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Novel ruthenium(II) complexes with chelating 1,2,4-triazole NHC ligands and their catalytic activity in the transfer hydrogenation of ketones

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S1. General information and materials

General Procedures. Solvents were purified and dried according to standard methods and stored over activated 3Å molecular sieves prior to use. Column chromatography was conducted on silica gel 60 (230−400 mesh, Merck).

Instrumentation.

^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance Neo 300 (300 and 75 MHz, respectively) spectrometer. Chemical shifts are given relative to the residual signals of protons of chloroform-*d* or DMSO-*d*$_6$ (7.26 and 2.50 ppm for ^{1}H NMR, respectively) or carbon signals in chloroform-*d* or DMSO-*d*$_6$ (77.16 and 39.52 ppm for ^{13}C NMR, respectively).

High-resolution mass spectra (HRMS) were recorded on a Bruker maXis Q-TOF instrument (Bruker Daltonik GmbH, Bremen, Germany) equipped with an electrospray ionization (ESI) ion source. The measurements were performed in a positive (+) MS ion mode (HV Capillary: 4500 V; Spray Shield: –500 V) with a scan range of *m/z* 50 – 1500. External calibration of the mass spectrometer was achieved using a low-concentration tuning mix solution (Agilent Technologies). Direct syringe injection was implemented for the analyzed solutions at a flow rate 3 μl min^{-1}. Nitrogen was used as nebulizer gas (0.4 bar) and dry gas (4.0 dm^3 min^{-1}). The dry temperature was established at 250 °C. All the spectra were recorded with 1 Hz frequency and processed using the Bruker Data Analysis 4.0 software package.

GC-MS analyses were accomplished using an Agilent 7890A gas chromatograph equipped with an Agilent 5975C mass-selective detector (EI, 70 eV) and an HP-5MS column (30 m × 0.25 mm × 0.25 μm film) using He as the carrier gas at a flow rate of 1.0 ml·min^{-1}.

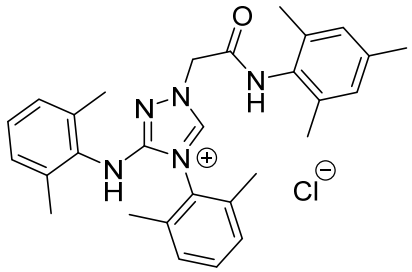
Melting points were determined in open capillary tubes using a Thiele apparatus and are uncorrected.

Materials.

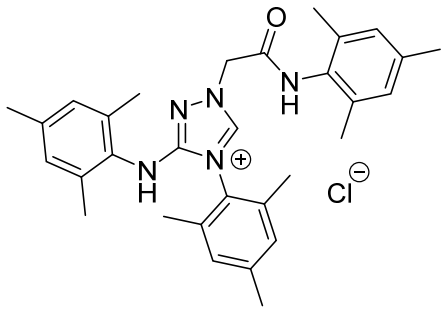
Starting compounds **1a-c** were were synthesized as described in the literature.[S1] All other chemicals were purchased from commercial sources.

S2. Synthetic procedures and characterization of isolated compounds

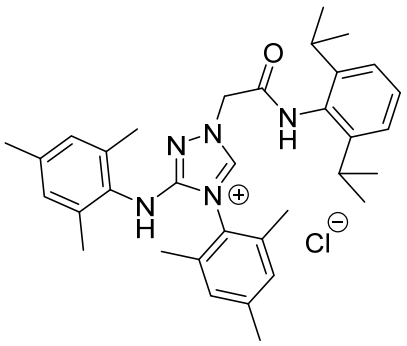
General procedure for the preparation of compounds 2a-c and 3a-c. A mixture of compound **1a-c** (1.24 mmol), the corresponding *N*-aryl-2-chloroacetamide or methyl chloroacetate (1.35 mmol) and DMF (6 ml) was heated at 90 °C within 16 h in a sealed vial. Then, the reaction mixture was evaporated to dryness in vacuo. A residue obtained was recrystallized from a MeCN : EtOAc (1 : 4 vol.) mixture, then dried *in vacuo* at 50 °C overnight.



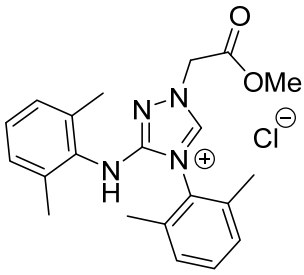
4-(2,6-Dimethylphenyl)-3-[(2,6-dimethylphenyl)amino]-1-{2-oxo-2-[(2,4,6-trimethylphenyl)amino]ethyl}-1*H*-1,2,4-triazol-4-ium chloride (2a). Yield 444 mg (71%), white crystals, mp 306-308 °C. ^{1}H NMR (DMSO-d_6, 300 MHz): δ 2.05 (s, 6H), 2.16 (s, 6H), 2.22 (s, 3H), 2.26 (s, 6H), 5.26 (s, 2H), 6.88 (s, 2H), 7.12-7.17 (m, 3H), 7.43 (d, J = 7.6 Hz, 2H), 7.52-7.57 (m, 1H), 9.04 (s, 1H), 10.20 (s, 1H), 10.21 (s, 1H). ^{13}C{^{1}H} NMR (DMSO-d_6, 75 MHz): δ 17.1, 17.7, 17.9, 20.5, 53.8, 127.7, 128.3, 128.4, 129.3, 131.46, 131.53, 134.0, 134.7, 135.8, 135.9, 136.2, 142.3, 151.9, 162.5 (signals of two aromatic carbons overlap). ESI-MS(TOF) *m/z*: [M - Cl]$^+$ calcd. For $C_{29}H_{34}N_5O^+$ 468.2758, found *m/z* 468.2767.



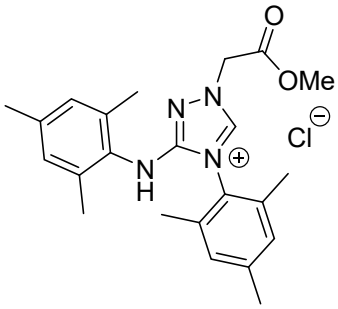
1-{2-Oxo-2-[(2,4,6-trimethylphenyl)amino]ethyl}-4-(2,4,6-trimethylphenyl)-3-[(2,4,6-trimethylphenyl)-amino]-1*H*-1,2,4-triazol-4-ium chloride (2b). Yield 535 mg (81%), white crystals, mp >310 °C. ^{1}H NMR (DMSO-d_6, 300 MHz): δ 2.04 (s, 6H), 2.10 (s, 6H), 2.19 (s, 6H), 2.22 (s, 3H), 2.24 (s, 3H), 2.37 (s, 3H), 5.20 (s, 2H), 6.88 (s, 2H), 6.93 (s, 2H), 7.24 (s, 2H), 8.86 (s, 1H), 10.02 (s, 1H), 10.08 (s, 1H). ^{13}C{^{1}H} NMR (DMSO-d_6, 75 MHz): δ 17.0, 17.6, 17.9, 20.5, 20.7, 53.7, 125.8, 128.4, 129.0, 129.8, 131.4, 131.5, 134.7, 135.4, 135.8, 135.9, 136.9, 141.3, 142.3, 152.2, 162.5 (signals of two aliphatic carbons overlap). ESI-MS(TOF) *m/z*: [M - Cl]$^+$ calcd. For $C_{31}H_{38}N_5O^+$ 496.3071, found *m/z* 496.3089.



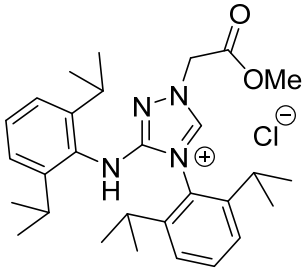
1-(2-{[2,6-Di(propan-2-yl)phenyl]amino}-2-oxoethyl)-4-(2,4,6-trimethylphenyl)-3-[(2,4,6-trimethylphenyl)amino]-1*H*-1,2,4-triazol-4-ium chloride (2c). Yield 548 mg (77%), white crystals, mp 298-300 °C. ^{1}H NMR (DMSO-d_6, 300 MHz): δ 1.06 (dd, J = 13.5, 6.8 Hz, 12H), 2.10 (s, 6H), 2.19 (s, 6H), 2.25 (s, 3H), 2.37 (s, 3H), 2,97 (hept, J = 6.8 Hz, 2H), 5.28 (s, 2H), 6.94 (s, 2H), 7.14-7.17 (m, 2H), 7.24-7.30 (m, 3H), 8.86 (s, 1H), 10.13 (s, 1H), 10.24 (s, 1H). ^{13}C{^{1}H} NMR (DMSO-d_6, 75 MHz): δ 17.0, 17.6, 20.5, 20.7, 23.1, 23.8, 27.9, 53.6, 123.1, 125.8, 127.9, 129.0, 129.8, 131.4, 131.5, 135.4, 135.8, 136.8, 141.3, 142.2, 145.7, 152.2, 163.6. ESI-MS(TOF) *m/z*: [M - Cl]$^{+}$ calcd. For $C_{34}H_{44}N_5O^{+}$ 538.3540, found *m/z* 538.3546.



4-(2,6-Dimethylphenyl)-3-[(2,6-dimethylphenyl)amino]-1-(2-methoxy-2-oxoethyl)-1*H*-1,2,4-triazol-4-ium chloride (3a). Yield 269 mg (67%), white crystals, mp 241-243 °C. ^{1}H NMR (DMSO-d_6, 300 MHz): δ 2.17 (s, 6H), 2.25 (s, 6H), 3.74 (s, 3H), 5.35 (s, 2H), 7.11-7.16 (m, 3H), 7.45 (d, J = 7.6 Hz, 2H), 7.53-7.58 (m, 1H), 9.09 (s, 1H), 10.10 (s, 1H). ^{13}C{^{1}H} NMR (DMSO-d_6, 75 MHz): δ 17.1, 17.7, 52.2, 53.0, 127.8, 128.2, 128.5, 129.4, 131.7, 133.9, 135.7, 136.1, 142.5, 151.9, 166.5. ESI-MS(TOF) *m/z*: [M - Cl]$^{+}$ calcd. For $C_{21}H_{25}N_4O_2^{+}$ 365.1972, found *m/z* 365.1979.



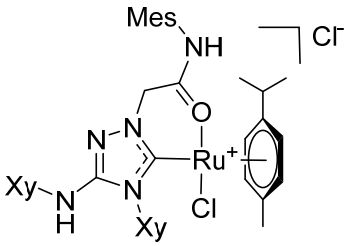
1-(2-Methoxy-2-oxoethyl)-4-(2,4,6-trimethylphenyl)-3-[(2,4,6-trimethylphenyl)amino]-1*H*-1,2,4-triazol-4-ium chloride (3b). Yield 313 mg (73%), white crystals, mp 247-249 °C. ^{1}H NMR (DMSO-d_6, 300 MHz): δ 2.11 (s, 6H), 2.19 (s, 6H), 2.23 (s, 3H), 2.37 (s, 3H), 3.74 (s, 3H), 5.33 (s, 2H), 6.94 (s, 2H), 7.25 (s, 2H), 8.93 (s, 1H), 10.06 (s, 1H). ^{13}C{^{1}H} NMR (DMSO-d_6, 75 MHz): δ 17.0, 17.6, 20.5, 20.7, 52.2, 53.0, 125.7, 129.0, 129.9, 131.4, 135.3, 135.7, 136.9, 141.4, 142.4, 152.2, 166.5. ESI-MS(TOF) *m/z*: [M - Cl]$^{+}$ calcd. For $C_{23}H_{29}N_4O_2^{+}$ 393.2285, found *m/z* 393.2288.



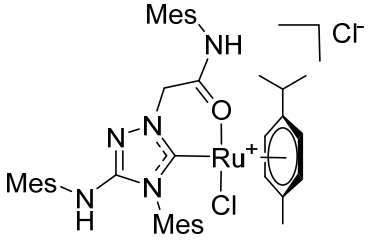
4-[2,6-Di(propan-2-yl)phenyl]-3-{[2,6-di(propan-2-yl)phenyl]amino}-1-(2-methoxy-2-oxoethyl)-1*H*-1,2,4-triazol-4-ium chloride (3c). Yield 375 mg (73%), white crystals, mp 238-240 °C. ^{1}H NMR (DMSO-d_6, 300 MHz): δ 1.10 (d, J = 5.3 Hz, 12H), 1.20 (d, J = 6.7 Hz, 6H), 1.37 (d, J = 6.8 Hz, 6H), 2.53-2.62 (m, 2H), 2.96-3.06 (m,

2H), 3.70 (s, 3H), 5.35 (s, 2H), 7.22 (d, J = 7.6 Hz, 2H), 7.31-7.36 (m, 1H), 7.57 (d, J = 7.7 Hz, 2H), 7.70-7.75 (m, 1H), 9.19 (s, 1H), 10.23 (s, 1H). $^{13}C\{^1H\}$ NMR (DMSO-d_6, 75 MHz): δ 22.26, 23.33, 23.8, 24.7, 28.0, 28.7, 52.4, 53.0, 123.8, 123.9, 125.2, 128.8, 131.0, 132.5, 142.5, 146.27, 146.33, 154.0, 166.2. ESI-MS(TOF) *m/z*: $[M - Cl]^+$ calcd. For $C_{29}H_{41}N_4O_2^+$ 477.3224, found *m/z* 477.3228.

General procedure for the preparation of compounds 4a-c and 5a-c. A mixture of azolium salt **2a-c** or **3a-c** (0.2 mmol), Ag_2O (0.1 mmol) and dry CH_2Cl_2 (3 ml) was stirred at room temperature under an argon atmosphere in the absence of light for 24 h. Then a solution of $[RuCl_2(p\text{-cymene})]_2$ (0.1 mmol) in dry CH_2Cl_2 (3 ml) was added to the reaction mixture. The resulting mixture was further stirred for 24 h, filtered through a short pad of Celite® and evaporated *in vacuo*. The crude product was chromatographed on a SiO_2 column using a 1:1 mixture of CH_2Cl_2 - EtOAc as eluent.

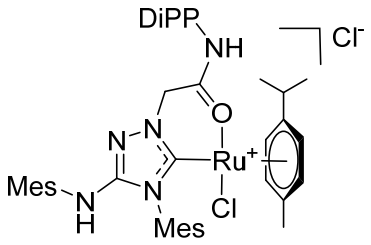


Chloro[η⁶-1-methyl-4-(propan-2-yl)benzene][4-(2,6-dimethylphenyl)-5-[(2,6-dimethylphenyl)amino]-2-{2-(oxo-κ*O*)-2-[(2,4,6-trimethylphenyl)amino]ethyl}-2,4-dihydro-3*H*-1,2,4-triazol-3-ylidene-κ*C*³]ruthenium chloride (4a). Yield 0.067 g (45%), orange crystals, mp > 150 °C, decomp. ^1H NMR ($CDCl_3$, 300 MHz) (a mixture of diastereomers): δ 0.77 (d, J = 6.8 Hz, 3H), 0.89 (d, J = 7.0 Hz, 3H), 1.71-1.78 (m, 4H), 2.15 – 2.27 (m, 18H), 2.52 (s, 3H), 3.12 (d, J = 5.4 Hz, 1H), 4.88 (d, J = 5.5 Hz, 1H), 5.10 (d, J = 17.5 Hz, 1H), 5.18 (d, J = 6.9 Hz, 1H), 5.50 (s, 1H), 5.65 (d, J = 6.8 Hz, 1H), 5.84 (d, J = 17.5 Hz, 1H), 6.83 (d, J = 13.4 Hz, 2H), 7.08 (q, J = 5.3 Hz, 3H), 7.36 – 7.65 (m, 3H), 12.54 (s, 1H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75 MHz) (a mixture of diastereomers): δ 17.7, 18.2, 18.7, 18.9, 20.4, 21.1, 22.9, 29.8, 40.2, 40.4, 52.6, 92.6, 103.8, 124.7, 128.1, 129.0, 130.0, 130.8, 132.2, 133.2, 133.4, 135.4, 137.0, 137.3, 139.4, 151.7, 170.4. ESI-MS(TOF) calcd. for $C_{39}H_{47}N_5ORu$ $[M\text{-}Cl^-]^+$ *m/z* 703.2751, found *m/z* 703.2758.

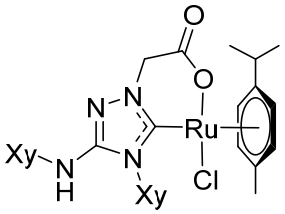


Chloro[η⁶-1-methyl-4-(propan-2-yl)benzene](2-{2-(oxo-κ*O*)-2-[(2,4,6-trimethylphenyl)amino]ethyl}-4-(2,4,6-trimethylphenyl)-5-[(2,4,6-trimethylphenyl)amino]-2,4-dihydro-3*H*-1,2,4-triazol-3-ylidene-κ*C*³)ruthenium chloride (4b). Yield 0.078 g (51%), orange crystals, mp > 150 °C, decomp. ^1H NMR ($CDCl_3$, 300 MHz) (a mixture of diastereomers): δ 0.77 (d, J = 6.8 Hz, 3H), 0.89 (d, J = 7.0 Hz,

3H), 1.72-1.74 (m, 4H), 2.12 – 2.28 (m, 21H), 2.46 (s, 6H), 3.23 (d, *J* = 5.3 Hz, 1H), 4.89 (d, *J* = 5.3 Hz, 1H), 5.08 (d, *J* = 17.6 Hz, 1H), 5.17 – 5.23 (m, 2H), 5.64 (d, *J* = 6.8 Hz, 1H), 5.79 (d, *J* = 17.6 Hz, 1H), 6.78 – 6.88 (m, 4H), 7.22 (s, 1H), 7.31 (s, 1H), 12.47 (s, 1H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75 MHz) (a mixture of diastereomers): δ 14.2, 17.7, 18.1, 18.5, 18.6, 18.8, 19.0, 20.4, 21.0, 21.1, 21.5, 22.9, 29.8, 52.6, 92.6, 97.8, 103.6, 128.5, 128.7, 129.7, 130.5, 130.6, 130.7, 130.8, 130.9, 134.8, 135.1, 135.4, 136.5, 137.2, 137.8, 138.9, 142.7, 151.9, 170.5, 171.7. ESI-MS(TOF) calcd. for $C_{41}H_{51}N_5ORu$ $[M\text{-}Cl^-]^+$ *m/z* 730.3064, found *m/z* 730.3064.

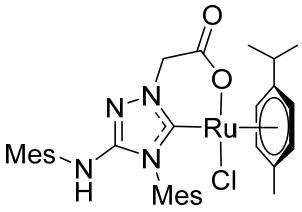


Chloro[η⁶-1-methyl-4-(propan-2-yl)benzene]{2-[2-{[2,6-di(propan-2-yl)phenyl]amino}-2-(oxo-κ*O*)ethyl]-4-(2,4,6-trimethylphenyl)-5-[(2,4,6-trimethylphenyl)amino]-2,4-dihydro-3*H*-1,2,4-triazol-3-ylidene-κC^3}ruthenium chloride (4c). Yield 0.066 g (41%), orange crystals, mp > 150 °C, decomp. ^{1}H NMR ($CDCl_3$, 300 MHz) (a mixture of diastereomers): δ 0.83 (d, *J* = 6.7 Hz, 3H), 0.86 (d, *J* = 7.1 Hz, 3H), 1.01 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.7 Hz, 3H), 1.18 (d, *J* = 6.7 Hz, 3H), 1.30 (d, *J* = 6.7 Hz, 3H), 1.70 (s, 3H), 2.16 (s, 6H), 2.18 (s, 3H), 2.25 (s, 3H), 2.46 (s, 4H), 2.96 – 3.14 (m, 2H), 3.30 (d, *J* = 5.2 Hz, 1H), 4.96 (d, *J* = 5.5 Hz, 1H), 5.06 (d, *J* = 6.7 Hz, 1H), 5.21 (d, *J* = 17.9 Hz, 1H), 5.40 (s, 1H), 5.49 (d, *J* = 6.7 Hz, 1H), 5.72 (d, *J* = 18.0 Hz, 1H), 6.87 (s, 2H), 7.06 – 7.24 (m, 4H), 7.31 (s, 1H), 12.38 (s, 1H) (signal $CH^{i\text{-}Pr}$ of *p*-Cymene is overlapped with water). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75 MHz) (a mixture of diastereomers): δ 17.8, 18.1, 18.6, 18.7, 20.8, 21.5, 22.9, 23.4, 24.3, 25.1, 28.4, 28.6, 29.6, 40.1, 53.0, 93.5, 103.1, 123.0, 123.6, 128.6, 129.7, 130.4, 130.5, 130.6, 130.8, 135.1, 136.4, 137.7, 138.9, 142.7, 145.5, 146.2, 152.0, 171.8. ESI-MS(TOF) calcd. for $C_{44}H_{57}N_5ORu$ $[M\text{-}Cl^-]^+$ *m/z* 772.3535, found *m/z* 772.3558.

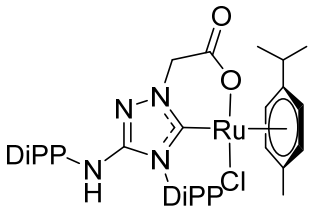


{2-[(Carboxylato-κ*O*)methyl]-4-(2,6-dimethylphenyl)-5-[(2,6-dimethylphenyl)amino]-2,4-dihydro-3*H*-1,2,4-triazol-3-ylidene-κC^3}(chloro[η⁶-1-methyl-4-(propan-2-yl)benzene]ruthenium (5a). Yield 0.040 g (32%), orange crystals, mp > 150 °C, decomp. ^{1}H NMR ($CDCl_3$, 300 MHz) (a mixture of diastereomers): δ 1.03 (d, *J* = 6.8 Hz, 3H), 1.17 (d, *J* = 7.0 Hz, 3H), 1.82 (s, 3H), 2.22 (s, 6H), 2.32 (s, 3H), 2.56 (s, 3H), 2.72 (hept, *J* = 6.9 Hz, 1H), 3.40 (s, 1H), 4.39 (d, *J* = 17.0 Hz, 1H), 4.77 (d, *J* = 17.0 Hz, 1H), 4.96 (d, *J* = 5.5 Hz, 1H), 5.15 (s, 1H), 5.51 (br. s, 1H), 5.62 (d, *J* = 6.7 Hz, 1H), 7.04 – 7.13 (m, 3H), 7.40 – 7.60 (m, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75 MHz) (a mixture of diastereomers): δ 18.0, 18.3, 18.6, 19.1, 20.6, 23.6, 29.6,

56.2, 93.6, 128.0, 129.0, 129.8, 130.1, 131.9, 133.7, 135.3, 137.1, 139.8, 151.0, 171.5. ESI-MS(TOF) calcd. for $C_{30}H_{35}N_4O_2Ru$ $[M\text{-}Cl^-]^+$ *m/z* 585.1804, found *m/z* 585.1810.



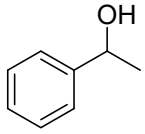
{2-[(Carboxylato-κ*O*)methyl]-4-(2,4,6-trimethylphenyl)-5-[(2,4,6-trimethylphenyl)amino]-2,4-dihydro-3*H*-1,2,4-triazol-3-ylidene-κ*C*^{3}}(chloro)[η^6-1-methyl-4-(propan-2-yl)benzene]ruthenium (5b). Yield 0.070 g (54%), orange crystals, mp > 150 °C, decomp. ^{1}H NMR ($CDCl_3$, 300 MHz) (a mixture of diastereomers): δ 1.03 (d, *J* = 6.8 Hz, 3H), 1.17 (d, *J* = 7.0 Hz, 3H), 1.83 (s, 3H), 2.16 (s, 6H), 2.25 (s, 3H), 2.26 (s, 3H), 2.47 (s, 3H), 2.50 (s, 3H), 2.73 (hept, *J* = 6.9 Hz, 1H), 3.35 (s, 1H), 4.40 (d, *J* = 17.1 Hz, 1H), 4.76 (d, *J* = 17.1 Hz, 1H), 4.97 (d, *J* = 5.5 Hz, 1H), 5.04 (s, 1H), 5.55 (s, 1H), 5.63 (d, *J* = 6.6 Hz, 1H), 6.88 (s, 2H), 7.21 (s, 1H), 7.29 (s, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz) (a mixture of diastereomers): δ 17.8, 18.2, 18.5, 18.6, 18.8, 19.0, 20.4, 21.06, 21.10, 21.5, 22.9, 29.8, 52.7, 92.6, 103.6, 128.5, 128.7, 129.7, 130.5, 130.6, 130.7, 130.8, 130.9, 134.8, 135.1, 135.4, 136.5, 137.2, 137.8, 138.9, 142.7, 151.9, 170.5, 171.7. ESI-MS(TOF) calcd. for $C_{32}H_{39}N_4O_2Ru$ $[M\text{-}Cl^-]^+$ *m/z* 613.2120, found *m/z* 613.2097.



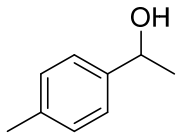
(2-[(Carboxylato-κ*O*)methyl]-4-[2,6-di(propan-2-yl)phenyl]-5-{[2,6-di(propan-2-yl)phenyl]amino}-2,4-dihydro-3*H*-1,2,4-triazol-3-ylidene-κ*C*^{3})(chloro)[η^6-1-methyl-4-(propan-2-yl)benzene]-ruthenium (5c). Yield 0.070 g (54%), orange crystals, mp > 150 °C, decomp. ^{1}H NMR ($CDCl_3$, 300 MHz) (a mixture of diastereomers): 1.05 – 1.15 (m, 18H), 1.22 (d, *J* = 7.0 Hz, 3H), 1.34 (d, *J* = 6.6 Hz, 3H), 1.46 (d, *J* = 6.6 Hz, 3H), 1.64-1.68 (m, 3H), 1.84 (s, 3H), 2.66 (hept, *J* = 6.8 Hz, 1H), 2.90 (hept, *J* = 6.7 Hz, 2H), 3.02 (hept, *J* = 6.8 Hz, 1H), 3.27 (hept, *J* = 6.6 Hz, 1H), 3.41 (d, *J* = 5.4 Hz, 1H), 4.39 (d, *J* = 17.1 Hz, 1H), 4.83 (d, *J* = 17.1 Hz, 1H), 5.07 (s, 1H), 5.24 (d, *J* = 5.4 Hz, 1H), 5.61 – 5.68 (m, 2H), 7.14 – 7.19 (m, 2H), 7.24 – 7.31 (m, 1H), 7.51-7.60 (m, 2H), 7.73 (t, *J* = 7.8 Hz, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz) (a mixture of diastereomers): δ 18.0, 18.2, 18.5, 18.9, 20.7, 21.1, 21.5, 23.6, 29.6, 56.1, 93.7, 102.7, 129.7, 130.4, 130.7, 130.8, 131.0, 135.1, 136.6, 137.7, 139.3, 142.2, 151.3, 171.5, 171.7. ESI-MS(TOF) calcd. for $C_{38}H_{51}N_4O_2Ru$ $[M\text{-}Cl^-]^+$ *m/z* 697.3056, found *m/z* 697.3070.

Catalytic activity study of complexes 4a-c or 5a-c in the transfer hydrogenation of ketones. All experiments were conducted in 4 ml screw-capped high-pressure glass vials equipped with a magnetic stirrer under an argon atmosphere. Powdered Bu^tOK (5.6 mg, 0.05 mmol) was added to a solution of acetophenone (60 mg, 0.5 mmol) in Pr^iOH (2 ml). Then a solution containing complex **4a-c** or **5a-c** (0.5-2.5 μmol) in Pr^iOH (100 μl) was added. The resulting mixture was then stirred at 80 °C for 3-10 h. Then, the reaction mixture was cooled to room temperature, and a solution of naphthalene (32 mg, 0.25 mmol) in Pr^iOH (1 ml) was added as an internal GC-MS standard. An aliquot (3 μl) of the reaction mixture was taken by a syringe, dissolved in acetonitrile (1 ml) and subjected to GC-MS analysis (see Tables 1).

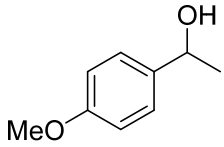
General procedure for the preparation of compounds 7a-h, 9a-d. A 4 ml screw-capped glass tube equipped with a magnetic stirring bar was charged with Bu^tOK (5.6 mg, 0.05 mmol), ketone **6a-h** or **8a-d** (0.5 mmol), and Pr^iOH (2 ml). A solution containing complex **4b** (2 mg, 0.0025 mmol) in Pr^iOH (100 μl) was then added. The tube was purged with argon, sealed with a screw cap fitted with a septum, additionally purged with argon through the septum, then placed in a thermostated oil bath and heated at 80 °C for 5 h. The reaction mixture was then cooled to room temperature and filtered through a short pad of Celite. The filtrate obtained was evaporated in vacuo to give a crude product, which was purified by column chromatography on silica gel (hexane-CH_2Cl_2 1:3 as the eluent).



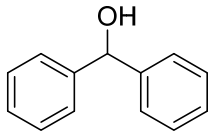
1-Phenylethanol (7a). Yield 49 mg (80%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.49 (d, J = 6.4 Hz, 3H), 2.42 (s, 1H), 4.87 (q, J = 6.5 Hz, 1H), 7.27-7.39 (m, 5H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75 MHz): δ 25.2, 70.4, 125.5, 127.5, 128.5, 145.9. (^{1}H and ^{13}C NMR spectral data of compound **7a** are in good agreement with those published earlier).[S2]



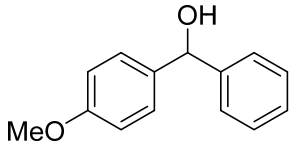
1-(4-Methylphenyl)ethanol (7b). Yield 59 mg (87%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.49 (d, J = 6.4 Hz, 3H), 1.87 (br.s, 1H), 2.35 (s, 3H), 4.87 (q, J = 6.5 Hz, 1H), 7.14-7.19 (m, 2H), 7.25-7.29 (m, 2H). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75 MHz): δ 21.2, 25.2, 70.4, 125.5, 129.3, 137.3, 143.0. (^{1}H and ^{13}C NMR spectral data of compound **7b** are in good agreement with those published earlier).[S2]



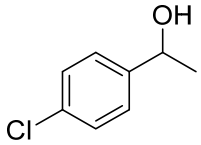
1-(4-Methoxyphenyl)ethanol (7c). Yield 60 mg (79%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.47 (d, J = 6.5 Hz, 3H), 2.03 (br.s, 1H), 3.80 (s, 3H), 4.84 (q, J = 6.4 Hz, 1H), 6.85-6.90 (m, 2H), 7.27-7.31 (m, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 25.1, 55.4, 70.0, 113.9, 126.8, 138.1, 159.1. (^{1}H and ^{13}C NMR spectral data of compound **7c** are in good agreement with those published earlier).[S2]



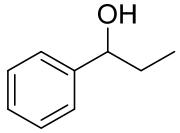
Diphenylmethanol (7d). Yield 89 mg (97%), yellowish oil. ^{1}H NMR (DMSO-d_6, 300 MHz): δ 5.71 (d, J = 3.7 Hz, 1H), 5.89 (d, J = 3.9 Hz, 1H), 7.17-7.23 (m, 2H), 7.27-7.33 (m, 4H), 7.36-7.40 (m, 4H). ^{13}C{^{1}H} NMR (DMSO-d_6, 75 MHz): δ 74.3, 126.2, 126.7, 128.1, 145.7. (^{1}H and ^{13}C NMR spectral data of compound **7d** are in good agreement with those published earlier).[S2]



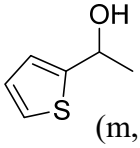
(4-Methoxyphenyl)(phenyl)methanol (7e). Yield 89 mg (83%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.25 (d, J = 3.3 Hz, 1H), 3.71 (s, 3H), 5.71 (d, J = 3.1 Hz, 1H), 6.77-6.81 (m, 2H), 7.17-7.32 (m, 7H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 55.4, 75.9, 114.0, 126.5, 127.5, 128.0, 128.5, 136.3, 144.1, 159.1. (^{1}H and ^{13}C NMR spectral data of compound **7e** are in good agreement with those published earlier).[S3]



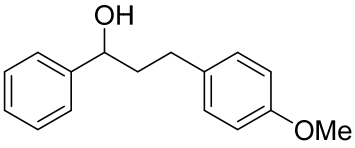
1-(4-Chlorophenyl)ethanol (7f). Yield 67 mg (86%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.43 (d, J = 6.4 Hz, 3H), 2.35 (br.s, 1H), 4.82 (q, J = 6.5 Hz, 1H), 7.24-7.31 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 25.3, 69.7, 126.9, 128.7, 133.1, 144.4. (^{1}H and ^{13}C NMR spectral data of compound **7f** are in good agreement with those published earlier).[S4]



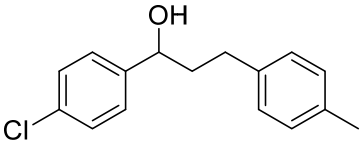
1-Phenylpropan-1-ol (7g). Yield 64 mg (94%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 0.82 (t, J = 7.4 Hz, 3H), 1.60-1.78 (m, 2H), 1.94 (br.s, 1H), 4.49 (t, J = 6.6 Hz, 1H), 7.16-7.27 (m, 5H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 10.3, 32.0, 76.1, 126.1, 127.6, 128.5, 144.7. (^{1}H and ^{13}C NMR spectral data of compound **7g** are in good agreement with those published earlier).[S3]



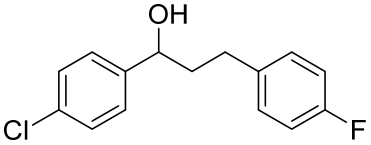
1-(Thiophen-2-yl)ethanol (7h). Yield 27 mg (42 %), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.61 (d, *J* = 6.4 Hz, 3H), 2.00 (d, *J* = 4.4 Hz, 1H), 5.10-5.18 (m, 1H), 6.95-7.00 (m, 2H), 7.24 (dd, *J* = 4.7, 1.6 Hz, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 25.4, 66.4, 123.3, 124.6, 126.8, 150.0. (^{1}H and ^{13}C NMR spectral data of compound **7h** are in good agreement with those published earlier).[S2]



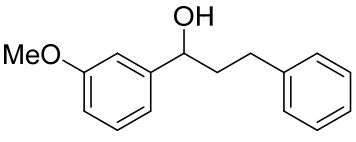
3-(4-Methoxyphenyl)-1-phenylpropan-1-ol (9a). Yield 69 mg (57%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.79 (d, *J* = 3.0 Hz, 1H), 1.95-2.21 (m, 2H), 2.59-2.78 (m, 2H), 3.81 (s, 3H), 4.62-4.67 (m, 1H), 6.87-6.92 (m, 2H), 7.16-7.21 (m, 3H), 7.26-7.31 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 32.3, 40.5, 55.4, 73.7, 114.0, 126.0, 127.4, 128.5, 128.6, 136.8, 142.0, 159.3. (^{1}H and ^{13}C NMR spectral data of compound **9a** are in good agreement with those published earlier).[S5]



1-(4-Chlorophenyl)-3-(4-methylphenyl)propan-1-ol (9b). Yield 56 mg (43%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.84-1.86 (m, 1H), 1.96-2.17 (m, 2H), 2,32 (s, 3H), 2.62-2.70 (m, 2H), 4.64-4.70 (m, 1H), 7.06-7.12 (m, 4H), 7.26-7.34 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 21.1, 31.6, 40.8, 73.3, 127.5, 128.4, 128.8, 129.3, 133.4, 135.6, 138.5, 143.2.



1-(4-Chlorophenyl)-3-(4-fluorophenyl)propan-1-ol (9c). Yield 62 mg (47%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.88-2.17 (m, 3H), 2.58-2.74 (m, 2H), 4.63-4.68 (m, 1H), 6.93-6.99 (m, 2H), 7.10-7.15 (m, 2H), 7.26-7.34 (m, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 31.2, 40.8, 73.2, 115.3 (d, *J* = 21.1 Hz), 127.4, 128.8, 129.9 (d, *J* = 7.7 Hz), 133.5, 137.2 (d, *J* = 3.2 Hz), 143.1, 161.5 (d, *J* = 243.6 Hz).



1-(3-Methoxyphenyl)-3-phenylpropan-1-ol (9d). Yield 82 mg (68%), yellowish oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.85 (br.s, 1H), 1.97-2.19 (m, 2H), 2.63-2.81 (m, 2H), 3.82 (s, 3H), 4.65-4.71 (m, 1H), 6.81-6.84 (m, 1H), 6.91-6.95 (m, 2H), 7.16-7.21 (m, 3H), 7.24-7.31 (m, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ 32.2, 40.6, 55.4, 74.0, 111.5, 113.2, 118.4, 126.0, 128.5, 128.6, 129.7, 141.9, 146.5, 160.0. (^{1}H and ^{13}C NMR spectral data of compound **9d** are in good agreement with those published earlier).[S6]

S3. X-Ray diffraction single-crystal studies

X-ray crystallographic data and refinement details.

A single crystal of compound **5b** was obtained from $CHCl_3$ by a slow evaporation at room temperature. X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix6000HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Mo K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program (CrysAlisPro. Version 1.171.42. *Rigaku Oxford Diffraction*, **2023**). The structure was solved by direct methods using SHELXT[7] and refined on F^2 using SHELXL-2018[S8] in the OLEX2 program.[S9] All non-hydrogen atoms were refined with individual anisotropic displacement parameters. A position of atom H4 was found from the electron density-difference map, all other hydrogen atoms were positioned geometrically and refined as riding atoms with relative isotropic displacement parameters.

Crystal data, data collection and structure refinement details for **5b** summarized in Table S1. The structure has been deposited at the Cambridge Crystallographic Data Center with the reference CCDC number 2306474, correspondingly; also contain the supplementary crystallographic data. These data can be obtained free of charge from the CCDC *via* https://www.ccdc.cam.ac.uk/structures/.

Table S1. Crystal data and structure refinement for **5b**.

Identification code	**5b•2CHCl$_3$**
Empirical formula	$C_{34}H_{41}Cl_7N_4O_2Ru$
Formula weight	886.93
Temperature, K	99.9(7)
Wavelength, Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$
a, Å	15.63046 (14)
b, Å	15.26918 (12)
c, Å	16.84325 (14)
β, °	97.6546 (8)
Volume, Å^3	3984.06 (6)
Z	4
Calculated density, g·cm^{-3}	1.479
Absorption coefficient, mm^{-1}	0.898
F(000)	1808
Crystal size, mm	0.59×0.43×0.27
θ range for data collection, °	2.137-35.410
Index ranges	-24≤*h*≤24, -24≤*k*≤23, -26≤*l*≤27
Reflections collected	96417
Independent reflections [$R_{(int)}$]	16732 [0.0455]
Observed reflections (with $I>2\sigma(I)$)	15303
Completeness to $\theta_{full}/\theta_{max}$, °	0.005
T_{max} / T_{min}	0.893 / 0.796
Data / restraints / parameters	16732/157/513
Goodness-of-fit on F^2	1.035
Final R_1 / wR_2 indices with $I>2\sigma(I)$	0.0264 / 0.0716
Final R_1 / wR_2 indices (all data)	0.0294 / 0.0731
Absolute structure parameter	-
Largest diff, peak / hole, ē·Å^3	1.183 / -1.386
CCDC number	2306474

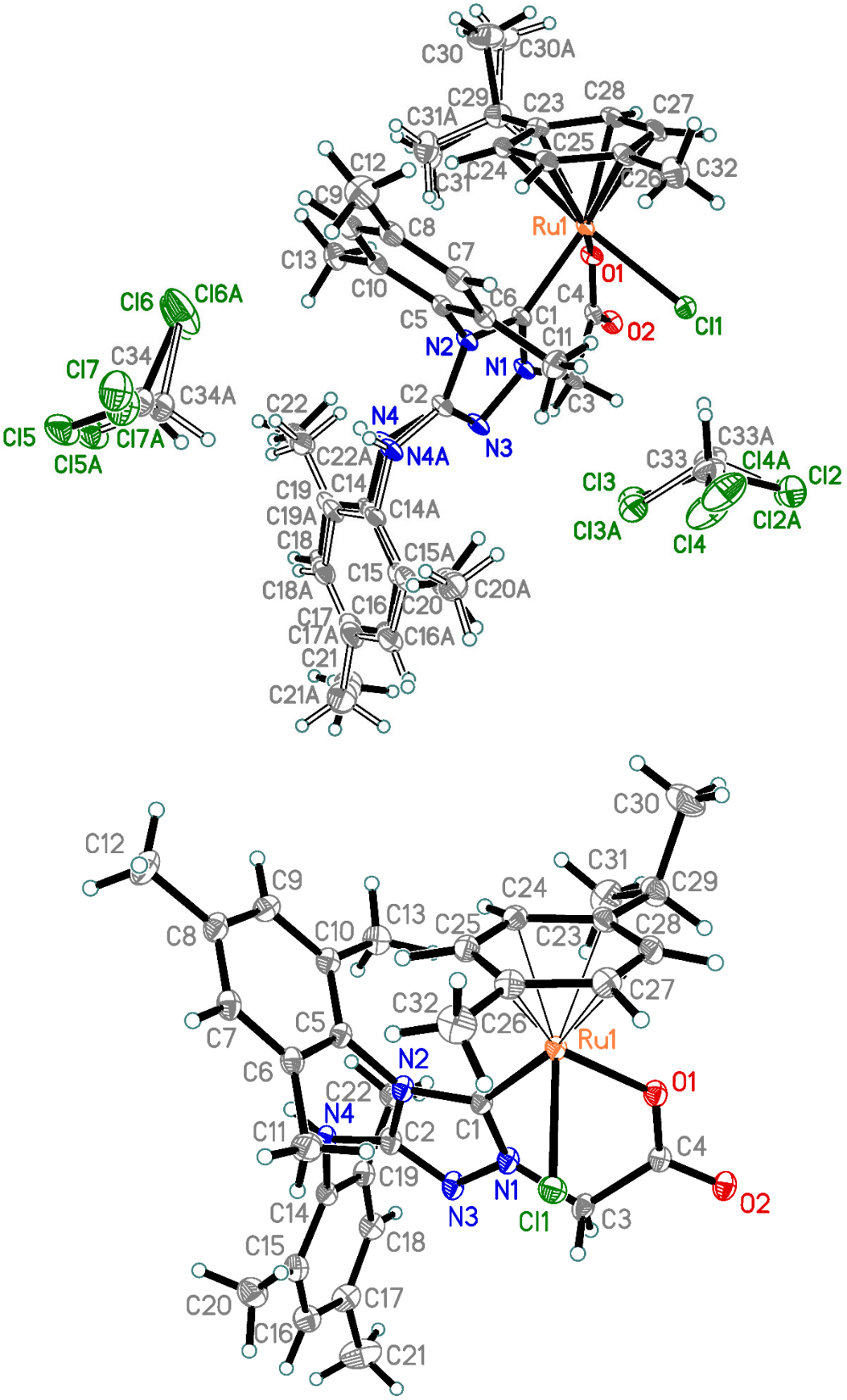


Figure S1. General view of complex **5b** in the representation of atoms *via* thermal ellipsoids at the 50% probability level.

Table S2. Selected bond lengths in **5b**, Å.

Ru1-Cl1	2.4137(2)	C8-C9	1.3958(15)	C19A-C22A	1.494(11)
Ru1-O1	2.1074(7)	C8-C12	1.5056(15)	C23-C24	1.4122(14)
Ru1-C1	2.0585(9)	C9-C10	1.3968(14)	C23-C28	1.4392(14)
Ru1-C23	2.1917(10)	C10-C13	1.5062(14)	C23-C29	1.5127(15)
Ru1-C24	2.1786(10)	N4-H4	0.788(19)	C24-C25	1.4280(14)
Ru1-C25	2.1995(9)	N4-C14	1.435(6)	C25-C26	1.4086(14)
Ru1-C26	2.2161(10)	C14-C15	1.414(4)	C26-C27	1.4358(15)
Ru1-C27	2.2467(9)	C14-C19	1.406(5)	C26-C32	1.5008(16)
Ru1-C28	2.2363(9)	C15-C16	1.398(5)	C27-C28	1.3929(15)
O1-C4	1.2756(12)	C15-C20	1.518(5)	C29-C30	1.545(4)
O2-C4	1.2421(12)	C16-C17	1.397(4)	C29-C31	1.527(5)
N1-N3	1.3881(11)	C17-C18	1.402(4)	C29-C30A	1.532(11)
N1-C1	1.3321(12)	C17-C21	1.513(4)	C29-C31A	1.524(13)
N1-C3	1.4561(12)	C18-C19	1.392(5)	Cl2-C33	1.759(2)
N2-C1	1.3857(12)	C19-C22	1.506(4)	Cl3-C33	1.760(2)
N2-C2	1.3795(12)	N4A-H4A	0.80(2)	Cl4-C33	1.7673(19)
N2-C5	1.4307(12)	N4A-C14A	1.443(12)	Cl2A-C33A	1.777(15)
N3-C2	1.3127(13)	C14A-C15A	1.364(11)	Cl3A-C33A	1.778(14)
C2-N4	1.364(6)	C14A-C19A	1.373(11)	Cl4A-C33A	1.778(14)
C2-N4A	1.363(12)	C15A-C16A	1.404(11)	Cl5-C34	1.7590(13)
C3-C4	1.5171(14)	C15A-C20A	1.460(12)	Cl6-C34	1.7612(14)
C5-C6	1.4002(13)	C16A-C17A	1.368(9)	Cl7-C34	1.7520(15)
C5-C10	1.3951(14)	C17A-C18A	1.366(9)	Cl5A-C34A	1.734(14)
C6-C7	1.3944(14)	C17A-C21A	1.513(10)	Cl6A-C34A	1.733(14)
C6-C11	1.5014(15)	C18A-C19A	1.415(11)	Cl7A-C34A	1.728(14)
C7-C8	1.3912(16)				

Table S3. Hydrogen bonds for **5b•2CHCl$_3$**, Å and °.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4)...O(2)#1	0.79	2.29	2.889(7)	133.5
N(4A)-H(4A)...O(2)#1	0.80	2.20	2.873(15)	141.5

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,y+1/2,-z+3/2

S4. ^{1}H and ^{13}C NMR spectra

Figure S2. ^{1}H NMR spectrum of compound **2a** (DMSO-d_6, 300 MHz).

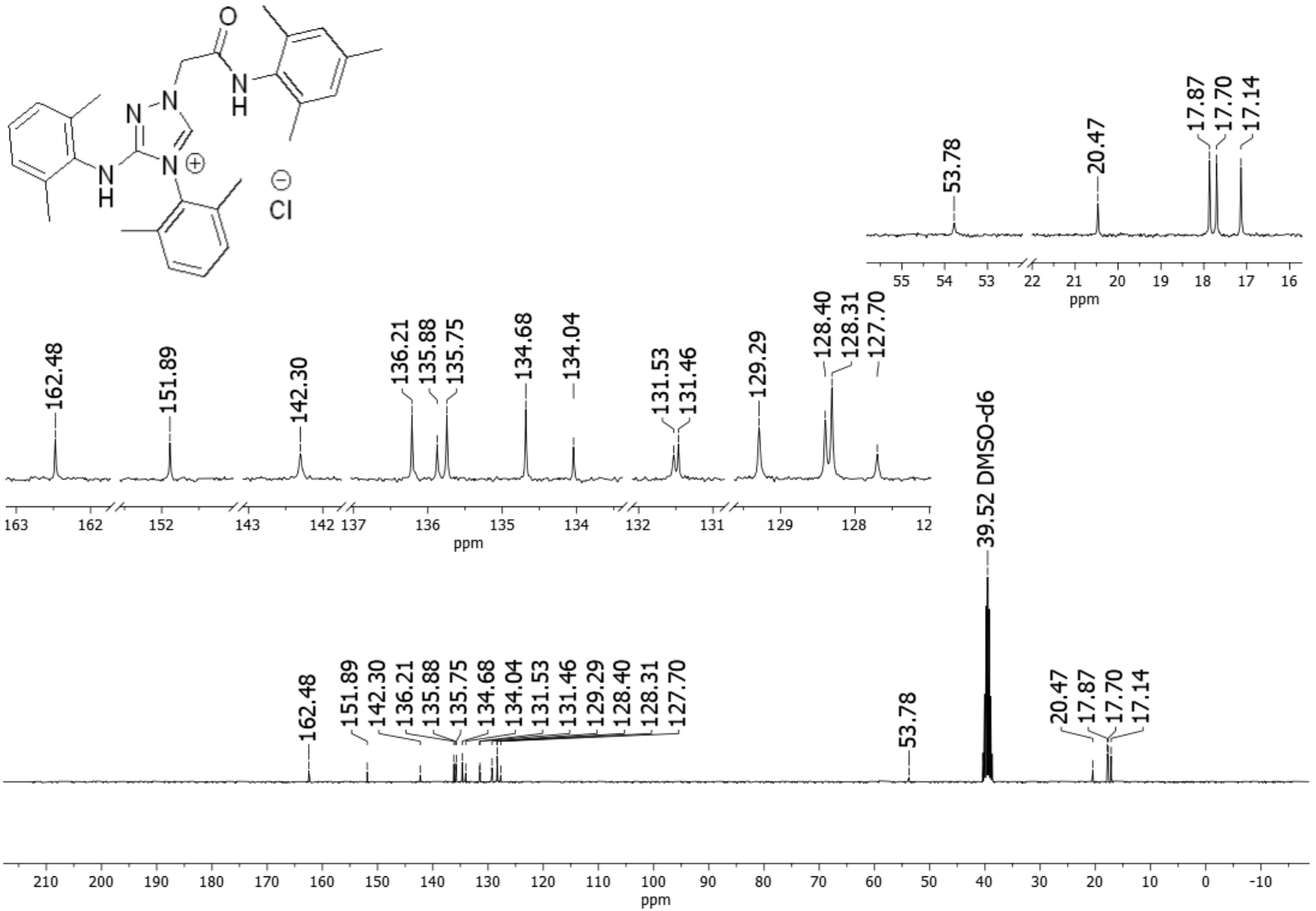


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of compound **2a** (DMSO-d_6, 75 MHz).

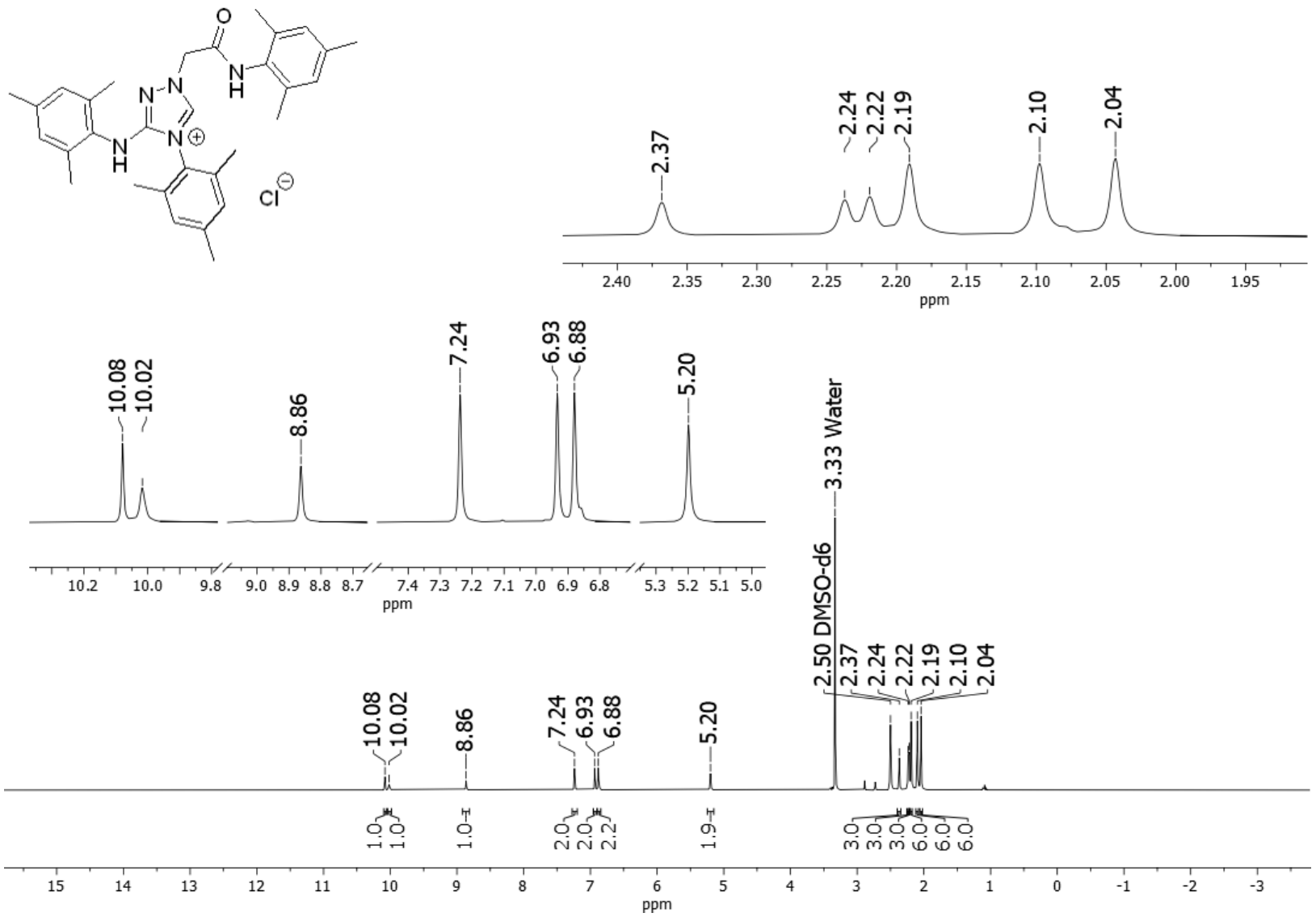


Figure S4. [1]H NMR spectrum of compound **2b** (DMSO-d_6, 300 MHz).

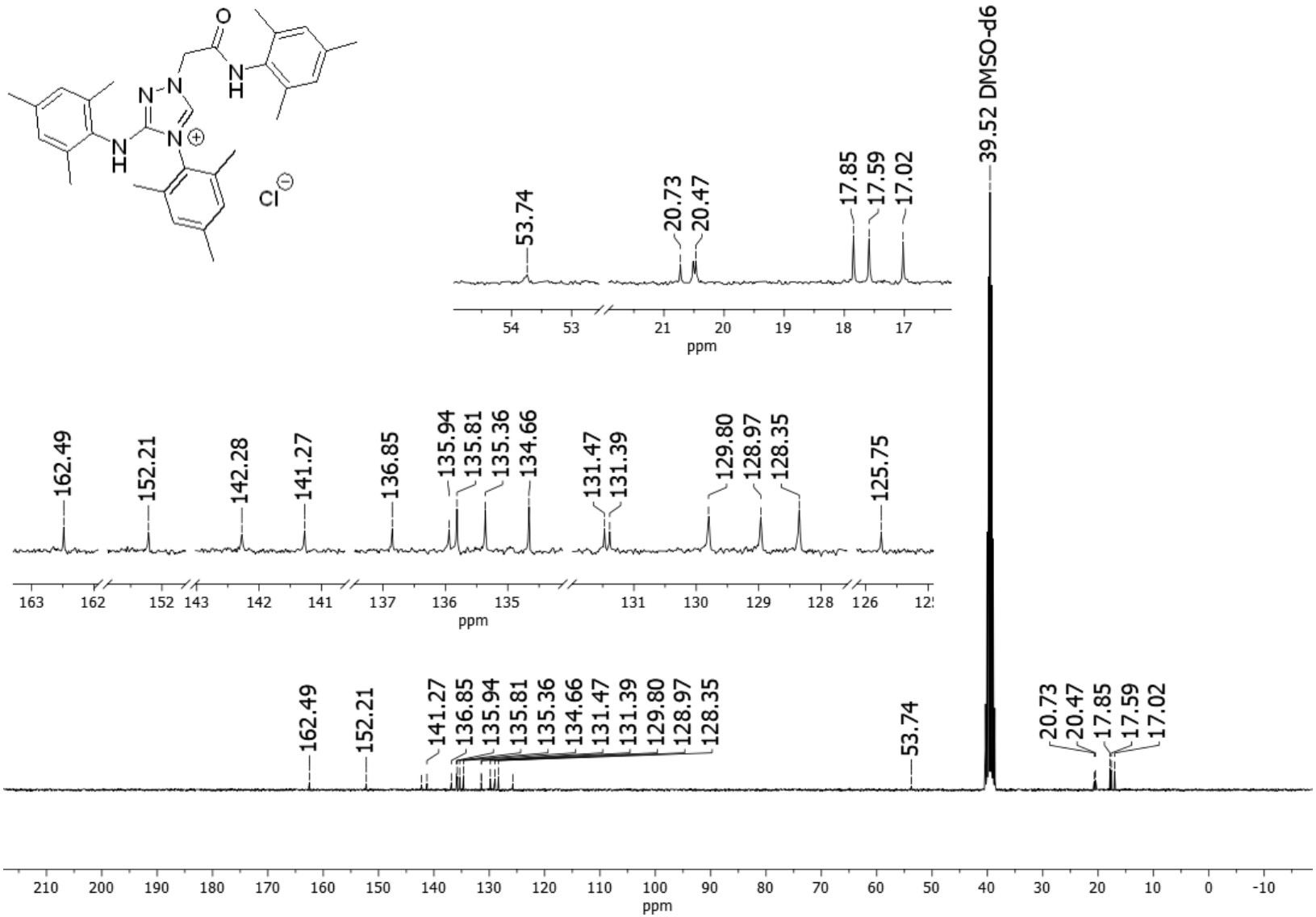


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of compound **2b** (DMSO-d_6, 75 MHz).

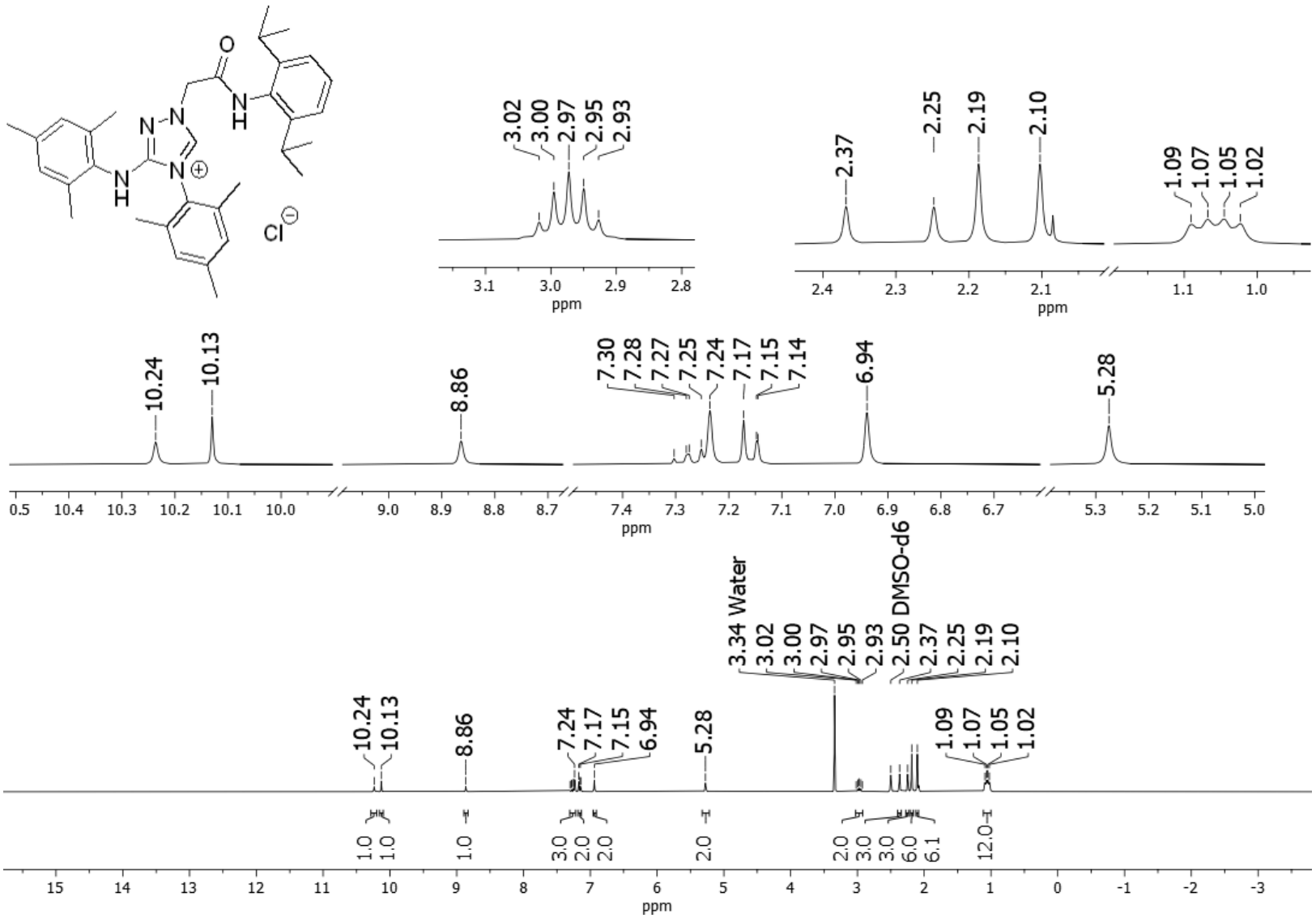


Figure S6. ^{1}H NMR spectrum of compound **2c** (DMSO-d_6, 300 MHz).

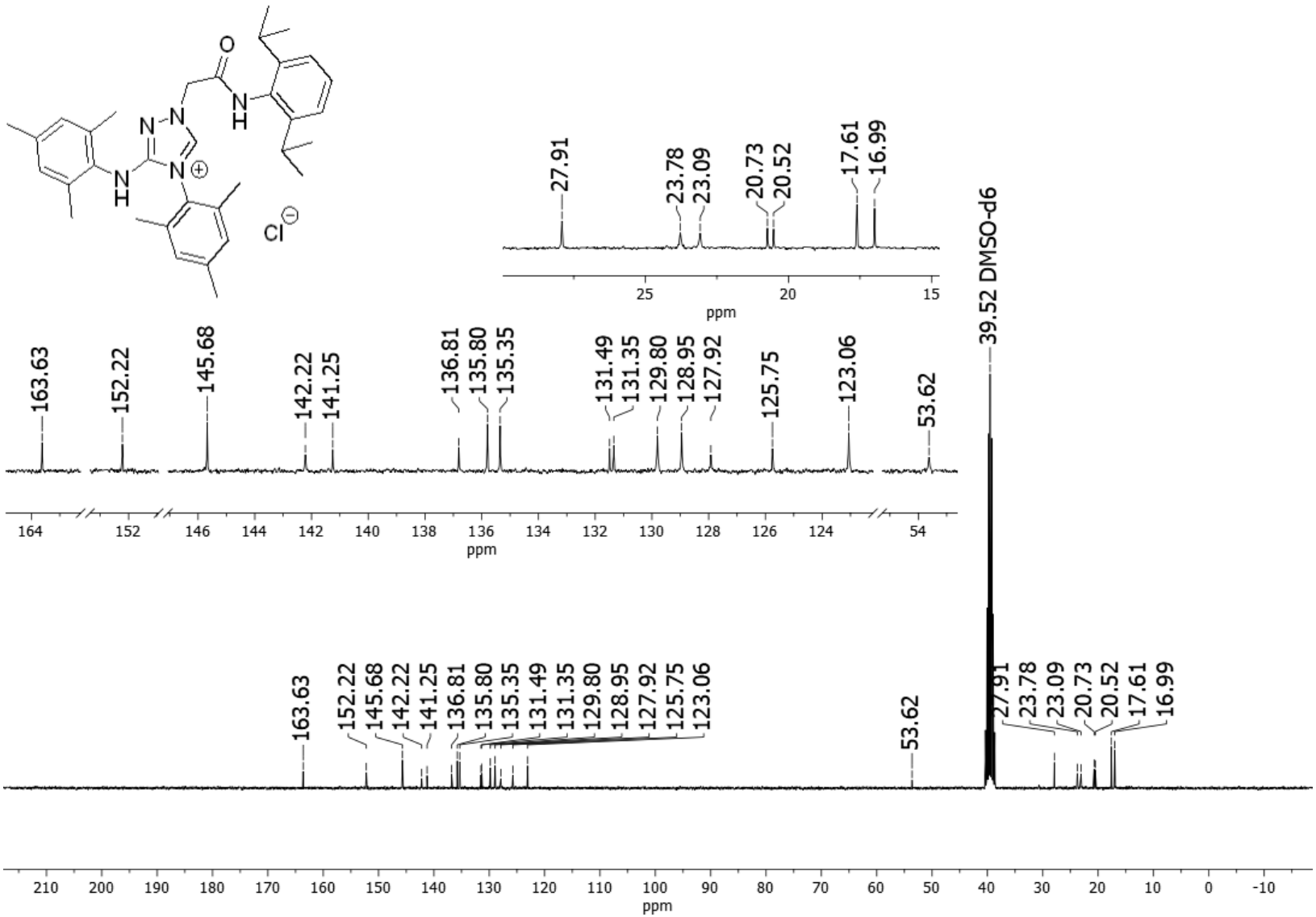


Figure S7. ^{13}C NMR spectrum of compound **2c** (DMSO-d_6, 75 MHz).

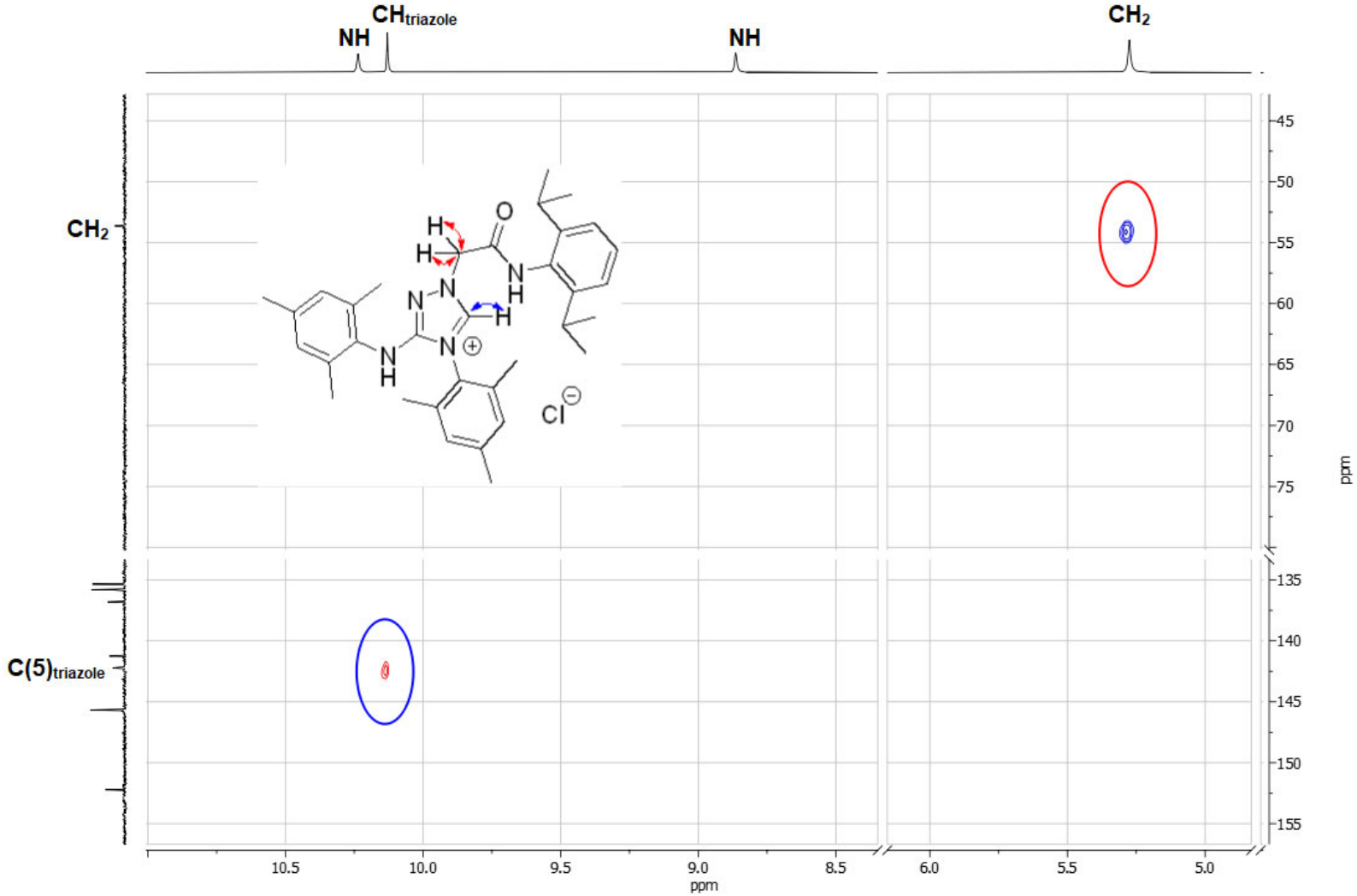


Figure S8. Fragment of ^{1}H-^{13}C HSQC spectrum of compound **2c** (DMSO-d_6).

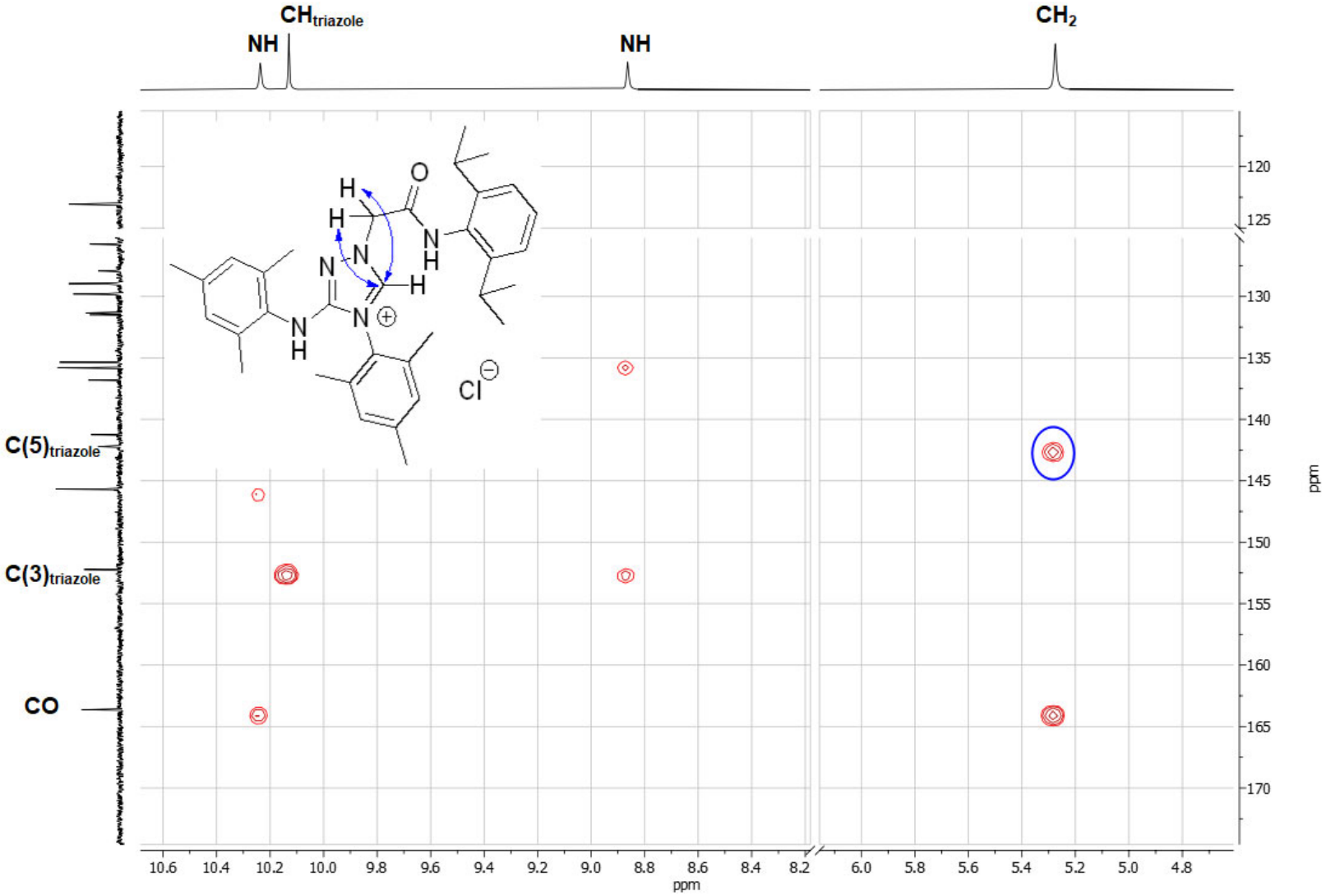


Figure S9. Fragment of ^{1}H-^{13}C HMBC spectrum of compound **2c** (DMSO-d_6).

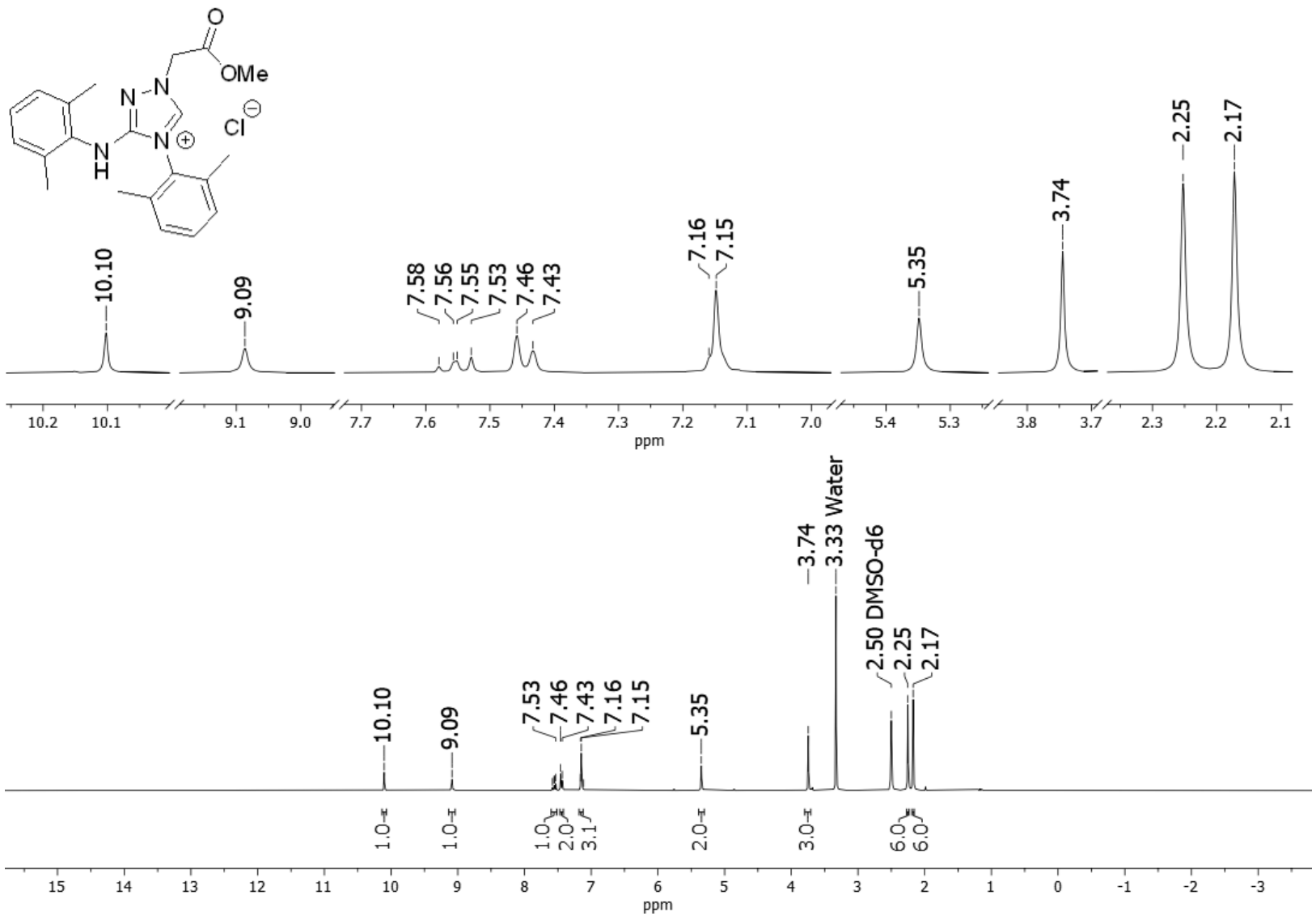


Figure S10. ^{1}H NMR spectrum of compound **3a** (DMSO-d_6, 300 MHz).

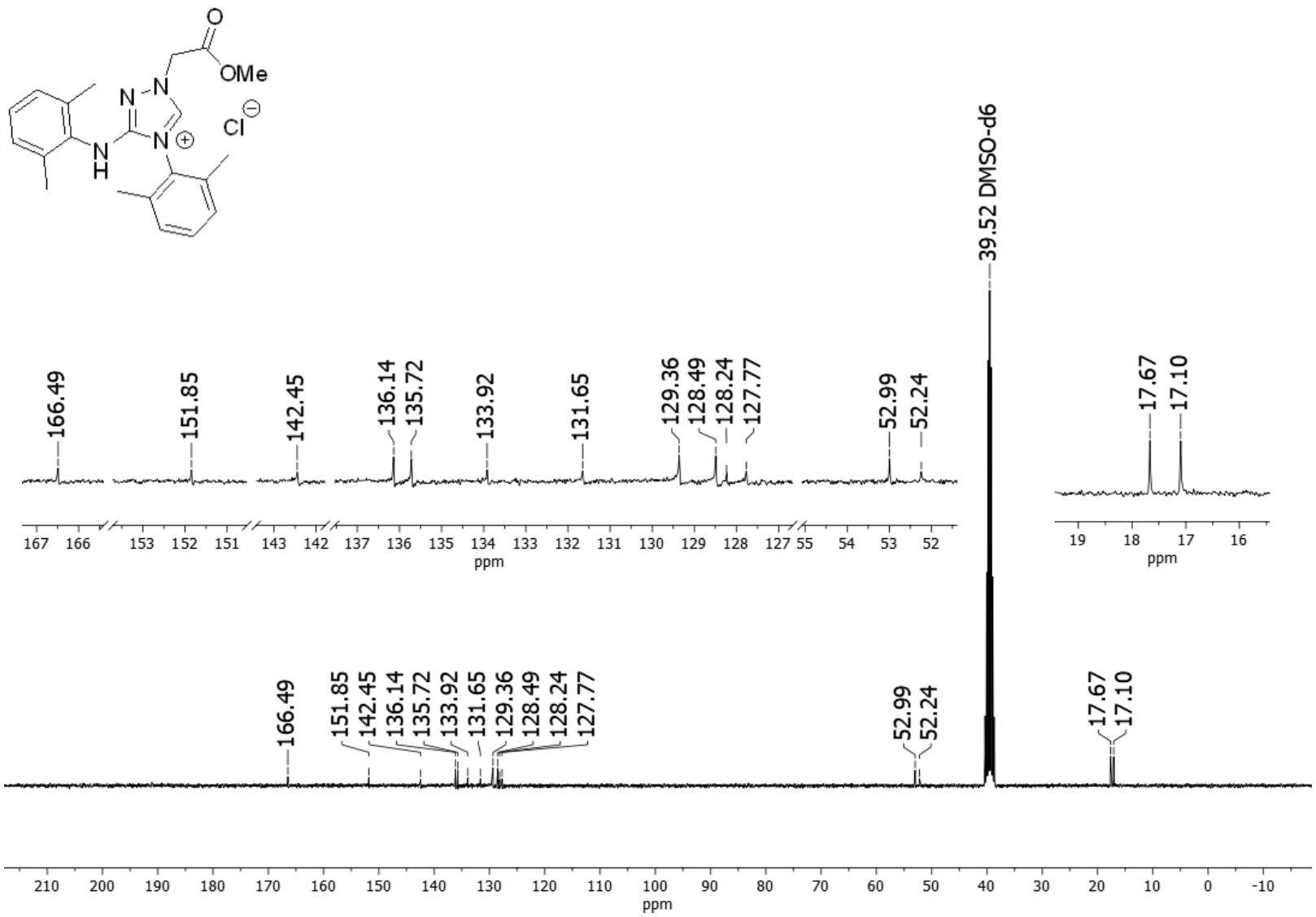


Figure S11. ^{13}C NMR spectrum of compound **3a** (DMSO-d_6, 75 MHz).

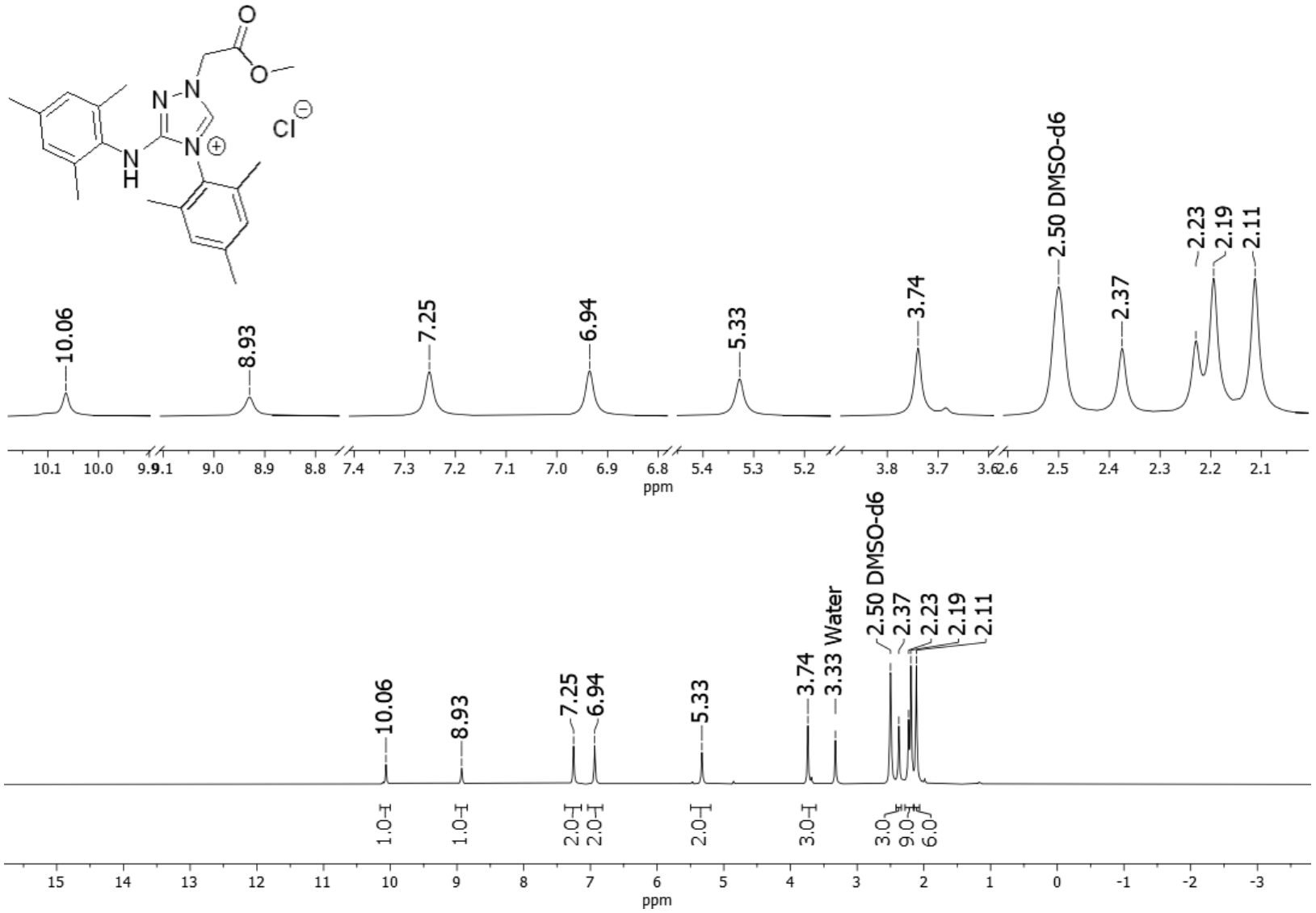


Figure S12. ^{1}H NMR spectrum of compound **3b** (DMSO-d_6, 300 MHz).

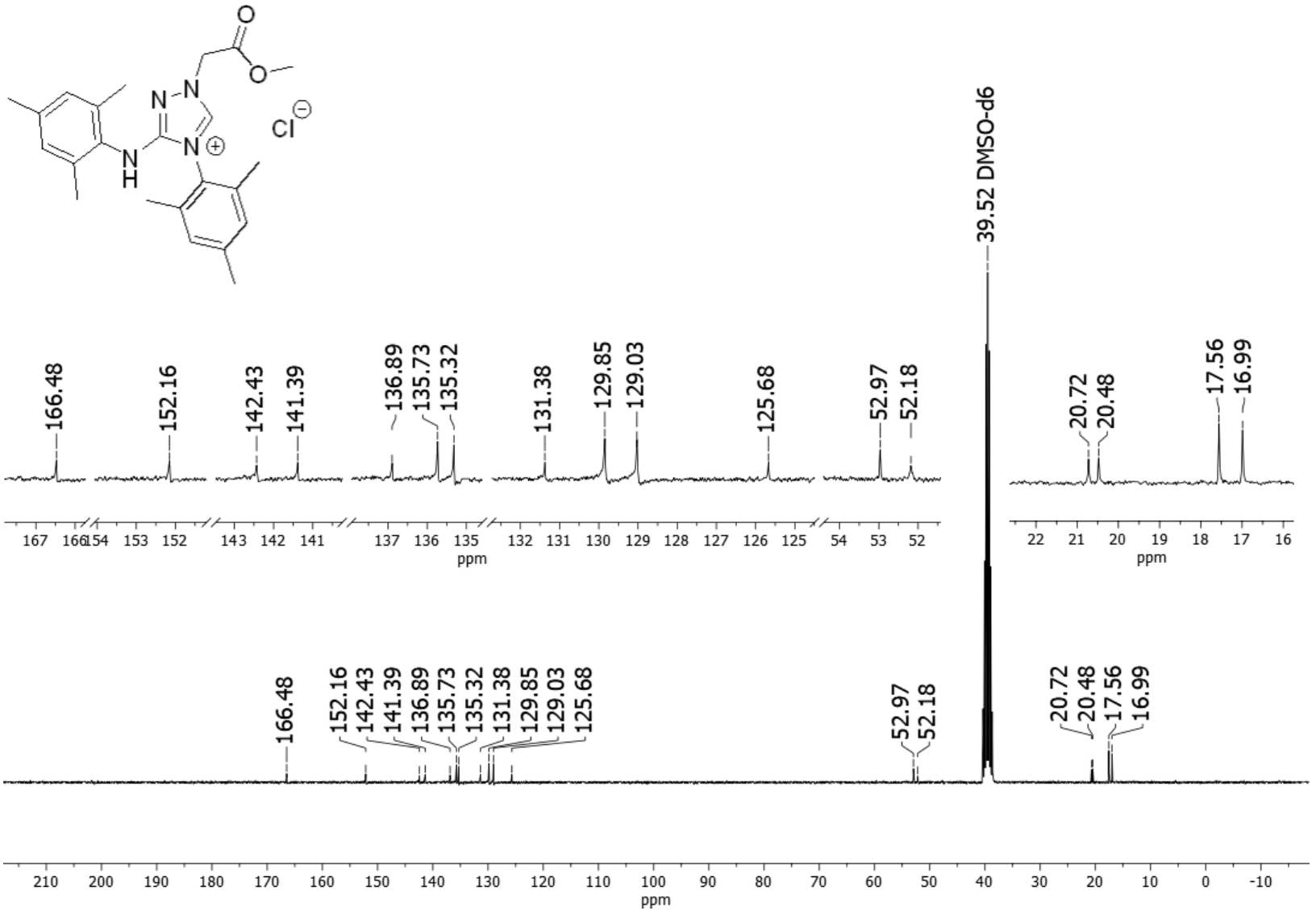


Figure S13. ^{13}C NMR spectrum of compound **3b** (DMSO-d_6, 75 MHz).

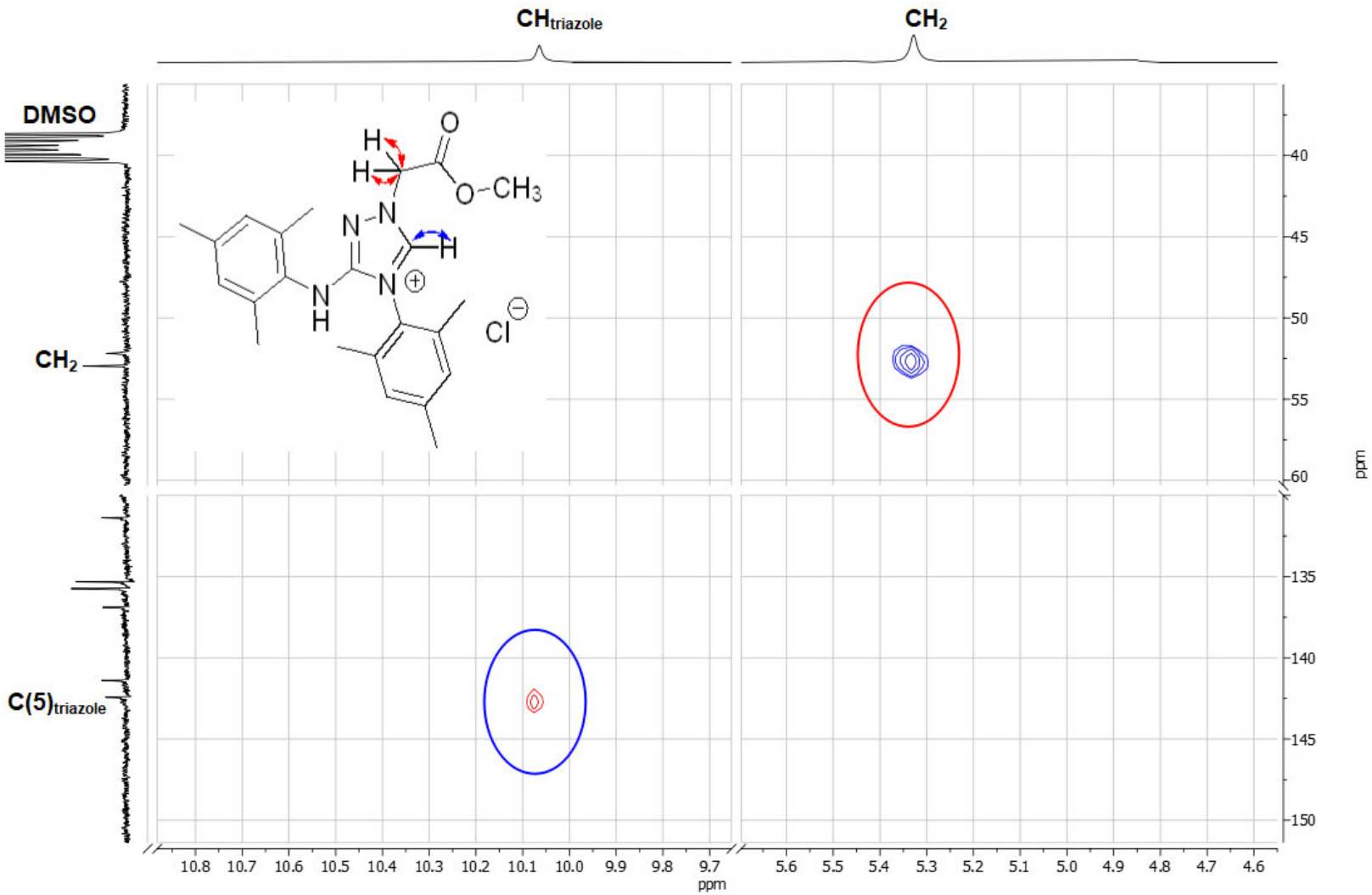


Figure S14. Fragment of ^{1}H-^{13}C HSQC spectrum of compound **3b** (DMSO-d_6).

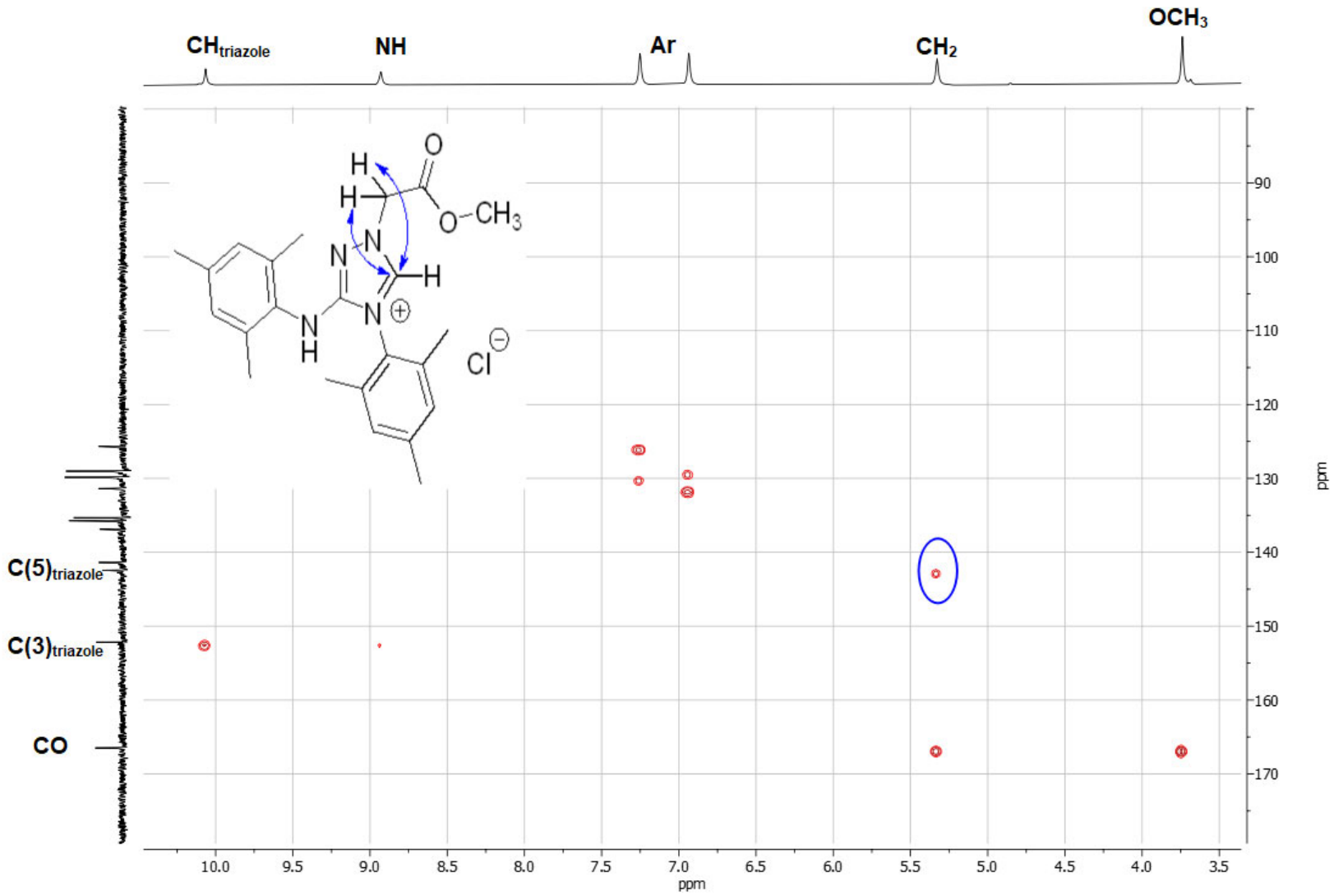


Figure S15. Fragment of ^{1}H-^{13}C HMBC spectrum of compound **3b** (DMSO-d_6).

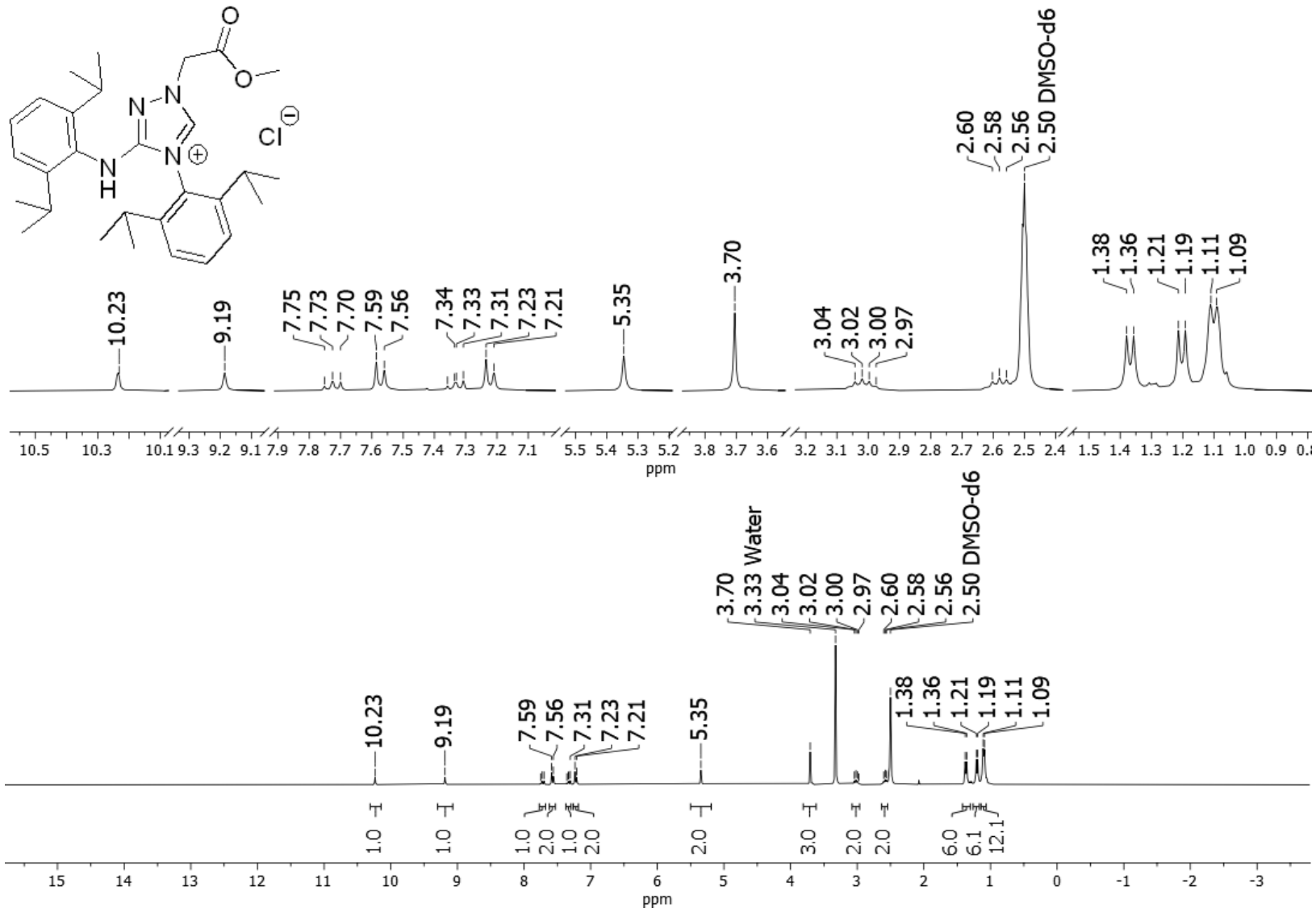


Figure S16. ^{1}H NMR spectrum of compound **3c** (DMSO-d_6, 300 MHz).

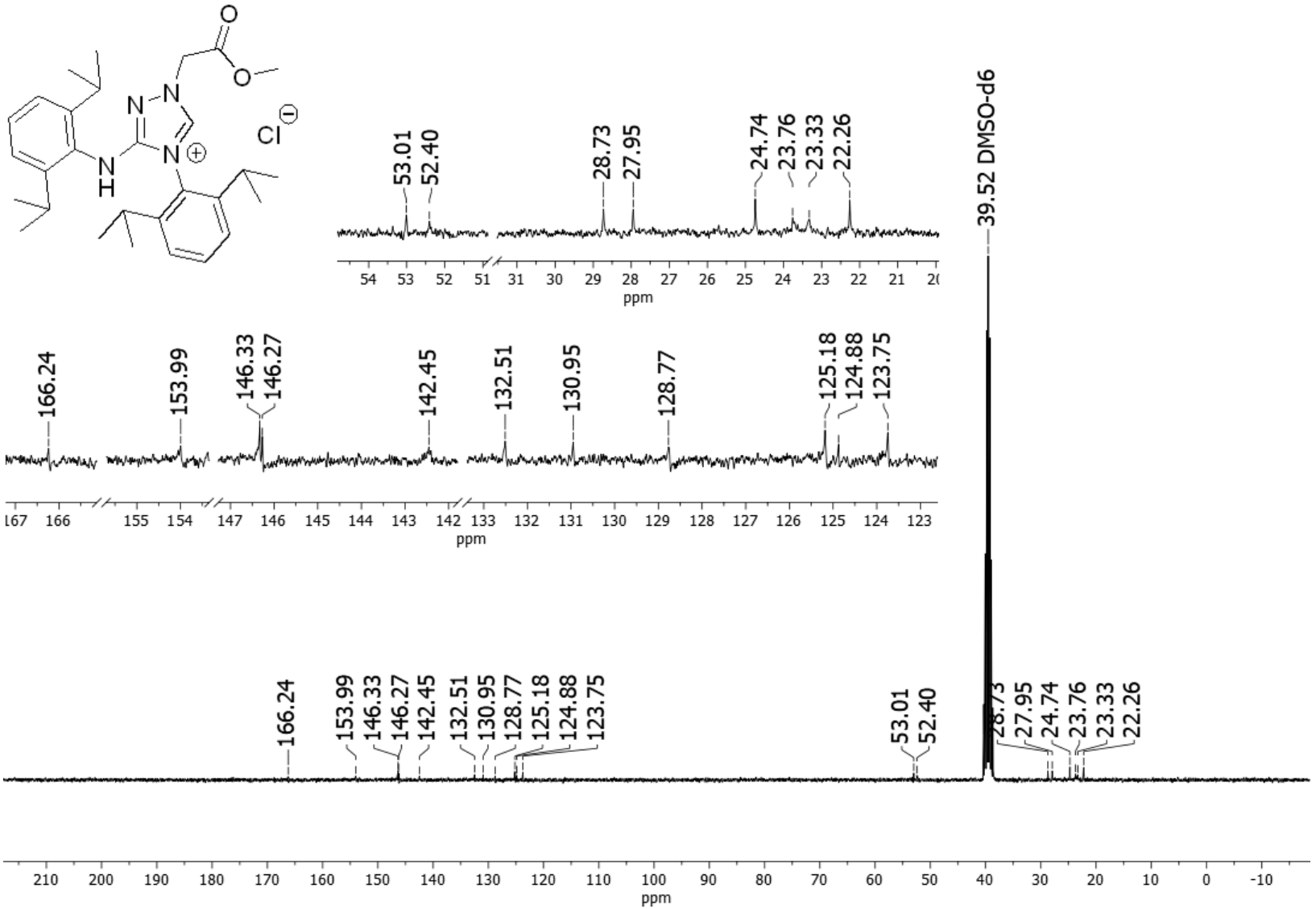


Figure S17. ^{13}C NMR spectrum of compound **3c** (DMSO-*d*$_6$, 75 MHz).

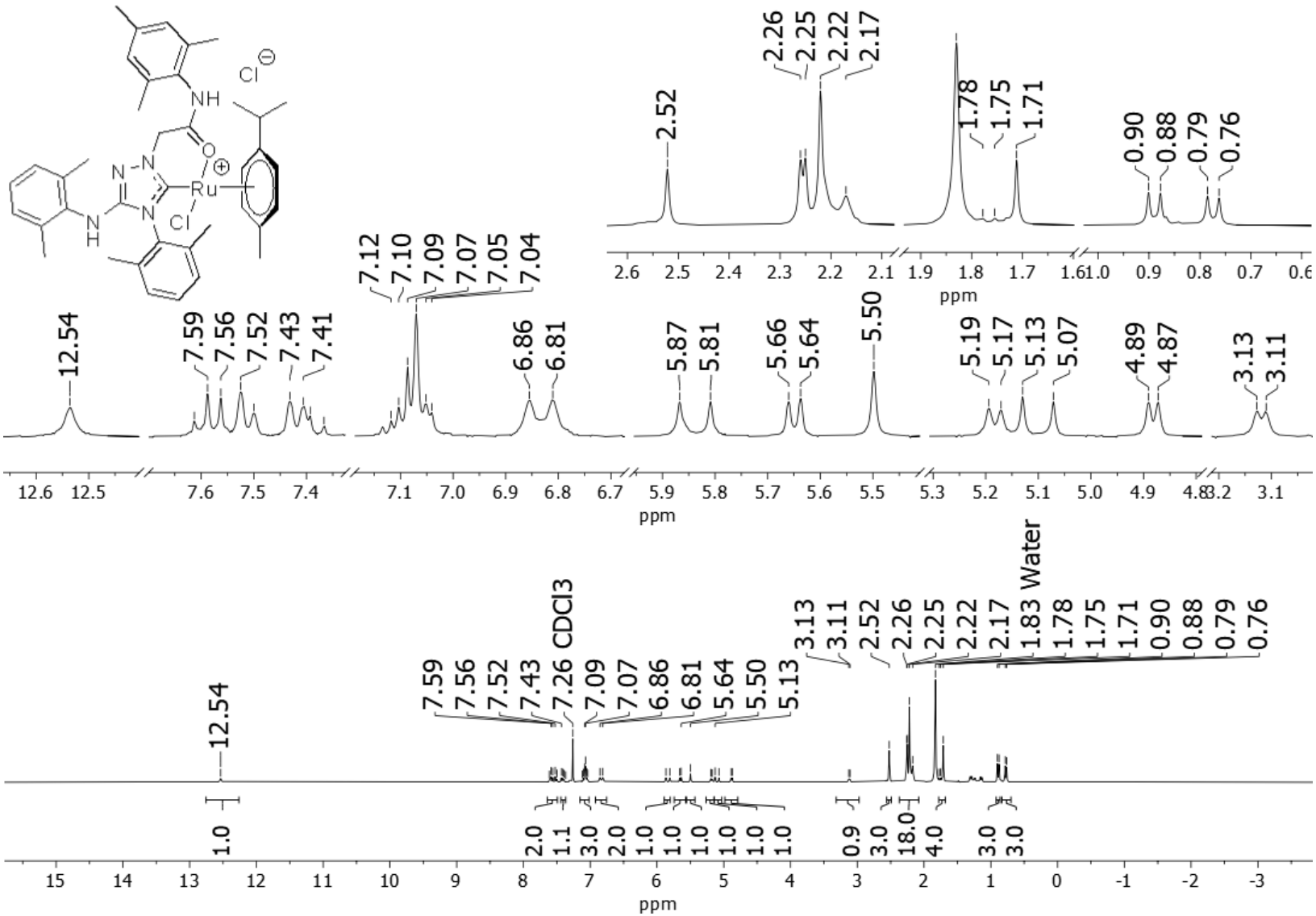


Figure S18. ^{1}H NMR spectrum of compound **4a** ($CDCl_3$, 300 MHz).

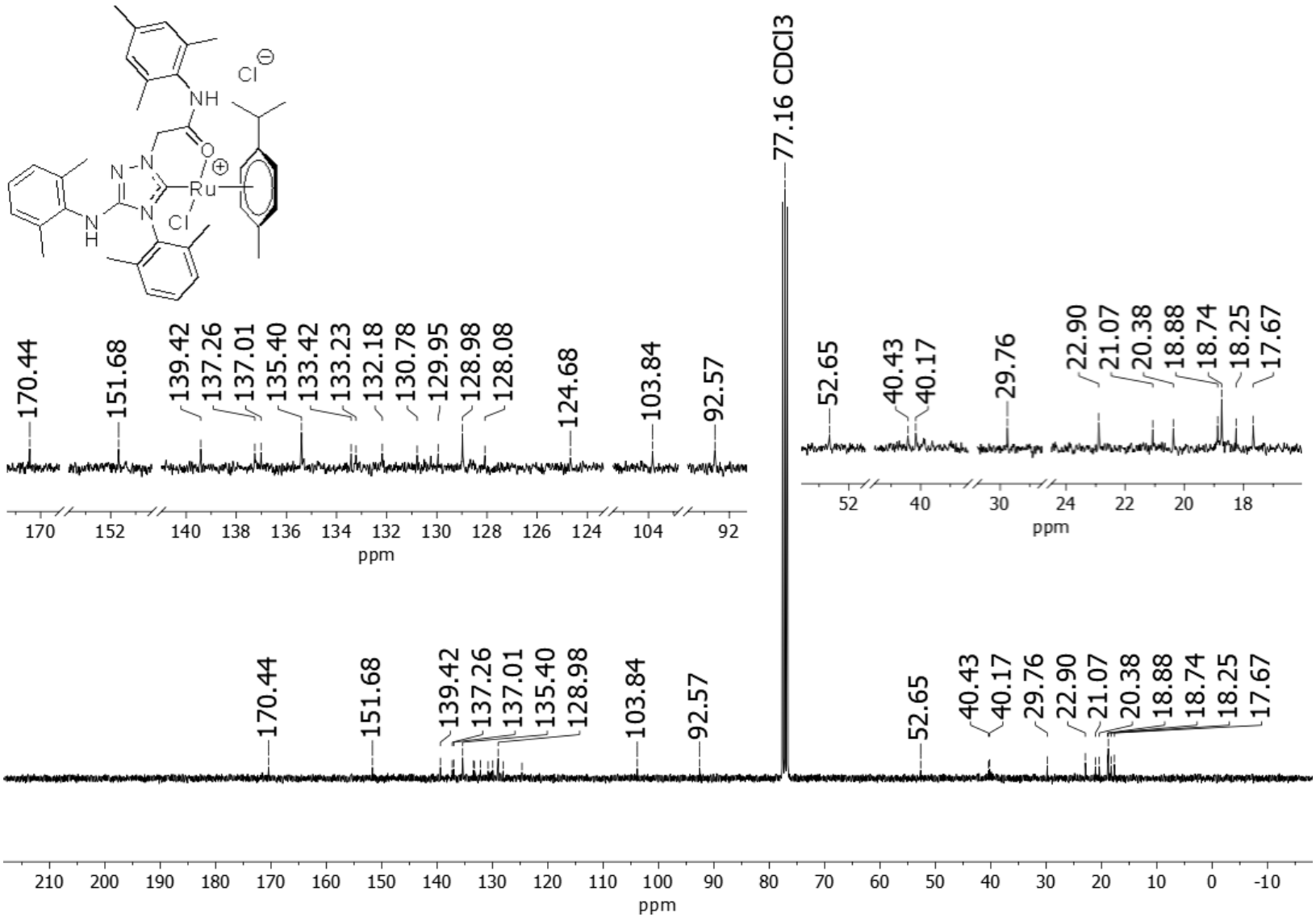


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4a** ($CDCl_3$, 300 MHz).

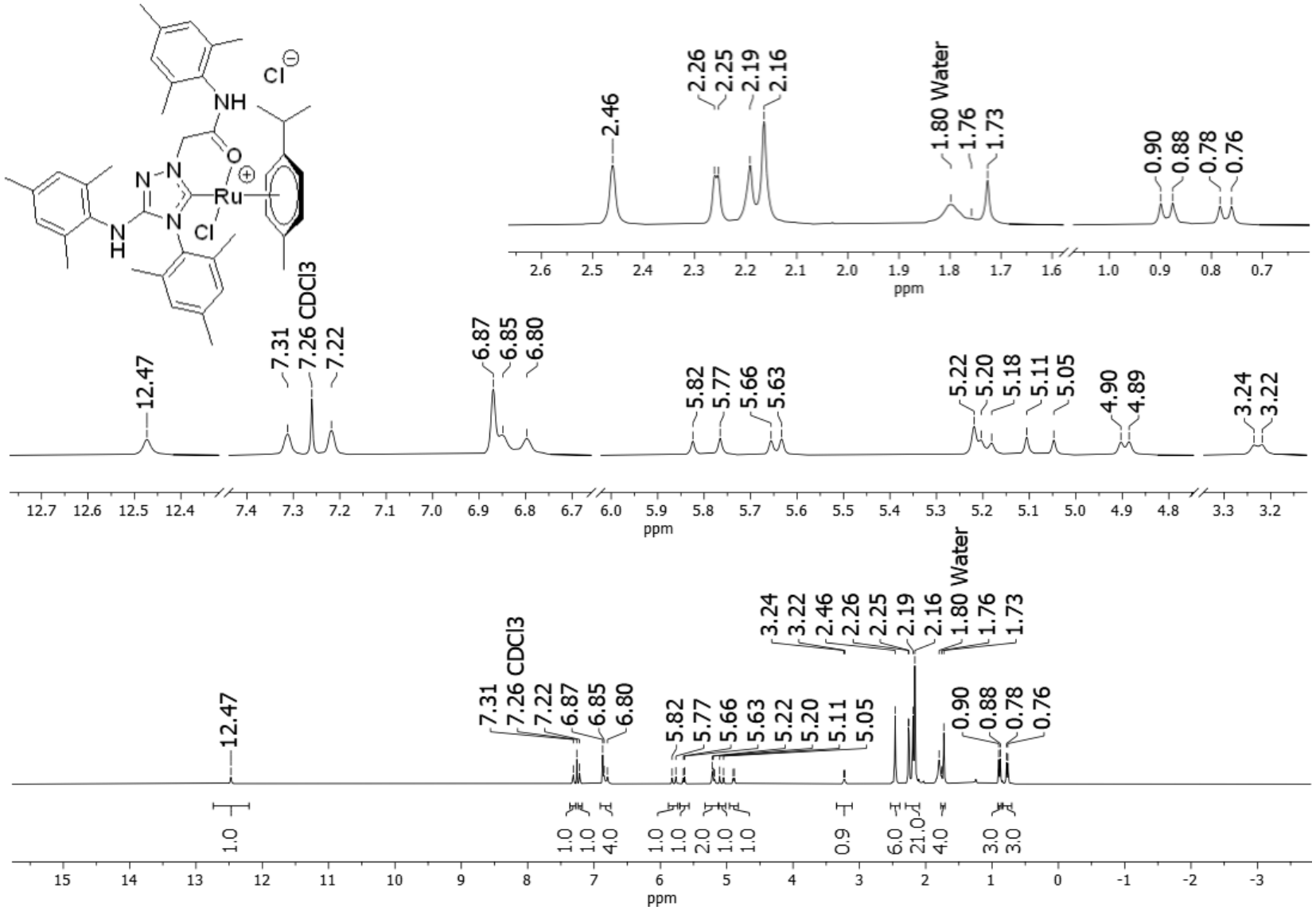


Figure S20. ^{1}H NMR spectrum of compound **4b** ($CDCl_3$, 300 MHz).

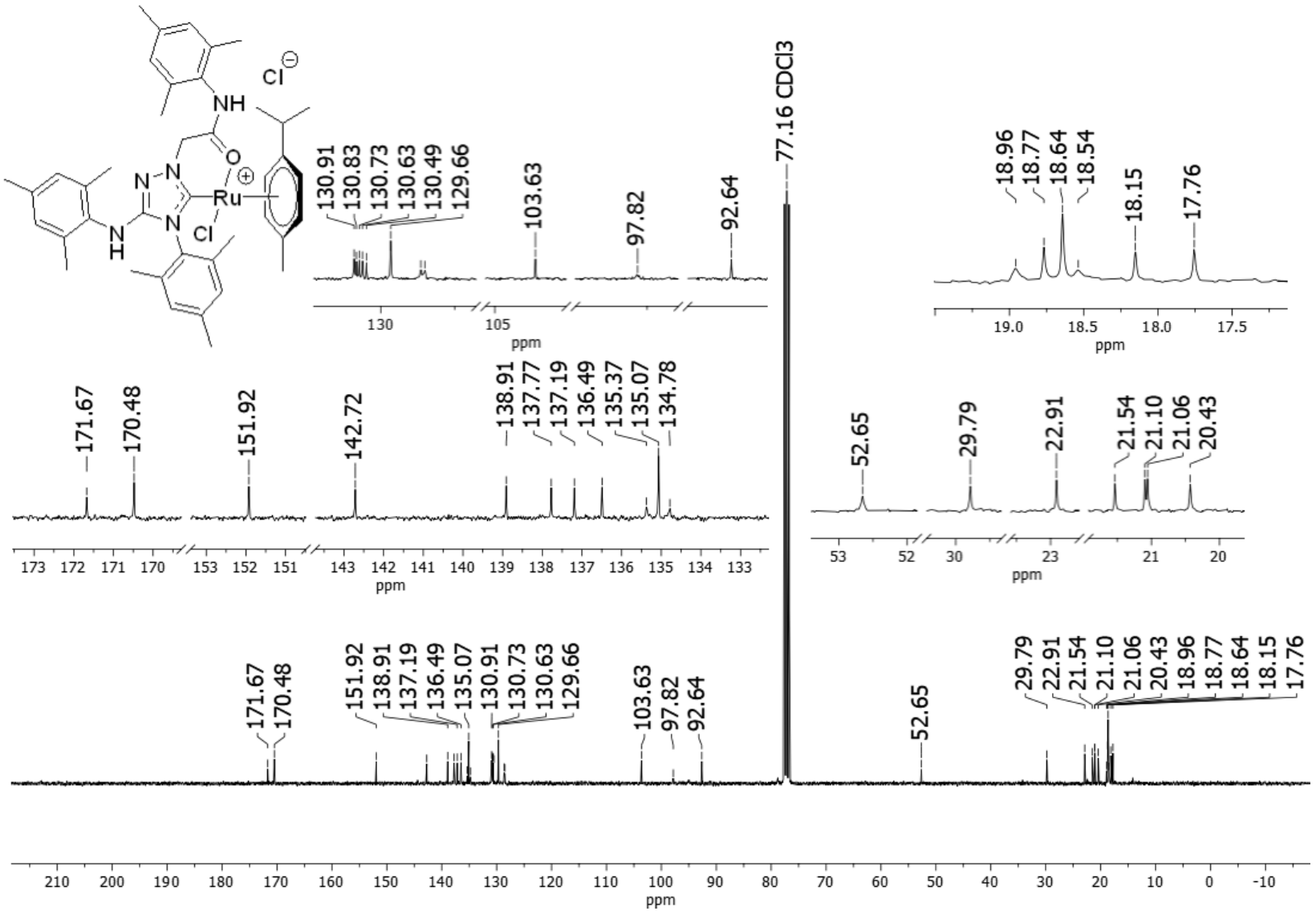


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4b** ($CDCl_3$, 300 MHz).

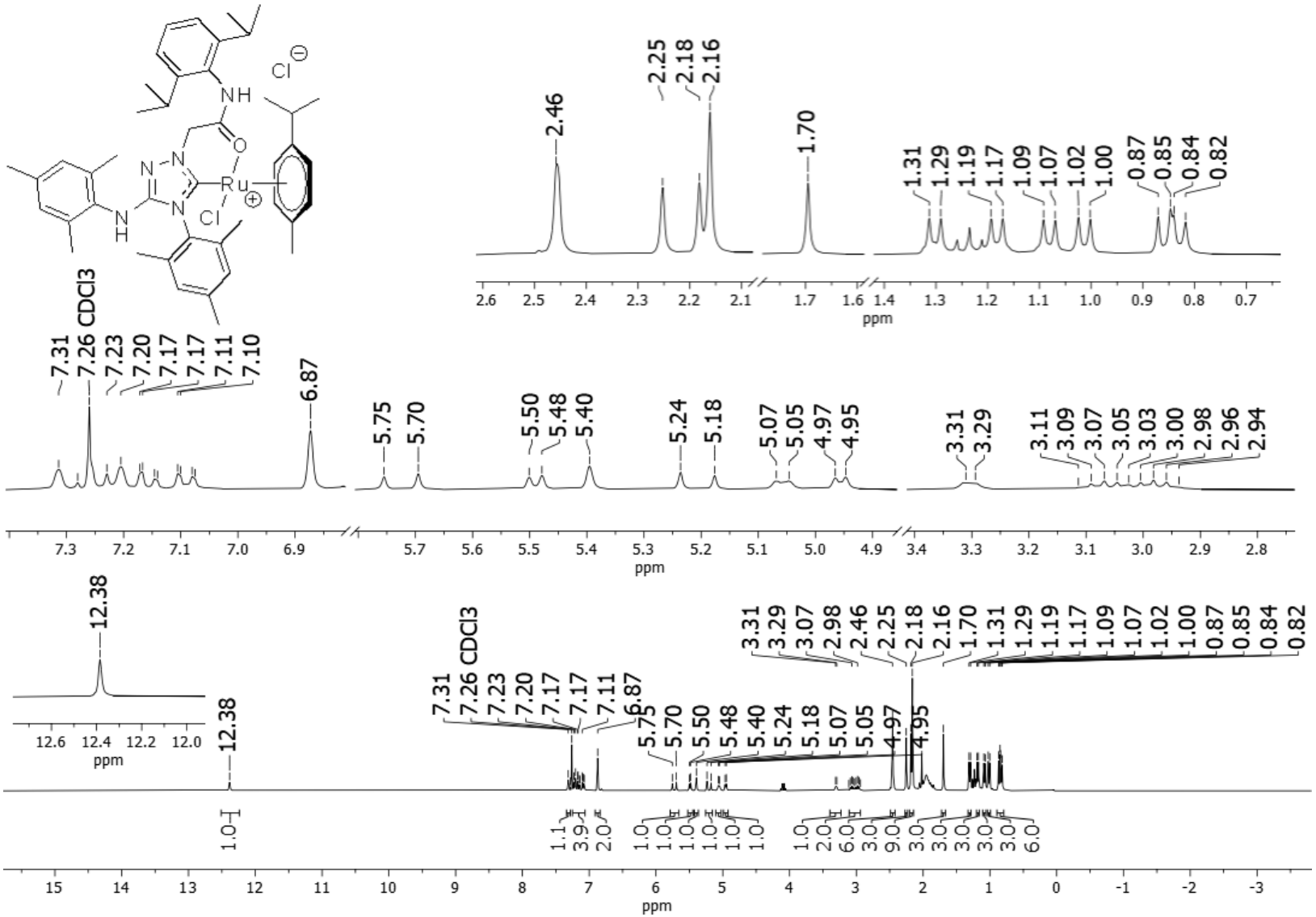


Figure S22. ^{1}H NMR spectrum of compound **4c** ($CDCl_3$, 300 MHz).

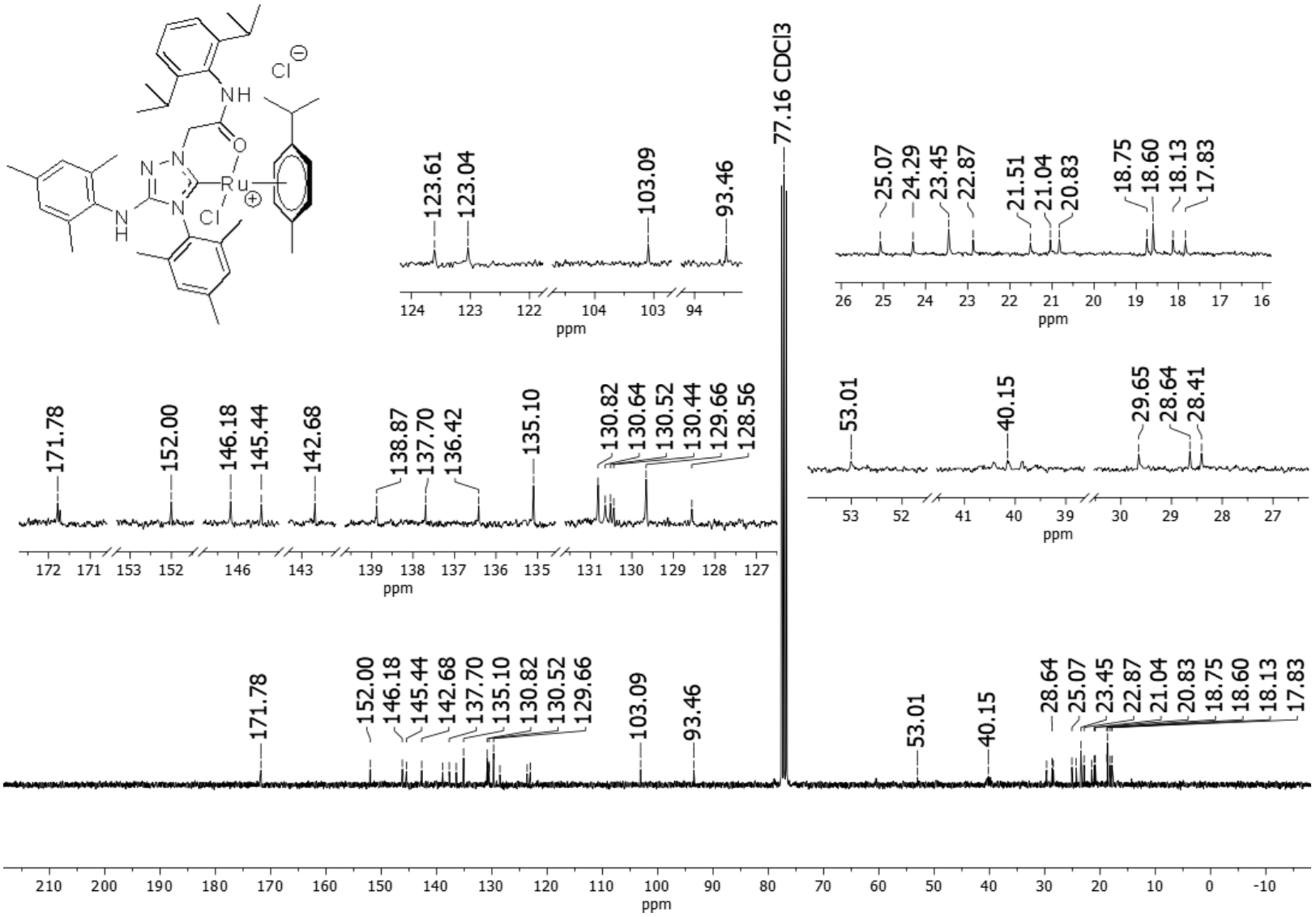


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4c** ($CDCl_3$, 300 MHz).

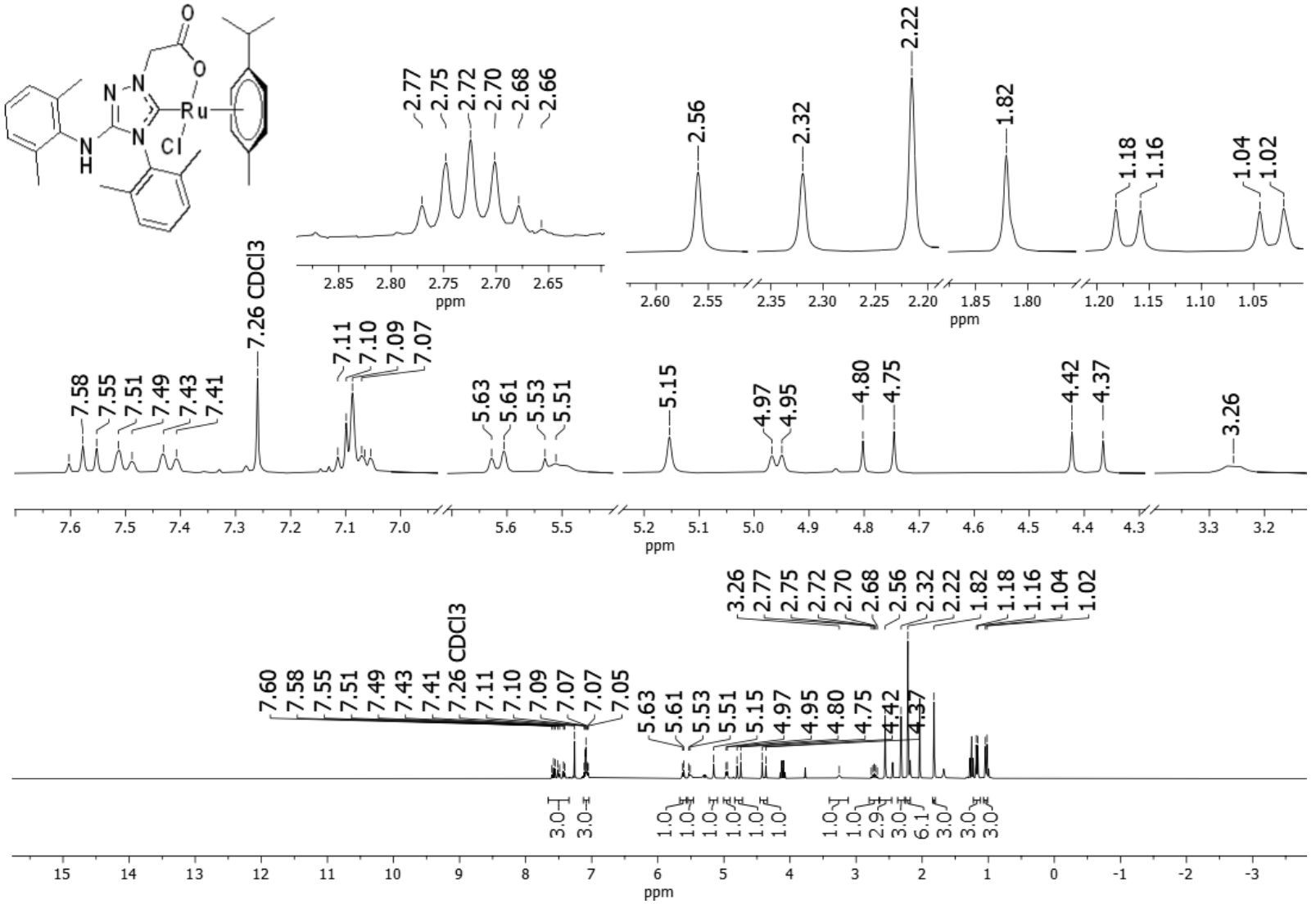


Figure S24. ^{1}H NMR spectrum of compound **5a** ($CDCl_3$, 300 MHz).

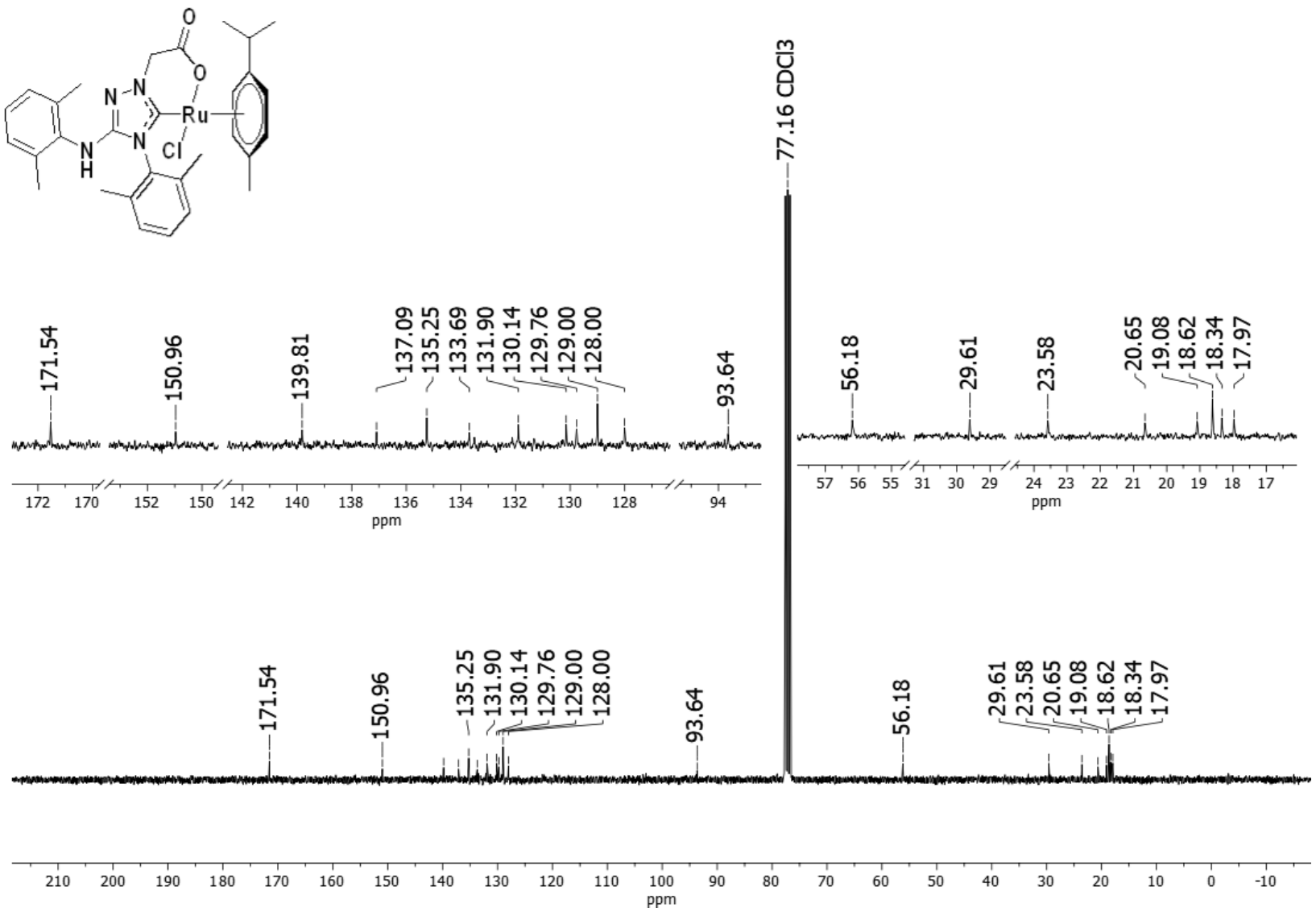


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of compound **5a** ($CDCl_3$, 300 MHz).

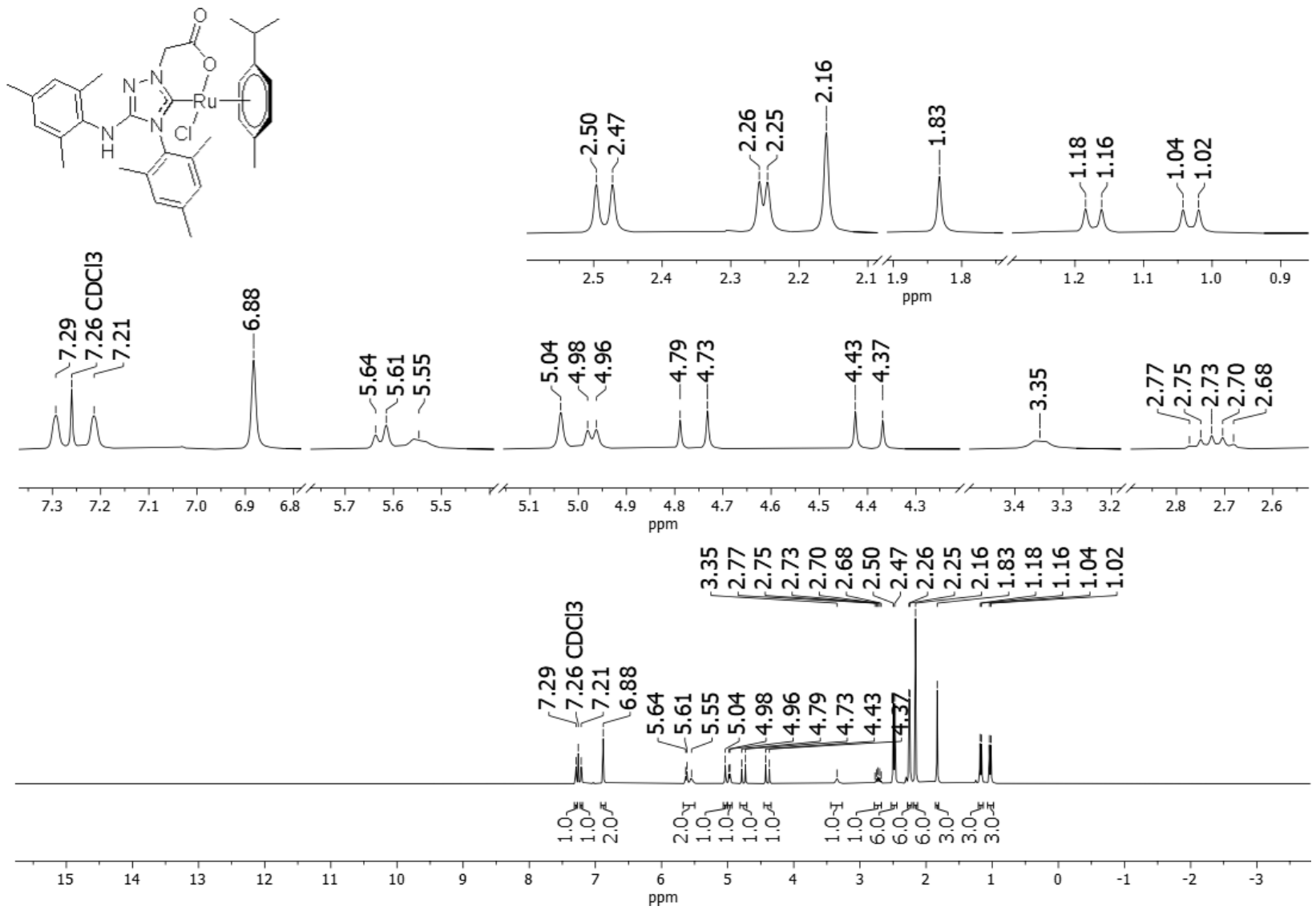


Figure S26. ^{1}H NMR spectrum of compound **5b** ($CDCl_3$, 300 MHz).

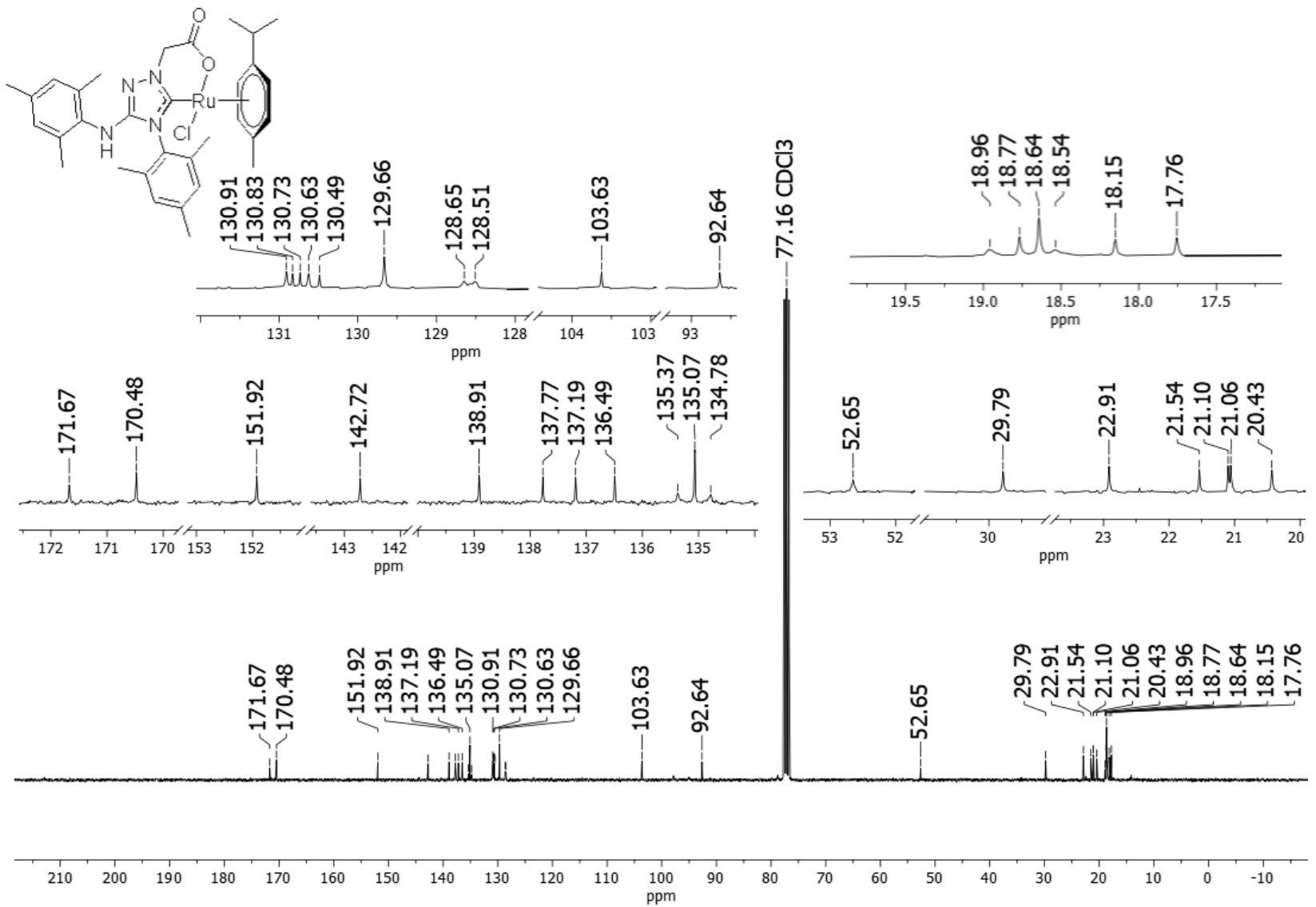


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of compound **5b** ($CDCl_3$, 300 MHz).

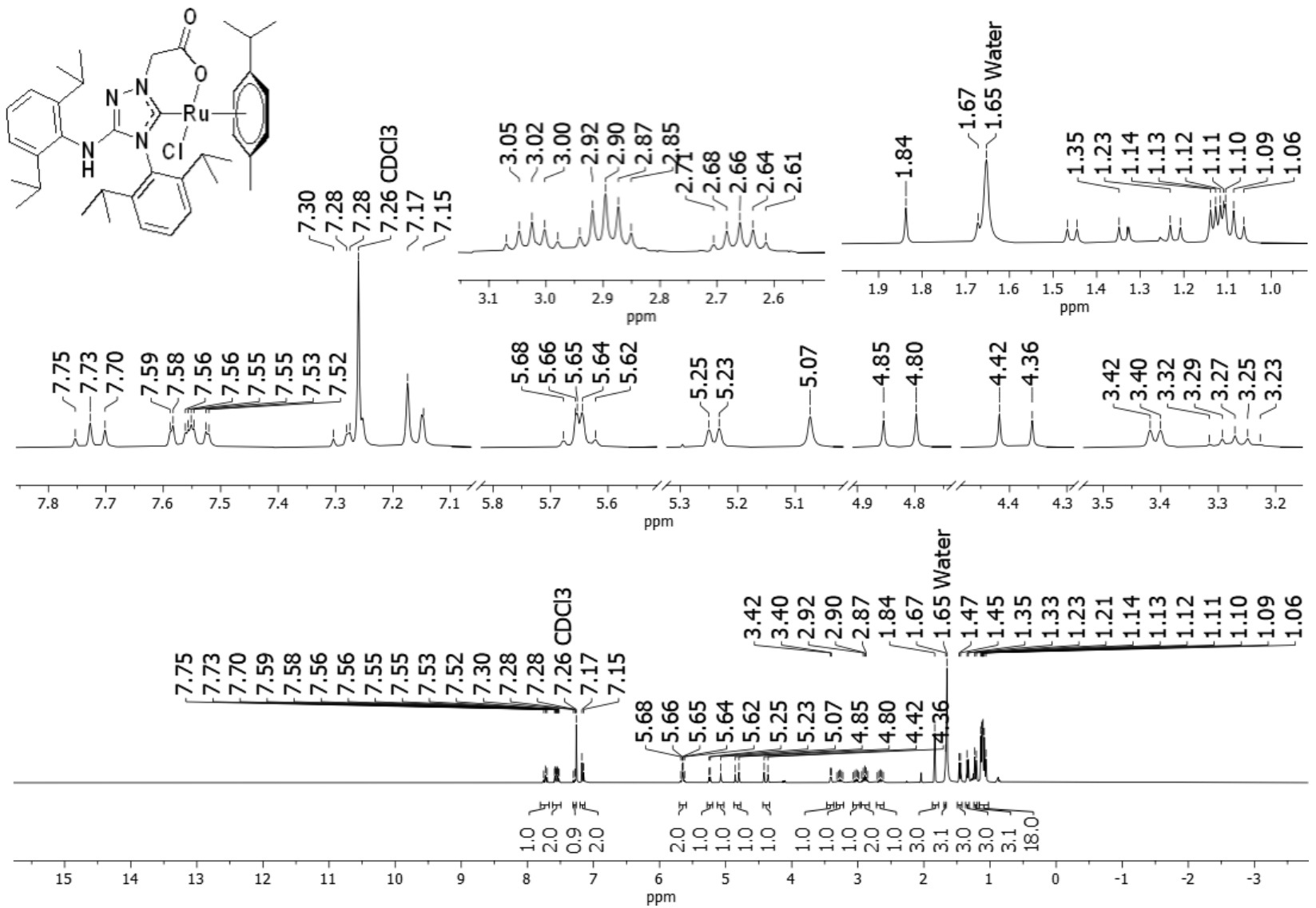


Figure S28. ^{1}H NMR spectrum of compound **5c** ($CDCl_3$, 300 MHz).

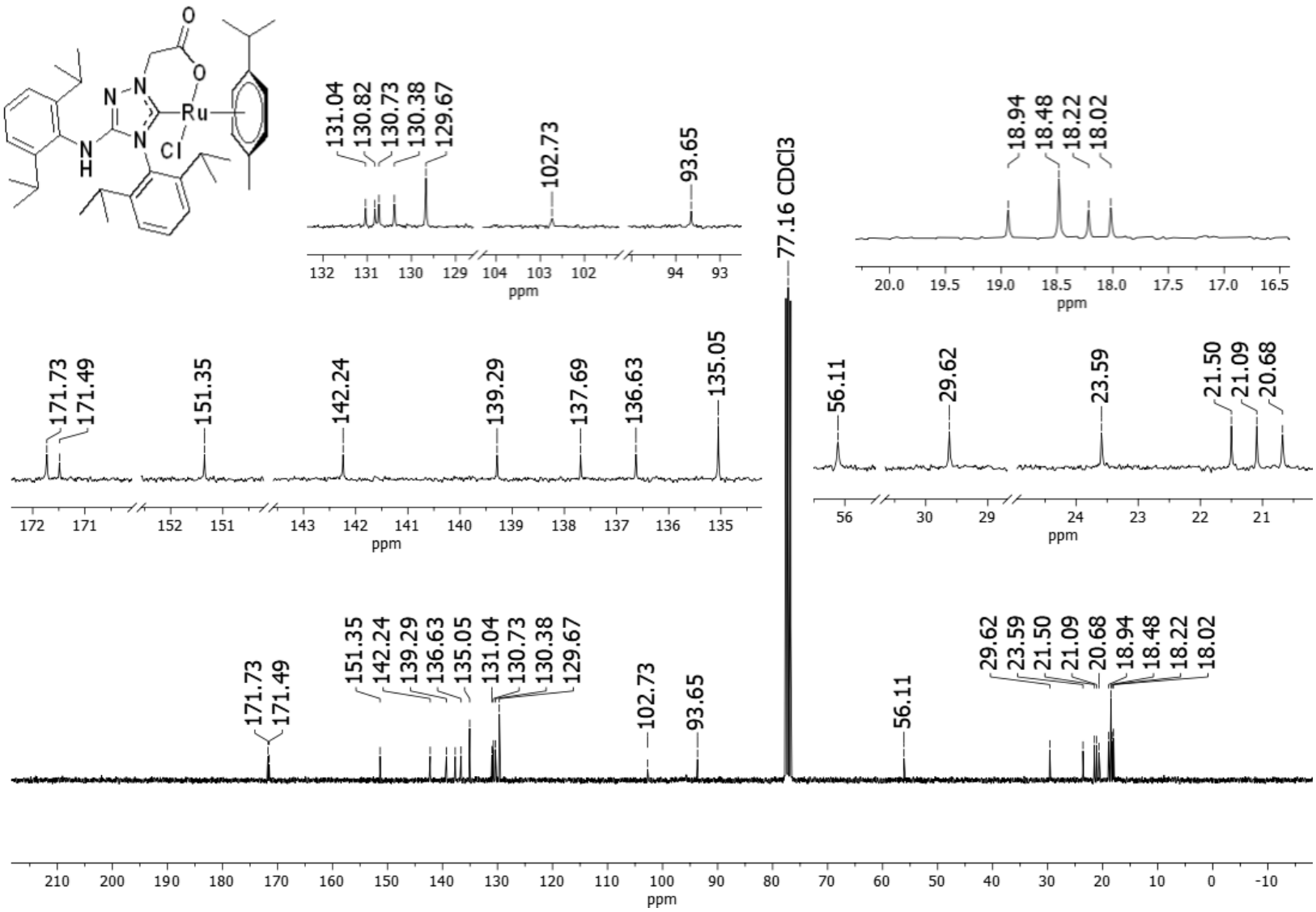


Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum of compound **5c** ($CDCl_3$, 300 MHz).

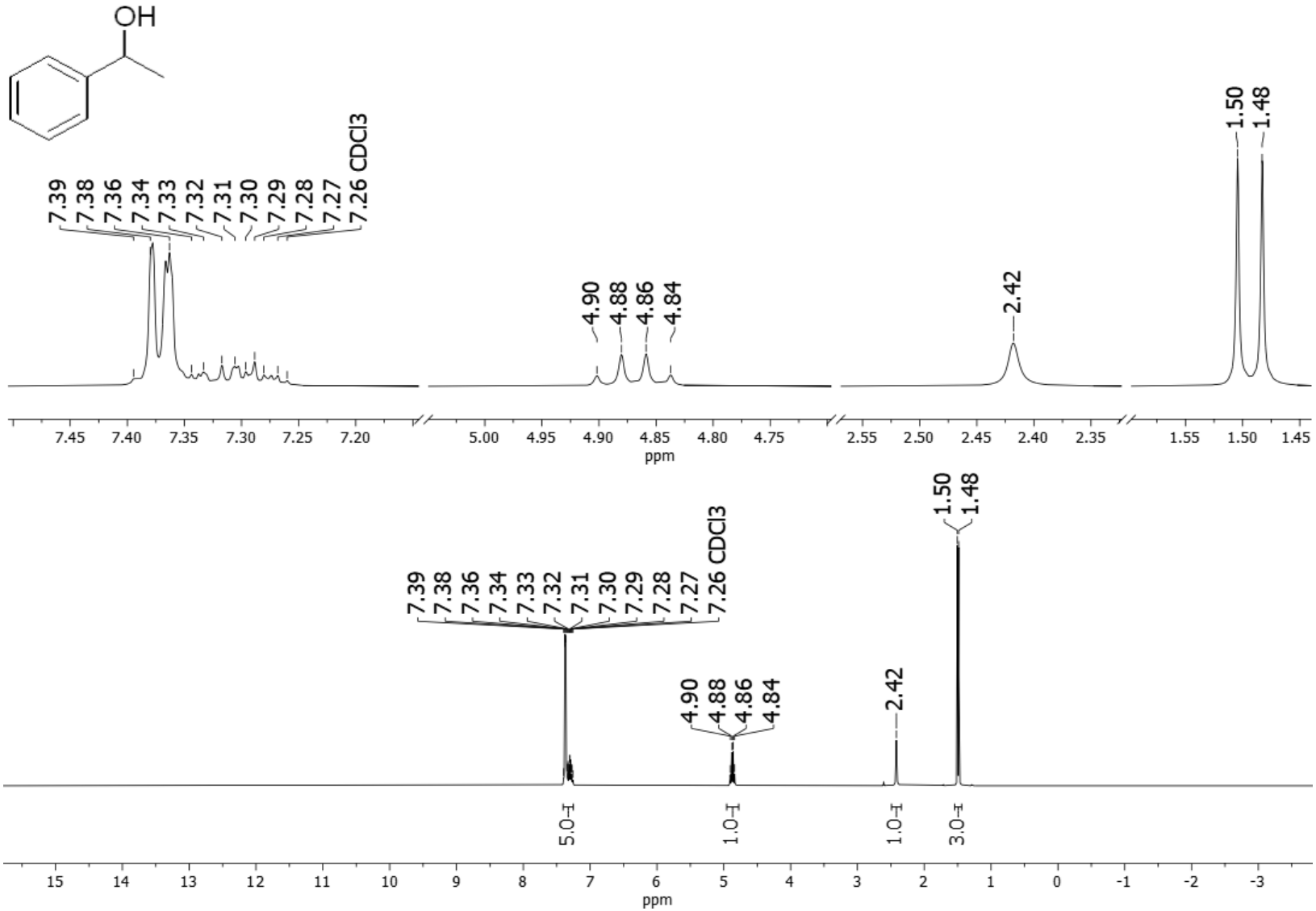


Figure S30. ^{1}H NMR spectrum of compound **7a** ($CDCl_3$, 300 MHz).

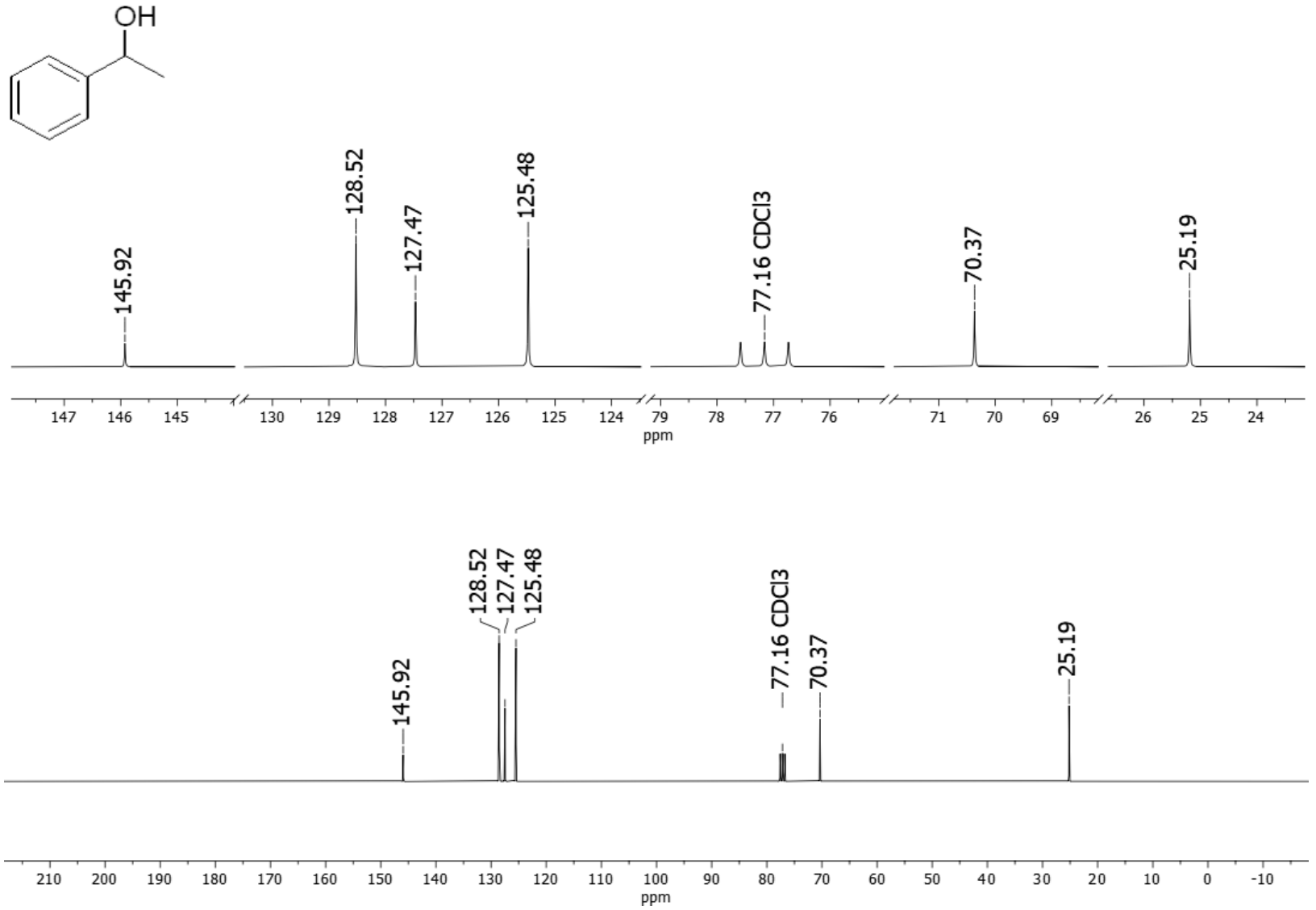


Figure S31. ^{13}C NMR spectrum of compound **7a** ($CDCl_3$, 75 MHz).

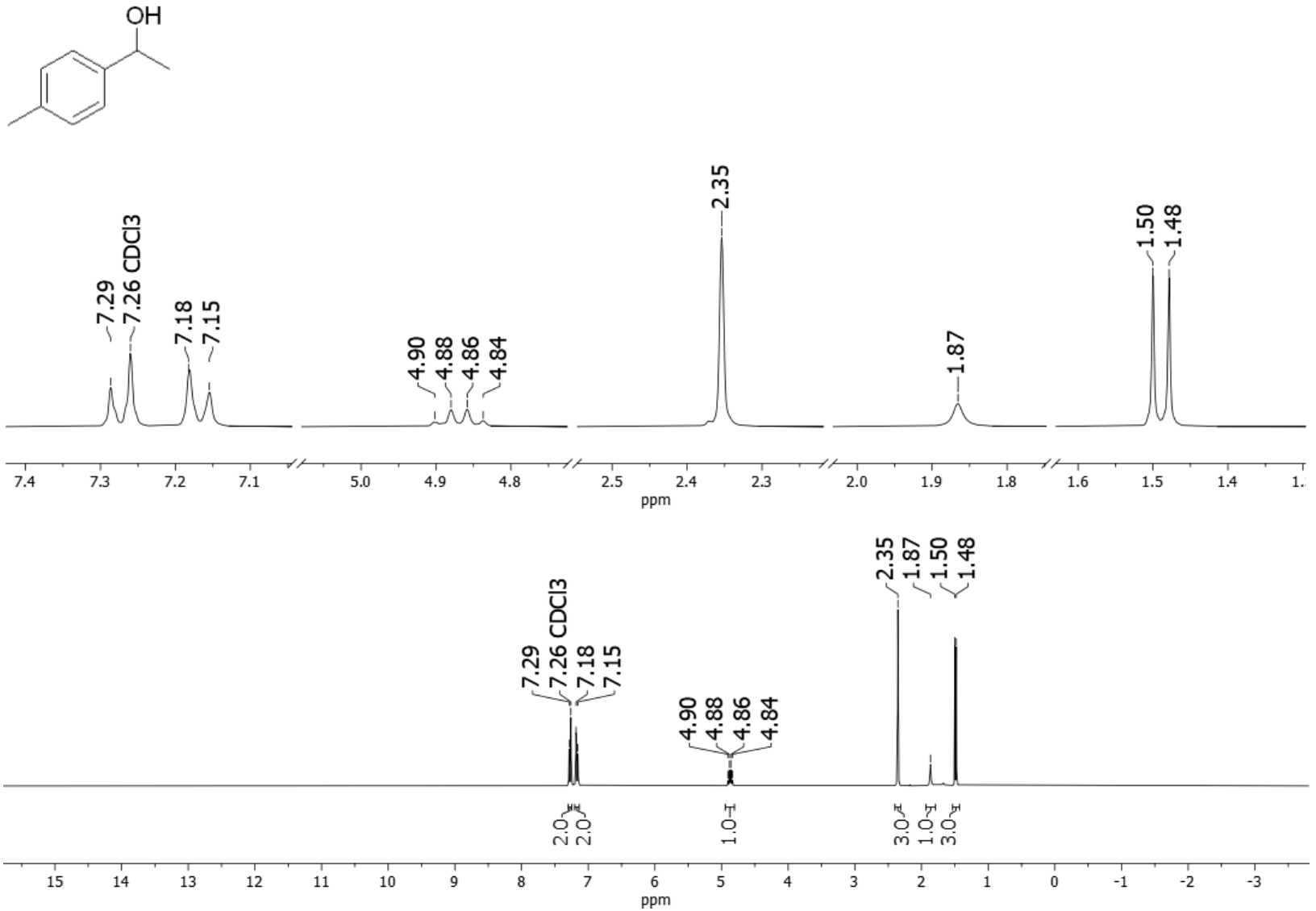


Figure S32. ^{1}H NMR spectrum of compound **7b** ($CDCl_3$, 300 MHz).

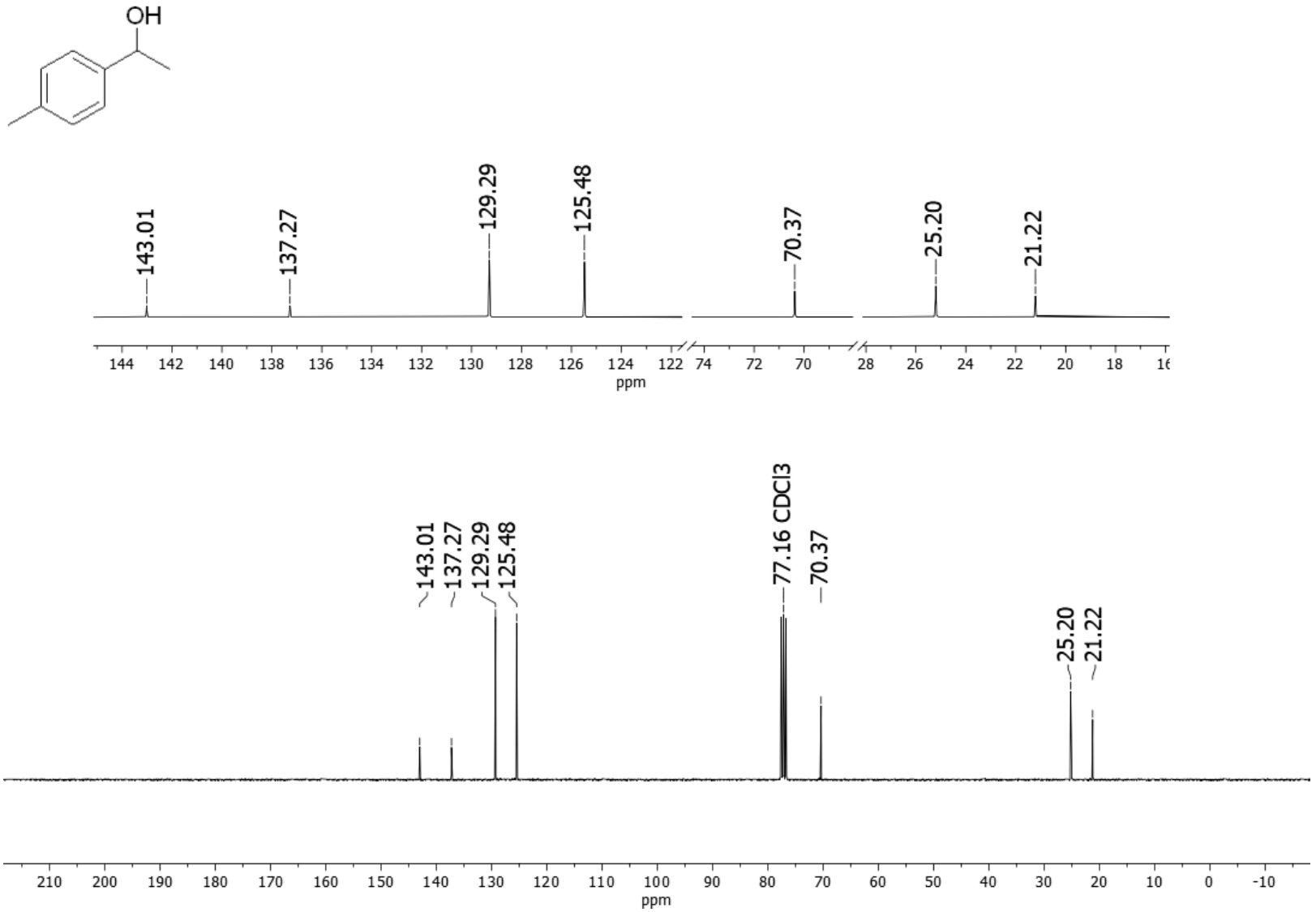


Figure S33. ^{13}C NMR spectrum of compound **7b** ($CDCl_3$, 75 MHz).

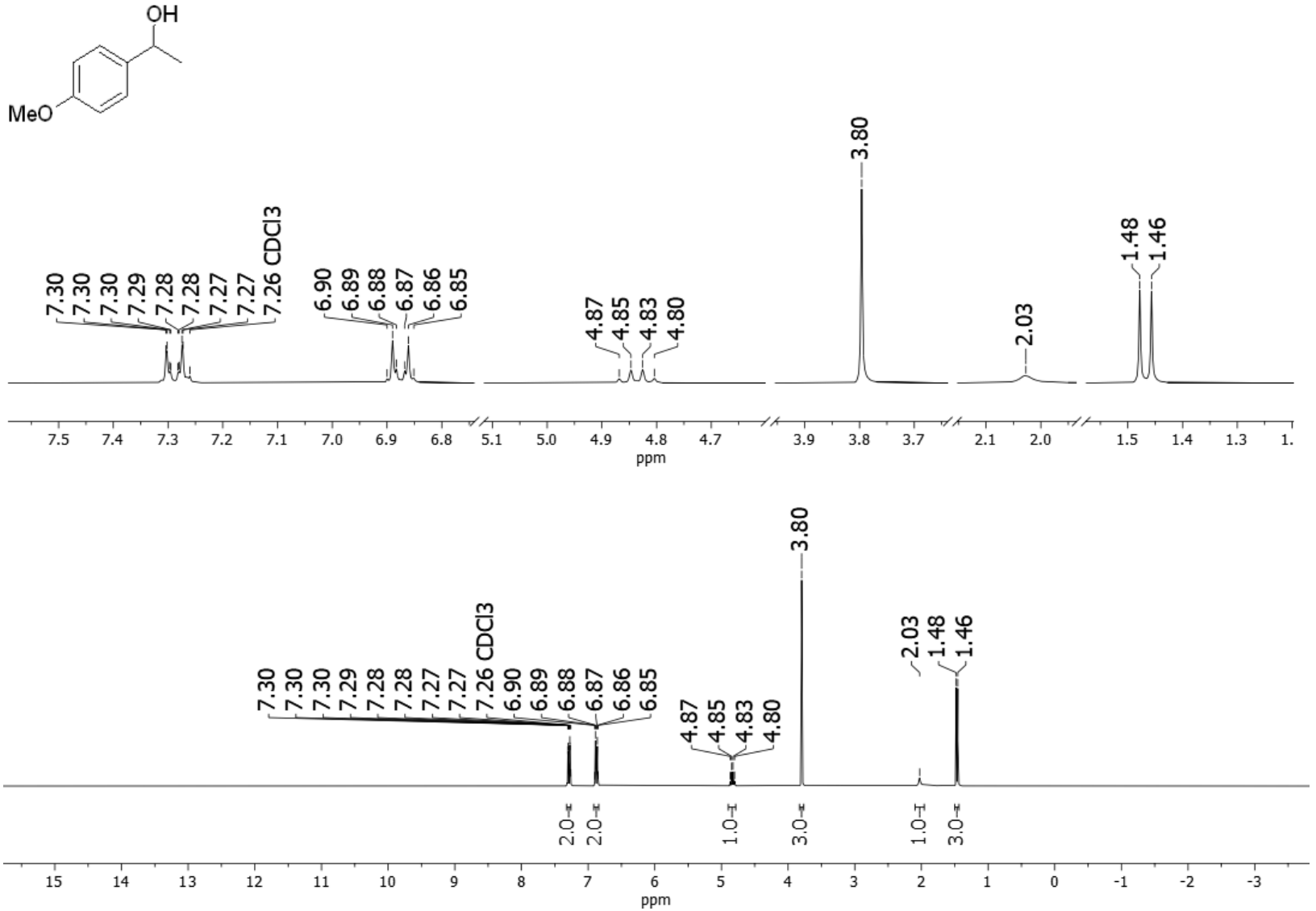


Figure S34. ^{1}H NMR spectrum of compound **7c** ($CDCl_3$, 300 MHz).

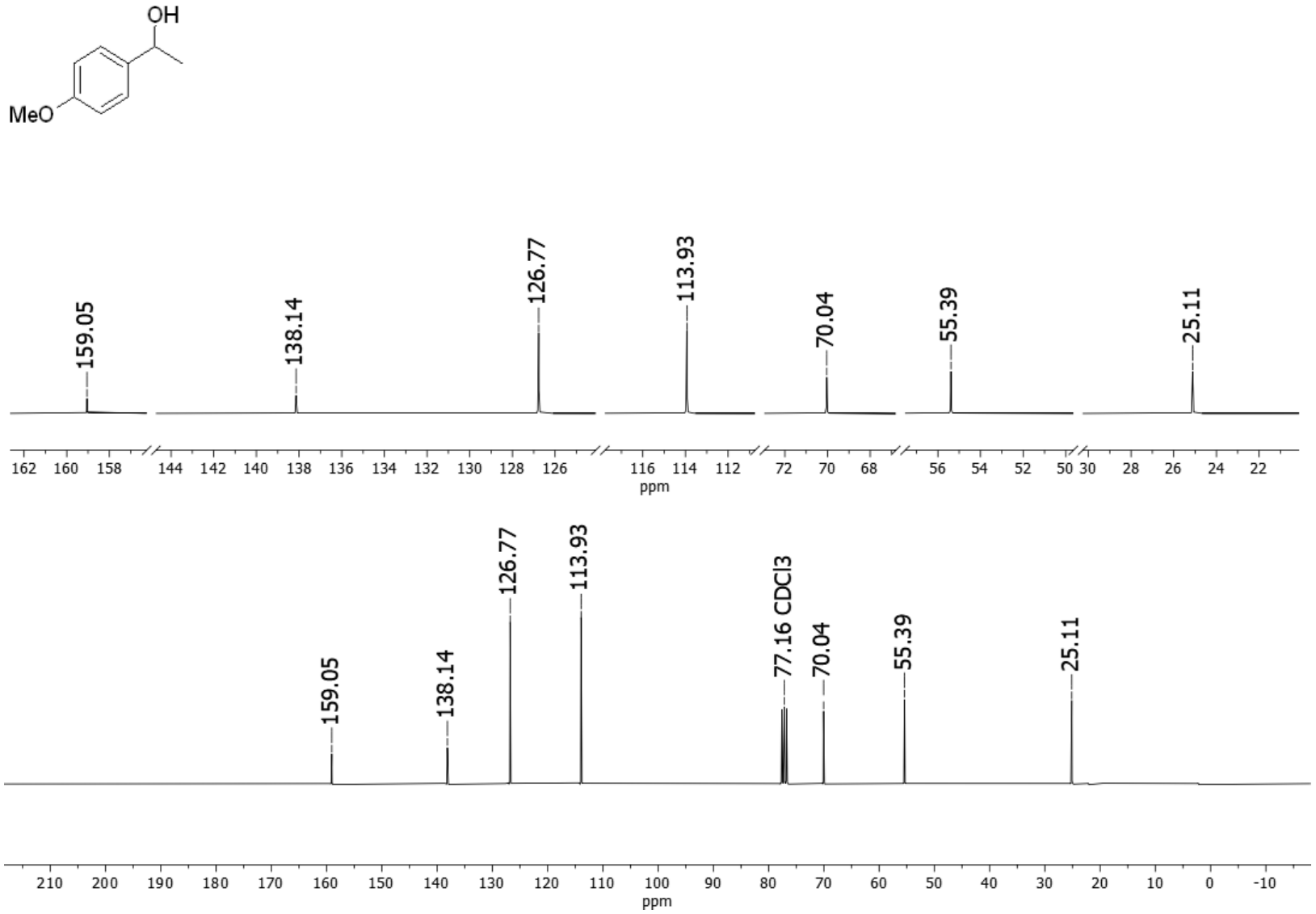


Figure S35. ^{13}C NMR spectrum of compound **7c** ($CDCl_3$, 75 MHz).

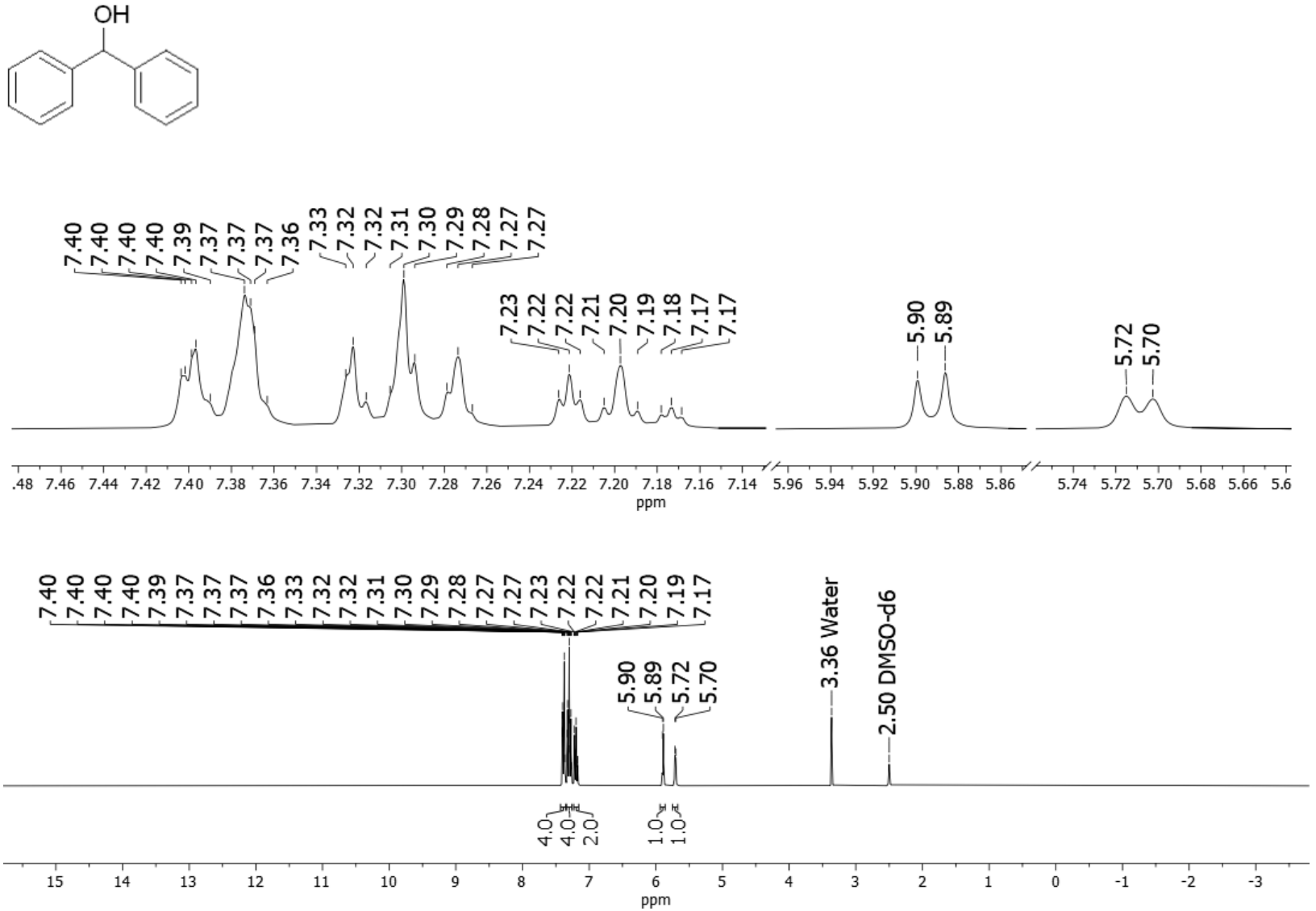


Figure S36. ^{1}H NMR spectrum of compound **7d** (DMSO-d_6, 300 MHz).

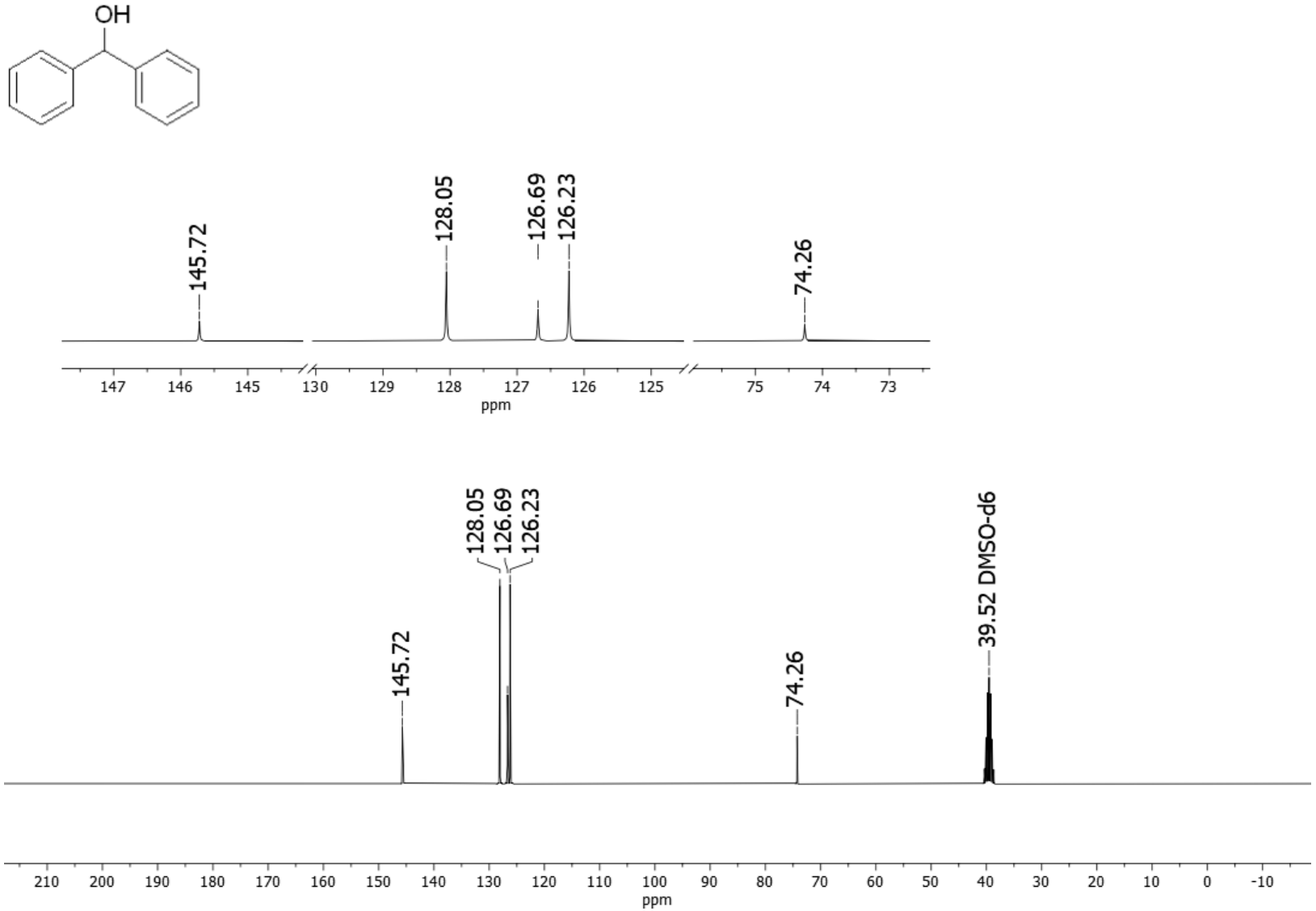


Figure S37. ^{13}C NMR spectrum of compound **7d** (DMSO-d_6, 75 MHz).

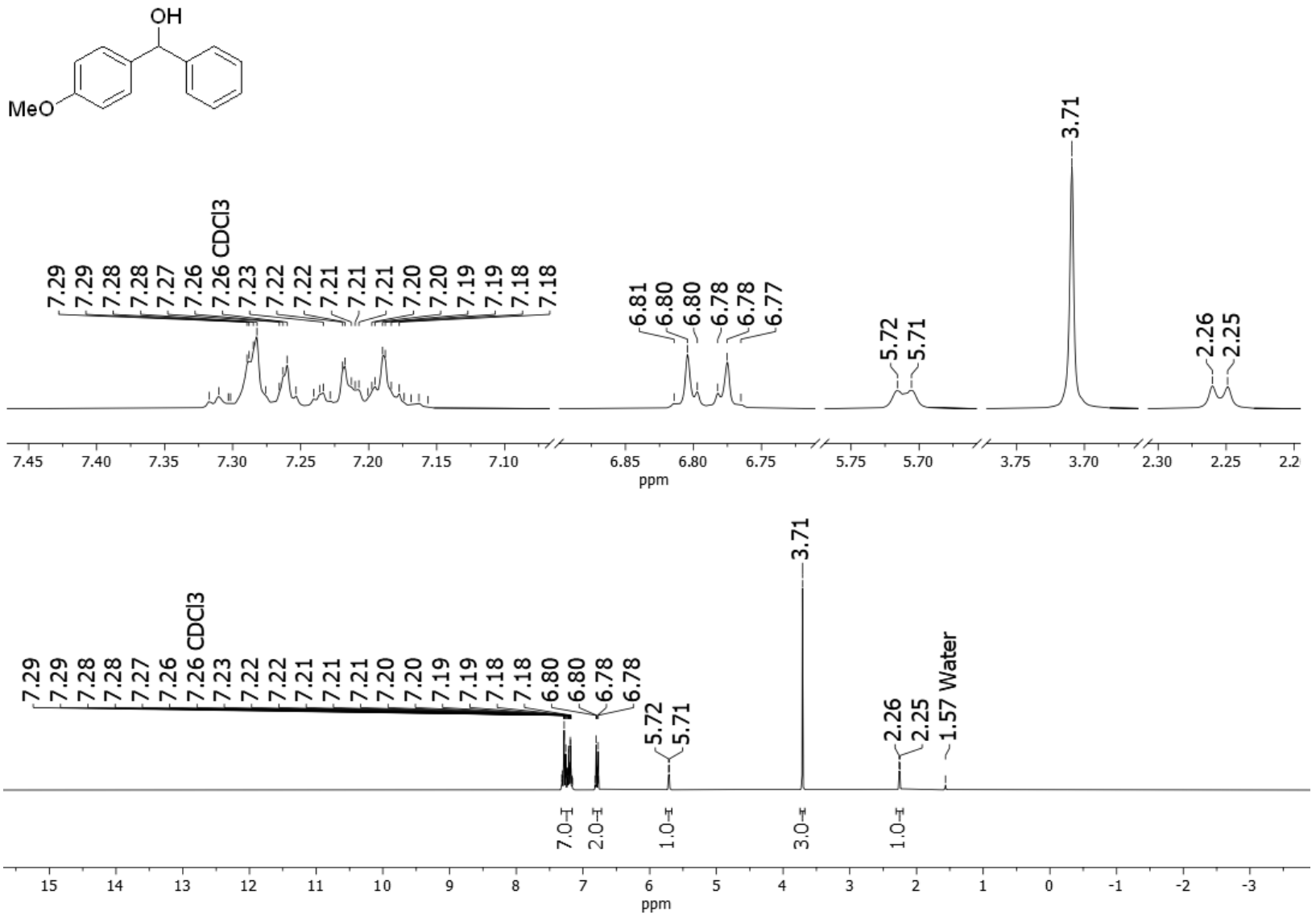


Figure S38. ^{1}H NMR spectrum of compound **7e** ($CDCl_3$, 300 MHz).

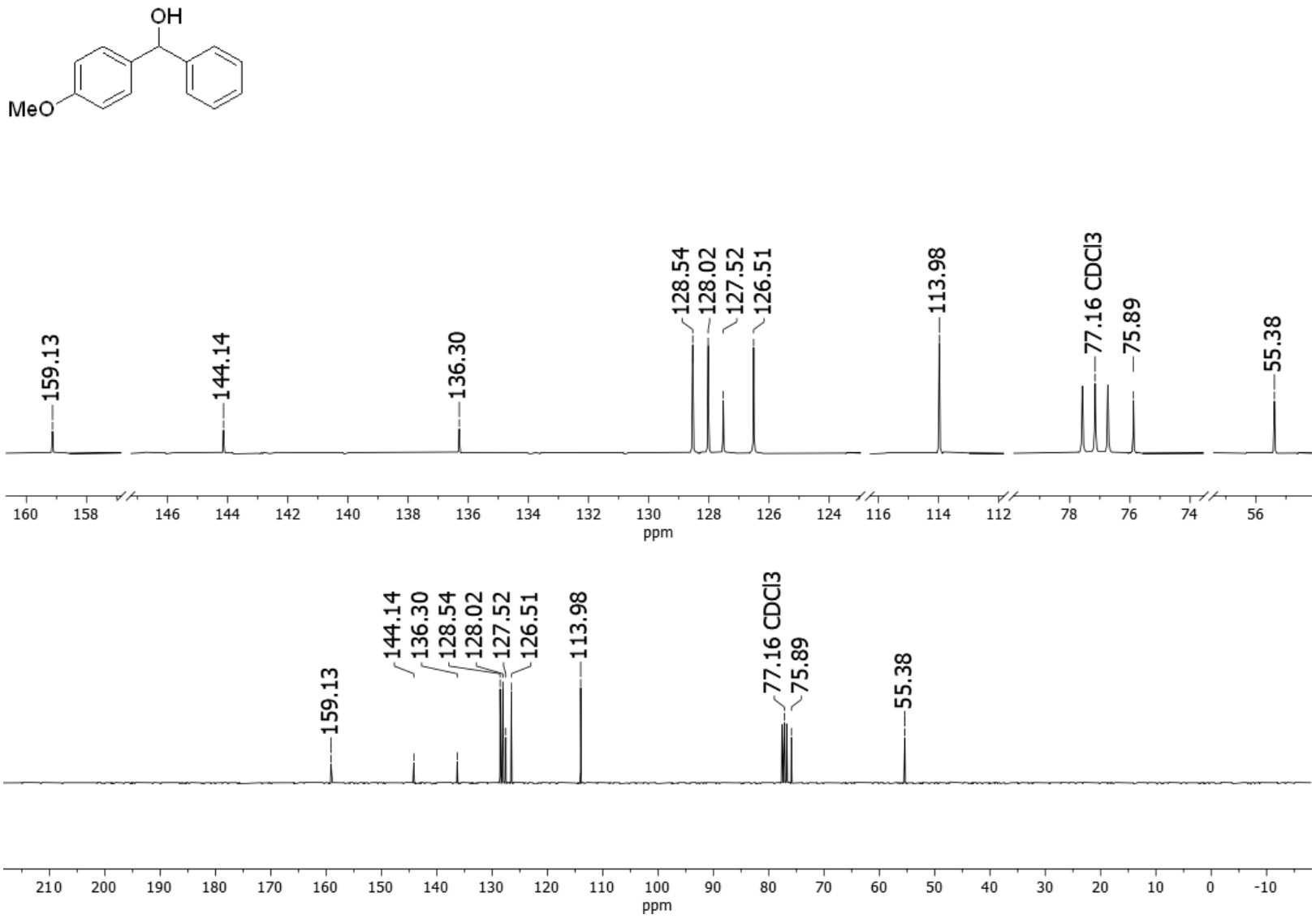


Figure S39. ^{13}C NMR spectrum of compound **7e** ($CDCl_3$, 75 MHz).

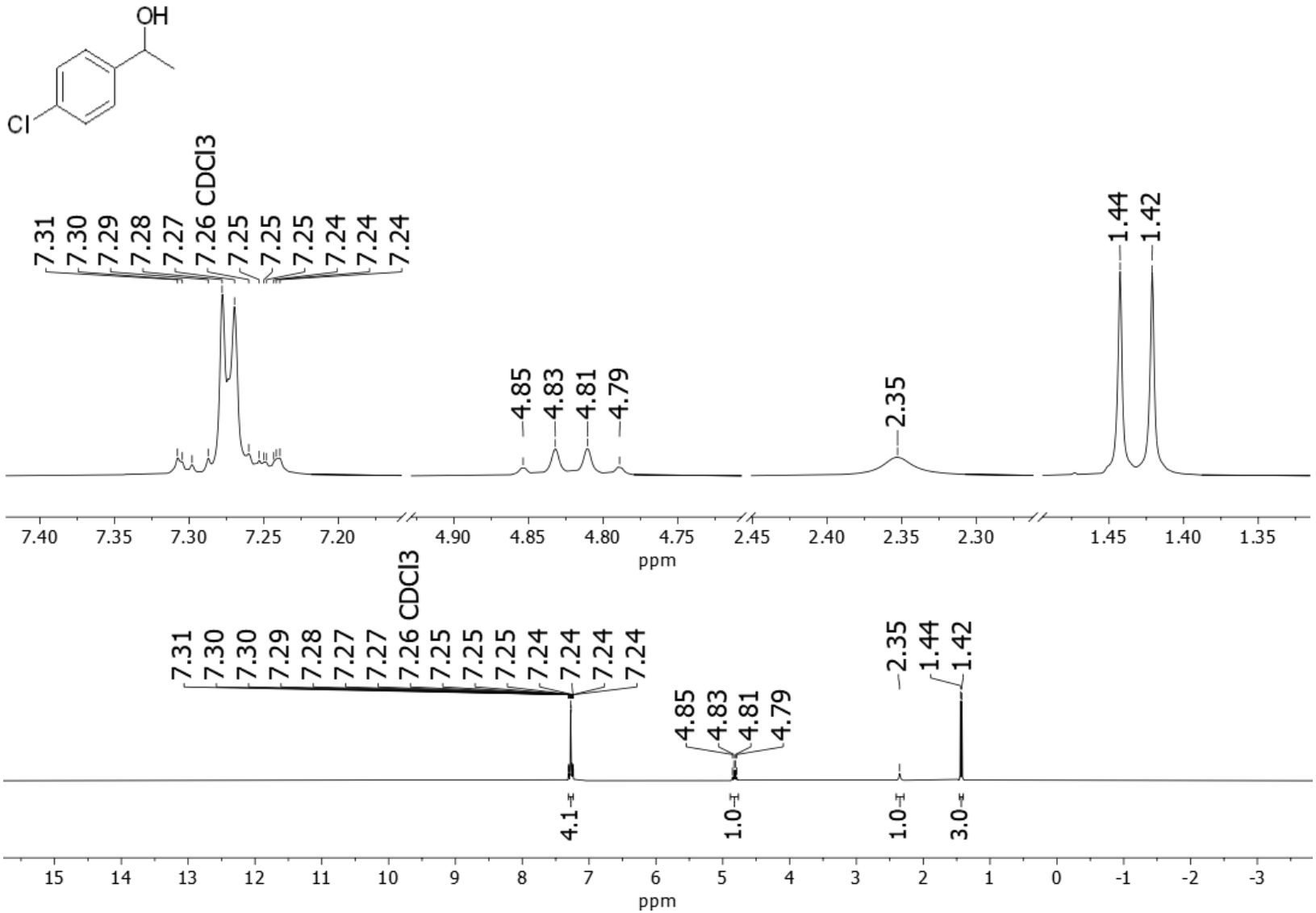


Figure S40. ^{1}H NMR spectrum of compound **7f** ($CDCl_3$, 300 MHz).

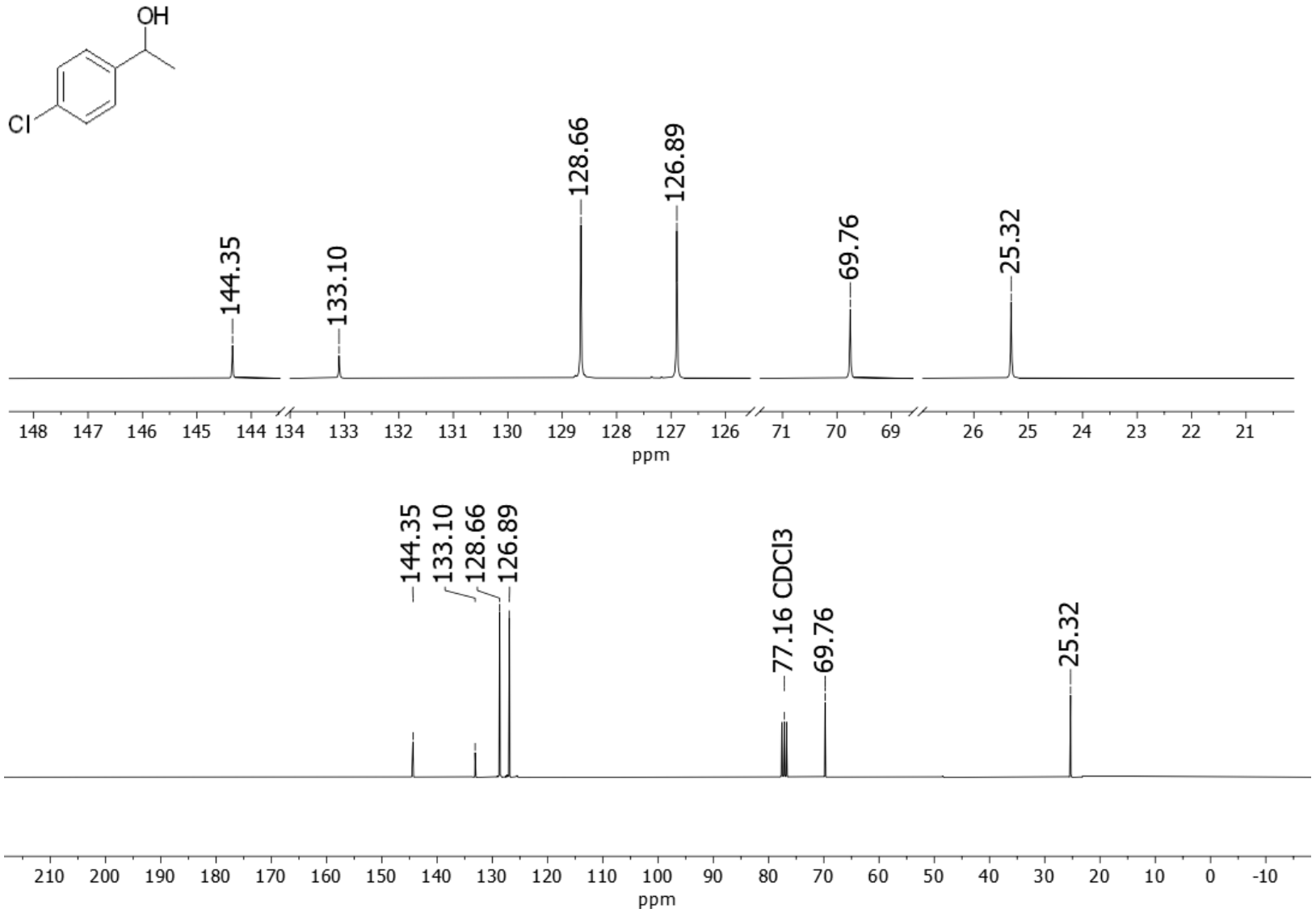


Figure S41. ^{13}C NMR spectrum of compound **7f** ($CDCl_3$, 75 MHz).

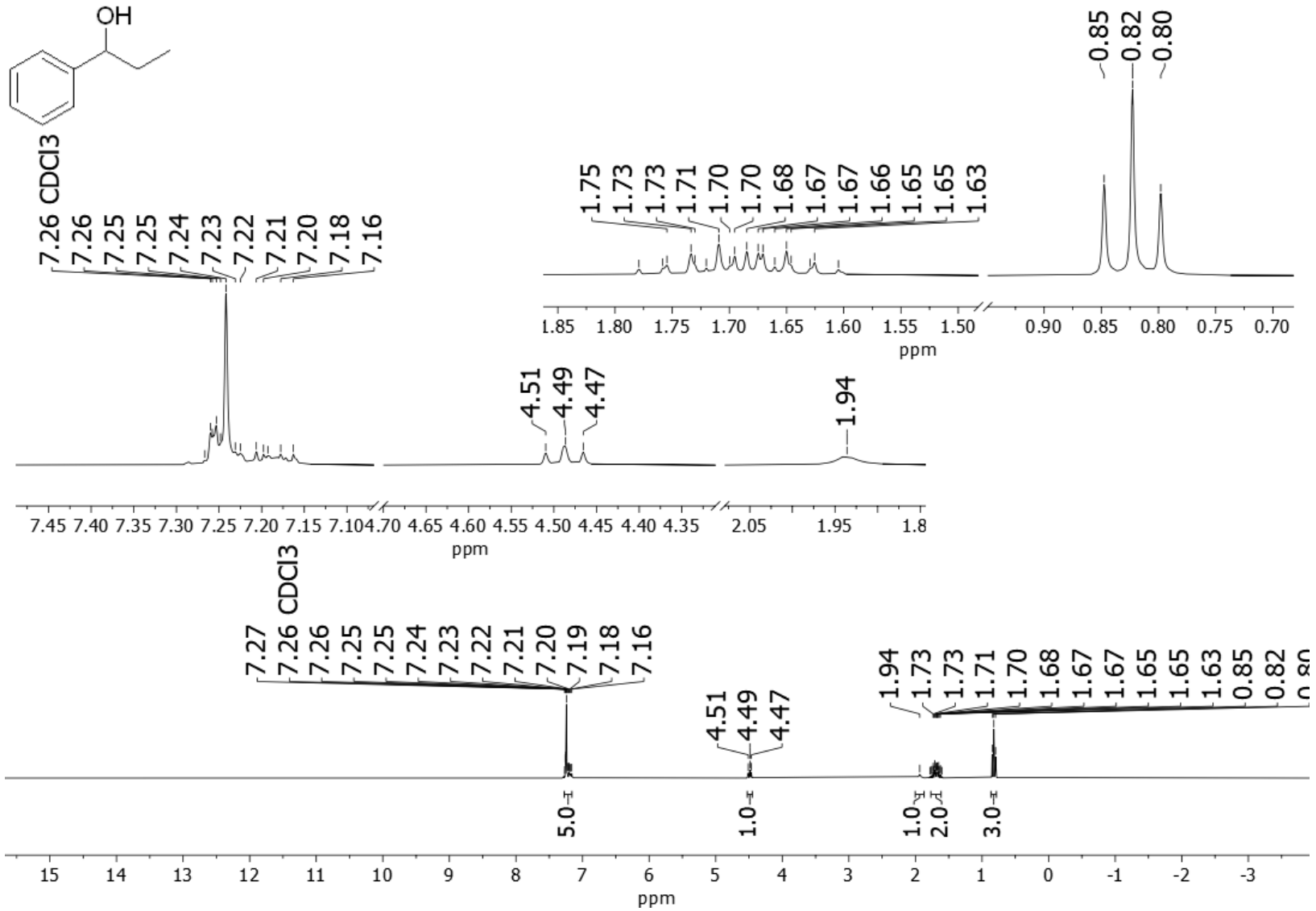


Figure S42. ^{1}H NMR spectrum of compound **7g** ($CDCl_3$, 300 MHz).

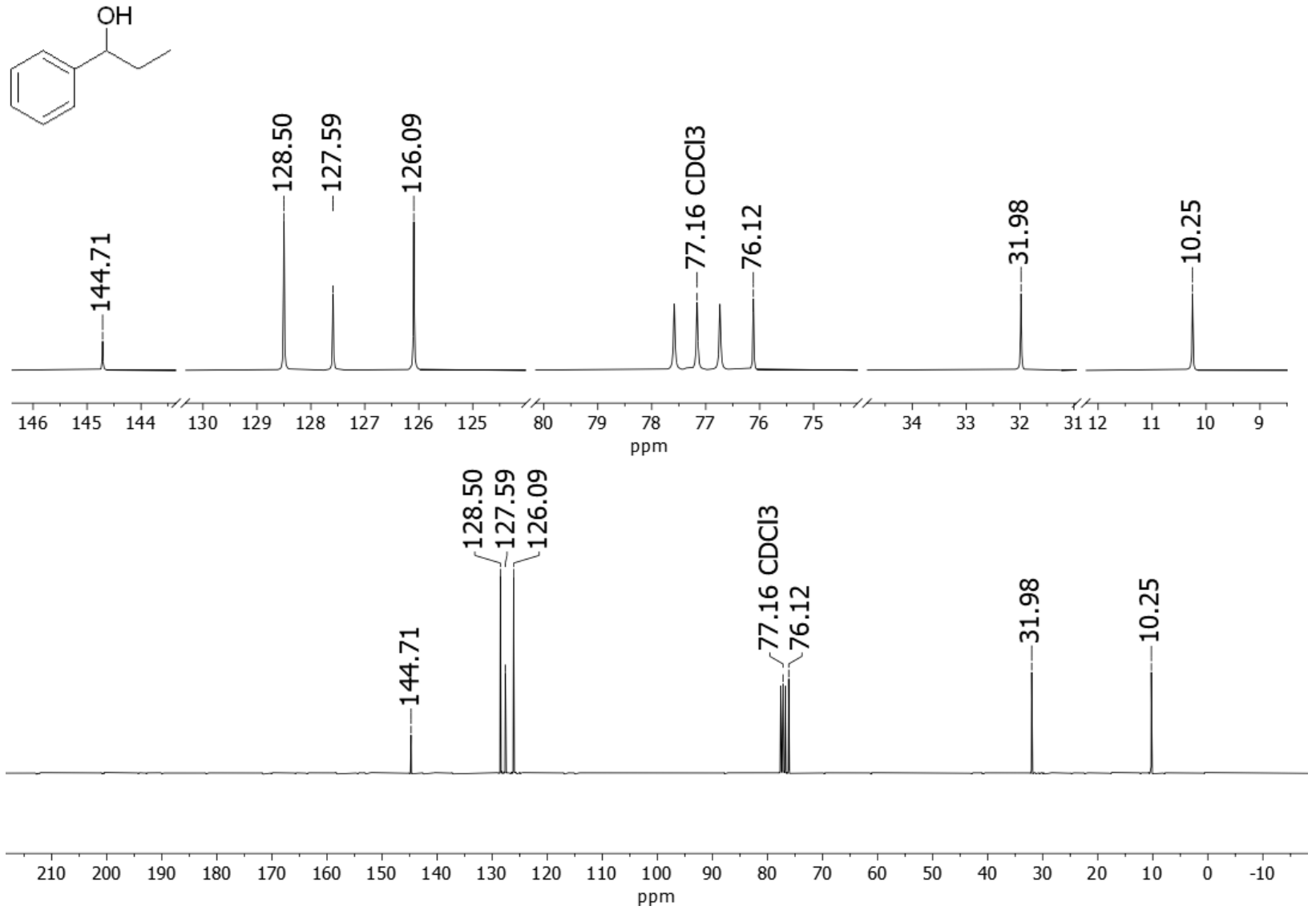


Figure S43. ^{13}C NMR spectrum of compound **7g** ($CDCl_3$, 75 MHz).

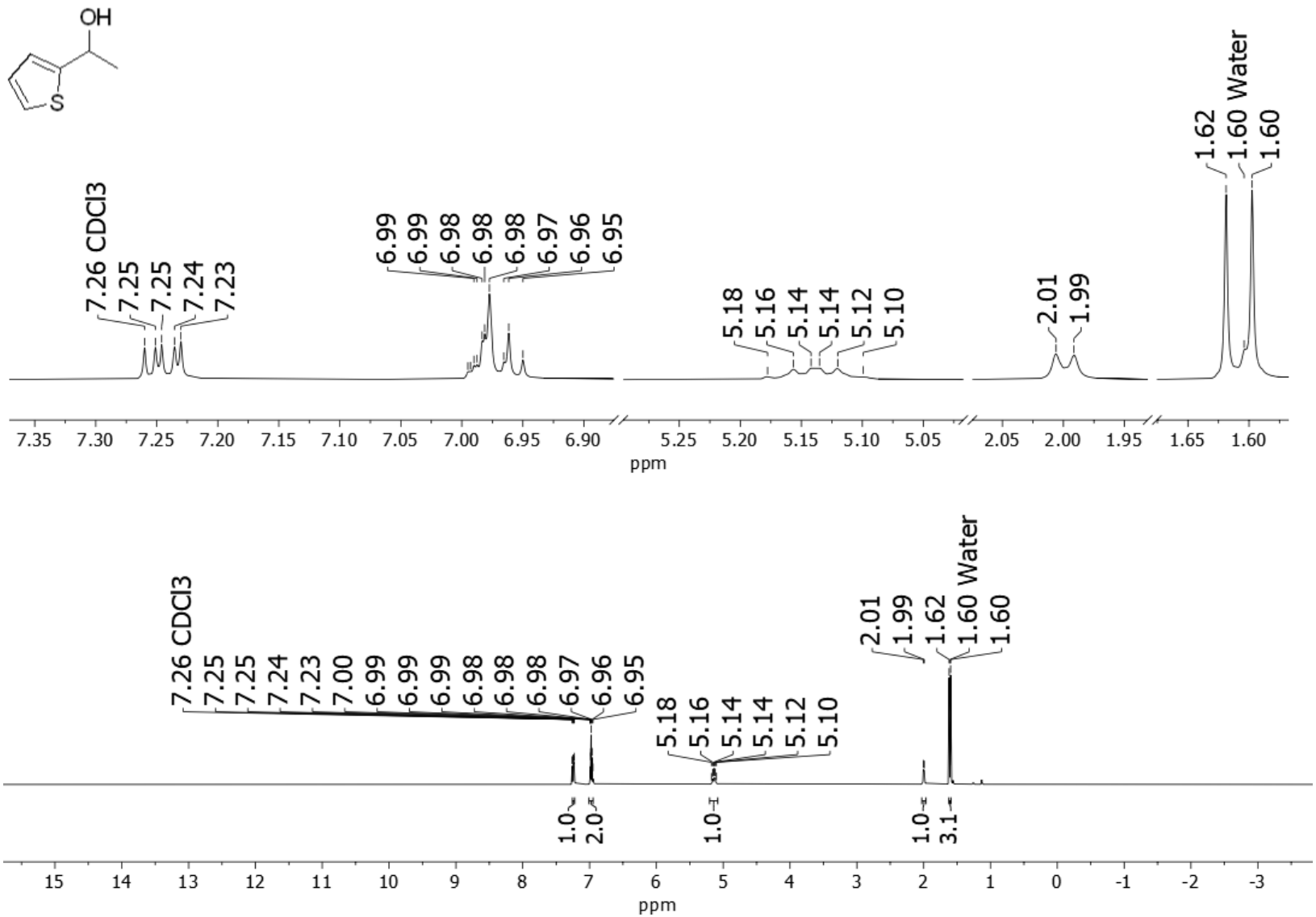


Figure S44. ^{1}H NMR spectrum of compound **7h** ($CDCl_3$, 300 MHz).

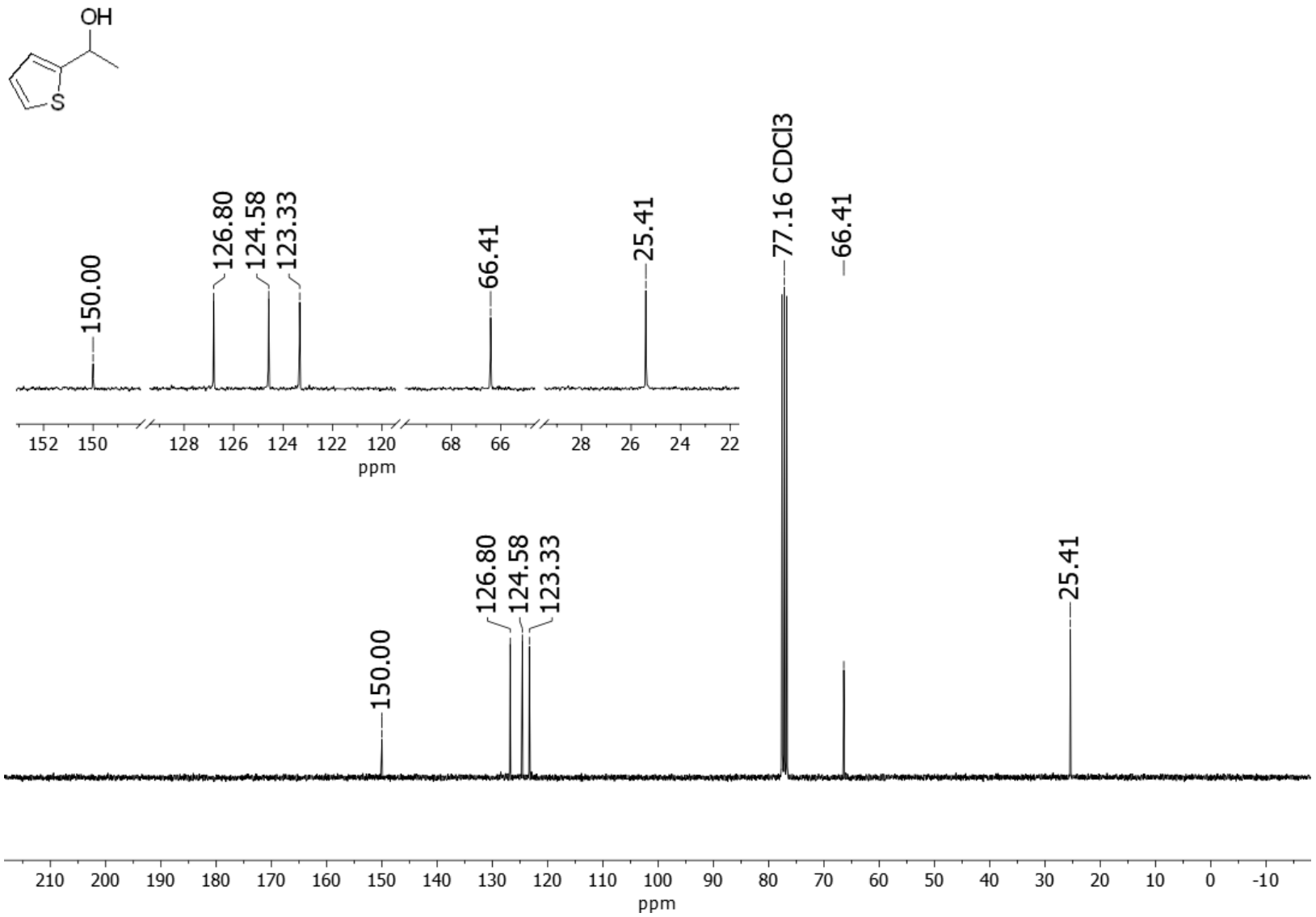


Figure S45. ^{13}C NMR spectrum of compound **7h** ($CDCl_3$, 75 MHz).

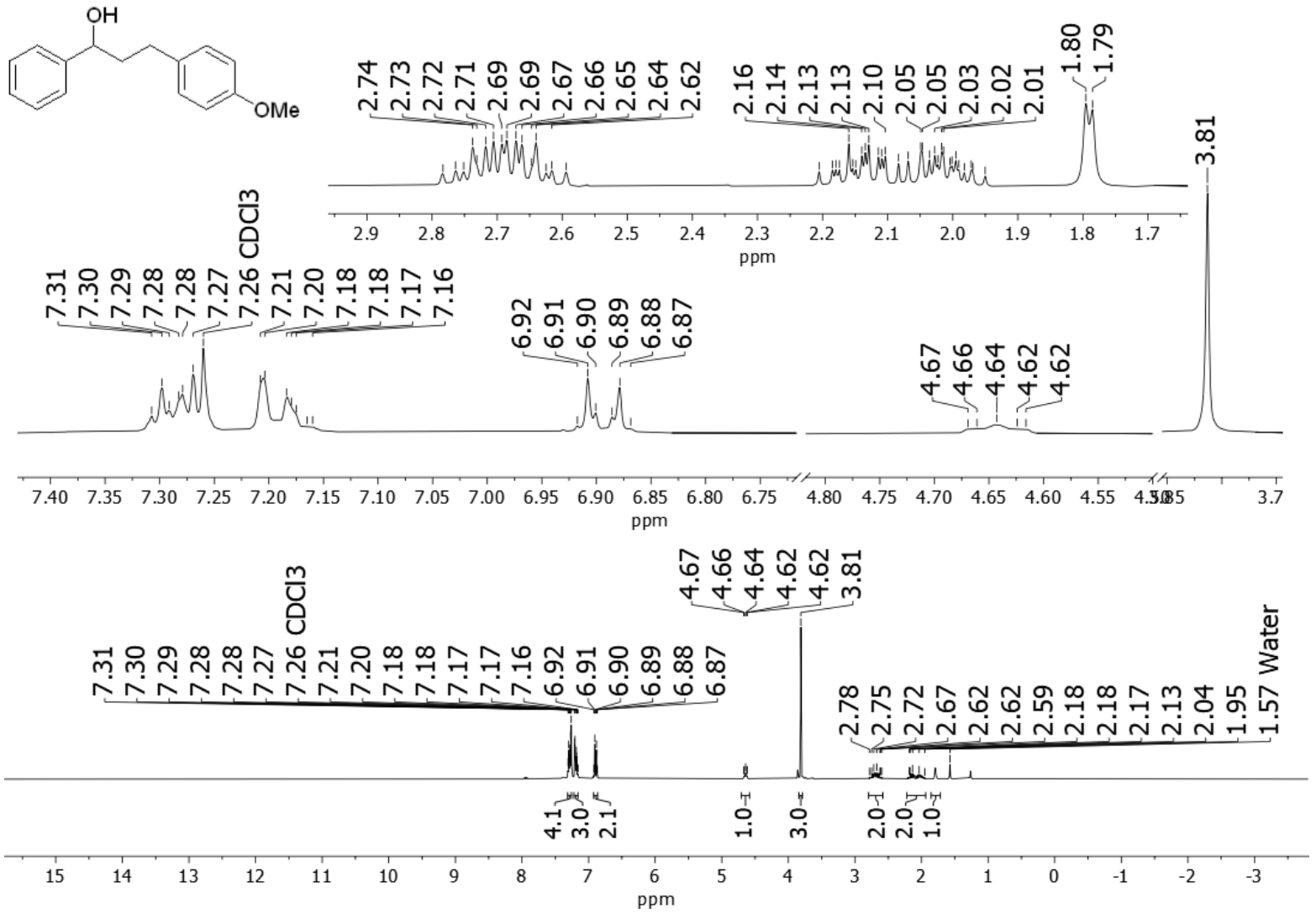


Figure S46. ^{1}H NMR spectrum of compound **9a** ($CDCl_3$, 300 MHz).

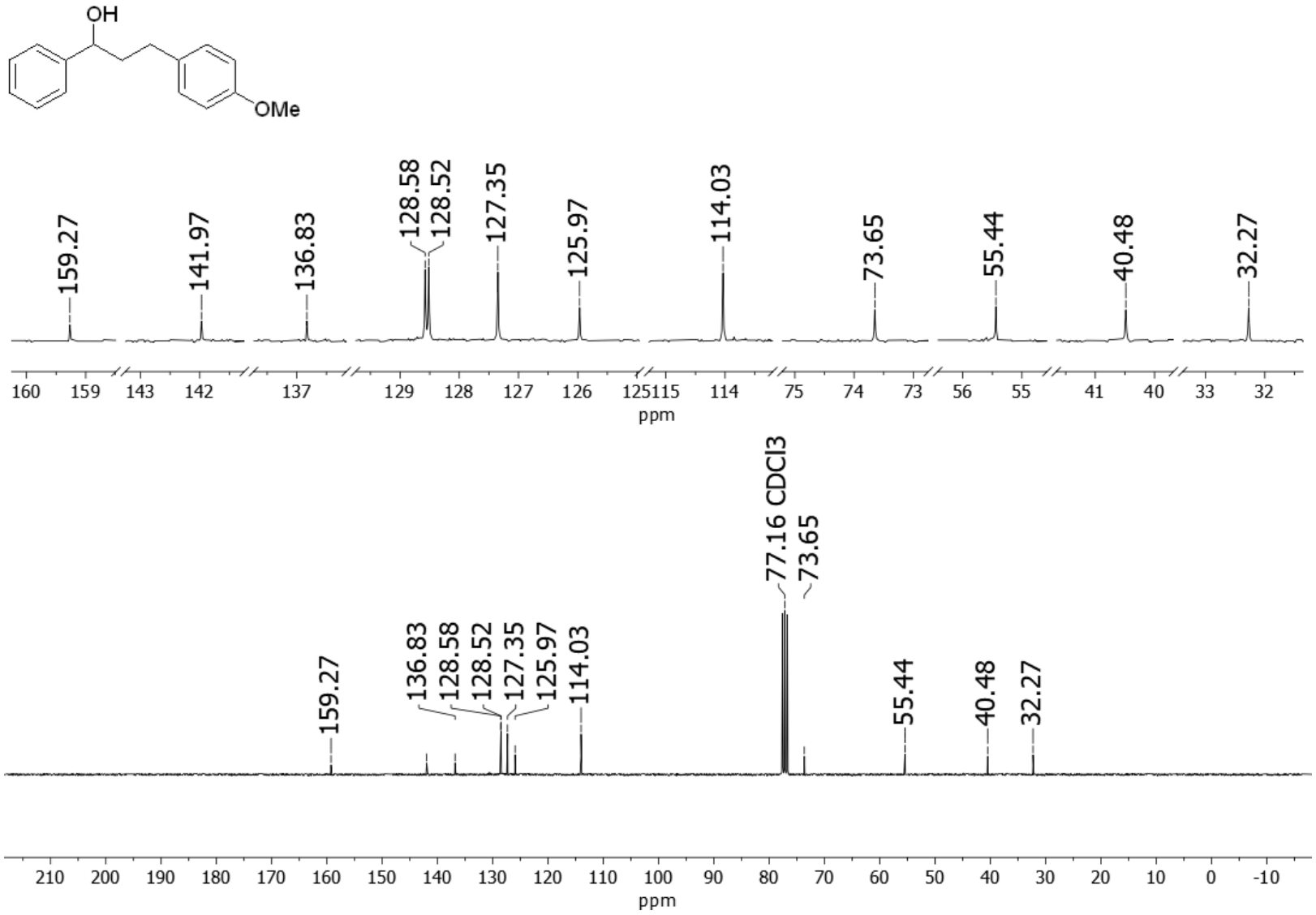


Figure S47. ^{13}C NMR spectrum of compound **9a** ($CDCl_3$, 75 MHz).

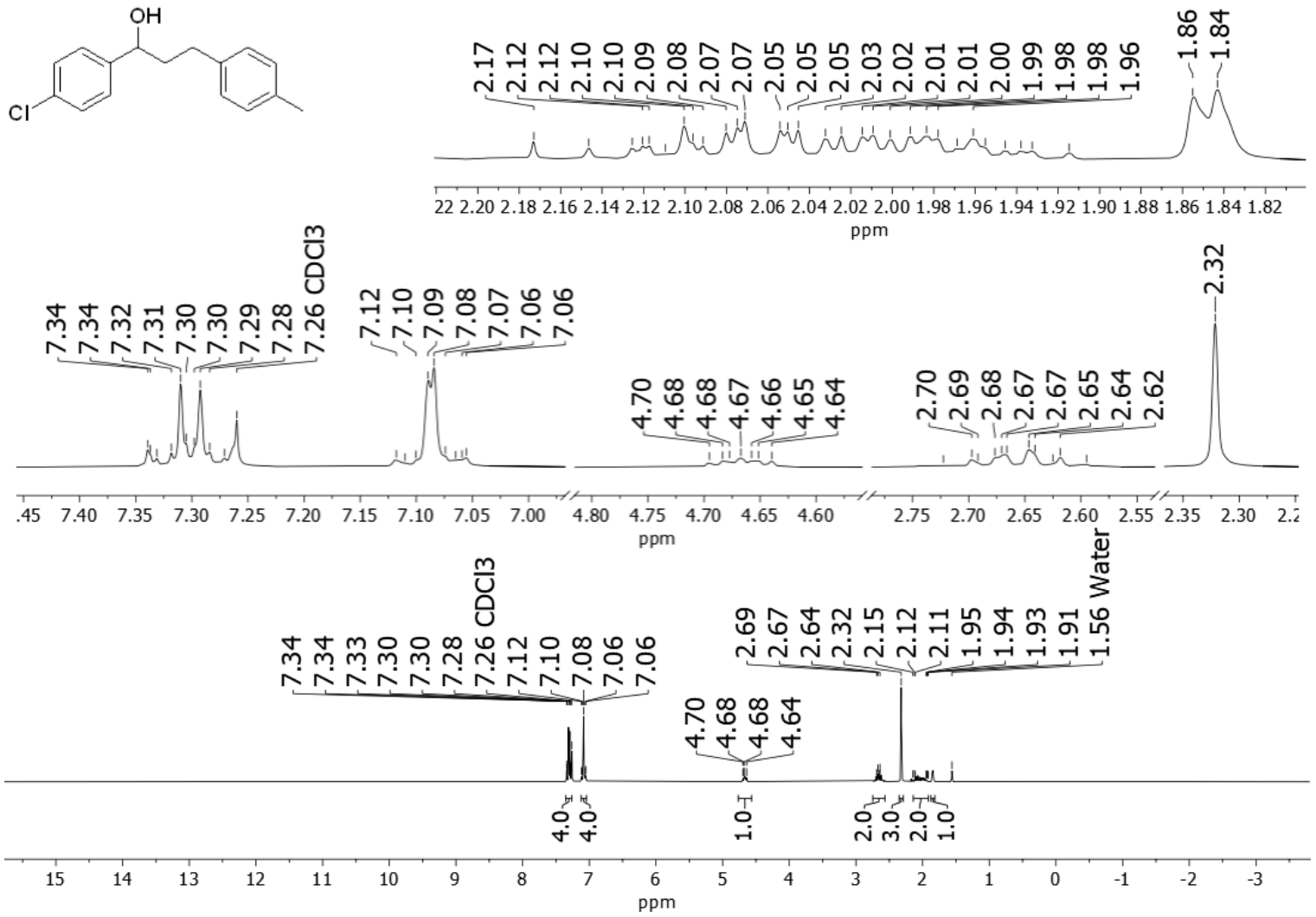


Figure S48. ^{1}H NMR spectrum of compound **9b** ($CDCl_3$, 300 MHz).

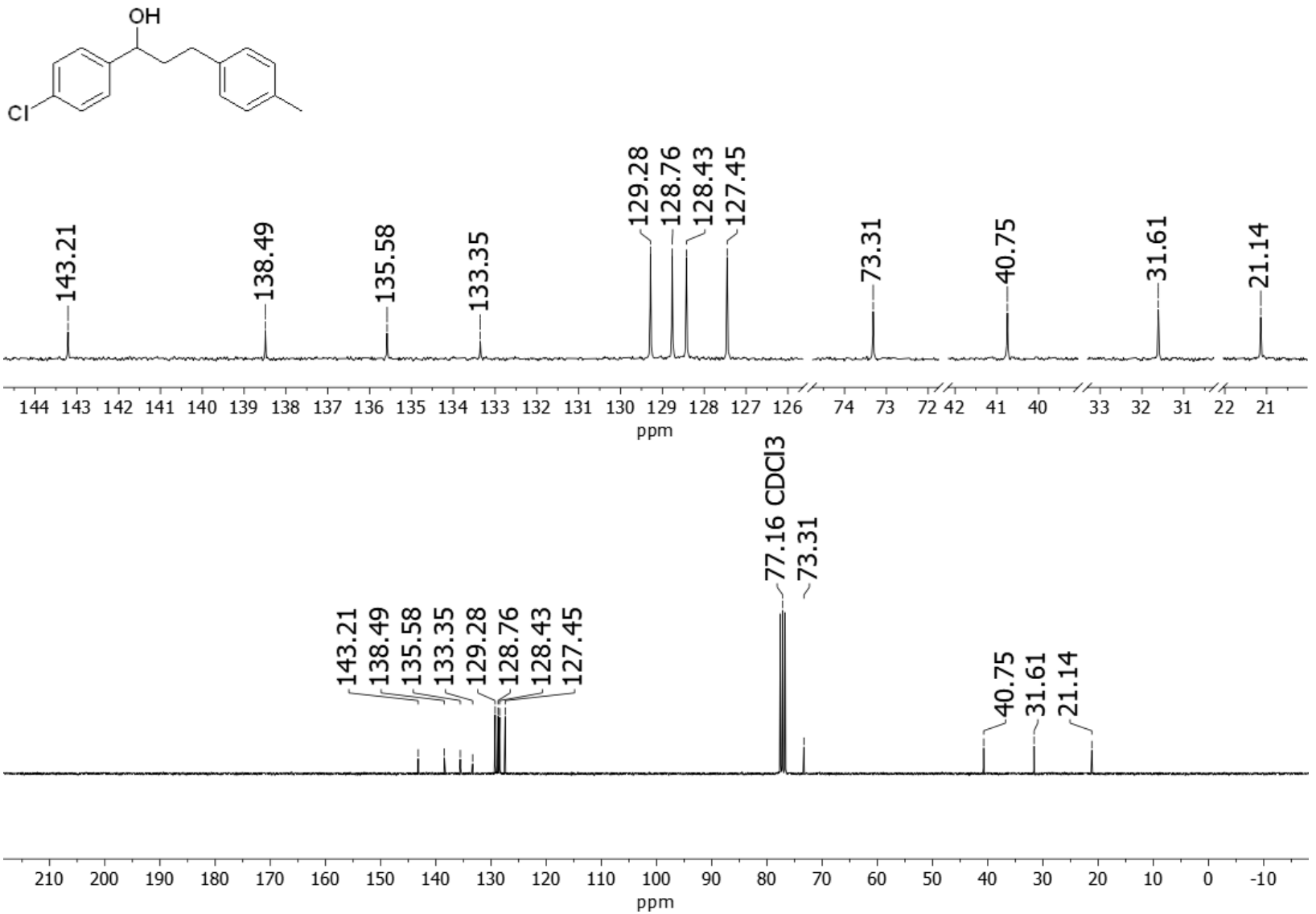


Figure S49. ^{13}C NMR spectrum of compound **9b** ($CDCl_3$, 75 MHz).

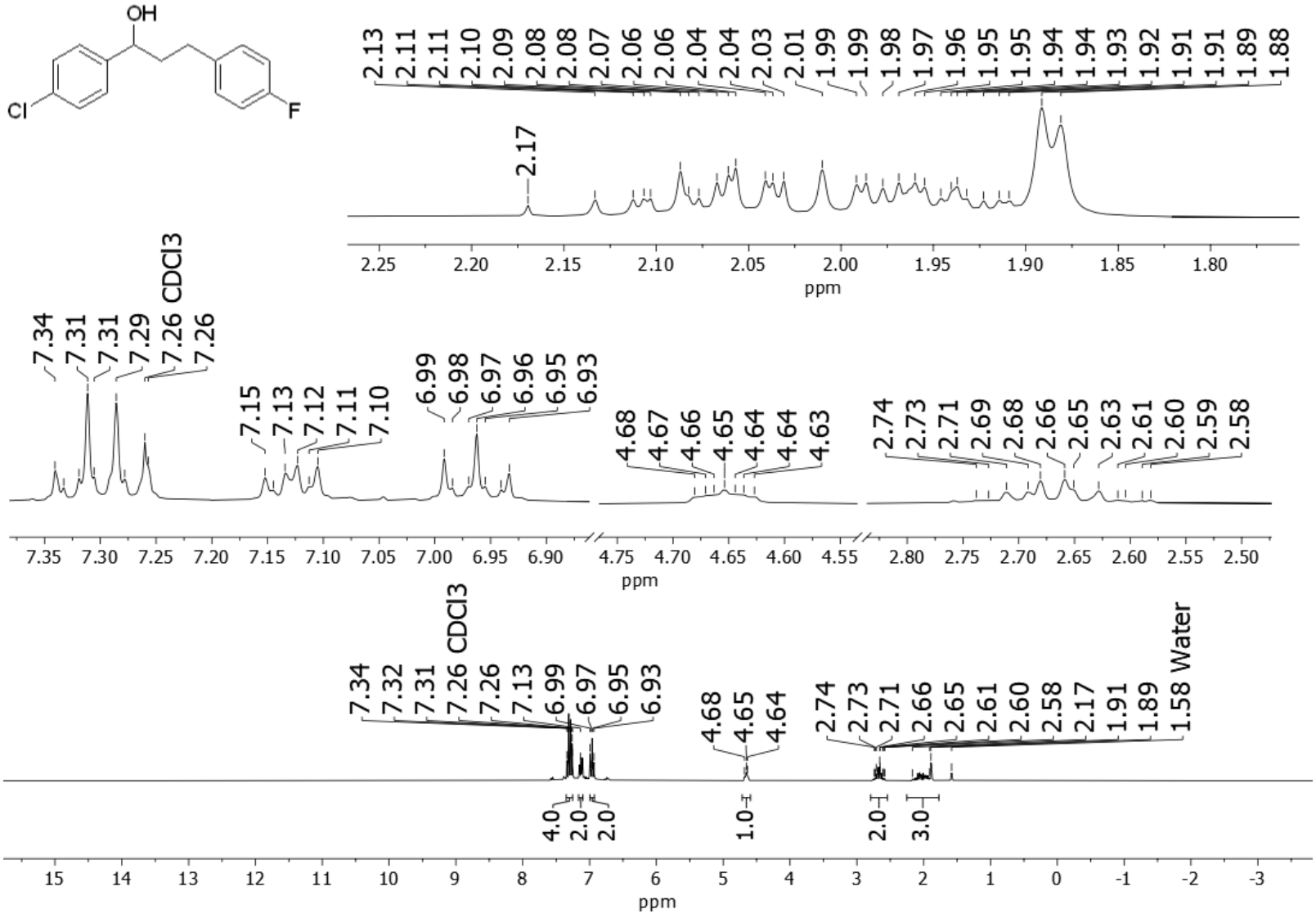


Figure S50. ^{1}H NMR spectrum of compound **9c** ($CDCl_3$, 300 MHz).

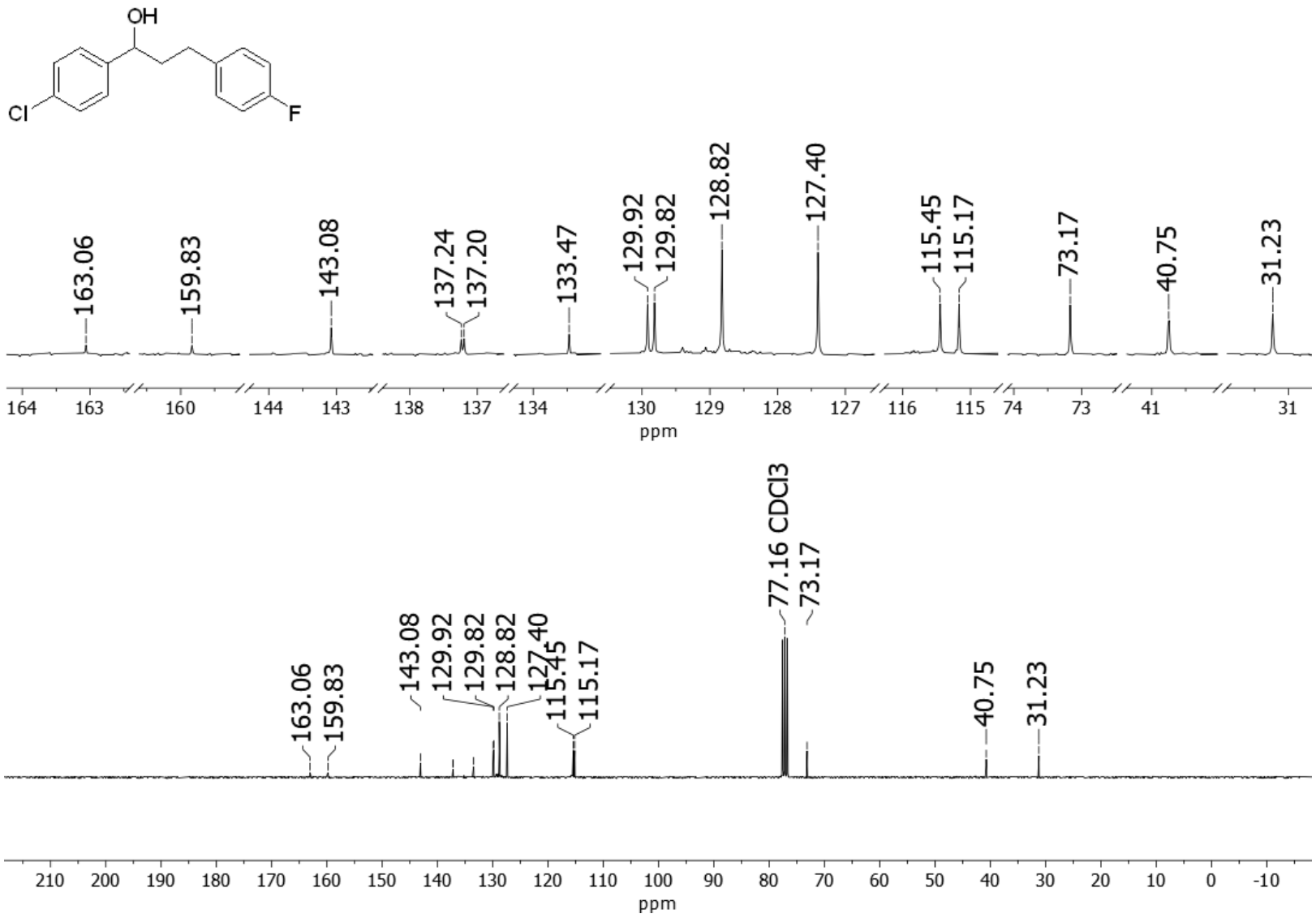


Figure S51. ^{13}C NMR spectrum of compound **9c** ($CDCl_3$, 75 MHz).

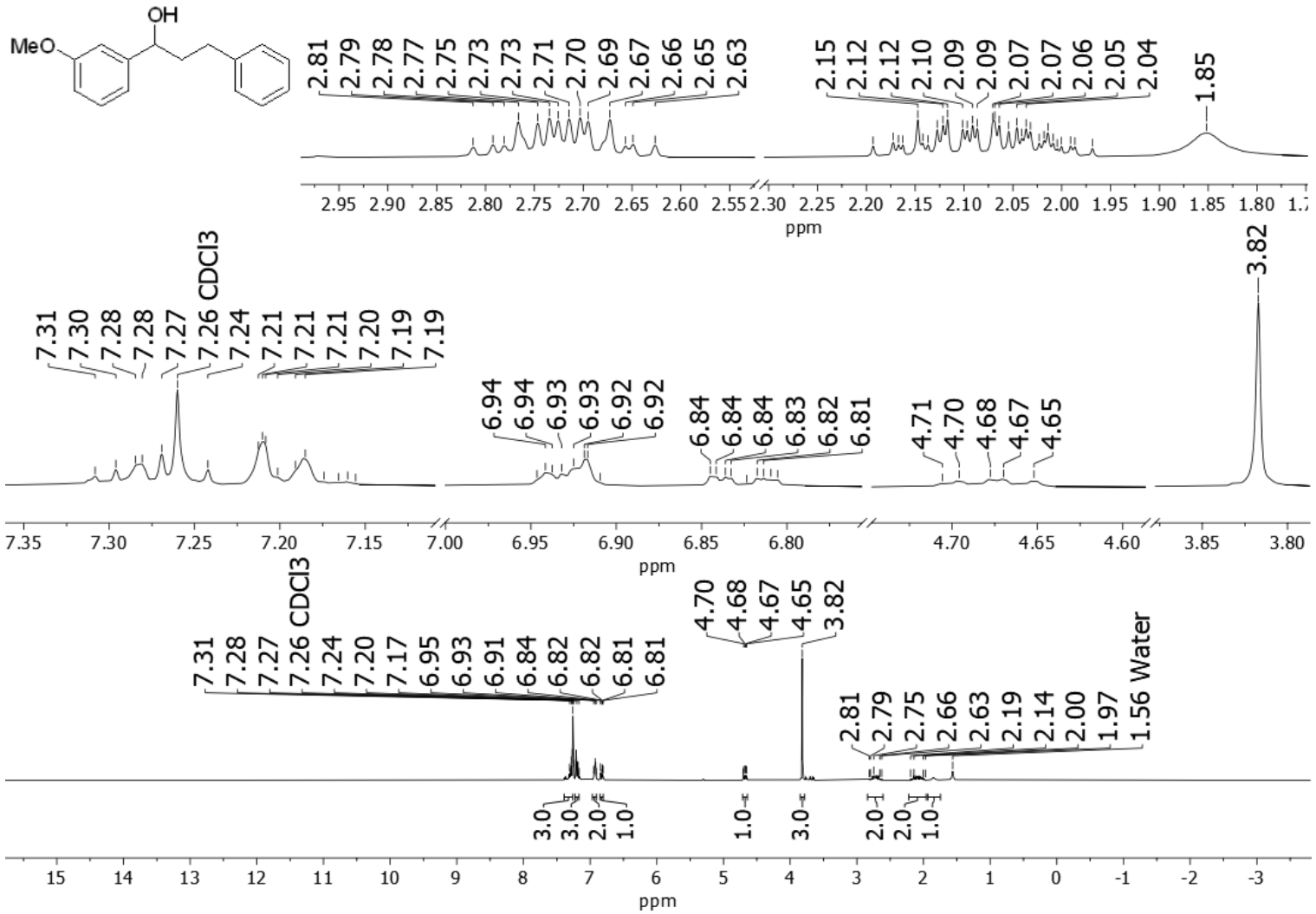


Figure S52. ^{1}H NMR spectrum of compound **9d** ($CDCl_3$, 300 MHz).

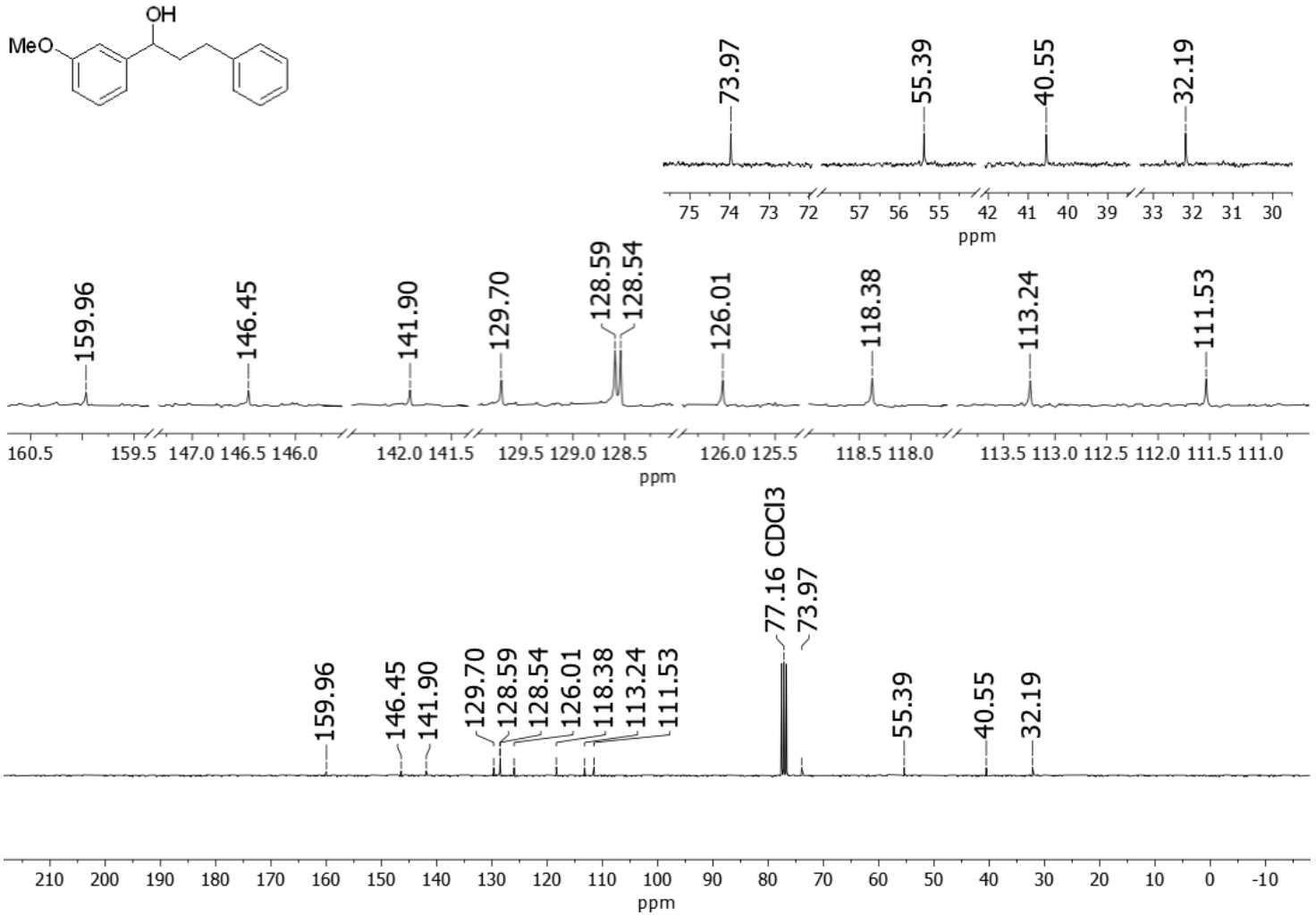


Figure S53. ^{13}C NMR spectrum of compound **9d** ($CDCl_3$, 75 MHz).

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