Supporting Information

Stereoselective Allylboration of Imines and Indoles under Mild Conditions. In Situ Isomerization of Imines by Allylboroxines

Rauful Alam,[a] Arindam Das,[a] Genping Huang, [a] Lars Eriksson,[b] Fahmi Himo[a] and Kálmán J. Szabó *[a]

[a]Department of Organic Chemistry, [b]Department of Inorganic and Structural Chemistry, SE-106 91 Stockholm, Sweden.
E-mail: kalman@organ.su.se. Fax: +46-8-15 49 08

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General Information

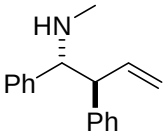
Allylboronic acids were synthesized according to previously described procedure[1]. Imine **1b**[2], **1c**[3] and **1e**[4] were prepared according to literature procedures preparation of **1i** is given in page S11. All other chemicals were obtained from commercial sources and used as received. Anhydrous DCM was purchased from commercial source and stored inside the glove box. Molecular sieves (pellets) were activated by several microwave heating/vacuum/Ar cycles. Dry $CDCl_3$, DCM, DMSO-d_6 and activated molecular sieves were stored in an argon-filled glove box. $CDCl_3$ and DMSO-d_6 were stored over molecular sieves (4Å) for several days before use. ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ (internal standard: 7.26 ppm, ^{1}H; 77.16 ppm, ^{13}C), CD_3CN (internal standard: 1.94 ppm, ^{1}H) and DMSO-d_6 (internal standard: 2.50 ppm, ^{1}H; 39.52 ppm, ^{13}C) using 400 MHz and 500 MHz spectrometers. High resolution mass data (HRMS) were obtained using ESI technique. For column chromatography, silica gel (35-70 microns) was used.

Experimental Procedures and Spectral Data

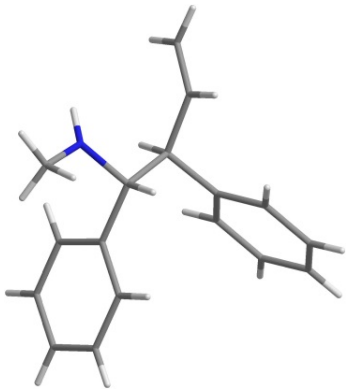
General Procedure A: Synthesis of Homoallylic Amine (Table 1). A Teflon coated screw capped glass vial (1.5 mL) was equipped with a magnetic stirrer and taken inside of an Ar-filled glove box. The vial was charged with molecular sieves (4 Å) (0.05-0.1 g) and boronic acid **2** (0.28 mmol), then CH_2Cl_2 (0.6 mL) was added and this mixture was stirred for 10-15 minutes. Then, the reaction vial was taken out from the glove box and imine **1** (0.20 mmol) was added to the boronic acid solution using a Hamilton syringe. The reaction mixture turned to pale yellow immediately but the yellow color disappeared within a few minutes. The mixture was stirred at room temperature for the reaction times given in Table 1. To establish the reaction time necessary for the completion (Table 1), the reactions were monitored by ^{1}H NMR. An aliquot from the reaction mixture was dissolved in dry $CDCl_3$ and analysed by ^{1}H NMR. When the imine was fully consumed, MeOH (0.1 mL) was added and the reaction mixture was stirred for a further 10-15 minutes. Then, the solvents were evaporated and the residue was purified by silica gel chromatography.

General Procedure B: Synthesis of 2-substituted Indoline (Table 2). Indole **4** (0.1 mmol) was placed in a screw capped glass vial (1.5 mL) under ambient conditions. Then the vial was taken inside an Ar-filled glove box. Allylboronic acid **2** (0.15 mmol) and CH_2Cl_2 (0.4 mL) were added sequentially, then the vial was sealed and it was taken outside of the glove box.

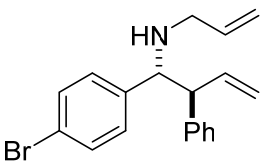
The reaction mixtures were stirred at the temperatures and reaction times given in Table 2. To establish the reaction time necessary for the completion (Table 2), the reactions were monitored by ^{1}H NMR. An aliquot from reaction mixture was dissolved in dry $CDCl_3$ analyzed by ^{1}H NMR. When the indole was consumed completely, MeOH (0.1 mL) was added to the reaction mixture and the mixture was stirred for further 10-15 minutes. Solvent was removed *in vacuo* to afford the crude product that was subsequently purified by flash column chromatography on silica gel.



***N*-methyl-1,2-diphenylbut-3-en-1-amine (3a).** The compound was prepared according to above general procedure A. Product **3a** was isolated in 73% yield (35.0 mg) as light yellow solid using pentane:Et_2O:Et_2NH (100:10:1) as eluent for silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17-7.04 (m, 8H), 6.98-6.95 (m, 2H), 6.17 (ddd, J = 18.3, 8.7, 8.3 Hz, 1H), 5.26-5.19 (m, 2H), 3.70 (d, J = 9.0 Hz, 1H), 3.46 (t, J = 9.2 Hz, 1H), 2.24 (s, 3H), 1.70 (bs, 1H, NH); ^{13}C NMR (101 MHz, $CDCl_3$): δ 141.7, 141.5, 139.4, 128.3(2), 128.3, 128.2(5), 127.9, 126.9, 126.3, 117.5, 69.7, 58.7, 34.8; HRMS (pos. ESI) m/z: Calcd for $C_{17}H_{20}N$ $[M+H]^+$ 238.1590. Found 238.1594.

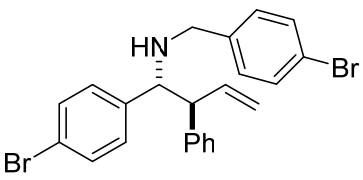


Chem3D diagram of compound **3a** from the X-ray diffraction data (cif file name: Compound_3a.cif)

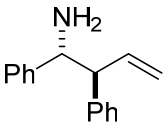


***N*-allyl-1-(4-bromophenyl)-2-phenylbut-3-en-1-amine (3b).** The compound was prepared according to above general procedure A. Product **3b** was isolated in 84% yield (58.0 mg) as colorless oil in a diastereomeric ratio of 98:2 using pentane:Et_2O:Et_2NH (100:10:1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.26-7.24 (m, 2H), 7.16-7.12 (m, 2H), 7.10-7.07 (m, 1H), 6.97-6.93 (m, 4H), 6.17-6.10 (m, 1H), 5.85-5.77 (m, 1H), 5.25 (ddd, J = 17.0,

1.6, 0.7 Hz, 1H), 5.21 (dd, *J* = 10.1, 1.6 Hz, 1H), 5.09-5.06 (m, 1H), 5.05 (t, *J* = 1.4 Hz, 1H), 3.83 (d, *J* = 9.1 Hz, 1H), 3.38 (t, *J* = 9.3 Hz, 1H), 3.07 (ddt, *J* = 14.3, 5.0, 1.6 Hz, 1H), 2.92 (ddt, *J* = 14.3, 7.0, 1.2 Hz, 1H), 1.75 (bs, 1H, NH); ^{13}C NMR (125 MHz, $CDCl_3$): δ 141.3, 140.8, 139.0, 136.8, 131.0, 130.0, 128.4, 128.2, 126.5, 120.6, 117.9, 116.0, 66.0, 58.7, 50.0; HRMS (pos. ESI) m/z: Calcd for $C_{19}H_{21}BrN$ $[M+H]^+$ 342.0852. Found 342.0837.

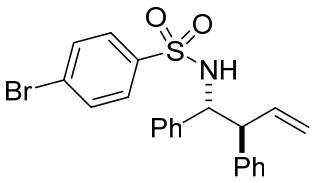


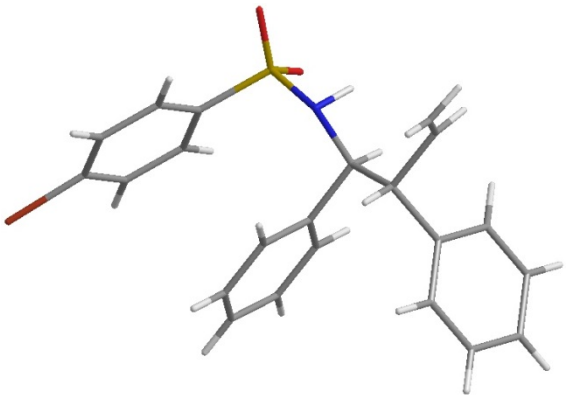
***N*-(4-bromobenzyl)-1-(4-bromophenyl)-2-phenylbut-3-en-1-amine (3c).** The compound was prepared according to above general procedure A. Product **3c** was isolated in 72% yield (68.0 mg) as colorless oil in a diastereomeric ratio of 91:9 using pentane:Et_2O:Et_2NH (100:10:1) as eluent for silica gel chromatography. ^{1}H NMR for major isomer (500 MHz, $CDCl_3$): δ 7.43-7.41 (m, 2H), 7.29-7.26 (m, 2H), 7.15-7.06 (m, 5H), 6.99-6.97 (m, 2H), 6.92-6.90 (m, 2H), 6.13-6.06 (m, 1H), 5.23-5.18 (m, 2H), 3.75 (d, *J* = 9.0 Hz, 1H), 3.58 (d, *J* = 13.7 Hz, 1H), 3.40 (d, *J* = 13.7 Hz, 2H), 2.10 (bs, 1H, NH); ^{13}C NMR for major isomer (125 MHz, $CDCl_3$): δ 141.1, 140.6, 139.4, 138.8, 131.6, 131.1, 130.0, 129.9, 128.4, 128.2, 126.6, 120.8, 118.1, 65.8, 58.6, 50.7; HRMS (pos. ESI) m/z: Calcd for $C_{23}H_{22}Br_2N$ $[M+H]^+$ 470.0114. Found 470.0121.



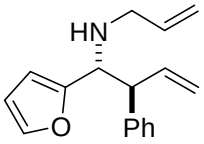
1,2-diphenylbut-3-en-1-amine (3d). The compound was prepared according to above general procedure A. Product **3d** was isolated in 78% yield (35.0 mg) as colorless oil using pentane:Et_2O:Et_3N (100:30:1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.19-7.07 (m, 8H), 7.02-7.00 (m, 2H), 6.19 (ddd, *J* = 18.2, 8.9, 8.1 Hz, 1H), 5.25-5.19 (m, 2H), 4.18 (d, *J* = 8.5 Hz, 1H), 3.46 (t, *J* = 8.8 Hz, 1H), 1.68 (bs, 2H, NH_2); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.8, 141.9, 139.0, 128.3, 128.2(7), 128.0, 127.4, 127.0, 126.4, 117.5, 60.5, 59.5; HRMS (pos. ESI) m/z: Calcd for $C_{16}H_{17}NNa$ $[M+Na]^+$ 246.1253. Found 246.1256.

Compound **3d** was not suitable for X-ray diffraction, so the sulfonamide derivative of **3d** was prepared.[5]

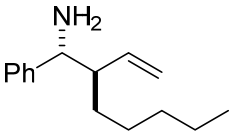




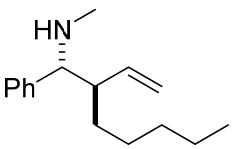
Chem3D diagram of compound **3d** sulfonamide derivative from the X-ray diffraction data (cif file name: Compound_3d_sulfonamide derivative.cif)



***N*-allyl-1-(furan-2-yl)-2-phenylbut-3-en-1-amine (3e).** The compound was prepared according to above general procedure A. Product **3e** was isolated in 92% yield (47.0 mg) as yellow liquid using pentane:Et_2O:Et_2NH (100:10:1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, CD_3CN): δ 7.28 (dd, J = 1.8, 0.8 Hz, 1H), 7.20-7.16 (m, 2H), 7.12-7.09 (m, 3H), 6.20-6.13 (m, 2H), 5.97 (dd, J = 3.2, 0.8 Hz, 1H), 5.90-5.78 (m, 1H), 5.16-5.07 (m, 3H), 5.04-5.00 (m, 1H), 3.99 (d, J = 9.6 Hz, 1H), 3.68 (t, J = 9.3 Hz, 1H), 3.09 (ddt, J = 14.3, 5.3, 1.6 Hz, 1H), 2.99 (ddt, J = 14.3, 6.5, 1.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.1, 141.6, 141.5, 139.1, 136.7, 128.3, 128.0, 126.5, 117.6, 116.2, 109.7, 108.4, 60.0, 55.7, 50.1; HRMS (pos. ESI) m/z: Calcd for $C_{17}H_{19}NONa$ $[M+Na]^+$ 276.1359. Found 276.1352.

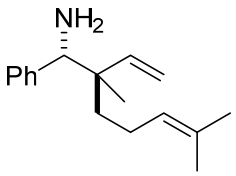


1-phenyl-2-vinylheptan-1-amine (3f). The compound was prepared according to general procedure A. Product **3f** was isolated in 80% yield (35.0 mg) as colorless oil in a diastereomeric ratio of 94:6 using pentane:Et_2O:Et_2NH (100:20:1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34-7.29 (m, 4H), 7.25-7.23 (m, 1H), 5.59 (ddd, J = 18.3, 9.0, 8.1 Hz, 1H), 5.18 (dd, J = 10.3, 2.0 Hz, 1H), 5.16-5.12 (m, 1H), 3.67 (d, J = 8.4 Hz, 1H), 2.22-2.16 (m, 1H), 1.28-1.06 (m, 8H), (t, J = 9.3 Hz, 1H), 0.81 (t, J = 7.1 Hz, 3H) ; ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.9, 140.5, 128.4, 127.5, 127.2, 117.7, 59.6, 52.6, 31.8, 31.3, 27.0, 22.7, 14.2; HRMS (pos. ESI) m/z: Calcd for $C_{15}H_{23}NNa$ $[M+Na]^+$ 240.1723. Found 240.1726.

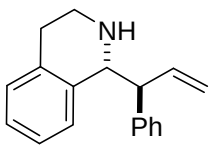


***N*-methyl-1-phenyl-2-vinylheptan-1-amine (3g).** The compound was prepared according to above general procedure A. Product **3g** was isolated in 74% yield (34.0 mg) as colorless oil using pentane:Et_2O:Et_2NH (100:20:1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34-7.31 (m, 2H), 7.29-7.24 (m, 3H), 5.57 (ddd, J = 18.4, 8.5, 8.5 Hz, 1H), 5.21-

5.15 (m, 2H), 3.19 (d, J = 9.0 Hz, 1H), 2.25-2.19 (m, 1H), 2.17 (s, 3H), 1.25-1.00 (m, 8H), 0.79 (t, J = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.5, 140.9, 128.5, 128.3, 127.2, 117.9, 69.2, 51.7, 34.7, 31.8, 31.2, 26.9, 22.6, 14.1; HRMS (pos. ESI) m/z: Calcd for $C_{16}H_{26}N$ $[M+H]^+$ 232.2060. Found 232.2061.

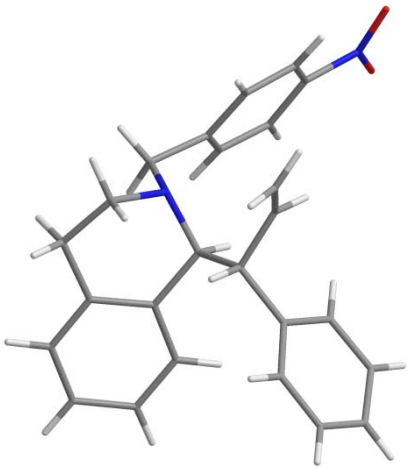


2,6-dimethyl-1-phenyl-2-vinylhept-5-en-1-amine (3h). Geranyl boronic acid was prepared according to previously described procedure[1] using $CDCl_3$ instead of $CHCl_3$ as a solvent. To a screw capped vial (1.5 mL) was added MS (4 Å) and activated by heating/vacuum/Ar cycles. Then, geranylboronic acid (**2c)** solution (0.9 mL, 0.3 M solution in $CDCl_3$) was added to the vial under Ar and stirred. Imine (0.2 mmol) was added to the boronic acid solution after 10 minutes by Hamilton syringe and allowed to stir at room temperature. The progess of the reaction was monitored by ^{1}H NMR. When the imine was fully consumed, the reaction mixture was quenched with MeOH (0.1 mL) and the solvent was evaporated *in vacuo* to afford crude product. Product **3h** was isolated in 66% yield (32.0 mg) as colorless oil in a diastereomeric ratio of 96:4 using pentane:Et_2O:Et_3N (100:10:1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.32-7.27 (m, 4H), 7.25-7.22 (m, 1H), 5.79 (dd, J = 17.6, 10.9 Hz, 1H), 5.22 (dd, J = 10.8, 1.4 Hz, 1H), 5.06-5.02 (m, 2H), 3.76 (s, 1H), 1.90-1.78 (m, 2H), 1.65 (s, 3H), 1.55 (s, 3H), 1.48 (bs, 2H, NH_2), 1.39-1.33 (m, 1H), 1.28-1.20 (m, 1H), 0.93 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.7, 142.7, 131.2, 128.9, 127.7, 127.1, 125.0, 114.9, 63.7, 45.1, 38.6, 25.8, 23.0, 17.8, 16.7; HRMS (pos. ESI) m/z: Calcd for $C_{17}H_{26}N$ $[M+H]^+$ 244.2060. Found 244.2069.

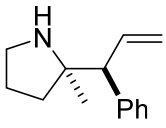


1-(-1-phenylallyl)-1,2,3,4-tetrahydroisoquinoline (3i). The compound was prepared according to above general procedure A. Product **3i** was isolated in 93% yield (46.0 mg) as colorless oil as a single diastereomer using pentane:EtOAc:Et_3N (100:10:0.5) as eluent for silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.24 (m, 5H), 7.14-7.11 (m, 2H), 7.04-7.01 (m, 1H), 6.85 (d, J = 7.7 Hz, 1H), 6.25-6.15 (m, 1H), 5.15 (d, J = 10.3 Hz, 1H), 5.07 (d, J = 17.3 Hz, 1H), 4.31 (d, J = 5.2 Hz, 1H), 4.00 (dd, J = 6.8, 6.8 Hz, 1H), 3.28-3.22 (m, 1H), 2.96-2.87 (m, 2H), 2.81-2.72 (m, 1H), 2.01(br, 1H, NH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.6, 137.6, 137.0, 136.0, 129.2, 128.8, 128.6, 127.1, 126.7, 126.1, 125.3, 117.8, 60.6, 54.8, 41.2, 30.0; HRMS (pos. ESI) m/z: Calcd for $C_{18}H_{20}N$ $[M+H]^+$ 250.1590. Found 250.1600.

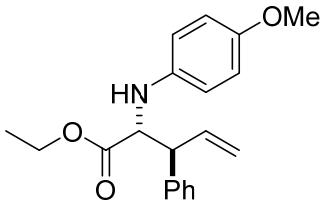
Compound **3i** was not suitable for X-ray diffraction, so the N-*para*-nitrobenzyl derivative of **3i** was prepared.



Chem3D diagram of compound **3i**_*p*-nitrobenzyl derivative from the X-ray diffraction data (cif file name: Compound_3i_ *p*-nitrobenzyl derivative.cif)

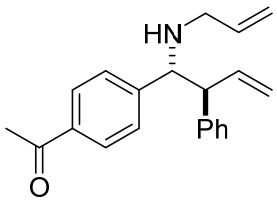


2,6-dimethyl-1-phenyl-2-vinylhept-5-en-1-amine (3j). The compound was prepared according to above general procedure A. Product **3j** was isolated in 65% yield (26.0 mg) as light yellow oil using DCM:Et_2O:Et_3N (90:30:1) as eluent for silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.28 (m, 4H), 7.24-7.18 (m, 1H), 6.33 (ddd, J = 18.3, 8.9, 8.1 Hz, 1H), 5.16-5.07 (m, 2H), 3.29 (d, J = 9.4 Hz, 1H), 3.02-2.96 (m, 1H), 2.95-2.89 (m, 1H), 1.86-1.70 (m, 3H), 1.40-1.34 (m, 1H), 1.07 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.4, 138.9, 129.2, 128.2, 126.4, 117.0, 64.2, 59.7, 45.9, 36.3, 25.4, 25.3; HRMS (pos. ESI) m/z: Calcd for $C_{14}H_{20}N$ $[M+H]^+$ 202.1590. Found 202.1586.

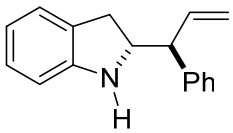


Ethyl-2-((4-methoxyphenyl)amino)-3-phenylpent-4-enoate (3k). The compound was prepared according to above general procedure A. Product **3k** was isolated in 72% yield (47.0 mg) as colorless oil as a single diastereomer using pentane:EtOAc:Et_3N (100:10:0.2) as eluent for silica gel chromatography. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.35-7.24 (m, 5H), 6.74 (d, J = 8.9 Hz, 2H), 6.56 (d, J = 8.9 Hz, 2H), 6.22 (ddd, J = 17.0, 10.2, 8.7 Hz, 1H), 5.24-5.18 (m, 2H), 4.20 (t, J = 8.1 Hz, 1H), 4.00 (d, J = 7.8 Hz, 1H), 3.93 (dq, J = 7.1, 1.9 Hz, 2H), 3.75-3.70 (m, 1H), 3.71 (s, 3H), 1.01 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 173.3, 153.4, 141.6, 140.6, 138.0, 129.0, 128.9, 127.7, 118.1, 115.3, 63.4,

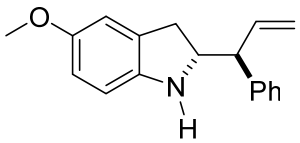
61.4, 56.1, 53.8, 14.3; HRMS (pos. ESI) m/z: Calcd for $C_{20}H_{23}NNaO_3$ $[M+Na]^+$ 348.1570. Found 348.1582.



1-(4-(-1-(allylamino)-2-phenylbut-3-en-1-yl)phenyl)ethan-1-one (3l). The compound was prepared according to above general procedure A. Product **3l** was isolated in 71% yield (44.0 mg) as colorless oil in a diastereomeric ratio of 91:9 using pentane:EtOAc:Et_3N (100:10:0.2) as eluent for silica gel chromatography. ^{1}H NMR for major isomer (400 MHz, $CDCl_3$): δ 7.73 (d, J = 8.3 Hz, 2H), 7.19 (d, J = 8.3 Hz, 2H), 7.14-7.05 (m, 3H), 6.96-6.94 (m, 2H), 6.16 (dt, J = 16.9, 9.8 Hz, 1H), 5.87-5.77 (m, 1H), 5.29-5.21 (m, 2H), 5.10-5.07 (m, 1H), 5.05 (t, J = 1.3 Hz, 1H), 3.94 (d, J = 9.1 Hz, 1H), 3.44 (t, J = 9.3 Hz, 1H), 3.07 (ddt, J = 14.4, 5.1, 1.6 Hz, 1H), 2.94 (ddt, J = 14.2, 6.9, 1.1 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR for major isomer (100 MHz, $CDCl_3$): δ 198.0, 147.7, 141.1, 138.9, 136.7, 136.0, 128.5, 128.4, 128.2, 128.0, 126.6, 118.0, 116.1, 66.3, 58.5, 50.1, 26.6; HRMS (pos. ESI) m/z: Calcd for $C_{21}H_{24}NO$ $[M+H]^+$ 306.1852. Found 306.1860.

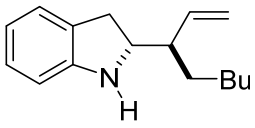


2-(1-phenylallyl) indoline (3m). The compound was prepared according to above general procedure B. Product **3m** was isolated in 90% yield (21.0 mg) as light yellow oil using Pentane:Et_2O (80:10) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.36-7.33 (m, 2H), 7.27-7.23 (m, 1H), 7.22-7.20 (m, 2H), 7.03-7.00 (m, 2H), 6.69-6.66 (m, 1H), 6.62 (d, J = 7.7 Hz, 1H), 6.10-6.03 (m, 1H), 5.21-5.17 (m, 2H), 4.17 (s, 1H), 4.09 (td, J = 9.0, 6.7 Hz, 1H), 3.34 (t, J = 9.1 Hz, 1H), 2.87 (dd, J = 15.9, 8.7 Hz, 1H), 2.69 (dd, J = 15.9, 6.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 150.5, 141.8, 139.6, 128.9, 128.3, 128.1, 127.5, 126.9, 124.9, 118.6, 117.1, 109.1, 62.8, 56.2, 34.3. HRMS (pos. ESI) m/z: Calcd for $C_{17}H_{18}N$ $[M+H]^+$ 236.1434. Found 236.1435.

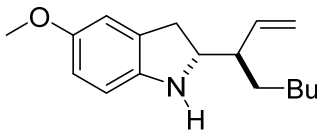


5-methoxy-2-(1-phenylallyl) indoline (3n). The compound was prepared according to above general procedure B. Product **3n** was isolated in 96% yield (26.0 mg) as light yellow oil using pentane:Et_2O:Et_3N (100:10:1) as eluent for silica gel chromatography. This reaction was scaled up to 0.5 mmol and isolated in 97% yield ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.36-7.32 (m, 2H), 7.26-7.20 (m, 3H), 6.65-6.54 (m, 3H), 6.10-6.03 (m, 1H), 5.20-5.16 (m, 2H), 4.09-4.04 (m, 1H), 3.96 (bs, 1H, NH), 3.72 (s, 3H), 3.33 (t, J = 9.1 Hz, 1H), 2.84 (dd, J = 16.0, 8.5 Hz,

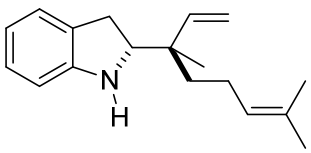
1H), 2.66 (dd, J = 16.0, 6.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.5, 144.4, 141.8, 139.7, 130.0, 128.9, 128.1, 126.8, 117.0, 112.2, 111.9, 109.7, 63.4, 56.1(3), 56.0(8), 34.8; HRMS (pos. ESI) m/z: Calcd for $C_{18}H_{20}NO$ $[M+H]^+$ 266.1539. Found 266.1553.



2-(oct-1-en-3-yl) indoline (3o). The compound was prepared according to above general procedure B. Product **3o** was isolated in 95% yield (22.0 mg) as colorless oil using pentane:Et_2O:Et_2NH (100:5:1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.06-7.04 (m, 1H), 7.00-6.97 (m, 1H), 6.66 (dt, J = 7.4, 1.0 Hz, 1H), 6.58-6.56 (m, 1H), 5.59 (ddd, J = 18.4, 9.0, 8.1 Hz, 1H), 5.15 (dd, J = 10.3, 2.1 Hz, 1H), 5.10 (ddd, J = 17.1, 2.1, 0.7 Hz, 1H), 3.66 (q, J = 8.4 Hz, 1H), 3.08 (dd, J = 15.5, 8.7 Hz, 1H), 2.81 (dd, J = 15.5, 8.4 Hz, 1H), 2.14-2.08 (m, 1H), 1.52-1.47 (m, 1H), 1.39-1.20 (m, 7H), 0.89 (t, J = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 150.9, 140.4, 128.8, 127.4, 124.8, 118.4, 117.5, 109.0, 63.1, 50.3, 34.3, 32.0, 31.4, 27.0, 22.7, 14.2; HRMS (pos. ESI) m/z: Calcd for $C_{16}H_{24}N$ $[M+H]^+$ 230.1903. Found 230.1894.

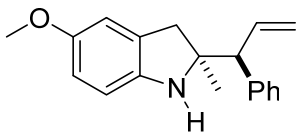


5-methoxy-2-(oct-1-en-3-yl) indoline (3p). The compound was prepared according to above general procedure B. Product **3p** was isolated in 85% yield (22.0 mg) as colorless oil using pentane:Et_2O:Et_2NH (100:10:1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.70 (m, 1H), 6.58-6.51 (m, 2H), 5.59 (ddd, J = 18.4, 8.9, 8.2 Hz, 1H), 5.14 (dd, J = 10.3, 2.1 Hz, 1H), 5.09 (ddd, J = 17.1, 2.1, 0.5 Hz, 1H), 3.73 (s, 3H), 3.65 (q, J = 8.4 Hz, 1H), 3.05 (dd, J = 15.6, 8.5 Hz, 1H), 2.79 (dd, J = 15.7, 8.5 Hz, 1H), 2.14-2.08 (m, 1H), 1.52-1.46 (m, 1H), 1.39-1.21 (m, 7H), 0.88 (t, J = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.4, 144.7, 140.4, 130.6, 117.4, 112.2, 111.8, 109.6, 63.7, 59.1, 50.2, 34.8, 32.0, 31.5, 27.0, 22.7, 14.2; HRMS (pos. ESI) m/z: Calcd for $C_{17}H_{26}NO$ $[M+H]^+$ 260.2009. Found 260.2009.



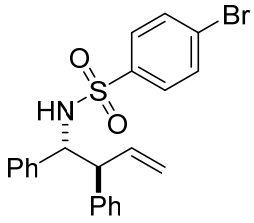
2-(3,7-dimethylocta-1,6-dien-3-yl) indoline (3q). The compound was prepared according to above general procedure B. Product **3q** was isolated in 74% yield (19.0 mg) as colorless oil using pentane:Et_2O:Et_3N (40:1:0.1) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.04-7.03 (m, 1H), 7.00-6.96 (m, 1H), 6.65 (dt, J = 7.4, 1.0 Hz, 1H), 6.56 (d, J = 7.7 Hz, 1H), 5.83 (dd, J = 17.7, 10.9 Hz, 1H), 5.17 (dd, J = 10.9, 1.5 Hz, 1H), 5.13-5.09

(m, 1H), 5.06 (dd, *J* = 17.6, 1.5 Hz, 1H), 3.78 (t, *J* = 9.5 Hz, 1H), 2.95 (dd, *J* = 15.8, 9.3 Hz, 1H), 2.87 (dd, *J* = 15.8, 9.7 Hz, 1H), 1.98-1.85 (m, 2H), 1.69 (s, 3H), 1.60 (s, 3H), 1.42-1.38 (m, 2H), 1.00 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.1, 144.2, 131.6, 129.0, 127.3, 124.8, 124.7, 118.3, 114.5, 108.7, 67.4, 43.8, 38.5, 31.2, 25.8, 22.9, 17.8, 17.3; HRMS (pos. ESI) m/z: Calcd for $C_{18}H_{26}N$ $[M+H]^+$ 256.2060. Found 256.2054.

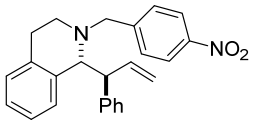


5-methoxy-2-methyl-2-(1-phenylallyl) indoline (3r). The compound was prepared according to above general procedure B, but the reaction was not quenched with MeOH. In addition the column chromatography was performed without evaporating solvent. Note, that compound **3r** easily decomposes under both acidic and basic conditions. Product **3r** was isolated in 75% yield (21.0 mg) as a light yellow oil using pentane:Et_2O (100:20) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, DMSO-d_6): δ 7.33-7.28 (m, 4H), 7.22-7.19 (m, 1H), 6.61 (d, *J* = 2.4 Hz, 1H), 6.48 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.42 (d, *J* = 8.4 Hz, 1H), 6.31 (ddd, *J* = 18.3, 8.9, 8.1 Hz, 1H), 5.10-5.04 (m, 2H), 4.82 (bs, 1H, NH), 3.61 (s, 3H), 3.38 (d, *J* = 9.4 Hz, 1H), 3.05 (d, *J* = 15.9 Hz, 1H), 2.48 (d, *J* = 15.9 Hz, 1H), 1.05 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.4, 144.1, 141.7, 138.5, 130.0, 129.1, 128.4, 126.7, 117.8, 112.3, 112.1, 109.8, 66.7, 59.1, 56.1, 41.8, 25.3; HRMS (pos. ESI) m/z: Calcd for $C_{19}H_{22}NO$ $[M+H]^+$ 280.1696. Found 280.1708.

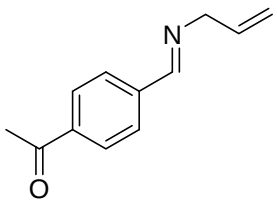
Derivatives for the X-ray Crystallography (see Chem3D Figures above)



4-bromo-N-(1,2-diphenylbut-3-en-1-yl)benzenesulfonamide (3d_sulfonamide derivative). The compound was prepared according to literature method.[5] Product **3d_sulfonamide derivative** was isolated in 78% yield as colorless oil using pentane:EtOAc:Et_3N (100:10:0.2) as eluent for silica gel chromatography. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.34-7.29 (m, 3H), 7.14-7.10 (m, 3H), 7.05-7.01 (m, 1H), 6.97-6.94 (m, 2H), 6.90-6.88 (m, 2H), 6.76-6.74 (m, 2H), 6.07 (ddd, *J* = 16.9, 10.1, 9.3 Hz, 1H), 5.29-5.23 (m, 2H), 5.10 (d, *J* = 5.4 Hz, 1H), 4.57 (dd, *J* = 9.2, 5.4 Hz, 1H), 3.48 (t, *J* = 9.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.6, 139.3, 137.9, 137.7, 131.8, 128.7, 128.6, 128.4, 127.9, 127.8, 127.5, 127.2, 127.1, 119.2, 62.1, 57.5; HRMS (pos. ESI) m/z: Calcd for $C_{22}H_{20}BrNNaO_2S$ $[M+Na]^+$ 464.0290. Found 464.0299.



2-(4-nitrobenzyl)-1-(-1-phenylallyl)-1,2,3,4-tetrahydroisoquinoline (3i_*p*-nitrobenzyl derivative). The compound was prepared according to literature methode.[6] Product **3i_*p*-nitrobenzyl derivative** was isolated in 82% yield as yellow color solid using pentane:EtOAc (100:10) as eluent for silica gel chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, J = 8.8 Hz, 2H), 7.53 (d, J = 8.8 Hz, 2H), 7.24-7.19 (m, 3H), 7.13-7.08 (m, 2H), 6.97-6.95 (m, 2H), 6.86-6.82 (m, 1H), 6.34 (ddd, J = 17.1, 10.2, 8.8 Hz, 1H), 6.23 (d, J = 7.7 Hz, 1H), 5.09 (dd, J = 10.2, 0.9 Hz, 1H), 4.98 (dt, J = 17.0, 1.2 Hz, 1H), 3.87-3.75 (m, 3H), 3.60 (dd, J = 8.6, 8.6 Hz, 1H), 3.43-3.36 (m, 1H), 2.97-2.89 (m, 1H), 2.82-2.77 (m, 1H), 2.60-2.54 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.9, 147.2, 142.6, 140.0, 135.6, 134.5, 129.4, 129.1, 128.9, 128.4, 126.6, 126.5, 125.0, 123.6, 114.9, 66.7, 57.9, 57.5, 43.2, 23.7; HRMS (pos. ESI) m/z: Calcd for $C_{25}H_{25}N_2O_2$ $[M+H]^+$ 385.1916. Found 385.1920.



1-(4-((allylimino)methyl)phenyl)ethan-1-one (1i). 4-acetyl-benzaldehyde (275 mg, 1.86 mmol) and allylamime (117 mg, 2.04 mmol) were taken in dry dichloromethane and molecular sieves were added. The reaction mixture was stirred for one hour. After removing the suspension by filtration, the solvent was evaporated under reduced pressure to provide imine (341 mg, 98%) as yellow colour oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (s, 1H), 8.00 (d, J = 8.5 Hz, 2H), 7.85 (d, J = 8.5 Hz, 2H), 6.08 (ddt, J = 17.1, 10.4, 5.7 Hz, 1H), 5.25 (ddt, J = 17.2, 1.7, 1.7 Hz, 1H), 5.18 (ddt, J = 10.3, 1.5, 1.5 Hz, 1H), 4.30 (ddd, J = 5.7, 1.7, 1.5 Hz, 2H), 2.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.8, 161.1, 140.2, 138.7, 135.6, 128.7, 128.4, 116.6, 63.8, 26.9; HRMS (pos. ESI) m/z: Calcd for $C_{12}H_{14}NO$ $[M+H]^+$ 188.1070. Found 188.1063.

^{1}H NMR Studies for E/Z Isomerization of 1a with Aryl Boroxine (Figure 1)

The *E/Z* isomerization of imine **1a** was studied in the presence of arylboroxine **5** in $CDCl_3$ using ^{1}H NMR (Figure 1). The E and Z geometry of the imine was assigned on the basis of dNOE experiments at 30 ^oC.

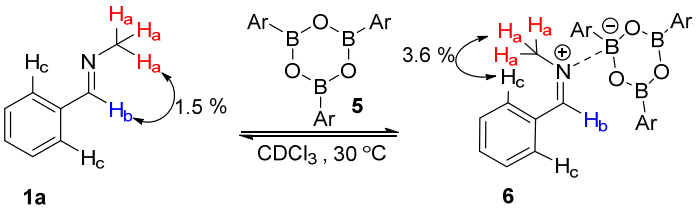


Figure 1. Isomerization of imine (**1a**) in the presence of aryl-boroxine. Major dNOE observations are shown for clarity.

The isolated imine **1a** (i.e. in the absence of boroxine) has three characteristic peaks H_a (N-methyl) at 3.52 ppm, H_b (imine C-H) at 8.29 ppm and H_c at 7.90 ppm as shown in Figure 2. When H_a was irradiated a 1.5% dNOE effect was observed at H_b (Figure 2). This shows that H_a and H_b are close to each other and thus the Ph and N-methyl group are in E geometry.

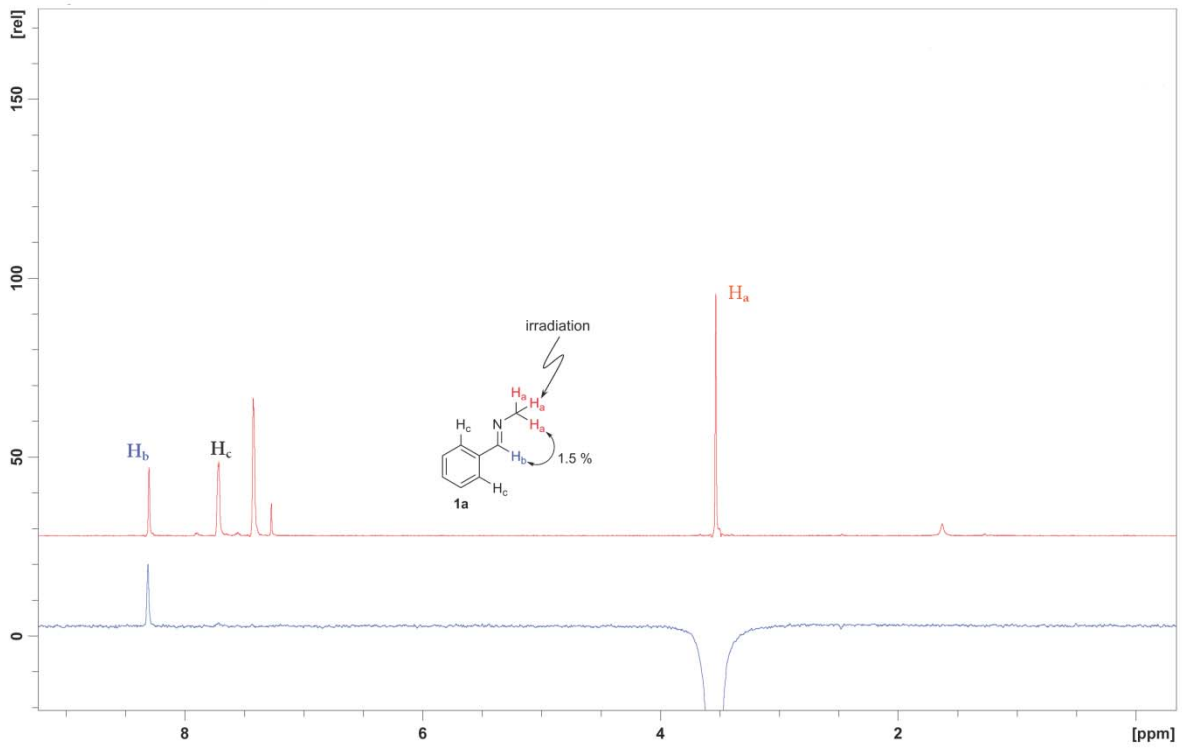


Figure 2. Observed dNOE between methyl proton (Ha) and imine proton (H_b) in pure imine (**1a**).

The boroxine of 4-fluorophenylboronic acid **5** was prepared according to the following procedure. A dry glass vial was charged with 4-fluorophenylboronic acid (0.3 mmol, 42.0 mg) and was taken inside a glove box. Molecular sieves 4 Å (0.1 g) and dry $CDCl_3$ (0.5 mL) were added sequentially and this mixture was stirred overnight. Formation of boroxine **5** was indicated by systematic changes of the ^{1}H NMR shifts.

To the solution of boroxine **5** prepared by the above procedure, imine **1a** (0.01 mmol) was added under inert conditions, and then the ^{1}H NMR spectrum was recorded at 30 ^{o}C (under Ar). When imine **1a** was added to boroxine **5**, a new species **6** was observed, which displayed characteristic new ^{1}H NMR peaks at 9.10 ppm and at 7.66-7.53 ppm (Figures 3-4). The new peak at 9.10 is the imine proton of **6** (Scheme 4), while the peak at 8.29 ppm corresponds imine proton H_b in **1a** (see also Figure 2). The other new peak at 7.66-7.53 ppm belongs to the aromatic protons (H_c) of the Ph group in **6** (Figure 4). According to integration the ratio of **1a** to **6** is 45:55 (at 30 ^{o}C). The N-methyl protons for the two different species (**1a** and **6**) are overlapping at 3.52 ppm. Under the experiment imine **1a** was also underwent partial hydrolysis to benzaldehyde. The (O=C)-H proton was observed at 10.03 ppm (Figure 3).

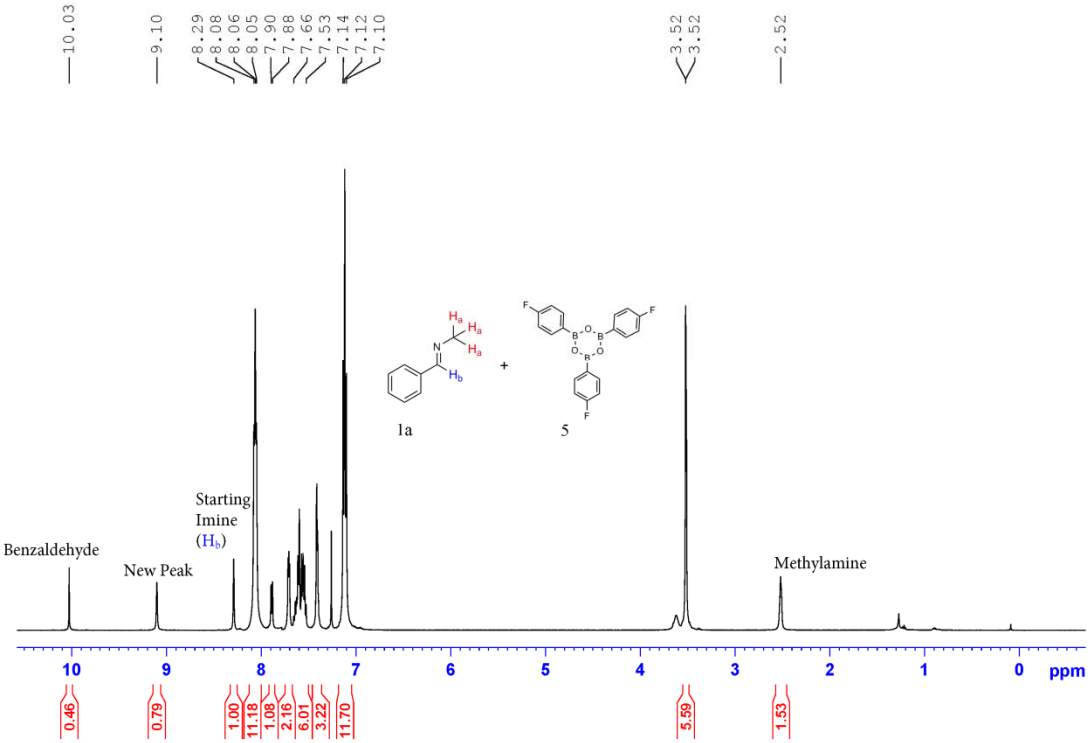


Figure 3. ^{1}H NMR ($CDCl_3$, 500 MHz) spectra for the mixture of **1a** and **5**.

When the N-methyl proton H_a of **6** (overlapping with the N-methyl proton of **1a**, see above) was irradiated a dNOE (3.6%) was observed with the aromatic (probably the ortho) H_c protons of **6** indicating that the phenyl and the N-methyl groups in **6** are in Z-geometry (Figure 4).

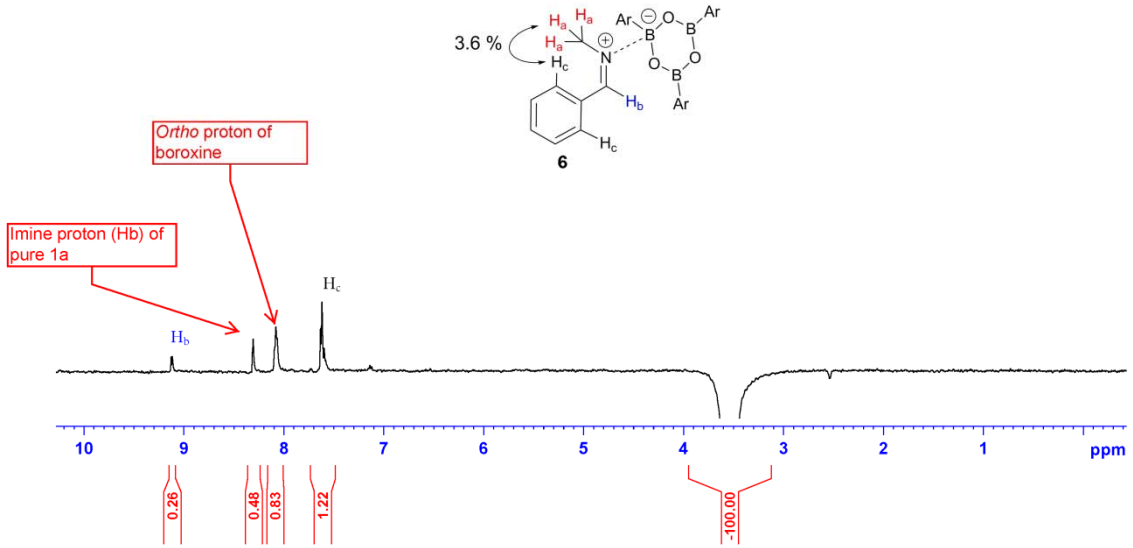


Figure 4. Observed dNOE between methyl proton Ha and aromatic proton H_c in complex **6.**

Formation of arylboroxine **5** is an equilibrium process. When water was added to the dry $CDCl_3$ solution of **5**, formation of 4-fluorophenylboronic acid was observed by ^1H NMR.

It is interesting to note that the reaction of phenyl boroxine and **1a** leads to similar changes in the ^1H NMR spectrum as described for **5** and **1a**. Appearance of new peaks indicates the formation of imine-boroxine complex similar to **6**. However, the extensive overlap of the ^1H NMR peaks in the aromatic area hindered the detection of the dNOE effects, when the N-methyl group was irradiated.

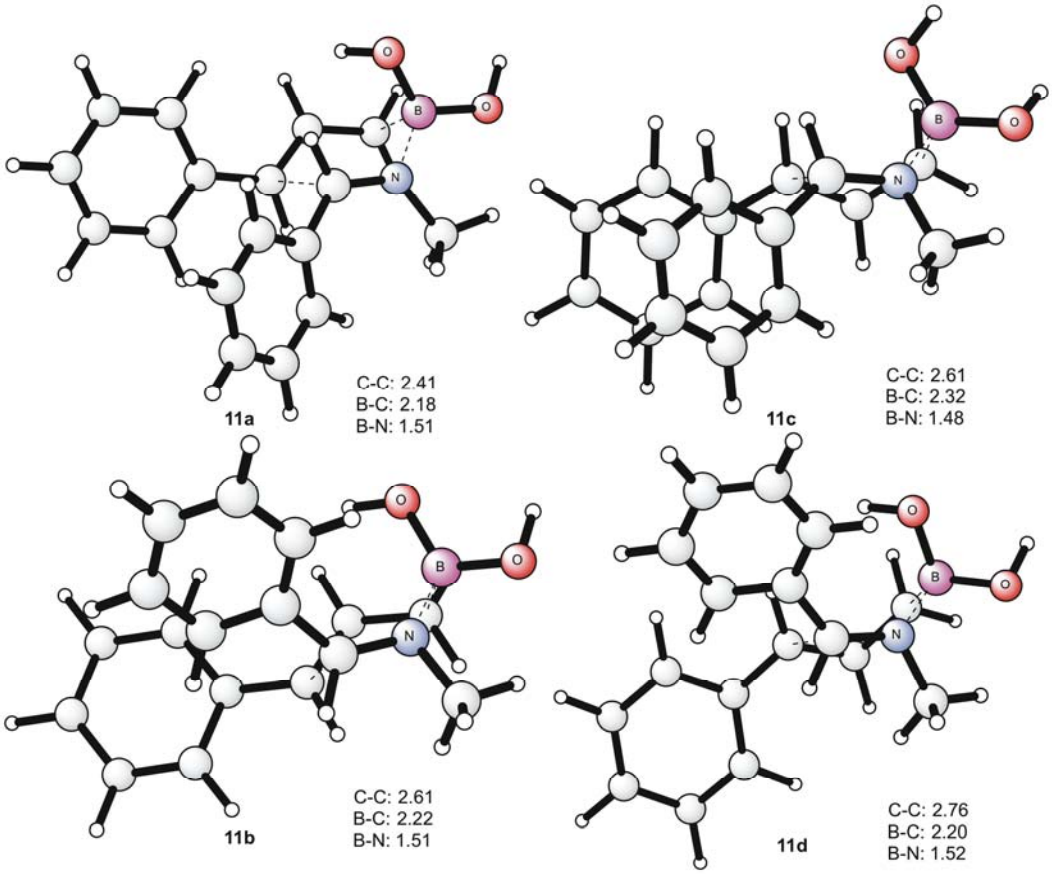
Computational Details

All the calculations were performed using the B3LYP functional[7] as implemented in the Gaussian09 software package[8]. Geometry optimizations were carried out with the 6-31G(*d*,*p*) basis set. Frequencies were computed analytically at the same level of theory to confirm the nature of the stationary points. Selected transition state structures were confirmed to connect the correct reactants and products by intrinsic reaction coordinate (IRC) calculations. To obtain more accurate final energy values, energies were recalculated on the basis of the optimized geometries using single-point calculations with the larger 6-311+G(*2d*,*2p*) basis set. Solvation effects were evaluated by performing single-point self-consistent reaction field calculations with the polarizable continuum model (PCM),[9] as implemented in Gaussian09. The parameters for dichloromethane ($\varepsilon = 8.93$), corresponding to the experimental conditions, and the default UFF atom radii were used in these calculations.

The final free energies reported in the article are the large basis set single-point energies corrected by gas-phase Gibbs free energy corrections (at 298.15 K), solvation corrections, and dispersion effects using the DFT-D2 method of Grimme.[10]

Optimized TS structures for the Allylboration of 1a with Allylboronic Acid 2a

(Distances are in Å)



Calculated Energies and Energy Corrections of the Stationary Points

Stationary point	Single-point basis set energy 6-311+G(*2d,2p*) (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)	Optimization basis set energy 6-31G(*d,p*) (a.u.)	Solvation energy (DCM) (a.u.)	Dispersion Correction (kcal/mol)
1a	-365.119080	0.117476	-365.021923	-0.00364775	-9.401853
1a$_c$	-365.107961	0.117611	-365.010809	-0.00445979	-10.762613
2a	-525.162586	0.146958	-525.003415	-0.0064436	-14.371365
11a	-890.246128	0.290314	-889.995645	-0.009454	-42.134927
10a	-890.270687	0.285560	-890.018184	-0.011306	-33.568335
12a	-890.295369	0.289599	-890.043430	-0.009196	-39.758261
11c	-890.239845	0.288493	-889.987581	-0.010610	-40.572281
11b	-890.243864	0.290437	-889.994384	-0.008011	-42.169155
10b	-890.264283	0.288052	-890.014001	-0.010971	-33.888353
12b	-890.291414	0.292743	-890.041658	-0.007557	-41.430760
11d	-890.238535	0.289119	-889.988779	-0.008004	-40.422804
2a$_b$	-1346.071992	0.410349	-1345.707557	-0.010146	-42.130097
8a	-1711.173531	0.557921	-1710.720621	-0.011435	-72.064705
7a	-1711.201490	0.555506	-1710.747298	-0.013015	-66.932136
9a	-1711.219197	0.556491	-1710.763435	-0.011082	-68.087883
8b	-1711.163608	0.560290	-1710.711656	-0.010936	-74.754754
7b	-1711.190265	0.556851	-1710.736567	-0.012568	-68.949080
9b	-1711.215688	0.559794	-1710.761395	-0.010606	-71.269832
8c	-1711.164100	0.556268	-1710.709173	-0.011610	-71.442405
8d	-1711.158818	0.557164	-1710.706045	-0.010592	-73.584989

Cartesian Coordinates

1a

C	-1.49865000	0.39184700	-0.03751100
H	-0.98301000	-0.57739600	-0.15326300
N	-0.85381400	1.48500800	0.07062100
C	-2.97044600	0.32324200	-0.01869700
C	-3.60460100	-0.92082700	-0.14243100
C	-3.75494600	1.48035300	0.12047400
C	-4.99619200	-1.01263700	-0.12778900
H	-3.00146500	-1.81922200	-0.25056300
C	-5.14231400	1.38763700	0.13493500
H	-3.25210400	2.43689900	0.21517600
C	-5.76738600	0.14164200	0.01098500
H	-5.47679500	-1.98173100	-0.22453100
H	-5.74277500	2.28637800	0.24284900
H	-6.85136900	0.07342900	0.02271800
C	0.59309200	1.42753900	0.03823400
H	0.96227100	2.05219200	-0.78377800
H	0.99379100	1.85763200	0.96382000
H	0.99973100	0.41005900	-0.08242400

$1a_c$

C	-1.35406800	0.33466800	0.07851600
H	-2.43730000	0.27795400	0.24019300
N	-0.85231700	1.50156300	0.19583500
C	-0.73714500	-0.98803300	-0.21151500
C	-1.32104100	-2.12121100	0.38016400
C	0.35066300	-1.17417500	-1.08145400

C	-0.80954300	-3.39568800	0.14964500
H	-2.18062200	-1.99238600	1.03320400
C	0.85347800	-2.45196000	-1.32482700
H	0.78481100	-0.32432600	-1.59518400
C	0.28329700	-3.56403200	-0.70344400
H	-1.26704400	-4.25749100	0.62660400
H	1.68927000	-2.57931100	-2.00662900
H	0.68004100	-4.55716500	-0.89239200
C	0.57692900	1.74489500	0.09369500
H	0.81555300	2.12522000	-0.90812700
H	0.83798600	2.54028200	0.79924800
H	1.21536200	0.87426000	0.29269500

$2a_b$

B	-2.09094900	-1.67836300	0.56005800
C	-1.82152000	-0.80356300	-0.72342000
C	-1.49287600	-1.57778600	-1.96827400
C	-0.37364200	-1.41711200	-2.68956900
H	-2.74768500	-0.22098800	-0.88101700
H	-1.04893500	-0.05775600	-0.50262100
H	-2.22762400	-2.32367200	-2.26558600
H	0.34203200	-0.66376900	-2.35801500
C	0.02282500	-2.14363700	-3.90577700
C	1.24089800	-1.81291600	-4.52533600
C	-0.75568100	-3.15970700	-4.49202200
C	1.66730800	-2.46445800	-5.68149000
H	1.85880900	-1.03177500	-4.08931900
C	-0.33168800	-3.81051300	-5.64636100
H	-1.70095400	-3.44479200	-4.04077600

C	0.88215300	-3.46761200	-6.24912400
H	2.61325800	-2.18747800	-6.13819900
H	-0.95080000	-4.59123900	-6.07947000
H	1.20993700	-3.97824400	-7.14972500
B	-2.22295600	-1.85188700	2.96022300
C	-2.10870500	-1.19231800	4.38775900
C	-1.06508600	-0.11571100	4.49552100
C	-0.04216200	-0.13236000	5.36289500
H	-3.10517500	-0.76185900	4.59614300
H	-1.95933900	-1.96937400	5.14550500
H	-1.16809900	0.70980100	3.79383500
H	0.02603600	-0.97218300	6.05543600
O	-1.96113500	-1.11959400	1.81805400
C	1.02312700	0.87167300	5.50959600
C	1.94947600	0.72921700	6.55767200
C	1.17055100	1.97699200	4.65018600
C	2.97619200	1.65251800	6.74862600
H	1.85680300	-0.11939100	7.23096700
C	2.19438800	2.89984300	4.84004900
H	0.48291000	2.11307900	3.82115300
C	3.10346100	2.74465100	5.89061700
H	3.67670800	1.51745400	7.56786800
H	2.28737300	3.74416600	4.16262900
H	3.90248400	3.46586800	6.03450100
B	-2.76606600	-3.75304300	1.58274100
C	-3.26221800	-5.24250700	1.43821700
C	-2.90268400	-6.13853800	2.59028200
C	-2.18549600	-7.26656100	2.48010100
H	-4.36203700	-5.18064700	1.34702200

H	-2.91269700	-5.65793000	0.48643300
H	-3.24965300	-5.80908300	3.56788900
H	-1.85988800	-7.56817500	1.48382200
O	-2.49937800	-2.99423900	0.45843100
O	-2.62801400	-3.16664900	2.82649200
C	-1.77951600	-8.17930700	3.56005700
C	-1.11855300	-9.37415600	3.22484300
C	-2.01562600	-7.92116700	4.92374400
C	-0.71524100	-10.27949700	4.20498200
H	-0.92250100	-9.59218700	2.17791700
C	-1.61423500	-8.82423300	5.90319300
H	-2.51155300	-7.00266400	5.22197700
C	-0.96231500	-10.00960900	5.55082000
H	-0.20733500	-11.19536300	3.91626300
H	-1.80719600	-8.60157400	6.94895000
H	-0.64870900	-10.71112100	6.31817600

7a

C	0.23263900	-2.49917900	-1.53417600
C	1.04797200	-3.62603600	-1.55904300
C	2.22441400	-3.64925700	-0.80724600
C	2.58217200	-2.54158100	-0.03465500
C	1.75770600	-1.42068400	0.01334800
C	0.56026500	-1.39152500	-0.72741200
C	-0.37282000	-0.26345500	-0.78223700
B	-1.68950900	1.87850900	-0.26611000
C	-0.80145600	3.24886600	-0.31460700
C	0.31702700	3.22373400	-1.30396600
C	1.62395000	3.34386000	-1.00934700

O	-2.65924300	1.89459900	0.82599200
O	-2.27820500	1.54995900	-1.55746900
H	-1.52165400	4.03519100	-0.58835500
H	-0.42768400	3.50814300	0.68432100
H	0.01786800	3.05527800	-2.33877100
H	1.89428700	3.53821900	0.03019500
H	-0.95543900	-0.17534000	-1.69718500
H	2.06973100	-0.55815400	0.58833600
H	-0.67229800	-2.47644700	-2.13402000
H	3.51070100	-2.54790100	0.52760100
H	0.76865300	-4.47441900	-2.17550300
H	2.87008500	-4.52194500	-0.83397600
N	-0.65526100	0.63768900	0.09560500
C	-0.06798000	0.68407000	1.43533900
H	0.16653500	-0.31748700	1.79955900
H	0.84340200	1.29022600	1.41986400
H	-0.79587600	1.15870600	2.09254200
C	2.76516100	3.27282400	-1.93431600
C	4.06010800	3.51251000	-1.43931400
C	2.63757500	2.97252900	-3.30473400
C	5.17820400	3.46132400	-2.27012000
H	4.18478400	3.74799000	-0.38496700
C	3.75250600	2.92308800	-4.13581000
H	1.65590000	2.77389300	-3.72369300
C	5.03102300	3.16665100	-3.62550300
H	6.16482400	3.65408500	-1.85773500
H	3.62467000	2.69090000	-5.18964700
H	5.89880800	3.12617600	-4.27717600
B	-3.59752900	1.27788500	-1.70789500

C	-4.15054200	0.78278900	-3.11947800
C	-4.02779700	-0.71410400	-3.18022500
C	-3.12808000	-1.38897500	-3.91714800
H	-5.20259200	1.07587700	-3.22505900
H	-3.57573900	1.24243700	-3.93045800
H	-4.70594900	-1.26412200	-2.52746800
H	-2.46500800	-0.81173700	-4.56245400
C	-2.91697700	-2.84446000	-3.96310300
C	-1.86637400	-3.35360000	-4.75002900
C	-3.70625100	-3.77032000	-3.25182100
C	-1.60818700	-4.72243900	-4.82131500
H	-1.24833000	-2.66025800	-5.31526500
C	-3.45044200	-5.13612100	-3.32375300
H	-4.53203500	-3.41913600	-2.64091000
C	-2.39906900	-5.62266400	-4.10672400
H	-0.79313200	-5.08448100	-5.44191000
H	-4.07684300	-5.82767300	-2.76725300
H	-2.20525500	-6.68968300	-4.16241500
B	-3.97770200	1.66343500	0.63516800
C	-5.01226100	1.71870800	1.84159700
C	-6.16487700	2.64075000	1.55860400
C	-6.45105200	3.74922100	2.25950000
H	-5.39747200	0.69542400	1.98503800
H	-4.50207300	2.00580000	2.76671000
H	-6.77543000	2.37253300	0.69752400
H	-5.82122200	3.98513800	3.11809200
O	-4.46774000	1.35475900	-0.63352200
C	-7.54171700	4.70586100	2.01813100
C	-7.73282100	5.76068100	2.92863900

C	-8.41612700	4.62791600	0.91692900
C	-8.75311900	6.69443000	2.75593100
H	-7.06808700	5.84324500	3.78504000
C	-9.43602300	5.55858100	0.74377500
H	-8.29347700	3.83479500	0.18571000
C	-9.61271200	6.59797000	1.66183300
H	-8.87574200	7.49788900	3.47701500
H	-10.09631500	5.47569500	-0.11523600
H	-10.40875600	7.32343200	1.52219400

7b

C	0.43505500	-0.93188100	-0.24427800
B	-1.58409200	0.81815100	0.05800800
C	-0.71446600	2.21486200	0.13869400
C	0.41266300	2.31728600	-0.82846600
C	1.71618700	2.38424300	-0.49670500
O	-2.59138000	0.75698900	1.10628400
O	-2.12595600	0.60096600	-1.26746200
H	-1.46381200	2.99054900	-0.08188600
H	-0.36499100	2.40383900	1.16130200
H	0.12913100	2.29598500	-1.88026500
H	1.96825300	2.42150300	0.56441900
N	-0.48485800	-0.37054500	0.47193100
C	-0.34825100	-0.50139000	1.93493500
H	0.53187500	-1.09630000	2.18914100
H	-0.27280200	0.48680800	2.39035700
H	-1.24776000	-0.97591500	2.32974200
C	2.87295900	2.44532200	-1.40099100
C	4.16112900	2.58318900	-0.85046500

C	2.76868400	2.37052000	-2.80444400
C	5.29467200	2.65003300	-1.65855500
H	4.26736100	2.64443000	0.23004300
C	3.90012900	2.43931800	-3.61221600
H	1.79371300	2.25682800	-3.26718300
C	5.17072000	2.57942000	-3.04643800
H	6.27498500	2.76016300	-1.20324700
H	3.79044200	2.38399200	-4.69188900
H	6.05074000	2.63368300	-3.68045000
H	1.27771300	-1.35513600	0.30919300
C	0.52611800	-1.14672000	-1.69131800
C	-0.56736500	-1.50651400	-2.49732000
C	1.81742500	-1.13734800	-2.25384200
C	-0.36965500	-1.81972500	-3.83931300
H	-1.55782800	-1.55917400	-2.06986000
C	2.00415400	-1.42053000	-3.60266700
H	2.67069200	-0.87905100	-1.63369000
C	0.90904100	-1.76663000	-4.39774000
H	-1.22001900	-2.11530800	-4.44505700
H	3.00170900	-1.38103900	-4.02817700
H	1.05446000	-2.00878500	-5.44641600
B	-3.46026600	0.55314600	-1.50656700
C	-4.03406700	0.45552600	-2.98740600
C	-4.74026700	-0.85189300	-3.21571800
C	-4.42492300	-1.74337700	-4.17000700
H	-4.75785200	1.27756800	-3.10678400
H	-3.23986400	0.60176200	-3.72640500
H	-5.55628200	-1.06645200	-2.52658600
H	-3.62709200	-1.48050300	-4.86605900

C	-5.05776400	-3.04686900	-4.42267800
C	-4.70179200	-3.76388200	-5.57912600
C	-6.00865500	-3.62670100	-3.56099000
C	-5.27457500	-5.00032000	-5.87233200
H	-3.96837400	-3.33664000	-6.25899700
C	-6.58276300	-4.86004300	-3.85340900
H	-6.29556200	-3.11129100	-2.64960300
C	-6.22083500	-5.55532300	-5.01087800
H	-4.98144800	-5.52946200	-6.77482000
H	-7.31415300	-5.28537200	-3.17172300
H	-6.66908200	-6.51888900	-5.23429800
B	-3.91150000	0.61038100	0.85026700
C	-4.97295200	0.50155800	2.03007100
C	-4.37689000	0.16371100	3.36316900
C	-4.63027100	-0.95556100	4.05980200
H	-5.48397200	1.47798400	2.08214500
H	-5.75165100	-0.21896800	1.75119400
H	-3.65909400	0.88540000	3.75066600
H	-5.34175500	-1.66736100	3.63901400
O	-4.37294800	0.56220200	-0.46005000
C	-4.04809400	-1.36160600	5.34869200
C	-4.36959700	-2.62752500	5.87060300
C	-3.17787400	-0.54827900	6.10039400
C	-3.84318000	-3.06940600	7.08333300
H	-5.04288700	-3.27179300	5.31045000
C	-2.65155100	-0.98792100	7.31133700
H	-2.91649800	0.44123600	5.73780700
C	-2.97888300	-2.25177100	7.81121500
H	-4.11005800	-4.05304700	7.45973900

H	-1.98447200	-0.33910400	7.87248300
H	-2.56755900	-2.59062200	8.75745400

8a

C	2.85725300	-0.85043700	-1.05449100
C	4.09453300	-1.46402800	-0.86746300
C	4.86135600	-1.16322100	0.25804200
C	4.38337000	-0.23882900	1.18821300
C	3.14467100	0.37258700	1.00222800
C	2.35200300	0.06581800	-0.11733800
C	1.02147700	0.67192300	-0.40780300
B	-1.33236200	1.19144500	-0.01862700
C	-0.85394400	3.10879900	0.02735600
C	0.14768700	3.14067300	-0.94344100
C	1.46407400	2.68248300	-0.72871600
O	-2.41158500	1.08945700	0.90759800
O	-1.64134900	0.88860800	-1.38443300
H	-1.81145200	3.56360600	-0.21726600
H	-0.57502900	3.21431000	1.07466500
H	-0.16288300	3.30537500	-1.97362700
H	1.86084200	2.84007600	0.27357900
H	0.69860200	0.49535500	-1.42890300
H	2.80694900	1.10462200	1.72729700
H	2.26790200	-1.08604200	-1.93570000
H	4.97897700	0.01315900	2.06073400
H	4.45923900	-2.17384000	-1.60381700
H	5.82688400	-1.63753200	0.40580900
N	-0.02815800	0.63615300	0.46351900
C	0.17653500	0.51551500	1.90547300
H	0.87061000	-0.29767700	2.12595100

H	0.57259000	1.43967200	2.35034400
H	-0.78628500	0.30737700	2.36867300
C	2.48417700	2.74025100	-1.80418900
C	3.81676400	3.05830500	-1.49694800
C	2.16435500	2.45697200	-3.14402400
C	4.79129800	3.11353400	-2.49206500
H	4.08704900	3.27119200	-0.46623200
C	3.13757200	2.51414800	-4.13991400
H	1.14680100	2.18291600	-3.40958700
C	4.45585600	2.84490200	-3.81975400
H	5.81403900	3.36866400	-2.22943100
H	2.86637800	2.29432000	-5.16870000
H	5.21370000	2.88790500	-4.59630100
B	-2.91900700	0.64303900	-1.78426800
C	-3.25896300	0.35065100	-3.30610200
C	-4.23193600	-0.78019400	-3.48695000
C	-3.98016500	-1.90773700	-4.16954200
H	-3.70452400	1.27762400	-3.70723900
H	-2.34006100	0.17439100	-3.87526500
H	-5.19308900	-0.64994800	-2.99255300
H	-3.00902700	-2.00300700	-4.65689000
C	-4.87676600	-3.05850700	-4.35868500
C	-4.46590700	-4.10877800	-5.19882800
C	-6.13646100	-3.17181200	-3.73951200
C	-5.27587300	-5.22138400	-5.42018600
H	-3.49573700	-4.04479900	-5.68557400
C	-6.94664500	-4.28125300	-3.96040300
H	-6.48306800	-2.38722800	-3.07406300
C	-6.52301100	-5.31351600	-4.80257500

H	-4.93160400	-6.01645300	-6.07576800
H	-7.91411800	-4.34399100	-3.46982100
H	-7.15741900	-6.17866600	-4.97117900
B	-3.68924000	0.86950300	0.48873200
C	-4.89762900	0.84712800	1.51565700
C	-5.90155400	1.91852500	1.18481200
C	-6.17454700	2.97980700	1.96026700
H	-5.38255900	-0.13899200	1.44490700
H	-4.53052600	0.96305500	2.54036100
H	-6.40077200	1.80781000	0.22332800
H	-5.65698800	3.05695500	2.91708200
O	-3.95304000	0.67035500	-0.85883800
C	-7.11457200	4.07592000	1.68095600
C	-7.30416800	5.07174900	2.65583000
C	-7.84281700	4.18908400	0.48095500
C	-8.18359300	6.13311200	2.44850000
H	-6.75131600	5.00598500	3.58973500
C	-8.72185000	5.24735300	0.27297500
H	-7.71839500	3.44396200	-0.29874900
C	-8.89879700	6.22672600	1.25477100
H	-8.30955900	6.88700300	3.22063600
H	-9.27175500	5.31106200	-0.66196400
H	-9.58475100	7.05204000	1.08833800

8b

C	0.69709500	-0.36680800	-0.44188400
B	-1.63667200	0.42887300	0.19343000
C	-0.84352200	2.29646100	0.44300000
C	0.06873200	2.31793800	-0.60204900

C	1.33491700	1.69916800	-0.53346400
O	-2.57453800	0.34174700	1.26137200
O	-2.19359300	0.49563000	-1.11165500
H	-1.76020500	2.87199800	0.34387200
H	-0.47938500	2.20140800	1.46359000
H	-0.28021900	2.66250600	-1.57315700
H	1.74800100	1.62589500	0.47231500
N	-0.37310900	-0.34273200	0.41581700
C	-0.00380900	-0.57732500	1.82273200
H	0.48636400	-1.54977400	1.91861700
H	0.68478900	0.19509100	2.19484200
H	-0.89905300	-0.57082300	2.44014100
C	2.36845100	1.90094500	-1.57087600
C	3.72493600	1.90778900	-1.19923000
C	2.05781300	2.08714900	-2.93005700
C	4.73184600	2.10563700	-2.14234100
H	3.98831900	1.76711300	-0.15347400
C	3.06344700	2.29364300	-3.87190100
H	1.02317900	2.05477300	-3.25650800
C	4.40513200	2.30407800	-3.48515000
H	5.77138900	2.11200600	-1.82697700
H	2.79776600	2.43741100	-4.91529100
H	5.18688000	2.46218600	-4.22203400
H	1.62670500	-0.61378600	0.06733300
C	0.66757400	-0.97243100	-1.79780300
C	-0.47962800	-1.54268400	-2.37713500
C	1.89381400	-1.12538500	-2.47483100
C	-0.40625600	-2.20271200	-3.60245100
H	-1.42576800	-1.48893100	-1.86085500

C	1.96394200	-1.78076300	-3.70116400
H	2.80273300	-0.73401600	-2.03096700
C	0.81114500	-2.31784700	-4.27521600
H	-1.30581800	-2.64444900	-4.02072000
H	2.92287300	-1.87984600	-4.20119500
H	0.86446900	-2.83891200	-5.22677100
B	-3.53822300	0.58660300	-1.31728000
C	-4.13311700	0.70444800	-2.78278800
C	-4.67358700	-0.62789200	-3.23093300
C	-4.16390800	-1.35993600	-4.23495100
H	-4.94745400	1.44309400	-2.76982800
H	-3.36417000	1.05348600	-3.47940300
H	-5.52559300	-1.00396500	-2.66556300
H	-3.32629300	-0.94067000	-4.79274700
C	-4.61558900	-2.68002400	-4.70013000
C	-4.07392200	-3.20245200	-5.88878900
C	-5.56506500	-3.46169200	-4.01430900
C	-4.46851300	-4.44567100	-6.38081200
H	-3.33889300	-2.61590600	-6.43465700
C	-5.96129000	-4.70162300	-4.50574400
H	-5.98974300	-3.10012200	-3.08286000
C	-5.41682500	-5.20184800	-5.69232100
H	-4.03488700	-4.82257400	-7.30286700
H	-6.69507400	-5.28577600	-3.95733800
H	-5.72618000	-6.17152900	-6.07084700
B	-3.91931000	0.39984300	1.05027900
C	-4.95364300	0.32918300	2.24915600
C	-4.35598900	0.10912000	3.60646300
C	-4.62805500	-0.93199900	4.40774600

H	-5.51089200	1.28122000	2.22858600
H	-5.70455000	-0.43934000	2.02169200
H	-3.63846000	0.86184900	3.93050900
H	-5.35094400	-1.66915300	4.05598400
O	-4.40998900	0.54522400	-0.23945900
C	-4.06505800	-1.21329500	5.73747800
C	-4.51025900	-2.34931100	6.43662300
C	-3.09633300	-0.40199600	6.35907400
C	-4.01531500	-2.66474200	7.70099300
H	-5.25772800	-2.99095400	5.97651900
C	-2.60173300	-0.71495000	7.62138700
H	-2.72534800	0.48205300	5.84974500
C	-3.05739100	-1.84811400	8.30156500
H	-4.37915600	-3.54911600	8.21655500
H	-1.85504100	-0.07170400	8.07898800
H	-2.66874300	-2.08941400	9.28648900

8c

C	0.16072200	0.23444500	-4.65606500
C	1.02092300	-0.02598100	-5.71838400
C	2.39380200	-0.14127200	-5.49487600
C	2.89359800	0.02209900	-4.20223400
C	2.03465000	0.28092200	-3.13699400
C	0.64267400	0.36912400	-3.33799300
C	-0.35998700	0.63512500	-2.29879900
B	-1.56627100	0.36438800	-0.20268300
C	-0.76286100	2.41479100	0.45842600
C	0.17894800	2.77730500	-0.48874900
C	-0.09619100	2.96266100	-1.85332700

O	-1.67045700	-0.31680700	1.02105700
O	-2.75680000	0.77471200	-0.83805800
H	-1.80040700	2.69383700	0.30637800
H	-0.45786100	2.27514200	1.49082300
H	1.22553800	2.75471200	-0.18316900
H	-1.14645900	3.09092800	-2.10846100
H	-1.34041600	0.89258000	-2.68015900
H	2.45497100	0.44374000	-2.15303100
H	-0.90706100	0.31721400	-4.83882200
H	3.96270300	-0.03904500	-4.02151800
H	0.61886800	-0.13835800	-6.72089700
H	3.06878800	-0.34320200	-6.32100500
N	-0.42814500	0.05253000	-1.07498700
C	0.73790400	-0.58698300	-0.46514700
H	1.21109200	-1.26441700	-1.17793200
H	1.47433300	0.15814300	-0.13987400
H	0.40656600	-1.14928400	0.40569200
C	0.83479400	3.52478900	-2.83589300
C	0.33718800	3.94414000	-4.08603100
C	2.21724300	3.67760000	-2.60580600
C	1.17190900	4.49411200	-5.05485100
H	-0.72617800	3.84261100	-4.28885500
C	3.05177800	4.23092100	-3.57331400
H	2.64588200	3.37560200	-1.65513300
C	2.53727300	4.64251600	-4.80471400
H	0.75445800	4.81199000	-6.00625400
H	4.11196600	4.34372600	-3.36331400
H	3.19073700	5.07531100	-5.55622000
B	-3.97214700	0.59209500	-0.23351500

C	-5.30107200	1.12313000	-0.90819700
C	-6.45938400	0.17145900	-0.79517500
C	-7.13342700	-0.33699100	-1.83783100
H	-5.55213200	2.06196600	-0.38331200
H	-5.11456400	1.39535000	-1.95239300
H	-6.72975800	-0.11701200	0.21908500
H	-6.83962000	-0.01869900	-2.83884200
C	-8.25831800	-1.28414100	-1.80165100
C	-8.90991600	-1.60947800	-3.00455300
C	-8.72491500	-1.89089500	-0.61984900
C	-9.98559000	-2.49552500	-3.03104400
H	-8.56467900	-1.15507800	-3.93003400
C	-9.79912800	-2.77494600	-0.64459400
H	-8.23895700	-1.67449400	0.32651000
C	-10.43759700	-3.08282100	-1.84951600
H	-10.47017900	-2.72654300	-3.97556100
H	-10.13953800	-3.23032600	0.28129600
H	-11.27465400	-3.77451400	-1.86488100
B	-2.88596300	-0.50823400	1.61946900
C	-3.01319900	-1.23389600	3.01947100
C	-1.79609900	-1.99083900	3.46326700
C	-1.76366400	-3.30873000	3.71187400
H	-3.25011900	-0.44024200	3.74981900
H	-3.89873500	-1.88151100	3.00809200
H	-0.88447700	-1.40266600	3.55710900
H	-2.68950300	-3.87245800	3.59051500
O	-4.03261100	-0.03535100	1.00003000
C	-0.60546600	-4.11546500	4.12667200
C	-0.74781600	-5.51165800	4.21497500

C	0.65004500	-3.56466200	4.44725700
C	0.31605700	-6.32738500	4.59666500
H	-1.70952200	-5.95901100	3.97609900
C	1.71306200	-4.37754800	4.82864400
H	0.79444500	-2.48938900	4.40549100
C	1.55430800	-5.76435500	4.90480900
H	0.17626100	-7.40323000	4.65391400
H	2.67136400	-3.92728900	5.07270100
H	2.38570200	-6.39551000	5.20441500

8d

C	0.25765400	-0.23157300	-1.96939900
B	-1.39024000	0.19685900	-0.09422800
C	-1.24118500	2.31543100	-0.53322100
C	-0.16177000	2.51997700	-1.38722800
C	-0.05965500	1.97091400	-2.67305300
O	-1.50093700	0.15894900	1.31626100
O	-2.55418600	-0.11847400	-0.83091900
H	-2.22250500	2.18707200	-0.97787900
H	-1.23140300	2.79682000	0.44067100
H	0.72862700	2.99658300	-0.97680000
H	-0.99301800	1.68819700	-3.15466900
N	-0.06585100	-0.20403700	-0.65046800
C	1.08067800	0.05846900	0.23389400
H	1.87741600	-0.65802500	0.02174100
H	1.46891700	1.07421700	0.08011900
H	0.76981900	-0.04521900	1.27104000
C	1.04456900	2.30520500	-3.59316900
C	0.79007800	2.43142200	-4.97217700

C	2.36682900	2.50931400	-3.15205600
C	1.80668100	2.75670000	-5.86906000
H	-0.22286900	2.28274700	-5.33647000
C	3.38137000	2.83950400	-4.04712300
H	2.60519600	2.39969300	-2.09758400
C	3.10853700	2.96490400	-5.41169700
H	1.57901900	2.85277700	-6.92697600
H	4.39231100	2.99147200	-3.67933700
H	3.90187100	3.21812100	-6.10839200
H	1.31824300	-0.10346600	-2.16678300
C	-0.43262800	-1.05989000	-2.97983700
C	-1.36377100	-2.05763800	-2.63953900
C	-0.03512200	-0.95593900	-4.32770000
C	-1.90958800	-2.88662900	-3.61770400
H	-1.64124400	-2.20076600	-1.60506700
C	-0.58681200	-1.78083100	-5.30306700
H	0.71156300	-0.22185200	-4.60933700
C	-1.53359000	-2.74674100	-4.95411000
H	-2.62141700	-3.65335200	-3.32676800
H	-0.26843300	-1.67630000	-6.33624100
H	-1.95818700	-3.39666200	-5.71361500
B	-3.74542500	-0.37185200	-0.21241800
C	-5.04740200	-0.71080700	-1.04846000
C	-5.43850100	-2.15080500	-0.84421300
C	-5.43796500	-3.08750000	-1.80627800
H	-5.86111800	-0.05961600	-0.69487300
H	-4.88479200	-0.50436400	-2.11072800
H	-5.71397600	-2.42125900	0.17445900
H	-5.17991000	-2.77561900	-2.81867300

C	-5.76780100	-4.51397400	-1.66521200
C	-5.90409300	-5.29781900	-2.82522000
C	-5.94940100	-5.14846400	-0.42139900
C	-6.21925700	-6.65371300	-2.75176900
H	-5.76699300	-4.82906600	-3.79672100
C	-6.26590800	-6.50138800	-0.34683100
H	-5.83100700	-4.58034400	0.49611100
C	-6.40398200	-7.26313800	-1.51087100
H	-6.32079900	-7.23352700	-3.66488700
H	-6.39976800	-6.96754900	0.62540300
H	-6.64787600	-8.31950200	-1.44855600
B	-2.68822400	-0.10745300	1.93500800
C	-2.82046000	-0.10859600	3.51328600
C	-1.52816100	-0.03847800	4.27080000
C	-1.09360400	-0.96849500	5.13457100
H	-3.45305100	0.76081100	3.76350000
H	-3.41003200	-0.98226300	3.81974400
H	-0.91163100	0.83604500	4.06788600
H	-1.73124200	-1.83551100	5.31201400
O	-3.81817100	-0.36127300	1.17227300
C	0.16694000	-0.97086700	5.89298800
C	0.44720100	-2.05836300	6.73930100
C	1.11931700	0.06398200	5.82207000
C	1.62500100	-2.11616100	7.48258500
H	-0.27403800	-2.86877800	6.81085900
C	2.29533400	0.00810700	6.56361600
H	0.93807100	0.92244000	5.18254200
C	2.55706000	-1.08206000	7.39866600
H	1.81345500	-2.96976500	8.12765500

H	3.01328500	0.82055700	6.49171400
H	3.47591200	-1.12194400	7.97611900

9a

C	1.92297900	-1.12497500	-0.82910700
C	2.74994500	-2.22327300	-0.60065800
C	3.88970800	-2.08653900	0.19402500
C	4.19080400	-0.84551800	0.75344300
C	3.35950300	0.25231700	0.51999300
C	2.21263500	0.12988300	-0.27438800
C	1.23324800	1.27708700	-0.52546100
B	-1.19229500	1.06561700	0.08795500
C	0.73000000	4.84528800	-0.07180700
C	0.83366400	3.75129400	-0.82533100
C	1.89529600	2.68421500	-0.66166100
O	-2.21629300	1.06867300	1.03625400
O	-1.52914600	0.84375300	-1.25144100
H	-0.04021900	5.58974900	-0.24888500
H	1.41747100	5.04239100	0.74759000
H	0.12885500	3.59625700	-1.64232900
H	2.45218400	2.91370500	0.25333700
H	0.74656900	1.06939500	-1.47976800
H	3.61920800	1.20986600	0.95997100
H	1.03553000	-1.23765100	-1.44701600
H	5.07614500	-0.72697600	1.37162000
H	2.50728200	-3.18395400	-1.04583900
H	4.53838600	-2.93913000	0.37237500
N	0.14256400	1.27472900	0.46987200
C	0.50353100	1.52025900	1.86212300

H	1.25927600	0.80503900	2.20389000
H	0.89686400	2.53473100	2.00119600
H	-0.38343600	1.41373600	2.48553200
C	2.88397200	2.73229600	-1.82582800
C	4.21535300	3.10805900	-1.61018900
C	2.48227400	2.43951000	-3.13736700
C	5.12366500	3.18162300	-2.66655600
H	4.54506200	3.34712600	-0.60225300
C	3.38682800	2.51152800	-4.19643100
H	1.45297700	2.15621400	-3.34054300
C	4.71253300	2.88163300	-3.96522000
H	6.15212800	3.47321100	-2.47340300
H	3.05439600	2.27912900	-5.20419200
H	5.41718200	2.93687600	-4.78970800
B	-2.83397100	0.64251800	-1.62911800
C	-3.21561300	0.41545000	-3.14627800
C	-4.21224500	-0.69428700	-3.34258400
C	-3.98777000	-1.80258500	-4.06455500
H	-3.65330500	1.36400600	-3.50275100
H	-2.31396800	0.24492000	-3.74372700
H	-5.16269200	-0.56441900	-2.82811100
H	-3.02432200	-1.89679800	-4.56702200
C	-4.90329600	-2.93399000	-4.27849700
C	-4.50041500	-3.98064800	-5.12669000
C	-6.17256300	-3.03089200	-3.67673700
C	-5.32670900	-5.07646300	-5.37031300
H	-3.52355700	-3.92796300	-5.60114900
C	-6.99881400	-4.12369900	-3.91957500
H	-6.51575600	-2.24605000	-3.00981200

C	-6.58225300	-5.15371800	-4.76802700
H	-4.98867200	-5.86971500	-6.03115000
H	-7.97371600	-4.17459100	-3.44269300
H	-7.22954100	-6.00554900	-4.95426900
B	-3.52327100	0.86929000	0.67091100
C	-4.67908500	0.85356900	1.74847000
C	-5.87473900	1.66833200	1.33546700
C	-6.34866300	2.72483200	2.01323200
H	-4.98184800	-0.20101100	1.86725200
H	-4.29571900	1.18151600	2.72006300
H	-6.35077400	1.36190300	0.40563300
H	-5.85371300	2.99514300	2.94667300
O	-3.82648900	0.66021700	-0.66509000
C	-7.49226900	3.57799800	1.65526400
C	-7.92826700	4.54876000	2.57445600
C	-8.18059500	3.47950300	0.43104800
C	-9.01052900	5.38063000	2.29246900
H	-7.40850900	4.64547800	3.52452600
C	-9.26172700	4.30863900	0.14849200
H	-7.86218000	2.75322300	-0.31037300
C	-9.68493800	5.26394000	1.07718700
H	-9.32606000	6.12036600	3.02286500
H	-9.77571700	4.21317300	-0.80396800
H	-10.52766900	5.91088700	0.85228500

9b

C	1.26096500	-0.20497000	-1.53286300
B	-0.61485700	0.58332800	0.05249300
C	1.24249600	0.45909000	-5.06171200

C	1.78571100	0.63101400	-3.85793900
C	1.00994700	0.91861000	-2.58968800
O	-1.03040100	0.79249000	1.37028000
O	-1.52513300	0.87503700	-0.96683600
H	1.85233000	0.27371000	-5.94080900
H	0.16649700	0.49294400	-5.21272400
H	2.87051400	0.58956200	-3.75358900
H	-0.05334700	0.92675000	-2.83656400
N	0.67177600	0.08068000	-0.20734700
C	1.53602800	-0.32752600	0.89917600
H	1.79572300	-1.39063600	0.81715000
H	2.46742200	0.25378300	0.89972700
H	1.02820800	-0.16695900	1.84883700
C	1.38482900	2.30116700	-2.05597300
C	0.45750700	3.34977500	-2.10142600
C	2.66635100	2.57428600	-1.55497000
C	0.79197200	4.62817700	-1.65185000
H	-0.53694400	3.16016000	-2.49500900
C	3.00492100	3.84964900	-1.10343600
H	3.41426600	1.78656000	-1.51842100
C	2.06759900	4.88304000	-1.14864500
H	0.05470000	5.42493200	-1.69685400
H	4.00338600	4.03675200	-0.71824600
H	2.33051700	5.87656900	-0.79766600
H	2.34525900	-0.21574200	-1.36707300
C	0.89594100	-1.59879400	-2.04172600
C	-0.43124000	-1.95829700	-2.32019200
C	1.89919600	-2.55590600	-2.23218900
C	-0.74048300	-3.23764300	-2.77934200

H	-1.22781600	-1.23648200	-2.17510100
C	1.59319700	-3.83952400	-2.68992600
H	2.93395300	-2.29465100	-2.02225400
C	0.27096600	-4.18343700	-2.96580900
H	-1.77421900	-3.49490200	-2.99267400
H	2.38795800	-4.56729000	-2.82768700
H	0.02769200	-5.18053600	-3.32138100
B	-2.79686400	1.31251100	-0.68625700
C	-3.84551200	1.50631800	-1.85491000
C	-4.57308300	0.19886000	-2.05169400
C	-4.36875200	-0.64286500	-3.07824900
H	-4.55851200	2.29670300	-1.58974700
H	-3.33595900	1.79411100	-2.78087400
H	-5.27591500	-0.06915100	-1.26386800
H	-3.65477300	-0.34277400	-3.84587300
C	-5.00026700	-1.95121400	-3.30674700
C	-4.61252300	-2.70144000	-4.43198800
C	-5.97840500	-2.50226700	-2.45693600
C	-5.17187400	-3.95048900	-4.69863300
H	-3.86172000	-2.29368000	-5.10429200
C	-6.53830300	-3.74775700	-2.72327600
H	-6.30660500	-1.95227700	-1.58039500
C	-6.13881400	-4.48062800	-3.84477300
H	-4.85276600	-4.50729400	-5.57511400
H	-7.29162300	-4.15070000	-2.05220500
H	-6.57818800	-5.45249100	-4.04874700
B	-2.28697100	1.26074000	1.66289900
C	-2.72305000	1.47546800	3.16739200
C	-2.80463600	0.15202500	3.88440400

C	-3.93569400	-0.39217400	4.35965800
H	-1.96864700	2.10943000	3.65716000
H	-3.68331300	1.99821200	3.21578800
H	-1.86189400	-0.38342200	3.98756900
H	-4.85827300	0.18011600	4.25751000
O	-3.17078500	1.51882100	0.62845700
C	-4.08644500	-1.68750200	5.03982300
C	-5.31524300	-1.99416900	5.65102500
C	-3.06103900	-2.64949900	5.11060600
C	-5.51189400	-3.20260900	6.31722400
H	-6.12310700	-1.26805600	5.60349500
C	-3.25567800	-3.85583400	5.77625400
H	-2.10641600	-2.45710200	4.63066000
C	-4.48130700	-4.14007300	6.38527300
H	-6.47122600	-3.41153000	6.78232900
H	-2.44907000	-4.58260400	5.81524200
H	-4.63075900	-5.08389900	6.90117700

2a

B	-0.78461400	-0.32423900	-0.01282400
C	-1.02691400	0.87246400	-1.04030000
C	-0.74121500	2.22123200	-0.44595400
C	-1.66645900	3.04496400	0.07820000
H	-0.42490000	0.69944700	-1.93990500
H	-2.07817300	0.81312100	-1.35773700
H	0.30968700	2.50827900	-0.40706000
H	-2.71233600	2.74198900	0.00674600
O	-0.52679300	-1.57225000	-0.50243600
O	-0.85858400	-0.14701800	1.34222300

C	-1.45098500	4.35036600	0.72289800
C	-2.57147200	5.10448000	1.11365500
C	-0.17573700	4.89085600	0.97539300
C	-2.43027200	6.34911900	1.72496200
H	-3.56595100	4.70527100	0.93023700
C	-0.03343400	6.13373000	1.58454100
H	0.71368100	4.33382200	0.69704000
C	-1.15909300	6.87118100	1.96303200
H	-3.31401000	6.91021600	2.01498600
H	0.96142500	6.52950100	1.76845300
H	-1.04379500	7.83992200	2.43988200
H	-0.43564800	-2.21442000	0.21422900
H	-1.03430400	0.77910000	1.56072700

10a

C	3.29838800	-2.36164200	-0.42609300
C	4.61772900	-2.79223900	-0.32562400
C	5.57483300	-1.96818700	0.27058900
C	5.20596900	-0.71434700	0.76162300
C	3.88125600	-0.28994900	0.68440700
C	2.90465300	-1.11739700	0.10093100
C	1.49142300	-0.74886000	-0.06406300
B	-0.85965500	0.31846900	0.21776100
C	-0.87463800	1.91617600	-0.16873600
C	0.16172700	2.34321400	-1.15346600
C	1.12497700	3.25709600	-0.93541400
O	-1.68004800	0.08507300	1.37559500
O	-1.07171900	-0.59856800	-0.88603300
H	-1.88030300	2.09403300	-0.58501600

H	-0.81710700	2.53025900	0.73876800
H	0.13841400	1.82538400	-2.11427300
H	1.11202900	3.78896300	0.01758200
H	0.97650100	-1.15382900	-0.93441800
H	3.61706900	0.69932100	1.03717300
H	2.55558400	-2.99280200	-0.90601000
H	5.95338100	-0.06060200	1.20034200
H	4.90241000	-3.76178400	-0.72236400
H	6.60785000	-2.29571400	0.33886600
N	0.72922800	-0.03153800	0.68264200
C	1.14063400	0.55526100	1.95542800
H	1.93020300	-0.02639300	2.43505600
H	1.49185500	1.57934100	1.78990100
H	0.25052100	0.58650000	2.58455000
H	-1.72384900	-0.23695500	-1.49361500
H	-1.95713400	-0.83927600	1.36185400
C	2.19930800	3.66646500	-1.85213800
C	3.00116400	4.77240700	-1.51438500
C	2.48073600	3.00583900	-3.06421000
C	4.02793600	5.20948000	-2.34944900
H	2.80553600	5.29810100	-0.58277900
C	3.50394400	3.44244200	-3.90030800
H	1.89661300	2.13673600	-3.35140200
C	4.28506100	4.54762200	-3.55024800
H	4.62670700	6.06939900	-2.06169200
H	3.69775400	2.91420600	-4.83004500
H	5.08419000	4.88427200	-4.20409200

10b

C	3.03207800	-0.79021100	-1.69004600
C	3.45864000	-0.69253800	-3.01024500
C	2.52192800	-0.49119400	-4.02614700
C	1.16392500	-0.39104900	-3.71296600
C	0.73075400	-0.47152000	-2.39237000
C	1.66777400	-0.66035200	-1.35979000
C	1.34724200	-0.78797500	0.06397800
B	-1.08262200	0.56012600	0.31608600
C	-0.44824700	2.01079900	-0.10909400
C	-1.54858500	2.88724100	-0.61259200
C	-1.77215400	3.18867200	-1.90626400
O	-1.83975600	0.67909400	1.52590800
O	-1.75420700	-0.18678400	-0.72301600
H	0.01131400	2.46426300	0.77984500
H	0.33193300	1.90975500	-0.87228600
H	-2.24818600	3.23661700	0.14613800
H	-1.05003600	2.83178700	-2.64248500
H	2.15792300	-1.25392100	0.63268300
H	-0.32079600	-0.41727900	-2.13216100
H	3.76029500	-0.95885500	-0.90064300
H	0.43457700	-0.25447600	-4.50581100
H	4.51419600	-0.78167200	-3.24745300
H	2.84870100	-0.42388900	-5.05977600
N	0.30793300	-0.43458200	0.74303900
C	0.33292300	-0.75936300	2.17649900
H	1.26942200	-1.25271300	2.45296400
H	0.19153900	0.15187600	2.75741500
H	-0.50785100	-1.41745600	2.40734300
H	-2.27352800	0.44377000	-1.24087500

H	-2.54414400	0.02014300	1.50019600
C	-2.87247200	3.98857000	-2.46494600
C	-2.87835400	4.26993400	-3.84352500
C	-3.93495200	4.49758400	-1.69236600
C	-3.89157600	5.02809100	-4.42770400
H	-2.06917000	3.88739600	-4.46113500
C	-4.94610900	5.25625800	-2.27390200
H	-3.97121000	4.29538300	-0.62633300
C	-4.93268000	5.52759700	-3.64526200
H	-3.86652700	5.22913700	-5.49527500
H	-5.75312400	5.63728000	-1.65388700
H	-5.72466500	6.11881800	-4.09546400

11a

C	3.65772300	-0.65934900	-1.08395700
C	5.02300500	-0.89810800	-0.95545500
C	5.67987100	-0.58807800	0.23572300
C	4.95730600	-0.02314700	1.28860400
C	3.59027100	0.21331800	1.16442900
C	2.90469000	-0.11847300	-0.02255200
C	1.47196300	0.09188900	-0.27347300
B	-0.96217300	0.15409300	0.11305300
C	-0.76651700	2.30194900	0.39672800
C	0.11529900	2.61329900	-0.63493800
C	1.50643800	2.48491000	-0.57619800
O	-1.93285900	-0.23860300	1.03266500
O	-1.29109500	-0.00910800	-1.24081000
H	-1.82024700	2.53626500	0.27557400
H	-0.41566900	2.31287400	1.42555500

H	-0.32819000	2.82129300	-1.61075300
H	1.96521100	2.53164100	0.40862800
H	1.18770100	-0.02283100	-1.31339900
H	3.06548200	0.68196800	1.98735400
H	3.15732500	-0.90107900	-2.01690600
H	5.46150700	0.24212900	2.21333000
H	5.57370200	-1.32391300	-1.78879800
H	6.74472800	-0.77281500	0.33963200
N	0.45306600	-0.08572100	0.57956300
C	0.66274700	-0.28717500	2.01530200
H	1.48665700	-0.98363100	2.18084200
H	0.88608600	0.65323500	2.53414300
H	-0.25426900	-0.69779200	2.43294300
H	-0.80819400	0.58085200	-1.82599100
H	-2.78291600	-0.29511800	0.58234700
C	2.41432500	2.74252100	-1.69756900
C	3.76630900	3.05003700	-1.44533400
C	2.00908900	2.66720300	-3.04693100
C	4.66249400	3.29067500	-2.48405000
H	4.10948300	3.10431300	-0.41592200
C	2.90358100	2.91339100	-4.08480300
H	0.98148900	2.41126700	-3.29001700
C	4.23700300	3.22901900	-3.81199900
H	5.69706800	3.53058600	-2.25455300
H	2.55912400	2.85322600	-5.11369500
H	4.93351900	3.41896600	-4.62311600

11b

C	1.32519800	-0.19726100	-0.19905800

B	-1.18488700	0.15237700	0.12047100
C	-0.76011200	2.32909700	0.24687100
C	0.19657600	2.51734500	-0.74632300
C	1.57140300	2.37648700	-0.56579900
O	-2.14674300	-0.05583600	1.10538600
O	-1.62149500	0.01659000	-1.19319200
H	-1.79359700	2.58672800	0.03805100
H	-0.46920800	2.40622500	1.29066800
H	-0.16950500	2.66662300	-1.76259800
H	1.93116800	2.38955900	0.46167600
N	0.22580100	-0.16342500	0.56849200
C	0.48912500	-0.03032600	2.01255200
H	0.92558000	-0.95872700	2.39288100
H	1.19093300	0.78974500	2.20516200
H	-0.44408700	0.16156500	2.53598900
H	-0.94780300	0.22378300	-1.84900300
H	-3.02273200	-0.00163000	0.70735400
C	2.59756300	2.61545900	-1.57483000
C	3.93334500	2.82293900	-1.16612800
C	2.33596600	2.63938800	-2.96184200
C	4.94988400	3.05303600	-2.08848000
H	4.16500100	2.81164800	-0.10354000
C	3.35229300	2.87864100	-3.88297500
H	1.32766700	2.46536100	-3.32392600
C	4.66605100	3.08632900	-3.45640300
H	5.96609100	3.21423400	-1.73914000
H	3.11751100	2.89538700	-4.94375500
H	5.45639200	3.26938300	-4.17807000
H	2.26148600	-0.02093400	0.32239100

C	1.46350300	-0.84757200	-1.50156300
C	0.52594000	-1.77285700	-2.01376900
C	2.65782700	-0.64480000	-2.22849800
C	0.75896800	-2.42226100	-3.22397300
H	-0.37066700	-1.99872700	-1.45214000
C	2.88260300	-1.29868200	-3.43485700
H	3.40740300	0.03566700	-1.84065100
C	1.93046300	-2.18460000	-3.94508200
H	0.02616700	-3.13297900	-3.59498400
H	3.80524000	-1.11590400	-3.97739500
H	2.10824800	-2.69790600	-4.88538800

11c

C	-0.03495200	0.44281000	-4.74875000
C	0.68496900	0.34249400	-5.93313100
C	2.07337300	0.19746900	-5.89991300
C	2.72740100	0.17064900	-4.66729500
C	2.01063100	0.26891400	-3.47795200
C	0.60279500	0.38468800	-3.48858700
C	-0.27022400	0.49272500	-2.32713900
B	-1.16413800	0.22763200	-0.07950400
C	-0.20466800	2.24018000	0.54370700
C	0.51317700	2.71291800	-0.55054800
C	-0.03061400	3.03860000	-1.79244000
O	-1.08294100	-0.54135400	1.08282000
O	-2.37817300	0.70944900	-0.58141900
H	-1.25113700	2.51043500	0.64283700
H	0.32284900	2.03832000	1.47147300
H	1.60103100	2.69332400	-0.46886700

H	-1.11621500	3.09549400	-1.84759900
H	-1.29155000	0.78044600	-2.54191800
H	2.55581100	0.28360600	-2.54399900
H	-1.11501100	0.55279400	-4.78574000
H	3.80954200	0.08533500	-4.62909800
H	0.16222400	0.38022100	-6.88430000
H	2.63982300	0.12026000	-6.82290500
N	-0.13078300	-0.05044300	-1.10801900
C	1.11362100	-0.68471200	-0.67296100
H	1.47578000	-1.36685600	-1.44460400
H	1.88847400	0.06115600	-0.46212400
H	0.91171200	-1.24069400	0.24018900
H	-3.11827500	0.47857300	-0.01156900
H	-1.60024800	-0.17957300	1.80841800
C	0.67724400	3.62842800	-2.92044900
C	-0.06326800	4.07905800	-4.03544200
C	2.08046600	3.78114600	-2.97750100
C	0.55711200	4.65410900	-5.14023800
H	-1.14607000	3.97976600	-4.01853900
C	2.69915700	4.35807200	-4.08216800
H	2.69369500	3.45715300	-2.14233500
C	1.94561000	4.79885700	-5.17322400
H	-0.04583700	4.99406700	-5.97813900
H	3.78060300	4.46664000	-4.09174100
H	2.43282600	5.25040300	-6.03227700

11d

C	0.29161800	-0.46008500	-1.82060000
B	-1.40803500	0.14146300	-0.00440200

C	-1.13088100	2.26381000	-0.50825300
C	-0.03745200	2.52055000	-1.35336500
C	0.04790300	2.15197800	-2.68358600
O	-1.48897800	0.09323600	1.38653400
O	-2.58957300	-0.15556800	-0.68467600
H	-2.11786100	2.20501200	-0.95845700
H	-1.11844400	2.69962700	0.48671900
H	0.85954900	2.92916400	-0.88688700
H	-0.86962800	1.83209500	-3.17508600
N	-0.04135800	-0.24372500	-0.55018900
C	1.09421100	0.07326800	0.33520100
H	1.66146600	-0.84078900	0.53398300
H	1.75647500	0.80290300	-0.14163000
H	0.72291300	0.47378000	1.27481300
H	-2.52106500	-0.10289000	-1.64336800
H	-2.41515400	0.13265800	1.64975800
C	1.17672800	2.39863100	-3.57966300
C	0.98366300	2.31111200	-4.97542500
C	2.47600900	2.72052200	-3.12826200
C	2.02762500	2.53363400	-5.87129000
H	-0.00834600	2.07719000	-5.35355900
C	3.51527400	2.94870400	-4.02389300
H	2.67534200	2.78640400	-2.06264500
C	3.30209500	2.85553400	-5.40287700
H	1.84211100	2.46216300	-6.93960600
H	4.50305800	3.19557000	-3.64406600
H	4.11717500	3.03101400	-6.09832000
H	1.32534500	-0.25235200	-2.08198100
C	-0.46877300	-1.20756400	-2.81995900

C	-1.47781100	-2.14003300	-2.49232900
C	-0.08752000	-1.08756300	-4.17511300
C	-2.10896400	-2.87914800	-3.49167500
H	-1.75045400	-2.29579900	-1.45660700
C	-0.72182700	-1.82895600	-5.16434300
H	0.70240900	-0.39317600	-4.44323900
C	-1.74270200	-2.72428600	-4.82911500
H	-2.88074300	-3.59263800	-3.21814900
H	-0.41765200	-1.71257500	-6.20040000
H	-2.23507900	-3.30666300	-5.60205100

12a

C	3.08298200	-1.33178900	-0.89858500
C	4.31258900	-1.97485100	-0.76610800
C	5.33871600	-1.37545300	-0.03369300
C	5.12084800	-0.13389800	0.56281000
C	3.88745700	0.50589100	0.42646500
C	2.85132900	-0.08150800	-0.30920300
C	1.46102300	0.54317300	-0.45059500
B	-0.71610300	-0.56668600	0.23718300
C	-0.78496800	3.20240900	-0.02596900
C	0.06810600	2.61657400	-0.86584000
C	1.45056500	2.11278500	-0.50998600
O	-1.42468300	-1.21643200	1.22595800
O	-1.27656900	-0.55763800	-1.03019700
H	-1.76188000	3.54558900	-0.35291300
H	-0.53674200	3.36281600	1.02000200
H	-0.21749000	2.49629200	-1.91315900
H	1.69078800	2.48747200	0.49139600

H	1.07917700	0.18929600	-1.41468900
H	3.74244600	1.47450800	0.89328300
H	2.28575200	-1.80780700	-1.46465100
H	5.91202100	0.34200600	1.13511200
H	4.47007500	-2.94135900	-1.23629500
H	6.29959100	-1.87110800	0.06941200
N	0.53880400	0.02553600	0.56689300
C	0.97030400	0.09988300	1.95904300
H	1.85584300	-0.51739000	2.14982600
H	1.21267600	1.12942300	2.25592100
H	0.16006800	-0.25268900	2.59591300
H	-0.91976000	0.12732300	-1.60322900
H	-2.28175000	-1.49425900	0.88304800
C	2.46261800	2.70358300	-1.48814900
C	3.26147100	3.78745400	-1.10187900
C	2.58007700	2.23178000	-2.80331600
C	4.15728000	4.37754600	-1.99348300
H	3.17701300	4.17588700	-0.08973300
C	3.47481800	2.81784700	-3.69862600
H	1.97504100	1.39349600	-3.13768000
C	4.26807800	3.89343600	-3.29724900
H	4.76735200	5.21577100	-1.66899300
H	3.55285300	2.43168700	-4.71096400
H	4.96531700	4.34937900	-3.99388700

12b

C	1.35267000	0.31565500	-0.47620600
B	-1.07252700	-0.22792500	0.19241800
C	-0.76359900	3.19577700	-0.92969500

C	0.09157600	2.32376000	-1.46415600
C	1.36208800	1.86240800	-0.79019300
O	-1.97303000	-0.26037200	1.23874300
O	-1.57770400	-0.44997900	-1.06957100
H	-1.67448300	3.48854900	-1.44315200
H	-0.58713500	3.64559400	0.04443300
H	-0.13685000	1.90300800	-2.44164300
H	1.36187600	2.32238600	0.20712900
N	0.31107500	-0.00821000	0.50421300
C	0.71466300	0.18533900	1.89308900
H	1.58959100	-0.43377000	2.13601000
H	0.97800000	1.23047200	2.11591300
H	-0.10491700	-0.09711500	2.55245800
H	-0.89874300	-0.55090300	-1.74660200
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C	2.64576100	2.35807800	-1.47293700
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C	2.60675400	3.24404700	-2.55906000
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H	1.64732300	3.57659200	-2.94178400
C	5.02376600	3.33326300	-2.65105600
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H	5.93762500	3.70519600	-3.10476700
H	2.30344300	0.12177800	0.03705200
C	1.35866300	-0.65591500	-1.66733400
C	1.22610000	-2.03057500	-1.39617800

C	1.56799400	-0.26969300	-2.99896500
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H	1.05837400	-2.34729200	-0.37172000
C	1.62807200	-1.22078100	-4.02257900
H	1.70869500	0.77350100	-3.25013700
C	1.49010700	-2.57667100	-3.73695600
H	1.18379700	-4.03250900	-2.17384400
H	1.78806600	-0.89183300	-5.04528900
H	1.53698200	-3.31348100	-4.53334100

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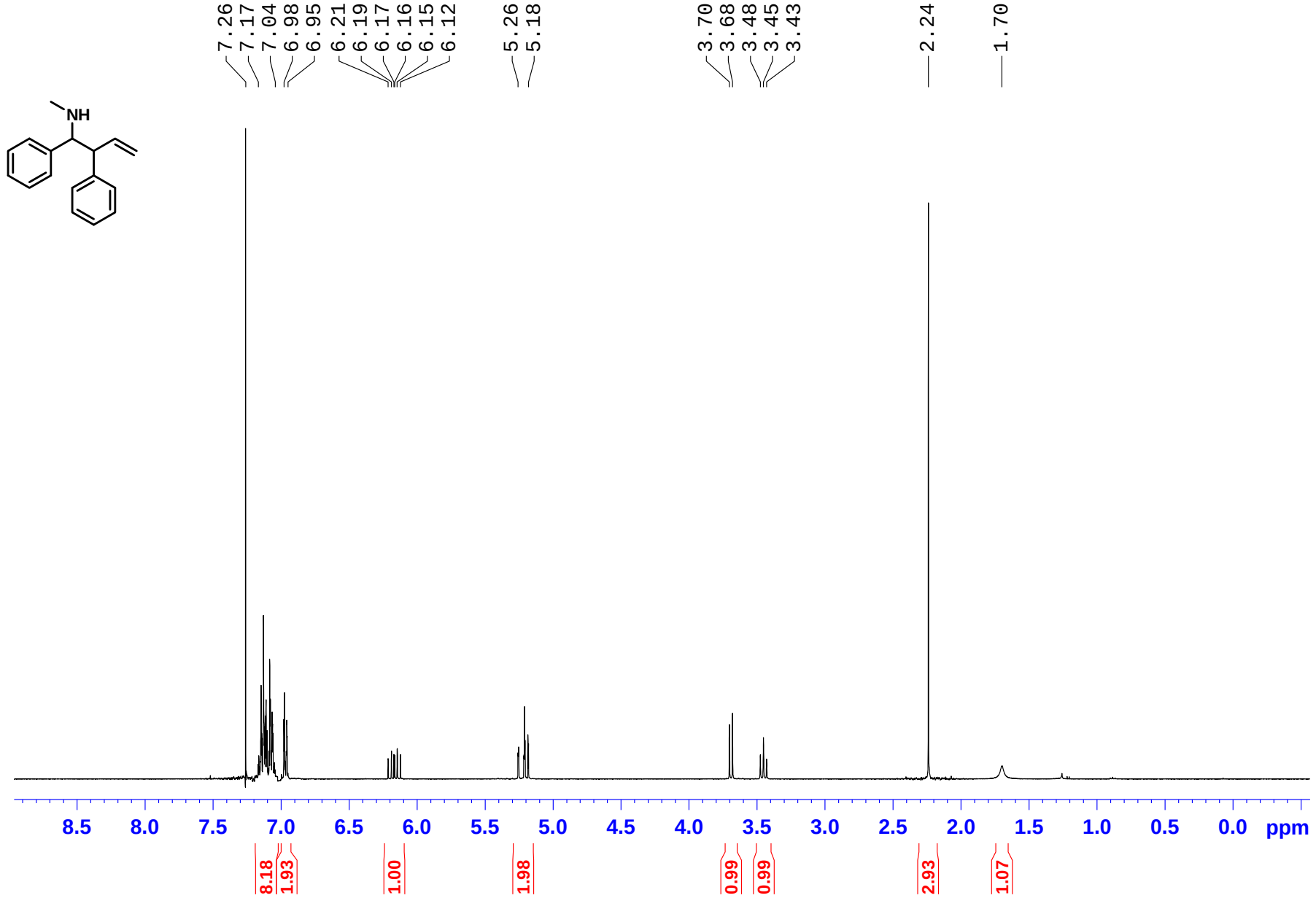
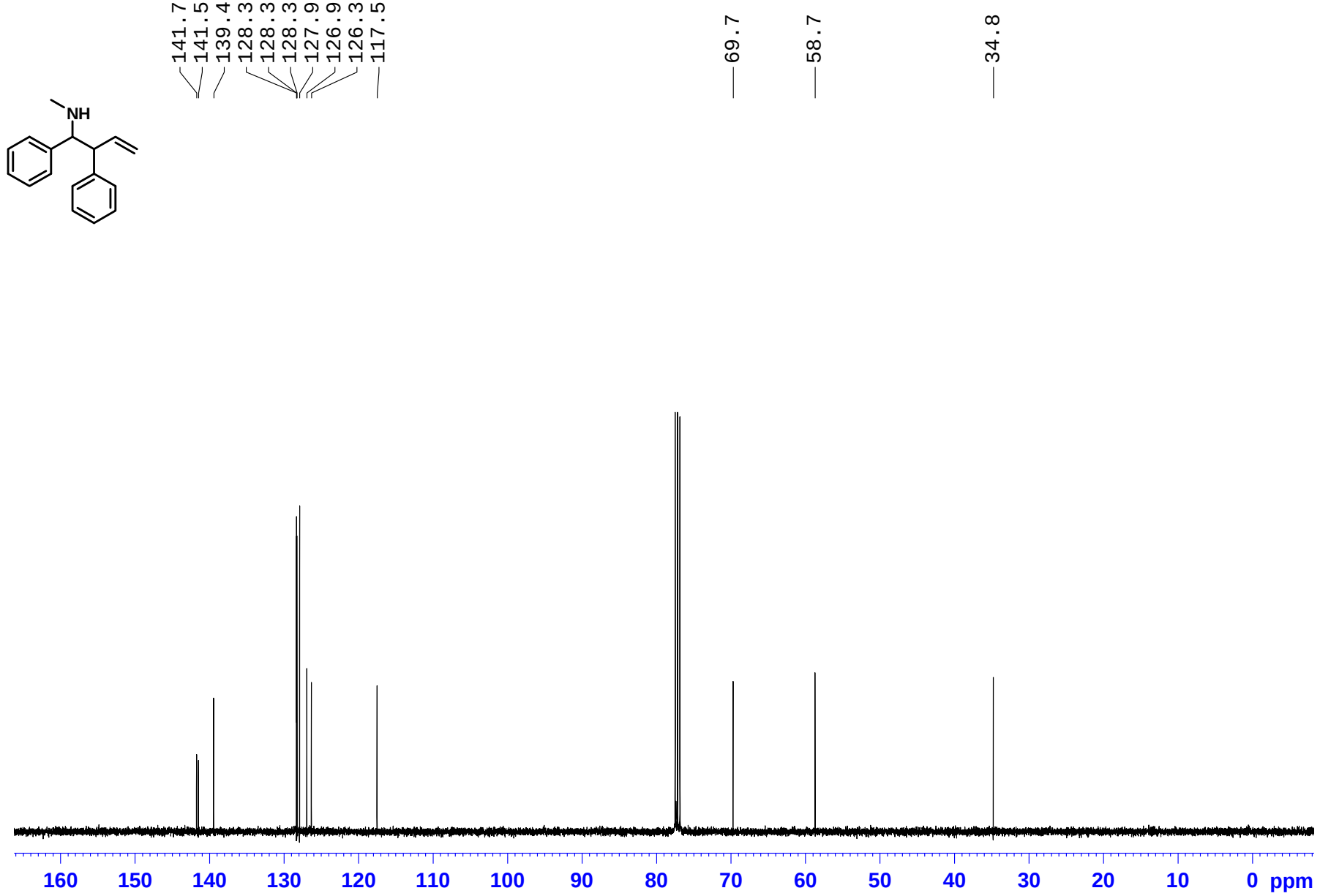
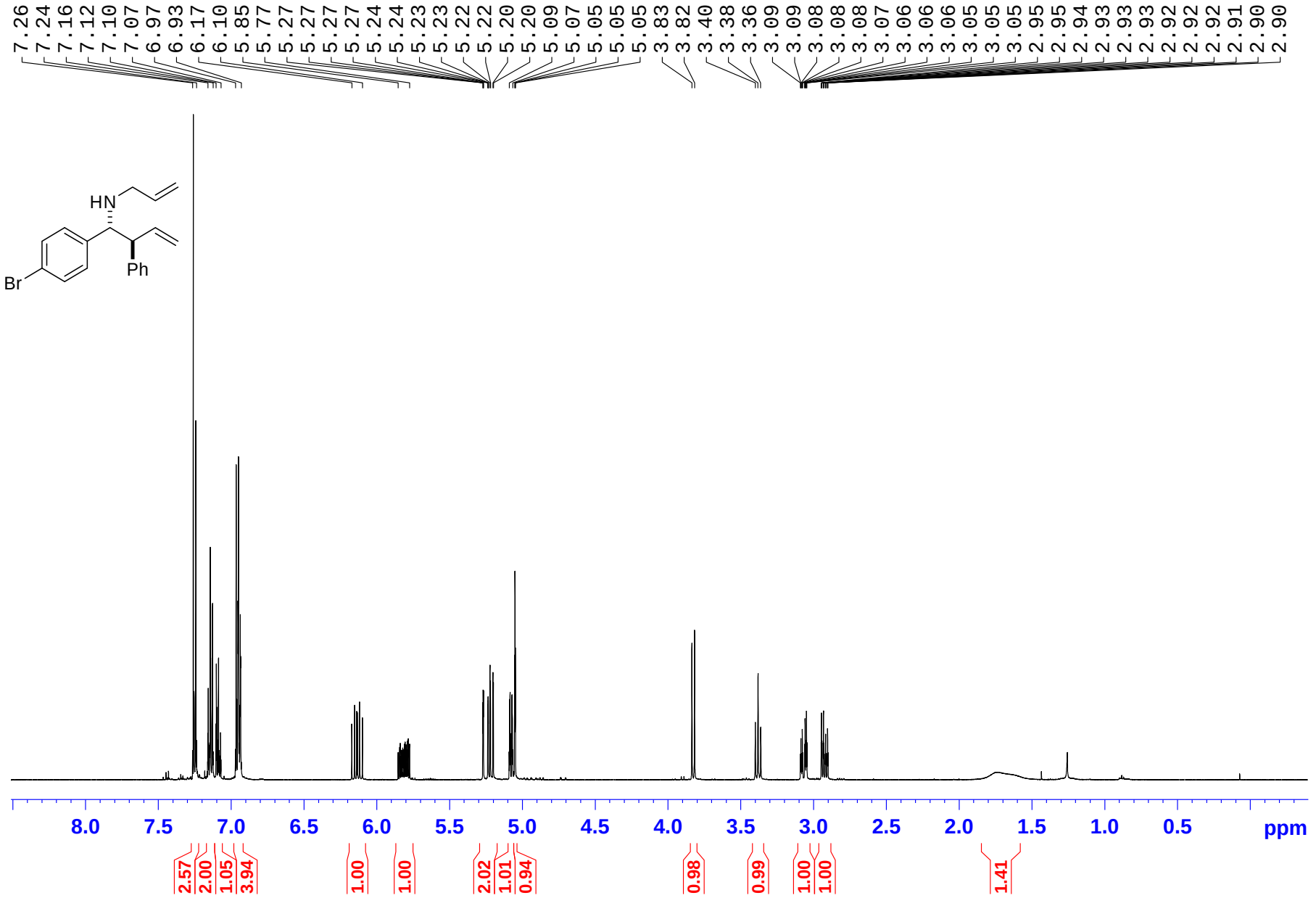
^{1}H NMR ($CDCl_3$, 400 MHz) of compound **3a**



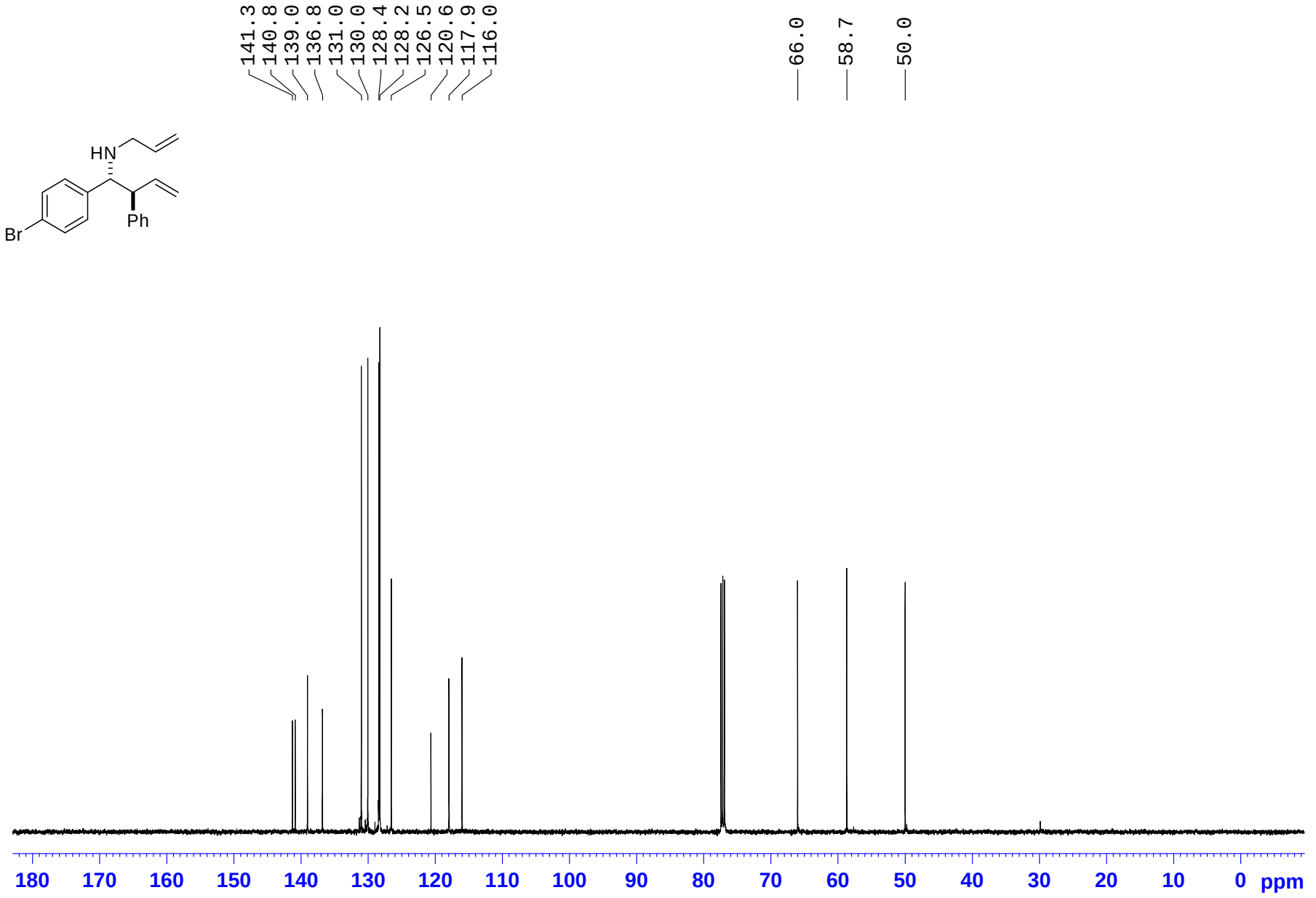
^{13}C NMR ($CDCl_3$, 101 MHz) of compound **3a**



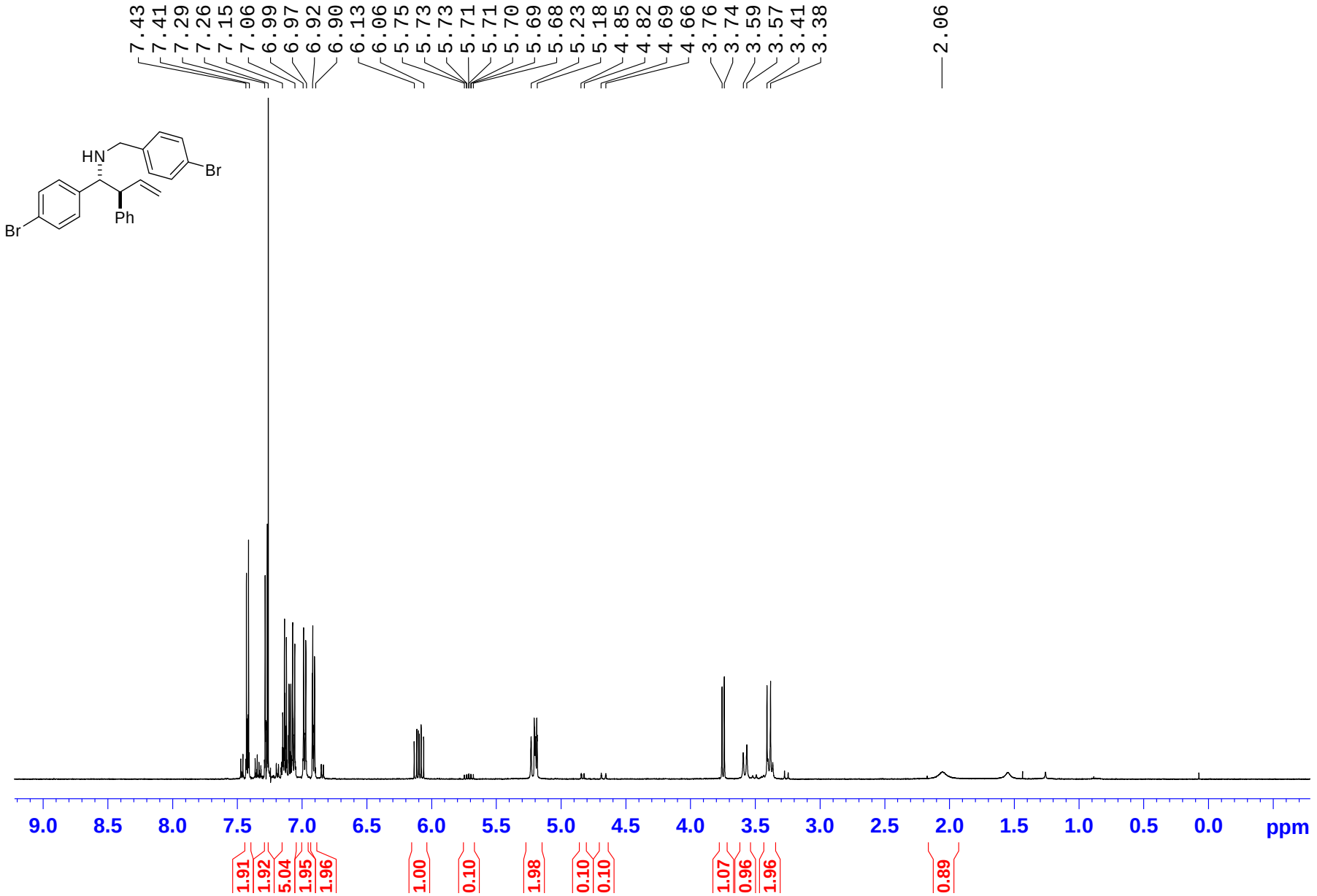
^{1}H NMR ($CDCl_3$, 500 MHz) of compound **3b**



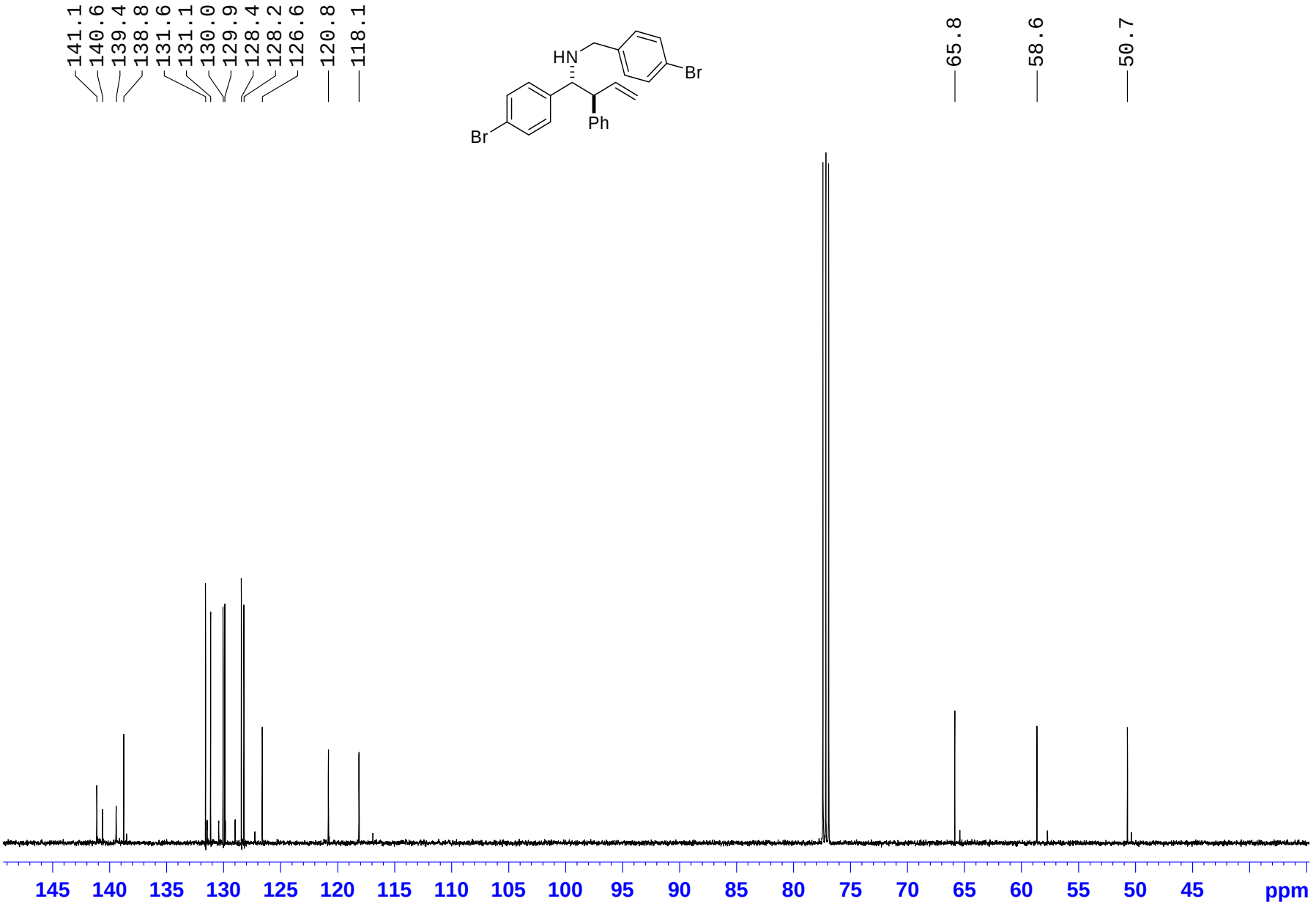
^{13}C NMR ($CDCl_3$, 125 MHz) of compound **3b**



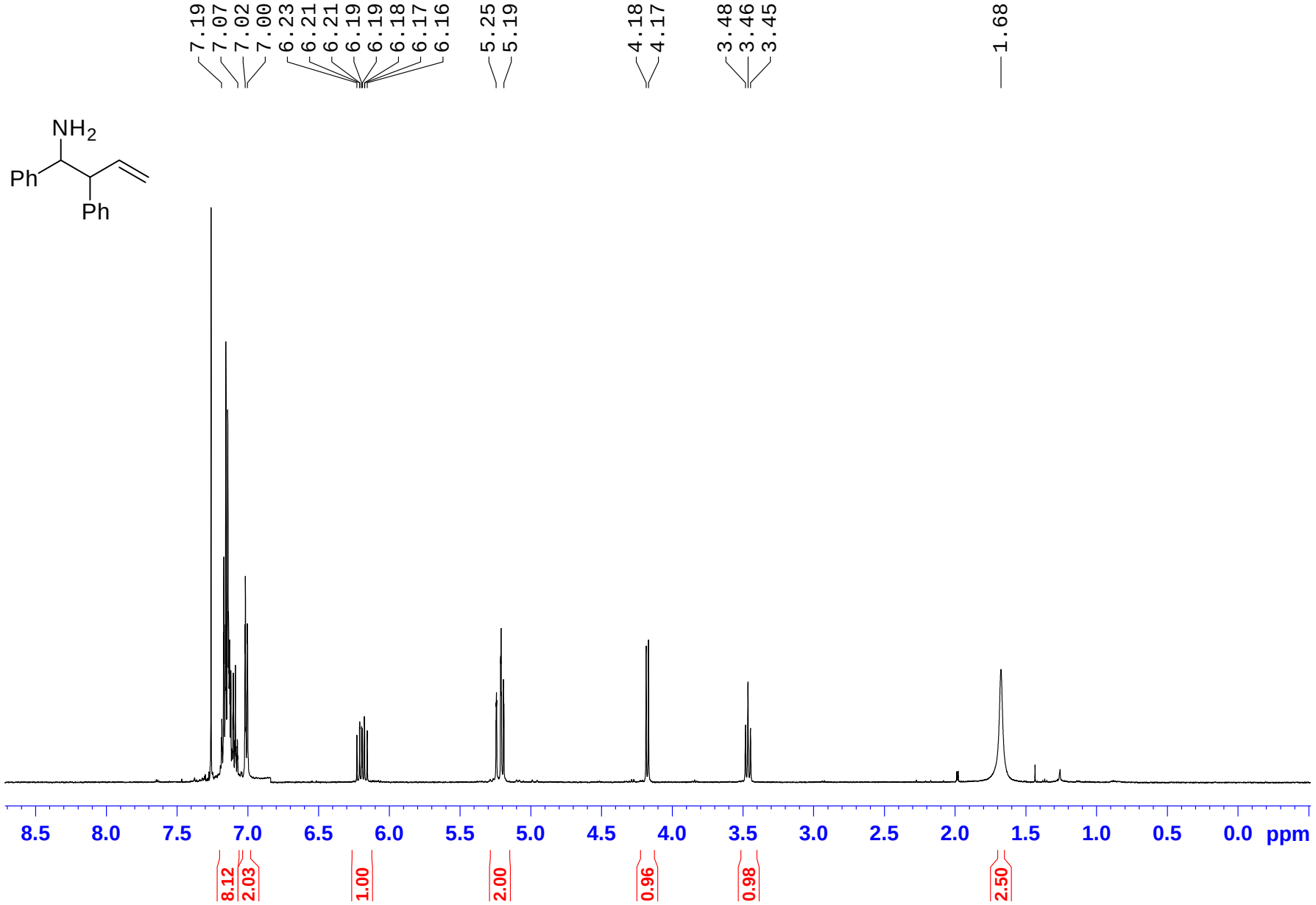
^{1}H NMR ($CDCl_3$, 500 MHz) of compound **3c**



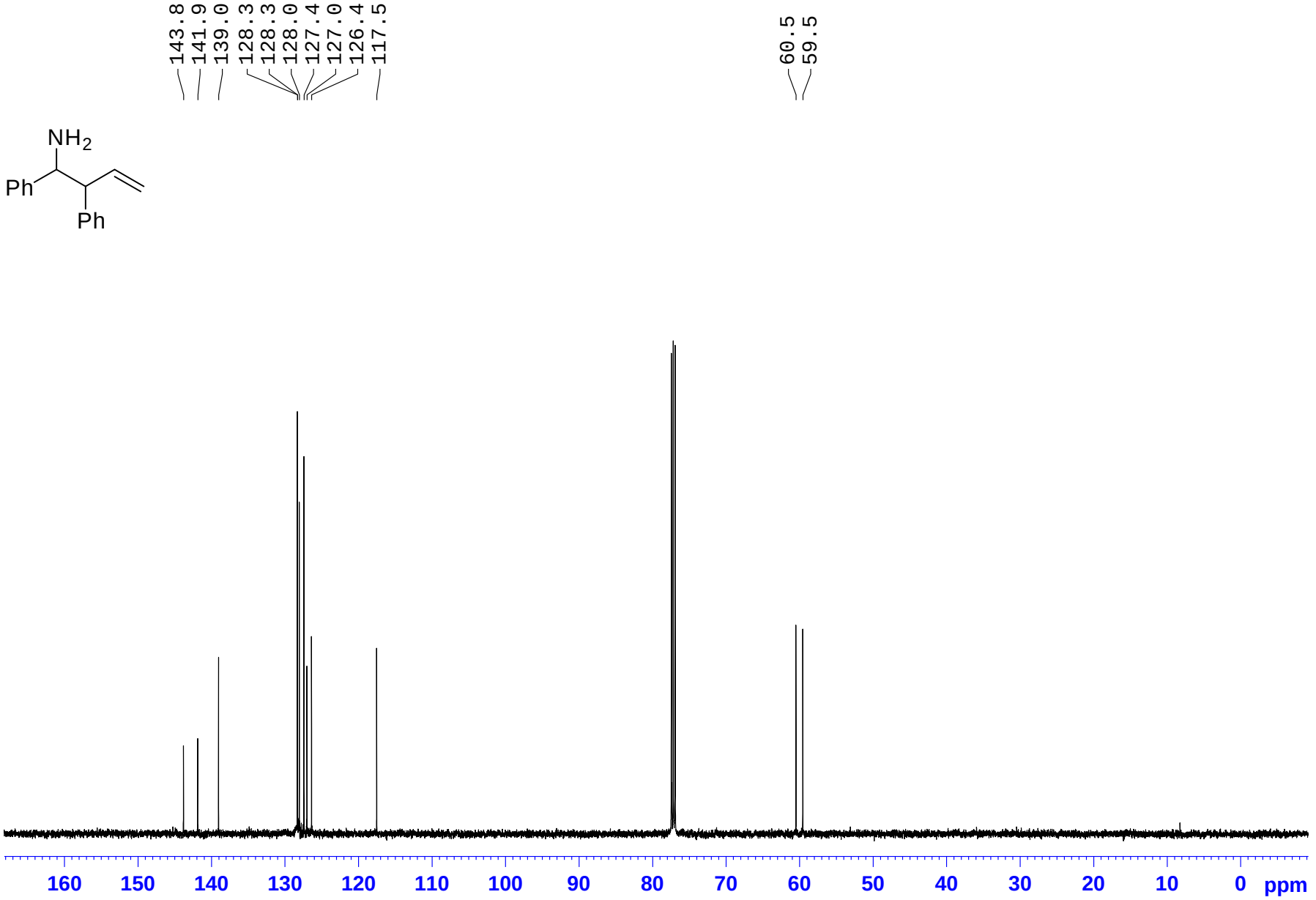
^{13}C NMR ($CDCl_3$, 125 MHz) of compound 3c



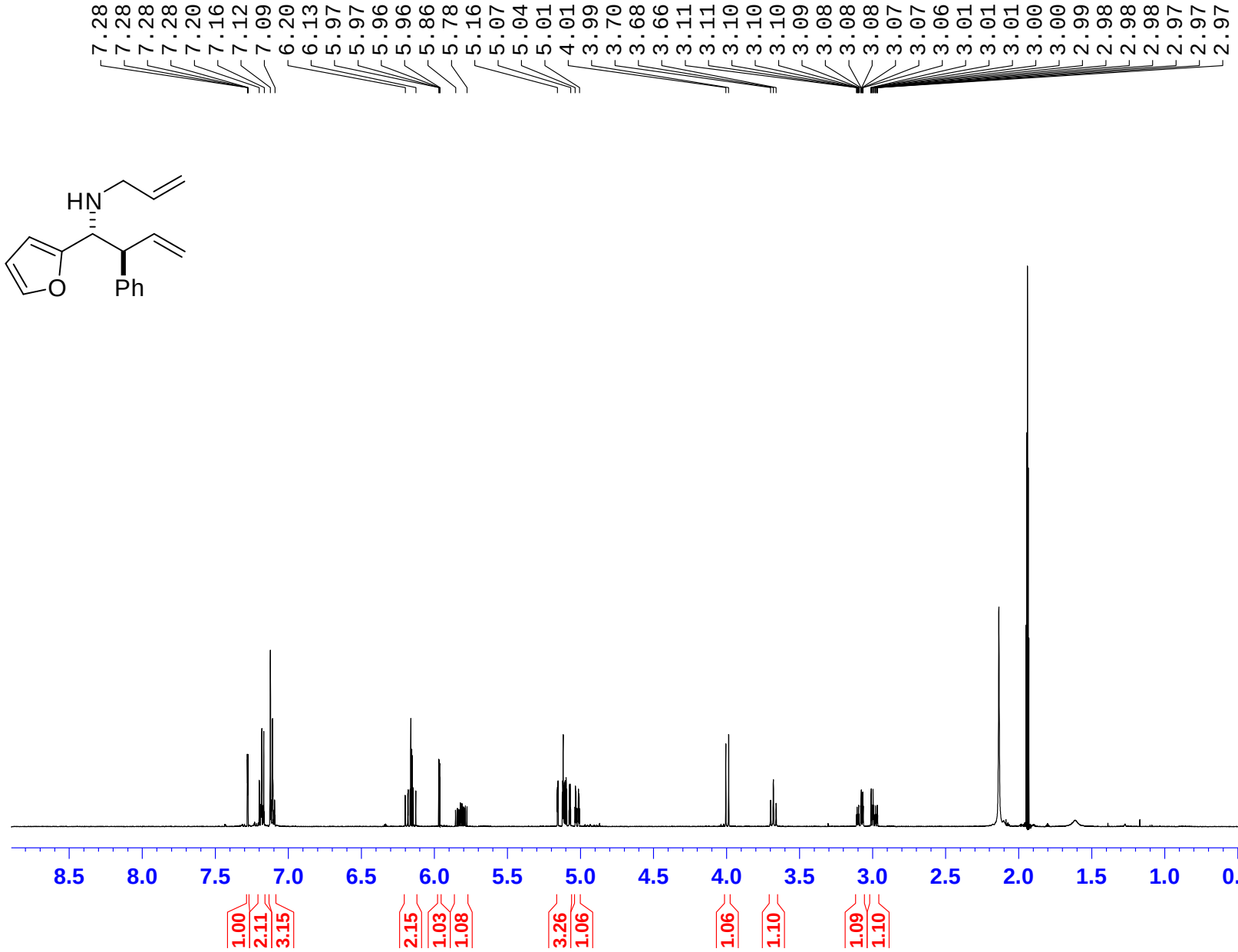
^{1}H NMR ($CDCl_3$, 500 MHz) of compound **3d**



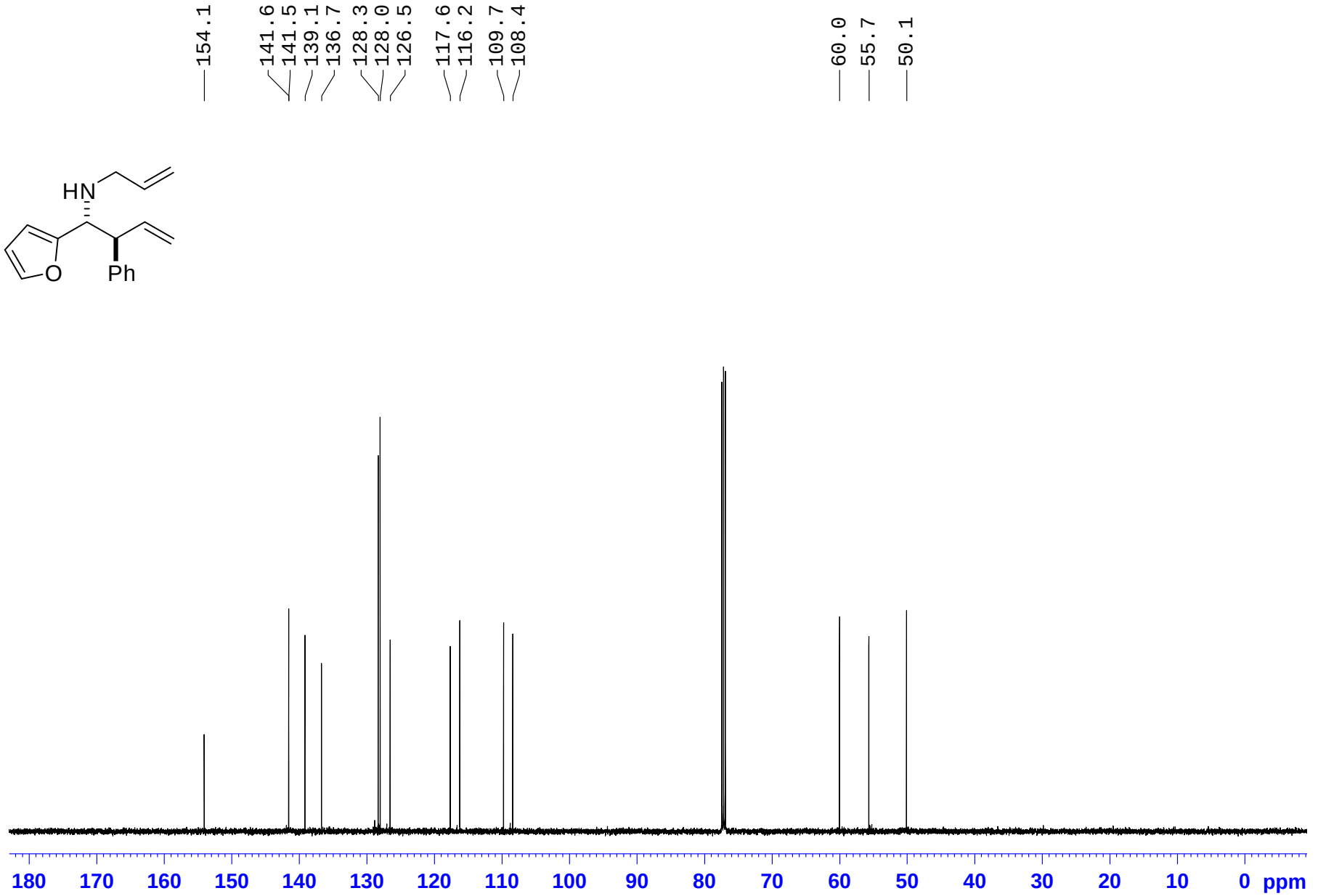
^{13}C NMR ($CDCl_3$, 125 MHz) of compound **3d**



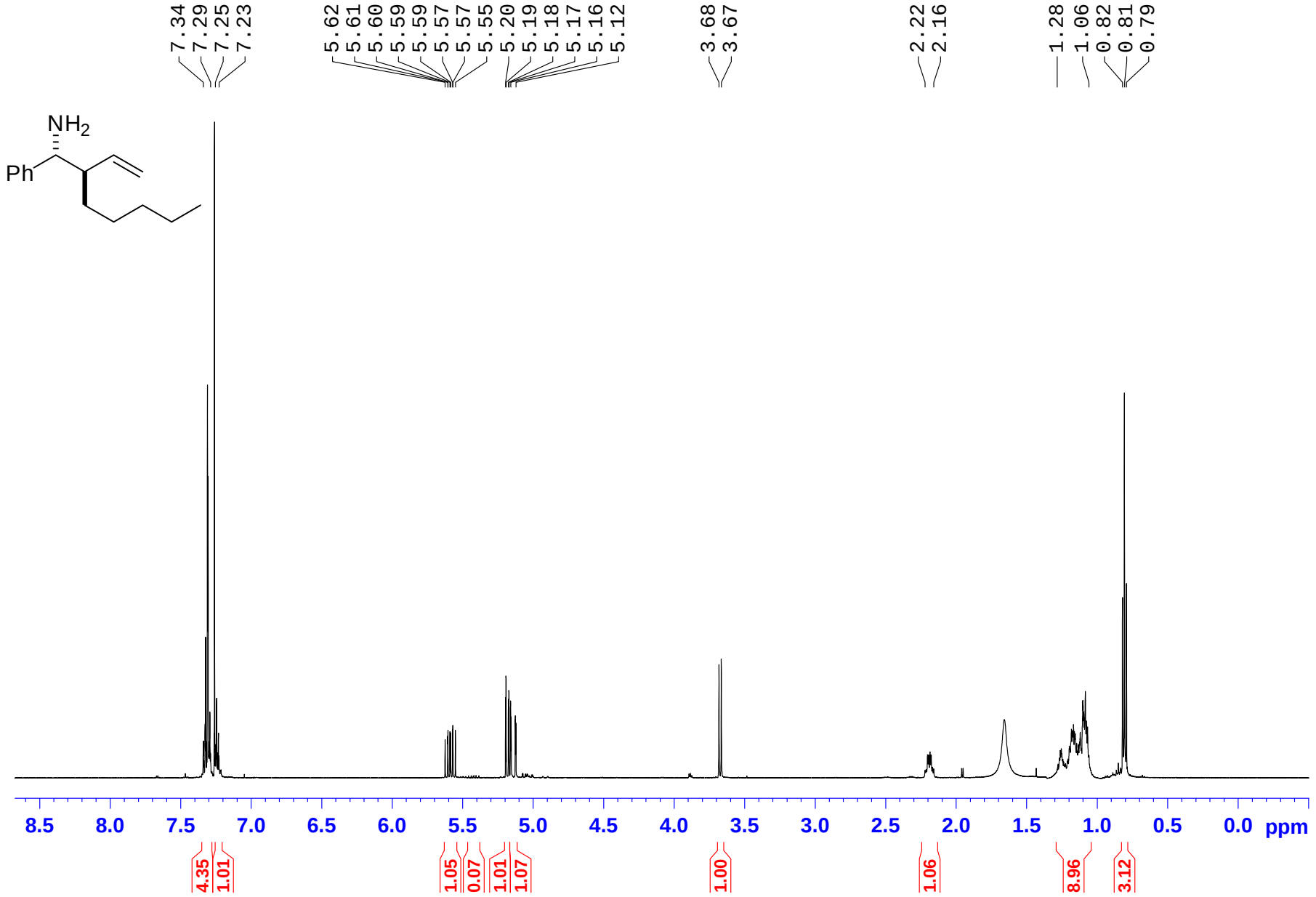
^{1}H NMR (CD_3CN, 500 MHz) of compound **3e**



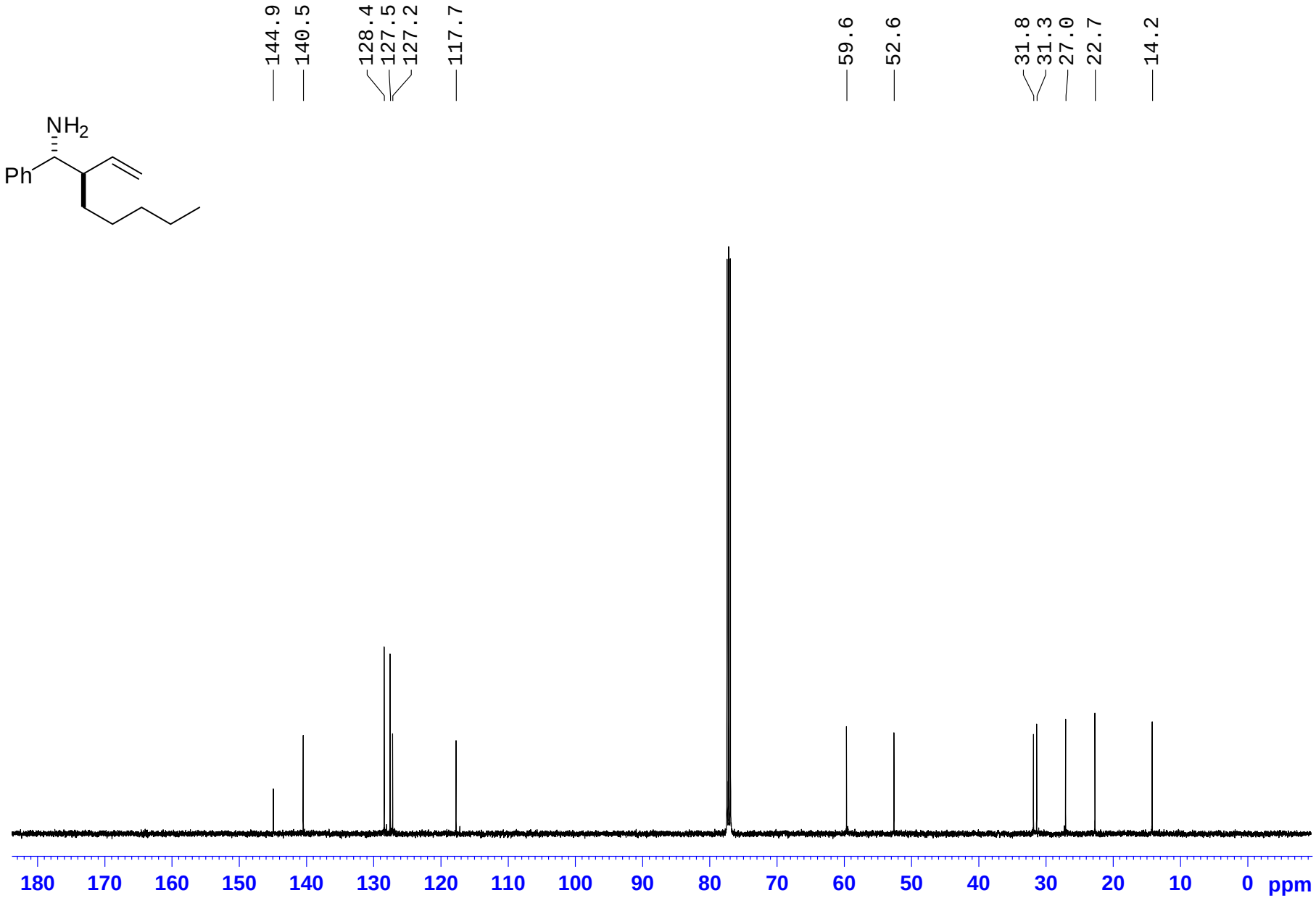
^{13}C NMR ($CDCl_3$, 125 MHz) of compound **3e**



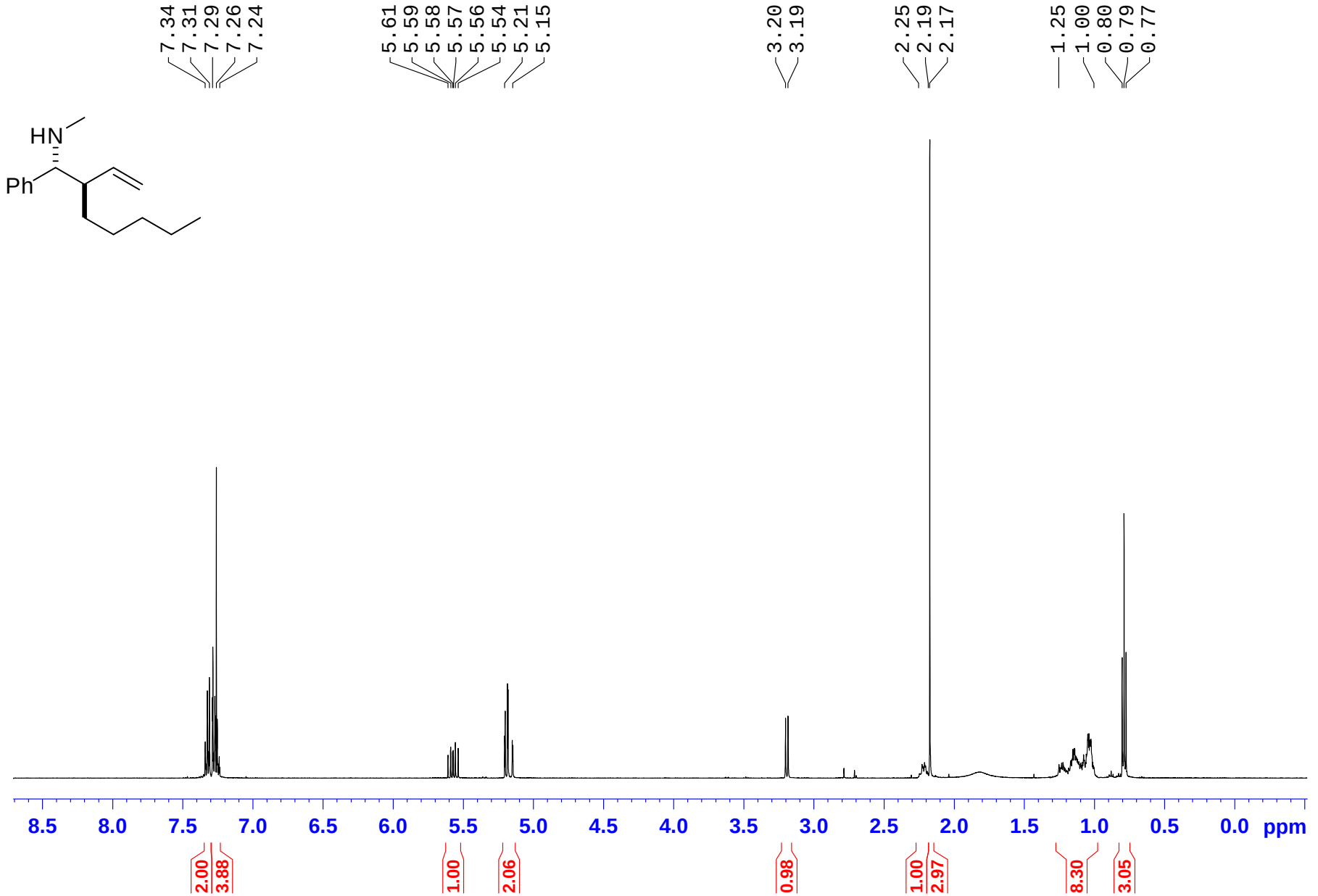
^{1}H NMR ($CDCl_3$, 500 MHz) of compound **3f**



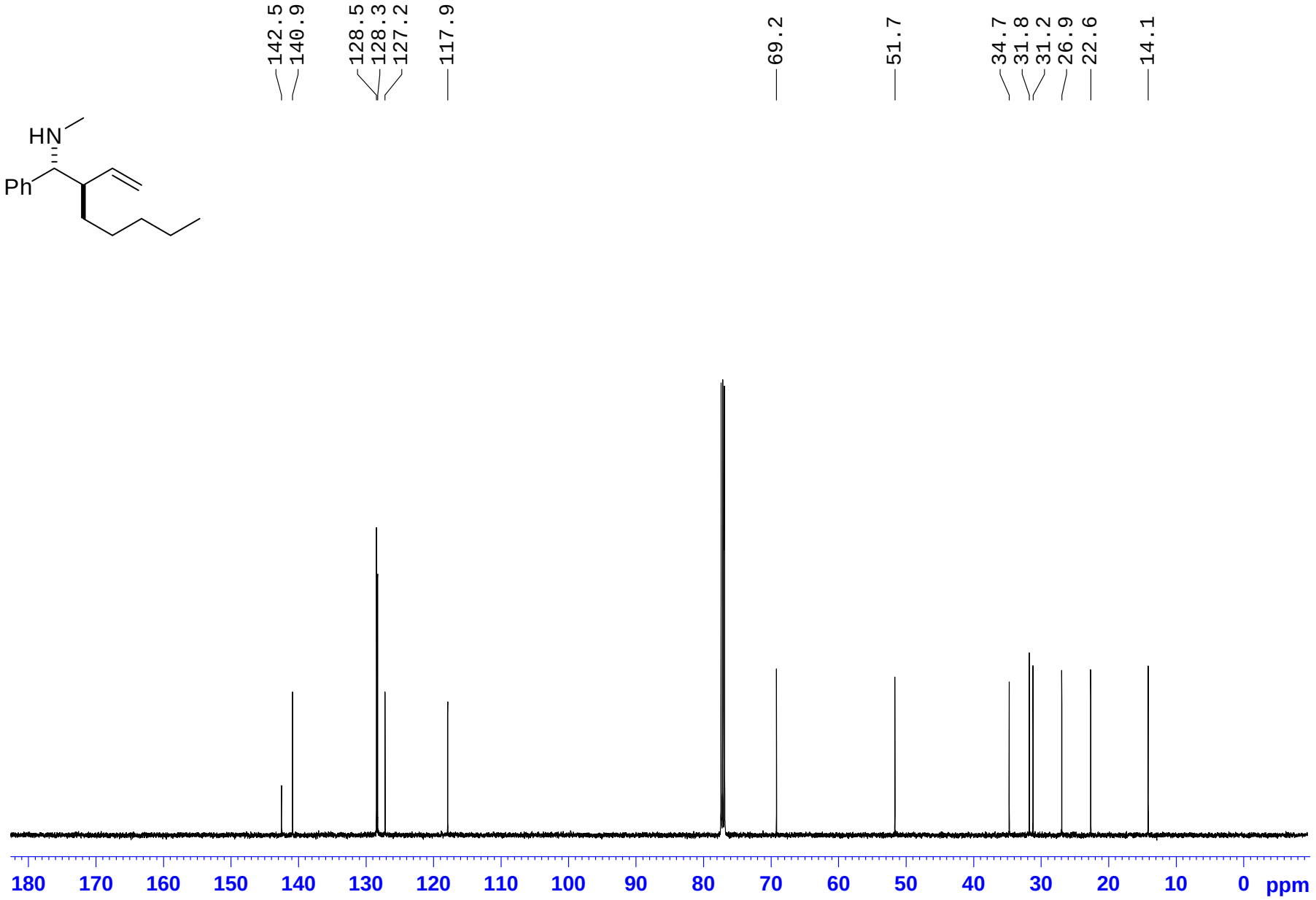
^{13}C NMR ($CDCl_3$, 125 MHz) of compound **3f**



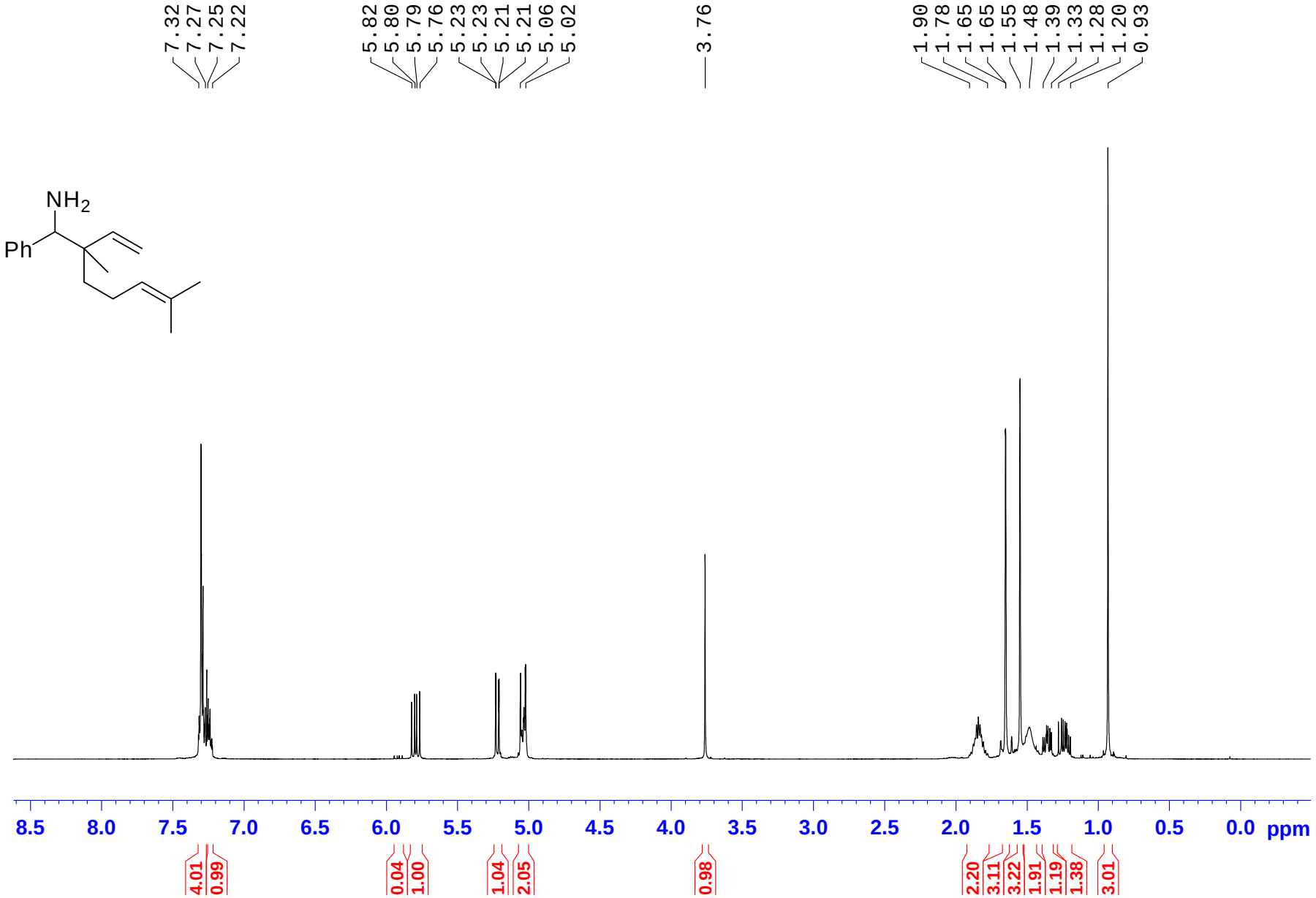
^{1}H NMR ($CDCl_3$, 500 MHz) of compound **3g**



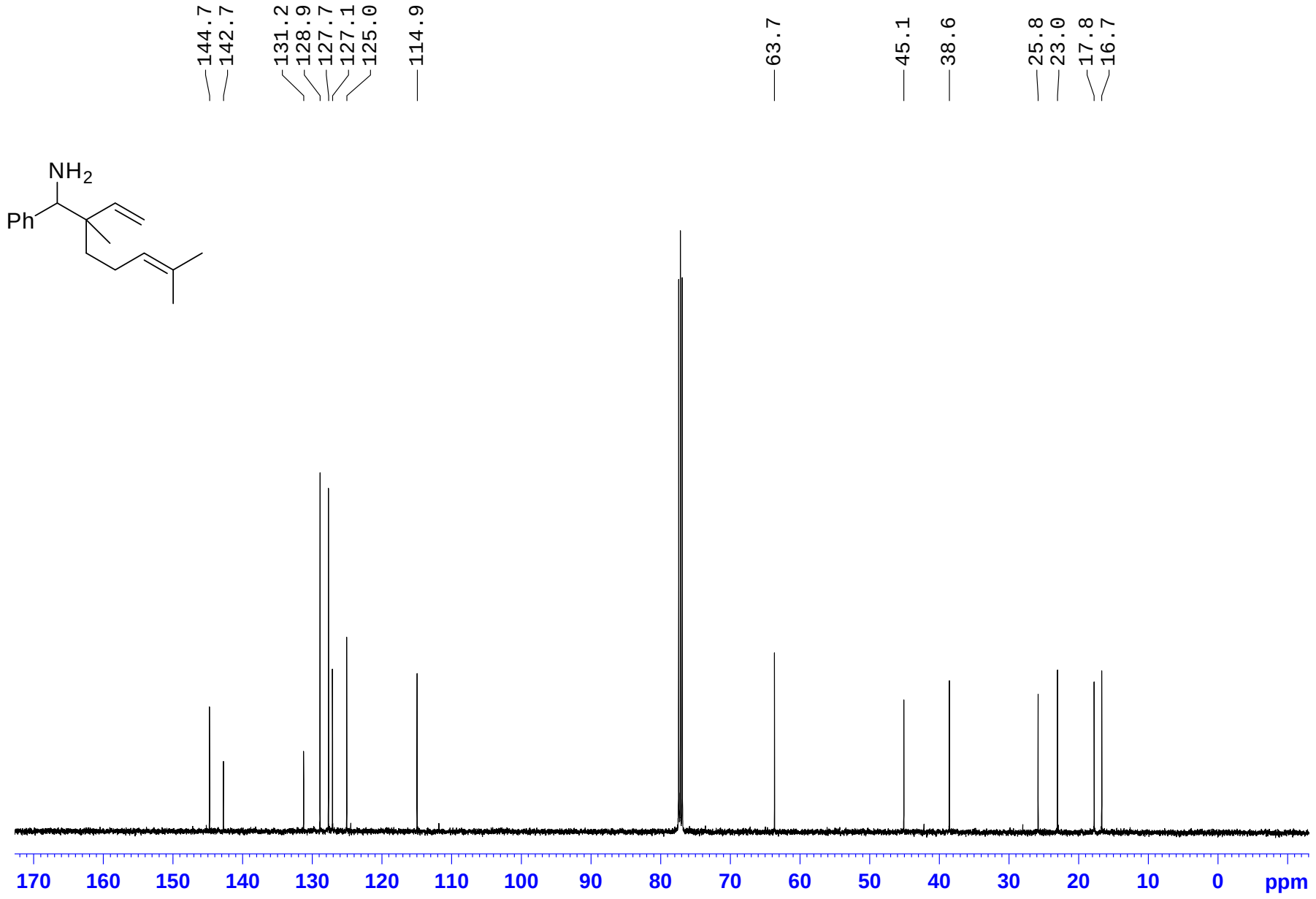
^{13}C NMR ($CDCl_3$, 125 MHz) of compound **3g**



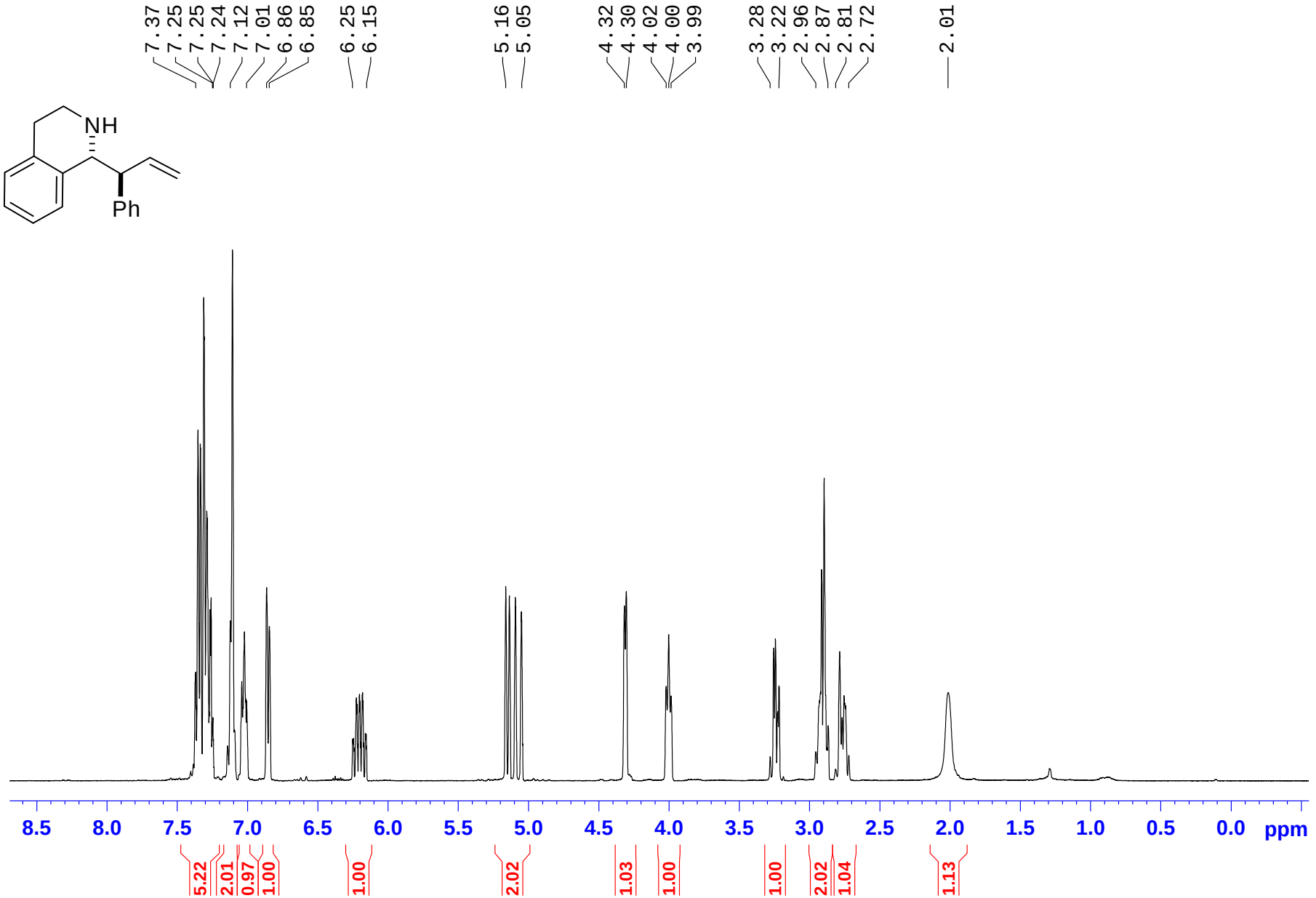
^{1}H NMR ($CDCl_3$, 500 MHz) of compound **3h**



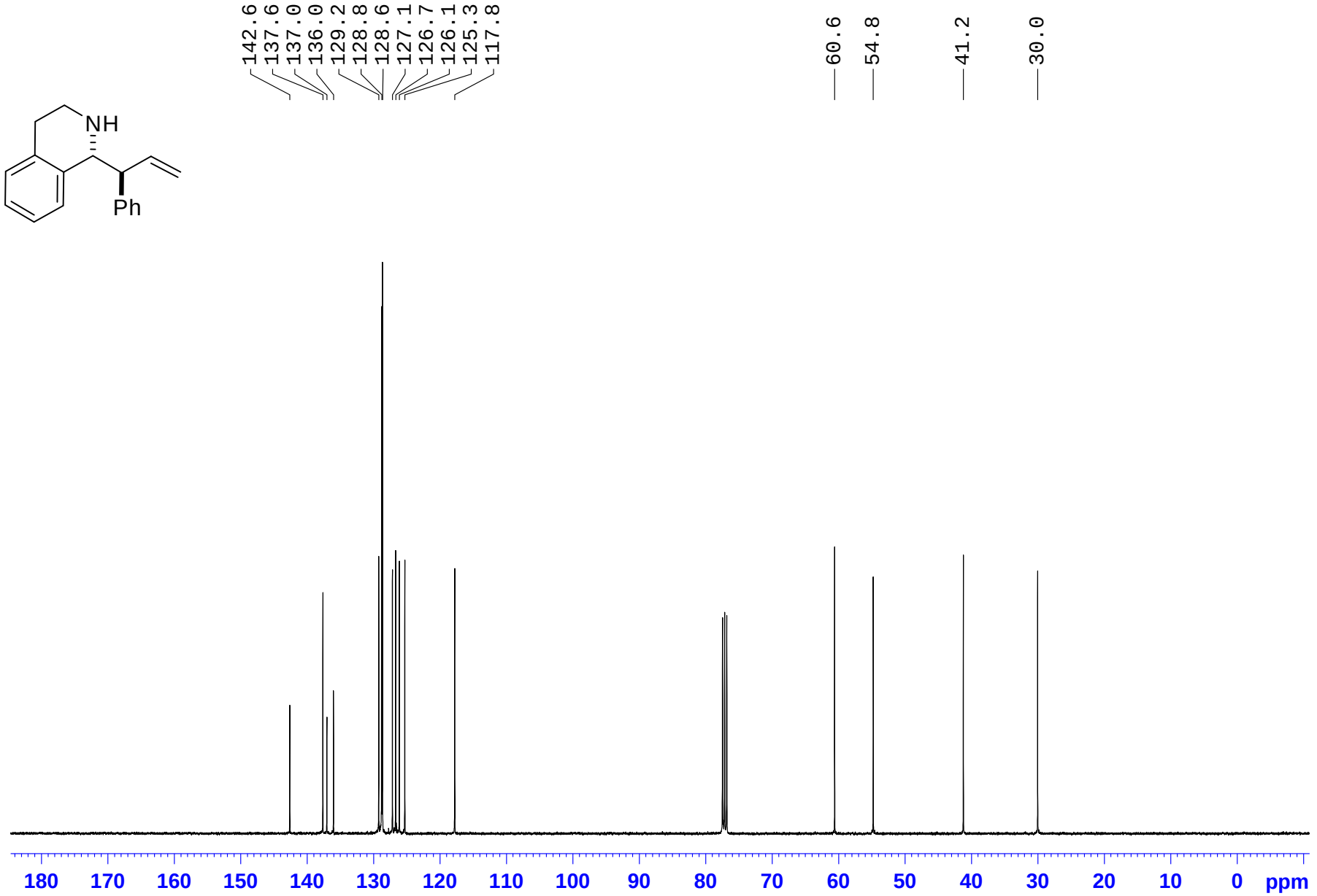
^{13}C NMR ($CDCl_3$, 125 MHz) of compound **3h**



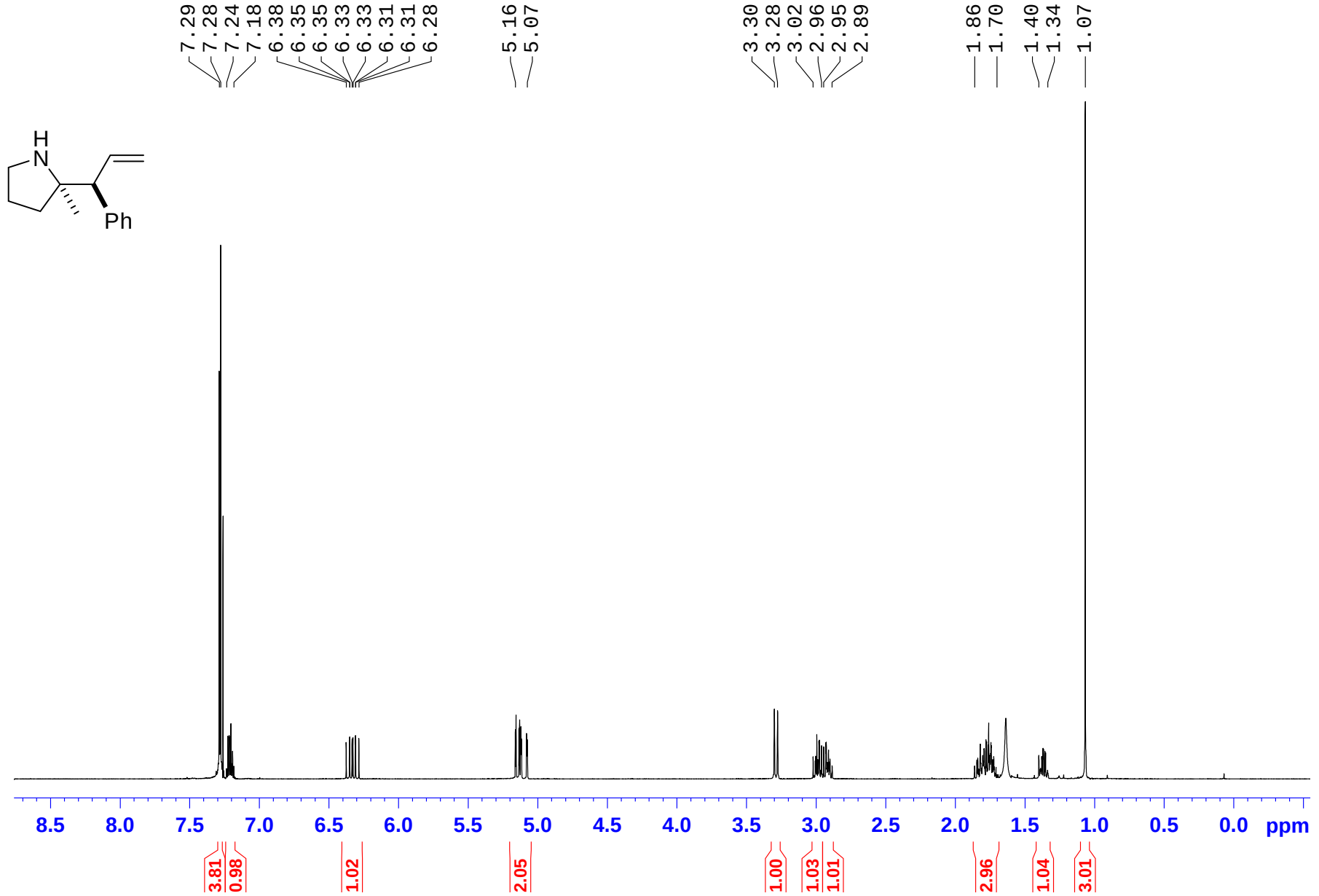
^{1}H NMR ($CDCl_3$, 400 MHz) of compound **3i**



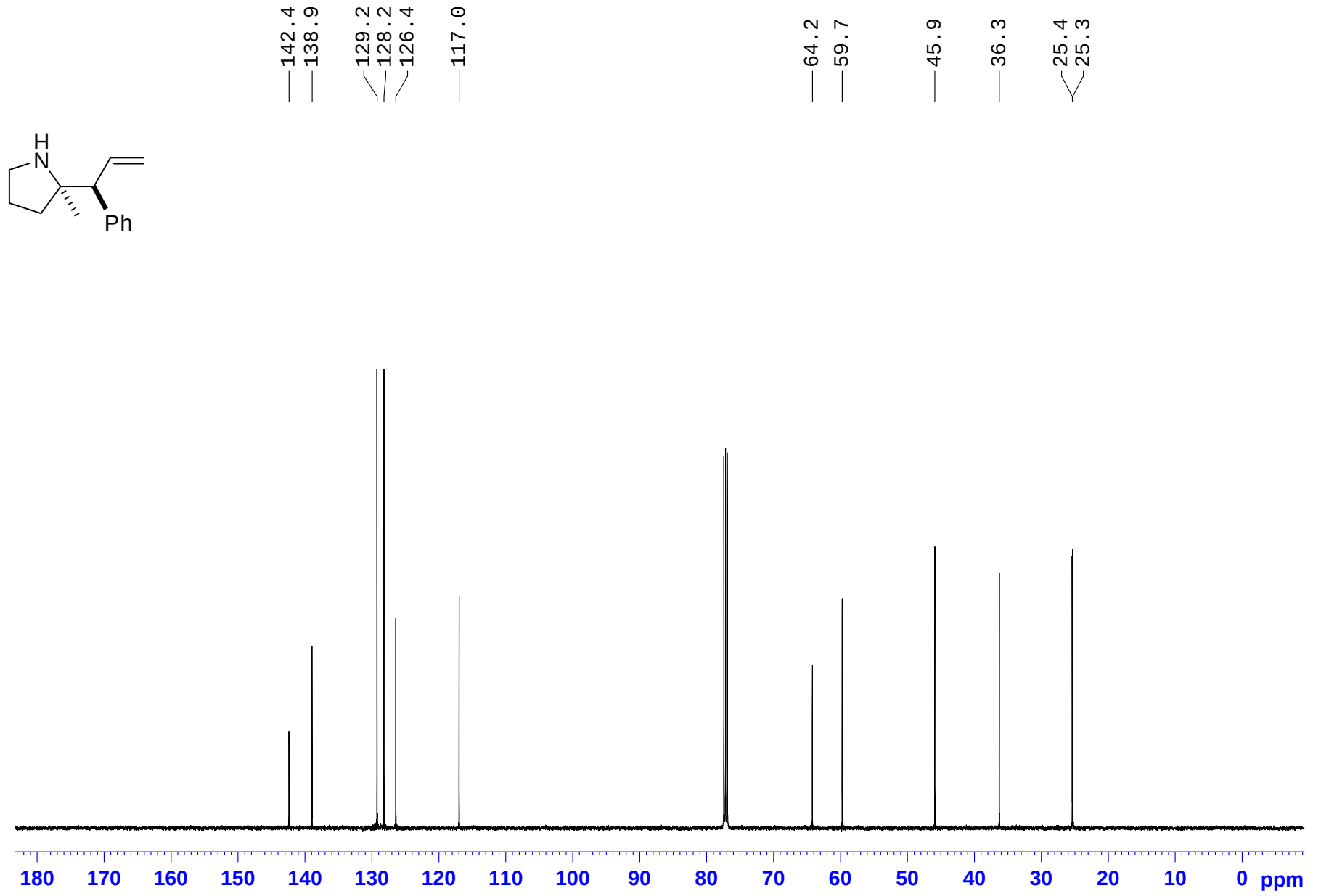
^{13}C NMR ($CDCl_3$, 100 MHz) of compound 3i



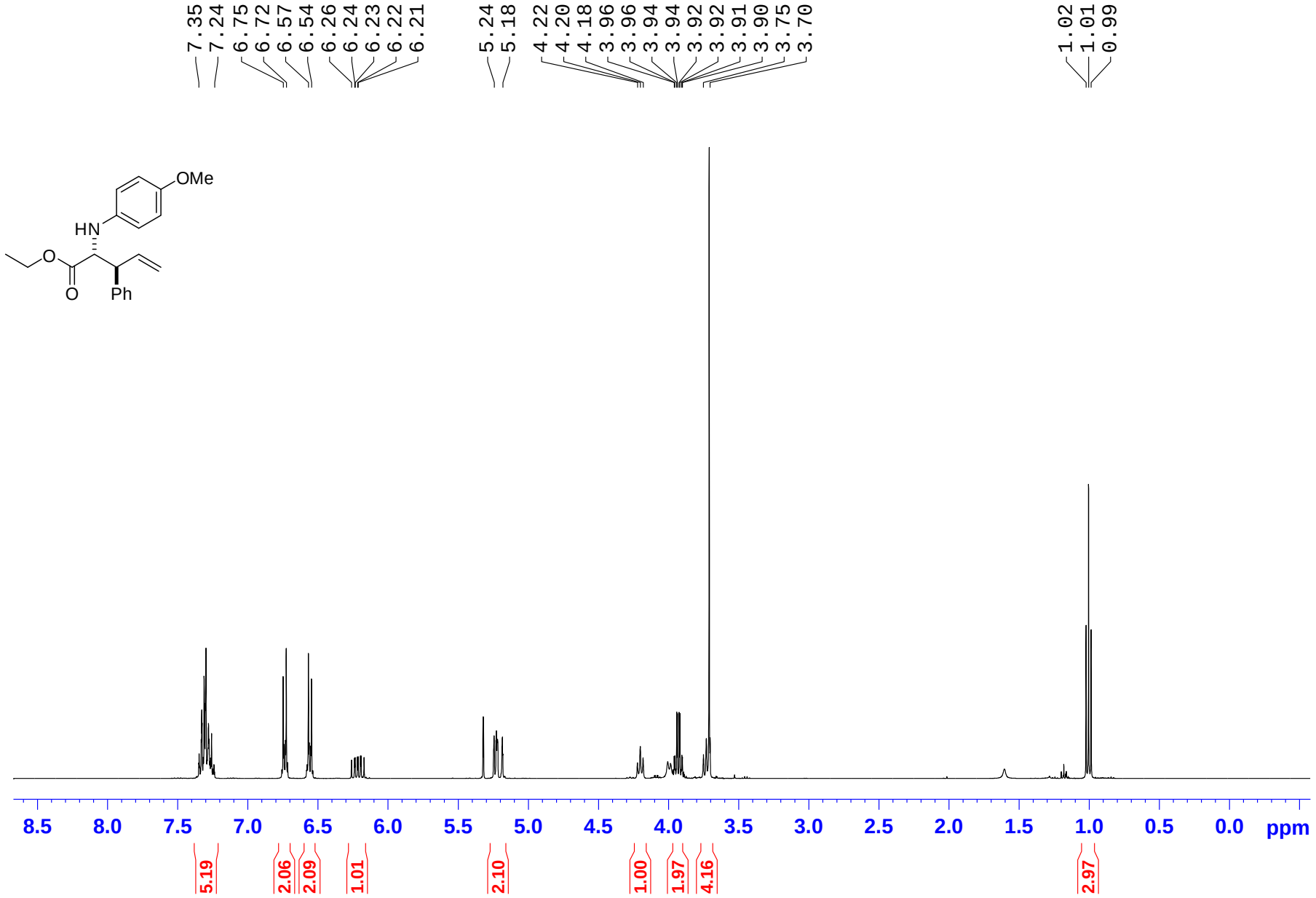
^{1}H NMR ($CDCl_3$, 400 MHz) of compound **3j**



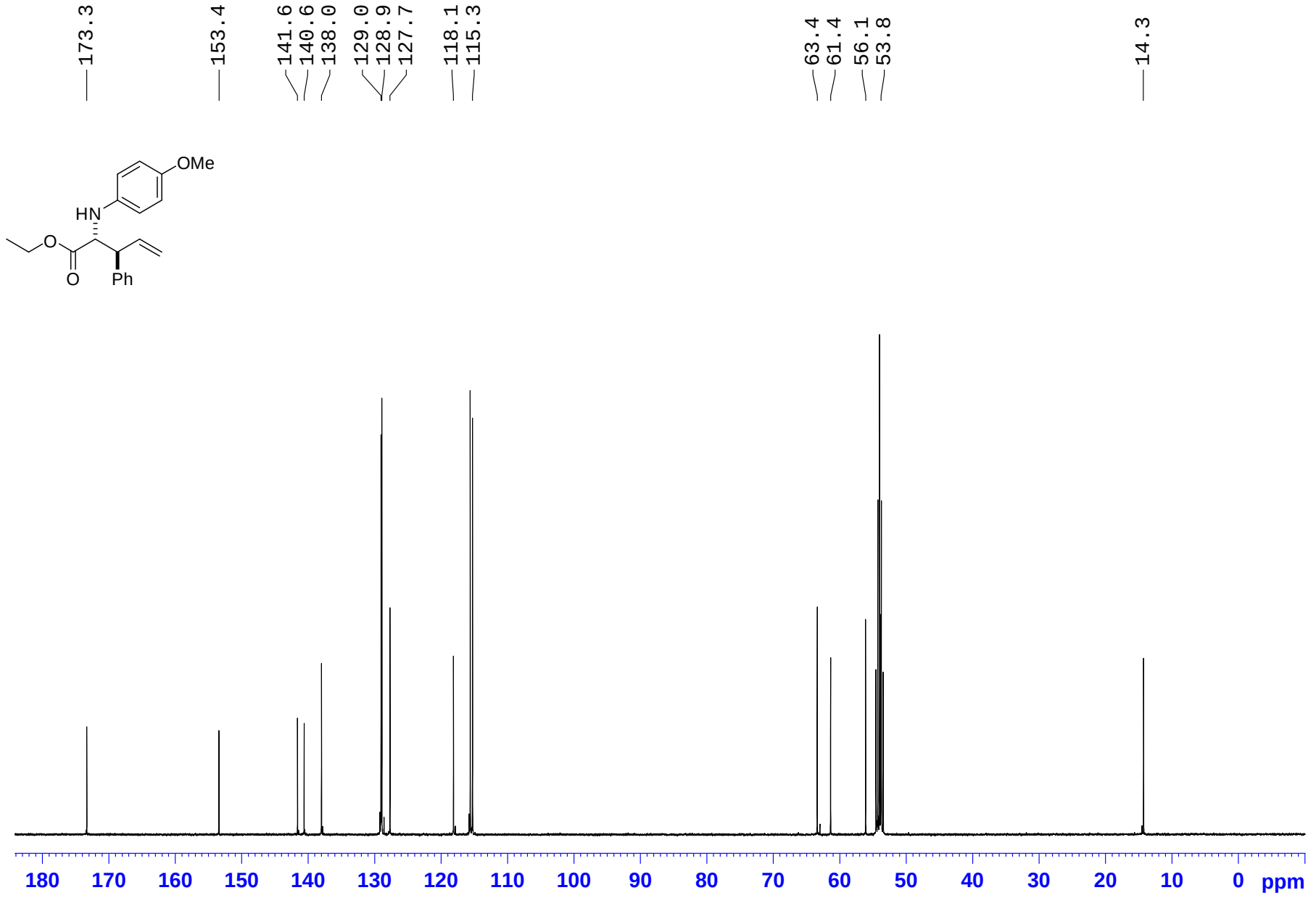
^{13}C NMR ($CDCl_3$, 125 MHz) of compound **3j**



^{1}H NMR (CD_2Cl_2, 400 MHz) of compound **3k**



^{13}C NMR (CD_2Cl_2, 400 MHz) of compound **3k**



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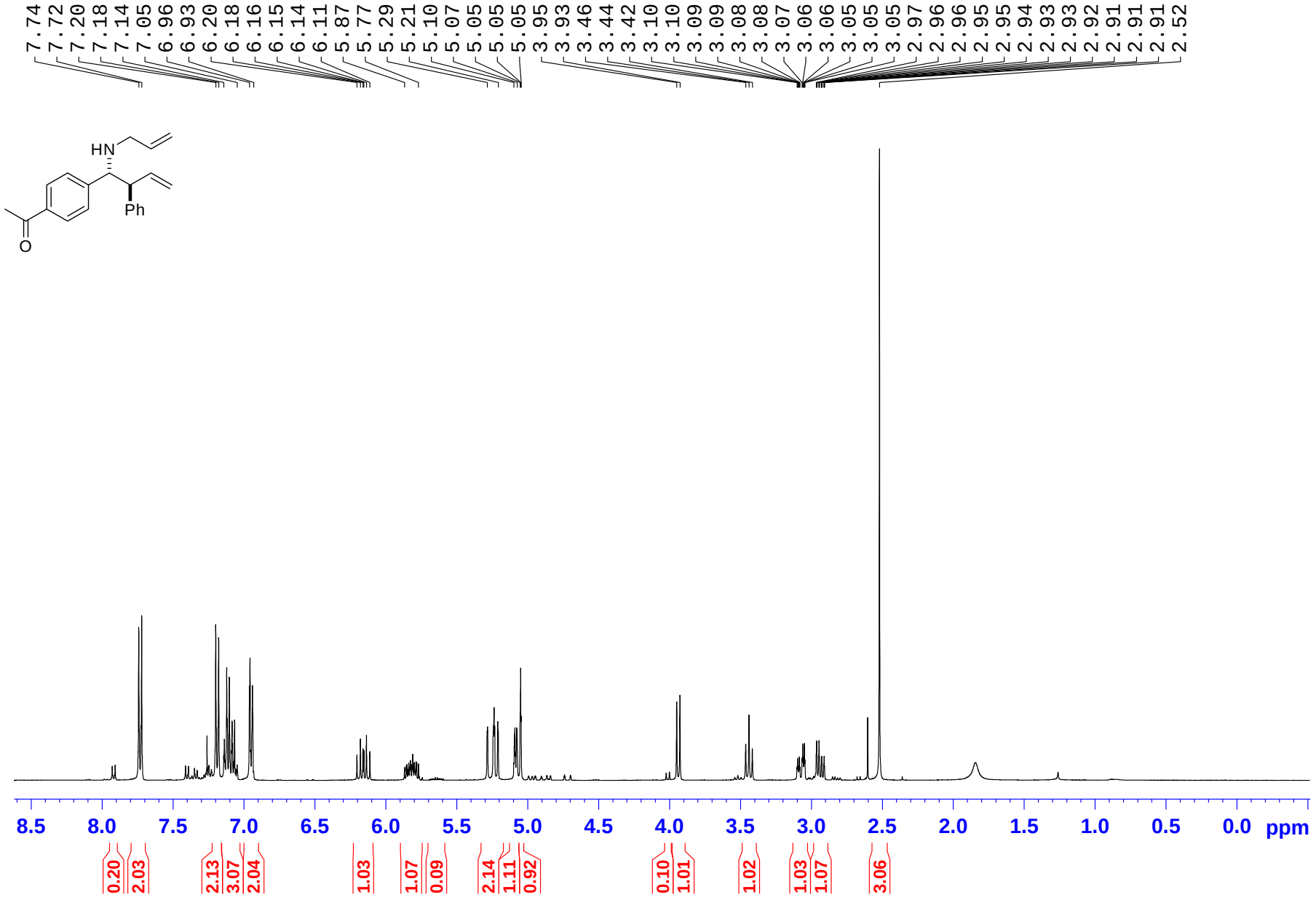

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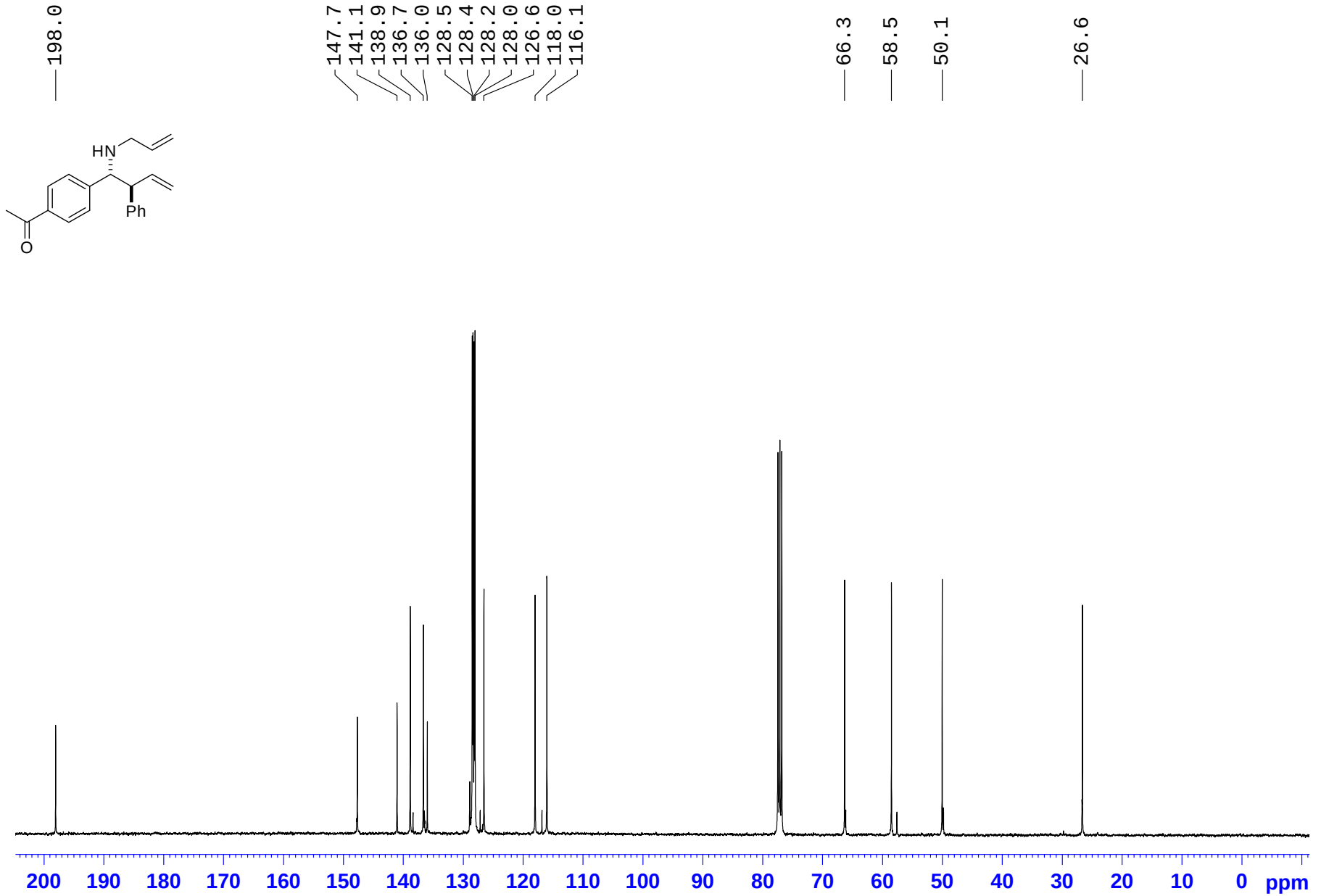
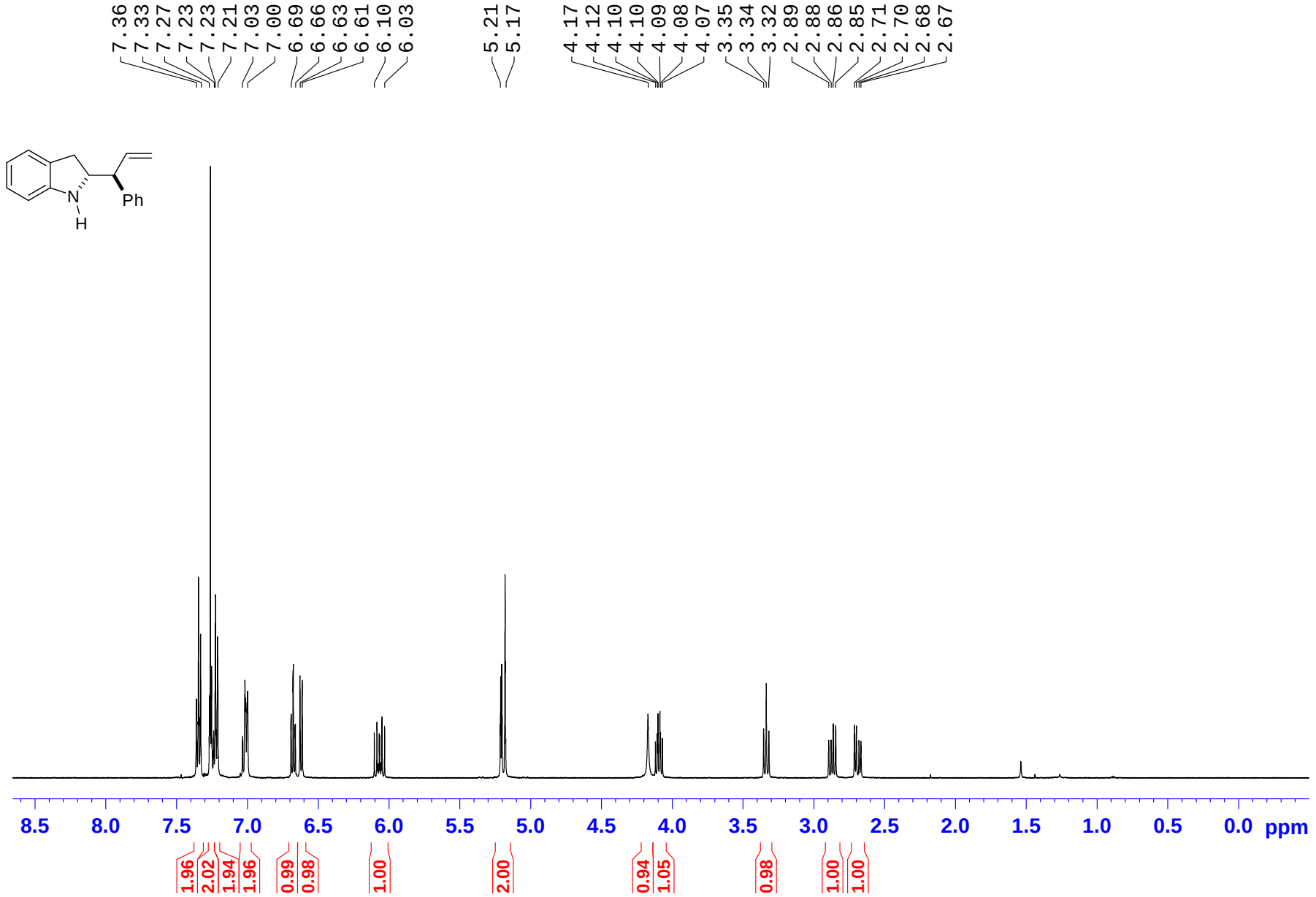
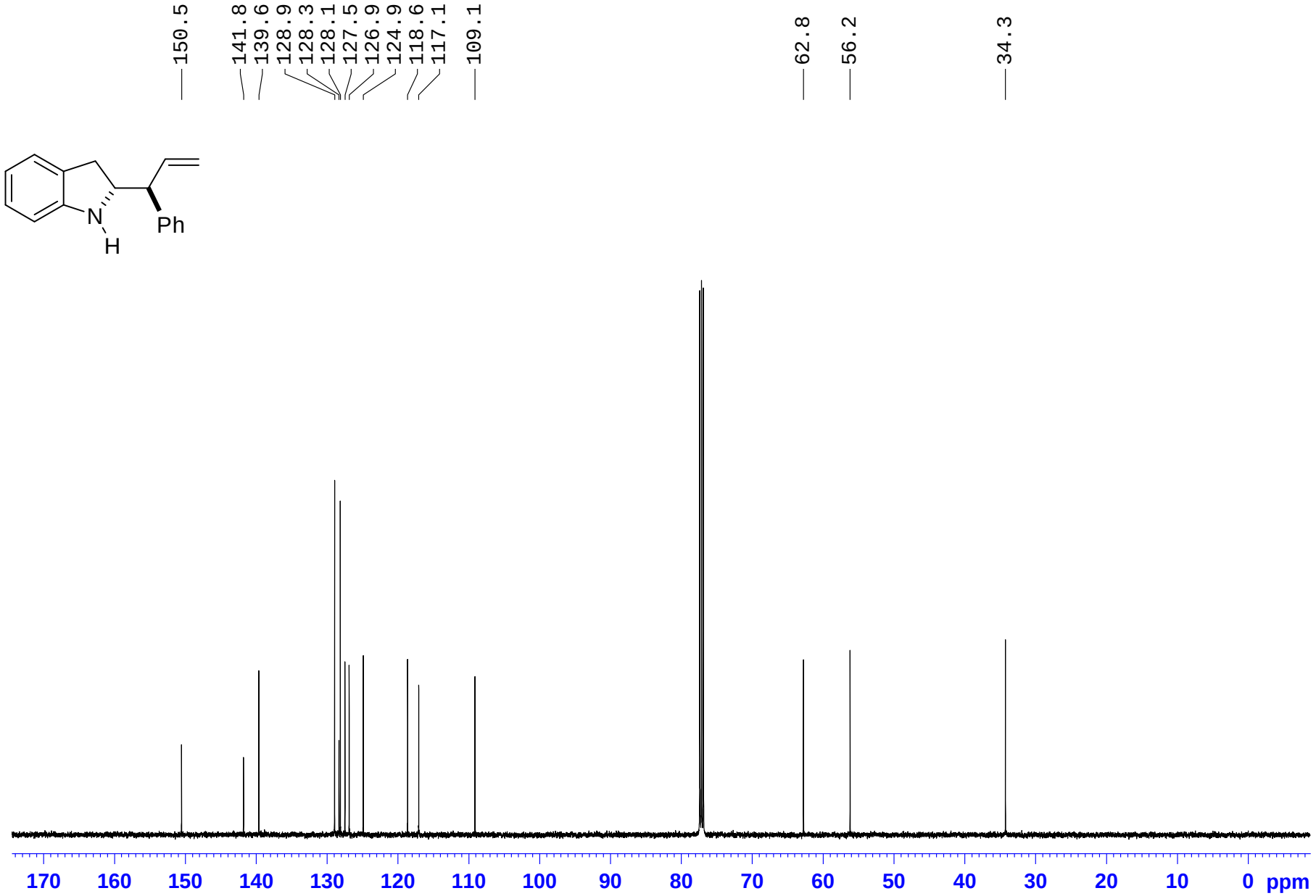


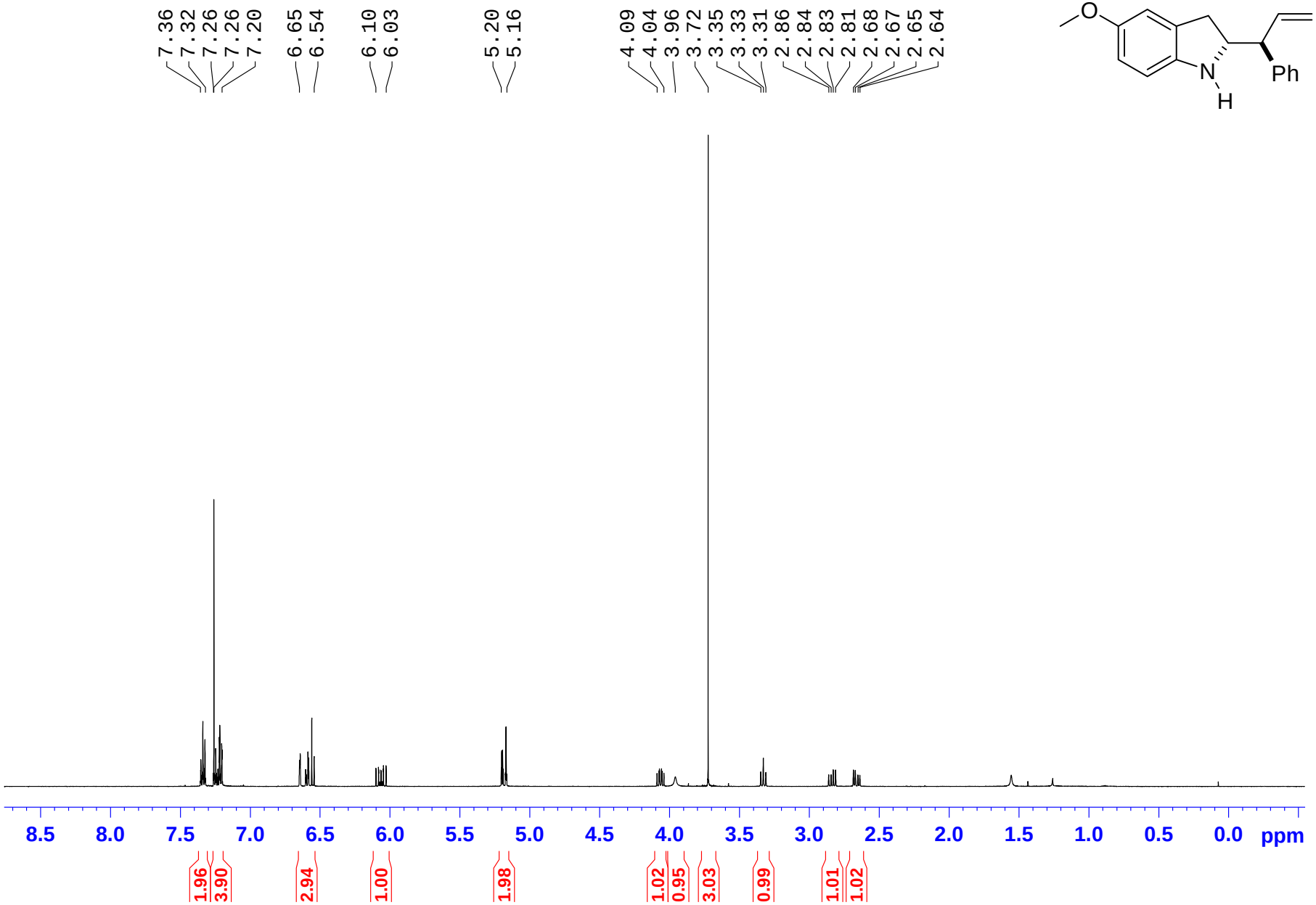
^{1}H NMR ($CDCl_3$, 500 MHz) of compound 3m



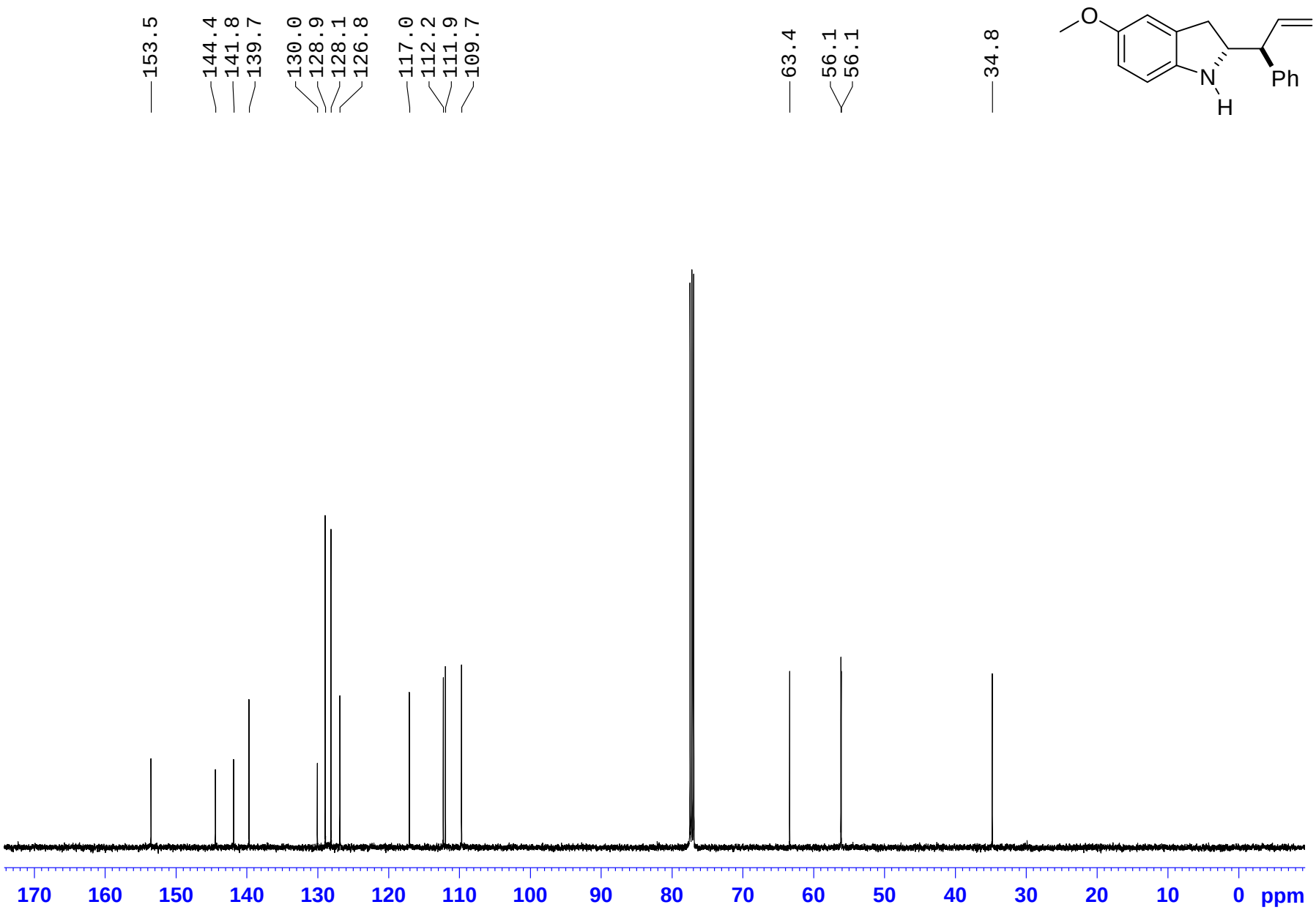
^{13}C NMR ($CDCl_3$, 125 MHz) of compound 3m



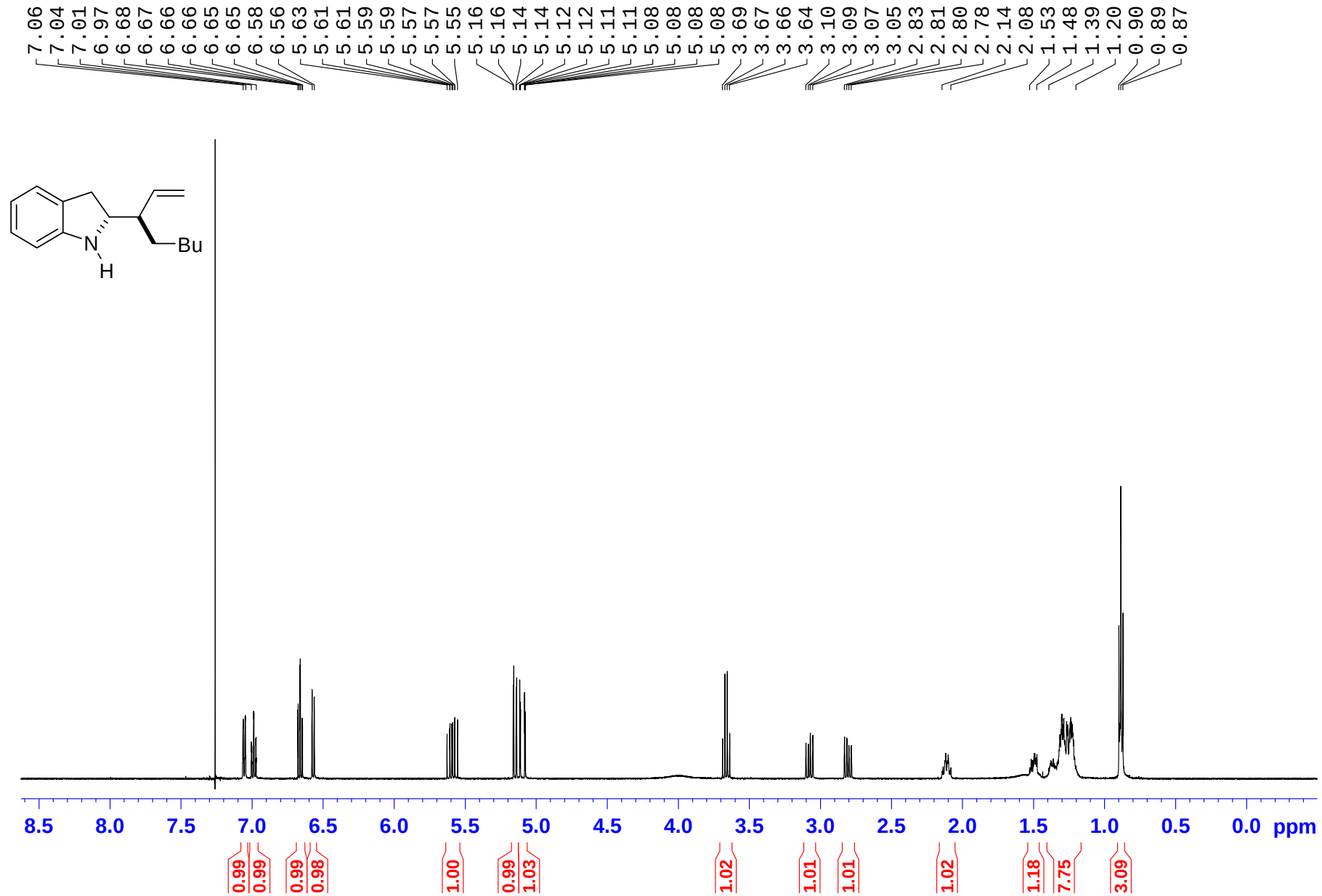
^{1}H NMR ($CDCl_3$, 500 MHz) of compound 3n



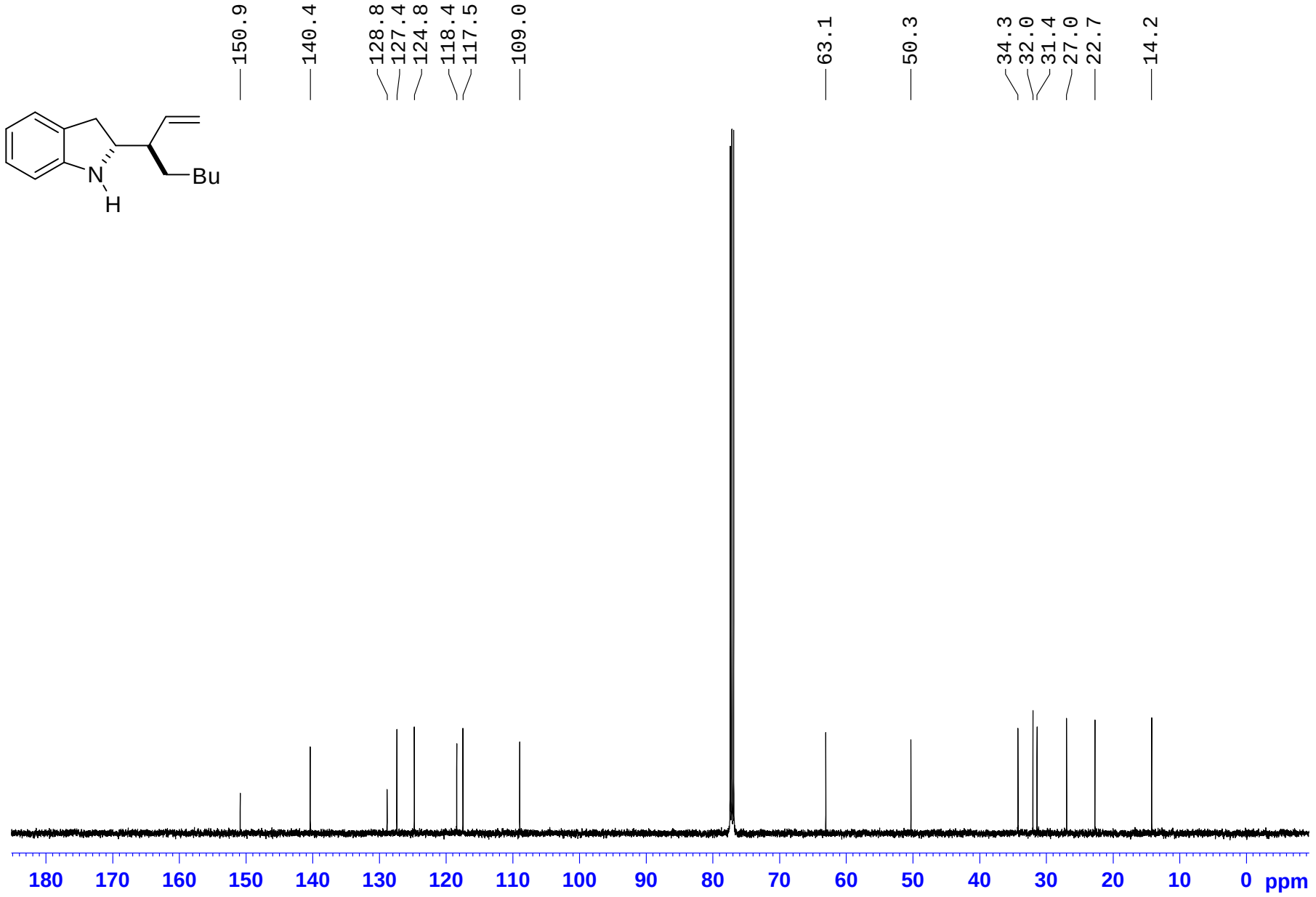
^{13}C NMR ($CDCl_3$, 125 MHz) of compound 3n



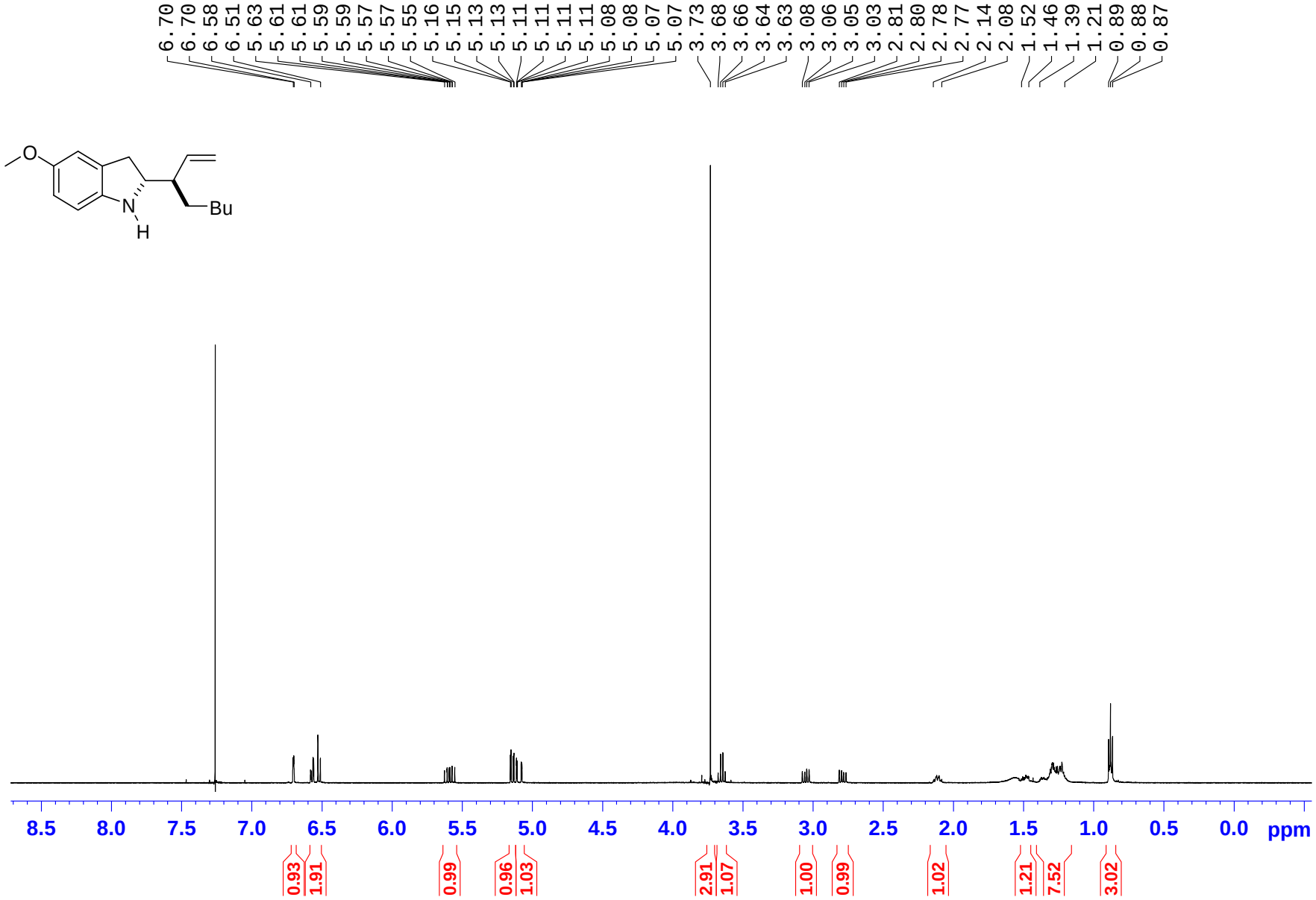
^{1}H NMR ($CDCl_3$, 500 MHz) of compound 3o



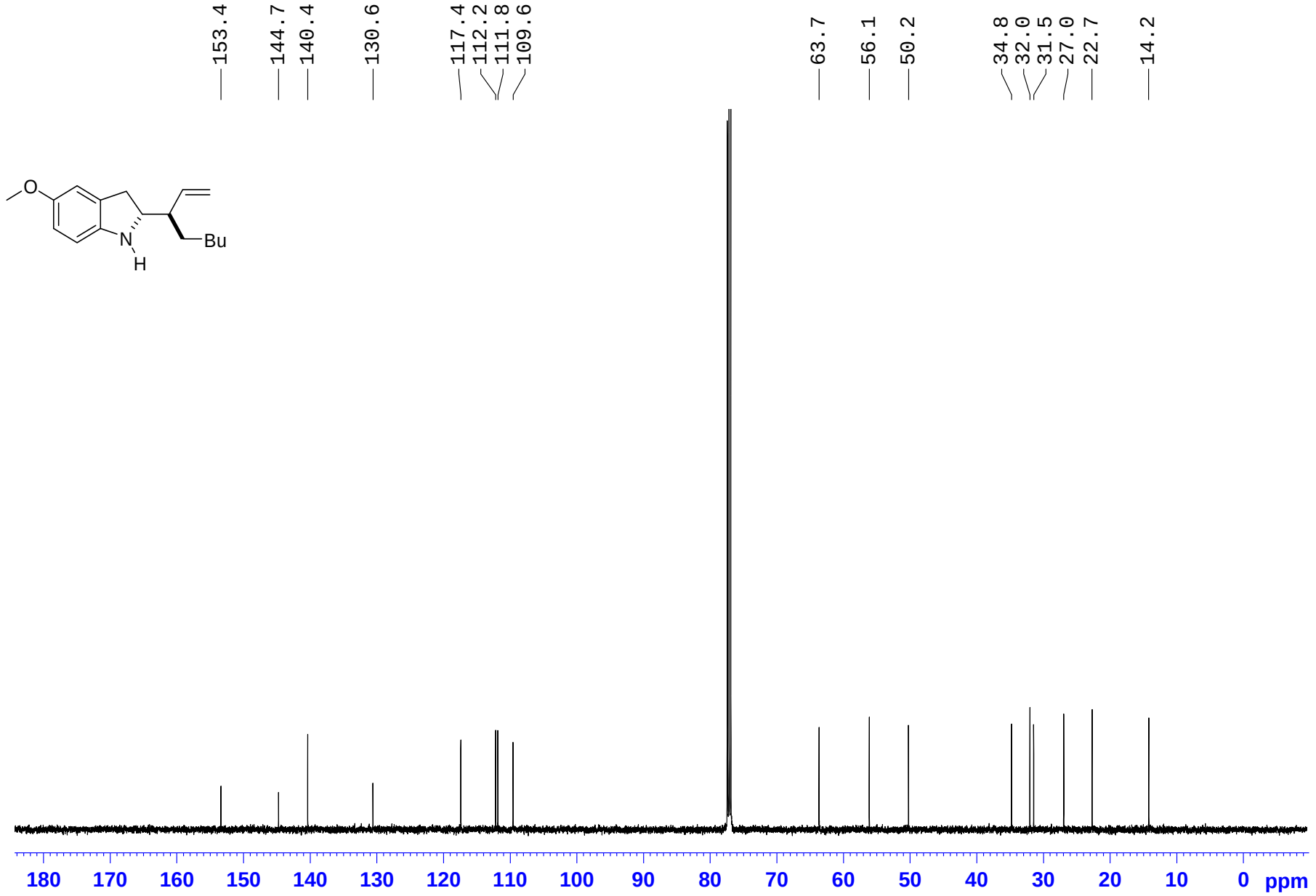
^{13}C NMR ($CDCl_3$, 125 MHz) of compound 3o



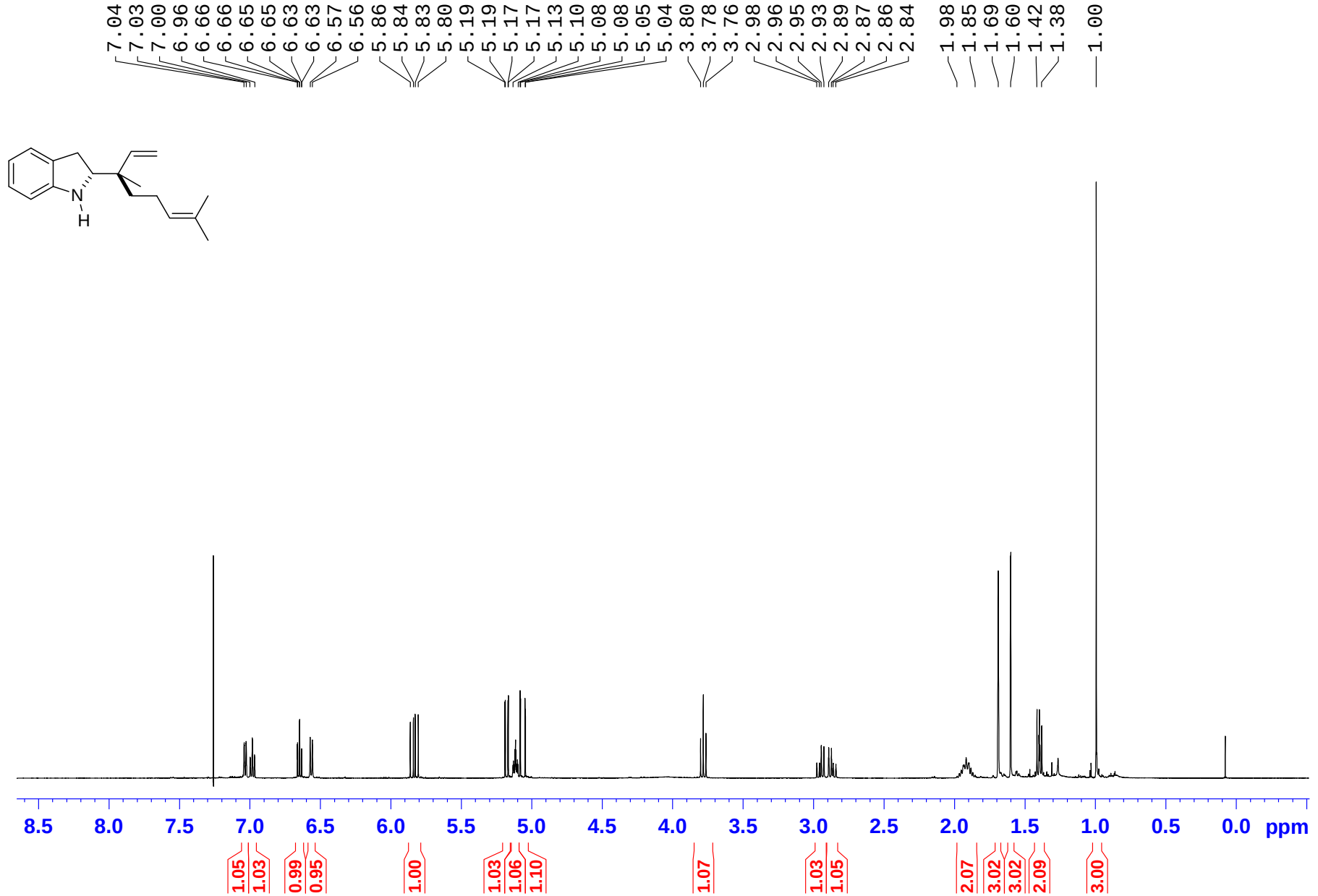
^{1}H NMR ($CDCl_3$, 500 MHz) of compound 3p



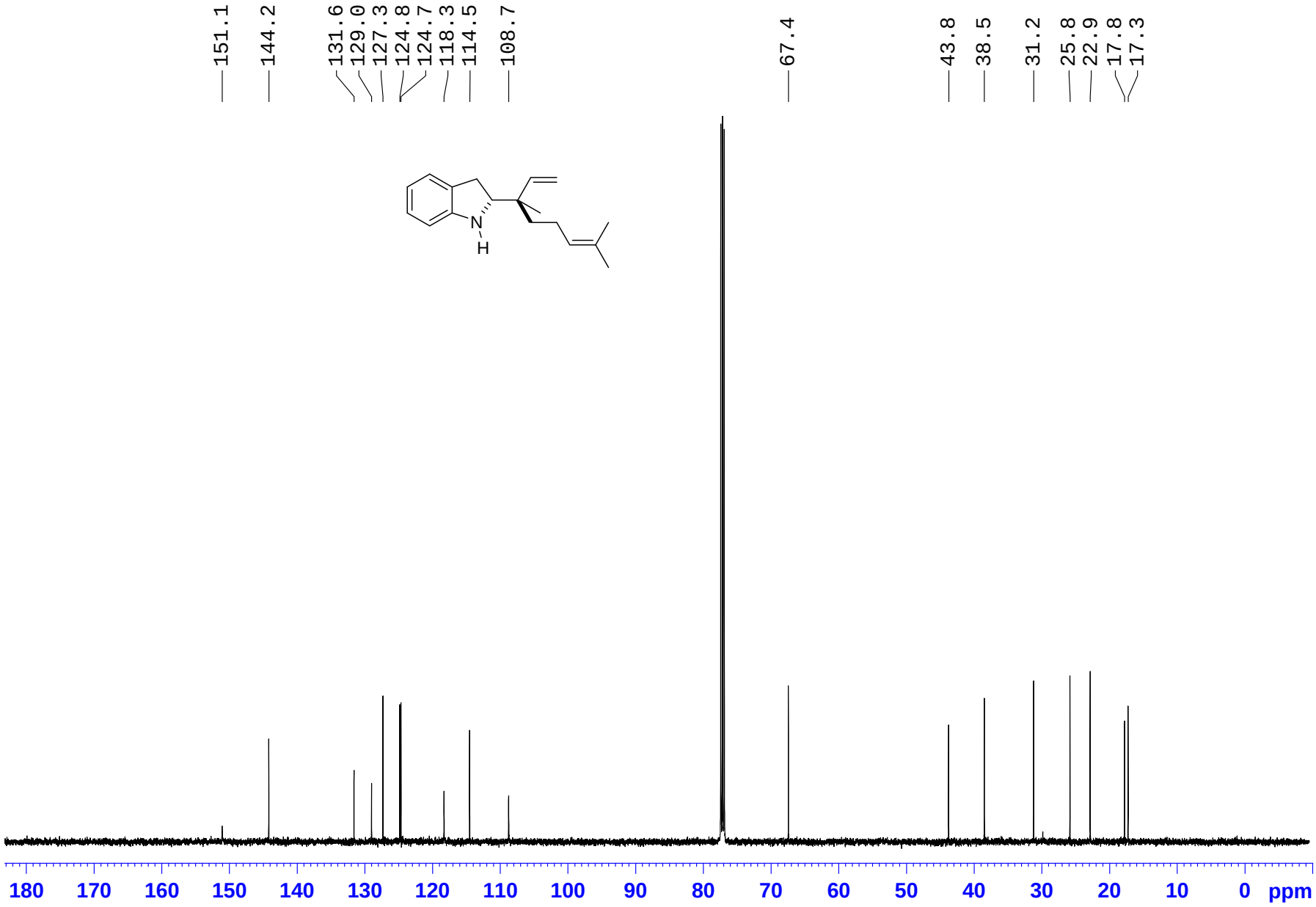
^{13}C NMR ($CDCl_3$, 125 MHz) of compound 3p



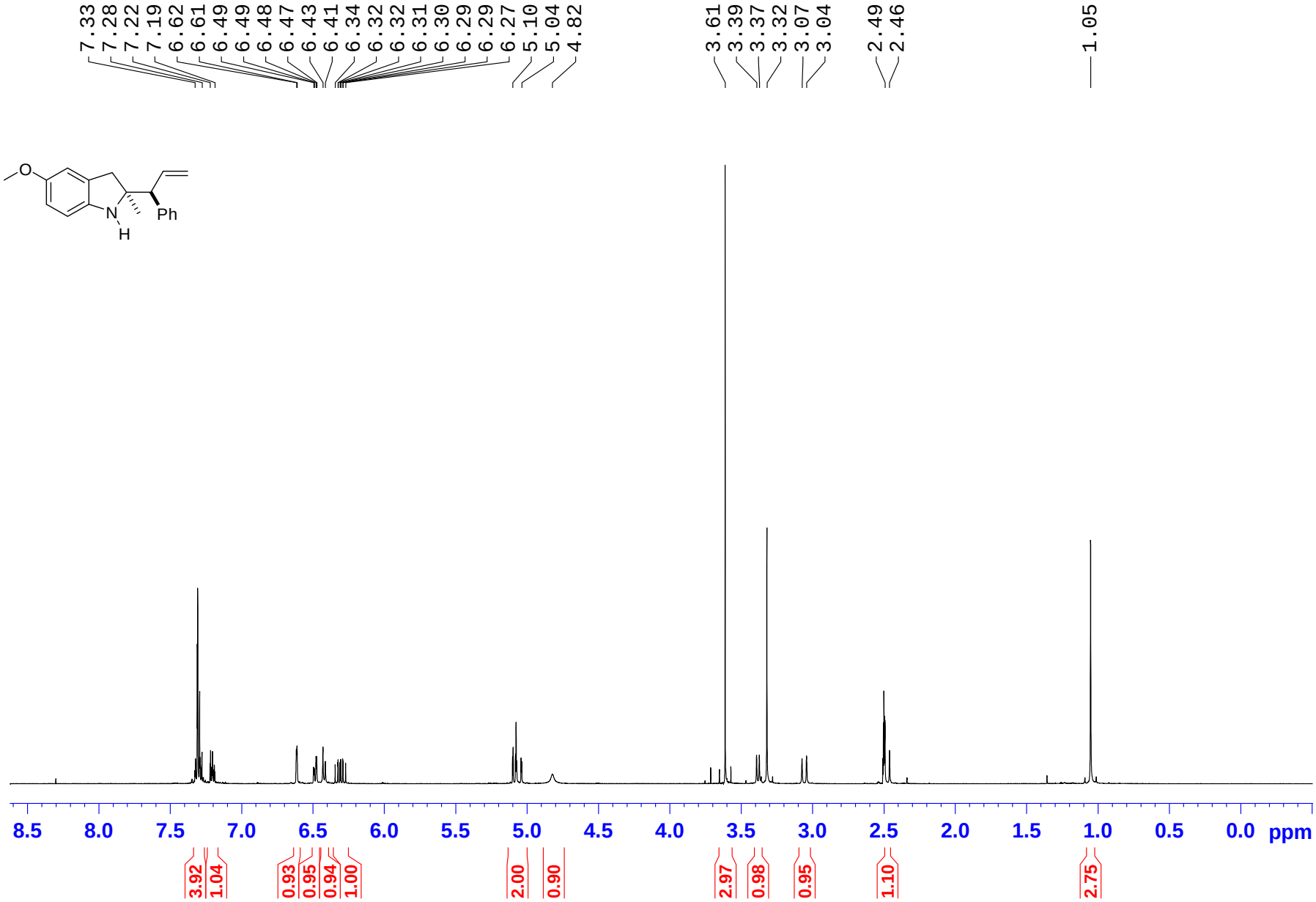
^{1}H NMR ($CDCl_3$, 500 MHz) of compound 3q



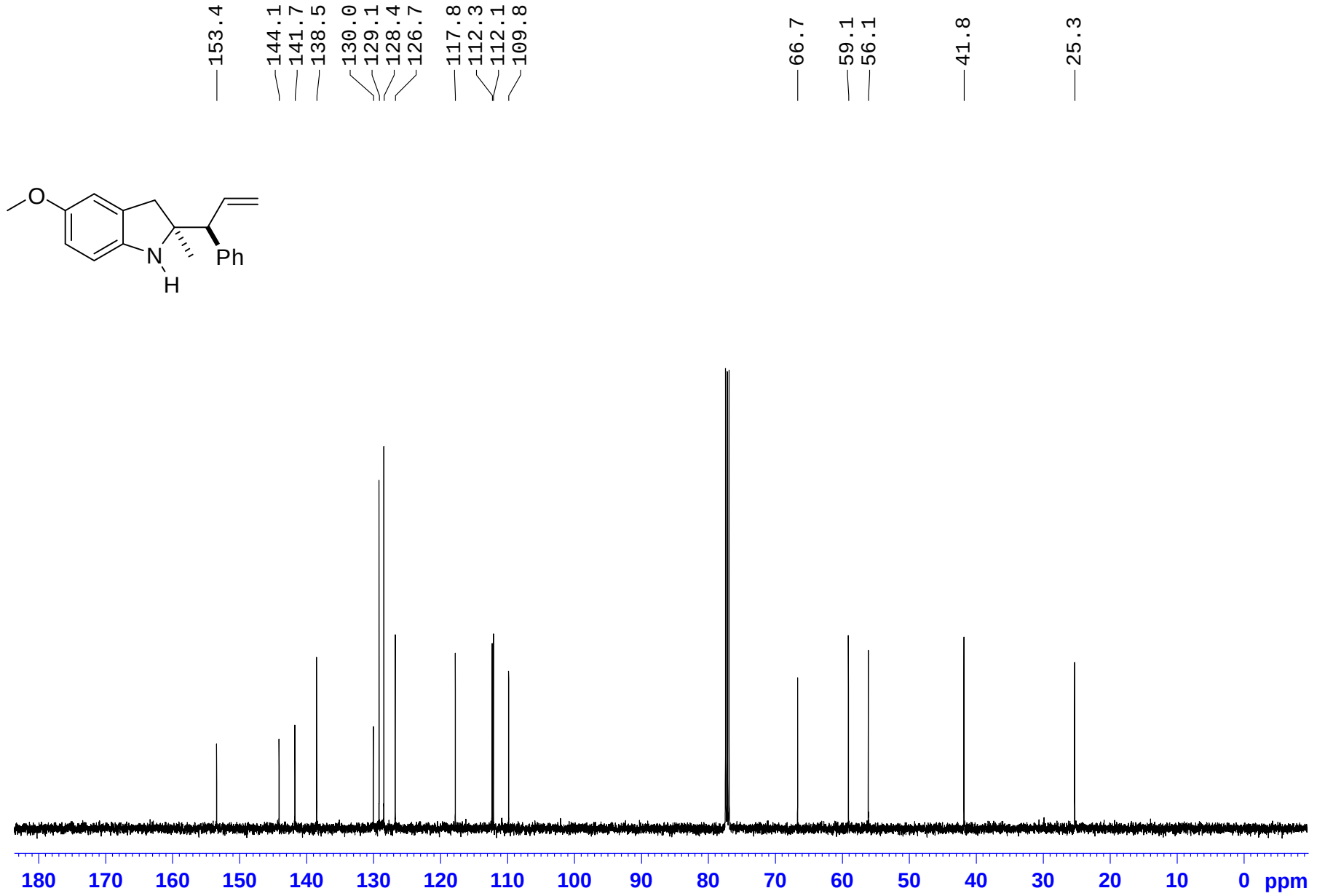
^{13}C NMR ($CDCl_3$, 125 MHz) of compound 3q



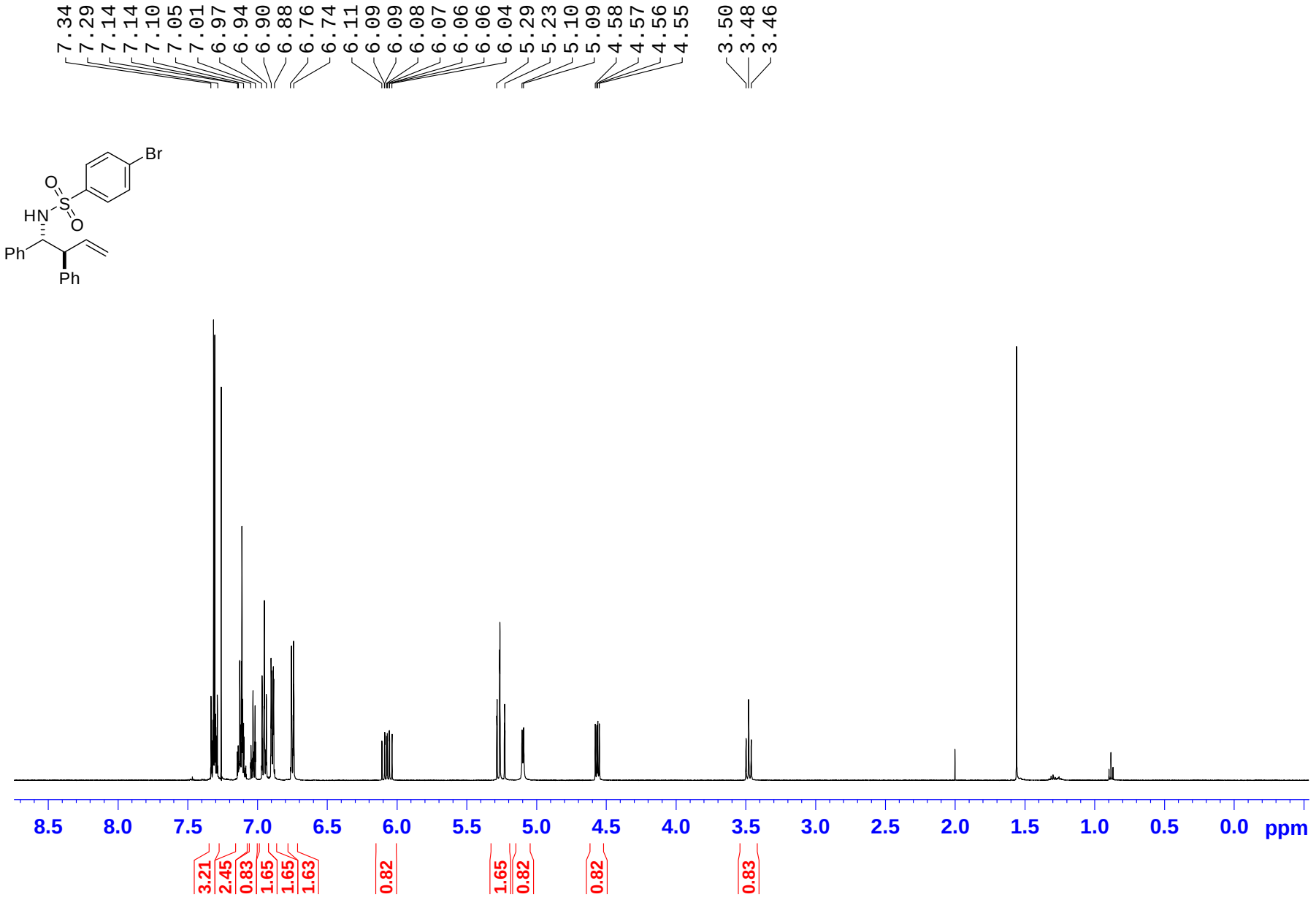
^{1}H NMR (DMSO-d_6, 500 MHz) of compound 3r



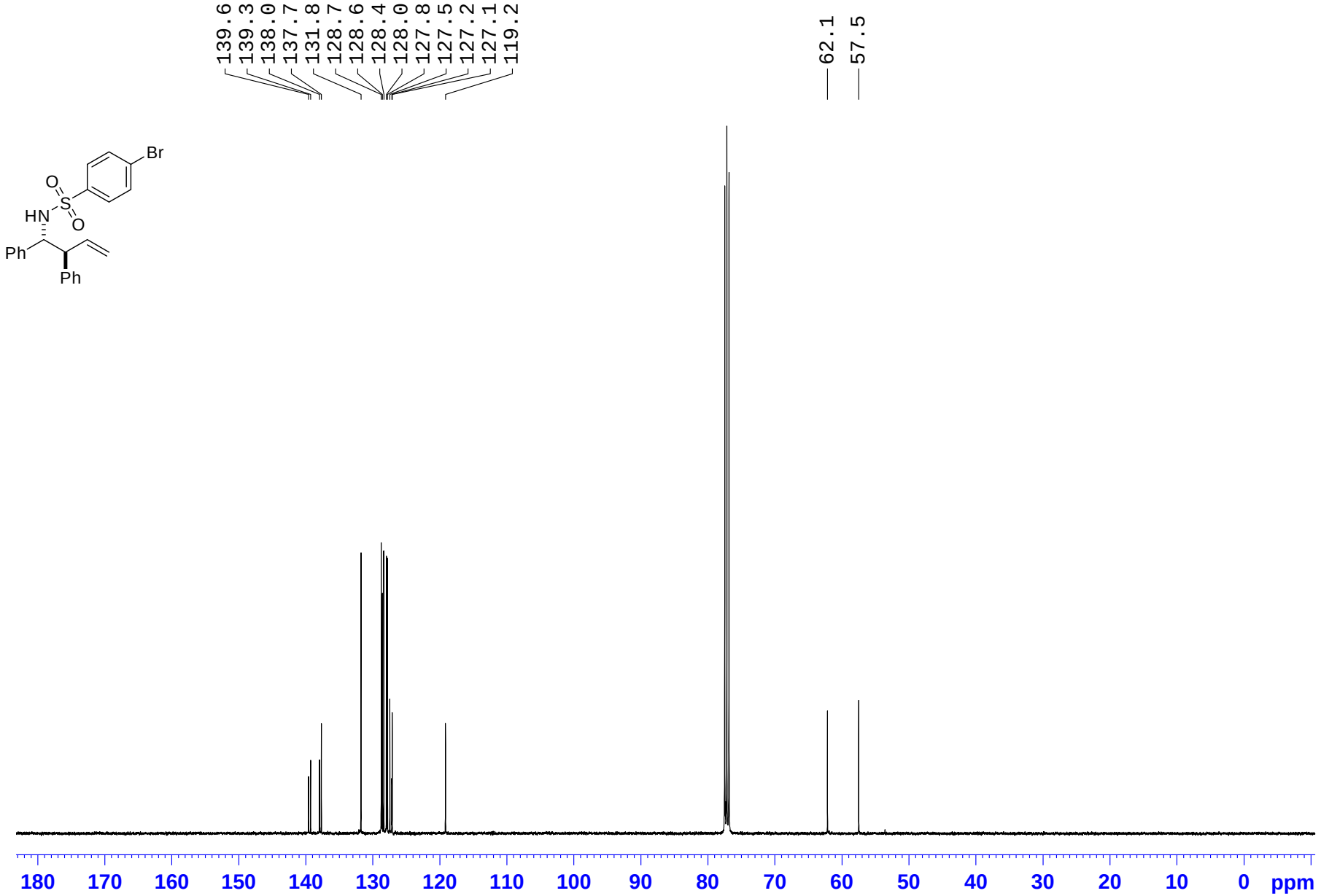
^{13}C NMR ($CDCl_3$, 125 MHz) of compound 3r



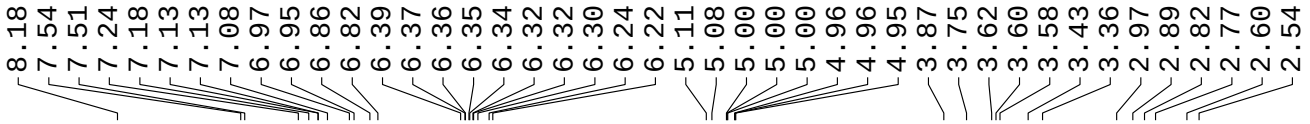
^{1}H NMR ($CDCl_3$, 500 MHz) of compound 3d_sulfonamide derivative

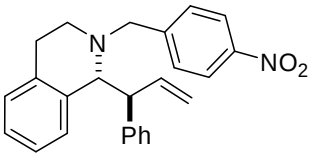


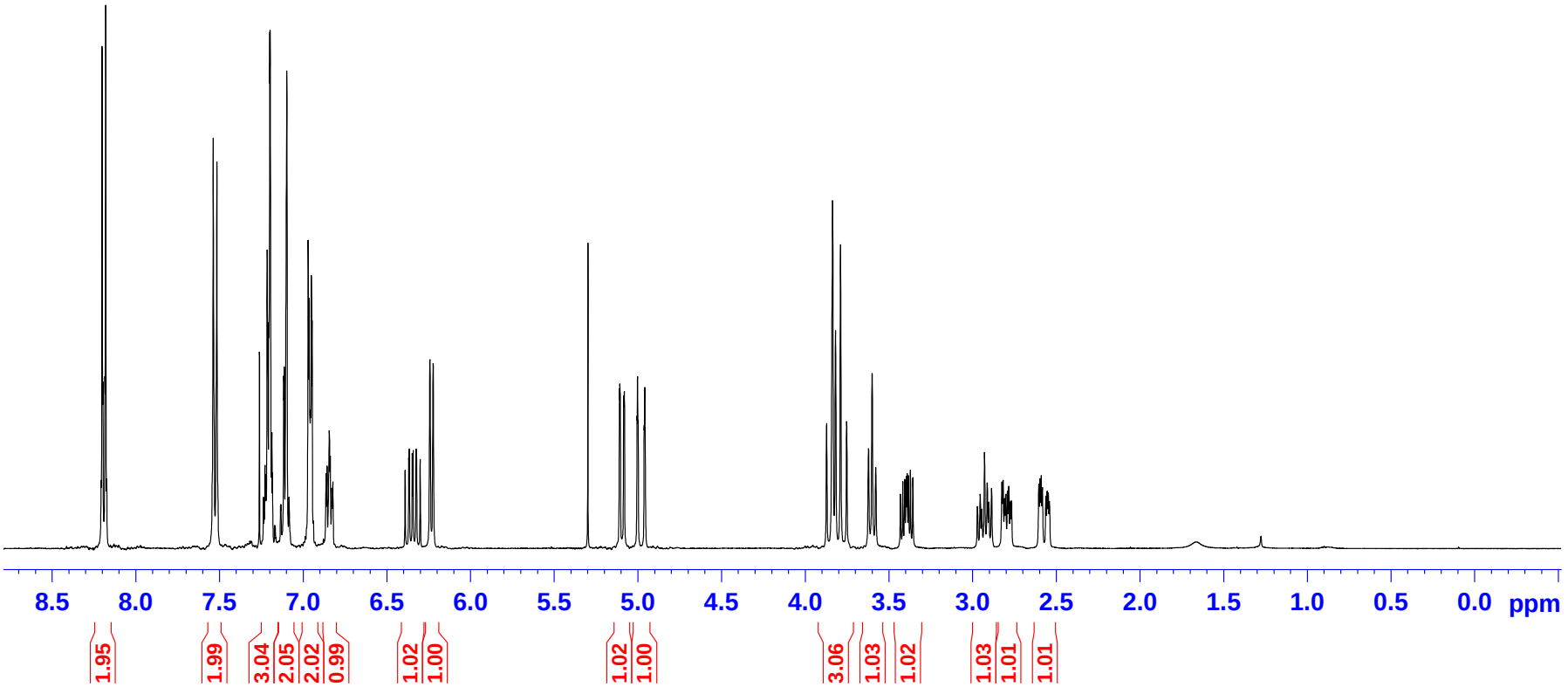
^{13}C NMR ($CDCl_3$, 100 MHz) of compound 3d_sulfonamide derivative



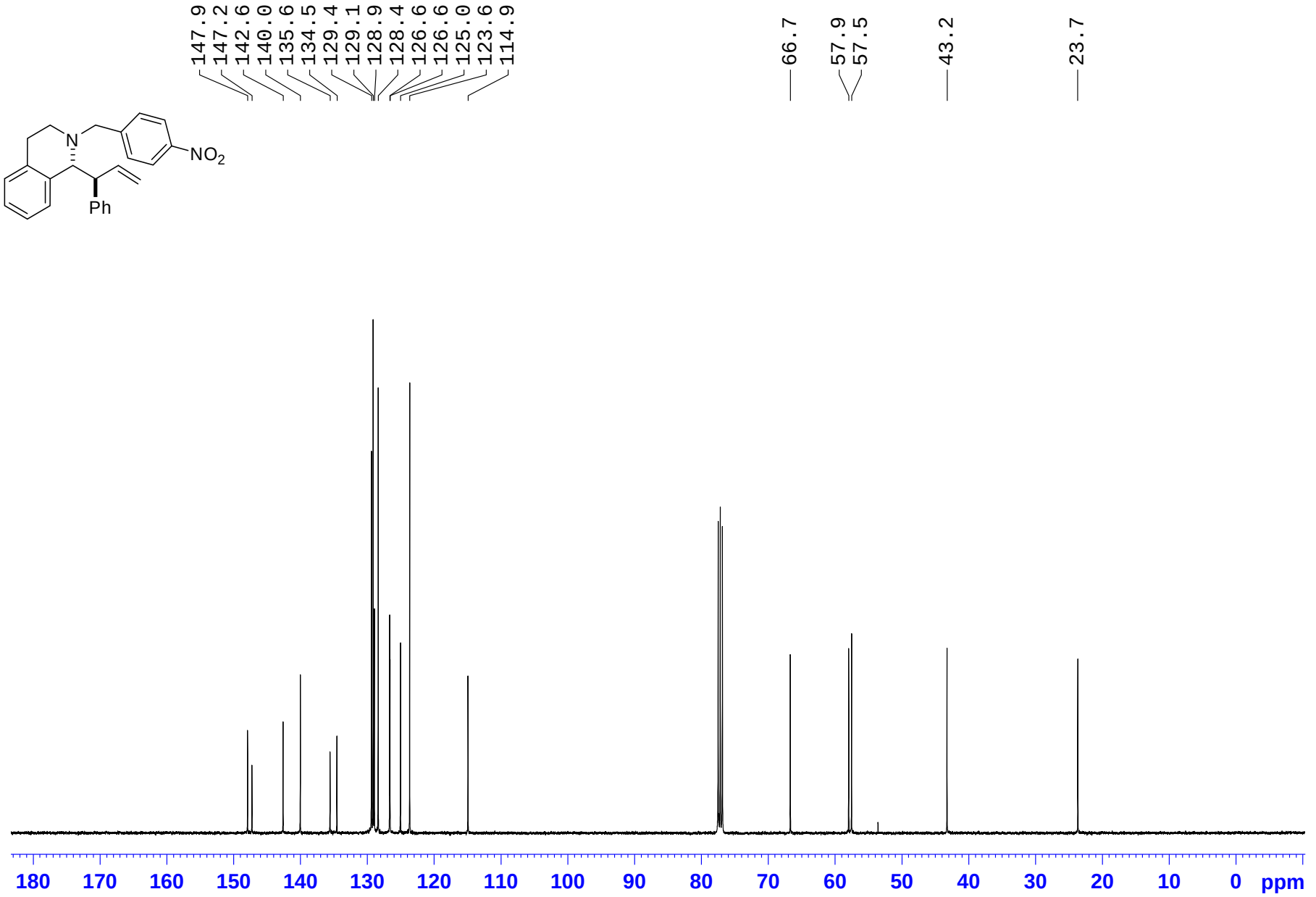
^{1}H NMR ($CDCl_3$, 400 MHz) of compound 3i_*p*-nitrobenzyl derivative



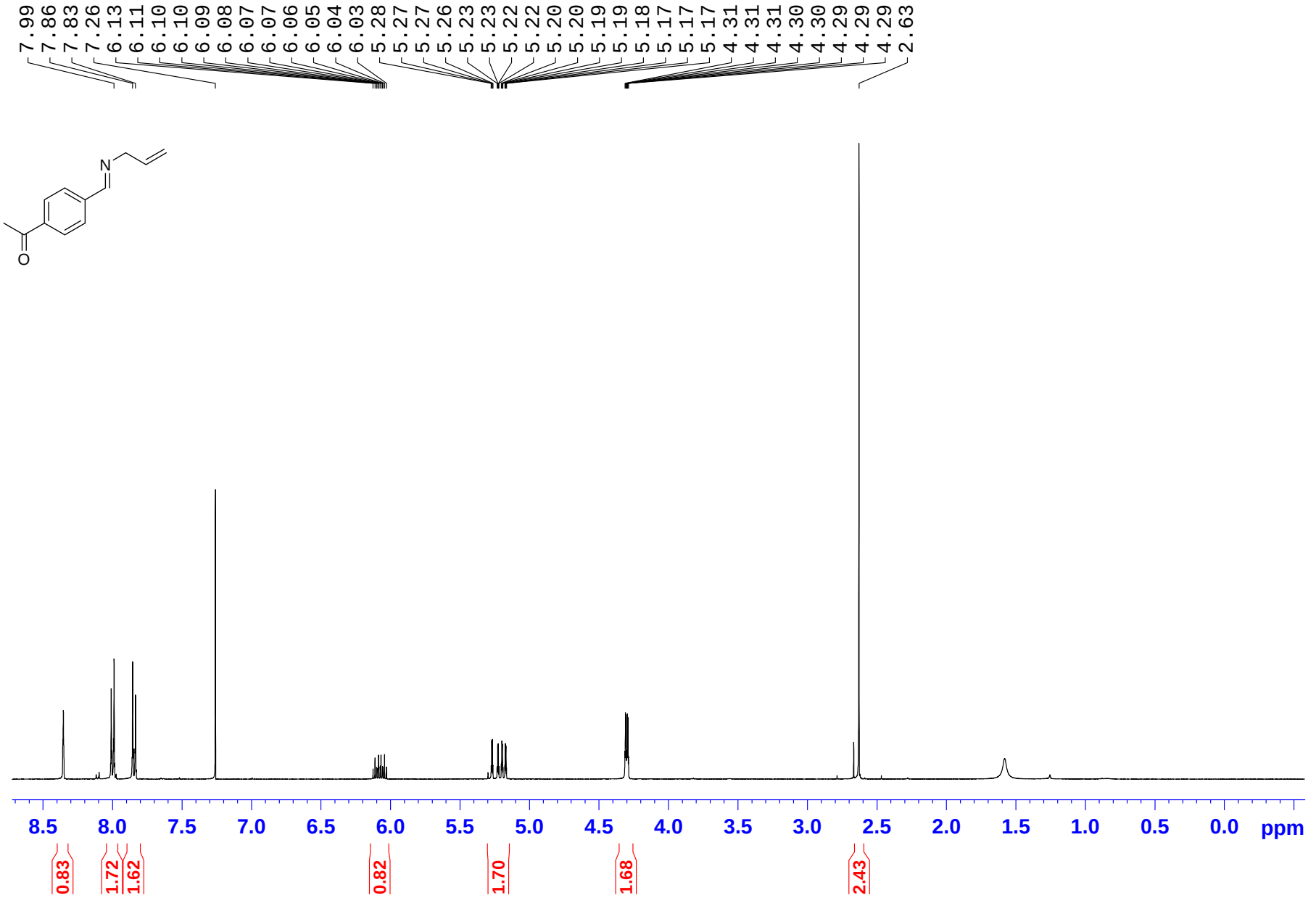




^{13}C NMR ($CDCl_3$, 100 MHz) of compound 3i_*p*-nitrobenzyl derivative



^{1}H NMR ($CDCl_3$, 400 MHz) of compound 1i



^{13}C NMR ($CDCl_3$, 100 MHz) of compound 1i