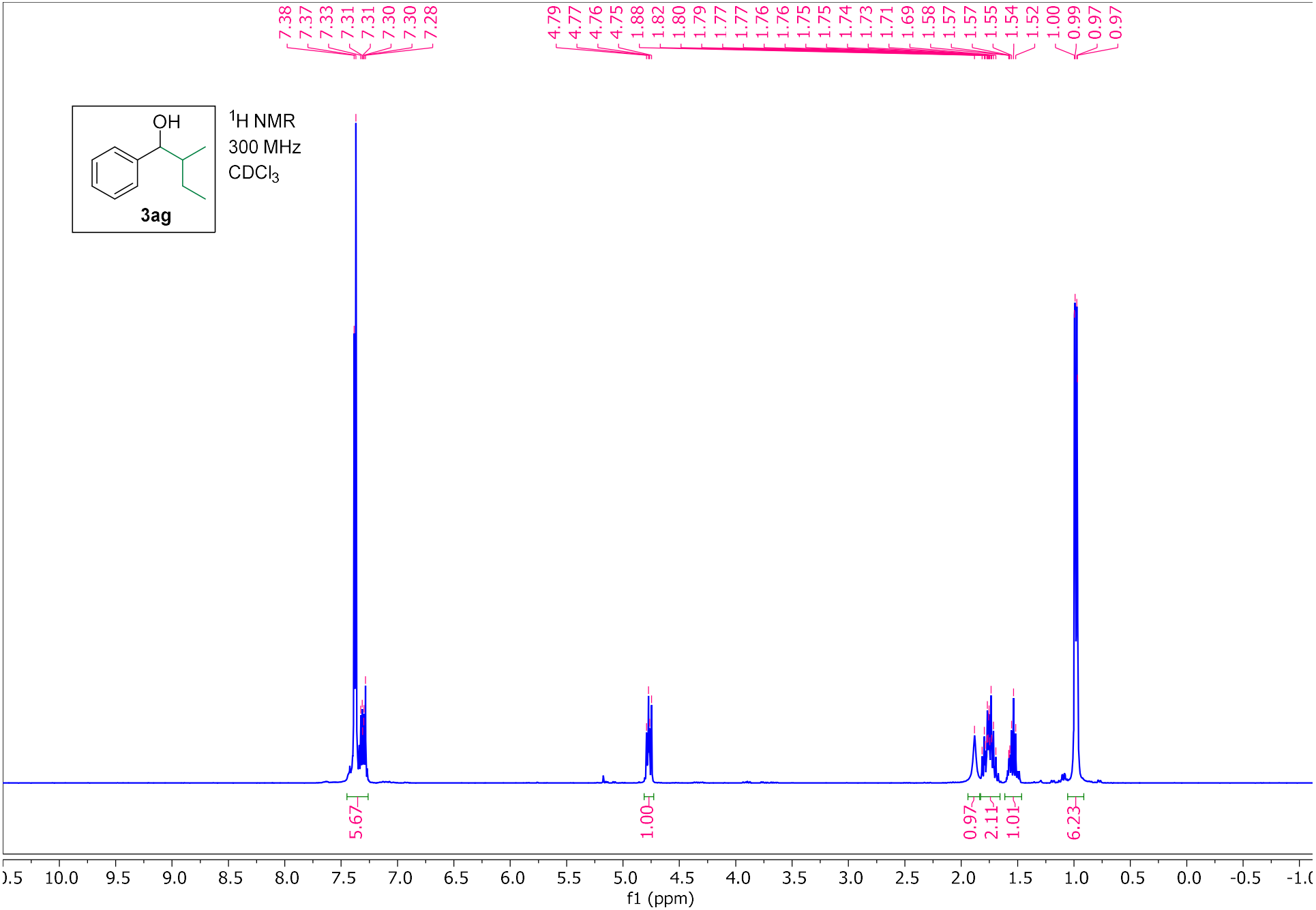
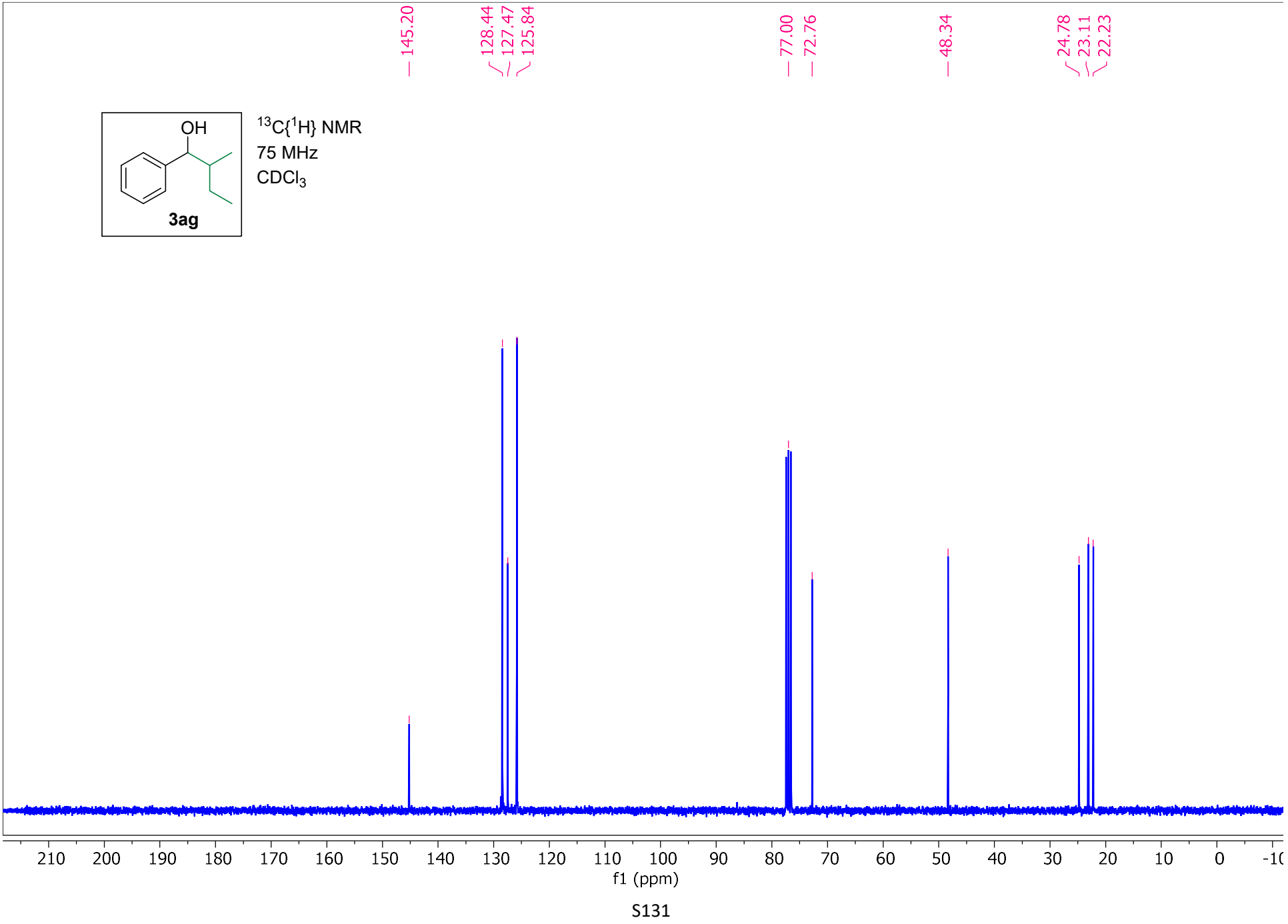
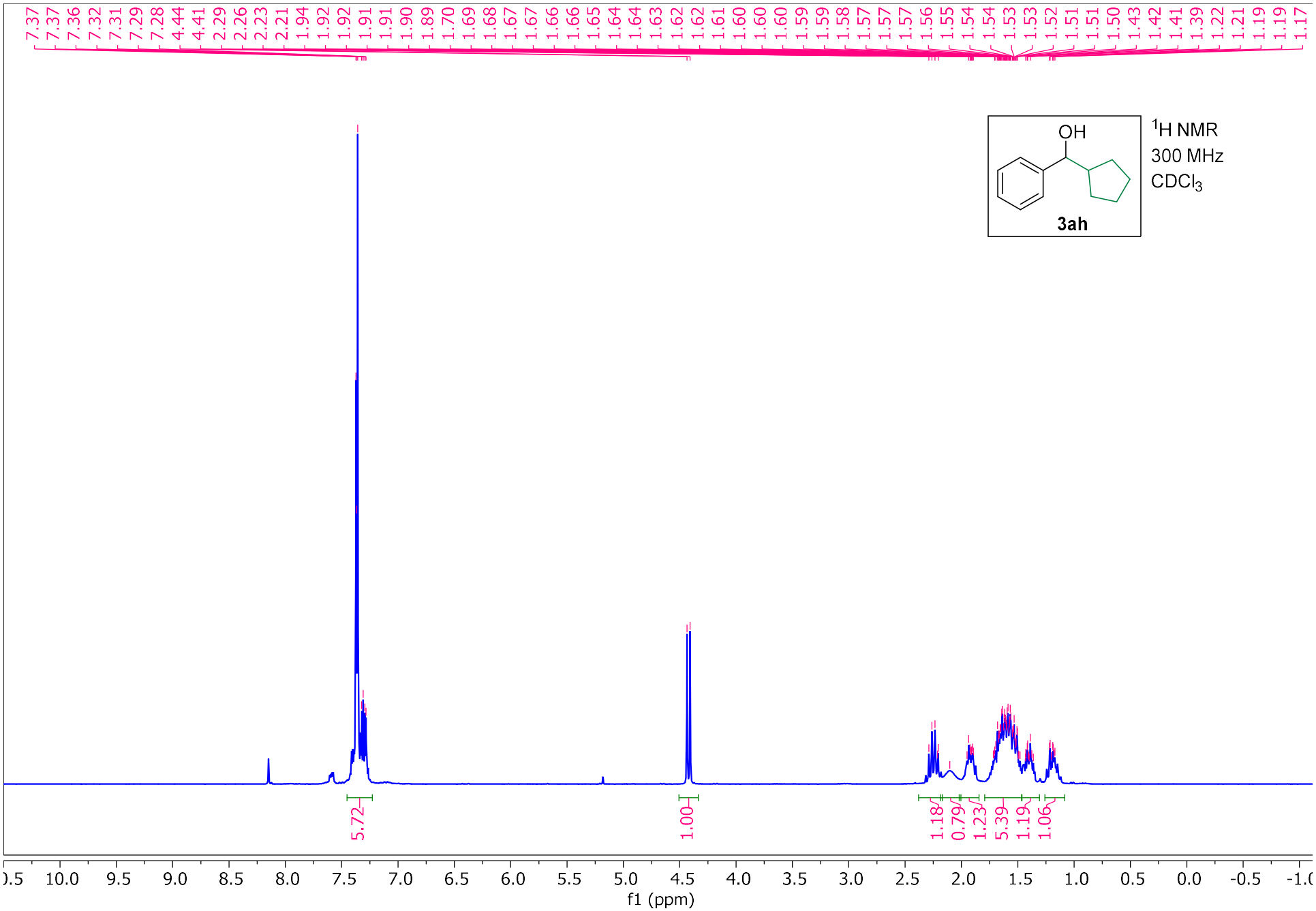
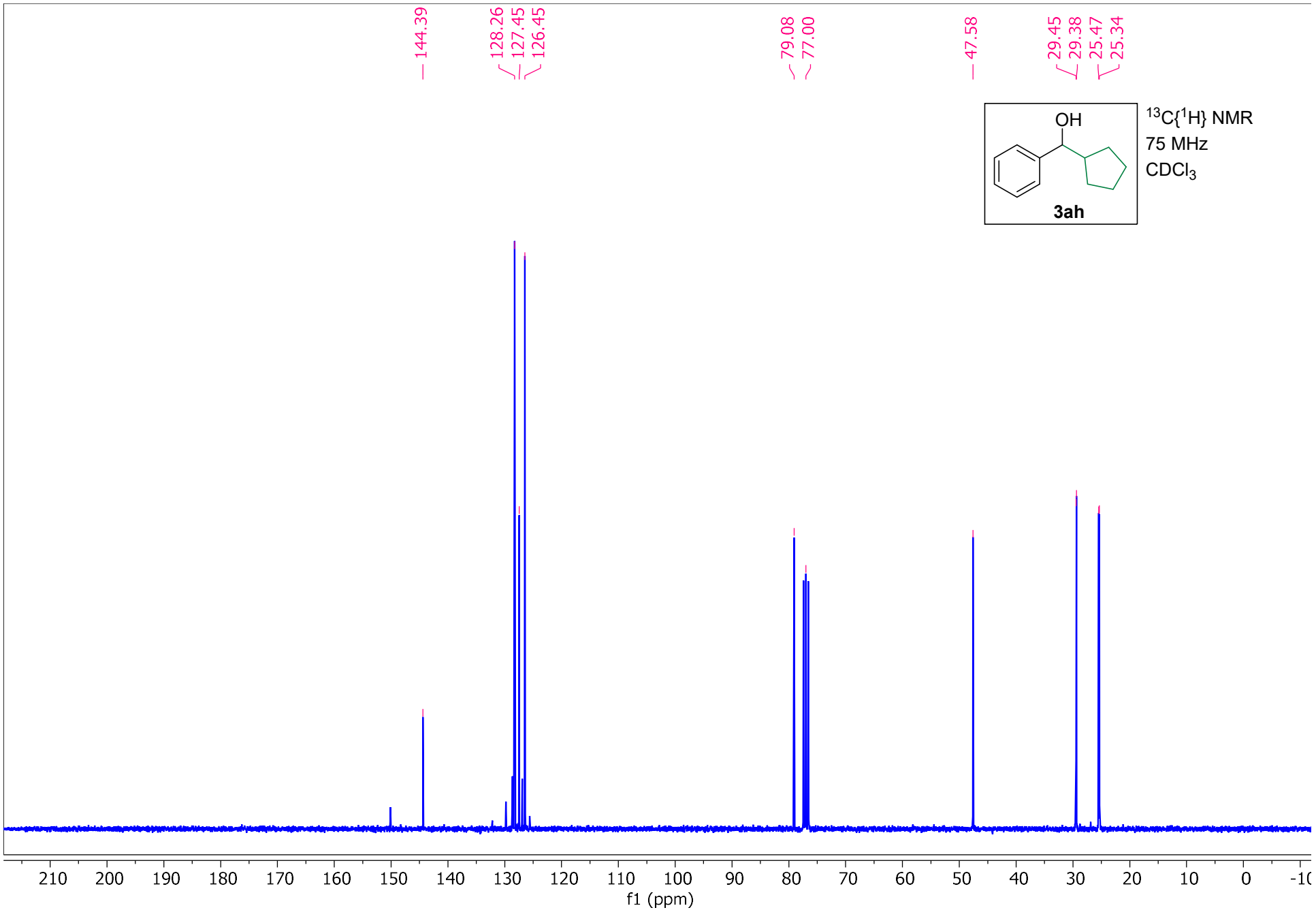
7.38
7.38
7.37
7.36
7.26
4.86
4.85
4.83
4.82
3.52
3.51
3.49
3.48
3.44
3.41
3.40
3.37
2.49
OH
I
3af
1H NMR
300 MHz
CDCl3
4.90
4.85
4.80
f1 (ppm)
1.00
3.56 3.54 3.52 3.50 3.48 3.46 3.44 3.42 3.40 3.38 3.36
f1 (ppm)
1.01
1.02
5.16
1.00
1.02
1.02
0.97
f1 (ppm)

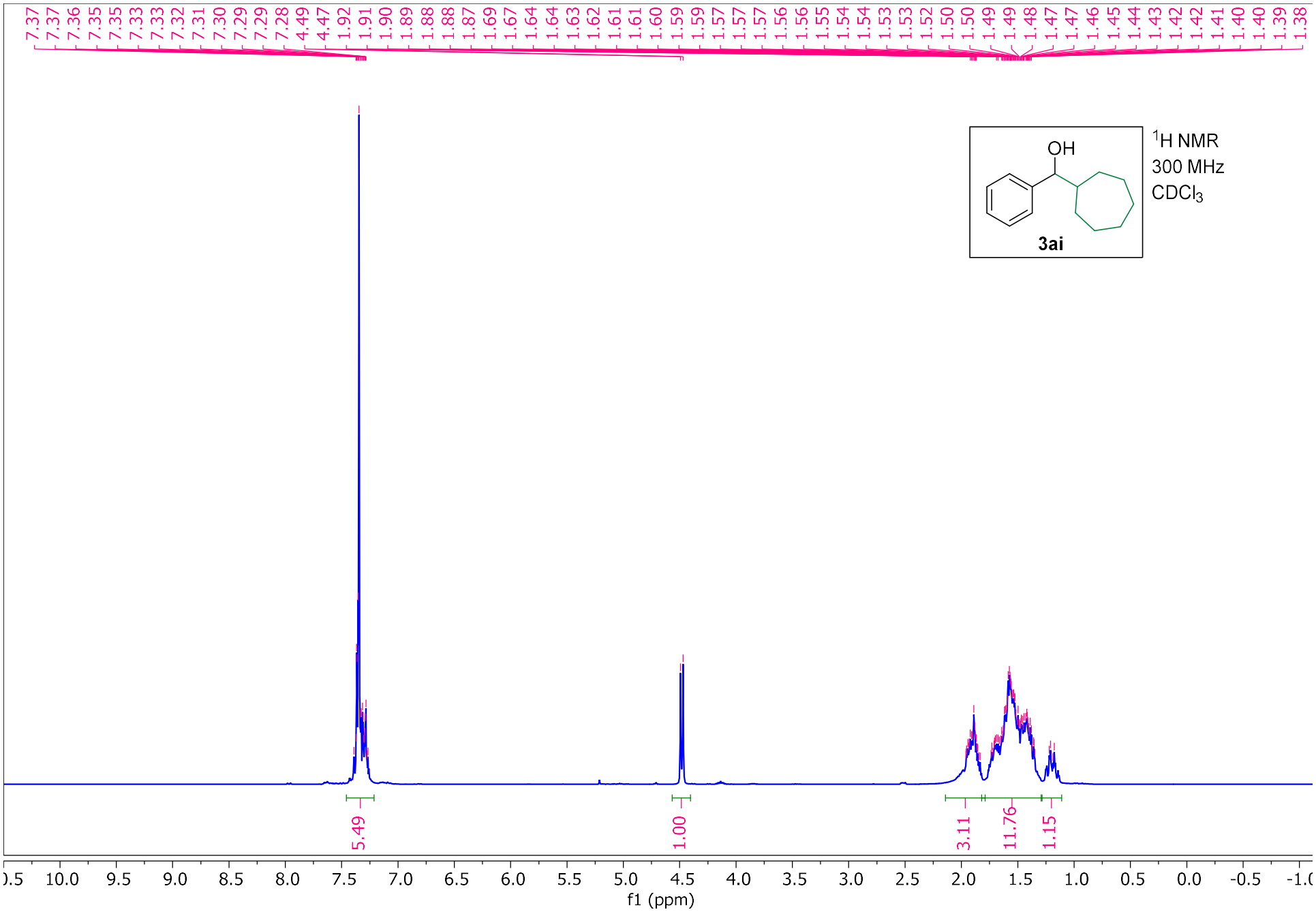

141.07
128.68
128.36
125.72
77.00
74.02
15.34
OH
I
3af
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

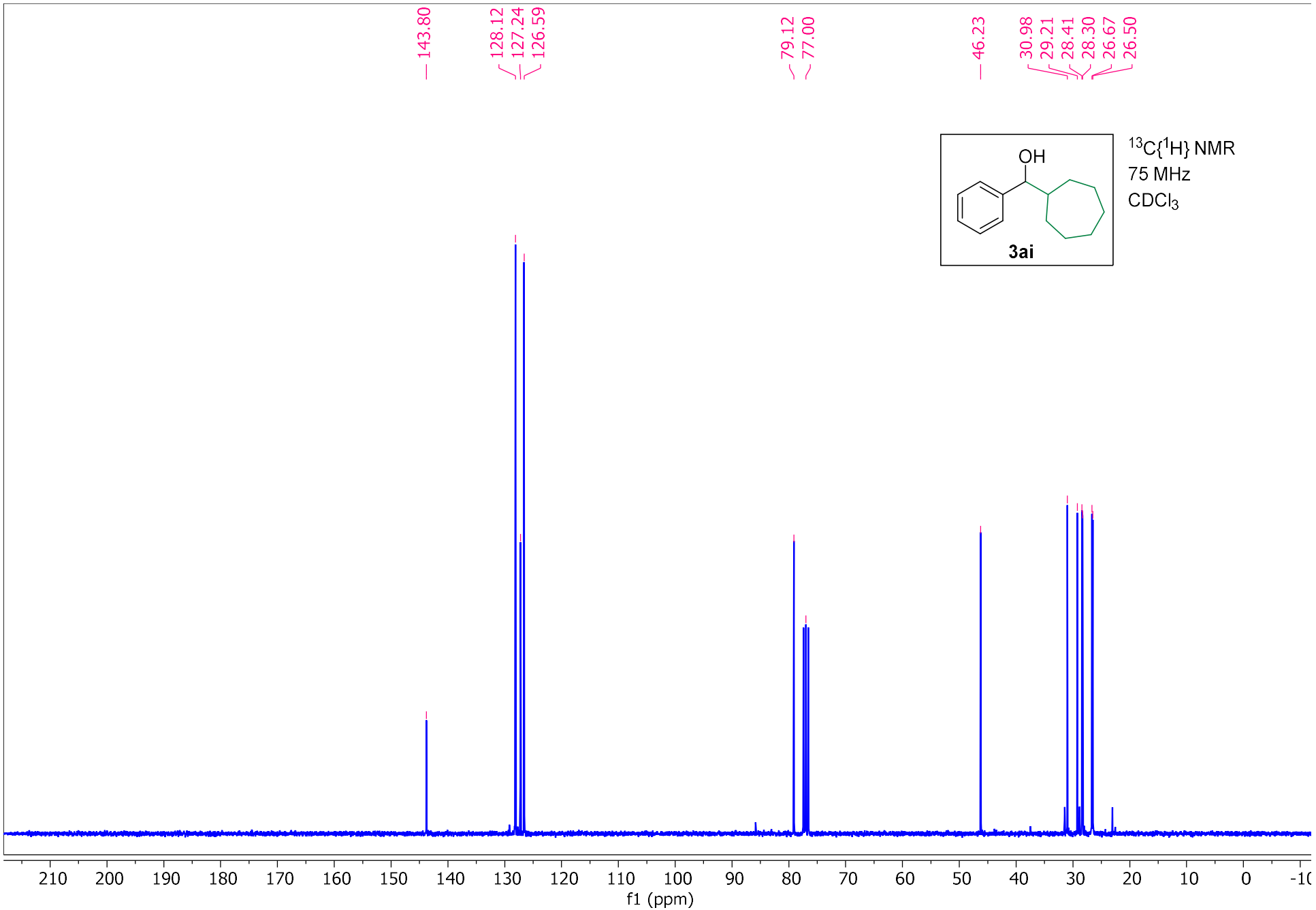

7.38
7.37
7.33
7.31
7.31
7.30
7.30
7.28
4.79
4.77
4.76
4.75
1.88
1.82
1.80
1.79
1.77
1.77
1.76
1.76
1.75
1.75
1.74
1.73
1.71
1.69
1.58
1.57
1.57
1.55
1.54
1.52
1.00
0.99
0.97
0.97
OH
3ag
1H NMR
300 MHz
CDCl3
5.67
1.00
0.97
2.11
1.01
6.23
f1 (ppm)

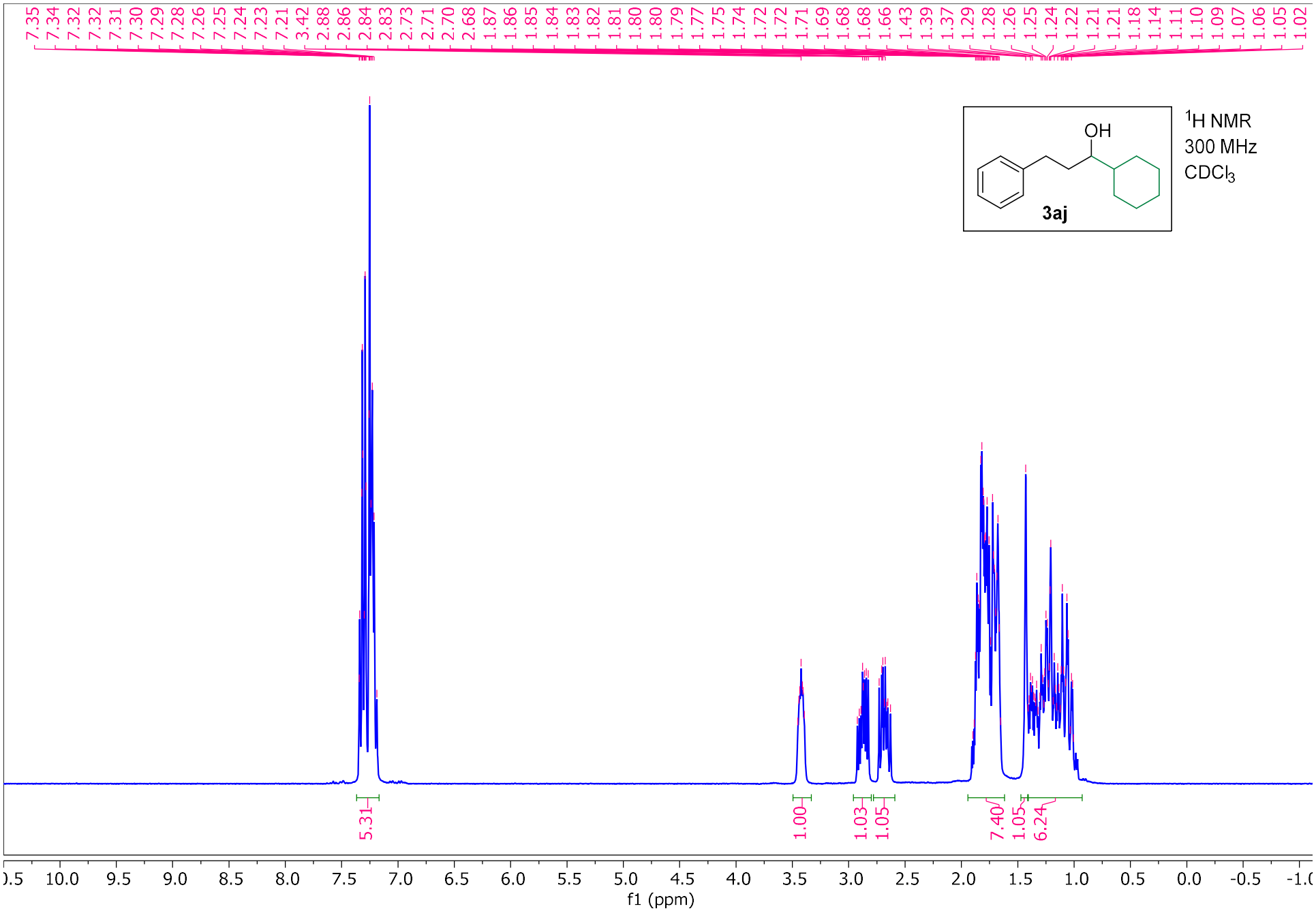

145.20
128.44
127.47
125.84
77.00
72.76
48.34
24.78
23.11
22.23
OH
3ag
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

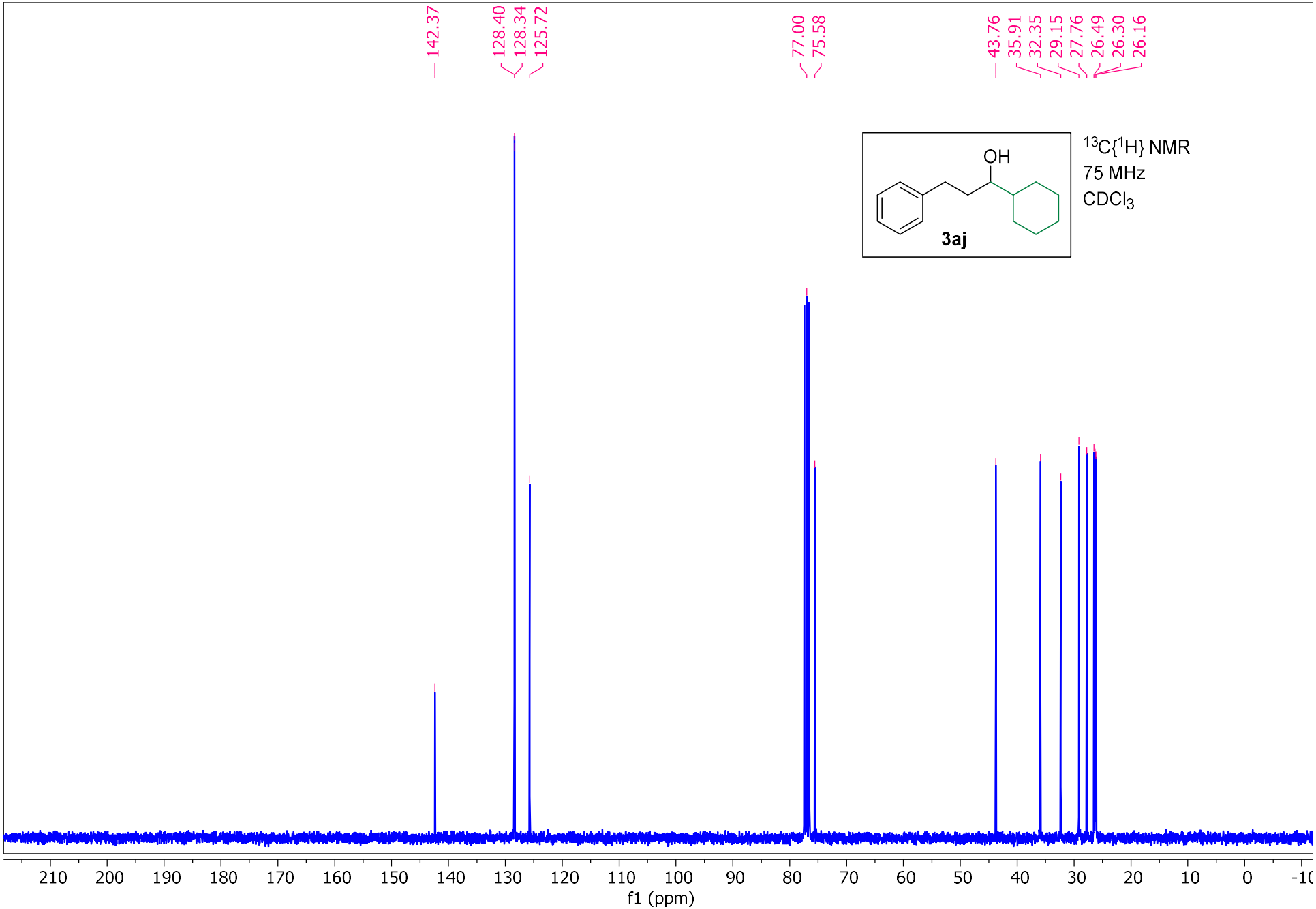

7.37 7.37 7.36 7.32 7.31 7.29 7.28 4.44 4.41 2.29 2.26 2.23 2.21 1.94 1.92 1.92 1.91 1.91 1.90 1.89 1.70 1.69 1.68 1.67 1.67 1.66 1.66 1.65 1.64 1.64 1.63 1.62 1.62 1.61 1.60 1.60 1.60 1.59 1.59 1.58 1.57 1.57 1.57 1.56 1.55 1.54 1.54 1.53 1.53 1.52 1.51 1.51 1.50 1.43 1.42 1.41 1.39 1.22 1.21 1.19 1.19 1.17
OH
3ah
1H NMR
300 MHz
CDCl3
5.72
1.00
1.18
0.79
1.23
5.39
1.19
1.06
f1 (ppm)

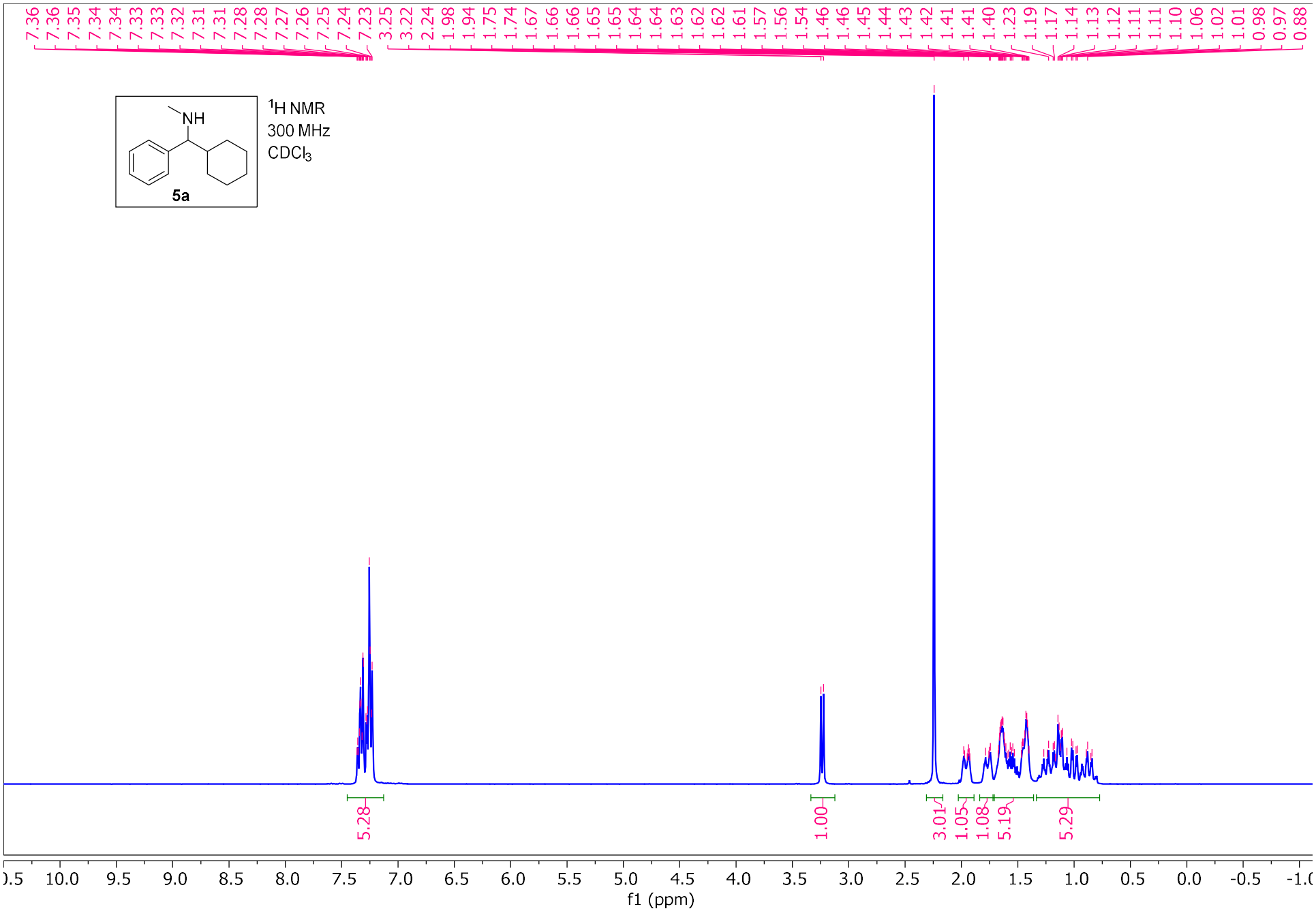

144.39
128.26
127.45
126.45
79.08
77.00
47.58
29.45
29.38
25.47
25.34
OH
3ah
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

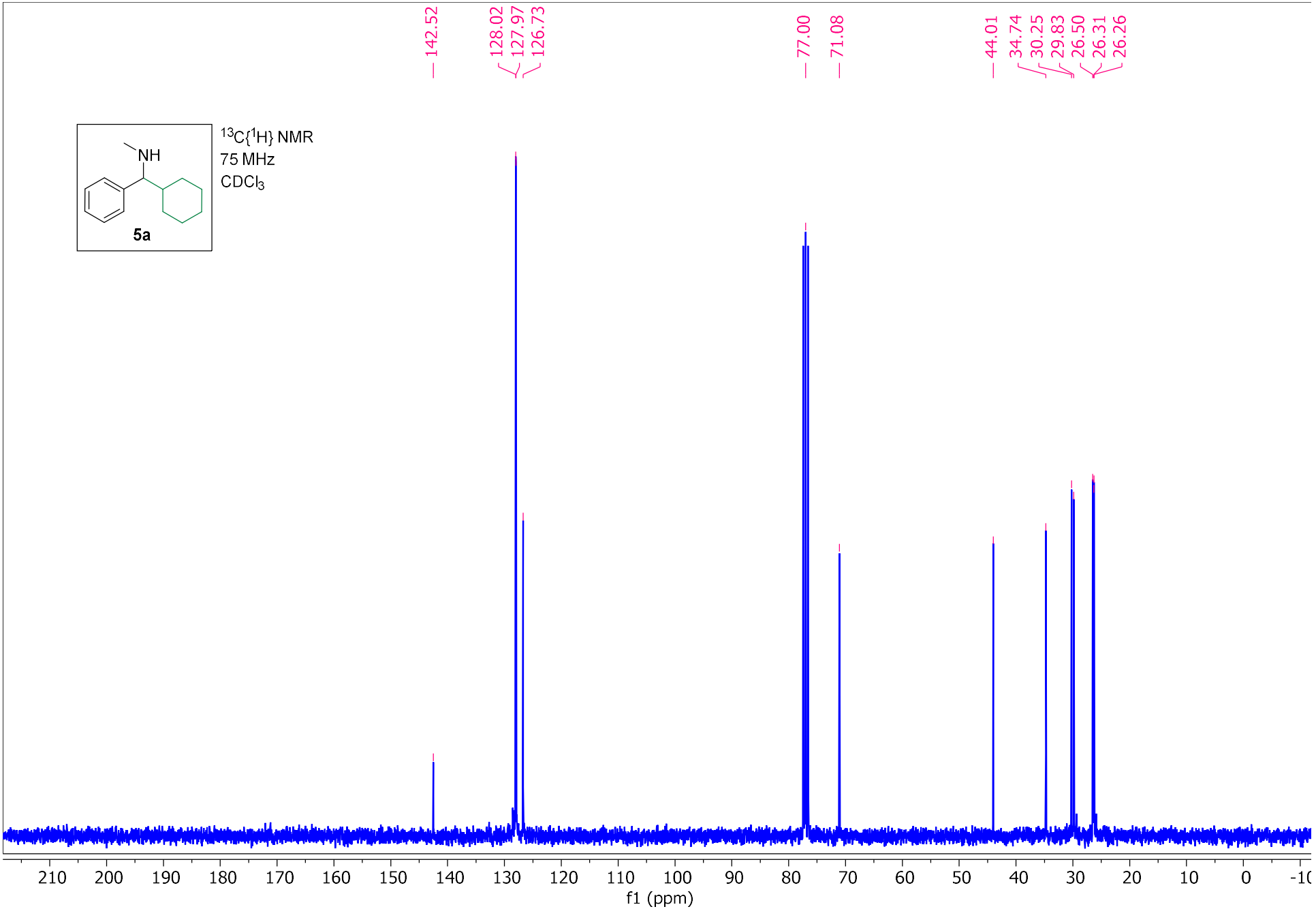

7.37 7.37 7.36 7.35 7.35 7.33 7.33 7.32 7.31 7.30 7.29 7.29 7.28 4.49 4.47 1.92 1.91 1.90 1.89 1.88 1.88 1.87 1.69 1.67 1.64 1.64 1.63 1.62 1.61 1.61 1.60 1.59 1.59 1.57 1.57 1.57 1.56 1.56 1.55 1.54 1.54 1.53 1.53 1.52 1.50 1.50 1.49 1.49 1.48 1.47 1.47 1.46 1.45 1.44 1.43 1.42 1.42 1.41 1.40 1.40 1.39 1.38
OH
3ai
1H NMR
300 MHz
CDCl3
5.49
1.00
3.11
11.76
1.15
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 -0.5
f1 (ppm)

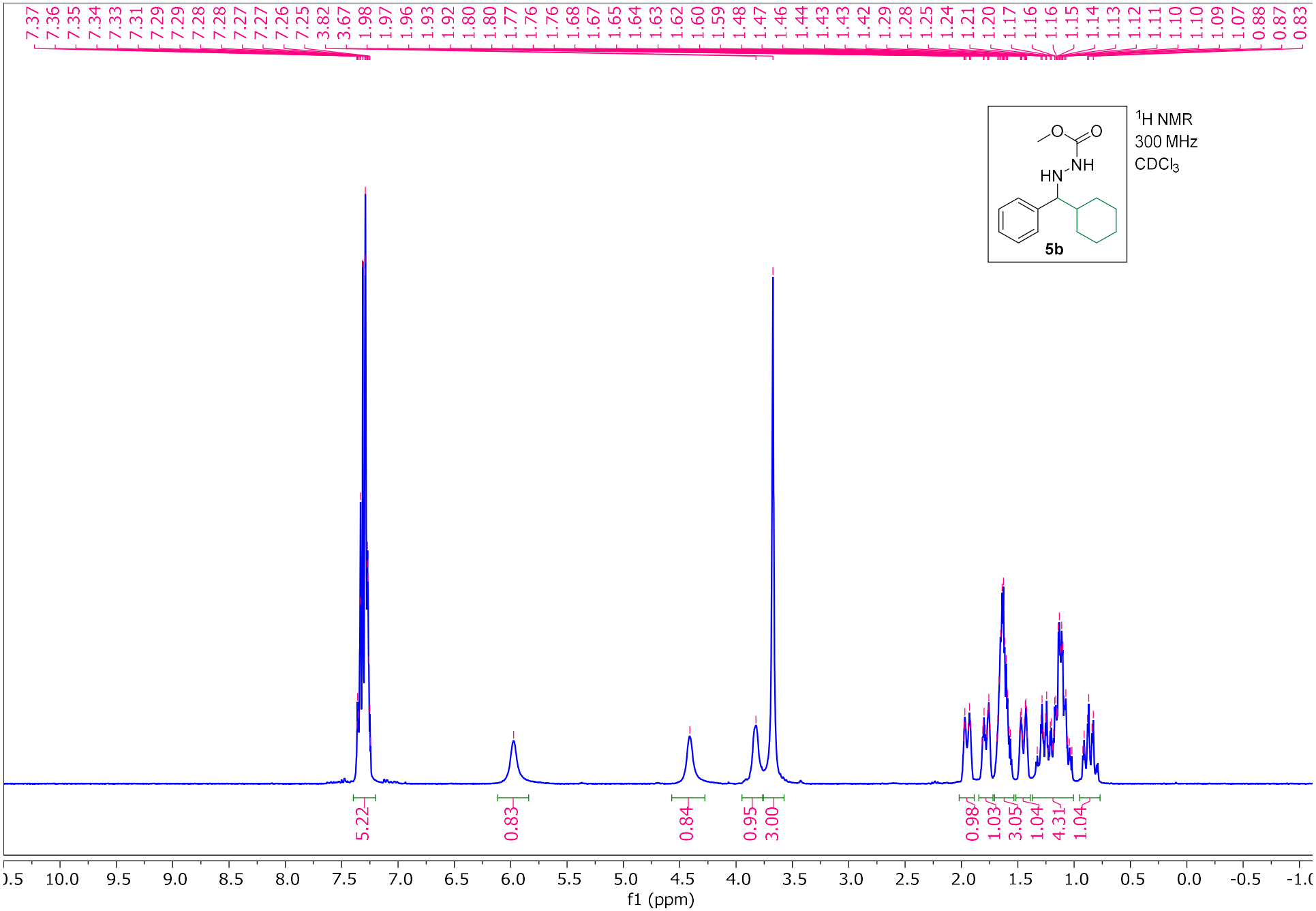

143.80
128.12
127.24
126.59
79.12
77.00
46.23
30.98
29.21
28.41
28.30
26.67
26.50
OH
3ai
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

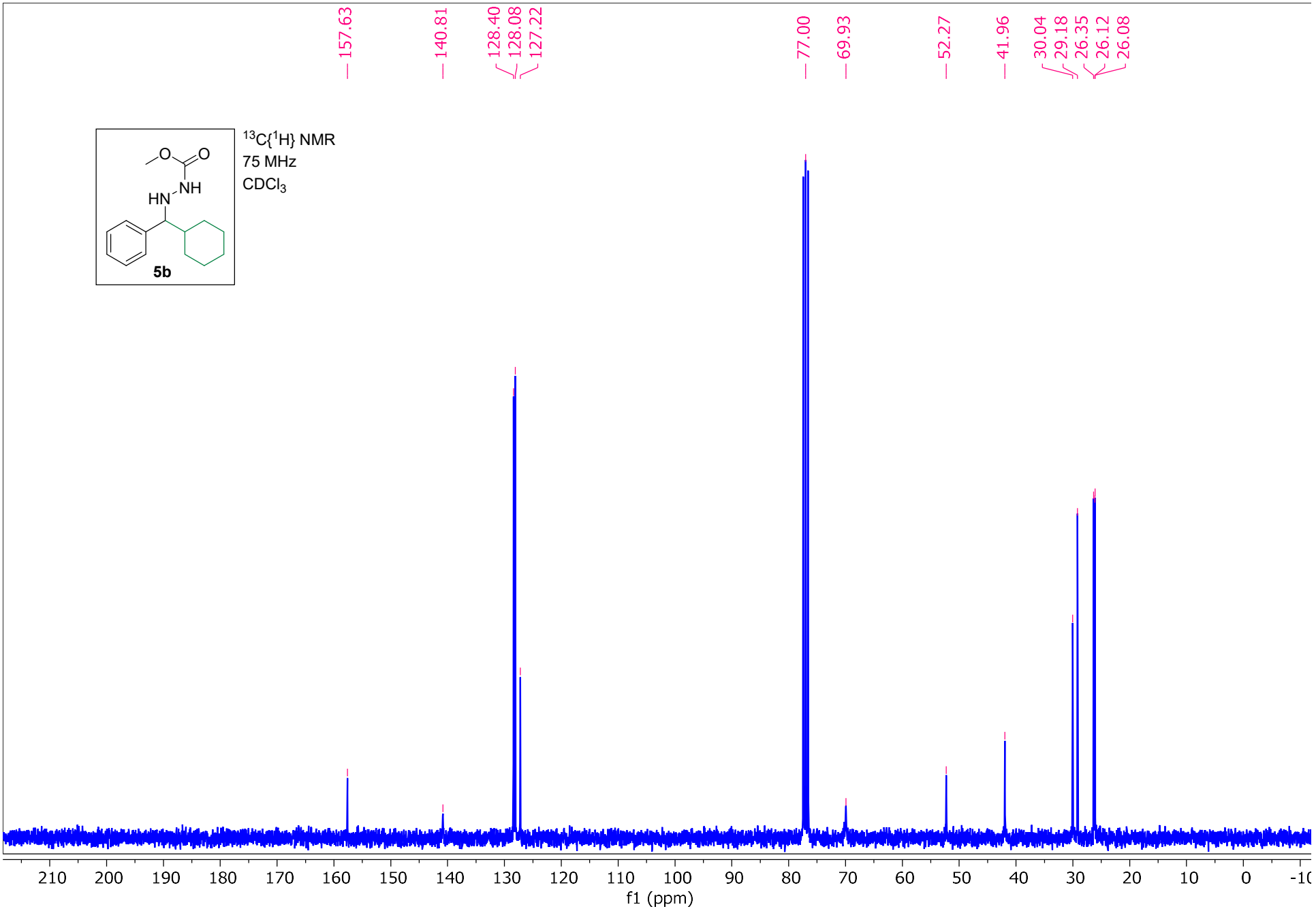

7.35 7.34 7.32 7.32 7.31 7.30 7.29 7.28 7.26 7.25 7.24 7.23 7.21 3.42 2.88 2.86 2.84 2.83 2.73 2.71 2.70 2.68 1.87 1.86 1.85 1.84 1.83 1.82 1.81 1.80 1.80 1.79 1.77 1.75 1.74 1.72 1.72 1.71 1.69 1.68 1.68 1.66 1.43 1.39 1.37 1.29 1.28 1.26 1.25 1.24 1.22 1.21 1.21 1.18 1.14 1.11 1.10 1.09 1.07 1.06 1.05 1.02
OH
3aj
1H NMR
300 MHz
CDCl3
5.31
1.00
1.03
1.05
7.40
1.05
6.24
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 -0.5
f1 (ppm)

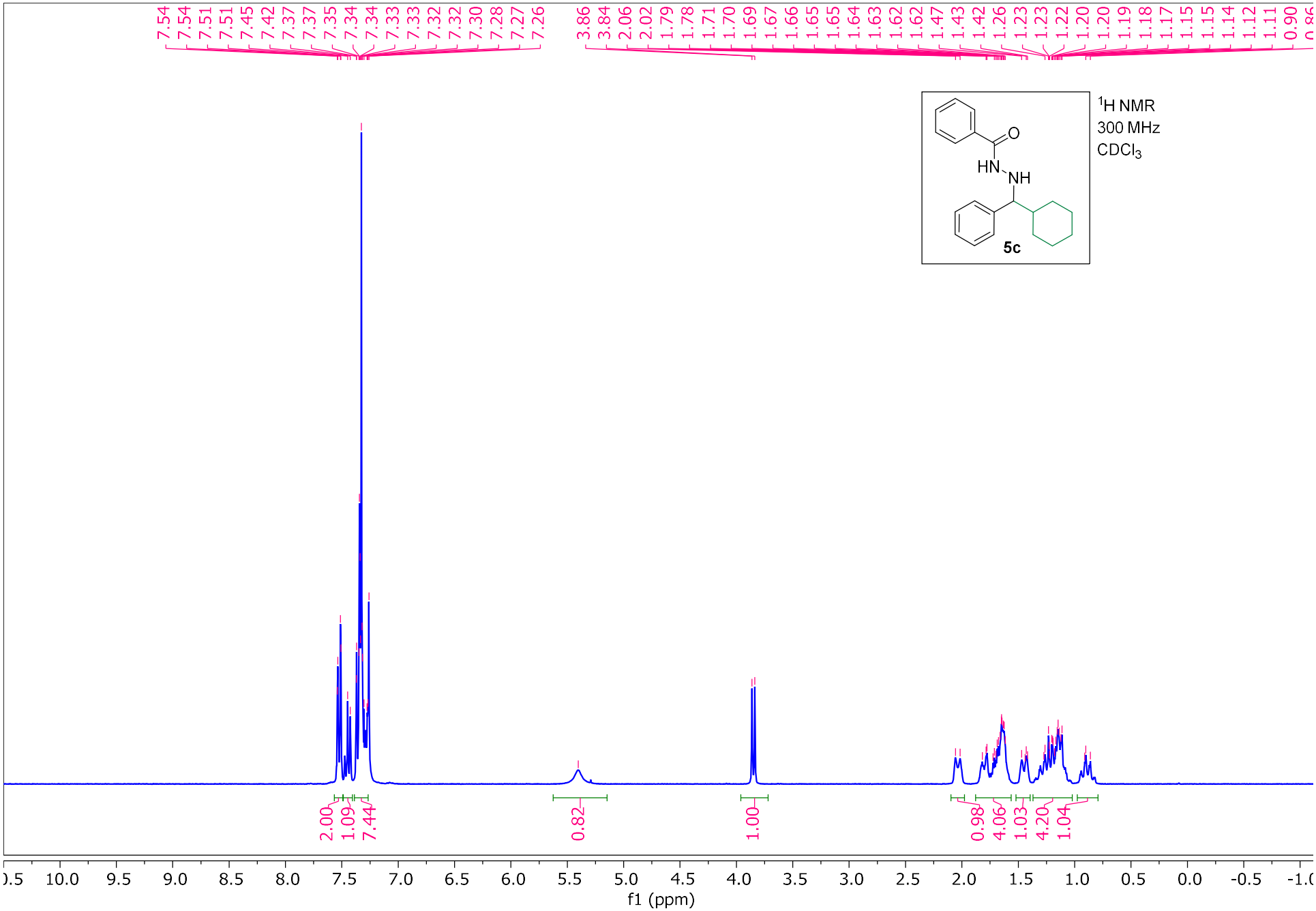

142.37
128.40
128.34
125.72
77.00
75.58
43.76
35.91
32.35
29.15
27.76
26.49
26.30
26.16
OH
3aj
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

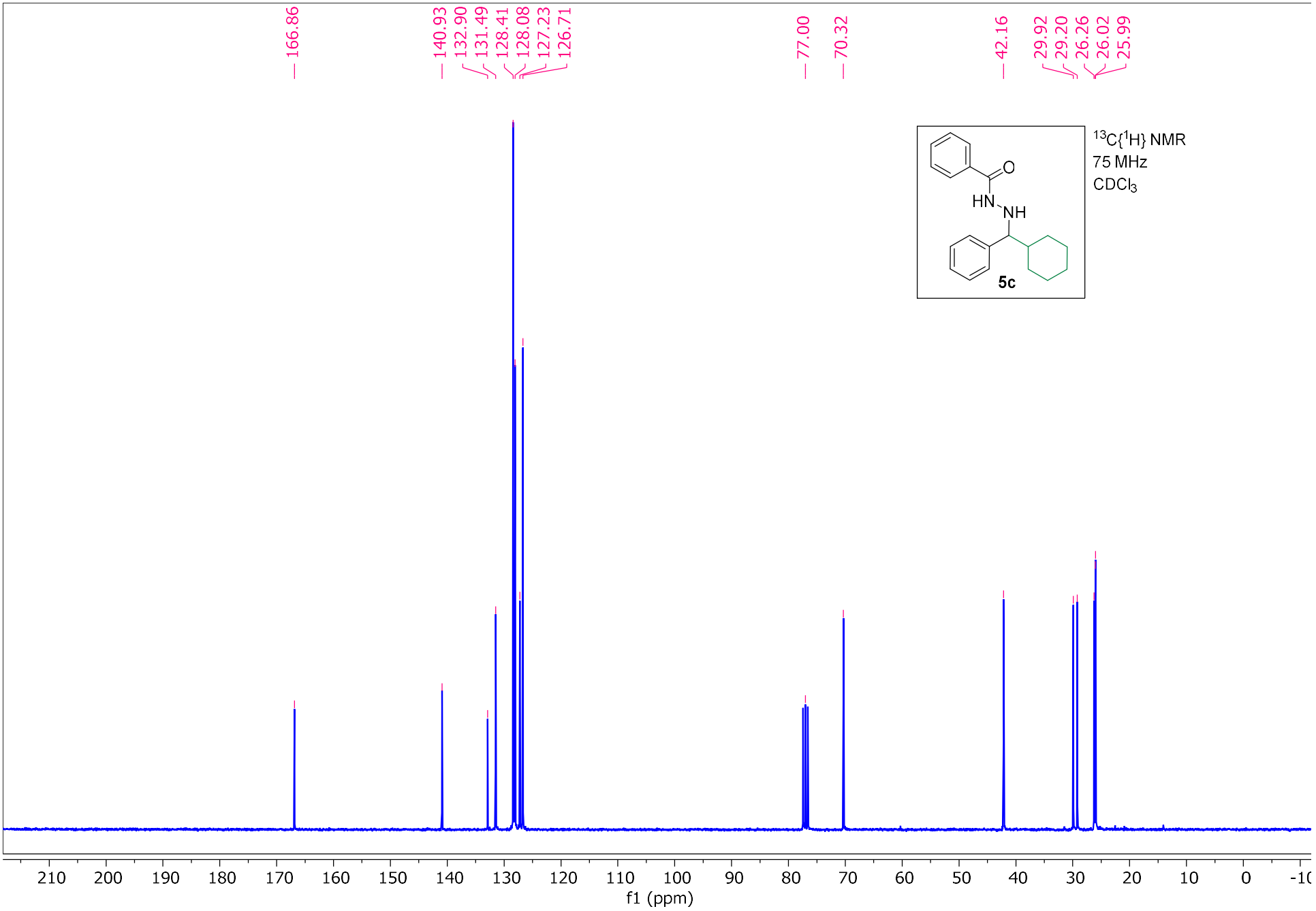

7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.31 7.31 7.28 7.28 7.27 7.26 7.25 7.24 7.23 3.25 3.22 2.24 1.98 1.94 1.75 1.74 1.67 1.66 1.66 1.65 1.65 1.64 1.64 1.63 1.62 1.62 1.61 1.57 1.56 1.54 1.46 1.46 1.45 1.44 1.43 1.42 1.41 1.41 1.40 1.23 1.19 1.17 1.14 1.13 1.12 1.11 1.11 1.10 1.06 1.02 1.01 0.98 0.97 0.88
NH
5a
1H NMR
300 MHz
CDCl3
5.28
1.00
3.01
1.05
1.08
5.19
5.29
f1 (ppm)

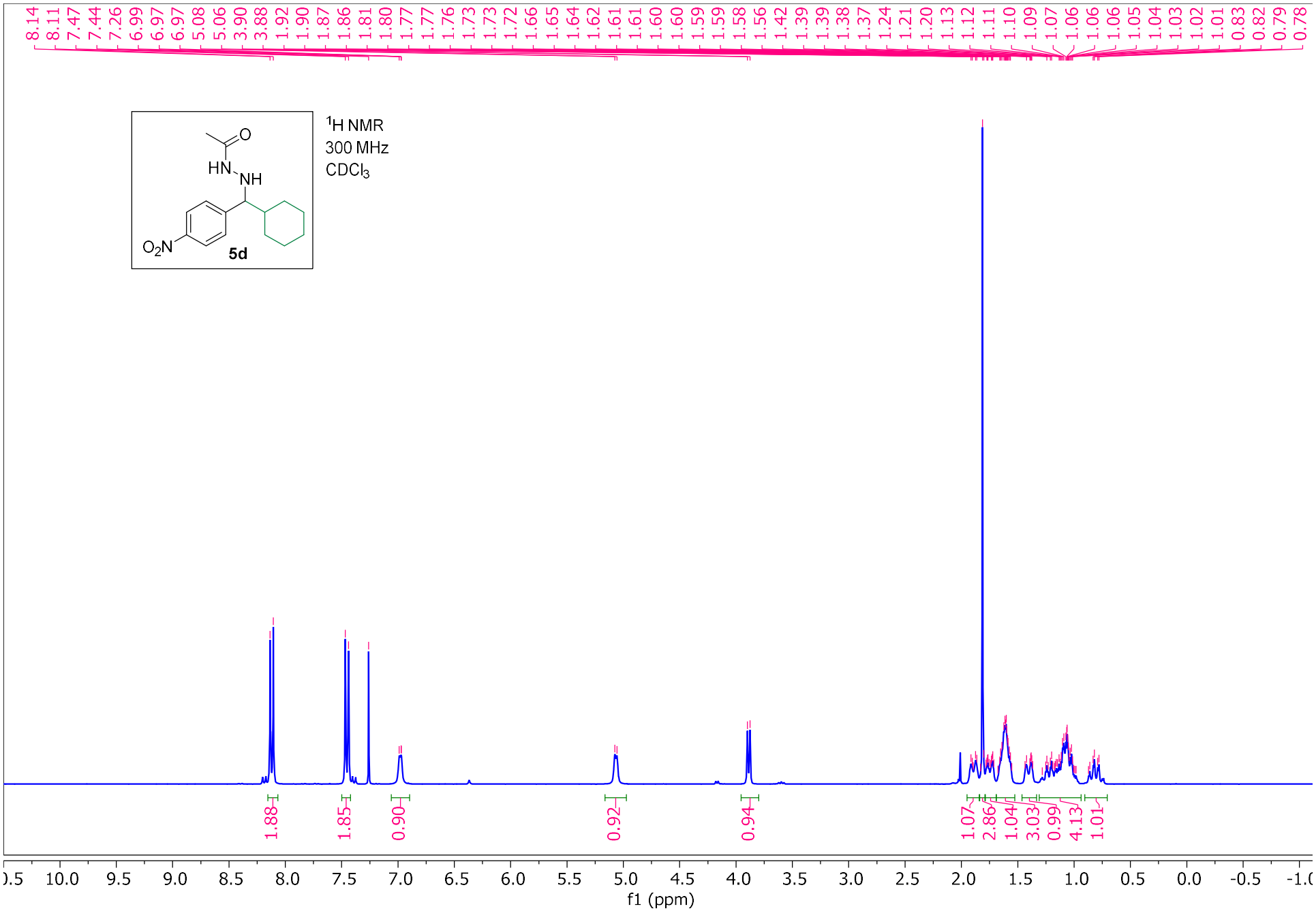

142.52
128.02
127.97
126.73
77.00
71.08
44.01
34.74
30.25
29.83
26.50
26.31
26.26
NH
5a
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

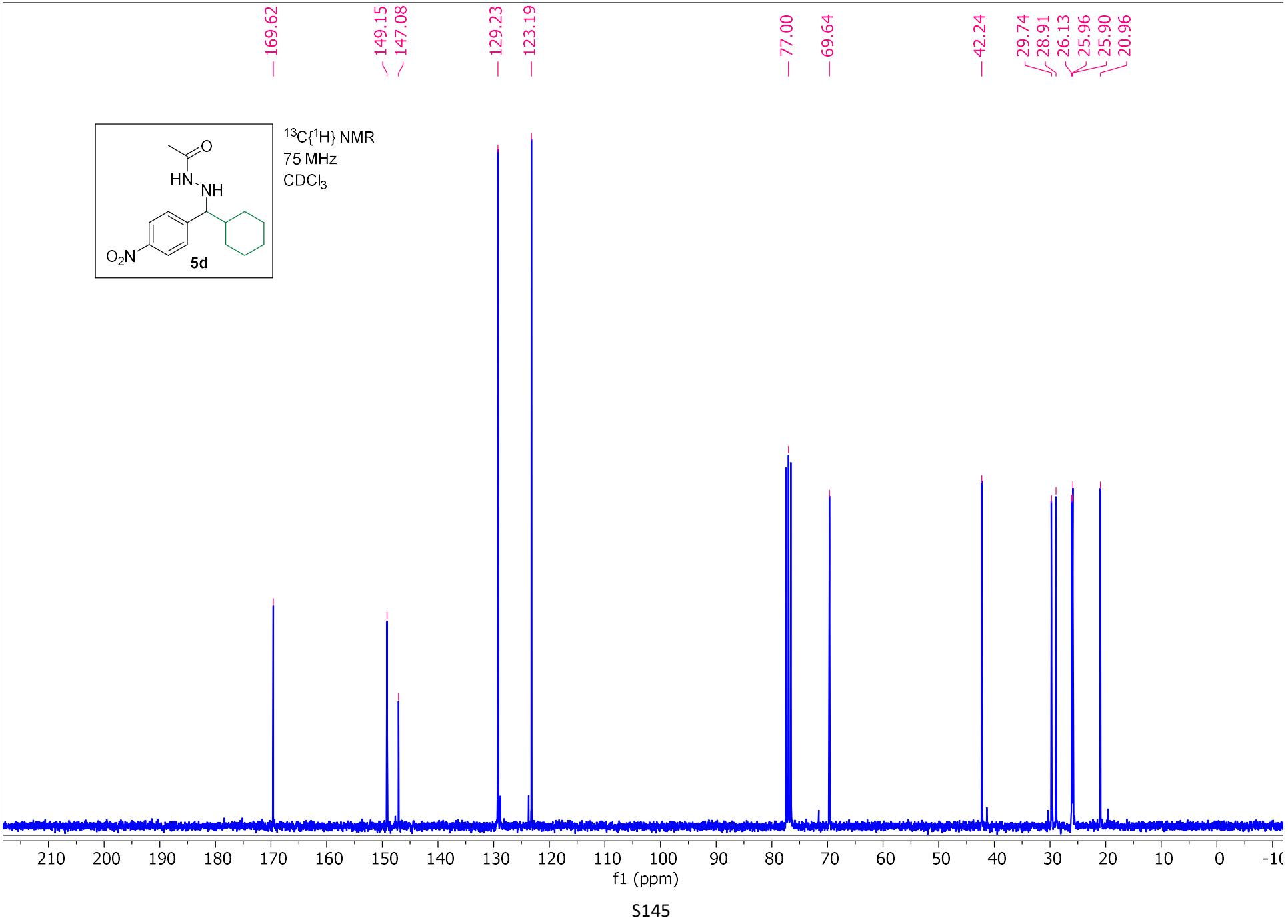

7.37 7.36 7.35 7.34 7.33 7.31 7.29 7.29 7.28 7.28 7.27 7.27 7.26 7.25 3.82 3.67 1.98 1.97 1.96 1.93 1.92 1.80 1.80 1.77 1.76 1.76 1.68 1.67 1.65 1.64 1.63 1.62 1.60 1.59 1.48 1.47 1.46 1.44 1.43 1.43 1.42 1.29 1.28 1.25 1.24 1.21 1.20 1.17 1.16 1.16 1.15 1.14 1.13 1.12 1.11 1.10 1.10 1.09 1.07 0.88 0.87 0.83
O
O
NH
HN
5b
1H NMR
300 MHz
CDCl3
5.22
0.83
0.84
0.95
3.00
0.98
1.03
3.05
1.04
4.31
1.04
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 -0.5
f1 (ppm)

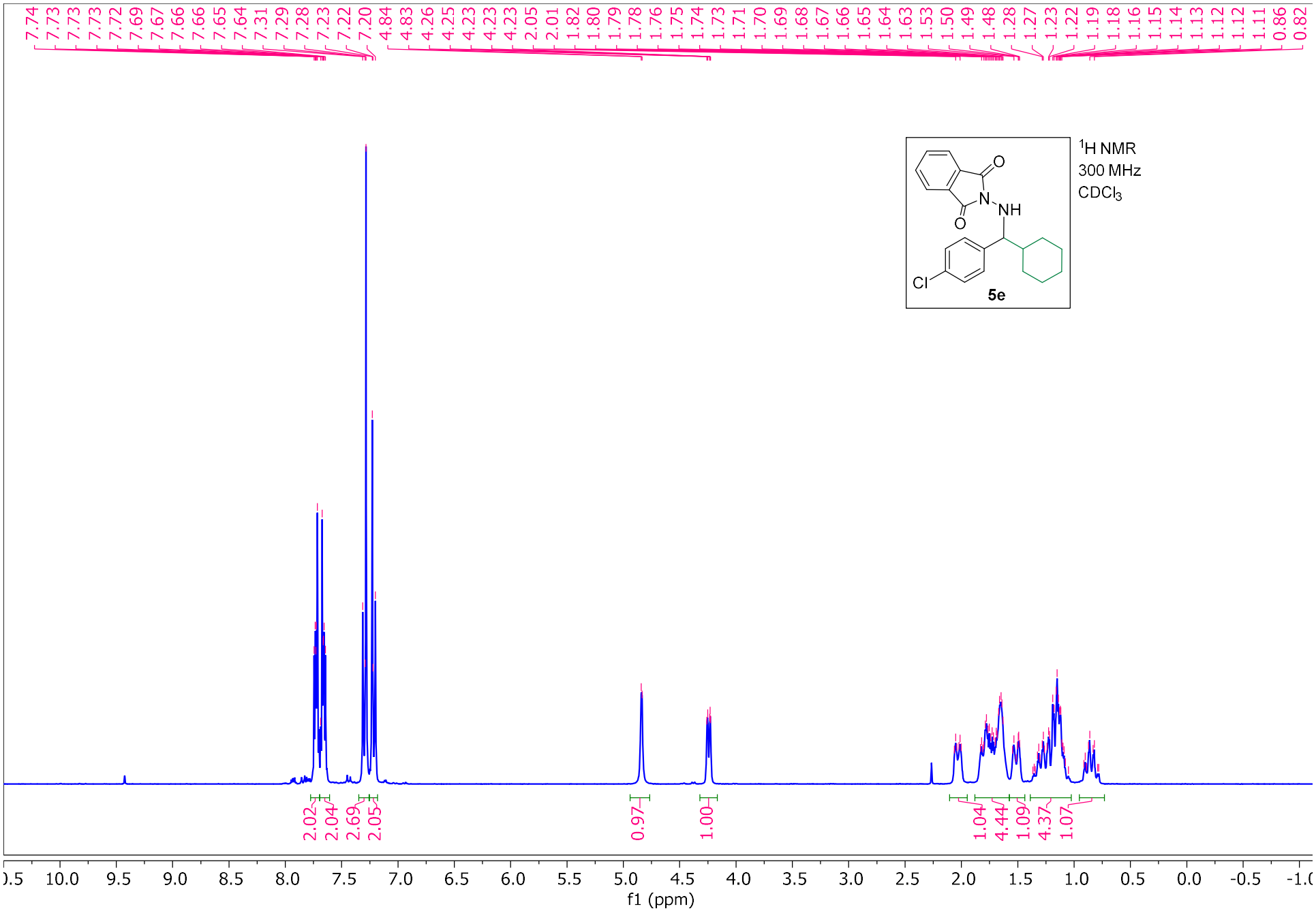

157.63
140.81
128.40
128.08
127.22
77.00
69.93
52.27
41.96
30.04
29.18
26.35
26.12
26.08
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
5b
f1 (ppm)

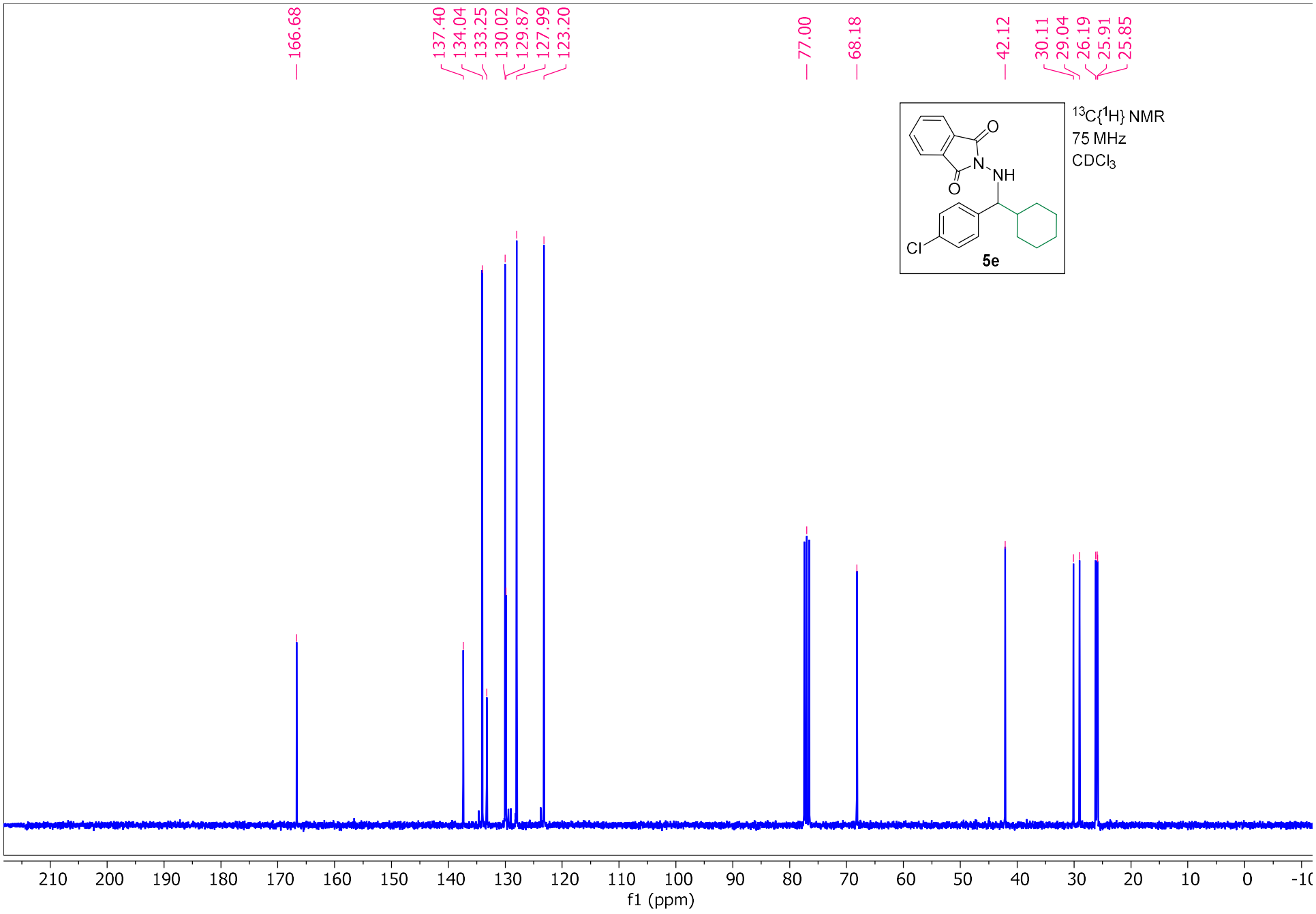

7.54 7.54 7.51 7.51 7.45 7.42 7.37 7.37 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.30 7.28 7.27 7.26
3.86 3.84 2.06 2.02 1.79 1.78 1.71 1.70 1.69 1.67 1.66 1.65 1.65 1.64 1.63 1.62 1.62 1.47 1.43 1.42 1.26 1.23 1.23 1.22 1.20 1.20 1.19 1.18 1.17 1.15 1.15 1.14 1.12 1.11 0.90
O
HN
NH
5c
1H NMR
300 MHz
CDCl3
2.00
1.09
7.44
0.82
1.00
0.98
4.06
1.03
4.20
1.04
f1 (ppm)

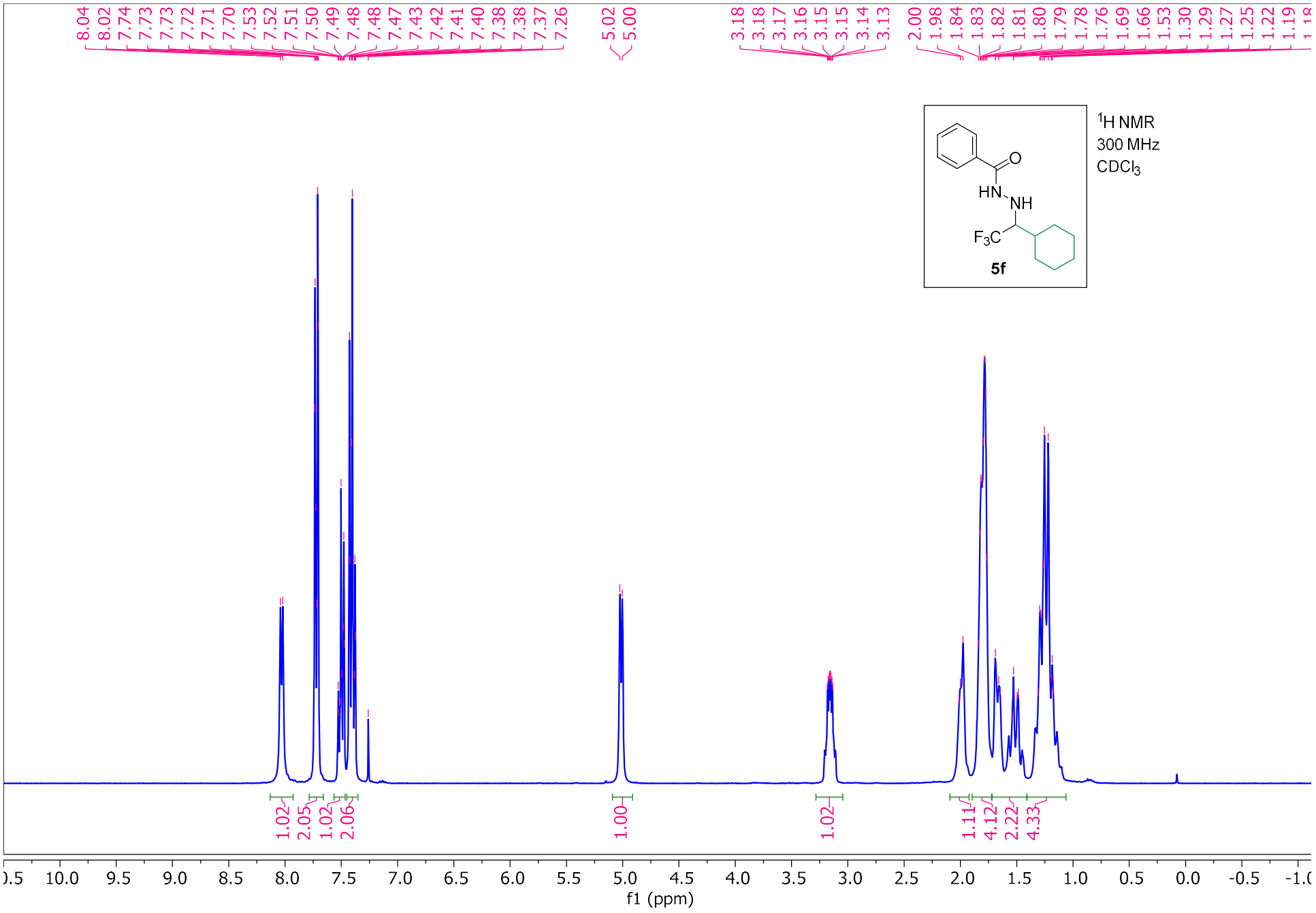

166.86
140.93
132.90
131.49
128.41
128.08
127.23
126.71
77.00
70.32
42.16
29.92
29.20
26.26
26.02
25.99
O
HN
NH
5c
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

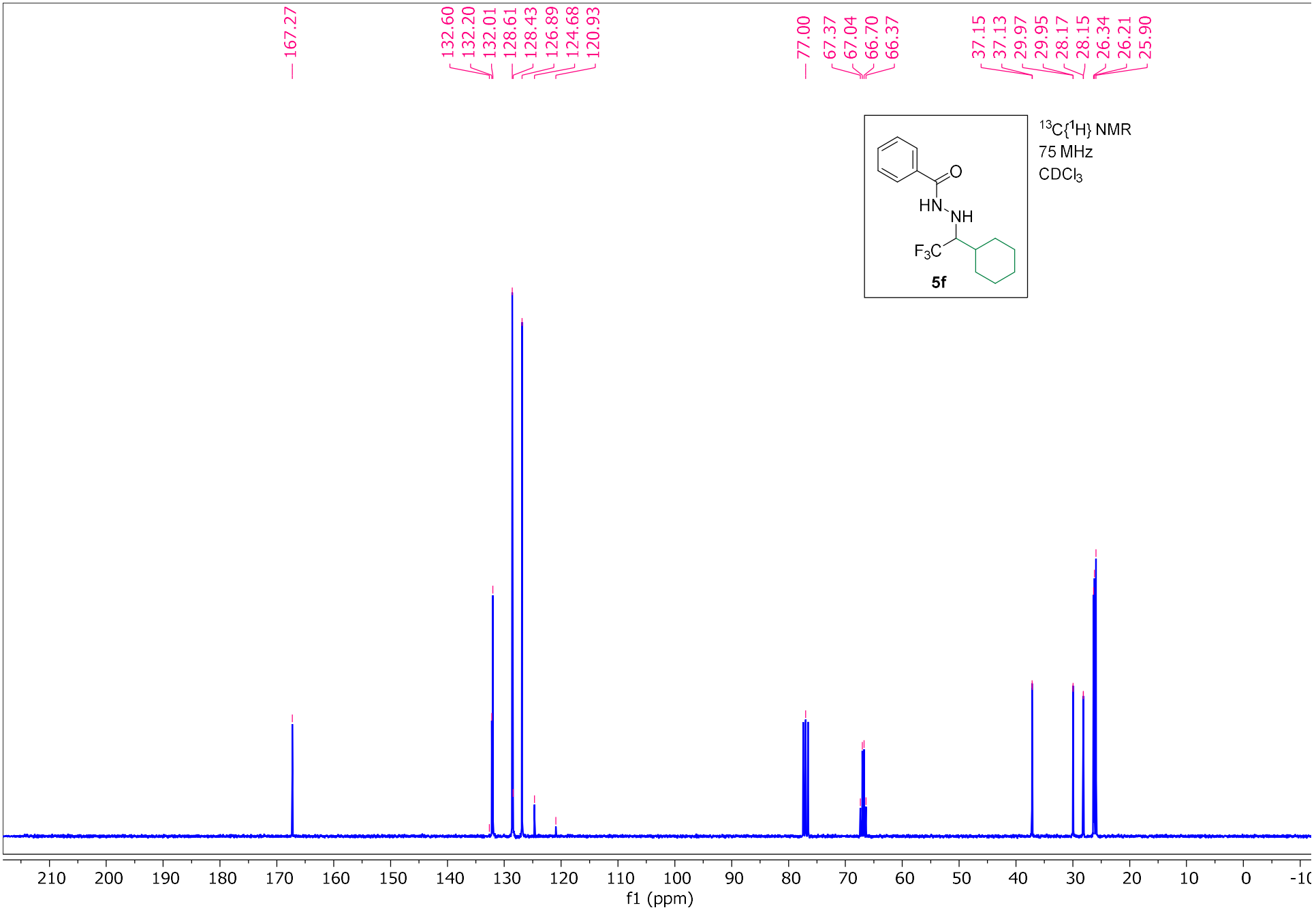

8.14 8.11 7.47 7.44 7.26 6.99 6.97 6.97 5.08 5.06 3.90 3.88 1.92 1.90 1.87 1.86 1.81 1.80 1.77 1.77 1.76 1.73 1.73 1.72 1.66 1.65 1.64 1.62 1.61 1.61 1.60 1.60 1.59 1.59 1.58 1.56 1.42 1.39 1.39 1.38 1.37 1.24 1.21 1.20 1.13 1.12 1.11 1.10 1.09 1.07 1.06 1.06 1.06 1.05 1.04 1.03 1.02 1.01 0.83 0.82 0.79 0.78
O
HN
NH
O2N
5d
1H NMR
300 MHz
CDCl3
1.88 1.85 0.90 0.92 0.94 1.07 2.86 1.04 3.03 0.99 4.13 1.01
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 -0.5
f1 (ppm)

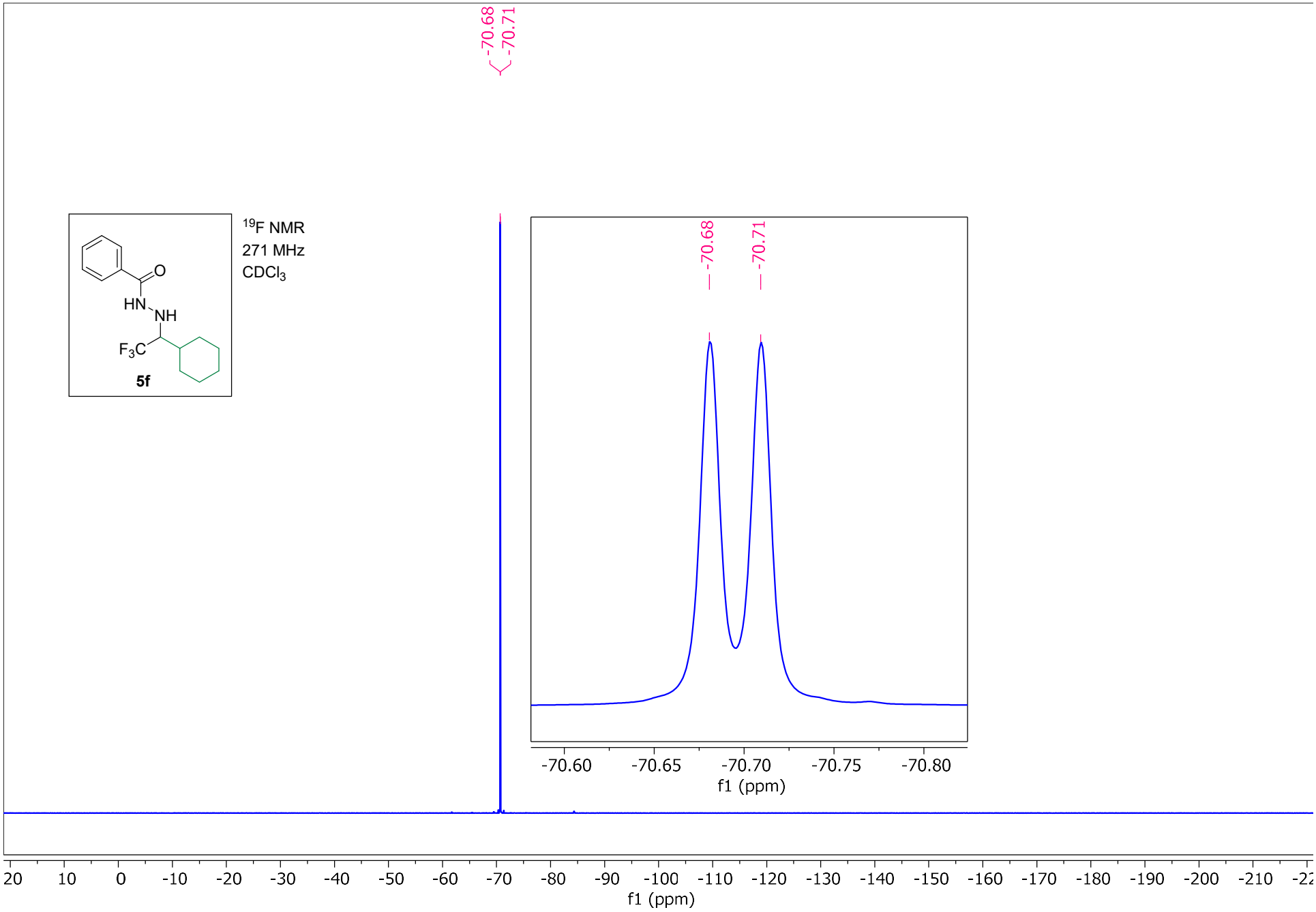

169.62
149.15
147.08
129.23
123.19
77.00
69.64
42.24
29.74
28.91
26.13
25.96
25.90
20.96
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
HN
NH
O
O_2N
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

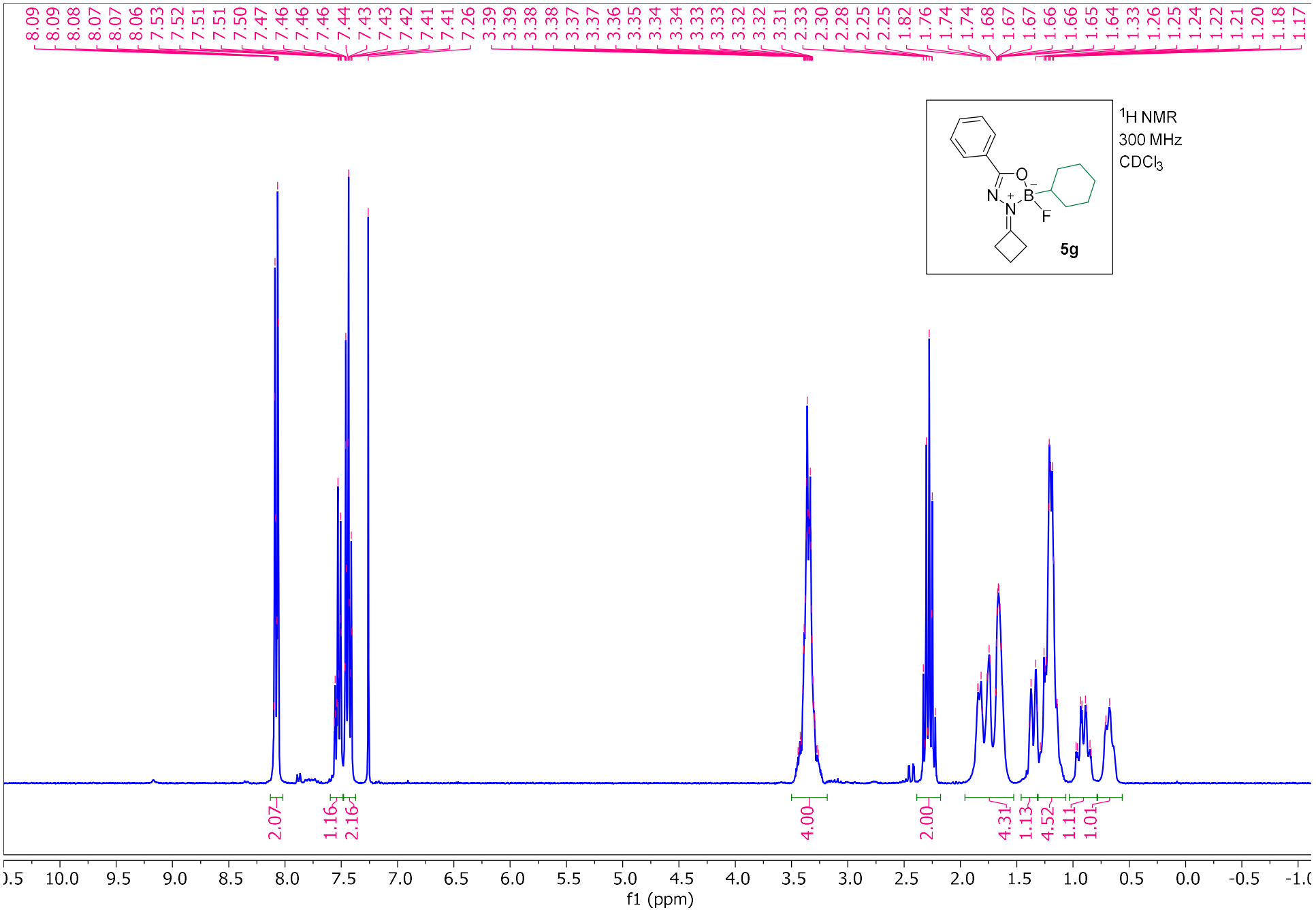

7.74 7.73 7.73 7.73 7.72 7.69 7.67 7.66 7.66 7.65 7.64 7.31 7.29 7.28 7.23 7.22 7.20 4.84 4.83 4.26 4.25 4.23 4.23 4.23 2.05 2.01 1.82 1.80 1.79 1.78 1.76 1.75 1.74 1.73 1.71 1.70 1.69 1.68 1.67 1.66 1.65 1.64 1.63 1.53 1.50 1.49 1.48 1.28 1.27 1.23 1.22 1.19 1.18 1.16 1.15 1.14 1.13 1.12 1.12 1.11 0.86 0.82
O
N
NH
O
Cl
5e
1H NMR
300 MHz
CDCl3
2.02 2.04 2.69 2.05 0.97 1.00 1.04 4.44 1.09 4.37 1.07
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 -0.5
f1 (ppm)

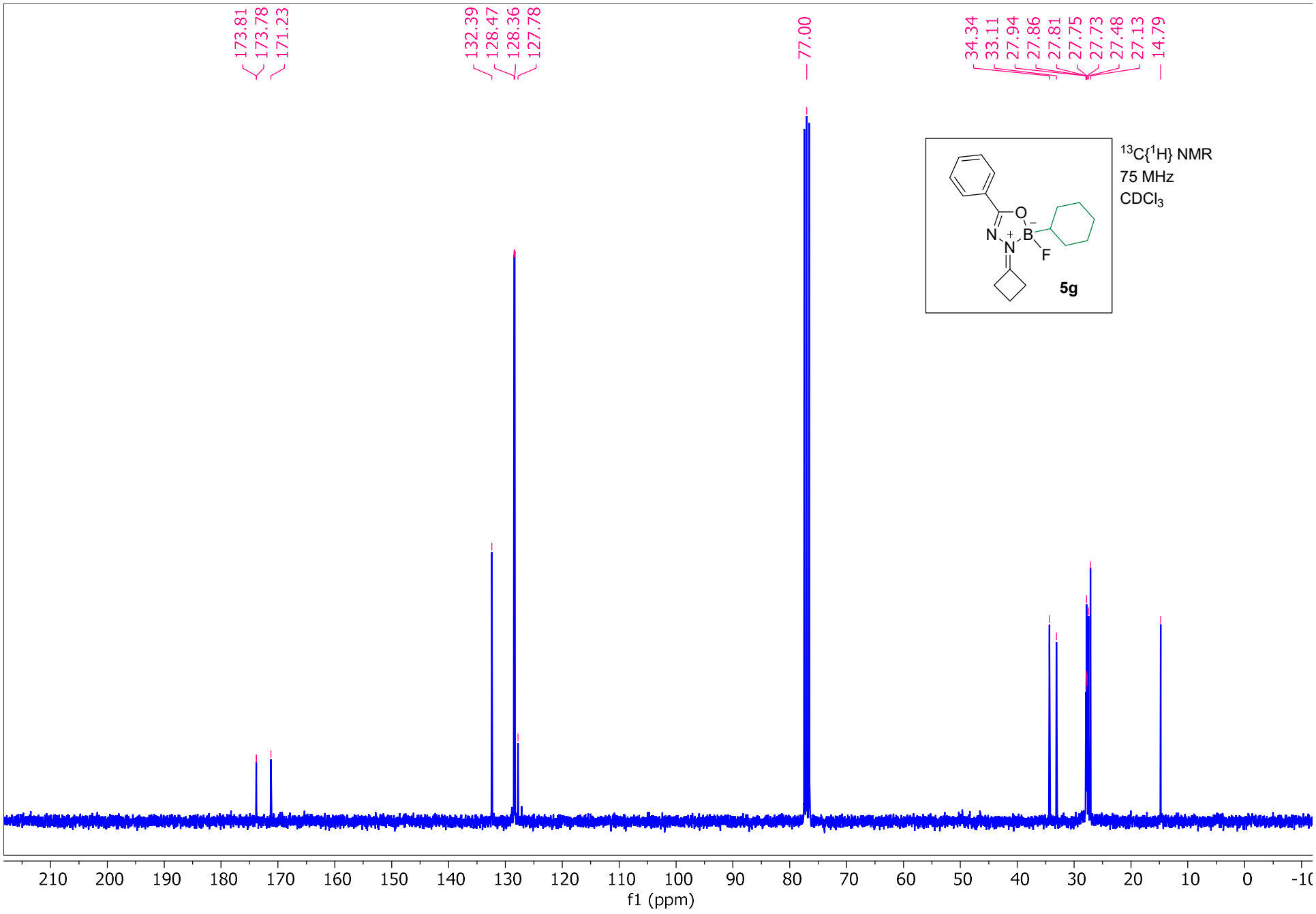

166.68
137.40
134.04
133.25
130.02
129.87
127.99
123.20
77.00
68.18
42.12
30.11
29.04
26.19
25.91
25.85
O
N
NH
O
Cl
5e
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

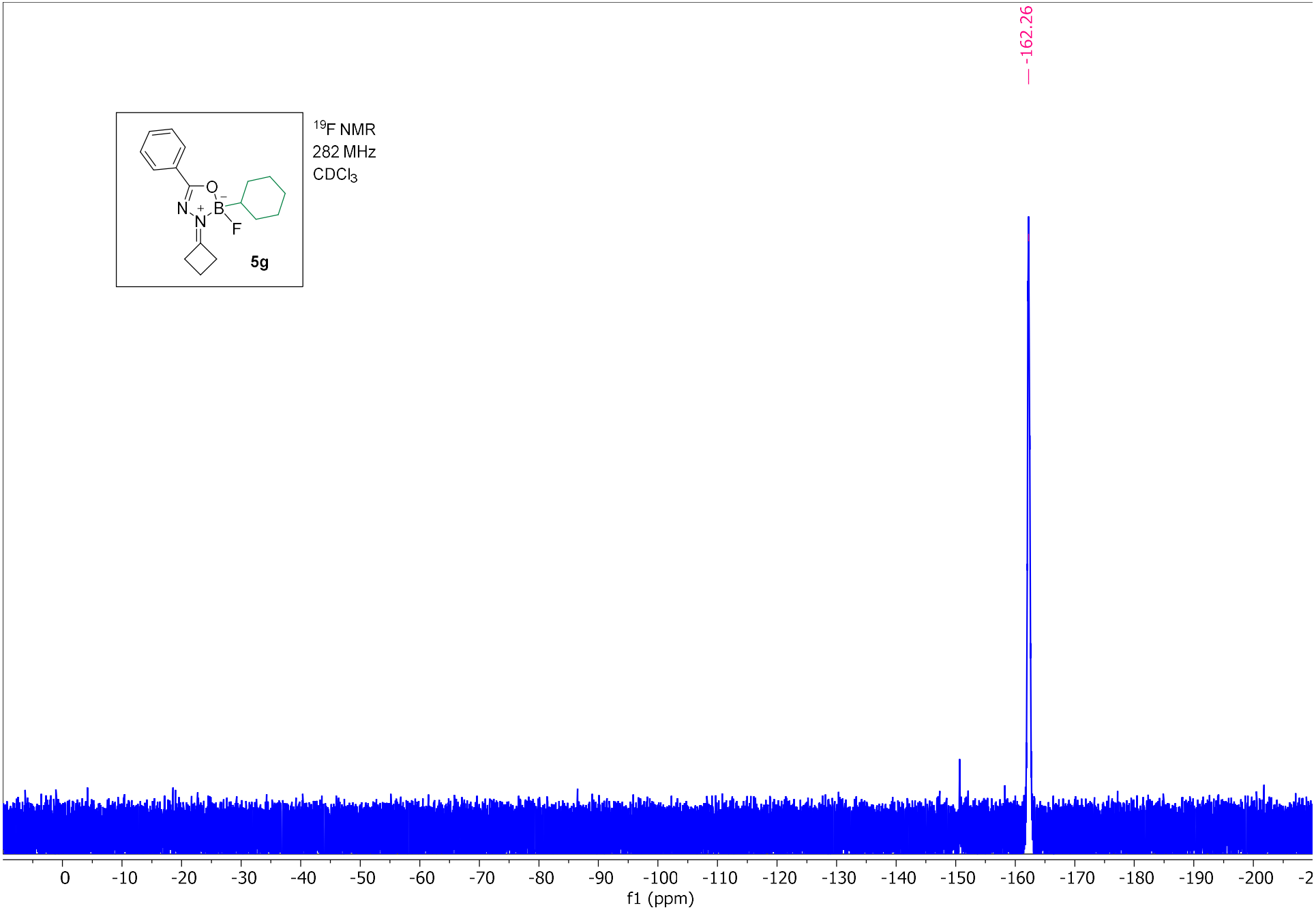

8.04 8.02 7.74 7.73 7.73 7.72 7.71 7.70 7.53 7.52 7.51 7.50 7.49 7.48 7.48 7.47 7.43 7.42 7.41 7.40 7.38 7.38 7.37 7.26
5.02 5.00
3.18 3.18 3.17 3.16 3.15 3.15 3.14 3.13
2.00 1.98 1.84 1.83 1.82 1.81 1.80 1.79 1.78 1.76 1.69 1.66 1.53 1.30 1.29 1.27 1.25 1.22 1.19
O
HN
NH
F3C
5f
1H NMR
300 MHz
CDCl3
1.02 2.05 1.02 2.06 1.00 1.02 1.11 4.12 2.22 4.33
f1 (ppm)

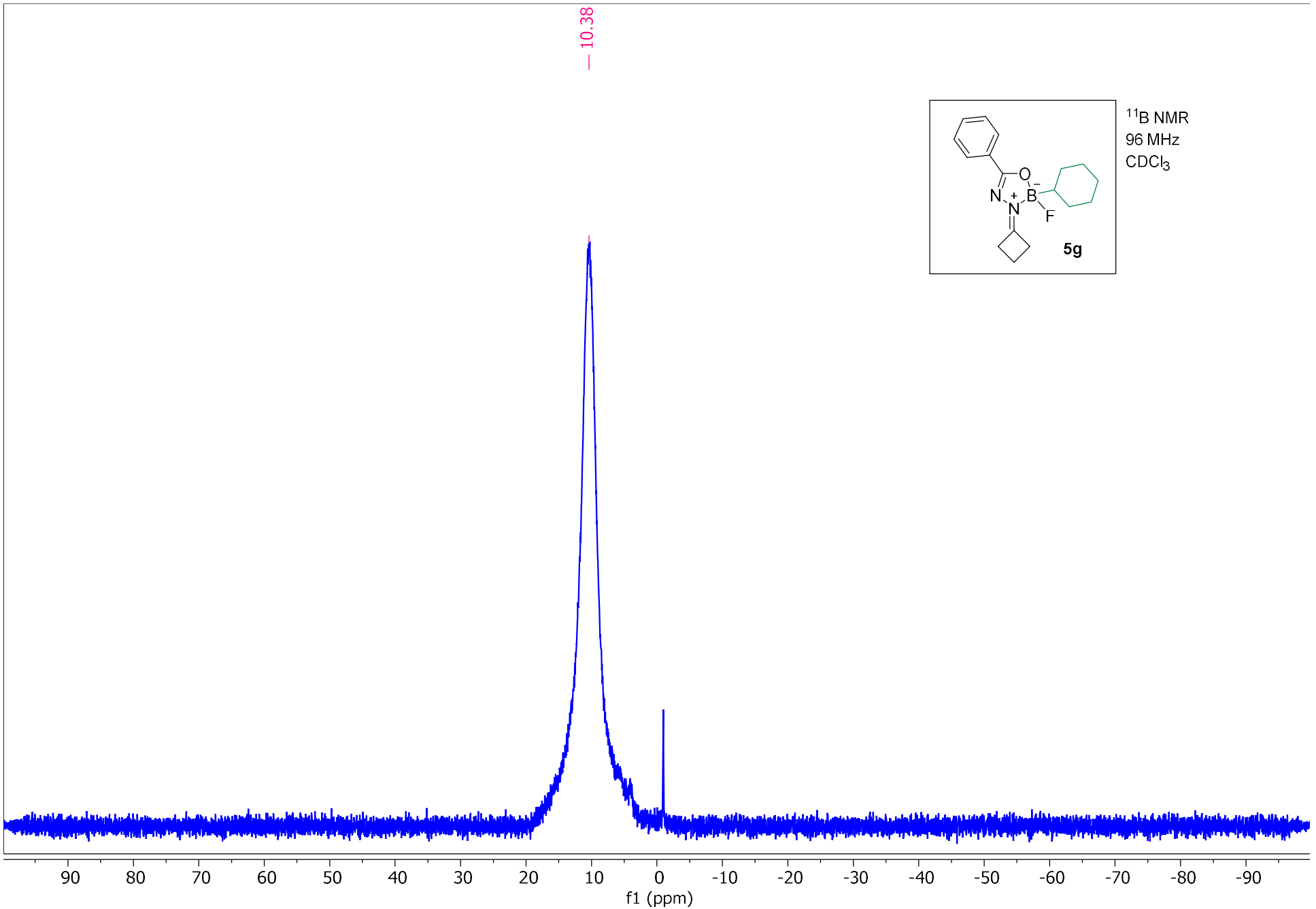

167.27
132.60
132.20
132.01
128.61
128.43
126.89
124.68
120.93
77.00
67.37
67.04
66.70
66.37
37.15
37.13
29.97
29.95
28.17
28.15
26.34
26.21
25.90
O
HN
NH
F3C
5f
13C{1H} NMR
75 MHz
CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

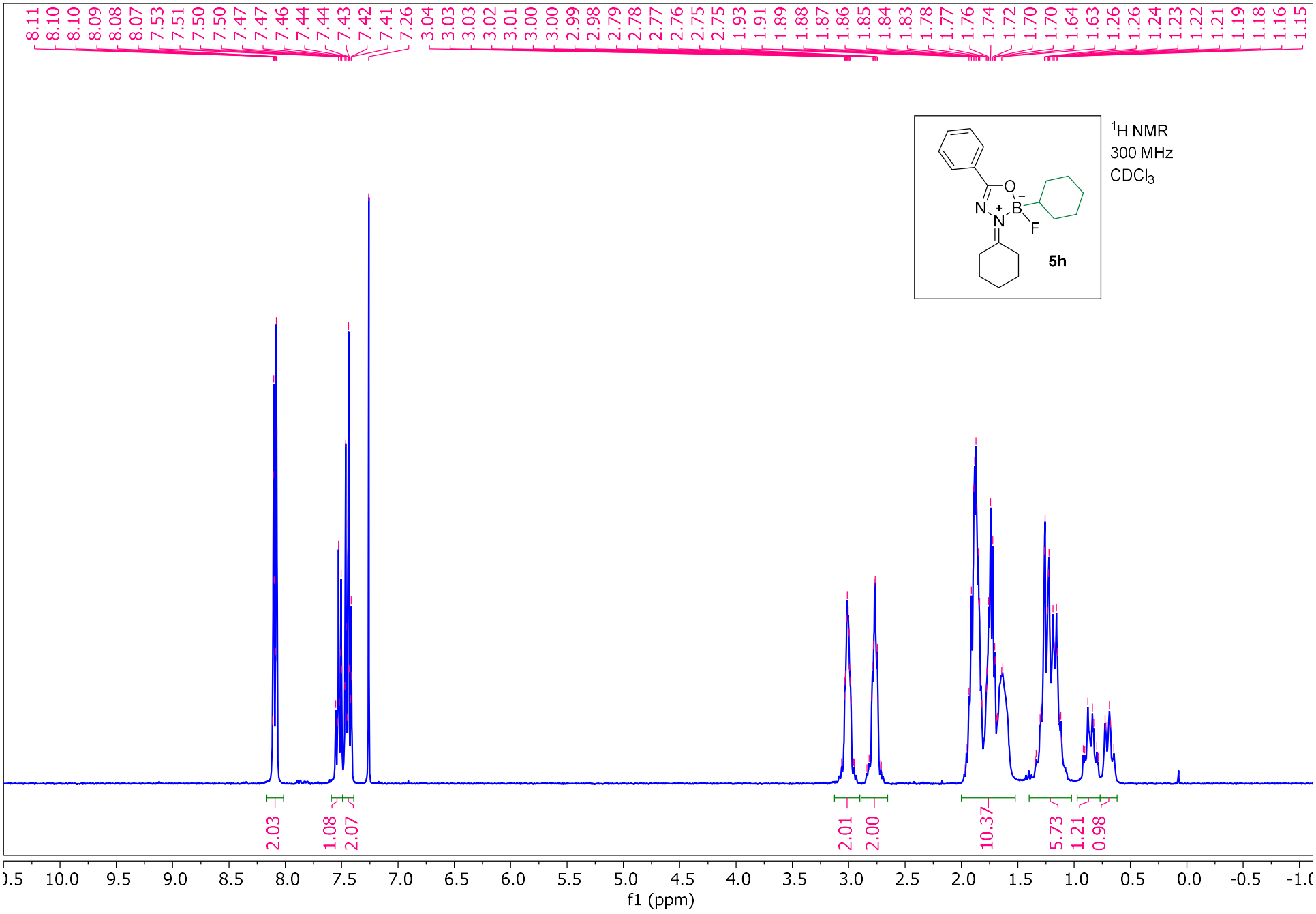

-70.68
-70.71
O
HN
NH
F3C
5f
19F NMR
271 MHz
CDCl3
-70.68
-70.71
-70.60
-70.65
-70.70
-70.75
-70.80
f1 (ppm)
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

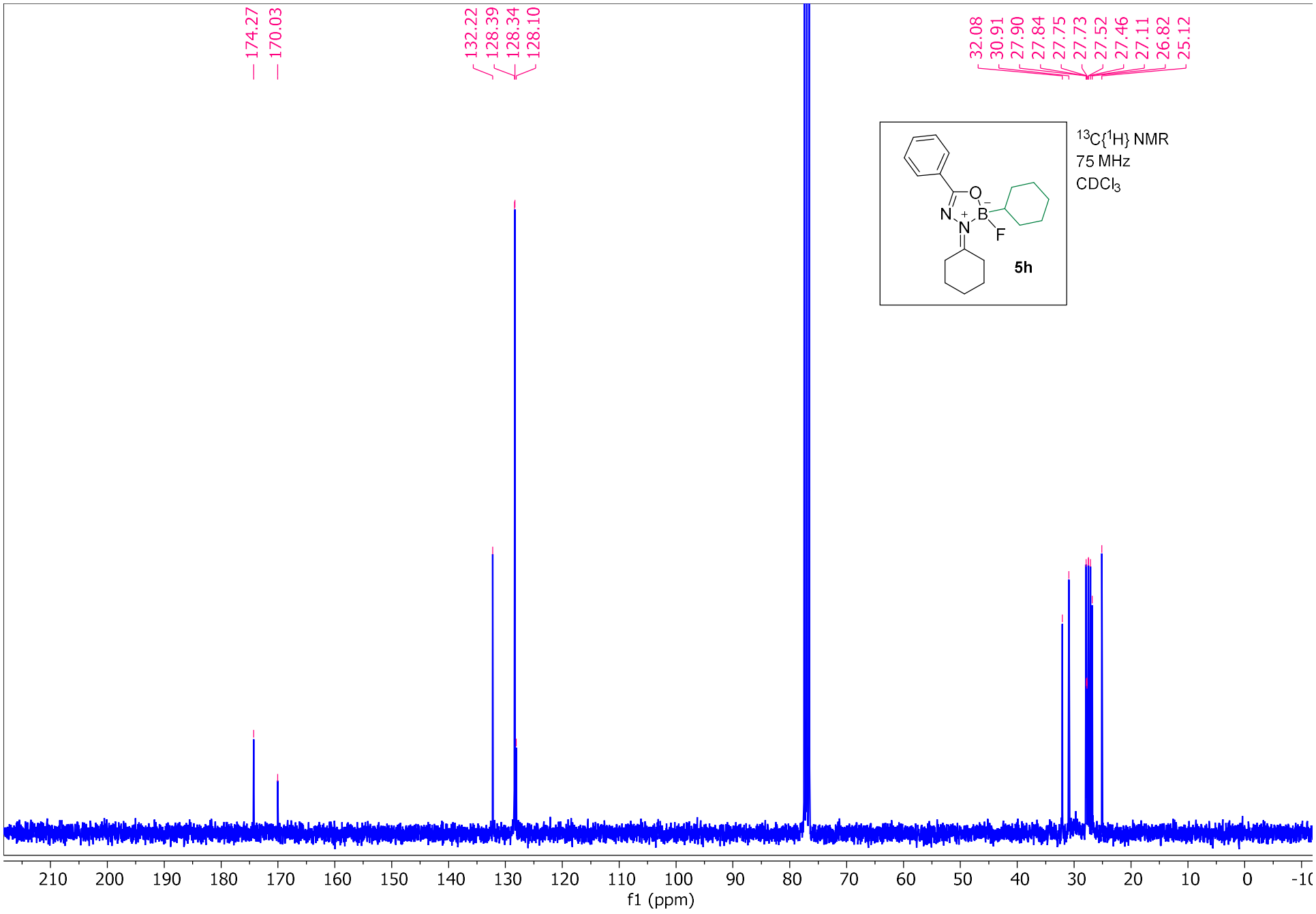

8.09 8.09 8.08 8.07 8.07 8.06 7.53 7.52 7.51 7.51 7.50 7.47 7.46 7.46 7.46 7.44 7.43 7.43 7.42 7.41 7.41 7.26
3.39 3.39 3.38 3.38 3.37 3.37 3.36 3.35 3.34 3.34 3.33 3.33 3.32 3.32 3.31 2.33 2.30 2.28 2.25 2.25 1.82 1.76 1.74 1.74 1.68 1.67 1.67 1.66 1.66 1.65 1.64 1.33 1.26 1.25 1.24 1.22 1.21 1.20 1.18 1.17
1H NMR
300 MHz
CDCl3
5g
2.07
1.16
2.16
4.00
2.00
4.31
1.13
4.52
1.11
1.01
f1 (ppm)

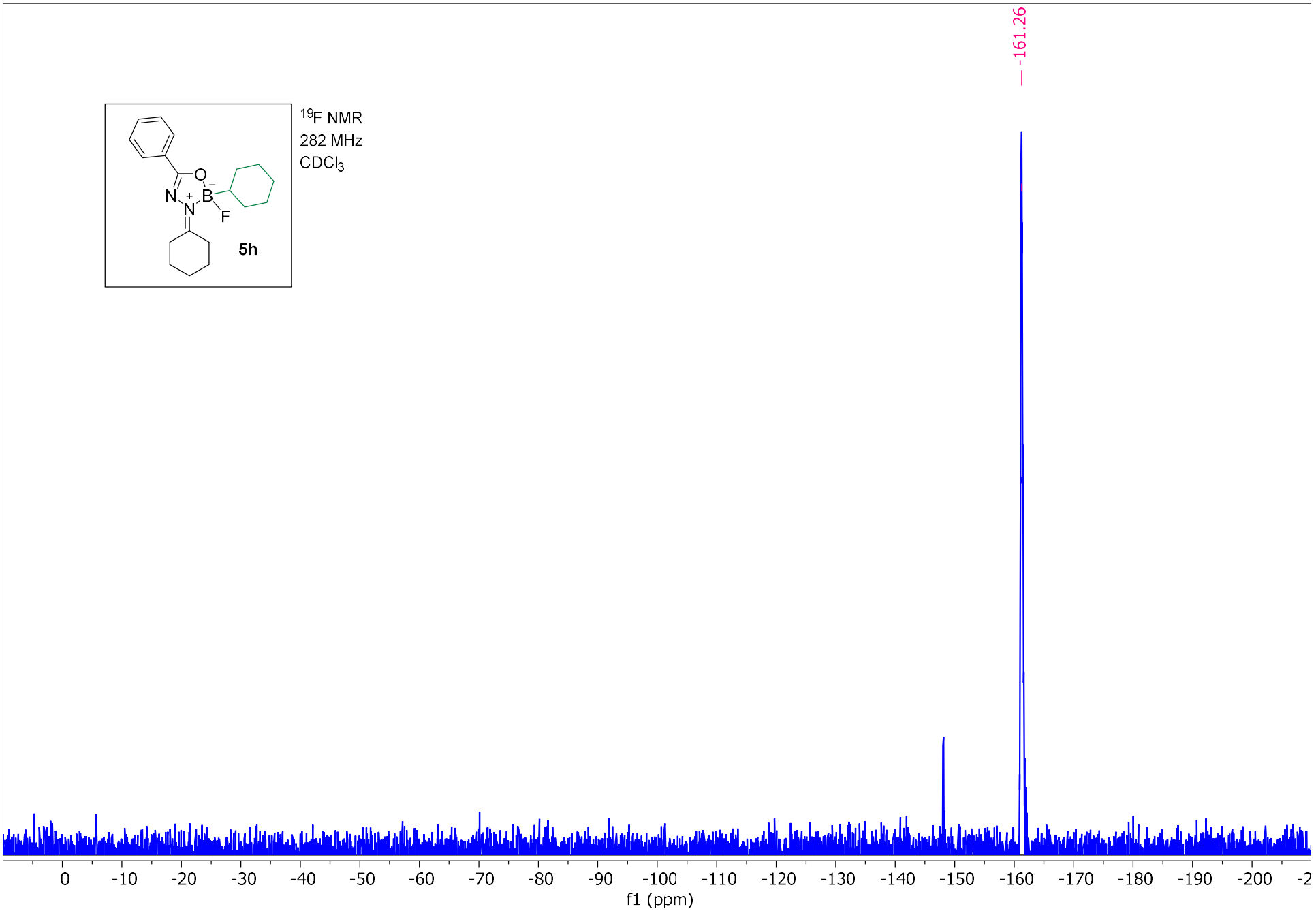

173.81
173.78
171.23
132.39
128.47
128.36
127.78
77.00
34.34
33.11
27.94
27.86
27.81
27.75
27.73
27.48
27.13
14.79
$^{13}C\{^{1}H\}$ NMR
75 MHz
$CDCl_3$
5g
f1 (ppm)

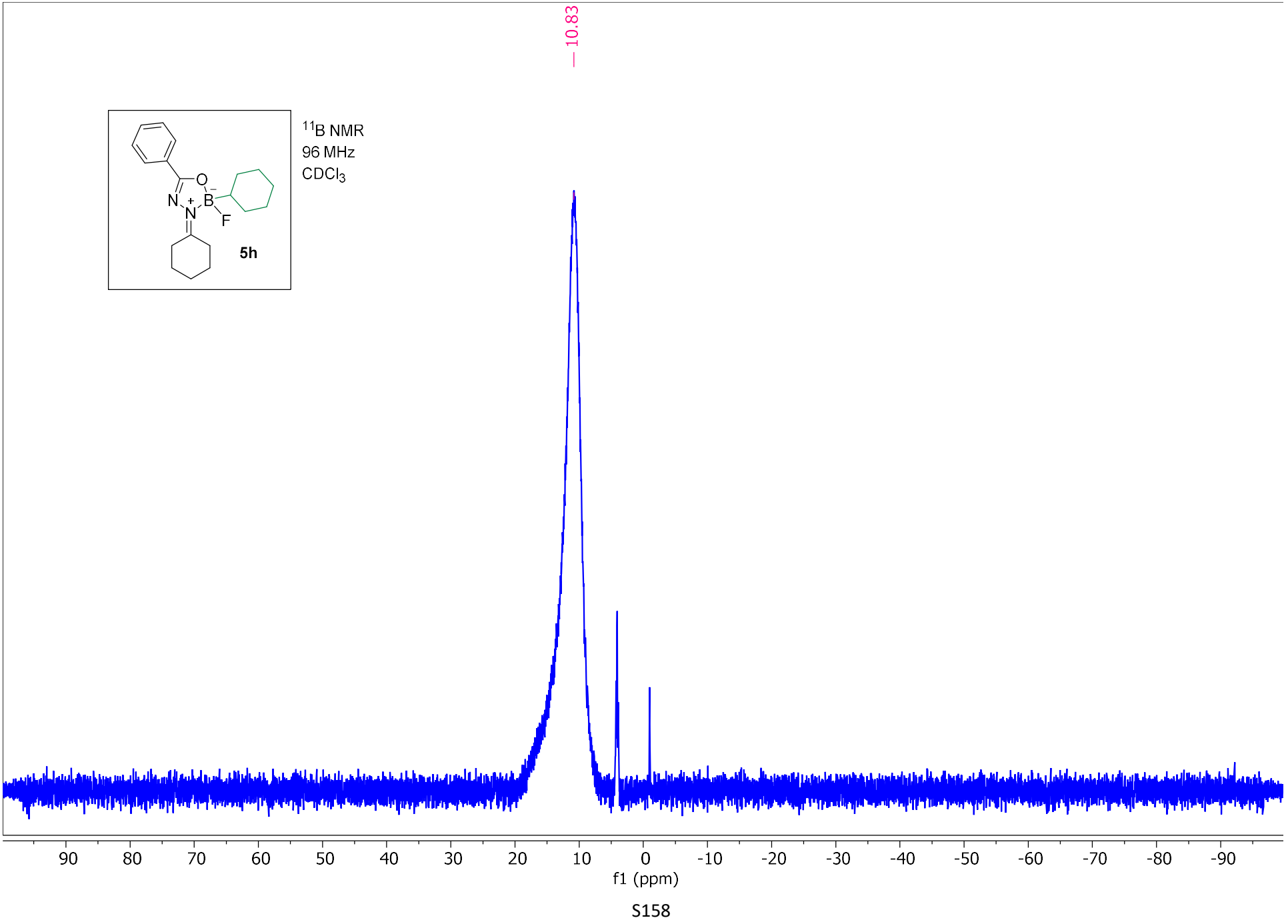

-162.26
5g
19F NMR
282 MHz
CDCl3
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


10.38
11B NMR
96 MHz
CDCl3
5g
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)


8.11 8.10 8.10 8.09 8.08 8.07 7.53 7.51 7.50 7.50 7.47 7.47 7.46 7.44 7.44 7.43 7.42 7.41 7.26
3.04 3.03 3.03 3.02 3.01 3.00 3.00 2.99 2.98 2.79 2.78 2.77 2.76 2.75 2.75 1.93 1.91 1.89 1.88 1.87 1.86 1.85 1.84 1.83 1.78 1.77 1.76 1.74 1.72 1.70 1.70 1.64 1.63 1.26 1.26 1.24 1.23 1.22 1.21 1.19 1.18 1.16 1.15
1H NMR
300 MHz
CDCl3
5h
2.03
1.08
2.07
2.01
2.00
10.37
5.73
1.21
0.98
f1 (ppm)


174.27
170.03
132.22
128.39
128.34
128.10
32.08
30.91
27.90
27.84
27.75
27.73
27.52
27.46
27.11
26.82
25.12
13C{1H} NMR
75 MHz
CDCl3
5h
f1 (ppm)


-161.26
19F NMR
282 MHz
CDCl3
5h
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)


10.83
11B NMR
96 MHz
CDCl3
5h
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)