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Palladium-Catalyzed N1-Selective Allylation of Indoles with Allylic Alcohols Promoted by Titanium Tetraisopropoxide

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Supporting Information

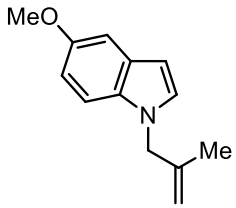
Table of Contents

Experimental Section

General Information. All reactions were carried out in flame-dried glassware under a positive nitrogen (N_2) atmosphere with standard Schlenk line technique. Transfer of anhydrous solvents and reagents was accomplished with oven-dried syringes or cannula. Tetrahydrofuran (THF) and dichloromethane (CH_2Cl_2) were first purged with nitrogen and then dried over activated alumina using a solvent purification system. Dimethyl sulfoxide (DMSO, anhydrous grade) was purchased and used without distillation. All other solvents (ACS grade) were used as received. Commercially available reagents were used as received without further purification. Thin layer chromatography (TLC) analysis was conducted on glass plates precoated with 0.25 mm silica gel, visualized with 254 nm UV lamp, and stained with potassium permaganate followed by heating until development of color. Flash chromatography was performed on 230−400 mesh silica gel with the indicated eluents. Nuclear magnetic resonance (NMR) spectra were recorded in indicated deuterated solvents and are reported in ppm with residual protiated solvent used as a reference. Coupling constants (*J*) are reported in Hertz (Hz). Infrared (IR) spectra were recorded neat and reported in cm−1. HRMS were recorded on a TOF mass spectrometer by using ionization methods (FD, ESI or FI) as specified in each case.

General Procedure for the Allylation Reaction of Indoles. To a stirring mixture of $Pd_2(dba)_3$ (18 mg, 0.02 mmol), dppf (33 mg, 0.06 mmol) in anhydrous DMSO (4 mL) was sequentially added indole (0.5 mmol), DBU (0.04 mL, 0.25 mmol), methallyl alcohol (90 mg, 2.5 mmol) and Ti(O*i*-Pr)$_4$ (0.225 mL, 0.75 mmol). The resulting mixture was brought up to 80°C (oil bath) and then stirred for 2-3 h. After being cooled to room temperature, the mixture was poured into 2 N of aqueous hydrochloric acid solution (15 mL) and extracted with ether (15 mL x 2). The combined organic layer was dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography.

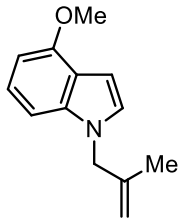
5-methoxy-1-(2-methylallyl)-1*H*-indole (**2a**)



The reaction was conducted with 0.5 mmol of 5-methoxyindole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc

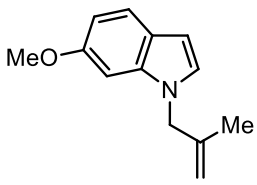
= 50:1) to afford **2b** (97 mg, 96%) as a pale yellow oil. R_f = 0.5 (hexanes/ EtOAc = 10:1). IR (film): 3078, 2954, 2918, 2849, 1657, 1621, 1510, 1486, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.9 Hz, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 7.06 (d, *J* = 3.1 Hz, 1H), 6.87 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.45 (dd, *J* = 3.1, 0.8 Hz, 1H), 4.91 (dqt, *J* = 1.4, 1.4, 1.4 Hz, 1H), 4.73 (qt, *J* = 1.6, 0.8 Hz, 1H), 4.61 (s, 2H), 3.86 (s, 3H), 1.67 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 154.0, 141.3, 131.6, 128.9, 128.8, 112.5, 111.8, 100.4, 102.5, 100.8, 55.8, 52.7, 19.8; HRMS (FI, $[M]^+$) for $C_{13}H_{15}NO$ calcd. 201.1148, found: 201.1149.

4-methoxy-1-(2-methylallyl)-1*H*-indole (**2b**)



The reaction was conducted with 0.5 mmol of 4-methoxyindole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2c** (96 mg, 95%) as a pale yellow oil. R_f = 0.5 (hexanes/ EtOAc = 10:1). IR (film): 3076, 2955, 2916, 2838, 1658, 1612, 1582, 1497, 1465, 1449 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.13 (t, *J* = 8.0 Hz, 1H), 7.00 (d, *J* = 3.2 Hz, 1H), 6.96 (d, *J* = 8.3 Hz, 1H), 6.63 (dd, *J* = 3.2, 0.8 Hz, 1H), 6.53 (d, *J* = 7.7 Hz, 1H), 4.91 (dqt, *J* = 1.4, 1.4, 1.4 Hz, 1H), 4.72 (qt, *J* = 1.6, 0.8 Hz, 1H), 4.62 (s, 2H), 3.97 (s, 3H), 1.68 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 153.4, 141.2, 137.8, 126.8, 122.3, 119.1, 112.5, 103.2, 99.2, 98.6, 55.3, 52.7, 19.8; HRMS (CI, $[M]^+$) for $C_{13}H_{15}NO$ calcd. 201.1148, found: 201.1157.

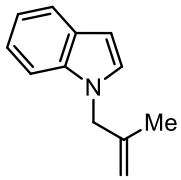
6-methoxy-1-(2-methylallyl)-1*H*-indole (**2c**)



The reaction was conducted with 0.5 mmol of 6-methoxyindole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2d** (84 mg, 83%) as a pale yellow oil. R_f = 0.5 (hexanes/EA = 10:1). IR (film): 3076, 2992, 2938, 2833, 1658, 1623, 1513, 1492, 1467 cm^{-1}; ^1H NMR (400

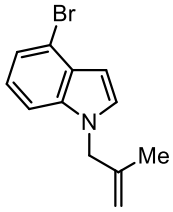
MHz, $CDCl_3$) δ 7.57 – 7.49 (m, 1H), 7.00 (d, *J* = 3.2 Hz, 1H), 6.86 – 6.79 (m, 2H), 6.48 (d, *J* = 3.1 Hz, 1H), 4.94 (dqt, *J* = 1.3, 1.3, 1.3 Hz, 1H), 4.76 (qd, *J* = 1.6, 0.8 Hz, 1H), 4.60 (s, 2H), 3.88 (s, 3H), 1.71 (dd, *J* = 1.5, 0.8 Hz, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 156.1, 141.0, 137.0, 127.2, 122.9, 121.3, 112.5, 109.1, 101.1, 93.4 , 55.6, 52.5, 19.8; HRMS (CI, $[M]^+$) for $C_{13}H_{15}NO$ calcd. 201.1148, found: 201.1158.

1-(2-methylallyl)-1*H*-indole (**2d**)



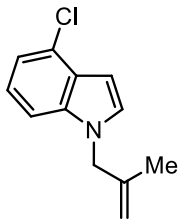
The reaction was conducted with 0.5 mmol of indole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2a** (70 mg, 82%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3056, 2956, 2924, 2853, 1658, 1613, 1512, 1463 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 1H), 7.09 (d, *J* = 3.0 Hz, 1H), 6.52 (d, *J* = 3.1 Hz, 1H), 4.91 (dq, *J* = 1.4, 1.4 Hz, 1H), 4.75 – 4.71 (m, 1H), 4.65 (s, 2H), 1.68 (s, 3H) ; ^{13}C NMR (400 MHz, $CDCl_3$) δ 141.1, 136.3, 128.6, 128.2, 121.4, 120.9, 119.3, 112.6, 109.6, 101.3, 52.5, 19.8; HRMS (EI, $[M]^+$) for $C_{12}H_{13}N$ calcd. 171.1076, found: 171.1072.

4-bromo-1-(2-methylallyl)-1*H*-indole (**2e**)



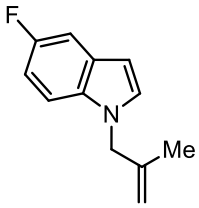
The reaction was conducted with 0.5 mmol of 4-bromoindole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2e** (112 mg, 90%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3102, 2973, 2922, 2852, 1659, 1607, 1558, 1508, 1479, 1432 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 7.14 (d, *J* = 3.2 Hz, 1H), 7.10 – 7.01 (m, 1H), 6.59 (dd, *J* = 3.2, 0.8 Hz, 1H), 4.93 (dq, *J* = 1.3, 1.3 Hz, 1H), 4.72 (qt, *J* = 1.6, 0.8 Hz, 1H), 4.63 (s, 2H), 1.70 – 1.66 (m, 3H) ; ^{13}C NMR (400 MHz, $CDCl_3$) δ 140.7, 136.6, 129.2, 128.8, 122.4, 122.3, 114.8, 112.9, 108.9, 101.7, 52.8, 19.8; HRMS (FI, $[M]^+$) for $C_{12}H_{12}Br^{79}N$ calcd. 249.0148, found: 249.0151.

4-chloro-1-(2-methylallyl)-1*H*-indole (**2f**)



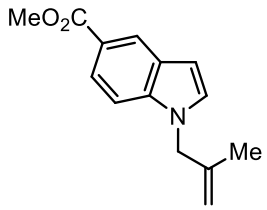
The reaction was conducted with 0.5 mmol of 4-chloroindole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2f** (89 mg, 87%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3078, 2954, 2923, 2869, 2852, 1659, 1608, 1564, 1509, 1482, 1398 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.18 (m, 1H), 7.14 – 7.08 (m, 3H), 6.62 (dd, *J* = 3.2, 0.8 Hz, 1H), 4.92 (dqt, *J* = 1.4, 1.4, 1.4 Hz, 1H), 4.71 (m, 1H), 4.64 (s, 2H), 1.67 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 140.7, 137.0, 128.8, 127.3, 126.1, 122.1, 119.1, 112.9, 108.4, 100.0, 52.8, 19.8; HRMS (FI, $[M]^+$) for $C_{12}H_{12}Cl^{35}N$ calcd. 205.0653, found: 205.0652.

5-fluoro-1-(2-methylallyl)-1*H*-indole (**2g**)



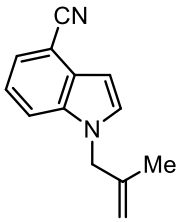
The reaction was conducted with 0.5 mmol of 5-fluoroindole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2g** (84 mg, 89%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3077, 3056, 2956, 2924, 2853, 1658, 1613, 1512, 1463 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 9.6, 2.4 Hz, 1H), 7.23 (dd, *J* = 8.9, 4.4 Hz, 1H), 7.13 (d, *J* = 3.1 Hz, 1H), 6.95 (td, *J* = 9.1, 2.4 Hz, 1H), 6.48 (d, *J* = 3.1 Hz, 1H), 4.93 (t, *J* = 1.6 Hz, 1H), 4.72 (s, 1H), 4.63 (s, 2H), 1.68 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 157.8 (d, *J* = 233.9 Hz), 140.9, 132.9 , 129.9 , 128.8 (d, *J* = 10.2 Hz), 112.7 , 110.3 (d, *J* = 9.8 Hz), 109.9 (d, *J* = 26.3 Hz), 105.5 (d, *J* = 23.3 Hz), 101.2 (d, *J* = 4.7 Hz), 52.8, 19.8; HRMS (CI, $[M]^+$) for $C_{12}H_{12}FN$ calcd. 189.0948, found: 189.0953.

methyl 1-(2-methylallyl)-1*H*-indole-5-carboxylate (**2h**)



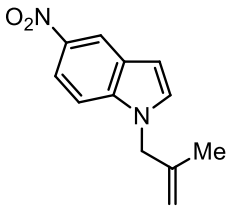
The reaction was conducted with 0.5 mmol of methyl indole-5-carboxylate following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 30:1) to afford **2h** (105 mg, 92%) as a pale yellow oil. R_f = 0.4 (hexanes/ EtOAc = 10:1). IR (film): 3081, 2949, 2917, 2852, 1711, 1613, 1514, 1487, 1450, 1435 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.92 (d, *J* = 8.7 Hz, 1H), 7.31 (d, *J* = 8.7 Hz, 1H), 7.13 (d, *J* = 2.9 Hz, 1H), 6.61 (d, *J* = 2.6 Hz, 1H), 4.92 (s, 1H), 4.69 (s, 1H), 4.63 (s, 2H), 3.93 (s, 3H), 1.67 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 168.1, 140.6, 138.7, 129.6, 128.0, 123.9, 122.8, 121.4, 112.8, 109.2, 102.9, 52.5, 51.7, 19.7; HRMS (CI, $[M]^+$) for $C_{14}H_{15}NO_2$ calcd. 229.1097, found: 229.1090.

1-(2-methylallyl)-1*H*-indole-4-carbonitrile (**2i**)



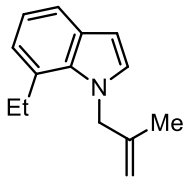
The reaction was conducted with 0.5 mmol of 4-cyanoindole following the general procedure. The crude product was purified by flash chromatography (hexanes/CH_2Cl_2 = 2:1) to afford **2i** (85 mg, 87%) as a pale yellow oil. R_f = 0.3 (hexanes/ EtOAc = 10:1). IR (film): 3101, 3082, 2974, 2918, 2223, 1657, 1605, 1505, 1488, 1435, 1402 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.3 Hz, 1H), 7.46 (d, *J* = 7.4 Hz, 1H), 7.26 (d, *J* = 3.3 Hz, 1H), 7.24 – 7.19 (m, 1H), 6.73 (d, *J* = 3.2 Hz, 1H), 4.94 (s, 1H), 4.70 (s, 1H), 4.68 (s, 2H), 1.67 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 140.3, 135.9, 130.9, 129.8, 124.9, 121.1, 118.7, 114.5, 113.2, 103.2, 100.4, 52.8, 19.7; HRMS (CI, $[M]^+$) for $C_{13}H_{12}N_2$ calcd. 196.0995, found: 196.1000.

1-(2-methylallyl)-5-nitro-1*H*-indole (**2j**)



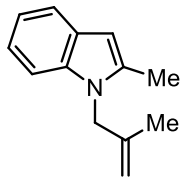
The reaction was conducted with 0.5 mmol of 5-nitroindole following the general procedure. The crude product was purified by flash chromatography (hexanes/CH_2Cl_2 = 2:1) to afford **2j** (97 mg, 90%) as a yellow solid. R_f = 0.3 (hexanes/ EtOAc = 10:1). IR (film): 3066, 2968, 2909, 2851, 1656, 1593, 1570, 1487, 1462, 1443, 1365 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 2.1 Hz, 1H), 8.10 (dd, *J* = 9.1, 2.2 Hz, 1H), 7.33 (d, *J* = 9.1 Hz, 1H), 7.23 (d, *J* = 3.2 Hz, 1H), 6.70 (d, *J* = 3.1 Hz, 1H), 4.96 (dq, *J* = 1.4, 1.4 Hz, 1H), 4.71 (s, 1H), 4.69 (s, 2H), 1.69 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 141.4, 140.1, 139.0, 131.5, 127.6, 118.0, 117.0, 113.1, 109.5, 103.9, 52.7, 19.6; HRMS (CI, $[M]^+$) for $C_{12}H_{12}N_2O_2$ calcd. 216.0893, found: 216.0898. m.p. = 64-65 °C.

7-ethyl-1-(2-methylallyl)-1*H*-indole (**2k**)



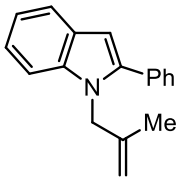
The reaction was conducted with 0.5 mmol of 5-methoxyindole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 70:1) to afford **2k** (72 mg, 73%) as a pale yellow oil. R_f = 0.7 (hexanes/ EtOAc = 10:1). IR (film): 3084, 3059, 2965, 2930, 2873, 1692, 1601, 1525, 1486, 1443, 1422 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.06 – 7.01 (m, 1H), 7.00 (d, *J* = 3.2 Hz, 1H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.51 (d, *J* = 3.2 Hz, 1H), 4.82 (dqt, *J* = 1.5, 1.5, 1.5 Hz, 1H), 4.77 (s, 2H), 4.24 (m, 1H), 2.94 (q, *J* = 7.5 Hz, 2H), 1.76 (s, 3H), 1.33 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 142.8, 134.2, 130.1, 129.8, 127.5, 122.4, 119.7, 118.9, 111.0, 101.7, 54.4, 25.0, 19.9, 16.1; HRMS (CI, $[M]^+$) for $C_{14}H_{17}N$ calcd. 199.1356, found: 199.1357.

2-methyl-1-(2-methylallyl)-1*H*-indole (**2l**)



To a stirring solution of $Pd_2(dba)_3$ (18 mg, 0.02 mmol), dppf (33 mg, 0.06 mmol) in anhydrous DMSO (4 mL) was sequentially added 2-methylindole (0.5 mmol), DBU (0.08 mL, 0.5 mmol), methallyl alcohol (90 mg, 2.5 mmol) and Ti(O-*i*Pr)$_4$ (0.075 mL, 0.025 mmol). The resulting mixture was brought up to 80°C and then stirred for 24 h. After cooled to room temperature, the mixture was pooled into 2 N of aqueous hydrochloric acid solution (15 mL) and extracted with ether (15 mL x 2). The organic layer was dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography (hexanes/EtOAc = 70:1) to afford **2l** (58 mg, 63%) as a brown oil. R_f = 0.7 (hexanes/ EtOAc = 10:1). IR (film): 3085, 3056, 3029, 2923, 2855, 1658, 1612, 1554, 1479, 1464 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 8.1 Hz, 1H), 7.17 – 7.11 (m, 1H), 7.11 – 7.05 (m, 1H), 6.30 (s, 1H), 4.85 (dqt, *J* = 1.5, 1.5, 1.5 Hz, 1H), 4.59 (s, 2H), 4.44 – 4.39 (m, 1H), 2.41 (s, 3H), 1.75 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 140.9, 137.0, 136.7, 128.0, 120.5, 119.6, 119.3, 111.2, 109.1, 100.0, 48.6, 20.0, 12.5; HRMS (CI, $[M]^+$) for $C_{13}H_{15}N$ calcd. 185.1199, found: 185.1205.

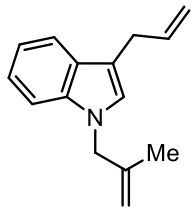
1-(2-methylallyl)-2-phenyl-1*H*-indole (**2m**)



The reaction was conducted with 0.5 mmol of 2-phenylindole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 70:1) to afford an inseparable mixture of **2m** and **2m'** (97% combined yield) as a pale yellow oil. R_f = 0.7 (hexanes/ EtOAc = 10:1). Spectral data of the major product **2m**. IR (film): 3059, 2971, 2930, 1658, 1604, 1490, 1475, 1462, 1444 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.8 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.52 – 7.41 (m, 3H), 7.29 – 7.23 (m, 1H), 7.22 – 7.16 (m, 1H), 6.65 (s, 1H), 4.96 (dqt, *J* = 1.5, 1.5, 1.5 Hz, 1H), 4.64 (s, 2H), 4.62 (s, 1H), 1.75 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 141.6,

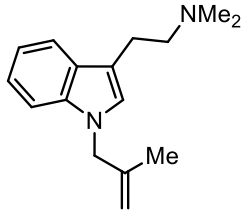
129.0, 128.5, 127.9, 121.7, 120.4, 120.0, 111.4, 110.4, 101.9, 49.8, 20.1 (Partial spectral data of **2m**); HRMS (EI, $[M]^+$) for $C_{18}H_{17}N$ calcd. 247.1356, found: 247.1351.

3-allyl-1-(2-methylallyl)-1*H*-indole (**2n**)



The reaction was conducted with 0.5 mmol of 3-allyl-1*H*-indole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2n** (95 mg, 90%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3076, 3056, 3003, 2913, 2852, 1639, 1614, 1581, 1554, 1481, 1466, 1437 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 6.89 (s, 1H), 6.10 (ddt, *J* = 16.6, 10.0, 6.4 Hz, 1H), 5.18 (dq, *J* = 17.1, 1.8 Hz, 1H), 5.09 (dq, *J* = 10.0, 1.5 Hz, 1H), 4.92 (dq, *J* = 1.4, 1.4 Hz, 1H), 4.79 – 4.73 (m, 1H), 4.61 (s, 2H), 3.55 (d, *J* = 6.4 Hz, 2H), 1.69 (s, 3H)); ^{13}C NMR (400 MHz, $CDCl_3$) δ 141.3, 137.4, 136.8, 128.0, 125.9, 121.5, 119.2, 118.7, 115.0, 113.2, 112.5, 109.6, 52.3, 29.7, 19.9; HRMS (FD, $[M]^+$) for $C_{15}H_{17}N$ calcd. 211.1356, found: 211.1363.

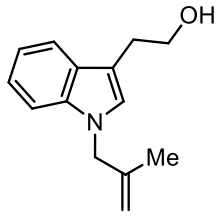
N,*N*-dimethyl-2-(1-(2-methylallyl)-1*H*-indol-3-yl)ethanamine (**2o**)



The reaction was conducted with 0.5 mmol of 2-(1*H*-indol-3-yl)-*N*,*N*-dimethylethanamine following the general procedure. The crude product was purified by flash chromatography (CH_2Cl_2/MeOH = 40:1) to afford **2o** (82 mg, 68%) as a brown oil. R_f = 0.5 (CH_2Cl_2/MeOH = 10:1). IR (film): 3073, 3054, 2952, 2925, 2854, 1657, 1614, 1467, 1443, 1376 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 1H), 7.28 (d, *J* = 8.2 Hz, 1H), 7.19 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.10 (ddd, *J* = 8.0, 6.9, 1.1 Hz, 1H), 6.93 (s, 1H), 4.89 (dq, *J* = 1.4, 1.4 Hz, 1H), 4.74 – 4.69 (dq, *J* = 1.4, 1.4 Hz, 1H), 4.59 (s, 2H), 3.09 – 2.99 (m, 2H), 2.84 –

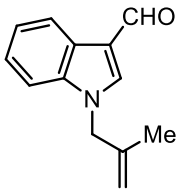
2.74 (m, 2H), 2.46 (s, 6H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 141.3, 136.6, 128.0, 125.6, 121.5, 118.9, 118.7, 113.2, 112.4, 109.6, 60.6, 52.3, 45.5, 23.7, 19.9; HRMS (EI, $[M]^+$) for $C_{16}H_{22}N_2$ calcd. 242.1778, found: 242.1775.

2-(1-(2-methylallyl)-1*H*-indol-3-yl)ethanol (**2p**)



The reaction was conducted with 0.5 mmol of tryptophol following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 3:1) to afford **2p** (104 mg, 97%) as a pale yellow oil. R_f = 0.3 (hexanes/ EtOAc = 2:1). IR (film): 3547, 3357, 3054, 2954, 2925, 2871, 1658, 1614, 1481, 1467, 1443, 1376 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (m, 1H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.21 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.12 (ddd, *J* = 8.0, 6.9, 1.1 Hz, 1H), 6.98 (s, 1H), 4.91 (dqt, *J* = 1.4, 1.4, 1.4 Hz, 1H), 4.73 (qt, *J* = 1.5, 0.7 Hz, 1H), 4.61 (s, 2H), 3.90 (t, *J* = 6.4 Hz, 2H), 3.04 (t, *J* = 6.7 Hz, 2H), 1.68 (s, 3H), 1.50 (br, 1H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 141.1, 136.8, 127.9, 126.6, 121.7, 118.9, 118.9, 112.6, 111.0, 109.7, 62.6, 52.3, 28.6, 19.8; HRMS (CI, $[M]^+$) for $C_{14}H_{17}NO$ calcd. 215.1305, found: 215.1309.

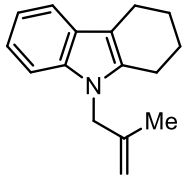
1-(2-methylallyl)-1*H*-indole-3-carbaldehyde (**2q**)



The reaction was conducted with 0.5 mmol of indole-3-carboxaldehyde following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 6:1) to afford **2q** (87 mg, 87%) as a pale yellow oil. R_f = 0.5 (hexanes/ EtOAc = 2:1). IR (film): 3103, 3054, 2974, 2917, 2853, 2808, 2753, 2729, 1660, 1614, 1577, 1531, 1485, 1466, 1442, 1401 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.00 (s, 1H), 8.36 – 8.27 (m, 1H), 7.69 (s, 1H), 7.38 – 7.28 (m, 3H), 5.00 (dqt, *J* = 1.3, 1.3, 1.3 Hz, 1H), 4.80 (dq, *J* = 1.2, 1.2 Hz, 1H), 4.69 (s, 2H), 1.71 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 184.5, 139.4, 138.6, 137.4, 125.3, 124.0, 122.9, 122.0, 118.3, 114.3, 110.3, 53.2, 19.8; HRMS (CI, $[M]^+$) for $C_{13}H_{13}NO$ calcd. 199.0992,

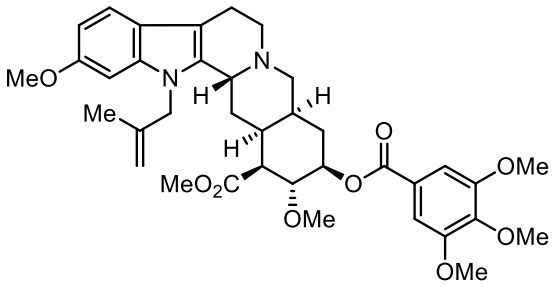
found: 199.0995.

9-(2-methylallyl)-2,3,4,9-tetrahydro-1*H*-carbazole (**2r**)



The reaction was conducted with 0.5 mmol of 1,2,3,4-tetrahydrocarbazole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2r** (104 mg, 92%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3052, 2925, 2853, 1469, 1443, 1375 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.14 (td, *J* = 8.1, 7.6, 1.3 Hz, 1H), 7.08 (td, *J* = 7.4, 1.2 Hz, 1H), 4.83 (dqt, *J* = 1.5, 1.5, 1.5 Hz, 1H), 4.54 (s, 2H), 4.49 (qd, *J* = 1.7, 0.8 Hz, 1H), 2.76 (tt, *J* = 5.9, 1.6 Hz, 2H), 2.68 (tt, *J* = 6.2, 1.6 Hz, 2H), 1.99 – 1.91 (m, 2H), 1.91 – 1.83 (m, 2H), 1.71 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 141.4, 136.5, 135.6, 127.3, 120.5, 118.6, 117.6, 111.2, 109.4, 108.9, 48.5, 23.27, 23.23, 22.0, 21.1, 20.0; HRMS (FD, $[M]^+$) for $C_{16}H_{19}N$ calcd. 225.1520, found: 225.1521.

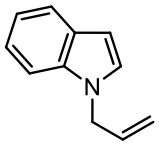
(1S,2R,3R,4aS,13bR,14aS)-methyl-2,11-dimethoxy-13-(2-methylallyl)-3-((3,4,5-tri-methoxybenzoyl)oxy)-1,2,3,4,4a,5,7,8,13,13b,14,14a-dodecahydroindolo[2',3':3,4]-pyrido[1,2-b]isoquinoline-1-carboxylate (**2s**)



The reaction was conducted with 0.5 mmol of Reserpine following the general procedure (In this case, ethyl acetate was used as a solvent for the extraction). The crude product was purified by flash chromatography (hexanes/EtOAc = 1.5:1) to afford **2t** (218 mg, 66%) as a pale yellow solid. R_f = 0.3 (hexanes/ EtOAc = 1.5:1). IR (film): 3079, 2936, 2839, 1734, 1714, 1621, 1589, 1504, 1492, 1460, 1437, 1416, 1364, 1225, 1257, 1228 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.30 (m, 3H),

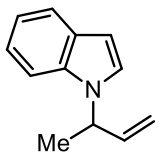
6.77 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.70 (d, *J* = 2.1 Hz, 1H), 5.05 (ddd, *J* = 11.9, 9.2, 5.1 Hz, 1H), 4.84 (s, 1H), 4.61 (d, *J* = 18.2 Hz, 1H), 4.45 (s, 1H), 4.39 (br, 1H), 4.23 (d, *J* = 18.1 Hz, 1H), 3.91 (s, 9H), 3.85 (s, 3H), 3.78 (s, 3H), 3.49 (s, 3H), 3.19 (dd, *J* = 11.8, 4.0 Hz, 1H), 3.11 (dd, *J* = 16.7, 5.3 Hz, 1H), 3.07 – 2.95 (m, 1H), 2.69 (dd, *J* = 11.3, 4.3 Hz, 1H), 2.58 – 2.49 (m, 1H), 2.48 – 2.40 (m, 1H), 2.39 – 2.30 (m, 1H), 2.24 (td, *J* = 14.5, 5.0 Hz, 1H), 2.18 – 1.92 (m, 6H), 1.74 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 172.5, 165.4, 156.3, 152.9, 142.2, 140.6, 138.3, 131.9, 125.4, 121.3, 118.4, 111.2, 109.1, 108.5, 106.8, 93.7, 78.2, 77.7, 60.9, 60.8, 56.2, 55.9, 55.6, 51.8, 49.9, 49.8, 34.0, 32.3, 30.2, 24.6, 20.0, 17.5; HRMS (ESI, $[M+H]^+$) for $C_{37}H_{47}N_2O_9$ calcd. 633.3276, found: 633.3290. m.p. = 97-98 ˚C.

1-allyl-1*H*-indole (**2t**)



The reaction was conducted with 0.5 mmol of indole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **2t** (70 mg, 89%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3055, 2955, 2923, 2869, 1644, 1613, 1511, 1483, 1463 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dt, *J* = 8.2, 1.1 Hz, 1H), 7.35 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.23 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.17 – 7.10 (m, 2H), 6.55 (dd, *J* = 3.1, 0.9 Hz, 1H), 6.02 (ddt, *J* = 17.1, 10.3, 5.4 Hz, 1H), 5.22 (dtd, *J* = 10.3, 1.5, 1.5 Hz, 1H), 5.11 (dtd, *J* = 17.1, 1.8, 1.3 Hz, 1H), 4.75 (dt, *J* = 5.4, 1.7 Hz 2H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 136.1, 133.5, 128.6, 127.8, 121.5, 120.9, 119.4, 117.2, 109.5, 101.4, 48.8; HRMS (FI, $[M]^+$) for $C_{11}H_{11}N$ calcd. 157.0886, found: 157.0883.

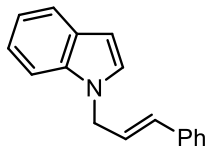
1-(but-3-en-2-yl)-1*H*-indole (**2u**)



The reaction was conducted with 0.5 mmol of indole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford an inseparable mixture of three isomers **2u**, **2u'(*trans*)** and **2u'(*cis*)** (63 mg, 74%) in a ratio of 5:3:1 (determine by ^{1}H NMR) as a pale yellow oil. R_f = 0.6

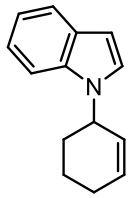
(hexanes/ EtOAc = 10:1). Spectral data of the major product **2u**. IR (film): 3049, 2919, 2857, 1641, 1511, 1483, 1462 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 8.6 Hz, 1H), 7.24 – 7.18 (m, 2H), 7.15 – 7.09 (m, 1H), 6.53 (d, *J* = 12.4 Hz, 1H), 6.13 – 6.01 (dddd, *J* = 15.3, 10.5, 4.9, 1.3 Hz, 1H), 5.20 (d, *J* = 10.4 Hz, 1H), 5.14 – 5.05 (m, 2H), 1.66 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 138.7, 135.7, 128.7, 124.6, 121.2, 120.9, 119.4, 115.4, 109.7, 101.4, 53.0, 19.7; HRMS (FI, $[M]^+$) for $C_{12}H_{13}N$ calcd. 171.1043, found: 171.1045.

1-cinnamyl-1*H*-indole (**2v**)



The reaction was conducted with 0.5 mmol of indole following the general procedure. The crude product was purified by flash chromatography (hexanes) to afford **2v** (63 mg, 54%) as a light yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3056, 3026, 2953, 2923, 2853, 1612, 1598, 1577, 1511, 1496, 1483, 1463, 1448, 1398 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.65 (dt, *J* = 7., 1.0 Hz, 1H), 7.39 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.36 – 7.27 (m, 4H), 7.26 – 7.19 (m, 2H), 7.16 (d, *J* = 3.2 Hz, 1H), 7.15 – 7.09 (m, 1H), 6.54 (dd, *J* = 3.1, 0.9 Hz, 1H), 6.50 (dt, *J* = 15.8, 1.5 Hz,1H), 6.36 (dt, *J* = 15.9, 5.7 Hz, 2H), 4.91 (dd, *J* = 5.8, 1.5 Hz, 2H) ; ^{13}C NMR (400 MHz, $CDCl_3$) δ 136.2, 136.1, 132.3, 128.7, 128.5, 127.8, 127.7, 126.4, 124.9, 121.6, 120.9, 119.4, 109.6, 101.5, 48.3; HRMS (FD, $[M]^+$) for $C_{17}H_{15}N$ calcd. 233.1199, found: 233.1198.

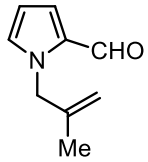
1-(cyclohex-2-en-1-yl)-1*H*-indole (**2w**)



The reaction was conducted with 0.5 mmol of indole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 70:1) to afford **2w** (30 mg, 30%) as a colorless oil. R_f = 0.7 (hexanes/ EtOAc = 10:1). IR (film): 3051, 2951, 2923, 1654, 1611, 1509, 1460, 1403 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.24 – 7.16 (m, 2H), 7.10 (ddd, *J* = 7.8, 7.0, 0.8 Hz, 1H), 6.48 (d, *J* = 3.2 Hz, 1H), 6.12 (dtd, *J* = 9.8, 3.7, 2.0 Hz,

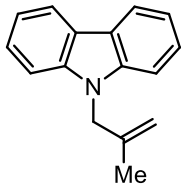
1H), 5.84 (ddt, *J* = 10.0, 2.5, 2.5 Hz, 1H), 5.07 – 5.0 (m, 1H), 2.28 – 2.04 (m, 3H), 1.99 – 1.88 (m, 1H), 1.79 – 1.66 (m, 2H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 135.4, 132.2, 129.0, 126.7, 126.2, 121.1, 121.0, 119.3, 109.6, 100.6, 51.2, 29.9, 24.9, 19.9; HRMS (EI, $[M]^+$) for $C_{14}H_{15}N$ calcd. 197.1199, found: 197.1195.

1-(2-methylallyl)-1*H*-pyrrole-2-carbaldehyde (**3a**)



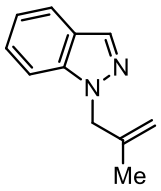
The reaction was conducted with 0.5 mmol of 1*H*-pyrrole-2-carbaldehyde following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 10:1) to afford **3a** (33 mg, 44%) as a light yellow oil. R_f = 0.5 (hexanes/ EtOAc = 4:1). IR (film): 2958, 2925, 2870, 2855, 2721, 1712, 1668, 1621, 1600, 1451, 1406 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.54 (d, *J* = 0.8 Hz, 1H), 6.98 – 6.91 (m, 2H), 6.26 (dd, *J* = 3.8, 2.7 Hz, 1H), 4.90 (s, 2H), 4.84 (dq, *J* = 1.4, 1.4 Hz, 1H), 4.49 (dq, *J* = 1.6, 0.8 Hz, 1H), 1.68 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 179.3, 142.0, 131.6, 131.4, 124.4, 111.6, 109.8, 53.8, 19.9; HRMS (FI, $[M]^+$) for $C_9H_{11}NO$ calcd. 149.0835, found: 149.0831.

9-(2-methylallyl)-9*H*-carbazole (**3b**)



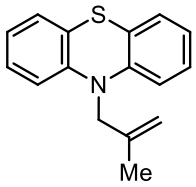
The reaction was conducted with 0.5 mmol of carbazole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **3b** (102 mg, 92%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3051, 2953, 2853, 1627, 1598, 1484, 1460, 1377, 1325 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 7.8 Hz, 2H), 7.47 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.26 (ddd, *J* = 7.9, 6.8, 1.0 Hz, 2H), 4.91 (dq, *J* = 1.4, 1.4 Hz, 1H), 4.84 (s, 2H), 4.75 – 4.69 (m, 1H), 1.75 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 140.7, 140.2, 125.7, 122.9, 120.3, 119.0, 112.0, 108.9, 48.9, 20.0; HRMS (CI, $[M]^+$) for $C_{16}H_{15}N$ calcd. 221.1199, found: 221.1194. m.p. = 62-63°C.

1-(2-methylallyl)-1*H*-indazole (**3c**)



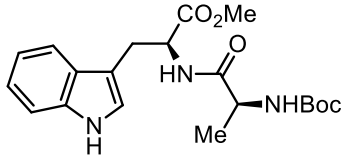
The reaction was conducted with 0.5 mmol of indazole following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 30:1) to afford **3c** (54 mg, 63%) as a pale yellow oil. R_f = 0.3 (hexanes/ EtOAc = 10:1). IR (film): 3079, 2955, 2924, 2869, 1659, 1617, 1500, 1465, 1437, 1419, 1332 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.46 – 7.30 (m, 2H), 7.15 (ddd, *J* = 7.8, 6.5, 1.1 Hz, 1H), 4.96 (s, 2H), 4.94 (s, 1H), 4.78 (s, 1H), 1.66 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 140.7, 139.7, 133.1, 126.2, 124.2, 121.1, 120.5, 113.1, 109.3, 55.3, 19.8; HRMS (FI, $[M]^+$) for $C_{11}H_{12}N_2$ calcd. 172.0995, found: 172.0997.

10-(2-methylallyl)-10*H*-phenothiazine (**3d**)



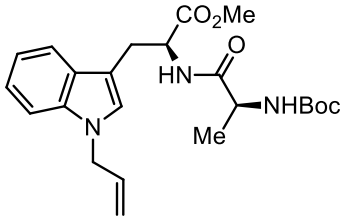
The reaction was conducted with 0.5 mmol of 10*H*-phenothiazine following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 50:1) to afford **3d** (115 mg, 90%) as a pale yellow oil. R_f = 0.6 (hexanes/ EtOAc = 10:1). IR (film): 3067, 2968, 2909, 2851, 1656, 1593, 1570, 1487, 1462, 1443, 1365, 1317 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.11 – 7.02 (m, 4H), 6.91 – 6.84 (m, 2H), 6.78 – 6.74 (m, 2H), 5.04 (dqt, *J* = 1.6, 1.6, 1.6 Hz, 1H), 4.88 (dq, *J* = 1.9, 0.9 Hz, 1H), 4.29 (s, 2H), 1.85 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 144.3, 138.3, 127.0, 126.6 122.8, 122.3, 115.3, 112.9, 55.1, 19.9; HRMS (CI, $[M]^+$) for $C_{16}H_{15}NS$ calcd. 253.0920, found: 253.0926.

(*S*)-methyl-2-((*S*)-2-((*tert*-butoxycarbonyl)amino)propanamido)-3-(1*H*-indol-3-yl) propanoate (**4**)



To a flask wrapped with aluminum foil was added L-tryptophan methyl ester (1.26 g, 5 mmol), dichloromethane (30mL), *N*-(*tert*-butoxycarbonyl)-L-alanine (1.23 g, 6.5 mmol), and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (1.14 mL, 6.5 mmol), and the resulting mixture was stirred at room temperature. After 4 h, the solution was sequentially washed with 1 N aqueous hydrochloric solution (30 mL) and 1 N aqueous sodium bicarbonate solution (30 mL) and then the combined organic layers were dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The residue was purified by flash chromatography (hexanes/EtOAc = 1:1) to afford **4** (1.8 g, 93%) as a white foam. R_f = 0.3 (hexanes/ EtOAc = 1:1). IR (film): 3326, 3059, 2979, 2930, 1741, 1697, 1664, 1518, 1458, 1369 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.12 (br, 1H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.9 Hz, 1H), 7.23 – 7.15 (m, 1H), 7.14 – 7.08 (m, 1H), 7.03 (s, 1H), 6.52 (m, 1H), 4.90 (dt, *J* = 7.9, 5.4 Hz, 2H), 4.13 (br, 1H), 3.67 (s, 3H), 3.33 (d, *J* = 5.4 Hz, 2H), 1.41 (s, 9H), 1.30 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 172.4, 172.1, 155.3, 136.1, 127.5, 123.1, 122.1, 119.5, 118.4, 111.3, 109.5, 80.0, 52.9, 52.3, 50.1, 28.2, 27.5, 18.3; HRMS (CI, $[M]^+$) for $C_{20}H_{27}N_3O_5$ calcd. 389.1945, found: 389.1950. m.p. = 124-125 ˚C. α_D^{22} = +71 (c=0.017, $CHCl_3$).

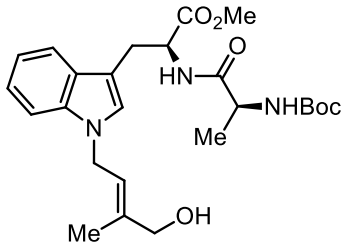
(*S*)-methyl-3-(1-allyl-1*H*-indol-3-yl)-2-((*S*)-2-((*tert*-butoxycarbonyl)amino) propaneido)propanoate (**2x**)



The reaction was conducted with 2.68 mmol of **4** following the general procedure. The crude product was purified by flash chromatography (hexanes/EtOAc = 4:1) to afford **2x** (722 mg, 63%) as a white foam. R_f = 0.5 (hexanes/ EtOAc = 1:1). IR (film):

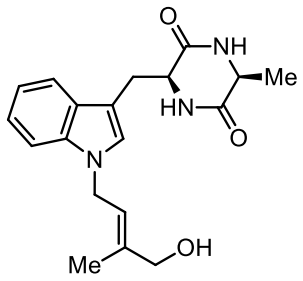
3310, 3056, 2955, 2926, 1743, 1713, 1667, 1516, 1468, 1391 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 7.8, 2.8 Hz, 1H), 7.29 – 7.25 (m, 1H), 7.23 – 7.14 (m, 1H), 7.14 – 7.06 (m, 1H), 6.92 (d, *J* = 10.4 Hz, 1H), 6.79 – 6.57 (m, 1H), 5.96 (ddt, *J* = 17.1, 10.4, 5.3 Hz, 1H), 5.17 (dd, *J* = 10.2, 1.4 Hz, 1H), 5.13 – 4.94 (m, 2H), 4.89 (dt, *J* = 7.7, 5.5 Hz, 1H), 4.72 – 4.63 (m, 2H), 4.14 (br, 1H), 3.65 (d, *J* = 3.8 Hz, 3H), 3.33 – 3.26 (m, 2H), 1.40 (d, *J* = 3.0 Hz, 8H), 1.32 – 1.24 (m, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 172.2, 171.9, 155.1, 136.1, 133.3, 128.1, 126.7, 121.7, 119.1, 118.6, 116.9, 109.6, 108.6, 79.8, 52.9, 52.1, 50.0, 48.5, 28.1, 27.5, 18.3; HRMS (CI, $[M]^+$) for $C_{23}H_{31}N_3O_5$ calcd. 429.2258, found: 429.2255. m.p. = 47-49 °C. α_D^{22} = +24.3 (c=0.016, $CHCl_3$).

(*S*)-methyl-2-((*S*)-2-((*tert*-butoxycarbonyl)amino)propanamido)-3-(1-((*E*)-4-hydroxy-3-methylbut-2-en-1-yl)-1*H*-indol-3-yl)propanoate (**5**)



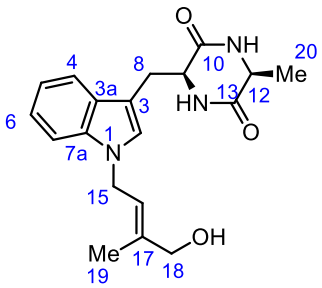
To a stirring solution of compound **2x** (125 mg, 0.291 mmol) in degassed 1,2-dichloroethane (1.5 mL) was added methallyl alcohol (0.26 mL, 2.91 mmol) and Hoveyda-Grubbs catalyst 2nd generation (38 mg, 0.058 mmol) at room temperature. The resulting mixture was brought up to 40 °C (oil bath) and stirred for 3.5 h. The organic solvent was removed by reduced pressure and the residue was purified by flash chromatography (hexanes/EtOAc = 1:1) to afford **5** (102 mg, 74%) as a brown foam. R_f = 0.2 (hexanes/ EtOAc = 1:1). IR (film): 3313, 2956, 2925, 2870, 1742, 1666, 1614, 1467, 1457, 1366 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.44 (m, 1H), 7.32 – 7.26 (m, 1H), 7.22 – 7.13 (m, 1H), 7.08 (ddd, *J* = 8.0, 6.9, 1.0 Hz, 1H), 6.98 – 6.91 (m, 1H), 6.79 – 6.61 (m, 1H), 5.67 – 5.59 (m, 1H), 5.27 – 5.11 (m, 1H), 4.86 (tt, *J* = 9.4, 5.5 Hz, 1H), 4.76 – 4.64 (m, 2H), 4.25 – 4.10 (m, 1H), 4.01 (s, 2H), 3.65 (s, 3H), 3.28 (d, *J* = 5.4 Hz, 3H), 1.79 (s, 3H), 1.38 (s, 9H), 1.31 – 1.20 (m, 3H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 172.4, 172.0, 155.4, 139.2, 136.1, 128.0, 125.9, 121.5, 119.3, 118.5, 109.4, 108.4, 79.8, 67.0, 52.6, 52.2, 49.9, 43.1, 28.1, 27.4, 18.1, 13.7; HRMS (CI, $[M]^+$) for $C_{25}H_{35}N_3O_6$ calcd. 473.2520, found: 473.2519. m.p. = 53-54 °C. α_D^{23} = +44.0 (c=0.01, $CHCl_3$).

N-(4'-hydroxyprenyl)-cyclo(alanyltryptophyl) (**6**)



To a stirring mixture of compound **5** (60 mg, 0.126 mmol), phenol (0.3 mL), *p*-cresol (0.3 mL), and dichloromethane (0.5 mL) was added trifluoroacetic acid (0.4 mL) at 0 °C, and the resulting solution was stirred at room temperature. After 20 min, the reaction mixture was concentrated, and then dichloromethane (1.5 mL) and morpholine (0.6 mL) were added. The resulting mixture was stirred at room temperature for 48 h. The organic solvent was removed under reduced pressure and the residue was directly purified by flash chromatography (CH_2Cl_2/ MeOH = 20:1) to afford **6** (24 mg, 58%) as a white solid. R_f = 0.3 (CH_2Cl_2/ MeOH = 10:1). IR (film): 3402, 3325, 3206, 3052, 2918, 2955, 1668, 1466, 1372 cm^{-1}; ^1H NMR (400 MHz, Acetone-d_6) δ 7.62 (d, *J* = 8.1 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.15 – 7.09 (m, 2H), 7.06 (d, *J* = 10.4 Hz, 1H), 7.00 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 5.62 (ddd, *J* = 7.2, 6.2, 1.4 Hz, 1H), 4.80 (d, *J* = 6.9 Hz, 2H), 4.25 (br, 1H), 3.96 (s, 2H), 3.85 – 3.77 (m, 1H), 3.32 (dd, *J* = 14.6, 5.3, 1H), 3.24 (dd, *J* = 14.5, 4.4 Hz, 1H), 1.83 (s, 3H), 0.70 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (400 MHz, Acetone-d_6) δ 169.1, 168.0, 140.4, 137.3, 129.5, 128.6, 122.1, 120.2, 119.8, 110.4, 109.5, 67.4, 56.8, 51.5, 44.0, 30.1, 20.4, 13.9; HRMS (EI, $[M]^+$) for $C_{19}H_{23}N_3O_3$ calcd. 341.1734, found: 341.1726. m.p. = 170-171° C. α_D^{21} = +5.9 (c=0.02, MeOH).

Table S1. Spectral Data of N-(4'-hydroxyprenyl)-cyclo(alanyltryptophyl) (**6**)



6

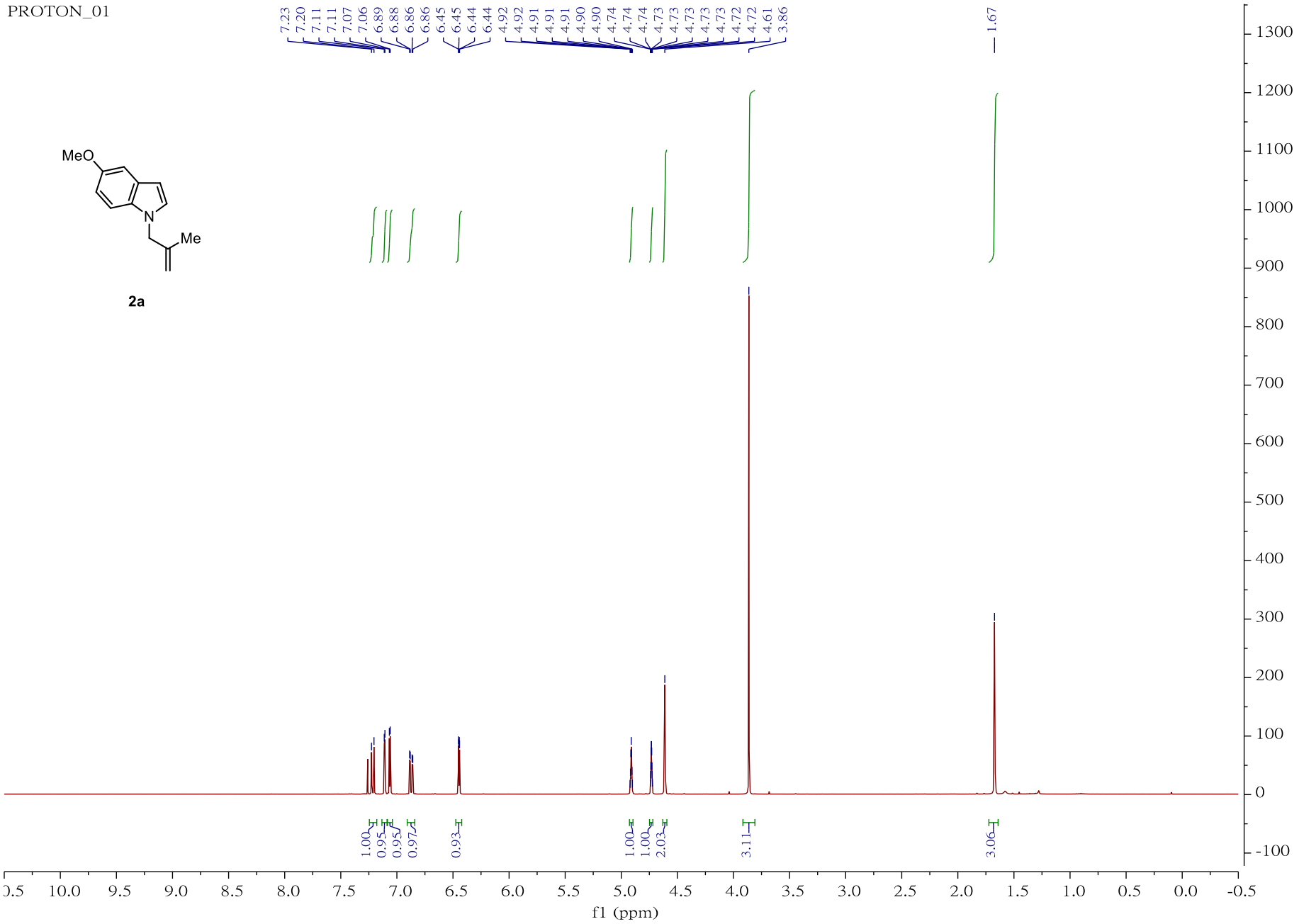
#	^{1}H NMR (in Acetone-d_6, 400 MHz)		^{13}C NMR (in Acetone-d_6, 100 MHz)	
	Natural [Ref.]	Synthetic	Natural [Ref.]	Synthetic
1				
2	7.13 (s)	7.13 (s)	128.6	128.5
3			109.6	109.5
3a			129.6	129.5
4	7.62 (d, J = 8.0)	7.62 (d, J = 8.1)	120.2	120.2
5	7.0 (t, J = 7.8)	7.0 (ddd, J = 8.0, 7.0, 1.0)	119.7	119.8
6	7.12 (t, J = 7.8)	7.15-7.09 (m)	122.2	122.1
7	7.36 (d, J = 8.2)	7.36 (d, J = 8.2)	110.4	110.4
7a			137.3	137.3
8	3.32 (dd, J = 14.6, 8.5)	3.32 (dd, J = 14.6, 5.3)	30.2	30.1
8’	3.24 (dd, J = 14.6, 4.1)	3.24 (dd, J = 14.6, 4.4)		
9	4.25 (br)	4.25 (br)	56.8	56.8
10			167.9	168.0
11				
12	3.81 (m)	3.85-3.77 (m)	51.5	51.5
13	2.63 (d, J = 17.7)	2.63 (d, J = 17.8)	169.0	169.1
14				
15	4.80 (d, J = 6.9)	4.80 (d, J = 6.9)	44.0	44.0
16	5.62 (t, J = 6.9)	5.62 (ddd, J = 7.2, 6.2, 1.4)	120.2	120.2
17			140.4	140.4
18	3.95 (s)	3.96 (s)	67.5	67.4
19	1.84 (s)	1.83 (s)	13.9	13.9
20	0.71 (d, J = 6.9)	0.70 (d, J = 7.0)	20.3	20.4

Ref: Du, F.-Y.; Li, X.; Li, X.-M.; Zhu, L.-W.; Wang, B.-G. *Mar. Drugs* **2017**, *15*, 24.

Table S2. Other Analytic Data of N-(4'-hydroxyprenyl)-cyclo(alanyltryptophyl) (**6**)

#	Optical Value		Molecular Mass	
	Natural [Ref.]	Synthetic	Natural HRESI $[M+Na]^+$	Synthetic HREIMS $[M]^+$
1	α_D^{20}= +6.0 (c=0.5, MeOH)	α_D^{21}= +5.9 (c=0.02, MeOH)	364.1633 (Calcd for $C_{19}H_{23}N_3O_3Na^+$, 364.1637)	341.1726 (Calcd for $C_{19}H_{23}N_3O_3$, 341.1734)

Ref: Du, F.-Y.; Li, X.; Li, X.-M.; Zhu, L.-W.; Wang, B.-G. *Mar. Drugs* **2017**, *15*, 24.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7.11
7.11
7.07
7.06
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6.88
6.86
6.86
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6.44
6.44
4.92
4.92
4.91
4.91
4.91
4.90
4.90
4.74
4.74
4.73
4.73
4.73
4.73
4.72
4.72
4.61
3.86
1.67
MeO
N
Me
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0.95
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0.93
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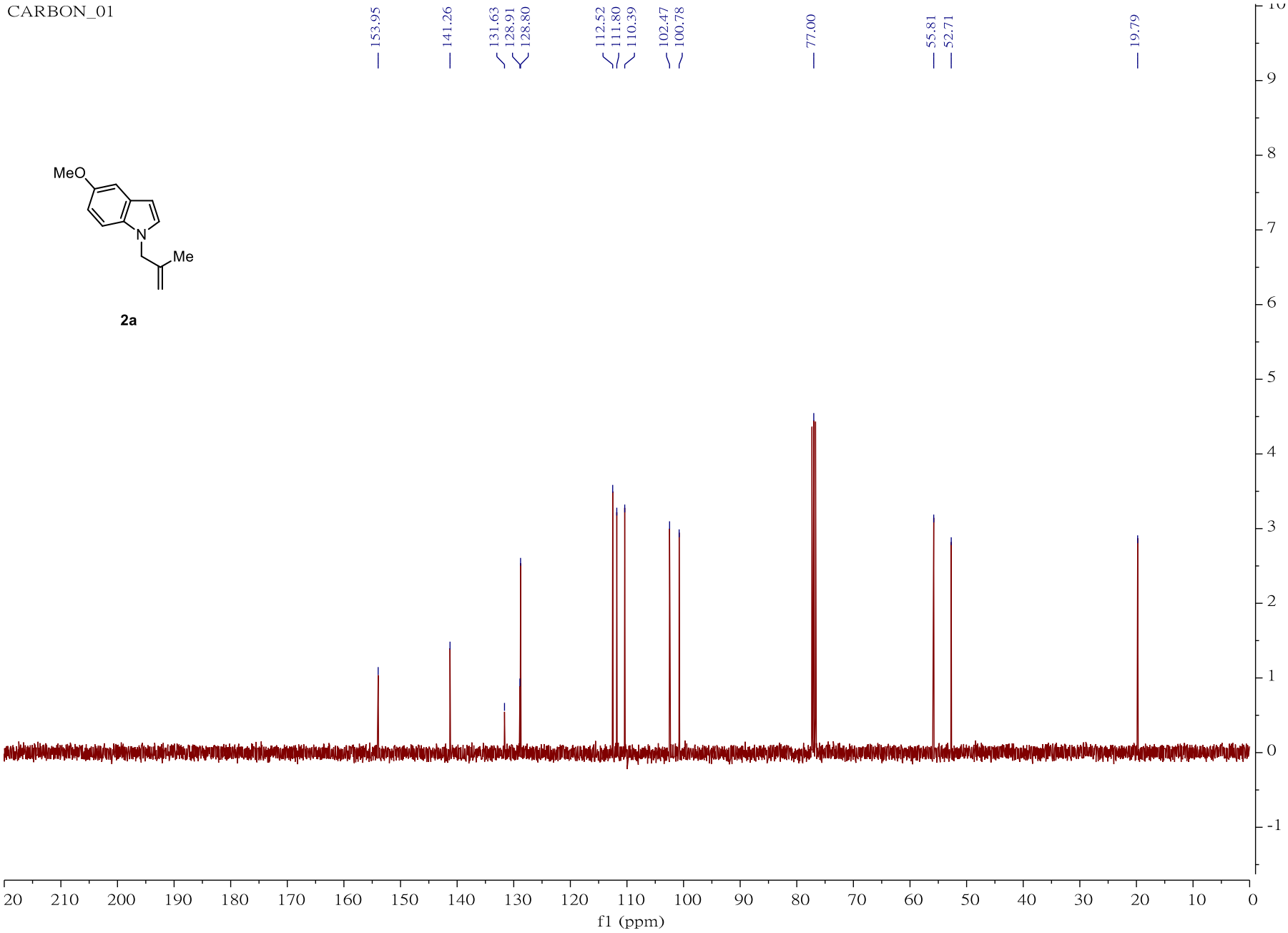
f1 (ppm)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19.79
MeO
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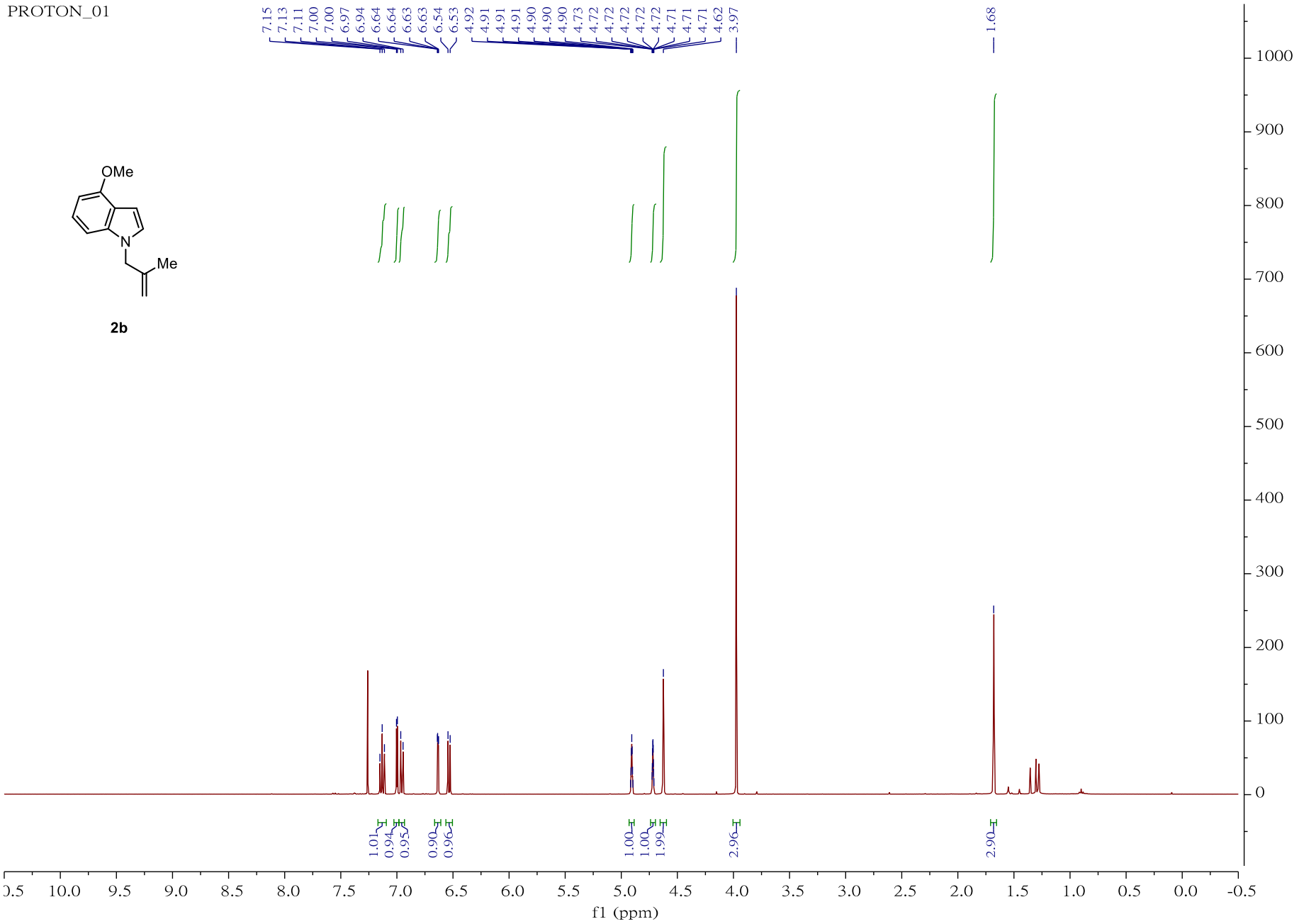
Me
2a
f1 (ppm)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4.72
4.71
4.71
4.62
3.97
1.68
OMe
N
Me
2b
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0.96
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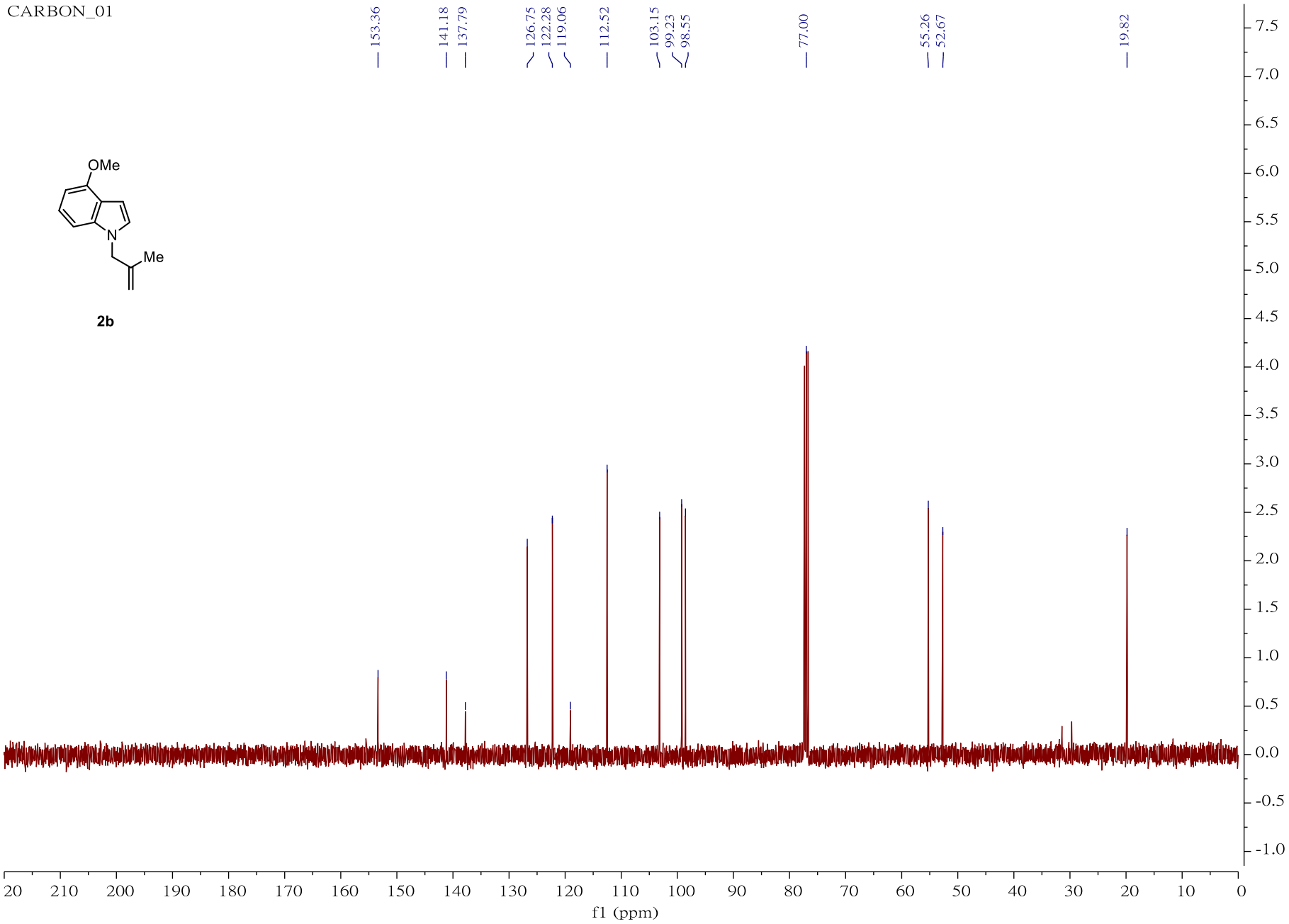
2.90
f1 (ppm)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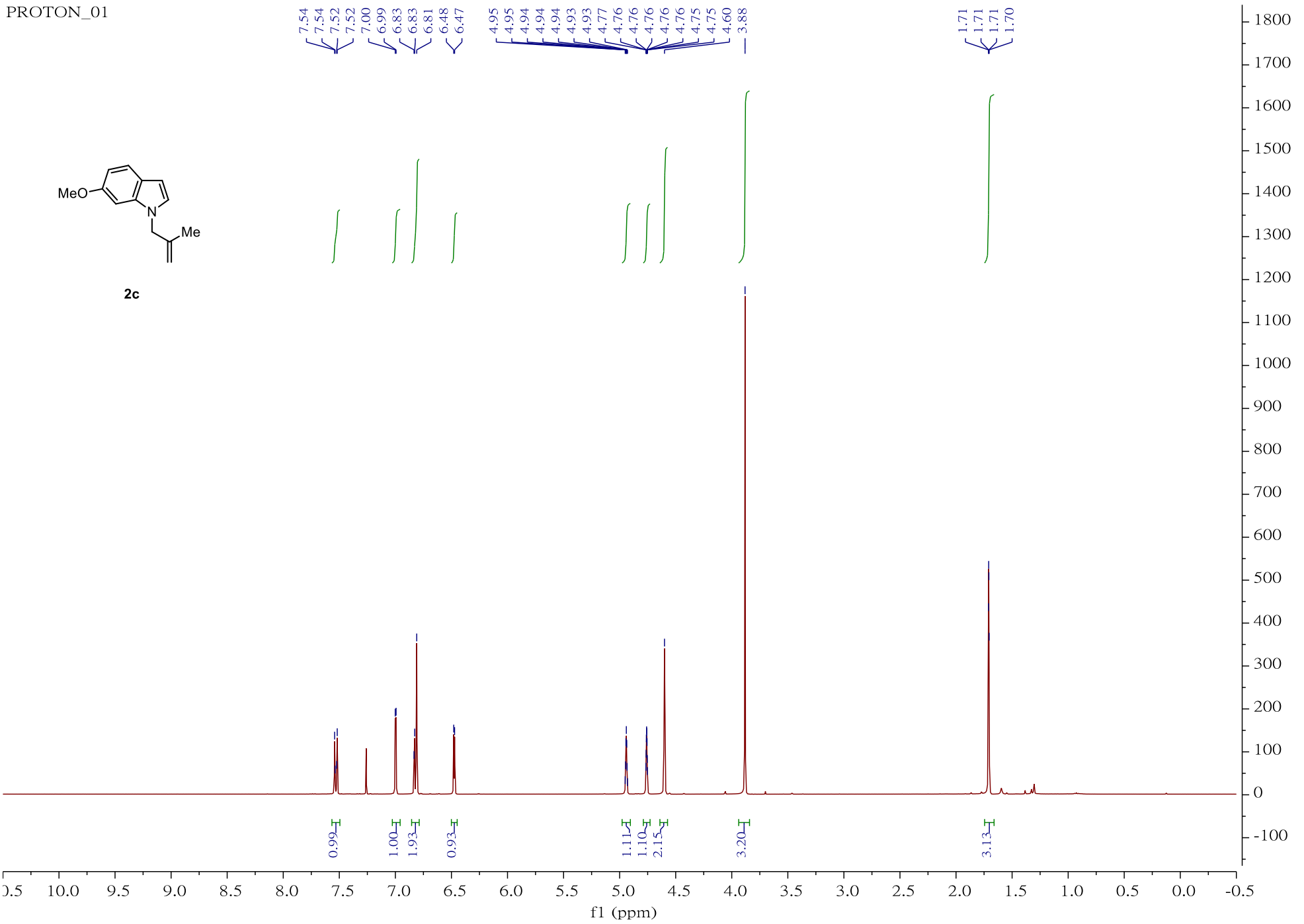
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4.76
4.76
4.75
4.75
4.60
3.88
1.71
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1.71
1.70
MeO
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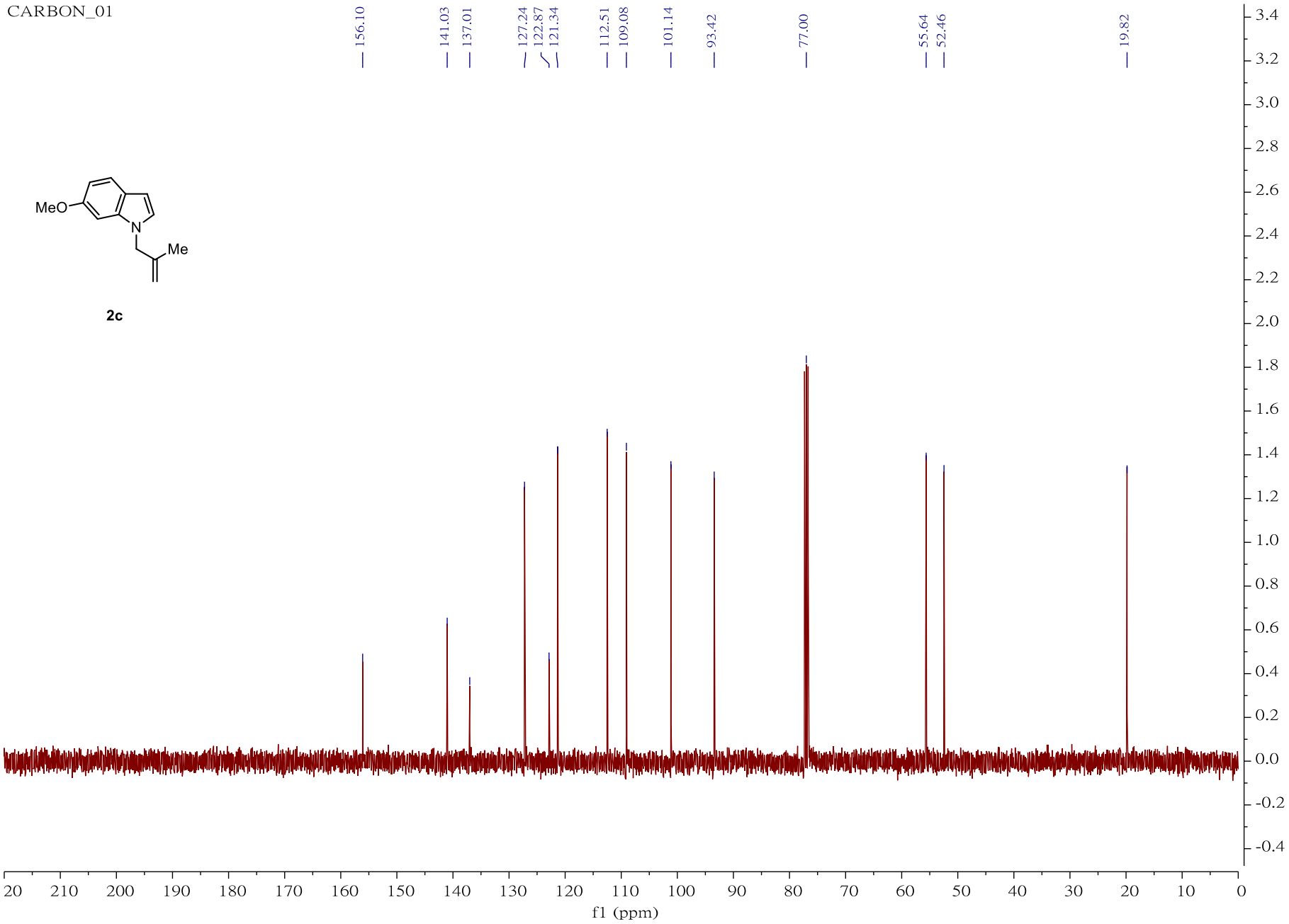
f1 (ppm)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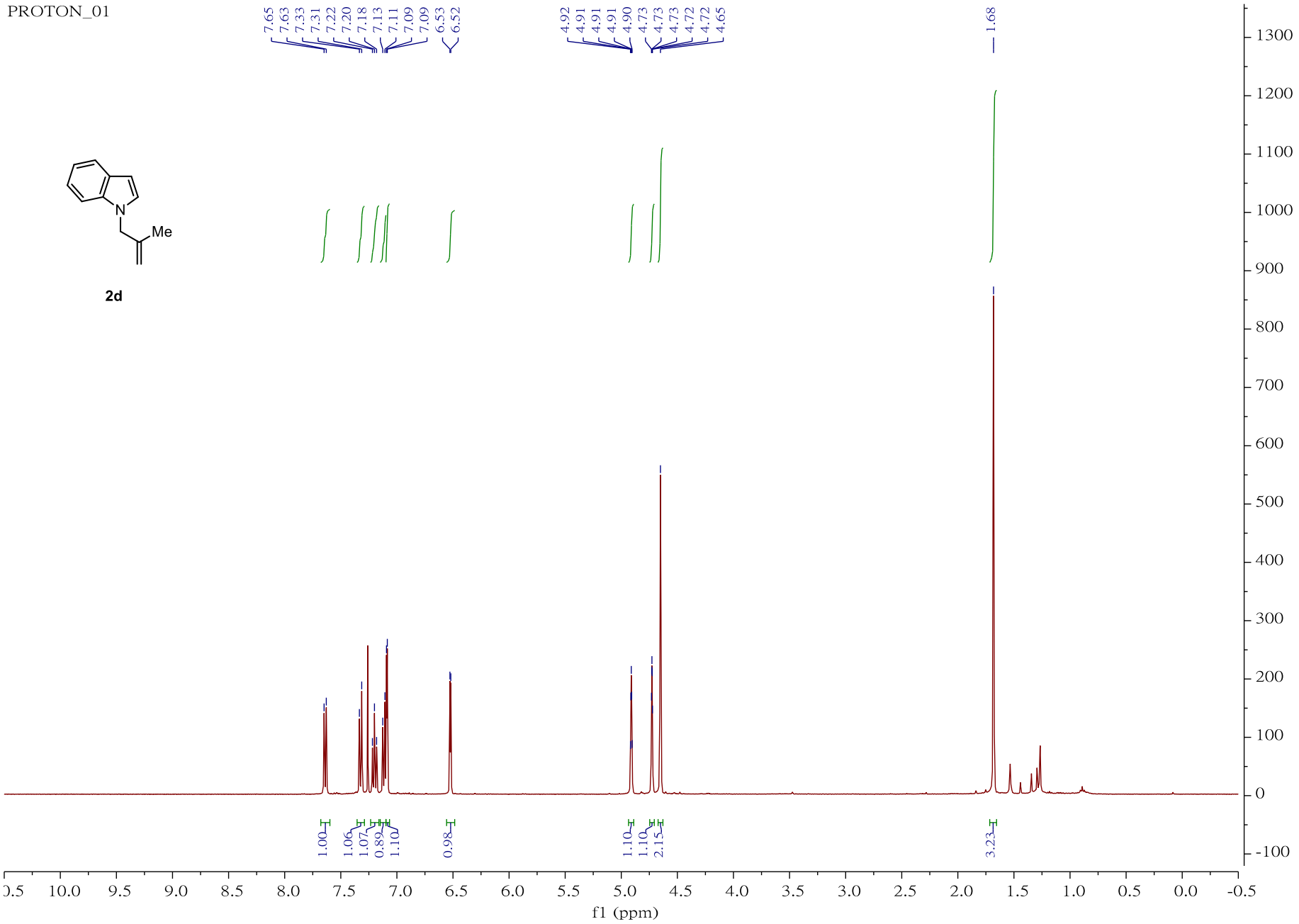
Me
2c
f1 (ppm)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4.73
4.73
4.73
4.72
4.72
4.65
1.68
N
Me
2d
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1.10
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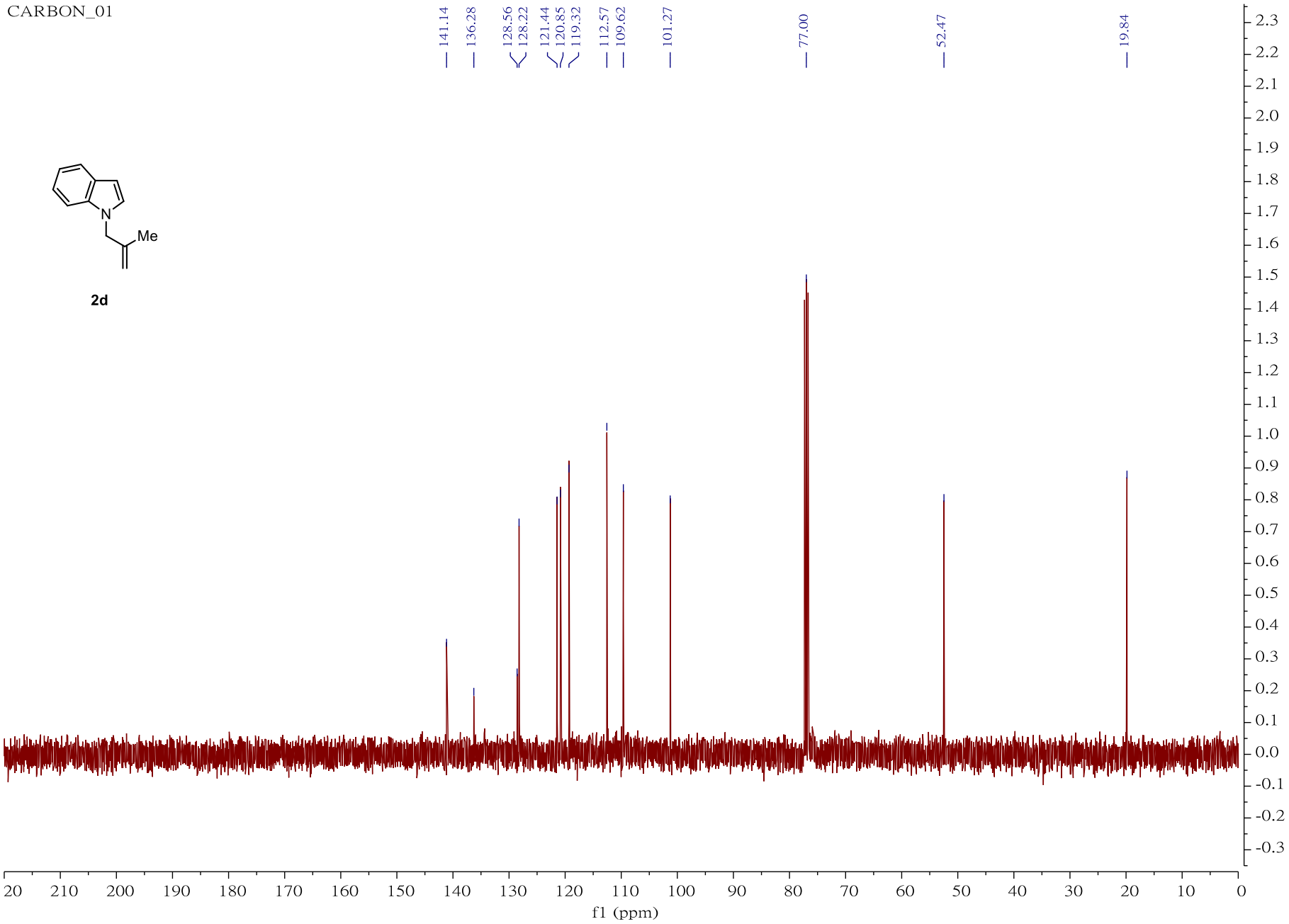
f1 (ppm)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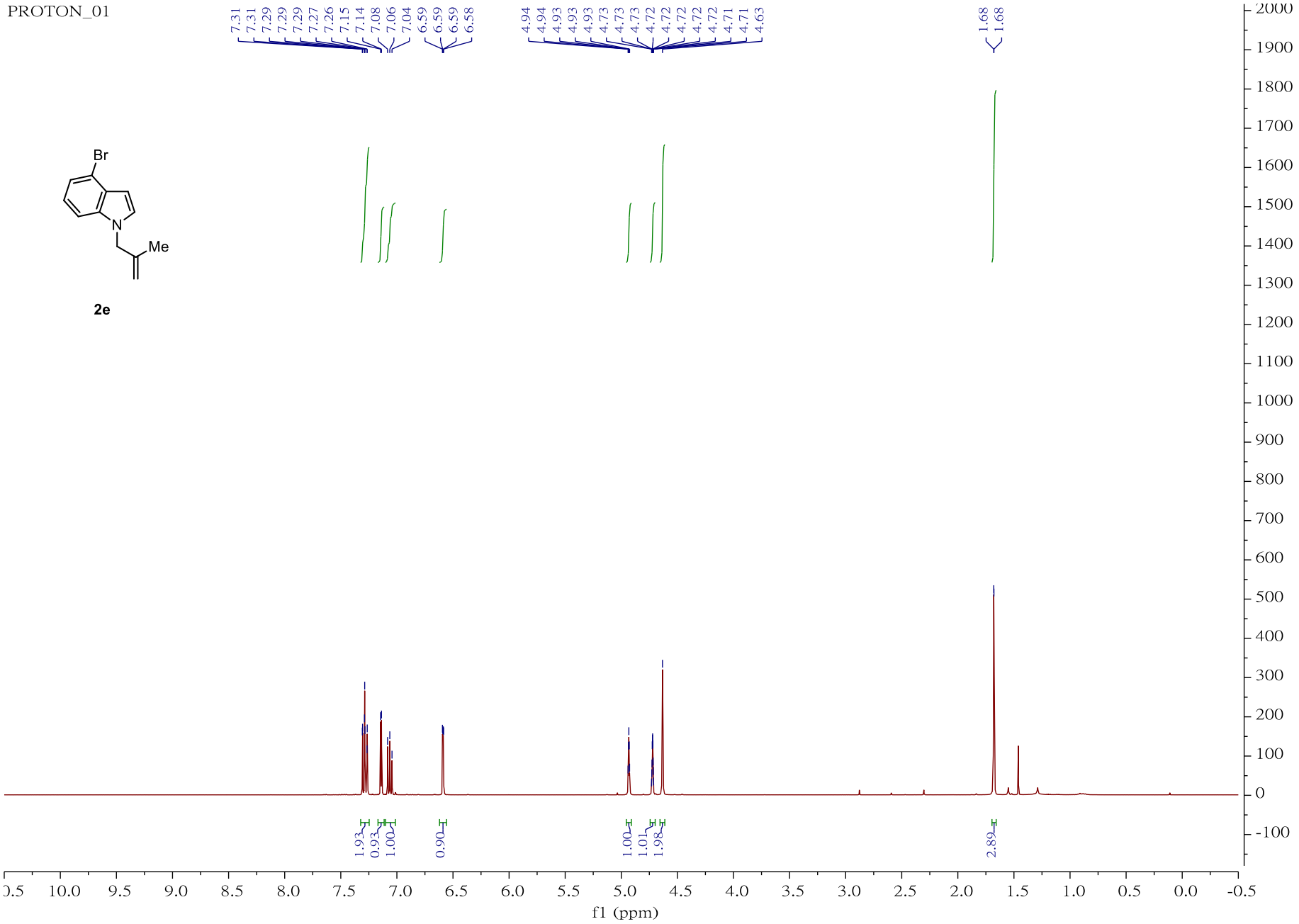
Me
2d
f1 (ppm)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7.29
7.29
7.27
7.26
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7.14
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6.59
6.58
4.94
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4.72
4.72
4.71
4.63
1.68
1.68
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N
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1.00
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1.01
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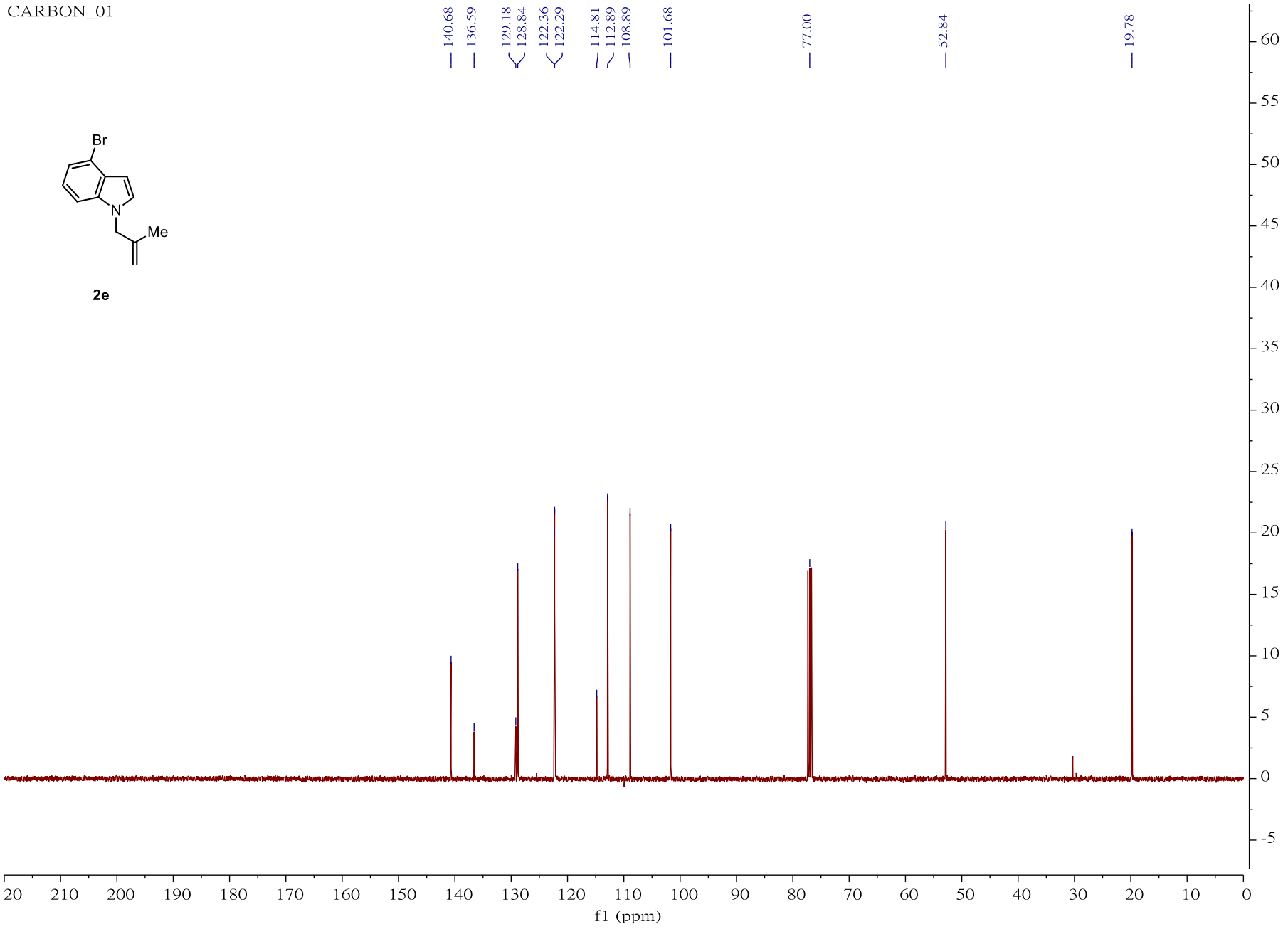
2.89
f1 (ppm)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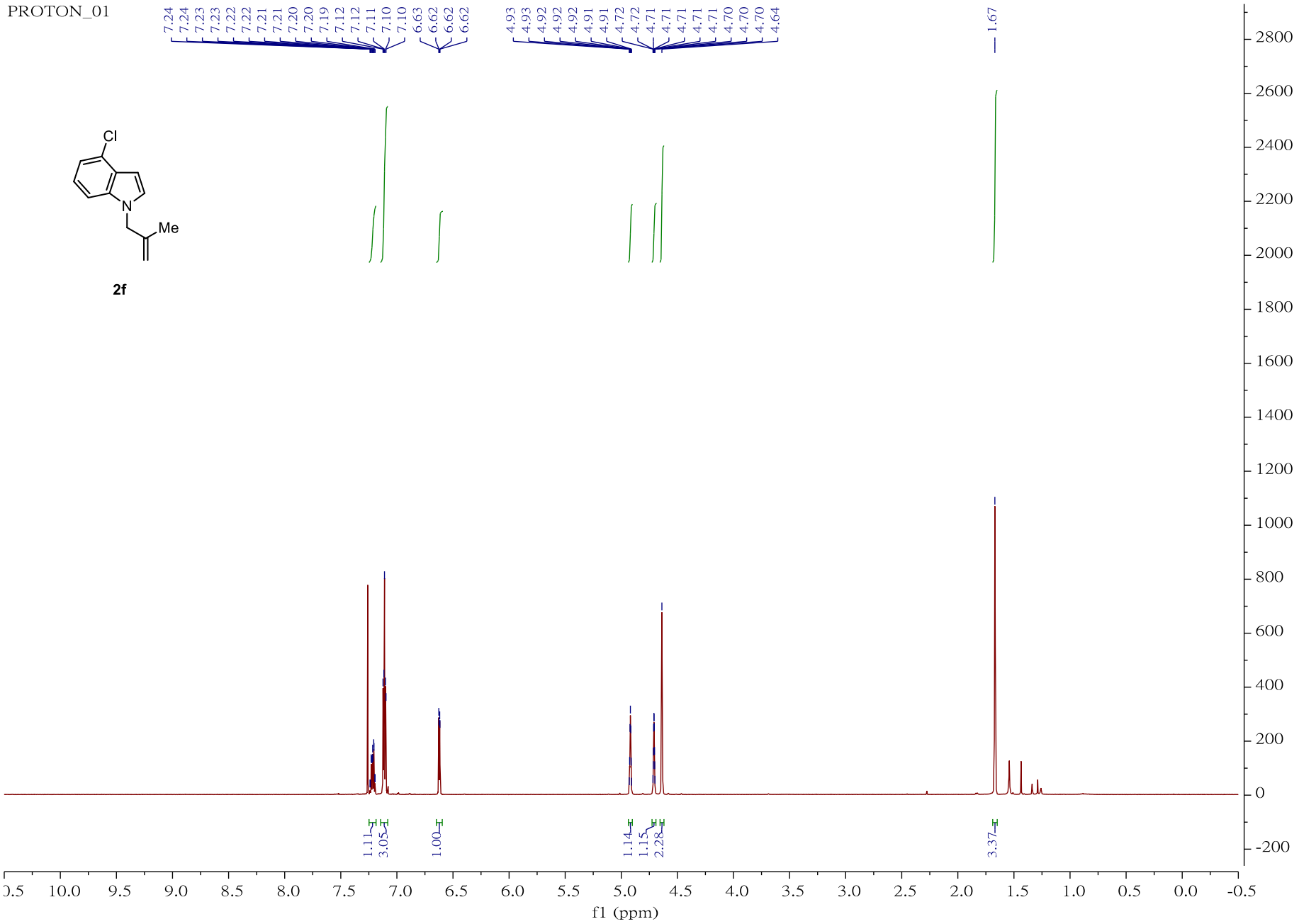
19.78
Br
N
Me
2e
f1 (ppm)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7.10
6.63
6.62
6.62
6.62
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4.91
4.91
4.72
4.72
4.71
4.71
4.71
4.71
4.70
4.70
4.64
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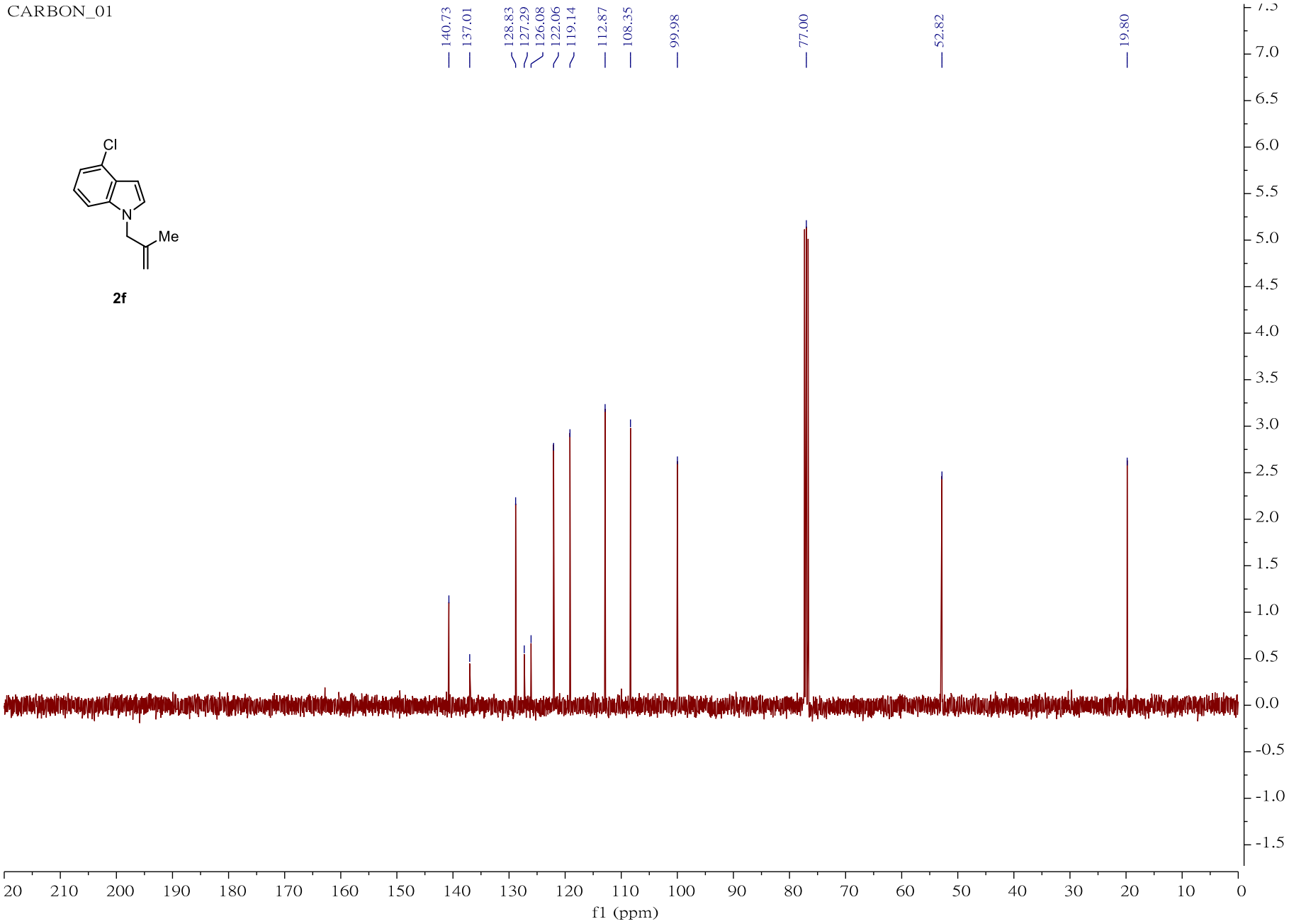
f1 (ppm)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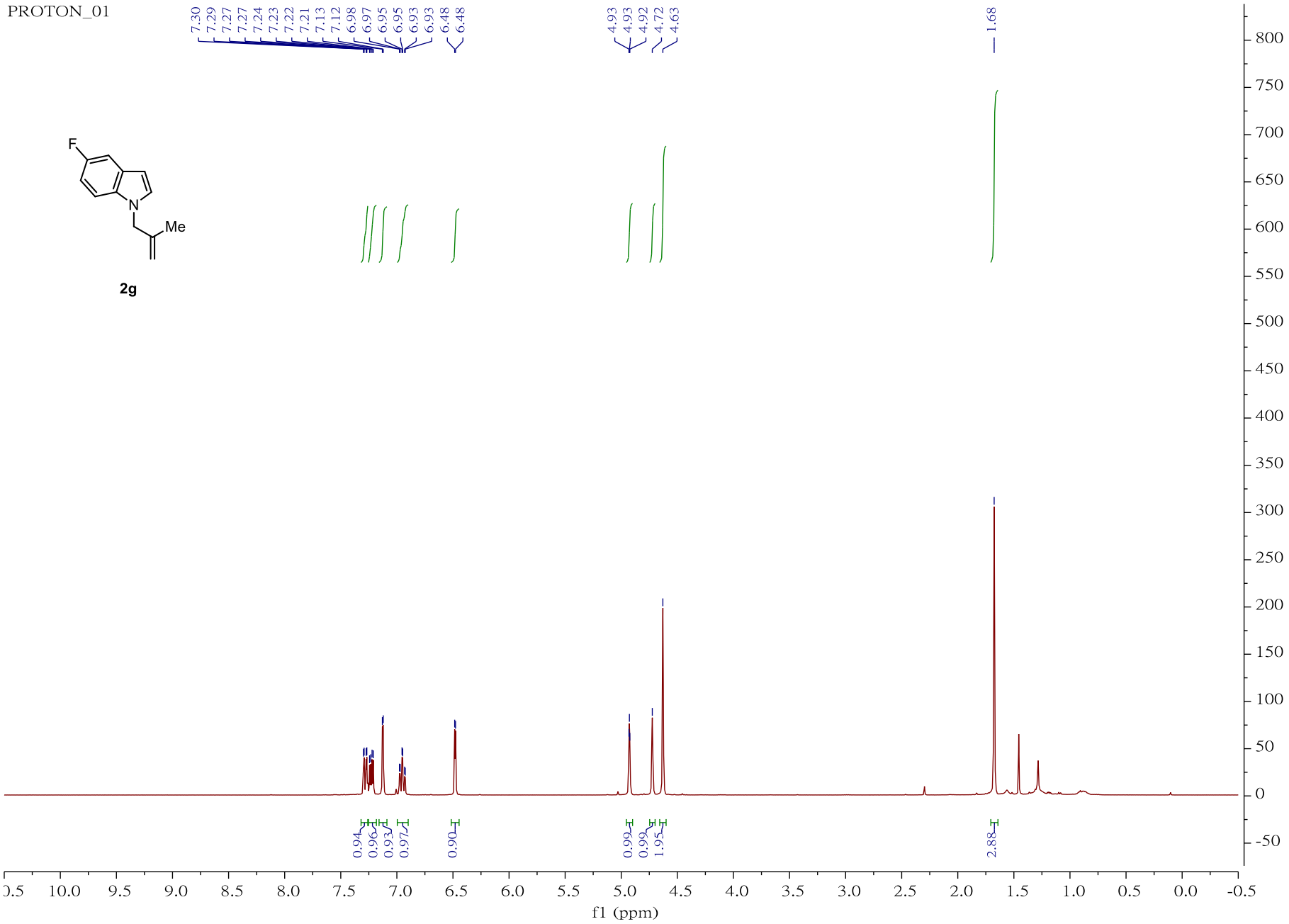
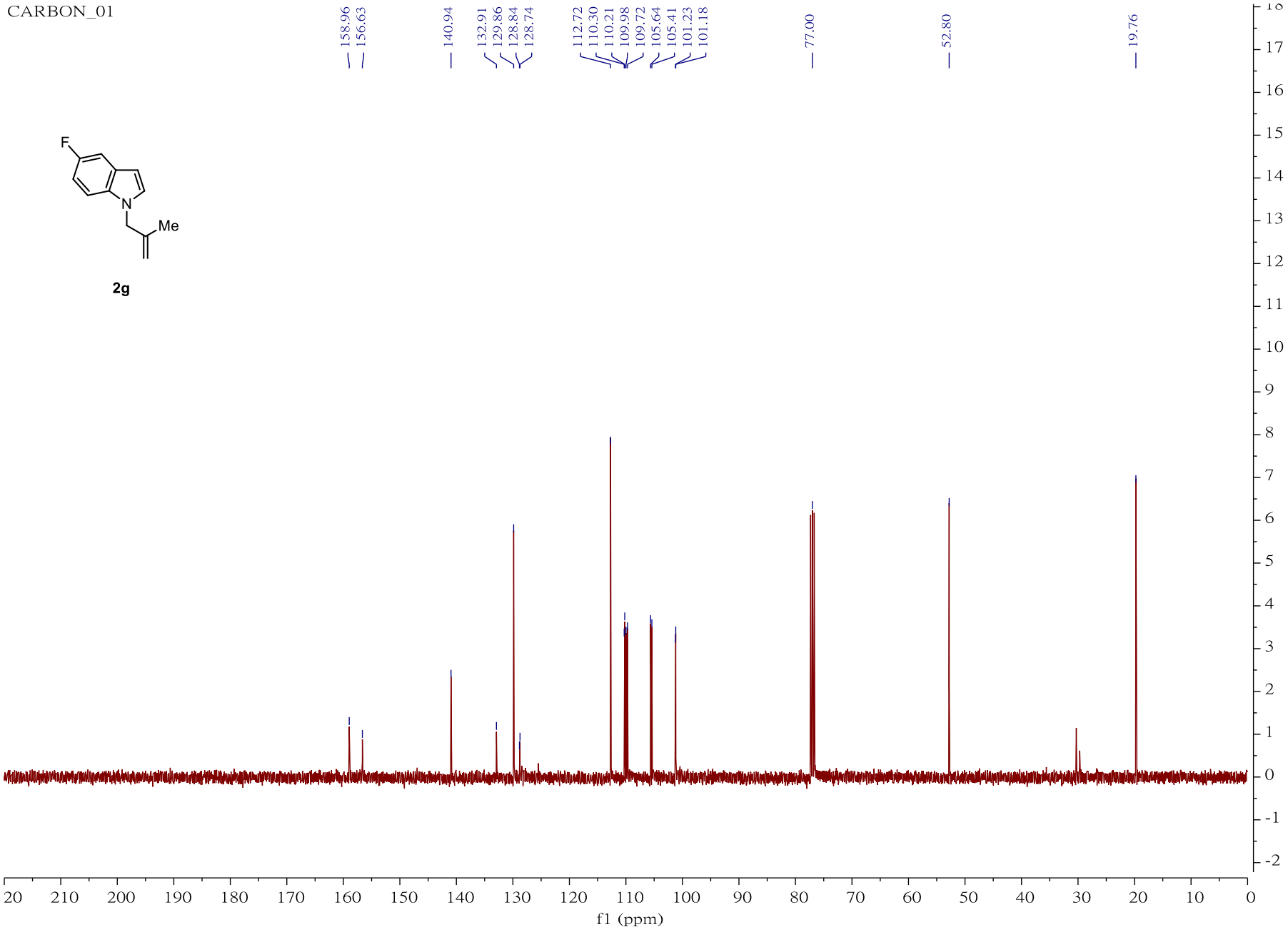
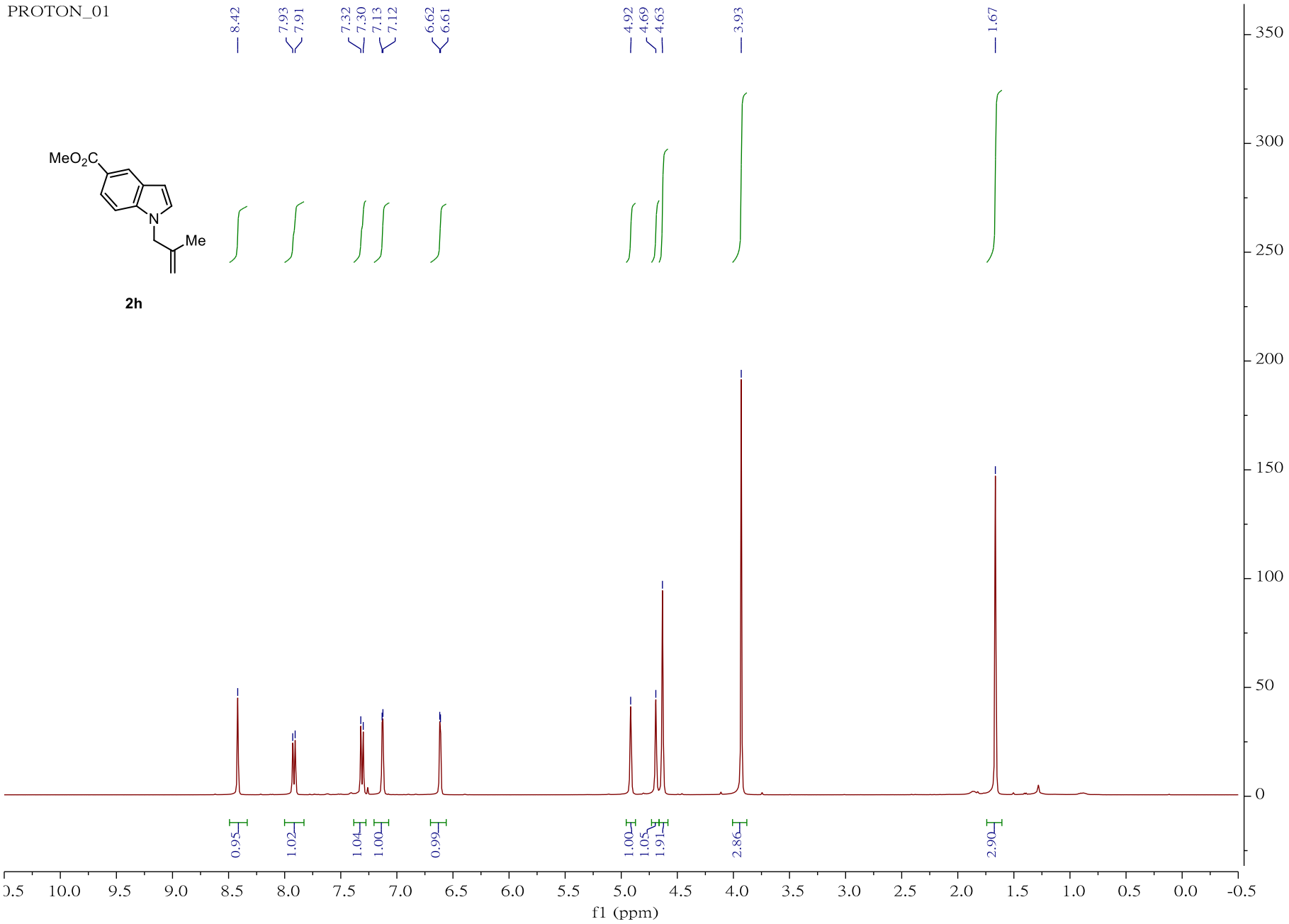
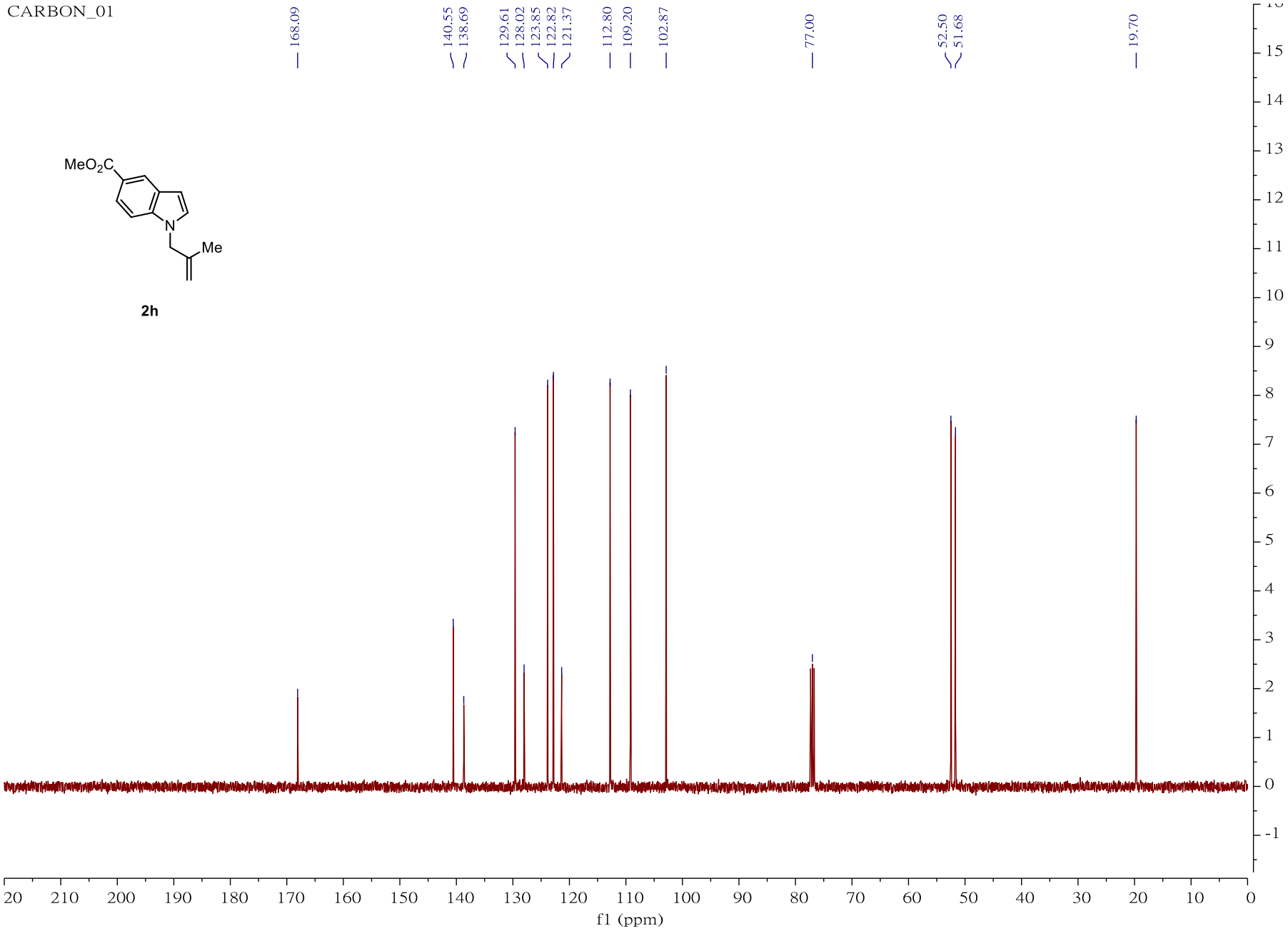
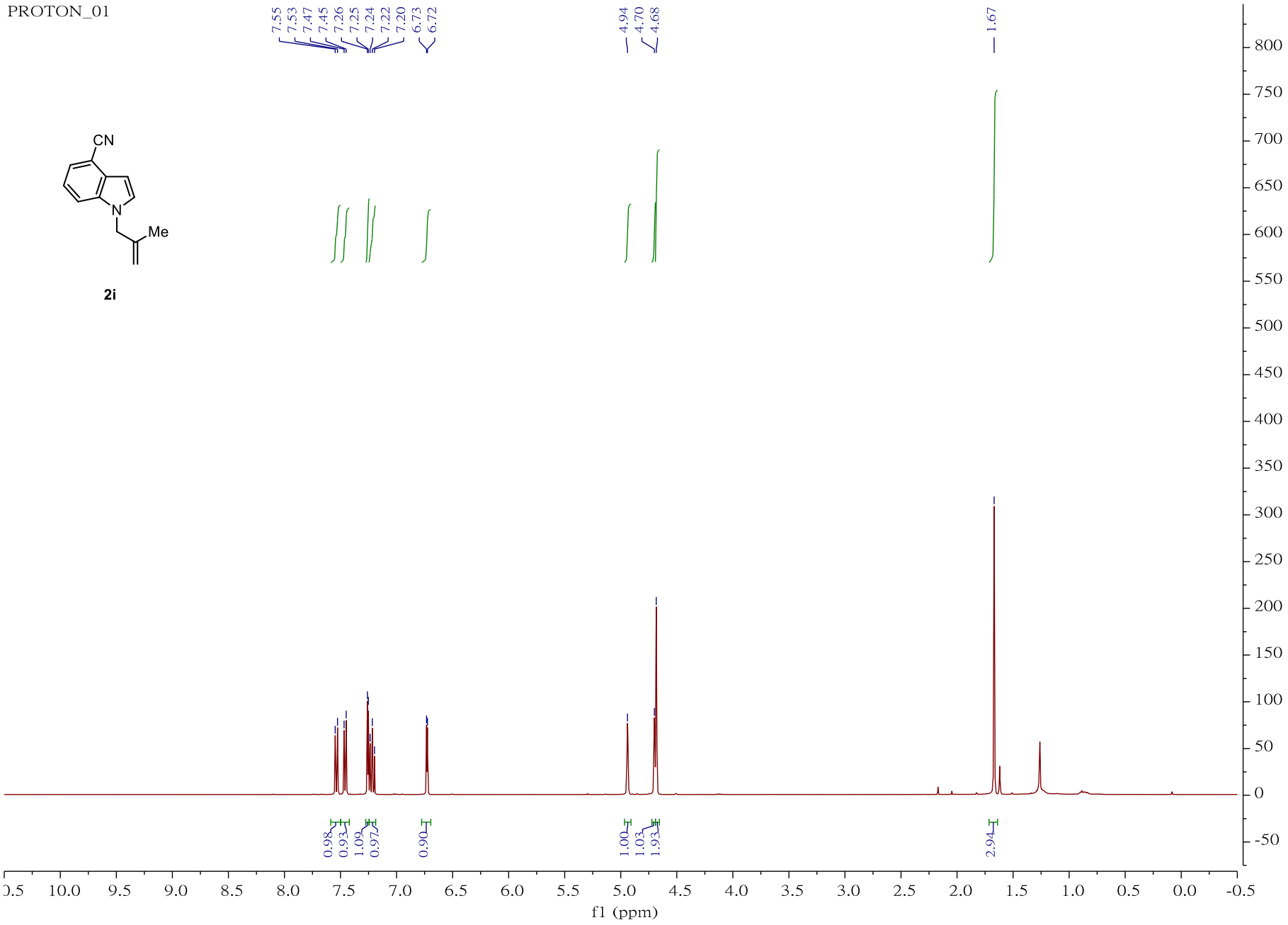
127.29
126.08
122.06
119.14
112.87
108.35
99.98
77.00
52.82
19.80
Cl
N
Me
2f
f1 (ppm)

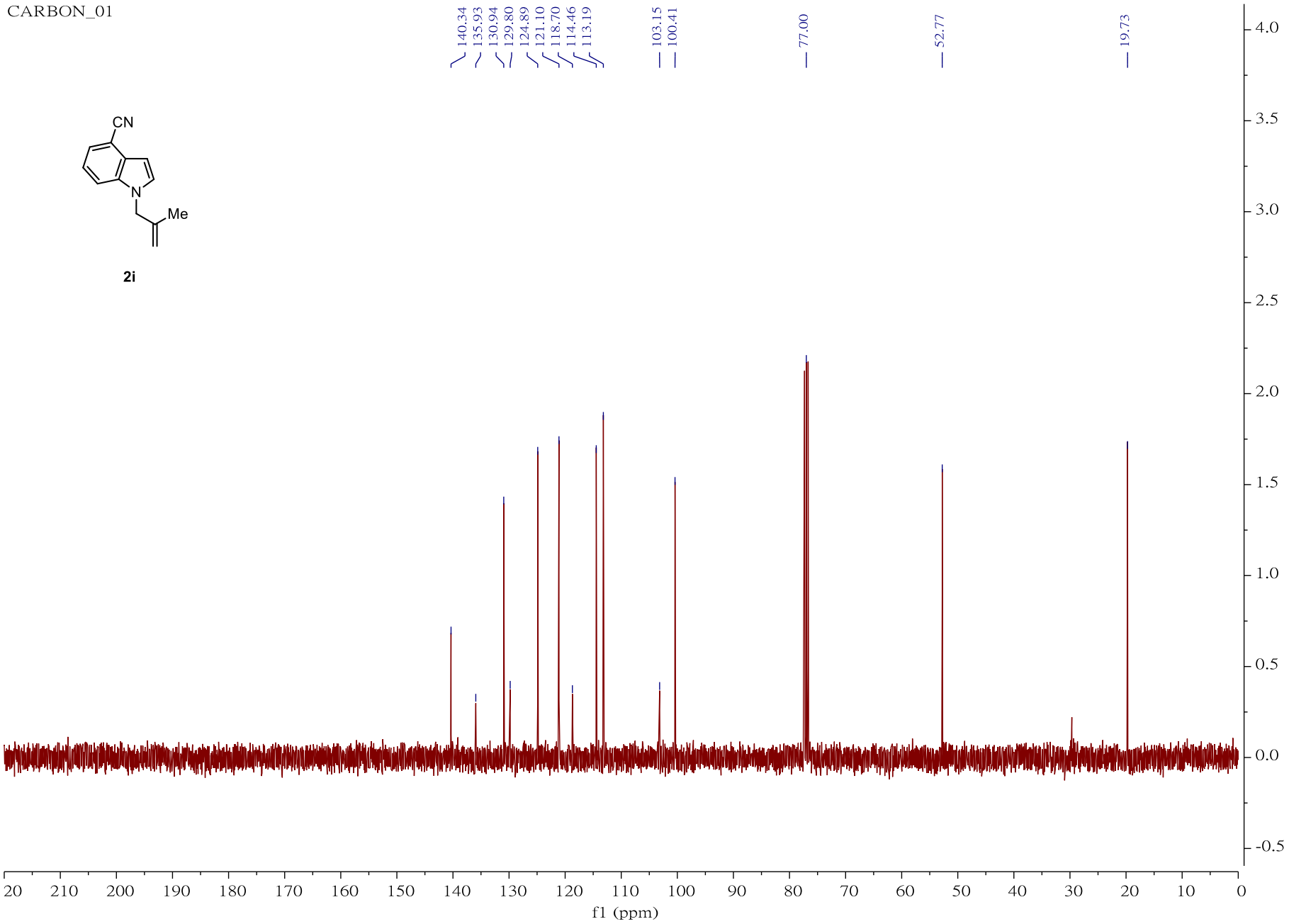

PROTON_01
7.30
7.29
7.27
7.27
7.24
7.23
7.22
7.21
7.13
7.12
6.98
6.97
6.95
6.95
6.93
6.93
6.48
6.48
4.93
4.93
4.92
4.72
4.63
1.68
F
N
Me
2g
0.94
0.96
0.93
0.97
0.90
0.99
0.99
1.95
2.88
f1 (ppm)

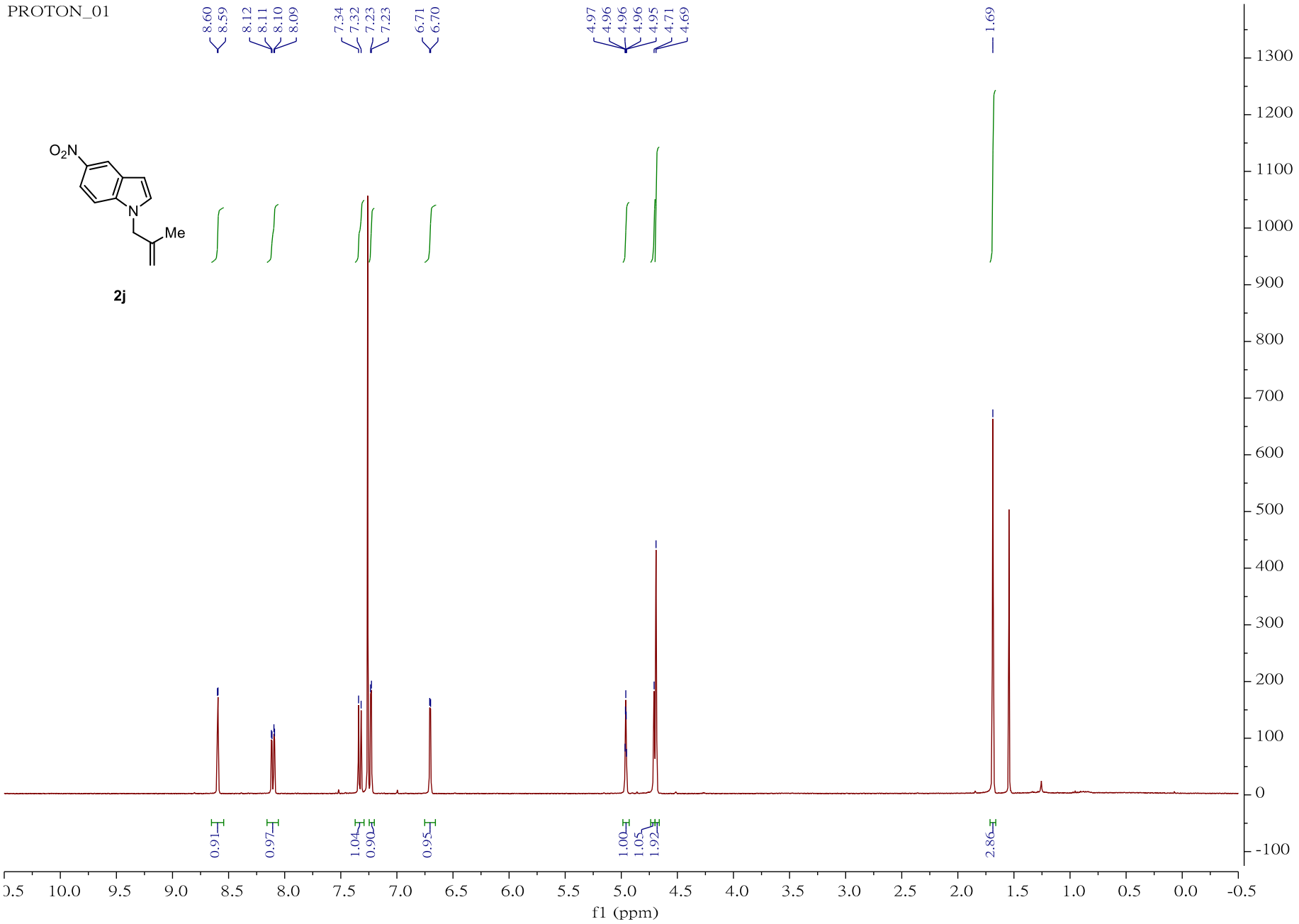

CARBON_01
158.96
156.63
140.94
132.91
129.86
128.84
128.74
112.72
110.30
110.21
109.98
109.72
105.64
105.41
101.23
101.18
77.00
52.80
19.76
F
N
Me
2g
f1 (ppm)

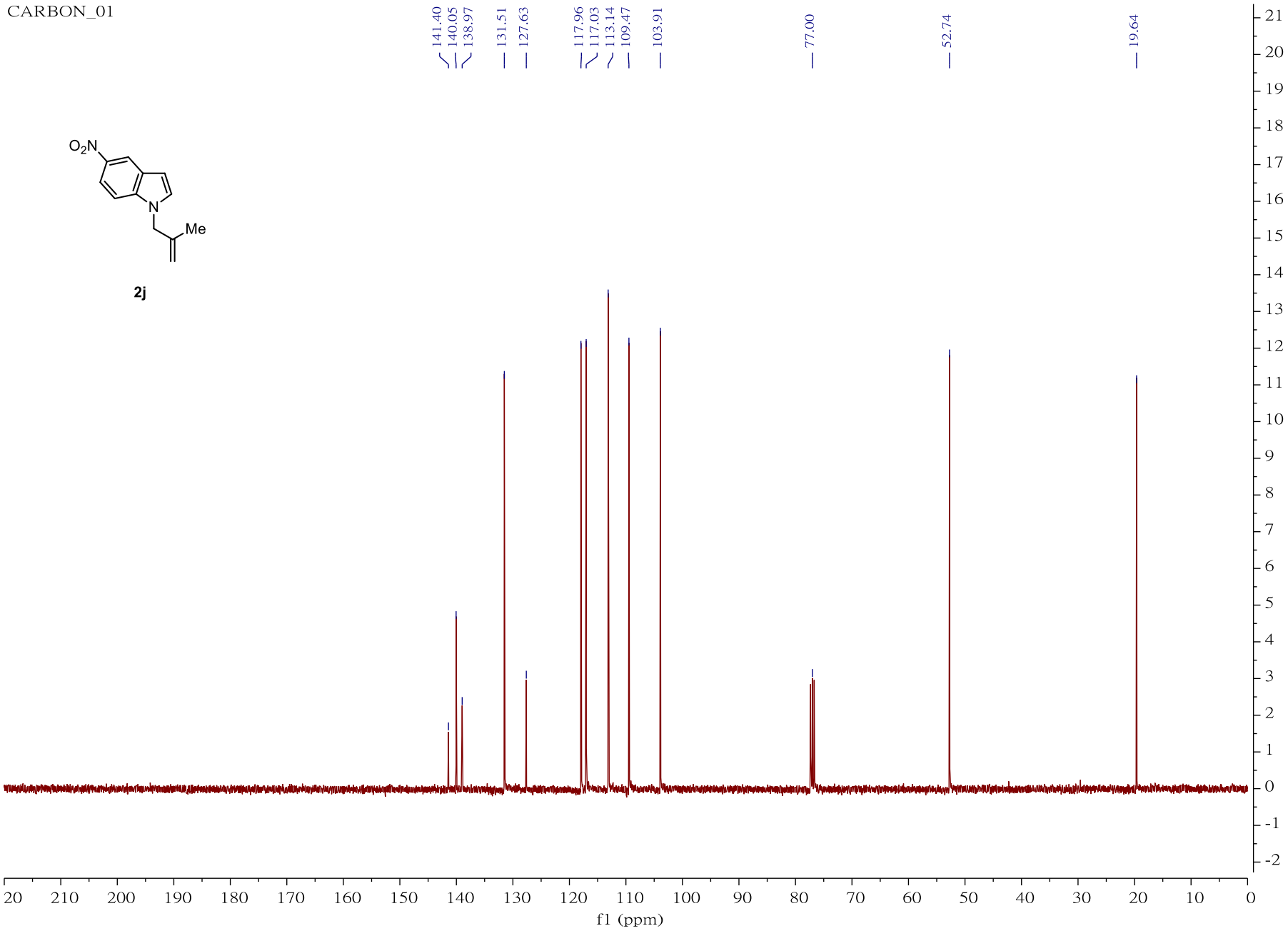

PROTON_01
8.42
7.93
7.91
7.32
7.30
7.13
7.12
6.62
6.61
4.92
4.69
4.63
3.93
1.67
MeO2C
N
Me
2h
0.95
1.02
1.04
1.00
0.99
1.00
1.05
1.91
2.86
2.90
f1 (ppm)

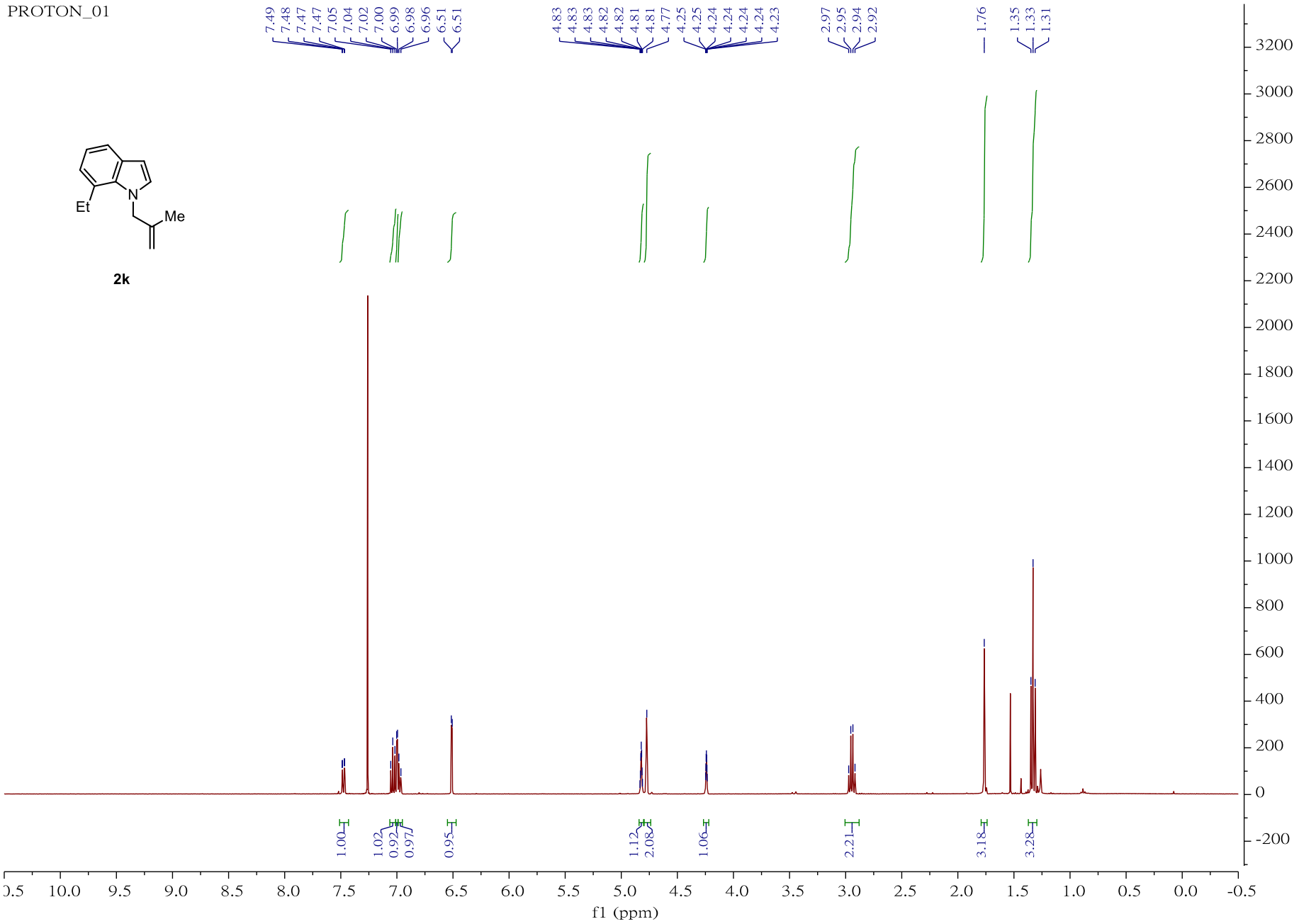

CARBON_01
168.09
140.55
138.69
129.61
128.02
123.85
122.82
121.37
112.80
109.20
102.87
77.00
52.50
51.68
19.70
MeO2C
N
Me
2h
f1 (ppm)

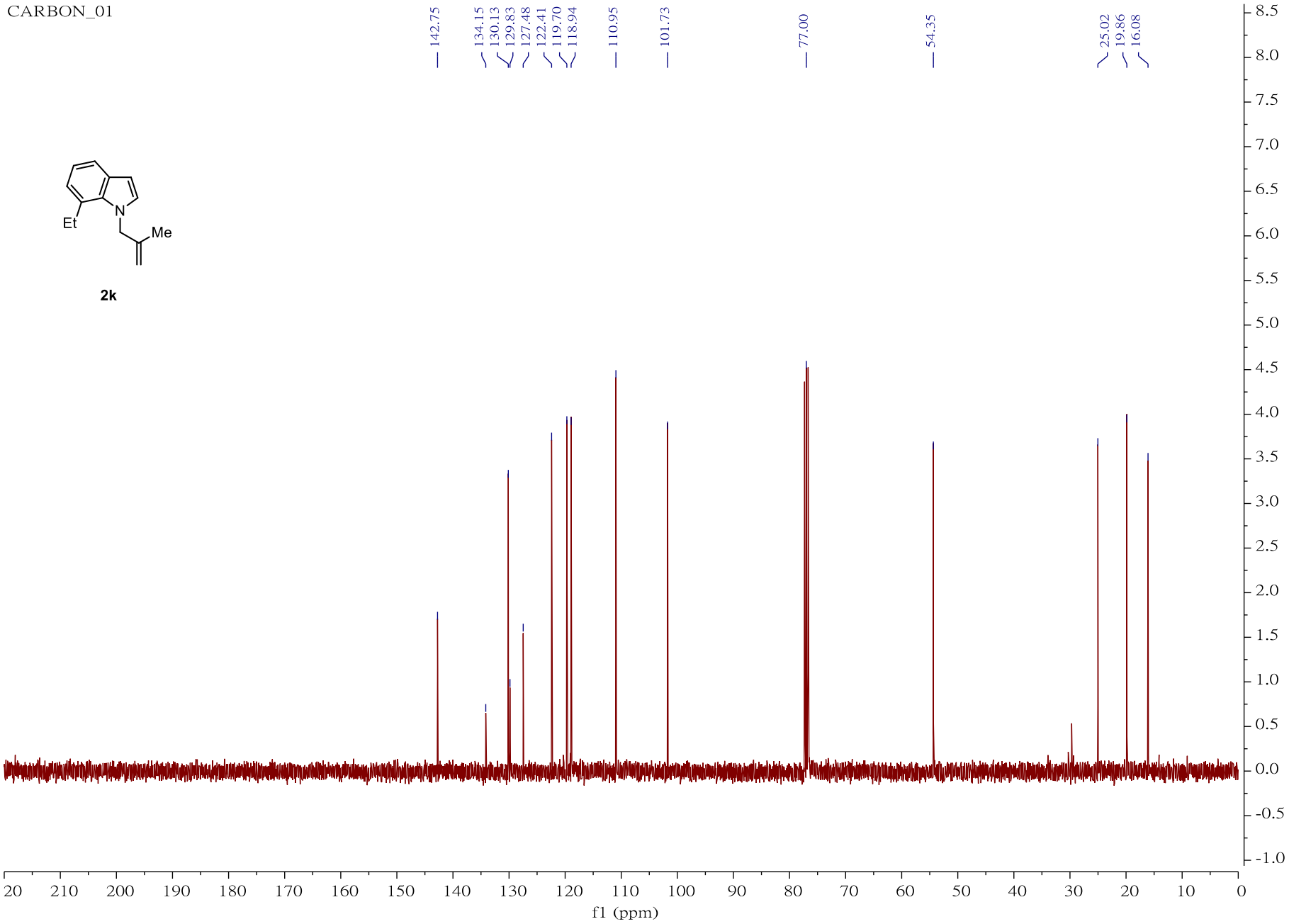

PROTON_01
7.55
7.53
7.47
7.45
7.26
7.25
7.24
7.22
7.20
6.73
6.72
4.94
4.70
4.68
1.67
CN
N
Me
2i
0.98
0.93
1.09
0.97
0.90
1.00
1.03
1.93
2.94
f1 (ppm)

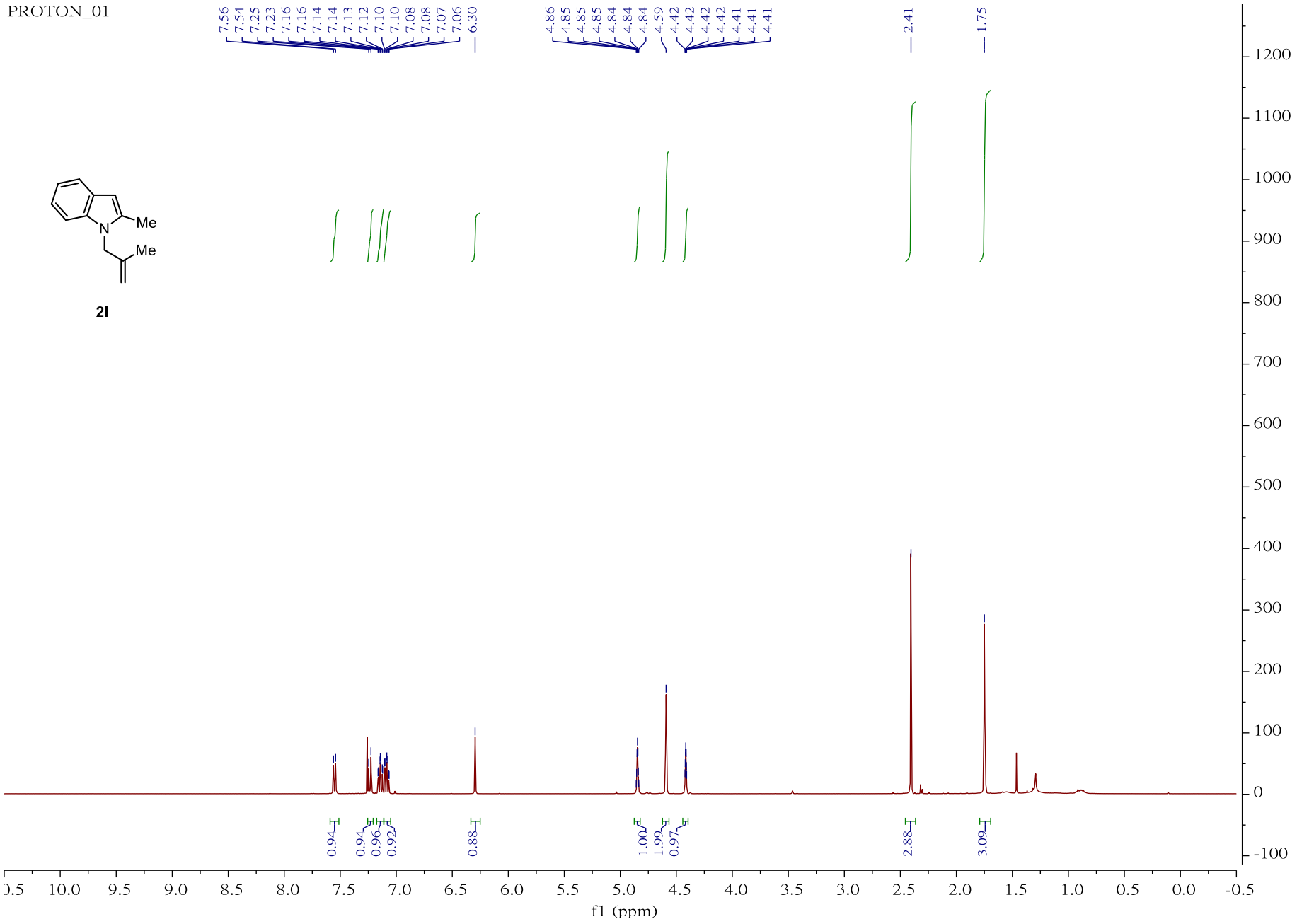

CARBON_01
140.34
135.93
130.94
129.80
124.89
121.10
118.70
114.46
113.19
103.15
100.41
77.00
52.77
19.73
CN
N
Me
2i
f1 (ppm)

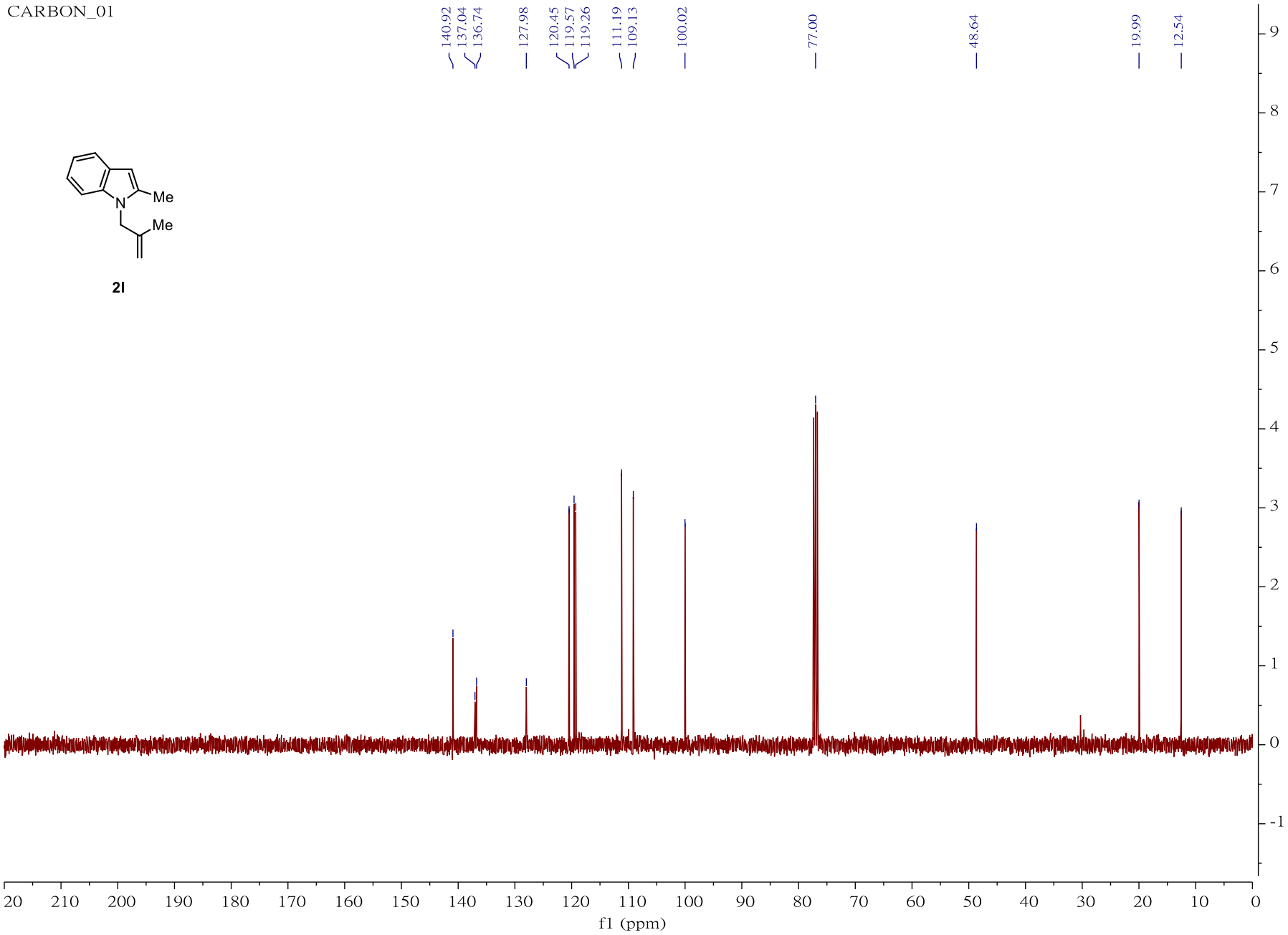

PROTON_01
8.60
8.59
8.12
8.11
8.10
8.09
7.34
7.32
7.23
7.23
6.71
6.70
4.97
4.96
4.96
4.96
4.95
4.71
4.69
1.69
O2N
N
Me
2j
0.91
0.97
1.04
0.90
0.95
1.00
1.05
1.92
2.86
f1 (ppm)

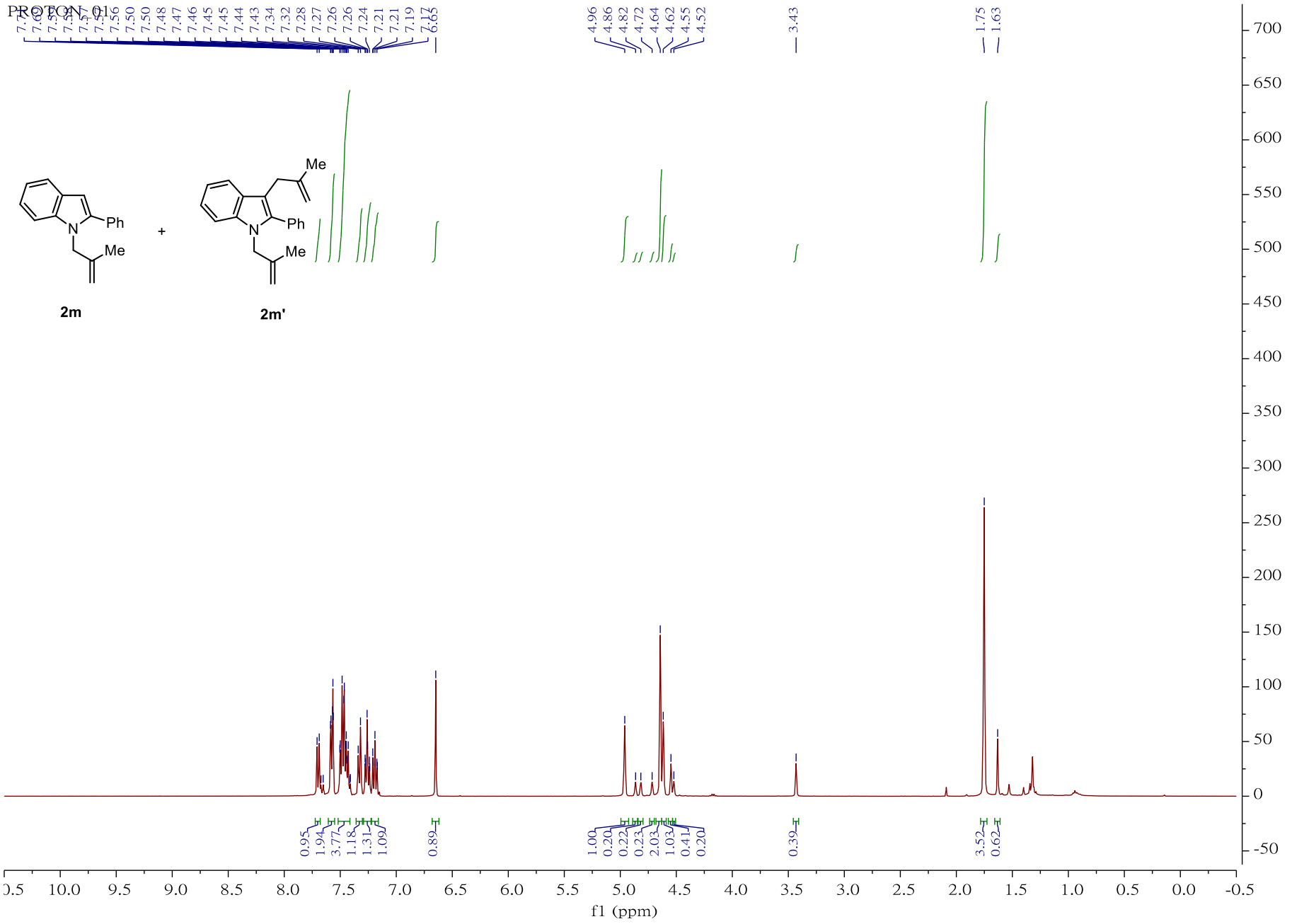

CARBON_01
141.40
140.05
138.97
131.51
127.63
117.96
117.03
113.14
109.47
103.91
77.00
52.74
19.64
O2N
N
Me
2j
f1 (ppm)

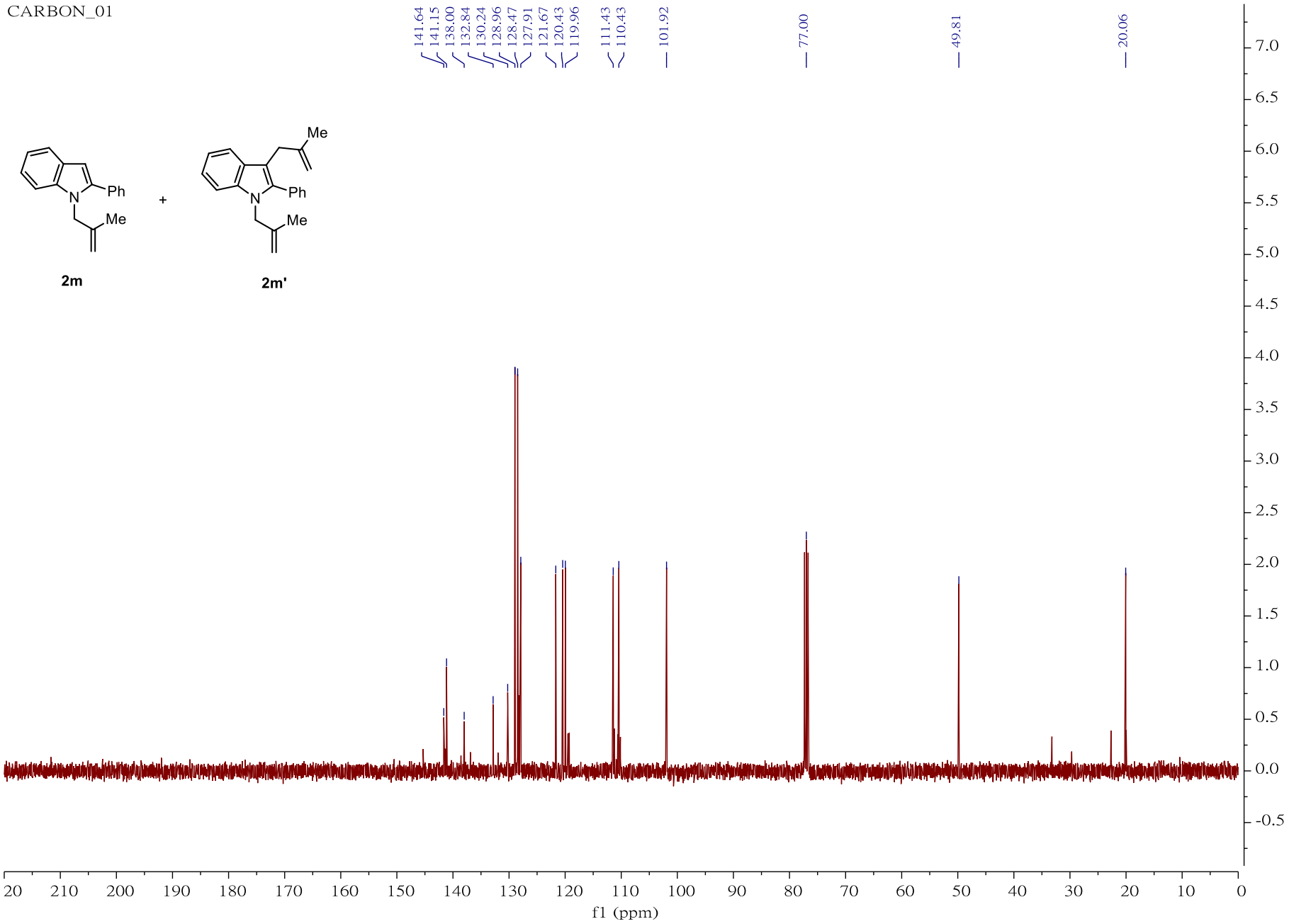

PROTON_01
7.49
7.48
7.47
7.47
7.05
7.04
7.02
7.00
6.99
6.98
6.96
6.51
6.51
4.83
4.83
4.83
4.82
4.82
4.81
4.81
4.77
4.25
4.25
4.24
4.24
4.24
4.24
4.23
2.97
2.95
2.94
2.92
1.76
1.35
1.33
1.31
Et
N
Me
2k
1.00
1.02
0.92
0.97
0.95
1.12
2.08
1.06
2.21
3.18
3.28
f1 (ppm)


CARBON_01
142.75
134.15
130.13
129.83
127.48
122.41
119.70
118.94
110.95
101.73
77.00
54.35
25.02
19.86
16.08
Et
N
Me
2k
f1 (ppm)


PROTON_01
7.56
7.54
7.25
7.23
7.16
7.16
7.14
7.14
7.13
7.12
7.10
7.10
7.08
7.08
7.07
7.06
6.30
4.86
4.85
4.85
4.85
4.84
4.84
4.84
4.59
4.42
4.42
4.42
4.42
4.41
4.41
4.41
2.41
1.75
Me
Me
N
2l
0.94
0.94
0.96
0.92
0.88
1.00
1.99
0.97
2.88
3.09
f1 (ppm)

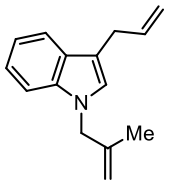

CARBON_01
140.92
137.04
136.74
127.98
120.45
119.57
119.26
111.19
109.13
100.02
77.00
48.64
19.99
12.54
Me
Me
N
2l
f1 (ppm)


PROTON_01
7.70 7.68 7.57 7.56 7.56 7.50 7.50 7.48 7.47 7.46 7.45 7.45 7.44 7.43 7.34 7.32 7.28 7.27 7.26 7.26 7.24 7.21 7.21 7.19 7.17 6.85
4.96 4.86 4.82 4.72 4.64 4.62 4.55 4.52
3.43
1.75 1.63
Ph
Me
+
Me
Ph
Me
2m
2m'
0.95 1.94 3.77 1.18 1.31 1.09 0.89 1.00 0.20 0.22 0.23 2.03 1.03 0.41 0.20 0.39 3.52 0.62
f1 (ppm)

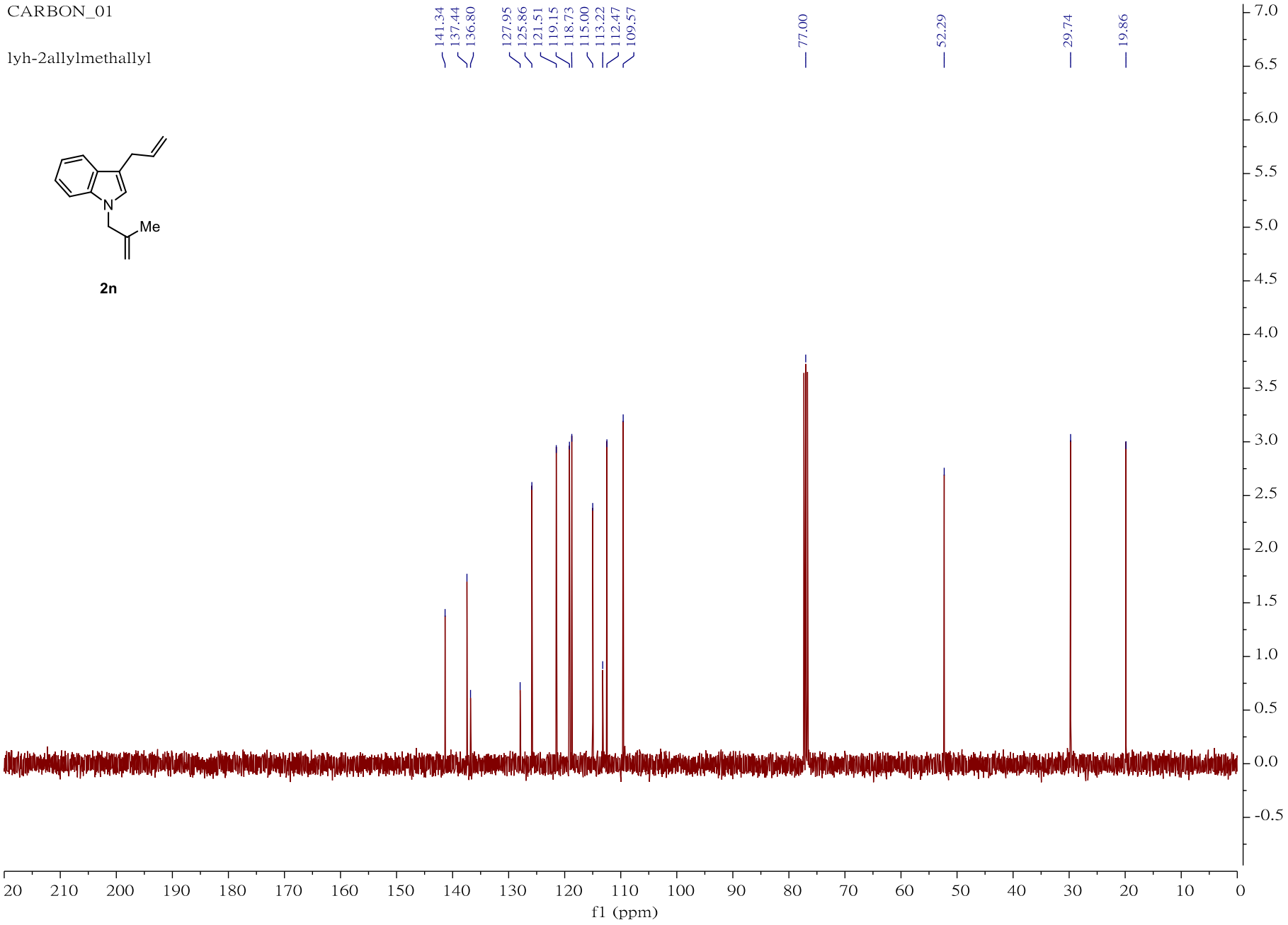

CARBON_01
141.64
141.15
138.00
132.84
130.24
128.96
128.47
127.91
121.67
120.43
119.96
111.43
110.43
101.92
77.00
49.81
20.06
Ph
Me
Me
Ph
Me
2m
2m'
f1 (ppm)

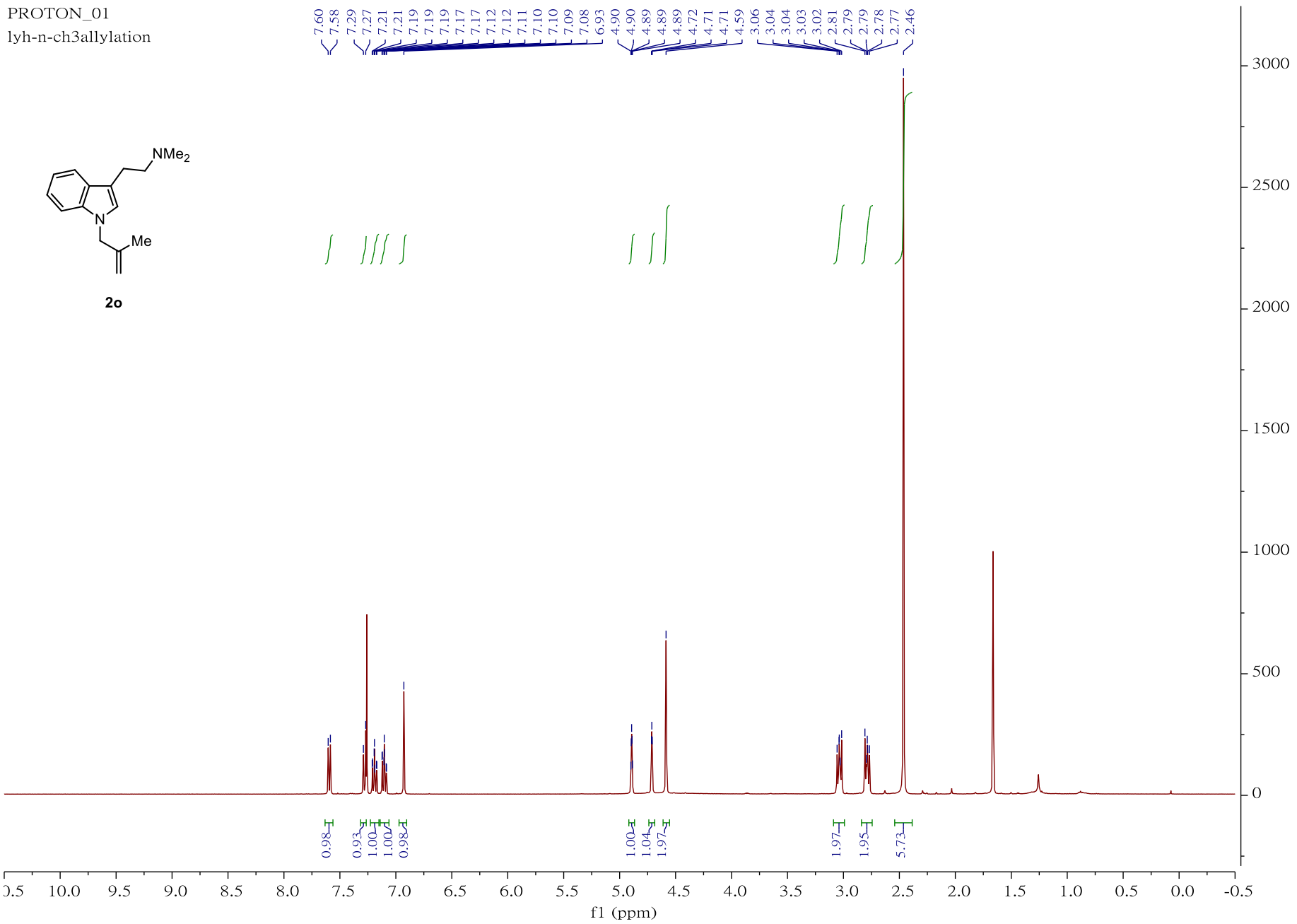
PROTON_01

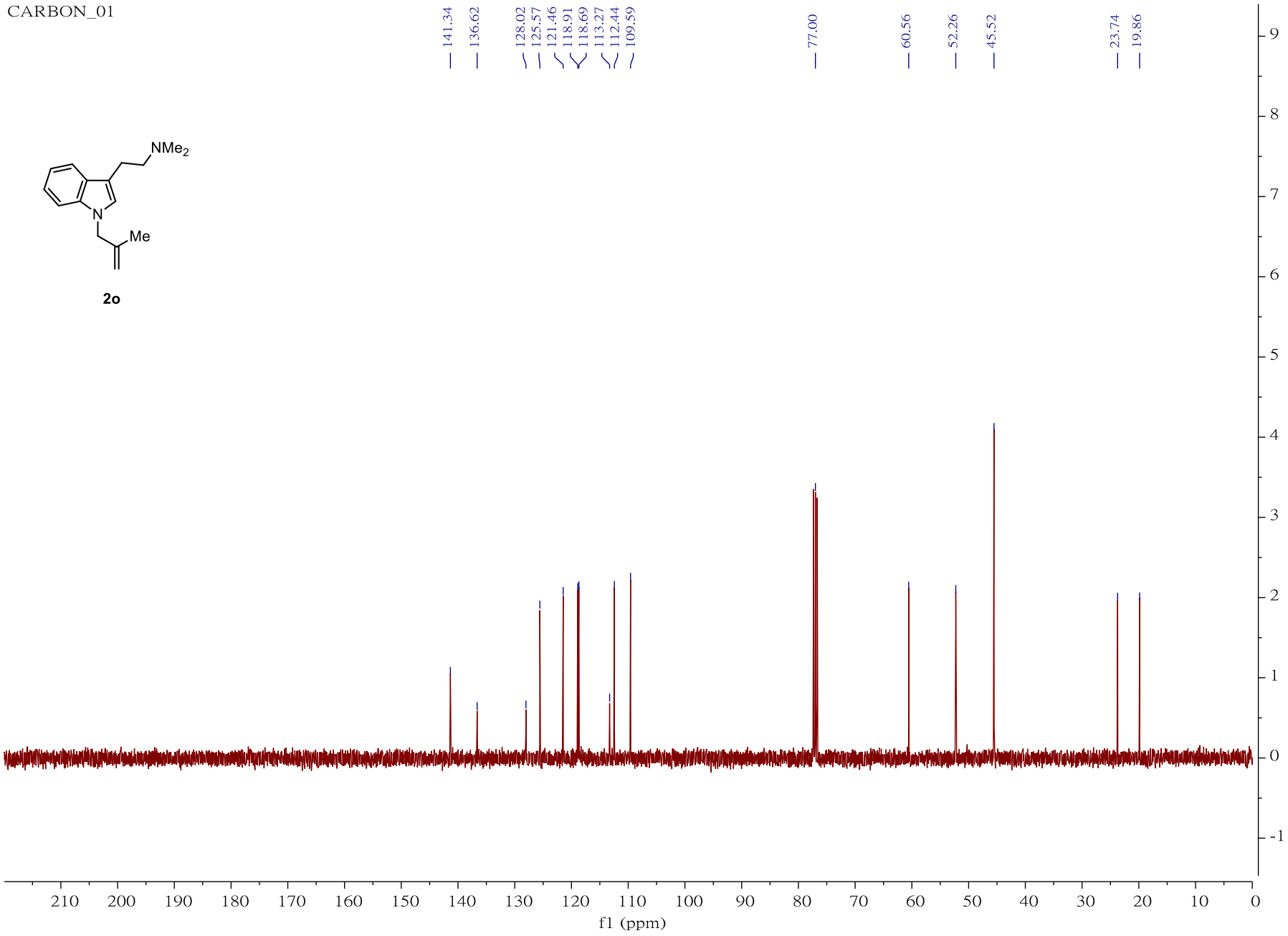
lyh-2allylmethallyl

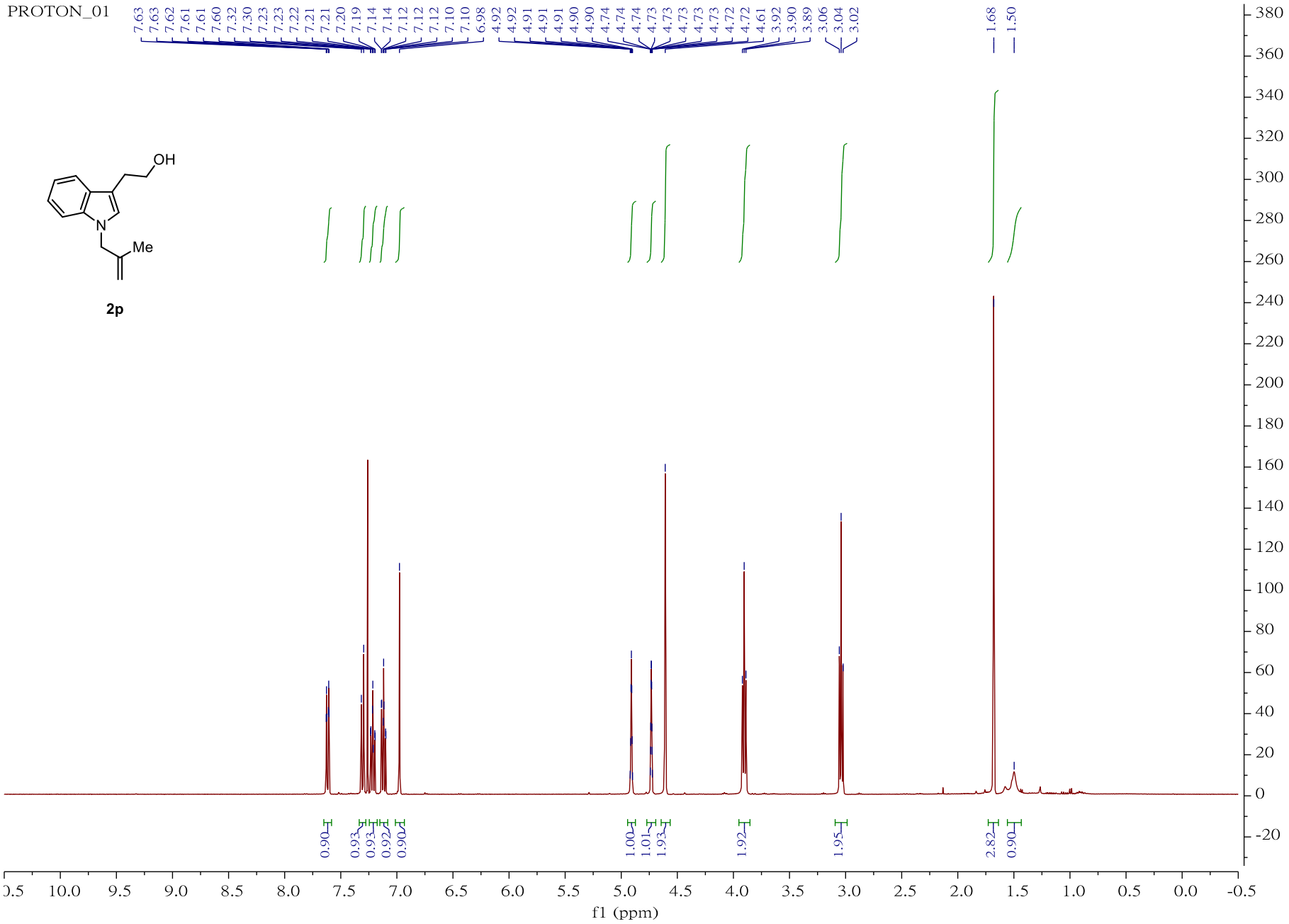


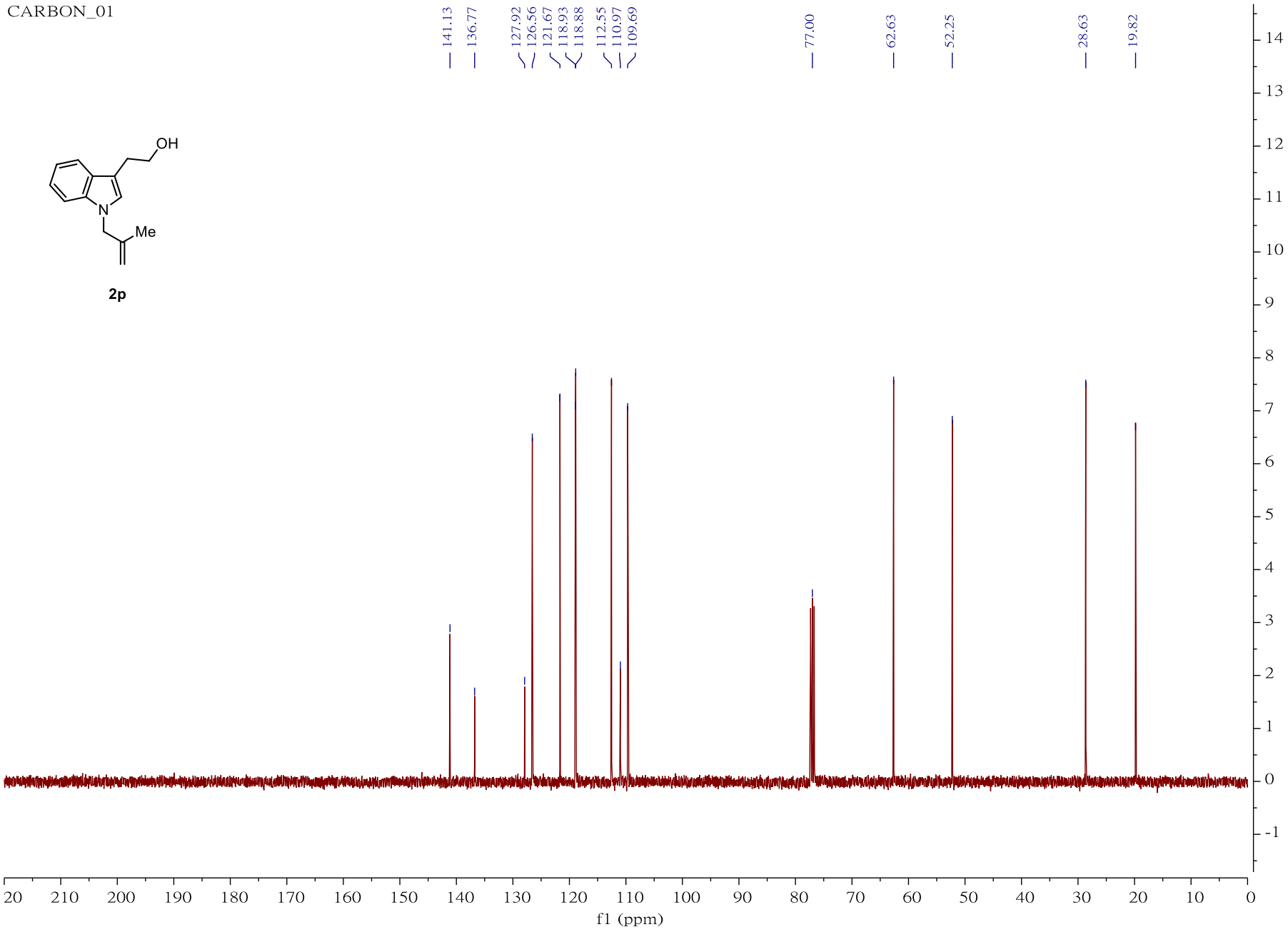
2n

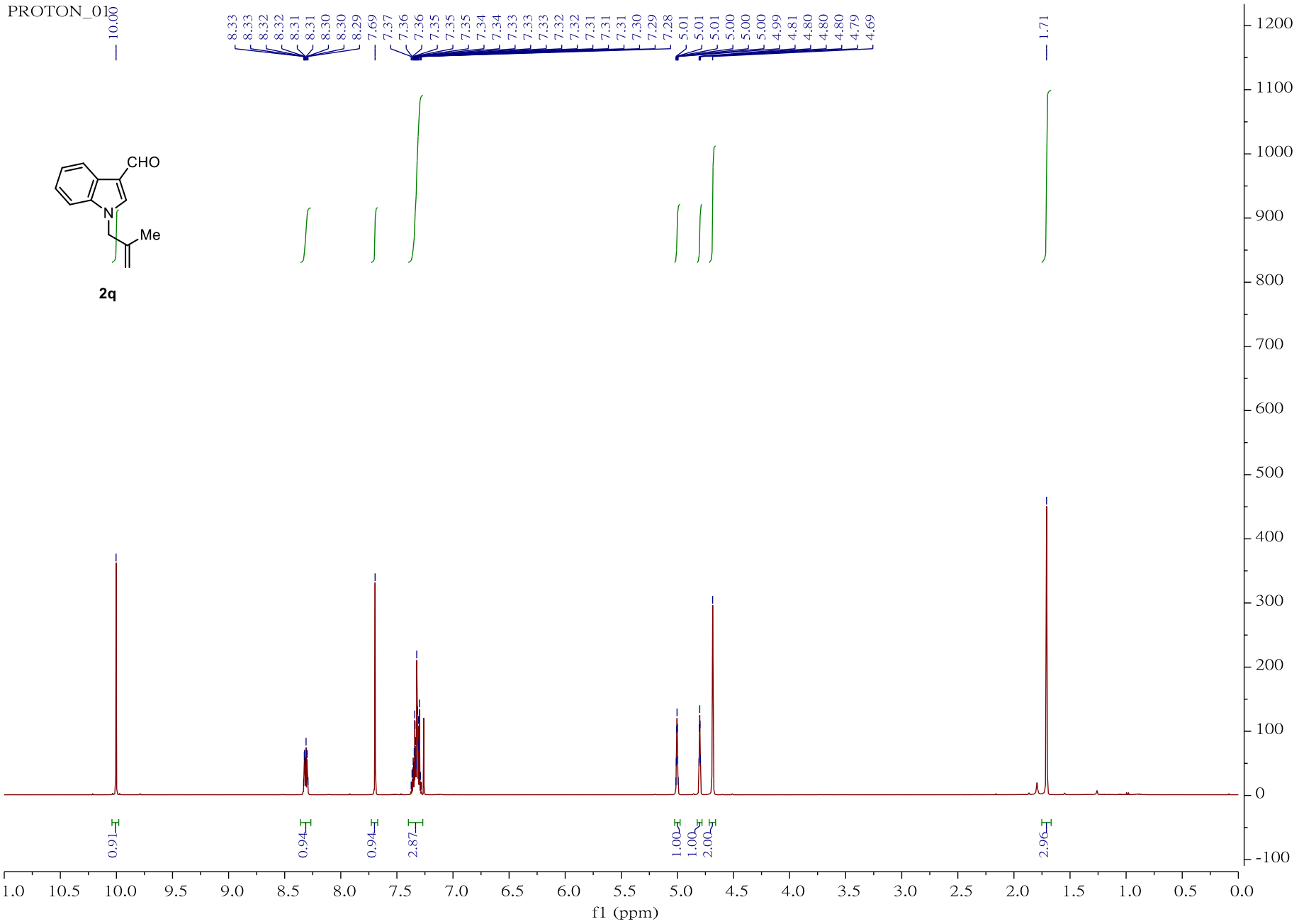

CARBON_01
lyh-2allylmethallyl
141.34
137.44
136.80
127.95
125.86
121.51
119.15
118.73
115.00
113.22
112.47
109.57
77.00
52.29
29.74
19.86
N
Me
2n
f1 (ppm)

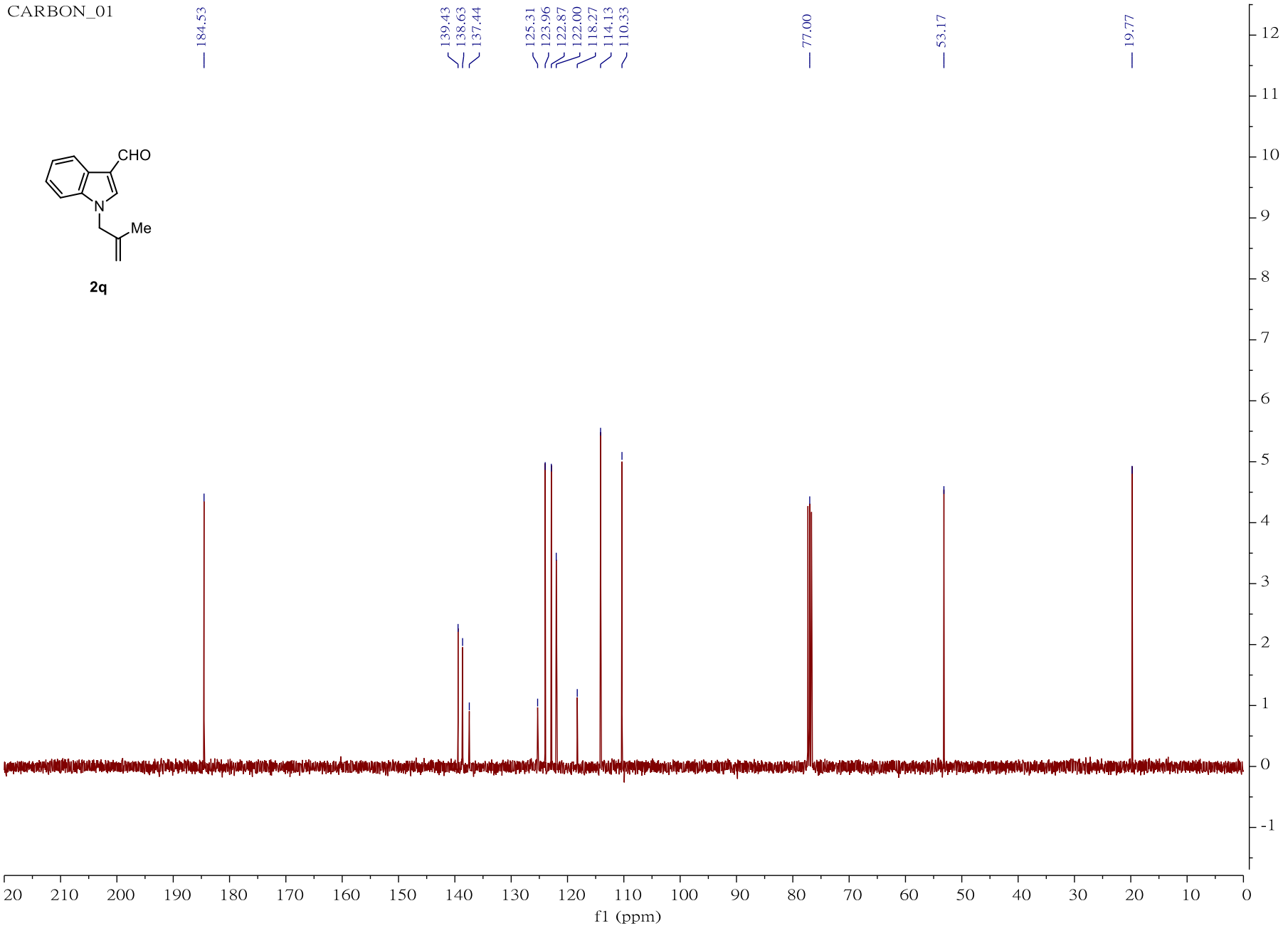

PROTON_01
lyh-n-ch3allylation
7.60
7.58
7.29
7.27
7.21
7.21
7.19
7.19
7.19
7.17
7.17
7.12
7.12
7.11
7.10
7.10
7.09
7.08
6.93
4.90
4.90
4.89
4.89
4.89
4.72
4.71
4.71
4.59
3.06
3.04
3.04
3.03
3.02
2.81
2.79
2.79
2.78
2.77
2.46
NMe2
N
Me
2o
3000
2500
2000
1500
1000
500
0
0.98
0.93
1.00
1.00
0.98
1.00
1.04
1.97
1.97
1.95
5.73
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

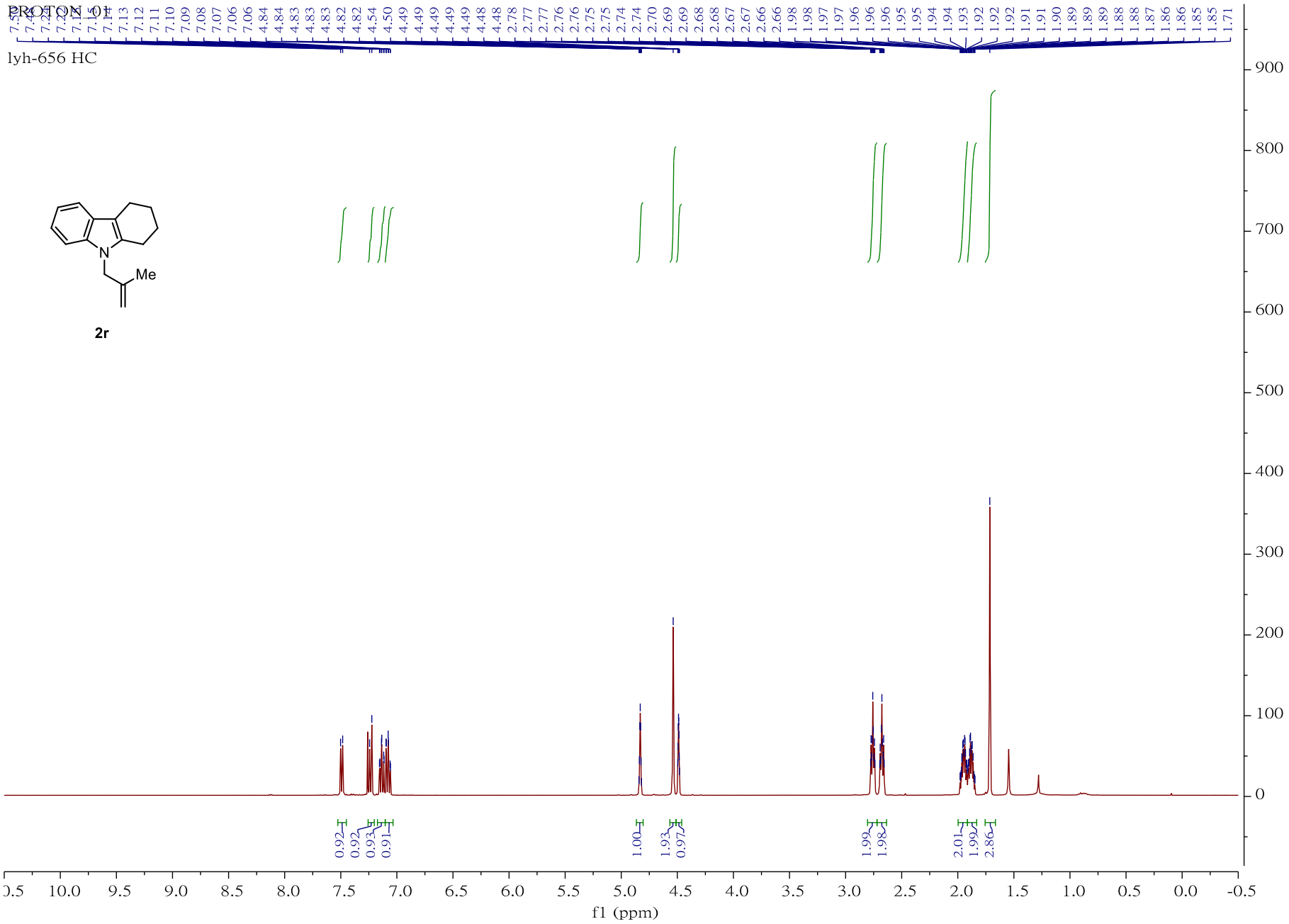

CARBON_01
141.34
136.62
128.02
125.57
121.46
118.91
118.69
113.27
112.44
109.59
77.00
60.56
52.26
45.52
23.74
19.86
NMe2
N
Me
2o
f1 (ppm)

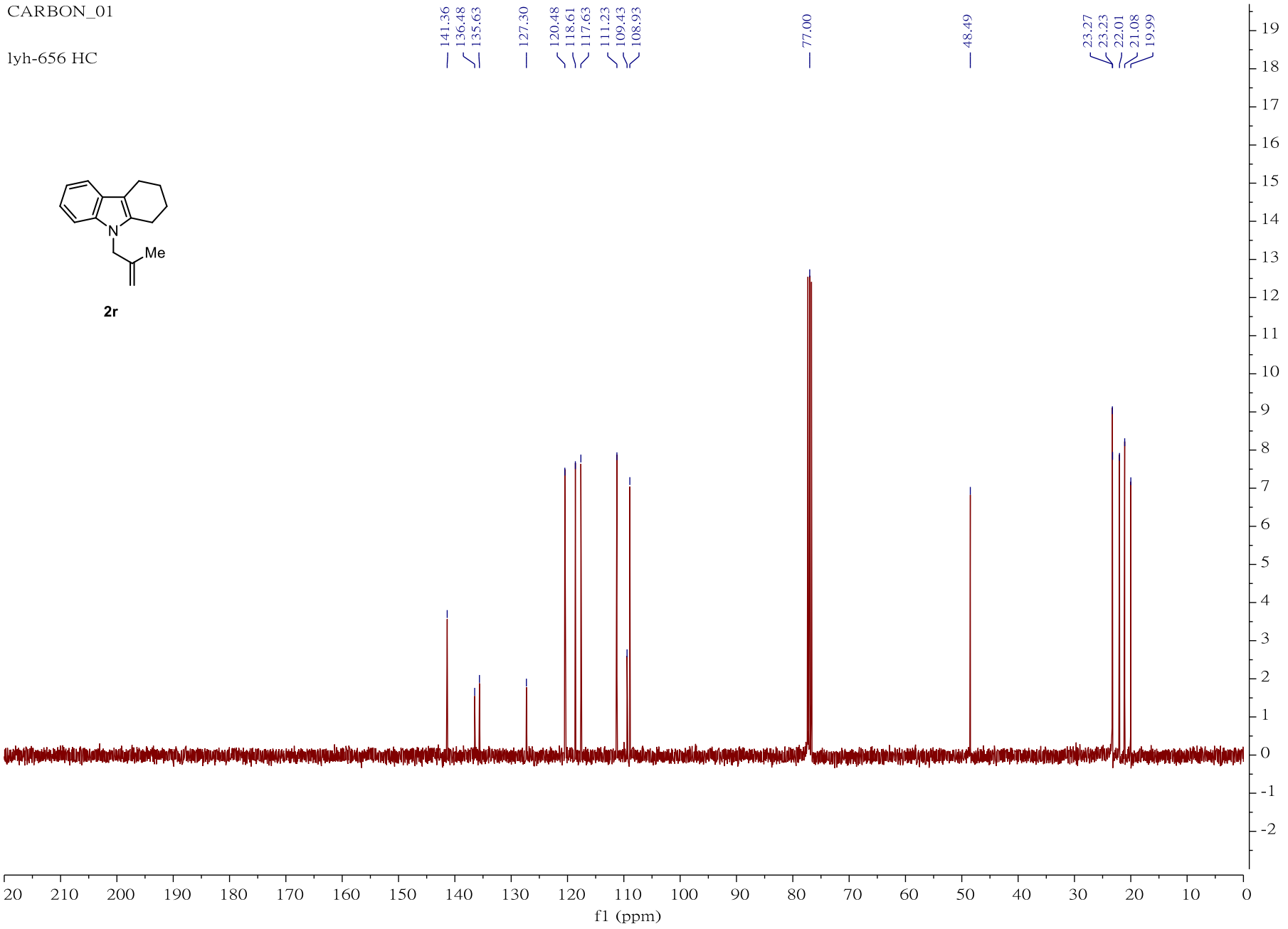

PROTON_01
7.63 7.63 7.62 7.61 7.61 7.60 7.32 7.30 7.23 7.23 7.22 7.21 7.21 7.20 7.19 7.14 7.14 7.12 7.12 7.12 7.10 7.10 6.98
4.92 4.92 4.91 4.91 4.91 4.90 4.90 4.74 4.74 4.74 4.73 4.73 4.73 4.73 4.73 4.72 4.72 4.61 3.92 3.90 3.89 3.06 3.04 3.02
1.68 1.50
OH
N
Me
2p
0.90 0.93 0.93 0.92 0.90 1.00 1.01 1.93 1.92 1.95 2.82 0.90
f1 (ppm)

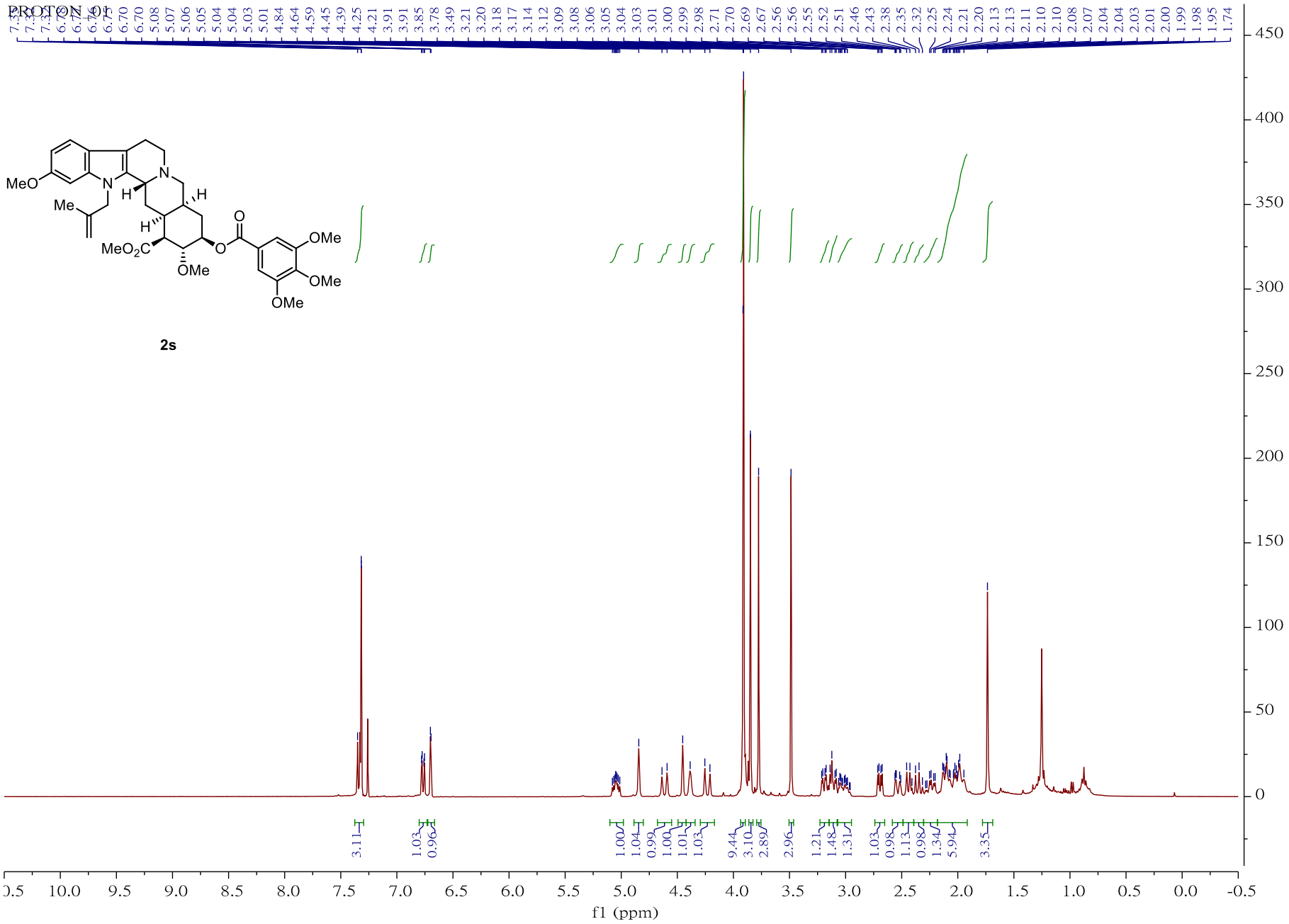

CARBON_01
141.13
136.77
127.92
126.56
121.67
118.93
118.88
112.55
110.97
109.69
77.00
62.63
52.25
28.63
19.82
OH
N
Me
2p
f1 (ppm)

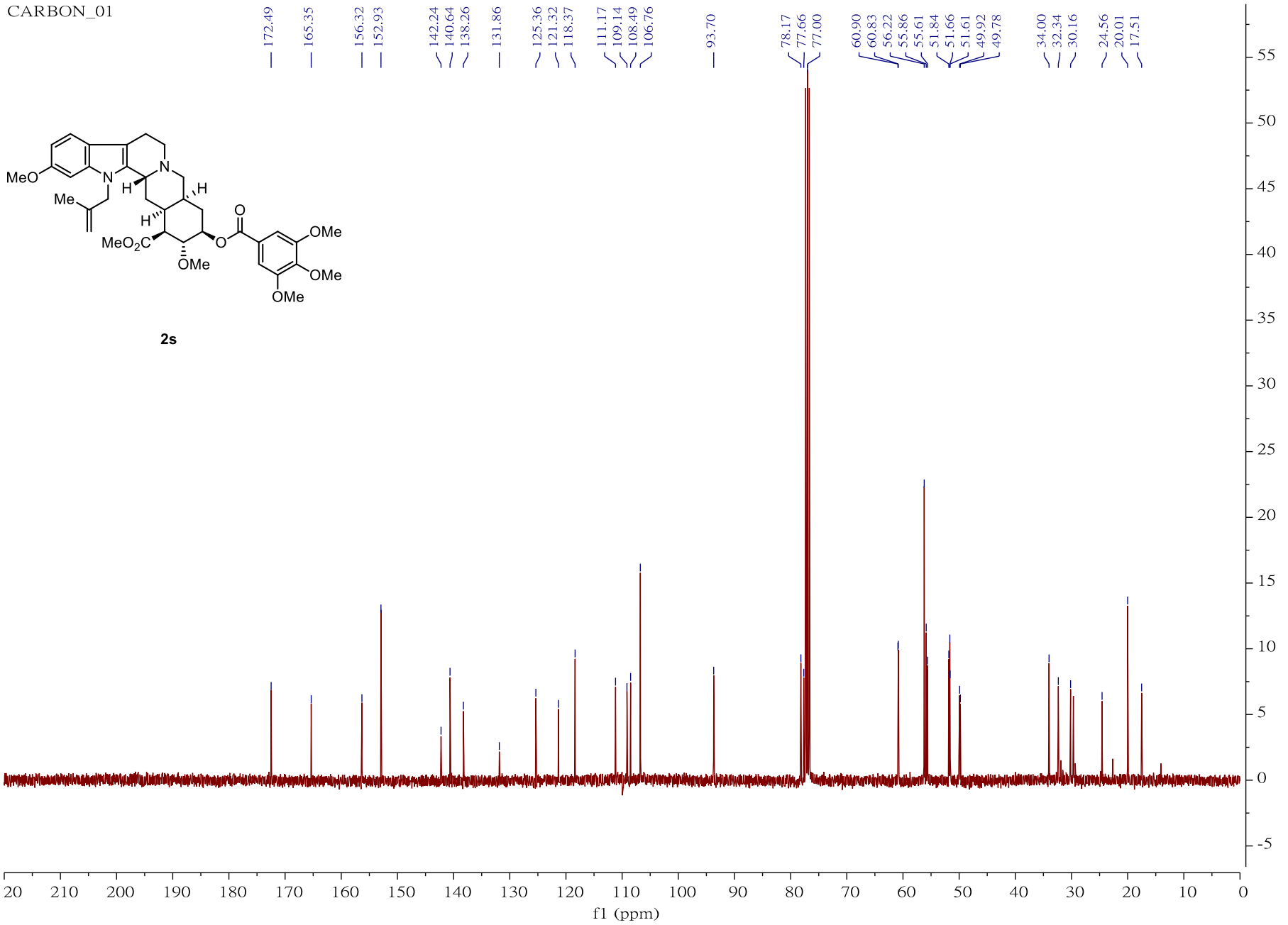

PROTON_01
10.00
8.33 8.33 8.32 8.32 8.31 8.31 8.30 8.30 8.29
7.69
7.37 7.36 7.36 7.35 7.35 7.35 7.34 7.34 7.33 7.33 7.33 7.32 7.32 7.31 7.31 7.31 7.30 7.29 7.28
5.01 5.01 5.01 5.00 5.00 5.00 4.99 4.81 4.80 4.80 4.80 4.79 4.69
1.71
CHO
N
Me
2q
0.91
0.94
0.94
2.87
1.00
1.00
2.00
2.96
f1 (ppm)

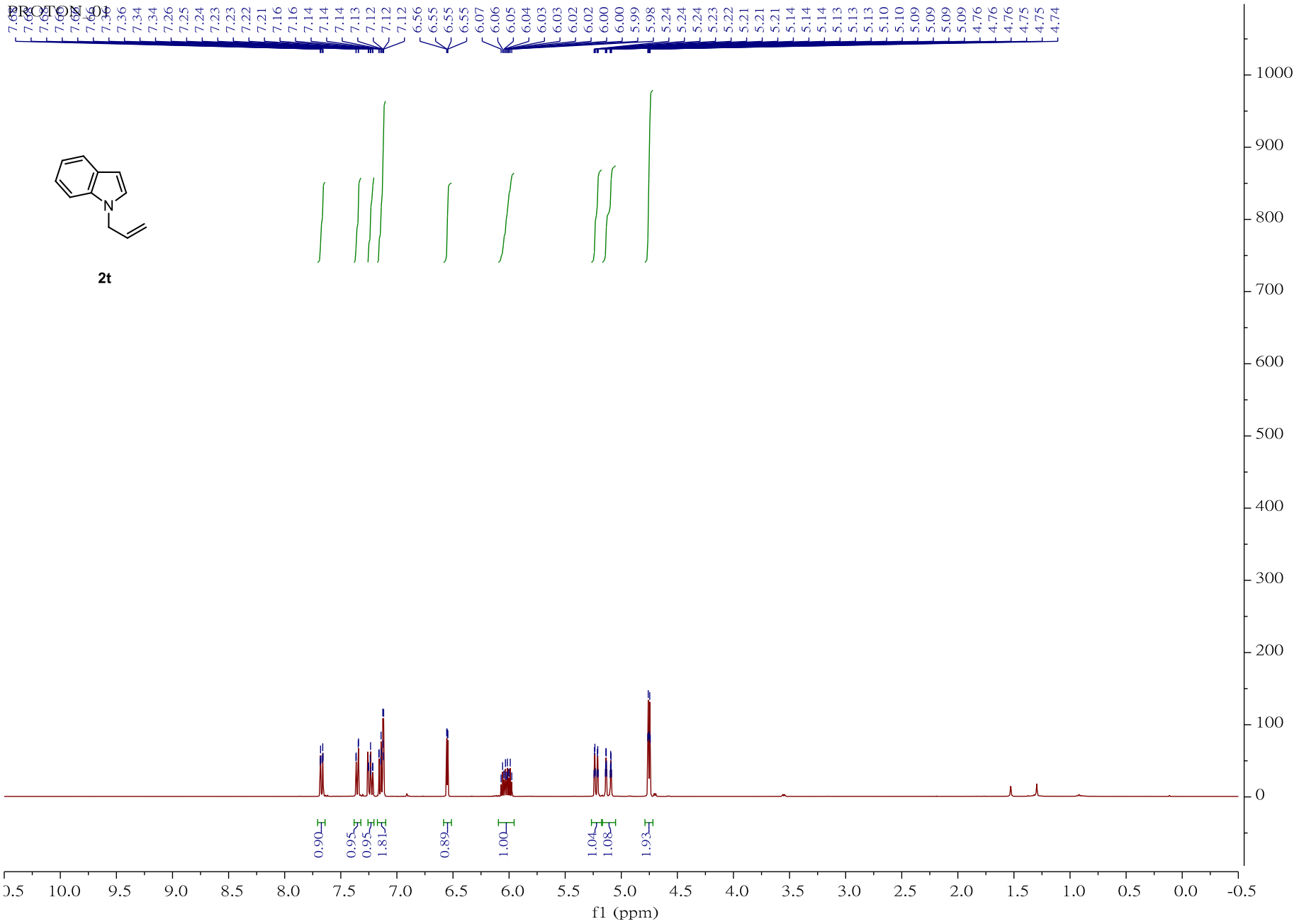

CARBON_01
184.53
139.43
138.63
137.44
125.31
123.96
122.87
122.00
118.27
114.13
110.33
77.00
53.17
19.77
CHO
N
Me
2q
f1 (ppm)

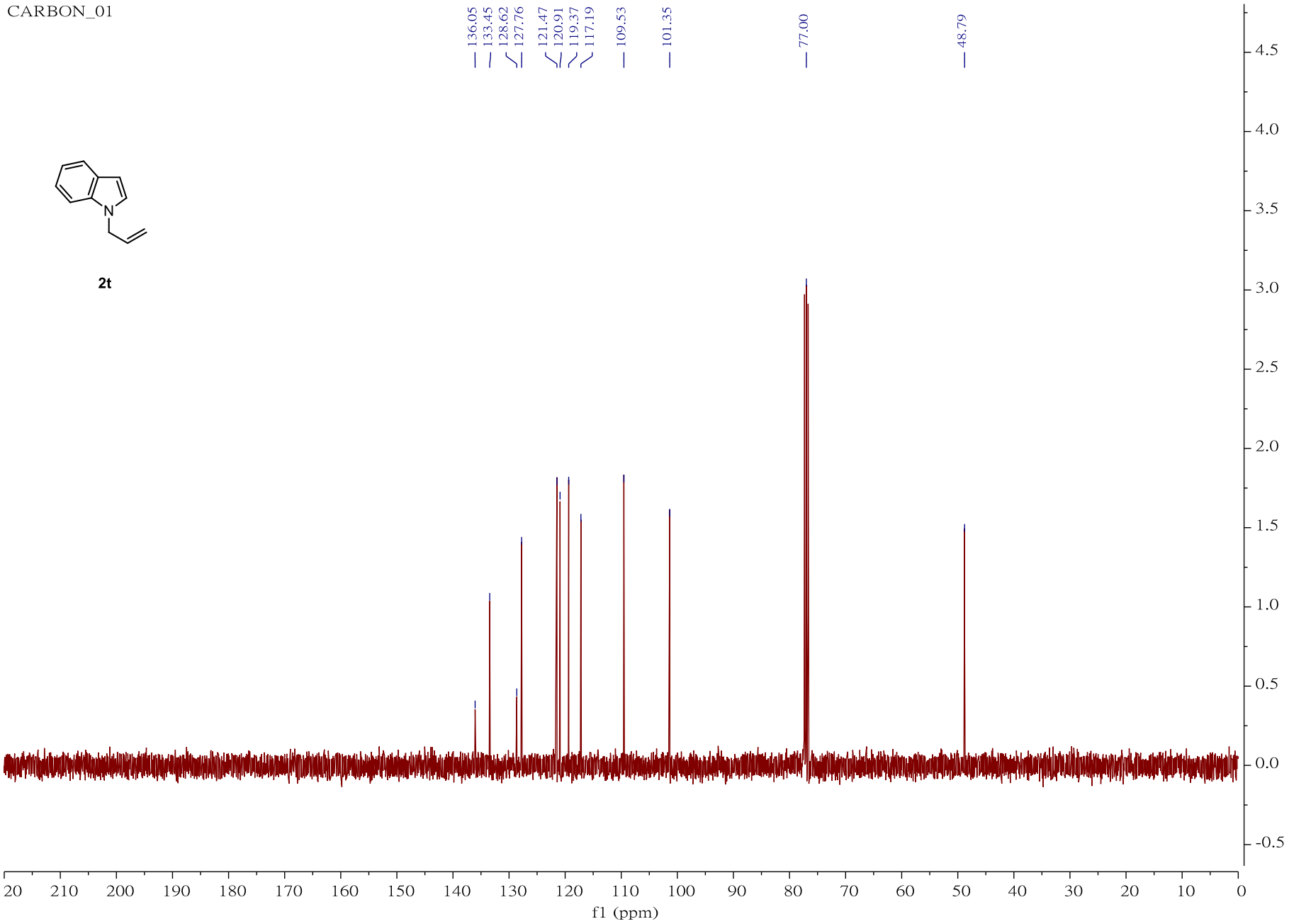

PROTON-01
lyh-656 HC
Me
2r
f1 (ppm)

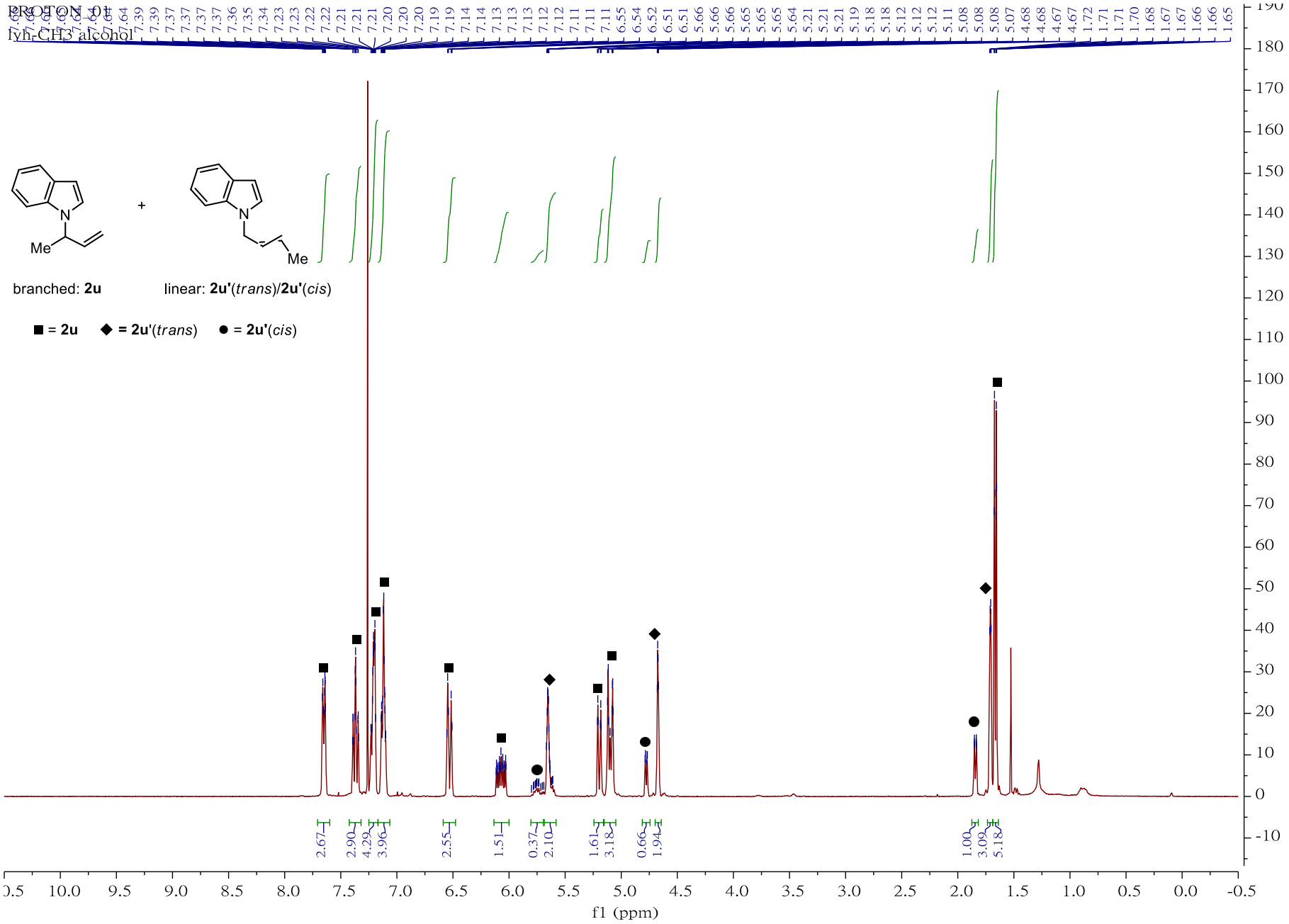

CARBON_01
lyh-656 HC
141.36
136.48
135.63
127.30
120.48
118.61
117.63
111.23
109.43
108.93
77.00
48.49
23.27
23.23
22.01
21.08
19.99
Me
2r
f1 (ppm)

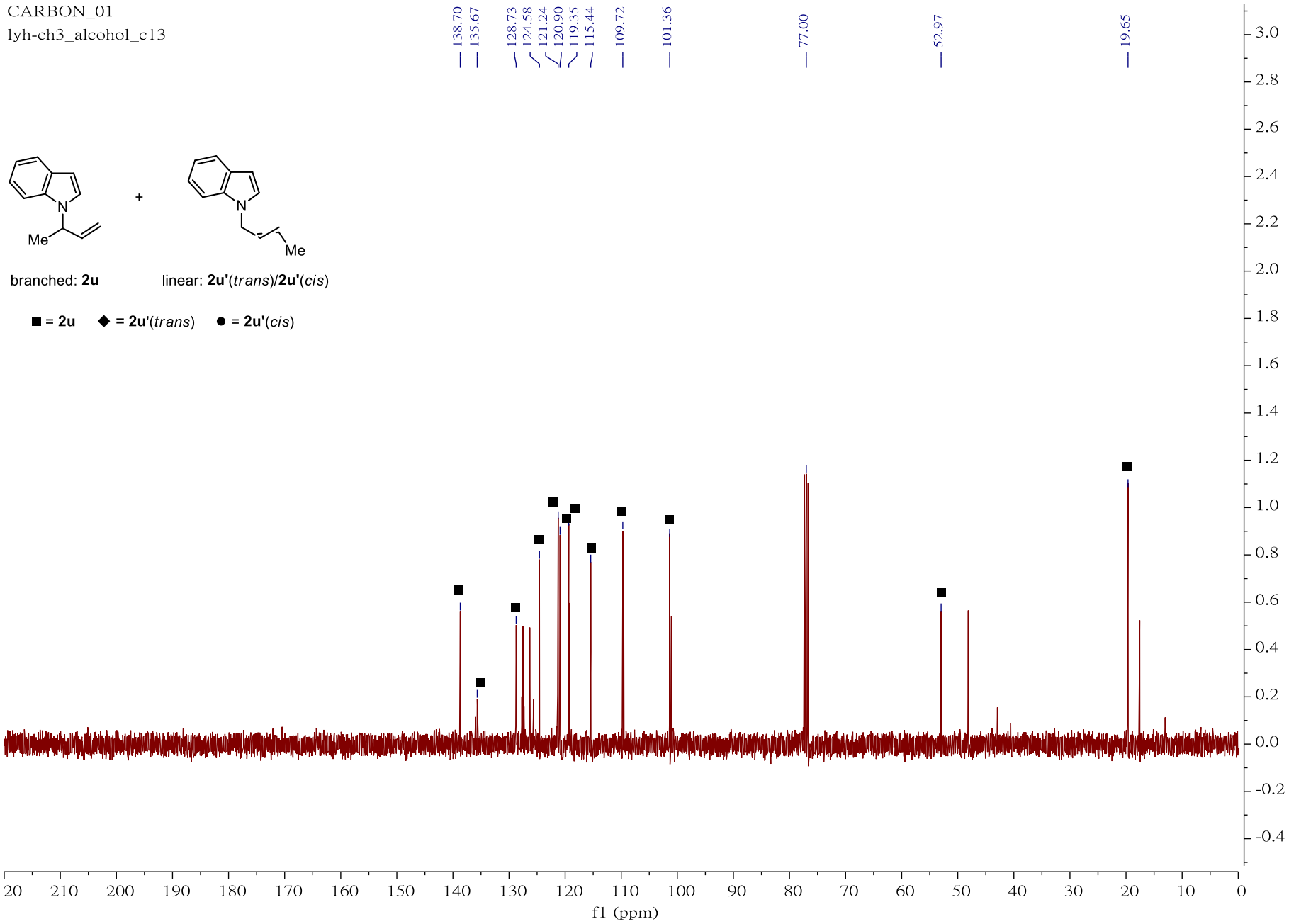

PROTON_01
MeO
Me
H
N
N
H
H
O
MeO2C
OMe
O
OMe
OMe
OMe
2s
f1 (ppm)

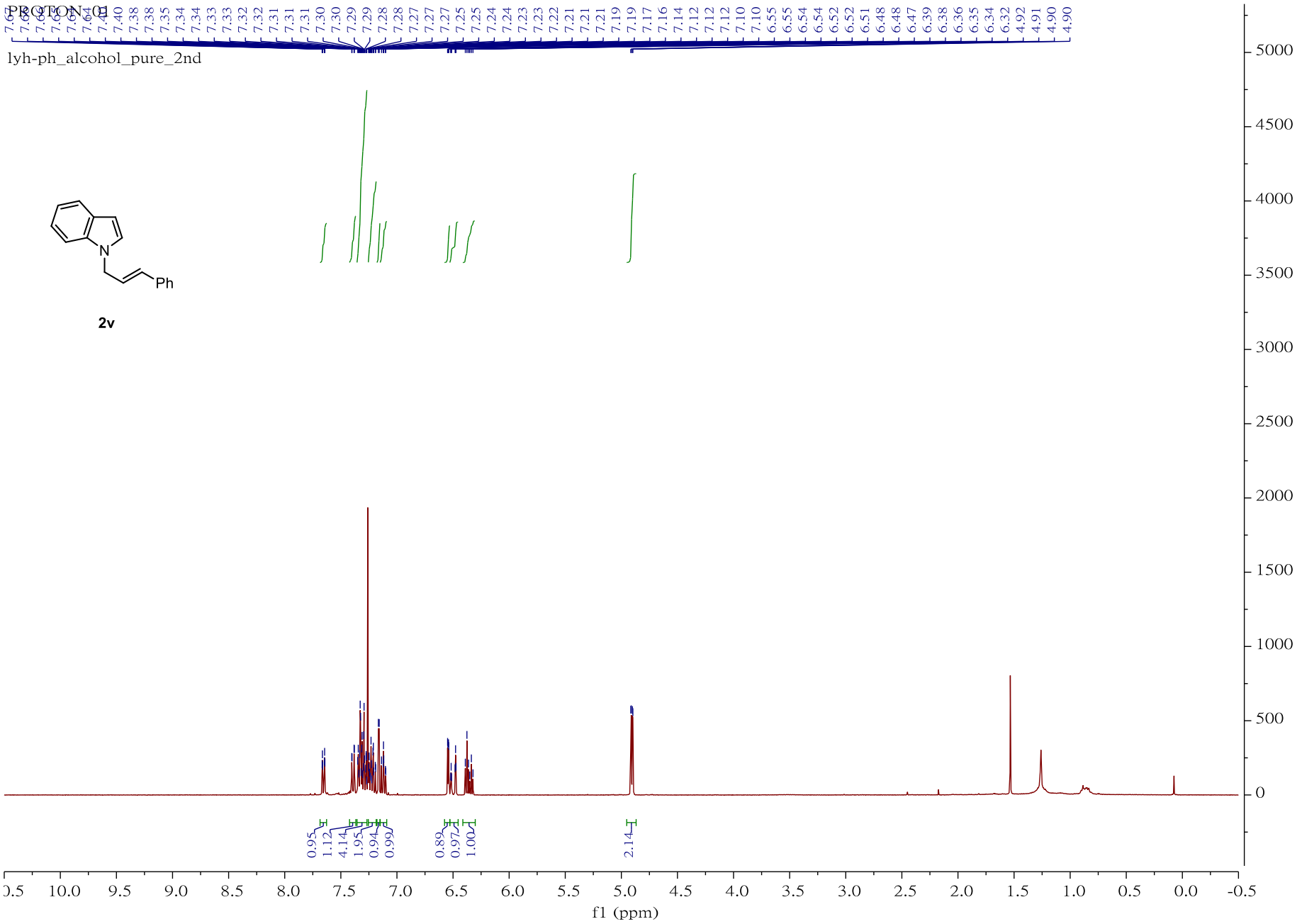

CARBON_01
172.49
165.35
156.32
152.93
142.24
140.64
138.26
131.86
125.36
121.32
118.37
111.17
109.14
108.49
106.76
93.70
78.17
77.66
77.00
60.90
60.83
56.22
55.86
55.61
51.84
51.66
51.61
49.92
49.78
34.00
32.34
30.16
24.56
20.01
17.51
MeO
N
H
N
H
H
Me
MeO2C
OMe
O
O
OMe
OMe
OMe
2s
f1 (ppm)


PROTON_01
2t
f1 (ppm)


CARBON_01
136.05
133.45
128.62
127.76
121.47
120.91
119.37
117.19
109.53
101.35
77.00
48.79
N
2t
f1 (ppm)

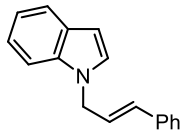

PROTON_01
lyh-CH3 alcohol
Me
+
N
Me
branched: 2u
linear: 2u'(trans)/2u'(cis)
■ = 2u ◆ = 2u'(trans) ● = 2u'(cis)
2.67
2.90
4.29
3.96
2.55
1.51
0.37
2.10
1.61
3.18
0.66
1.94
1.00
3.09
5.18
f1 (ppm)


CARBON_01
lyh-ch3_alcohol_c13
138.70
135.67
128.73
124.58
121.24
120.90
119.35
115.44
109.72
101.36
77.00
52.97
19.65
Me
+
Me
branched: 2u
linear: 2u'(trans)/2u'(cis)
■ = 2u ◆ = 2u'(trans) ● = 2u'(cis)
f1 (ppm)

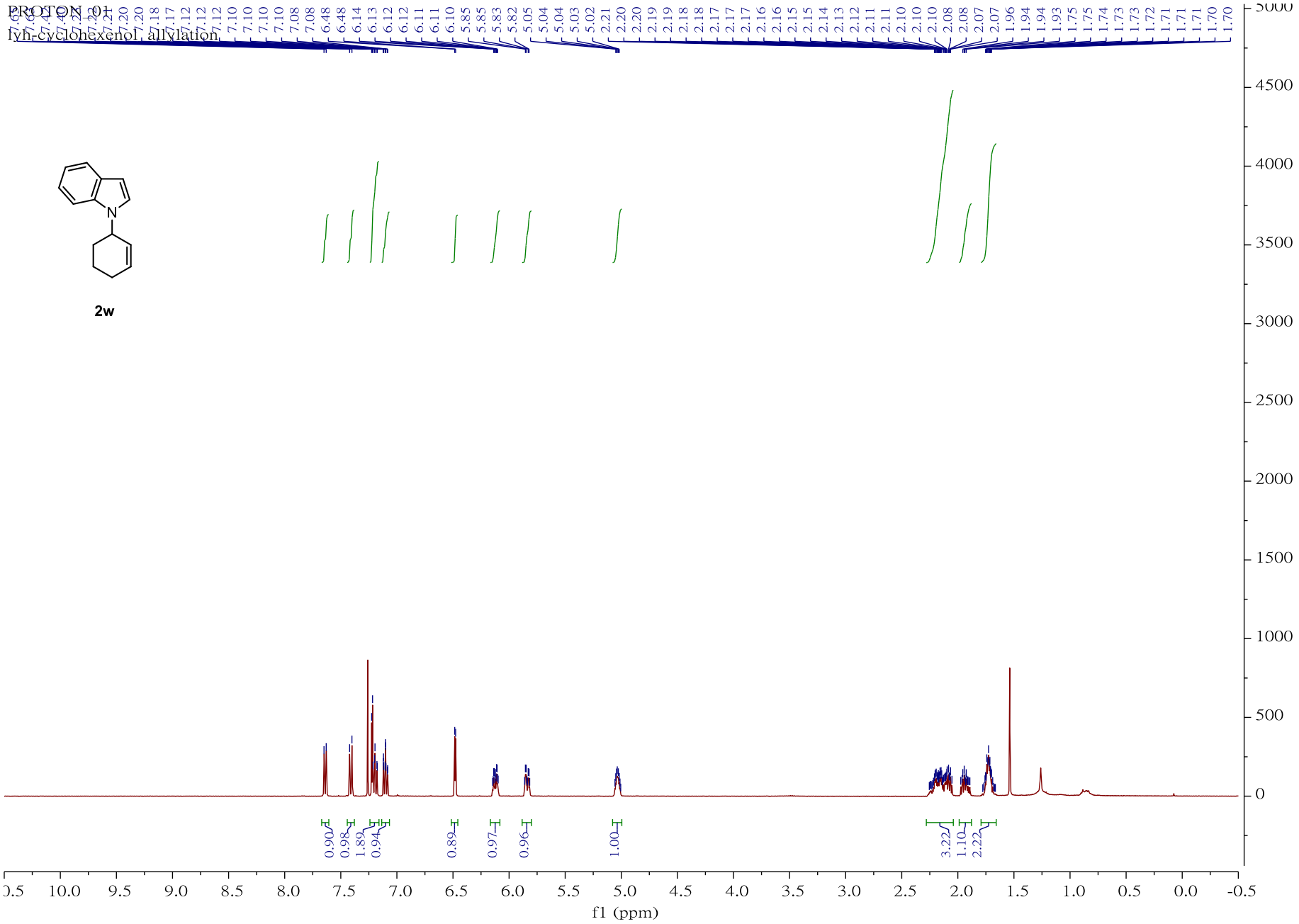

PROTON-01
lyh-ph_alcohol_pure_2nd
N
Ph
2v
f1 (ppm)

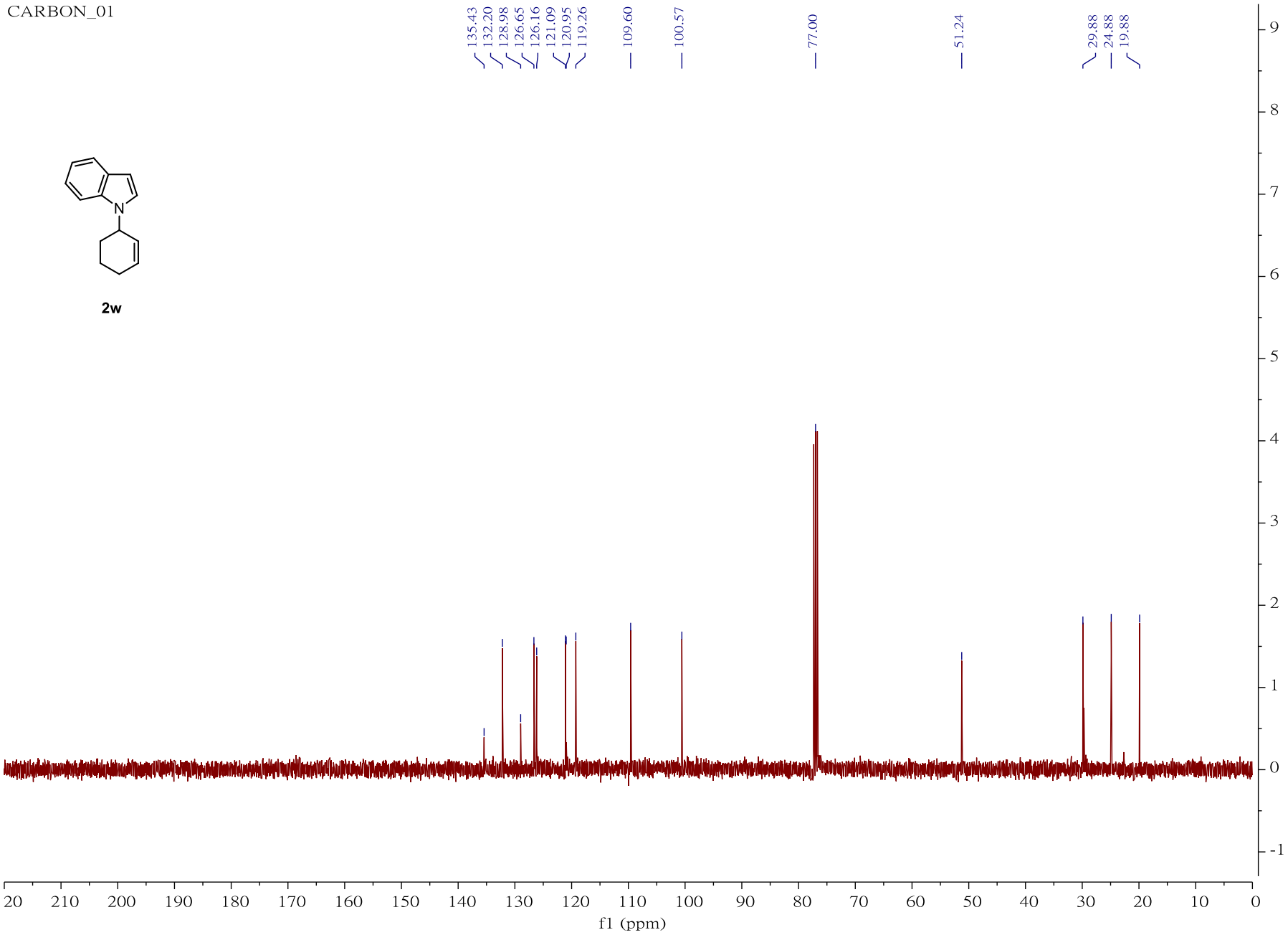
CARBON_01

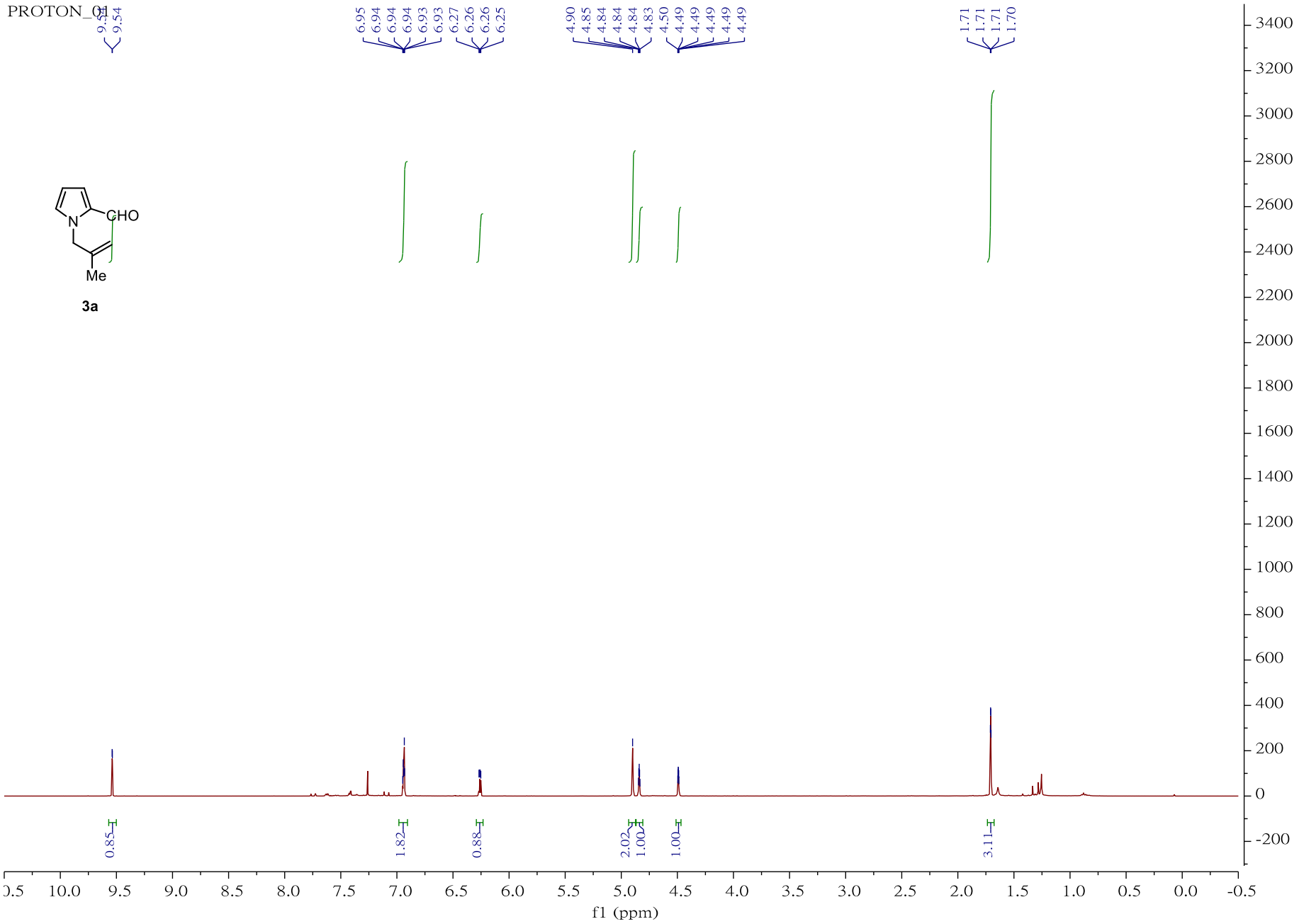
lyh-cinnamary

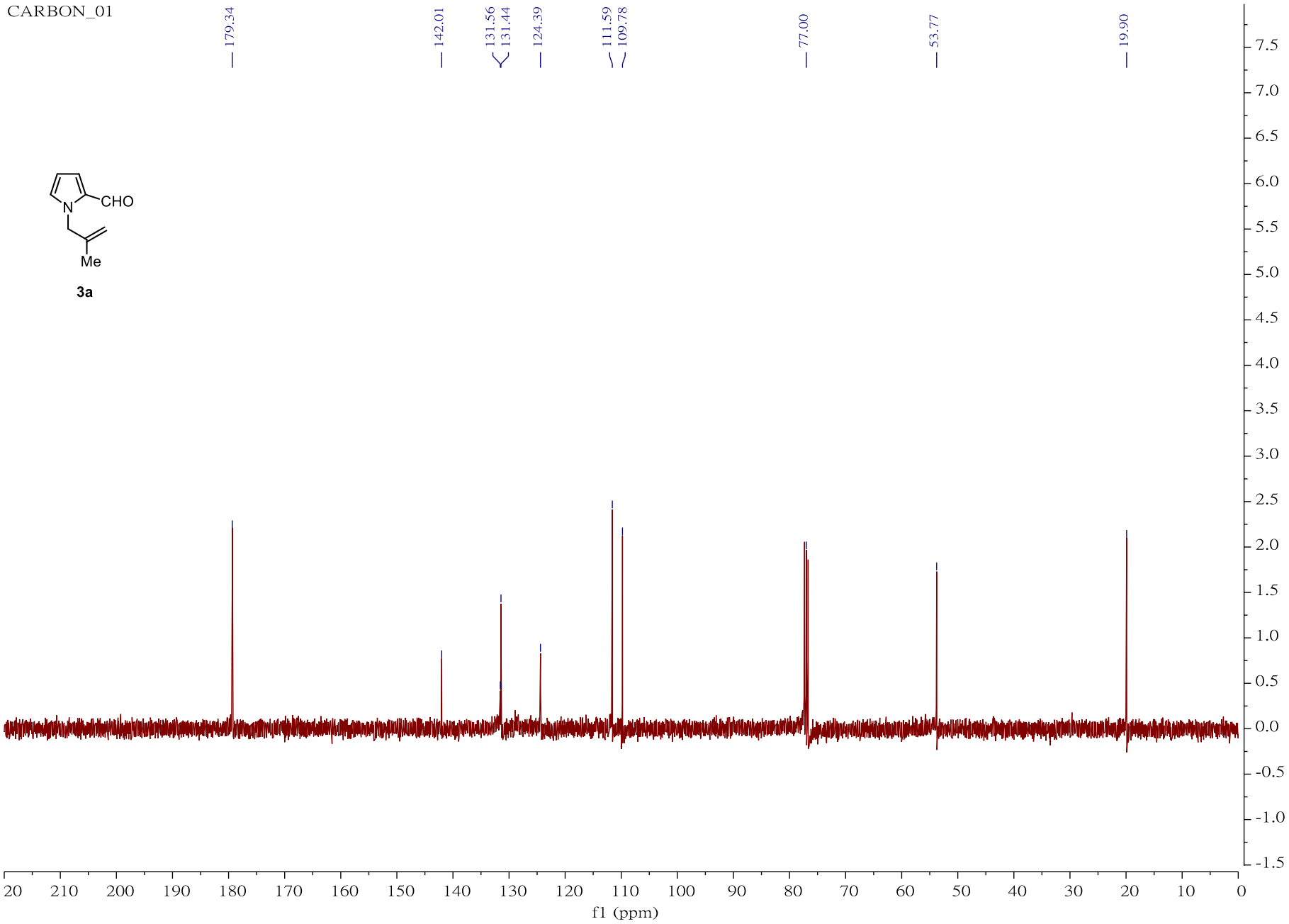


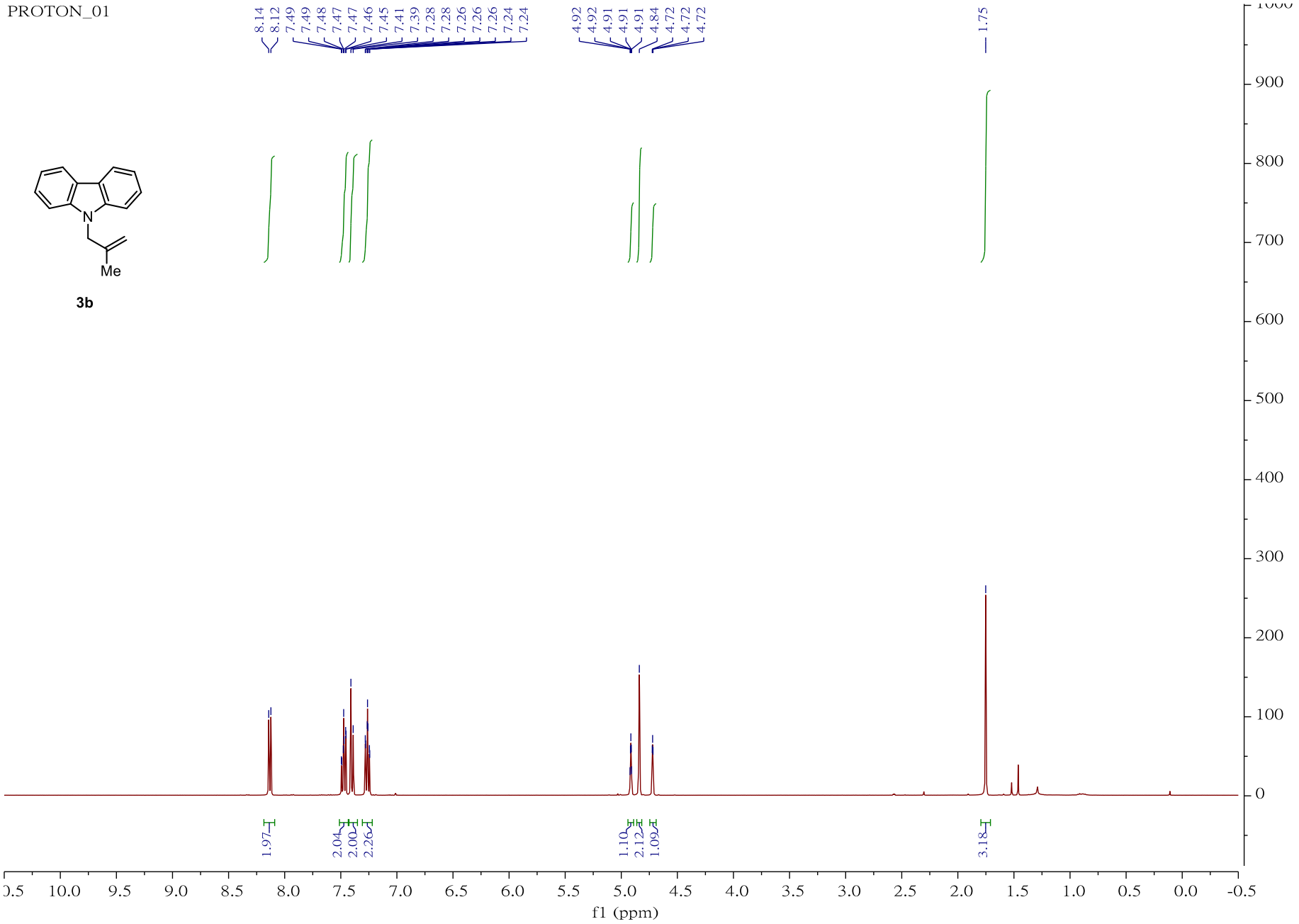
2v

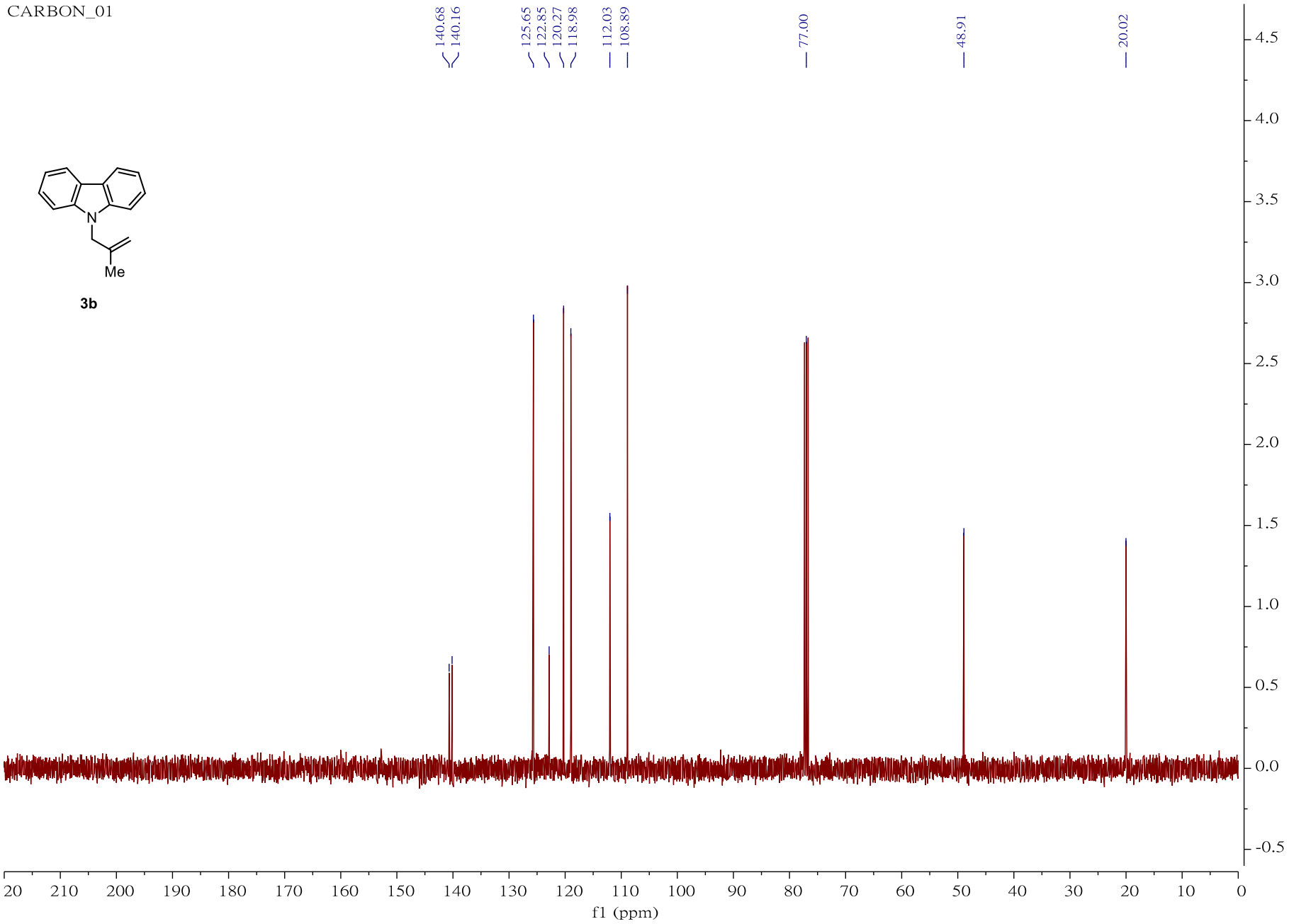

PROTON-01
lyh-cyclohexenol_allylation
2w
f1 (ppm)

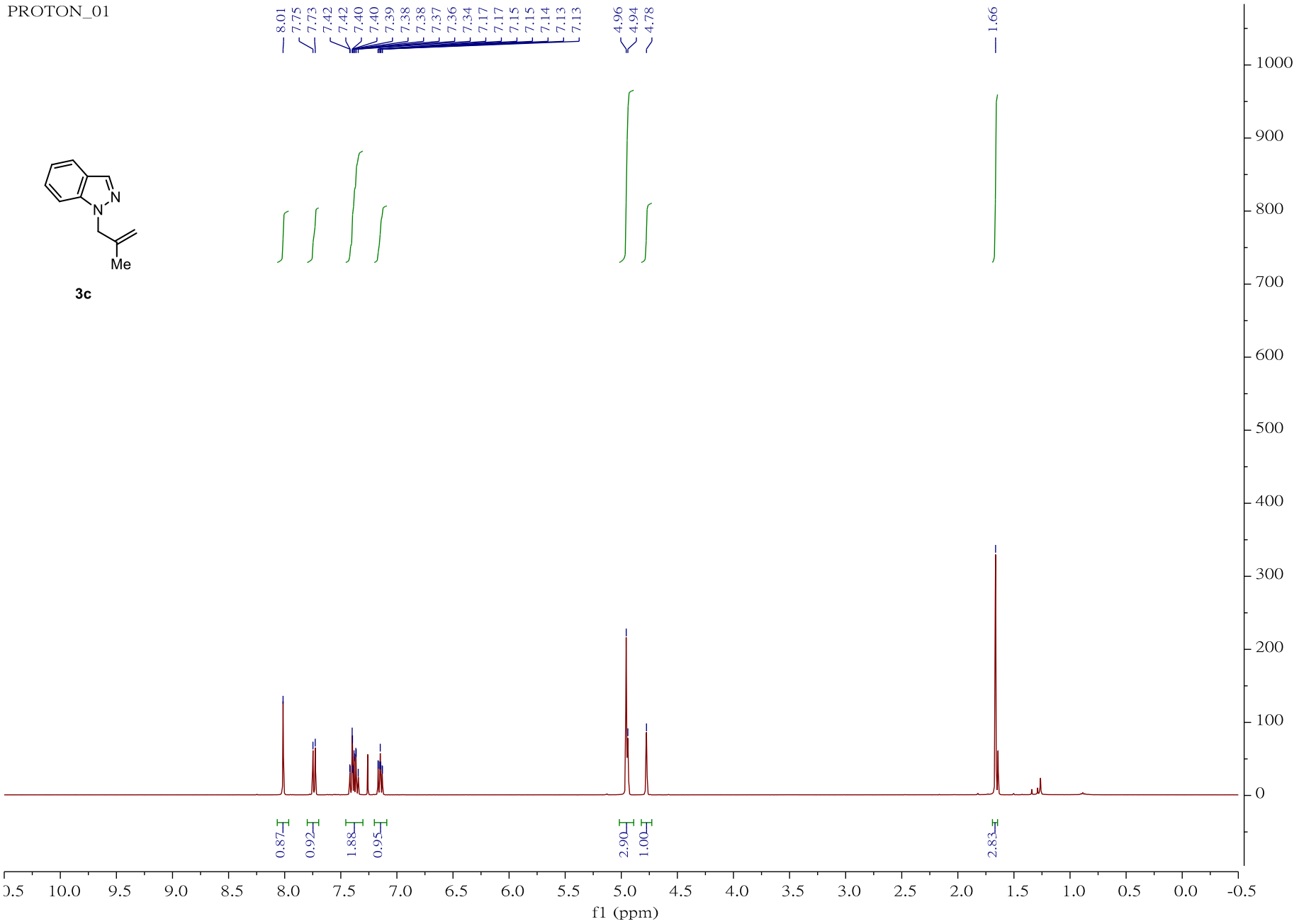

CARBON_01
135.43
132.20
128.98
126.65
126.16
121.09
120.95
119.26
109.60
100.57
77.00
51.24
29.88
24.88
19.88
N
2w
f1 (ppm)

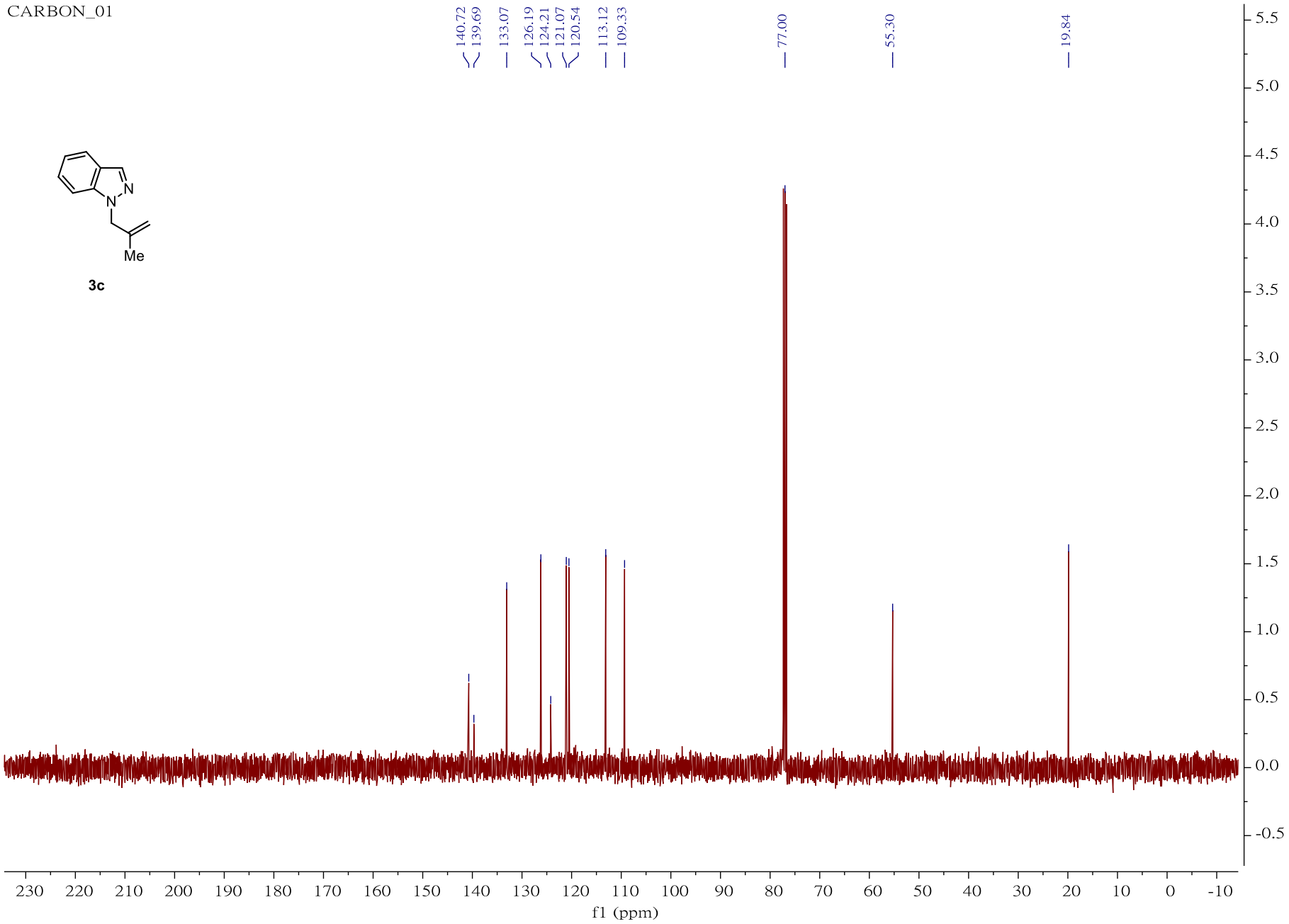

PROTON_01
9.55
9.54
6.95
6.94
6.94
6.94
6.93
6.93
6.27
6.26
6.26
6.25
4.90
4.85
4.84
4.84
4.84
4.83
4.50
4.49
4.49
4.49
4.49
4.49
1.71
1.71
1.71
1.70
CHO
N
Me
3a
0.85
1.82
0.88
2.02
1.00
1.00
3.11
f1 (ppm)

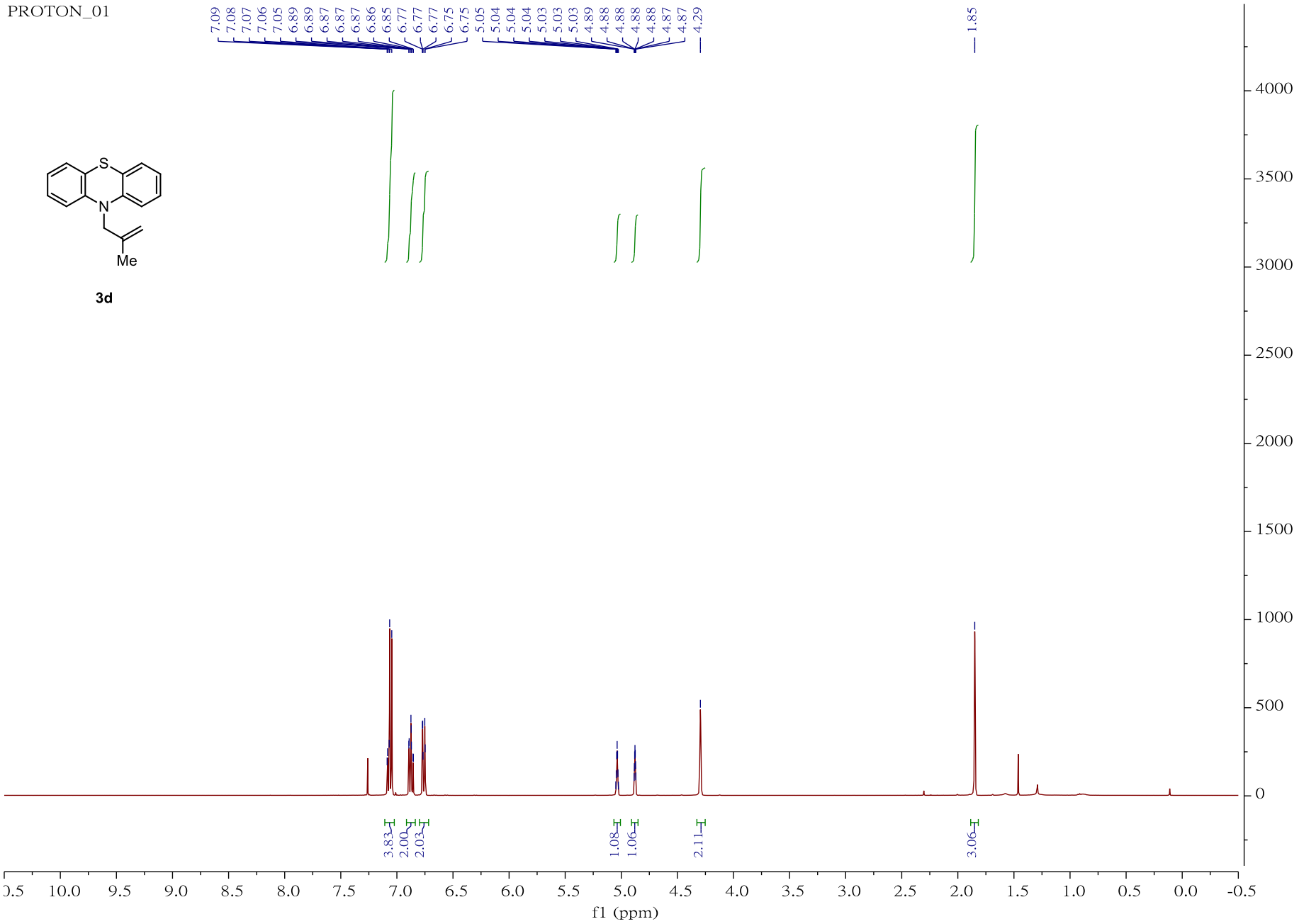

CARBON_01
179.34
142.01
131.56
131.44
124.39
111.59
109.78
77.00
53.77
19.90
CHO
N
Me
3a
f1 (ppm)

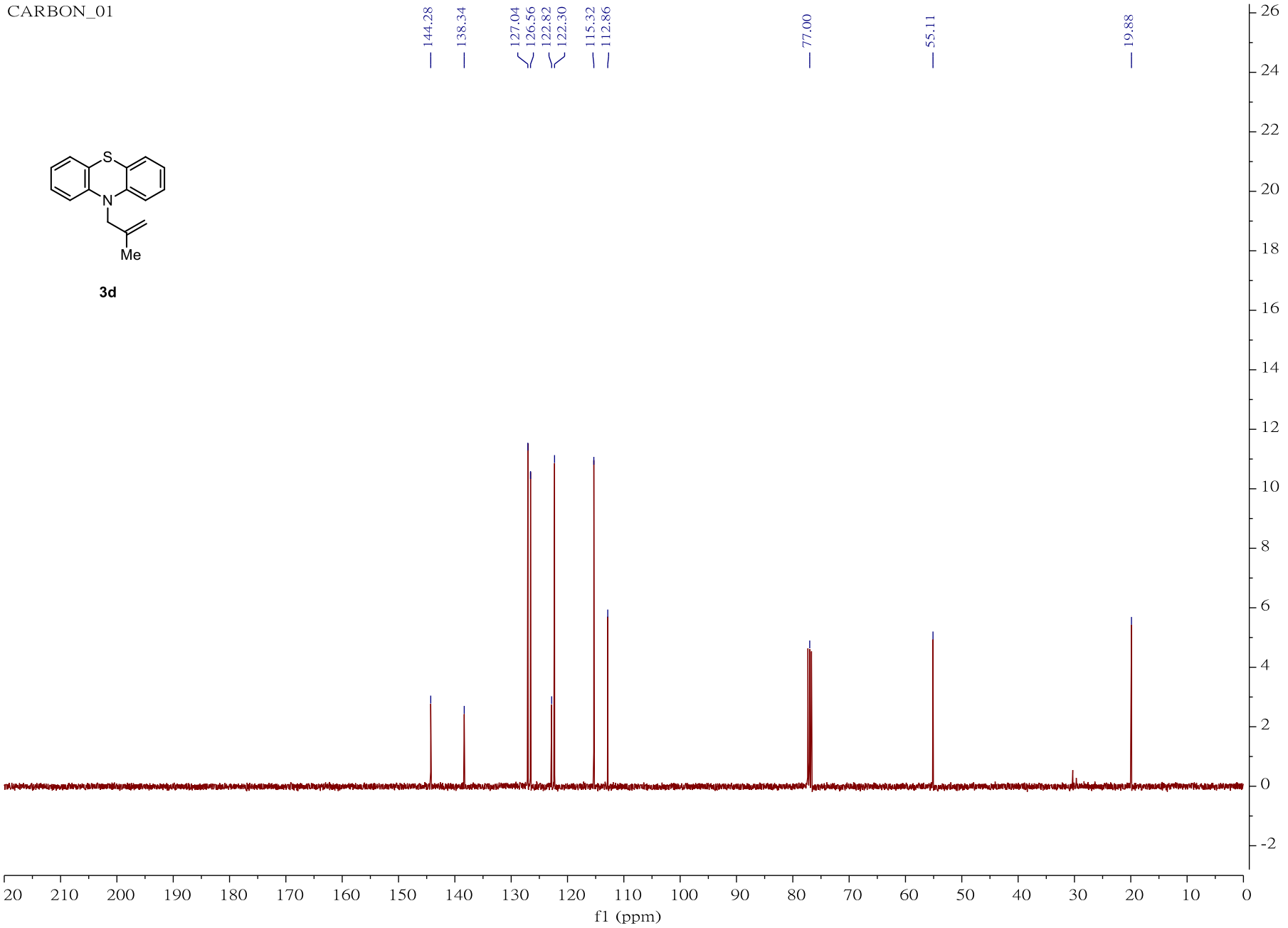

PROTON_01
8.14
8.12
7.49
7.48
7.47
7.47
7.46
7.45
7.41
7.39
7.28
7.26
7.26
7.26
7.24
7.24
4.92
4.92
4.91
4.91
4.91
4.84
4.72
4.72
4.72
1.75
N
Me
3b
1.97
2.04
2.00
2.26
1.10
2.12
1.09
3.18
f1 (ppm)

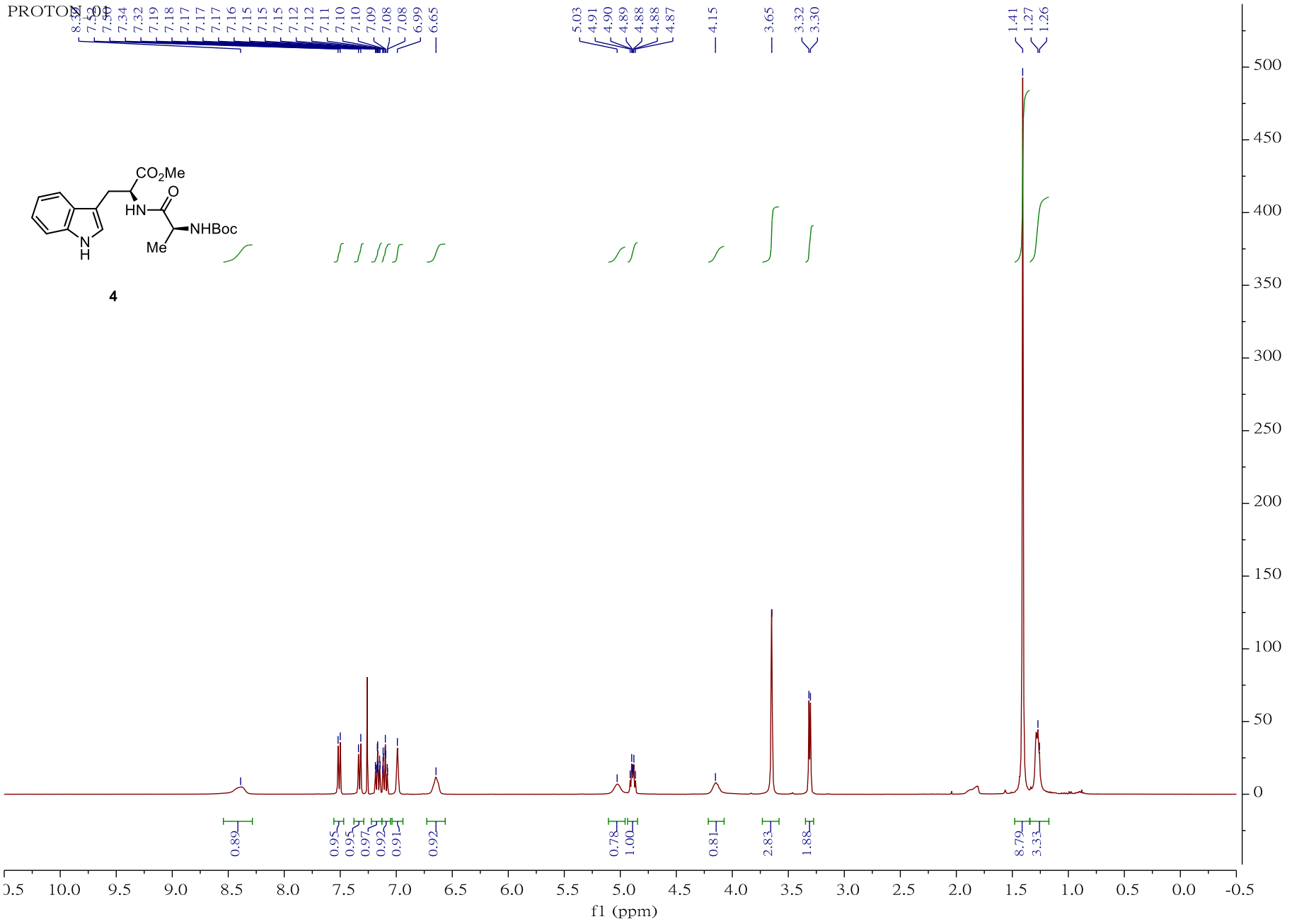

CARBON_01
140.68
140.16
125.65
122.85
120.27
118.98
112.03
108.89
77.00
48.91
20.02
Me
3b
f1 (ppm)

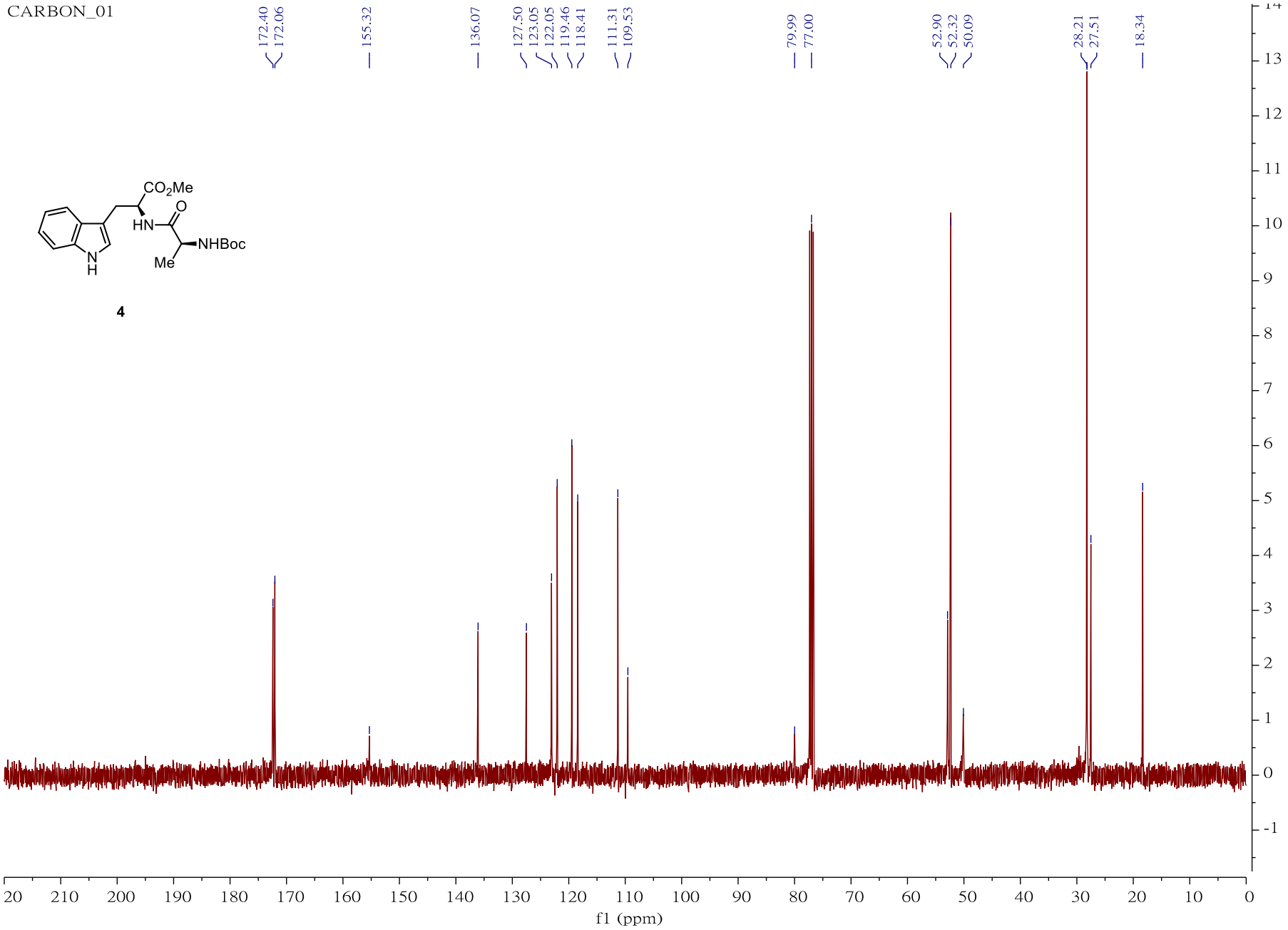

PROTON_01
8.01
7.75
7.73
7.42
7.42
7.40
7.40
7.39
7.38
7.38
7.37
7.36
7.34
7.17
7.17
7.15
7.15
7.14
7.13
7.13
4.96
4.94
4.78
1.66
N
N
Me
3c
0.87
0.92
1.88
0.95
2.90
1.00
2.83
f1 (ppm)

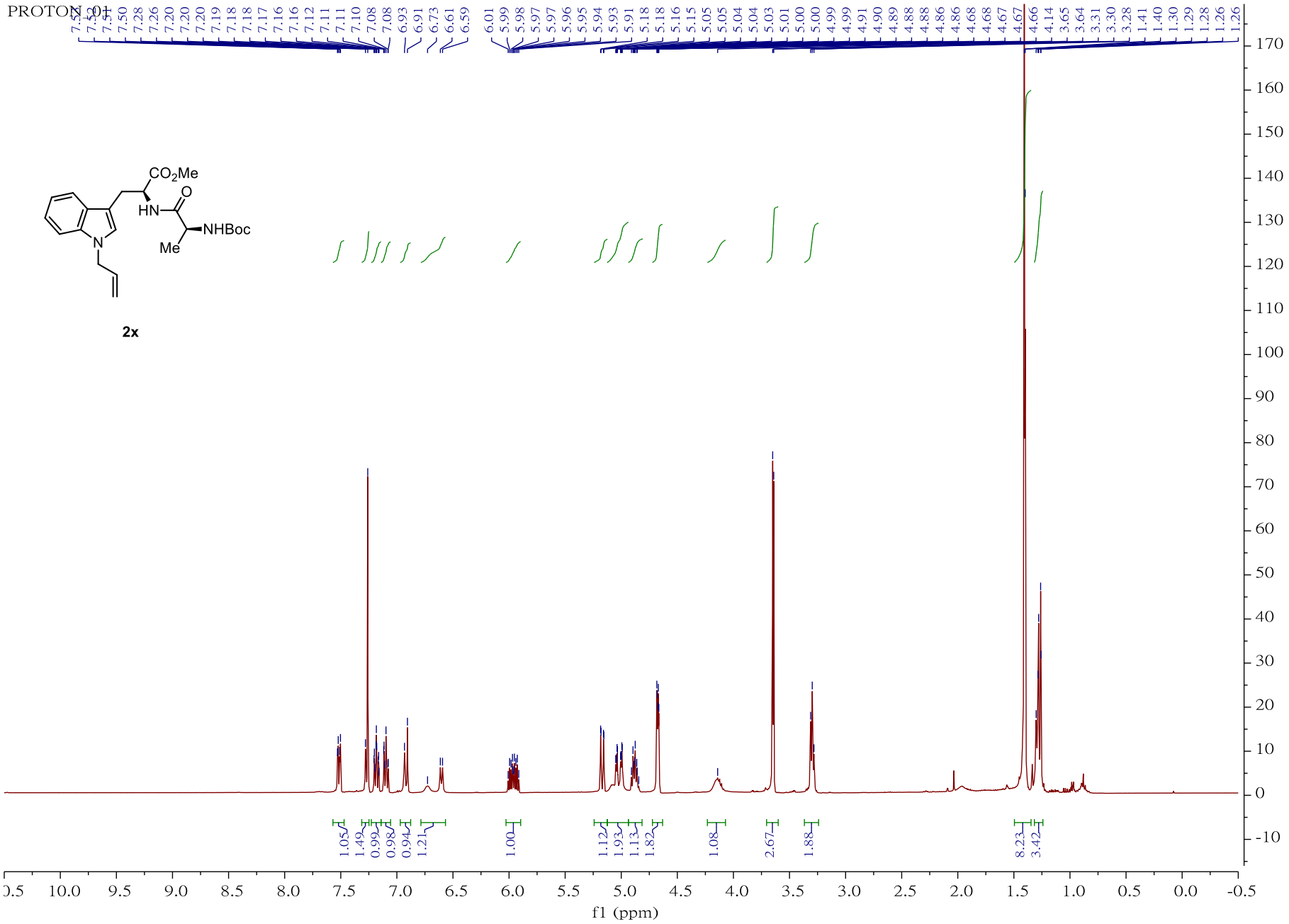

CARBON_01
140.72
139.69
133.07
126.19
124.21
121.07
120.54
113.12
109.33
77.00
55.30
19.84
N
N
Me
3c
f1 (ppm)

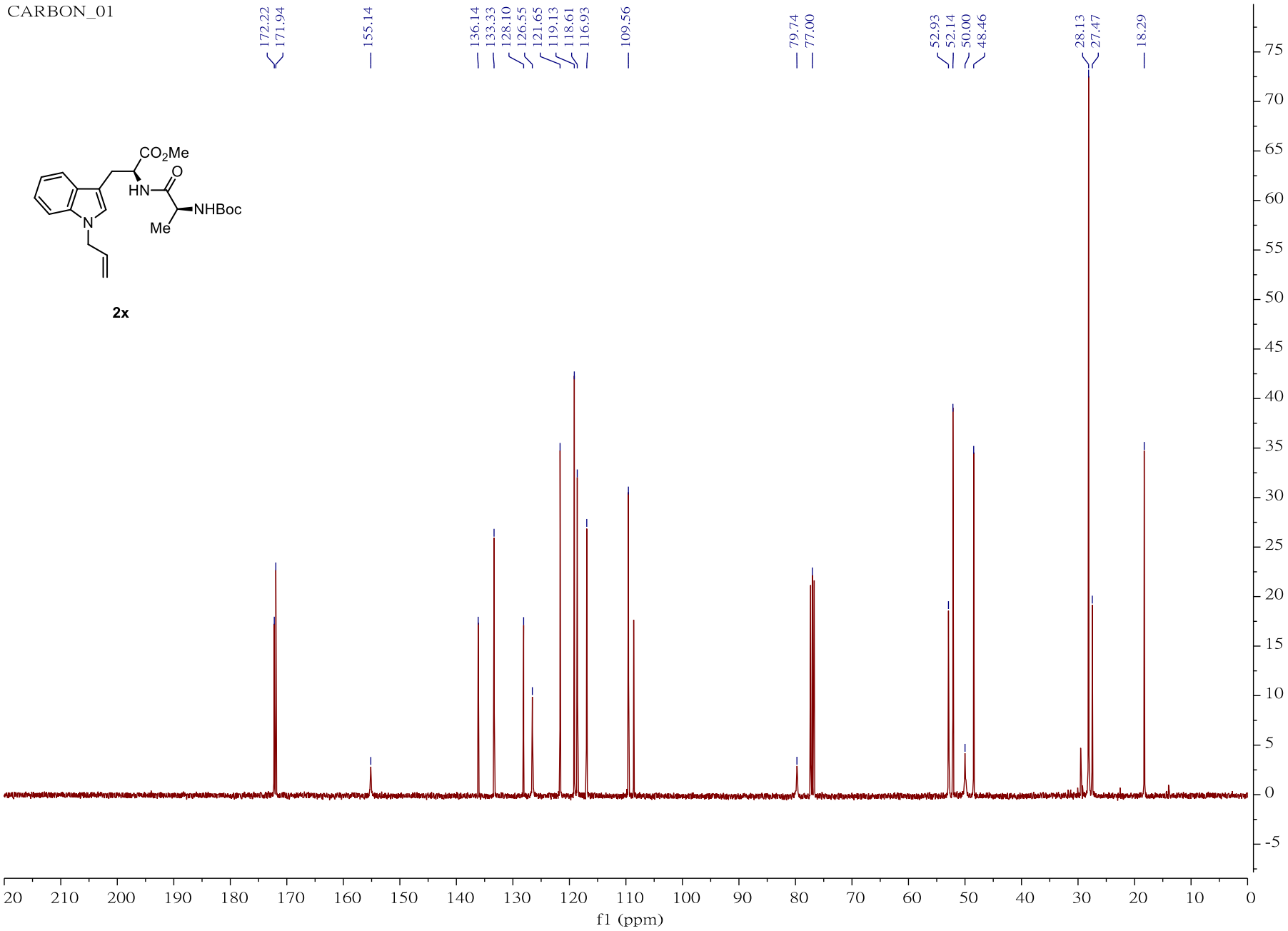

PROTON_01
7.09
7.08
7.07
7.06
7.05
6.89
6.89
6.87
6.87
6.87
6.86
6.85
6.77
6.77
6.77
6.75
6.75
5.05
5.04
5.04
5.04
5.03
5.03
5.03
4.89
4.88
4.88
4.88
4.88
4.87
4.87
4.29
1.85
S
N
Me
3d
4000
3500
3000
2500
2000
1500
1000
500
0
3.83
2.00
2.03
1.08
1.06
2.11
3.06
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

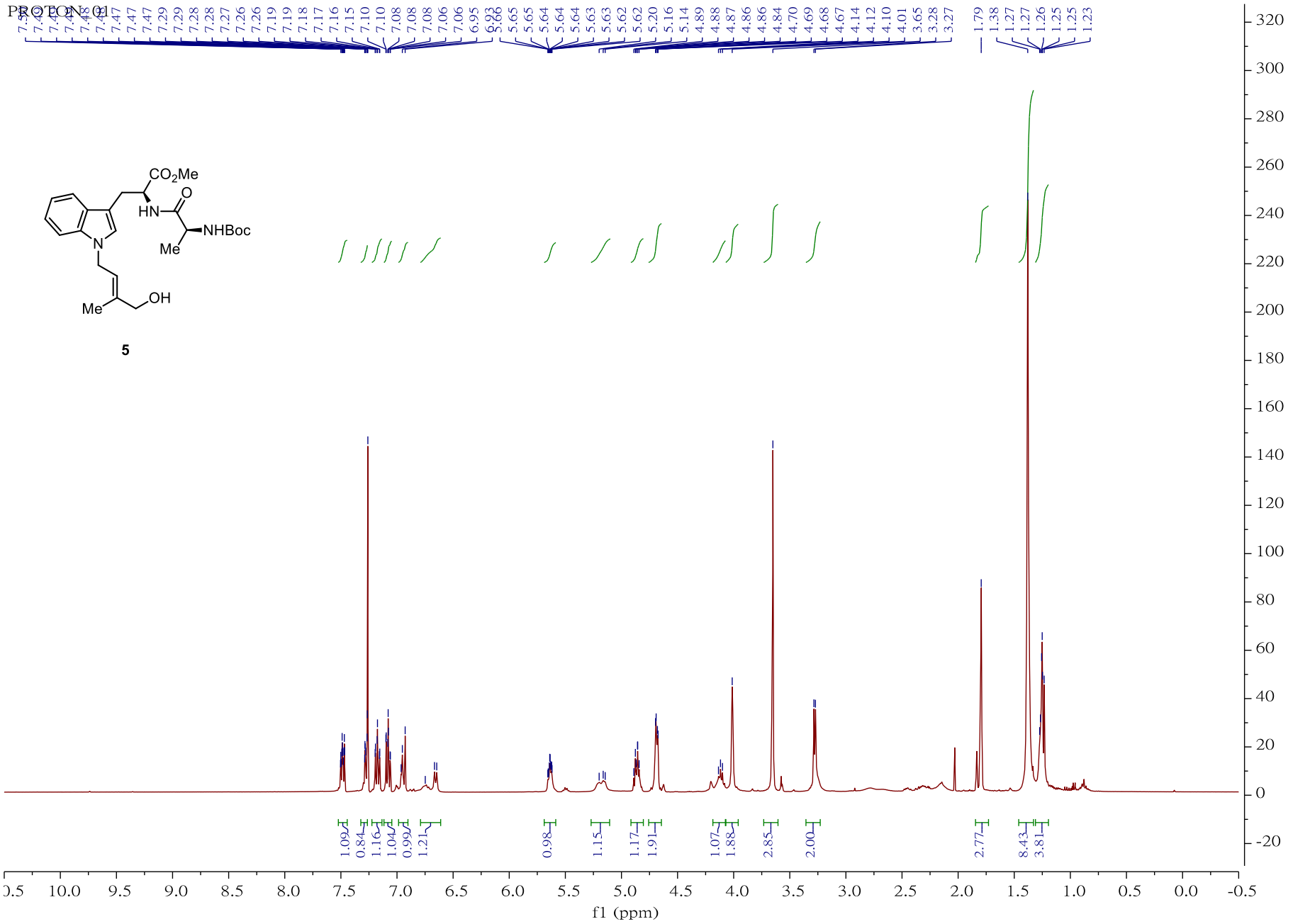

CARBON_01
144.28
138.34
127.04
126.56
122.82
122.30
115.32
112.86
77.00
55.11
19.88
S
N
Me
3d
f1 (ppm)

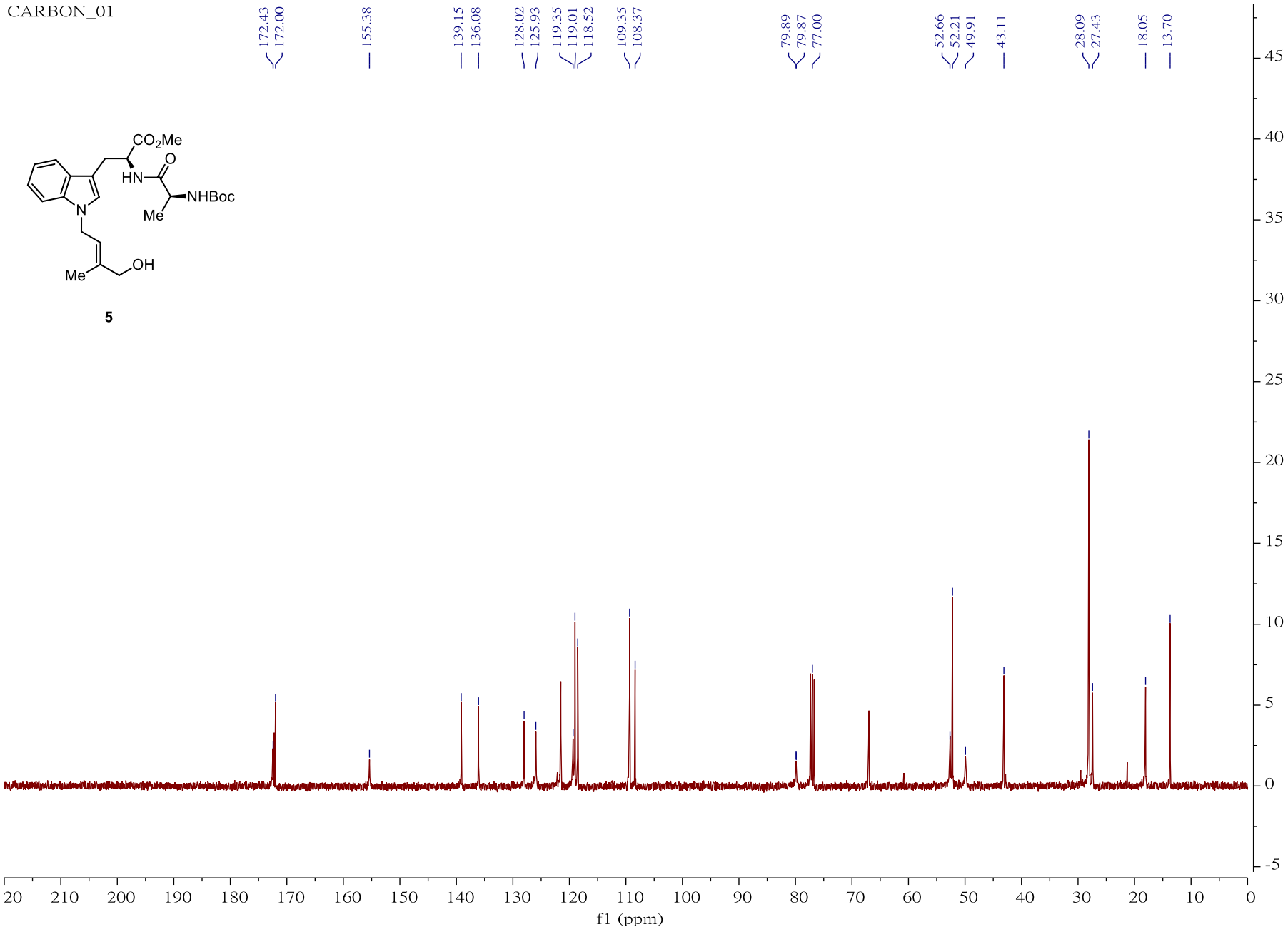

PROTON.01
8.15
7.50
7.50
7.34
7.32
7.19
7.18
7.17
7.17
7.17
7.16
7.15
7.15
7.15
7.12
7.12
7.11
7.10
7.10
7.09
7.08
7.08
6.99
6.65
5.03
4.91
4.90
4.89
4.88
4.88
4.87
4.15
3.65
3.32
3.30
1.41
1.27
1.26
CO2Me
HN
O
NHBoc
Me
N
H
4
0.89
0.95
0.95
0.97
0.92
0.91
0.92
0.78
1.00
0.81
2.83
1.88
8.79
3.33
f1 (ppm)

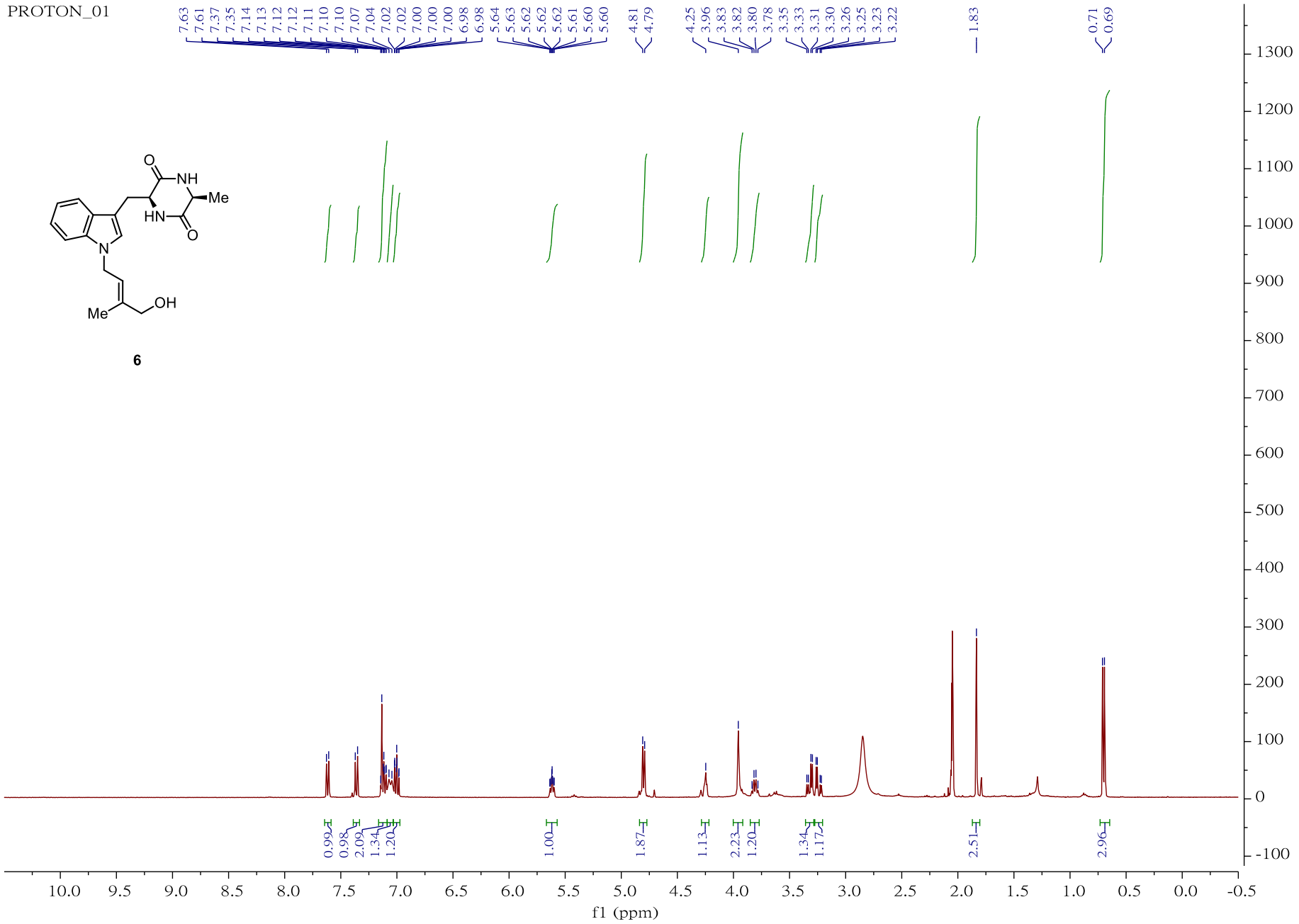

CARBON_01
172.40
172.06
155.32
136.07
127.50
123.05
122.05
119.46
118.41
111.31
109.53
79.99
77.00
52.90
52.32
50.09
28.21
27.51
18.34
CO2Me
HN
O
NHBoc
Me
N
H
4
f1 (ppm)

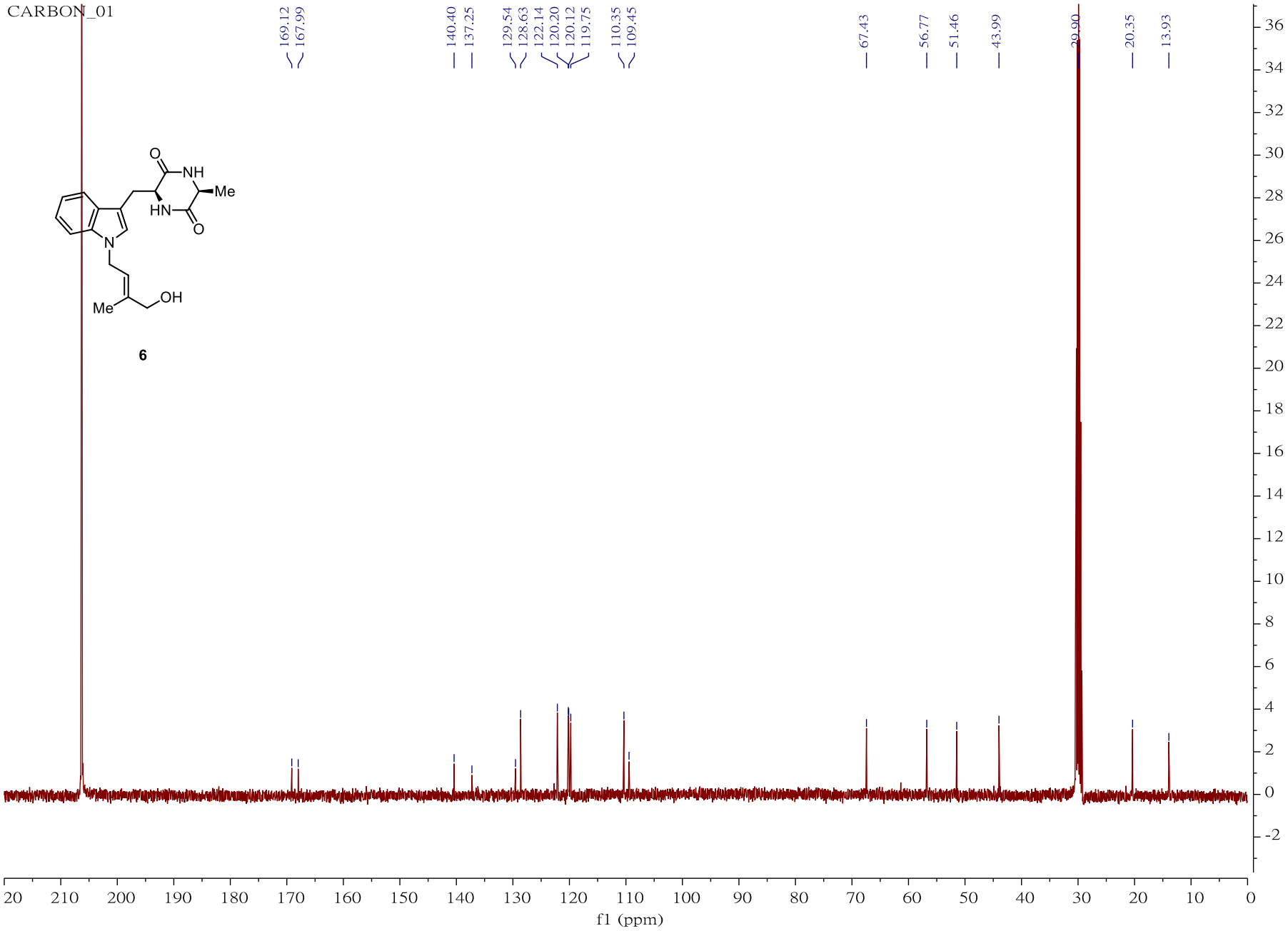

PROTON_01
CO2Me
HN
O
NHBoc
Me
N
2x
f1 (ppm)

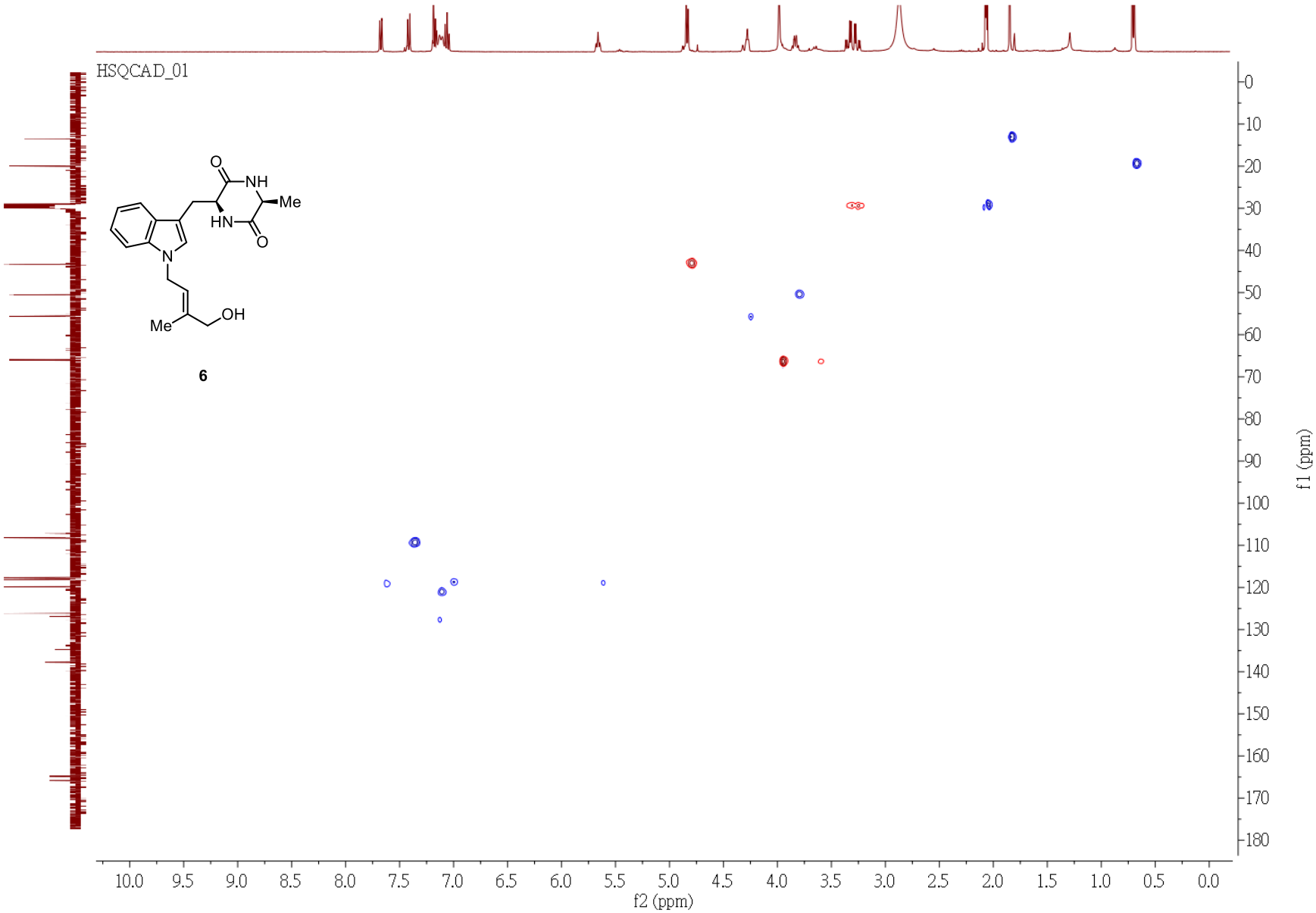

CARBON_01
172.22
171.94
155.14
136.14
133.33
128.10
126.55
121.65
119.13
118.61
116.93
109.56
79.74
77.00
52.93
52.14
50.00
48.46
28.13
27.47
18.29
CO2Me
HN
O
NHBoc
Me
N
2x
f1 (ppm)


PROTON_01
CO2Me
HN
O
NHBoc
Me
N
Me
OH
5
f1 (ppm)


CARBON_01
172.43
172.00
155.38
139.15
136.08
128.02
125.93
119.35
119.01
118.52
109.35
108.37
79.89
79.87
77.00
52.66
52.21
49.91
43.11
28.09
27.43
18.05
13.70
CO2Me
HN
O
NHBoc
Me
N
Me
OH
5
f1 (ppm)


PROTON_01
7.63 7.61 7.37 7.35 7.14 7.13 7.12 7.12 7.11 7.10 7.10 7.07 7.04 7.02 7.02 7.00 7.00 7.00 6.98 6.98 5.64 5.63 5.62 5.62 5.62 5.61 5.60 5.60 4.81 4.79 4.25 3.96 3.83 3.82 3.80 3.78 3.35 3.33 3.31 3.30 3.26 3.25 3.23 3.22 1.83 0.71 0.69
O
NH
Me
HN
O
N
Me
OH
6
0.99 0.98 2.09 1.34 1.20 1.00 1.87 1.13 2.23 1.20 1.34 1.17 2.51 2.96
f1 (ppm)


CARBON_01
169.12
167.99
140.40
137.25
129.54
128.63
122.14
120.20
120.12
119.75
110.35
109.45
67.43
56.77
51.46
43.99
29.90
20.35
13.93
O
NH
Me
HN
O
N
Me
OH
6
f1 (ppm)


HSQCAD_01
O
NH
Me
HN
O
N
OH
Me
6
f2 (ppm)
f1 (ppm)