Supplementary Materials for

Iron(II)-Based Metalloradical System for Intramolecular Amination of C(sp^2)-H and C(sp^3)-H bonds: Synthetic Applications and Mechanistic Studies

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Experimental Part Contents:

Details of Computational Part Contents:

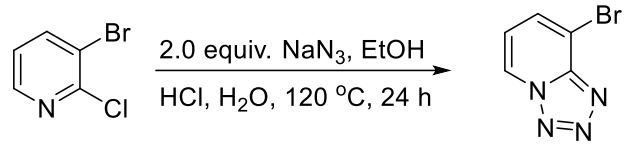
General Information:

All commercially available chemicals were used as received unless otherwise indicated. Benzene (PhH), Tetrahydrofuran (THF), Chlorobenzene (PhCl), Toluene (PhMe) and 1,4-Dioxane were refluxed over sodium/benzophenone ketyl, distilled and degassed twice before reaction. DMF was stirred over CaH_2 for overnight, distilled and degassed twice before reaction. Column chromatography was performed on flash silica gel (ACME). Thin layer chromatography was performed on 0.25 mm thick aluminum-backed silica gel plates purchased from Merck and visualized with ultraviolet light (λ = 254 nm).

^{1}H and ^{13}Cwere recorded on Bruker 400 MHz NMR spectrometers. All coupling constants are apparent J values measured at the indicated field strengths in Hertz (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, bs = broad singlet, dt = doublet of triplets, td = triplet of doublets, ddd = doublet of doublet of doublets, ttt = triplet of triplet of triplets). High-resolution mass spectra (HRMS) were obtained at the Centre of Biomedical Research Mass Spectrometry Service Center using a Waters GCT Premier instrument run on electron ionization (EI) direct probe or a Waters QTOF Ultima instrument run on electrospray ionization (ESI+). GC-MS & GC (Agilent Technology) were obtained from Centre of Biomedical Research Institute and for the analysis, RAM temperature was used 50 ^{o}C for each sample.

Preparation of Starting Materials:

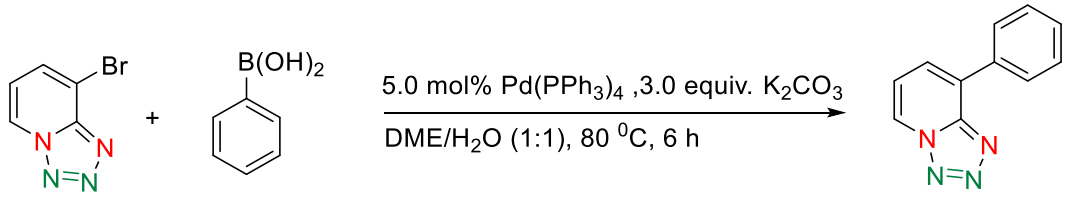
Preparation of 8-bromotetrazolo[1,5-a]pyridine:



25.0 mmol Yield: 82%

An oven dried 100 mL seal-tube was charged with 3-bromo-2-chloro pyridine (4.8 g, 25.0 mmol), ethanol (10.0 mL), H_2O (30.0 mL), HCl (4.0 mL) and NaN_3 (3.25 g, 2.0 equiv.). The seal-tube wascapped tightly and heated at 120 °C for 24 h. Then, the reaction mixture was cooled to 0 °C. A white precipitate was appeared which was isolated through filtration and dried in high vacuum to afford 4.08 g (82%) 8-bromotetrazolo[1,5-a]pyridine as white solid.(**Caution:Tetrazole preparation step was done very carefully under fume hood.).** Spectral data are in accordance with reported literature data. [1]

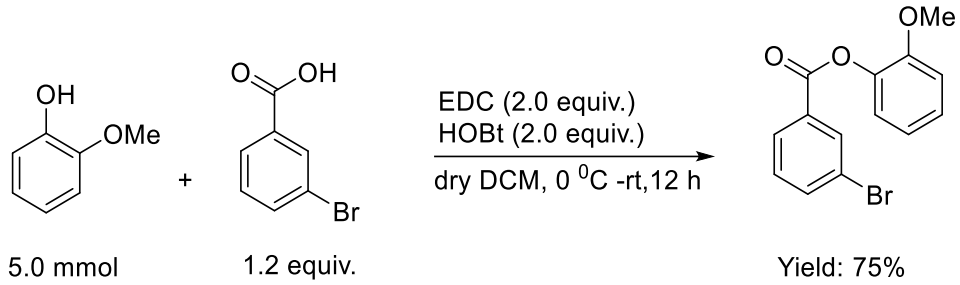
*Preparation of 8-phenyltetrazolo [1, 5-a] pyridine (**1a**):*



1.0 mmol 1.2 equiv. **1a**: 92%

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with 8-bromotetrazolo[1,5-a]pyridine (199.0 mg, 1.0 mmol), phenylboronic acid (146.3 mg, 1.2 equiv.), K_2CO_3 (414.0 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well and DME and water 5.0 mL each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 °C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with silica gel (20% ethyl acetate in hexane as eluent) gave 180.5 mg (92%) of 8-phenyltetrazolo[1,5-a]pyridine (**1a**) as white solid. Spectral data are in accordance with reported data.[1]

Preparation of 2-methoxyphenyl 3-bromobenzoate:



An oven dried 2-necked 100 mL round bottom flask equipped with a condenser and a magnetic stirbar under an argon atmosphere was charged with 3-bromo benzoic acid (744.8 mg, 5.0 mmol), and dry DCM (30.0 mL). Then, reaction mixture was cooled to 0 ^{o}C. After that, EDC (1.91g, 2.0 equiv.) and HOBt (1.3 g, 2.0 equiv.) were added. Then, reaction mixture was stirred for 30 min at 0 ^{o}C. After 30 min stirring, 2-methoxy phenol (620.5 mg, 5.0 mmol) in 10 ml dry DCM was added into the flask via a syringe. Then, the reaction mixture was warmed to rt and stirred for 12 h. min. Upon completion (judged by TLC), the reaction mixture was worked up by DCM (100 mL) and water (50 mL). Dichloromethane layer was washed two times by saturated $NaHCO_3$ solution and then concentrated in vaccuo to afford the crude product. The crude product was purified by silica gel column chromatography (30% ethyl acetate in hexane as eluent) to afford 1.1g (75%) of the 2-methoxyphenyl 3-bromobenzoate as white solid.

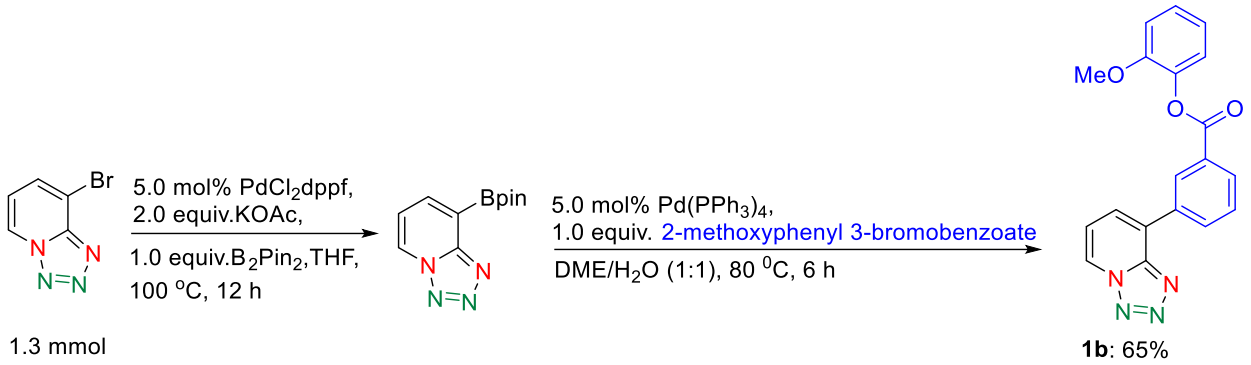
Melting Point: 152-154 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49 (s, 1H), 8.27 (d, J = 7.6 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.51 (t, J = 8.0 Hz, 1H), 7.39 (m, 1H), 7.27 (dd, J = 6.8 Hz, J = 1.2 Hz, 1H), 7.16 – 7.10 (m, 2H), 3.94 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 163.4, 151.1, 139.7, 136.3, 133.2, 131.3, 130.0, 128.8, 127.1, 122.7, 122.5, 120.8, 112.5, 55.8.

HRMS (ESI) *m/z* calcd for $C_{14}H_{11}BrO_3$ $[M+Na]^{+}$328.9789, found 328.9786.

*Preparation of 3-(tetrazolo[1,5-a]pyridin-8-yl)phenyl 2-methoxybenzoate (**1b**):*



1.3 mmol

1b: 65%

Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

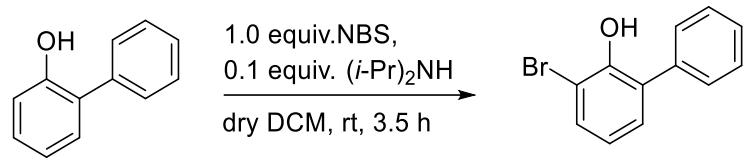
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 2-methoxyphenyl 3-bromobenzoate (307.1 mg, 1.0 mmole.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ° C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with silica gel (30% ethyl acetate in hexane as eluent) gave 225.1 mg (65%) of 3-(tetrazolo[1,5-a]pyridin-8-yl)phenyl 2-methoxybenzoate (**1b**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.12 (d, J = 6.8 Hz, 1H), 9.07 (s, 1H), 8.88 (d, J = 7.6 Hz, 1H), 8.62 (d, J = 7.6 Hz, 1H), 8.22 (d, J = 7.2 Hz, 1H), 8.00 (t, J = 7.6 Hz, 1H), 7.63 (t, J = 7.2 Hz, 1H), 7.52 (t, J = 8.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.29 (dd, J = 8.0 Hz, J = 4.8 Hz, 2H), 4.10 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.2, 151.2, 147.8, 139.7, 133.9, 133.9, 131.3, 130.3, 129.7, 129.4, 129.0, 128.6, 127.1, 124.4, 122.8, 120.8, 116.9, 112.4, 55.8.

HRMS (ESI) *m/z* calcd for $C_{19}H_{14}N_4O_3$ $[M+H]^+$ 347.1144, found 347.1138.

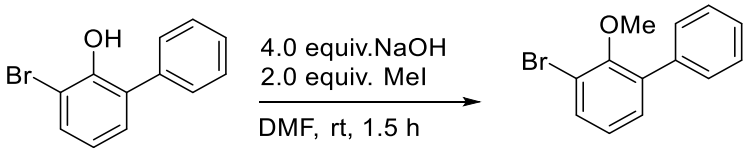
Preparation of 3-bromo-[1,1'-biphenyl]-2-ol:



10.0 mmol Yield: 65%

A 250 mL 2 necked round bottom flask was charged with 2-phenylphenol (1.7g, 10.0 mmol) and 20.8 mL dry DCM. $(i\text{-Pr})_2NH$ (166.0 µL, 0.1 equiv.) was added to the above solution. To the mixture was added a solution of NBS (1.7 g, 1.0 equiv.) in 50.0 mL dry DCM dropwise by syringe over 30 min. After stirring at rt about 3.5 h, H_2O was added and the mixture was acidified to pH = 2 with 1 (M) HCl. The organic layer was separated, and the aqueous layer was extracted with DCM (3×20 mL). The combined organic layers were washed with brine (50 mL), dried over Na_2SO_4 and concentrated in vacuo. The resultant oil was purified by silica gel (using 10% ethyl acetate in hexane) to afford product 3-bromo-[1,1'-biphenyl]-2-ol (1.6 g, 65%) as a pale-yellow oil. Spectral data are in accordance with reported literature data.[2]

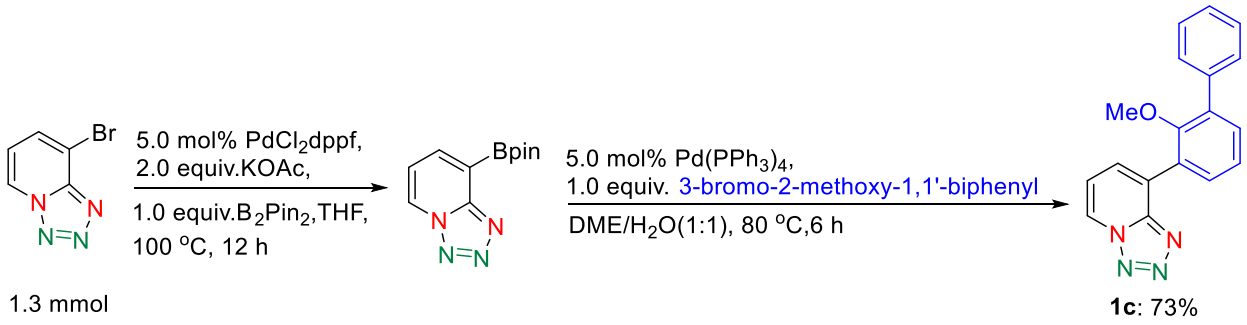
Preparation of 3-bromo-2-methoxy-1,1'-biphenyl:



4.0 mmol Yield: 85%

An oven dried 100 mL round bottom flask was charged with 3-bromo-[1,1'-biphenyl]-2-ol (997 mg, 4.0 mmol) and NaOH (645 mg ,4.0 equiv.) were dissolved in 5.0 mL of DMF. After 30 minutes of stirring, methyl iodide (0.50 mL, 4.0 equiv.) was added and the mixture was stirred for an additional 1.5 hours. Upon completion (checked by TLC), reaction mixture was transferred to a separatory funnel with 20 mL of diethyl ether and 10 mL of cold water. The organic layer was obtained and washed with 10%(w/v) NaOH (aq) (2 x 30 mL), cold water (4 x 20 mL) and 20 mL of brine. The solution was dried with Na_2SO_4 then solvent was removed under reduced pressure to yield 894.7 mg (85%) of 3-bromo-2-methoxy-1,1'-biphenyl as golden oil.[3]

*Preparation of 8-(2-methoxy-[1,1'-biphenyl]-3-yl)tetrazolo[1,5-a]pyridine (**1c**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 3-bromo-2-methoxy-1,1'-biphenyl (263.1 mg, 1.0 mmol.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ° C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with silica gel (30% ethyl acetate in hexane as eluent) gave 220.7 mg (73%) of 8-(2-methoxy-[1,1'-biphenyl]-3-yl)tetrazolo[1,5-a]pyridine (**1c**) as white solid.

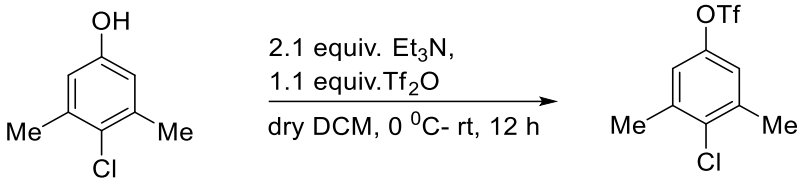
Melting Point: 144-146 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.82 (d, J = 6.0 Hz, 1H), 7.94 (d, J = 6.0 Hz, 1H), 7.75 (d, J = 6.4 Hz, 1H), 7.61 (d, J = 6.0 Hz, 2H), 7.46 -7.30 (m, 6H), 3.19 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 155.4, 148.6, 138.1, 125.6, 132.7, 131.9, 130.6, 129.0, 128.3, 127.6, 127.4, 127.1, 124.3, 123.9, 116.7, 60.8.

HRMS (ESI) *m/z* calcd for $C_{18}H_{14}N_4O$ $[M+H]^+$ 303.1246, found 303.1240.

Preparation of 4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate:



Yield: 95%

To an oven dried 250 mL round-bottomed flask was added the 4-chloro-3,5-dimethylphenol (1.4 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at0 ^{0}C for 30minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (2% ethyl acetate in hexane as eluent) gave 2.5 g (95%) of 4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate as a colorless oil. Spectral data are in accordance with reported data.[4]

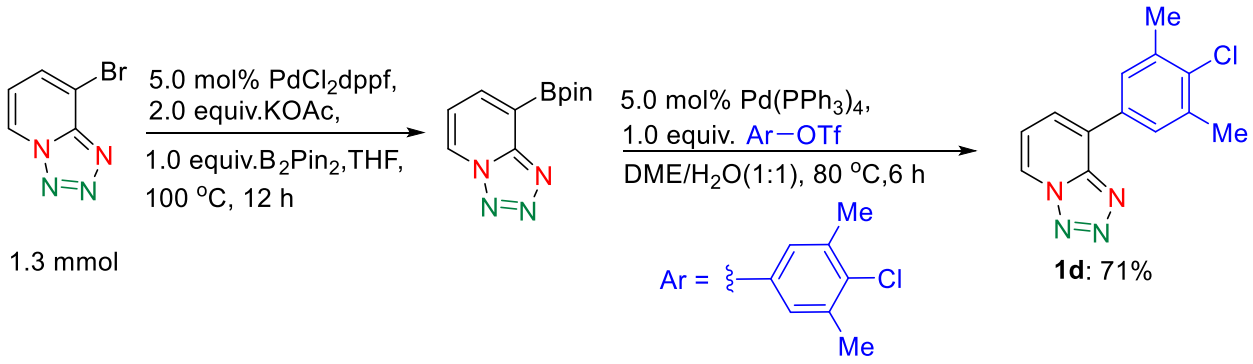
^{1}H NMR (800 MHz, $CDCl_3$): δ 7.01 (s, 2H), 2.41 (s, 6H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 146.9, 138.7, 134.5, 120.8, 118.7 (q, J = 318.8 HZ), 20.9, 20.8.

^{19}F NMR (376 MHz, $CDCl_3$): -72.9.

HRMS (ESI) *m/z* calcd for $C_9H_8ClF_3O_3S$ $[M+H]^+$ 288.9913, found 288.9916.

*Preparation of 8-(4-chloro-3,5-dimethylphenyl)tetrazolo[1,5-a]pyridine(**1d**):*



1.3 mmol

1d: 71%

Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate (288.7 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 183.7 mg (71%) of 8-(4-chloro-3,5-dimethylphenyl) tetrazolo[1,5-a] pyridine (**1d**) as white solid.

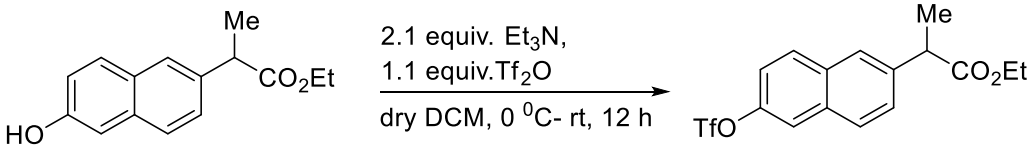
Melting Point: 196=5-197 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (d, J = 6.8 Hz, 1H), 7.85 (s, 2H), 7.79 (d, J = 7.2 Hz, 1H), 7.30 (t, J = 7.2 Hz, 1H), 2.49 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 147.9, 137.0, 136.5, 131.1, 129.1, 128.3, 123.7, 116.9, 20.9.

HRMS (ESI) *m/z* calcd for $C_{13}H_{11}ClN_4$ $[M+H]^+$ 259.0750, found 259.0742.

Preparation of ethyl 2-(6-(((trifluoromethyl)sulfonyl)oxy)naphthalen-2-yl)propanoate:



Yield: 72%

To an oven dried 250 mL round-bottomed flask was added the ethyl 2-(6-hydroxynaphthalen-2-yl)propanoate (2.2 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere.

Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (10% ethyl acetate in hexane as eluent) gave 2.4 g (72%) of ethyl 2-(6-(((trifluoromethyl)sulfonyl)oxy)naphthalen-2-yl)propanoateas a colorless oil.

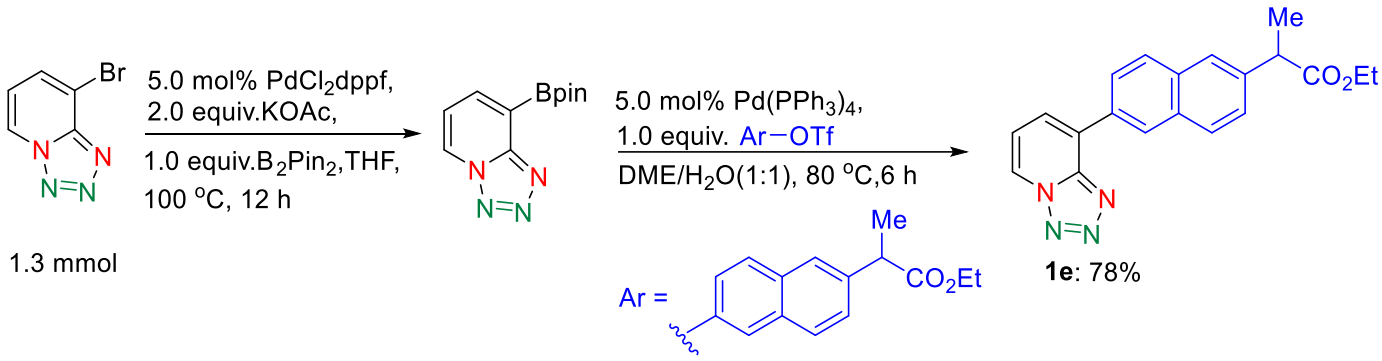
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 (d, J = 8.8 Hz, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.80 (s, 1H), 7.73 (d, J = 2.0 Hz, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.37 (dd, J = 9.0 Hz, J = 2.4 Hz, 1H), 4.21-4.08 (m, 2H), 3.90 (q, J = 7.2 Hz, 1H), 1.59 (d, J = 7.2 Hz, 3H), 1.21 (t, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 174.1, 147.0, 139.8, 132.4, 132.4, 130.5, 128.4, 127.6, 126.1, 119.8, 119.0, 118.8 (J = 319.0 Hz), 61.0, 45.6, 18.5, 14.1.

^{19}F NMR (376 MHz, $CDCl_3$): -72.8

HRMS (ESI) *m/z*calcd for $C_{16}H_{15}F_3O_5S$ $[M+H]^+$ 377.0671, found 377.0666.

*Preparation of ethyl 2-(6-(tetrazolo[1,5-a]pyridin-8-yl)naphthalen-2-yl)propanoate (**1e**):*



1.3 mmol

Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, ethyl 2-(6-(((trifluoromethyl)sulfonyl)oxy)naphthalen-2-yl)propanoate (376.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 270.2 mg (78%) of ethyl 2-(6-(tetrazolo[1,5-a]pyridin-8-yl)naphthalen-2-yl)propanoate (**1e**) as brown solid.

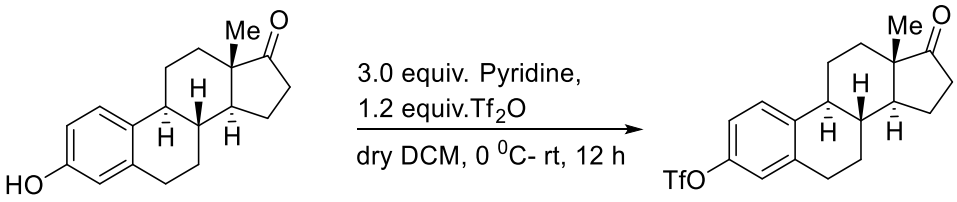
Melting Point: 132-134 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (d, J = 7.2 Hz, 2H), 8.12 (d, J = 8.4 Hz, 1H), 7.97 – 7.92 (m, 3H), 7.79 (s, 1H), 7.53 (d, J = 8.8 Hz, 1H), 7.32 (t, J = 6.8 Hz, 1H), 4.22 – 4.10 (m, 2H), 3.91 (q, J = 6.8 Hz, 1H), 1.61 (d, J = 7.2 Hz, 3H), 1.22 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 174.3, 148.0, 139.7, 129.2, 128.6, 128.5, 126.7, 125.8, 125.3, 123.7, 117.0, 60.9, 45.7, 18.5, 14.1.

HRMS (ESI) *m/z*calcd for $C_{20}H_{18}N_4O_2$ $[M+H]^+$ 347.1508, found 347.1499.

Preparation of (8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-benzo[a]cyclopenta[f]naphthalen-3-yl trifluoromethanesulfonate:



quantitative yield

To an oven dried 250 mL round-bottomed flask was added the estrone (2.0 g, 7.5 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, pyridine (1.8 mL, 3.0 equiv.) was added dropwise over a period of 10 min at 0 ^{o}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.5 mL, 1.2 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction

mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (10% ethyl acetate in hexane as eluent) gave quantitative (8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-benzo[a]cyclopenta[f]naphthalen-3 yltrifluoromethan-esulfonateas a white solid. Spectral data are in accordance with reported data.[5]

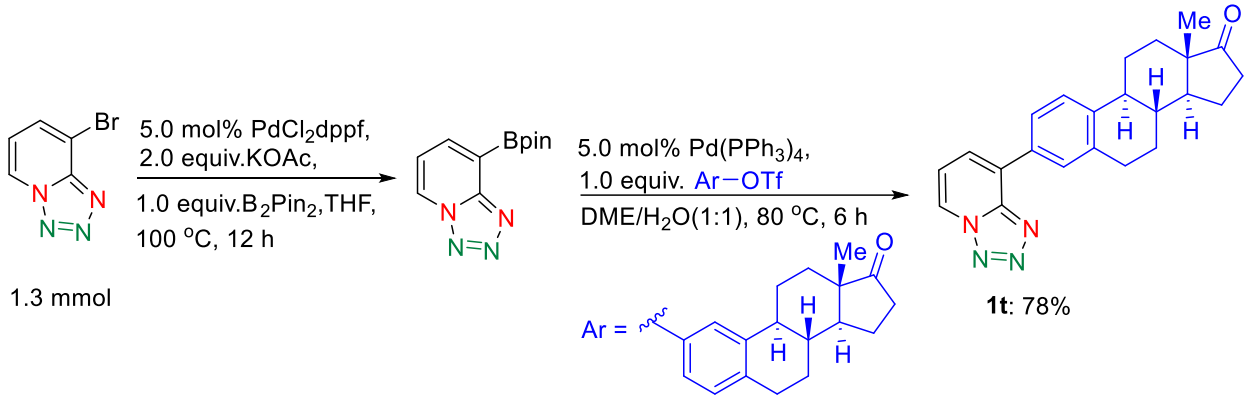
^{1}H NMR (800 MHz, $CDCl_3$): δ 7.34 (d, J = 8.8 Hz, 1H), 7.03 – 7.02 (m, 1H), 6.99 (s, 1H), 2.94 – 2.93 (m, 2H), 2.53 – 2.49 (m, 1H), 2.40-2.39 (m, 1H), 2.29 (t, J = 10.4 Hz, 1H), 2.17 – 2.13 (m, 1H), 2.07 – 2.03 (m, 2H), 1.98 – 1.97 (m, 1H), 1.65-1.60 (m, 2H), 1.56 – 1.45 (m, 4H), 0.91 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 220.4, 147.5, 140.2, 139.3, 127.2, 121.2, 118.7 (q, J = 318.8 Hz), 118.3, 50.3, 47.8, 44.1, 37.7, 35.8, 31.4, 29.4, 26.0, 25.6, 21.5, 13.8.

^{19}F NMR (376 MHz, $CDCl_3$): -73.0.

HRMS (ESI) *m/z* calcd for $C_{19}H_{21}F_3O_4S$ $[M+H]^+$ 403.1191, 403.1186.

*Preparation of (8R,9S,13S,14S)-13-methyl-2-(tetrazolo[1,5-a]pyridin-8 yl)6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one(**1t**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, (8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-benzo[a]cyclopenta[f]naphthalen-3-yl trifluoromethanesulfonate (402.4 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 290.5 mg (78%) of (8R,9S,13S,14S)-13-methyl-2-(tetrazolo[1,5-a]pyridin-8-yl)6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one(**1t**) as brown solid.

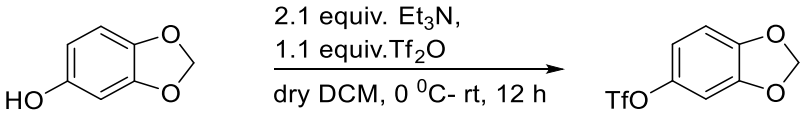
Melting Point: >200 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.78 (d, J = 6.8 Hz, 1H), 7.93 (s, 1H), 7.88 (d, J = 12.3 Hz, 1H), 7.80 (d, J = 7.2 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.29 (t, J = 7.2 Hz, 1H), 3.07-3.03 (m, 2H), 2.57 – 2.47 (m, 2H), 2.42-2.37 (m, 1H), 2.20 – 2.00 (m, 4H), 1.71 – 1.64 (m, 2H), 1.60-1.47 (m, 4H), 0.94 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 220.8, 148.0, 141.8, 137.3, 129.8, 129.1, 128.0, 126.1,125.7, 123.5, 116.9, 50.4, 47.9, 44.5, 37.9, 35.8, 31.5, 29.5, 26.3, 25.6, 21.5, 13.8.

HRMS (ESI) *m/z*calcd for $C_{23}H_{24}N_4O$ $[M+H]^+$ 373.2028, found 373.2022.

Preparation of (benzo[d][1,3]dioxol-5-yl trifluoromethanesulfonate:



Yield: 81%

To an oven dried 250 mL round-bottomed flask was added the sesamol (1.2 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room

temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (5% ethyl acetate in hexane as eluent) gave 2.0 g (81%) of benzo[d][1,3]dioxol-5-yl trifluoromethanesulfonateasa colorless oil. Spectral data are in accordance with reported data.[6]

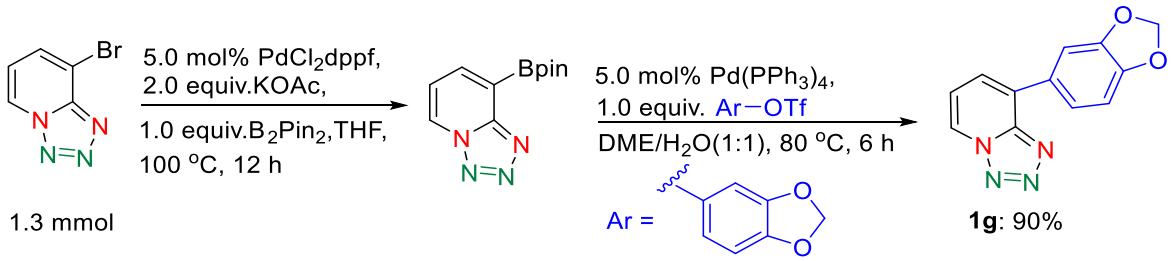
^{1}H NMR (800 MHz, $CDCl_3$): δ 6.80 (d, J = 8.0 Hz, 1H), 6.77 – 6.74 (m, 2H), 6.05 (s, 2H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 148.5, 147.4, 143.5, 118.7 (q, J = 318.8 Hz), 114.4, 108.2, 103.3, 102.5.

^{19}F NMR (376 MHz, $CDCl_3$): -77.7.

HRMS (ESI) *m/z* calcd for $C_8H_5F_3O_5S$ $[M+H]^+$ 270.9888, found 270.9884.

*Preparation of 8-(benzo[d][1,3]dioxol-5-yl)tetrazolo[1,5-a]pyridine(**1g**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, benzo[d][1,3]dioxol-5-yl trifluoromethanesulfonate (270.2 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ° C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and

extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% dichloromethane in hexane as eluent) gave 216.2 mg (90%) of (8-(benzo[d][1,3]dioxol-5-yl)tetrazolo[1,5-a]pyridine (**1g**) as white solid.

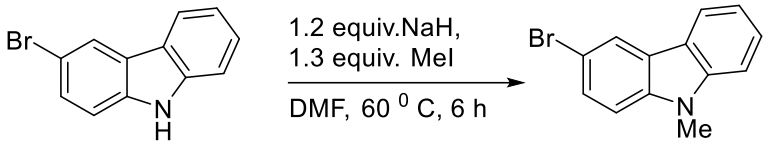
Melting Point: >200 ^{o}C

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.26 (d, J = 6.4 Hz, 1H), 8.09 (d, J = 6.8 Hz, 1H), 7.87 – 7.76 (m, 2H), 7.50 (t, J = 6.8 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 6.14 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 148.6, 148.1, 147.6, 129.2, 127.5, 124.9, 123.2, 118.0, 108.9, 108.6, 101.9, 31.0.

HRMS (ESI) *m/z* calcd for $C_{12}H_8N_4O_2$ $[M+H]^+$ 241.0726, found 241.0705.

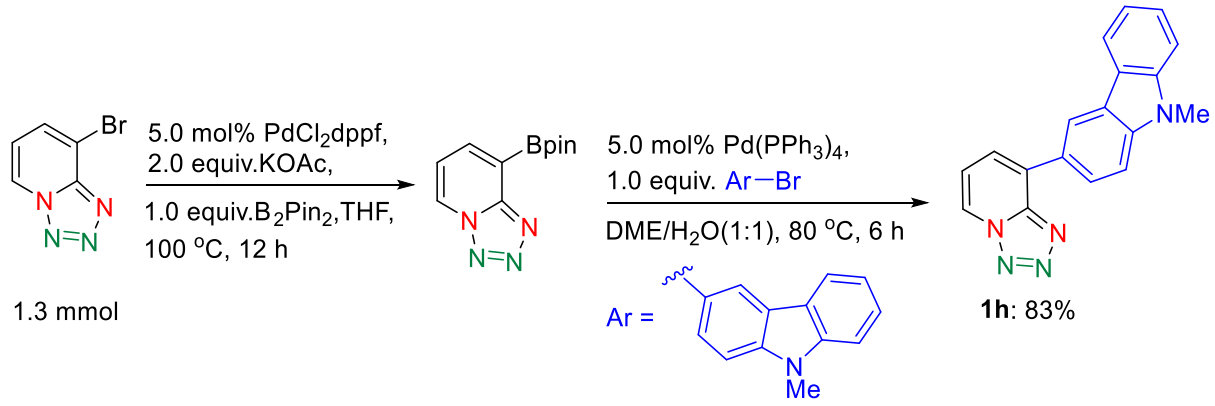
Preparation of 3-bromo-9-methyl-9H-carbazole:



4.0 mmol Yield: 98%

A mixture of 3-bromocarbazole (1.00 g, 4.0 mmol) in dry DMF (3.5 mL) in a pressure tube was treated with 60% NaH (0.2 g, 1.2 equiv.) and then methyl iodide (0.34 mL, 1.3equiv.). The tube was sealed and the reaction was stirred at 60°C for 6 h. The mixture was cooled, poured into 25 mL H_2O and extracted with EtOAc. The extracts were washed with brine, dried (Na_2SO_4) and concentrated to yield 1.02 g (98%) of 3-Bromo-9-methyl-9H-carbazole as a yellow oil. Spectral data are in accordance with reported data.[7]

*Preparation of 9-methyl-3-(tetrazolo[1,5-a]pyridin-8-yl)-9H-carbazole(**1u**):*



1.3 mmol **1h**: 83%

Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 3-Bromo-9-methyl-9H-carbazole (260.1 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (50% dichloromethane in hexane as eluent) gave 248.5 mg (83 %) of 9-methyl-3-(tetrazolo[1,5-a]pyridin-8-yl)-9H-carbazole (**1u**) as white solid.

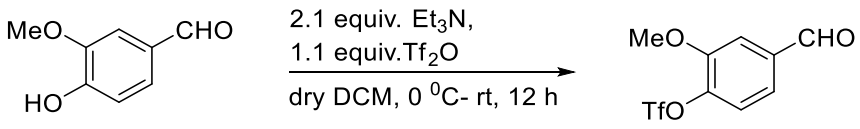
Melting Point: 129-131 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.90 (s, 1H), 8.73 (d, J = 6.8 Hz, 1H), 8.28 (d, J = 12.8 Hz, 1H), 8.19 (d, J = 8.0 Hz, 1H), 7.88 (d, J = 7.2 Hz, 1H), 7.52 (t, J = 8.4 Hz, 2H), 7.43 (d, J = 8.0 Hz, 1H), 7.29 (t, J = 7.2 Hz, 2H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.2, 141.6, 141.4, 130.7, 127.3, 126.3, 126.2, 124.2, 123.2, 122.7,122.5, 120.8, 120.6, 119.5, 117.1, 108.8, 108.7, 29.2.

HRMS (ESI) *m/z* calcd for $C_{18}H_{13}N_5$ $[M+H]^+$ 300.1249, found 300.1243.

Preparation of 4-formyl-2-methoxyphenyl trifluoromethanesulfonate:

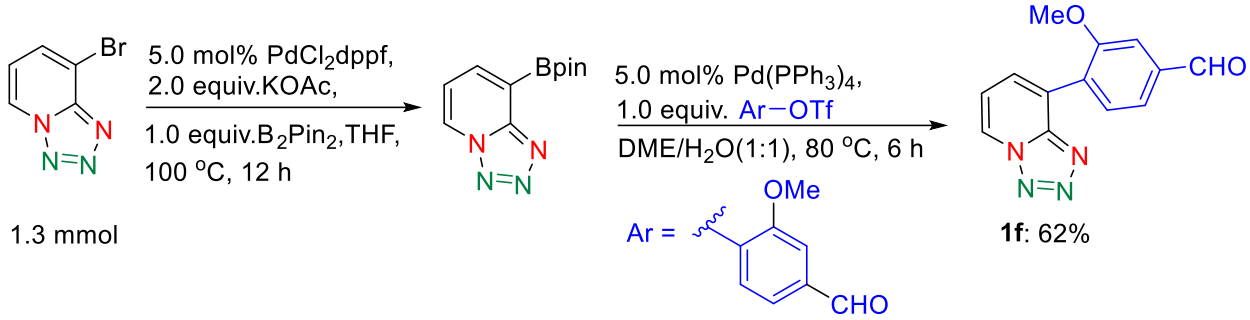


9.0 mmol

Yield: 65%

To an oven dried 250 mL round-bottomed flask was added the vaniline (1.4 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (5% ethyl acetate in hexane as eluent) gave 1.7 g (65%) of 4-formyl-2-methoxyphenyl trifluoromethanesulfonateasa colorless oil. Spectral data are in accordance with reported data.[8]

*Preparation of 3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)benzaldehyde(**1f**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 4-formyl-2-methoxyphenyl trifluoromethanesulfonate (284.2 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C

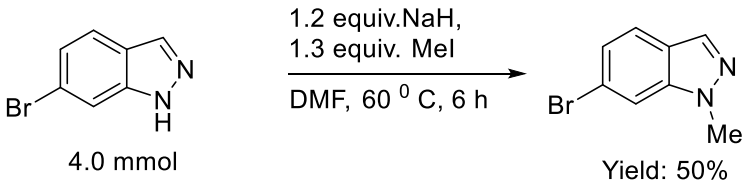
for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 157.6 mg (62%) of 3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)benzaldehyde (**1f**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.10 (s, 1H), 9.35 (d, J = 6.4Hz, 1H), 7.98 (d, J = 7.2 Hz, 1H), 7.89 (d, J = 7.6 Hz, 1H), 7.71 (s, 2H), 7.55 (t, J = 6.8 Hz, 1H), 3.86 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 192.7, 157.3, 147.6, 138.1, 133.1, 132.1, 128.6, 125.9, 124.6, 122.5, 117.3, 111.2, 56.0.

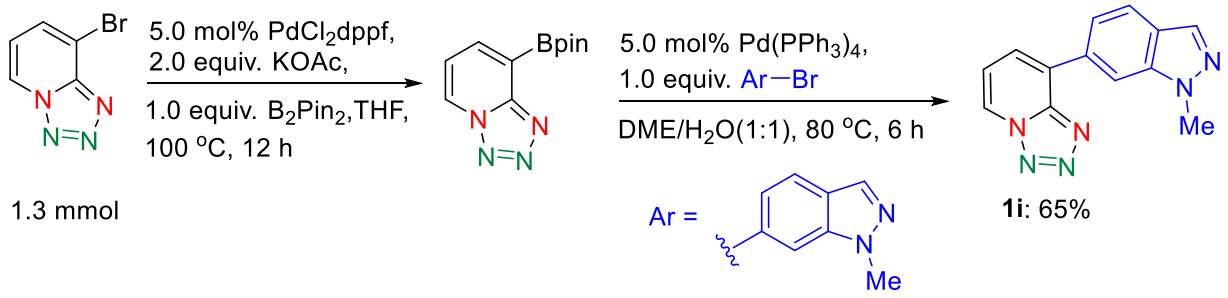
HRMS (ESI) *m/z* calcd for $C_{13}H_{10}N_4O_2$ $[M+H]^+$ 255.0882, found 255.0861.

Preparation of 6-bromo-1-methyl-1H-indazole:



A mixture of 6-bromo -1H-indazole (788 mg, 4.0 mmol) in dry DMF (3.5 mL) in a pressure tube was treated with 60% NaH (0.2 g, 1.2 equiv.) and then methyl iodide (0.34 mL, 1.3equiv.). The tube was sealed and the reaction was stirred at 60°C for 6 h. The mixture was cooled, poured into 25 mL H_2O and extracted with EtOAc. The extracts were washed with brine, dried (Na_2SO_4) and concentrated to yield 422.2 mg (50%) of 5-bromo-1-methyl-1H-indazoleas a yellow oil. Spectral data are in accordance with reported data.[9]

*Preparation of 8-(1-methyl-1H-indazol-6-yl)tetrazolo[1,5-a]pyridine (**1i**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was

sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 6-bromo-1-methyl-1H-indazole (211.1 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (50% dichloromethane in hexane as eluent) gave 162.7 mg (65%) of 8-(1-methyl-1H-indazol-6-yl)tetrazolo[1,5-a]pyridine (**1i**) as white solid.

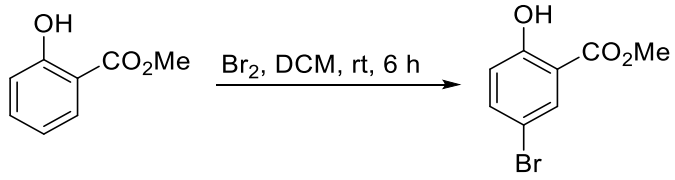
Melting Point: >200 ^{o}C

^{1}H NMR (400 MHz, DMSO-d_6): δ 9.35 (d, J = 6.8 Hz, 1H), 8.51 (s, 1H), 8.27 (d, J = 7.2 Hz, 1H), 8.14 (s, 1H), 7.95 (s, 2H), 7.59 (t, J = 7.2 Hz, 1H), 4.14 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 147.5, 139.7, 132.4, 131.3, 130.4, 128.0, 125.3, 123.7, 121.2, 120.7, 117.7, 109.9, 35.5.

HRMS (ESI) *m/z*calcd for $C_{13}H_{10}N_6$ $[M+H]^+$ 251.1045, found 251.1032.

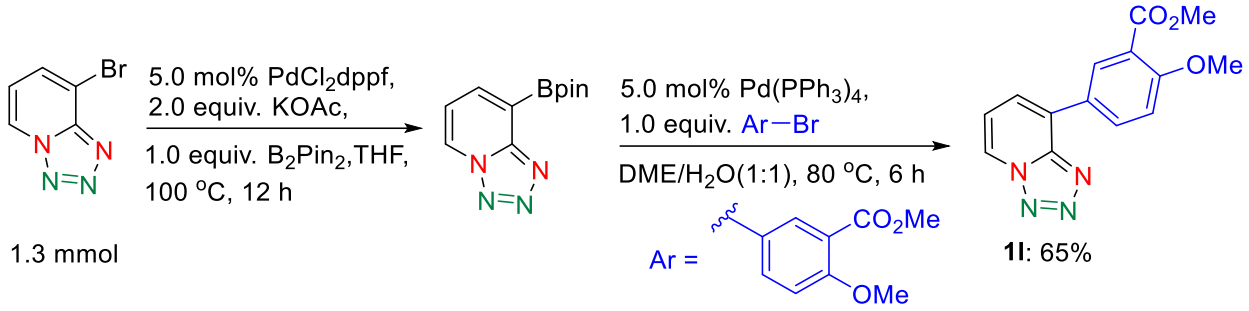
Preparation of methyl 5-bromo-2-hydroxybenzoate:



10.0 mmol Yield: 90%

To a solution of methyl salicylate (1.52 g, 10.0 mmol) in dichloromethane (100 mL) was added dropwise bromine [1(N)solution in dichloromethane, 1.1 equiv] for 6h. After that, the reaction mass was poured into thesaturated sodium sulphite solution nd worked up by DCM (100 mL) and water (100 mL). Then organic layer was evaporated in vaccum and then crude solid materialwashed with hexane to obtain the desired 2.1 g (90%) methyl 5-bromo-2-hydroxybenzoateas light yellow solid. Spectral data are in accordance with the reported data.[10]

*Preparation of methyl 2-methoxy-5-(tetrazolo[1,5-a]pyridin-8-yl)benzoate(1**l**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, methyl 5-bromo-2-hydroxybenzoate (245.0 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ° C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (50% dichloromethane in hexane as eluent) gave 184.8 mg (65%) of methyl 2-methoxy-5-(tetrazolo[1,5-a]pyridin-8-yl)benzoate (**1l**) as white solid.

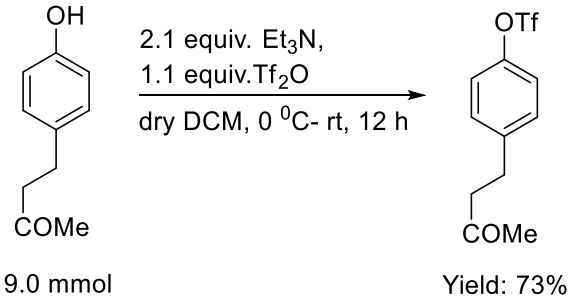
Melting Point: 191-193 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.78 (d, J = 6.8 Hz, 1H), 8.51 (d, J = 5.6 Hz, 2H), 7.83 (d, J = 7.2 Hz, 1H), 7.31 (t, J = 6.8 Hz, 1H), 7.21 – 7.17 (m, 1H), 4.00 (s, 3H), 3.94 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 160.2, 147.8, 134.0, 131.5, 1284, 127.5, 125.4, 123.5, 120.6, 116.9, 112.6, 56.3, 52.3.

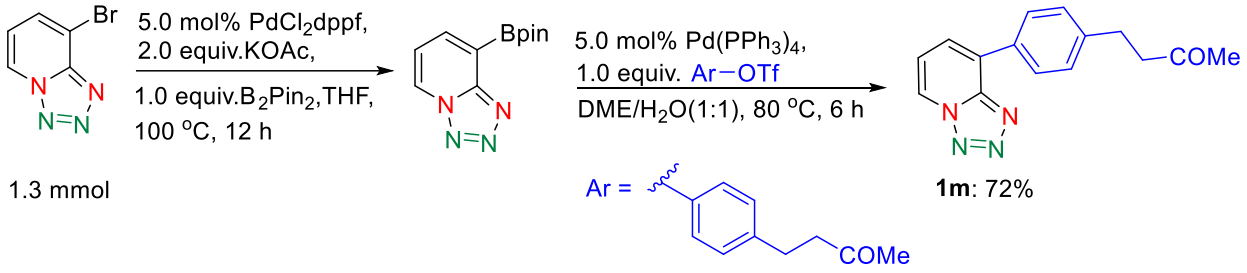
HRMS (ESI) *m/z* calcd for $C_{14}H_{12}N_4O_3$ $[M+H]^+$ 285.0988, found 285.0976.

Preparation of 4-(3-oxobutyl)phenyl trifluoromethanesulfonate:



To an oven dried 250 mL round-bottomed flask was added the 4-(4-hydroxyphenyl)butan-2-one (1.5 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (15% ethyl acetate in hexane as eluent) gave 1.9 g (73%) of 4-(3-oxobutyl)phenyl trifluoromethanesulfonateas a colorless oil. Spectral data are in accordance with reported data.[11]

*Preparation of 4-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)butan-2-one (**1m**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of

celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 4-(3-oxobutyl)phenyl trifluoromethanesulfonate (296.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 191.7 mg (72%) of 4-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)butan-2-one (**1m**) as white solid.

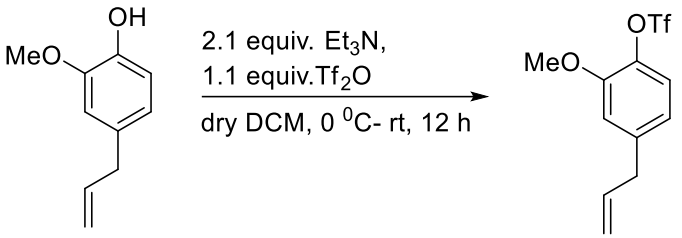
Melting Point: 115-117 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73 (d, J = 6.8 Hz, 1H), 7.98 (d, J = 7.6 Hz, 2H), 7.75 (d, J = 7.2 Hz, 1H), 7.34 – 7.28 (m, 3H), 2.91 (t, J = 7.2 Hz, 2H), 2.77 (t, J = 7.4 Hz, 2H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.6,147.7,142.8, 131.1, 129.3, 128.8, 128.4, 128.1, 123.5, 117.0, 44.5, 30.0, 29.2.

HRMS (ESI) *m/z* calcd for $C_{15}H_{14}N_4O$ $[M+H]^+$ 267.1246, found 267.1238.

Preparation of 4-allyl-2-methoxyphenyl trifluoromethanesulfonate:



9.0 mmol Yield: 86%

To an oven dried 250 mL round-bottomed flask was added the 4-(4-hydroxyphenyl)butan-2-one (1.5 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction

mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (15% ethyl acetate in hexane as eluent) gave 2.3 g (86%) of 4-allyl-2-methoxyphenyl trifluoromethanesulfonateas a colorless oil. Spectral data are in accordance with reported data.[12]

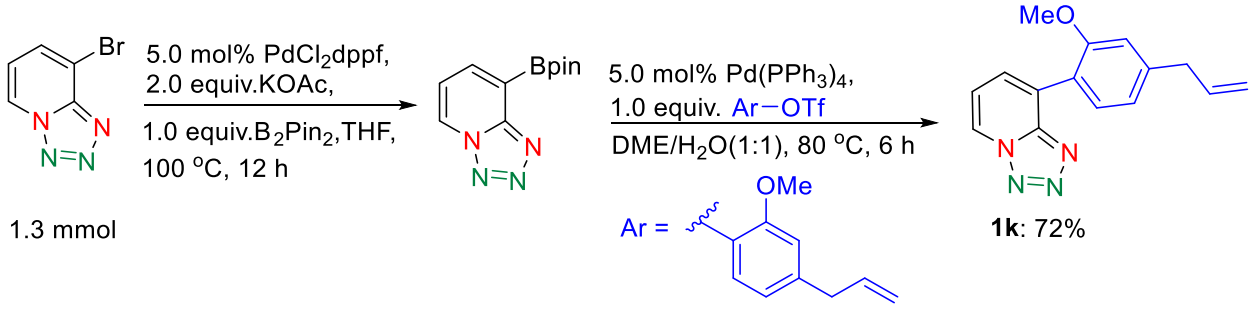
^{1}H NMR (800 MHz, $CDCl_3$): δ 7.14 (d, J = 8.8 Hz, 1H), 6.87 (s, 1H), 6.80 (dd, J = 8.8 Hz, J = 1.6 Hz, 1H), 5.98 – 5.93 (m, 1H), 5.15-5.12 (m, 2H), 3.89 (s, 3H), 3.40 (d, J = 6.4 Hz, 2H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 151.1, 141.8, 137.1, 136.2, 122.1, 120.7, 118.7 (q, J = 318.6 Hz), 116.7, 113.3, 56.0, 39.9.

^{19}F NMR (376 MHz, $CDCl_3$): -73.9.

HRMS (ESI) *m/z* calcd for $C_{11}H_{11}F_3O_4S$ $[M+H]^+$ 297.0408, found 297.0410.

*Preparation of 8-(4-allyl-2-methoxyphenyl)tetrazolo[1,5-a]pyridine (**1k**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 4-allyl-2-methoxyphenyl trifluoromethanesulfonate (296.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and

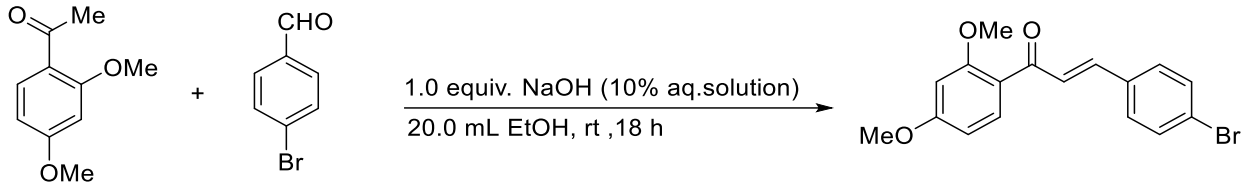
$Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (20% ethyl acetate in hexane as eluent) gave 191.7 mg (72%) of 8-(4-allyl-2-methoxyphenyl)tetrazolo[1,5-a]pyridine (**1k**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (d, J = 6.8 Hz, 1H), 7.81 (d, J = 7.2 Hz, 1H), 7.70 (d, J = 7.6 Hz, 1H), 7.28 – 7.24 (m, 1H), 6.97 (d, J = 8.0 Hz, 1H), 6.90 (s, 1H), 6.05-5.95 (m, 1H), 5.15 (t, J = 10.4 Hz, 2H), 3.82 (s, 3H), 3.47 (d, J = 6.4 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 143.7, 131.6, 131.5, 127.5, 123.5, 121.3, 120.5, 116.8, 116.6, 112.0, 58.8, 40.6.

HRMS (ESI) *m/z* calcd for $C_{15}H_{14}N_4O$ $[M+H]^+$ 267.1246, found 267.1239.

Preparation of (E)-3-(4-bromophenyl)-1-(2,4-dimethoxyphenyl)prop-2-en-1-one:



5.0 mmol 1.0 equiv. yield : 60%

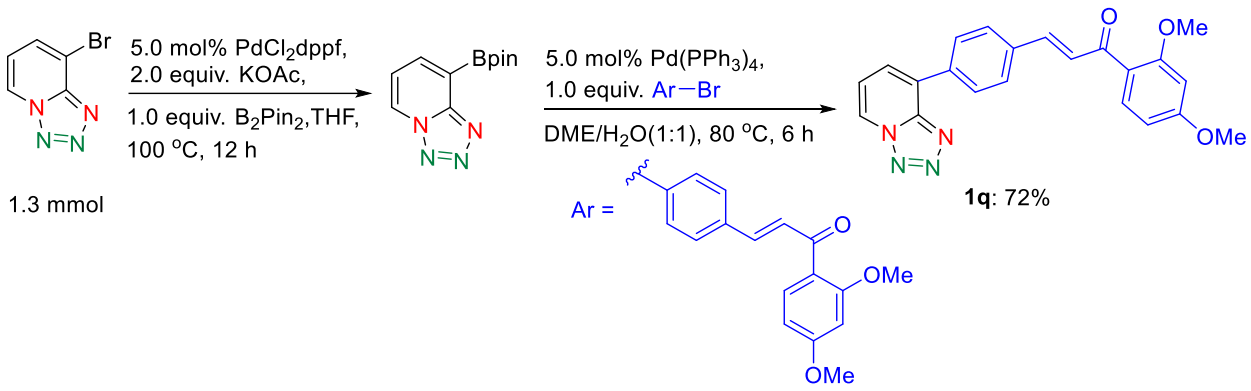
To an oven dried 250 mL round-bottomed flask was added the 1-(2,4-dimethoxyphenyl)ethan-1-one (901 mg, 5.0 mmol), 4-bromo benzaldehyde (926 mg, 1.0 equiv.) and 20 mL ethanol under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, 10% aq. solution of NaOH (1.0 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at room temperature for 18 h. After 18 h, ethanol was evaporated and then crude reaction mixture was worked up using ethyl acetate (200 mL) and water (50 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (15% ethyl acetate in hexane as eluent) gave 1.0 g (60%) of (E)-3-(4-bromophenyl)-1-(2,4-dimethoxyphenyl)prop-2-en-1-one as a white solid. Spectral data are in accordance with reported data.[13]

^{1}H NMR (800 MHz, $CDCl_3$): δ 7.77 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 16.0 Hz, 1H), 7.52 – 7.50 (m, 3H), 7.45 (d, J = 8.0 Hz, 2H), 6.57 (dd, J = 8.8 Hz, J = 2.4 Hz, 1H), 6.49 (d, J = 2.4 Hz, 1H), 3.90 (s, 3H), 3.87 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 190.0, 164.3, 160.5, 140.4, 134.4, 133.0, 132.0, 129.6, 127.7, 124.0, 122.0, 105.2, 98.6, 55.7, 55.5.

HRMS (ESI) *m/z* calcd for $C_{17}H_{15}BrO_3$ $[M+H]^+$ 347.0283, found 347.0281.

*Preparation of (E)-1-(2,4-dimethoxyphenyl)-3-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)prop-2-en-1-one (1**q**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, (*E*)-3-(4-bromophenyl)-1-(2,4-dimethoxyphenyl)prop-2-en-1-one (347.2 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under

reduced pressure and chromatographic separation with neutral silica gel (50% dichloromethane in hexane as eluent) gave 278.2 mg (72%) of (*E*)-1-(2,4-dimethoxyphenyl)-3-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)prop-2-en-1-one (**1q**) as white solid.

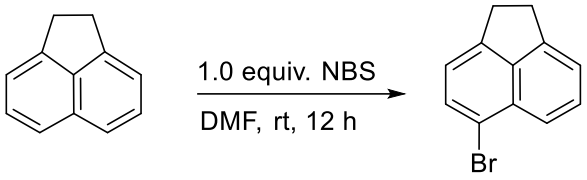
Melting Point: 145-147 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80 (d, J = 6.8 Hz, 1H), 8.19 (d, J = 8.4 Hz, 2H), 7.86 (d, J = 7.2 Hz, 1H), 7.80 – 7.73 (m, 3H), 7.70 – 7.59 (m, 2H), 7.32 (t, J = 7.2 Hz, 1H), 6.57 (d, J = 8.4 Hz, 1H), 6.50 (s, 1H), 3.92 (s, 3H), 3.87 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 190.0, 164.4, 160.5, 147.8, 140.4, 136.9, 134.6, 133.0, 128.9, 128.8, 128.4, 128.4, 124.0, 121.9, 116.9, 105.3, 98.5, 55.7, 55.5.

HRMS (ESI) *m/z* calcd for $C_{22}H_{18}N_4O_3$ $[M+H]^+$ 387.1457, found 387.1449.

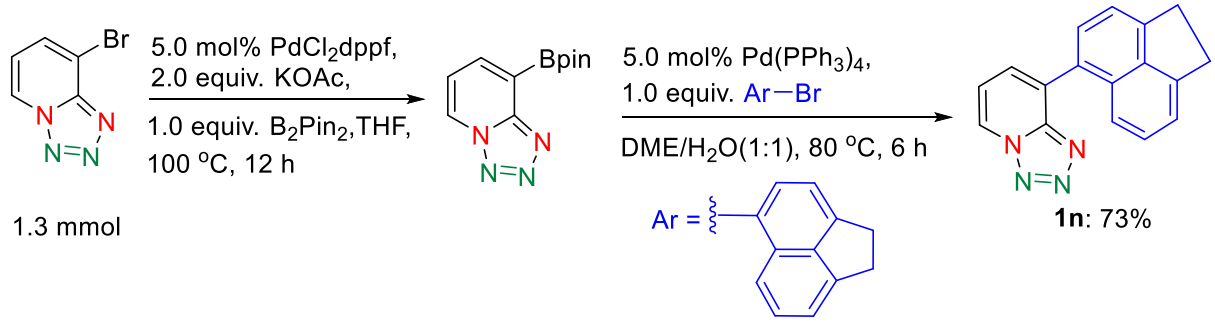
Preparation of 5-bromo-1,2-dihydroacenaphthylene:



Yield: 91%

An oven dried 500 mL round bottom flask was charged with accenaphthene (3.0 g, 19.45 mmol) and DMF (30 mL) were charged in a flask and *N*-bromosuccinimide (3.5 g, 1.0 equiv.) was added in several portions under stirring at room temperature. After further stirring overnight the reaction mixture was added to ice/water and filtered. The resulting solid was dissolved in dichloromethane, dried over sodium sulphate, filtered, and concentrated under reduced pressure to give 5-bromo-1, 2-dihydroacenaphthylene (4.1 g, 91%) as a pale-yellow solid. Spectral data are in accordance to reported literature data.[14]

*Preparation of (8-(1,2-dihydroacenaphthylen-5-yl)tetrazolo[1,5-a]pyridine (1**n**):*



1.3 mmol

1n: 73%

Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 5-bromo-1,2-dihydroacenaphthylene (233.1 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (50% dichloromethane in hexane as eluent) gave 198.8 mg (73%) of 8-(1,2-dihydroacenaphthylen-5-yl)tetrazolo[1,5-a]pyridine (**1n**) as white solid.

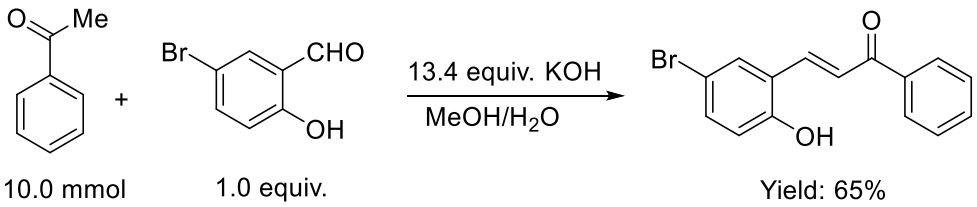
Melting Point: 163-165 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.85 (d, J = 6.8 Hz, 1H), 7.82 (d, J = 7.2 Hz, 2H), 7.51-7.42 (m, 3H), 7.35 (t, J = 6.8 Hz, 2H), 3.47 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 148.4, 146.6, 139.6, 131.4, 130.3, 129.3, 129.2, 128.8, 126.7, 123.8, 119.9, 119.7, 119.1, 116.7, 30.4, 30.2.

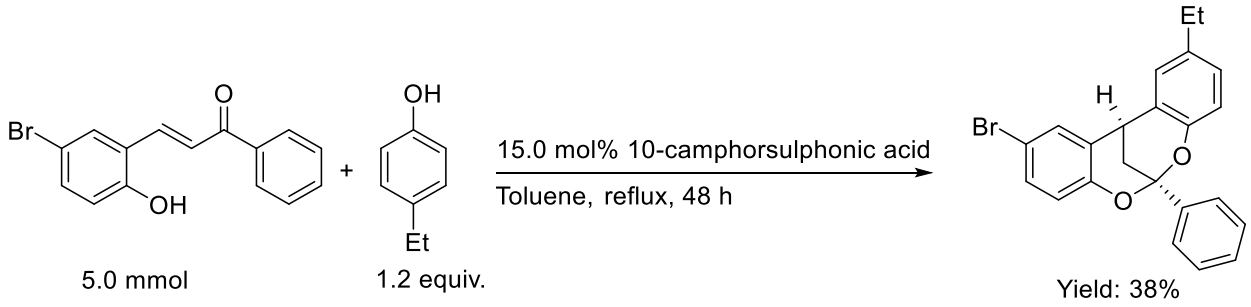
HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_4$ $[M+H]^+$ 273.1140, found 273.1135.

Preparation of (E)-3-(5-bromo-2-hydroxyphenyl)-1-phenylprop-2-en-1-one:



In an oven dried 100 mL round-bottom flask equipped with a magnetic stir bar in ice bath were added potassium hydroxide (7.5 g, 13.4 equiv.), water (1.3 mL), and methanol (6.3 mL). Then, acetophenone (1.2 mL, 10 mmol, 1.0 equiv.) was added and the reaction was stirred for 10 min. After that, 5-Bromosalicylaldehyde (2.01 g, 1.0 equiv.) was then added. The reaction mixture was then removed from ice bath and stirred for overnight. Upon completion, the dark red mixture was acidified with 3(M) HCl until pH ~ 2. The resulting yellow mixture was extracted with dichloromethane (3 x 20 mL). The combinedorganic layer was dried over sodium sulphate and concentrated in vacuo. Chromatographic separation with silica gel (10 - 40% ethyl acetate in hexane as eluent) yielded 1.97 g (65%) of (*E*)-3-(5-bromo-2-hydroxyphenyl)-1-phenylprop-2-en-1-one as yellow powder. Spectral data are in accordance to reported literature data.[15]

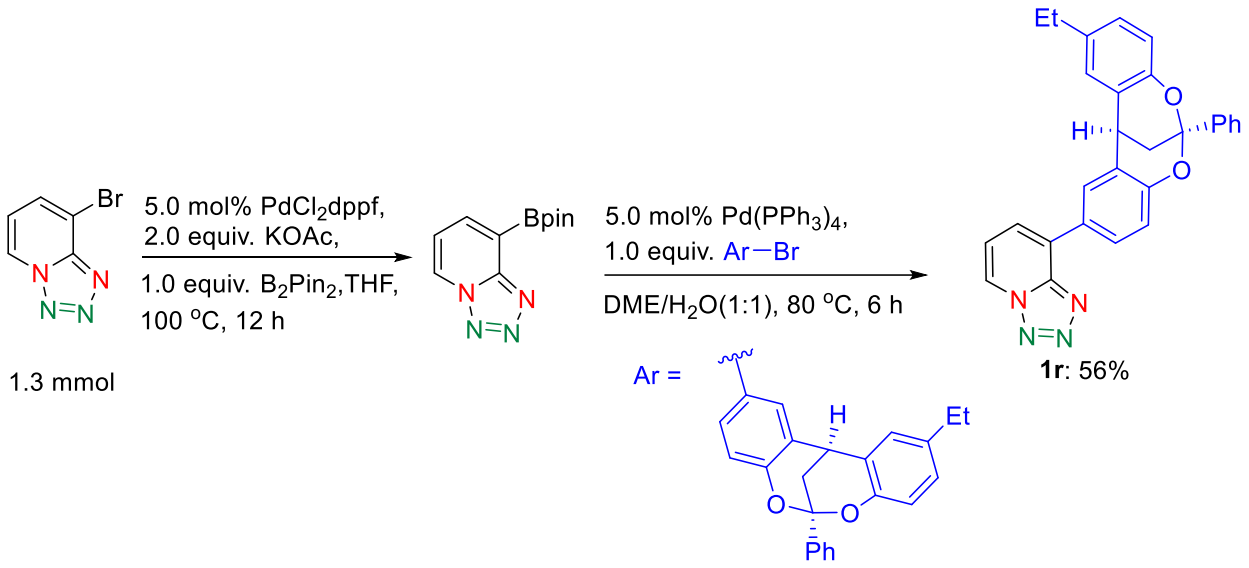
Preparation of 2-bromo-10-ethyl-6-phenyl-cis-12H-6,12-methanodibenzo[d,g][1,3]dioxocine [(±)]:



5.0 mmol 1.2 equiv. Yield: 38%

In a 100 mLseal tube were added (*E*)-3-(5-bromo-2-hydroxyphenyl)-1-phenylprop-2-en-1-one (1.5 g, 5.0 mmol), 4-ethylphenol (733 mg, 1.2 equiv.), DL-10-camphorsulfonic acid (174 mg, 15.0 mol%) and toluene (63 mL). The seal tube was capped tightly and refluxed for 48 h. The resulting dark green mixture was condensed via rotary evaporation. Purification by silica gel eluting with 0%→10% EtOAc/hexanes yielded the product as a light-yellow powder (772 mg, 38% yield). Spectral data are in accordance to reported literature data. [16]

*Preparation of 8-((6R,12R)-10-ethyl-6-phenyl-12H-6,12-methanodibenzo[d,g][1,3]dioxocin-2-yl)tetrazolo[1,5-a]pyridine(1**r**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, (6R,12R)-2-bromo-10-ethyl-6-phenyl-12H-6,12-methanodibenzo[d,g][1,3]dioxocine(407.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 °C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel

(30% ethyl acetate in hexane as eluent) gave 250.0 mg (56%) of 8-((6R,12R)-10-ethyl-6-phenyl-12H-6,12-methanodibenzo[d,g][1,3]dioxocin-2-yl)tetrazolo[1,5-a]pyridine (**1r**) as white solid.

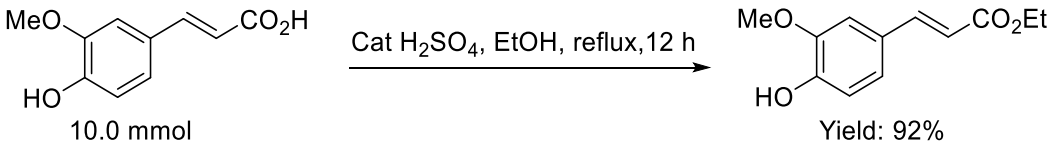
Melting Point: 184-186 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (d, J = 6.8 Hz, 1H), 8.27 (d, J = 2.0 Hz, 1H), 7.82 – 7.73 (m, 4H), 7.51 – 7.42 (m, 3H), 7.27 (d, J = 6.8 Hz, 1H), 7.20 – 7.14 (m, 2H), 7.02 – 6.96 (m, 2H), 4.27 (s, 1H), 2.56 (q, J = 7.6 Hz, 2H), 2.47 (d, J = 2.8 Hz, 2H), 1.19 (t, J = 7.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 153.7, 149.6, 148.0, 141.0, 137.6, 129.3, 128.9, 128.4, 128.0, 127.7, 127.4, 127.3, 126.7, 126.6, 125.7, 125.5, 123.1, 117.5, 117.0, 116.6, 99.0, 34.2, 33.2, 28.0, 15.8.

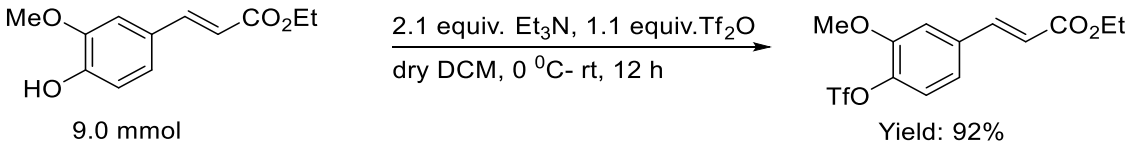
HRMS (ESI) *m/z*calcd for $C_{28}H_{22}N_4O_2$ $[M+H]^+$ 447.1821, found 447.1821.

Preparation of ethyl (E)-3-(4-hydroxy-3-methoxyphenyl)acrylate:



In a 100 mL seal tube were added Ferulic acid (1.94 g, 10.0 mmol), EtOH (15.0 mL) and catalytic amount of conc H_2SO_4.Then seal tube was capped tightly and refluxed for 12 h. After completion of the reaction, ethanol was removed under vacuum and the compound was extracted with dichloromethane (100 mL x 3). Organic layer was washed with aq. $NaHCO_3$ solution, water and dried over anhydrous sodium sulfate. The solvent was evaporated under vacuum to give the pure 2.0 g (92%) ethyl *(E)*-3-(4-hydroxy-3-methoxyphenyl) as white crystal. Spectral data are in accordance to reported literature data. [17]

Preparation of ethyl (E)-3-(3-methoxy-4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acrylate:



To an oven dried 250 mL round-bottomed flask was added the ethyl (*E*)-3-(4-hydroxy-3-methoxyphenyl)acrylate (2.0 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12

hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (15% ethyl acetate in hexane as eluent) gave 2.9 g (92%) of ethyl (*E*)-3-(3-methoxy-4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acrylateas a brown solid.

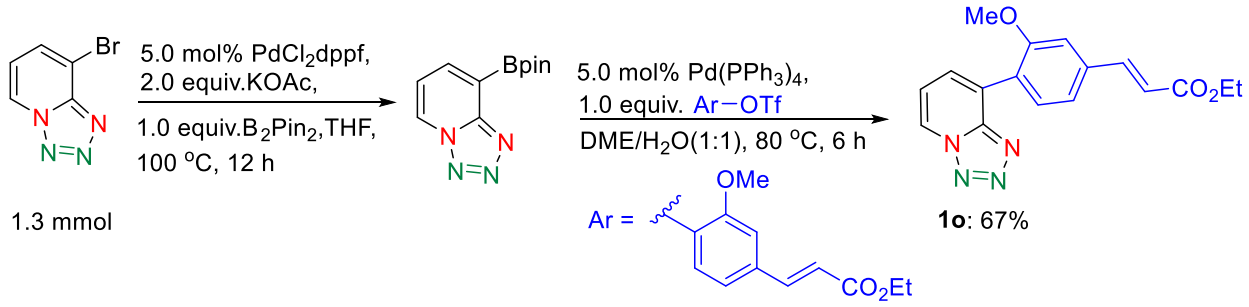
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, J = 16.0 Hz, 1H), 7.22 (d, J = 8.4 Hz, 1H), 7.12 (dd, J = 10.9 Hz, J = 2.4 Hz, 2H), 6.41 (d, J = 16.0 Hz, 1H), 4.27 (q, J = 7.2 Hz, 2H), 3.94 (s, 3H), 1.33 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.3, 151.6, 142.6, 139.6, 135.7, 123.5, 122.8, 120.8, 120.2, 117.1, 113.9, 60.7, 56.2, 14.2.

^{19}F NMR (376 MHz, $CDCl_3$): -73.8.

HRMS (ESI) *m/z* calcd for $C_{13}H_{13}F_3O_6S$ $[M+H]^+$355.0463, found 355.0477.

*Preparation of ethyl (E)-3-(3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acrylate (**1o**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, ethyl (*E*)-3-(3-methoxy-4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acrylate (354.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0

equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (20% ethyl acetate in hexane as eluent) gave 217.3 mg (67%) of ethyl (*E*)-3-(3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acrylate(**1o**) as white solid.

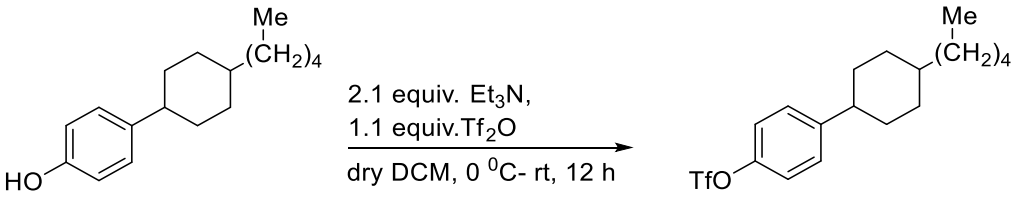
Melting Point: 95-97 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (d, J = 6.8 Hz, 1H), 7.86 (d, J = 7.2 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 16.0 Hz, 1H), 7.30-7.27 (m, 2H), 7.18 (s, 1H), 6.50 (d, J = 16.0 Hz, 1H), 4.28 (q, J = 7.2 Hz, 2H), 3.86 (s, 3H), 1.35 (t, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.7, 157.1, 148.3, 143.7, 137.0, 131.8, 126.4, 124.3, 123.9, 120.8, 119.5, 116.6, 110.5, 60.6, 55.7, 14.3.

HRMS (ESI) *m/z* calcd for $C_{17}H_{16}N_4O_3$ $[M+H]^+$ 325.1301, found 325.1295.

Preparation of 4-(4-pentylcyclohexyl)phenyl trifluoromethanesulfonate:

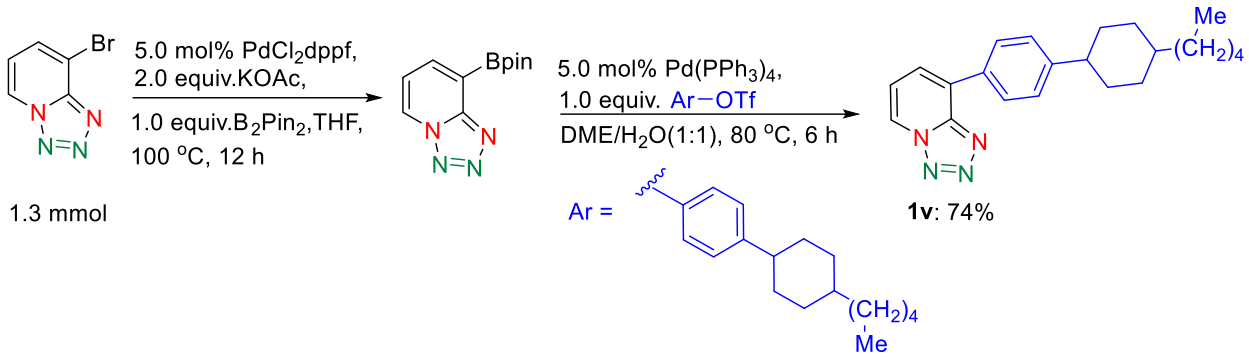


9.0 mmol

Yield: 73%

To an oven dried 250 mL round-bottomed flask was added the 4-(4-pentylcyclohexyl)phenol (2.2 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (5.0% ethyl acetate in hexane as eluent) gave 2.5g (73%) of 4-(4-pentylcyclohexyl)phenyl trifluoromethanesulfonate as a colorless solid. Spectral data are in accordance with reported data.[18]

*Preparation of 8-(4-(4-pentylcyclohexyl)phenyl)tetrazolo[1,5-a]pyridine (**1v**):*



Step I: In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 4-(4-pentylcyclohexyl)phenyl trifluoromethanesulfonate (378.5 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ° C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (20% ethyl acetate in hexane as eluent) gave 257.9 mg (74%) of 8-(4-(4-pentylcyclohexyl)phenyl)tetrazolo[1,5-a]pyridine (**1v**) as white solid.

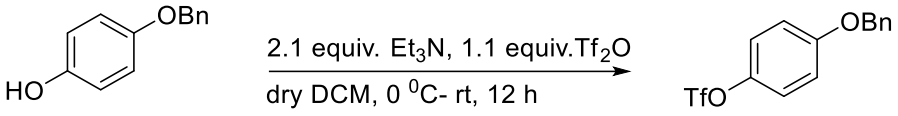
Melting Point: 139-141 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (d, J = 6.8 Hz, 1H), 8.05 (d, J = 8.0 Hz, 2H), 7.79 (d, J = 6.8 Hz, 1H), 7.39 (d, J = 8.0 Hz, 2H), 7.28 (t, J = 7.2 Hz, 1H), 2.55 (t, J = 12.0 Hz, 1H), 1.91 (t, J = 13.6 Hz, 4H), 1.54 – 1.45 (m, 2H), 1.35 -1.24 (m, 9H), 1.09 (t, J = 12.4 Hz, 2H), 0.90 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 149.9, 148.0, 130.9, 129.9, 128.4, 127.8, 127.6, 123.3, 116.9, 44.5, 37.3, 37.2, 34.1, 33.5, 32.2, 26.6, 22.7, 14.1.

HRMS (ESI) *m/z*calcd for $C_{22}H_{28}N_4$ $[M+H]^+$ 349.2392, found 349.2387.

Preparation of 4-(benzyloxy)phenyl trifluoromethanesulfonate:



9.0 mmol Yield: 93%

To an oven dried 250 mL round-bottomed flask was added the 4-(benzyloxy)phenol(1.8 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (5.0% ethyl acetate in hexane as eluent) gave 2.8 g (93%) of 4-(benzyloxy)phenyl trifluoromethanesulfonate as white solid.

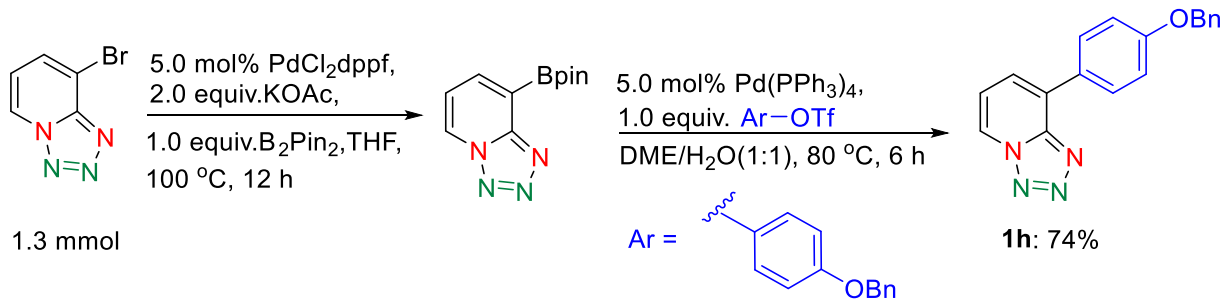
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 – 7.34 (m, 5H), 7.20 (d, J = 9.2 Hz, 2H), 7.01 (d, J = 9.2 Hz, 2H), 5.07 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 158.2, 143.1, 136.1, 128.7, 128.3, 127.5, 122.4, 120.3, 117.1, 115.9, 70.5.

^{19}F NMR (376 MHz, $CDCl_3$): -72.7.

HRMS (ESI) *m/z*calcd for $C_{14}H_{11}F_3O_4S$ $[M+H]^+$ 333.0408, found 333.0403.

*Preparation of 8-(4-(benzyloxy)phenyl)tetrazolo[1,5-a]pyridine (**1h**):*



1.3 mmol **1h**: 74%

Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 4-(benzyloxy)phenyl trifluoromethanesulfonate (332.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (20% ethyl acetate in hexane as eluent) gave 223.7 mg (74%) of 8-(4-(benzyloxy)phenyl)tetrazolo[1,5-a]pyridine(**1h**) as white solid.

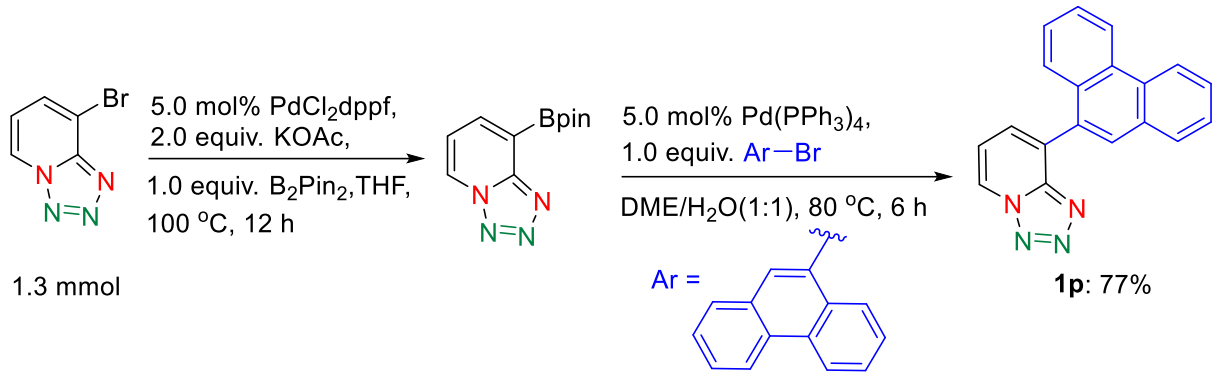
Melting Point: 161-163 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (d, J = 6.8 Hz, 1H), 8.11 (d, J = 8.8 Hz, 2H), 7.73 (d, J = 7.2 Hz, 1H), 7.43 (d, J = 7.6 Hz, 2H), 7.41 – 7.31 (m, 3H), 7.23 (d, J = 6.4 Hz, 1H), 7.12 (d, J = 8.8 Hz, 2H), 5.13 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.1, 147.9, 136.5, 129.9, 129.4, 128.6, 128.1, 127.5, 127.1, 126.1, 123.0, 116.9, 115.4, 70.1.

HRMS (ESI) *m/z*calcd for $C_{18}H_{14}N_4O$ $[M+H]^+$ 303.1246, found 303.1239.

*Preparation of 8-(phenanthren-9-yl)tetrazolo[1,5-a]pyridine (1**p**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 9-bromophenanthrene (257.1 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ° C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (70% dichloromethane in hexane as eluent) gave 228.2 mg (77%) of 8-(phenanthren-9-yl)tetrazolo[1,5-a]pyridine (**1p**) as white solid.

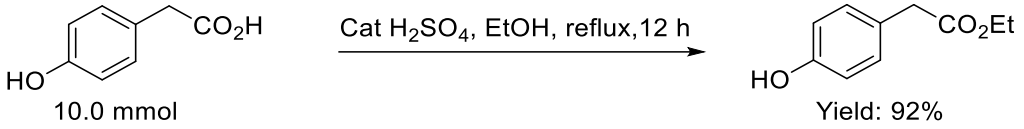
Melting Point: 197-199 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.92 (d, J = 6.8 Hz, 1H), 8.78 (dd, J = 22.8 Hz, J = 8.4 Hz, 2H), 7.97 – 7.89 (m, 2H), 7.80 – 7.60 (m, 5H), 7.51 (t, J = 7.6 Hz, 1H), 7.38 (t, J = 6.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 149.0, 132.3, 130.9, 130.8,130.8, 130.3,129.8, 129.6, 129.1,127.7, 127.1,126.9, 125.8, 124.5, 123.2, 122.6, 116.7.

HRMS (ESI) *m/z* calcd for $C_{19}H_{12}N_4$ $[M+H]^+$ 297.1140, found 297.1136.

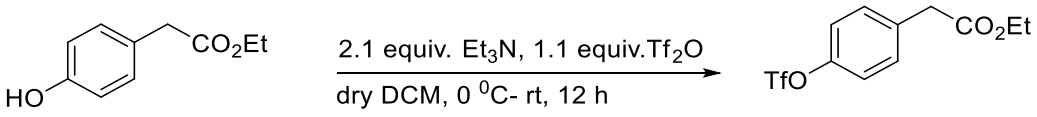
Preparation of ethyl 2-(4-hydroxyphenyl)acetate:



10.0 mmol Yield: 92%

In a 100 mL seal tube were added 2-(4-hydroxyphenyl) acetic acid (1.52 g, 10.0 mmol), EtOH (15.0 mL) and catalytic amount of conc H_2SO_4.Then, seal tube was capped tightly and refluxed for 12 h. After completion of the reaction, ethanol was removed under vacuum and the compound was extracted with dichloromethane (100 mL x 3). Organic layer was washed with aq. $NaHCO_3$ solution, water and dried over anhydrous sodium sulfate. The solvent was evaporated under vacuum to give the pure 1.6 g (92%) ethyl 2-(4-hydroxyphenyl) acetate as brown liquid. Spectral data are in accordance with reported data.[19]

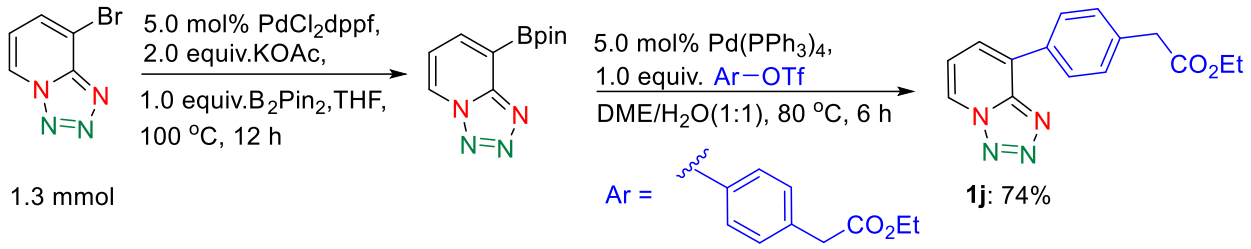
Preparation of ethyl 2-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acetate:



9.0 mmol Yield: 83%

To an oven dried 250 mL round-bottomed flask was added the ethyl 2-(4-hydroxyphenyl)acetate (1.6 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (5.0% ethyl acetate in hexane as eluent) gave 2.3 g (83%) of ethyl 2-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acetate as white solid. Spectral data are in accordance with reported data. [20]

*Preparation of ethyl 2-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetate (**1j**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

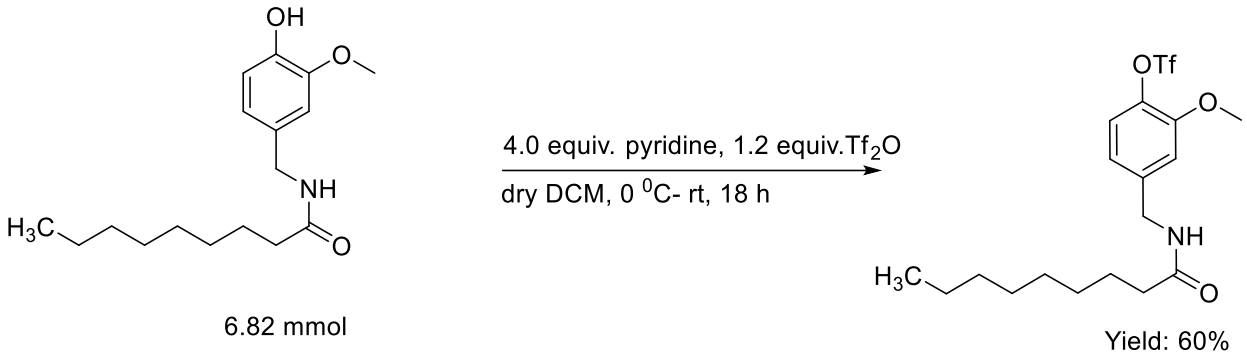
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, ethyl 2-(4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acetate (312.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 208.9 mg (74%) of ethyl 2-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetate (**1j**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (d, J = 6.8 Hz, 1H), 8.02 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 7.2 Hz, 1H), 7.39 (d, J = 8.4 Hz, 2H), 7.24 (t, J = 6.8 Hz, 1H), 4.11 (q, J = 7.2 Hz, 2H), 3.63 (s, 2H), 1.20 (t, J = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.0, 147.8, 135.8, 132.1, 129.8, 129.2, 128.5, 128.3, 123.7, 116.9, 60.9, 41.0, 14.1.

HRMS (ESI) *m/z* calcd for $C_{15}H_{14}N_4O_2$ $[M+H]^+$ 283.1195, found 283.1190.

Preparation of 2-methoxy-4-(nonanamidomethyl)phenyl trifluoromethanesulfonate:



To an oven dried 250 mL round-bottomed flask was added the N-(4-hydroxy-3-methoxybenzyl)nonanamide (2.0 g, 6.82 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, pyridine (2.2 mL, 4.0 equiv.) was added at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.4 mL, 1.2 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) and 20 mL 2(N) HCl was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (30.0% ethyl acetate in hexane as eluent) gave 1.7 g (60%) of 2-methoxy-4-(nonanamidomethyl)phenyl trifluoromethanesulfonate as white solid.

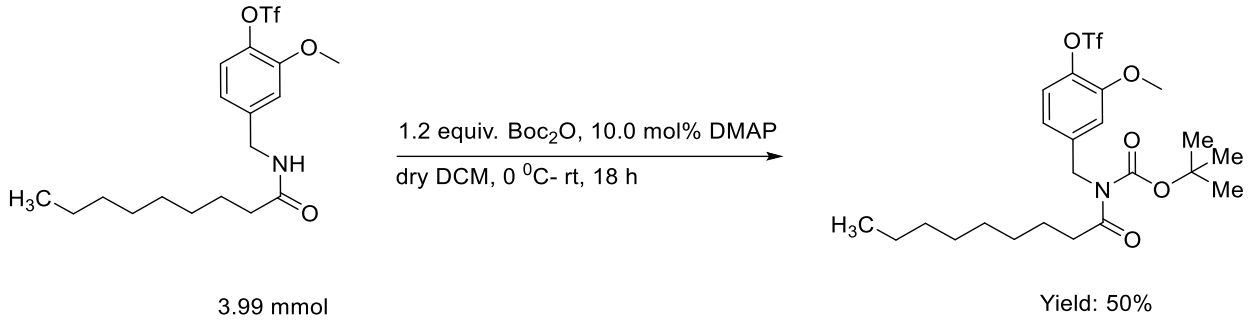
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.13 (d, J = 8.4 Hz, 1H), 6.94 (s, 1H), 6.84 (d, J = 8.0 Hz, 1H), 6.08 (s, 1H), 4.39 (d, J = 5.6 Hz, 2H), 3.87 (s, 3H), 2.21 (t, J = 7.6 Hz, 2H), 1.65-1.60 (m, 2H), 1.28-1.24 (dd, J = 9.8, 5.1 Hz, 10H), 0.86 (t, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 173.2, 151.4, 140.4, 137.8, 122.4, 119.7, 118.6 (q, J= 318.6 Hz), 112.5, 56.1, 42.9, 36.6, 21.7, 29.3, 29.2, 29.1, 25.7, 22.6, 14.0.

^{19}F NMR (376 MHz, $CDCl_3$): -73.9.

HRMS (ESI) *m/z* calcd for $C_{18}H_{26}F_3NO_5S$ $[M+H]^+$ 426.1562, found 426.1564.

Preparation of 4-((N-(tert-butoxycarbonyl)nonanamido)methyl)-2-methoxyphenyl trifluoromethanesulfonate:



3.99 mmol

Yield: 50%

To an oven dried 250 mL round-bottomed flask was added the 2-methoxy-4-(nonanamidomethyl)phenyl trifluoromethanesulfonate (1.7 g, 3.99 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, DMAP (48.7 mg, 10.0 mol%) was added at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, Boc_2O (1.0 g, 1.2 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 18 hours. After 18 h, water (50 mL) was added and the reaction mixture was extracted with ethyl aceatate (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (10.0% ethyl acetate in hexane as eluent) gave 1.0 g (50%) of 4-((N-(tert-butoxycarbonyl)nonanamido)methyl)-2-methoxyphenyl trifluoromethanesulfonate as colorless liquid.

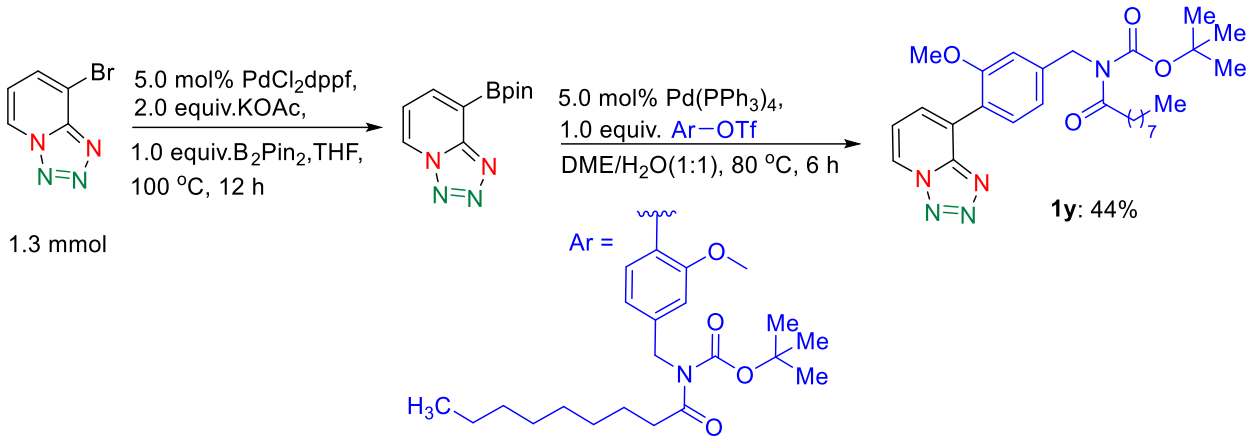
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.13 (d, J = 8.3 Hz, 1H), 6.97 (s, 1H), 6.87 (d, J = 8.4 Hz, 1H), 4.86 (s, 2H), 3.88 (s, 3H), 2.89 (t, J = 7.2 Hz, 2H), 1.64 (dd, J = 14.6 Hz, J = 6.8 Hz, 2H), 1.45 (s, 9H), 1.28 (d, J = 14.0 Hz, 10H), 0.87 (t, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 176.3, 152.8, 151.2, 140.1, 137.7, 120.1, 112.7, 83.6, 56.1, 47.0, 38.4, 31.8, 29.4, 29.2, 29.1, 27.9, 25.2, 22.6, 14.1.

^{19}F NMR (376 MHz, $CDCl_3$): -73.9.

HRMS (ESI) *m/z* calcd for $C_{23}H_{34}F_3NO_7S$ $[M+H]^+$ 525.2008, found 525.2001.

*Preparation of tert-butyl (3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)benzyl)(propionyl)carbamate (**1y**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

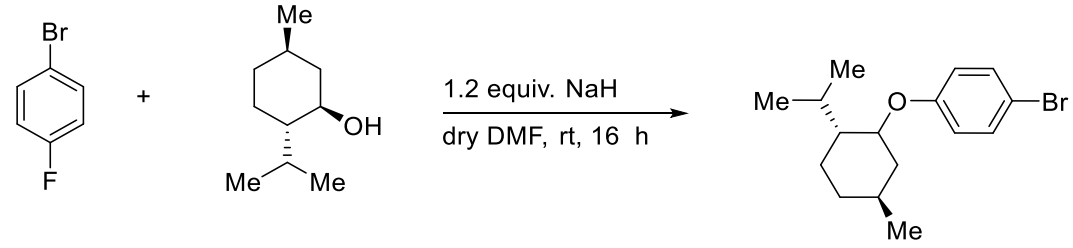
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 4-((N-(tert-butoxycarbonyl)nonanamido)methyl)-2-methoxyphenyl trifluoromethanesulfonate (525.6 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 °C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 218.1 mg (44%) of tert-butyl (3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)benzyl)(propionyl)carbamate (**1y**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73 (d, J = 6.8 Hz, 1H), 7.78 (d, J = 6.8 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.24 (t, J = 6.8 Hz, 1H), 7.00 (d, J = 8.8 Hz, 2H), 4.91 (s, 2H), 3.77 (s, 3H), 2.88 (t, J = 7.6 Hz, 2H), 1.65-1.60 (m, 2H), 1.47 (s, 9H), 1.28-1.22 (m, 10H), 0.82 (d, J = 6.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 176.1, 156.7, 152.9, 148.3, 141.5, 131.6, 131.1, 126.9, 123.4, 121.3, 120.0, 116.5, 111.0, 83.3, 55.5, 47.2, 38.3, 31.7, 29.3, 29.1, 29.0, 27.9, 25.1, 22.5, 13.9.

HRMS (ESI) *m/z*calcd for $C_{27}H_{37}N_5O_4$ $[M+H]^+$ 496.2924, found 496.2918.

Preparation of 1-bromo-4-(((2R,5S)-2-isopropyl-5-methylcyclohexyl)oxy)benzene:



10.0 mmol 1.1 equiv. Yield: 71%

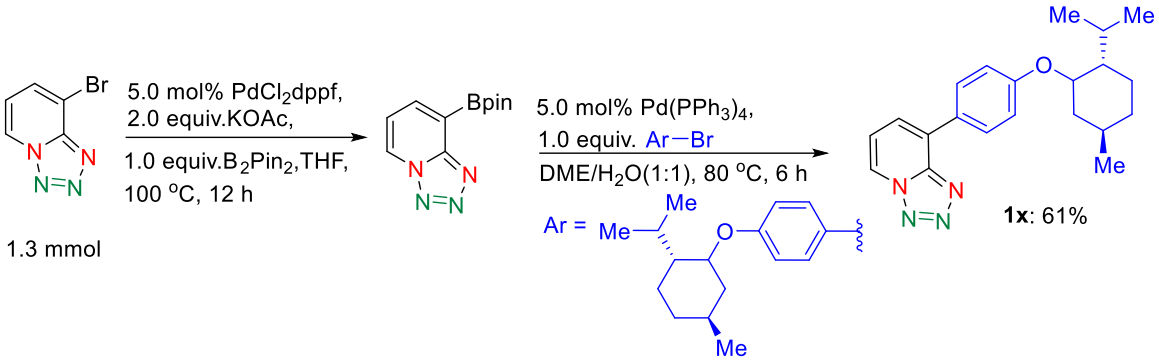
To a 100 mL oven dried round bottom flask with a stir bar were added L-menthol (1.7 g, 1.1 equiv), dry DMF (20 mL) and sodium hydride (0.48 g of a 60% w/w dispersion in mineral oil, 1.2 equiv), and the reaction was stirred at r.t. for 30 min. After that, 1-Bromo-4-fluorobenzene (1.1 mL, 1.0 equiv) was added and the reaction was stirred at r.t. for 16 h. After completion (judged by TLC), the reaction mixture was quenched with sat. aq. NH_4Cl solution and extracted with EtOAc (100 mL×3). The organic fractions were combined, washed with brine (100 mL×1), dried over Na_2SO_4, and concentrated. The crude residue was purified by flash column chromatography (eluent 0–5% ethyl acetate/hexanes) to yield the product 1-bromo-4-(((2R,5S)-2-isopropyl-5-methylcyclohexyl)oxy)benzene as a colourless oil (2.2 g, 71%). Spectral data are in accordance with reported data.[21]

^{1}H NMR (800 MHz, $CDCl_3$): δ 7.35 (d, J = 9.6 Hz, 2H), 6.78 (d, J = 8.8 Hz, 2H), 3.97 (td, J = 10.4 Hz, J = 4.0 Hz, 1H), 2.19-2.16 (m, 1H), 2.11 (d, J = 12.0 Hz, 1H), 1.72 (d, J = 12.0 Hz, 2H), 1.52 – 1.44 (m, 2H), 1.11 – 1.07 (m, 1H), 1.00 (dd, J = 23.2, 12.0 Hz, 1H), 0.94 – 0.92 (m, 7H), 0.76 (d, J = 7.2 Hz, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 157.5, 132.3, 117.5, 112.3, 77.9, 48.0, 40.1, 34.4, 31.4, 26.0, 23.7, 22.1, 20.7, 16.5.

HRMS (ESI) *m/z* calcd for $C_{16}H_{23}BrO$ $[M+H]^+$ 311.1011, found 311.1012.

*Preparation of 8-(4-(((2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)phenyl)tetrazolo[1,5-a]pyridine (**1x**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 1-bromo-4-(((2R,5S)-2-isopropyl-5-methylcyclohexyl)oxy)benzene (311.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 213.8 mg (61%) of 8-(4-(((2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)phenyl)tetrazolo[1,5-a]pyridine (**1x**) as white solid.

Melting Point: 130-132 ^{o}C

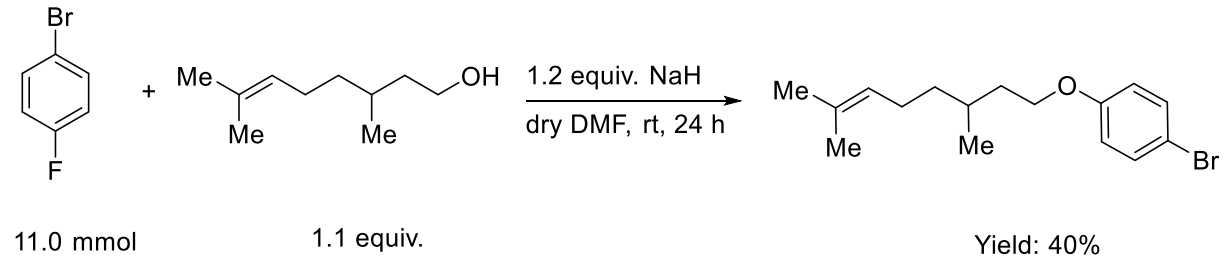
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (d, J = 6.4 Hz, 1H), 8.10 (d, J = 8.8 Hz, 2H), 7.75 (d, J = 6.8 Hz, 1H), 7.27 (t, J = 6.8 Hz, 1H), 7.07 (d, J = 8.8 Hz, 2H), 4.18 - 4.12 (m, 1H), 2.29 – 2.19 (m,

2H), 1.75 (d, J = 11.2 Hz, 2H), 1.59-1.51 (m, 2H), 1.14-0.97 (m, 3H), 0.94 (d, J = 6.8 Hz, 6H), 0.79 (d, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.8, 147.9, 129.9, 129.6, 126.9, 125.4, 122.8, 117.0, 115.9, 47.9, 40.1, 34.4, 31.3, 26.1, 23.7, 22.1, 20.6, 16.6.

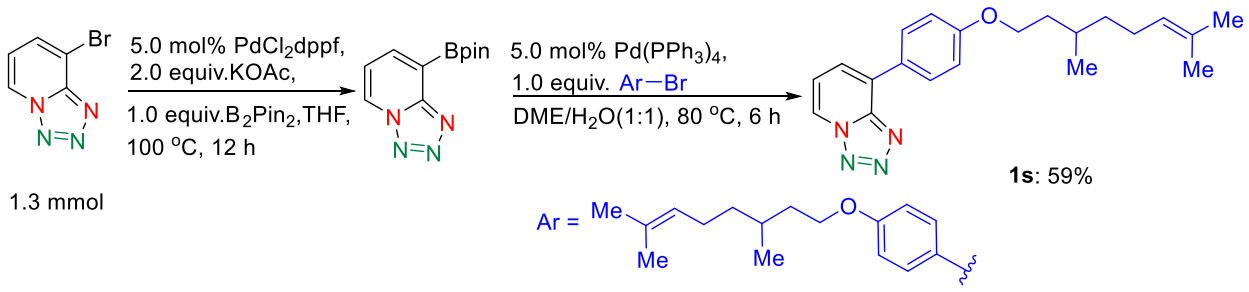
HRMS (ESI) *m/z* calcd for $C_{21}H_{26}N_4O$ $[M+H]^+$ 351.2185, found 351.2179.

Preparation of 1-bromo-4-((3,7-dimethyloct-6-en-1-yl)oxy)benzene:



To a 100 mL oven dried round bottom flask with a stir bar were added citronellol (2.0 mL, 1.1 equiv), dry DMF (20 mL) and sodium hydride (0.48 g of a 60% w/w dispersion in mineral oil, 1.2 equiv), and the reaction was stirred at r.t. for 30 min. After that, 1-Bromo-4-fluorobenzene (1.1 mL, 1.0 equiv) was added and the reaction was stirred at r.t. for 23 h 30 min. After completion (judged by TLC), the reaction mixture was quenched with sat. aq. NH_4Cl solution and extracted with EtOAc (100 mL×3). The organic fractions were combined, washed with brine (100 mL×1), dried over Na_2SO_4, and concentrated. The crude residue was purified by flash column chromatography (eluent 0-2% ethyl acetate/hexanes) to yield the product 1-bromo-4-((3,7-dimethyloct-6-en-1-yl)oxy)benzene as a colourless oil (1.2 g, 40%). Spectral data are in accordance with reported data.[21]

*Preparation of 8-(4-((3,7-dimethyloct-6-en-1-yl)oxy)phenyl)tetrazolo[1,5-a]pyridine (**1s**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-

bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 1-bromo-4-((3,7-dimethyloct-6-en-1-yl)oxy)benzene (311.3 mg, 1.0 equiv.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 206.8 mg (59%) of 8-(4-((3,7-dimethyloct-6-en-1-yl)oxy)phenyl)tetrazolo[1,5-a]pyridine (**1s**) as white solid.

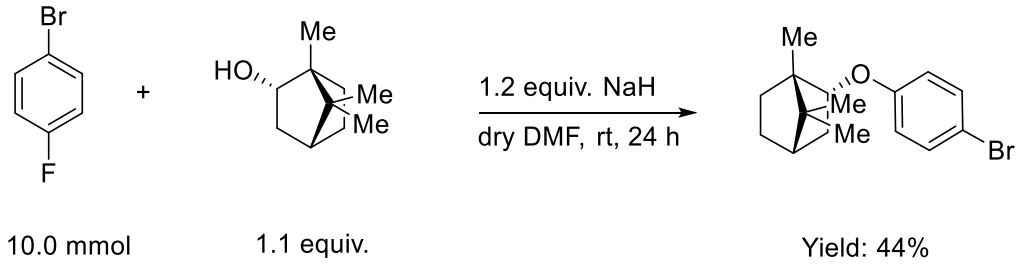
Melting Point: 59-61 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73 (d, J = 6.8 Hz, 1H), 8.12 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 8.0 Hz, 1H), 7.28 (t, J = 7.2 Hz, 1H), 7.06 (d, J = 8.8 Hz, 2H), 5.11 (t, J = 6.8 Hz, 1H), 4.12-4.08 (m, , 2H), 2.07-1.98 (m, 2H), 1.90-1.84 (dt, J = 12.7, 6.4 Hz, 1H), 1.75 – 1.67 (m, 4H), 1.62 (s, 3H), 1.47 – 1.38 (m, 1H), 1.28 – 1.21 (m, 1H), 0.97 (d, J = 6.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.4, 147.9, 131.3, 129.9, 129.5, 126.9, 125.6, 124.6, 122.9,117.0, 115.0, 66.4, 37.1, 36.0, 29.5, 25.7, 25.4, 19.5, 17.6.

HRMS (ESI) *m/z*calcd for $C_{21}H_{26}N_4O$ $[M+H]^+$ 351.2185, found 351.2177.

Preparation of (1S,2R,4S)-2-(4-bromophenoxy)-1,7,7-trimethylbicyclo[2.2.1]heptane:



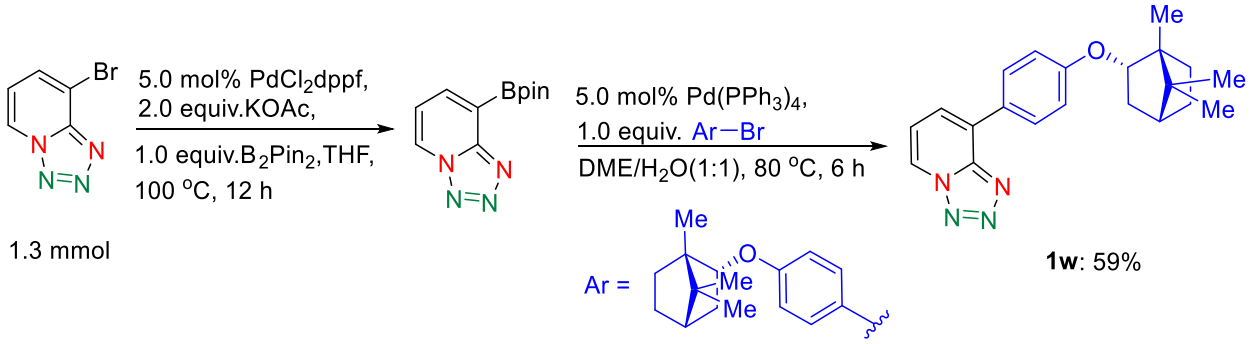
To a 100 mL oven dried round bottom flask with a stir bar were added borneol (1.7 g, 1.1 equiv), dry DMF (20 mL) and sodium hydride (0.48 g of a 60% w/w dispersion in mineral oil, 1.2 equiv), and the reaction was stirred at r.t. for 30 min. After that, 1-Bromo-4-fluorobenzene (1.1 mL, 1.0 equiv) was added and the reaction was stirred at r.t. for 23 h 30 min. After completion (judged by TLC), the reaction mixture was quenched with sat. aq. NH_4Cl solution and extracted with EtOAc (100 mL×3). The organic fractions were combined, washed with brine (100 mL×1), dried over Na_2SO_4, and concentrated. The crude residue was purified by flash column chromatography (eluent 0-2% ethyl acetate/hexanes) to yield the product (1S,2R,4S)-2-(4-bromophenoxy)-1,7,7-trimethylbicyclo[2.2.1]heptane as a colourless oil (1.4 g, 44%)**.**

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.32 (m, 2H), 6.74-6.71 (m, 2H), 4.29-4.26 (m, 1H), 2.38-2.31 (m, 1H), 2.24-2.17 (m, 1H), 1.80 – 1.74 (m, 2H), 1.36-1.30 (m, 2H), 1.08 (dd, J = 13.2 Hz, J = 3.2 Hz, 2H), 0.94 (s, 3H), 0.92 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 158.2, 132.1, 171.2, 83.1, 49.5, 47.6, 45.1, 36.6, 27.9, 26.7, 19.7, 18.9, 13.7.

HRMS (ESI) *m/z* calcd for $C_{16}H_{21}BrO$ $[M+H]^+$ 309.0854, found 309.0844.

*Preparation of 8-(4-(((1R,2S,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)phenyl)tetrazolo[1,5-a]pyridine (**1w**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

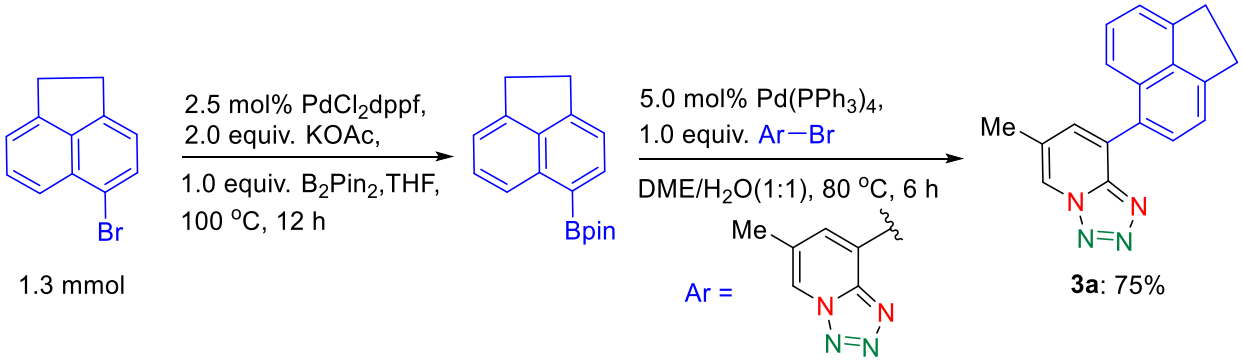
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, (1S,2R,4S)-2-(4-bromophenoxy)-1,7,7-trimethylbicyclo[2.2.1]heptane (309.2 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 205.6 mg (59%) of 8-(4-(((1R,2S,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)phenyl)tetrazolo[1,5-a]pyridine (**1w**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.70 (d, J = 6.8 Hz, 1H), 8.08 (d, J = 8.8 Hz, 2H), 7.72 (d, J = 7.2 Hz, 1H), 7.25 – 7.22 (m, 1H), 6.98 (d, J = 8.8 Hz, 2H), 4.39 (d, J = 8.8 Hz, 1H), 2.44-2.36 (m, 1H), 2.28 – 2.19 (m, 1H), 1.78 – 1.73 (m, 2H), 1.37-1.31 (m, 1H), 1.28-1.22 (m, 1H), 1.12 (dd, J = 13.2 Hz, J = 3.2 Hz, 1H), 0.95 – 0.91(m, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.6, 148.0, 129.8, 129.7, 126.8, 125.2, 122.8, 117.0, 115.9, 83.1, 49.5, 47.6, 45.1, 36.8, 27.9, 26.75, 19.7, 19.0, 13.7.

HRMS (ESI) *m/z*calcd for $C_{21}H_{24}N_4O$ $[M+H]^+$ 349.2028, found 349.2023.

*Preparation of 8-(1,2-dihydroacenaphthylen-5-yl)-6-methyltetrazolo[1,5-a]pyridine (**3a**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (23.7 mg, 2.5 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of

celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 8-bromo-6-methyltetrazolo[1,5-a]pyridine (213.0 mg, 1.0 equiv.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (Dichloromethane as eluent) gave 214.8 mg (75%) of 8-(1,2-dihydroacenaphthylen-5-yl)-6-methyltetrazolo[1,5-a]pyridine (**3a**) as white solid.

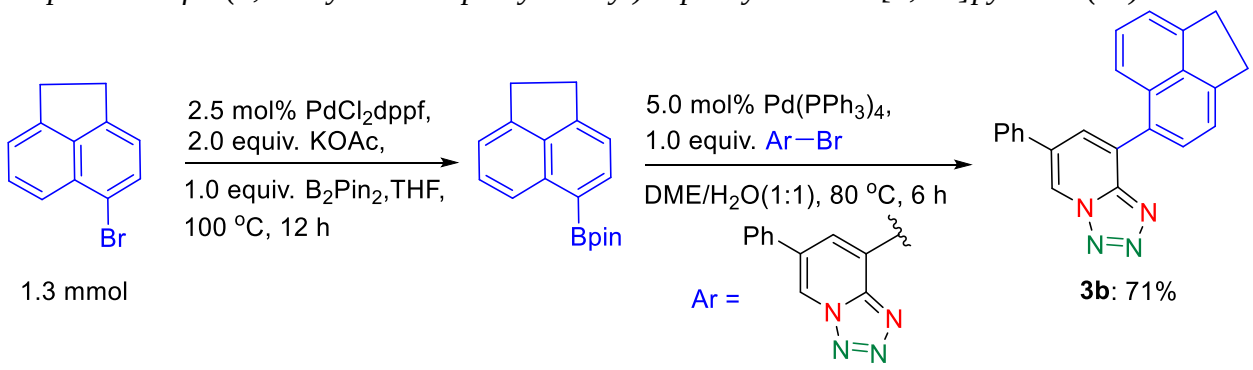
Melting Point: 167-169 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (s, 1H), 7.79 (d, J = 7.2 Hz, 1H), 7.65 (s, 1H), 7.50-7.41 (m, 3H), 7.34 (d, J = 6.4 Hz, 1H), 3.47 (s, 4H), 2.56 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.3, 148.0, 146.6, 139.6, 134.5, 130.2, 129.4, 128.7, 128.2, 127.2, 126.8, 121.4, 119.9, 119.8, 119.1, 30.5, 30.2, 18.2.

HRMS (ESI) *m/z*calcd for $C_{18}H_{14}N_4$ $[M+H]^+$ 287.1297, found 287.1288.

*Preparation of 8-(1,2-dihydroacenaphthylen-5-yl)-6-phenyltetrazolo[1,5-a]pyridine (**3b**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (23.7 mg, 2.5 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture

was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 8-bromo-6-methyltetrazolo[1,5-a]pyridine (275.1 mg, 1.0 equiv.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 247.4 mg (71%) of 8-(1,2-dihydroacenaphthylen-5-yl)-6-phenyltetrazolo[1,5-a]pyridine(**3b**) as white solid.

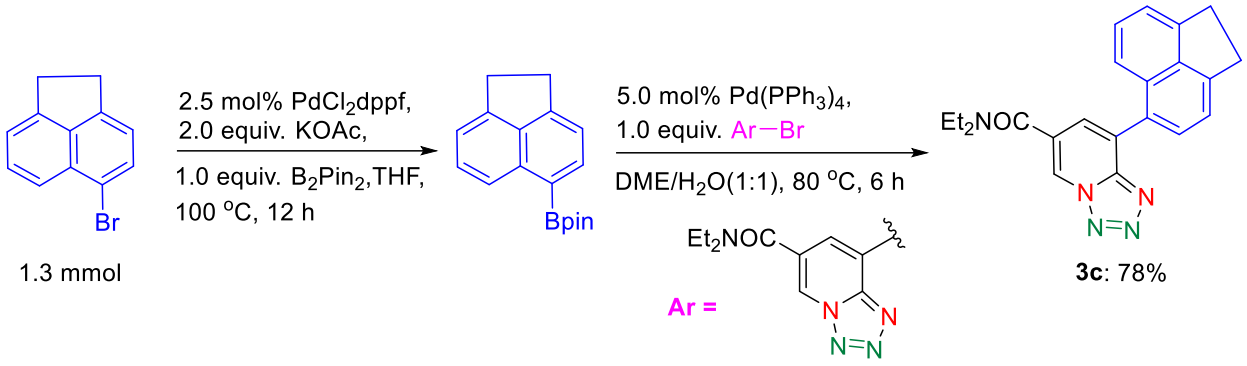
Melting Point: 177-179 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.00 (s, 1H), 8.09 (s, 1H), 7.88 (d, J = 7.2 Hz, 1H), 7.68 (d, J = 7.6 Hz, 2H), 7.59 – 7.44 (m, 7H), 7.36 (d, J = 6.8 Hz, 1H), 3.48 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.6, 148.2, 146.7, 139.7, 135.1, 132.3, 131.5, 130.4, 129.5, 129.4, 129.3, 128.9, 128.8,127.3, 126.7, 120.4, 119.9, 119.7, 119.2, 30.5, 20.3.

HRMS (ESI) *m/z*calcd for $C_{23}H_{16}N_4$ $[M+H]^+$ 349.1453, found 349.1447.

*Preparation of 8-(1,2-dihydroacenaphthylen-5-yl)-N,N-diethyltetrazolo[1,5-a]pyridine-6-carboxamide (**3c**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (23.7 mg, 2.5 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-

bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

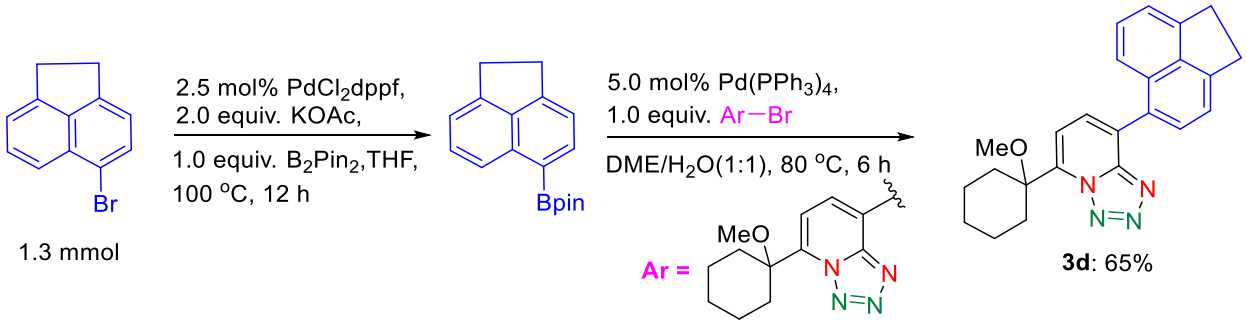
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 8-bromo-N,N-diethyltetrazolo[1,5-a]pyridine-6-carboxamide (298.1 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^oC for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 289.7 mg (78%) of 8-(1,2-dihydroacenaphthylen-5-yl)-*N*,*N*-diethyltetrazolo[1,5-a]pyridine-6-carboxamide (**3c**) as white solid.

^1H NMR (400 MHz, $CDCl_3$): δ 8.91 (s, 1H), 7.82 (s, 2H), 7.51 – 7.42 (m, 3H), 7.35 (d, J = 6.0 Hz, 1H), 3.59 (s, 2H), 3.46 (s, 6H), 1.27 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.6, 148.9, 148.5, 146.7, 139.6, 130.5, 130.3, 129.5, 129.1, 129.0, 127.0, 126.0, 121.8, 120.0, 119.5, 119.1, 43.7, 39.9, 30.4, 30.2, 14.4, 12.6.

HRMS (ESI) *m/z*calcd for $C_{22}H_{21}N_5O$ $[M+H]^+$ 372.1824, found 372.1818.

*Preparation of 8-(1,2-dihydroacenaphthylen-5-yl)-5-(1-methoxycyclohexyl)tetrazolo[1,5-a]pyridine (**3d**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (23.7 mg, 2.5 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-

bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 8-bromo-5-(1-methoxycyclohexyl)tetrazolo[1,5-a]pyridine (311.2 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then, the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^oC for 6 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (20% ethyl acetate in hexane as eluent) gave 250.0 mg (65%) of 8-(1,2-dihydroacenaphthylen-5-yl)-5-(1-methoxycyclohexyl)tetrazolo[1,5-a]pyridine (**3d**) as white solid.

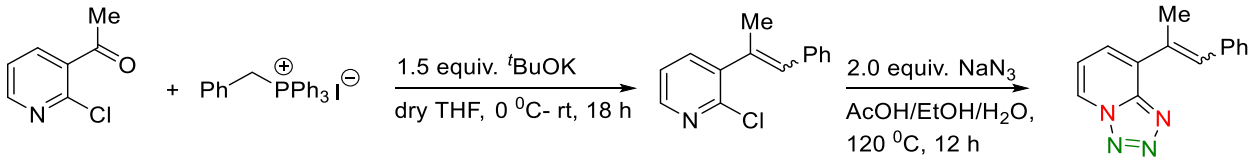
Melting Point: 133-135 ^oC

^1H NMR (400 MHz, $CDCl_3$): δ 7.82 (t, J = 6.8 Hz, 2H), 7.53 (d, J = 8.0 Hz, 1H), 7.44 (t, J = 7.2 Hz, 2H), 7.34 (t, J = 7.2 Hz, 2H), 3.47 (s, 4H), 3.27 (s, 3H), 2.47 – 2.34 (m, 4H), 1.87 – 1.74 (m, 4H), 1.65 – 1.40 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 150.0, 148.2, 146.6, 142.0, 139.7, 131.4, 130.4, 129.5, 128.6, 127.6, 127.0, 119.9, 119.8, 119.2, 114.3, 50.6, 31.6, 30.5, 30.3, 25.2, 21.4.

HRMS (ESI) *m/z*calcd for $C_{24}H_{24}N_4O$ $[M+H]^+$ 385.2028, found 385.2021.

*Preparation of 8-(1-phenylprop-1-en-2-yl)tetrazolo[1,5-a]pyridine (**5a**):*



2.0 mmol 1.2 equiv. **5a**: 30% yield

Step -I:

To a heterogeneous mixture of Wittig salt (1.1 g, 1.2 equiv.) in 10.0 mL dry THF, ^{t}BuOK (336.6 mg, 1.5 equiv.) was added in one portion at 0 ^oC and stirred for 30 min. Then, 1-(2-chloropyridin-

3-yl)ethan-1-one (311.2 mg, 2.0 mmol) in 5.0 mL THF was added slowly. Then reaction mixture was warmed to room temperature and stirred for another 4 h. Upon completion (judged by GC-MS), reaction mixture was quenched by slow addition of water, which was extracted with ethyl acetate (3 x 50 mL). Organic layer was washed with brine, dried over Na_2SO_4 and concentrated in vacuum. The crude product was used for the next step further any purification.

Step -II:

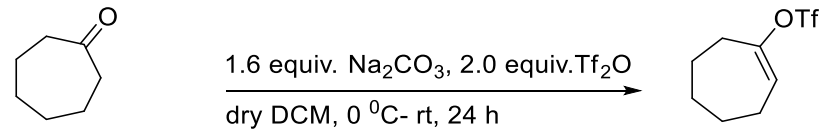
A 5.0 mL wheaton microreactor was charged with crude wittig product, NaN_3(260.0 mg, 2.0 equiv.). To this microreactor, H_2O (2.0 mL), EtOH (1.0 mL) and AcOH (500.0 µL) was added. The microreactor was capped with a Teflon pressure cap and placed into a preheated aluminum block at 120 ^oC. The reaction mixture was stirred for 24 h. After completion (checked by TLC) the reaction mixture was poured into water (50 mL) and neutralized with $NaHCO_3$. The reaction mixture was extracted with ethyl acetate (2 x 50 mL) and the organic layer was washed with brine (50 mL). Then the organic part was dried over Na_2SO_4 and concentrated under vacuum. The crude product was purified by column chromatography (30% ethyl acetate in hexane as eluent) to afford 141.8 mg (30%) of 8-(1-phenylprop-1-en-2-yl)tetrazolo[1,5-a]pyridine (5a) as white solid.

^1H NMR (400 MHz, $CDCl_3$): δ 8.75 (t, J = 6.0 Hz, 2H), 8.23 (s, 1H), 7.70 (d, J = 7.2 Hz, 1.32H), 7.51 – 7.42 (m, 4.79H), 7.36 – 7.27 (m, 3.23H), 7.12 – 7.04 (m, 3.82H), 6.94 – 6.87 (m, 3H), 2.48 (s, 3H), 2.47 (s, 2.87H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.0, 147.8, 137.2, 136.4,125.8, 132.3, 132.0, 131.7, 130.9, 130.9, 130.5, 129.5, 128.7, 128.2, 128.1, 127.4, 127.3, 126.9, 123.8, 123.1, 116.7, 116.6, 24.8, 16.8.

HRMS (ESI) m/z calcd for $C_{14}H_{12}N_4$ $[M+H]^+$ 237.1140, found 237.1134.

Preparation of cyclohept-1-en-1-yl trifluoromethanesulfonate:

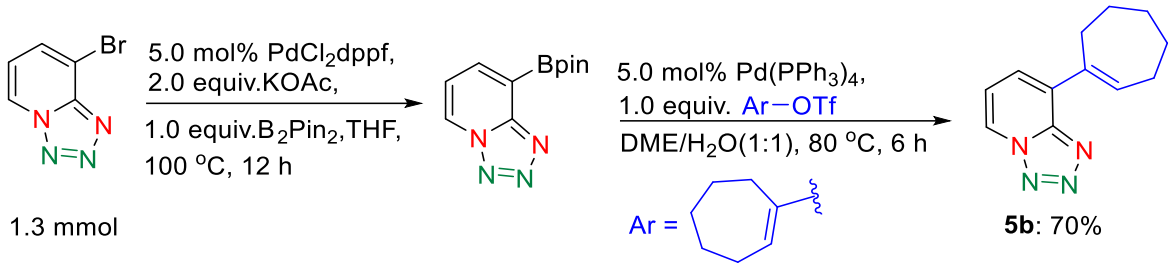


6.0 mmol Yield: 80%

To an oven dried 100 mL round-bottomed flask was added the cycloheptanone (673.0 mg, 6.0 mmol) and dry dichloromethane (15 mL) under an argon atmosphere. After that, oven dried Na_2CO_3 (639 mg, 1.6 equiv.) was added at rt. Then, trifluoromethanesulfonic anhydride (1.3mL, 2.0 equiv.) was added dropwise. The reaction mixture was then stirred at room temperature for 24

hours. After 24 h, reaction mixture was washed with saturated aqueous $NaHCO_3$ solution (2 x 20.0 mL), with water (2 x 20.0 mL), filtered, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel chromatography eluting with pentane to afford cyclohept-1-en-1-yl trifluoromethanesulfonate (1.2 g, 80 %) as a pale brown oil. Spectral data are in accordance with reported data.[22]

*Preparation of 8-(cyclohept-1-en-1-yl)tetrazolo[1,5-a]pyridine (**5b**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

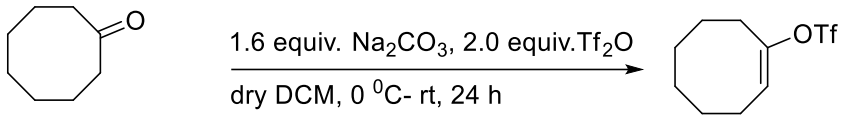
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, cyclohept-1-en-1-yl trifluoromethanesulfonate (244.2 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 °C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 150.0 mg (70%) of 8-(cyclohept-1-en-1-yl)tetrazolo[1,5-a]pyridine (**5b**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.65 (d, J = 6.8 Hz, 1H), 7.44 (d, J = 7.2 Hz, 1H), 7.15 (t, J = 7.2 Hz, 1H), 6.98 (t, J = 6.8 Hz, 1H), 2.79 – 2.75 (m, 2H), 2.46 – 2.41 (m, 2H), 1.91 – 1.86 (m, 2H), 1.77 – 1.73 (m, 2H), 1.65– 1.59 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 147.8, 138.9, 138.3, 133.4, 126.4, 122.6, 116.7, 32.3, 31.8, 29.1, 26.5, 26.3.

HRMS (ESI) *m/z* calcd for $C_{12}H_{14}N_4$ $[M+H]^+$ 215.1297, found 215.1289.

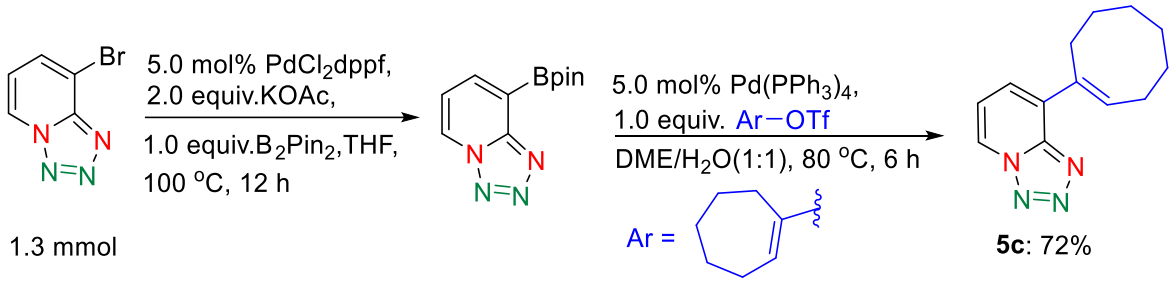
Preparation of (E)-cyclooct-1-en-1-yl trifluoromethanesulfonate:



6.0 mmol Yield: 75%

To an oven dried 100 mL round-bottomed flask was added the cyclooctanone (757.2 mg, 6.0 mmol) and dry dichloromethane (15 mL) under an argon atmosphere. After that, oven dried Na_2CO_3 (639 mg, 1.6 equiv.) was added at rt. Then, trifluoromethanesulfonic anhydride (1.3 mL, 2.0 equiv.) was added dropwise. The reaction mixture was then stirred at room temperature for 24 hours. After 24 h, reaction mixture was washed with saturated aqueous $NaHCO_3$ solution (2 x 20.0 mL), with water (2 x 20.0 mL), filtered, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel chromatography eluting with pentane to afford (*E*)-cyclooct-1-en-1-yl trifluoromethanesulfonate (1.16 g, 75 %) as a pale brown oil. Spectral data are in accordance with reported literature data.[23]

*Preparation of (E)-8-(cyclooct-1-en-1-yl)tetrazolo[1,5-a]pyridine (**5c**):*



1.3 mmol **5c**: 72%

Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture

was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, (*E*)-cyclooct-1-en-1-yl trifluoromethanesulfonate (258.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^oC for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 164.4 mg (72%) of (*E*)-8-(cyclooct-1-en-1-yl)tetrazolo[1,5-a]pyridine (**5c**) as white solid.

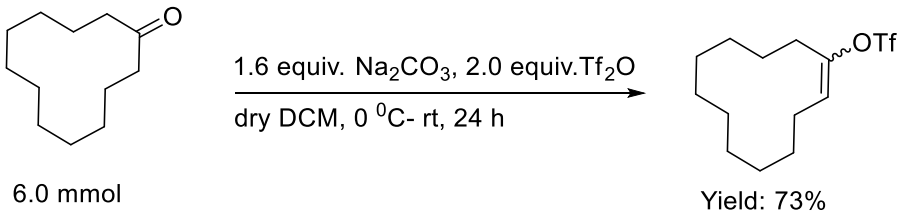
Melting Point: 132-134 ^oC

^1H NMR (400 MHz, $CDCl_3$): δ 8.64 (d, J = 6.8 Hz, 1H), 7.51 (d, J = 7.2 Hz, 1H), 7.37 (t, J = 8.4 Hz, 1H), 7.17 (t, J = 6.8 Hz, 1H), 2.81 (t, J = 6.4 Hz, 2H), 2.44 (q, J = 8.0 Hz, 2H), 1.65 (s, 4H), 1.53 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 147.9, 137.9, 133.9, 131.0, 126.4, 122.4, 116.7, 29.7, 29.0, 27.8, 27.1, 26.9, 25.9.

HRMS (ESI) *m/z* calcd for $C_{13}H_{16}N_4$ $[M+H]^+$ 229.1453, found 229.1445.

Preparation of cyclododec-1-en-1-yl trifluoromethanesulfonate:



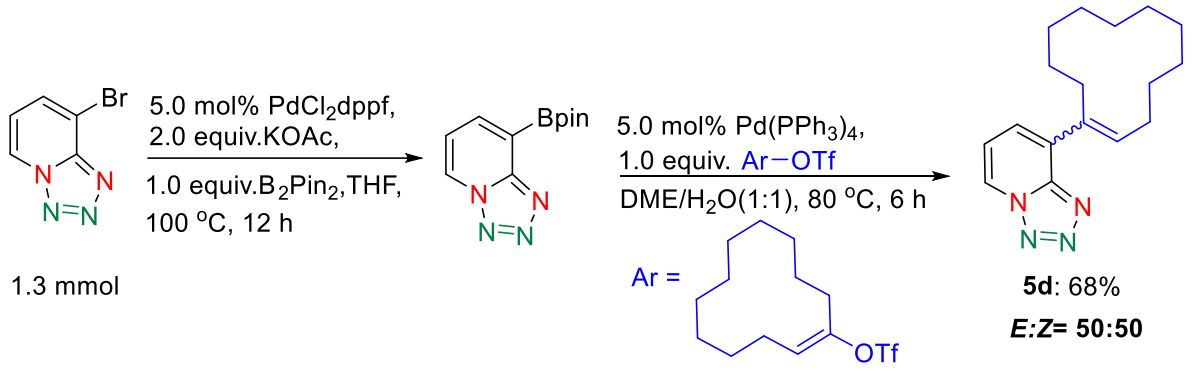
6.0 mmol

Yield: 73%

To an oven dried 100 mL round-bottomed flask was added the cyclododecanone (1.09 g, 6.0 mmol) and dry dichloromethane (15 mL) under an argon atmosphere. After that, oven dried Na_2CO_3 (639 mg, 1.6 equiv.) was added at rt. Then, trifluoromethanesulfonic anhydride (1.3 mL, 2.0 equiv.) was added dropwise. The reaction mixture was then stirred at room temperature for 24 hours. After 24 h, reaction mixture was washed with saturated aqueous $NaHCO_3$ solution (2 x 20.0 mL), with water (2 x 20.0 mL), filtered, dried over Na_2SO_4 and concentrated under reduced pressure. The

residue was purified by silica gel chromatography eluting with pentane to afford cyclododec-1-en-1-yl trifluoromethanesulfonate (1.4 g, 73 %) as a pale brown oil. Spectral data are in accordance with reported literature data.[24]

*Preparation of (E)-8-(cyclododec-1-en-1-yl)tetrazolo[1,5-a]pyridine (**5d**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

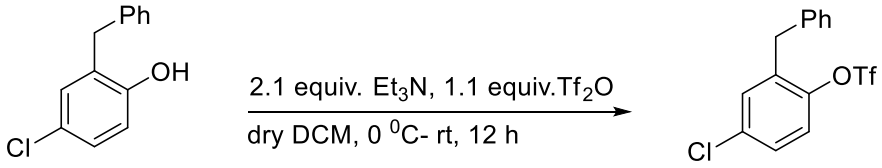
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, (*E*)-cyclododec-1-en-1-yl trifluoromethanesulfonate (314.4 mg, 1.0 equiv.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ° C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 193.4 mg (68%) of 8-(cyclododec-1-en-1-yl)tetrazolo[1,5-a]pyridine (**5d**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.78 (d, J = 6.8 Hz, 1H), 8.71 (d, J = 6.8 Hz, 1H), 7.54 (t, J = 6.4 Hz, 2H), 7.28 (t, J = 7.2 Hz, 1H), 7.21 (t, J = 7.2 Hz, 1H), 6.40 (t, J = 7.6 Hz, 1H), 6.13 (t, J = 8.0 Hz, 1H), 2.93 (t, J = 6.8 Hz, 2H), 2.78 (s, 2H), 2.38 (q, J = 6.8 Hz, 2H), 1.97 (d, J = 7.6 Hz, 2H), 1.67 – 1.36 (m, 30H), 1.24-1.19 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.0, 147.9, 136.9, 135.3, 134.9, 132.3, 131.9, 130.2, 129.4, 128.1, 123.5, 122.8, 116.7, 116.4, 34.9, 29.3, 27.5, 26.9, 26.8, 26.1, 25.8, 25.5, 25.4, 24.9, 24.7, 24.5, 24.3, 24.2, 24.1, 23.5, 23.5, 23.0, 22.2, 22.2.

HRMS (ESI) *m/z* calcd for $C_{17}H_{24}N_4$ $[M+H]^+$ 285.2079, found 285.2075.

Preparation of 2-benzyl-4-chlorophenyl trifluoromethanesulfonate:



9.0 mmol Yield: 61%

To an oven dried 250 mL round-bottomed flask was added the 2-benzyl-4-chlorophenol (2.0 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (2.0% ethyl acetate in hexane as eluent) gave 1.92 g (61%) of 2-benzyl-4-chlorophenyl trifluoromethanesulfonate as colourless liquid.

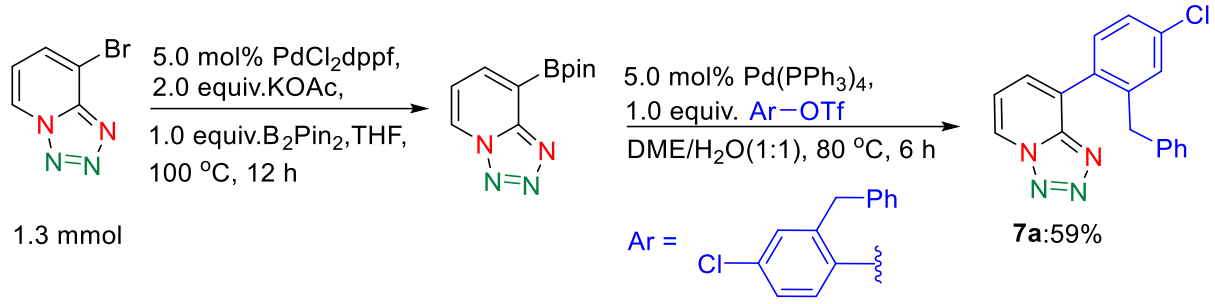
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (t, J = 7.2 Hz, 2H), 7.33-7.28 (m, 2H), 7.25 – 7.20 (m, 3H), 4.09 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 146.1, 137.5, 136.0, 134.1, 131.5, 129.1, 128.8, 128.2, 127.0, 122.6, 115.3(q, J= 318.3 Hz), 35.6.

^{19}F NMR (376 MHz, $CDCl_3$): -73.6.

HRMS (ESI) *m/z* calcd for $C_{14}H_{10}ClF_3O_3S$ $[M+K]^+$ 388.9628, found 388.9648.

*Preparation of 8-(2-benzyl-4-chlorophenyl)tetrazolo[1,5-a]pyridine (**7a**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then, the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 2-benzyl-4-chlorophenyl trifluoromethanesulfonate (350.7 mg, 1.0 mmol.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 °C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 189.3 mg (59%) 8-(2-benzyl-4-chlorophenyl)tetrazolo[1,5-a]pyridine (**7a**) as white solid.

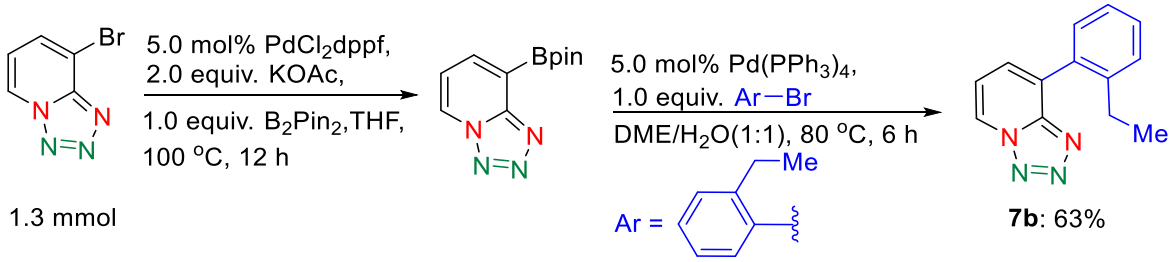
Melting Point: 101-103 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (d, J = 6.8 Hz, 1H), 7.38 – 7.29 (m, 4H), 7.17 – 7.05 (m, 4H), 6.76 (d, J = 7.2 Hz, 2H), 3.94 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.0, 141.6, 139.4, 135.5, 132.3, 131.7, 131.6, 130.8, 129.3, 128.5, 128.3, 127.0, 126.2, 124.3, 116.4, 39.6.

HRMS (ESI) *m/z* calcd for $C_{18}H_{13}ClN_4$ $[M+H]^+$ 321.0907, found 321.0901.

*Preparation of 8-(2-ethylphenyl)tetrazolo[1,5-a]pyridine (**7b**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then, the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 2-bromo ethyl benzene (185.1 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 °C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 141.3 mg (63%) 8-(2-ethylphenyl)tetrazolo[1,5-a]pyridine (**7b**) as white solid.

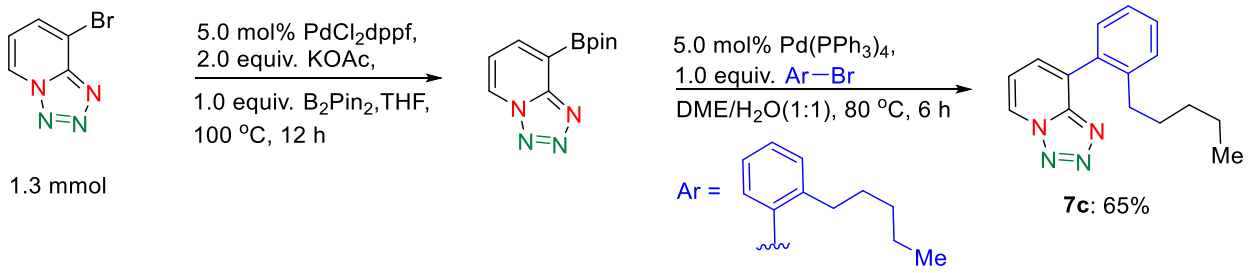
Melting Point: 64-66 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.86 (d, J = 6.8 Hz, 1H), 7.56 (d, J = 7.2 Hz, 1H), 7.47 – 7.43 (m, 2H), 7.35-7.24 (m Hz, 3H), 2.57 (q, J = 7.6 Hz, 2H), 1.10 (t, J = 7.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.6, 142.4, 133.2, 131.3, 130.9, 130.1, 129.6, 128.9, 126.1, 124.1, 116.5, 26.3, 15.1.

HRMS (ESI) *m/z* calcd for $C_{13}H_{12}N_4$ $[M+H]^+$ 225.1140, found 225.1135.

*Preparation of 8-(2-pentylphenyl)tetrazolo[1,5-a]pyridine (**7c**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then, the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

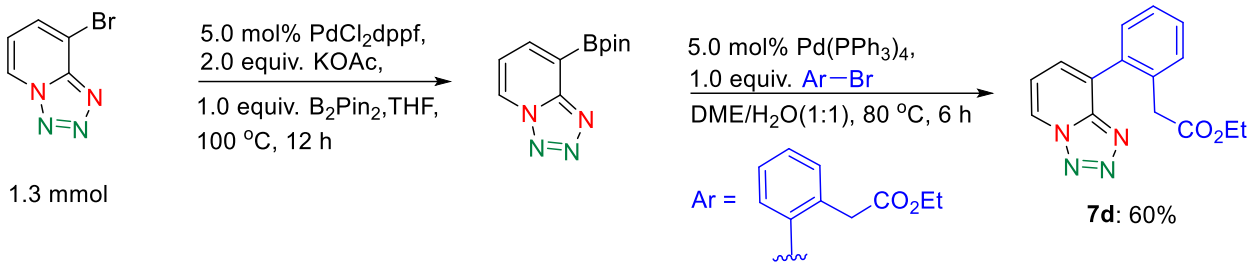
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 1-bromo-2-pentylbenzene (227.1 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ° C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 173.1 mg (65%) 8-(2-pentylphenyl)tetrazolo[1,5-a]pyridine (**7c**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.84 (d, J = 6.8 Hz, 1H), 7.54 (d, J = 6.8 Hz, 1H), 7.41 – 7.26 (m, 5H), 2.50 (t, J = 8.0 Hz 2H), 1.46-1.38 (m, 2H), 1.11 – 1.02 (m, 4H), 0.71 (t, J = 6.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.4, 141.1, 133.2, 131.4, 130.5, 130.0, 129.4, 129.2, 129.2, 125.8, 124.0, 116.6, 33.0, 31.2, 30.4, 22.0, 13.6.

HRMS (ESI) *m/z* calcd for $C_{16}H_{18}N_4$ $[M+H]^+$ 267.1610, found 267.1601.

*Preparation of ethyl 2-(2-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetate (**7d**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then, the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, ethyl 2-(2-bromophenyl)acetate (243.0 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 °C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 169.4 mg (60%) ethyl 2-(2-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetate (**7d**) as white solid.

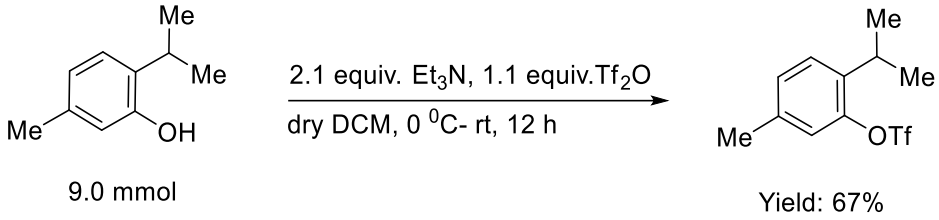
Melting Point: 89-91 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.82 (d, J = 6.8 Hz, 1H), 7.62 (d, J = 6.8 Hz, 1H), 7.44 – 7.38 (m, 4H), 7.30 (t, J = 6.8 Hz, 1H), 3.94 (q, J = 7.2 Hz, 2H), 3.58 (s, 2H), 1.06 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.0, 148.1, 134.0, 132.8, 132.1, 131.0, 130.5, 129.5, 127.5, 124.0, 116.7, 60.7, 39.2, 13.8.

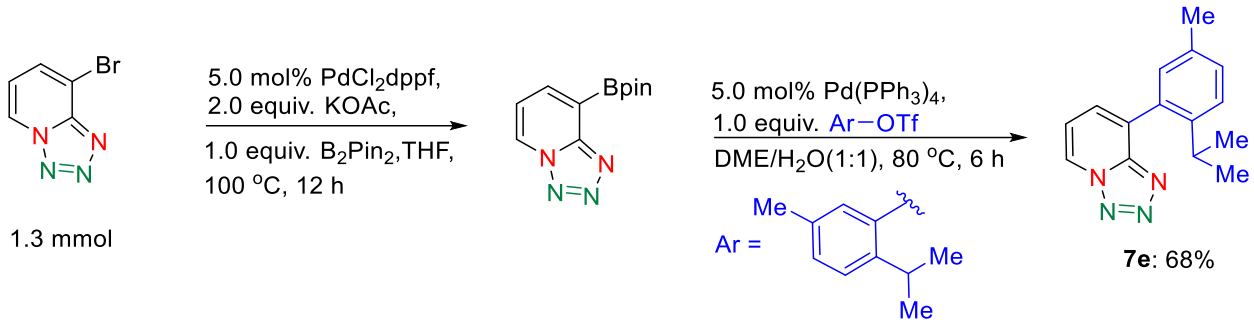
HRMS (ESI) *m/z* calcd for $C_{15}H_{14}N_4O_2$ $[M+H]^+$ 283.1195, found 283.1188.

Preparation of 2-isopropyl-5-methylphenyl trifluoromethanesulfonate:



To an oven dried 250 mL round-bottomed flask was added the 2-isopropyl-5-methylphenol (1.4 g, 9.0 mmol) and dry dichloromethane (20 mL) under an argon atmosphere. Then, reaction mixture was cooled to 0 ^{0}C. After that, dry triethylamine (2.6 mL, 2.1 equiv.) was added dropwise over a period of 10 min at 0 ^{0}C. The mixture was stirred at 0 ^{0}C for 30 minutes. Then, trifluoromethanesulfonic anhydride (1.7 mL, 1.1 equiv.) was added dropwise. The reaction mixture was then allowed to warm to room temperature and stirred for an additional 12 hours. After 12 h, water (50 mL) was added and the reaction mixture was extracted with diethyl ether (200 mL). The combined organic layers were concentrated under reduced pressure and chromatographic separation with silica gel (2.0% ethyl acetate in hexane as eluent) gave 1.7 g (67%) of 2-isopropyl-5-methylphenyl trifluoromethanesulfonateas colourless liquid. Spectral data are accordance with reported data.[25]

*Preparation of 8-(2-isopropyl-5-methylphenyl)tetrazolo[1,5-a]pyridine (**7e**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then, the reaction mixture was passed through a short pad of

celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 2-isopropyl-5-methylphenyl trifluoromethanesulfonate (282.3 mg, 1.0 mmole), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 171.6 mg (68%) 8-(2-isopropyl-5-methylphenyl)tetrazolo[1,5-a]pyridine (**7e**) as white solid.

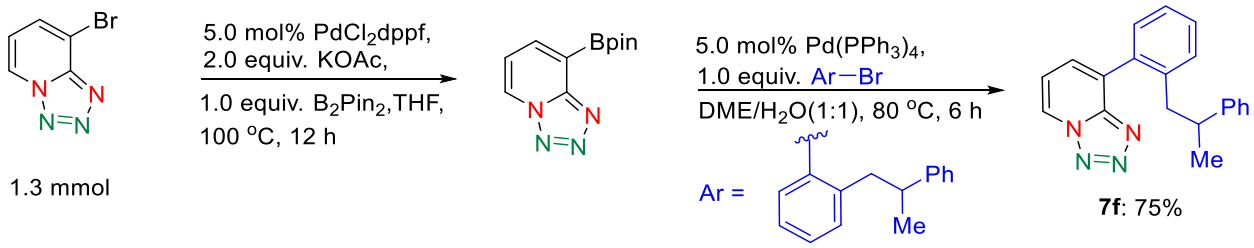
Melting Point: 129-131 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.83 (d, J = 6.8 Hz, 1H), 7.50 (d, J = 6.8 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.30 (t, J = 6.4 Hz, 2H), 7.10 (s, 1H), 2.72-2.65 (m, 1H), 2.36 (s, 3H), 1.15 (d, J = 6.8 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 144.2, 135.4, 132.3, 131.3, 131.1, 130.6, 130.4, 126.0, 116.5, 30.0, 24.2, 20.8.

HRMS (ESI) *m/z* calcd for $C_{15}H_{16}N_4$ $[M+H]^+$ 253.1453, found 253.1447.

*Preparation of 8-(2-(2-phenylpropyl)phenyl)tetrazolo[1,5-a]pyridine (**7f**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture

was cooled to room temperature. Then, the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 1-bromo-2-(2-phenylpropyl)benzene (275.2 mg, 1.0 equiv.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 235.8 mg (75%) 8-(2-(2-phenylpropyl)phenyl)tetrazolo[1,5-a]pyridine (**7f**) as white solid.

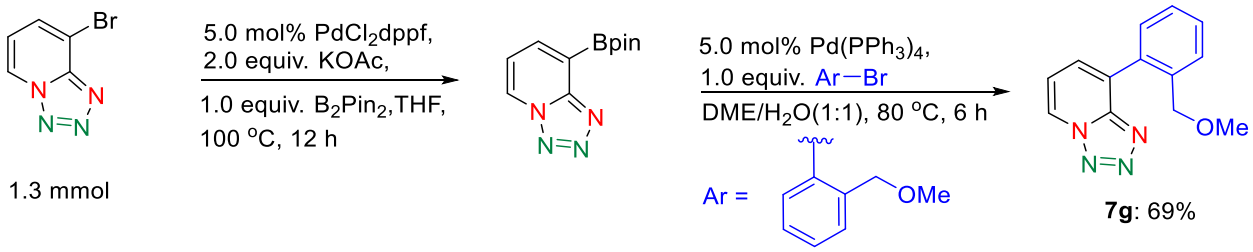
Melting Point: 112-114 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (d, J = 6.8 Hz, 1H), 7.38 (t, J = 7.6 Hz, 1H), 7.33 – 7.24 (m, 3H), 7.18 (t, J = 6.8 Hz, 1H), 7.11 (d, J = 6.8 Hz, 1H), 7.06 (d, J = 6.0 Hz, 3H), 6.76 – 6.71 (m, 2H), 2.85 – 2.76 (m, 3H), 1.10 (d, J = 6.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.3, 145.7, 139.1, 133.7, 131.4, 130.5, 130.3, 130.0, 129.1, 127.9, 126.6, 125.8, 123.8, 116.5, 42.3, 41.6, 21.2.

HRMS (ESI) *m/z* calcd for $C_{20}H_{18}N_4$ $[M+H]^+$ 315.1610, found 315.1604.

*Preparation of 8-(2-(methoxymethyl)phenyl)tetrazolo[1,5-a]pyridine (**7g**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture

was cooled to room temperature. Then, the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 1-bromo-2-(methoxymethyl)benzene (201.1 mg, 1.0 equiv.), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 165.8 mg (69%) 8-(2-(methoxymethyl)phenyl)tetrazolo[1,5-a]pyridine (**7g**) as white solid.

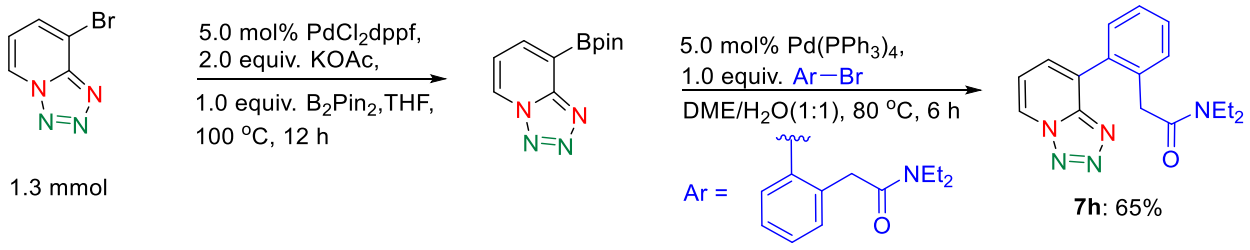
Melting Point: 99-101 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.84 (d, J = 7.2 Hz, 1H), 7.71 (d, J = 6.8 Hz, 1H), 7.60-7.44 (m, 4H), 7.32 (t, J = 6.8 Hz, 1H), 4.38 (s, 2H), 3.22 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.4, 136.4, 133.5, 131.4, 130.6, 129.9, 129.8, 129.5, 128.2, 124.2, 116.6, 72.8, 57.9.

HRMS (ESI) *m/z* calcd for $C_{13}H_{12}N_4O$ $[M+H]^+$ 241.1089, found 241.1078.

*Preparation of N,N-diethyl-2-(2-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetamide (**7h**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture

was cooled to room temperature. Then, the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 2-(2-bromophenyl)-N,N-diethylacetamide (270.2 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 201.1 mg (65%) *N*, *N*-diethyl-2-(2-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetamide (**7h**) as white solid.

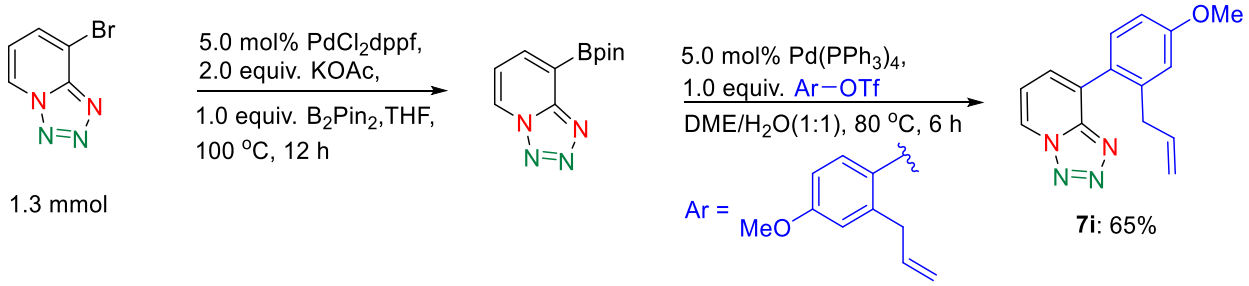
Melting Point: 124-126 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.83 (d, J = 6.8 Hz, 1H), 7.66 (d, J = 6.8 Hz, 1H), 7.46-7.43 (m, 1H), 7.40 (d, J = 3.2 Hz, 2H), 7.35 (d, J = 7.6 Hz, 1H), 7.29 (d, J = 7.2 Hz, 1H), 3.65 (s, 2H), 3.23 (q, J = 7.1 Hz, 2H), 3.10 (q, J = 6.8 Hz, 2H), 0.97 (t, J = 7.2 Hz, 3H), 0.87 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 169.6, 148.0, 134.5, 134.0, 132.4, 130.5, 130.2, 130.1, 129.7, 127.2, 124.2, 116.8, 42.1, 40.2, 38.7, 14.0, 12.9.

HRMS (ESI) *m/z* calcd for $C_{17}H_{19}N_5O$ $[M+H]^+$ 310.1668, found 310.1662.

*Preparation of 8-(2-allyl-4-methoxyphenyl)tetrazolo[1,5-a]pyridine (**7i**):*



Step I:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with $PdCl_2$•dppf (47.5 mg, 5.0 mol %), KOAc (255.2 mg, 2.0 equiv.), B_2pin_2 (330.1 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (258.7 mg, 1.3 mmol) and dry THF (4.0 mL). The microreactor was

sealed and heated at 100 °C for 12 h. After completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then, the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then, solvent was evaporated and without any further purification the crude product was used for next step.

Step II:

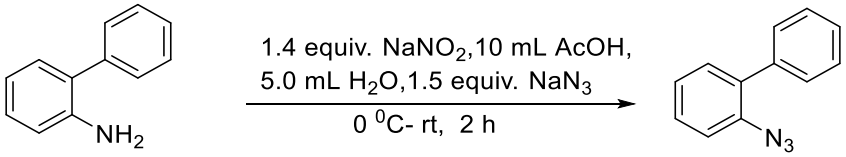
An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, 2-allyl-4-methoxyphenyl trifluoromethanesulfonate (296.3 mg, 1.0 mmol), K_2CO_3 (414 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (57.8 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water (5.0 mL) each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 6 h. After completion (judged by TLC), reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with neutral silica gel (30% ethyl acetate in hexane as eluent) gave 173.1 mg (65%) 8-(2-allyl-4-methoxyphenyl)tetrazolo[1,5-a]pyridine (**7i**) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.81 (d, J = 6.8 Hz, 1H), 7.53 (d, J = 6.8 Hz, 1H), 7.38 (d, J = 8.4 Hz, 1H), 7.30 – 7.23 (m, 1H), 6.93-6.89 (m, 2H), 5.87-5.77 (m, 1H), 4.95 (d, J = 10.4 Hz, 1H), 4.81 (dd, J = 18.0 Hz, J = 1.2Hz, 1H), 3.87 (s, 3H), 3.32 (d, J = 6.4 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.4, 148.7, 139.8, 136.7, 131.7, 131.3, 130.3, 126.0, 123.8, 116.5, 116.4, 115.8, 112.0, 55.4, 38.0.

HRMS (ESI) *m/z* calcd for $C_{15}H_{14}N_4O$ $[M+H]^+$ 267.1246, found 267.1238.

Preparation of 2-azido-1,1'-biphenyl (9a):



1.48 mmol **9a**: 80%

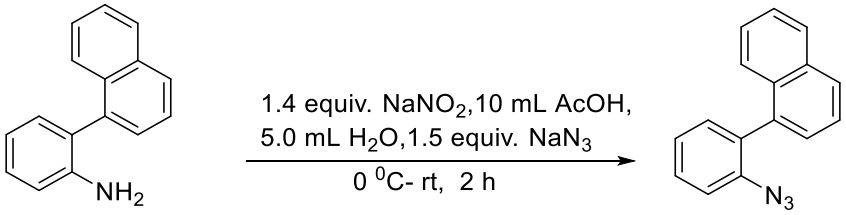
To a 100 mL oven dried round bottom flask with a stir bar were added 2-aminobiphenyl (0.250 g, 1.48 mmol) ,10 mL of HOAc and 5 mL of H_2O and then reaction mixture was cooled in an ice bath. Then, $NaNO_2$ (142 mg, 2.07 mmol) was added slowly, and the resulting mixture was stirred at 0 °C for one hour. After that, NaN_3 (144 mg, 1.5 equiv) was then added slowly, and the resulting mixture was warmed to ambient temperature, and stirred for additional one hours. The

solution was diluted with 20 mL of water and 20 mL of DCM and basified by the slow addition of K_2CO_3 until bubbling ceased. The organic layer was separated and the aqueous layer was extracted with an additional DCM (2 × 20 mL). The combined organic layers were washed with water (1 × 20 mL) and brine solution (1 × 20 mL). The resulting organic phase dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo and the crude residue was purified by flash column chromatography (eluent 1% ethyl acetate/hexanes) to yield the product 2-azido-1,1'-biphenyl (**9a**) as a colourless oil (231.2 mg, 80%). Spectral data are in accordance with reported data.[26]

^{1}H NMR (800 MHz, $CDCl_3$): δ 7.47-7.46 (m, 4H), 7.42 – 7.36 (m, 3H), 7.28 (d, J = 7.2 Hz, 1H), 7.23 (t, J = 6.4 Hz, 1H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 138.1, 137.1, 133.7, 131.2, 129.4, 128.7, 128.1, 127.5, 124.9, 118.7.

Preparation of 1-(2-azidophenyl)naphthalene (9b):



1.48 mmol **9b**: 70%

To a 100 mL oven dried round bottom flask with a stir bar were added 2-(naphthalen-1-yl)aniline (324.6 mg, 1.48 mmol) ,10 mL of HOAc and 5 mL of H_2O and then reaction mixture was cooled in an ice bath. Then, $NaNO_2$ (142 mg, 2.07 mmol) was added slowly, and the resulting mixture was stirred at 0 °C for one hour. After that, NaN_3 (144 mg, 1.5 equiv) was then added slowly, and the resulting mixture was warmed to ambient temperature, and stirred for additional one hours. The

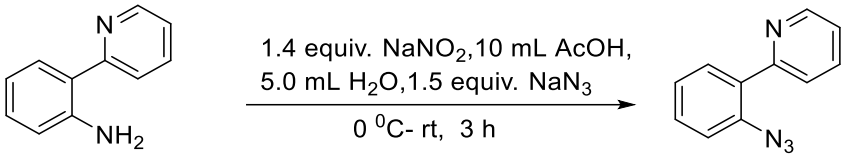
solution was diluted with 20 mL of water and 20 mL of DCM and basified by the slow addition of K_2CO_3 until bubbling ceased. The organic layer was separated and the aqueous layer was extracted with an additional DCM (2 × 20 mL). The combined organic layers were washed with water (1 × 20 mL) and brine solution (1 × 20 mL). The resulting organic phase dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo and the crude residue was purified by flash column chromatography (eluent 1% ethyl acetate/hexanes) to yield the product 1-(2-azidophenyl)naphthalene (**9b**) as a colourless oil (254.1 mg, 70%). Spectral data are in accordance with reported data.[26]

^{1}H NMR (800 MHz, $CDCl_3$): δ 8.12 (d, J = 7.2 Hz, 1H), 8.05 (d, J = 8.8 Hz, 1H), 7.87 (dd, J = 12.0 Hz, J= 8.0 Hz, 2H), 7.69 (s, 1H), 7.57-7.55 (m, 1H), 7.54 – 7.52 (m, 2H), 3.99 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 163.9, 133.5, 131.6, 129.8, 129.4, 128.8, 128.2, 127.1, 126.7, 126.0, 125.2, 123.4, 122.4, 77.16, 53.0.

HRMS (ESI) *m/z*calcd for $C_{16}H_{11}N$ $[M+H]^{+}(-N_2)$ 218.0970, found 218.0963.

Preparation of 2-(2-azidophenyl)pyridine (9c):



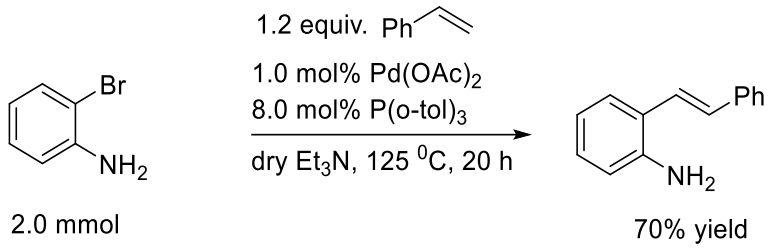
1.48 mmol **9c**: 80%

To a 100 mL oven dried round bottom flask with a stir bar were added 2-(pyridin-2-yl)aniline (251.9 mg, 1.48 mmol) ,10 mL of HOAc and 5 mL of H_2O and then reaction mixture was cooled in an ice bath. Then, $NaNO_2$ (142 mg, 2.07 mmol) was added slowly, and the resulting mixture was stirred at 0 °C for 1.5 hour. After that, NaN_3 (144 mg, 1.5 equiv) was then added slowly and the resulting mixture was warmed to ambient temperature, and stirred for additional 1.5 h. The solution was diluted with 20 mL of water and 20 mL of DCM and basified by the slow addition of K_2CO_3 until pH of the reaction mixture reached to 8. The organic layer was separated and the aqueous layer was extracted with an additional DCM (2 × 20 mL). The combined organic layers were washed with water (1 × 20 mL) and brine solution (1 × 20 mL). The resulting organic phase dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo and the crude residue was purified by flash column chromatography (eluent 5% ethyl acetate/hexanes) to yield the product 2-(2-azidophenyl)pyridine (**9c**) as a colourless oil (232.3 mg, 80%). Spectral data are in accordance with reported data.[27]

^{1}H NMR (800 MHz, $CDCl_3$): δ 8.71 (s, 1H), 7.74 (s, 1H), 7.68 (s, 2H), 7.44 (s, 1H), 7.26 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 155.8, 149.5, 137.2, 135.8, 132.2, 131.4, 129.8, 125.0, 124.8, 122.2, 118.8.

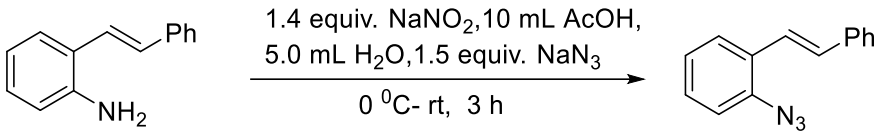
Preparation of (E)-2-styrylaniline:



2.0 mmol — 70% yield

In an argon filled glove box, a 20 mL oven dried seal tube with a stir bar were charged with 2-bromoaniline (344.0 mg, 2.0 mmol), 1.9 mL dry Et_3N, $Pd(OAc)_2$ (4.5 mg, 1 mol%), P(*o*-Tol)$_3$ (51.3 mg, 8 mol%), and styrene (249.8 mg, 1.2 equiv). The seal-tube was capped tightly and placed into a preheated oil bath at 125 ^oC for 20 h. After being stirred at 120 °C, the reaction mixture was poured into water and then the product was extracted with DCM (three times). The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel (eluent 20% ethyl acetate in hexane) to afford the corresponding 2-styrylaniline product with 70% (273.4 mg) isolated yield. Spectral data are in accordance with reported data.[26]

Preparation of (E)-1-azido-2-styrylbenzene (*9d*)*:*



1.48 mmol — **9d**: 80%

To a 100 mL oven dried round bottom flask with a stir bar were added (*E*)-2-styrylaniline (289.0 mg, 1.48 mmol) ,10 mL of HOAc and 5 mL of H_2O and then reaction mixture was cooled in an ice bath. Then, $NaNO_2$ (142 mg, 2.07 mmol) was added slowly, and the resulting mixture was stirred at 0 °C for 1.5 hour. After that, NaN_3 (144 mg, 1.5 equiv) was then added slowly and the resulting mixture was warmed to ambient temperature, and stirred for additional 1.5 h. The solution was diluted with 20 mL of water and 20 mL of DCM and basified by the slow addition of K_2CO_3 until pH of the reaction mixture reached to 8. The organic layer was separated and the aqueous layer was extracted with an additional DCM (2 × 20 mL). The combined organic layers were washed with water (1 × 20 mL) and brine solution (1 × 20 mL). The resulting organic phase dried over Na_2SO_4 and filtered. The filtrate was concentrated in vacuo and the crude residue was purified by flash column chromatography (eluent 5% ethyl acetate/hexanes) to yield the product *(E)*-1-

azido-2-styrylbenzene (**9d**) as a yellow solid (262.0 mg, 80%). Spectral data are in accordance with reported data.[26]

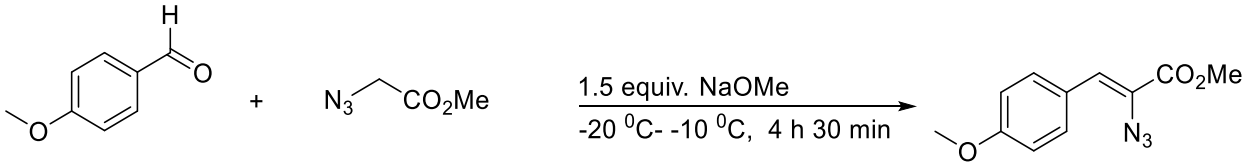
Melting Point: 93-95 ^{o}C

^{1}H NMR (800 MHz, $CDCl_3$): δ 7.66 (d, J = 8.0 Hz, 1H), 7.54 (d, J = 7.2 Hz, 2H), 7.38 – 7.36 (m, 3H), 7.30 (dt, J = 21.6Hz, J = 7.2 Hz, 2H), 7.18 (d, J = 8.0 Hz, 1H), 7.15 (t, J = 7.2 Hz, 1H), 7.10 (d, J = 16.0 Hz, 1H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 137.3, 137.2, 130.3, 129.1, 128.7, 128.7, 127.8, 126.7, 126.3, 124.9, 122.9, 118.5.

HRMS (ESI) *m/z*calcd for $C_{15}H_{14}N_2O$ $[M+H]^+$ ($-N_2$) 194.0970, found 194.0957.

Preparation of methyl (Z)-2-azido-3-(4-methoxyphenyl)acrylate (9f):



7.4 mmol 3.0 equiv. **9f**: 40%

To a 100 mL oven dried round bottom flask with a stir bar were added a solution of NaOMe (601 mg, 1.5 equiv) in 4.0 mL dry MeOH and then reaction mixtrure was cooled to -20 °C. After that, a solution of 4-methoxybenzaldehyde (1.0 g, 7.4 mmol) and methyl azidoacetate (2.53 g, 3.0 equiv.) were added dropwise over 30 minutes. After 4 h, the heterogeneous mixture was diluted with 20 mL of water and 20 mL of diethyl ether. The organic and aqueous layers were separated and the resulting aquesous layer was extracted with an additional 2 × 20 mL of diethyl ether. The combined organic layers were washed with 2 × 20 mL of distilled water and 1 × 20 mL of brine. The resulting organic layer was dried over Na_2SO_4 and the heterogeneous mixture was filtered. Purification of crude residue by flash chromatography (4% ethyl acetate in hexane) afforded desired methyl (Z)-2-azido-3-(4-methoxyphenyl)acrylate (**9f**) as a pale-yellow low melting solid (690.3 mg, 40%).[28]

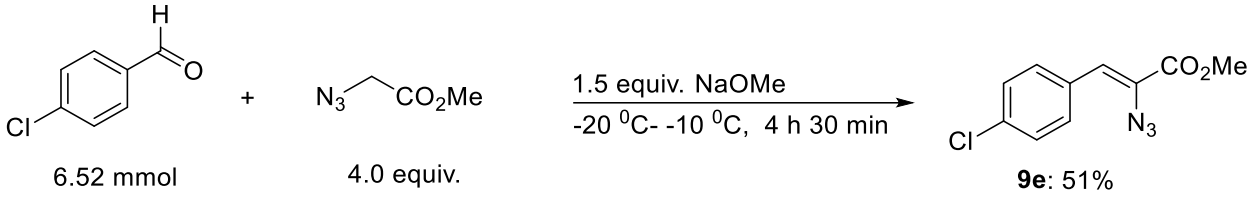
Melting Point: 46-48 ^{o}C

^{1}H NMR (800 MHz, $CDCl_3$): δ 7.78 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 8.8 Hz, 2H), 6.87 (s, 1H), 3.88 (s, 3H), 3.82 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 164.2, 160.4, 132.3, 125.9, 125.6, 122.9, 113.8, 55.2, 52.7.

HRMS (ESI) *m/z*calcd for $C_{11}H_{11}NO_3$ $[M+H]^+$ ($-N_2$)206.0817, found 206.0808.

*Preparation of methyl (Z)-2-azido-3-(4-chlorophenyl)acrylate (**9e**):*



6.52 mmol 4.0 equiv. **9e**: 51%

To a 100 mL oven dried round bottom flask with a stir bar were added a solution of NaOMe (405 mg, 1.5 equiv) in 4.0 mL dry MeOH and then reaction mixtrure was cooled to -20 °C. After that, a solution of 4-chloro benzaldehyde (0.917 g, 6.52 mmol) and methyl azidoacetate (3.0 g, 4.0 equiv.) were added dropwise over 30 minutes. After 4 h, the heterogeneous mixture was diluted with 20 mL of water and 20 mL of diethyl ether. The organic and aqueous layers were separated and the resulting aquesous layer was extracted with an additional 2 × 20 mL of diethyl ether. The combined organic layers were washed with 2 × 20 mL of distilled water and 1 × 20 mL of brine. The resulting organic layer was dried over Na_2SO_4 and the heterogeneous mixture was filtered. Purification of crude residue by flash chromatography (1% ethyl acetate in hexane) afforded desired methyl methyl (*Z*)-2-azido-3-(4-chlorophenyl)acrylate (**9e**) as a pale-yellow solid (790.0 mg, 51%).[28]

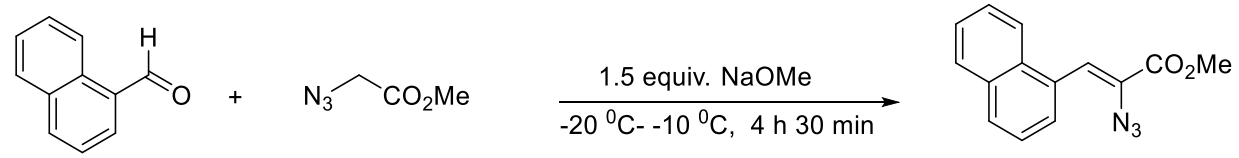
Melting Point: 47-49 ^oC

^1H NMR (800 MHz, $CDCl_3$): δ 7.75 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.8 Hz, 2H), 6.84 (s, 1H), 3.91 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 163.8, 135.2, 131.8, 131.6, 128.7, 125.7, 123.9, 77.16, 53.0.

HRMS (ESI) *m/z*calcd for $C_{10}H_8ClN_3O_2$ $[M+H]^+$ 238.0383, found 238.0401.

*Preparation of methyl (Z)-2-azido-3-(naphthalen-1-yl)acrylate (**9g**):*



7.36 mmol 4.0 equiv. **9g**: 35%

To a 100 mL oven dried round bottom flask with a stir bar were added a solution of NaOMe (596.2 mg, 1.5 equiv) in 4.0 mL dry MeOH and then reaction mixtrure was cooled to -20 °C. After that, a solution of 1-naphthaldehyde (1.0 mL, 7.36 mmol) and methyl azidoacetate (3.4 g, 4.0 equiv.) were added dropwise over 30 minutes. After 4 h, the heterogeneous mixture was diluted with 20 mL of water and 20 mL of diethyl ether. The organic and aqueous layers were separated and the

resulting aquesous layer was extracted with an additional 2 × 20 mL of diethyl ether. The combined organic layers were washed with 2 × 20 mL of distilled water and 1 × 20 mL of brine. The resulting organic layer was dried over Na_2SO_4 and the heterogeneous mixture was filtered. Purification of crude residue by flash chromatography (1% ethyl acetate in hexane) afforded desired methyl (*Z*)-2-azido-3-(naphthalen-1-yl)acrylate (**9g**) as a pale-yellow solid (652.5 mg, 35%).[28]

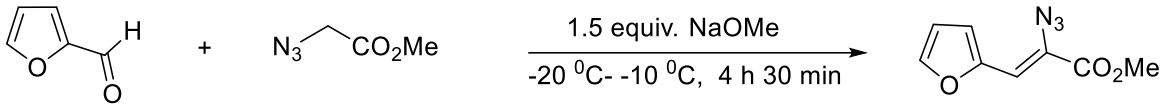
Melting Point: 93-95 ^oC

^1H NMR (800 MHz, $CDCl_3$): δ 7.91 – 7.88 (m, 4H), 7.61 (dd, J = 8.8 Hz, J = 1.6 Hz, 1H), 7.53 – 7.51 (m, 2H), 7.47 – 7.43 (m, 2H), 7.31 (d, J = 8.0 Hz, 1H), 7.27 – 7.25 (m, 1H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 137.3, 135.7, 133.7, 133.2, 132.6, 131.5, 128.8, 128.3, 128.2, 127.7, 127.6, 127.5, 126.2, 126.2, 125.0, 118.8.

HRMS (ESI) *m/z*calcd for $C_{14}H_{11}NO_2$ $[M+H]^+$ ($-N_2$) 226.0868, found 226.0867.

*Preparation of methyl (Z)-2-azido-3-(furan-2-yl)acrylate (**9h**):*



10.4 mmol 3.0 equiv. **9h**: 10%

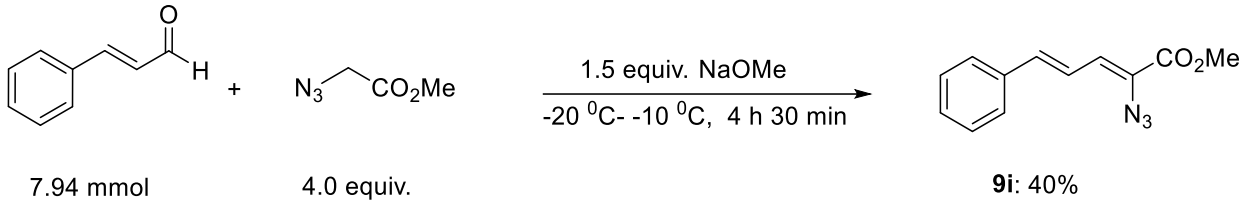
To a 100 mL oven dried round bottom flask with a stir bar were added a solution of NaOMe (844 mg, 1.5 equiv) in 6.0 mL dry MeOH and then reaction mixtrure was cooled to -20 °C. After that, a solution of 2-furaldehyde (0.863 mL, 7.36 mmol) and methyl azidoacetate (3.59 g, 3.0 equiv.) were added dropwise over 30 minutes. After 4 h, the heterogeneous mixture was diluted with 20 mL of water and 20 mL of diethyl ether. The organic and aqueous layers were separated and the resulting aquesous layer was extracted with an additional 2 × 20 mL of diethyl ether. The combined organic layers were washed with 2 × 20 mL of distilled water and 1 × 20 mL of brine. The resulting organic layer was dried over Na_2SO_4 and the heterogeneous mixture was filtered. Purification of crude residue by flash chromatography (1% ethyl acetate in hexane) afforded desired methyl (*Z*)-2-azido-3-(furan-2-yl)acrylate (**9h**) as a pale-yellow low melting solid (201.0 mg, 10%).[28]

^1H NMR (800 MHz, $CDCl_3$): δ 7.49 (s, 1H), 7.10 (d, J = 3.2 Hz, 1H), 6.86 (s, 1H), 6.52 (s, 1H), 3.88 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 163.6, 149.4, 143.9, 122.6, 115.3, 113.6, 112.6, 52.8.

HRMS (ESI) *m/z*calcd for $C_8H_7NO_3$ $[M+H]^+$ ($-N_2$) 166.0504, found 166.0487.

*Preparation of methyl (2Z,4E)-2-azido-5-phenylpenta-2,4-dienoate (**9i**):*



7.94 mmol 4.0 equiv. **9i**: 40%

To a 100 mL oven dried round bottom flask with a stir bar were added a solution of NaOMe (493mg, 1.5 equiv) in 3.0 mL dry MeOH and then reaction mixtrure was cooled to -20 °C. After that, a solution of cinnamaldehyde (1.0 mL, 7.94 mmol) and methyl azidoacetate (3.66 g, 4.0 equiv.) were added dropwise over 30 minutes. After 4 h, the heterogeneous mixture was diluted with 20 mL of water and 20 mL of diethyl ether. The organic and aqueous layers were separated and the resulting aquesous layer was extracted with an additional 2 × 20 mL of diethyl ether. The combined organic layers were washed with 2 × 20 mL of distilled water and 1 × 20 mL of brine. The resulting organic layer was dried over Na_2SO_4 and the heterogeneous mixture was filtered. Purification of crude residue by flash chromatography (1% ethyl acetate in hexane) afforded desired methyl (*2Z,4E*)-2-azido-5-phenylpenta-2,4-dienoate (**9i**) as a yellow solid (727.9 mg, 40%).[28]

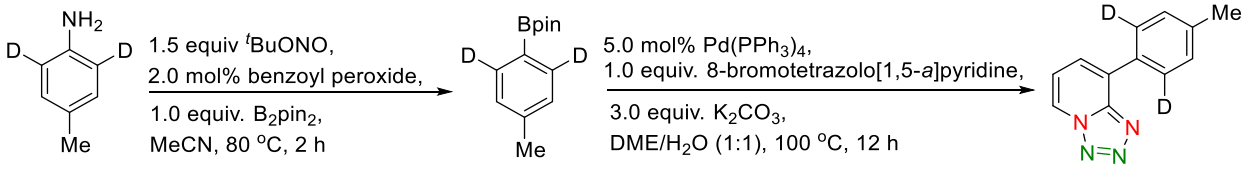
Melting Point: 140-142 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (d, J = 7.6 Hz, 2H), 7.38-7.28 (m, 3H), 7.17 (dd, J = 16.0 Hz, J = 11.6 Hz, 1H), 6.79 (dd, J = 19.6 Hz, J = 10.8 Hz, 2H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 163.6, 139.1, 136.3, 129.0, 128.8, 127.2, 127.1, 125.4, 122.2, 52.7.

HRMS (ESI) *m/z*calcd for $C_{12}H_{11}NO_2$ $[M+H]^+$ ($-N_2$) 202.0868, found 202.0856.

Preparation of 8-(4-methylphenyl-2,6-d$_2$)tetrazolo[1,5-a]pyridine:



93.5% D
1.3 mmol

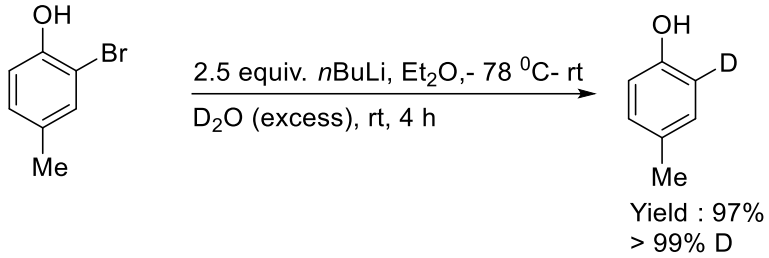
13-d_2: Yield: 70%

Step-I: In an argon-filled glovebox, a 5 mL wheaton microreactor was charged with ^{t}BuONO (270.0 mg, 1.5 equiv.), benzoyl peroxide (6.3 mg, 2.0 mol%), B_2pin_2 (330.2 mg, 1.0 equiv.), 2,6-*d*$_2$-*p*-toluidine (141.7 mg, 1.3 mmol) and dry MeCN (2 mL). The microreactor was sealed and heated at 80 °C for 2 h. After completion (judged by GC/MS), the reaction mixture was cooled to

room temperature. Then the reaction mixture was passed through a short pad of celite and eluted with ethyl acetate (50 mL). Then solvent was evaporated and without any further purification the crude product was used for next step.

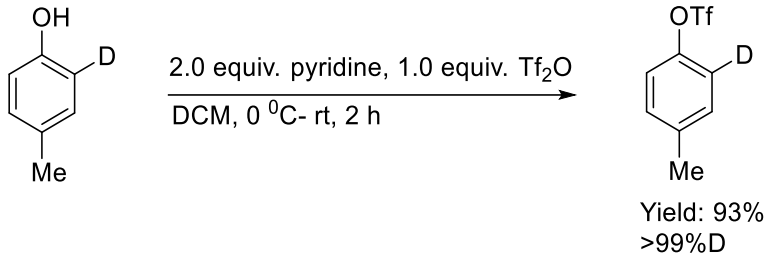
Step-II: An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stir bar under an argon atmosphere was charged with borylated crude product, bromotetrazolo[1,5-*a*]pyridine (238.8 mg, 1.0 equiv.), K_2CO_3 (496.8 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (69.3 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water 5.0 mL each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 100 ^oC for 12 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with silica gel (30% ethyl acetate in hexane as eluent) gave 178.3 mg (70%) of 8-(4-methylphenyl-2,6-d_2)tetrazolo[1,5-*a*]pyridine (**13-*d*$_2$)** as brown solid. Spectral data are in accordance with reported literature data.[1]

Preparation of 2-d-4-methylphenol:



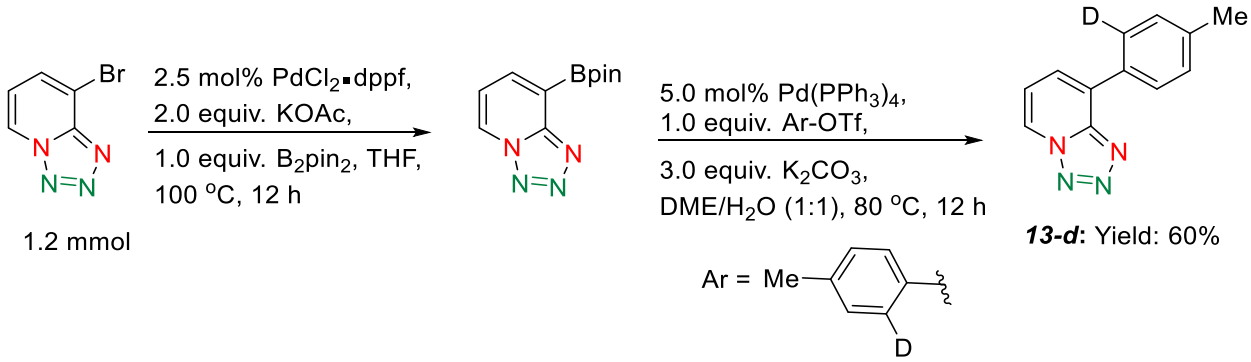
An oven dried 2-neck 250 mL round bottom flask was charged with 2-bromo-4-methylphenol (1.8 g, 10.0 mmol) and degassed with argon for three times. Then, dry diethyl ether (50 mL) was added via a syringe and cooled to -78 ^oC in a dry ice acetone bath. After that, *n*-BuLi (2.5 M in hexane) (10.0 mL, 2.5 equiv.) was added very slowly and the resulting solution was warmed to rt and stirred for 3 h. Then, D_2O (5.0 mL) was added dropwise to the solution, resulting in the formation of a white precipitate. Upon completion (monitored by GC-MS), 10% aqueous HCl (20 mL) was added slowly and then reaction mixture was extracted with diethyl ether (100 mL) and washed with water (100 mL). Organic layer was dried over Na_2SO_4 and evaporated under reduced pressure. The crude mixture was purified by column chromatography (5% ethyl acetate in hexane) to afford 1.06 g (97%) of 2-*d*-4-methylphenol as yellow liquid. Spectral data are in accordance with reported literature data.[1]

Preparation of 4-methylphenyl-2-d trifluoromethanesulfonate:



An oven dried 2-neck 100 mL round bottom flask was charged with 2-d-4-methylphenol (1.0 g, 10.0 mmol) and degassed with argon for three times. Then, dry dichloromethane (50 mL) was added via a syringe and cooled to 0 ^{0}C. After that, pyridine (1.6 mL, 2.0 equiv.) was added dropwise and stirred at 0 ^{0}C for 30 min. Then, Tf_2O (1.7 mL, 1.0 equiv.) was added dropwise and the resulting solution was warmed to rt and stirred for 2 h. Upon completion (monitored by GCMS), the mixture was poured into water and extracted with diethyl ether (200 mL). Then, ether layer was washed sequentially with water (20 mL x 2), 10 % aqueous hydrochloric acid solution (20 mL x 2). Organic layer was dried over Na_2SO_4 and evaporated under reduced pressure. The crude mixture was purified by column chromatography (10 % ethyl acetate in hexane) to afford 2.24 g (93%) of 4-methylphenyl-2-d-trifluoromethanesulfonate as yellow liquid. Spectral data are in accordance with reported literature data.[1]

Preparation of 8-(4-methylphenyl-2-d)tetrazolo[1,5-a]pyridine (13-d):

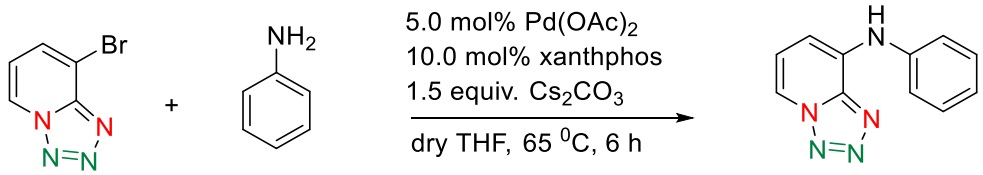


Step-I: In an argon-filled glove box, a 5 mL wheaton microreactor was charged with $PdCl_2$•dppf (10.9 mg, 1.5 mol %), KOAc (196.0 mg, 2.0 equiv.), B_2pin_2 (304.8 mg, 1.0 equiv.), 8-bromotetrazolo[1,5-a]pyridine (238.8 mg, 1.2 mmol) and dry THF (4.0 mL). The microreactor was sealed and heated at 100 °C for 12 h. Upon completion (judged by GC/MS), the reaction mixture was cooled to room temperature. Then the reaction mixture was passed through a short pad of

celite and eluted with ethyl acetate (50 mL). Then solvent was evaporated and without any further purification the crude product was used for next step.

Step-II: An oven dried 2-neck 50 mL round bottom flask equipped with a condenser and a magnetic stirrer under an argon atmosphere was charged with borylated crude product, 4-methylphenyl-2-d trifluoromethanesulfonate (289.4 mg,1.0 equiv.), K_2CO_3 (496.8 mg, 3.0 equiv.) and $Pd(PPh_3)_4$ (69.3 mg, 5.0 mol%). Then the system was degassed well. After that, DME and water 5.0 mL each (1:1) was added into the flask via a syringe. Reaction mixture was heated at 80 ^{o} C for 12 h. After completion (judged by TLC), the reaction mixture was cooled to room temperature and extracted with ethyl acetate (20 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and chromatographic separation with silica gel (30% ethyl acetate in hexane as eluent) gave 152.0 mg (60%) of 8-(4-methylphenyl-2-d)tetrazolo[1,5-a]pyridine (**13-d)** as white solid. Spectral data are in accordance with reported literature data.[1]

Preparation of N-phenyltetrazolo[1,5-a]pyridin-8-amine (15):



1.0 mmol 1.0 equiv. 53% yield

In an argon filled glove box, a 5.0 mL wheaton micrreactor with a stir bar were charged with 8-bromotetrazolo[1,5-a]pyridine (199.0 mg, 1.0 mmol), $Pd(OAc)_2$ (11.2 mg, 5.0 mol%), xanthphos (58.0 mg, 10.0 mol%), and aniline (93.0 mg, 1.0 equiv). The seal-tube was capped tightly and placed into a preheated aluminium block at 65 ^{o}C for 6 h. After being stirred at 65 °C for 6 h, the reaction mixture was poured into water and then the product was extracted with ethyl acetate (three times). The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel (eluent 20% ethyl acetate in hexane) to afford the corresponding *N*-phenyltetrazolo[1,5-a]pyridin-8-amine (**15**) product with 53% (112.0 mg) isolated yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (d, J = 6.4 Hz, 1H), 7.43 (t, J = 7.2 Hz, 2H), 7.34 (d, J = 7.6 Hz, 3H), 7.18 (t, J = 7.6 Hz, 1H), 7.12 (d, J = 7.6 Hz, 1H), 7.03 (t, J = 7.2 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 143.5, 138.9, 133.0, 129.8, 124.6, 121.5, 118.0, 114.6, 105.2.

HRMS (ESI) *m/z*calcd for $C_{11}H_9N_5$ $[M+H]^+$ 212.0936, found 212.0925.

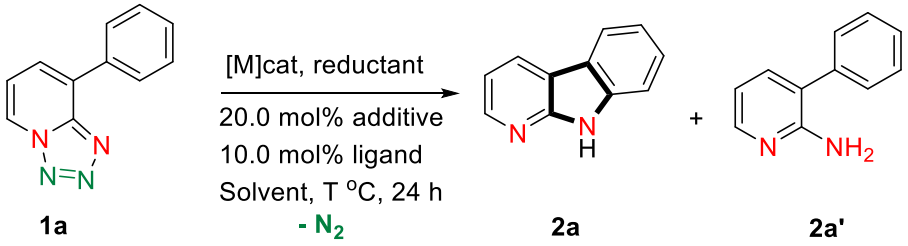
Preparation of (Z)-8-styryltetrazolo[1,5-a]pyridine (17):

(*Z*)-8-styryltetrazolo[1,5-a]pyridine (**17**) was prepared following the reported procedure.[1]

Reaction Optimization for C(sp^2)-H Amination:

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with 5.0 mol% catalyst, 20.0 mol% additive,10.0 mol% reductant and tetrazole **1a** (49.0 mg, 0.25 mmol), and dry solvent (1.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at mentioned temperature. The reaction mixture was stirred for 24 h and conversions were measured by NMR using 1,3,5-trimethoxybenzene as internal standard.

Initial Optimization:

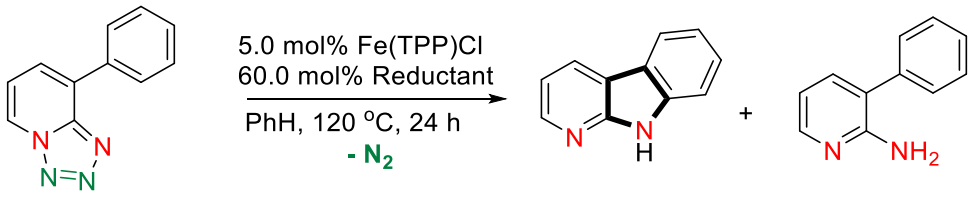


#	Catalyst (mol%)	Reductant (mol%)	Additive (mol%)	Ligand (mol%)	Solvent	T °C	2a/2a′
1	Mn(TPP)Cl (5)	-	-	-	PhH	120 °C	0/0
2	Mn(TPP)Cl (5)	-	-	-	PhMe	120 °C	0/0
3	Mn(TPP)Cl (5)	-	-	-	DCE	120 °C	0/0
4	Mn(TPP)Cl (5)	-	-	-	PhCl	120 °C	0/0
5	Mn(TPP)Cl (5)	-	-	-	PhCl	150 °C	0/0
6	Co(TPP) (5)	-	-	-	PhH	120 °C	0/0
7	Co(F_{20}TPP) (5)	-	-	-	PhH	120 °C	0/0
8	Mn(TPP)Cl (5)	-	$AgSbF_6$(20)	-	PhH	120 °C	0/0
9	Mn(TPP)Cl (5)	-	$AgBF_4$ (20)	-	PhH	120 °C	0/0
9	Mn(TPP)Cl (5)	-	AgOAc (20)	-	PhH	120 °C	0/0
10	Mn(TPP)Cl (5)	-	TMP (10)	-	PhH	120 °C	0/0
11	Mn(TPP)Cl (5)	-	bpy (10)	-	PhH	120 °C	0/0
12	Mn(TPP)Cl (5)	-	dtbpy (10)	-	PhH	120 °C	0/0
13	Fe(TPP)Cl (5)	-	-	-	PhH	120 °C	0/0
14	Fe(TPP)Cl (5)	-	-	-	PhMe	120 °C	0/0

15	Fe(TPP)Cl (5)	-	-	-	DCE	120 ^{0}C	0/0
16	Fe(TPP)Cl (5)	-	-	-	PhCl	120 ^{0}C	0/0
17	Fe(TPP)Cl (5)	-	-	-	PhCl	150 ^{0}C	0/0
18	Fe(TPP)Cl (5)	-	$AgSbF_6$(20)	-	PhH	120 ^{0}C	0/0
19	Fe(TPP)Cl (5)	-	$AgBF_4$ (20)	-	PhH	120 ^{0}C	0/0
20	Fe(TPP)Cl (5)	-	AgOAc (20)	-	PhH	120 ^{0}C	0/0
21	Fe(TPP)Cl (5)	-	TMP (10)	-	PhH	120 ^{0}C	0/0
22	Fe(TPP)Cl (5)	-	bpy (10)	-	PhH	120 ^{0}C	0/0
23	Fe(TPP)Cl (5)	-	dtbpy (10)	-	PhH	120 ^{0}C	0/0
24	Mn(TPP)Cl (5)	Zn (10)	-	-	PhH	120 ^{0}C	0/0
25	Mn(TPP)Cl (5)	Zn (10)	-	-	PhMe	120 ^{0}C	0/0
26	Mn(TPP)Cl (5)	Zn (10)	-	-	PhH	150 ^{0}C	0/10
27	Mn(TPP)Cl (5)	Zn (10)	-	-	PhMe	150 ^{0}C	0/10
28	Fe(TPP)Cl (5)	Zn (10)	-	-	PhH	120 ^{0}C	10/5
29	Fe(TPP)Cl (5)	Zn (10)	-	-	PhH	150 ^{0}C	15/10 (3%) [a]
30	Fe(TPP)Cl (5)	Zn (10)	-	-	PhMe	120 ^{0}C	20/50 (11%) [a]
31	Fe(TPP)Cl (5)	Zn (30)	-	-	PhH	120 ^{0}C	20/5 (20%) [a]
32	Fe(TPP)Cl (5)	Zn (40)	-	-	PhH	120 ^{0}C	40/5 (33%) [a]
33	Fe(TPP)Cl (5)	Zn (60)	-	-	PhH	120 ^{0}C	95/5 (92%) [a]
34	Fe(TPP)Cl (5)	-	-		PhH	120	0/0
35	-	Zn (10)	-		PhH	120	0/0
36	-	Zn (60)	-	-	PhH	120	0/7

TMP: 3,4,7,8-Tetramethyl-1,10-phenanthroline; dtbpy: 4,4′-Di-tert-butyl-2,2′-dipyridyl; bpy: bipyridine. [a]In parenthesis isolated yield is given.

Reductant Screening:

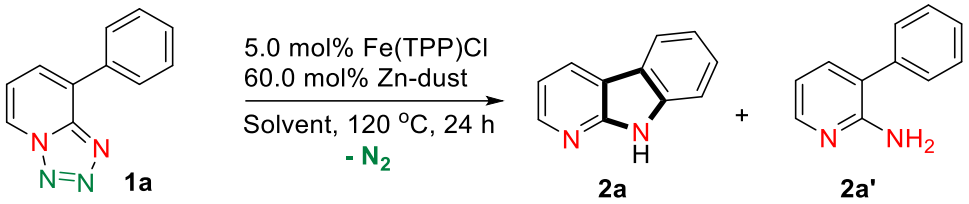


1a **2a** **2a'**

#	Catalyst	Reductant	Solvent	T °C	2a/2a′
1	Fe(TPP)Cl	Zn	PhH	120	95/5

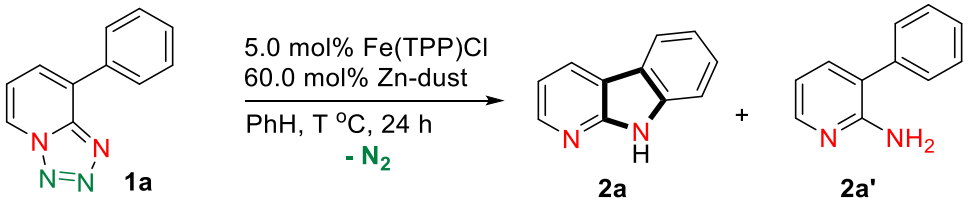
2	Fe(TPP)Cl	$NaBH_4$	PhH	120	0/0
3	Fe(TPP)Cl	$LiAlH_4$	PhH	120	0/0
4	Fe(TPP)Cl	Mn	PhH	120	0/0
5	Fe(TPP)Cl	Raney-Ni	PhH	120	0/0

Solvent Screening:



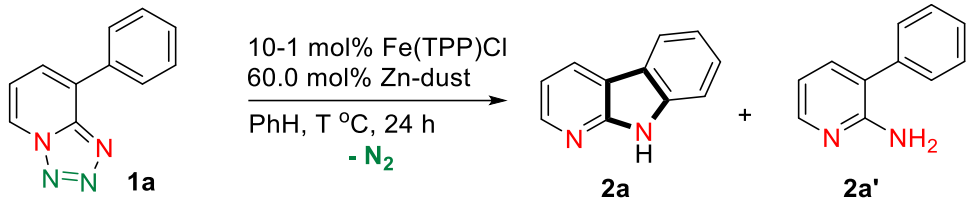
#	Catalyst	Reductant	Solvent	T °C	2a/2a′
1	Fe(TPP)Cl	Zn	PhH	120	95/5
2	Fe(TPP)Cl	Zn	PhMe	120	20/50
3	Fe(TPP)Cl	Zn	DCE	120	0/0
4	Fe(TPP)Cl	Zn	THF	120	0/0
5	Fe(TPP)Cl	Zn	1,4-dioxane	120	0/0

Temperature Screening:



#	Catalyst	Reductant	Solvent	T °C	2a/2a′
1	Fe(TPP)Cl	Zn	PhH	80	0/0
2	Fe(TPP)Cl	Zn	PhH	100	20/0
3	Fe(TPP)Cl	Zn	PhH	120	95/5
4	Fe(TPP)Cl	Zn	PhH	130	96/4
5	Fe(TPP)Cl	Zn	PhH	150	80/20

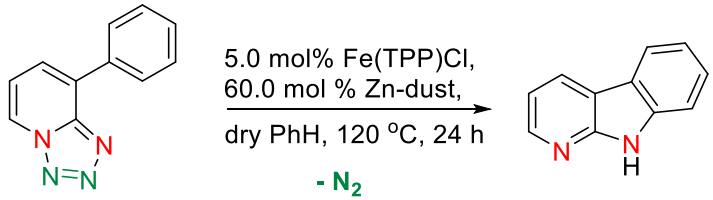
Catalyst Loading Studies:



#	Catalyst	mol%	Reductant	Solvent	T °C	Time (h)	2a/2a′
1	Fe(TPP)Cl	10.0	Zn	PhH	120	12	95/5
2	Fe(TPP)Cl	5.0	Zn	PhH	120	24	95/5
3	Fe(TPP)Cl	4.0	Zn	PhH	120	24	90/5
4	Fe(TPP)Cl	3.0	Zn	PhH	120	24	85/5
5	Fe(TPP)Cl	2.0	Zn	PhH	120	24	70/5
6	Fe(TPP)Cl	1.0	Zn	PhH	120	24	44/5

Intramolecular C(sp^2)–H Amination of Tetrazoles:

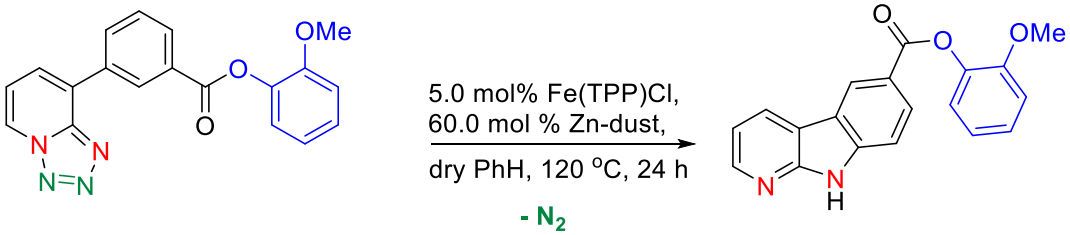
Amination reaction of tetrazole 1a:



1a: 0.25 mmol **2a:** 92%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (8.8 mg, 5.0 mol%), Zn-dust (9.8 mg, 60.0 mol%) and dry benzene (1.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1a)** (49.0 mg, 0.25 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (in DCM) gave 38.7 mg (92%) aminated product **(2a)** as white solid. Spectral data are in accordance with reported data.[1]

Amination reaction of tetrazole 1b:



1b: 0.5 mmol **2b:** 75%

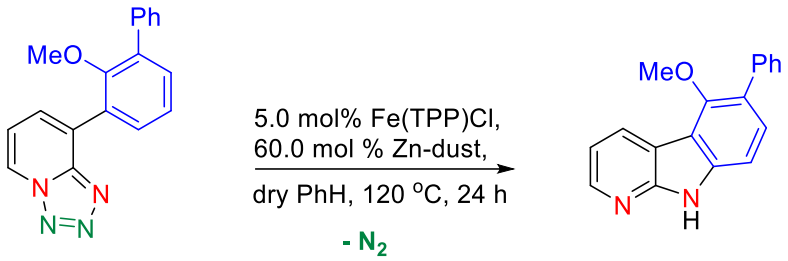
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1b)** (173.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (in 20 % ethyl acetate in DCM) gave 119.4 mg (75%) aminated product **(2b)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.38 (s, 1H), 9.03 (s, 1H), 8.73 (d, J = 7.6 Hz, 1H), 8.50 (d, J = 4.8 Hz, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.67 (d, J = 8.4 Hz, 1H), 7.31 – 7.24 (m, 3H), 7.19 (d, J = 8.0 Hz, 1H), 7.02 (t, J = 7.6 Hz, 1H), 3.76 (s, 3H)

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.7, 152.6, 151.2, 147.1, 142.3, 139.7, 129.6, 128.3, 127.0, 124.3, 123.2, 120.7, 120.5, 119.7, 116.1, 115.4, 112.9, 111.5, 52.1.

HRMS (ESI) *m/z*calcd for $C_{19}H_{14}N_2O_3$ $[M+H]^+$ 319.1083, found 319.1077.

Amination reaction of tetrazole 1c:



1c: 0.5 mmol **2c:** 92%

In an argon-filled glove box, a 5.0 mL wheatonmicroreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1c)** (151.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (in 10 % ethyl acetate in DCM) gave126.2 mg (92%) aminated product **(2c)** as white solid.

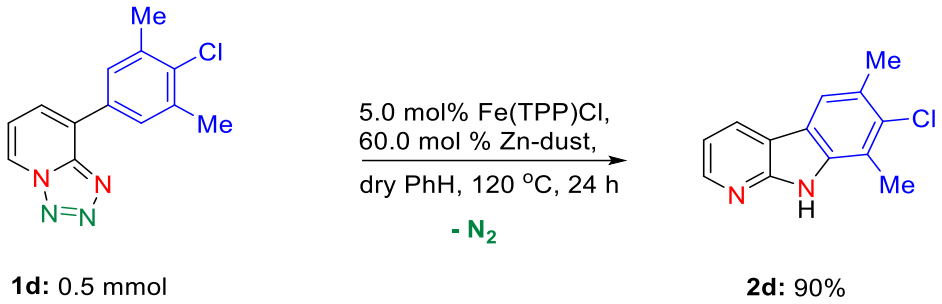
Melting Point: >200 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.99 (s, 1H), 8.45 (dd, J = 11.2 Hz, J = 8.0 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.48-7.44 (m, 3H), 7.37 – 7.32 (m, 2H), 7.25 (dd, J = 7.6 Hz, J = 4.4 Hz, 1H), 3.61 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0, 151.9, 146.0, 140.0, 138.4, 130.1, 129.5, 129.1, 128.4, 126.7, 124.8, 115.5, 113.9, 113.9, 107.7, 60.0.

HRMS (ESI) *m/z*calcd for $C_{18}H_{14}N_2O$ $[M+H]^+$ 275.1184, found 275.1166.

Amination reaction of tetrazole 1d:



1d: 0.5 mmol

2d: 90%

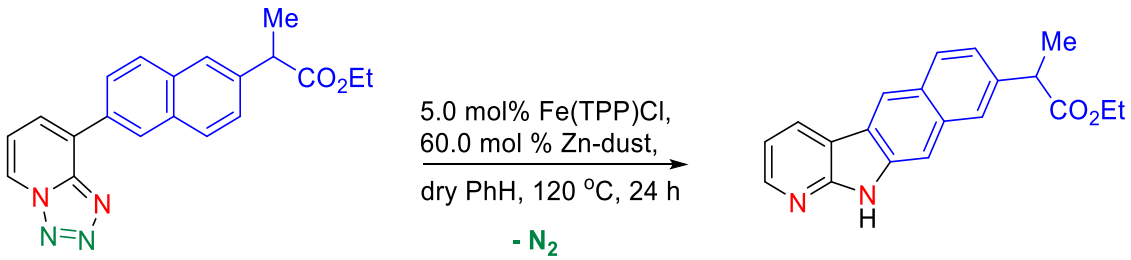
In an argon-filled glove box, a 5.0 mL wheatonmicroreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1d)** (129.3 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (in DCM) gave 103.8 mg (90%) aminated product **(2d)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.84 (s, 1H), 8.43 (t, J = 8.4 Hz, 2H), 7.97 (s, 1H), 7.21 (dd, J = 31.6, J = 8.8 Hz, 1H), 2.60 (s, 3H), 2.46 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 146.2, 137.3, 131.7, 128.5, 126.5, 120.0, 118.8, 118.6, 115.2, 115.1, 20.8, 14.9.

HRMS (ESI) *m/z*calcd for $C_{13}H_{11}ClN_2$ $[M+H]^+$ 231.0689, found 231.0677.

Amination reaction of tetrazole 1e:



1e: 0.5 mmol

2e: 81%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The

reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1e)** (173.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 20% ethyl acetate in DCM as eluent) gave 128.9 mg (81%) aminated product **(2e)** as white solid.

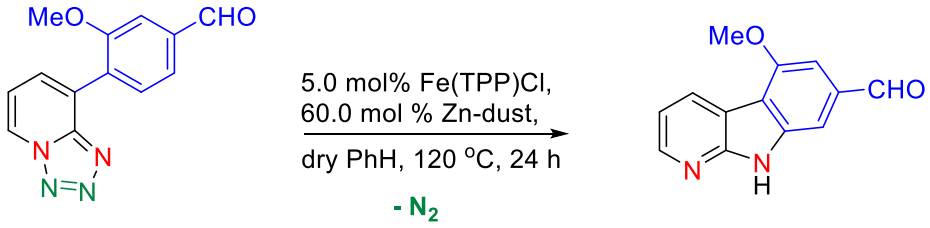
Melting Point: >200 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.74 (s, 1H), 8.57 (dd, J = 12.0 Hz, J = 8.8 Hz, 2H), 8.46 (d, J = 4.4 Hz, 1H), 8.22 (d, J = 8.4 Hz, 1H), 7.93 (s, 1H), 7.67 (d, J = 8.4 Hz, 1H), 7.57 (d, J = 8.4 Hz, 1H), 7.27 (dd, J = 7.6, J = 4.8 Hz, 1H), 4.12 – 4.04 (m, 2H), 3.99 (q, J = 7.2 Hz, 1H), 1.52 (d, J = 7.2 Hz, 3H), 1.13 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 173.9, 151.1, 145.3, 138.2, 134.6, 132.3, 128.0, 126.8, 125.5, 122.7, 120.1, 120.1, 119.9, 115.9, 115.6, 115.3, 60.4, 18.6, 14.0.

HRMS (ESI) *m/z* calcd for $C_{20}H_{18}N_2NaO_2$ $[M+Na]^+$ 341.1266, found 341.1256.

Amination reaction of tetrazole 1f:



1f: 0.5 mmol **2f:** 82%

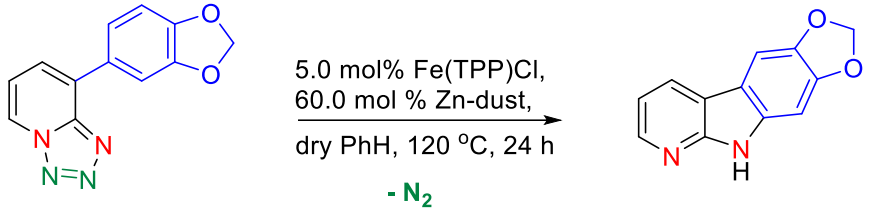
In an argon-filled glove box, a 5.0 mL wheatonmicroreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1f)** (127.1mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 92.8 mg (82%) aminated product **(2f)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.29 (s, 1H), 10.10 (s, 1H), 8.50 (d, J = 8.8 Hz, 2H), 7.73 (s, 1H), 7.30 – 7.27 (m, 2H), 4.11 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 193.0, 156.2, 152.2, 147.1, 139.3, 135.7, 131.0, 116.0, 114.1, 113.7, 108.6, 99.2, 55.9.

HRMS (ESI) *m/z*calcd for $C_{13}H_{10}N_2O_2$ $[M+H]^+$ 227.0821, found 227.0794.

Amination reaction of tetrazole 1g:



1g: 0.5 mmol

2g: 93%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1g)** (120.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 5% ethyl acetate in DCM) gave 98.7 mg (93%) aminated product **(2g)** as white solid.

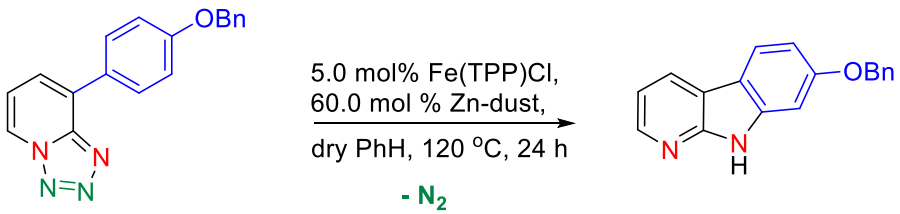
Melting Point: >200 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.64 (s, 1H), 8.30 (dd, J = 18.8 Hz, J = 3.6 Hz, 2H), 7.67 (s, 1H), 7.11 (dd, J = 6.8 Hz, J = 4.8 Hz, 1H), 7.02 (s, 1H), 6.05 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 151.6, 147.4, 144.2, 142.1, 134.4, 127.2, 115.7, 114.7, 113.2, 100.9, 100.3, 92.5.

HRMS (ESI) *m/z*calcd for $C_{12}H_8N_2O_2$ $[M+H]^+$ 213.0664, found 213.0652.

Amination reaction of tetrazole 1h:



1h: 0.5 mmol

2h: 88%

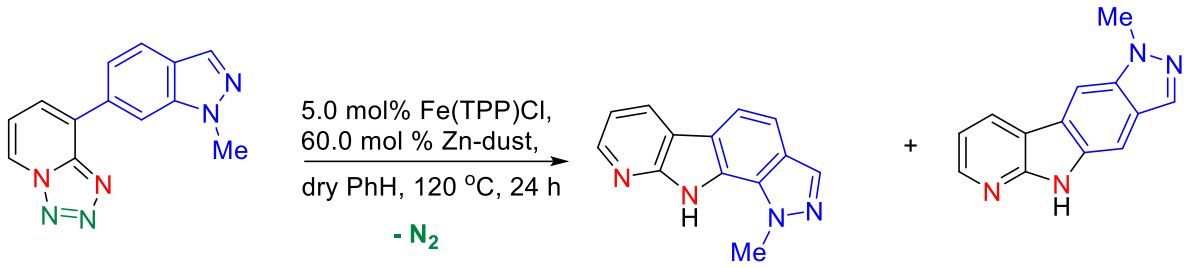
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1h)** (151.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 120.7 mg (88%) aminated product **(2h)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.68 (s, 1H), 8.34 (d, J = 7.6 Hz, 1H), 8.31 (d, J = 4.4 Hz, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.49 (d, J = 7.6 Hz, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.33 (t, J = 7.2 Hz, 1H), 7.14 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 7.07 (s, 1H), 6.92 (d, J = 7.6 Hz, 1H), 5.20 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 158.1, 152.1, 144.4, 140.2, 137.2, 128.4, 127.8, 127.6, 127.1, 122.1, 115.5, 115.0, 114.2, 109.2, 96.0, 69.5.

HRMS (ESI) *m/z* calcd for $C_{18}H_{14}N_2O$ $[M+H]^+$ 275.1184, found 275.1163.

Amination reaction of tetrazole 1i:

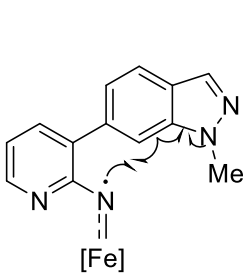


1i: 0.5 mmol **2i:** 83% **2i':** 0%

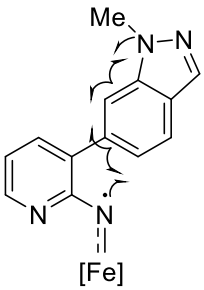
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1i)** (125.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 92.2 mg (83%) aminated product **(2i)** as white solid.

Note: From manuscript

In particular, tetrazole **1i** reacted differently from other tetrazoles. Generally, we noticed regioselectivity mainly governed by the steric effect (attack on nitrene happened from less hindered side). But in case of **1i** electronic might plays major roll rather steric effect. Here, the ortho stabilization (**Int-I**) win the race compare to the para-stabilization (**Int-II**) leading **2i** exclusively.



Int-I



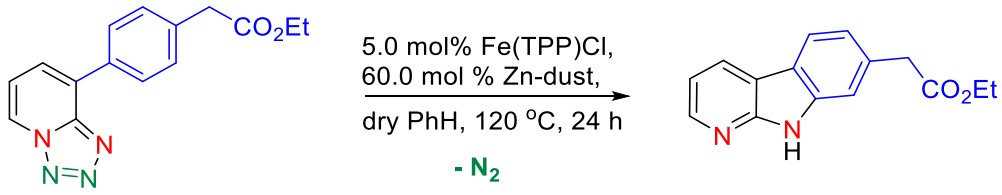
Int-II

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.46 (s, 1H), 8.54 (d, J = 7.6 Hz, 1H), 8.48 (d, J = 4.8Hz, 1H), 8.12 (s, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 8.4 Hz, 1H), 7.27 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 4.46 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 151.4, 145.4, 133.4, 128.4, 128.1, 123.6, 122.9, 117.4, 115.8, 115.8, 114.4, 112.6, 38.3.

HRMS (ESI) *m/z*calcd for $C_{13}H_{10}N_4$ $[M+H]^+$ 223.0984, found 223.0970.

Amination reaction of tetrazole 1j:



1j: 0.5 mmol

2j: 83%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1j)** (141.1 mg, 0.5 mmol). The microreactor was capped with a teflon

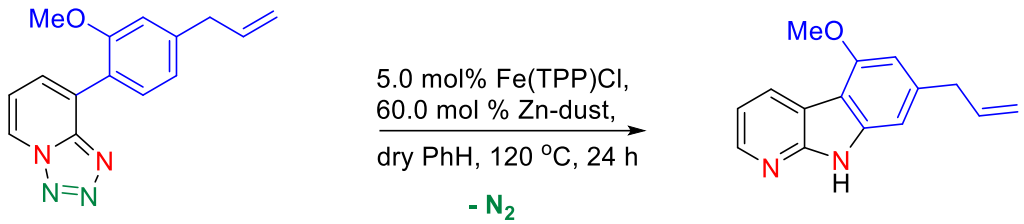
pressure cap and placed into a pre-heated aluminium block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 105.5 mg (83%) aminated product **(2j)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.77 (s, 1H), 8.46 (d, J = 7.6 Hz, 1H), 8.39 (d, J = 4.0 Hz, 1H), 8.08 (d, J = 8.0 Hz, 1H), 7.41 (s, 1H), 7.19 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 7.11 (d, J = 7.6 Hz, 1H), 4.09 (q, J = 7.2 Hz, 2H), 3.82 (s, 2H), 1.24-1.16 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.4, 152.1, 145.9, 139.0, 133.0, 128.3, 121.0, 121.0, 119.2, 115.1, 115.0, 111.9, 60.3, 14.1.

HRMS (ESI) *m/z*calcd for $C_{15}H_{14}N_2O_2$ $[M+H]^+$ 255.1134, found 255.1125.

Amination reaction of tetrazole 1k:



1k: 0.5 mmol

2k: 94%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1k)** (133.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using in DCM) gave 112.0 mg (94%) aminated product **(2k)** as white solid.

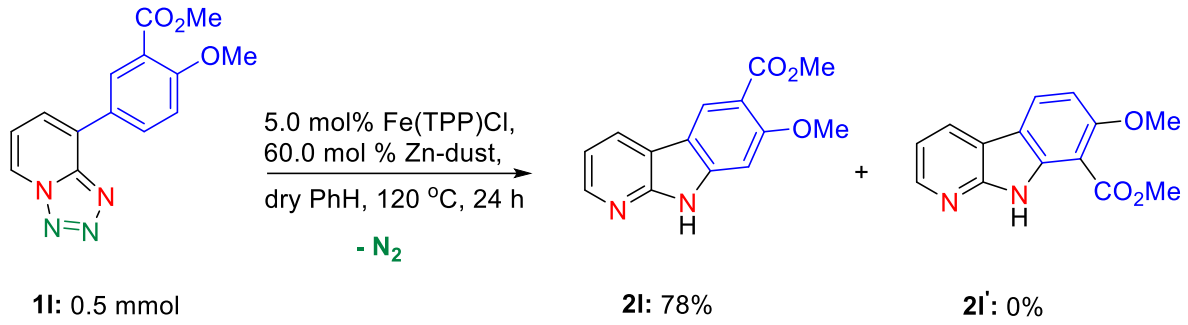
Melting Point: 165-167 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.63 (s, 1H), 8.50 (d, J = 7.2 Hz, 2H), 7.23 – 7.17 (m, 1H), 7.02 (s, 1H), 6.56 (s, 1H), 6.14-6.03 (m, 1H), 5.24 – 5.09 (m, 2H), 4.06 (s, 3H), 3.58 (d, J = 6.8 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 151.8, 143.5, 140.6, 140.4, 137.5, 130.4, 116.1, 115.9, 115.2, 108.6, 104.0, 101.7, 55.3, 41.2.

HRMS (ESI) *m/z*calcd for $C_{15}H_{14}N_2O$ $[M+H]^+$ 239.1184, found 239.1173.

Amination reaction of tetrazole 1l:



1l: 0.5 mmol **2l:** 78% **2l':** 0%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1l)** (142.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 99.9 mg (78%) aminated product **(2l)** as white solid.

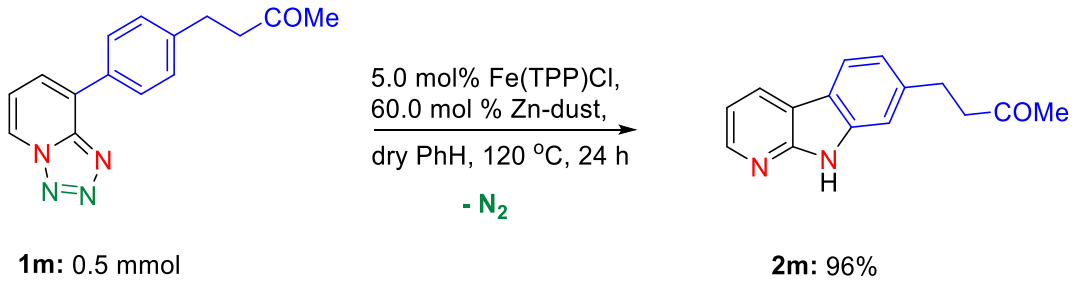
Note: We observed amination from less hindered site.

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.00 (s, 1H), 8.55 (s, 1H), 8.49 (d, J = 7.6 Hz, 1H), 8.35 (d, J = 4.8 Hz, 1H), 7.20 (dd, J = 7.5 Hz, J = 5.2 Hz, 1H), 7.07 (s, 1H), 3.91 (s, 3H), 3.81 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2, 158.6, 152.6, 145.2, 142.7, 128.0, 125.1, 115.8, 115.6, 113.2, 112.8, 94.1, 56.0, 51.7.

HRMS (ESI) *m/z* calcd for $C_{14}H_{12}N_2O_3$ $[M+H]^+$ 257.0926, found 257.0918.

Amination reaction of tetrazole 1m:



1m: 0.5 mmol **2m:** 96%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1m)** (133.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 114.4 mg (96%) aminated product **(2m)** as white solid.

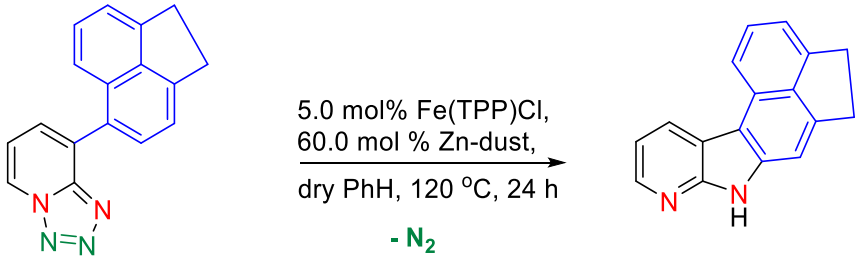
Melting Point: 167-169 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.67 (s, 1H), 8.50 (d, J = 4.8 Hz, 1H), 8.30 (d, J = 7.6 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.36 (s, 1H), 7.20 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 7.11 (d, J = 8.0 Hz, 1H), 3.09 (t, J = 7.6 Hz, 2H), 2.86 (t, J = 7.6 Hz, 2H), 2.16 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.9, 152.3, 145.0, 140.4, 139.1, 128.2, 121.0, 120.6, 119.3, 116.5, 115.2, 110.8, 45.5, 30.4, 30.1.

HRMS (ESI) *m/z*calcd for $C_{15}H_{14}N_2O$ $[M+H]^+$ 239.1184, found 239.1161.

Amination reaction of tetrazole 1n:



1n: 0.5 mmol **2n:** 97%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1n)** (136.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure

and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 118.5 mg (97%) aminated product **(2n)** as white solid.

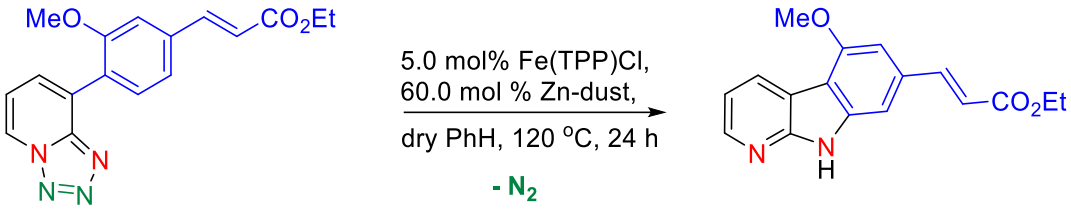
Melting Point: >200 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.15 (s, 1H), 8.79 (d, J = 7.6 Hz, 1H), 8.40 (d, J = 4.4 Hz, 1H), 8.30 (d, J = 8.4 Hz, 1H), 7.64 (t, J = 7.6 Hz, 1H), 7.51 (s, 1H), 7.32 – 7.28 (m, 2H), 3.45 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 150.5, 146.6, 146.1, 143.8, 139.4, 134.4, 129.1, 128.5, 127.0, 118.5, 117.4, 115.8, 115.6, 109.5, 106.6, 30.5, 29.6.

HRMS (ESI) *m/z*calcd for $C_{17}H_{12}N_2$ $[M+H]^+$ 245.1079, found 245.1069.

Amination reaction of tetrazole 1o:



1o: 0.5 mmol

2o: 76%

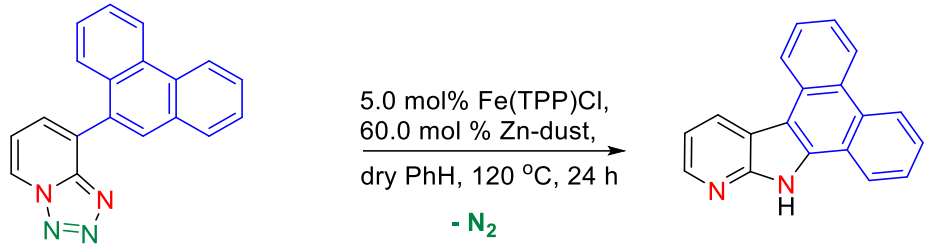
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 ^{o}C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1o)** (162.2mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 ^{o}C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 112.6 mg (76%) aminated product **(2o)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.01 (s, 1H), 8.40 -8.38 (m, 2H), 7.80 (d, J = 16.0 Hz, 1H), 7.40 (s, 1H), 7.23 – 7.17 (m, 2H), 6.76 (d, J = 15.6Hz, 1H), 4.21 (q, J = 6.8 Hz, 2H), 4.07 (s, 3H), 1.28 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.5, 156.1, 151.8, 145.9, 145.6, 139.9, 133.7, 130.1, 117.9, 115.7, 114.1, 111.3, 106.1, 99.7, 60.0, 55.9, 14.3.

HRMS (ESI) *m/z*calcd for $C_{17}H_{16}N_2O_3$ $[M+H]^+$ 297.1239, found 297.1226.

Amination reaction of tetrazole 1p:



1p: 0.5 mmol

2p: 91%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1p)** (148.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 122.1 mg (91%) aminated product **(2p)** as white solid.

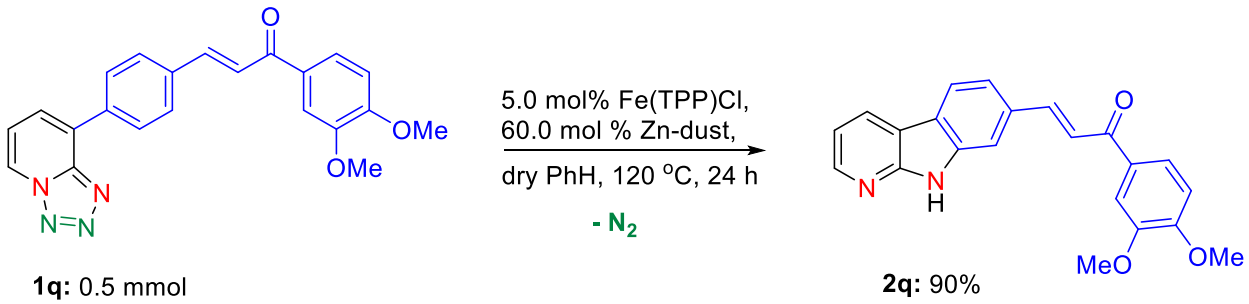
Melting Point: >200 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.96 (s, 1H), 8.96-8.90 (m, 3H), 8.76 (d, J = 8.0 Hz, 1H), 8.70 (d, J = 7.6 Hz, 1H), 8.50 (d, J = 4.8 Hz, 1H), 7.80 – 7.74 (m, 3H), 7.62 (t, J = 7.6 Hz, 1H), 7.37 (dd, J = 7.8 Hz, J = 4.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 144.5, 134.0, 129.7, 129.4, 129.1, 127.8, 127.2, 127.1, 126.4, 124.2, 124.1, 124.0, 123.5, 122.9, 122.3, 116.3, 116.2, 109.8.

HRMS (ESI) *m/z*calcd for $C_{19}H_{12}N_2$ $[M+H]^+$ 269.1079, found 269.1070.

Amination reaction of tetrazole 1q:



1q: 0.5 mmol

2q: 90%

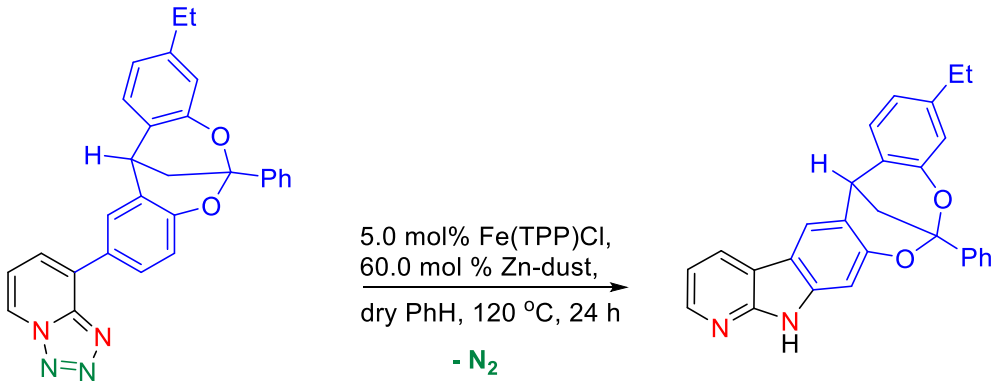
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1q)** (193.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 161.3 mg (90%) aminated product **(2q)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.96 (s, 1H), 8.54 (d, J = 7.6 Hz, 1H), 8.45 (d, J = 4.8 Hz, 1H), 8.21 (d, J = 8.4 Hz, 1H), 7.80 (s, 1H), 7.73 (d, J = 15.6 Hz, 1H), 7.66-7.61 (m, 3H), 7.23 (dd, J = 7.6 Hz, J = 5.2 Hz, 1H), 6.71 (s, 1H), 6.66 (d, J = 8.4 Hz, 1H), 3.93 (s, 3H), 3.86 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 189.3, 164.0, 160.3, 152.6, 146.9, 142.3, 139.0, 133.2, 132.1, 129.0, 126.6, 122.2, 121.7, 121.6, 119.6, 115.5, 114.9, 111.6, 106.1, 98.7, 56.1, 55.7.

HRMS (ESI) *m/z*calcd for $C_{22}H_{18}N_2O_3$ $[M+H]^+$ 359.1396, found 359.1388.

Amination reaction of tetrazole 1r:



1r: 0.5 mmol

2r: 72%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1r)** (223.3 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure

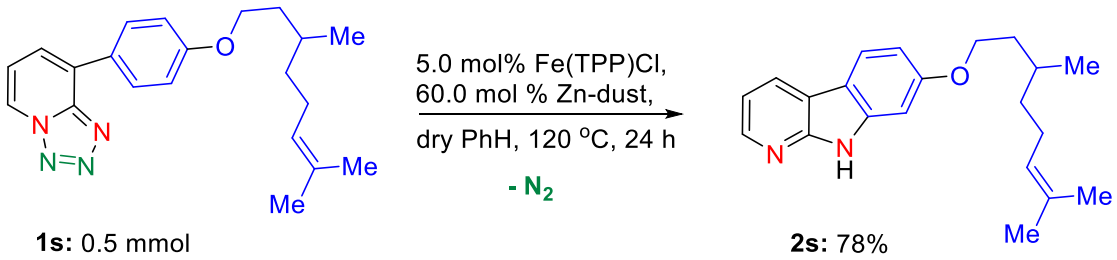
and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 150.7 mg (72%) aminated product **(2r)** as white solid.

^{1}H NMR (400 MHz, DMSO-d_6): δ 11.60 (s, 1H), 8.37 (d, J = 7.6 Hz, 1H), 8.31 (s, 1H), 8.18 (s, 1H), 7.76 (d, J = 7.2 Hz, 2H), 7.53 – 7.43 (m, 3H), 7.32 (s, 1H), 7.17 – 7.14 (m, 1H), 7.01 – 6.96 (m, 2H), 6.88 (d, J = 8.0 Hz, 1H), 5.75 (s, 1H), 5.29 (s, 1H), 4.38 (s, 1H), 2.47 – 2.41 (m, 2H), 1.15 (t, J = 7.6 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 152.4, 151.2, 149.2, 144.8, 141.4, 139.0, 136.8, 128.8, 128.3, 127.4, 127.0, 126.9, 125.6, 120.4, 119.6, 116.0, 115.3, 115.0, 114.9, 98.6, 97.8, 79.2, 33.1, 32.5, 27.4, 15.6.

HRMS (ESI) *m/z*calcd for $C_{28}H_{22}N_2O_2$ $[M+H]^+$ 419.1760, found 419.1737.

Amination reaction of tetrazole 1s:



1s: 0.5 mmol

2s: 78%

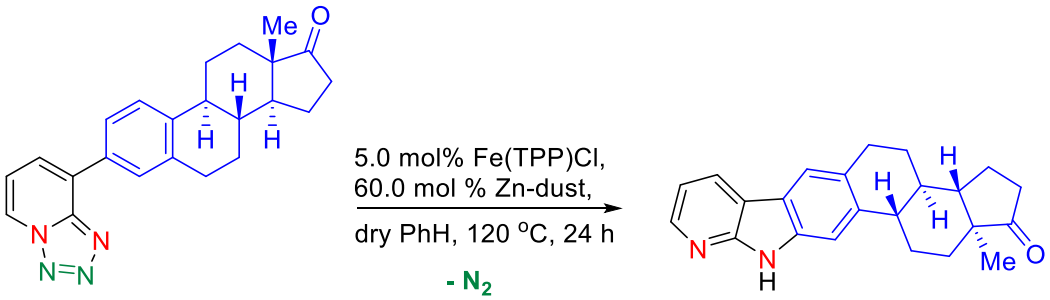
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1s)** (175.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 125.8 mg (78%) aminated product **(2s)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.37 (s, 1H), 8.42 (d, J = 4.4 Hz, 1H), 8.23 (d, J = 7.6 Hz, 1H), 7.92 (d, J = 8.4 Hz, 1H), 7.17 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 7.01 (d, J = 1.6 Hz, 1H), 6.89 (dd, J = 8.8 Hz, J = 2.0 Hz, 1H), 5.13 (t, J = 6.8 Hz, 1H), 4.14- 4.09 (m, 2H), 2.09 – 2.00 (m, 2H), 1.94 – 1.88 (m, 1H), 1.75 – 1.68 (m, 4H), 1.62 (s, 3H), 1.49-1.40 (m, , 1H), 1.30-1.21 (m, 2H), 1.00 (d, J = 6.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.2, 152.4, 143.8, 140.1, 131.3, 127.2, 124.7, 121.8, 116.8, 115.3, 114.6, 109.4, 95.9, 66.7, 37.2, 36.2, 29.6, 25.7, 25.5, 19.6, 17.7.

HRMS (ESI) *m/z*calcd for $C_{21}H_{26}N_2O$ $[M+H]^+$ 323.2123, found 323.2120.

Amination reaction of tetrazole 1t:



1t: 0.5 mmol

2t: 85%

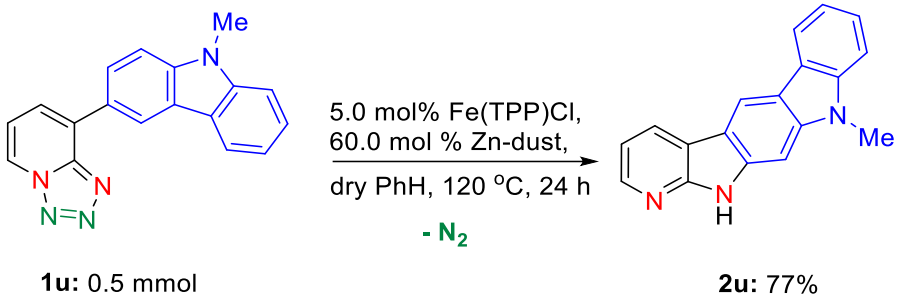
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1t)** (186.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 5% ethyl acetate in DCM) gave 146.4 mg (85%) aminated product **(2t)** as white solid.

^{1}H NMR (400 MHz, DMSO-d_6): δ 11.55 (s, 1H), 8.38 (d, J = 8.0Hz, 1H), 8.33 (d, J = 4.8 Hz, 1H), 7.83 (s, 1H), 7.37 (s, 1H), 7.13 (dd, J = 8.8 Hz, J = 8.4 Hz, 1H), 3.01 (dd, J = 8.3 Hz, J = 4.4 Hz, 2H), 2.43 – 2.39 (m, 2H), 2.11-1.96 (m, 4H), 1.82 (d, J = 12.4 Hz, 1H), 1.59 – 1.40 (m, 6H), 0.84 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 220.0, 152.4, 145.5, 139.3, 137.8, 128.0, 120.7, 118.6, 115.1, 114.8, 107.4, 50.0, 47.4, 44.4, 37.8, 35.5, 31.5, 29.1, 26.4, 25.7, 21.3, 13.6.

HRMS (ESI) *m/z*calcd for $C_{23}H_{24}N_2O$ $[M+H]^+$ 345.1967, found 345.1946.

Amination reaction of tetrazole 1u:



1u: 0.5 mmol

2u: 77%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1u)** (149.7 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 5% ethyl acetate in DCM) gave 104.5 mg (77%) aminated product **(2u)** as white solid.

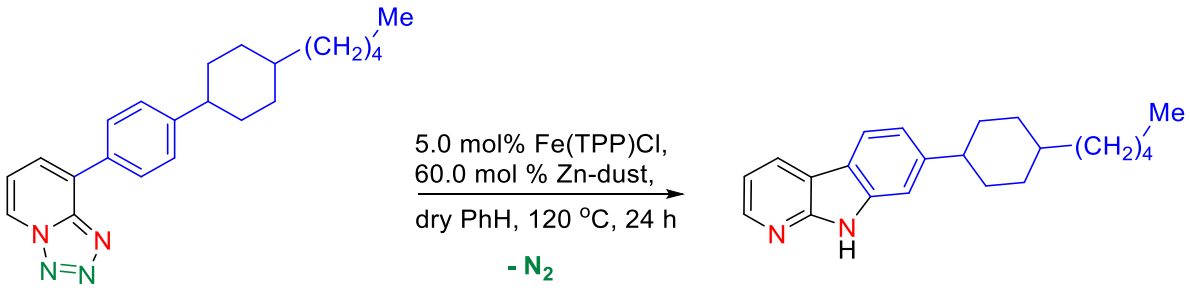
Melting Point: >200 °C

^{1}H NMR (400 MHz, DMSO-d_6): δ 11.81 (s, 1H), 8.91 (s, 1H), 8.50 (d, J = 7.2 Hz, 1H), 8.34 (d, J = 4.8 Hz, 1H), 8.19 (d, J = 7.6 Hz, 1H), 7.57 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 8.0 Hz, 2H), 7.21 (dd, J = 14.8 Hz, J = 8.0 Hz, 2H), 3.91 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 152.8, 144.5, 141.4, 141.2, 139.2, 127.0, 124.9, 122.7, 119.4, 118.7, 117.2, 116.2, 114.8, 112.7, 108.7, 89.6, 29.2.

HRMS (ESI) *m/z* calcd for $C_{18}H_{13}N_3$ $[M+H]^+$ 272.1188, found 272.1181.

Amination reaction of tetrazole 1v:



1v: 0.5 mmol

2v: 78%

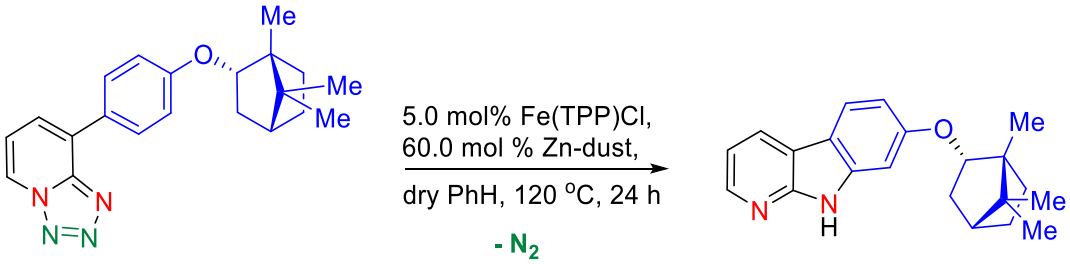
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1v)** (174.3 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 125.0 mg (78%) aminated product **(2v)** as white solid.

^{1}H NMR (400 MHz, DMSO-d_6): δ 11.64 (s, 1H), 8.40 (d, J = 7.6 Hz, 1H), 8.35 (d, J = 4.8 Hz, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.30 (s, 1H), 7.15(dd, J= 5.2 Hz, J= 7.6 Hz) 2.61 (t, J = 12.4 Hz, 1H), 1.86 (t, J = 12.8 Hz, 4H), 1.55-1.46 (m, 2H), 1.30 – 1.20 (m, 9H), 1.11-1.02 (m, 2H), 0.87 (t, J = 6.4Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 152.1, 146.5, 145.4, 139.2, 127.9, 127.4, 120.9, 119.0, 118.5, 115.3, 114.9, 108.8, 45.7, 44.5, 34.3, 33.2, 31.7, 26.1, 22.2, 14.0.

HRMS (ESI) *m/z* calcd for $C_{22}H_{28}N_2$ $[M+H]^+$ 321.2331, found 321.2309.

Amination reaction of tetrazole 1w:



1w: 0.5 mmol **2w:** 81%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1w)** (174.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure

and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 129.7 mg (81%) aminated product **(2w)** as white solid.

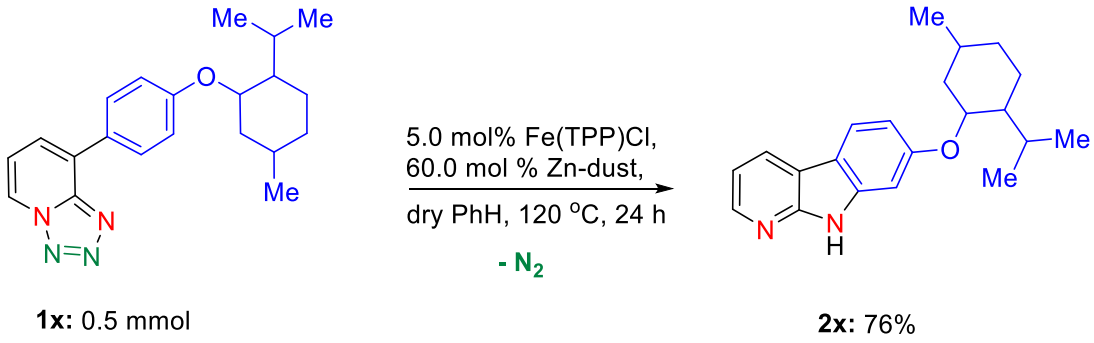
Melting Point: >200 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.78 (s, 1H), 8.42 (d, J = 4.8 Hz, 1H), 8.23 (d, J = 7.6 Hz, 1H), 7.91 (d, J = 8.8 Hz, 1H), 7.18 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 6.94 (s, 1H), 6.86 (dd, J = 8.4 Hz, J = 1.6 Hz, 1H), 4.46 (d, J = 8.4 Hz, 1H), 2.50-2.43 (m, J = 13.1, 8.9, 4.1 Hz, 1H), 2.37 – 2.27 (m, 1H), 1.85 – 1.76 (m, 2H), 1.44 -1.28 (m, 2H), 1.23 (dd, J = 13.2 Hz, J = 3.2 Hz, 1H), 1.01 (s, 3H), 0.99 (s, 3H), 0.95 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3, 152.5, 143.5, 140.3, 127.2, 121.7, 117.0, 115.2, 114.3, 110.1, 97.0, 83.3, 49.6, 47.6, 45.2, 37.0, 27.9, 26.8, 19.7, 19.0, 13.8.

HRMS (ESI) *m/z*calcd for $C_{21}H_{24}N_2O$ $[M+H]^+$ 321.1967, found 321.1963.

Amination reaction of tetrazole 1x:



1x: 0.5 mmol

2x: 76%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 ^{o}C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1x)** (175.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 ^{o}C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 122.5 mg (76%) aminated product **(2x)** as white solid.

Melting Point: >200 ^{o}C

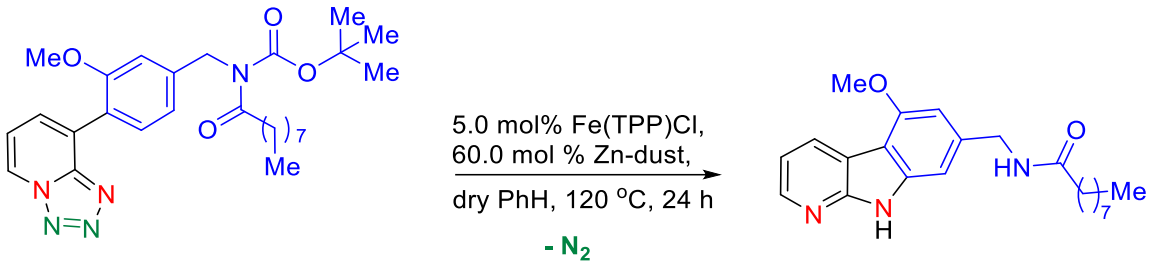
^{1}H NMR (400 MHz, $CDCl_3$): δ 10.08 (s, 1H), 8.40 (d, J = 4.8 Hz, 1H), 8.22 (d, J = 7.6 Hz, 1H), 7.91 (d, J = 8.8 Hz, 1H), 7.17 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 7.02 (d, J = 1.6 Hz, 1H), 6.89 (dd, J = 8.8 Hz, J = 1.6 Hz, 1H), 4.15 (td, J = 10.4 Hz, J = 4.0 Hz, 1H), 2.33 – 2.23 (m, 2H), 1.76 (d, J

= 11.6 Hz, 2H), 1.62 – 1.47 (m, 2H), 1.16-1.09 (m, 2H), 0.95 (t, J = 6.8 Hz, 7H), 0.82 (d, J = 8.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 158.5, 152.3, 148.7, 140.2, 127.2, 121.9, 116.9, 115.3, 114.7, 110.4, 97.5, 78.3, 48.2, 40.4, 34.5, 31.5, 26.2, 23.8, 22.1, 20.7, 16.6.

HRMS (ESI) *m/z*calcd for $C_{21}H_{26}N_2O$ $[M+H]^+$ 323.2123, found 323.2117.

Amination reaction of tetrazole 1y:



1y: 0.5 mmol

2y: 65%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1y)** (247.8 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 119.4 mg (65%) aminated product **(2y)** as white solid.

Note: Boc deprotection was observed after the reaction.

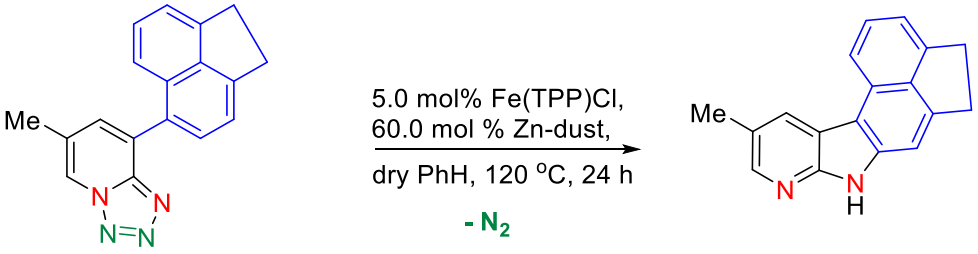
^{1}H NMR (400 MHz, DMSO-d_6): δ 11.76 (s, 1H), 8.40 (t, J = 5.2 Hz, 1H), 8.33 (s, 1H), 8.31 (d, J = 2.0 Hz, 1H), 7.18 – 7.14 (m, 1H), 6.99 (s, 1H), 6.68 (s, 1H), 4.40 (d, J = 6.0 Hz, 2H), 3.99 (s, 3H), 2.16 (t, J = 7.2 Hz, 2H), 1.57 – 1.52 (m, 2H), 1.25 – 1.20 (m, 10H), 0.82 (t, J = 6.0 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 172.2, 155.7, 151.4, 144.7, 140.2, 140.1, 129.2, 115.1, 114.4, 108.1, 102.7, 100.3, 55.4, 35.5, 31.2, 28.8, 28.7, 28.6, 25.4, 22.1, 13.9.

HRMS (ESI) *m/z* calcd for $C_{22}H_{29}N_3O_2$ $[M+H]^+$ 368.2338, found 368.2332.

Scope of Substituted Tetrazoles:

Amination reaction of tetrazole 3a:



3a: 0.5 mmol **4a:** 94%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(3a)** (143.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 121.4 mg (94%) aminated product **(4a)** as white solid.

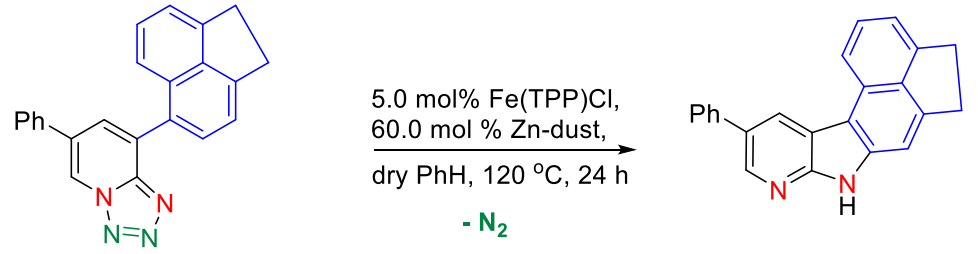
Melting Point: >200 °C

^{1}H NMR (400 MHz, DMSO-d_6): δ 12.00 (s, 1H), 8.63 (s, 1H), 8.30 (d, J = 8.0 Hz, 1H), 8.24 (s, 1H), 7.63 (t, J = 7.6 Hz, 1H), 7.48 (s, 1H), 7.30 (d, J = 6.8 Hz, 1H), 3.45 (s, 4H), 2.52 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 172.2, 155.7, 151.4, 144.7, 140.2, 140.1, 129.2, 115.1, 114.4, 108.1, 102.7, 100.3, 55.4, 35.5, 31.2, 28.8, 28.7, 28.6, 25.4, 22.1, 13.9.

HRMS (ESI) *m/z* calcd for $C_{18}H_{14}N_2$ $[M+H]^+$ 259.1235, found 259.1224.

Amination reaction of tetrazole 3b:



3b: 0.5 mmol **4b:** 90%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(3b)** (174.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 144.2 mg (90%) aminated product **(4b)** as white solid.

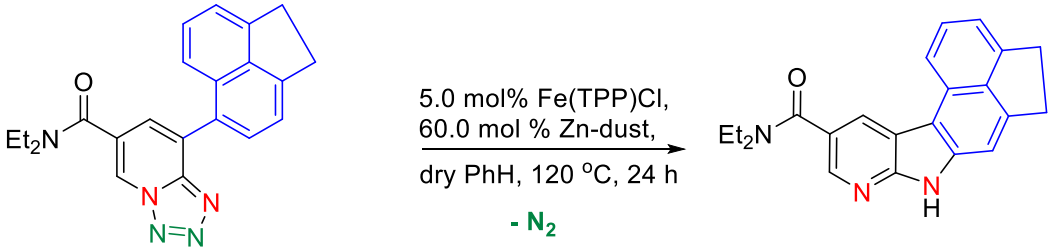
Melting Point: >200 °C

^{1}H NMR (400 MHz, DMSO-d_6): δ 12.24 (s, 1H), 8.98 (s, 1H), 8.71 (s, 1H), 8.47 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 7.6 Hz, 2H), 7.66 (t, J = 7.6 Hz, 1H), 7.54 (t, J = 6.0 Hz, 3H), 7.41 (t, J = 7.2 Hz, 1H), 7.33 (d, J = 6.8 Hz, 1H), 3.46 (s, 4H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 150.1, 146.6, 146.5, 142.7, 140.1, 138.9, 134.5, 129.2, 129.0, 128.3, 127.3, 127.1, 127.0, 126.3, 119.0, 117.6, 116.0, 109.7, 106.7, 30.5, 29.7

HRMS (ESI) *m/z* calcd for $C_{23}H_{16}N_2$ $[M+H]^+$ 321.1392, found 321.1385.

Amination reaction of tetrazole 3c:



3c: 0.5 mmol **4c:** 89%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(3c)** (185.7 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure

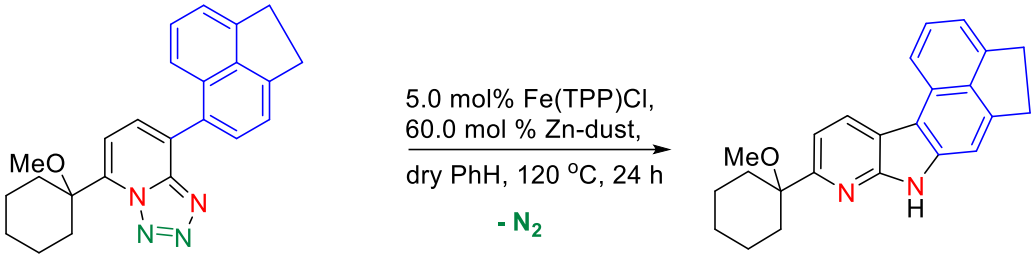
and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 152.8 mg (89%) aminated product **(4c)** as white solid.

^{1}H NMR (400 MHz, DMSO-d_6): δ 12.35 (s, 1H), 8.75 (s, 1H), 8.39 (s, 1H), 8.31 (t, J = 8.4 Hz 1H), 7.64 (t, J = 7.6Hz, 1H), 7.53 (s, 1H), 7.32 (d, J = 6.8 Hz, 1H), 3.44 (s, 8H), 1.18 (d, J = 6.8 Hz, 6H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 169.5, 150.6, 147.1, 146.9, 141.9, 140.5, 134.8, 129.5, 127.1, 126.7, 125.3, 118.9, 118.0, 115.2, 109.8, 106.9, 30.7, 29.9, 14.2, 14.0, 8.8, 7.4.

HRMS (ESI) *m/z* calcd for $C_{22}H_{21}N_3O$ $[M+H]^+$ 344.1763, found 344.1749.

Amination reaction of tetrazole 3d:



3d: 0.5 mmol **4d:** 84%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(3d)** (192.2mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 149.7 mg (89%) aminated product **(4d)** as white solid.

Melting Point: 190-192 °C

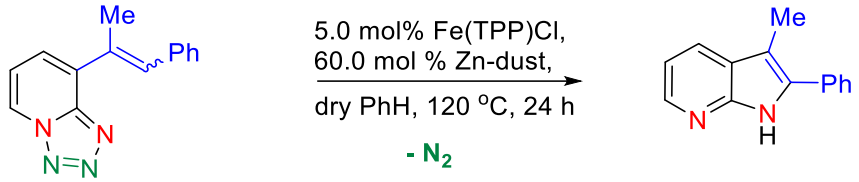
^{1}H NMR (400 MHz, DMSO-d_6): δ 12.13 (s, 1H), 8.76 (d, J = 8.4 Hz, 1H), 8.26 (t, J = 8.4 Hz, 1H), 7.62 (t, J = 8.0 Hz, 1H), 7.48 (s, 1H), 7.43 (d, J = 8.0 Hz, 1H), 7.30 (d, J = 6.8 Hz, 1H), 3.44 (s, 4H), 2.99 (s, 3H), 2.00 (s, 4H), 1.67-1.58 (m, 6H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 159.0, 149.9, 146.5, 145.7, 139.4, 134.4, 128.9, 127.0, 118.5, 117.3, 114.2, 109.6, 106.6, 79.1, 49.5, 34.2, 30.5, 29.6, 25.3.

HRMS (ESI) *m/z* calcd for $C_{24}H_{24}N_2O$ $[M+H]^+$ 357.1967, found 357.1934.

Scope of Substituted Alkenes:

Amination reaction of tetrazole 5a:



5a: 0.5 mmol **6a:** 82%

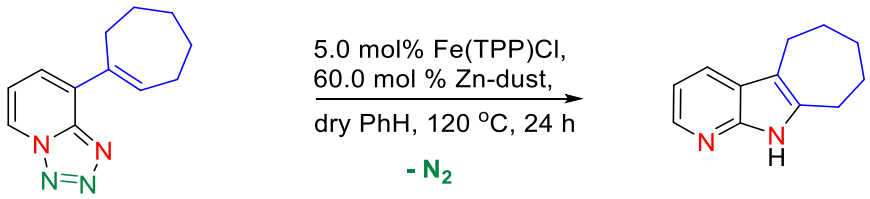
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(5a)** (118.1mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 85.4 mg (82%) aminated product **(6a)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.17 (s, 1H), 8.23 (s, 1H), 7.91 (d, J = 7.6 Hz, 1H), 7.73 (d, J = 7.6 Hz, 2H), 7.54 (t, J = 7.6 Hz, 2H), 7.41 (t, J = 7.2 Hz, 1H), 7.09 (s, 1H), 2.49 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.7, 142.4, 134.8, 132.9, 128.8, 128.0, 127.7, 127.0, 106.6, 29.7.

HRMS (ESI) *m/z*calcd for $C_{14}H_{12}N_2$ $[M+H]^+$ 209.1079, found 209.1073.

Amination reaction of tetrazole 5b:



5b: 0.5 mmol **6b:** 94%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(5b)** (107.0 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was

stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 87.5 mg (94%) aminated product **(6b)** as white solid.

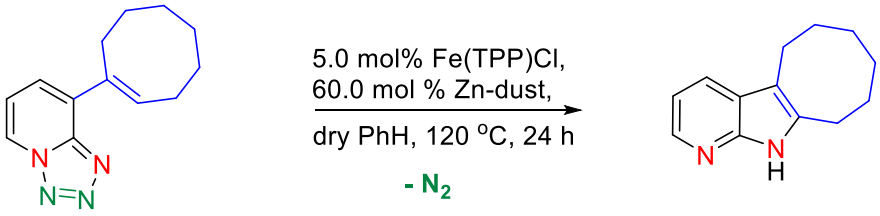
Melting Point: 157-159 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.23 (d, J = 22.8 Hz, 1H), 8.19 (d, J = 4.8 Hz, 1H), 7.77 (d, J = 7.6 Hz, 1H), 7.02 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 2.96 (t, J = 5.6 Hz, 2H), 2.80 (t, J = 5.6 Hz, 2H), 1.95 – 1.86 (m, 2H), 1.84-1.74 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 147.4, 140.2, 138.8, 125.5, 122.1, 114.8, 111.6, 31.7, 29.6, 28.7, 27.4, 24.6.

HRMS (ESI) *m/z*calcd for $C_{12}H_{14}N_2$ $[M+H]^+$ 187.1235, found 187.1239.

Amination reaction of tetrazole 5c:



5c: 0.5 mmol **6c:** 92%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 ^{o}C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(5c)** (114.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120^{o}C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 92.1 mg (92%) aminated product **(6c)** as white solid.

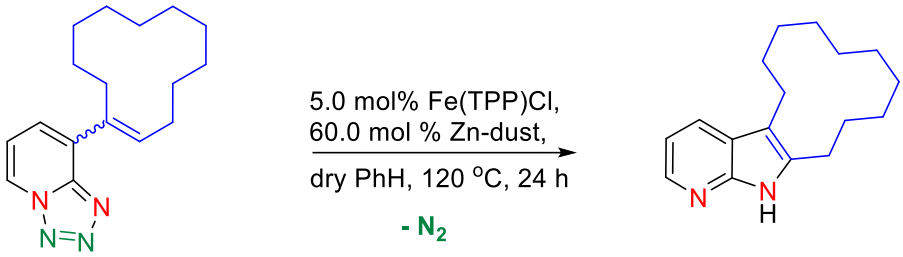
Melting Point: 156-158 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 11.21 (s, 1H), 8.20 (d, J = 4.4 Hz, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.03 (dd, J = 7.6 Hz, J = 5.6 Hz, 1H), 2.98 (t, J = 6.0 Hz, 2H), 2.86 (t, J = 6.0 Hz, 2H), 1.89 – 1.80 (m, 2H), 1.73-1.69 (m, 2H), 1.46-1.44 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.2, 140.2, 137.0, 125.4, 121.4, 114.8, 109.7, 29.9, 29.1, 26.0, 25.0, 25.7, 22.1.

HRMS (ESI) *m/z*calcd for $C_{13}H_{16}N_2$ $[M+H]^+$ 201.1392, found 201.1384.

Amination reaction of tetrazole 5d:



5d: 0.5 mmol
E:Z = 50:50

6d: 81%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(5d)** (142.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 103.8 mg (92%) aminated product **(6d)** as white solid.

Melting Point: 174-176 °C

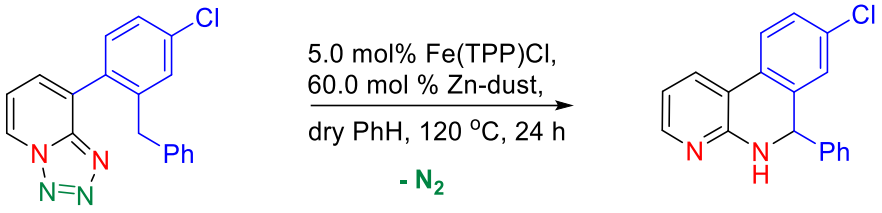
^{1}H NMR (400 MHz, $CDCl_3$): δ 10.43 (s, 1H), 8.19 (d, J = 4.4 Hz, 1H), 7.82 (d, J = 7.6 Hz, 1H), 7.00 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 2.83 (t, J = 7.2 Hz, 2H), 2.75 (t, J = 6.8 Hz, 2H), 1.92-1.86 (m, 2H), 1.83-1.77 (m, 2H), 1.47 (s, 4H), 1.34 (s, 6H), 1.29 – 1.24 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 140.9, 136.9, 126.6, 121.4, 114.8, 110.6, 27.8, 27.2, 24.8, 24.8, 24.7, 24.2, 22.8, 22.6, 22.3, 21.1.

HRMS (ESI) *m/z* calcd for $C_{17}H_{24}N_2$ $[M+H]^+$257.2018, found 257.2012.

Scope of C(sp^3)-H Amination Over C(sp^2)-H Amination:

Amination reaction of tetrazole 7a:



7a: 0.5 mmol **8a:** 92%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7a)** (160.4 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 134.7 mg (92%) aminated product **(8a)** as white solid.

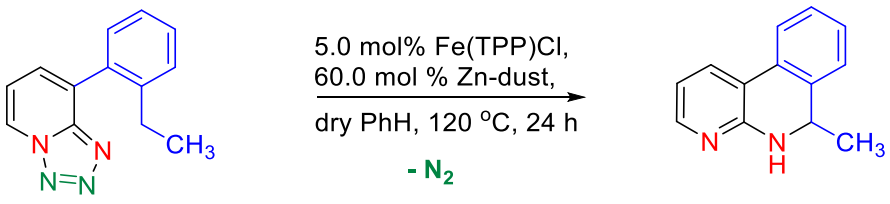
Melting Point: 197-199 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, J = 4.4 Hz, 1H), 7.77 (d, J = 7.2 Hz, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.26 (s, 4H), 7.19 (d, J = 6.0 Hz, 1H), 6.78 (s, 1H), 6.62 (dd, J = 7.2 Hz, J = 5.2 Hz, 1H), 5.66 (s, 1H), 5.49 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 155.3, 148.3, 142.8, 136.4, 133.7, 130.2, 129.0, 128.5, 128.3, 128.0, 127.4, 127.4, 123.7, 114.7, 114.2, 59.7.

HRMS (ESI) *m/z* calcd for $C_{18}H_{13}ClN_2$ $[M+H]^+$ 293.0846, found 293.0835.

Amination reaction of tetrazole 7b:



7b: 0.5 mmol **8b:** 90%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was

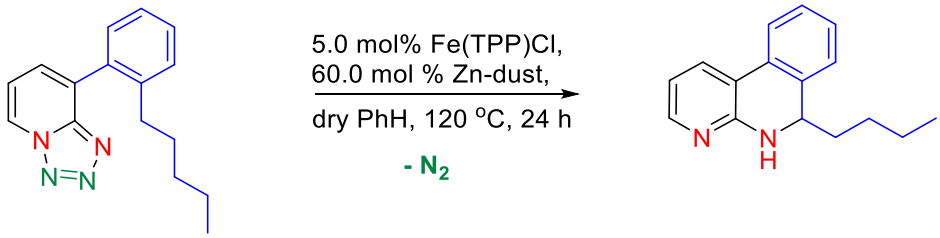
capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7b)** (112.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 88.3 mg (90%) aminated product **(8b)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (d, J = 4.8 Hz, 1H), 7.95 (d, J = 7.6 Hz, 1H), 7.77 (d, J = 7.6 Hz, 1H), 7.44-7.34 (m, 2H), 7.23 (d, J = 7.2 Hz, 1H), 6.83 – 6.77 (m, 1H), 5.17 (s, 1H), 4.85 (q, J = 6.8 Hz, 1H), 1.55 (d, J = 6.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 155.5, 147.9, 136.5, 130.1, 129.5, 128.0, 127.5, 125.8, 122.4, 115.2, 114.4, 51.1, 51.1, 24.6.

HRMS (ESI) *m/z* calcd for $C_{13}H_{12}N_2$ $[M+H]^+$ 197.1079, found 197.1073.

Amination reaction of tetrazole 7c:



7c: 0.5 mmol

8c: 97%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7c)** (133.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 115.6 mg (90%) aminated product **(8c)** as white solid.

Melting Point: 100-102 °C

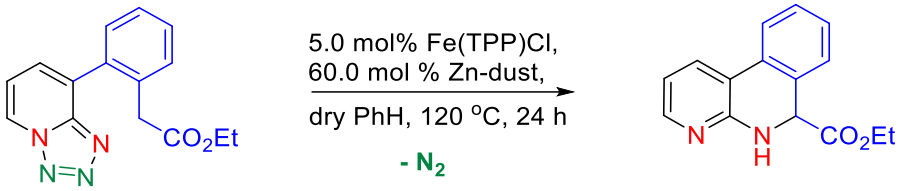
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, J = 4.8 Hz, 1H), 7.87 (d, J = 7.2 Hz, 1H), 7.70 (d, J = 7.6 Hz, 1H), 7.30 (dt, J = 20.8 Hz, J = 7.6 Hz, 2H), 7.13 (d, J = 7.2 Hz, 1H), 6.70 (dd, J = 7.2 Hz, J =

5.2 Hz, 1H), 5.57 (d, J = 17.2 Hz, 1H), 4.54 (t, J = 6.4 Hz, 1H), 1.83 – 1.73 (m, 1H), 1.68 – 1.58 (m, 1H), 1.44 – 1.27 (m, 4H), 0.87 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 155.5, 147.8, 125.5, 130.0, 129.6, 127.6, 127.3, 126.5, 122.3, 115.1, 114.0, 55.6, 38.6, 27.3, 22.4, 13.9.

HRMS (ESI) *m/z* calcd for $C_{16}H_{18}N_2$ $[M+H]^+$ 239.1548, found 239.1541.

Amination reaction of tetrazole 7d:



7d: 0.5 mmol

8d: 85%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7d)** (141.0 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 108.1 mg (85%) aminated product **(8d)** as white solid.

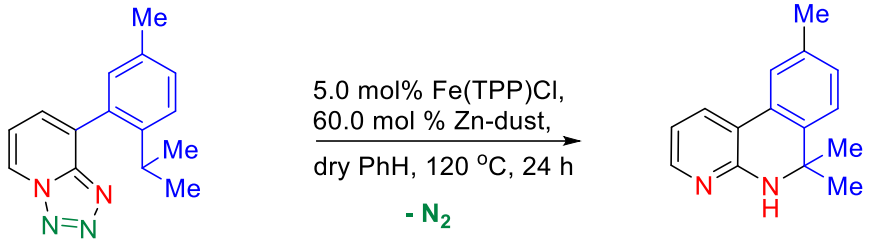
Melting Point: 107-109 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, J = 4.8 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.35 (t, J = 10.0 Hz, 2H), 7.28 (d, J = 7.6 Hz, 1H), 6.73 (dd, J = 7.2 Hz, J = 5.2 Hz, 1H), 5.84 (d, J = 17.2 Hz, 1H), 5.17 (s, 1H), 4.10- 4.01 (m, 2H), 1.12 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.8, 155.3, 148.0, 130.3, 130.0, 128.9, 128.6, 128.3, 127.8, 122.5, 115.0, 114.8, 61.5, 58.3, 13.9.

HRMS (ESI) *m/z* calcd for $C_{15}H_{14}N_2O_2$ $[M+H]^+$ 255.1134, found 255.1125.

Amination reaction of tetrazole 7e:



7e: 0.5 mmol **8e:** 90%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7e)** (126.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in DCM) gave 100.9 mg (90%) aminated product **(8e)** as white solid.

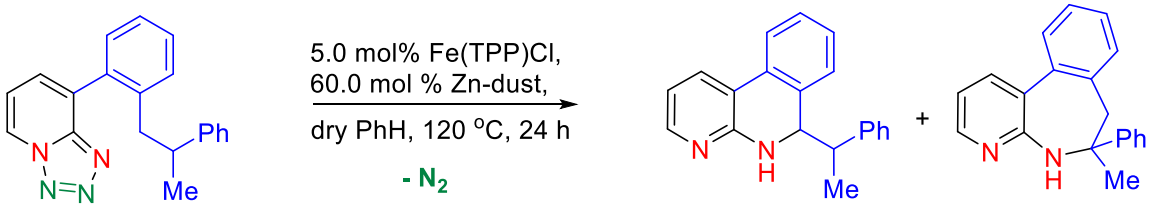
Melting Point: 162-164 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, J = 4.8 Hz, 1H), 7.88 (d, J = 7.6 Hz, 1H), 7.51 (s, 1H), 7.19 (d, J = 7.6 Hz, 1H), 7.11 (d, J = 8.0 Hz, 1H), 6.69 (dd, J = 7.2 Hz, J = 4.8 Hz, 1H), 4.95 (s, 1H), 2.38 (s, 3H), 1.54 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 155.2, 147.8, 137.6, 136.7, 129.9, 128.9, 123.7, 123.0, 115.3, 114.2, 54.2, 30.9, 21.2

HRMS (ESI) *m/z* calcd for $C_{15}H_{16}N_2$ $[M+H]^+$ 225.1392, found 225.1384.

Amination reaction of tetrazole 7f:



7f: 0.5 mmol **8f:** 15% **8f':** 77%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was

capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7f)** (157.2 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using DCM as eluent) gave 21.5 mg (15%) aminated six membered product **(8f)** as white solid and 110.3 mg (77%) seven membered product (**8f'**) as white solid.

Melting Point of **8f'**: 132-134 °C

NMR Data of 8f:

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, J = 4.8 Hz, 1H), 7.80 (d, J = 7.6 Hz, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.27 – 7.09 (m, 7H), 6.86 (d, J = 7.6 Hz, 1H), 6.62 (dd, J = 7.6 Hz, J = 4.8 Hz, 1H), 5.19 (s, 1H), 4.66 (d, J = 4.8 Hz, 1H), 3.13 – 3.01 (m, 1H), 1.20 (d, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 155.5, 147.9, 142.5, 133.3, 130.3, 129.7, 128.4, 127.9, 127.5, 127.4, 127.3, 126.6, 122.0, 115.0, 113.9, 61.5, 48.3, 14.0

HRMS (ESI) *m/z*calcd for $C_{20}H_{18}N_2$ $[M+H]^+$ 287.1548, found 287.1545.

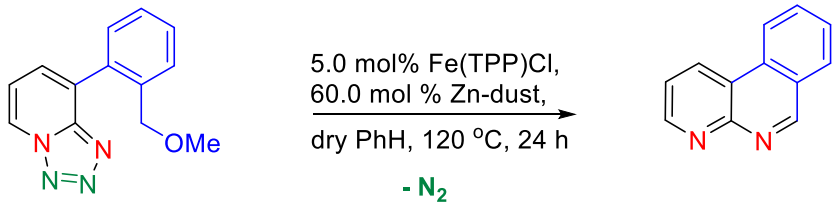
NMR Data of 8f':

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33 (d, J = 4.8 Hz, 1H), 7.80 (d, J = 7.2 Hz, 1H), 7.56 (d, J = 7.6 Hz, 2H), 7.46 (d, J = 7.6 Hz, 1H), 7.38-7.34 (m, 3H), 7.28 (t, J = 7.2 Hz, 1H), 7.20 (d, J = 7.6 Hz, 1H), 7.04 (dd, J = 7.2 Hz, J = 4.8 Hz, 1H), 6.91 (d, J = 7.6 Hz, 1H), 4.89 (s, 1H), 3.14 (s, 2H), 1.86 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 148.2, 147.9, 137.8, 137.5, 136.6, 129.5, 128.4, 128.0, 127.1, 127.0, 126.5, 125.6, 123.4, 116.2, 69.3, 46.8, 30.9.

HRMS (ESI) *m/z* calcd for $C_{20}H_{18}N_2$ $[M+H]^+$ 287.1548, found 287.1545.

Amination reaction of tetrazole 7g:



7g: 0.5 mmol

8g: 89%

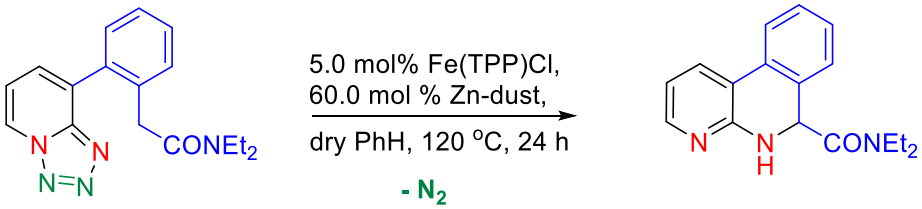
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7g)** (120.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using DCM as eluent) gave 80.2 mg (89%) aminated product **(8g)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.47 (s, 1H), 9.05 (d, J = 3.2 Hz, 1H), 8.86 (d, J = 8.4 Hz, 1H), 8.52 (d, J = 8.0 Hz, 1H), 8.06 (d, J = 7.6 Hz, 1H), 7.86 (t, J = 7.6 Hz, 1H), 7.72 (t, J = 7.6 Hz, 1H), 7.58 (dd, J = 8.4 Hz, J = 4.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 153.8, 151.2, 132.5, 131.5, 131.4, 128.8,128.2, 126.3, 122.2, 121.8, 118.8.

HRMS (ESI) *m/z*calcd for $C_{12}H_8N_2$ $[M+H]^+$ 181.0766, found 181.0755.

Amination reaction of tetrazole 7h:



7h: 0.5 mmol

8h: 83%

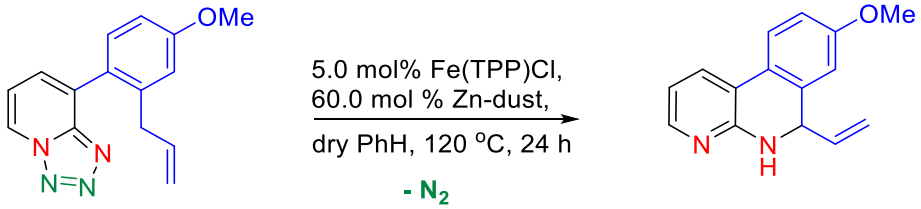
In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7h)** (154.7 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using DCM as eluent) gave 116.8 mg (83%) aminated product **(8h)** as white solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, J = 4.8 Hz, 1H), 7.87 (d, J = 7.6 Hz, 1H), 7.72 (d, J = 7.6 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 7.27 (t, J = 7.2 Hz, 1H),7.13 (d, J = 7.6 Hz, 1H) 6.70 (t, J =7.2 Hz, J = 5.2 Hz, 1H), 6.30 (s, 1H), 5.76 (s, 1H), 3.52 – 3.36 (m, 4H), 1.15 (t, J = 6.8 Hz, 3H), 1.07 (t, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 169.9, 154.9, 147.7, 130.1, 129.9, 129.7, 128.3, 128.1, 125.5, 122.6, 114.5, 114.4, 58.9, 41.7, 40.6, 14.0, 12.5.

HRMS (ESI) *m/z* calcd for $C_{17}H_{19}N_3O$ $[M+H]^+$ 282.1606, found 282.1600.

Amination reaction of tetrazole 7i:



7i: 0.5 mmol

8i: 81%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(7i)** (133.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using DCM as eluent) gave 96.5 mg (81%) aminated product **(8i)** as white solid.

Melting Point: 165-167 °C

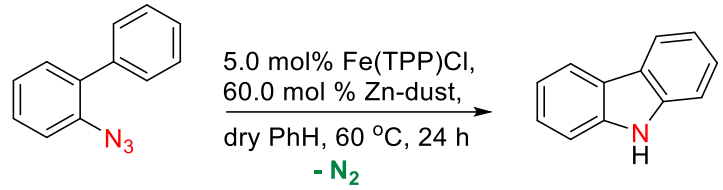
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, J = 4.4 Hz, 1H), 7.76 (d, J = 7.2 Hz, 1H), 7.61 (d, J = 8.8 Hz, 1H), 6.87 (dd, J = 8.8 Hz, J =1.2 Hz, 1H), 6.69- 6.60 (m, 2H), 6.05-5.97 (m, 1H), 5.36 (s, 1H), 5.22 (d, J = 16.8 Hz, 1H), 5.10 (dd, J = 15.6 Hz, J = 10.0 Hz, 2H), 3.82 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 154.8, 146.7, 139.1, 135.0,129.2, 123.9, 122.3, 115.8, 114.6, 113.7, 111.9, 58.8, 55.3.

HRMS (ESI) *m/z*calcd for $C_{15}H_{14}N_2O$ $[M+H]^+$ 239.1184, found 239.1178.

Scope of Organic Azides:

Amination of azide 9a:



9a: 0.5 mmol **10a:** 92%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9a)** (97.6 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60°C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in hexane as eluent) gave 76.9 mg (92%) aminated product **(10a)** as white solid. Spectral data are in accordance with reported literature data.[26]

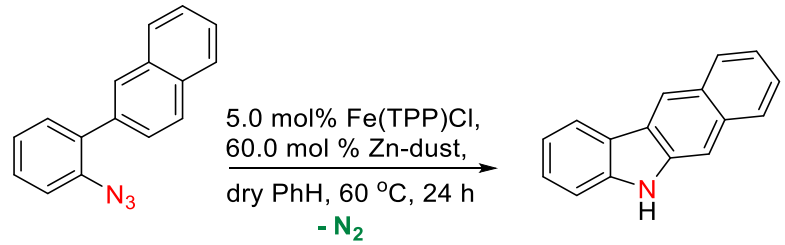
Melting Point: 140-142 °C

^{1}H NMR (800 MHz, DMSO-d_6): δ 11.27 (s, 1H), 8.11 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 7.39 (t, J = 8.0 Hz, 2H), 7.16 (t, J = 7.2 Hz, 2H).

^{13}C NMR (200 MHz, DMSO-d_6): δ 139.7, 125.5, 122.4, 120.2, 118.5, 110.9.

HRMS (ESI) *m/z*calcd for $C_{12}H_9N$ $[M+H]^+$ 168.0813, found 168.0801.

Amination of azide 9b:



9b: 0.5 mmol **10b:** 85%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The

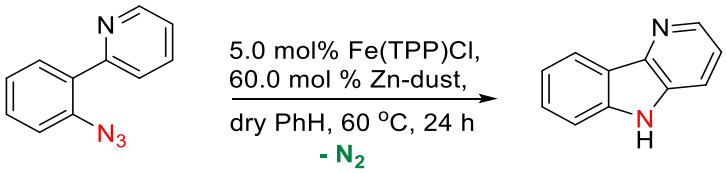
reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9b)** (122.6 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 10% ethyl acetate in hexane as eluent) gave 92.3 mg (85%) aminated product **(10b)** as white solid. Spectral data are in accordance with reported literature data.[26]

^{1}H NMR (800 MHz, $CDCl_3$): δ 8.82 (s, 1H), 8.14 (dd, J = 15.2 Hz, J = 8.0 Hz, 3H), 8.02 (d, J = 8.8 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.60 (t, J = 8.8 Hz, 2H), 7.55 (t, J = 7.2 Hz, 1H), 7.45 (t, J = 7.2 Hz, 1H), 7.32 (t, J = 7.2 Hz, 1H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 138.4, 134.8, 132.4, 129.0, 125.5, 125.2, 124.8, 124.2, 121.1, 120.5, 120.2, 120.0, 119.9, 119.3, 118.4, 111.0.

HRMS (ESI) *m/z*calcd for $C_{16}H_{11}N$ $[M+H]^+$ 218.0970, found 218.0962.

Amination of azide 9c:



9c: 0.5 mmol **10c:** 91%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9c)** (98.1 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 5% ethyl acetate in hexane as eluent) gave 76.5 mg (91%) aminated product **(10c)** as white solid. Spectral data are in accordance with reported literature data.[27]

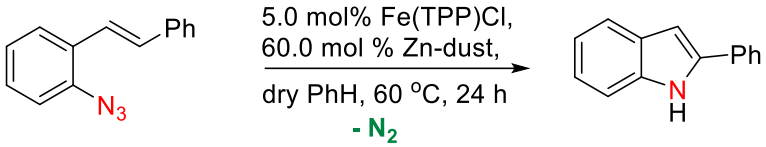
Melting Point: 82-84 °C

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (d, J = 6.8 Hz, 1H), 8.07 (dd, J = 8.0 Hz J = 3.2 Hz, 2H), 7.85 (d, J = 8.8 Hz, 1H), 7.56 (t, J = 8.0 Hz 1H), 7.31 (t, J = 8.0 Hz, 1H), 7.22 (t, J = 7.2 Hz, 1H), 7.14 (t, J = 6.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 149.6, 135.3, 128.4, 127.9, 121.8, 119.7, 119.6, 117.9, 116.2, 115.5, 115.1.

HRMS (ESI) *m/z*calcd for $C_{11}H_8N_2$ $[M+H]^+$ 169.0766, found 169.0759.

Amination of azide 9d:



9d: 0.5 mmol **10d:** 95%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9d)** (110.6 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 5% ethyl acetate in hexane as eluent) gave 91.8 mg (95%) aminated product **(10d)** as white solid. Spectral data are in accordance with reported literature data.[26]

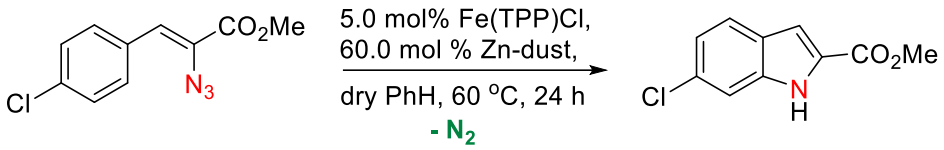
Melting Point: 187-189 °C

^{1}H NMR (800 MHz, $CDCl_3$): δ 8.30 (s, 1H), 7.70 – 7.67 (m, 3H), 7.47 (t, J = 8.0 Hz, 2H), 7.41 (d, J = 8.0 Hz, 1H), 7.36 (t, J = 7.2 Hz, 1H), 7.25 (t, J = 8.0 Hz, 1H), 7.19 (t, J = 7.2 Hz, 1H), 6.87 (s, 1H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 137.8, 136.7, 132.3, 129.2, 129.0, 127.7, 125.1, 122.3, 120.6, 120.2, 110.9, 99.9.

HRMS (ESI) *m/z*calcd for $C_{14}H_{11}N$ $[M+H]^+$ 194.0970, found 194.0961.

Amination of azide 9e:



9e: 0.5 mmol **10e:** 95%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9e)** (118.8mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 5% ethyl acetate in hexane as eluent) gave 99.6 mg (95%) aminated product **(10e)** as white solid. Spectral data are in accordance with reported literature data.[28]

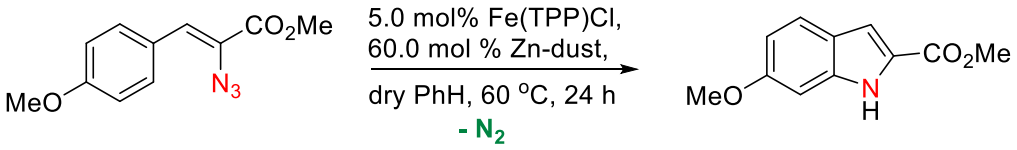
Melting Point: 175-177 °C

^{1}H NMR (800 MHz, $CDCl_3$): δ 9.23 (s, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.43 (s, 1H), 7.19 (s, 1H), 7.12 (d, J = 8.8 Hz, 1H), 3.97 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 162.3, 137.1, 131.3, 127.8, 126.0, 123.5, 121.9, 111.7, 108.8, 52.2.

HRMS (ESI) *m/z*calcd for $C_{10}H_8ClNO_2$ $[M+H]^+$ 210.0322, found 210.0315.

Amination of azide 9f:



9f: 0.5 mmol **10f:** 83%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9f)** (116.6 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure

and chromatographic separation with silica gel (using 5% ethyl acetate in hexane as eluent) gave 85.2 mg (83%) aminated product **(10f)** as white solid. Spectral data are in accordance with reported literature data.[28]

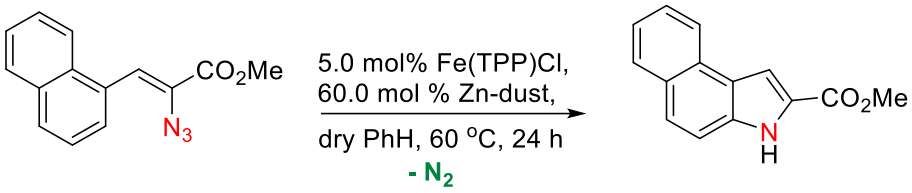
Melting Point: 173-175 ^{o}C

^{1}H NMR (800 MHz, $CDCl_3$): δ 8.92 (s, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.36 (s, 1H), 6.93 – 6.91 (m, 2H), 4.02 (s, 3H), 3.96 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 162.4, 158.9, 137.9, 126.0, 123.4, 121.8, 112.4, 109.2, 93.6, 55.5, 51.8.

HRMS (ESI) *m/z*calcd for $C_{11}H_{11}NO_3$ $[M+H]^+$ 206.0817, found 206.0810.

Amination of azide 9g:



9g: 0.5 mmol **10g:** 75%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 ^{o}C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9g)** (126.6 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60 ^{o}C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 5% ethyl acetate in hexane as eluent) gave 84.5mg (75%) aminated product **(10g)** as white solid. Spectral data are in accordance with reported literature data.[28]

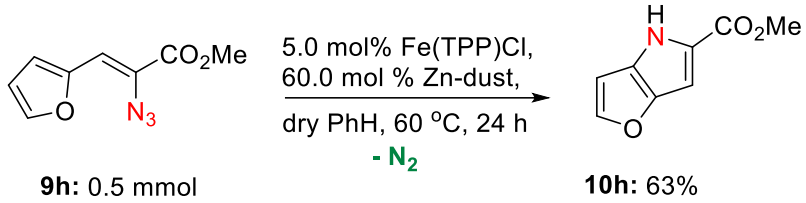
Melting Point: 190-192 ^{o}C

^{1}H NMR (800 MHz, $CDCl_3$): δ 9.83 (s, 1H), 8.25 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.77 (s, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.61 (t, J = 8.0 Hz, 1H), 7.52 (d, J = 8.8 Hz, 1H), 7.48 (t, J = 7.2 Hz, 1H), 4.02 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 162.6, 134.4, 129.3, 128.7, 128.6, 127.0, 126.7, 125.1, 124.2, 122.9, 122.8, 113.0, 107.9, 52.0.

HRMS (ESI) *m/z*calcd for $C_{14}H_{11}NO_2$ $[M+H]^+$ 226.0868, found 226.0865.

Amination of azide 9h:



9h: 0.5 mmol **10h:** 63%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9h)** (96.6 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure and chromatographic separation with silica gel (using 5% ethyl acetate in hexane as eluent) gave 52.0 mg (63%) aminated product **(10h)** as white solid. Spectral data are in accordance with reported literature data.[28]

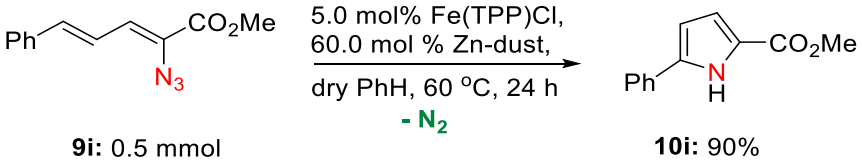
Melting Point: 135-137 °C

^{1}H NMR (800 MHz, $CDCl_3$): δ 8.81 (s, 1H), 7.52 (d, J = 1.6 Hz, 1H), 6.80 (s, 1H), 6.46 (s, 1H), 3.88 (s, 3H).

^{13}C NMR (200 MHz, $CDCl_3$): δ 162.5, 148.7, 148.0, 128.8, 123.8, 98.9, 97.0, 51.6.

HRMS (ESI) *m/z*calcd for $C_8H_7NO_3$ $[M+H]^+$ 166.0504, found 166.0506.

Amination of azide 9i:



9i: 0.5 mmol **10i:** 90%

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(9i)** (114.6 mg, 0.5 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 60 °C. The reaction mixture was stirred for 20 h. After completion (judged by TLC), benzene was removed under reduced pressure

and chromatographic separation with silica gel (using 5% ethyl acetate in hexane as eluent) gave 90.6 mg (90%) aminated product **(10i)** as white solid. Spectral data are in accordance with reported literature data.[28]

Melting Point: 141-143 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.52 (s, 1H), 7.59 (d, J = 8.0 Hz, 2H), 7.41 (t, J = 7.6 Hz, 2H), 7.30 (t, J = 7.6 Hz, 1H), 6.97 (t, J = 2.4 Hz 1H), 6.55 (t, J = 3.2 Hz, 1H), 3.88 (s, 3H).

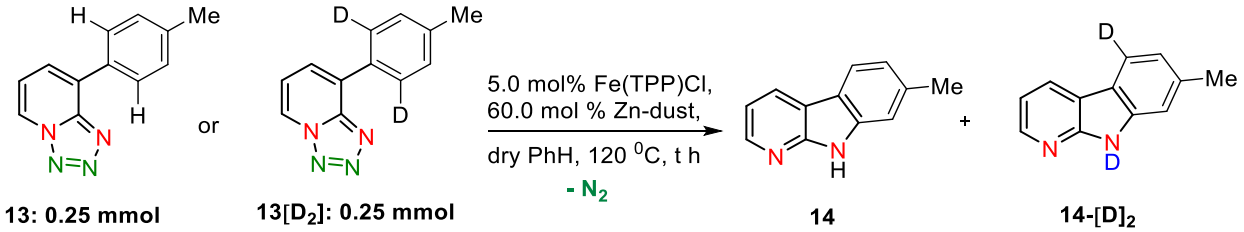
^{13}C NMR (100 MHz, $CDCl_3$): δ 161.7, 136.9, 131.3, 129.0, 127.8, 124.8, 123.0, 116.9, 108.0, 51.6.

HRMS (ESI) *m/z*calcd for $C_{12}H_{11}NO_2$ $[M+H]^+$ 202.0868, found 202.0834.

Mechanistic Studies/Control Experiments:

(A) KIE experiment:

Intermolecular



13: 0.25 mmol **13[D_2]: 0.25 mmol** **14** **14-[D]$_2$**

Separate Vessel

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (8.8 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (1.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(**either **13 or 13-[D_2])** (52.5 mg, 0.25 mmol or 53.0 mg, 0.25 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 ^{0}C. After different time interval 100 µL of aliquot was withdrawn and conversion was checked by ^{1}H-NMR spectroscopy (after evaporation of remaining benzene) in $CDCl_3$ (see below **Figure 1**).

Sl. No.	Time (h)	Conversion (%) k_H
1	3	34.6
2	6	40.8
3	9	42.8
4	12	48.9
5	15	55.6

Sl. No.	Time (h)	Conversion (%) k_D
1	3	29.0
2	6	34.6
3	9	36.7
4	12	42.8
5	15	49.5

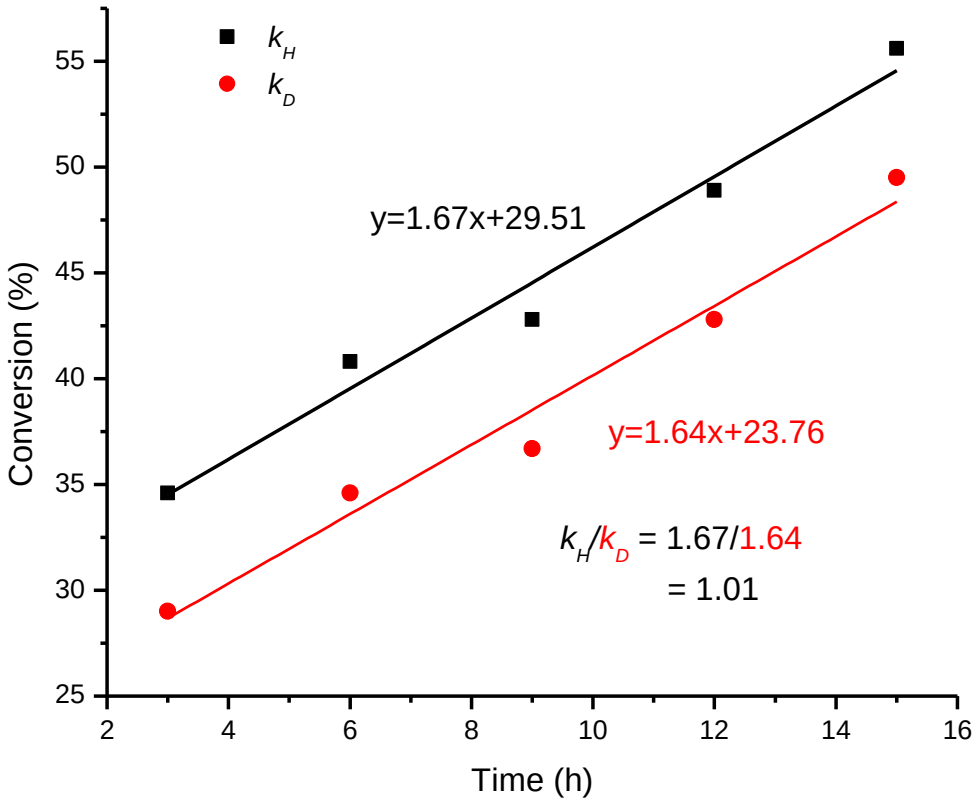
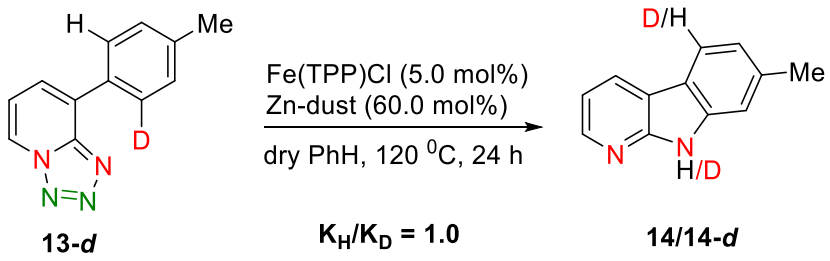


Figure 1. Intermolecular KIE experiment

Intramolecular kinetic experiment:



13-*d* **K_H/K_D = 1.0** **14/14-*d***

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole (**11-*d)*** (105.6 mg, 0.5 mmol). The micro reactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture

was stirred for 20 h. Then, the benzene was removed under reduced pressure and pass through a short pad of silica (DCM as eluent). The filtrate was concentrated *in vacuo,* and the reaction progress was analyzed using ^{1}H-NMR analysis.

The isotope effect was determined by comparison of the integration of the multiplet at 8.04 ppm (1.01 H) of tetrazole**(13-*d*)** relative to the multiplet at 7.94 ppm (0.5 H) of deuterated aminated product. The intramolecular KIE value is 1.0.

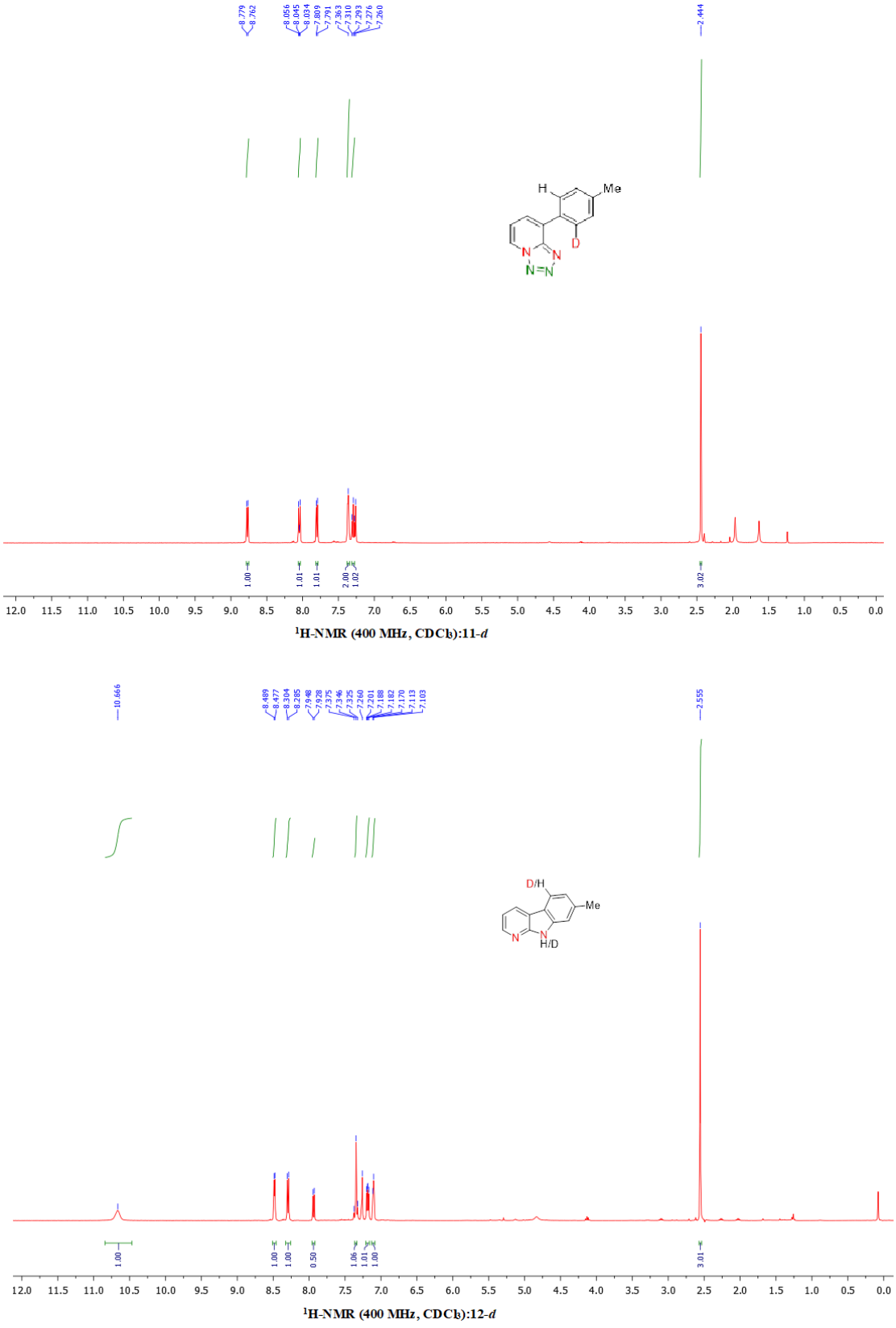
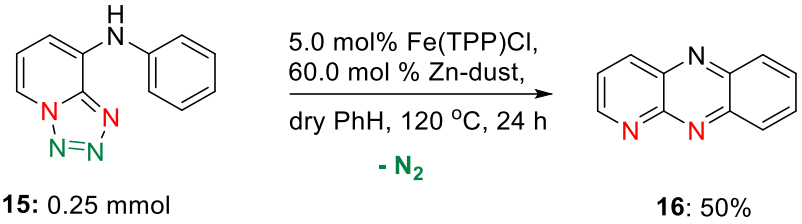


Figure 2. Intramolecular KIE experiment

B) Experiment with non-conjugated tetrazole:



15: 0.25 mmol

16: 50%

In an argon-filled glove box, a 5.0 mL wheatonmicroreactor was charged with Fe(TPP)Cl (8.8 mg, 5.0 mol%), Zn-dust (9.8 mg, 60.0 mol%) and dry benzene (1.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **15** (52.8 mg, 0.25 mmol). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. Then, the benzene was removed under reduced pressure and crude mixture was purified by silica gel (in 5% ethyl acetate in DCM) to afford 22.6 mg (50%) product **(16)** as brown solid.

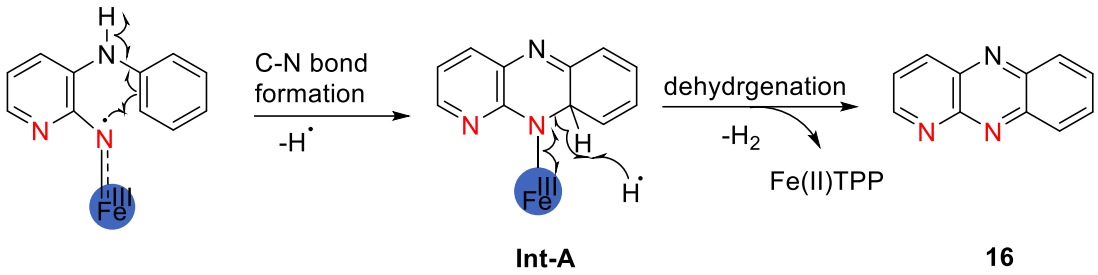
^{1}H NMR (400 MHz, $CDCl_3$): δ 9.37 (s, 1H), 8.62 (d, J = 8.4 Hz, 1H), 8.39 (dd, J = 6.8 Hz, J = 3.2 Hz, 1H), 8.29 (dd, J = 6.7, 3.4 Hz, 1H), 7.93 (dd, J = 6.8 Hz, J = 3.6 Hz, 2H), 7.79 (dd, J = 8.4 Hz, J = 3.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 156.5, 149.6, 145.0, 144.2, 139.2, 138.6, 131.6, 131.4, 130.4, 129.4, 125.5.

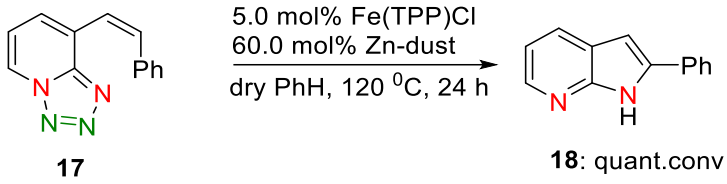
HRMS (ESI) *m/z* calcd for $C_{11}H_7N_3$ $[M+H]^+$ 182.0718, found 182.0710.

NOTE: From manuscript

We hypothesized that dehydrogenation might proceed via above arrow-pushing mechanism. In the mechanism, at first nitrene radical attacks at ortho position of adjacent phenyl ring by the generation of hydrogen radical. After that, hydrogen radical grabs another hydrogen atom to produce compound 16 as well as one molecule of hydrogen gas is liberated. Finally, active Fe(II)TPP catalyst also regenerated. The driving force behind dehydrogenation is the gaining of aromaticity.

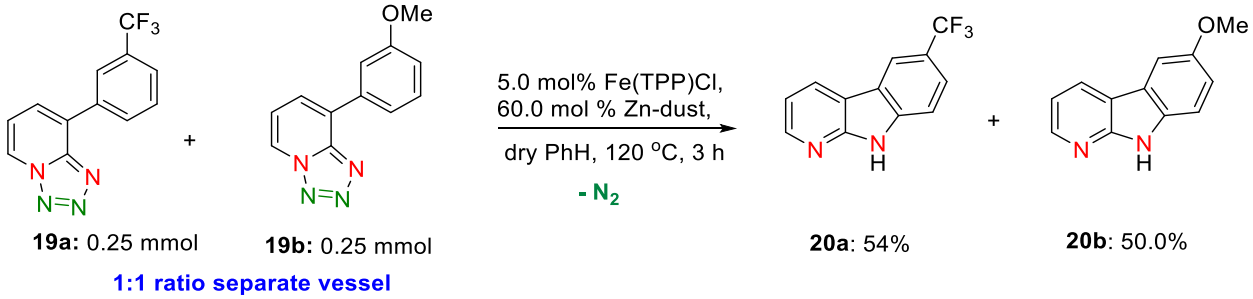


C) Experiment with conjugated Z-alkene:



In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole (**17**) (111.1 mg, 0.5 mmol). The micro reactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 20 h. Then, the benzene was removed under reduced pressure and chromatographic separation with neutral silica gel (10% ethyl acetate in DCM as eluent) afforded desired annulated product (**18**) quantitatively. Spectral data are in accordance with reported literature data.[1]

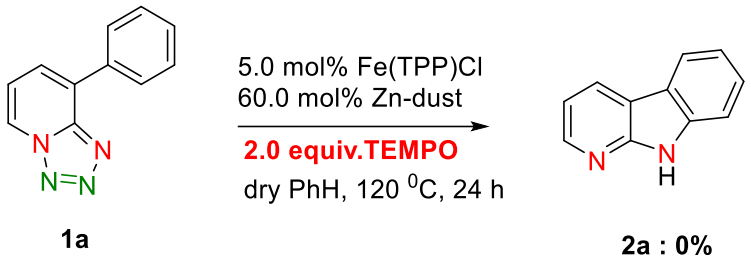
(D) Effect of substitutions on the aryl ring:



In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (2.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole (**19a or 19b**) (66.0 mg or 55.5 mg, 0.25 mmol) The micro reactor was

capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. After 3 h, 100.0 µL of aliquot was withdrawn and conversion was checked by ^{1}H-NMR spectroscopy (after evaporation of solvent) in $CDCl_3$ which showed 54% (**20a)** and 50% (**20b**).

(E) Experiment with TEMPO:



1a **2a : 0%**

In an argon-filled glove box, a 5.0 mL wheaton microreactor was charged with Fe(TPP)Cl (17.6 mg, 5.0 mol%), Zn-dust (19.6 mg, 60.0 mol%) and dry benzene (1.0 mL). The microreactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 4 h. After that, the microreactor was brought into the glove box and charged with tetrazole **(1a)** (98.1 mg, 0.5 mmol) and TEMPO (156.3 mg, 2.0 equiv.). The micro reactor was capped with a teflon pressure cap and placed into a pre-heated aluminum block at 120 °C. The reaction mixture was stirred for 8 h. The reaction was cooled to room temperature and benzene was removed under reduced pressure. Analyzing the crude reaction mixture by ^{1}H-NMR spectroscopy, we did not observe any desired product (**2a**) and this is because of radical trapping by the TEMPO.

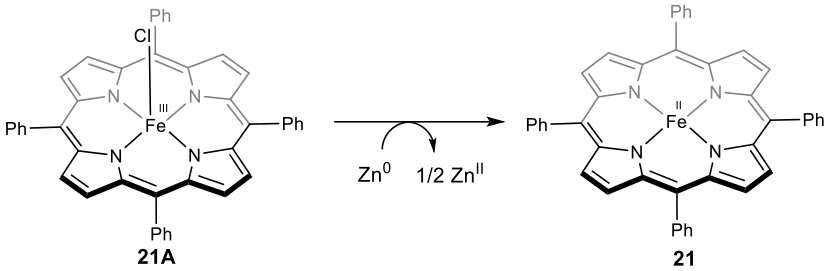
Computational Methods

All computations were performed using the Gaussian16 (Rev. B.01) suite of quantum chemical program.[29] Geometry optimizations of all stationary points (reactants, intermediates, transition states, and products) were carried out in the condensed phase. Depending on whether the species concerned bears a paired or unpaired electron, restricted or unrestricted (U)B3LYP-D3 hybrid density functional theory[30] is respectively used in conjunction with the 6-31G** basis set[31] for all elements except Fe. The SDD basis set with an effective core potential (ECP) for the 10 core electrons and explicit basis set for the 16 valence electrons were used for Fe.[32] In various mechanistic pathways examined, different likely spin states arising due to the presence of Fe were considered, as applicable. For instance, $Fe^{(III)}$ in the sextet and $Fe^{(II)}$ in singlet, triplet, and quintet states were considered. The *guess=mix* keyword was employed as the broken symmetry (BS) correction in the case of the open-shell singlet state calculations.[33]

All stationary points were characterized by using frequency calculations in order to verify that the transition states (TSs) have one and only one imaginary frequency for the desired reaction coordinate. The intrinsic reaction coordinate (IRC) calculations[34] were also performed on all the TSs to verify their connectivity to the desired minima on either side of the first-order saddle point. The effect of continuum solvation was incorporated through the SMD solvation model developed by Truhlar and Cramer.[35] The continuum dielectric of benzene (ε=2.28) was employed in our computations in view of the fact that our experimental studies were conducted in benzene solvent. The standard state of all solute species was considered as 1 mol/L in our calculations. The Gibbs free energies were evaluated at 393.15 K (in conformity with the reaction temperature) wherein the vibrational entropy contribution was computed using the free-rotor approximation for frequencies <100 cm^{-1}.[36] The discussions in the manuscript are presented on the basis of the Gibbs

free energies thus obtained at the $SMD_{(Benzene)}$/(U)B3LYP-D3/6-31G**,SDD(Fe) level of theory. The *energetic span model* was used to identify the turnover determining intermediate (TDI) and turnover determining transition state (TDTS).[37]

Generation of active catalyst



Scheme S1. The conversion of pre-catalyst to potential active catalyst

Table S1. Relative Gibbs free energies (in kcal/mol) for different spin states at the $SMD_{(Benzene)}$/UB3LYP-D3/6-31G**,SDD(Fe) level of theory for the generation of active catalyst with respect to the lower energy spin state

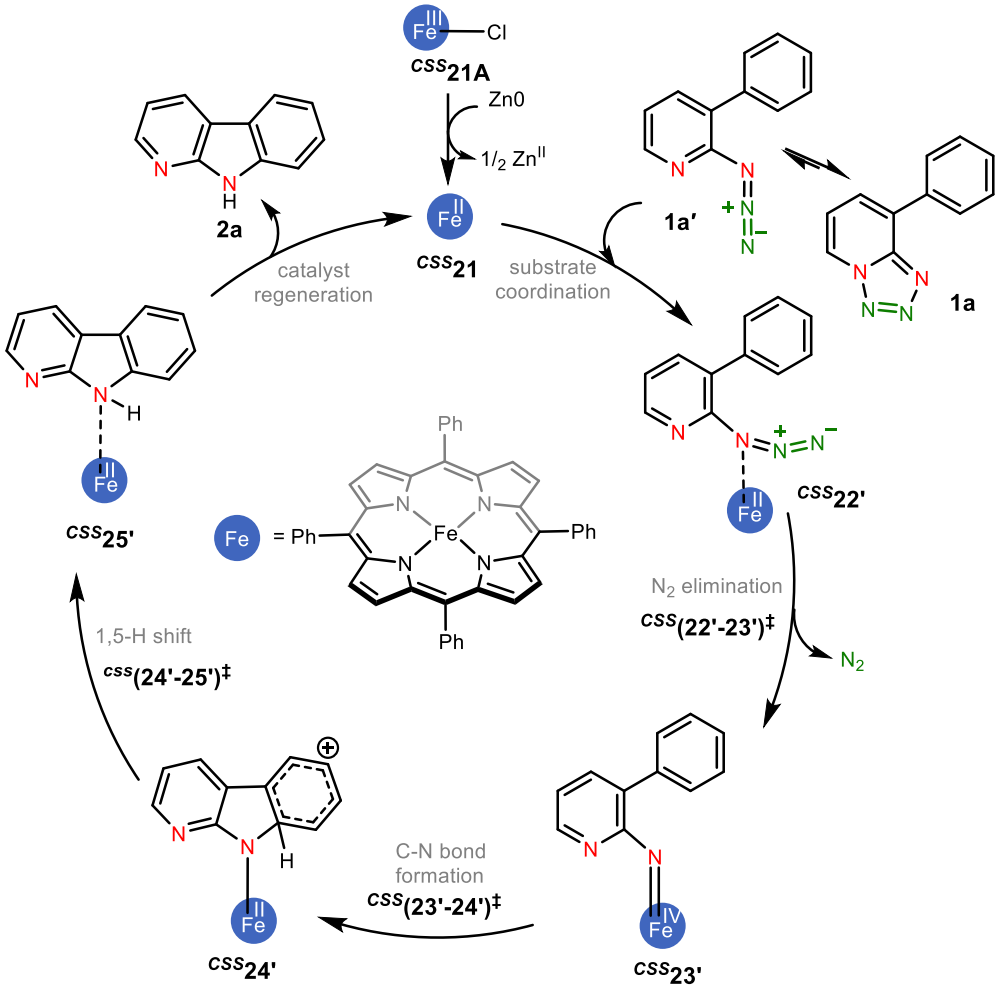
pre-catalyst	ΔG	active catalyst	ΔG
^{6}**21A**	0	^{3}**21**	0
^{4}**21A**	3.2	^{5}**21**	7.3
^{2}**21A**	19.3	^{OSS}**21**	11.9
		^{CSS}**21**	32.5

The Fe^{III}-porphyrin pre-catalyst (**21A**) has three different spin states; doublet, quartet and sextet. These spin-multiplets are referred to as the low, intermediate, and high spin state. The preferred ground state of **21A** is found to exhibit the sextet state (^{6}**21A**), followed by the quartet (^{4}**21A**), and doublet (^{2}**21A**) in their energetic order (Table S1). The Fe^{II}-porphyrin complex (**21**) with even number of unpaired electrons in the *d* orbitals have three spin-multiplets, singlet, triplet, and quintet. The triplet state (^{3}**21**) is lower in energy compared to quintet (^{5}**21**), open-shell singlet

(^{OSS}**21**), and closed-shell singlet (^{CSS}**21**) by 7.3, 11.9 and 32.5 kcal/mol respectively (Table S1). The triplet state ^{3}**21** of the active catalyst is found to be the ground state.

Electrophilic aromatic substitution (EAS) pathway

A. Catalytic cycle for EAS mechanism



Scheme S2. The key mechanistic steps involved in the electrophilic aromatic substitution (EAS) mechanism of Fe-catalyzed intramolecular C(sp^2)-H amination of fused 1,2,3,4-tetrazole.

B. Gibbs free energy profile for EAS pathway

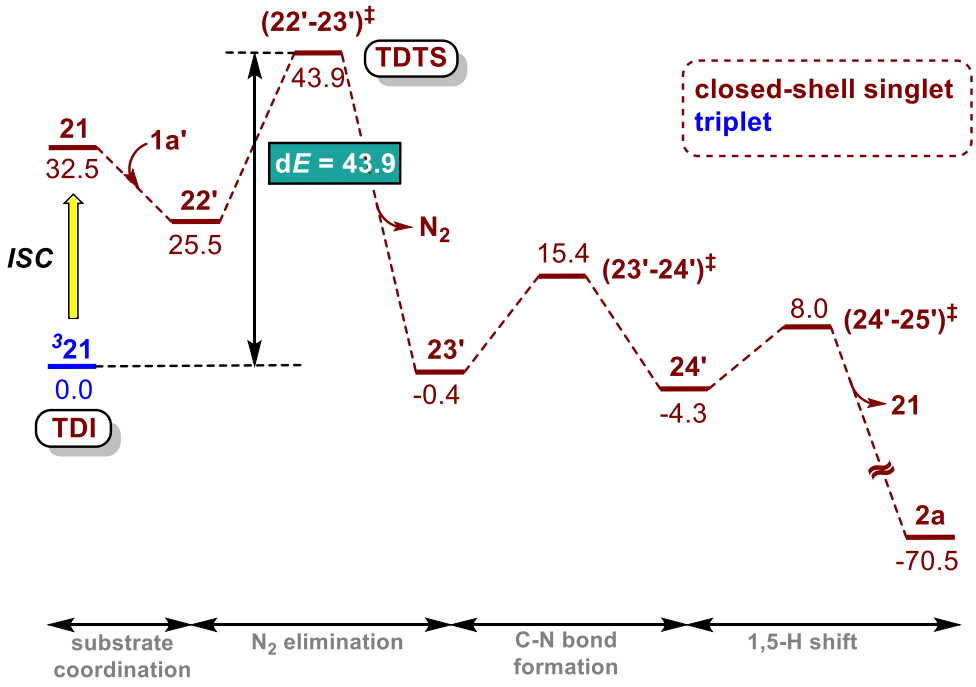


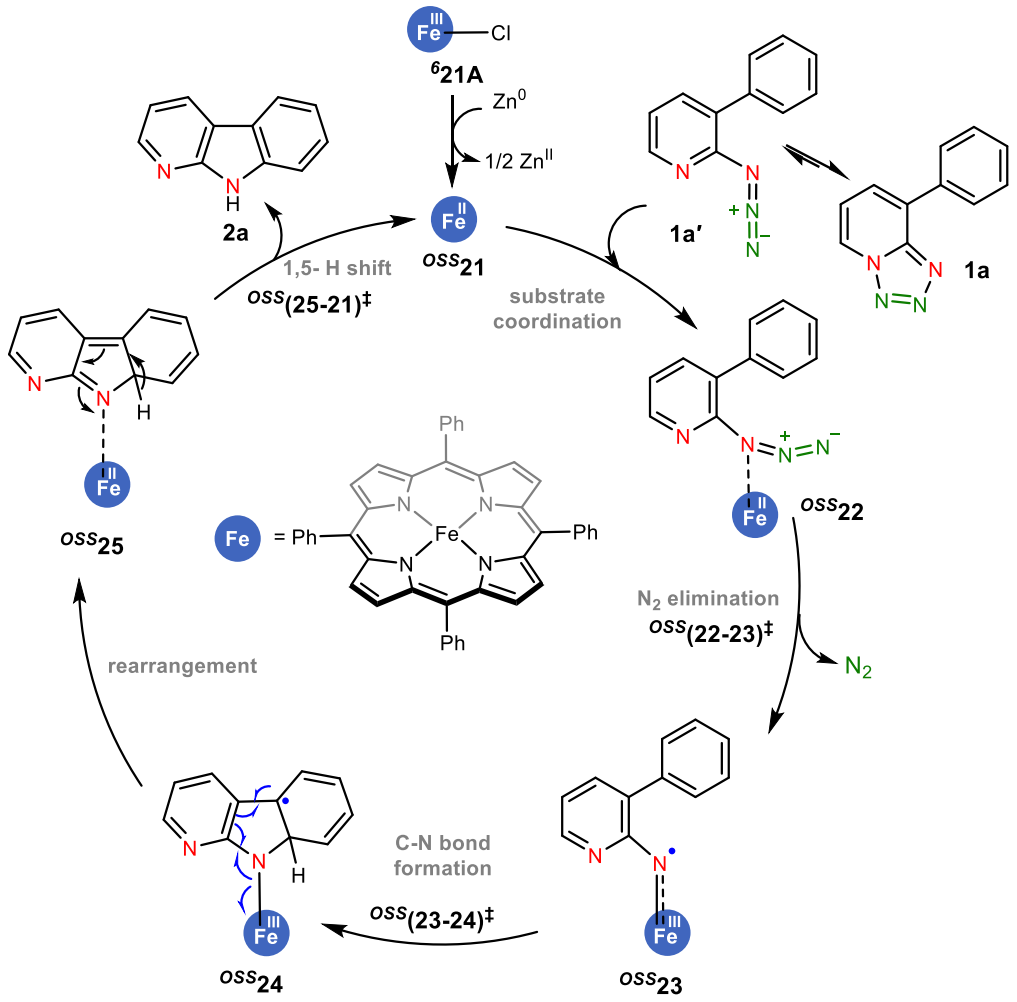
Figure S1. Gibbs free energy (kcal/mol) profile for electrophilic aromatic substitution mechanism obtained at the $SMD_{(Benzene)}$/B3LYP-D3/6-31G**,SDD(Fe) level of theory for Fe-catalyzed intramolecular C(sp^2)-H amination of fused 1,2,3,4-tetrazole.

In Figure S1, the relative Gibbs free energies are calculated with respect to the triplet state of the active catalyst (**^{3}21**). For the electrophilic aromatic substitution (EAS) pathway, an intersystem crossing (ISC) from the triplet state (**^{3}21**) to the closed-shell singlet state (**^{CSS}21**) would require as high as 32.5 kcal/mol energy, rendering this pathway much less likely. The N_2 elimination of intermediate **22'** leading to the generation of neutral intermediate **23'** has an activation barrier of 43.9 kcal/mol, which involves a concomitant oxidation of Fe^{II} to Fe^{IV}. The C-N bond formation transition state **(23'-24')**‡ generates a carbocation intermediate **24'** and Fe^{IV} is further reduced to Fe^{II}. The 1,5-H shift occurs within the $Fe^{(II)}$-porphyrin intermediate **24'** and gives catalyst bound product **25'**. The elementary step barrier for the C-N bond formation and the 1,5-H shift transition

states are 15.8 and 12.3 kcal/mol respectively. In the next step, the product precursor departs from **25'** and active catalyst (^{CSS}**21**) is regenerated. The application of the energetic span model to the Gibbs free energy profile shown in Figure S1 conveys that intermediate ^{3}**21** is the turn-over determining intermediate (TDI) and ^{CSS}**(22'-23')**‡ is the turn-over determining transition state (TDTS) in the EAS pathway and the energetic span is 43.9 kcal/mol. The computed free energy profile (Figure S1) indicates that the EAS pathway goes through a high energy route as compared to the MRA pathway (Figure 3 shown in the main manuscript) and is therefore considered unfavorable under the experimental condition.

4. Metalloradical activation (MRA) pathway

Catalytic cycle for MRA mechanism



Scheme S3. The key mechanistic steps involved in the metalloradical activation (MRA) mechanism in the open-shell singlet (OSS) state of Fe-catalyzed intramolecular C(sp^2)-H amination of fused 1,2,3,4-tetrazole.

5. Application of Energetic Span Model

The energies of the various stationary points are considered for the evaluation of the turnover frequency (TOF) of the catalytic cycle. The turnover frequency is determined by identifying the turnover determining intermediate (TDI) and turnover determining transition state (TDTS). The energetic span of the catalytic cycle can be calculated by using the following equations,

δE = TDTS – TDI, if TDTS appears after TDI

δE = TDTS – TDI + ΔG_{rxn}, if TDTS appears before TDI

where, ΔG_{rxn} is the Gibbs free energy of the reaction.

Table S2. Calculation of energetic span (δE, in kcal/mol) using different likely combinations of TDI and TDTS for the C(sp^2)-H amination of substrate **1a** for the triplet pathway (highlighted pair is the one found to give the maximum energetic span)

TDI	TDTS	δE	TDI	TDTS	δE
21	**[22-23]‡**	28.5	**22**	**[22-23]‡**	21.8
	[23-24]‡	9.3		**[23-24]‡**	2.6
	[25-2a]‡	-4.9		**[25-2a]‡**	-11.6
23	**[22-23]‡**	-32.7	**24**	**[22-23]‡**	-29.4
	[23-24]‡	19.6		**[23-24]‡**	-48.6
	[25-2a]‡	5.4		**[25-2a]‡**	7.5
25	**[22-23]‡**	-30.6			
	[23-24]‡	-49.8			
	[25-2a]‡	7.5			

Table S3. Calculation of energetic span (δ*E*, in kcal/mol) using different likely combinations of TDI and TDTS for the C(sp^2)-H amination of substrate **7a** for the triplet pathway (highlighted pair is the one found to give the maximum energetic span)

TDI	TDTS	δ*E*	TDI	TDTS	δ*E*
21	**[22b-23b]‡**	25.6	**22b**	**[22b-23b]‡**	21.2
	[23b-24b]‡	7.1		**[23b-24b]‡**	2.7
	[25b-8b]‡	-5.0		**[25b-8b]‡**	-9.4
23b	**[22b-23b]‡**	-31.5	**24b**	**[22b-23b]‡**	-32.0
	[23b-24b]‡	21.1		**[23b-24b]‡**	-50.5
	[25b-8b]‡	9.0		**[25b-8b]‡**	8.5
25b	**[22b-23b]‡**	-33.2			
	[23b-24b]‡	-51.7			
	[25b-8b]‡	7.3			

Table S4. Calculation of energetic span (δ*E*, in kcal/mol) using different likely combinations of TDI and TDTS for the C(sp^3)-H amination of substrate **7a** (highlighted pair is the one found to give the maximum energetic span)

TDI	TDTS	δ*E* (OSS)	δ*E* (triplet)	δ*E* (quintet)
21	**[22a-23a]‡**	21.8	29.3	21.5
	[23a-24a]‡	-8.9	-2.0	-15.6
	[25a-8a]‡	-16.7	-17.9	-24.9
22a	**[22a-23a]‡**	19.5	25.6	2.2
	[23a-24a]‡	-11.2	-5.7	-34.9
	[25a-8a]‡	-19.0	-21.6	-44.2
23a	**[22a-23a]‡**	-22.4	-18.0	-17.0
	[23a-24a]‡	10.1	13.9	9.1
	[25a-8a]‡	2.3	-2.0	-0.2
24a	**[22a-23a]‡**	-5.9	-9.2	-1.1
	[23a-24a]‡	-36.6	-40.5	-38.2
	[25a-8a]‡	18.8	6.8	15.7
25a	**[22a-23a]‡**	-11.5	-11.6	-8.2
	[23a-24a]‡	-42.2	-42.9	-45.3

	[25a-8a]‡	13.2	4.4	8.6

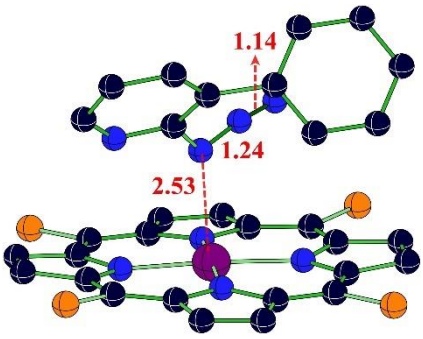
Table S5. Calculation of energetic span (δ*E*, in kcal/mol) using different likely combinations of TDI and TDTS for the C(sp^2)-H amination of substrate **1a** through electrophilic aromatic substitution (EAS) pathway (highlighted pair is the one found to give the maximum energetic span)

TDI	TDTS	δ*E*	TDI	TDTS	δ*E*
^{3}21	**[22'-23']‡**	43.9	**^{CSS}21**	**[22'-23']‡**	11.4
	[23'-24']‡	15.4		**[23'-24']‡**	-17.1
	[24'-25']‡	8.0		**[24'-25']‡**	-24.5
22'	**[22'-23']‡**	18.4	**23'**	**[22'-23']‡**	-26.2
	[23'-24']‡	-10.1		**[23'-24']‡**	15.8
	[24'-25']‡	-17.5		**[24'-25']‡**	8.4
24'	**[22'-23']‡**	-22.3			
	[23'-24']‡	-50.8			
	[24'-25']‡	12.3			

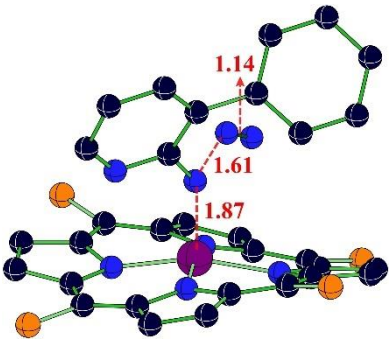
6. Optimized geometries of important transition states and intermediates

A. C(sp^2)-H amination

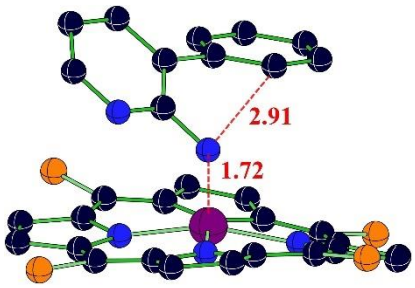
i) Metalloradical activation (MRA) pathway



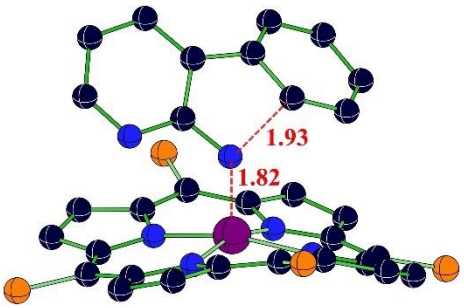
^{3}**22** (6.7)



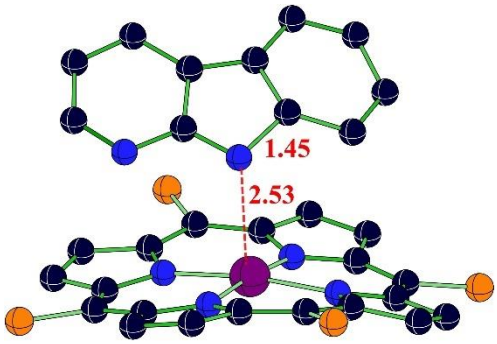
^{3}**(22-23)**‡ (28.5)



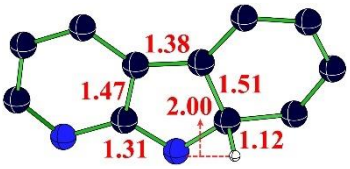
^{3}**23** (-10.3)

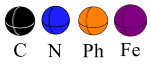


^{3}**(23-24)**‡ (9.3)

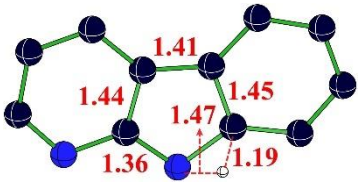


^{3}**24** (-13.6)

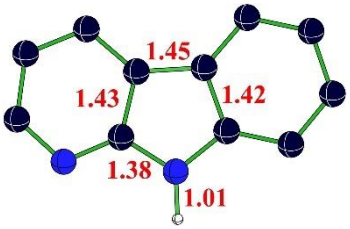




25 (-12.4)



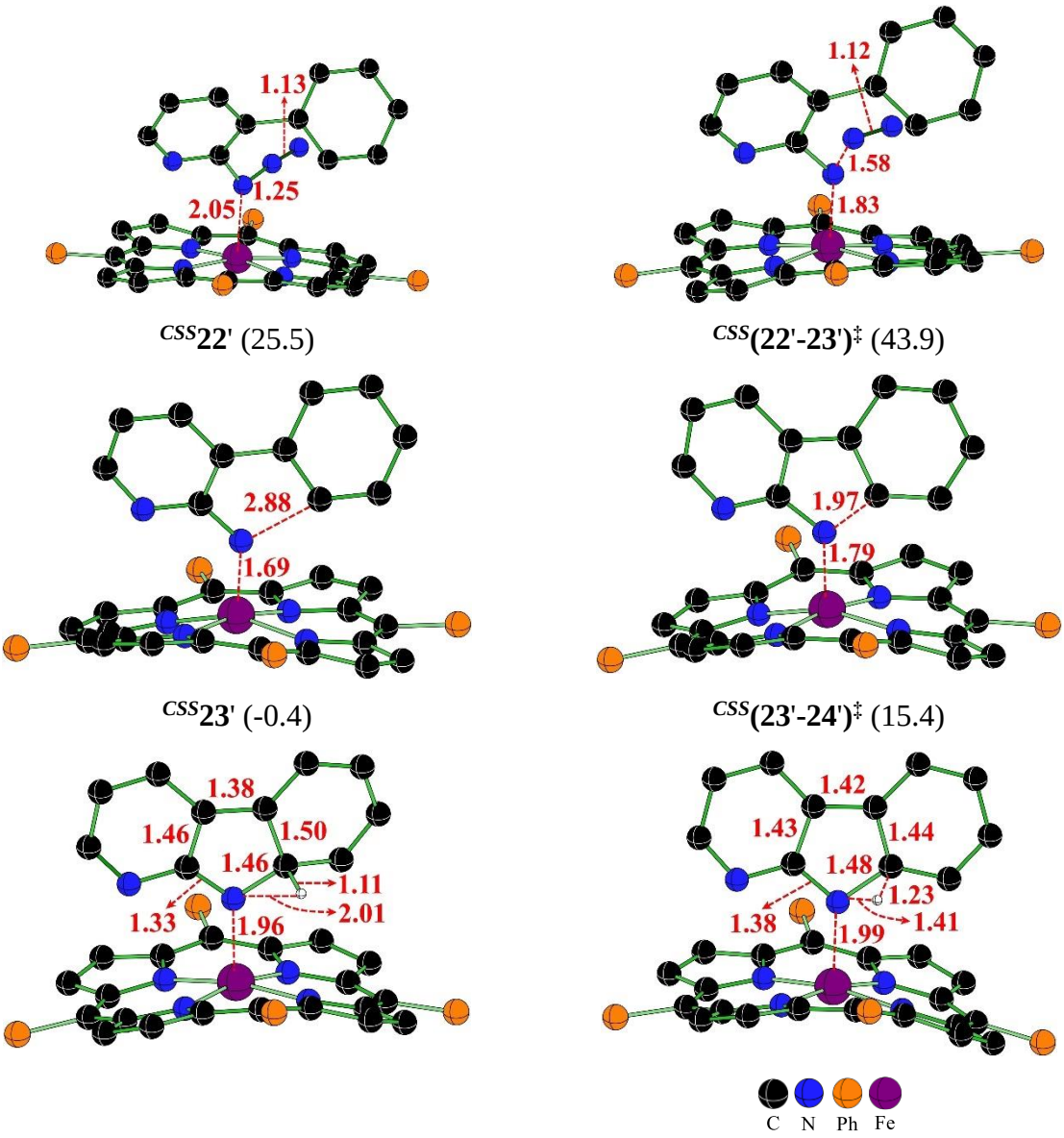
(25-2a)‡ (-4.9)



2a (-70.5)

Figure S2. Optimized intermediates and transition state geometries for the metalloradical activation pathway of substrate **1a** obtained at the $SMD_{(Benzene)}$/UB3LYP-D3/6-31G**,SDD(Fe) level of theory. Distances are in Å and relative Gibbs free energies (in kcal/mol) are given in parentheses.

ii) Electrophilic aromatic substitution (EAS) pathway



^{CSS}**22'** (25.5)

^{CSS}**(22'-23')**‡ (43.9)

^{CSS}**23'** (-0.4)

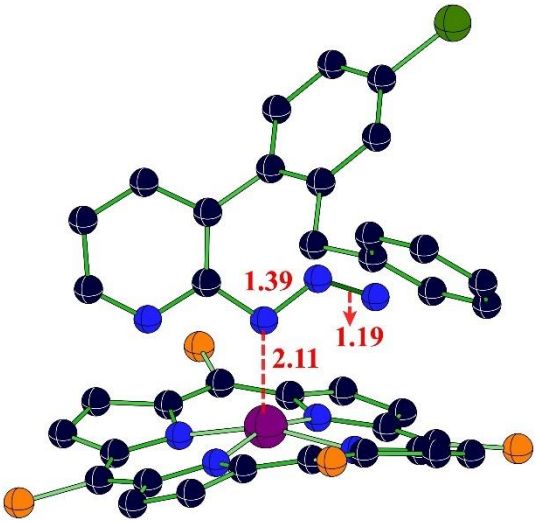
^{CSS}**(23'-24')**‡ (15.4)

^{CSS}**24'** (-4.3)

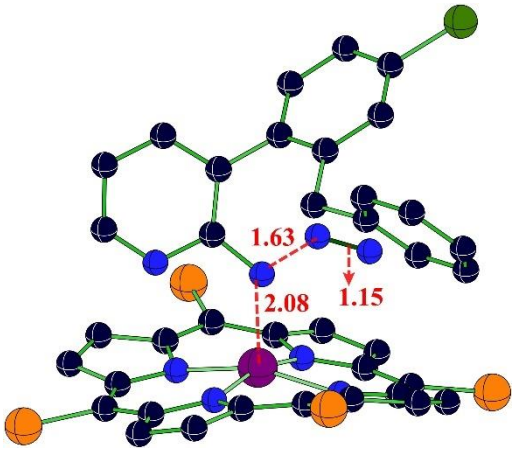
^{CSS}**(24'-25')**‡ (8.0)

Figure S3. Optimized intermediates and transition state geometries for the electrophilic aromatic substitution pathway of substrate **1a** obtained at the $SMD_{(Benzene)}$/B3LYP-D3/6-31G**,SDD(Fe) level of theory. Distances are in Å and relative Gibbs free energies (in kcal/mol) are given in parentheses.

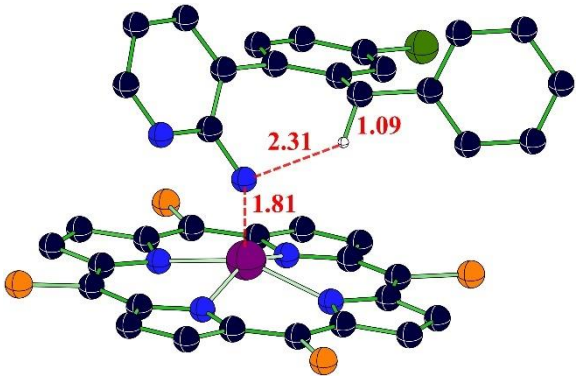
B. C(sp^3)-H amination via metalloradical activation pathway



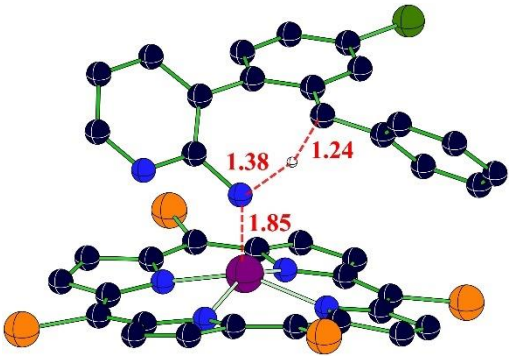
^{5}**22a** (26.6)



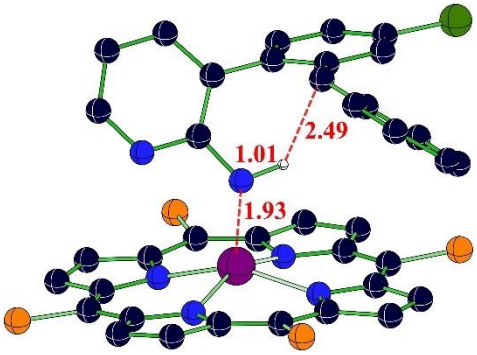
^{5}**(22a-23a)**‡ (28.8)



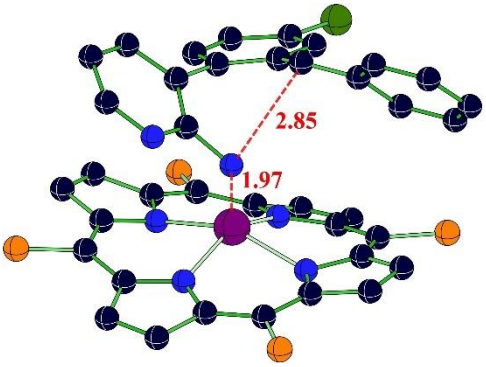
^{5}**23a** (-17.4)



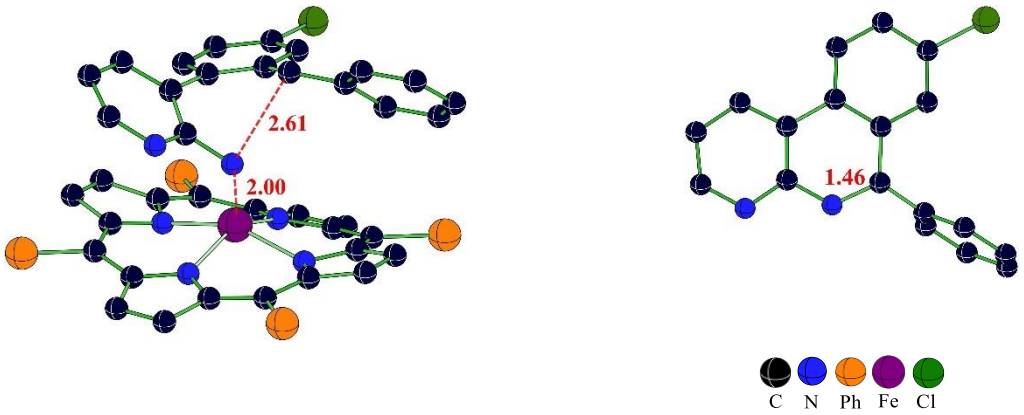
^{5}**(23a-24a)**‡ (-8.3)



^{5}**24a** (-33.3)



^{5}**25a** (-26.2)



^{5}**(25a-8a)**‡ (-17.6) **8a** (-63.2)

Figure S4. Optimized intermediates and transition state geometries for the metalloradical activation pathway of substrate **7a** obtained at the $SMD_{(Benzene)}$/UB3LYP-D3/6-31G**,SDD(Fe) level of theory. Distances are in Å and relative Gibbs free energies (in kcal/mol) are given in parenthesis.

7. Gibbs Free Energies of Important Stationary Points

Table S6. The corrected Gibbs free energies (in Hartree/Particle) of transition states and intermediates obtained by applying standard state corrections at 1 mol/L concentration and 393.15 K temperature[36]

Stationary points	Energy (**L1**)
^{OSS}**21**	-2036.217844
^{3}**21**	-2036.236849
^{5}**21**	-2036.225289
1a	-642.845459
1a'	-642.838629
^{OSS}**22**	-2679.053424
^{3}**22**	-2679.071607
^{5}**22**	-2679.036256
^{OSS}**(22-23)**‡	-2679.028916
^{3}**(22-23)**‡	-2679.036825
^{5}**(22-23)**‡	-2679.023624
^{OSS}**23**	-2569.559602
^{3}**23**	-2569.567899

N_2	-109.530807
^{OSS}(23-24)‡	-2569.533515
^{3}(23-24)‡	-2569.536749
^{OSS}24	-2569.559486
^{3}24	-2569.573244
^{OSS}25	-2569.564459
^{3}25	-533.334348
^{OSS}(25-21)‡	-2569.547393
^{CSS}(25-2a)‡	-533.322454
2a	-533.426978
7a	-1372.744402
^{OSS}22a	-3408.958653
^{3}22a	-3408.975368
^{5}22a	-3408.938802
^{OSS}(22a-23a)‡	-3408.927409
^{3}(22a-23a)‡	-3408.934528
^{5}(22a-23a)‡	-3408.935303
^{OSS}23a	-3299.461722
^{3}23a	-3299.475724
^{5}23a	-3299.478236
^{OSS}(23a-24a)‡	-3299.445652
^{3}(23a-24a)‡	-3299.453610
^{5}(23a-24a)‡	-3299.463697
^{OSS}24a	-3299.487994
^{3}24a	-3299.489809
^{5}24a	-3299.503458
^{OSS}25a	-3299.479178
^{3}25a	-3299.486043
^{5}25a	-3299.492174
^{OSS}(25a-8a)‡	-3299.458020
^{3}(25a-8a)‡	-3299.479125
^{5}(25a-8a)‡	-3299.478472
8a	-1263.314240
^{OSS}22b	-3408.961316
^{3}22b	-3408.974175
^{5}22b	-3408.935990
^{OSS}(22b-23b)‡	-3408.934702
^{3}(22b-23b)‡	-3408.940503
^{5}(22b-23b)‡	-3408.934702

^{OSS}**23b**	-3299.455550
^{3}**23b**	-3299.472791
^{OSS}**(23b-24b)‡**	-3299.433555
^{3}**(23b-24b)‡**	-3299.439202
^{OSS}**24b**	-3299.460335
^{3}**24b**	-3299.472009
^{OSS}**25b**	-3299.464841
^{3}**25b**	-1263.233298
^{OSS}**(25b-2a)‡**	-3299.446462
^{CSS}**(25b-8b)‡**	-1263.221579
8b	-1263.326962
(1a-1a')‡	-642.810885
^{3}**(21-22)‡**	-2679.046415

L1 = $SMD_{(Benzene)}$/UB3LYP-D3/6-31G**, SDD(Fe)

----------Part B----------

Cartesian Coordinates of the optimized geometries of various stationary points obtained at the $SMD_{(Benzene)}$/(U)B3LYP-D3/6-31G**,SDD(Fe) Level of Theory.

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^{2}21A

Number of imaginary frequencies : 0
Electronic energy : HF=-2496.9464132
Zero-point correction= 0.599920 (Hartree/Particle)
Thermal correction to Energy= 0.638644
Thermal correction to Enthalpy= 0.639588
Thermal correction to Gibbs Free Energy= 0.524027
Sum of electronic and zero-point Energies= -2496.346494
Sum of electronic and thermal Energies= -2496.307769
Sum of electronic and thermal Enthalpies= -2496.306825
Sum of electronic and thermal Free Energies= -2496.422387
.....
Cartesian Coordinates
.....
26 0.006455 0.000034 0.060094

17	-0.061143	-0.000263	2.264207
7	0.001693	1.973534	-0.216150
7	-2.013600	-0.000039	-0.149159
7	2.013615	0.000111	-0.108128
7	0.001654	-1.973412	-0.216222
6	1.102750	2.818825	-0.194161
6	0.678692	4.191227	-0.186793
6	-0.681151	4.189864	-0.194393
6	-1.101732	2.816854	-0.186134
6	-2.441407	2.428209	-0.140125
6	-3.491400	3.493585	-0.096197
6	-3.690205	4.246414	1.070691
6	-4.673421	5.235872	1.114776
6	-5.468441	5.485791	-0.006211
6	-2.850249	1.094880	-0.121524
6	-4.230740	0.678632	-0.062403
6	-4.230712	-0.678668	-0.061224
6	-2.850219	-1.094952	-0.119870
6	-2.441304	-2.428264	-0.137235
6	-3.491050	-3.493784	-0.091114
6	-3.688405	-4.245388	1.076807
6	-4.671164	-5.235207	1.122950
6	-5.467169	-5.486702	0.003015
6	2.851118	-1.096230	-0.132336
6	4.230974	-0.678377	-0.183552
6	4.230948	0.678810	-0.182425
6	2.851073	1.096517	-0.130681
6	2.443727	2.430488	-0.157752
6	3.496132	3.492906	-0.148510
6	4.277327	3.706966	0.997164
6	5.262718	4.695107	1.007366
6	5.482056	5.479482	-0.127354
6	3.723129	4.285708	-1.283721
6	4.710407	5.271950	-1.272980
6	-4.294826	3.749826	-1.216914
6	-5.276798	4.740815	-1.171955
6	-4.295467	-3.751587	-1.210761
6	-5.276979	-4.742938	-1.163741
6	-1.101644	-2.816820	-0.184501
6	-0.680959	-4.189794	-0.193168
6	0.678898	-4.191037	-0.187865
6	1.102817	-2.818595	-0.195793
6	2.443809	-2.430188	-0.160607
6	3.496247	-3.492592	-0.153505
6	4.278844	-3.707712	0.991017
6	5.264393	-4.695713	0.999033
6	5.482437	-5.478951	-0.136722
6	3.721877	-4.284335	-1.289727
6	4.709310	-5.270443	-1.281171
1	1.341871	5.042678	-0.172378
1	-1.346742	5.039668	-0.194832
1	-3.072439	4.047998	1.941527
1	-4.819798	5.808559	2.026226

1	-6.233386	6.256349	0.028725
1	-5.077460	1.347247	-0.023392
1	-5.077407	-1.347248	-0.021089
1	-3.069837	-4.045779	1.946801
1	-4.816398	-5.806953	2.035173
1	-6.231743	-6.257554	0.039548
1	5.077796	-1.345724	-0.237071
1	5.077744	1.346282	-0.234864
1	4.103771	3.096912	1.878638
1	5.856546	4.853432	1.903146
1	6.249890	6.247898	-0.119048
1	3.123527	4.122004	-2.174357
1	4.878437	5.875255	-2.160664
1	-4.144341	3.169668	-2.122702
1	-5.889808	4.931757	-2.048308
1	-4.146068	-3.172411	-2.117357
1	-5.890755	-4.935128	-2.039285
1	-1.346489	-5.039645	-0.192450
1	1.342192	-5.042419	-0.174480
1	4.106311	-3.098528	1.873292
1	5.859351	-4.854825	1.893922
1	6.250406	-6.247249	-0.130118
1	3.121143	-4.119859	-2.179459
1	4.876300	-5.872883	-2.169639

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^{4}21A

Number of imaginary frequencies : 0
Electronic energy : HF=-2496.970144
Zero-point correction= 0.599823 (Hartree/Particle)
Thermal correction to Energy= 0.638668
Thermal correction to Enthalpy= 0.639612
Thermal correction to Gibbs Free Energy= 0.522048
Sum of electronic and zero-point Energies= -2496.370321
Sum of electronic and thermal Energies= -2496.331476
Sum of electronic and thermal Enthalpies= -2496.330532
Sum of electronic and thermal Free Energies= -2496.448096

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Cartesian Coordinates

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26	-0.001951	0.000108	0.122900
17	-0.017394	0.000370	2.444526
7	-0.005182	1.997344	-0.161448
7	-1.998881	-0.003812	-0.172908
7	1.994716	0.003908	-0.151206
7	0.002379	-1.997120	-0.161047
6	1.094449	2.837407	-0.165007
6	0.669338	4.210604	-0.167017
6	-0.690420	4.207244	-0.175132
6	-1.108835	2.832224	-0.157130
6	-2.446017	2.434919	-0.142887
6	-3.505052	3.490875	-0.112324
6	-3.709639	4.256525	1.045511

6	-4.698575	5.240704	1.077249
6	-5.494419	5.472694	-0.046989
6	-2.838363	1.096188	-0.149185
6	-4.210948	0.672031	-0.102549
6	-4.208364	-0.687766	-0.099551
6	-2.834205	-1.106908	-0.144920
6	-2.436704	-2.444077	-0.135369
6	-3.491333	-3.504247	-0.099589
6	-3.689657	-4.267846	1.060680
6	-4.674094	-5.256359	1.097333
6	-5.471607	-5.494786	-0.024371
6	2.833448	-1.096044	-0.181440
6	4.205016	-0.671597	-0.254102
6	4.202449	0.688163	-0.251322
6	2.829264	1.107115	-0.177519
6	2.433102	2.444741	-0.166537
6	3.492306	3.500866	-0.161475
6	4.278645	3.709118	0.981712
6	5.269640	4.691734	0.989535
6	5.488236	5.477282	-0.144538
6	3.718979	4.294263	-1.296194
6	4.710820	5.276123	-1.287358
6	-4.309158	3.730314	-1.236697
6	-5.297398	4.715373	-1.203902
6	-4.297055	-3.750172	-1.221411
6	-5.280780	-4.739565	-1.183695
6	-1.098023	-2.836238	-0.152547
6	-0.674401	-4.209638	-0.171490
6	0.685388	-4.207758	-0.169150
6	1.105212	-2.832931	-0.168577
6	2.442358	-2.435184	-0.173322
6	3.505424	-3.487439	-0.173797
6	4.296006	-3.695761	0.966451
6	5.290725	-4.674633	0.968654
6	5.508759	-5.456434	-0.168115
6	3.731439	-4.277196	-1.311184
6	4.726993	-5.255323	-1.307970
1	1.333024	5.061850	-0.167309
1	-1.358415	5.055059	-0.189877
1	-3.092001	4.071370	1.919331
1	-4.849125	5.822926	1.981934
1	-6.263987	6.239003	-0.021541
1	-5.060745	1.336560	-0.064833
1	-5.055648	-1.355326	-0.058947
1	-3.070675	-4.077745	1.932485
1	-4.819808	-5.836952	2.003855
1	-6.237641	-6.264492	0.004890
1	5.053516	-1.336218	-0.314086
1	5.048430	1.356230	-0.308668
1	4.104653	3.098900	1.863025
1	5.868006	4.845172	1.883139
1	6.259986	6.241787	-0.137832
1	3.115453	4.134788	-2.185003

1	4.878079	5.880655	-2.174362
1	-4.153536	3.141693	-2.136148
1	-5.910468	4.892806	-2.083046
1	-4.146173	-3.163241	-2.122774
1	-5.895142	-4.922046	-2.060903
1	-1.339213	-5.060000	-0.183337
1	1.352360	-5.056433	-0.172026
1	4.122481	-3.088463	1.849869
1	5.892436	-4.828117	1.860001
1	6.283427	-6.218007	-0.165779
1	3.124533	-4.117745	-2.197694
1	4.893715	-5.856979	-2.197029

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^{6}21A

Number of imaginary frequencies : 0
Electronic energy : HF=-2496.9734611
Zero-point correction= 0.598231 (Hartree/Particle)
Thermal correction to Energy= 0.637392
Thermal correction to Enthalpy= 0.638336
Thermal correction to Gibbs Free Energy= 0.521048
Sum of electronic and zero-point Energies= -2496.375230
Sum of electronic and thermal Energies= -2496.336069
Sum of electronic and thermal Enthalpies= -2496.335125
Sum of electronic and thermal Free Energies= -2496.452413

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Cartesian Coordinates

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26	-0.007154	0.000012	0.343319
17	-0.066815	0.000041	2.599765
7	0.002231	2.034582	-0.143097
7	-2.034249	0.001405	-0.185401
7	2.035879	-0.001393	-0.094996
7	-0.000584	-2.034544	-0.143088
6	1.108496	2.861578	-0.159661
6	0.683364	4.238676	-0.185430
6	-0.678340	4.238525	-0.198458
6	-1.103820	2.861983	-0.160359
6	-2.444835	2.448137	-0.156033
6	-3.501190	3.507634	-0.136497
6	-3.679688	4.310837	1.000458
6	-4.665956	5.297768	1.022952
6	-5.485929	5.496203	-0.090278
6	-2.861086	1.107975	-0.163428
6	-4.237950	0.683852	-0.119732
6	-4.238898	-0.677941	-0.119326
6	-2.862628	-1.104006	-0.162847
6	-2.448217	-2.444740	-0.155006
6	-3.506011	-3.502785	-0.134655
6	-3.685216	-4.305182	1.002757
6	-4.672896	-5.290682	1.026111
6	-5.493566	-5.488493	-0.086714
6	2.860164	-1.107974	-0.151516

6	4.233897	-0.683705	-0.255654
6	4.234845	0.677960	-0.255208
6	2.861695	1.104071	-0.150897
6	2.448518	2.445228	-0.158047
6	3.511590	3.497761	-0.187555
6	4.344556	3.697217	0.924014
6	5.341335	4.673558	0.896288
6	5.520346	5.461964	-0.242683
6	3.699176	4.294635	-1.327430
6	4.696972	5.269871	-1.354469
6	-4.329989	3.714055	-1.249815
6	-5.315303	4.702167	-1.226586
6	-4.335480	-3.708607	-1.247585
6	-5.322203	-4.695292	-1.223496
6	-1.107776	-2.860431	-0.159729
6	-0.684207	-4.237555	-0.197960
6	0.677505	-4.239566	-0.185755
6	1.104533	-2.863051	-0.160215
6	2.445134	-2.448549	-0.159089
6	3.506678	-3.502598	-0.189458
6	4.339839	-3.703751	0.921656
6	5.335100	-4.681618	0.893108
6	5.512377	-5.469870	-0.246241
6	3.692518	-4.299328	-1.329721
6	4.688799	-5.276088	-1.357583
1	1.344016	5.092385	-0.198414
1	-1.339054	5.091641	-0.233265
1	-3.043664	4.152436	1.866303
1	-4.795610	5.908375	1.912045
1	-6.253460	6.264754	-0.072240
1	-5.090307	1.345352	-0.081580
1	-5.092176	-1.338228	-0.080791
1	-3.048648	-4.147257	1.868290
1	-4.803103	-5.900653	1.915560
1	-6.262209	-6.255916	-0.068001
1	5.082529	-1.345684	-0.340636
1	5.084396	1.338814	-0.339765
1	4.202748	3.084521	1.809358
1	5.975594	4.819635	1.766059
1	6.296955	6.221251	-0.263940
1	3.060920	4.141566	-2.192687
1	4.833234	5.875973	-2.245698
1	-4.195025	3.097315	-2.133511
1	-5.946854	4.853303	-2.097511
1	-4.199947	-3.092511	-2.131641
1	-5.954284	-4.845967	-2.094115
1	-1.346110	-5.089768	-0.232335
1	1.336989	-5.094172	-0.199108
1	4.199365	-3.091185	1.807303
1	5.969519	-4.829015	1.762538
1	6.287793	-6.230358	-0.268129
1	3.054084	-4.144960	-2.194616
1	4.823710	-5.882071	-2.249099

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^{CSS}21

Number of imaginary frequencies : 0
Electronic energy : HF=-2036.6934914
Zero-point correction= 0.599037 (Hartree/Particle)
Thermal correction to Energy= 0.635496
Thermal correction to Enthalpy= 0.636440
Thermal correction to Gibbs Free Energy= 0.528277
Sum of electronic and zero-point Energies= -2036.094454
Sum of electronic and thermal Energies= -2036.057996
Sum of electronic and thermal Enthalpies= -2036.057051
Sum of electronic and thermal Free Energies= -2036.165215

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Cartesian Coordinates

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6	2.659175	1.497784	-0.036285
7	1.278738	1.554266	-0.012937
1	4.265131	3.064374	-0.095945
6	0.959703	2.898314	-0.027206
6	2.162583	3.694289	-0.083377
1	2.192018	4.772890	-0.118475
6	3.211282	2.830295	-0.075856
6	-0.332087	3.435987	0.018153
7	-1.552660	1.278083	0.002077
6	-2.895625	0.957390	0.049734
6	-3.689175	2.157185	0.167257
1	-4.765291	2.184061	0.249610
6	-2.825331	3.206153	0.168941
1	-3.057450	4.257220	0.252764
6	-1.495617	2.657725	0.054267
6	3.435341	0.333931	0.001718
1	3.069174	-4.261917	0.117123
6	2.833254	-3.208927	0.083935
6	1.499923	-2.659007	0.029058
1	4.775588	-2.186894	0.096998
7	1.554823	-1.278344	0.015804
6	2.898354	-0.957801	0.039466
6	3.696425	-2.159525	0.077617
6	-3.434397	-0.334124	-0.001466
1	-2.181470	-4.766786	-0.253337
6	-2.155222	-3.690700	-0.169890
6	-3.204532	-2.827210	-0.168791
1	-4.255534	-3.059929	-0.251450
6	-2.656461	-1.497441	-0.051679
7	-1.276554	-1.554159	-0.003140
6	-0.955591	-2.896813	-0.054365
6	0.336138	-3.435862	-0.016529
26	0.001187	-0.000039	0.000596
6	4.925678	0.477814	0.000888
6	5.671045	0.203900	1.157676
6	5.603019	0.886684	-1.157842
6	7.060720	0.334263	1.155413

1	5.153711	-0.112063	2.058917
6	6.992549	1.018583	-1.159877
1	5.032726	1.098915	-2.057504
6	7.725279	0.742246	-0.003354
1	7.623334	0.120293	2.059923
1	7.502046	1.333665	-2.066285
1	8.806834	0.843888	-0.005110
6	-0.478345	4.925037	0.034195
6	-0.054134	5.674866	1.142374
6	-1.042933	5.599539	-1.059569
6	-0.189142	7.063806	1.155647
1	0.381405	5.160491	1.993952
6	-1.178020	6.988532	-1.046525
1	-1.372978	5.026941	-1.921349
6	-0.751128	7.724727	0.061000
1	0.141666	7.628616	2.022794
1	-1.613014	7.495212	-1.903551
1	-0.855724	8.805950	0.071042
6	-4.923332	-0.477829	-0.001461
6	-5.585769	-1.070584	1.084969
6	-5.686605	-0.019048	-1.086666
6	-6.975236	-1.200527	1.086594
1	-5.003227	-1.426013	1.929750
6	-7.075996	-0.149265	-1.085432
1	-5.181990	0.439203	-1.932111
6	-7.724447	-0.740160	0.001429
1	-7.472163	-1.657516	1.937849
1	-7.651022	0.208084	-1.935153
1	-8.806092	-0.840771	0.002893
6	0.477643	-4.925484	-0.032242
6	1.031074	-5.581456	-1.142814
6	0.053553	-5.694790	1.062471
6	1.157714	-6.971226	-1.158136
1	1.359075	-4.993911	-1.995248
6	0.179971	-7.084546	1.047348
1	-0.375455	-5.194951	1.925976
6	0.732522	-7.726803	-0.063077
1	1.584589	-7.463248	-2.027677
1	-0.150482	-7.664616	1.904514
1	0.830369	-8.808638	-0.075287

***oss*21**

Number of imaginary frequencies : 0
Electronic energy : HF=-2036.7249672
Zero-point correction= 0.598447 (Hartree/Particle)
Thermal correction to Energy= 0.635178
Thermal correction to Enthalpy= 0.636122
Thermal correction to Gibbs Free Energy= 0.526564
Sum of electronic and zero-point Energies= -2036.126520
Sum of electronic and thermal Energies= -2036.089789
Sum of electronic and thermal Enthalpies= -2036.088845
Sum of electronic and thermal Free Energies= -2036.198403

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Cartesian Coordinates
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6	2.781939	-1.259526	0.039598
7	1.410368	-1.436508	0.012929
1	4.517608	-2.679505	0.101580
6	1.209788	-2.802944	0.024850
6	2.477178	-3.489973	0.082083
1	2.600894	-4.561967	0.116411
6	3.447526	-2.537615	0.078652
6	-0.029988	-3.452384	-0.021411
7	-1.434623	-1.409426	-0.000956
6	-2.801995	-1.206963	-0.048159
6	-3.487086	-2.469910	-0.166366
1	-4.556767	-2.590770	-0.248175
6	-2.533930	-3.439605	-0.170544
1	-2.674404	-4.506672	-0.256438
6	-1.257304	-2.778308	-0.055326
6	3.453229	-0.032204	0.005406
1	2.685913	4.512470	-0.116989
6	2.541893	3.443075	-0.080982
6	1.261821	2.779831	-0.026785
1	4.566933	2.594969	-0.089752
7	1.437182	1.409687	-0.010526
6	2.805155	1.207415	-0.031949
6	3.494368	2.472900	-0.070943
6	-3.451919	0.032167	0.003515
1	-2.589537	4.556515	0.249591
6	-2.469316	3.486770	0.166291
6	-3.440259	2.534896	0.167959
1	-4.507284	2.676040	0.251922
6	-2.778990	1.259148	0.051448
7	-1.407995	1.436287	0.000334
6	-1.205397	2.801524	0.050471
6	0.034193	3.452464	0.014035
26	0.001309	0.000022	0.000252
6	4.950610	-0.045790	0.008344
6	5.670091	0.286173	-1.149545
6	5.659396	-0.390082	1.169175
6	7.065837	0.274881	-1.146473
1	5.127776	0.552257	-2.052208
6	7.055154	-0.402805	1.171887
1	5.108867	-0.646884	2.069539
6	7.762085	-0.069890	0.014201
1	7.608447	0.532292	-2.051886
1	7.589612	-0.669129	2.079559
1	8.848409	-0.078965	0.016516
6	-0.045816	-4.948197	-0.041213
6	0.441555	-5.655105	-1.151673
6	-0.551348	-5.672235	1.049840
6	0.424551	-7.050428	-1.170186
1	0.831629	-5.102371	-2.001238
6	-0.568171	-7.067590	1.031499

1	-0.928885	-5.132805	1.913546
6	-0.080236	-7.760733	-0.078590
1	0.802081	-7.581865	-2.039355
1	-0.959189	-7.612573	1.886207
1	-0.093331	-8.846913	-0.092997
6	-4.947713	0.045237	0.008007
6	-5.662480	0.575626	-1.077439
6	-5.664226	-0.473061	1.098166
6	-7.057938	0.587477	-1.072909
1	-5.115721	0.976095	-1.926024
6	-7.059659	-0.460653	1.103055
1	-5.118823	-0.883406	1.942888
6	-7.760581	0.069518	0.017453
1	-7.595609	0.997909	-1.923117
1	-7.598598	-0.861901	1.956839
1	-8.846891	0.078825	0.021117
6	0.044738	4.948404	0.024577
6	0.543167	5.654311	1.130711
6	-0.447440	5.673660	-1.071799
6	0.550747	7.049827	1.139576
1	0.922255	5.100706	1.984678
6	-0.439703	7.069164	-1.063114
1	-0.834110	5.135014	-1.931941
6	0.059613	7.761303	0.042540
1	0.936576	7.580568	2.005518
1	-0.820608	7.614979	-1.921848
1	0.065402	8.847623	0.049436

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^{3}21

Number of imaginary frequencies : 0
Electronic energy : HF=-2036.7432458
Zero-point correction= 0.598783 (Hartree/Particle)
Thermal correction to Energy= 0.635379
Thermal correction to Enthalpy= 0.636323
Thermal correction to Gibbs Free Energy= 0.526457
Sum of electronic and zero-point Energies= -2036.144463
Sum of electronic and thermal Energies= -2036.107867
Sum of electronic and thermal Enthalpies= -2036.106923
Sum of electronic and thermal Free Energies= -2036.216789

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Cartesian Coordinates

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6	-2.791972	-1.221486	0.092220
7	-1.424077	-1.415875	0.017873
1	-4.530156	-2.609509	0.380850
6	-1.236862	-2.782694	0.090991
6	-2.504457	-3.447836	0.264348
1	-2.634693	-4.513285	0.380876
6	-3.464142	-2.484521	0.264874
6	-0.009293	-3.450301	0.000156
7	1.416429	-1.423529	-0.017839
6	2.785346	-1.236511	-0.092372

6	3.450688	-2.503165	-0.264957
1	4.516002	-2.633907	-0.381034
6	2.485830	-3.461298	-0.264220
1	2.610315	-4.527444	-0.380650
6	1.221852	-2.789326	-0.090799
6	-3.452241	0.009296	-0.000145
1	-2.610310	4.527436	-0.380695
6	-2.485826	3.461291	-0.264254
6	-1.221849	2.789323	-0.090808
1	-4.515998	2.633894	-0.381065
7	-1.416425	1.423527	-0.017848
6	-2.785341	1.236508	-0.092378
6	-3.450684	2.503158	-0.264981
6	3.452246	-0.009298	-0.000147
1	2.634704	4.513272	0.380919
6	2.504465	3.447827	0.264369
6	3.464153	2.484515	0.264858
1	4.530170	2.609501	0.380820
6	2.791978	1.221484	0.092217
7	1.424083	1.415874	0.017871
6	1.236868	2.782694	0.090982
6	0.009297	3.450301	0.000150
26	0.000002	-0.000001	0.000024
6	-4.947410	0.013308	-0.000284
6	-5.661974	0.603293	1.054392
6	-5.664912	-0.572872	-1.055086
6	-7.057376	0.606511	1.054552
1	-5.114869	1.056673	1.875638
6	-7.060311	-0.568693	-1.055490
1	-5.120074	-1.029170	-1.876223
6	-7.760685	0.020767	-0.000528
1	-7.594525	1.063475	1.881009
1	-7.599733	-1.022812	-1.882035
1	-8.847060	0.023652	-0.000623
6	-0.013306	-4.945085	0.000274
6	0.580612	-5.662990	1.050687
6	-0.611049	-5.659984	-1.050019
6	0.576409	-7.058356	1.051077
1	1.042506	-5.118239	1.868725
6	-0.614280	-7.055352	-1.050178
1	-1.070016	-5.112915	-1.868158
6	-0.020803	-7.758763	0.000505
1	1.036449	-7.597753	1.874361
1	-1.077183	-7.592424	-1.873377
1	-0.023704	-8.845136	0.000596
6	4.947416	-0.013302	-0.000286
6	5.661983	-0.603232	1.054418
6	5.664910	0.572833	-1.055118
6	7.057386	-0.606452	1.054570
1	5.114881	-1.056570	1.875688
6	7.060310	0.568645	-1.055533
1	5.120068	1.029082	-1.876278
6	7.760688	-0.020764	-0.000545

1	7.594540	-1.063369	1.881049
1	7.599729	1.022712	-1.882108
1	8.847064	-0.023652	-0.000648
6	0.013301	4.945086	0.000272
6	0.610994	5.659992	-1.050044
6	-0.580583	5.662984	1.050709
6	0.614217	7.055361	-1.050199
1	1.069935	5.112929	-1.868202
6	-0.576388	7.058350	1.051103
1	-1.042441	5.118227	1.868763
6	0.020779	7.758764	0.000511
1	1.077083	7.592439	-1.873414
1	-1.036399	7.597741	1.874407
1	0.023673	8.845137	0.000606

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^{5}21

Number of imaginary frequencies : 0
Electronic energy : HF=-2036.7300487
Zero-point correction= 0.597328 (Hartree/Particle)
Thermal correction to Energy= 0.633962
Thermal correction to Enthalpy= 0.634906
Thermal correction to Gibbs Free Energy= 0.525604
Sum of electronic and zero-point Energies= -2036.132721
Sum of electronic and thermal Energies= -2036.096087
Sum of electronic and thermal Enthalpies= -2036.095143
Sum of electronic and thermal Free Energies= -2036.204444

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Cartesian Coordinates

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6	-2.886796	1.109790	0.032768
7	-2.073651	-0.000120	-0.016450
1	-5.120075	1.337302	0.209917
6	-2.886681	-1.110108	0.032642
6	-4.265053	-0.682402	0.131710
1	-5.119938	-1.337904	0.209738
6	-4.265120	0.681906	0.131797
6	-2.454414	-2.455263	0.024127
7	0.000131	-2.074958	-0.000020
6	1.110320	-2.889400	-0.008387
6	0.682371	-4.271158	0.002532
1	1.336847	-5.130212	0.010729
6	-0.681879	-4.271226	-0.002727
1	-1.336257	-5.130351	-0.010968
6	-1.109989	-2.889513	0.008314
6	-2.454667	2.454999	0.024407
1	1.336265	5.130359	0.011549
6	0.681893	4.271231	0.003233
6	1.110011	2.889522	-0.007951
1	-1.336840	5.130209	-0.010094
7	-0.000103	2.074962	0.000401
6	-1.110298	2.889398	0.008772
6	-0.682359	4.271158	-0.001999

6	2.454689	-2.455006	-0.024204
1	5.119879	1.337897	-0.210638
6	4.265026	0.682405	-0.132185
6	4.265095	-0.681906	-0.132250
1	5.120019	-1.337292	-0.210769
6	2.886812	-1.109788	-0.032679
7	2.073691	0.000123	0.016975
6	2.886696	1.110112	-0.032575
6	2.454435	2.455275	-0.023961
26	0.000015	0.000002	0.000511
6	-3.516671	3.510102	0.037403
6	-3.673028	4.361605	1.142637
6	-4.380871	3.665375	-1.058251
6	-4.665063	5.343119	1.151056
1	-3.012473	4.246117	1.996866
6	-5.373450	4.646196	-1.049815
1	-4.266590	3.012103	-1.918271
6	-5.518291	5.488576	0.054814
1	-4.773881	5.990878	2.016495
1	-6.030617	4.754369	-1.908247
1	-6.290680	6.252493	0.061480
6	-3.516414	-3.510365	0.037260
6	-3.672738	-4.361772	1.142577
6	-4.380890	-3.665491	-1.058195
6	-4.664925	-5.343128	1.151215
1	-3.012037	-4.246330	1.996699
6	-5.373621	-4.646155	-1.049540
1	-4.266697	-3.012235	-1.918239
6	-5.518379	-5.488488	0.055136
1	-4.773702	-5.990822	2.016709
1	-6.030985	-4.754232	-1.907834
1	-6.290923	-6.252246	0.061997
6	3.516677	-3.510109	-0.037446
6	4.381287	-3.665242	1.057908
6	3.672601	-4.361798	-1.142603
6	5.373837	-4.646088	1.049253
1	4.267345	-3.011835	1.917871
6	4.664607	-5.343337	-1.151242
1	3.011731	-4.246426	-1.996604
6	5.518244	-5.488645	-0.055299
1	6.031321	-4.754144	1.907457
1	4.773083	-5.991232	-2.016623
1	6.290608	-6.252586	-0.062133
6	3.516421	3.510377	-0.037379
6	3.672316	4.361920	-1.142654
6	4.381309	3.665404	1.057770
6	4.664488	5.343288	-1.151557
1	3.011289	4.246574	-1.996537
6	5.374023	4.646081	1.048851
1	4.267442	3.012059	1.917790
6	5.518356	5.488537	-0.055787
1	4.772923	5.991083	-2.017019
1	6.031706	4.754071	1.906912

1	6.290887	6.252307	-0.062855

1a

Number of imaginary frequencies : 0
Electronic energy : HF=-642.9734257
Zero-point correction= 0.175326 (Hartree/Particle)
Thermal correction to Energy= 0.185571
Thermal correction to Enthalpy= 0.186515
Thermal correction to Gibbs Free Energy= 0.138570
Sum of electronic and zero-point Energies= -642.798100
Sum of electronic and thermal Energies= -642.787855
Sum of electronic and thermal Enthalpies= -642.786910
Sum of electronic and thermal Free Energies= -642.834856

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Cartesian Coordinates

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6	1.163297	-0.422462	-0.060415
6	2.927651	1.238902	0.134155
6	1.971892	2.204764	0.274877
6	0.591001	1.868914	0.252751
6	0.142526	0.569529	0.078752
1	3.999147	1.387208	0.141221
1	2.277703	3.235012	0.414555
1	-0.133305	2.662594	0.398846
6	-1.294107	0.216455	0.034304
6	-2.229401	1.133886	-0.479245
6	-1.759839	-1.021876	0.512267
6	-3.588860	0.830858	-0.498069
1	-1.888652	2.078153	-0.893063
6	-3.121423	-1.319795	0.492779
1	-1.055203	-1.750412	0.894992
6	-4.041218	-0.396541	-0.008125
1	-4.293792	1.549430	-0.906257
1	-3.462940	-2.279034	0.870794
1	-5.100903	-0.634438	-0.025460
7	2.485834	-0.045796	-0.026611
7	1.137453	-1.750192	-0.238349
7	2.418382	-2.144030	-0.306395
7	3.256735	-1.154884	-0.185761

1a'

Number of imaginary frequencies : 0
Electronic energy : HF=-642.9622872
Zero-point correction= 0.173099 (Hartree/Particle)
Thermal correction to Energy= 0.184518
Thermal correction to Enthalpy= 0.185463
Thermal correction to Gibbs Free Energy= 0.134587
Sum of electronic and zero-point Energies= -642.789188
Sum of electronic and thermal Energies= -642.777769
Sum of electronic and thermal Enthalpies= -642.776825
Sum of electronic and thermal Free Energies= -642.827700

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Cartesian Coordinates
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6	1.335627	0.085815	-0.014500
6	0.204006	-0.757833	0.091258
6	0.480687	-2.124899	0.220745
6	1.795382	-2.587943	0.248376
6	2.822288	-1.652692	0.145747
1	-0.347159	-2.820681	0.318409
1	2.017018	-3.644340	0.355950
1	3.865366	-1.960568	0.168417
7	2.599912	-0.340510	0.013987
6	-1.198238	-0.270568	0.049437
6	-2.144261	-0.947069	-0.739603
6	-1.624357	0.830882	0.811029
6	-3.476316	-0.535027	-0.768402
1	-1.826805	-1.788586	-1.348915
6	-2.956714	1.239884	0.782712
1	-0.910717	1.361396	1.431602
6	-3.887602	0.560200	-0.006479
1	-4.190504	-1.066062	-1.391431
1	-3.268846	2.090158	1.382536
1	-4.924433	0.883344	-0.028824
7	1.110014	1.472538	-0.182973
7	2.120178	2.186420	-0.280294
7	2.953191	2.953102	-0.380673

N_2

Number of imaginary frequencies : 0
Electronic energy : HF=-109.515205
Zero-point correction= 0.005605 (Hartree/Particle)
Thermal correction to Energy= 0.007966
Thermal correction to Enthalpy= 0.008910
Thermal correction to Gibbs Free Energy= -0.012843
Sum of electronic and zero-point Energies= -109.509600
Sum of electronic and thermal Energies= -109.507239
Sum of electronic and thermal Enthalpies= -109.506295
Sum of electronic and thermal Free Energies= -109.528048

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Cartesian Coordinates
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7	0.000000	0.000000	0.552489
7	0.000000	0.000000	-0.552489

***oss*22**

Number of imaginary frequencies : 1
Electronic energy : HF=-2679.716677
Zero-point correction= 0.772446 (Hartree/Particle)
Thermal correction to Energy= 0.821506
Thermal correction to Enthalpy= 0.822451
Thermal correction to Gibbs Free Energy= 0.687180

Sum of electronic and zero-point Energies= -2678.944231
Sum of electronic and thermal Energies= -2678.895171
Sum of electronic and thermal Enthalpies= -2678.894227
Sum of electronic and thermal Free Energies= -2679.029497

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Cartesian Coordinates

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6	0.293165	3.306498	-0.667966
7	-0.632253	2.281899	-0.652724
1	0.117111	5.542842	-0.576119
6	-1.862205	2.887980	-0.508058
6	-1.705972	4.323432	-0.465985
1	-2.514940	5.034307	-0.387353
6	-0.374624	4.581613	-0.562770
6	-3.097905	2.231699	-0.420515
7	-2.260028	-0.065255	-0.820524
6	-2.872119	-1.299502	-0.845751
6	-4.282389	-1.161657	-0.569359
1	-4.988138	-1.976689	-0.511655
6	-4.520391	0.163225	-0.383631
1	-5.458465	0.640941	-0.143610
6	-3.257405	0.845083	-0.547643
6	1.682569	3.156655	-0.762791
1	4.947274	-0.056222	-1.312377
6	3.991774	0.436159	-1.209685
6	2.708091	-0.222928	-1.253567
1	4.474656	2.557671	-0.914469
7	1.695961	0.696265	-1.063565
6	2.321957	1.923083	-0.938237
6	3.753031	1.760355	-1.009939
6	-2.235214	-2.529899	-1.049264
1	1.918368	-4.355550	-1.889301
6	1.124715	-3.663345	-1.650405
6	-0.205173	-3.922627	-1.539006
1	-0.710666	-4.867616	-1.671048
6	-0.854151	-2.669827	-1.233267
7	0.078916	-1.654337	-1.167535
6	1.300589	-2.250394	-1.410018
6	2.543608	-1.604121	-1.429922
6	-2.430230	-2.207649	2.811042
6	-1.701405	-2.970004	3.722483
6	-0.346749	-2.687249	3.880626
6	0.258820	-1.663949	3.138081
6	-0.600753	-0.940321	2.279569
1	-3.484256	-2.400883	2.628703
1	-2.176939	-3.770505	4.279464
1	0.265633	-3.277530	4.555689
7	0.607250	0.997770	1.940277
7	1.281578	1.861599	2.235433
26	-0.279585	0.302039	-0.837212
7	-0.134992	0.131925	1.441418
6	1.714337	-1.398201	3.262055
6	2.522645	-1.283004	2.119331

6	2.309759	-1.283321	4.528369
6	3.891145	-1.049215	2.240017
1	2.077094	-1.376894	1.136503
6	3.680458	-1.052406	4.646922
1	1.691960	-1.355955	5.419185
6	4.474301	-0.932393	3.503884
1	4.494089	-0.959161	1.342306
1	4.126248	-0.956880	5.632970
1	5.540130	-0.745239	3.597518
7	-1.889926	-1.205100	2.110954
6	2.530625	4.383303	-0.648880
6	3.253578	4.867602	-1.749668
6	2.616909	5.070820	0.571899
6	4.043726	6.012295	-1.632964
1	3.189618	4.341684	-2.697757
6	3.407248	6.214989	0.688476
1	2.064000	4.696310	1.428287
6	4.122670	6.689137	-0.413680
1	4.594125	6.377035	-2.495862
1	3.466974	6.733500	1.641444
1	4.737609	7.580193	-0.323153
6	3.770351	-2.439770	-1.617411
6	4.167740	-3.348871	-0.623620
6	4.551438	-2.326198	-2.777814
6	5.318914	-4.121325	-0.784864
1	3.573244	-3.436988	0.280384
6	5.701768	-3.099902	-2.939715
1	4.249191	-1.627627	-3.552432
6	6.089300	-3.999177	-1.943520
1	5.615059	-4.815179	-0.002950
1	6.292972	-3.002335	-3.846043
1	6.985332	-4.600418	-2.069539
6	-3.070003	-3.769890	-1.032551
6	-4.023908	-4.016900	-2.031770
6	-2.915163	-4.710796	-0.001494
6	-4.803836	-5.174033	-2.000684
1	-4.147895	-3.295748	-2.834236
6	-3.695225	-5.867401	0.029953
1	-2.182196	-4.523146	0.777450
6	-4.642068	-6.102636	-0.969860
1	-5.534758	-5.351743	-2.784700
1	-3.565256	-6.583462	0.836930
1	-5.249022	-7.003377	-0.946413
6	-4.317977	3.062701	-0.181447
6	-4.487170	3.754087	1.028618
6	-5.316807	3.168921	-1.162285
6	-5.625235	4.530037	1.252495
1	-3.720309	3.674881	1.793514
6	-6.454681	3.945408	-0.939063
1	-5.192272	2.639890	-2.102508
6	-6.612459	4.628222	0.269175
1	-5.742081	5.054660	2.196784
1	-7.215603	4.019967	-1.711090

1	-7.498325	5.232540	0.443283

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^{CSS}22'

Number of imaginary frequencies : 0
Electronic energy : HF=-2679.7043219
Zero-point correction= 0.773063 (Hartree/Particle)
Thermal correction to Energy= 0.822634
Thermal correction to Enthalpy= 0.823578
Thermal correction to Gibbs Free Energy= 0.686064
Sum of electronic and zero-point Energies= -2678.931259
Sum of electronic and thermal Energies= -2678.881688
Sum of electronic and thermal Enthalpies= -2678.880744
Sum of electronic and thermal Free Energies= -2679.018258

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Cartesian Coordinates

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6	2.479764	1.577447	-1.172537
7	1.130514	1.734900	-0.920855
1	4.179942	3.024506	-1.417433
6	0.939144	3.091338	-0.747413
6	2.183312	3.798840	-0.936825
1	2.301219	4.871024	-0.887187
6	3.133395	2.864670	-1.205134
6	-0.273187	3.714469	-0.422332
7	-1.693010	1.698804	-0.613709
6	-3.050553	1.490297	-0.509526
6	-3.720145	2.721213	-0.156214
1	-4.783188	2.826798	0.001837
6	-2.760562	3.677755	-0.053050
1	-2.885983	4.718956	0.203798
6	-1.499891	3.041735	-0.362412
6	3.145685	0.358651	-1.348241
1	2.402896	-4.196528	-1.390466
6	2.252923	-3.127553	-1.368067
6	0.974664	-2.468020	-1.242088
1	4.264257	-2.269557	-1.554498
7	1.146175	-1.097576	-1.215140
6	2.503454	-0.886440	-1.357316
6	3.196130	-2.150612	-1.451140
6	-3.708401	0.268632	-0.693464
1	-2.888723	-4.225911	-1.317978
6	-2.761718	-3.162395	-1.179619
6	-3.724656	-2.207937	-1.091433
1	-4.795606	-2.338178	-1.138730
6	-3.047667	-0.941983	-0.925190
7	-1.681177	-1.123917	-0.961035
6	-1.489110	-2.482455	-1.094010
6	-0.253430	-3.136981	-1.162977
6	-2.514993	-1.939071	2.801875
6	-1.829833	-2.685043	3.760134
6	-0.457862	-2.486186	3.890583
6	0.207580	-1.569749	3.064128

6	-0.608714	-0.860258	2.156300
1	-3.584064	-2.065685	2.650102
1	-2.354372	-3.405215	4.379288
1	0.120403	-3.058014	4.610120
7	0.708151	0.966191	1.769859
7	1.404568	1.775542	2.147456
26	-0.267192	0.287685	-0.787362
7	-0.052977	0.120794	1.244944
6	1.678300	-1.383609	3.167734
6	2.495582	-1.511296	2.034646
6	2.268768	-1.086184	4.405945
6	3.874547	-1.335728	2.135980
1	2.048459	-1.751119	1.079155
6	3.649198	-0.909229	4.504447
1	1.640679	-0.976079	5.285692
6	4.454668	-1.029878	3.369429
1	4.489550	-1.434674	1.247442
1	4.093870	-0.670110	5.466284
1	5.528758	-0.886302	3.445388
7	-1.915637	-1.031303	2.025323
6	4.634402	0.383440	-1.488129
6	5.257781	-0.003455	-2.684253
6	5.437936	0.786462	-0.408702
6	6.649002	0.008783	-2.797768
1	4.643758	-0.312871	-3.524891
6	6.828907	0.797168	-0.521905
1	4.961408	1.084555	0.520153
6	7.438643	0.407812	-1.716887
1	7.115482	-0.290061	-3.732431
1	7.435590	1.107671	0.324403
1	8.521339	0.416466	-1.805793
6	-0.253894	-4.632137	-1.157433
6	-0.652010	-5.328271	-0.004890
6	0.132777	-5.366691	-2.288815
6	-0.658972	-6.723458	0.016780
1	-0.953417	-4.765228	0.873843
6	0.125439	-6.762322	-2.267312
1	0.435621	-4.835451	-3.186292
6	-0.269745	-7.444713	-1.114458
1	-0.965801	-7.247222	0.918034
1	0.423767	-7.316041	-3.153280
1	-0.275476	-8.531004	-1.098218
6	-5.200839	0.254972	-0.595182
6	-5.991379	0.871196	-1.577157
6	-5.837760	-0.366746	0.489955
6	-7.383761	0.861640	-1.479003
1	-5.506183	1.355993	-2.419249
6	-7.229529	-0.375765	0.589527
1	-5.228979	-0.834631	1.257647
6	-8.006860	0.237806	-0.395774
1	-7.981286	1.339549	-2.250445
1	-7.706740	-0.858020	1.438348
1	-9.090548	0.230836	-0.319235

6	-0.246143	5.179919	-0.126801
6	0.422682	5.655334	1.012547
6	-0.876212	6.104799	-0.973698
6	0.457268	7.020440	1.299490
1	0.912834	4.943949	1.671186
6	-0.840711	7.470369	-0.687283
1	-1.390874	5.745358	-1.859867
6	-0.174536	7.932059	0.450292
1	0.975685	7.371212	2.187637
1	-1.329680	8.173606	-1.355794
1	-0.147141	8.995092	0.672846

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^{3}22

Number of imaginary frequencies : 0
Electronic energy : HF=-2679.7310921
Zero-point correction= 0.772497 (Hartree/Particle)
Thermal correction to Energy= 0.822577
Thermal correction to Enthalpy= 0.823521
Thermal correction to Gibbs Free Energy= 0.682659
Sum of electronic and zero-point Energies= -2678.958595
Sum of electronic and thermal Energies= -2678.908515
Sum of electronic and thermal Enthalpies= -2678.907571
Sum of electronic and thermal Free Energies= -2679.048433

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Cartesian Coordinates

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6	0.160645	3.330073	-0.612365
7	-0.719226	2.265937	-0.655185
1	-0.113306	5.551876	-0.465038
6	-1.978854	2.815925	-0.539581
6	-1.885928	4.254375	-0.460368
1	-2.727257	4.927859	-0.394043
6	-0.564104	4.571240	-0.497171
6	-3.185788	2.105914	-0.493661
7	-2.228161	-0.152185	-0.848313
6	-2.779686	-1.416593	-0.852802
6	-4.197421	-1.342583	-0.595187
1	-4.861499	-2.190678	-0.523487
6	-4.503254	-0.027092	-0.447782
1	-5.466525	0.409762	-0.230903
6	-3.274099	0.712926	-0.608490
6	1.556249	3.244869	-0.674593
1	4.961309	0.205475	-1.325294
6	3.984617	0.650397	-1.206152
6	2.733735	-0.065431	-1.276733
1	4.369630	2.778078	-0.822117
7	1.679224	0.798870	-1.056936
6	2.249857	2.048058	-0.881099
6	3.685874	1.952915	-0.952490
6	-2.082560	-2.615589	-1.039954
1	2.143448	-4.222879	-1.947701
6	1.319372	-3.571743	-1.696874

6	0.007653	-3.900379	-1.554067
1	-0.450316	-4.871551	-1.667979
6	-0.699741	-2.682888	-1.243171
7	0.180780	-1.617743	-1.200706
6	1.427764	-2.152287	-1.463273
6	2.636891	-1.447010	-1.488766
6	-2.427970	-2.329230	2.866657
6	-1.639566	-3.141580	3.680156
6	-0.289818	-2.823885	3.812299
6	0.250412	-1.715968	3.145217
6	-0.665688	-0.945768	2.390017
1	-3.480032	-2.548753	2.702840
1	-2.065241	-4.006198	4.178571
1	0.369501	-3.450566	4.405558
7	0.504029	1.034875	2.111963
7	1.201347	1.891605	2.381318
26	-0.273624	0.316516	-0.894213
7	-0.283467	0.205467	1.631708
6	1.702288	-1.418226	3.231953
6	2.458096	-1.186516	2.070877
6	2.349542	-1.397917	4.477821
6	3.825942	-0.932657	2.155539
1	1.972604	-1.205990	1.102357
6	3.719096	-1.146004	4.559852
1	1.771849	-1.562280	5.383239
6	4.460547	-0.911058	3.399658
1	4.388285	-0.752070	1.245569
1	4.204919	-1.124809	5.531291
1	5.525718	-0.708547	3.464725
7	-1.951496	-1.249002	2.240517
6	2.345237	4.502671	-0.494653
6	3.052042	5.074100	-1.563377
6	2.386906	5.132506	0.758971
6	3.783934	6.248986	-1.383107
1	3.021393	4.592723	-2.536493
6	3.119162	6.306752	0.938821
1	1.846557	4.689057	1.590116
6	3.819154	6.868438	-0.131696
1	4.322733	6.682064	-2.221360
1	3.145552	6.780518	1.916246
1	4.388447	7.783106	0.008375
6	3.901824	-2.215956	-1.704634
6	4.359715	-3.116007	-0.728818
6	4.659798	-2.044394	-2.872986
6	5.546948	-3.825145	-0.916819
1	3.783662	-3.245908	0.182064
6	5.846469	-2.754770	-3.061312
1	4.311171	-1.351154	-3.632821
6	6.293606	-3.646760	-2.083758
1	5.890003	-4.513331	-0.149195
1	6.419567	-2.613279	-3.973445
1	7.217867	-4.198563	-2.230410
6	-2.848308	-3.898573	-0.991280

6	-3.792149	-4.220991	-1.978308
6	-2.634184	-4.805554	0.059350
6	-4.506120	-5.418774	-1.915444
1	-3.960598	-3.526638	-2.796142
6	-3.348400	-6.002651	0.122334
1	-1.908728	-4.559510	0.828890
6	-4.286784	-6.312835	-0.864933
1	-5.230416	-5.654955	-2.690079
1	-3.173752	-6.691815	0.944142
1	-4.842677	-7.244987	-0.816668
6	-4.451652	2.877632	-0.298465
6	-4.699071	3.557541	0.904500
6	-5.418017	2.934025	-1.315165
6	-5.881607	4.276075	1.085552
1	-3.958381	3.514057	1.697467
6	-6.600239	3.653232	-1.134581
1	-5.233491	2.411799	-2.249355
6	-6.835449	4.326591	0.066336
1	-6.059175	4.792880	2.024661
1	-7.335386	3.690266	-1.933796
1	-7.755924	4.886181	0.207227

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^{5}22

Number of imaginary frequencies : 0
Electronic energy : HF=-2679.6946082
Zero-point correction= 0.771113 (Hartree/Particle)
Thermal correction to Energy= 0.820916
Thermal correction to Enthalpy= 0.821861
Thermal correction to Gibbs Free Energy= 0.682863
Sum of electronic and zero-point Energies= -2678.923495
Sum of electronic and thermal Energies= -2678.873692
Sum of electronic and thermal Enthalpies= -2678.872748
Sum of electronic and thermal Free Energies= -2679.011746

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Cartesian Coordinates

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6	0.613089	3.239326	-0.901545
7	-0.388668	2.319709	-0.646649
1	0.663040	5.475865	-0.943853
6	-1.503807	3.059506	-0.309218
6	-1.201416	4.463199	-0.371778
1	-1.907676	5.255415	-0.173817
6	0.097223	4.573967	-0.765498
6	-2.776232	2.551184	-0.028828
7	-2.265156	0.244519	-0.768002
6	-3.045463	-0.881506	-0.939435
6	-4.403013	-0.603937	-0.553984
1	-5.211509	-1.318652	-0.583993
6	-4.438862	0.681596	-0.111442
1	-5.283512	1.224267	0.284697
6	-3.115082	1.218983	-0.272595
6	1.950813	2.942647	-1.166070

1	4.831246	-0.649228	-1.202349
6	3.934717	-0.048292	-1.209377
6	2.593834	-0.566901	-1.184128
1	4.637996	2.032470	-1.278432
7	1.683492	0.477189	-1.159388
6	2.438350	1.634738	-1.211518
6	3.837413	1.308781	-1.251845
6	-2.601755	-2.152232	-1.311859
1	1.314372	-4.533208	-1.816115
6	0.605323	-3.738566	-1.638686
6	-0.752454	-3.788048	-1.730811
1	-1.368414	-4.634530	-1.993800
6	-1.246886	-2.476141	-1.412961
7	-0.187337	-1.619597	-1.174307
6	0.956348	-2.385437	-1.307983
6	2.275232	-1.926750	-1.229158
6	-2.339580	-2.394722	2.426929
6	-1.737385	-3.089301	3.472397
6	-0.427861	-2.743027	3.802522
6	0.243279	-1.722284	3.119194
6	-0.501486	-1.024932	2.118159
1	-3.344534	-2.647113	2.092699
1	-2.259525	-3.888169	3.988891
1	0.105653	-3.299271	4.568375
7	0.777145	0.901548	2.160350
7	1.402976	1.835790	1.762756
26	-0.261482	0.320147	-0.653353
7	0.005236	0.055380	1.384026
6	1.681646	-1.485760	3.413818
6	2.625071	-1.390957	2.376641
6	2.142185	-1.431716	4.739003
6	3.981864	-1.249440	2.653632
1	2.284691	-1.415492	1.349416
6	3.502198	-1.286404	5.017634
1	1.426573	-1.483191	5.554896
6	4.428531	-1.196500	3.977040
1	4.688593	-1.178819	1.831726
1	3.836228	-1.236371	6.050555
1	5.486638	-1.080157	4.194235
7	-1.747325	-1.389187	1.779896
6	2.925621	4.065473	-1.305406
6	3.567880	4.308893	-2.528659
6	3.228855	4.879213	-0.202367
6	4.487884	5.351502	-2.649855
1	3.338907	3.679195	-3.383572
6	4.150809	5.919244	-0.324931
1	2.745498	4.678344	0.748863
6	4.780891	6.159172	-1.548638
1	4.973885	5.533058	-3.604427
1	4.381380	6.537918	0.537798
1	5.498236	6.969604	-1.642834
6	3.375911	-2.936614	-1.238509
6	3.510483	-3.833673	-0.166466

6	4.281954	-3.018119	-2.307636
6	4.535702	-4.780100	-0.158856
1	2.818007	-3.773088	0.666841
6	5.304597	-3.967435	-2.300083
1	4.176128	-2.335923	-3.145905
6	5.435345	-4.849600	-1.224850
1	4.632363	-5.459886	0.682902
1	5.995853	-4.020490	-3.136491
1	6.233020	-5.587015	-1.218565
6	-3.617760	-3.229174	-1.506035
6	-4.548504	-3.154854	-2.553629
6	-3.673347	-4.323384	-0.627069
6	-5.508142	-4.154044	-2.722587
1	-4.512432	-2.310721	-3.235997
6	-4.634390	-5.320589	-0.795816
1	-2.963867	-4.378124	0.192994
6	-5.553476	-5.239466	-1.844759
1	-6.218304	-4.085309	-3.541853
1	-4.668031	-6.158139	-0.104631
1	-6.301325	-6.016329	-1.976211
6	-3.812796	3.496126	0.481633
6	-3.647442	4.103403	1.736698
6	-4.948383	3.813640	-0.280417
6	-4.601163	4.998850	2.221790
1	-2.769639	3.862916	2.329068
6	-5.900241	4.710934	0.205065
1	-5.075568	3.358944	-1.258344
6	-5.729931	5.304627	1.457933
1	-4.462613	5.455606	3.197639
1	-6.771250	4.950664	-0.398414
1	-6.471288	6.003106	1.835604

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^{oss}(22-23)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2679.6876248
Zero-point correction= 0.769423 (Hartree/Particle)
Thermal correction to Energy= 0.819110
Thermal correction to Enthalpy= 0.820054
Thermal correction to Gibbs Free Energy= 0.682519
Sum of electronic and zero-point Energies= -2678.918202
Sum of electronic and thermal Energies= -2678.868515
Sum of electronic and thermal Enthalpies= -2678.867571
Sum of electronic and thermal Free Energies= -2679.005106

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Cartesian Coordinates

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6	1.535444	2.805875	-1.027219
7	0.317966	2.229450	-0.706383
1	2.245756	4.928275	-1.139037
6	-0.505738	3.273522	-0.343400
6	0.198724	4.524794	-0.453453
1	-0.229219	5.494670	-0.247945

6	1.448141	4.238187	-0.909224
6	-1.865500	3.171326	-0.025578
7	-2.092604	0.822257	-0.759697
6	-3.182736	-0.003541	-0.947718
6	-4.393742	0.682005	-0.578258
1	-5.384850	0.256595	-0.626467
6	-4.032387	1.909655	-0.118387
1	-4.672021	2.685034	0.275090
6	-2.603528	2.009523	-0.264902
6	2.711169	2.111733	-1.320256
1	4.383197	-2.179610	-1.163828
6	3.709123	-1.337092	-1.198204
6	2.274255	-1.421422	-1.119212
1	5.003547	0.423870	-1.429544
7	1.721395	-0.153184	-1.155144
6	2.787641	0.715764	-1.296926
6	4.023508	-0.019445	-1.336478
6	-3.145063	-1.355850	-1.298377
1	-0.146461	-4.855651	-1.522859
6	-0.582386	-3.873424	-1.416052
6	-1.884008	-3.510801	-1.569915
1	-2.722982	-4.141593	-1.821662
6	-1.956488	-2.089717	-1.336787
7	-0.693851	-1.585053	-1.096252
6	0.159167	-2.668259	-1.142790
6	1.555050	-2.620138	-1.068625
6	-2.878114	-1.649808	2.467223
6	-2.427601	-2.346949	3.584897
6	-1.070034	-2.267791	3.889661
6	-0.198212	-1.513844	3.095710
6	-0.779520	-0.798417	2.003562
1	-3.922797	-1.692038	2.163732
1	-3.108085	-2.942586	4.184730
1	-0.664868	-2.830253	4.726011
7	0.898655	0.956393	2.073586
7	1.738586	1.664819	1.743000
26	-0.173660	0.301900	-0.672506
7	-0.009997	0.011759	1.153676
6	1.255059	-1.525480	3.406372
6	2.210665	-1.738478	2.399022
6	1.701834	-1.372582	4.729150
6	3.567950	-1.798504	2.702482
1	1.881958	-1.841296	1.374321
6	3.062537	-1.430513	5.033641
1	0.979137	-1.185685	5.518633
6	4.001343	-1.644131	4.022181
1	4.284383	-1.961488	1.902415
1	3.389108	-1.299792	6.061762
1	5.060835	-1.684352	4.259114
7	-2.085012	-0.884151	1.715564
6	3.968026	2.881416	-1.562397
6	4.597755	2.840462	-2.815665
6	4.551945	3.636876	-0.533151

6	5.780017	3.547921	-3.038543
1	4.152642	2.253810	-3.614041
6	5.735193	4.341717	-0.756715
1	4.074765	3.656721	0.441997
6	6.351153	4.300736	-2.010006
1	6.253202	3.512024	-4.015855
1	6.178735	4.918154	0.050321
1	7.272162	4.850225	-2.183354
6	2.298208	-3.913091	-0.978959
6	2.179925	-4.702001	0.176457
6	3.108057	-4.368462	-2.030757
6	2.865566	-5.912804	0.281033
1	1.558279	-4.353302	0.995263
6	3.790556	-5.581206	-1.926154
1	3.193702	-3.768883	-2.932111
6	3.672527	-6.355520	-0.769444
1	2.770803	-6.507837	1.184973
1	4.410258	-5.923005	-2.750459
1	4.205190	-7.298816	-0.688181
6	-4.442543	-2.061736	-1.518900
6	-5.266295	-1.716394	-2.601329
6	-4.875479	-3.061129	-0.632126
6	-6.489329	-2.359664	-2.797002
1	-4.939948	-0.941925	-3.289187
6	-6.099011	-3.702523	-0.827362
1	-4.247818	-3.323319	0.214090
6	-6.908937	-3.354549	-1.911104
1	-7.112939	-2.084484	-3.642989
1	-6.421921	-4.470189	-0.129645
1	-7.861543	-3.854122	-2.063027
6	-2.549402	4.386352	0.507984
6	-2.172923	4.904408	1.757496
6	-3.548604	5.046426	-0.224622
6	-2.790173	6.047222	2.267153
1	-1.396682	4.400949	2.326181
6	-4.163681	6.190570	0.284993
1	-3.833360	4.661700	-1.199326
6	-3.787714	6.692889	1.532962
1	-2.492116	6.431790	3.238497
1	-4.932065	6.692777	-0.296156
1	-4.267131	7.583500	1.929356

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^{CSS}(22'-23')‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2679.6717501
Zero-point correction= 0.770311 (Hartree/Particle)
Thermal correction to Energy= 0.819768
Thermal correction to Enthalpy= 0.820712
Thermal correction to Gibbs Free Energy= 0.682360
Sum of electronic and zero-point Energies= -2678.901439
Sum of electronic and thermal Energies= -2678.851982
Sum of electronic and thermal Enthalpies= -2678.851038

Sum of electronic and thermal Free Energies= -2678.989390

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Cartesian Coordinates

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6	2.370178	1.717708	-1.259775
7	1.018628	1.773379	-0.974861
1	3.939796	3.285379	-1.596279
6	0.729337	3.113436	-0.813055
6	1.902543	3.912792	-1.067582
1	1.934827	4.991802	-1.043105
6	2.915889	3.050555	-1.346433
6	-0.503205	3.638946	-0.407377
7	-1.762756	1.518940	-0.579934
6	-3.104562	1.216344	-0.492322
6	-3.852157	2.381583	-0.084158
1	-4.918441	2.407547	0.083363
6	-2.959948	3.396953	0.058808
1	-3.155309	4.415253	0.359598
6	-1.663805	2.866966	-0.290875
6	3.133666	0.554462	-1.402173
1	2.756714	-4.040312	-1.262586
6	2.523045	-2.986581	-1.284562
6	1.195871	-2.426460	-1.189255
1	4.460648	-1.976911	-1.500024
7	1.257722	-1.046322	-1.219067
6	2.594290	-0.735013	-1.360106
6	3.385945	-1.941836	-1.402050
6	-3.681069	-0.033690	-0.745302
1	-2.510943	-4.447310	-1.389503
6	-2.468075	-3.380220	-1.229175
6	-3.498801	-2.495032	-1.197858
1	-4.551232	-2.699405	-1.324448
6	-2.926728	-1.189774	-0.968056
7	-1.548312	-1.275382	-0.924122
6	-1.255212	-2.616508	-1.062211
6	0.024162	-3.184216	-1.097079
6	-2.646215	-1.411785	2.816195
6	-2.052170	-2.168062	3.831120
6	-0.668239	-2.136498	3.953725
6	0.100215	-1.375991	3.057920
6	-0.612077	-0.674280	2.049048
1	-3.727561	-1.387795	2.701119
1	-2.662423	-2.758858	4.506847
1	-0.169071	-2.710204	4.728734
7	0.705216	1.314055	1.803077
7	1.662058	1.899793	1.930827
26	-0.239852	0.232378	-0.705816
7	0.144538	0.032773	1.075405
6	1.573882	-1.293615	3.218867
6	2.450522	-1.426061	2.128220
6	2.116848	-1.072907	4.496793
6	3.828705	-1.330459	2.311861
1	2.049760	-1.608458	1.141803

6	3.496495	-0.975237	4.677161
1	1.452026	-0.948864	5.347142
6	4.357049	-1.100937	3.584439
1	4.485622	-1.434192	1.453664
1	3.897353	-0.791611	5.670053
1	5.431410	-1.019739	3.723560
7	-1.945685	-0.680294	1.951932
6	4.615659	0.694660	-1.541487
6	5.270022	0.344075	-2.731764
6	5.379372	1.168660	-0.462505
6	6.656446	0.464808	-2.841474
1	4.684670	-0.021905	-3.570222
6	6.765509	1.286770	-0.572178
1	4.876078	1.436188	0.461974
6	7.407720	0.935586	-1.762135
1	7.148854	0.193827	-3.771314
1	7.343417	1.650871	0.272816
1	8.486724	1.028605	-1.848046
6	0.127810	-4.674180	-1.060365
6	-0.275955	-5.373966	0.088156
6	0.613693	-5.401724	-2.157810
6	-0.189650	-6.765590	0.139907
1	-0.653365	-4.815950	0.940422
6	0.698612	-6.793829	-2.106277
1	0.919121	-4.868287	-3.053057
6	0.298241	-7.479586	-0.957155
1	-0.500943	-7.291939	1.038024
1	1.072501	-7.342555	-2.966258
1	0.364632	-8.563210	-0.917521
6	-5.171620	-0.135610	-0.736083
6	-5.940992	0.575897	-1.671187
6	-5.836643	-0.931649	0.210737
6	-7.333799	0.492276	-1.660770
1	-5.437161	1.193544	-2.408619
6	-7.229220	-1.014907	0.222524
1	-5.251135	-1.486925	0.936515
6	-7.982748	-0.302976	-0.713544
1	-7.911449	1.045815	-2.395863
1	-7.725518	-1.632563	0.966047
1	-9.067156	-0.367416	-0.704910
6	-0.572289	5.098474	-0.093625
6	0.143703	5.614570	0.998622
6	-1.337038	5.977859	-0.875628
6	0.091257	6.974932	1.304109
1	0.739103	4.938470	1.605517
6	-1.387863	7.338871	-0.570797
1	-1.887373	5.587425	-1.726471
6	-0.674853	7.841022	0.520254
1	0.647263	7.357380	2.155613
1	-1.980820	8.007190	-1.189047
1	-0.714857	8.900523	0.757184

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^{3}(22-23)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2679.693839
Zero-point correction= 0.769403 (Hartree/Particle)
Thermal correction to Energy= 0.819122
Thermal correction to Enthalpy= 0.820066
Thermal correction to Gibbs Free Energy= 0.680826
Sum of electronic and zero-point Energies= -2678.924436
Sum of electronic and thermal Energies= -2678.874717
Sum of electronic and thermal Enthalpies= -2678.873773
Sum of electronic and thermal Free Energies= -2679.013013

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Cartesian Coordinates

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6	1.559641	2.783573	-1.023340
7	0.332135	2.225074	-0.708485
1	2.297161	4.896106	-1.154671
6	-0.482062	3.283095	-0.368920
6	0.237522	4.525505	-0.489182
1	-0.181560	5.503070	-0.302901
6	1.488771	4.218514	-0.925361
6	-1.846007	3.202109	-0.058089
7	-2.107921	0.843227	-0.751067
6	-3.207350	0.024136	-0.905823
6	-4.406405	0.728523	-0.532400
1	-5.401768	0.311065	-0.554363
6	-4.027610	1.963966	-0.109075
1	-4.654787	2.753796	0.275568
6	-2.599599	2.046398	-0.275013
6	2.729286	2.072077	-1.297462
1	4.337234	-2.247576	-1.216974
6	3.677248	-1.393358	-1.230508
6	2.240747	-1.455463	-1.147744
1	4.998638	0.351822	-1.423563
7	1.707230	-0.179978	-1.156051
6	2.786323	0.674521	-1.282370
6	4.012011	-0.078096	-1.337679
6	-3.187105	-1.334401	-1.236470
1	-0.224949	-4.861213	-1.521751
6	-0.649356	-3.875204	-1.403750
6	-1.950794	-3.500537	-1.527446
1	-2.800467	-4.123611	-1.761769
6	-2.005918	-2.079269	-1.292380
7	-0.733205	-1.586675	-1.076255
6	0.109458	-2.678242	-1.145032
6	1.506027	-2.645384	-1.098966
6	-2.828730	-1.704415	2.507224
6	-2.327986	-2.458191	3.565036
6	-0.964002	-2.363408	3.833217
6	-0.131901	-1.545767	3.059102
6	-0.761451	-0.786520	2.025255
1	-3.882284	-1.748098	2.236501
1	-2.976038	-3.103167	4.149496

1	-0.521451	-2.960329	4.625523
7	0.917106	0.986591	2.103703
7	1.622904	1.831240	1.803281
26	-0.197521	0.290651	-0.669446
7	-0.060052	0.098214	1.186664
6	1.326490	-1.528538	3.345279
6	2.272354	-1.660243	2.315368
6	1.789355	-1.428579	4.667777
6	3.635434	-1.695107	2.596043
1	1.931087	-1.723531	1.291977
6	3.155798	-1.461265	4.949830
1	1.074075	-1.303921	5.476043
6	4.084567	-1.595359	3.915746
1	4.343156	-1.795343	1.778220
1	3.494310	-1.373491	5.978640
1	5.148305	-1.616468	4.135505
7	-2.076187	-0.878817	1.778007
6	3.998618	2.826688	-1.522543
6	4.646085	2.778918	-2.766550
6	4.574457	3.578052	-0.485740
6	5.838479	3.474360	-2.972466
1	4.206607	2.196490	-3.571086
6	5.767953	4.270738	-0.692198
1	4.081995	3.605704	0.481662
6	6.402055	4.222188	-1.936115
1	6.325407	3.433242	-3.942793
1	6.204840	4.844129	0.120619
1	7.330929	4.762349	-2.096299
6	2.236537	-3.946532	-1.024789
6	2.145803	-4.724580	0.140230
6	3.009692	-4.417071	-2.096954
6	2.821018	-5.942193	0.232970
1	1.553778	-4.361598	0.974900
6	3.681958	-5.636569	-2.003979
1	3.075429	-3.823836	-3.004212
6	3.590358	-6.401359	-0.838557
1	2.747980	-6.529701	1.143839
1	4.273222	-5.990845	-2.843767
1	4.114936	-7.349933	-0.766555
6	-4.493919	-2.031398	-1.427932
6	-5.338607	-1.681500	-2.492860
6	-4.914010	-3.028854	-0.532738
6	-6.569291	-2.317370	-2.662545
1	-5.022231	-0.909198	-3.187738
6	-6.145146	-3.663011	-0.701983
1	-4.269877	-3.295843	0.299362
6	-6.976000	-3.309936	-1.768044
1	-7.208886	-2.038477	-3.495274
1	-6.457459	-4.429155	0.002199
1	-7.934530	-3.803840	-1.899849
6	-2.516329	4.434061	0.453822
6	-2.133550	4.970818	1.693580
6	-3.510250	5.090454	-0.289191

6	-2.739249	6.128292	2.183480
1	-1.361254	4.470321	2.270181
6	-4.113755	6.249357	0.200571
1	-3.800229	4.690830	-1.256323
6	-3.731526	6.770285	1.438949
1	-2.436486	6.527122	3.147597
1	-4.878144	6.748328	-0.388582
1	-4.202039	7.672285	1.819963

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^{5}(22-23)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2679.6784501
Zero-point correction= 0.768222 (Hartree/Particle)
Thermal correction to Energy= 0.818392
Thermal correction to Enthalpy= 0.819336
Thermal correction to Gibbs Free Energy= 0.679379
Sum of electronic and zero-point Energies= -2678.910228
Sum of electronic and thermal Energies= -2678.860058
Sum of electronic and thermal Enthalpies= -2678.859114
Sum of electronic and thermal Free Energies= -2678.999071

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Cartesian Coordinates

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6	1.127610	3.090197	-0.721785
7	-0.019844	2.323670	-0.611316
1	1.492233	5.299123	-0.641234
6	-1.060365	3.204283	-0.383682
6	-0.551365	4.551471	-0.351161
1	-1.154082	5.437958	-0.222908
6	0.790646	4.481633	-0.571338
6	-2.427025	2.886637	-0.319784
7	-2.228438	0.497286	-0.917081
6	-3.125667	-0.532944	-1.010653
6	-4.467147	-0.048294	-0.768899
1	-5.360773	-0.654125	-0.770942
6	-4.360359	1.277680	-0.490020
1	-5.150467	1.963895	-0.224817
6	-2.955916	1.613971	-0.583554
6	2.429146	2.619597	-0.949479
1	4.820953	-1.301836	-1.476154
6	4.015138	-0.591402	-1.365854
6	2.615957	-0.929754	-1.271160
1	4.994335	1.374150	-1.303577
7	1.868449	0.216453	-1.117013
6	2.758815	1.268638	-1.125882
6	4.102391	0.766024	-1.281232
6	-2.795869	-1.888898	-1.165822
1	0.808288	-4.746483	-1.557826
6	0.207723	-3.863047	-1.400984
6	-1.149769	-3.765869	-1.399497
1	-1.865907	-4.557065	-1.560557
6	-1.482916	-2.380827	-1.184941

7	-0.316251	-1.640707	-1.069394
6	0.731359	-2.535630	-1.214641
6	2.100034	-2.232316	-1.281359
6	-2.881796	-1.965971	2.596254
6	-2.286313	-2.803573	3.539232
6	-0.918497	-2.662456	3.764292
6	-0.171166	-1.716922	3.051800
6	-0.888245	-0.891428	2.131495
1	-3.943357	-2.046062	2.370018
1	-2.872025	-3.544350	4.074116
1	-0.411880	-3.316919	4.467790
7	0.596832	1.090803	2.369498
7	1.246098	1.977333	2.079628
26	-0.126466	0.306968	-0.563412
7	-0.280608	0.094643	1.363289
6	1.293088	-1.615700	3.275332
6	2.190215	-1.504254	2.198619
6	1.818179	-1.668555	4.577748
6	3.564938	-1.455913	2.415222
1	1.801071	-1.445662	1.192433
6	3.195578	-1.615729	4.795380
1	1.141158	-1.728828	5.425254
6	4.074692	-1.510103	3.715704
1	4.233724	-1.370089	1.563839
1	3.580438	-1.648299	5.810991
1	5.146681	-1.464475	3.885853
7	-2.213579	-1.021160	1.933473
6	3.542308	3.617794	-0.963885
6	4.252368	3.889028	-2.143190
6	3.900009	4.292047	0.214337
6	5.296194	4.815673	-2.145197
1	3.978724	3.371508	-3.058043
6	4.944142	5.217655	0.211189
1	3.356177	4.078373	1.129679
6	5.644492	5.482358	-0.968293
1	5.834017	5.019170	-3.067025
1	5.212782	5.728996	1.131389
1	6.457073	6.203440	-0.970171
6	3.065788	-3.371487	-1.363084
6	3.256020	-4.209095	-0.252716
6	3.798393	-3.619089	-2.533553
6	4.161757	-5.268974	-0.312256
1	2.700121	-4.013778	0.659172
6	4.703135	-4.680416	-2.592187
1	3.651384	-2.977093	-3.397140
6	4.887077	-5.507843	-1.481927
1	4.303022	-5.904943	0.557166
1	5.260550	-4.862956	-3.506705
1	5.591629	-6.333485	-1.528003
6	-3.917223	-2.871331	-1.262457
6	-4.820503	-2.822798	-2.336120
6	-4.098671	-3.851544	-0.272808
6	-5.877087	-3.730665	-2.418583

1	-4.686386	-2.069892	-3.107133
6	-5.156018	-4.757971	-0.355272
1	-3.408263	-3.890754	0.563625
6	-6.048481	-4.700706	-1.428390
1	-6.563856	-3.681997	-3.259020
1	-5.284757	-5.506530	0.421689
1	-6.871590	-5.406767	-1.492549
6	-3.374133	3.988867	0.027829
6	-3.318861	4.596090	1.292533
6	-4.326316	4.442617	-0.898640
6	-4.197448	5.628177	1.623560
1	-2.585813	4.247902	2.014089
6	-5.203556	5.476002	-0.567369
1	-4.369939	3.983153	-1.881619
6	-5.142075	6.071228	0.694766
1	-4.145758	6.083448	2.608618
1	-5.931235	5.819262	-1.297453
1	-5.825212	6.875624	0.952464

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^{oss}23

Number of imaginary frequencies : 0
Electronic energy : HF=-2570.2156537
Zero-point correction= 0.763391 (Hartree/Particle)
Thermal correction to Energy= 0.810824
Thermal correction to Enthalpy= 0.811768
Thermal correction to Gibbs Free Energy= 0.678578
Sum of electronic and zero-point Energies= -2569.452263
Sum of electronic and thermal Energies= -2569.404830
Sum of electronic and thermal Enthalpies= -2569.403886
Sum of electronic and thermal Free Energies= -2569.537076

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Cartesian Coordinates

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6	-2.576473	2.059099	-0.567916
7	-2.104716	0.769441	-0.739673
1	-4.630058	2.953135	-0.514799
6	-3.231422	-0.027471	-0.831399
6	-4.420076	0.782545	-0.765615
1	-5.429349	0.404660	-0.827420
6	-4.016709	2.068959	-0.600937
6	-3.251637	-1.420853	-0.869919
7	-0.798335	-1.712046	-0.889306
6	0.015792	-2.832666	-0.907223
6	-0.783618	-4.028265	-0.824506
1	-0.392647	-5.034405	-0.808275
6	-2.084868	-3.635518	-0.816426
1	-2.966365	-4.258244	-0.796251
6	-2.091198	-2.195653	-0.848235
6	-1.803353	3.209746	-0.396251
1	2.589457	4.606113	-0.531054
6	1.696379	4.000301	-0.564460
6	1.666194	2.587176	-0.849783

1	0.047661	5.370421	-0.089387
7	0.370575	2.115755	-0.798053
6	-0.410304	3.212902	-0.502279
6	0.412521	4.386202	-0.341542
6	1.400385	-2.834568	-1.080087
1	4.923532	0.048167	-1.802096
6	3.941853	-0.351248	-1.596072
6	3.555127	-1.655207	-1.568077
1	4.156245	-2.534062	-1.747418
6	2.146735	-1.666594	-1.262758
7	1.671487	-0.376349	-1.140517
6	2.775277	0.439740	-1.294563
6	2.804626	1.825424	-1.118875
26	-0.211759	0.181551	-0.620433
6	-2.504282	4.497721	-0.106081
6	-2.495756	5.548944	-1.035973
6	-3.188242	4.673245	1.107115
6	-3.154211	6.747761	-0.758616
1	-1.972858	5.418227	-1.978789
6	-3.845243	5.872670	1.384357
1	-3.197429	3.863338	1.830532
6	-3.830074	6.913137	0.452487
1	-3.142247	7.550512	-1.490646
1	-4.365982	5.994943	2.329986
1	-4.342201	7.846583	0.668440
6	4.128405	2.518002	-1.173667
6	5.080378	2.299068	-0.165419
6	4.438520	3.397944	-2.221141
6	6.316214	2.945486	-0.206887
1	4.837819	1.627682	0.653155
6	5.676373	4.041767	-2.262940
1	3.705117	3.571118	-3.003295
6	6.618120	3.816994	-1.256255
1	7.041572	2.771678	0.583148
1	5.905158	4.716705	-3.082999
1	7.580849	4.319330	-1.288465
6	2.131014	-4.139377	-1.074755
6	1.982697	-5.061143	-2.121773
6	2.991593	-4.453164	-0.010965
6	2.677699	-6.271529	-2.104485
1	1.322756	-4.821079	-2.950212
6	3.684350	-5.664314	0.006396
1	3.108252	-3.744065	0.803621
6	3.529510	-6.576340	-1.040325
1	2.556304	-6.974009	-2.924330
1	4.342956	-5.895816	0.838860
1	4.070117	-7.518544	-1.027339
6	-4.575259	-2.116305	-0.862708
6	-5.002027	-2.809629	0.280656
6	-5.413566	-2.082868	-1.986699
6	-6.239069	-3.454968	0.298479
1	-4.354062	-2.838174	1.151328
6	-6.652026	-2.726934	-1.967432

1	-5.088726	-1.549538	-2.875364
6	-7.067963	-3.414708	-0.825287
1	-6.556716	-3.986114	1.191546
1	-7.289410	-2.694467	-2.846694
1	-8.031396	-3.916438	-0.811108
6	2.399480	-1.001135	2.165153
6	-0.661371	-0.533211	2.091718
6	3.781892	-0.824612	2.217553
6	1.592218	-0.718294	3.280751
6	0.124704	-0.912219	3.235349
6	4.387454	-0.361449	3.388465
1	4.377821	-1.048719	1.337648
6	2.215552	-0.257171	4.454058
6	-2.610392	-1.250468	3.101559
6	-0.561376	-1.471636	4.315491
6	3.598020	-0.079833	4.506545
1	5.463932	-0.219932	3.429662
1	1.608667	-0.009579	5.320406
6	-1.944414	-1.642446	4.265342
1	-3.689750	-1.370568	3.016282
1	-0.002095	-1.788844	5.191224
1	4.057916	0.289033	5.419238
1	-2.489707	-2.077512	5.096368
7	-2.001946	-0.725626	2.040156
7	-0.039244	0.119801	1.074491
1	1.940955	-1.366910	1.257227

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Number of imaginary frequencies : 0
Electronic energy : HF=-2570.2089661
Zero-point correction= 0.763418 (Hartree/Particle)
Thermal correction to Energy= 0.810685
Thermal correction to Enthalpy= 0.811629
Thermal correction to Gibbs Free Energy= 0.679717
Sum of electronic and zero-point Energies= -2569.445548
Sum of electronic and thermal Energies= -2569.398282
Sum of electronic and thermal Enthalpies= -2569.397337
Sum of electronic and thermal Free Energies= -2569.529249

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Cartesian Coordinates

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6	-2.651573	1.969819	-0.550550
7	-2.120863	0.702743	-0.738650
1	-4.740809	2.775171	-0.537098
6	-3.213446	-0.141513	-0.861635
6	-4.433779	0.620507	-0.821436
1	-5.425412	0.203951	-0.912677
6	-4.088285	1.919559	-0.624240
6	-3.184112	-1.536244	-0.874331
7	-0.730844	-1.731162	-0.816905
6	0.129222	-2.811290	-0.838060
6	-0.614010	-4.044460	-0.742529

1	-0.177948	-5.031895	-0.720403
6	-1.931291	-3.709541	-0.746699
1	-2.784766	-4.370459	-0.732492
6	-1.998048	-2.269164	-0.796121
6	-1.937337	3.148590	-0.315285
1	2.392635	4.743344	-0.426893
6	1.525422	4.100741	-0.459634
6	1.547513	2.694005	-0.785522
1	-0.173505	5.387170	0.071784
7	0.278668	2.168677	-0.721378
6	-0.544527	3.220881	-0.394907
6	0.229931	4.425614	-0.208124
6	1.504423	-2.741197	-1.065613
1	4.850151	0.306017	-1.928202
6	3.894226	-0.137047	-1.692385
6	3.567262	-1.457628	-1.659129
1	4.201959	-2.307352	-1.861645
6	2.175166	-1.536894	-1.301499
7	1.643661	-0.265643	-1.164355
6	2.708981	0.601278	-1.340500
6	2.700366	1.981552	-1.119714
26	-0.221523	0.206150	-0.576649
6	-2.704511	4.390700	0.004628
6	-2.719687	5.478490	-0.882159
6	-3.427790	4.486111	1.203995
6	-3.438924	6.634654	-0.576055
1	-2.167184	5.409686	-1.814553
6	-4.145344	5.642967	1.510256
1	-3.419363	3.647619	1.894069
6	-4.152959	6.720432	0.621272
1	-3.444378	7.466282	-1.275204
1	-4.695902	5.703088	2.444945
1	-4.712304	7.620709	0.859770
6	3.996466	2.722460	-1.196600
6	4.991442	2.508046	-0.229692
6	4.235538	3.648867	-2.222431
6	6.199629	3.203261	-0.290949
1	4.803545	1.801651	0.573669
6	5.445753	4.341800	-2.284332
1	3.468367	3.819600	-2.972041
6	6.430710	4.120512	-1.319153
1	6.958605	3.032040	0.467439
1	5.619020	5.052671	-3.087481
1	7.371877	4.661068	-1.366687
6	2.306098	-4.003624	-1.069583
6	2.168385	-4.950944	-2.094987
6	3.222630	-4.251105	-0.035383
6	2.928743	-6.121541	-2.085608
1	1.465068	-4.761922	-2.900614
6	3.980683	-5.422571	-0.025863
1	3.331397	-3.521881	0.762346
6	3.836104	-6.360512	-1.050968
1	2.814635	-6.844214	-2.888805

1	4.682598	-5.602850	0.783606
1	4.427465	-7.271814	-1.044146
6	-4.481179	-2.278760	-0.909439
6	-4.919932	-2.992009	0.217068
6	-5.283138	-2.273133	-2.060487
6	-6.131719	-3.683437	0.192365
1	-4.301616	-2.999461	1.109486
6	-6.496423	-2.963036	-2.083944
1	-4.949185	-1.725137	-2.936735
6	-6.923973	-3.670304	-0.958053
1	-6.458528	-4.229093	1.073310
1	-7.104865	-2.951282	-2.983978
1	-7.867726	-4.207985	-0.977053
6	2.468250	-0.923035	2.095509
6	-0.593156	-0.566507	2.045033
6	3.844823	-0.710070	2.171501
6	1.653281	-0.800947	3.233731
6	0.194092	-1.023357	3.157687
6	4.435434	-0.371256	3.390603
1	4.446293	-0.812258	1.272864
6	2.263019	-0.464359	4.456868
6	-2.538348	-1.371249	2.997980
6	-0.483471	-1.696372	4.180013
6	3.638128	-0.249901	4.532842
1	5.506946	-0.202521	3.452445
1	1.650457	-0.337245	5.344833
6	-1.863316	-1.869609	4.116421
1	-3.619006	-1.476691	2.912361
1	0.078795	-2.087335	5.023112
1	4.087322	0.023179	5.483667
1	-2.403520	-2.382750	4.905389
7	-1.931762	-0.767627	1.980124
7	0.018027	0.213482	1.096384
1	2.021646	-1.201671	1.152924

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Number of imaginary frequencies : 0
Electronic energy : HF=-2570.2250105
Zero-point correction= 0.763802 (Hartree/Particle)
Thermal correction to Energy= 0.810654
Thermal correction to Enthalpy= 0.811598
Thermal correction to Gibbs Free Energy= 0.681720
Sum of electronic and zero-point Energies= -2569.461208
Sum of electronic and thermal Energies= -2569.414357
Sum of electronic and thermal Enthalpies= -2569.413412
Sum of electronic and thermal Free Energies= -2569.543290

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Cartesian Coordinates

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6	0.476905	-2.637023	-1.023728
7	1.134485	-1.419602	-0.972202
1	1.167624	-4.749077	-1.285141

6	2.483761	-1.723711	-1.044967
6	2.662435	-3.139855	-1.218154
1	3.617305	-3.632321	-1.324096
6	1.425415	-3.704794	-1.191315
6	3.541912	-0.836809	-0.846614
7	2.143540	1.161059	-0.469980
6	2.438046	2.462552	-0.113155
6	3.860195	2.616402	0.075722
1	4.350955	3.532231	0.368358
6	4.429776	1.416752	-0.210571
1	5.477730	1.157220	-0.201005
6	3.357193	0.509167	-0.532454
6	-0.903678	-2.836502	-0.938424
1	-4.832792	-0.431064	-1.105745
6	-3.789158	-0.702811	-1.068758
6	-2.692085	0.232909	-1.050713
1	-3.769093	-2.893000	-0.943329
7	-1.490819	-0.442907	-0.965864
6	-1.819937	-1.783554	-0.947090
6	-3.251352	-1.947089	-0.983193
6	1.518836	3.509088	-0.021886
1	-2.880175	4.474754	-0.989720
6	-1.962135	3.943893	-0.788127
6	-0.753942	4.464289	-0.443475
1	-0.489997	5.502873	-0.311391
6	0.159974	3.358179	-0.319351
7	-0.487418	2.169509	-0.591634
6	-1.803826	2.513177	-0.842390
6	-2.857094	1.619884	-1.059079
26	0.318940	0.319545	-0.488356
6	-1.411431	-4.238791	-0.842822
6	-2.157549	-4.821550	-1.878001
6	-1.141188	-4.997220	0.307940
6	-2.630744	-6.129718	-1.761913
1	-2.362096	-4.244204	-2.774743
6	-1.616714	-6.303986	0.423511
1	-0.559632	-4.552549	1.109545
6	-2.363819	-6.873641	-0.610320
1	-3.204137	-6.568641	-2.573647
1	-1.403520	-6.876265	1.322236
1	-2.733391	-7.891256	-0.520584
6	-4.235904	2.160471	-1.259112
6	-4.894844	2.856352	-0.233519
6	-4.905026	1.962468	-2.477165
6	-6.189066	3.342532	-0.421230
1	-4.385547	3.007324	0.712493
6	-6.198689	2.450495	-2.665671
1	-4.402715	1.424289	-3.275548
6	-6.844819	3.141355	-1.638065
1	-6.686381	3.874746	0.384898
1	-6.700139	2.292893	-3.616485
1	-7.852376	3.520269	-1.784277
6	2.006656	4.871684	0.353154

6	2.852927	5.596738	-0.500138
6	1.606392	5.455720	1.564899
6	3.292741	6.873205	-0.147222
1	3.159680	5.154548	-1.443378
6	2.047834	6.731595	1.918057
1	0.950102	4.900496	2.228538
6	2.892180	7.443720	1.063169
1	3.944326	7.423302	-0.820422
1	1.733453	7.167798	2.862096
1	3.234832	8.437386	1.337739
6	4.934158	-1.383548	-0.860890
6	5.624379	-1.569310	0.346819
6	5.562012	-1.732845	-2.064537
6	6.918719	-2.090647	0.348727
1	5.134323	-1.302922	1.278658
6	6.856892	-2.255572	-2.061257
1	5.031187	-1.592260	-3.001735
6	7.538107	-2.435102	-0.855367
1	7.441652	-2.230984	1.290743
1	7.333623	-2.519596	-3.001167
1	8.545710	-2.841286	-0.853656
6	-2.314092	0.188109	2.625927
6	0.437537	-1.103803	1.947350
6	-3.626748	0.654185	2.589347
6	-2.041034	-1.190649	2.572488
6	-0.656193	-1.714284	2.642792
6	-4.694688	-0.240559	2.487365
1	-3.814866	1.722538	2.641664
6	-3.125246	-2.081065	2.473014
6	1.925634	-2.686958	2.734552
6	-0.365924	-2.860135	3.393020
6	-4.437441	-1.611289	2.430734
1	-5.715347	0.128961	2.444821
1	-2.934902	-3.147091	2.389321
6	0.930613	-3.367033	3.441956
1	2.954350	-3.043663	2.749085
1	-1.163780	-3.346976	3.946666
1	-5.257648	-2.317551	2.335945
1	1.169033	-4.253073	4.021197
7	1.699621	-1.590723	2.013886
7	0.218077	0.017132	1.197652
1	-1.493374	0.892293	2.697081

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Number of imaginary frequencies : 0
Electronic energy : HF=-2679.6926029
Zero-point correction= 0.766335 (Hartree/Particle)
Thermal correction to Energy= 0.817603
Thermal correction to Enthalpy= 0.818548
Thermal correction to Gibbs Free Energy= 0.676665
Sum of electronic and zero-point Energies= -2678.926268
Sum of electronic and thermal Energies= -2678.875000

Sum of electronic and thermal Enthalpies= -2678.874055
Sum of electronic and thermal Free Energies= -2679.015938

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Cartesian Coordinates

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6	2.668412	0.821472	-1.467016
7	1.390545	1.230616	-1.118230
1	4.511508	1.907816	-2.081982
6	1.438879	2.606990	-1.104982
6	2.711324	3.069123	-1.520794
1	2.999283	4.104122	-1.626535
6	3.483498	1.946322	-1.755009
6	0.369249	3.458754	-0.673492
7	-1.370219	1.717659	-0.773603
6	-2.741602	1.759026	-0.663249
6	-3.167124	3.070183	-0.233799
1	-4.189122	3.356509	-0.037474
6	-2.049825	3.832532	-0.111232
1	-1.982701	4.864345	0.198533
6	-0.929577	3.006581	-0.496980
6	3.137067	-0.519358	-1.414220
1	1.679871	-4.790823	-0.446513
6	1.703068	-3.739101	-0.688308
6	0.540153	-2.896587	-0.859022
1	3.831690	-3.244765	-0.868956
7	0.934744	-1.587342	-1.101333
6	2.309486	-1.617365	-1.164321
6	2.791896	-2.956414	-0.901609
6	-3.604233	0.691430	-0.922537
1	-3.487845	-3.896151	-1.551277
6	-3.189357	-2.871698	-1.387248
6	-3.980198	-1.733484	-1.454430
1	-5.034411	-1.675669	-1.678802
6	-3.142870	-0.634961	-1.152291
7	-1.836222	-1.063318	-0.977302
6	-1.884176	-2.440372	-1.070212
6	-0.776799	-3.328461	-0.851106
6	-2.995265	-0.046468	3.012110
6	-2.486947	-0.323774	4.286448
6	-1.116500	-0.556002	4.408457
6	-0.286084	-0.500748	3.288833
6	-0.908867	-0.181632	2.024673
1	-4.061237	0.131159	2.872658
1	-3.146272	-0.369946	5.146916
1	-0.686955	-0.804488	5.374939
7	2.268487	1.919693	1.881645
7	3.264420	1.533134	1.599234
26	-0.224756	0.064337	-0.740417
7	-0.104163	-0.046622	0.958322
6	1.172076	-0.736099	3.402392
6	1.869287	-1.518091	2.463098
6	1.896094	-0.163074	4.463072
6	3.245452	-1.702444	2.573502

1	1.332495	-1.977191	1.642482
6	3.273678	-0.351371	4.573808
1	1.379030	0.463693	5.184103
6	3.955506	-1.115841	3.624820
1	3.761797	-2.300248	1.828461
1	3.816039	0.114060	5.392238
1	5.030456	-1.252907	3.701998
7	-2.251344	0.019294	1.913889
6	4.595961	-0.764145	-1.578947
6	5.070918	-1.580229	-2.619443
6	5.522275	-0.200726	-0.683670
6	6.437046	-1.822869	-2.764960
1	4.361481	-2.015780	-3.316624
6	6.886066	-0.454456	-0.824947
1	5.160908	0.420621	0.128421
6	7.348395	-1.262653	-1.867062
1	6.788604	-2.448145	-3.580856
1	7.588595	-0.022066	-0.117910
1	8.411846	-1.454862	-1.978180
6	-1.085202	-4.765835	-0.640807
6	-1.935792	-5.154664	0.410477
6	-0.553666	-5.760233	-1.480025
6	-2.223365	-6.500286	0.629873
1	-2.358864	-4.392199	1.057120
6	-0.852768	-7.105999	-1.265420
1	0.081843	-5.469266	-2.310517
6	-1.683659	-7.480811	-0.207713
1	-2.869594	-6.784190	1.455660
1	-0.440601	-7.860527	-1.929511
1	-1.913551	-8.529063	-0.039308
6	-5.068882	0.932171	-0.873582
6	-5.674747	1.879668	-1.716719
6	-5.876448	0.228100	0.038615
6	-7.048223	2.114840	-1.651592
1	-5.061352	2.422663	-2.429216
6	-7.246796	0.472521	0.109378
1	-5.413925	-0.501754	0.695106
6	-7.838119	1.414414	-0.737242
1	-7.501211	2.843324	-2.318155
1	-7.853637	-0.070999	0.828196
1	-8.907081	1.600521	-0.684717
6	0.685308	4.894224	-0.446528
6	1.659153	5.263567	0.498523
6	0.036760	5.905292	-1.175914
6	1.957548	6.606395	0.721821
1	2.169129	4.489391	1.061938
6	0.345019	7.248642	-0.958451
1	-0.700470	5.629103	-1.923340
6	1.302768	7.603645	-0.006608
1	2.702146	6.874847	1.465929
1	-0.160201	8.016758	-1.537224
1	1.540711	8.649700	0.164429

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^{oss}(23-24)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2570.1891835
Zero-point correction= 0.761316 (Hartree/Particle)
Thermal correction to Energy= 0.807921
Thermal correction to Enthalpy= 0.808865
Thermal correction to Gibbs Free Energy= 0.678905
Sum of electronic and zero-point Energies= -2569.427867
Sum of electronic and thermal Energies= -2569.381263
Sum of electronic and thermal Enthalpies= -2569.380318
Sum of electronic and thermal Free Energies= -2569.510278

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Cartesian Coordinates

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6	-1.429501	2.657548	-0.587164
7	-1.505696	1.303948	-0.837547
1	-2.946439	4.309300	-0.600784
6	-2.830579	1.041367	-1.118406
6	-3.591937	2.265748	-1.085857
1	-4.650548	2.341632	-1.284466
6	-2.732710	3.258810	-0.731462
6	-3.400434	-0.227328	-1.255766
7	-1.323445	-1.482461	-0.795055
6	-1.056499	-2.811941	-0.533510
6	-2.282859	-3.571705	-0.547100
1	-2.361521	-4.630642	-0.352562
6	-3.276663	-2.711961	-0.898644
1	-4.321936	-2.935827	-1.048467
6	-2.682517	-1.403508	-1.016915
6	-0.258482	3.380892	-0.325922
1	4.295665	2.938279	-0.940131
6	3.241529	2.727734	-0.837309
6	2.631455	1.437502	-1.044525
1	2.337578	4.624067	-0.197368
7	1.274960	1.515345	-0.814903
6	1.018084	2.830963	-0.488085
6	2.250218	3.579909	-0.457651
6	0.221445	-3.370183	-0.418262
1	4.543895	-2.326171	-1.630763
6	3.512446	-2.242475	-1.323250
6	2.667692	-3.245203	-0.954938
1	2.872036	-4.304833	-0.911856
6	1.388471	-2.640763	-0.686286
7	1.465303	-1.273032	-0.857727
6	2.776640	-1.007936	-1.218293
6	3.345290	0.266479	-1.330957
26	-0.029597	0.013738	-0.582916
6	-0.395552	4.818158	0.056563
6	0.030500	5.848242	-0.796414
6	-0.982709	5.157326	1.285875
6	-0.118161	7.185133	-0.424554
1	0.471599	5.594190	-1.755639

6	-1.129811	6.494268	1.657383
1	-1.317981	4.363961	1.947430
6	-0.697171	7.511802	0.803844
1	0.212900	7.971084	-1.097716
1	-1.581169	6.740242	2.614535
1	-0.812709	8.552670	1.092778
6	4.798316	0.394883	-1.653029
6	5.781529	-0.106901	-0.784721
6	5.206667	1.054600	-2.822981
6	7.136536	0.039385	-1.083298
1	5.476961	-0.607569	0.129544
6	6.561942	1.199397	-3.122270
1	4.453054	1.450691	-3.497210
6	7.530816	0.691679	-2.253807
1	7.883716	-0.351103	-0.398003
1	6.860227	1.707725	-4.034920
1	8.585864	0.805455	-2.486268
6	0.369898	-4.823670	-0.105905
6	-0.068548	-5.815600	-0.997220
6	0.989161	-5.217707	1.090761
6	0.096532	-7.167440	-0.692728
1	-0.531512	-5.519636	-1.933757
6	1.153059	-6.569536	1.395422
1	1.337879	-4.456464	1.782699
6	0.705796	-7.548297	0.505097
1	-0.245196	-7.922607	-1.395076
1	1.629128	-6.857207	2.328650
1	0.834097	-8.600836	0.741411
6	-4.865425	-0.311244	-1.539429
6	-5.765645	-0.745545	-0.553450
6	-5.369015	0.073280	-2.791263
6	-7.134784	-0.801514	-0.816534
1	-5.381817	-1.036136	0.419720
6	-6.738926	0.018307	-3.053641
1	-4.679534	0.415408	-3.557578
6	-7.625452	-0.420173	-2.067658
1	-7.818631	-1.137292	-0.041844
1	-7.112462	0.316228	-4.029412
1	-8.691592	-0.462450	-2.271944
6	1.451756	-0.598080	2.322104
6	-1.035286	-0.151526	2.108649
6	2.801675	-0.144222	2.161542
6	0.805794	-0.348080	3.594474
6	-0.627329	-0.382291	3.473555
6	3.467580	0.444446	3.215418
1	3.304490	-0.317585	1.219881
6	1.524776	0.211052	4.658154
6	-3.243717	-0.155510	2.732136
6	-1.608959	-0.467956	4.463708
6	2.850381	0.595090	4.480545
1	4.497235	0.767501	3.083970
1	1.014403	0.419177	5.595065
6	-2.944036	-0.360460	4.090218

1	-4.283574	-0.067497	2.417805
1	-1.326375	-0.628852	5.500818
1	3.399717	1.050389	5.299104
1	-3.744111	-0.441450	4.818748
7	-2.341425	-0.063844	1.759666
7	-0.023316	0.072896	1.227066
1	1.201857	-1.522452	1.801442

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^{CSS}(23'-24')‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2570.1834333
Zero-point correction= 0.762064 (Hartree/Particle)
Thermal correction to Energy= 0.808527
Thermal correction to Enthalpy= 0.809471
Thermal correction to Gibbs Free Energy= 0.679545
Sum of electronic and zero-point Energies= -2569.421369
Sum of electronic and thermal Energies= -2569.374906
Sum of electronic and thermal Enthalpies= -2569.373962
Sum of electronic and thermal Free Energies= -2569.503889

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Cartesian Coordinates

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6	-2.306855	2.023199	-0.730844
7	-1.880180	0.724202	-0.909530
1	-4.312264	3.021027	-0.878915
6	-3.018869	-0.013043	-1.164814
6	-4.170200	0.856800	-1.222487
1	-5.179851	0.535814	-1.431622
6	-3.733640	2.110830	-0.934639
6	-3.108799	-1.407199	-1.161797
7	-0.710198	-1.829127	-0.782895
6	0.034568	-2.974708	-0.580434
6	-0.838194	-4.123038	-0.496565
1	-0.517828	-5.138839	-0.319902
6	-2.100421	-3.675890	-0.735900
1	-3.008940	-4.256560	-0.794508
6	-2.016805	-2.243899	-0.902570
6	-1.497289	3.120939	-0.413858
1	2.949121	4.350949	-0.606166
6	2.034660	3.776437	-0.595779
6	1.939258	2.361061	-0.871016
1	0.462107	5.207812	-0.048902
7	0.634299	1.941899	-0.753070
6	-0.098992	3.068363	-0.455275
6	0.776913	4.208875	-0.311382
6	1.432948	-3.035256	-0.603256
1	5.053795	-0.409471	-1.750776
6	4.066107	-0.731436	-1.456438
6	3.639682	-2.002631	-1.212478
1	4.208770	-2.918212	-1.277551
6	2.238659	-1.920950	-0.886730
7	1.816322	-0.607329	-0.928553

6	2.941075	0.141721	-1.231588
6	3.028830	1.539364	-1.179693
26	-0.043060	0.048239	-0.608770
6	-2.170402	4.409212	-0.069485
6	-2.065354	5.538356	-0.896474
6	-2.943176	4.498860	1.099731
6	-2.710335	6.729256	-0.559004
1	-1.480415	5.473904	-1.809102
6	-3.586603	5.689907	1.437518
1	-3.032100	3.625624	1.739559
6	-3.471323	6.809087	0.609489
1	-2.622866	7.592717	-1.212711
1	-4.176669	5.743795	2.348299
1	-3.973311	7.736263	0.871580
6	4.355936	2.188934	-1.401812
6	5.421744	1.976234	-0.512925
6	4.553738	3.045888	-2.496022
6	6.653994	2.598303	-0.715668
1	5.272385	1.325906	0.343544
6	5.786637	3.666975	-2.700318
1	3.733605	3.218906	-3.186526
6	6.840567	3.444740	-1.811138
1	7.466270	2.426433	-0.014785
1	5.923815	4.322920	-3.555490
1	7.799966	3.929202	-1.969484
6	2.117187	-4.345809	-0.388320
6	1.953444	-5.415999	-1.282030
6	2.967297	-4.515388	0.716733
6	2.613513	-6.627147	-1.069885
1	1.311701	-5.288483	-2.148502
6	3.625994	-5.726786	0.929499
1	3.107765	-3.689113	1.407742
6	3.450025	-6.786978	0.037235
1	2.479283	-7.443411	-1.774248
1	4.275833	-5.842123	1.792554
1	3.963717	-7.730031	0.201505
6	-4.456936	-2.027656	-1.345624
6	-5.119406	-2.625183	-0.261882
6	-5.090661	-2.007735	-2.596845
6	-6.382789	-3.194287	-0.427413
1	-4.634962	-2.636840	0.709927
6	-6.355809	-2.574594	-2.761683
1	-4.584982	-1.545206	-3.439507
6	-7.004886	-3.170390	-1.678039
1	-6.883166	-3.652011	0.421632
1	-6.832264	-2.553297	-3.737927
1	-7.988969	-3.612282	-1.806877
6	1.478745	-0.643306	2.241304
6	-0.987222	-0.217620	2.086319
6	2.855887	-0.263340	2.104606
6	0.860102	-0.490366	3.539297
6	-0.553286	-0.456179	3.446533
6	3.564912	0.148526	3.207357

1	3.349245	-0.384027	1.150686
6	1.631357	-0.113184	4.659751
6	-3.183995	-0.216163	2.754408
6	-1.520042	-0.517220	4.467551
6	2.964331	0.204748	4.495457
1	4.618158	0.396471	3.106104
1	1.150195	0.003897	5.626537
6	-2.849494	-0.393227	4.122407
1	-4.232397	-0.138633	2.466910
1	-1.216698	-0.676359	5.498525
1	3.555309	0.527746	5.347313
1	-3.636913	-0.453506	4.866536
7	-2.314087	-0.159502	1.765680
7	-0.023700	0.070358	1.186489
1	1.177972	-1.508769	1.647212

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^{3}(23-24)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2570.1913721
Zero-point correction= 0.761163 (Hartree/Particle)
Thermal correction to Energy= 0.807764
Thermal correction to Enthalpy= 0.808709
Thermal correction to Gibbs Free Energy= 0.678646
Sum of electronic and zero-point Energies= -2569.430209
Sum of electronic and thermal Energies= -2569.383608
Sum of electronic and thermal Enthalpies= -2569.382664
Sum of electronic and thermal Free Energies= -2569.512726

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Cartesian Coordinates

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6	-1.109086	2.492899	-0.826150
7	-1.340708	1.139134	-0.949698
1	-2.434159	4.295583	-0.981242
6	-2.686032	1.001187	-1.211312
6	-3.307370	2.301202	-1.283009
1	-4.352776	2.476661	-1.488546
6	-2.339812	3.220305	-1.017310
6	-3.388841	-0.207424	-1.257847
7	-1.470953	-1.638799	-0.635792
6	-1.366288	-2.953070	-0.220020
6	-2.666794	-3.575589	-0.237218
1	-2.871661	-4.594927	0.053104
6	-3.543988	-2.653488	-0.717293
1	-4.601466	-2.777046	-0.895431
6	-2.805664	-1.432438	-0.920838
6	0.142055	3.096274	-0.655150
1	4.596893	2.057003	-1.286656
6	3.529435	1.981908	-1.142485
6	2.781981	0.750133	-1.127645
1	2.857817	4.040234	-0.777350
7	1.444427	1.014504	-0.911247
6	1.343073	2.385420	-0.778689

6	2.648310	2.986354	-0.879927
6	-0.173706	-3.622590	0.073920
1	4.308086	-3.227348	-0.912243
6	3.277838	-2.991053	-0.692225
6	2.307117	-3.830305	-0.238045
1	2.386997	-4.885857	-0.023699
6	1.089285	-3.060453	-0.161256
7	1.332135	-1.754032	-0.517883
6	2.675076	-1.687813	-0.836891
6	3.371497	-0.520203	-1.170616
26	-0.033895	-0.277934	-0.504405
6	0.178958	4.565860	-0.392978
6	0.695572	5.473811	-1.330098
6	-0.333872	5.061138	0.816975
6	0.712063	6.842689	-1.058042
1	1.076318	5.100981	-2.276227
6	-0.316518	6.429649	1.087977
1	-0.744108	4.364092	1.541277
6	0.208514	7.324285	0.152458
1	1.111824	7.533190	-1.795510
1	-0.713044	6.796618	2.030665
1	0.221273	8.389956	0.363213
6	4.832786	-0.600099	-1.470804
6	5.753486	-1.000964	-0.489196
6	5.314707	-0.240353	-2.739165
6	7.119204	-1.048740	-0.771255
1	5.392187	-1.270241	0.498943
6	6.680477	-0.289072	-3.021472
1	4.609991	0.075865	-3.502555
6	7.586662	-0.694032	-2.038806
1	7.817909	-1.357774	0.001185
1	7.035821	-0.012307	-4.010147
1	8.649878	-0.731095	-2.258519
6	-0.222623	-5.037287	0.553299
6	-0.681276	-6.075323	-0.272947
6	0.228444	-5.351800	1.844635
6	-0.699664	-7.393157	0.185717
1	-1.015761	-5.842883	-1.279568
6	0.209159	-6.669666	2.303376
1	0.590053	-4.554379	2.487320
6	-0.255962	-7.693907	1.475597
1	-1.054329	-8.185454	-0.467661
1	0.556184	-6.895317	3.307884
1	-0.270157	-8.719984	1.832094
6	-4.856192	-0.150978	-1.535893
6	-5.786534	-0.401169	-0.514378
6	-5.328649	0.187154	-2.812692
6	-7.156496	-0.323102	-0.767090
1	-5.423464	-0.655135	0.476988
6	-6.699508	0.265601	-3.064867
1	-4.614825	0.387247	-3.606508
6	-7.616914	0.010008	-2.043361
1	-7.863899	-0.516947	0.034505

1	-7.049840	0.524498	-4.060201
1	-8.683597	0.071504	-2.239941
6	1.361952	0.210705	2.518585
6	-1.097337	0.493609	2.079199
6	2.721149	0.313959	2.080466
6	0.789398	1.340368	3.221901
6	-0.654942	1.277153	3.204123
6	3.456415	1.449286	2.353228
1	3.171819	-0.529851	1.572782
6	1.568895	2.459057	3.517166
6	-3.286778	0.950740	2.579963
6	-1.603846	1.926034	3.989654
6	2.898234	2.514567	3.094748
1	4.486909	1.515775	2.015942
1	1.112946	3.316829	4.004735
6	-2.952877	1.760954	3.674661
1	-4.334656	0.805784	2.318782
1	-1.292851	2.542020	4.829704
1	3.495121	3.397617	3.302340
1	-3.733049	2.233441	4.262159
7	-2.408613	0.316383	1.800968
7	-0.107969	-0.015123	1.291112
1	1.053582	-0.785952	2.836652

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^{oss}24

Number of imaginary frequencies : 0
Electronic energy : HF=-2570.2160871
Zero-point correction= 0.762214 (Hartree/Particle)
Thermal correction to Energy= 0.808993
Thermal correction to Enthalpy= 0.809937
Thermal correction to Gibbs Free Energy= 0.680174
Sum of electronic and zero-point Energies= -2569.453873
Sum of electronic and thermal Energies= -2569.407094
Sum of electronic and thermal Enthalpies= -2569.406150
Sum of electronic and thermal Free Energies= -2569.535913

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Cartesian Coordinates

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6	-1.389282	2.729037	-0.392288
7	-1.473797	1.394768	-0.726528
1	-2.901325	4.382005	-0.267382
6	-2.798606	1.161025	-1.030299
6	-3.556614	2.381780	-0.899201
1	-4.615446	2.476067	-1.088741
6	-2.693084	3.342755	-0.474810
6	-3.368987	-0.088530	-1.289062
7	-1.308445	-1.386453	-0.870533
6	-1.058456	-2.729403	-0.669817
6	-2.284727	-3.480037	-0.784270
1	-2.374236	-4.548497	-0.657973
6	-3.260067	-2.594950	-1.125942
1	-4.298673	-2.803623	-1.333194

6	-2.659011	-1.284124	-1.133961
6	-0.206119	3.436338	-0.148097
1	4.301848	3.016093	-1.061458
6	3.256484	2.799774	-0.898501
6	2.642284	1.508684	-1.078480
1	2.388895	4.684609	-0.179082
7	1.295984	1.581312	-0.773657
6	1.057993	2.893037	-0.410530
6	2.287325	3.643489	-0.445973
6	0.209483	-3.297971	-0.508341
1	4.583951	-2.259139	-1.522119
6	3.540968	-2.176143	-1.255798
6	2.680827	-3.178317	-0.924839
1	2.880540	-4.238646	-0.876164
6	1.391583	-2.571383	-0.708780
7	1.478891	-1.203981	-0.868974
6	2.800383	-0.941381	-1.184441
6	3.360137	0.332053	-1.331479
26	-0.007336	0.081938	-0.558158
6	-0.319575	4.853043	0.311024
6	0.053414	5.926106	-0.513354
6	-0.835218	5.128098	1.587443
6	-0.074677	7.242132	-0.066874
1	0.436101	5.722307	-1.508955
6	-0.962268	6.444291	2.033234
1	-1.131503	4.301774	2.226929
6	-0.580982	7.504820	1.208133
1	0.214806	8.062072	-0.718277
1	-1.357867	6.640187	3.025929
1	-0.680466	8.529442	1.555190
6	4.816725	0.454394	-1.640271
6	5.782729	0.027263	-0.715100
6	5.242715	1.027736	-2.847858
6	7.142662	0.161537	-0.996623
1	5.457725	-0.402433	0.227855
6	6.603401	1.161171	-3.128830
1	4.500653	1.365539	-3.565379
6	7.556734	0.727409	-2.204887
1	7.878271	-0.170934	-0.269495
1	6.917983	1.602226	-4.070548
1	8.615663	0.831826	-2.423821
6	0.333350	-4.758807	-0.219856
6	-0.027625	-5.728450	-1.167999
6	0.849093	-5.179632	1.015834
6	0.113145	-7.087236	-0.882247
1	-0.411571	-5.409989	-2.132566
6	0.988697	-6.538454	1.301287
1	1.133995	-4.434189	1.752835
6	0.620004	-7.495859	0.353518
1	-0.167482	-7.825825	-1.627948
1	1.384240	-6.848407	2.264498
1	0.729572	-8.553693	0.575209
6	-4.827223	-0.139827	-1.611517

6	-5.751097	-0.664668	-0.693713
6	-5.301441	0.369089	-2.830192
6	-7.114028	-0.687507	-0.991664
1	-5.390953	-1.050615	0.254973
6	-6.665039	0.346657	-3.127586
1	-4.593781	0.782022	-3.543184
6	-7.575003	-0.182492	-2.209805
1	-7.816340	-1.094013	-0.269144
1	-7.015336	0.741036	-4.077397
1	-8.636337	-0.199188	-2.440995
6	1.187688	-0.481331	2.089287
6	-1.090128	-0.320238	2.098673
6	2.430251	0.360544	2.093758
6	0.693047	-0.769200	3.487583
6	-0.718001	-0.762072	3.421020
6	3.267258	0.278198	3.162705
1	2.694707	0.918277	1.208975
6	1.597761	-0.865812	4.548055
6	-3.303024	-0.391489	2.632221
6	-1.736470	-1.020006	4.353214
6	2.901170	-0.414824	4.369197
1	4.223875	0.794465	3.132221
1	1.258693	-1.193214	5.527966
6	-3.050670	-0.834296	3.946194
1	-4.330369	-0.232510	2.307134
1	-1.496921	-1.352473	5.359443
1	3.611578	-0.465443	5.188803
1	-3.880437	-1.019689	4.620660
7	-2.364879	-0.140122	1.718426
7	-0.002343	-0.085477	1.299377
1	1.499471	-1.454244	1.655960

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^{CSS}24'

Number of imaginary frequencies : 0
Electronic energy : HF=-2570.2159212
Zero-point correction= 0.763216 (Hartree/Particle)
Thermal correction to Energy= 0.809930
Thermal correction to Enthalpy= 0.810875
Thermal correction to Gibbs Free Energy= 0.681107
Sum of electronic and zero-point Energies= -2569.452705
Sum of electronic and thermal Energies= -2569.405991
Sum of electronic and thermal Enthalpies= -2569.405047
Sum of electronic and thermal Free Energies= -2569.534815

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Cartesian Coordinates

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6	-1.547258	2.682274	-0.429316
7	-1.557916	1.336351	-0.716180
1	-3.154374	4.254021	-0.355165
6	-2.866003	1.017403	-1.003074
6	-3.697118	2.197564	-0.901519
1	-4.761580	2.226175	-1.081322

6	-2.886754	3.221432	-0.525009
6	-3.362968	-0.272272	-1.231232
7	-1.229135	-1.461865	-0.863147
6	-0.894876	-2.791802	-0.726095
6	-2.077508	-3.615201	-0.851523
1	-2.100979	-4.691810	-0.772319
6	-3.111218	-2.777918	-1.133269
1	-4.139457	-3.042075	-1.329980
6	-2.584714	-1.431124	-1.104332
6	-0.405511	3.460678	-0.189524
1	4.156456	3.286957	-0.905657
6	3.119940	3.011888	-0.777502
6	2.583414	1.681430	-0.955125
1	2.116457	4.862287	-0.156026
7	1.228686	1.681405	-0.690847
6	0.899548	2.984828	-0.384298
6	2.086040	3.809124	-0.392460
6	0.408849	-3.288299	-0.587582
1	4.740110	-1.975861	-1.474778
6	3.690775	-1.958298	-1.220786
6	2.881760	-3.018939	-0.951411
1	3.139396	-4.068021	-0.951718
6	1.555360	-2.490369	-0.731517
7	1.572618	-1.113612	-0.824369
6	2.879576	-0.767324	-1.109813
6	3.368660	0.543958	-1.206670
26	-0.004646	0.097016	-0.581896
6	-0.607262	4.891638	0.193550
6	-0.272458	5.938333	-0.680088
6	-1.165688	5.210168	1.441590
6	-0.479848	7.268181	-0.310856
1	0.145546	5.701170	-1.653854
6	-1.373753	6.539857	1.810866
1	-1.434575	4.405446	2.119726
6	-1.029780	7.573207	0.936357
1	-0.218086	8.065534	-1.001038
1	-1.803432	6.768134	2.782439
1	-1.192078	8.608482	1.223095
6	4.819946	0.752115	-1.496911
6	5.806647	0.319182	-0.596126
6	5.223797	1.410201	-2.669356
6	7.159530	0.531596	-0.863746
1	5.503546	-0.183978	0.317266
6	6.576747	1.623586	-2.937079
1	4.467804	1.751769	-3.370206
6	7.549039	1.184242	-2.035691
1	7.908847	0.191624	-0.154056
1	6.870855	2.130703	-3.851877
1	8.602208	1.350201	-2.244343
6	0.613581	-4.755492	-0.383847
6	0.298900	-5.686279	-1.386513
6	1.158423	-5.225435	0.821504
6	0.512011	-7.050609	-1.184143

1	-0.108165	-5.330992	-2.328375
6	1.371978	-6.589555	1.024641
1	1.411174	-4.512824	1.601603
6	1.047740	-7.506733	0.022535
1	0.265572	-7.756358	-1.972620
1	1.790164	-6.935473	1.965994
1	1.214250	-8.568765	0.179448
6	-4.823350	-0.414407	-1.518667
6	-5.688025	-1.003536	-0.581961
6	-5.363847	0.064251	-2.722216
6	-7.054072	-1.115695	-0.843558
1	-5.277452	-1.373417	0.352711
6	-6.730506	-0.046247	-2.983977
1	-4.703764	0.524414	-3.451649
6	-7.579992	-0.636872	-2.045857
1	-7.708467	-1.572233	-0.105845
1	-7.130511	0.326973	-3.922754
1	-8.643669	-0.722712	-2.249654
6	1.137821	-0.458977	2.156960
6	-1.084375	-0.351209	2.159816
6	2.422428	0.298633	2.117448
6	0.680399	-0.812657	3.537809
6	-0.704816	-0.801254	3.494848
6	3.275391	0.182776	3.164448
1	2.694455	0.813690	1.209607
6	1.628392	-0.970328	4.580842
6	-3.289020	-0.465932	2.700994
6	-1.724140	-1.083330	4.442138
6	2.902112	-0.501364	4.380946
1	4.257073	0.644379	3.109765
1	1.321353	-1.359700	5.547045
6	-3.021883	-0.909678	4.040595
1	-4.327322	-0.327513	2.398762
1	-1.473863	-1.417788	5.444831
1	3.634051	-0.575606	5.180182
1	-3.854862	-1.100032	4.709017
7	-2.389465	-0.207549	1.782743
7	-0.041217	-0.106332	1.366042
1	1.436743	-1.426475	1.689925

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Number of imaginary frequencies : 0
Electronic energy : HF=-2570.2278033
Zero-point correction= 0.762434 (Hartree/Particle)
Thermal correction to Energy= 0.809632
Thermal correction to Enthalpy= 0.810576
Thermal correction to Gibbs Free Energy= 0.677931
Sum of electronic and zero-point Energies= -2569.465369
Sum of electronic and thermal Energies= -2569.418171
Sum of electronic and thermal Enthalpies= -2569.417227
Sum of electronic and thermal Free Energies= -2569.549873
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Cartesian Coordinates

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6	-2.028223	1.666876	-1.043287
7	-1.662971	0.340183	-1.007765
1	-3.987083	2.712195	-1.386843
6	-2.821301	-0.380410	-1.203535
6	-3.933505	0.516706	-1.410474
1	-4.952270	0.210928	-1.596622
6	-3.446506	1.781645	-1.296105
6	-2.953593	-1.766598	-1.064585
7	-0.584610	-2.237259	-0.536197
6	0.091313	-3.373146	-0.149840
6	-0.832151	-4.479048	-0.029759
1	-0.569046	-5.479506	0.279371
6	-2.055903	-4.016459	-0.399432
1	-2.984039	-4.565437	-0.454699
6	-1.901055	-2.612267	-0.697606
6	-1.166698	2.764168	-0.893738
1	3.337673	3.777500	-1.036143
6	2.401734	3.241517	-0.985934
6	2.266119	1.806023	-0.991200
1	0.866744	4.800437	-0.814894
7	0.933522	1.458516	-0.879133
6	0.230047	2.646962	-0.853723
6	1.148103	3.759588	-0.870813
6	1.478605	-3.478637	0.022038
1	5.349136	-1.150645	-0.922382
6	4.317601	-1.391613	-0.713745
6	3.799516	-2.596338	-0.349452
1	4.326372	-3.528596	-0.208666
6	2.371439	-2.425643	-0.230727
7	2.028964	-1.118332	-0.501031
6	3.215342	-0.462727	-0.781870
6	3.348219	0.913385	-1.016658
26	0.163859	-0.379279	-0.615472
6	-1.779944	4.125088	-0.816985
6	-1.578357	5.080020	-1.826023
6	-2.591344	4.464901	0.277944
6	-2.162553	6.344549	-1.737144
1	-0.965216	4.821670	-2.684174
6	-3.175645	5.728813	0.366251
1	-2.761996	3.728233	1.056666
6	-2.961381	6.673968	-0.639755
1	-1.998917	7.069742	-2.529544
1	-3.797922	5.975527	1.222410
1	-3.416401	7.658144	-0.571316
6	4.714906	1.482000	-1.221916
6	5.683918	1.420657	-0.206690
6	5.049853	2.114200	-2.430069
6	6.951879	1.972031	-0.395119
1	5.435774	0.935652	0.732892
6	6.317650	2.665807	-2.619214
1	4.307438	2.168151	-3.220748

6	7.272892	2.596605	-1.602524
1	7.687118	1.917115	0.403048
1	6.559808	3.146839	-3.562854
1	8.259845	3.026007	-1.749865
6	2.060110	-4.797879	0.416751
6	1.972286	-5.914628	-0.430040
6	2.731030	-4.935584	1.642408
6	2.532258	-7.137244	-0.057395
1	1.466706	-5.814610	-1.385795
6	3.290801	-6.158221	2.015637
1	2.806257	-4.076020	2.301977
6	3.192444	-7.263281	1.167102
1	2.458134	-7.989481	-0.727299
1	3.801506	-6.247849	2.970505
1	3.628656	-8.215135	1.456898
6	-4.326898	-2.348234	-1.181955
6	-5.017238	-2.751182	-0.027464
6	-4.957888	-2.475511	-2.427372
6	-6.308541	-3.272511	-0.118508
1	-4.528123	-2.648715	0.936952
6	-6.250831	-2.995586	-2.517762
1	-4.429932	-2.163899	-3.324034
6	-6.929156	-3.395556	-1.364346
1	-6.831059	-3.579340	0.783551
1	-6.726361	-3.090661	-3.490108
1	-7.934836	-3.800421	-1.435694
6	0.651845	0.895749	2.585229
6	-1.461555	0.436855	2.220877
6	2.013524	1.252353	2.116683
6	-0.136035	2.008018	3.215427
6	-1.466922	1.646920	3.048106
6	2.588289	2.388972	2.583213
1	2.545092	0.531424	1.510493
6	0.532406	3.147945	3.723938
6	-3.737696	0.386780	2.214250
6	-2.708143	2.217034	3.430724
6	1.858643	3.321384	3.407534
1	3.612157	2.627607	2.312215
1	-0.013742	3.914120	4.266443
6	-3.846808	1.590293	2.994136
1	-4.657586	-0.103548	1.895421
1	-2.747098	3.117879	4.037202
1	2.374966	4.213064	3.752356
1	-4.833613	1.969339	3.237989
7	-2.622561	-0.196733	1.848048
7	-0.255721	0.033990	1.848910
1	0.913724	0.253921	3.464857

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^{oss}25

Number of imaginary frequencies : 0
Electronic energy : HF=-2570.2204472
Zero-point correction= 0.762531 (Hartree/Particle)

Thermal correction to Energy= 0.809599
Thermal correction to Enthalpy= 0.810543
Thermal correction to Gibbs Free Energy= 0.679270
Sum of electronic and zero-point Energies= -2569.457916
Sum of electronic and thermal Energies= -2569.410848
Sum of electronic and thermal Enthalpies= -2569.409904
Sum of electronic and thermal Free Energies= -2569.541177

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Cartesian Coordinates

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6	-1.475306	2.790189	-0.392559
7	-1.545349	1.445099	-0.673254
1	-3.024925	4.415508	-0.246237
6	-2.874474	1.171410	-0.902029
6	-3.661493	2.378214	-0.756993
1	-4.732038	2.441737	-0.883476
6	-2.800010	3.374630	-0.426462
6	-3.423160	-0.094512	-1.144317
7	-1.317341	-1.368365	-0.922286
6	-1.022449	-2.711621	-0.850274
6	-2.234819	-3.489910	-0.967526
1	-2.292314	-4.567574	-0.930939
6	-3.251628	-2.608145	-1.167536
1	-4.295659	-2.830817	-1.329291
6	-2.679081	-1.282679	-1.102837
6	-0.299911	3.531551	-0.204025
1	4.264301	3.191522	-0.862949
6	3.215279	2.955135	-0.762602
6	2.633894	1.646675	-0.952301
1	2.266241	4.843066	-0.168025
7	1.274271	1.699212	-0.725310
6	0.986722	3.011620	-0.418193
6	2.201275	3.791983	-0.406801
6	0.266212	-3.256741	-0.745048
1	4.664302	-2.078204	-1.483744
6	3.609639	-2.029868	-1.257465
6	2.753766	-3.066896	-1.053074
1	2.971839	-4.124302	-1.087129
6	1.442004	-2.495722	-0.843989
7	1.514525	-1.118128	-0.883694
6	2.839362	-0.812852	-1.126954
6	3.381182	0.479542	-1.185459
26	-0.023111	0.150757	-0.621342
6	-0.439113	4.973730	0.165551
6	-0.084197	5.994229	-0.730937
6	-0.951824	5.331589	1.422552
6	-0.229269	7.336273	-0.376493
1	0.301079	5.726961	-1.710426
6	-1.097857	6.673540	1.776995
1	-1.234379	4.547752	2.119278
6	-0.735593	7.680212	0.879044
1	0.047167	8.112901	-1.084370
1	-1.493015	6.932152	2.755595

1	-0.849487	8.725001	1.154378
6	4.851140	0.629613	-1.411356
6	5.774864	0.152824	-0.466829
6	5.336995	1.271663	-2.561066
6	7.146632	0.308219	-0.669275
1	5.406362	-0.339572	0.428415
6	6.709040	1.427946	-2.763665
1	4.630090	1.645824	-3.295706
6	7.618162	0.946217	-1.819048
1	7.846842	-0.064938	0.073188
1	7.067426	1.923327	-3.661815
1	8.686069	1.067685	-1.977392
6	0.415780	-4.737835	-0.601962
6	0.063189	-5.614116	-1.640413
6	0.940772	-5.277661	0.582878
6	0.221925	-6.992958	-1.493658
1	-0.331113	-5.205157	-2.565812
6	1.100442	-6.656184	0.730239
1	1.220677	-4.607315	1.390683
6	0.739996	-7.518467	-0.307668
1	-0.053276	-7.656008	-2.309237
1	1.504502	-7.056281	1.656188
1	0.864327	-8.591751	-0.194260
6	-4.898513	-0.181875	-1.373239
6	-5.742154	-0.777067	-0.421579
6	-5.472312	0.350932	-2.538111
6	-7.120353	-0.841587	-0.630450
1	-5.305638	-1.190181	0.482576
6	-6.850958	0.288248	-2.747132
1	-4.828396	0.815598	-3.279031
6	-7.679512	-0.308546	-1.794259
1	-7.757951	-1.303676	0.118448
1	-7.276836	0.703314	-3.656504
1	-8.752552	-0.357308	-1.957068
6	1.176097	-0.550167	2.170795
6	-1.032725	-0.447393	2.238808
6	2.467627	0.192400	2.154695
6	0.760312	-1.054453	3.516647
6	-0.627444	-1.046738	3.508703
6	3.355624	-0.037036	3.153763
1	2.709712	0.794604	1.291073
6	1.743319	-1.323090	4.503390
6	-3.225737	-0.635866	2.800833
6	-1.627536	-1.443761	4.433836
6	3.012111	-0.837684	4.306065
1	4.341286	0.417209	3.113499
1	1.471366	-1.811094	5.434624
6	-2.932687	-1.232324	4.074803
1	-4.270770	-0.469441	2.538467
1	-1.360462	-1.892076	5.386608
1	3.769777	-0.996524	5.068269
1	-3.754033	-1.504451	4.729109
7	-2.346755	-0.265539	1.901135

7	-0.013105	-0.114819	1.455163
1	1.457191	-1.468371	1.599541

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^{CSS}25

Number of imaginary frequencies : 0
Electronic energy : HF=-533.4528061
Zero-point correction= 0.162677 (Hartree/Particle)
Thermal correction to Energy= 0.171444
Thermal correction to Enthalpy= 0.172388
Thermal correction to Gibbs Free Energy= 0.128645
Sum of electronic and zero-point Energies= -533.290129
Sum of electronic and thermal Energies= -533.281362
Sum of electronic and thermal Enthalpies= -533.280418
Sum of electronic and thermal Free Energies= -533.324162

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Cartesian Coordinates

.....

6	-3.008505	1.099156	-0.127900
6	-3.293285	-0.314664	-0.170966
6	-1.100541	-0.890263	0.039975
6	-0.709722	0.528061	0.100189
6	-1.716714	1.527211	0.013630
1	-3.833767	1.799491	-0.204695
1	-4.335475	-0.617218	-0.283185
1	-1.465348	2.583695	0.054287
6	1.062757	-0.907985	0.333637
6	2.422467	-1.240340	-0.183779
6	3.331499	-0.242467	-0.300447
6	2.970689	1.145320	-0.094680
6	1.678511	1.539136	0.138780
6	0.670115	0.539179	0.207736
1	2.678468	-2.284153	-0.336614
1	4.355695	-0.470389	-0.581520
1	3.749944	1.896515	-0.189021
1	1.417197	2.592912	0.176270
7	-2.419018	-1.283762	-0.084612
7	-0.100130	-1.739559	0.112265
1	1.223701	-1.031667	1.433868

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^{OSS}(25-21)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2570.2005397
Zero-point correction= 0.759512 (Hartree/Particle)
Thermal correction to Energy= 0.806335
Thermal correction to Enthalpy= 0.807279
Thermal correction to Gibbs Free Energy= 0.676369
Sum of electronic and zero-point Energies= -2569.441028
Sum of electronic and thermal Energies= -2569.394205
Sum of electronic and thermal Enthalpies= -2569.393261
Sum of electronic and thermal Free Energies= -2569.524171

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Cartesian Coordinates

.....

6	-1.469835	2.714984	-0.490864
7	-1.526219	1.366346	-0.756085
1	-3.032581	4.331000	-0.404045
6	-2.847581	1.078752	-1.010068
6	-3.644046	2.282705	-0.903808
1	-4.711709	2.337655	-1.056082
6	-2.796451	3.289511	-0.565539
6	-3.381591	-0.197599	-1.233364
7	-1.274557	-1.448382	-0.912104
6	-0.974670	-2.785092	-0.769551
6	-2.181275	-3.573799	-0.875687
1	-2.236448	-4.648311	-0.785386
6	-3.196251	-2.708581	-1.145287
1	-4.234912	-2.945014	-1.320983
6	-2.632299	-1.378419	-1.128724
6	-0.301591	3.463165	-0.278931
1	4.271885	3.139127	-0.881083
6	3.223244	2.898553	-0.787412
6	2.650246	1.585798	-0.971881
1	2.261485	4.784873	-0.208676
7	1.289763	1.633369	-0.752934
6	0.991572	2.947024	-0.460517
6	2.203007	3.732342	-0.442735
6	0.316005	-3.318001	-0.622281
1	4.692225	-2.143270	-1.478592
6	3.643502	-2.091082	-1.227189
6	2.798694	-3.124915	-0.965283
1	3.022340	-4.181656	-0.969241
6	1.489070	-2.554511	-0.747272
7	1.553927	-1.179249	-0.831381
6	2.871836	-0.874185	-1.115151
6	3.403652	0.421428	-1.207196
26	0.001791	0.087512	-0.656424
6	-0.456979	4.906672	0.078093
6	-0.084248	5.924511	-0.814120
6	-1.004436	5.267811	1.319466
6	-0.245707	7.267440	-0.470255
1	0.327339	5.654652	-1.782103
6	-1.166531	6.610607	1.663316
1	-1.300876	4.485986	2.012708
6	-0.786199	7.614732	0.770003
1	0.044890	8.042084	-1.174594
1	-1.588296	6.871836	2.630018
1	-0.912643	8.660215	1.037044
6	4.864078	0.583815	-1.479727
6	5.827941	0.101169	-0.579251
6	5.301298	1.248310	-2.636793
6	7.189595	0.272273	-0.831184
1	5.500799	-0.409949	0.321363
6	6.662962	1.420261	-2.889074
1	4.563965	1.627646	-3.338051

6	7.611665	0.932393	-1.987514
1	7.920315	-0.105561	-0.121283
1	6.982256	1.932985	-3.792203
1	8.671680	1.066385	-2.184040
6	0.476389	-4.790614	-0.419728
6	0.116596	-5.712538	-1.415642
6	1.024850	-5.276371	0.777959
6	0.288741	-7.082631	-1.213689
1	-0.292295	-5.346066	-2.352382
6	1.197548	-6.646244	0.980514
1	1.314454	-4.570468	1.551362
6	0.828026	-7.554040	-0.014464
1	0.007914	-7.781182	-1.997050
1	1.619213	-7.003839	1.915896
1	0.962528	-8.620651	0.142015
6	-4.848830	-0.298583	-1.504291
6	-5.720583	-0.870018	-0.563467
6	-5.387025	0.201614	-2.700262
6	-7.091391	-0.944193	-0.813657
1	-5.312143	-1.256921	0.364903
6	-6.758276	0.129113	-2.950603
1	-4.721333	0.648495	-3.432846
6	-7.614912	-0.444440	-2.008383
1	-7.751158	-1.387446	-0.072668
1	-7.156301	0.518477	-3.883632
1	-8.682239	-0.500713	-2.203149
6	1.099957	-0.268048	2.397337
6	-1.136107	-0.321475	2.308955
6	2.461745	0.110291	2.170015
6	0.642718	-0.557074	3.739143
6	-0.773374	-0.589992	3.669101
6	3.340381	-0.013746	3.220603
1	2.778792	0.428557	1.189206
6	1.578279	-0.673262	4.783601
6	-3.343531	-0.502430	2.766386
6	-1.801600	-0.826664	4.602145
6	2.910718	-0.417161	4.514510
1	4.388095	0.224928	3.063374
1	1.250198	-0.920375	5.788847
6	-3.101171	-0.771061	4.138996
1	-4.370681	-0.455519	2.408308
1	-1.577516	-1.037037	5.643912
1	3.643980	-0.494635	5.311768
1	-3.942057	-0.934050	4.805185
7	-2.404762	-0.301201	1.855441
7	-0.051712	-0.088372	1.498652
1	0.840243	-1.196160	1.652269

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^{CSS}(24'-25')‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2570.1936246
Zero-point correction= 0.760277 (Hartree/Particle)

Thermal correction to Energy= 0.806701
Thermal correction to Enthalpy= 0.807645
Thermal correction to Gibbs Free Energy= 0.678531
Sum of electronic and zero-point Energies= -2569.433348
Sum of electronic and thermal Energies= -2569.386924
Sum of electronic and thermal Enthalpies= -2569.385979
Sum of electronic and thermal Free Energies= -2569.515094

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Cartesian Coordinates

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6	-1.582107	2.569191	-0.537964
7	-1.557795	1.217459	-0.794716
1	-3.224444	4.105311	-0.540058
6	-2.850735	0.860734	-1.103990
6	-3.708476	2.024962	-1.052467
1	-4.768527	2.025947	-1.258897
6	-2.929971	3.075442	-0.679514
6	-3.313158	-0.447496	-1.302487
7	-1.165599	-1.575238	-0.836615
6	-0.807689	-2.888540	-0.621786
6	-1.971331	-3.741081	-0.729599
1	-1.977535	-4.811927	-0.591833
6	-3.012973	-2.941345	-1.083147
1	-4.030345	-3.237409	-1.290603
6	-2.514635	-1.583879	-1.110624
6	-0.461504	3.374739	-0.281965
1	4.111007	3.282513	-0.948345
6	3.079440	2.988783	-0.821464
6	2.570747	1.645227	-0.982227
1	2.036543	4.827250	-0.230058
7	1.216673	1.622373	-0.722925
6	0.857195	2.923369	-0.441605
6	2.028111	3.770558	-0.452185
6	0.505258	-3.347896	-0.437075
1	4.790266	-1.987438	-1.461763
6	3.747583	-1.978731	-1.181261
6	2.968165	-3.042502	-0.843285
1	3.248137	-4.085133	-0.805057
6	1.635982	-2.532514	-0.616935
7	1.623294	-1.161928	-0.767150
6	2.916077	-0.799990	-1.098516
6	3.375940	0.519960	-1.232643
26	0.017658	0.020836	-0.604201
6	-0.703132	4.805462	0.077135
6	-0.365734	5.849697	-0.798390
6	-1.303972	5.125212	1.305126
6	-0.611635	7.178615	-0.450000
1	0.084188	5.611396	-1.757508
6	-1.550401	6.453894	1.653531
1	-1.575243	4.322159	1.984352
6	-1.203272	7.485007	0.777615
1	-0.347310	7.974040	-1.141410
1	-2.012516	6.683182	2.609855

1	-1.395433	8.519559	1.047993
6	4.813592	0.756216	-1.565087
6	5.838921	0.345838	-0.697441
6	5.165120	1.422771	-2.749908
6	7.177343	0.587832	-1.008999
1	5.578700	-0.164049	0.225395
6	6.503407	1.665478	-3.061910
1	4.379334	1.747682	-3.425411
6	7.514061	1.248109	-2.192893
1	7.956596	0.265391	-0.323843
1	6.756075	2.178509	-3.985743
1	8.555976	1.437108	-2.435576
6	0.744610	-4.795857	-0.153399
6	0.436966	-5.791845	-1.093937
6	1.322164	-5.180725	1.067045
6	0.686262	-7.136275	-0.814767
1	0.008850	-5.503193	-2.049064
6	1.571827	-6.524870	1.346883
1	1.573562	-4.416420	1.797117
6	1.252338	-7.507381	0.407127
1	0.445010	-7.893211	-1.555936
1	2.014854	-6.803991	2.298949
1	1.446793	-8.554109	0.623401
6	-4.762853	-0.629835	-1.619328
6	-5.638553	-1.204014	-0.683474
6	-5.283481	-0.201157	-2.850155
6	-6.995688	-1.350913	-0.972632
1	-5.243647	-1.534422	0.272445
6	-6.641285	-0.346587	-3.139543
1	-4.615072	0.247850	-3.578972
6	-7.501662	-0.922411	-2.202167
1	-7.658848	-1.795059	-0.235200
1	-7.025816	-0.012025	-4.099130
1	-8.558453	-1.035388	-2.427411
6	1.070380	-0.106844	2.337193
6	-1.173448	-0.210894	2.202217
6	2.438298	0.237069	2.104457
6	0.574345	-0.201691	3.691054
6	-0.838273	-0.266429	3.591158
6	3.282514	0.273694	3.190135
1	2.792272	0.408911	1.102227
6	1.473652	-0.158721	4.771083
6	-3.388427	-0.360161	2.639008
6	-1.882966	-0.377996	4.528705
6	2.814515	0.063300	4.514526
1	4.334412	0.490977	3.029896
1	1.109094	-0.261206	5.788811
6	-3.173883	-0.413509	4.039647
1	-4.406192	-0.386936	2.253122
1	-1.676043	-0.426256	5.593807
1	3.520995	0.107058	5.337931
1	-4.026022	-0.487655	4.707343
7	-2.429143	-0.281927	1.729806

7	-0.063344	-0.077293	1.388691
1	0.809642	-1.139270	1.725540

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^{CSS}(25-2a)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-533.4386105
Zero-point correction= 0.159956 (Hartree/Particle)
Thermal correction to Energy= 0.168433
Thermal correction to Enthalpy= 0.169377
Thermal correction to Gibbs Free Energy= 0.126269
Sum of electronic and zero-point Energies= -533.278654
Sum of electronic and thermal Energies= -533.270178
Sum of electronic and thermal Enthalpies= -533.269234
Sum of electronic and thermal Free Energies= -533.312342

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Cartesian Coordinates

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6	-3.033768	1.091192	-0.055610
6	-3.325090	-0.302756	-0.059599
6	-1.130345	-0.861008	-0.000903
6	-0.723562	0.521478	0.021044
6	-1.722941	1.516474	-0.005257
1	-3.853610	1.801772	-0.083916
1	-4.367100	-0.619247	-0.093805
1	-1.468640	2.572644	0.009896
6	1.078010	-0.873304	0.109938
6	2.456020	-1.236242	-0.101442
6	3.386842	-0.227376	-0.116183
6	3.008930	1.144637	-0.020585
6	1.683795	1.527305	0.065371
6	0.689467	0.528782	0.083727
1	2.731671	-2.282804	-0.178196
1	4.439422	-0.474262	-0.220111
1	3.786066	1.902903	-0.042683
1	1.409436	2.578176	0.079533
7	-2.424717	-1.268873	-0.016085
7	-0.094132	-1.741691	-0.003611
1	0.750543	-1.380332	1.144155

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^{CSS}25'

Number of imaginary frequencies : 0
Electronic energy : HF=-2570.2869024
Zero-point correction= 0.766527 (Hartree/Particle)
Thermal correction to Energy= 0.812877
Thermal correction to Enthalpy= 0.813822
Thermal correction to Gibbs Free Energy= 0.685093
Sum of electronic and zero-point Energies= -2569.520375
Sum of electronic and thermal Energies= -2569.474025
Sum of electronic and thermal Enthalpies= -2569.473081
Sum of electronic and thermal Free Energies= -2569.601809

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Cartesian Coordinates

.....

6	-2.285415	1.674546	-0.872962
7	-1.852370	0.366102	-0.823943
1	-4.300764	2.620518	-1.181614
6	-2.985452	-0.409294	-0.959445
6	-4.146581	0.431414	-1.138679
1	-5.156070	0.074591	-1.279283
6	-3.715096	1.718782	-1.082653
6	-3.048872	-1.799100	-0.814843
7	-0.627532	-2.182441	-0.503164
6	0.127994	-3.313886	-0.261813
6	-0.734730	-4.464776	-0.117734
1	-0.402585	-5.470630	0.091509
6	-2.006796	-4.033376	-0.329288
1	-2.914473	-4.618553	-0.328766
6	-1.937126	-2.609615	-0.560552
6	-1.476951	2.811655	-0.738746
1	2.971328	4.047860	-0.738649
6	2.060693	3.467671	-0.735542
6	1.992604	2.027527	-0.828619
1	0.447217	4.939940	-0.529264
7	0.680970	1.608353	-0.751102
6	-0.077793	2.758684	-0.682302
6	0.782960	3.918484	-0.626754
6	1.528389	-3.361625	-0.233516
1	5.212359	-0.748079	-1.186361
6	4.206425	-1.067637	-0.958931
6	3.773565	-2.329205	-0.689942
1	4.355059	-3.238846	-0.661568
6	2.345159	-2.250078	-0.490902
7	1.917463	-0.945522	-0.632223
6	3.053353	-0.201204	-0.887602
6	3.112290	1.196687	-0.964742
26	0.026171	-0.278093	-0.535173
6	-2.144359	4.149292	-0.708378
6	-1.941009	5.083776	-1.736609
6	-3.001663	4.491688	0.349504
6	-2.571105	6.328503	-1.703722
1	-1.288263	4.824788	-2.564820
6	-3.631328	5.736522	0.382966
1	-3.168036	3.771416	1.143400
6	-3.417177	6.659931	-0.642826
1	-2.405209	7.037077	-2.510554
1	-4.288568	5.985501	1.211879
1	-3.907948	7.628856	-0.617713
6	4.440851	1.848478	-1.178298
6	5.460157	1.750795	-0.218213
6	4.688956	2.586366	-2.346991
6	6.693925	2.370066	-0.421254
1	5.272088	1.190878	0.691456
6	5.922833	3.205186	-2.551492
1	3.906081	2.669174	-3.095080

6	6.929728	3.098776	-1.589274
1	7.469362	2.287101	0.335474
1	6.098325	3.767479	-3.464492
1	7.890335	3.580787	-1.748037
6	2.199591	-4.673471	0.020698
6	2.085413	-5.735764	-0.890222
6	2.977043	-4.859571	1.174827
6	2.725266	-6.952377	-0.649711
1	1.494836	-5.597959	-1.790946
6	3.616802	-6.076039	1.416355
1	3.076210	-4.042196	1.883446
6	3.491925	-7.126836	0.504817
1	2.628955	-7.762083	-1.367755
1	4.210469	-6.203230	2.317423
1	3.990082	-8.074024	0.691606
6	-4.397986	-2.445875	-0.853373
6	-4.995800	-2.891812	0.335673
6	-5.092118	-2.605422	-2.061182
6	-6.258593	-3.485730	0.316168
1	-4.459134	-2.766624	1.271688
6	-6.356644	-3.197460	-2.080272
1	-4.634957	-2.262281	-2.984800
6	-6.942862	-3.639530	-0.892166
1	-6.709298	-3.825192	1.244857
1	-6.881609	-3.316160	-3.024170
1	-7.926317	-4.100981	-0.907659
6	1.090159	0.478777	2.196276
6	-1.183444	0.320088	2.136649
6	2.442471	0.168724	2.230082
6	0.580223	1.656649	2.781814
6	-0.870821	1.556621	2.737763
6	3.301155	1.096802	2.826270
1	2.819322	-0.753472	1.806047
6	1.454730	2.590623	3.342317
6	-3.389347	0.519185	2.521114
6	-1.931969	2.317530	3.225818
6	2.819632	2.303708	3.352698
1	4.362968	0.876325	2.877694
1	1.075488	3.508927	3.780149
6	-3.217010	1.783426	3.098242
1	-4.381634	0.084044	2.438611
1	-1.767053	3.281286	3.697846
1	3.515736	3.012821	3.790395
1	-4.082774	2.329752	3.457996
7	-2.379784	-0.227529	2.041095
7	0.012816	-0.287003	1.625744
1	0.059583	-1.295810	1.766689

2a

Number of imaginary frequencies : 0
Electronic energy : HF=-533.5484637
Zero-point correction= 0.165451 (Hartree/Particle)

Thermal correction to Energy= 0.174118
Thermal correction to Enthalpy= 0.175062
Thermal correction to Gibbs Free Energy= 0.131672
Sum of electronic and zero-point Energies= -533.383013
Sum of electronic and thermal Energies= -533.374346
Sum of electronic and thermal Enthalpies= -533.373401
Sum of electronic and thermal Free Energies= -533.416791

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Cartesian Coordinates

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6	-3.054215	1.085697	0.000297
6	-3.340706	-0.287598	0.000589
6	-1.154601	-0.820994	-0.000344
6	-0.729126	0.540155	-0.000431
6	-1.725477	1.515595	0.000122
1	-3.869365	1.801829	0.000395
1	-4.375439	-0.624261	0.000614
1	-1.479010	2.573669	-0.000038
6	1.103071	-0.847291	-0.000282
6	2.445638	-1.232787	0.000296
6	3.407046	-0.223984	0.000636
6	3.044778	1.135804	0.000304
6	1.704995	1.515808	-0.000475
6	0.717641	0.523193	-0.000526
1	2.727828	-2.281395	-0.000020
1	4.458901	-0.495270	0.001097
1	3.820800	1.895361	0.000654
1	1.427638	2.566173	-0.000553
7	-2.411483	-1.256062	0.000127
7	-0.039206	-1.632127	-0.000881
1	-0.070788	-2.640378	0.002013

7a

Number of imaginary frequencies : 0
Electronic energy : HF=-1372.9594021
Zero-point correction= 0.275045 (Hartree/Particle)
Thermal correction to Energy= 0.292462
Thermal correction to Enthalpy= 0.293406
Thermal correction to Gibbs Free Energy= 0.228118
Sum of electronic and zero-point Energies= -1372.684357
Sum of electronic and thermal Energies= -1372.666940
Sum of electronic and thermal Enthalpies= -1372.665996
Sum of electronic and thermal Free Energies= -1372.731285

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Cartesian Coordinates

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6	-1.305399	-1.493849	-0.272476
6	-3.177375	-1.418141	1.269806
6	-2.333121	-0.957148	2.239921
6	-0.957400	-0.733014	1.956398
6	-0.415310	-0.973335	0.708231
1	-4.238324	-1.601189	1.375794

1	-2.727871	-0.741953	3.225763
1	-0.320073	-0.323853	2.733085
6	1.015006	-0.702518	0.411453
6	1.977365	-1.309015	1.231741
6	1.429793	0.180947	-0.614226
6	3.339999	-1.078213	1.058994
1	1.649973	-1.989990	2.011621
6	2.800096	0.412707	-0.778888
6	3.734680	-0.213019	0.043777
1	4.073938	-1.560864	1.694194
1	3.140148	1.094407	-1.551306
7	-2.631642	-1.668105	0.041093
7	-1.152754	-1.838935	-1.557600
7	-2.370035	-2.202882	-1.992078
7	-3.282812	-2.116068	-1.066379
6	0.454805	0.907190	-1.527235
17	5.449179	0.110537	-0.202373
1	1.028426	1.588794	-2.165629
6	-0.625861	1.695992	-0.805625
6	-0.291102	2.600170	0.211999
6	-1.976122	1.531125	-1.139756
6	-1.281539	3.315544	0.884791
1	0.752813	2.731926	0.485430
6	-2.970566	2.246095	-0.467872
1	-2.251172	0.824478	-1.918555
6	-2.626783	3.138709	0.548647
1	-1.004273	4.010567	1.672875
1	-4.013024	2.099178	-0.737011
1	-3.399129	3.692960	1.074613
1	-0.013755	0.176987	-2.193868

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^{oss}22b

Number of imaginary frequencies : 0
Electronic energy : HF=-3409.7124934
Zero-point correction= 0.872700 (Hartree/Particle)
Thermal correction to Energy= 0.929557
Thermal correction to Enthalpy= 0.930501
Thermal correction to Gibbs Free Energy= 0.776603
Sum of electronic and zero-point Energies= -3408.839793
Sum of electronic and thermal Energies= -3408.782937
Sum of electronic and thermal Enthalpies= -3408.781992
Sum of electronic and thermal Free Energies= -3408.935890

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Cartesian Coordinates

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6	2.082487	0.896672	-2.269114
7	0.783655	1.202898	-1.911024
1	3.825568	2.138515	-2.947863
6	0.698104	2.578897	-1.949329
6	1.948906	3.141100	-2.404642
1	2.137779	4.193384	-2.556115
6	2.802343	2.102297	-2.604756

6	-0.411583	3.343358	-1.563243
7	-1.971875	1.450483	-1.235288
6	-3.301700	1.370609	-0.882771
6	-3.828225	2.690177	-0.630423
1	-4.846124	2.909443	-0.344198
6	-2.804441	3.566758	-0.816961
1	-2.824256	4.640470	-0.705417
6	-1.654031	2.791783	-1.219260
6	2.661401	-0.376735	-2.237074
1	1.650802	-4.782001	-1.293650
6	1.566991	-3.721186	-1.477387
6	0.341606	-2.961545	-1.422645
1	3.613419	-3.059097	-1.927041
7	0.598341	-1.630558	-1.681285
6	1.953480	-1.547252	-1.930942
6	2.562491	-2.847564	-1.797216
6	-4.053386	0.194050	-0.783158
1	-3.610983	-4.393270	-0.759423
6	-3.403045	-3.336569	-0.839501
6	-4.280865	-2.302677	-0.761193
1	-5.347083	-2.346326	-0.595452
6	-3.516041	-1.088407	-0.933844
7	-2.186593	-1.388616	-1.140662
6	-2.094470	-2.761463	-1.059046
6	-0.915866	-3.513130	-1.136165
6	-2.502826	-1.565912	2.782298
6	-1.780981	-2.236868	3.768930
6	-0.393062	-2.099691	3.771328
6	0.238594	-1.317157	2.800908
6	-0.602889	-0.684149	1.859560
1	-3.586305	-1.641608	2.730822
1	-2.287907	-2.847474	4.508530
1	0.213707	-2.604233	4.517547
7	0.931346	0.788453	0.942111
7	1.835674	1.467838	0.863796
26	-0.681822	-0.086998	-1.413915
7	-0.106844	0.110768	0.784914
6	1.718117	-1.146687	2.769825
6	2.448960	-1.777410	1.752974
6	2.378586	-0.309868	3.696889
6	3.825400	-1.598797	1.633015
1	1.932893	-2.400636	1.028935
6	3.763770	-0.147347	3.583232
6	4.466942	-0.783145	2.561468
1	4.378487	-2.072966	0.830879
1	4.293696	0.490885	4.282489
7	-1.927549	-0.799774	1.850477
6	4.135120	-0.488029	-2.463414
6	4.652206	-1.141694	-3.591815
6	5.029329	0.048171	-1.522281
6	6.031320	-1.257028	-3.775424
1	3.966213	-1.557707	-4.323920
6	6.407762	-0.070529	-1.704501

1	4.633015	0.549959	-0.644557
6	6.912300	-0.723205	-2.831971
1	6.416882	-1.762194	-4.656743
1	7.085335	0.342386	-0.962701
1	7.985383	-0.815545	-2.974402
6	-0.999110	-4.982639	-0.872583
6	-1.317093	-5.451577	0.412315
6	-0.757732	-5.918024	-1.890516
6	-1.390528	-6.820568	0.672293
1	-1.503013	-4.733026	1.205361
6	-0.831718	-7.287453	-1.630622
1	-0.514347	-5.563622	-2.887818
6	-1.147909	-7.742734	-0.348593
1	-1.634047	-7.166780	1.673086
1	-0.646274	-7.998226	-2.431180
1	-1.205138	-8.808649	-0.146565
6	-5.499956	0.309701	-0.416225
6	-6.507636	0.075767	-1.362869
6	-5.868539	0.644440	0.896053
6	-7.853964	0.173304	-1.005581
1	-6.229393	-0.183254	-2.380364
6	-7.214165	0.744829	1.252524
1	-5.089208	0.826053	1.630601
6	-8.210797	0.508522	0.302424
1	-8.623482	-0.008967	-1.750674
1	-7.484047	1.004461	2.272610
1	-9.258470	0.585543	0.579485
6	-0.240679	4.825571	-1.478909
6	0.656938	5.372582	-0.546370
6	-0.960825	5.696536	-2.310811
6	0.821735	6.754186	-0.442424
1	1.216197	4.702255	0.098893
6	-0.794013	7.078733	-2.208103
1	-1.650156	5.282464	-3.040648
6	0.095633	7.611861	-1.272620
1	1.516276	7.160373	0.288012
1	-1.356382	7.738593	-2.862963
1	0.224166	8.687674	-1.192971
17	6.208472	-0.536421	2.440951
6	1.619571	0.511180	4.734566
1	0.850283	-0.097470	5.216963
1	2.319236	0.822131	5.516982
6	0.976224	1.736951	4.097374
6	1.767045	2.825610	3.704126
6	-0.392718	1.762579	3.800955
6	1.209484	3.896525	3.005496
1	2.832139	2.818953	3.921025
6	-0.950242	2.822354	3.079652
1	-1.024121	0.935946	4.112339
6	-0.148663	3.890079	2.673783
1	1.839489	4.727690	2.700825
1	-2.004905	2.802469	2.820866
1	-0.573949	4.705222	2.096669

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^{3}22b

Number of imaginary frequencies : 0
Electronic energy : HF=-3409.7236294
Zero-point correction= 0.872932 (Hartree/Particle)
Thermal correction to Energy= 0.929789
Thermal correction to Enthalpy= 0.930733
Thermal correction to Gibbs Free Energy= 0.775123
Sum of electronic and zero-point Energies= -3408.850698
Sum of electronic and thermal Energies= -3408.793840
Sum of electronic and thermal Enthalpies= -3408.792896
Sum of electronic and thermal Free Energies= -3408.948507

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Cartesian Coordinates

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6	0.728809	2.481693	-2.054379
7	-0.431277	1.881377	-1.602573
1	1.292157	4.611177	-2.484069
6	-1.314489	2.909403	-1.352536
6	-0.708928	4.175560	-1.690101
1	-1.196119	5.136213	-1.613640
6	0.548916	3.910410	-2.134472
6	-2.622337	2.772198	-0.866505
7	-2.718906	0.299897	-0.971644
6	-3.706602	-0.617960	-0.684556
6	-4.885228	0.056146	-0.196719
1	-5.795344	-0.432053	0.117962
6	-4.603473	1.385835	-0.185440
1	-5.240618	2.194722	0.139240
6	-3.258371	1.537000	-0.688023
6	1.935140	1.826441	-2.327056
1	3.901695	-2.332968	-2.053861
6	3.170734	-1.538787	-2.071917
6	1.754815	-1.703090	-1.841518
1	4.325700	0.276664	-2.510150
7	1.123026	-0.476698	-1.897333
6	2.109945	0.442741	-2.202847
6	3.386988	-0.216790	-2.308071
6	-3.588565	-2.010720	-0.773338
1	-0.446231	-5.318474	-1.457157
6	-0.923652	-4.357047	-1.339812
6	-2.244061	-4.100134	-1.140380
1	-3.052877	-4.810674	-1.059237
6	-2.386197	-2.666594	-1.061914
7	-1.161503	-2.057641	-1.257607
6	-0.249264	-3.082280	-1.404707
6	1.129790	-2.938147	-1.614233
6	-2.357722	-1.522549	3.084054
6	-1.589727	-2.118705	4.083468
6	-0.204366	-1.975730	4.014231
6	0.379266	-1.247433	2.973571
6	-0.508007	-0.659607	2.042362

1	-3.441041	-1.619675	3.075437
1	-2.058737	-2.686772	4.879767
1	0.439260	-2.441295	4.755075
7	0.986846	0.752131	0.971250
7	1.904358	1.392760	0.783904
26	-0.794745	-0.088897	-1.390509
7	-0.085088	0.116784	0.933676
6	1.858800	-1.137153	2.834536
6	2.480144	-1.834087	1.788571
6	2.634035	-0.326259	3.691148
6	3.853475	-1.755509	1.575328
1	1.874346	-2.426612	1.111613
6	4.017332	-0.263746	3.486948
6	4.608983	-0.970194	2.441488
1	4.317764	-2.287126	0.753399
1	4.632743	0.353653	4.132891
7	-1.831598	-0.803658	2.088714
6	3.130615	2.657154	-2.667032
6	3.716717	2.594422	-3.939824
6	3.697154	3.503817	-1.700535
6	4.840721	3.365027	-4.242497
1	3.284260	1.939364	-4.690548
6	4.821264	4.272701	-2.003550
1	3.252400	3.544872	-0.710548
6	5.395430	4.206447	-3.275570
1	5.280780	3.309426	-5.234356
1	5.252201	4.919565	-1.244249
1	6.270769	4.805323	-3.511149
6	1.974239	-4.171954	-1.606924
6	2.083923	-4.951479	-0.443136
6	2.674800	-4.579987	-2.753762
6	2.881720	-6.096209	-0.421793
1	1.537918	-4.653833	0.447038
6	3.471064	-5.725631	-2.733603
1	2.587922	-3.992320	-3.662613
6	3.579820	-6.485915	-1.566820
1	2.959038	-6.681239	0.490447
1	4.003088	-6.026573	-3.631823
1	4.201353	-7.376720	-1.551202
6	-4.795447	-2.838523	-0.470178
6	-5.927470	-2.790525	-1.298507
6	-4.825128	-3.668798	0.662328
6	-7.057975	-3.554427	-1.004448
1	-5.913624	-2.150780	-2.175981
6	-5.955430	-4.432018	0.956930
1	-3.954726	-3.705832	1.310736
6	-7.075407	-4.377694	0.123715
1	-7.923725	-3.508893	-1.659351
1	-5.962597	-5.066088	1.839365
1	-7.955580	-4.971975	0.352566
6	-3.377481	4.017981	-0.532403
6	-2.940967	4.849777	0.511287
6	-4.526941	4.386657	-1.248856

6	-3.636938	6.014751	0.834995
1	-2.051624	4.570081	1.066458
6	-5.222973	5.552742	-0.926649
1	-4.868329	3.754006	-2.062753
6	-4.781170	6.369726	0.116674
1	-3.287081	6.642661	1.649853
1	-6.108303	5.825049	-1.494594
1	-5.324016	7.276817	0.367126
6	1.997513	0.584007	4.733828
1	1.198572	0.062600	5.266868
1	2.753851	0.859018	5.476108
6	1.439543	1.836650	4.070321
6	0.066124	1.983337	3.840697
6	2.310363	2.821592	3.583485
6	-0.424553	3.067483	3.106448
1	-0.624731	1.235283	4.218060
6	1.823750	3.911425	2.863018
1	3.380009	2.716095	3.745010
6	0.454156	4.030138	2.609118
1	-1.490941	3.147559	2.916429
1	2.514472	4.659081	2.483214
1	0.079686	4.865889	2.025587
17	6.351489	-0.852002	2.204585

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[5]22b

Number of imaginary frequencies : 1
Electronic energy : HF=-3409.686177
Zero-point correction= 0.871285 (Hartree/Particle)
Thermal correction to Energy= 0.927090
Thermal correction to Enthalpy= 0.928034
Thermal correction to Gibbs Free Energy= 0.777703
Sum of electronic and zero-point Energies= -3408.814892
Sum of electronic and thermal Energies= -3408.759087
Sum of electronic and thermal Enthalpies= -3408.758143
Sum of electronic and thermal Free Energies= -3408.908474

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Cartesian Coordinates

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6	0.647721	2.715076	-2.164244
7	-0.397267	2.027432	-1.573301
1	0.937551	4.863100	-2.723930
6	-1.332389	2.978637	-1.226155
6	-0.892234	4.278013	-1.655810
1	-1.453516	5.192119	-1.532889
6	0.315956	4.110313	-2.263029
6	-2.555382	2.732577	-0.587325
7	-2.507352	0.299878	-1.013969
6	-3.451383	-0.698845	-0.890404
6	-4.628688	-0.180735	-0.248282
1	-5.508080	-0.760480	-0.011161
6	-4.390740	1.130756	0.032133
1	-5.041072	1.828667	0.536973

6	-3.090422	1.444864	-0.493489
6	1.897417	2.177114	-2.480035
1	4.260869	-1.737969	-1.886912
6	3.455917	-1.024830	-1.980197
6	2.059882	-1.327492	-1.812735
1	4.433702	0.876793	-2.491364
7	1.311292	-0.169031	-1.945364
6	2.209434	0.831500	-2.262054
6	3.544166	0.298883	-2.290393
6	-3.291808	-2.038581	-1.262960
1	0.113245	-5.059483	-1.999883
6	-0.440269	-4.146357	-1.838570
6	-1.792222	-3.973345	-1.829269
1	-2.555648	-4.721901	-1.977605
6	-2.038896	-2.581279	-1.563278
7	-0.836757	-1.899628	-1.505443
6	0.151484	-2.851457	-1.644211
6	1.532218	-2.612004	-1.654498
6	-1.951233	-2.529718	2.203523
6	-1.168033	-3.158952	3.167502
6	0.132250	-2.681501	3.341031
6	0.613706	-1.615740	2.579822
6	-0.276461	-1.042652	1.620759
1	-2.975719	-2.850564	2.021399
1	-1.553179	-3.987735	3.752254
1	0.794220	-3.142329	4.069716
7	1.043052	0.824362	1.245661
7	1.555435	1.733100	0.671394
26	-0.540733	0.061684	-1.229681
7	0.052050	-0.001418	0.753868
6	2.014027	-1.146760	2.791687
6	2.992445	-1.443361	1.834766
6	2.373177	-0.426673	3.952809
6	4.311593	-1.021695	1.984636
1	2.711502	-1.991564	0.942078
6	3.699022	-0.007721	4.104823
6	4.647580	-0.302177	3.126881
1	5.056706	-1.244003	1.229172
1	3.992460	0.555568	4.984785
7	-1.524589	-1.512358	1.455215
6	2.981709	3.083001	-2.959498
6	3.538566	2.914290	-4.236677
6	3.480157	4.099654	-2.128960
6	4.562422	3.752719	-4.679575
1	3.160102	2.125893	-4.880830
6	4.506493	4.934247	-2.572034
1	3.066243	4.215607	-1.132060
6	5.048062	4.765060	-3.848752
1	4.979161	3.615797	-5.673501
1	4.887890	5.712000	-1.916438
1	5.846694	5.416209	-4.192838
6	2.448306	-3.783201	-1.540005
6	2.416567	-4.574927	-0.379291

6	3.339256	-4.128338	-2.568960
6	3.267485	-5.672194	-0.244678
1	1.726922	-4.317316	0.418802
6	4.186449	-5.228679	-2.434524
1	3.356173	-3.534668	-3.477852
6	4.155571	-6.001371	-1.271118
1	3.237760	-6.267525	0.663449
1	4.866512	-5.485546	-3.241783
1	4.817745	-6.856115	-1.166801
6	-4.491308	-2.924910	-1.232494
6	-5.597591	-2.645179	-2.051635
6	-4.555829	-4.032898	-0.370622
6	-6.733046	-3.455052	-2.016152
1	-5.558121	-1.789915	-2.719592
6	-5.692459	-4.840867	-0.334066
1	-3.711676	-4.249797	0.276023
6	-6.784079	-4.555410	-1.157428
1	-7.576802	-3.227024	-2.661337
1	-5.727218	-5.689654	0.343188
1	-7.669015	-5.184760	-1.128691
6	-3.315209	3.900458	-0.058638
6	-2.723098	4.732723	0.907177
6	-4.605401	4.212893	-0.516899
6	-3.411539	5.833901	1.416198
1	-1.723816	4.498847	1.259513
6	-5.291754	5.316713	-0.009311
1	-5.062329	3.592693	-1.281904
6	-4.699223	6.127832	0.961173
1	-2.941992	6.459975	2.169649
1	-6.287175	5.547012	-0.378502
1	-5.235361	6.985775	1.356732
6	1.350698	-0.068257	5.023147
1	0.909163	-0.983385	5.430870
1	1.877282	0.414476	5.854330
6	0.231454	0.842841	4.540581
6	-1.100483	0.411848	4.550281
6	0.517673	2.125658	4.056200
6	-2.123593	1.235151	4.077315
1	-1.334549	-0.589403	4.900958
6	-0.502429	2.954213	3.589211
1	1.550123	2.462579	4.015850
6	-1.827545	2.510332	3.594018
1	-3.148058	0.873481	4.071691
1	-0.258757	3.942619	3.208520
1	-2.619561	3.149006	3.215379
17	6.311937	0.250242	3.348548

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^{oss}(22b-23b)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3409.6807654
Zero-point correction= 0.869685 (Hartree/Particle)
Thermal correction to Energy= 0.926272

Thermal correction to Enthalpy= 0.927216
Thermal correction to Gibbs Free Energy= 0.775647
Sum of electronic and zero-point Energies= -3408.811080
Sum of electronic and thermal Energies= -3408.754494
Sum of electronic and thermal Enthalpies= -3408.753550
Sum of electronic and thermal Free Energies= -3408.905118

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Cartesian Coordinates

.....

6	2.074066	1.031216	-2.270180
7	0.770371	1.269738	-1.869279
1	3.720539	2.345980	-3.026873
6	0.620392	2.643242	-1.910679
6	1.817784	3.261472	-2.417546
1	1.943519	4.320965	-2.583052
6	2.714337	2.264796	-2.643528
6	-0.503214	3.354943	-1.480691
7	-1.962701	1.375671	-1.230278
6	-3.300501	1.227495	-0.917238
6	-3.887206	2.508290	-0.623576
1	-4.921360	2.668500	-0.357695
6	-2.897415	3.434837	-0.738201
1	-2.964050	4.500410	-0.579246
6	-1.708978	2.732518	-1.148111
6	2.724723	-0.202519	-2.242560
1	1.939414	-4.644069	-1.293141
6	1.802169	-3.589427	-1.478237
6	0.542696	-2.894954	-1.413061
1	3.807869	-2.822197	-1.945876
7	0.725468	-1.549074	-1.680966
6	2.076628	-1.400837	-1.932054
6	2.748577	-2.666886	-1.806543
6	-4.005392	0.024705	-0.892376
1	-3.331108	-4.524958	-0.915139
6	-3.174887	-3.457825	-0.967035
6	-4.107081	-2.469724	-0.944910
1	-5.179264	-2.565222	-0.859887
6	-3.395300	-1.220131	-1.045546
7	-2.039681	-1.447683	-1.168778
6	-1.889165	-2.816460	-1.094312
6	-0.678395	-3.512545	-1.129543
6	-2.656237	-1.527251	2.614441
6	-1.965442	-2.156407	3.648309
6	-0.577456	-2.016802	3.670149
6	0.080885	-1.292166	2.675369
6	-0.721703	-0.698841	1.655281
1	-3.740972	-1.593975	2.547300
1	-2.490525	-2.727948	4.406468
1	0.011131	-2.488199	4.452496
7	1.002670	0.939267	1.164199
7	1.739299	1.631105	0.635281
26	-0.572086	-0.064649	-1.238505
7	-0.178524	0.013847	0.580722

6	1.563400	-1.152646	2.704816
6	2.320414	-1.779650	1.706183
6	2.213927	-0.366039	3.683237
6	3.703304	-1.634869	1.638964
1	1.813460	-2.369363	0.951173
6	3.606009	-0.232700	3.621513
6	4.330220	-0.853740	2.605875
1	4.273354	-2.107884	0.847822
1	4.125293	0.373633	4.356490
7	-2.060898	-0.803375	1.664628
6	4.202349	-0.232257	-2.462822
6	4.762773	-0.842026	-3.594463
6	5.054229	0.336439	-1.502102
6	6.148149	-0.882110	-3.762592
1	4.107563	-1.282489	-4.340417
6	6.438633	0.288642	-1.667819
1	4.621026	0.802695	-0.622232
6	6.988644	-0.319547	-2.799030
1	6.570150	-1.352752	-4.646236
1	7.085190	0.721021	-0.909600
1	8.066640	-0.355913	-2.928721
6	-0.697339	-4.978996	-0.845072
6	-1.036560	-5.436476	0.438380
6	-0.383623	-5.918820	-1.838645
6	-1.056551	-6.802589	0.721410
1	-1.279697	-4.712858	1.210982
6	-0.405960	-7.285149	-1.554830
1	-0.126861	-5.571623	-2.835125
6	-0.741327	-7.730470	-0.274137
1	-1.315846	-7.141590	1.720530
1	-0.165565	-8.001170	-2.335723
1	-0.757831	-8.794084	-0.053712
6	-5.468918	0.062226	-0.582705
6	-6.427337	-0.131662	-1.586681
6	-5.897358	0.280522	0.735693
6	-7.789188	-0.108792	-1.278372
1	-6.100597	-0.300635	-2.608721
6	-7.258616	0.306115	1.042224
1	-5.152940	0.430629	1.512366
6	-8.207817	0.110557	0.035789
1	-8.522224	-0.259101	-2.066064
1	-7.577437	0.475719	2.066995
1	-9.267503	0.129228	0.274320
6	-0.387652	4.837612	-1.350443
6	0.516275	5.380748	-0.421791
6	-1.160260	5.709207	-2.132831
6	0.633802	6.762803	-0.271914
1	1.113263	4.707889	0.185741
6	-1.038410	7.091864	-1.984589
1	-1.852738	5.296763	-2.860627
6	-0.143729	7.622234	-1.052329
1	1.331923	7.167672	0.455617
1	-1.639794	7.754123	-2.601085

1	-0.051163	8.698424	-0.936519
17	6.081691	-0.634786	2.540656
6	1.444462	0.436267	4.728431
1	0.669489	-0.180070	5.190598
1	2.137525	0.724743	5.525744
6	0.808368	1.682050	4.125461
6	1.602612	2.785088	3.786254
6	-0.557012	1.718667	3.814609
6	1.053187	3.883987	3.126053
1	2.665650	2.768129	4.013452
6	-1.108035	2.810796	3.139704
1	-1.188637	0.874142	4.072975
6	-0.303170	3.894608	2.787046
1	1.686440	4.726832	2.862057
1	-2.160785	2.802294	2.872185
1	-0.723760	4.736246	2.245090

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^{3}(22b-23b)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3409.6883048
Zero-point correction= 0.869569 (Hartree/Particle)
Thermal correction to Energy= 0.926198
Thermal correction to Enthalpy= 0.927143
Thermal correction to Gibbs Free Energy= 0.774754
Sum of electronic and zero-point Energies= -3408.818735
Sum of electronic and thermal Energies= -3408.762106
Sum of electronic and thermal Enthalpies= -3408.761162
Sum of electronic and thermal Free Energies= -3408.913551

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Cartesian Coordinates

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6	2.080185	0.954127	-2.260542
7	0.783693	1.225869	-1.859916
1	3.752428	2.223769	-3.041305
6	0.659648	2.600534	-1.927183
6	1.869037	3.186692	-2.446201
1	2.015755	4.240228	-2.631261
6	2.745610	2.168764	-2.654952
6	-0.452908	3.341454	-1.513772
7	-1.957588	1.400963	-1.231904
6	-3.293314	1.284838	-0.905761
6	-3.850727	2.582151	-0.623236
1	-4.878404	2.768022	-0.348952
6	-2.843027	3.485870	-0.761435
1	-2.886353	4.554776	-0.617278
6	-1.672271	2.751610	-1.169497
6	2.701233	-0.296041	-2.226163
1	1.812869	-4.719290	-1.273359
6	1.700796	-3.661781	-1.459403
6	0.457080	-2.937423	-1.400954
1	3.725750	-2.941889	-1.918248
7	0.672574	-1.598146	-1.666281

6	2.026836	-1.479772	-1.912752
6	2.669767	-2.761471	-1.784065
6	-4.022059	0.095540	-0.856374
1	-3.456547	-4.470826	-0.875726
6	-3.273986	-3.408047	-0.931026
6	-4.181286	-2.397228	-0.893511
1	-5.253897	-2.467423	-0.790901
6	-3.442462	-1.164604	-1.006884
7	-2.094451	-1.426794	-1.149358
6	-1.974205	-2.800092	-1.076408
6	-0.780973	-3.525173	-1.119479
6	-2.639211	-1.456895	2.662079
6	-1.943902	-2.093302	3.688744
6	-0.554456	-1.968199	3.696631
6	0.101419	-1.255528	2.691738
6	-0.705563	-0.650430	1.681967
1	-3.725172	-1.512947	2.606336
1	-2.467138	-2.657929	4.453302
1	0.036856	-2.444047	4.474184
7	1.060478	0.974543	1.151073
7	1.788785	1.662634	0.624178
26	-0.610141	-0.088427	-1.236893
7	-0.173452	0.053822	0.596848
6	1.585140	-1.132856	2.703068
6	2.323499	-1.775367	1.699615
6	2.256847	-0.351208	3.671336
6	3.708206	-1.656143	1.622518
1	1.800821	-2.360098	0.951302
6	3.650759	-0.242716	3.598818
6	4.356327	-0.882860	2.582228
1	4.264232	-2.142742	0.829717
1	4.185944	0.357761	4.327124
7	-2.047604	-0.734552	1.708940
6	4.176579	-0.360320	-2.453135
6	4.717600	-1.002078	-3.576768
6	5.046599	0.209888	-1.509617
6	6.100594	-1.072257	-3.753576
1	4.048688	-1.443179	-4.310013
6	6.428659	0.132300	-1.683847
1	4.629186	0.701696	-0.636081
6	6.958783	-0.507820	-2.806840
1	6.506940	-1.567353	-4.631172
1	7.088951	0.566907	-0.938883
1	8.034917	-0.567226	-2.943290
6	-0.833996	-4.991003	-0.835816
6	-1.178307	-5.441339	0.448906
6	-0.544761	-5.937482	-1.830464
6	-1.228093	-6.806699	0.731857
1	-1.401654	-4.712315	1.222547
6	-0.596694	-7.303087	-1.546788
1	-0.283358	-5.595902	-2.827687
6	-0.937520	-7.741182	-0.265052
1	-1.491119	-7.140070	1.731921

1	-0.375042	-8.024149	-2.328599
1	-0.977038	-8.804226	-0.044747
6	-5.479902	0.167910	-0.526154
6	-6.457628	-0.018103	-1.512942
6	-5.883754	0.412657	0.795399
6	-7.813853	0.038180	-1.184699
1	-6.150126	-0.207258	-2.537411
6	-7.239316	0.471722	1.121915
1	-5.124524	0.556676	1.558789
6	-8.207725	0.283620	0.132506
1	-8.561823	-0.106462	-1.959320
1	-7.538775	0.661546	2.148994
1	-9.263027	0.328303	0.386564
6	-0.308374	4.823843	-1.412901
6	0.612906	5.368908	-0.502489
6	-1.071173	5.694369	-2.206265
6	0.757292	6.751223	-0.381241
1	1.202932	4.697632	0.113523
6	-0.922589	7.077146	-2.086813
1	-1.776936	5.280549	-2.920342
6	-0.010509	7.609350	-1.172628
1	1.468770	7.157383	0.332517
1	-1.516667	7.738013	-2.711835
1	0.103107	8.685718	-1.079417
17	6.110996	-0.699334	2.506540
6	1.509839	0.472541	4.715990
1	0.722187	-0.123335	5.183411
1	2.212017	0.749884	5.509162
6	0.901362	1.728158	4.105304
6	1.719141	2.812188	3.760047
6	-0.462181	1.790169	3.789944
6	1.194006	3.916671	3.089374
1	2.780844	2.775687	3.991137
6	-0.988848	2.887645	3.104022
1	-1.112014	0.961637	4.054467
6	-0.161054	3.952049	2.745945
1	1.844848	4.744594	2.821022
1	-2.040585	2.898070	2.832942
1	-0.562861	4.797560	2.195944

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^{5}(22b-23b)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3409.6788874
Zero-point correction= 0.868676 (Hartree/Particle)
Thermal correction to Energy= 0.925918
Thermal correction to Enthalpy= 0.926862
Thermal correction to Gibbs Free Energy= 0.770343
Sum of electronic and zero-point Energies= -3408.810212
Sum of electronic and thermal Energies= -3408.752969
Sum of electronic and thermal Enthalpies= -3408.752025
Sum of electronic and thermal Free Energies= -3408.908544
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Cartesian Coordinates

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6	-0.496732	-2.511134	-2.281781
7	0.538529	-1.807018	-1.694241
1	-0.739012	-4.653132	-2.886002
6	1.520059	-2.735927	-1.415439
6	1.104660	-4.038242	-1.860148
1	1.699662	-4.935742	-1.780603
6	-0.126984	-3.893659	-2.423334
6	2.773448	-2.468295	-0.852644
7	2.601683	-0.012482	-1.085181
6	3.496698	1.017517	-0.885678
6	4.747149	0.496602	-0.399429
1	5.611826	1.094681	-0.154281
6	4.595472	-0.848290	-0.266144
1	5.314778	-1.563656	0.102282
6	3.270185	-1.169487	-0.724607
6	-1.759490	-2.000385	-2.590133
1	-4.277140	1.801606	-1.939057
6	-3.443682	1.121401	-2.025710
6	-2.068979	1.459527	-1.767480
1	-4.328098	-0.782122	-2.675060
7	-1.271508	0.338315	-1.927374
6	-2.118731	-0.673442	-2.336917
6	-3.470012	-0.186148	-2.403069
6	3.233027	2.383980	-1.010810
1	-0.327710	5.289384	-1.399434
6	0.269677	4.392718	-1.329734
6	1.626308	4.291631	-1.265099
1	2.351383	5.091423	-1.265694
6	1.943521	2.890234	-1.196108
7	0.783522	2.142762	-1.271561
6	-0.253092	3.053389	-1.342157
6	-1.613228	2.750005	-1.480056
6	2.466997	1.728605	2.793207
6	1.762929	2.118241	3.931749
6	0.404989	1.799148	3.986874
6	-0.207001	1.100869	2.945442
6	0.616651	0.707205	1.841997
1	3.521708	1.977288	2.681118
1	2.249514	2.668371	4.730403
1	-0.200036	2.127386	4.828083
7	-0.917165	-1.139157	1.253274
7	-1.553254	-1.776930	0.544881
26	0.601660	0.137823	-1.220251
7	0.141806	0.027626	0.745980
6	-1.680860	0.887122	2.954185
6	-2.442245	1.490772	1.942668
6	-2.336720	0.121362	3.943136
6	-3.827768	1.374348	1.893965
1	-1.930213	2.040384	1.161934
6	-3.732512	0.012737	3.901501
6	-4.459866	0.635146	2.890024

1	-4.398016	1.847791	1.103062
1	-4.252268	-0.571882	4.653616
7	1.926288	1.036546	1.790140
6	-2.808785	-2.929737	-3.105175
6	-3.329126	-2.775458	-4.398947
6	-3.306919	-3.958384	-2.289618
6	-4.318973	-3.638357	-4.871875
1	-2.950299	-1.978297	-5.032013
6	-4.298397	-4.818248	-2.762957
1	-2.918221	-4.066244	-1.281580
6	-4.805198	-4.662044	-4.055504
1	-4.708532	-3.511680	-5.878111
1	-4.679360	-5.606196	-2.119302
1	-5.576716	-5.332601	-4.423363
6	-2.598872	3.868494	-1.383243
6	-2.745127	4.580101	-0.180917
6	-3.384663	4.241303	-2.485957
6	-3.665405	5.624152	-0.079502
1	-2.138169	4.306459	0.676268
6	-4.301495	5.287961	-2.384883
1	-3.266664	3.708784	-3.424805
6	-4.447225	5.980261	-1.180448
1	-3.772148	6.156597	0.861294
1	-4.898225	5.565434	-3.249261
1	-5.163229	6.793324	-1.101521
6	4.365571	3.340220	-0.831569
6	5.430255	3.367052	-1.745590
6	4.397685	4.210558	0.270411
6	6.497626	4.248192	-1.566803
1	5.413475	2.694743	-2.598372
6	5.465983	5.089945	0.449099
1	3.583673	4.182694	0.988491
6	6.518196	5.112255	-0.469636
1	7.311656	4.260895	-2.286169
1	5.478754	5.753577	1.309233
1	7.349549	5.797473	-0.330358
6	3.607590	-3.626619	-0.418984
6	3.144855	-4.458234	0.613737
6	4.839641	-3.920413	-1.023567
6	3.902949	-5.547883	1.042203
1	2.190975	-4.233087	1.078805
6	5.595782	-5.013097	-0.596529
1	5.197044	-3.292532	-1.834248
6	5.131457	-5.827807	0.438793
1	3.535441	-6.176336	1.848790
1	6.545311	-5.230926	-1.077422
1	5.721996	-6.676923	0.770995
6	-1.570202	-0.686508	4.981320
1	-0.795647	-0.079545	5.454857
1	-2.263611	-0.986827	5.774409
6	-0.933119	-1.924406	4.366501
6	0.450550	-2.007131	4.173922
6	-1.738413	-2.985401	3.931090

6	1.019054	-3.123604	3.554776
1	1.085336	-1.186059	4.494157
6	-1.175828	-4.102743	3.317063
1	-2.816379	-2.923313	4.057253
6	0.207035	-4.174436	3.125709
1	2.093688	-3.165819	3.400960
1	-1.815189	-4.914940	2.982230
1	0.644154	-5.046501	2.647308
17	-6.218800	0.472931	2.868180

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^{oss}23b

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2011435
Zero-point correction= 0.863475 (Hartree/Particle)
Thermal correction to Energy= 0.917929
Thermal correction to Enthalpy= 0.918873
Thermal correction to Gibbs Free Energy= 0.770398
Sum of electronic and zero-point Energies= -3299.337668
Sum of electronic and thermal Energies= -3299.283215
Sum of electronic and thermal Enthalpies= -3299.282270
Sum of electronic and thermal Free Energies= -3299.430746

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Cartesian Coordinates

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6	2.319262	-2.235186	-1.208110
7	2.269789	-0.850719	-1.144320
1	3.992687	-3.719848	-1.149339
6	3.581286	-0.441627	-0.962905
6	4.460531	-1.581447	-0.972512
1	5.533368	-1.534192	-0.863318
6	3.682041	-2.686552	-1.109477
6	4.012029	0.852442	-0.670041
7	1.768444	1.873491	-0.698793
6	1.319087	3.162381	-0.489741
6	2.409536	4.013048	-0.077894
1	2.322041	5.061890	0.162793
6	3.535164	3.252786	-0.115583
1	4.550418	3.559193	0.086052
6	3.130787	1.922057	-0.499229
6	1.237817	-3.103361	-1.374503
1	-3.261029	-3.006505	-2.399951
6	-2.248836	-2.719050	-2.157982
6	-1.781006	-1.359018	-2.031148
1	-1.152732	-4.605261	-1.905625
7	-0.444736	-1.341023	-1.703888
6	-0.060046	-2.659970	-1.637896
6	-1.184453	-3.526047	-1.907328
6	0.031341	3.623864	-0.767574
1	-3.974479	2.219428	-2.556911
6	-2.968468	2.233758	-2.165567
6	-2.247870	3.307714	-1.743878

1	-2.546065	4.345294	-1.725145
6	-0.962911	2.812344	-1.322953
7	-0.888008	1.445144	-1.523083
6	-2.136454	1.071331	-1.991288
6	-2.588489	-0.233605	-2.203221
26	0.628657	0.230632	-0.998613
6	1.486538	-4.574849	-1.279419
6	1.406435	-5.401795	-2.409738
6	1.796664	-5.151052	-0.037344
6	1.626589	-6.775871	-2.300035
1	1.172064	-4.960895	-3.374220
6	2.013376	-6.525530	0.071662
1	1.851110	-4.516988	0.841947
6	1.928897	-7.341345	-1.059077
1	1.564506	-7.403472	-3.184702
1	2.244991	-6.957445	1.041266
1	2.098291	-8.411079	-0.974180
6	-4.019234	-0.438585	-2.585705
6	-5.041173	-0.178986	-1.659635
6	-4.362212	-0.903225	-3.864032
6	-6.377753	-0.377904	-2.006283
1	-4.780586	0.170586	-0.665928
6	-5.700088	-1.099469	-4.210721
1	-3.574836	-1.106614	-4.584063
6	-6.710801	-0.837369	-3.282850
1	-7.156583	-0.177849	-1.276004
1	-5.952015	-1.455157	-5.205958
1	-7.751787	-0.991773	-3.552722
6	-0.298326	5.059663	-0.504108
6	0.256656	6.083350	-1.286930
6	-1.184453	5.402880	0.528815
6	-0.064275	7.419120	-1.040409
1	0.937706	5.824230	-2.092154
6	-1.504029	6.738682	0.775930
1	-1.618603	4.617830	1.140860
6	-0.944908	7.750325	-0.008104
1	0.370719	8.200024	-1.657890
1	-2.188556	6.988097	1.581849
1	-1.194672	8.790087	0.183255
6	5.473149	1.084386	-0.455850
6	5.966113	1.383402	0.823966
6	6.377759	0.996376	-1.524623
6	7.330502	1.590913	1.029458
1	5.269586	1.452282	1.653813
6	7.742812	1.202662	-1.318504
1	6.003897	0.765727	-2.517911
6	8.223039	1.500570	-0.041301
1	7.696610	1.818479	2.026826
1	8.430204	1.134088	-2.157051
1	9.285458	1.661178	0.118703
6	-1.967666	1.651923	1.740918
6	0.826264	0.251143	1.749407
6	-3.328862	1.785578	1.486489

6	-1.473463	0.728399	2.675029
6	-0.000549	0.626234	2.855217
6	-4.209479	0.962945	2.185201
1	-3.687404	2.496267	0.751431
6	-2.380153	-0.103584	3.367371
6	2.726619	0.348444	3.046607
6	0.632365	0.915376	4.064571
6	-3.751084	0.027176	3.107198
6	2.014905	0.769959	4.173969
1	3.803685	0.198097	3.101494
1	0.041250	1.245540	4.914134
1	-4.458541	-0.619280	3.616285
1	2.530651	0.975467	5.106265
7	2.168183	0.123782	1.859068
7	0.171337	-0.092682	0.590284
1	-1.265827	2.271306	1.197677
6	-1.933060	-1.201702	4.311944
1	-1.005597	-0.911789	4.815318
1	-2.681617	-1.314907	5.103960
6	-1.705644	-2.560489	3.655580
6	-1.804661	-3.718284	4.441322
6	-1.348943	-2.692333	2.307272
6	-1.542331	-4.977747	3.901102
1	-2.087679	-3.630527	5.488284
6	-1.086117	-3.953591	1.766562
1	-1.264816	-1.817607	1.669460
6	-1.177990	-5.099251	2.557804
1	-1.626326	-5.861920	4.527735
1	-0.808322	-4.033868	0.721602
1	-0.969608	-6.076043	2.129893
17	-5.944844	1.104772	1.890110

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^{3}23b

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.217385
Zero-point correction= 0.862425 (Hartree/Particle)
Thermal correction to Energy= 0.916321
Thermal correction to Enthalpy= 0.917265
Thermal correction to Gibbs Free Energy= 0.769995
Sum of electronic and zero-point Energies= -3299.354960
Sum of electronic and thermal Energies= -3299.301064
Sum of electronic and thermal Enthalpies= -3299.300120
Sum of electronic and thermal Free Energies= -3299.447390

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Cartesian Coordinates

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6	-0.388265	-2.799611	-1.468519
7	0.726086	-2.066906	-1.097734
1	-0.807286	-4.997332	-1.614238
6	1.681659	-2.999831	-0.751557
6	1.158451	-4.334191	-0.898322
1	1.715582	-5.239740	-0.709896

6	-0.114482	-4.211003	-1.355820
6	3.004587	-2.724288	-0.405416
7	2.865194	-0.272652	-0.746386
6	3.795512	0.744592	-0.589803
6	5.065778	0.198439	-0.193570
1	5.954979	0.780211	-0.003511
6	4.907290	-1.146938	-0.089203
1	5.641672	-1.881702	0.203834
6	3.542824	-1.439776	-0.431725
6	-1.605006	-2.281352	-1.914706
1	-3.839369	1.726863	-2.290685
6	-3.060577	0.988465	-2.174621
6	-1.691546	1.276678	-1.834498
1	-4.035213	-0.942300	-2.556774
7	-0.962615	0.105522	-1.739839
6	-1.859274	-0.909352	-2.014403
6	-3.159756	-0.361566	-2.308159
6	3.562289	2.113347	-0.728427
1	0.120704	5.082018	-1.499557
6	0.690853	4.178504	-1.343667
6	2.026742	4.054982	-1.130816
1	2.768200	4.837609	-1.074260
6	2.300447	2.644705	-1.002546
7	1.145176	1.913974	-1.175178
6	0.144150	2.843910	-1.371264
6	-1.198377	2.568587	-1.635808
26	0.897913	-0.072630	-0.919420
6	-2.707041	-3.230202	-2.262908
6	-3.168208	-3.333564	-3.584558
6	-3.313056	-4.017203	-1.271410
6	-4.211102	-4.203162	-3.906508
1	-2.703639	-2.728019	-4.357272
6	-4.358658	-4.883451	-1.593283
1	-2.973468	-3.932844	-0.244806
6	-4.810239	-4.979375	-2.911364
1	-4.554387	-4.274626	-4.934791
1	-4.825060	-5.473651	-0.809657
1	-5.624665	-5.653303	-3.161837
6	-2.144101	3.721823	-1.741955
6	-2.487939	4.453253	-0.595629
6	-2.693758	4.095297	-2.977734
6	-3.368530	5.532204	-0.682912
1	-2.071458	4.161714	0.363082
6	-3.571965	5.176483	-3.064053
1	-2.426204	3.535343	-3.869136
6	-3.912034	5.897013	-1.916522
1	-3.635503	6.080201	0.215758
1	-3.987713	5.457130	-4.027817
1	-4.598065	6.736727	-1.983495
6	4.708284	3.055255	-0.539933
6	5.755455	3.101171	-1.472781
6	4.756546	3.906996	0.574377
6	6.825129	3.980130	-1.296524

1	5.724041	2.444850	-2.337575
6	5.826449	4.785505	0.750339
1	3.950963	3.872469	1.301923
6	6.863347	4.824731	-0.184767
1	7.626477	4.006971	-2.029647
1	5.851277	5.436220	1.620010
1	7.695873	5.509019	-0.047776
6	3.870543	-3.860724	0.032711
6	3.627359	-4.481460	1.267726
6	4.926169	-4.325869	-0.765036
6	4.425341	-5.543032	1.696171
1	2.812459	-4.119467	1.887474
6	5.723689	-5.388101	-0.335683
1	5.115676	-3.851914	-1.723721
6	5.475522	-5.999006	0.895650
1	4.228123	-6.012294	2.656082
1	6.535852	-5.740572	-0.965401
1	6.096290	-6.825954	1.228842
6	-1.117795	2.483404	3.252719
6	0.973564	-0.129453	1.956494
6	-2.261052	3.262265	3.089865
6	-1.064573	1.145280	2.829753
6	0.202144	0.397829	3.054845
6	-3.372016	2.676651	2.488246
1	-2.286975	4.295100	3.418975
6	-2.208429	0.565189	2.235006
6	2.604793	-0.904997	3.401149
6	0.727545	0.253837	4.336739
6	-3.354873	1.351035	2.067199
6	1.943888	-0.406082	4.529474
1	3.551302	-1.433843	3.507774
1	0.174797	0.653851	5.182633
1	-4.242909	0.920279	1.619628
1	2.365204	-0.536647	5.520702
7	2.151846	-0.779892	2.157980
7	0.471939	0.055104	0.725349
1	-0.236097	2.925289	3.707504
6	-2.224127	-0.885290	1.769878
1	-1.956723	-0.904305	0.708989
1	-1.430628	-1.431779	2.286106
6	-3.540603	-1.600854	1.987715
6	-3.858897	-2.139751	3.242836
6	-4.469917	-1.732471	0.948168
6	-5.071368	-2.796802	3.451744
1	-3.146646	-2.041873	4.058945
6	-5.685644	-2.390342	1.152595
1	-4.232176	-1.323070	-0.028730
6	-5.989856	-2.924930	2.405187
1	-5.299766	-3.211852	4.429810
1	-6.387369	-2.490866	0.329163
1	-6.933173	-3.439362	2.566525
17	-4.839047	3.632153	2.263020

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^{oss}(23b-24b)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3300.1791151
Zero-point correction= 0.861685 (Hartree/Particle)
Thermal correction to Energy= 0.915377
Thermal correction to Enthalpy= 0.916321
Thermal correction to Gibbs Free Energy= 0.771157
Sum of electronic and zero-point Energies= -3299.317430
Sum of electronic and thermal Energies= -3299.263738
Sum of electronic and thermal Enthalpies= -3299.262794
Sum of electronic and thermal Free Energies= -3299.407958

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Cartesian Coordinates

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6	-0.172202	-2.448308	-1.636880
7	0.976371	-1.732446	-1.384197
1	-0.556083	-4.599496	-2.146499
6	2.015756	-2.635946	-1.448427
6	1.511413	-3.937685	-1.810094
1	2.118162	-4.820125	-1.948400
6	0.158276	-3.827971	-1.900420
6	3.332559	-2.390054	-1.049497
7	2.951886	-0.048642	-0.356426
6	3.701270	0.864171	0.362980
6	4.951672	0.264683	0.758563
1	5.715043	0.749084	1.348367
6	4.987760	-0.979813	0.209249
1	5.787577	-1.702842	0.262840
6	3.725758	-1.187340	-0.454324
6	-1.470493	-1.920283	-1.703023
1	-3.493723	2.169727	-2.433040
6	-2.771464	1.398218	-2.211952
6	-1.367797	1.625088	-1.976521
1	-3.937689	-0.457170	-2.085358
7	-0.740862	0.433259	-1.688924
6	-1.716999	-0.542777	-1.761450
6	-2.995311	0.066514	-2.031683
6	3.368602	2.210198	0.555271
1	0.649181	5.349734	-1.439909
6	1.032805	4.416512	-1.056558
6	2.115098	4.228830	-0.250851
1	2.788430	4.976416	0.141827
6	2.261905	2.807337	-0.067124
7	1.247505	2.140217	-0.719095
6	0.462505	3.117121	-1.311465
6	-0.772743	2.894950	-1.932709
26	1.035618	0.161702	-0.814029
6	-2.608231	-2.882468	-1.773285
6	-3.472690	-2.934400	-2.878597
6	-2.818243	-3.779115	-0.711570
6	-4.527847	-3.847159	-2.913564
1	-3.306032	-2.262820	-3.715048

6	-3.874433	-4.689882	-0.746044
1	-2.150783	-3.748042	0.144467
6	-4.733747	-4.725778	-1.846915
1	-5.184398	-3.876603	-3.778656
1	-4.030383	-5.364129	0.090969
1	-5.556549	-5.434478	-1.874307
6	-1.544106	4.043979	-2.490776
6	-1.963362	5.115206	-1.685130
6	-1.892176	4.050611	-3.851827
6	-2.700074	6.168067	-2.227940
1	-1.730005	5.106874	-0.626240
6	-2.626510	5.105110	-4.394929
1	-1.578004	3.223538	-4.481614
6	-3.031607	6.168171	-3.584727
1	-3.023379	6.983440	-1.586905
1	-2.880472	5.096186	-5.451205
1	-3.605560	6.988417	-4.006536
6	4.273428	3.093132	1.350532
6	5.587099	3.364405	0.935388
6	3.798999	3.700704	2.524068
6	6.408658	4.209112	1.682727
1	5.956061	2.916845	0.017555
6	4.621144	4.544356	3.271901
1	2.781044	3.504291	2.847960
6	5.929204	4.799536	2.854302
1	7.421196	4.411610	1.344954
1	4.239539	5.001070	4.180788
1	6.569360	5.457043	3.435653
6	4.311888	-3.515911	-1.133737
6	4.757359	-4.165199	0.028566
6	4.776790	-3.963717	-2.379100
6	5.653602	-5.231433	-0.053159
1	4.392912	-3.826300	0.993651
6	5.672332	-5.031591	-2.460375
1	4.432373	-3.469445	-3.282869
6	6.113909	-5.667440	-1.298040
1	5.987486	-5.725381	0.855185
1	6.026303	-5.364602	-3.432068
1	6.810735	-6.498441	-1.361683
6	-0.569581	1.116198	1.968631
6	0.542669	-1.125847	1.739069
6	-1.356887	2.180478	1.432746
6	-1.207531	0.091587	2.777771
6	-0.316911	-1.047547	2.901124
6	-2.710799	2.173049	1.673122
1	-0.883520	2.985994	0.889813
6	-2.597757	0.119259	2.982180
6	1.475536	-3.077643	2.501006
6	-0.211424	-2.046534	3.868948
6	-3.340390	1.175742	2.436753
6	0.699315	-3.084208	3.668301
1	2.190019	-3.880966	2.322776
1	-0.807574	-2.003609	4.775027

1	-4.416908	1.197849	2.556909
1	0.824470	-3.872262	4.403449
7	1.431600	-2.129684	1.565593
7	0.324233	-0.162657	0.808921
1	0.447260	1.399470	2.237984
6	-3.347263	-1.003226	3.686411
1	-2.711268	-1.891864	3.718722
1	-3.536227	-0.722904	4.730248
6	-4.653211	-1.375677	3.009647
6	-5.880646	-1.269201	3.671655
6	-4.640420	-1.836305	1.684159
6	-7.071658	-1.618779	3.026965
1	-5.906732	-0.909425	4.697598
6	-5.823989	-2.187458	1.038568
1	-3.695447	-1.909825	1.154290
6	-7.046319	-2.078714	1.710008
1	-8.017021	-1.528418	3.555269
1	-5.788987	-2.549914	0.015419
1	-7.971160	-2.349433	1.208042
17	-3.712081	3.482638	1.037452

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^{3}(23b-24b)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3300.1840309
Zero-point correction= 0.861693 (Hartree/Particle)
Thermal correction to Energy= 0.915229
Thermal correction to Enthalpy= 0.916173
Thermal correction to Gibbs Free Energy= 0.771648
Sum of electronic and zero-point Energies= -3299.322338
Sum of electronic and thermal Energies= -3299.268802
Sum of electronic and thermal Enthalpies= -3299.267858
Sum of electronic and thermal Free Energies= -3299.412382

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Cartesian Coordinates

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6	-0.198175	-2.383086	-1.438669
7	0.989600	-1.728477	-1.209310
1	-0.695151	-4.475647	-2.074153
6	1.989306	-2.665536	-1.378176
6	1.413503	-3.913674	-1.814414
1	1.973179	-4.798787	-2.076624
6	0.061532	-3.752304	-1.808415
6	3.332238	-2.483173	-1.032889
7	3.092154	-0.133225	-0.296762
6	3.894269	0.719637	0.441196
6	5.103611	0.035746	0.825827
1	5.887995	0.455447	1.437441
6	5.060999	-1.200808	0.257616
1	5.799100	-1.986423	0.321972
6	3.797500	-1.309732	-0.425796
6	-1.475354	-1.801151	-1.412363
1	-3.308577	2.383517	-2.104182

6	-2.620435	1.578358	-1.897285
6	-1.203033	1.737109	-1.697726
1	-3.882613	-0.203452	-1.699096
7	-0.630871	0.514552	-1.414865
6	-1.658723	-0.411909	-1.452405
6	-2.910034	0.263448	-1.687218
6	3.631578	2.074301	0.670446
1	1.014470	5.366273	-1.214188
6	1.356593	4.412955	-0.841470
6	2.456336	4.164204	-0.077193
1	3.185591	4.872513	0.287542
6	2.530875	2.734975	0.099433
7	1.458605	2.128831	-0.510860
6	0.707366	3.145338	-1.073236
6	-0.548846	2.979309	-1.671817
26	1.157980	0.146191	-0.616221
6	-2.647842	-2.721150	-1.394131
6	-3.635128	-2.709887	-2.392997
6	-2.767307	-3.650240	-0.343605
6	-4.721894	-3.584031	-2.330032
1	-3.539257	-2.023562	-3.228166
6	-3.852693	-4.524061	-0.283335
1	-2.006055	-3.673382	0.429982
6	-4.837419	-4.489921	-1.273283
1	-5.474237	-3.561932	-3.113460
1	-3.933387	-5.224621	0.542866
1	-5.686771	-5.164844	-1.222929
6	-1.265708	4.155078	-2.245017
6	-1.582450	5.285934	-1.474191
6	-1.661180	4.132061	-3.593478
6	-2.264800	6.364045	-2.037573
1	-1.313707	5.305535	-0.424241
6	-2.342776	5.210847	-4.156994
1	-1.424591	3.261646	-4.198145
6	-2.645761	6.331610	-3.380955
1	-2.508327	7.225569	-1.422103
1	-2.634551	5.175765	-5.202909
1	-3.178134	7.171518	-3.818316
6	4.605835	2.898088	1.444682
6	5.927129	3.080076	1.004811
6	4.194176	3.540825	2.623488
6	6.815912	3.872576	1.731875
1	6.248811	2.605108	0.083006
6	5.083869	4.331558	3.351388
1	3.172017	3.410898	2.966740
6	6.397864	4.498816	2.908386
1	7.833009	4.006736	1.374250
1	4.750421	4.815870	4.264938
1	7.090335	5.115842	3.473960
6	4.292111	-3.614590	-1.195192
6	4.122950	-4.816592	-0.488839
6	5.404823	-3.481320	-2.041001
6	5.036579	-5.860973	-0.633176

1	3.273413	-4.920577	0.178820
6	6.317610	-4.526793	-2.186401
1	5.546432	-2.552972	-2.586539
6	6.135520	-5.720168	-1.484024
1	4.893254	-6.782563	-0.075841
1	7.169393	-4.409303	-2.850483
1	6.846637	-6.533707	-1.596480
6	-0.702791	0.868637	2.099036
6	0.473323	-1.311877	1.774241
6	-1.302724	2.062895	1.592622
6	-1.543629	-0.262060	2.437676
6	-0.725178	-1.453727	2.565235
6	-2.670598	2.098028	1.470358
1	-0.690616	2.927341	1.371244
6	-2.941445	-0.181516	2.294048
6	1.161047	-3.423296	2.341811
6	-0.937230	-2.661143	3.233295
6	-3.494942	1.010546	1.817123
6	0.020968	-3.668822	3.119300
1	1.928087	-4.191807	2.250654
1	-1.820952	-2.810550	3.843747
1	-4.564906	1.094887	1.677717
1	-0.096416	-4.616767	3.633797
7	1.406921	-2.284976	1.692754
7	0.593704	-0.142445	1.082555
1	0.167930	1.043231	2.731465
6	-3.830451	-1.386062	2.582158
1	-3.374943	-2.262088	2.105912
1	-3.818592	-1.584749	3.661019
6	-5.262992	-1.257021	2.113267
6	-6.274900	-0.845570	2.989585
6	-5.595993	-1.516199	0.775849
6	-7.590742	-0.698104	2.543765
1	-6.029356	-0.636638	4.028247
6	-6.909054	-1.371890	0.327903
1	-4.821790	-1.835450	0.086878
6	-7.911588	-0.961224	1.210619
1	-8.363446	-0.378981	3.237910
1	-7.147575	-1.585613	-0.710338
1	-8.934692	-0.849010	0.862636
17	-3.456432	3.572977	0.903538

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^{oss}24b

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2061682
Zero-point correction= 0.862706 (Hartree/Particle)
Thermal correction to Energy= 0.916617
Thermal correction to Enthalpy= 0.917561
Thermal correction to Gibbs Free Energy= 0.770926
Sum of electronic and zero-point Energies= -3299.343462
Sum of electronic and thermal Energies= -3299.289551
Sum of electronic and thermal Enthalpies= -3299.288607

Sum of electronic and thermal Free Energies= -3299.435242

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Cartesian Coordinates

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6	1.321603	1.560640	-2.090716
7	-0.002370	1.617266	-1.721555
1	2.772587	3.099937	-2.836982
6	-0.393632	2.929521	-1.876639
6	0.703852	3.705885	-2.401159
1	0.661062	4.759603	-2.633553
6	1.774539	2.870008	-2.493645
6	-1.593256	3.478809	-1.412342
7	-2.391084	1.412286	-0.318175
6	-3.378533	1.142903	0.609467
6	-4.077548	2.360194	0.941269
1	-4.883406	2.441217	1.654998
6	-3.562207	3.342722	0.151917
1	-3.870734	4.375814	0.098775
6	-2.478891	2.760026	-0.599836
6	2.087623	0.390637	-2.195200
1	1.246217	-4.090644	-2.952691
6	1.149162	-3.055352	-2.661381
6	-0.058596	-2.449998	-2.160015
1	3.161844	-2.205902	-2.892724
7	0.173373	-1.120770	-1.868075
6	1.497223	-0.879720	-2.181555
6	2.121692	-2.100611	-2.623110
6	-3.746728	-0.137388	1.044362
1	-3.533969	-4.417643	-0.648038
6	-3.284824	-3.398312	-0.393989
6	-3.906456	-2.586531	0.506753
1	-4.767254	-2.810335	1.119643
6	-3.251256	-1.304260	0.441276
7	-2.201360	-1.359367	-0.449397
6	-2.196684	-2.645352	-0.965187
6	-1.216200	-3.167323	-1.820469
26	-0.979657	0.142092	-0.862503
6	3.556535	0.537470	-2.409020
6	4.179973	0.162939	-3.609239
6	4.337977	1.097477	-1.384600
6	5.554934	0.334262	-3.777534
1	3.579433	-0.249955	-4.414176
6	5.711790	1.271592	-1.556472
1	3.862812	1.388342	-0.452274
6	6.324542	0.888443	-2.752049
1	6.022659	0.043345	-4.714001
1	6.299917	1.707000	-0.753941
1	7.393952	1.024983	-2.885872
6	-1.317407	-4.583916	-2.281057
6	-1.255460	-5.649860	-1.369244
6	-1.439677	-4.869961	-3.649594
6	-1.326632	-6.969594	-1.816077
1	-1.133168	-5.437477	-0.311933

6	-1.513184	-6.190438	-4.095089
1	-1.480163	-4.050172	-4.360939
6	-1.458437	-7.243665	-3.179464
1	-1.270124	-7.783401	-1.098584
1	-1.614017	-6.395535	-5.157210
1	-1.513605	-8.271592	-3.526543
6	-4.805930	-0.295002	2.085478
6	-6.130841	0.108817	1.855817
6	-4.487104	-0.895301	3.313789
6	-7.107527	-0.068567	2.836543
1	-6.392153	0.552438	0.899876
6	-5.463826	-1.071295	4.294663
1	-3.466583	-1.219127	3.496233
6	-6.776474	-0.656446	4.059596
1	-8.129005	0.245773	2.641418
1	-5.198394	-1.531944	5.242090
1	-7.537392	-0.794194	4.822556
6	-1.839019	4.930994	-1.661326
6	-1.776122	5.862355	-0.612281
6	-2.098657	5.393050	-2.960377
6	-1.978945	7.221103	-0.856009
1	-1.561798	5.511466	0.392698
6	-2.301093	6.752633	-3.203544
1	-2.142233	4.679526	-3.778102
6	-2.243209	7.670077	-2.152232
1	-1.923859	7.929561	-0.034076
1	-2.505601	7.093909	-4.214519
1	-2.400363	8.728127	-2.341928
6	0.272161	-0.961325	1.620787
6	0.469905	1.292099	1.376751
6	0.580595	-2.309066	1.057013
6	1.314481	-0.469169	2.607787
6	1.301030	0.945403	2.507004
6	1.382598	-3.127717	1.776645
1	0.057743	-2.659021	0.186679
6	2.123193	-1.371821	3.314602
6	0.862953	3.517231	1.675595
6	1.942197	1.990713	3.195540
6	2.109040	-2.715358	2.938045
6	1.717900	3.293395	2.769336
1	0.670340	4.534816	1.338000
1	2.602859	1.792078	4.029782
1	2.734775	-3.434591	3.454488
1	2.188927	4.133484	3.269235
7	0.243579	2.556180	0.989937
7	-0.022493	0.188609	0.733197
1	-0.674720	-1.099969	2.192432
6	3.128700	-0.909358	4.346746
1	2.659000	-0.209941	5.047693
1	3.435363	-1.774446	4.948375
6	4.379217	-0.260239	3.758256
6	5.135896	0.622620	4.542201
6	4.812343	-0.534808	2.455082

6	6.296358	1.213844	4.040838
1	4.809586	0.850850	5.554757
6	5.974448	0.053561	1.951078
1	4.234878	-1.204069	1.825303
6	6.720609	0.930719	2.740249
1	6.865824	1.898177	4.664073
1	6.287654	-0.170899	0.935813
1	7.622461	1.391191	2.346197
17	1.612820	-4.802996	1.236843

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^{3}24b

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2179526
Zero-point correction= 0.863252 (Hartree/Particle)
Thermal correction to Energy= 0.917247
Thermal correction to Enthalpy= 0.918191
Thermal correction to Gibbs Free Energy= 0.772726
Sum of electronic and zero-point Energies= -3299.354700
Sum of electronic and thermal Energies= -3299.300706
Sum of electronic and thermal Enthalpies= -3299.299762
Sum of electronic and thermal Free Energies= -3299.445226

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Cartesian Coordinates

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6	-0.301552	-2.302463	-1.383920
7	0.919436	-1.730165	-1.112409
1	-0.913286	-4.363619	-2.037243
6	1.860534	-2.730638	-1.261222
6	1.215393	-3.943211	-1.705351
1	1.719333	-4.866524	-1.947810
6	-0.121380	-3.689138	-1.746954
6	3.215359	-2.625189	-0.918413
7	3.155267	-0.241487	-0.258335
6	4.037700	0.586438	0.401260
6	5.212014	-0.161536	0.788040
1	6.041971	0.230840	1.356355
6	5.062630	-1.420009	0.293050
1	5.742895	-2.253621	0.384333
6	3.772838	-1.466781	-0.354190
6	-1.543041	-1.639693	-1.397297
1	-3.177905	2.647046	-1.967712
6	-2.527446	1.807353	-1.777170
6	-1.105767	1.895035	-1.559892
1	-3.869591	0.080895	-1.659110
7	-0.595716	0.639250	-1.288850
6	-1.658600	-0.239835	-1.384781
6	-2.876586	0.500793	-1.617429
6	3.873616	1.967761	0.577458
1	1.303436	5.408475	-1.114499
6	1.629045	4.433027	-0.786464
6	2.769970	4.119155	-0.112030
1	3.554178	4.788724	0.209498

6	2.785777	2.685557	0.051082
7	1.645288	2.140194	-0.493080
6	0.907662	3.199657	-0.990532
6	-0.387818	3.101455	-1.522140
26	1.257974	0.190501	-0.687207
6	-2.772813	-2.479460	-1.499871
6	-3.697481	-2.334810	-2.548337
6	-3.021175	-3.466299	-0.528384
6	-4.846012	-3.126509	-2.604015
1	-3.504333	-1.607190	-3.329826
6	-4.166464	-4.260602	-0.586178
1	-2.303111	-3.602733	0.272506
6	-5.089072	-4.087889	-1.620401
1	-5.546469	-2.997802	-3.424507
1	-4.341096	-5.009396	0.181538
1	-5.985553	-4.699518	-1.662445
6	-1.073154	4.333067	-2.015802
6	-1.330929	5.424173	-1.169601
6	-1.496199	4.409469	-3.353209
6	-1.985058	6.559590	-1.648158
1	-1.029899	5.369803	-0.129100
6	-2.150858	5.544741	-3.832193
1	-1.304040	3.570919	-4.015936
6	-2.396796	6.624460	-2.981317
1	-2.180836	7.390232	-0.975649
1	-2.465654	5.586061	-4.871281
1	-2.907225	7.508441	-3.353233
6	4.941382	2.746694	1.272413
6	6.246557	2.821797	0.759048
6	4.643054	3.447574	2.452499
6	7.227776	3.567584	1.413295
1	6.483364	2.298123	-0.162112
6	5.624362	4.192540	3.107319
1	3.635400	3.397950	2.854380
6	6.920472	4.254012	2.590360
1	8.230897	3.618032	0.998856
1	5.376586	4.722970	4.022671
1	7.684795	4.834626	3.099269
6	4.103813	-3.814887	-1.078311
6	3.856327	-5.013389	-0.388976
6	5.231518	-3.744873	-1.913149
6	4.706183	-6.110227	-0.534092
1	2.992875	-5.076029	0.265114
6	6.081581	-4.841576	-2.059422
1	5.434785	-2.822260	-2.448605
6	5.821588	-6.028562	-1.370798
1	4.500276	-7.026768	0.012098
1	6.945602	-4.769040	-2.714169
1	6.484020	-6.882201	-1.483409
6	-0.741697	0.444348	2.101751
6	0.354485	-1.446176	1.999093
6	-1.218096	1.732806	1.551504
6	-1.765220	-0.642286	2.298675

6	-1.019600	-1.817651	2.356768
6	-2.548738	1.966541	1.613238
1	-0.494507	2.474407	1.241436
6	-3.154367	-0.330538	2.294110
6	1.048799	-3.602857	2.193019
6	-1.296281	-3.179681	2.655268
6	-3.511404	0.959417	1.971296
6	-0.259153	-4.071041	2.557637
1	1.858844	-4.330088	2.140424
1	-2.285887	-3.503211	2.959460
1	-4.560543	1.227268	1.927136
1	-0.398445	-5.125165	2.772961
7	1.374740	-2.360891	1.932433
7	0.521397	-0.159604	1.730081
1	-0.536595	0.754593	3.158541
6	-4.189835	-1.425302	2.501661
1	-3.836130	-2.315188	1.970417
1	-4.221555	-1.692249	3.566171
6	-5.576568	-1.088045	2.000560
6	-6.569430	-0.614134	2.865817
6	-5.872488	-1.213900	0.634860
6	-7.834819	-0.273733	2.379780
1	-6.350777	-0.510551	3.926073
6	-7.134925	-0.876915	0.148139
1	-5.110541	-1.582382	-0.044834
6	-8.120365	-0.404078	1.019510
1	-8.595658	0.091349	3.064184
1	-7.348538	-0.988448	-0.911297
1	-9.104178	-0.141322	0.640932
17	-3.188388	3.549040	1.172696

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^{oss}25b

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2090982
Zero-point correction= 0.862275 (Hartree/Particle)
Thermal correction to Energy= 0.916735
Thermal correction to Enthalpy= 0.917679
Thermal correction to Gibbs Free Energy= 0.768952
Sum of electronic and zero-point Energies= -3299.346823
Sum of electronic and thermal Energies= -3299.292363
Sum of electronic and thermal Enthalpies= -3299.291419
Sum of electronic and thermal Free Energies= -3299.440146

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Cartesian Coordinates

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6	-4.055867	-0.468816	0.059017
7	-2.913658	-0.864530	-0.596241
1	-5.960307	-1.529962	0.612329
6	-3.076605	-2.203825	-0.865983
6	-4.374796	-2.649723	-0.411214
1	-4.759567	-3.653448	-0.514017
6	-4.979297	-1.577619	0.163417

6	-2.093116	-3.066015	-1.369959
7	-0.329290	-1.364584	-1.683225
6	0.994167	-1.428351	-2.059753
6	1.377619	-2.802781	-2.290299
1	2.362301	-3.136456	-2.581669
6	0.262091	-3.560193	-2.105765
1	0.161101	-4.629255	-2.220574
6	-0.796094	-2.661180	-1.707768
6	-4.310626	0.811615	0.570585
1	-2.651870	5.123041	0.459892
6	-2.770339	4.058420	0.323677
6	-1.868810	3.208023	-0.418283
1	-4.597938	3.544423	1.425262
7	-2.301447	1.901575	-0.366588
6	-3.475903	1.917584	0.353414
6	-3.755768	3.257922	0.813276
6	1.842102	-0.320663	-2.241780
1	1.718279	4.291238	-2.477312
6	1.461030	3.261672	-2.279063
6	2.197200	2.150909	-2.551694
1	3.168451	2.095933	-3.020976
6	1.414374	1.013398	-2.129090
7	0.213899	1.431914	-1.597605
6	0.239906	2.813970	-1.648867
6	-0.709728	3.665043	-1.068848
26	-1.280836	0.250822	-0.909234
6	-5.553514	1.004316	1.378411
6	-6.602860	1.816347	0.920668
6	-5.691006	0.360068	2.618625
6	-7.758490	1.983695	1.685277
1	-6.507576	2.311961	-0.040885
6	-6.846064	0.528202	3.383169
1	-4.882314	-0.271242	2.974987
6	-7.883163	1.340941	2.919060
1	-8.563228	2.612414	1.314176
1	-6.934639	0.026307	4.342828
1	-8.782815	1.471522	3.513993
6	-0.458354	5.138676	-1.099379
6	0.642531	5.693947	-0.427074
6	-1.327290	5.997577	-1.791099
6	0.869360	7.070495	-0.448431
1	1.318731	5.039866	0.115410
6	-1.099564	7.374170	-1.813530
1	-2.181530	5.576709	-2.313144
6	-0.000564	7.914944	-1.142118
1	1.723855	7.482726	0.081161
1	-1.779457	8.023458	-2.358247
1	0.176303	8.986743	-1.158883
6	3.278239	-0.559452	-2.581550
6	3.664790	-1.159806	-3.789872
6	4.278474	-0.174124	-1.673068
6	5.013505	-1.379549	-4.075928
1	2.901001	-1.448936	-4.505473

6	5.626589	-0.394271	-1.957774
1	3.992128	0.299819	-0.739178
6	5.998124	-1.000701	-3.160267
1	5.294554	-1.842403	-5.017859
1	6.381230	-0.095779	-1.235848
1	7.047142	-1.172934	-3.384404
6	-2.423992	-4.522458	-1.466343
6	-1.874184	-5.434312	-0.551594
6	-3.296638	-5.000813	-2.454586
6	-2.187267	-6.792322	-0.625598
1	-1.201074	-5.067993	0.218172
6	-3.611614	-6.359015	-2.527457
1	-3.726860	-4.300904	-3.165018
6	-3.057547	-7.258553	-1.613878
1	-1.754705	-7.485586	0.090775
1	-4.287485	-6.714269	-3.300454
1	-3.302348	-8.315458	-1.671545
6	1.063618	0.167126	1.090566
6	-0.438910	-1.316772	1.706202
6	1.518707	1.581019	1.169742
6	1.768906	-0.793212	1.987127
6	0.822219	-1.756235	2.312475
6	2.795807	1.767627	1.568338
1	0.885875	2.374111	0.797972
6	3.146837	-0.565216	2.292674
6	-1.535534	-3.121011	2.550727
6	0.832050	-2.966320	3.059063
6	3.636359	0.697053	2.053770
6	-0.352480	-3.645784	3.173738
1	-2.468337	-3.673089	2.663378
1	1.740720	-3.329645	3.526917
1	4.675131	0.921178	2.267947
1	-0.421162	-4.571903	3.734564
7	-1.605236	-2.021104	1.839553
7	-0.330415	-0.194731	1.001874
1	1.461813	-0.134224	0.086653
6	3.996951	-1.670963	2.898298
1	3.742528	-1.771818	3.961834
1	3.707209	-2.616134	2.424513
6	5.487440	-1.466278	2.734698
6	6.283413	-1.024395	3.797475
6	6.087172	-1.679060	1.484198
6	7.652500	-0.805356	3.619720
1	5.829366	-0.849880	4.769888
6	7.452648	-1.461614	1.304090
1	5.477153	-2.004542	0.645538
6	8.240381	-1.023768	2.373112
1	8.257008	-0.464263	4.455497
1	7.901550	-1.636248	0.330179
1	9.304343	-0.854690	2.233900
17	3.507382	3.382534	1.530189

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^{CSS}25b

Number of imaginary frequencies : 0
Electronic energy : HF=-1263.4379502
Zero-point correction= 0.262786 (Hartree/Particle)
Thermal correction to Energy= 0.278847
Thermal correction to Enthalpy= 0.279791
Thermal correction to Gibbs Free Energy= 0.217382
Sum of electronic and zero-point Energies= -1263.175164
Sum of electronic and thermal Energies= -1263.159103
Sum of electronic and thermal Enthalpies= -1263.158159
Sum of electronic and thermal Free Energies= -1263.220568

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Cartesian Coordinates

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6	3.705151	-2.660603	-0.356862
6	4.827262	-1.754819	-0.292175
6	3.498395	0.049059	0.107896
6	2.284862	-0.790627	0.058615
6	2.434855	-2.189229	-0.175647
1	3.895922	-3.712386	-0.543272
1	5.824374	-2.171561	-0.440407
1	1.577756	-2.853356	-0.208396
6	1.847599	1.407481	0.540962
6	1.051726	2.598593	0.124084
6	-0.276658	2.417439	-0.027484
6	-0.921538	1.122343	0.038448
6	-0.206811	-0.042198	0.151108
6	1.219102	0.071821	0.245511
1	1.527752	3.570622	0.073537
1	-2.000137	1.087410	-0.059554
7	4.767129	-0.470015	-0.062009
7	3.274468	1.323523	0.325067
1	1.791004	1.474802	1.655591
6	-0.850119	-1.416766	0.067349
1	-0.464340	-1.910502	-0.834597
1	-0.489103	-2.015392	0.913213
6	-2.361750	-1.422489	0.043059
6	-3.058718	-1.385983	-1.171812
6	-3.092230	-1.421289	1.239012
6	-4.454415	-1.354935	-1.192485
1	-2.502659	-1.380422	-2.106206
6	-4.487385	-1.391016	1.222283
1	-2.561778	-1.443749	2.187964
6	-5.172444	-1.357791	0.005298
1	-4.980028	-1.329762	-2.142936
1	-5.039146	-1.394647	2.158179
1	-6.258412	-1.335468	-0.009181
17	-1.325510	3.797994	-0.367547

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^{oss}25b

Number of imaginary frequencies : 1
Electronic energy : HF=-3300.1882584

Zero-point correction= 0.859385 (Hartree/Particle)
Thermal correction to Energy= 0.913605
Thermal correction to Enthalpy= 0.914549
Thermal correction to Gibbs Free Energy= 0.766492
Sum of electronic and zero-point Energies= -3299.328873
Sum of electronic and thermal Energies= -3299.274654
Sum of electronic and thermal Enthalpies= -3299.273710
Sum of electronic and thermal Free Energies= -3299.421766

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Cartesian Coordinates

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6	-4.106739	-0.277815	0.277005
7	-3.033962	-0.752163	-0.440717
1	-6.039062	-1.208707	0.951775
6	-3.307907	-2.074984	-0.706971
6	-4.605471	-2.429005	-0.176340
1	-5.065623	-3.402591	-0.256340
6	-5.094561	-1.321628	0.440595
6	-2.422121	-3.000692	-1.274192
7	-0.539156	-1.435969	-1.610369
6	0.776639	-1.598371	-1.994357
6	1.052847	-2.997892	-2.222009
1	2.009102	-3.406856	-2.511742
6	-0.119044	-3.666762	-2.043668
1	-0.300634	-4.724418	-2.162857
6	-1.104003	-2.692989	-1.635671
6	-4.257677	1.028165	0.765658
1	-2.392077	5.238526	0.374163
6	-2.571367	4.176895	0.291576
6	-1.756652	3.251795	-0.459919
1	-4.349948	3.803445	1.522366
7	-2.251565	1.972405	-0.326779
6	-3.379145	2.078096	0.458307
6	-3.562630	3.448789	0.874163
6	1.694604	-0.555712	-2.208655
1	1.829593	4.041402	-2.652692
6	1.516672	3.038615	-2.404026
6	2.190435	1.876579	-2.623822
1	3.155038	1.747071	-3.091850
6	1.351132	0.805725	-2.143858
7	0.179425	1.316817	-1.628235
6	0.281123	2.691381	-1.741999
6	-0.607420	3.618536	-1.179853
26	-1.370080	0.259933	-0.888412
6	-5.445020	1.317909	1.626419
6	-6.467725	2.175129	1.190390
6	-5.560976	0.720226	2.891764
6	-7.574542	2.432548	2.000578
1	-6.390653	2.634409	0.209384
6	-6.667556	0.978036	3.701892
1	-4.774486	0.054009	3.233858
6	-7.677411	1.835518	3.259122
1	-8.358888	3.095425	1.645648

1	-6.739064	0.510870	4.680278
1	-8.539120	2.036159	3.889616
6	-0.291607	5.075166	-1.298044
6	0.855743	5.616222	-0.695595
6	-1.150009	5.934118	-2.002815
6	1.138774	6.978564	-0.798970
1	1.523793	4.963300	-0.142001
6	-0.866182	7.296432	-2.107123
1	-2.040551	5.524540	-2.470363
6	0.279192	7.822896	-1.505527
1	2.028833	7.380129	-0.322465
1	-1.538953	7.945587	-2.660731
1	0.499617	8.883678	-1.585821
6	3.112077	-0.889199	-2.545807
6	3.457727	-1.554116	-3.732598
6	4.137411	-0.515653	-1.660760
6	4.791817	-1.848177	-4.020342
1	2.674855	-1.831685	-4.431981
6	5.471023	-0.807890	-1.948944
1	3.882667	0.007252	-0.744486
6	5.801953	-1.478322	-3.129143
1	5.041832	-2.359916	-4.945605
1	6.246130	-0.513229	-1.247478
1	6.839823	-1.706031	-3.355747
6	-2.885575	-4.416782	-1.412676
6	-2.374264	-5.422477	-0.577230
6	-3.853988	-4.761739	-2.367353
6	-2.817010	-6.740554	-0.696861
1	-1.629102	-5.160202	0.167691
6	-4.298528	-6.079773	-2.485762
1	-4.256398	-3.989159	-3.016091
6	-3.780969	-7.073183	-1.651548
1	-2.412460	-7.506619	-0.040838
1	-5.047278	-6.330255	-3.232166
1	-4.126976	-8.098833	-1.744111
6	1.190437	0.266362	1.306813
6	-0.235178	-1.386598	1.733527
6	1.713878	1.578646	1.086544
6	1.942875	-0.726907	2.040182
6	1.019855	-1.773085	2.317146
6	3.037887	1.750661	1.396382
1	1.107352	2.352435	0.638909
6	3.318183	-0.506704	2.300512
6	-1.259689	-3.286734	2.411253
6	1.078260	-3.015418	2.983581
6	3.846223	0.729421	1.962315
6	-0.078657	-3.769638	3.029871
1	-2.168331	-3.884791	2.451977
1	1.989833	-3.363237	3.456459
1	4.896859	0.932112	2.131464
1	-0.098451	-4.728607	3.537364
7	-1.352704	-2.136867	1.761024
7	-0.190411	-0.163340	1.110511

1	0.930938	-0.219025	0.219071
6	4.166181	-1.602689	2.927702
1	3.927903	-1.666153	3.997748
1	3.857414	-2.558513	2.489616
6	5.656869	-1.432209	2.733454
6	6.466563	-0.895872	3.741213
6	6.244174	-1.775705	1.506812
6	7.835602	-0.708208	3.531603
1	6.022328	-0.621518	4.694974
6	7.609989	-1.589950	1.294629
1	5.623793	-2.180627	0.711561
6	8.410616	-1.054379	2.307883
1	8.450580	-0.292037	4.324652
1	8.049447	-1.865900	0.339930
1	9.474697	-0.909815	2.144106
17	3.796674	3.308600	1.072042

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^{CSS}(25b-8b)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-1263.4233937
Zero-point correction= 0.259762 (Hartree/Particle)
Thermal correction to Energy= 0.275606
Thermal correction to Enthalpy= 0.276551
Thermal correction to Gibbs Free Energy= 0.214372
Sum of electronic and zero-point Energies= -1263.163631
Sum of electronic and thermal Energies= -1263.147787
Sum of electronic and thermal Enthalpies= -1263.146843
Sum of electronic and thermal Free Energies= -1263.209022

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Cartesian Coordinates

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6	3.761462	-2.654133	-0.143434
6	4.864548	-1.755778	-0.101461
6	3.504261	0.050427	0.025167
6	2.312114	-0.764276	0.003496
6	2.473201	-2.166961	-0.080221
1	3.951574	-3.720185	-0.215574
1	5.874532	-2.161603	-0.146047
1	1.622052	-2.838561	-0.098107
6	1.805175	1.449956	0.186451
6	0.992172	2.625860	0.011431
6	-0.360183	2.423298	-0.017674
6	-0.962165	1.133186	0.022464
6	-0.198882	-0.019596	0.062179
6	1.213289	0.124361	0.094608
1	1.441594	3.610679	-0.024529
1	-2.042867	1.065831	-0.002407
7	4.767333	-0.442423	-0.001489
7	3.257807	1.385394	0.080164
1	2.370137	1.584336	1.235469
6	-0.814642	-1.409400	0.025049
1	-0.427707	-1.924134	-0.864179

1	-0.433659	-1.973892	0.885908
6	-2.325912	-1.449716	0.017449
6	-3.035023	-1.438465	-1.190958
6	-3.045202	-1.455559	1.220031
6	-4.430994	-1.438981	-1.198807
1	-2.487772	-1.427179	-2.130472
6	-4.440993	-1.456229	1.216280
1	-2.505745	-1.458074	2.164164
6	-5.137849	-1.447990	0.005727
1	-4.965819	-1.433091	-2.144456
1	-4.983841	-1.464082	2.157360
1	-6.224155	-1.449545	0.001223
17	-1.435916	3.816981	-0.136221

8b

Number of imaginary frequencies : 0
Electronic energy : HF=-1263.5344898
Zero-point correction= 0.265476 (Hartree/Particle)
Thermal correction to Energy= 0.281455
Thermal correction to Enthalpy= 0.282399
Thermal correction to Gibbs Free Energy= 0.220255
Sum of electronic and zero-point Energies= -1263.269014
Sum of electronic and thermal Energies= -1263.253035
Sum of electronic and thermal Enthalpies= -1263.252091
Sum of electronic and thermal Free Energies= -1263.314234

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Cartesian Coordinates

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6	3.780880	-2.667428	-0.000065
6	4.866177	-1.780532	-0.000342
6	3.497239	0.005177	-0.000197
6	2.306061	-0.782679	0.000089
6	2.475764	-2.169868	0.000175
1	3.963824	-3.736873	-0.000027
1	5.883293	-2.166768	-0.000559
1	1.629155	-2.847382	0.000486
6	1.767688	1.450998	0.000019
6	0.991181	2.611294	-0.000016
6	-0.384891	2.422784	0.000244
6	-0.987152	1.155008	0.000469
6	-0.205369	-0.000201	0.000472
6	1.195726	0.148156	0.000255
1	1.431669	3.601364	-0.000082
1	-2.067322	1.081051	0.000614
7	4.747971	-0.443709	-0.000407
7	3.145455	1.338026	-0.000212
1	3.806781	2.100440	-0.000344
6	-0.814429	-1.394342	0.000766
1	-0.428341	-1.933499	-0.874220
1	-0.428917	-1.932837	0.876413
6	-2.325393	-1.446044	0.000248
6	-3.039778	-1.449549	-1.205227

6	-3.040664	-1.451004	1.205153
6	-4.435599	-1.463963	-1.207999
1	-2.496025	-1.438651	-2.146800
6	-4.436513	-1.465425	1.206863
1	-2.497637	-1.441240	2.147157
6	-5.138158	-1.472199	-0.000824
1	-4.973951	-1.469443	-2.151747
1	-4.975551	-1.472042	2.150212
1	-6.224458	-1.484604	-0.001243
17	-1.430184	3.845834	0.000233

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^{oss}22a

Number of imaginary frequencies : 0
Electronic energy : HF=-3409.7105326
Zero-point correction= 0.873197 (Hartree/Particle)
Thermal correction to Energy= 0.930040
Thermal correction to Enthalpy= 0.930985
Thermal correction to Gibbs Free Energy= 0.777743
Sum of electronic and zero-point Energies= -3408.837335
Sum of electronic and thermal Energies= -3408.780492
Sum of electronic and thermal Enthalpies= -3408.779548
Sum of electronic and thermal Free Energies= -3408.932790

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Cartesian Coordinates

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6	1.903651	2.505907	-1.413362
7	0.540831	2.378101	-1.232808
1	3.294815	4.264198	-1.454846
6	0.069303	3.653371	-1.001033
6	1.152336	4.605030	-1.098007
1	1.051220	5.674814	-0.993271
6	2.287712	3.893513	-1.332713
6	-1.245644	3.985572	-0.645301
7	-2.205684	1.704757	-0.818945
6	-3.442439	1.176526	-0.514051
6	-4.302815	2.206168	0.016705
1	-5.313523	2.056190	0.364699
6	-3.590640	3.364025	0.002563
1	-3.908054	4.340803	0.335848
6	-2.281835	3.048163	-0.520074
6	2.805303	1.456553	-1.621886
1	2.912480	-3.035059	-2.664671
6	2.571901	-2.045373	-2.399076
6	1.192589	-1.666864	-2.207016
1	4.402451	-0.846272	-2.193425
7	1.112198	-0.334962	-1.853571
6	2.413454	0.132229	-1.846016
6	3.327243	-0.938971	-2.155344
6	-3.822976	-0.161640	-0.679296
1	-2.254584	-4.155513	-2.379091
6	-2.307013	-3.144469	-2.004196
6	-3.396791	-2.487402	-1.523870

1	-4.408444	-2.855261	-1.441488
6	-2.966108	-1.155305	-1.172189
7	-1.616976	-1.010323	-1.433499
6	-1.194881	-2.228708	-1.932164
6	0.118797	-2.564378	-2.282713
6	-2.692386	-0.691601	3.205134
6	-2.046028	-1.357788	4.244968
6	-0.652716	-1.351185	4.265927
6	0.057932	-0.677312	3.268593
6	-0.713982	0.017741	2.311446
1	-3.776304	-0.695882	3.123264
1	-2.616427	-1.888343	4.999807
1	-0.103847	-1.899480	5.025372
7	0.870536	1.474729	1.533587
7	1.750906	2.183901	1.641839
26	-0.533463	0.675878	-1.262087
7	-0.109129	0.764369	1.245729
6	1.544772	-0.716379	3.198989
6	2.301177	-0.062974	4.179128
6	2.198408	-1.369775	2.129070
6	3.692376	-0.008913	4.106839
1	1.790004	0.437437	4.996467
6	3.593628	-1.305837	2.053727
6	4.321109	-0.623704	3.027639
1	4.271024	0.511576	4.861483
1	4.110852	-1.782045	1.227706
7	-2.039642	-0.009681	2.256376
6	4.268781	1.765907	-1.580560
6	5.049548	1.776755	-2.745381
6	4.883007	2.036406	-0.347756
6	6.417231	2.049644	-2.678937
1	4.578188	1.570570	-3.702016
6	6.250967	2.303820	-0.281620
1	4.282359	2.025830	0.556850
6	7.021257	2.311546	-1.446970
1	7.009867	2.058006	-3.589591
1	6.714205	2.499906	0.681265
1	8.086285	2.520001	-1.395555
6	0.406560	-3.967603	-2.712413
6	0.261488	-5.034825	-1.811104
6	0.844276	-4.240631	-4.017944
6	0.546619	-6.341696	-2.208250
1	-0.070590	-4.831577	-0.798380
6	1.127847	-5.548502	-4.414204
1	0.958463	-3.420239	-4.720514
6	0.980407	-6.603106	-3.510054
1	0.433671	-7.154535	-1.496008
1	1.461061	-5.743071	-5.429908
1	1.201995	-7.621141	-3.818106
6	-5.213518	-0.561981	-0.310144
6	-6.330085	-0.017809	-0.964336
6	-5.427319	-1.506670	0.707932
6	-7.623276	-0.400078	-0.604520

1	-6.176593	0.704142	-1.760726
6	-6.719772	-1.888685	1.068245
1	-4.568336	-1.935670	1.213987
6	-7.822806	-1.334933	0.413800
1	-8.475096	0.028995	-1.124859
1	-6.865180	-2.617305	1.861207
1	-8.829837	-1.631613	0.693127
6	-1.552928	5.415042	-0.332715
6	-0.964473	6.049232	0.773292
6	-2.443611	6.147403	-1.133277
6	-1.256618	7.381176	1.069014
1	-0.277711	5.487770	1.399935
6	-2.735264	7.479866	-0.838143
1	-2.903675	5.664426	-1.990300
6	-2.142571	8.100782	0.263680
1	-0.795041	7.855162	1.930874
1	-3.422940	8.033499	-1.471462
1	-2.369714	9.138022	0.493430
17	6.075641	-0.537647	2.883705
6	1.427536	-2.122341	1.060346
1	0.802384	-1.422220	0.502377
1	2.143282	-2.516730	0.333235
6	0.564852	-3.261166	1.575618
6	1.134733	-4.316263	2.300827
6	-0.809531	-3.293608	1.308538
6	0.350316	-5.381442	2.744935
1	2.200103	-4.299514	2.517850
6	-1.596457	-4.361011	1.746535
1	-1.265178	-2.479106	0.756369
6	-1.019523	-5.408875	2.466467
1	0.808522	-6.193089	3.303847
1	-2.658428	-4.371457	1.517848
1	-1.629511	-6.240728	2.807757

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^{3}22a

Number of imaginary frequencies : 0
Electronic energy : HF=-3409.7265602
Zero-point correction= 0.873450 (Hartree/Particle)
Thermal correction to Energy= 0.930287
Thermal correction to Enthalpy= 0.931231
Thermal correction to Gibbs Free Energy= 0.777398
Sum of electronic and zero-point Energies= -3408.853110
Sum of electronic and thermal Energies= -3408.796273
Sum of electronic and thermal Enthalpies= -3408.795329
Sum of electronic and thermal Free Energies= -3408.949162

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Cartesian Coordinates

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6	0.936741	3.148657	-1.254936
7	-0.303424	2.547996	-1.143651
1	1.634838	5.275822	-1.116440
6	-1.194067	3.568245	-0.878962

6	-0.504505	4.836903	-0.880331
1	-0.972095	5.798018	-0.728133
6	0.814881	4.574213	-1.080717
6	-2.549308	3.409067	-0.558411
7	-2.641082	0.944142	-0.813714
6	-3.611284	0.003941	-0.532692
6	-4.781728	0.647206	0.012143
1	-5.674359	0.139135	0.344018
6	-4.529005	1.982552	0.025137
1	-5.173681	2.775949	0.372757
6	-3.190396	2.164853	-0.484606
6	2.149297	2.479734	-1.455442
1	3.809033	-1.619694	-2.746655
6	3.144425	-0.831066	-2.426900
6	1.716837	-0.964715	-2.263222
1	4.441540	0.915139	-2.105303
7	1.176952	0.231251	-1.834197
6	2.237237	1.115105	-1.748072
6	3.467239	0.449441	-2.096105
6	-3.497367	-1.374404	-0.747796
1	-0.662031	-4.472034	-2.657125
6	-1.060060	-3.562248	-2.233925
6	-2.304098	-3.352857	-1.724803
1	-3.121717	-4.055029	-1.659948
6	-2.360481	-1.975435	-1.302449
7	-1.151360	-1.353238	-1.552526
6	-0.334014	-2.323206	-2.103260
6	1.018567	-2.168202	-2.430229
6	-2.370143	-1.475572	3.244346
6	-1.538981	-2.042919	4.208903
6	-0.191506	-1.687367	4.206549
6	0.290348	-0.776806	3.262402
6	-0.664732	-0.220766	2.380918
1	-3.420611	-1.748196	3.178335
1	-1.928985	-2.761823	4.921320
1	0.505941	-2.143011	4.902637
7	0.531602	1.594531	1.634060
7	1.265292	2.459774	1.708792
26	-0.725525	0.585786	-1.288936
7	-0.318051	0.727686	1.371212
6	1.738363	-0.441751	3.162139
6	2.344764	0.329243	4.160870
6	2.495613	-0.859667	2.043966
6	3.677139	0.727816	4.062785
1	1.754995	0.647019	5.015641
6	3.830273	-0.452963	1.943406
6	4.400673	0.339103	2.938797
1	4.136267	1.337446	4.832621
1	4.419728	-0.748003	1.081903
7	-1.945233	-0.576173	2.349686
6	3.428019	3.243679	-1.316552
6	3.855883	4.153140	-2.293951
6	4.230664	3.034207	-0.183961

6	5.060727	4.842345	-2.140005
1	3.243086	4.313800	-3.176279
6	5.435328	3.721258	-0.032323
1	3.901366	2.333320	0.576991
6	5.853348	4.627259	-1.010120
1	5.382694	5.542094	-2.906383
1	6.043669	3.545884	0.850312
1	6.791811	5.161999	-0.892651
6	1.781941	-3.365722	-2.897565
6	1.982199	-4.458057	-2.037036
6	2.333216	-3.411986	-4.187610
6	2.717064	-5.566999	-2.457668
1	1.563309	-4.427630	-1.036195
6	3.067265	-4.522496	-4.607308
1	2.182455	-2.571968	-4.859186
6	3.262042	-5.602752	-3.743402
1	2.866830	-6.400383	-1.776887
1	3.484380	-4.544238	-5.610305
1	3.834864	-6.466234	-4.069958
6	-4.632757	-2.263862	-0.359583
6	-5.885271	-2.177362	-0.986150
6	-4.451243	-3.220506	0.653761
6	-6.931678	-3.018429	-0.603498
1	-6.031876	-1.448831	-1.777758
6	-5.497442	-4.060171	1.036995
1	-3.484994	-3.290569	1.143688
6	-6.741617	-3.961503	0.409079
1	-7.893916	-2.940369	-1.101875
1	-5.341534	-4.790603	1.826253
1	-7.556901	-4.615228	0.705816
6	-3.349067	4.628116	-0.226476
6	-3.062881	5.386512	0.919996
6	-4.411714	5.028920	-1.051426
6	-3.816666	6.518870	1.230679
1	-2.247174	5.078456	1.567371
6	-5.165230	6.161989	-0.741090
1	-4.640653	4.446257	-1.938907
6	-4.869622	6.910447	0.400537
1	-3.584116	7.091892	2.124063
1	-5.981367	6.461487	-1.392802
1	-5.456109	7.792446	0.642214
17	6.077806	0.855620	2.766885
6	1.896261	-1.727138	0.953386
1	1.098837	-1.178635	0.445977
1	2.661103	-1.900691	0.190867
6	1.358218	-3.064721	1.429297
6	2.175597	-3.954022	2.140094
6	0.042775	-3.445355	1.138490
6	1.688546	-5.196000	2.549475
1	3.197382	-3.666896	2.376173
6	-0.444983	-4.690754	1.539148
1	-0.602584	-2.759995	0.601344
6	0.375473	-5.570112	2.248007

1	2.335145	-5.874561	3.099551
1	-1.465581	-4.969554	1.291625
1	-0.001608	-6.539324	2.562663

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^{5}22a

Number of imaginary frequencies : 0
Electronic energy : HF=-3409.6856754
Zero-point correction= 0.870817 (Hartree/Particle)
Thermal correction to Energy= 0.927860
Thermal correction to Enthalpy= 0.928804
Thermal correction to Gibbs Free Energy= 0.773349
Sum of electronic and zero-point Energies= -3408.814859
Sum of electronic and thermal Energies= -3408.757816
Sum of electronic and thermal Enthalpies= -3408.756872
Sum of electronic and thermal Free Energies= -3408.912327

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Cartesian Coordinates

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6	-0.454139	2.886277	-2.012783
7	-1.272211	2.000950	-1.334182
1	-0.576118	5.085567	-2.406508
6	-2.290552	2.761043	-0.795303
6	-2.113774	4.141988	-1.151382
1	-2.783118	4.941181	-0.870160
6	-1.000437	4.213347	-1.932715
6	-3.399933	2.273022	-0.096661
7	-2.961701	-0.099613	-0.642973
6	-3.696828	-1.256945	-0.481783
6	-4.933075	-0.962213	0.190701
1	-5.686251	-1.692142	0.446214
6	-4.926151	0.368154	0.479483
1	-5.676204	0.935662	1.008924
6	-3.716064	0.912465	-0.072226
6	0.768850	2.575101	-2.609681
1	3.843071	-0.848718	-2.702811
6	2.922559	-0.295107	-2.604841
6	1.689329	-0.834530	-2.099090
1	3.385841	1.732302	-3.315788
7	0.726536	0.160169	-2.045072
6	1.331116	1.298526	-2.546943
6	2.691312	1.010810	-2.912523
6	-3.279688	-2.555692	-0.787631
1	0.600472	-4.877237	-1.697871
6	-0.109616	-4.084942	-1.513745
6	-1.455541	-4.187144	-1.330951
1	-2.056789	-5.083510	-1.331480
6	-1.959138	-2.855177	-1.130805
7	-0.927028	-1.942156	-1.255483
6	0.213663	-2.685542	-1.488965
6	1.483048	-2.181549	-1.793509
6	-2.170829	-2.088849	2.756337
6	-1.681819	-2.075553	4.058758

6	-0.579613	-1.259428	4.312677
6	-0.003166	-0.478981	3.305690
6	-0.637399	-0.512637	2.022540
1	-3.009973	-2.725147	2.478917
1	-2.126123	-2.690159	4.834502
1	-0.128250	-1.240629	5.301118
7	0.495763	1.356557	1.258967
7	1.109940	2.049436	0.510372
26	-1.006180	0.040677	-1.039043
7	-0.237438	0.230919	0.912585
6	1.219259	0.303704	3.654728
6	1.120103	1.298630	4.636493
6	2.486706	0.005563	3.101433
6	2.231748	2.022753	5.063974
1	0.145276	1.521966	5.060063
6	3.601315	0.731881	3.528100
6	3.464851	1.726670	4.494089
1	2.139184	2.798830	5.815606
1	4.578523	0.519741	3.111745
7	-1.672613	-1.333051	1.778659
6	1.569540	3.669298	-3.236167
6	1.799833	3.683481	-4.619804
6	2.125259	4.684487	-2.441663
6	2.562177	4.698760	-5.199707
1	1.375603	2.897100	-5.237435
6	2.888808	5.697291	-3.023083
1	1.962455	4.662306	-1.368329
6	3.107447	5.708070	-4.402965
1	2.728592	4.701428	-6.273303
1	3.318048	6.474107	-2.396607
1	3.701925	6.497276	-4.854550
6	2.624991	-3.139101	-1.877130
6	3.066709	-3.796762	-0.719390
6	3.270094	-3.404975	-3.095282
6	4.141340	-4.684216	-0.773895
1	2.575893	-3.591914	0.225934
6	4.341447	-4.296898	-3.149805
1	2.923649	-2.911888	-3.998636
6	4.782258	-4.935777	-1.988473
1	4.483900	-5.168366	0.135516
1	4.829326	-4.494623	-4.100171
1	5.620579	-5.625392	-2.030276
6	-4.264241	-3.666664	-0.627630
6	-5.411619	-3.720205	-1.434658
6	-4.079963	-4.658150	0.350287
6	-6.347502	-4.742547	-1.272602
1	-5.563194	-2.956019	-2.191263
6	-5.017143	-5.678839	0.512955
1	-3.199930	-4.617751	0.984693
6	-6.153051	-5.724649	-0.298713
1	-7.227436	-4.772354	-1.909019
1	-4.862202	-6.434686	1.277765
1	-6.882646	-6.519381	-0.171859

6	-4.300405	3.259795	0.567850
6	-3.813119	4.036995	1.631100
6	-5.623440	3.451539	0.139157
6	-4.634387	4.974323	2.258371
1	-2.788816	3.895983	1.963345
6	-6.442910	4.390752	0.766302
1	-6.001570	2.867425	-0.694505
6	-5.951363	5.152990	1.828609
1	-4.244933	5.563608	3.083675
1	-7.462933	4.531452	0.419882
1	-6.589940	5.884061	2.316267
17	4.898251	2.623711	5.010342
6	2.619487	-1.102555	2.064792
1	2.285529	-2.042323	2.522936
1	1.913283	-0.902938	1.251556
6	3.996457	-1.280605	1.470651
6	4.413508	-0.456335	0.416116
6	4.877673	-2.257206	1.949622
6	5.673667	-0.619678	-0.159546
1	3.740157	0.311123	0.045032
6	6.140045	-2.423840	1.375622
1	4.567482	-2.897783	2.772014
6	6.539814	-1.607951	0.315444
1	5.976942	0.023064	-0.981603
1	6.808614	-3.192736	1.753455
1	7.518694	-1.740495	-0.136804

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^{oss}(22a-23a)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3409.6765459
Zero-point correction= 0.869795 (Hartree/Particle)
Thermal correction to Energy= 0.926337
Thermal correction to Enthalpy= 0.927281
Thermal correction to Gibbs Free Energy= 0.775580
Sum of electronic and zero-point Energies= -3408.806751
Sum of electronic and thermal Energies= -3408.750209
Sum of electronic and thermal Enthalpies= -3408.749265
Sum of electronic and thermal Free Energies= -3408.900966

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Cartesian Coordinates

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6	-0.645137	2.895627	-1.935408
7	-1.400261	1.947965	-1.267513
1	-0.917551	5.088263	-2.309126
6	-2.458252	2.635699	-0.710970
6	-2.378673	4.031628	-1.054446
1	-3.098710	4.781320	-0.761927
6	-1.278939	4.185108	-1.841141
6	-3.528103	2.064300	-0.011902
7	-2.935332	-0.263926	-0.584430
6	-3.607944	-1.463498	-0.467682
6	-4.871178	-1.260237	0.191880

1	-5.586322	-2.038489	0.411873
6	-4.944533	0.059033	0.516665
1	-5.735110	0.568814	1.046164
6	-3.758230	0.686087	-0.004670
6	0.605825	2.674368	-2.516417
1	3.912498	-0.531227	-2.601154
6	2.958835	-0.038740	-2.492092
6	1.757402	-0.663581	-2.002522
1	3.294461	2.019349	-3.186043
7	0.732180	0.266342	-1.944764
6	1.264135	1.443825	-2.439858
6	2.645661	1.252659	-2.789926
6	-3.107952	-2.725269	-0.802694
1	0.918772	-4.785146	-1.706211
6	0.159472	-4.043318	-1.509079
6	-1.177141	-4.233748	-1.346866
1	-1.722085	-5.164842	-1.380120
6	-1.764709	-2.936896	-1.123150
7	-0.792784	-1.957389	-1.208871
6	0.392886	-2.622664	-1.443158
6	1.628542	-2.029970	-1.729765
6	-1.988476	-2.285358	2.742913
6	-1.431244	-2.204043	4.014853
6	-0.397323	-1.286690	4.194830
6	0.054885	-0.484688	3.142200
6	-0.640765	-0.600505	1.895109
1	-2.782440	-2.997189	2.521819
1	-1.776078	-2.839362	4.823796
1	0.102088	-1.204963	5.156311
7	0.217221	1.570951	1.216431
7	0.851320	2.305168	0.598552
26	-1.007490	0.015949	-0.992640
7	-0.319847	0.148912	0.757409
6	1.211972	0.416357	3.410946
6	1.069291	1.402563	4.399689
6	2.456808	0.271856	2.757560
6	2.110564	2.263616	4.734196
1	0.111557	1.507510	4.900786
6	3.502428	1.138571	3.092067
6	3.321087	2.119951	4.062060
1	1.983535	3.028874	5.491737
1	4.463341	1.041087	2.600823
7	-1.619575	-1.502230	1.730340
6	1.331165	3.822188	-3.139274
6	1.586911	3.839006	-4.518578
6	1.792018	4.886948	-2.348935
6	2.279586	4.903444	-5.097646
1	1.237153	3.014867	-5.133581
6	2.486249	5.949207	-2.929005
1	1.609839	4.866845	-1.278715
6	2.730005	5.961232	-4.304585
1	2.465674	4.906412	-6.168021
1	2.841745	6.764228	-2.304802

1	3.270250	6.788888	-4.755481
6	2.824446	-2.916990	-1.841167
6	3.278407	-3.619816	-0.714498
6	3.509330	-3.076644	-3.056424
6	4.404322	-4.438755	-0.792057
1	2.755143	-3.503361	0.227912
6	4.632481	-3.900712	-3.135414
1	3.152632	-2.555725	-3.939819
6	5.086483	-4.579299	-2.002170
1	4.755067	-4.952701	0.097337
1	5.149677	-4.015346	-4.083969
1	5.965668	-5.214550	-2.062321
6	-4.028435	-3.895913	-0.694510
6	-5.153969	-3.992886	-1.527826
6	-3.807179	-4.902968	0.259427
6	-6.031182	-5.072398	-1.415590
1	-5.334492	-3.217086	-2.266000
6	-4.685556	-5.981047	0.372495
1	-2.944011	-4.830294	0.913896
6	-5.799628	-6.069615	-0.465520
1	-6.894313	-5.134749	-2.072382
1	-4.502229	-6.748727	1.119081
1	-6.483555	-6.908991	-0.377554
6	-4.487507	2.982739	0.669003
6	-4.047486	3.769860	1.745384
6	-5.819991	3.102152	0.243724
6	-4.922925	4.645039	2.389059
1	-3.015839	3.685997	2.074453
6	-6.694046	3.979379	0.886933
1	-6.162948	2.510832	-0.599949
6	-6.248714	4.751400	1.962445
1	-4.568869	5.242802	3.224244
1	-7.720967	4.064342	0.542673
1	-6.929812	5.434151	2.462492
17	4.662805	3.199893	4.453336
6	2.647154	-0.774237	1.670520
1	2.022413	-1.641424	1.908336
1	2.242171	-0.373325	0.733982
6	4.073107	-1.228847	1.458145
6	4.859000	-0.674712	0.440415
6	4.632902	-2.221656	2.273876
6	6.166516	-1.115869	0.226521
1	4.434132	0.096874	-0.194788
6	5.938903	-2.664968	2.064388
1	4.033834	-2.654409	3.071802
6	6.708773	-2.116142	1.034867
1	6.757671	-0.682840	-0.575790
1	6.355408	-3.440955	2.701169
1	7.723203	-2.466137	0.865593

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^{3}(22a-23a)‡

Number of imaginary frequencies : 1

Electronic energy : HF=-3409.6821196
Zero-point correction= 0.869824 (Hartree/Particle)
Thermal correction to Energy= 0.926423
Thermal correction to Enthalpy= 0.927367
Thermal correction to Gibbs Free Energy= 0.774667
Sum of electronic and zero-point Energies= -3408.812295
Sum of electronic and thermal Energies= -3408.755697
Sum of electronic and thermal Enthalpies= -3408.754753
Sum of electronic and thermal Free Energies= -3408.907453

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Cartesian Coordinates

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6	-0.698974	2.873478	-1.898053
7	-1.464648	1.903696	-1.271341
1	-1.067160	5.019622	-2.425825
6	-2.615169	2.547250	-0.865929
6	-2.596530	3.921671	-1.294253
1	-3.394922	4.630292	-1.132054
6	-1.421867	4.117019	-1.951614
6	-3.675755	1.962635	-0.161797
7	-2.936689	-0.366141	-0.527709
6	-3.528644	-1.588350	-0.286399
6	-4.770372	-1.407160	0.418225
1	-5.419291	-2.205871	0.744427
6	-4.926579	-0.069809	0.615507
1	-5.731534	0.435198	1.127686
6	-3.805495	0.580566	-0.010256
6	0.622171	2.716661	-2.320972
1	3.952663	-0.466640	-2.519523
6	2.998364	0.020925	-2.392678
6	1.779362	-0.639776	-2.004714
1	3.368201	2.140483	-2.839645
7	0.754748	0.282280	-1.883989
6	1.305566	1.498671	-2.244800
6	2.702970	1.340746	-2.550693
6	-2.995383	-2.839595	-0.613173
1	0.978681	-4.779574	-1.913383
6	0.226749	-4.060402	-1.625586
6	-1.086608	-4.282418	-1.356926
1	-1.617143	-5.222001	-1.380459
6	-1.675611	-3.005464	-1.040544
7	-0.731056	-2.002310	-1.168496
6	0.442969	-2.639858	-1.519400
6	1.658041	-2.022599	-1.833169
6	-1.278976	-2.625835	2.762841
6	-0.455353	-2.606868	3.883645
6	0.440125	-1.544201	3.996349
6	0.518680	-0.555697	3.010397
6	-0.401410	-0.656839	1.917964
1	-2.002014	-3.425801	2.614023
1	-0.509786	-3.386794	4.635734
1	1.116886	-1.484329	4.844297
7	-0.163075	1.731957	1.474571

7	-0.196806	2.761278	0.993604
26	-1.011987	-0.029551	-0.944217
7	-0.457055	0.257163	0.857033
6	1.504362	0.547073	3.206701
6	1.365787	1.354210	4.349665
6	2.584244	0.786047	2.330985
6	2.250349	2.390607	4.630614
1	0.530441	1.174601	5.019857
6	3.474427	1.829096	2.613217
6	3.301864	2.618088	3.744841
1	2.122935	3.012182	5.509843
1	4.310541	2.014240	1.946610
7	-1.269900	-1.676368	1.826751
6	1.362443	3.917034	-2.813301
6	1.808207	3.994337	-4.141691
6	1.636236	4.983742	-1.942124
6	2.508434	5.115121	-4.590289
1	1.599002	3.172388	-4.820026
6	2.339622	6.101953	-2.390906
1	1.298285	4.923614	-0.911771
6	2.776410	6.171092	-3.716097
1	2.842168	5.163949	-5.623025
1	2.549502	6.916949	-1.703917
1	3.323010	7.042584	-4.065265
6	2.850900	-2.891260	-2.063148
6	3.371354	-3.664031	-1.013816
6	3.466129	-2.960996	-3.323532
6	4.487450	-4.475796	-1.215538
1	2.912962	-3.606673	-0.032956
6	4.580458	-3.775958	-3.525429
1	3.061800	-2.376234	-4.144371
6	5.095604	-4.534077	-2.471180
1	4.887243	-5.049724	-0.385436
1	5.042459	-3.822103	-4.507704
1	5.965728	-5.165457	-2.627898
6	-3.861272	-4.041721	-0.431027
6	-5.061033	-4.167482	-1.150570
6	-3.511118	-5.058642	0.472834
6	-5.884799	-5.279626	-0.974064
1	-5.340701	-3.387340	-1.852166
6	-4.335835	-6.169587	0.650795
1	-2.587656	-4.969465	1.035956
6	-5.525235	-6.284026	-0.072576
1	-6.806130	-5.362378	-1.543753
1	-4.051133	-6.943238	1.358408
1	-6.167449	-7.149152	0.065759
6	-4.718970	2.867693	0.403155
6	-4.364441	3.810610	1.382101
6	-6.052040	2.815613	-0.034027
6	-5.322268	4.671306	1.918456
1	-3.333030	3.858854	1.719070
6	-7.008587	3.679371	0.500839
1	-6.330794	2.100380	-0.801933

6	-6.647060	4.607747	1.479849
1	-5.033407	5.390426	2.679759
1	-8.034854	3.630832	0.147693
1	-7.392394	5.279571	1.896115
17	4.436386	3.931969	4.064205
6	2.843788	-0.059634	1.099721
1	1.937335	-0.590698	0.811868
1	3.083041	0.601162	0.262824
6	3.975310	-1.052640	1.296123
6	5.171014	-0.933764	0.579048
6	3.836110	-2.117480	2.199060
6	6.206151	-1.855505	0.755199
1	5.286217	-0.119275	-0.131372
6	4.867683	-3.038464	2.378668
1	2.909808	-2.222304	2.757178
6	6.058658	-2.909902	1.656892
1	7.124232	-1.751433	0.183540
1	4.742893	-3.858340	3.081176
1	6.862190	-3.627914	1.795327

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^{5}(22a-23a)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3409.6800834
Zero-point correction= 0.868682 (Hartree/Particle)
Thermal correction to Energy= 0.925762
Thermal correction to Enthalpy= 0.926706
Thermal correction to Gibbs Free Energy= 0.771220
Sum of electronic and zero-point Energies= -3408.811402
Sum of electronic and thermal Energies= -3408.754322
Sum of electronic and thermal Enthalpies= -3408.753377
Sum of electronic and thermal Free Energies= -3408.908863

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Cartesian Coordinates

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6	-0.319685	2.803152	-2.071788
7	-1.183705	1.949223	-1.409959
1	-0.361543	5.001652	-2.487113
6	-2.198102	2.744871	-0.914356
6	-1.968811	4.116294	-1.277698
1	-2.623645	4.937662	-1.027944
6	-0.827121	4.147333	-2.019475
6	-3.343355	2.298275	-0.246966
7	-2.941677	-0.099837	-0.704341
6	-3.702304	-1.236859	-0.517348
6	-4.952590	-0.893397	0.105097
1	-5.726394	-1.599093	0.367162
6	-4.929974	0.447234	0.338325
1	-5.684771	1.049349	0.820759
6	-3.692007	0.946362	-0.195353
6	0.907593	2.449991	-2.636750
1	3.879476	-1.064064	-2.639329
6	2.974415	-0.481838	-2.563989

6	1.717119	-0.976808	-2.069636
1	3.509257	1.520423	-3.295507
7	0.781398	0.043672	-2.054668
6	1.428241	1.155965	-2.558526
6	2.787033	0.825031	-2.895054
6	-3.301024	-2.554548	-0.754322
1	0.546715	-4.983388	-1.512638
6	-0.151549	-4.171560	-1.373632
6	-1.499987	-4.242645	-1.194415
1	-2.116627	-5.127613	-1.152770
6	-1.981994	-2.893498	-1.065273
7	-0.934768	-2.005762	-1.225140
6	0.194927	-2.777595	-1.413134
6	1.475897	-2.308577	-1.724399
6	-2.348680	-1.798831	2.883338
6	-1.927920	-1.604797	4.196931
6	-0.803434	-0.803179	4.392457
6	-0.134962	-0.217401	3.313531
6	-0.701472	-0.413671	2.010404
1	-3.200905	-2.439208	2.658679
1	-2.443212	-2.074797	5.027962
1	-0.404969	-0.653469	5.392532
7	0.490553	1.563207	1.120939
7	1.333748	2.003832	0.472422
26	-0.979215	-0.014043	-1.079457
7	-0.170029	0.095877	0.841941
6	1.108684	0.554827	3.595225
6	1.024774	1.671937	4.438919
6	2.374228	0.161615	3.097441
6	2.147568	2.422832	4.780471
1	0.051234	1.970658	4.816576
6	3.500505	0.916069	3.437734
6	3.378044	2.030694	4.264215
1	2.066119	3.292876	5.422375
1	4.475895	0.632628	3.061457
7	-1.774864	-1.213709	1.833704
6	1.755568	3.516134	-3.250073
6	2.011433	3.519579	-4.629264
6	2.329005	4.515305	-2.447959
6	2.817049	4.507961	-5.197070
1	1.573273	2.745838	-5.253083
6	3.135562	5.501395	-3.017047
1	2.145894	4.502264	-1.377748
6	3.380073	5.501242	-4.392591
1	3.003081	4.502335	-6.267425
1	3.577890	6.265709	-2.384322
1	4.008233	6.269450	-4.834670
6	2.602617	-3.287871	-1.754592
6	3.030730	-3.890690	-0.562229
6	3.251601	-3.620718	-2.953766
6	4.096791	-4.789987	-0.565472
1	2.538741	-3.632509	0.369036
6	4.313963	-4.525360	-2.956848

1	2.916738	-3.168371	-3.882518
6	4.741793	-5.108945	-1.762122
1	4.430163	-5.228800	0.369812
1	4.805366	-4.775352	-3.893012
1	5.573648	-5.807648	-1.764024
6	-4.302494	-3.643221	-0.549680
6	-5.426509	-3.743604	-1.384006
6	-4.153442	-4.566653	0.498171
6	-6.374947	-4.746936	-1.180109
1	-5.550145	-3.031605	-2.194720
6	-5.103086	-5.568264	0.702324
1	-3.290993	-4.487985	1.153077
6	-6.215873	-5.661916	-0.136919
1	-7.236659	-4.814607	-1.838207
1	-4.975834	-6.272020	1.520142
1	-6.954922	-6.442039	0.021912
6	-4.244365	3.320389	0.361916
6	-3.783672	4.103186	1.432705
6	-5.542684	3.536755	-0.126077
6	-4.606952	5.071263	2.008656
1	-2.778591	3.942058	1.811357
6	-6.364399	4.506344	0.449914
1	-5.899839	2.946375	-0.964590
6	-5.899471	5.274778	1.519700
1	-4.238616	5.664869	2.840566
1	-7.365176	4.665239	0.058190
1	-6.539730	6.029353	1.967733
17	4.824594	2.962058	4.668751
6	2.490153	-1.065291	2.203946
1	2.085983	-1.926655	2.750534
1	1.821911	-0.916991	1.347268
6	3.873559	-1.384822	1.690201
6	4.375135	-0.709787	0.567821
6	4.674635	-2.356417	2.302269
6	5.639100	-1.010681	0.060666
1	3.762789	0.048614	0.088382
6	5.940289	-2.662011	1.795886
1	4.299147	-2.883009	3.176639
6	6.424589	-1.992209	0.670552
1	6.007614	-0.482662	-0.814695
1	6.545742	-3.424674	2.278440
1	7.405705	-2.233547	0.271314

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^{oss}23a

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2053267
Zero-point correction= 0.862262 (Hartree/Particle)
Thermal correction to Energy= 0.916981
Thermal correction to Enthalpy= 0.917925
Thermal correction to Gibbs Free Energy= 0.768160
Sum of electronic and zero-point Energies= -3299.343065
Sum of electronic and thermal Energies= -3299.288346

Sum of electronic and thermal Enthalpies= -3299.287401
Sum of electronic and thermal Free Energies= -3299.437166

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Cartesian Coordinates

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6	-1.992047	-0.158611	-2.211563
7	-0.845111	-0.763517	-1.730484
1	-3.877041	-0.958435	-3.130437
6	-1.097436	-2.119895	-1.765067
6	-2.384751	-2.370202	-2.360609
1	-2.805520	-3.347552	-2.542366
6	-2.927094	-1.159234	-2.659194
6	-0.242850	-3.131588	-1.305828
7	1.724545	-1.669971	-1.028798
6	3.052354	-1.918820	-0.769340
6	3.249926	-3.316519	-0.474953
1	4.197258	-3.769137	-0.222461
6	2.031661	-3.914605	-0.563819
1	1.790698	-4.953904	-0.399696
6	1.088181	-2.893412	-0.951495
6	-2.270762	1.212595	-2.169643
1	-0.453947	5.146251	-0.570746
6	-0.580306	4.122013	-0.887634
6	0.448066	3.111657	-0.868394
1	-2.661457	3.988323	-1.572279
7	-0.062645	1.903511	-1.292729
6	-1.370003	2.153045	-1.654453
6	-1.696764	3.536198	-1.397903
6	4.066610	-0.957026	-0.763254
1	4.621572	3.596785	-0.478608
6	4.183940	2.617728	-0.604258
6	4.824009	1.423700	-0.723762
1	5.887013	1.236038	-0.709513
6	3.809053	0.412340	-0.852199
7	2.558828	1.005243	-0.921137
6	2.773949	2.354120	-0.701291
6	1.793949	3.343260	-0.576025
6	2.978245	0.630893	3.153151
6	2.439904	0.029912	4.301839
6	1.189767	-0.584695	4.199835
6	0.510066	-0.575345	2.985078
6	1.158366	0.044366	1.850837
1	3.946809	1.128010	3.203220
1	2.984605	0.049257	5.240047
1	0.734894	-1.062462	5.063230
26	0.817053	0.118496	-0.995269
7	0.475921	0.011539	0.700999
6	-0.797314	-1.267329	2.822350
6	-0.833949	-2.654819	3.012471
6	-1.984265	-0.580240	2.476702
6	-2.008168	-3.386546	2.841356
1	0.081521	-3.176100	3.276689
6	-3.157854	-1.316677	2.291747

6	-3.157498	-2.698825	2.466947
1	-2.022590	-4.461772	2.977631
1	-4.076514	-0.809198	2.022844
7	2.385148	0.637917	1.967556
6	-3.604432	1.698635	-2.636739
6	-3.693269	2.614994	-3.697503
6	-4.791237	1.272827	-2.016949
6	-4.932439	3.092018	-4.125787
1	-2.782572	2.948888	-4.185707
6	-6.030272	1.752857	-2.442871
1	-4.735857	0.575516	-1.187825
6	-6.104835	2.663992	-3.498823
1	-4.981337	3.796632	-4.951246
1	-6.935677	1.417160	-1.945193
1	-7.069356	3.037368	-3.830890
6	2.218595	4.701454	-0.124198
6	2.727775	4.871684	1.173337
6	2.126673	5.819278	-0.967342
6	3.127864	6.131499	1.619234
1	2.800077	4.006341	1.825718
6	2.529561	7.078961	-0.521347
1	1.743920	5.693584	-1.975829
6	3.029411	7.238701	0.773008
1	3.514023	6.249019	2.627941
1	2.457150	7.934307	-1.187297
1	3.341505	8.219787	1.119777
6	5.473043	-1.421633	-0.566615
6	6.112068	-2.193644	-1.548895
6	6.170381	-1.117153	0.613077
6	7.420179	-2.642118	-1.360285
1	5.577927	-2.436312	-2.462877
6	7.477214	-1.567405	0.802509
1	5.675178	-0.530763	1.380896
6	8.106310	-2.329850	-0.184590
1	7.903342	-3.233415	-2.133087
1	8.002289	-1.326662	1.722756
1	9.124356	-2.679433	-0.037947
6	-0.778487	-4.523855	-1.244212
6	-1.876880	-4.815123	-0.418712
6	-0.220762	-5.558750	-2.012358
6	-2.393514	-6.108739	-0.350679
1	-2.317502	-4.020806	0.172564
6	-0.739300	-6.852590	-1.945379
1	0.615499	-5.341005	-2.669810
6	-1.824985	-7.132439	-1.112186
1	-3.240211	-6.314147	0.298210
1	-0.298854	-7.640259	-2.550355
1	-2.227622	-8.140143	-1.060623
17	-4.654857	-3.598984	2.200951
6	-1.983009	0.931855	2.297081
1	-1.309896	1.366966	3.045840
1	-1.523830	1.147571	1.326301
6	-3.337492	1.597270	2.389675

6	-3.947352	2.127146	1.247411
6	-4.019815	1.680625	3.612674
6	-5.208348	2.724369	1.316811
1	-3.425158	2.075889	0.298511
6	-5.277184	2.279315	3.688707
1	-3.561885	1.267000	4.508148
6	-5.877281	2.802382	2.538839
1	-5.662872	3.121432	0.413330
1	-5.790782	2.337437	4.644663
1	-6.857787	3.266709	2.598341

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^{3}23a

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2180632
Zero-point correction= 0.862428 (Hartree/Particle)
Thermal correction to Energy= 0.917242
Thermal correction to Enthalpy= 0.918186
Thermal correction to Gibbs Free Energy= 0.767055
Sum of electronic and zero-point Energies= -3299.355635
Sum of electronic and thermal Energies= -3299.300822
Sum of electronic and thermal Enthalpies= -3299.299877
Sum of electronic and thermal Free Energies= -3299.451009

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Cartesian Coordinates

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6	-1.250656	-1.956793	-1.722226
7	0.055708	-1.657948	-1.396124
1	-2.391876	-3.877845	-1.915613
6	0.665339	-2.868849	-1.155459
6	-0.277460	-3.947892	-1.324184
1	-0.045555	-4.996162	-1.209392
6	-1.460227	-3.383885	-1.683624
6	2.023679	-3.047908	-0.886474
7	2.622036	-0.639081	-0.909821
6	3.829417	0.029925	-0.792034
6	4.910873	-0.917368	-0.735666
1	5.957439	-0.658704	-0.683239
6	4.357298	-2.159325	-0.731974
1	4.862978	-3.111118	-0.672289
6	2.934030	-1.989137	-0.848581
6	-2.228863	-1.034654	-2.095578
1	-3.041183	3.495762	-2.172029
6	-2.555270	2.536435	-2.077340
6	-1.240457	2.329261	-1.529143
1	-3.999889	1.071321	-2.851071
7	-0.903713	0.992208	-1.584601
6	-2.025098	0.347987	-2.076788
6	-3.037831	1.312001	-2.424200
6	3.996724	1.406607	-0.635139
1	1.483051	5.216537	0.009798
6	1.784679	4.207554	-0.227427
6	3.037686	3.680229	-0.201011

1	3.960206	4.171363	0.069706
6	2.921788	2.295793	-0.582238
7	1.604777	1.983337	-0.843464
6	0.897721	3.162048	-0.670508
6	-0.447611	3.349948	-0.989609
6	3.016190	0.344790	3.241587
6	2.468264	-0.326084	4.337453
6	1.204767	-0.906023	4.186140
6	0.527411	-0.792888	2.976304
6	1.185028	-0.089955	1.909011
1	3.997214	0.812060	3.320442
1	3.012077	-0.392880	5.273843
1	0.740663	-1.447318	5.006397
26	0.811516	0.155067	-0.915254
7	0.502694	0.014015	0.748032
6	-0.788705	-1.455259	2.750462
6	-0.828496	-2.854900	2.726285
6	-1.983062	-0.721805	2.558163
6	-2.012890	-3.551923	2.488842
1	0.094077	-3.408188	2.876555
6	-3.173418	-1.420366	2.335551
6	-3.174079	-2.814020	2.292725
1	-2.028156	-4.635219	2.450753
1	-4.102096	-0.881223	2.193667
7	2.413828	0.462716	2.058735
6	-3.586894	-1.544015	-2.463133
6	-4.026352	-1.540105	-3.794495
6	-4.445545	-2.023571	-1.462598
6	-5.302537	-2.004815	-4.118440
1	-3.363976	-1.172285	-4.572910
6	-5.719455	-2.490087	-1.788138
1	-4.108400	-2.030159	-0.431147
6	-6.151770	-2.480317	-3.116455
1	-5.631109	-1.998342	-5.154022
1	-6.371840	-2.858373	-1.001649
1	-7.144209	-2.842402	-3.369894
6	-1.083278	4.683212	-0.769141
6	-2.143538	4.798951	0.145244
6	-0.662449	5.826024	-1.466759
6	-2.762687	6.029953	0.360997
1	-2.480114	3.919244	0.683738
6	-1.283843	7.056987	-1.250278
1	0.147398	5.741923	-2.185396
6	-2.334492	7.162639	-0.335525
1	-3.580488	6.097741	1.072888
1	-0.951062	7.931979	-1.801731
1	-2.817708	8.121435	-0.169379
6	5.369816	1.950361	-0.411305
6	5.951662	2.827986	-1.338848
6	6.090553	1.614429	0.745983
6	7.226385	3.351837	-1.118071
1	5.398652	3.095066	-2.234596
6	7.364092	2.139365	0.966852

1	5.640317	0.940735	1.468359
6	7.936040	3.008944	0.034937
1	7.665320	4.025910	-1.848334
1	7.907525	1.873047	1.869206
1	8.927770	3.417716	0.206762
6	2.517462	-4.440546	-0.655873
6	2.175610	-5.116071	0.525480
6	3.306035	-5.100720	-1.609825
6	2.617680	-6.420332	0.750731
1	1.558738	-4.610458	1.262619
6	3.749549	-6.404711	-1.383361
1	3.565740	-4.586944	-2.530787
6	3.407228	-7.067545	-0.202576
1	2.346824	-6.929996	1.671238
1	4.357449	-6.904139	-2.132592
1	3.751444	-8.082919	-0.027651
17	-4.695946	-3.659783	1.986170
6	-1.947122	0.800087	2.621861
1	-1.572333	1.096611	3.608942
1	-1.194402	1.134071	1.899738
6	-3.237318	1.527416	2.323710
6	-3.761977	1.511575	1.022487
6	-3.910517	2.262091	3.306906
6	-4.926254	2.212186	0.710746
1	-3.244706	0.951012	0.251952
6	-5.074609	2.971484	2.997774
1	-3.515598	2.286743	4.319693
6	-5.586389	2.948485	1.698812
1	-5.306232	2.192047	-0.306442
1	-5.580192	3.541441	3.772677
1	-6.490561	3.500460	1.457484

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^{5}23a

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2174357
Zero-point correction= 0.860196 (Hartree/Particle)
Thermal correction to Energy= 0.915572
Thermal correction to Enthalpy= 0.916516
Thermal correction to Gibbs Free Energy= 0.764652
Sum of electronic and zero-point Energies= -3299.357240
Sum of electronic and thermal Energies= -3299.301864
Sum of electronic and thermal Enthalpies= -3299.300919
Sum of electronic and thermal Free Energies= -3299.452784

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Cartesian Coordinates

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6	-1.943833	-0.587686	-1.885633
7	-0.666685	-0.988632	-1.563793
1	-3.766485	-1.715494	-2.568806
6	-0.633847	-2.356835	-1.699570
6	-1.927526	-2.830911	-2.139281
1	-2.175784	-3.859903	-2.351420

6	-2.735132	-1.741782	-2.251014
6	0.485012	-3.180530	-1.479679
7	2.135740	-1.394325	-0.976778
6	3.476257	-1.389382	-0.649292
6	3.963682	-2.746913	-0.609753
1	4.981948	-3.036017	-0.396431
6	2.910910	-3.562323	-0.897846
1	2.909545	-4.640625	-0.952028
6	1.766862	-2.715075	-1.137227
6	-2.414596	0.736702	-1.906607
1	-1.032562	5.125882	-1.398378
6	-1.045548	4.046675	-1.427226
6	0.088481	3.192582	-1.169776
1	-3.112428	3.532426	-1.953513
7	-0.286693	1.873880	-1.315383
6	-1.622660	1.874578	-1.658307
6	-2.102097	3.235780	-1.715844
6	4.267683	-0.254385	-0.401599
1	4.074088	4.357927	-0.113535
6	3.814894	3.323226	-0.281213
6	4.620645	2.233307	-0.160336
1	5.661894	2.210008	0.124557
6	3.813402	1.073670	-0.467074
7	2.533601	1.470418	-0.774702
6	2.505414	2.841881	-0.663728
6	1.376846	3.659241	-0.846350
6	2.774185	-0.745267	3.763773
6	2.014473	-1.600983	4.586532
6	0.711528	-1.909823	4.204553
6	0.189041	-1.372315	3.025972
6	1.043215	-0.514037	2.238019
1	3.795438	-0.490139	4.044464
1	2.442349	-2.001692	5.499834
1	0.095018	-2.562911	4.815739
26	0.832130	0.210979	-0.677070
7	0.594024	0.003225	1.102619
6	-1.176199	-1.737044	2.567529
6	-1.444183	-3.097774	2.354752
6	-2.205466	-0.786690	2.364447
6	-2.686254	-3.540582	1.902719
1	-0.651307	-3.821975	2.517570
6	-3.453533	-1.237449	1.924106
6	-3.675652	-2.590134	1.678253
1	-2.875538	-4.593172	1.725166
1	-4.260393	-0.529532	1.782221
7	2.324602	-0.211297	2.641530
6	-3.862915	0.948695	-2.215823
6	-4.269880	1.616664	-3.381497
6	-4.845726	0.477518	-1.331107
6	-5.624955	1.817082	-3.648672
1	-3.517449	1.975218	-4.077633
6	-6.200202	0.678444	-1.597641
1	-4.538418	-0.044236	-0.432334

6	-6.593936	1.351239	-2.756433
1	-5.923342	2.333205	-4.556982
1	-6.944166	0.311282	-0.896393
1	-7.648383	1.508919	-2.965083
6	1.556165	5.136196	-0.689938
6	0.940034	5.821061	0.369308
6	2.341988	5.863088	-1.597829
6	1.106891	7.198559	0.517225
1	0.332733	5.264575	1.077095
6	2.507975	7.240814	-1.449926
1	2.819005	5.340441	-2.421661
6	1.891096	7.912403	-0.391966
1	0.626813	7.712786	1.345142
1	3.115956	7.789422	-2.163959
1	2.020644	8.984852	-0.276759
6	5.691436	-0.480848	-0.002226
6	6.748056	-0.118724	-0.850952
6	5.989618	-1.058235	1.242039
6	8.072858	-0.329411	-0.464591
1	6.524149	0.326617	-1.815890
6	7.313885	-1.269171	1.627394
1	5.172239	-1.334414	1.901075
6	8.359395	-0.905176	0.775168
1	8.880428	-0.047253	-1.134389
1	7.529518	-1.714177	2.594973
1	9.390570	-1.069138	1.075205
6	0.295598	-4.656866	-1.628296
6	-0.551178	-5.354730	-0.752906
6	0.949995	-5.370743	-2.644562
6	-0.735970	-6.731087	-0.886782
1	-1.064423	-4.804877	0.028676
6	0.765090	-6.747546	-2.778487
1	1.600734	-4.837846	-3.331480
6	-0.077459	-7.432241	-1.899559
1	-1.393720	-7.255788	-0.199071
1	1.275281	-7.283924	-3.573706
1	-0.221870	-8.503762	-2.005165
17	-5.252060	-3.101302	1.074654
6	-1.976104	0.697376	2.632322
1	-1.421851	0.798582	3.573062
1	-1.310014	1.076051	1.849811
6	-3.229621	1.540673	2.682242
6	-3.667263	2.225389	1.541413
6	-4.001718	1.619030	3.849731
6	-4.849782	2.967680	1.561788
1	-3.081372	2.169871	0.629765
6	-5.181232	2.364454	3.876454
1	-3.675980	1.087527	4.740942
6	-5.610435	3.039824	2.730275
1	-5.174879	3.483317	0.662446
1	-5.766398	2.417274	4.790656
1	-6.530308	3.617699	2.749689

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^{OSS}(23a-24a)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3300.1871614
Zero-point correction= 0.857478 (Hartree/Particle)
Thermal correction to Energy= 0.911183
Thermal correction to Enthalpy= 0.912127
Thermal correction to Gibbs Free Energy= 0.767785
Sum of electronic and zero-point Energies= -3299.329684
Sum of electronic and thermal Energies= -3299.275978
Sum of electronic and thermal Enthalpies= -3299.275034
Sum of electronic and thermal Free Energies= -3299.419376

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Cartesian Coordinates

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6	-1.900015	-0.749641	-2.234455
7	-0.661180	-1.026005	-1.692471
1	-3.518998	-2.056153	-3.080780
6	-0.568135	-2.398768	-1.623897
6	-1.758980	-2.998740	-2.168132
1	-1.931919	-4.061202	-2.256423
6	-2.561956	-1.981277	-2.587433
6	0.552473	-3.127645	-1.200887
7	2.067004	-1.185483	-1.124855
6	3.433750	-1.045679	-1.053957
6	4.052468	-2.339990	-0.907890
1	5.115175	-2.512332	-0.823875
6	3.048118	-3.257818	-0.850288
1	3.134267	-4.325667	-0.716910
6	1.811069	-2.539369	-1.032897
6	-2.477401	0.525000	-2.315507
1	-1.919866	4.702888	-0.448933
6	-1.726928	3.708691	-0.820654
6	-0.497449	2.977248	-0.643541
1	-3.566303	3.129465	-1.864058
7	-0.619191	1.713356	-1.185690
6	-1.878413	1.657898	-1.749864
6	-2.559216	2.913247	-1.544275
6	4.128794	0.169772	-0.996191
1	3.318891	4.542475	0.216882
6	3.190958	3.516645	-0.096364
6	4.151040	2.625458	-0.467645
1	5.218405	2.781761	-0.507618
6	3.481103	1.389847	-0.786439
7	2.112181	1.569111	-0.706123
6	1.920222	2.860152	-0.263446
6	0.685137	3.507212	-0.120383
6	3.288525	-0.397785	2.794210
6	2.876279	-1.095587	3.928023
6	1.542492	-1.502805	3.989157
6	0.670000	-1.222761	2.937008
6	1.187911	-0.469921	1.828975
1	4.323562	-0.074020	2.692408

1	3.571622	-1.314457	4.731725
1	1.175850	-2.054430	4.850557
26	0.685817	0.234908	-0.929151
7	0.342007	-0.208762	0.775707
6	-0.715070	-1.765265	2.956649
6	-0.900294	-3.113286	3.288608
6	-1.852098	-0.958985	2.678943
6	-2.170065	-3.688405	3.363742
1	-0.029637	-3.736104	3.469933
6	-3.126458	-1.530998	2.783627
6	-3.270910	-2.876477	3.115125
1	-2.295180	-4.737223	3.608439
1	-4.009688	-0.926305	2.622954
7	2.476451	-0.071753	1.788131
6	-3.827993	0.680964	-2.933317
6	-3.995890	1.505094	-4.057703
6	-4.957438	0.039436	-2.398011
6	-5.255177	1.680114	-4.632893
1	-3.129860	2.007333	-4.478462
6	-6.216706	0.213558	-2.973579
1	-4.844813	-0.591205	-1.522043
6	-6.369867	1.035134	-4.092795
1	-5.363768	2.318718	-5.505057
1	-7.078431	-0.288587	-2.542675
1	-7.350329	1.171529	-4.540123
6	0.663858	4.844757	0.542997
6	0.945974	4.933824	1.915641
6	0.380418	6.021842	-0.166429
6	0.929137	6.168194	2.566090
1	1.174563	4.026404	2.467265
6	0.365187	7.256410	0.484544
1	0.179055	5.963881	-1.231851
6	0.636546	7.332820	1.852569
1	1.143992	6.219508	3.629890
1	0.147047	8.159248	-0.079129
1	0.623925	8.294134	2.358377
6	5.621102	0.119178	-1.021208
6	6.292481	-0.318740	-2.173677
6	6.379276	0.467334	0.108419
6	7.685704	-0.395322	-2.199958
1	5.713749	-0.596643	-3.049669
6	7.772015	0.389564	0.082429
1	5.866546	0.793983	1.007750
6	8.429659	-0.040479	-1.072477
1	8.189480	-0.730660	-3.102237
1	8.342770	0.658739	0.966905
1	9.514112	-0.101272	-1.092539
6	0.381912	-4.594766	-0.986993
6	-0.471053	-5.038906	0.037150
6	1.029015	-5.547014	-1.789430
6	-0.659012	-6.402647	0.261980
1	-0.978057	-4.307432	0.658781
6	0.838162	-6.911312	-1.564319

1	1.673189	-5.212028	-2.596865
6	-0.004074	-7.343068	-0.536944
1	-1.318104	-6.728808	1.061991
1	1.341725	-7.636612	-2.197425
1	-0.152066	-8.405258	-0.363339
17	-4.895557	-3.562230	3.216152
6	-1.628391	0.463834	2.279859
1	-0.949830	0.963490	2.977926
1	-0.802668	0.254781	1.309796
6	-2.736779	1.353395	1.869665
6	-3.740426	0.957641	0.963519
6	-2.792536	2.665162	2.381298
6	-4.791256	1.814019	0.640416
1	-3.683559	-0.022737	0.502597
6	-3.838062	3.524656	2.050783
1	-2.010243	3.002984	3.056053
6	-4.851990	3.096973	1.190175
1	-5.552316	1.485624	-0.060419
1	-3.862196	4.527389	2.468508
1	-5.672278	3.762141	0.935806

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^{3}(23a-24a)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3300.1941866
Zero-point correction= 0.858004 (Hartree/Particle)
Thermal correction to Energy= 0.911673
Thermal correction to Enthalpy= 0.912617
Thermal correction to Gibbs Free Energy= 0.767115
Sum of electronic and zero-point Energies= -3299.336183
Sum of electronic and thermal Energies= -3299.282513
Sum of electronic and thermal Enthalpies= -3299.281569
Sum of electronic and thermal Free Energies= -3299.427072

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Cartesian Coordinates

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6	-2.012924	-0.616099	-2.026760
7	-0.770131	-0.964648	-1.531945
1	-3.754291	-1.819706	-2.774632
6	-0.753488	-2.342522	-1.487199
6	-2.007324	-2.868570	-1.964181
1	-2.247002	-3.917723	-2.049943
6	-2.769968	-1.804198	-2.332631
6	0.355864	-3.142711	-1.182820
7	1.972718	-1.275316	-1.050209
6	3.352604	-1.217690	-1.024918
6	3.897917	-2.550921	-1.030089
1	4.949818	-2.792167	-1.041844
6	2.846672	-3.413558	-0.988343
1	2.878715	-4.491776	-0.953534
6	1.645755	-2.619787	-1.045322
6	-2.493953	0.690997	-2.168449
1	-1.506768	4.955419	-0.719422

6	-1.430676	3.908701	-0.971994
6	-0.289977	3.071887	-0.698491
1	-3.323159	3.420702	-1.968892
7	-0.525784	1.789072	-1.144079
6	-1.789712	1.806804	-1.701426
6	-2.345488	3.133958	-1.613950
6	4.119600	-0.054137	-0.908733
1	3.605868	4.285136	0.523311
6	3.406319	3.308070	0.110273
6	4.304976	2.338636	-0.209674
1	5.378789	2.366386	-0.100602
6	3.551990	1.201375	-0.674123
7	2.206568	1.501017	-0.689369
6	2.099974	2.799644	-0.223551
6	0.917598	3.543315	-0.166958
6	3.288900	-0.785978	2.829367
6	2.821401	-1.610947	3.851219
6	1.464599	-1.927843	3.851163
6	0.610070	-1.435051	2.858434
6	1.190805	-0.557564	1.880271
1	4.342100	-0.513433	2.773427
1	3.491201	-1.988032	4.616905
1	1.055508	-2.569322	4.626858
26	0.692593	0.230562	-0.842595
7	0.411411	0.013877	0.899776
6	-0.802590	-1.894804	2.818463
6	-1.073994	-3.256479	3.017644
6	-1.890746	-1.005478	2.609302
6	-2.374158	-3.761073	3.008055
1	-0.246728	-3.946672	3.150351
6	-3.197710	-1.511815	2.606849
6	-3.423496	-2.871404	2.797978
1	-2.563100	-4.819498	3.148518
1	-4.039647	-0.843112	2.480972
7	2.507958	-0.264578	1.884360
6	-3.840033	0.912368	-2.778060
6	-3.959910	1.660086	-3.960610
6	-5.007979	0.403572	-2.186008
6	-5.210269	1.892308	-4.534878
1	-3.063673	2.057651	-4.427403
6	-6.258602	0.635860	-2.760250
1	-4.933701	-0.172759	-1.269664
6	-6.364083	1.381633	-3.936401
1	-5.281293	2.469870	-5.452268
1	-7.150078	0.236791	-2.284550
1	-7.337590	1.562534	-4.383074
6	0.931417	4.923318	0.402242
6	0.147246	5.211160	1.531394
6	1.683336	5.956452	-0.178893
6	0.128383	6.496054	2.074125
1	-0.451335	4.420532	1.973241
6	1.663531	7.241581	0.364934
1	2.274461	5.748798	-1.065742

6	0.888424	7.514659	1.494345
1	-0.480558	6.701133	2.950349
1	2.247702	8.031208	-0.099433
1	0.873088	8.515609	1.916310
6	5.610214	-0.158943	-0.900923
6	6.366272	0.439039	-1.920749
6	6.283079	-0.824076	0.136703
6	7.760064	0.365447	-1.909046
1	5.853687	0.960461	-2.723846
6	7.676319	-0.897019	0.148258
1	5.704062	-1.278687	0.934496
6	8.419014	-0.303479	-0.875291
1	8.330250	0.829566	-2.708941
1	8.181677	-1.412240	0.960450
1	9.503852	-0.359885	-0.865832
6	0.144750	-4.619983	-1.107769
6	-0.672643	-5.151930	-0.098237
6	0.714124	-5.495238	-2.046176
6	-0.898793	-6.526090	-0.016532
1	-1.129458	-4.479116	0.619127
6	0.487207	-6.869859	-1.963782
1	1.326793	-5.091388	-2.846525
6	-0.316968	-7.390147	-0.946964
1	-1.531609	-6.920149	0.774150
1	0.932127	-7.533306	-2.700182
1	-0.493778	-8.460233	-0.884736
17	-5.082437	-3.476881	2.776650
6	-1.582106	0.439610	2.425920
1	-0.903882	0.792488	3.208775
1	-0.725964	0.376508	1.459060
6	-2.613443	1.450127	2.104705
6	-3.574212	1.260577	1.093667
6	-2.617979	2.676567	2.798593
6	-4.526754	2.240042	0.818897
1	-3.553490	0.347424	0.509436
6	-3.563541	3.660627	2.515966
1	-1.877255	2.846584	3.576044
6	-4.529422	3.442248	1.530337
1	-5.254529	2.070844	0.031352
1	-3.549346	4.595835	3.069034
1	-5.269539	4.206144	1.310031

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^{5}(23a-24a)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3300.2017007
Zero-point correction= 0.856447 (Hartree/Particle)
Thermal correction to Energy= 0.910542
Thermal correction to Enthalpy= 0.911486
Thermal correction to Gibbs Free Energy= 0.765223
Sum of electronic and zero-point Energies= -3299.345254
Sum of electronic and thermal Energies= -3299.291159
Sum of electronic and thermal Enthalpies= -3299.290215

Sum of electronic and thermal Free Energies= -3299.436478

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Cartesian Coordinates

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6	-2.090117	-0.648509	-1.910795
7	-0.818215	-1.003164	-1.515620
1	-3.859594	-1.857351	-2.594070
6	-0.754468	-2.376808	-1.565207
6	-2.028435	-2.904723	-1.995383
1	-2.252132	-3.950863	-2.141316
6	-2.844679	-1.839772	-2.226611
6	0.396215	-3.159034	-1.352549
7	2.016931	-1.298504	-1.082446
6	3.390191	-1.226665	-0.969848
6	3.941816	-2.559100	-1.020883
1	4.993026	-2.801340	-0.984703
6	2.895682	-3.427552	-1.107869
1	2.939179	-4.505506	-1.142609
6	1.690383	-2.637866	-1.174802
6	-2.582655	0.664581	-2.012881
1	-1.451209	5.055815	-1.089974
6	-1.406166	3.984388	-1.214384
6	-0.263149	3.158452	-0.910737
1	-3.371464	3.436245	-2.017648
7	-0.557016	1.843454	-1.199887
6	-1.850528	1.818238	-1.676348
6	-2.379248	3.161102	-1.694788
6	4.145948	-0.056997	-0.772221
1	3.661751	4.412625	0.306206
6	3.459196	3.406648	-0.029276
6	4.348459	2.386089	-0.177910
1	5.410206	2.403250	0.017673
6	3.600045	1.228492	-0.611764
7	2.273911	1.565186	-0.745327
6	2.161082	2.897127	-0.407732
6	0.976593	3.652626	-0.459947
6	3.217321	-1.234776	3.038460
6	2.658284	-2.152976	3.926444
6	1.281972	-2.363232	3.859665
6	0.497993	-1.676120	2.927213
6	1.170523	-0.720118	2.094690
1	4.288711	-1.040272	3.046020
1	3.276085	-2.679611	4.646166
1	0.805738	-3.070983	4.532690
26	0.661469	0.228043	-0.656542
7	0.482633	0.031634	1.174977
6	-0.944008	-2.008990	2.785818
6	-1.321273	-3.360036	2.773033
6	-1.956097	-1.018367	2.679341
6	-2.653190	-3.755794	2.653134
1	-0.551018	-4.123063	2.827821
6	-3.295013	-1.415535	2.579065
6	-3.627207	-2.767356	2.557573

1	-2.923432	-4.805496	2.626918
1	-4.080876	-0.672214	2.534471
7	2.506159	-0.524161	2.162332
6	-3.988941	0.850859	-2.488020
6	-4.249873	1.520985	-3.694068
6	-5.075827	0.369361	-1.739698
6	-5.559862	1.710962	-4.135621
1	-3.416607	1.891093	-4.283844
6	-6.386286	0.560517	-2.180751
1	-4.891732	-0.155146	-0.807059
6	-6.632654	1.233358	-3.379466
1	-5.741266	2.228967	-5.073224
1	-7.213237	0.184856	-1.584721
1	-7.652437	1.382026	-3.722871
6	1.023022	5.087123	-0.045582
6	0.248989	5.522747	1.043132
6	1.810597	6.024758	-0.732106
6	0.271342	6.860008	1.439643
1	-0.370261	4.804721	1.572919
6	1.831314	7.362367	-0.334774
1	2.399434	5.699607	-1.584553
6	1.063305	7.783666	0.753148
1	-0.329489	7.179605	2.286651
1	2.442416	8.076259	-0.880080
1	1.079736	8.825125	1.061826
6	5.630966	-0.187533	-0.657821
6	6.471035	0.425252	-1.601180
6	6.215559	-0.905520	0.397823
6	7.858442	0.318939	-1.494660
1	6.027692	0.983359	-2.420529
6	7.602566	-1.011479	0.504338
1	5.572010	-1.378004	1.132536
6	8.428578	-0.400011	-0.441787
1	8.493171	0.795053	-2.236848
1	8.038057	-1.567443	1.330056
1	9.508586	-0.482436	-0.358498
6	0.220943	-4.643879	-1.372706
6	-0.562688	-5.265321	-0.387148
6	0.802767	-5.439789	-2.371974
6	-0.746946	-6.648126	-0.391552
1	-1.028119	-4.652960	0.378113
6	0.618139	-6.823218	-2.375749
1	1.394034	-4.966669	-3.150216
6	-0.154768	-7.432176	-1.384351
1	-1.353752	-7.112614	0.381077
1	1.072329	-7.424022	-3.158767
1	-0.298763	-8.508925	-1.388839
17	-5.323378	-3.230018	2.401280
6	-1.539666	0.418107	2.695435
1	-0.912520	0.631902	3.566997
1	-0.678639	0.433099	1.805731
6	-2.471814	1.532027	2.401170
6	-3.377577	1.487327	1.325520

6	-2.407999	2.712110	3.166981
6	-4.218717	2.563111	1.052171
1	-3.399221	0.612369	0.687297
6	-3.243147	3.792719	2.887990
1	-1.701514	2.772523	3.990944
6	-4.158615	3.719302	1.833999
1	-4.907905	2.499612	0.215760
1	-3.183474	4.690846	3.496614
1	-4.810989	4.560223	1.616991

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^{oss}24a

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2338317
Zero-point correction= 0.863066 (Hartree/Particle)
Thermal correction to Energy= 0.917553
Thermal correction to Enthalpy= 0.918497
Thermal correction to Gibbs Free Energy= 0.771636
Sum of electronic and zero-point Energies= -3299.370765
Sum of electronic and thermal Energies= -3299.316279
Sum of electronic and thermal Enthalpies= -3299.315335
Sum of electronic and thermal Free Energies= -3299.462196

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Cartesian Coordinates

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6	-1.697083	-1.306502	-1.985136
7	-0.376631	-1.382403	-1.583800
1	-3.213481	-2.843966	-2.589233
6	-0.094217	-2.731179	-1.491516
6	-1.233008	-3.507512	-1.912596
1	-1.260018	-4.584974	-1.973704
6	-2.220305	-2.627139	-2.226025
6	1.113986	-3.292149	-1.063871
7	2.365109	-1.159499	-0.931489
6	3.689544	-0.863765	-0.674800
6	4.418580	-2.066728	-0.369643
1	5.467313	-2.107818	-0.116884
6	3.531839	-3.095813	-0.430472
1	3.716884	-4.142114	-0.240420
6	2.260586	-2.534544	-0.809869
6	-2.460371	-0.137992	-2.071448
1	-2.212108	4.353868	-1.109144
6	-1.941178	3.331512	-1.319768
6	-0.620113	2.774362	-1.174783
1	-3.814216	2.365723	-1.918152
7	-0.633238	1.425934	-1.478530
6	-1.944084	1.133944	-1.808311
6	-2.753740	2.323417	-1.728437
6	4.255674	0.413681	-0.640081
1	2.995544	4.841202	-0.478417
6	2.978372	3.764722	-0.561841
6	4.033463	2.908370	-0.591285
1	5.084553	3.147011	-0.531325

6	3.492097	1.578583	-0.716778
7	2.115754	1.634108	-0.834007
6	1.786425	2.968590	-0.713024
6	0.501028	3.513452	-0.790390
6	2.853711	-0.281133	3.113327
6	2.277090	-0.940660	4.196419
6	0.937085	-1.321685	4.077918
6	0.222229	-1.034488	2.918265
6	0.914277	-0.346255	1.862684
1	3.898973	0.024569	3.149925
1	2.850934	-1.154196	5.091828
1	0.439257	-1.851572	4.886053
26	0.836948	0.123736	-1.015005
7	0.257720	-0.041373	0.706549
6	-1.168114	-1.542836	2.739511
6	-1.355934	-2.928296	2.715399
6	-2.300385	-0.675485	2.556248
6	-2.608172	-3.509198	2.505389
1	-0.489137	-3.570581	2.838453
6	-3.573036	-1.281176	2.381982
6	-3.703550	-2.659984	2.343129
1	-2.729429	-4.585774	2.470398
1	-4.462789	-0.670072	2.332179
7	2.207153	0.015313	1.984044
6	-3.927559	-0.265781	-2.326365
6	-4.521764	0.279455	-3.473660
6	-4.744402	-0.914704	-1.384490
6	-5.900415	0.183433	-3.672441
1	-3.897246	0.780193	-4.207639
6	-6.122205	-1.007679	-1.582034
1	-4.290864	-1.342580	-0.495173
6	-6.704347	-0.457150	-2.726753
1	-6.345522	0.607646	-4.568157
1	-6.737673	-1.509191	-0.840513
1	-7.777093	-0.529171	-2.882182
6	0.326881	4.958299	-0.451576
6	0.551731	5.396258	0.863430
6	-0.065640	5.897030	-1.417877
6	0.374710	6.737224	1.206337
1	0.859393	4.674404	1.614037
6	-0.240502	7.238618	-1.075163
1	-0.231682	5.568377	-2.439471
6	-0.024058	7.662009	0.238170
1	0.547025	7.058631	2.229836
1	-0.542083	7.953438	-1.835716
1	-0.161841	8.706198	0.504470
6	5.727322	0.526688	-0.409852
6	6.640601	0.064577	-1.369914
6	6.222138	1.075985	0.784071
6	8.015057	0.154385	-1.144454
1	6.265543	-0.363870	-2.294716
6	7.596138	1.163974	1.009736
1	5.519063	1.430022	1.532004

6	8.496622	0.704096	0.045767
1	8.709134	-0.203236	-1.899932
1	7.962893	1.587502	1.940641
1	9.566471	0.772631	0.221659
6	1.171551	-4.774883	-0.886427
6	0.379149	-5.394382	0.093564
6	1.997391	-5.575176	-1.691002
6	0.418864	-6.777525	0.270693
1	-0.269430	-4.780310	0.710721
6	2.035900	-6.959064	-1.514316
1	2.604996	-5.105570	-2.458755
6	1.248583	-7.564046	-0.531992
1	-0.197221	-7.240719	1.036533
1	2.677184	-7.564838	-2.148463
1	1.279365	-8.641227	-0.394821
17	-5.307377	-3.358254	2.095899
6	-2.107781	0.746847	2.590886
1	-1.161225	1.061493	3.019712
1	-0.709222	-0.341468	0.713701
6	-2.930237	1.823971	2.122930
6	-4.098221	1.693455	1.323404
6	-2.512640	3.148173	2.437510
6	-4.825684	2.809236	0.926928
1	-4.408227	0.722855	0.961262
6	-3.234651	4.258388	2.024102
1	-1.601939	3.283392	3.014837
6	-4.409988	4.097580	1.278790
1	-5.711280	2.671298	0.312551
1	-2.879331	5.253774	2.274907
1	-4.979228	4.965224	0.958365

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^{3}24a

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2337017
Zero-point correction= 0.862668 (Hartree/Particle)
Thermal correction to Energy= 0.917333
Thermal correction to Enthalpy= 0.918277
Thermal correction to Gibbs Free Energy= 0.769840
Sum of electronic and zero-point Energies= -3299.371034
Sum of electronic and thermal Energies= -3299.316369
Sum of electronic and thermal Enthalpies= -3299.315425
Sum of electronic and thermal Free Energies= -3299.463861

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Cartesian Coordinates

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6	-1.703495	-1.405172	-1.820773
7	-0.365577	-1.431206	-1.471543
1	-3.216879	-3.006233	-2.241365
6	-0.042644	-2.768187	-1.341669
6	-1.187984	-3.589127	-1.643346
1	-1.194064	-4.668590	-1.642180
6	-2.210932	-2.747962	-1.947724

6	1.217970	-3.284591	-1.028720
7	2.390675	-1.105661	-0.893971
6	3.720036	-0.765961	-0.722829
6	4.527396	-1.953959	-0.617744
1	5.600744	-1.966814	-0.504821
6	3.681162	-3.015940	-0.670090
1	3.928507	-4.064407	-0.602747
6	2.354244	-2.488219	-0.863311
6	-2.477435	-0.257501	-2.016166
1	-2.254380	4.320819	-1.560272
6	-1.989510	3.275725	-1.607151
6	-0.699424	2.731801	-1.266419
1	-3.813682	2.255205	-2.268893
7	-0.692700	1.364471	-1.455382
6	-1.976228	1.038155	-1.854346
6	-2.777678	2.230372	-1.969406
6	4.226371	0.529428	-0.599408
1	2.765072	4.856403	-0.029644
6	2.798932	3.801729	-0.256953
6	3.882424	2.981503	-0.257503
1	4.906511	3.232753	-0.026041
6	3.411254	1.662456	-0.592915
7	2.048940	1.683174	-0.815178
6	1.661931	2.997847	-0.629681
6	0.376102	3.508228	-0.822709
6	2.879495	-0.151988	3.170717
6	2.335964	-0.848872	4.247892
6	1.014249	-1.289114	4.128005
6	0.284615	-1.016886	2.974501
6	0.942225	-0.287496	1.923193
1	3.906231	0.210596	3.213075
1	2.920309	-1.042853	5.140968
1	0.542387	-1.850049	4.930793
26	0.816577	0.125943	-0.964293
7	0.268534	0.010646	0.773902
6	-1.085015	-1.568077	2.778307
6	-1.235079	-2.953914	2.678764
6	-2.232135	-0.722497	2.608975
6	-2.461889	-3.549511	2.379682
1	-0.357275	-3.580558	2.804512
6	-3.477856	-1.340684	2.323085
6	-3.568142	-2.717633	2.197356
1	-2.554111	-4.624847	2.279718
1	-4.375434	-0.741005	2.250622
7	2.220019	0.122354	2.043384
6	-3.931329	-0.422376	-2.323895
6	-4.468716	0.006346	-3.546863
6	-4.791161	-0.996725	-1.372733
6	-5.833565	-0.126166	-3.808033
1	-3.810302	0.445074	-4.290789
6	-6.155533	-1.127201	-1.633449
1	-4.381663	-1.346260	-0.429855
6	-6.681186	-0.689926	-2.851491

1	-6.233468	0.208324	-4.761215
1	-6.804476	-1.570951	-0.883863
1	-7.743352	-0.791093	-3.055602
6	0.127199	4.960007	-0.565783
6	-0.721577	5.347744	0.482956
6	0.713113	5.952983	-1.365648
6	-0.972591	6.697969	0.728387
1	-1.186517	4.584649	1.099068
6	0.460999	7.303469	-1.118866
1	1.363218	5.659531	-2.184637
6	-0.381813	7.679836	-0.070496
1	-1.630368	6.982196	1.545133
1	0.918817	8.060636	-1.749401
1	-0.578270	8.731113	0.120772
6	5.692760	0.715649	-0.378230
6	6.483440	1.359406	-1.342252
6	6.300468	0.270660	0.806565
6	7.849723	1.549413	-1.129368
1	6.019805	1.709118	-2.260038
6	7.666198	0.461197	1.019226
1	5.691933	-0.223497	1.557668
6	8.444947	1.100691	0.051670
1	8.448832	2.045780	-1.887721
1	8.120749	0.114521	1.943177
1	9.508166	1.249538	0.217810
6	1.352999	-4.769281	-0.901506
6	0.752201	-5.440975	0.174114
6	2.061450	-5.517649	-1.853816
6	0.863758	-6.826153	0.299680
1	0.192771	-4.866919	0.905836
6	2.173688	-6.903188	-1.727954
1	2.521240	-5.006482	-2.694464
6	1.576523	-7.561218	-0.650357
1	0.395187	-7.330649	1.140228
1	2.723227	-7.468518	-2.475468
1	1.663819	-8.639656	-0.553172
17	-5.133270	-3.439939	1.811885
6	-2.097457	0.695763	2.787206
1	-1.221087	1.009224	3.347646
1	-0.696192	-0.295378	0.797048
6	-2.949964	1.757763	2.336130
6	-3.898992	1.636416	1.287290
6	-2.811352	3.036589	2.942431
6	-4.686477	2.715703	0.904497
1	-3.977452	0.709874	0.733371
6	-3.607339	4.107832	2.559086
1	-2.074950	3.164575	3.731532
6	-4.557649	3.954411	1.540772
1	-5.393332	2.592128	0.089022
1	-3.489398	5.068726	3.052459
1	-5.175625	4.794305	1.237509

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^{5}24a

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2410807
Zero-point correction= 0.859775 (Hartree/Particle)
Thermal correction to Energy= 0.915317
Thermal correction to Enthalpy= 0.916261
Thermal correction to Gibbs Free Energy= 0.762784
Sum of electronic and zero-point Energies= -3299.381305
Sum of electronic and thermal Energies= -3299.325764
Sum of electronic and thermal Enthalpies= -3299.324820
Sum of electronic and thermal Free Energies= -3299.478297

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Cartesian Coordinates

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6	-1.705308	-1.305355	-1.892421
7	-0.368021	-1.394016	-1.575094
1	-3.262145	-2.854977	-2.368572
6	-0.054667	-2.735407	-1.541712
6	-1.228223	-3.512394	-1.868618
1	-1.260687	-4.589226	-1.941799
6	-2.243902	-2.632063	-2.086684
6	1.210999	-3.282863	-1.270668
7	2.454435	-1.158707	-0.952872
6	3.770523	-0.846441	-0.683946
6	4.546764	-2.061257	-0.623858
1	5.611287	-2.111897	-0.450926
6	3.686254	-3.100148	-0.816057
1	3.917478	-4.154731	-0.821035
6	2.377134	-2.533773	-1.032158
6	-2.442510	-0.116371	-2.024660
1	-2.044585	4.482414	-1.714135
6	-1.820578	3.426598	-1.709344
6	-0.546776	2.847247	-1.358663
1	-3.697351	2.459976	-2.304576
7	-0.616507	1.475008	-1.486498
6	-1.908104	1.175488	-1.866332
6	-2.660176	2.398110	-2.012788
6	4.288594	0.441471	-0.461393
1	3.013630	4.874453	-0.096511
6	3.003046	3.811113	-0.283189
6	4.041928	2.936800	-0.171452
1	5.057156	3.153822	0.125368
6	3.533831	1.626546	-0.502612
7	2.195729	1.720087	-0.813959
6	1.849046	3.049526	-0.698915
6	0.575249	3.590023	-0.947442
6	2.656513	-0.961674	3.359694
6	2.009014	-1.746006	4.314110
6	0.640937	-1.972931	4.143374
6	-0.036868	-1.412548	3.062449
6	0.724032	-0.616049	2.140230
1	3.723641	-0.760702	3.447387
1	2.552744	-2.164354	5.154305

1	0.090665	-2.589273	4.849755
26	0.835005	0.141228	-0.764620
7	0.155259	-0.058239	1.033755
6	-1.461896	-1.748658	2.794970
6	-1.793505	-3.087628	2.562778
6	-2.483171	-0.746859	2.694805
6	-3.086663	-3.485102	2.220576
1	-1.008362	-3.835668	2.622429
6	-3.797683	-1.164210	2.364414
6	-4.073069	-2.502198	2.127511
1	-3.320248	-4.525098	2.024015
1	-4.604012	-0.442489	2.343412
7	2.050037	-0.412781	2.306428
6	-3.908034	-0.235288	-2.300813
6	-4.462182	0.205273	-3.512118
6	-4.759564	-0.787404	-1.329796
6	-5.835616	0.106311	-3.741528
1	-3.810007	0.624752	-4.272471
6	-6.132329	-0.885446	-1.559011
1	-4.337707	-1.143459	-0.395436
6	-6.674699	-0.436302	-2.765217
1	-6.248917	0.449177	-4.686018
1	-6.771863	-1.313903	-0.792972
1	-7.743330	-0.511956	-2.945355
6	0.383864	5.059612	-0.746866
6	-0.470369	5.520914	0.267952
6	1.036830	5.997824	-1.560773
6	-0.664666	6.888465	0.462970
1	-0.980622	4.800893	0.900148
6	0.841825	7.365921	-1.363919
1	1.693367	5.647931	-2.352002
6	-0.009420	7.815147	-0.351694
1	-1.327439	7.229179	1.253799
1	1.350516	8.080011	-2.005601
1	-0.161606	8.880080	-0.199719
6	5.738819	0.557971	-0.115185
6	6.636165	1.197033	-0.984641
6	6.225465	0.036185	1.093873
6	7.987534	1.309589	-0.654257
1	6.267405	1.602127	-1.922400
6	7.576297	0.149302	1.424029
1	5.533651	-0.455839	1.770625
6	8.461393	0.786106	0.550770
1	8.670236	1.802819	-1.340580
1	7.936293	-0.255941	2.365657
1	9.513239	0.874130	0.807799
6	1.315512	-4.775008	-1.223459
6	0.701735	-5.487831	-0.181505
6	2.014461	-5.487344	-2.209448
6	0.788153	-6.879240	-0.124766
1	0.156263	-4.940032	0.581517
6	2.101466	-6.879346	-2.152115
1	2.486237	-4.943183	-3.022313

6	1.489305	-7.578935	-1.109734
1	0.310337	-7.416304	0.689974
1	2.643322	-7.416937	-2.925248
1	1.556873	-8.662280	-1.066041
17	-5.721300	-2.975566	1.705768
6	-2.162747	0.627864	2.974906
1	-1.286068	0.781769	3.597853
1	-0.851981	-0.182018	1.012550
6	-2.807810	1.822672	2.517263
6	-3.716677	1.879268	1.426217
6	-2.475452	3.051666	3.151837
6	-4.282443	3.084782	1.029124
1	-3.936933	0.984623	0.856700
6	-3.050977	4.250024	2.752682
1	-1.762405	3.039927	3.971921
6	-3.965787	4.275957	1.691127
1	-4.961696	3.097706	0.181941
1	-2.786031	5.170696	3.265408
1	-4.409826	5.214646	1.373480

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^{oss}25a

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2265177
Zero-point correction= 0.863441 (Hartree/Particle)
Thermal correction to Energy= 0.917591
Thermal correction to Enthalpy= 0.918535
Thermal correction to Gibbs Free Energy= 0.773978
Sum of electronic and zero-point Energies= -3299.363077
Sum of electronic and thermal Energies= -3299.308927
Sum of electronic and thermal Enthalpies= -3299.307983
Sum of electronic and thermal Free Energies= -3299.452539

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Cartesian Coordinates

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6	-2.186773	-0.580855	-1.576122
7	-0.900660	-1.022021	-1.322642
1	-4.020129	-1.579725	-2.393468
6	-0.905465	-2.377538	-1.618105
6	-2.193563	-2.765391	-2.129591
1	-2.451734	-3.752096	-2.482330
6	-2.989416	-1.663564	-2.084342
6	0.152229	-3.263221	-1.387661
7	1.814017	-1.524036	-0.815050
6	3.127923	-1.576508	-0.387954
6	3.502040	-2.938661	-0.109002
1	4.456684	-3.253240	0.284259
6	2.439872	-3.719412	-0.449525
1	2.360371	-4.794372	-0.388580
6	1.396520	-2.837091	-0.905105
6	-2.658360	0.730048	-1.418190
1	-1.061997	5.034757	-0.933451
6	-1.124707	3.961517	-1.032034

6	0.003391	3.072716	-1.151229
1	-3.267034	3.505714	-0.955311
7	-0.426202	1.762491	-1.209590
6	-1.805637	1.818972	-1.199396
6	-2.241212	3.186318	-1.046234
6	3.995967	-0.483948	-0.329450
1	4.151456	4.012534	-1.348426
6	3.799228	3.011318	-1.151117
6	4.536193	1.906553	-0.854736
1	5.609436	1.827214	-0.766376
6	3.612932	0.812962	-0.693730
7	2.324260	1.242753	-0.933950
6	2.416625	2.607204	-1.144139
6	1.336115	3.494237	-1.205562
6	2.949538	-1.060236	3.246169
6	2.343004	-2.237342	3.679329
6	1.027471	-2.470203	3.282482
6	0.370417	-1.569666	2.436434
6	1.124828	-0.463516	1.951716
1	3.953769	-0.801891	3.576665
1	2.863799	-2.921395	4.341117
1	0.483447	-3.329367	3.664957
26	0.667630	0.120446	-0.824351
7	0.578756	0.417771	1.025495
6	-1.077287	-1.762585	2.165867
6	-1.514697	-3.015249	1.725223
6	-2.046054	-0.744156	2.451242
6	-2.866239	-3.314778	1.550873
1	-0.773579	-3.773277	1.493663
6	-3.415556	-1.068553	2.290089
6	-3.800361	-2.323879	1.845453
1	-3.188229	-4.291061	1.207862
1	-4.174622	-0.350838	2.572028
7	2.369901	-0.201518	2.402935
6	-4.124088	0.974438	-1.556203
6	-4.627391	1.876753	-2.509024
6	-5.037363	0.292092	-0.734250
6	-5.999057	2.105856	-2.618871
1	-3.936316	2.391535	-3.169123
6	-6.408362	0.524938	-0.840557
1	-4.662675	-0.421316	-0.009847
6	-6.894084	1.435928	-1.781012
1	-6.368873	2.804108	-3.364571
1	-7.093437	-0.007592	-0.187263
1	-7.961735	1.617918	-1.865493
6	1.610334	4.960447	-1.286024
6	2.268187	5.628882	-0.241085
6	1.199848	5.699325	-2.407053
6	2.512412	7.000435	-0.317394
1	2.580710	5.066105	0.633385
6	1.447188	7.070378	-2.484318
1	0.689022	5.189734	-3.218622
6	2.104023	7.724804	-1.439730

1	3.017621	7.503484	0.502354
1	1.128840	7.626213	-3.361819
1	2.295362	8.792515	-1.499238
6	5.394615	-0.689869	0.147146
6	6.299397	-1.511138	-0.542690
6	5.823759	-0.042882	1.318386
6	7.600218	-1.688220	-0.068436
1	5.979278	-2.003736	-1.455922
6	7.123257	-0.222842	1.792468
1	5.121792	0.592072	1.849737
6	8.014902	-1.046920	1.101021
1	8.291064	-2.322860	-0.616469
1	7.438867	0.279760	2.702611
1	9.027382	-1.185960	1.469507
6	-0.030350	-4.718278	-1.668744
6	-1.044675	-5.466783	-1.049748
6	0.828339	-5.373939	-2.568358
6	-1.194140	-6.827878	-1.316400
1	-1.716528	-4.971851	-0.359476
6	0.677778	-6.734163	-2.837334
1	1.612356	-4.805949	-3.059705
6	-0.332969	-7.466947	-2.210741
1	-1.982384	-7.388826	-0.822006
1	1.348177	-7.220303	-3.540521
1	-0.449473	-8.526653	-2.419252
17	-5.522561	-2.681849	1.664874
6	-1.638925	0.531183	2.978926
1	-0.687984	0.541111	3.501167
6	-2.313838	1.792325	2.922877
6	-3.392950	2.087531	2.047389
6	-1.847142	2.849193	3.752928
6	-3.990101	3.341890	2.039685
1	-3.727456	1.344183	1.337414
6	-2.446848	4.100850	3.737432
1	-1.006911	2.660703	4.416676
6	-3.531021	4.356391	2.887148
1	-4.810477	3.533045	1.352914
1	-2.071111	4.885244	4.388904
1	-3.999670	5.336109	2.875717
1	1.048086	1.314376	1.151678

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^{3}25a

Number of imaginary frequencies : 0
Electronic energy : HF=-3300.2300517
Zero-point correction= 0.862282 (Hartree/Particle)
Thermal correction to Energy= 0.916827
Thermal correction to Enthalpy= 0.917772
Thermal correction to Gibbs Free Energy= 0.770950
Sum of electronic and zero-point Energies= -3299.367770
Sum of electronic and thermal Energies= -3299.313224
Sum of electronic and thermal Enthalpies= -3299.312280
Sum of electronic and thermal Free Energies= -3299.459101

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Cartesian Coordinates
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6	-2.204411	-0.548787	-1.625917
7	-0.922524	-0.994987	-1.370318
1	-4.032391	-1.536044	-2.463273
6	-0.917055	-2.342116	-1.691873
6	-2.201447	-2.722823	-2.216644
1	-2.455778	-3.704918	-2.585015
6	-3.001686	-1.623336	-2.154772
6	0.141686	-3.227647	-1.463585
7	1.800740	-1.488700	-0.864777
6	3.108273	-1.541438	-0.408162
6	3.468296	-2.902413	-0.121208
1	4.412404	-3.218868	0.294965
6	2.411401	-3.681340	-0.487382
1	2.327614	-4.755965	-0.426230
6	1.378718	-2.800730	-0.961702
6	-2.676605	0.757547	-1.435445
1	-1.047950	5.042388	-0.908946
6	-1.115626	3.970776	-1.020865
6	0.008133	3.084747	-1.166320
1	-3.260158	3.524582	-0.914777
7	-0.432801	1.775325	-1.232738
6	-1.815368	1.836812	-1.205207
6	-2.237788	3.200456	-1.025494
6	3.987946	-0.457985	-0.342243
1	4.163626	4.030297	-1.404284
6	3.808686	3.032096	-1.196181
6	4.544578	1.927291	-0.890616
1	5.617721	1.845171	-0.802174
6	3.618856	0.838753	-0.718508
7	2.332191	1.275420	-0.948013
6	2.424403	2.632720	-1.176857
6	1.338819	3.514696	-1.236327
6	2.995500	-1.139882	3.327476
6	2.395712	-2.339802	3.705084
6	1.074561	-2.550604	3.306865
6	0.409028	-1.609674	2.517555
6	1.153412	-0.464121	2.087509
1	4.005704	-0.902446	3.658303
1	2.922889	-3.057163	4.325048
1	0.536178	-3.432329	3.644501
26	0.648139	0.141680	-0.813661
7	0.609312	0.425100	1.197446
6	-1.031570	-1.804243	2.213771
6	-1.452854	-3.044242	1.720176
6	-2.017159	-0.801831	2.501879
6	-2.798560	-3.347717	1.508545
1	-0.702929	-3.790553	1.478308
6	-3.379801	-1.126903	2.294549
6	-3.746570	-2.371854	1.807017
1	-3.106570	-4.316930	1.134110

1	-4.149304	-0.419811	2.575860
7	2.409302	-0.230011	2.545934
6	-4.143493	1.003699	-1.542102
6	-4.666652	1.928434	-2.462204
6	-5.038248	0.299293	-0.718224
6	-6.040536	2.157610	-2.538122
1	-3.989909	2.459863	-3.124029
6	-6.411300	0.532245	-0.791094
1	-4.647798	-0.428921	-0.017072
6	-6.917091	1.465359	-1.698762
1	-6.426709	2.873165	-3.258668
1	-7.082020	-0.016836	-0.136691
1	-7.986434	1.647641	-1.756667
6	1.604908	4.981088	-1.327829
6	2.286063	5.654755	-0.300983
6	1.165915	5.715408	-2.441366
6	2.525087	7.026522	-0.387949
1	2.618939	5.096301	0.568679
6	1.408061	7.086648	-2.529048
1	0.637965	5.201895	-3.239389
6	2.088308	7.746032	-1.502684
1	3.047864	7.533593	0.418135
1	1.067704	7.638739	-3.400596
1	2.275598	8.813953	-1.570298
6	5.378696	-0.673168	0.151643
6	6.290170	-1.492324	-0.531606
6	5.791167	-0.034459	1.333235
6	7.584455	-1.673763	-0.041436
1	5.980975	-1.979339	-1.451661
6	7.084188	-0.219522	1.822833
1	5.079209	0.590692	1.863044
6	7.984045	-1.039572	1.137171
1	8.281773	-2.306283	-0.583652
1	7.387863	0.275158	2.741282
1	8.991409	-1.182149	1.518116
6	-0.032294	-4.680099	-1.757777
6	-1.049389	-5.435242	-1.151685
6	0.837687	-5.326755	-2.653045
6	-1.192476	-6.794810	-1.428863
1	-1.724784	-4.946230	-0.460689
6	0.693340	-6.685530	-2.932280
1	1.624574	-4.753145	-3.133228
6	-0.321476	-7.424969	-2.320106
1	-1.982473	-7.361761	-0.944325
1	1.371705	-7.165414	-3.632065
1	-0.432870	-8.483584	-2.536679
17	-5.462335	-2.736173	1.575201
6	-1.636223	0.460992	3.078530
1	-0.709506	0.461153	3.642497
6	-2.323075	1.715898	3.025654
6	-3.356595	2.023051	2.100571
6	-1.920884	2.752015	3.913087
6	-3.974877	3.267272	2.099621

1	-3.638475	1.296402	1.351244
6	-2.541495	3.993704	3.904525
1	-1.115182	2.554919	4.615886
6	-3.581924	4.260094	3.004242
1	-4.761035	3.467045	1.376133
1	-2.216513	4.761894	4.601110
1	-4.067528	5.231617	2.999389
1	1.145746	1.290550	1.273467

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^{5}25a

Number of imaginary frequencies : 0 Electronic energy : HF=-3300.2340432
Zero-point correction= 0.861313 (Hartree/Particle)
Thermal correction to Energy= 0.916029
Thermal correction to Enthalpy= 0.916973
Thermal correction to Gibbs Free Energy= 0.769113
Sum of electronic and zero-point Energies= -3299.372730
Sum of electronic and thermal Energies= -3299.318014
Sum of electronic and thermal Enthalpies= -3299.317070
Sum of electronic and thermal Free Energies= -3299.464930

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Cartesian Coordinates

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6	-2.496983	-0.082285	-1.575718
7	-1.326376	-0.746692	-1.282707
1	-4.429309	-0.745914	-2.510695
6	-1.524070	-2.069536	-1.624794
6	-2.841098	-2.224600	-2.195592
1	-3.244080	-3.139701	-2.601298
6	-3.445696	-1.005686	-2.149677
6	-0.603013	-3.115886	-1.427029
7	1.372063	-1.693856	-0.950643
6	2.691871	-1.951230	-0.630254
6	2.850410	-3.358550	-0.365329
1	3.765611	-3.834457	-0.046636
6	1.645376	-3.952432	-0.610630
1	1.399621	-5.000336	-0.523820
6	0.727550	-2.913315	-1.005504
6	-2.737349	1.295456	-1.396218
1	-0.462313	5.275281	-0.714342
6	-0.691727	4.232661	-0.876777
6	0.282073	3.188096	-1.081375
1	-2.880100	4.125342	-0.769061
7	-0.365776	1.976654	-1.205395
6	-1.720845	2.240512	-1.155783
6	-1.923042	3.647780	-0.910814
6	3.735029	-1.006916	-0.664797
1	4.547457	3.476279	-1.493256
6	4.053728	2.533071	-1.312633
6	4.628530	1.309026	-1.152274
1	5.679939	1.064076	-1.178014
6	3.557129	0.359330	-0.951730
7	2.349161	1.009566	-1.042555

6	2.623762	2.348210	-1.199535
6	1.674618	3.386267	-1.155538
6	3.421301	-0.297138	3.399574
6	3.050164	-1.528488	3.935786
6	1.773863	-2.006693	3.634150
6	0.927843	-1.283315	2.791234
6	1.444520	-0.081738	2.217980
1	4.383313	0.146033	3.652842
1	3.717098	-2.071908	4.596524
1	1.411369	-2.926366	4.085312
26	0.466726	0.150552	-0.599960
7	0.702908	0.624979	1.295166
6	-0.459206	-1.741402	2.538220
6	-0.676258	-3.071560	2.172199
6	-1.583266	-0.865070	2.700619
6	-1.955296	-3.574155	1.932527
1	0.179310	-3.725878	2.039277
6	-2.871531	-1.376144	2.419587
6	-3.035193	-2.699597	2.035287
1	-2.100368	-4.610567	1.655845
1	-3.744196	-0.753535	2.569594
7	2.655821	0.408391	2.560824
6	-4.144235	1.771673	-1.527926
6	-4.482269	2.814493	-2.408859
6	-5.175627	1.173123	-0.780459
6	-5.799310	3.259847	-2.519313
1	-3.705488	3.266313	-3.017326
6	-6.492355	1.619468	-0.889942
1	-4.938153	0.356044	-0.107216
6	-6.808708	2.668600	-1.756189
1	-6.037727	4.064421	-3.209268
1	-7.269413	1.148649	-0.294553
1	-7.833865	3.017613	-1.840865
6	2.175081	4.793735	-1.158472
6	3.000832	5.263392	-0.123761
6	1.822971	5.676291	-2.192739
6	3.462837	6.579840	-0.124921
1	3.271744	4.589859	0.683762
6	2.287589	6.991852	-2.194659
1	1.187164	5.320571	-2.997973
6	3.108642	7.447613	-1.160641
1	4.095874	6.928356	0.686320
1	2.011177	7.659096	-3.006276
1	3.469567	8.472240	-1.161703
6	5.124717	-1.479340	-0.390980
6	5.743845	-2.439985	-1.206934
6	5.841449	-0.956022	0.697900
6	7.043285	-2.870820	-0.936898
1	5.202391	-2.840229	-2.058799
6	7.139352	-1.389332	0.968616
1	5.364593	-0.213713	1.329060
6	7.744105	-2.348517	0.152694
1	7.510026	-3.610135	-1.581835

1	7.677111	-0.979245	1.819027
1	8.755476	-2.684970	0.362822
6	-1.041790	-4.512726	-1.713952
6	-2.219540	-5.041766	-1.155212
6	-0.288768	-5.334969	-2.572460
6	-2.618629	-6.349720	-1.428464
1	-2.822289	-4.420887	-0.503523
6	-0.688643	-6.642677	-2.846470
1	0.608479	-4.936049	-3.034912
6	-1.852895	-7.157558	-2.271996
1	-3.528560	-6.736304	-0.977990
1	-0.093249	-7.256557	-3.516534
1	-2.163382	-8.176641	-2.484433
17	-4.661569	-3.296794	1.680426
6	-1.388991	0.459981	3.231092
1	-0.505985	0.584724	3.850119
6	-2.200680	1.630150	3.093072
6	-3.197975	1.796313	2.097224
6	-1.962790	2.728551	3.964500
6	-3.936524	2.970329	2.009184
1	-3.346686	1.017381	1.361906
6	-2.703646	3.898381	3.870967
1	-1.187506	2.637471	4.721214
6	-3.703933	4.025904	2.897979
1	-4.687258	3.066342	1.230539
1	-2.503966	4.718049	4.555882
1	-4.283040	4.941853	2.824522
1	1.063273	1.580574	1.271762

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^{oss}(25a-8a)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3300.2088385
Zero-point correction= 0.864899 (Hartree/Particle)
Thermal correction to Energy= 0.917692
Thermal correction to Enthalpy= 0.918636
Thermal correction to Gibbs Free Energy= 0.777879
Sum of electronic and zero-point Energies= -3299.343939
Sum of electronic and thermal Energies= -3299.291146
Sum of electronic and thermal Enthalpies= -3299.290202
Sum of electronic and thermal Free Energies= -3299.430960

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Cartesian Coordinates

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6	-2.428726	0.541171	-1.676131
7	-1.414129	-0.325709	-1.300407
1	-4.433243	0.228902	-2.636977
6	-1.912202	-1.599527	-1.521516
6	-3.222527	-1.521442	-2.115571
1	-3.811480	-2.366223	-2.438212
6	-3.538287	-0.203222	-2.216238
6	-1.259449	-2.803964	-1.225306
7	0.957171	-1.784095	-0.869786

6	2.220045	-2.316737	-0.712514
6	2.130709	-3.732884	-0.451468
1	2.968965	-4.380661	-0.243233
6	0.813749	-4.066674	-0.532095
1	0.368695	-5.041596	-0.402532
6	0.091334	-2.857367	-0.851501
6	-2.419943	1.934187	-1.523996
1	0.430858	5.333931	-0.218930
6	0.034063	4.372422	-0.508192
6	0.811985	3.169816	-0.692299
1	-2.123636	4.693787	-0.745465
7	-0.018822	2.111546	-0.998792
6	-1.283196	2.643602	-1.110715
6	-1.258621	4.049845	-0.781899
6	3.417492	-1.608925	-0.869923
1	5.006353	2.710050	-1.106131
6	4.351207	1.852753	-1.063232
6	4.685283	0.537837	-1.166669
1	5.667499	0.112749	-1.307899
6	3.466075	-0.218854	-1.034207
7	2.386835	0.641697	-0.955559
6	2.921418	1.913965	-0.899207
6	2.209900	3.099678	-0.665891
6	3.480154	-0.831652	2.726721
6	3.088070	-2.056027	3.259849
6	1.747875	-2.422775	3.136507
6	0.852925	-1.597933	2.448246
6	1.388513	-0.422796	1.855494
1	4.495335	-0.464754	2.863646
1	3.795702	-2.680511	3.794947
1	1.383872	-3.326469	3.616166
26	0.466784	0.166436	-0.789787
7	0.543731	0.406215	1.087982
6	-0.599224	-1.885714	2.426451
6	-1.056621	-3.201070	2.316429
6	-1.548003	-0.827857	2.574746
6	-2.415689	-3.512372	2.344497
1	-0.338402	-4.000719	2.169998
6	-2.918193	-1.145440	2.587324
6	-3.328791	-2.468516	2.469373
1	-2.754647	-4.535825	2.240219
1	-3.655744	-0.368234	2.740344
7	2.656820	-0.034239	2.033601
6	-3.667069	2.695588	-1.824006
6	-3.655089	3.753648	-2.749207
6	-4.884261	2.376338	-1.195895
6	-4.816709	4.473733	-3.029295
1	-2.727001	4.002682	-3.254228
6	-6.046094	3.095981	-1.475135
1	-4.912552	1.561233	-0.479867
6	-6.016136	4.149740	-2.391691
1	-4.784844	5.284593	-3.751689
1	-6.973284	2.835319	-0.972404

1	-6.920491	4.710712	-2.609601
6	2.990139	4.341355	-0.385788
6	3.810385	4.410577	0.752641
6	2.927524	5.453078	-1.240688
6	4.543301	5.564373	1.031523
1	3.863483	3.551648	1.415313
6	3.662899	6.606042	-0.962327
1	2.303420	5.404363	-2.127920
6	4.471658	6.665632	0.174924
1	5.168568	5.603584	1.919235
1	3.608003	7.455576	-1.637412
1	5.043394	7.563688	0.391485
6	4.696542	-2.381827	-0.863948
6	4.942130	-3.353689	-1.848109
6	5.673197	-2.163990	0.120890
6	6.129925	-4.085719	-1.847514
1	4.195043	-3.527541	-2.616692
6	6.860125	-2.897337	0.123180
1	5.490282	-1.419146	0.887091
6	7.092734	-3.860670	-0.860981
1	6.304196	-4.829012	-2.620543
1	7.601741	-2.718235	0.896867
1	8.017260	-4.431177	-0.859686
6	-2.014382	-4.080403	-1.396339
6	-3.237542	-4.289728	-0.735890
6	-1.535069	-5.095338	-2.243419
6	-3.945785	-5.480264	-0.897563
1	-3.629113	-3.512026	-0.092062
6	-2.243748	-6.285947	-2.406664
1	-0.606519	-4.939817	-2.783659
6	-3.449443	-6.485646	-1.730381
1	-4.884779	-5.619369	-0.368950
1	-1.856752	-7.054217	-3.070364
1	-4.000254	-7.413431	-1.857037
17	-5.057534	-2.834148	2.472064
6	-1.058237	0.522680	2.804474
1	-0.177484	0.571204	3.437781
6	-1.751652	1.777227	2.685534
6	-2.882032	1.998885	1.862490
6	-1.244989	2.883553	3.416640
6	-3.503312	3.243544	1.830096
1	-3.243489	1.199949	1.226450
6	-1.861332	4.126355	3.368367
1	-0.362211	2.742675	4.035502
6	-3.005904	4.310602	2.584353
1	-4.367642	3.391875	1.191804
1	-1.454898	4.952964	3.944431
1	-3.495388	5.279447	2.547762
1	0.843024	1.371887	1.228522

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^{3}(25a-8a)‡

Number of imaginary frequencies : 1

Electronic energy : HF=-3300.2251457
Zero-point correction= 0.862772 (Hartree/Particle)
Thermal correction to Energy= 0.916268
Thermal correction to Enthalpy= 0.917213
Thermal correction to Gibbs Free Energy= 0.773301
Sum of electronic and zero-point Energies= -3299.362374
Sum of electronic and thermal Energies= -3299.308877
Sum of electronic and thermal Enthalpies= -3299.307933
Sum of electronic and thermal Free Energies= -3299.451844

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Cartesian Coordinates

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6	-2.439647	0.455590	-1.696848
7	-1.402380	-0.384294	-1.333290
1	-4.430147	0.102075	-2.669275
6	-1.848699	-1.666919	-1.596019
6	-3.157659	-1.619849	-2.197023
1	-3.711991	-2.476981	-2.547077
6	-3.521739	-0.312144	-2.259319
6	-1.155984	-2.850170	-1.315035
7	1.030057	-1.750146	-0.941197
6	2.303135	-2.239688	-0.700527
6	2.235573	-3.642912	-0.402018
1	3.078352	-4.258565	-0.126654
6	0.931626	-4.019603	-0.536963
1	0.509018	-5.002577	-0.394448
6	0.189430	-2.849775	-0.917699
6	-2.471912	1.843528	-1.519003
1	0.318865	5.299516	-0.250260
6	-0.054457	4.331240	-0.547811
6	0.757991	3.168355	-0.783113
1	-2.233091	4.577886	-0.678181
7	-0.049541	2.085454	-1.087167
6	-1.341209	2.575185	-1.130021
6	-1.348708	3.966917	-0.770604
6	3.494434	-1.511114	-0.815811
1	4.969930	2.840216	-1.218843
6	4.341825	1.966442	-1.129874
6	4.713874	0.659039	-1.169782
1	5.706872	0.254928	-1.296667
6	3.514999	-0.125200	-1.002750
7	2.415299	0.705414	-0.943771
6	2.910244	1.992021	-0.959350
6	2.158876	3.158797	-0.775062
6	3.460983	-0.797471	2.854668
6	3.078486	-2.045526	3.338077
6	1.739620	-2.416170	3.190984
6	0.844118	-1.573996	2.530244
6	1.367085	-0.361717	1.985453
1	4.475020	-0.432814	3.011322
1	3.788200	-2.683967	3.853457
1	1.379396	-3.341688	3.631399
26	0.473937	0.166460	-0.797372

7	0.528496	0.454268	1.240063
6	-0.603080	-1.881259	2.459845
6	-1.032353	-3.196045	2.260950
6	-1.580333	-0.850731	2.634649
6	-2.385069	-3.535090	2.219387
1	-0.293246	-3.973826	2.100735
6	-2.943059	-1.194885	2.568980
6	-3.322755	-2.515766	2.357844
1	-2.697460	-4.558440	2.051221
1	-3.701793	-0.440696	2.734877
7	2.639982	0.026354	2.191246
6	-3.750211	2.569023	-1.765101
6	-3.801784	3.650728	-2.661256
6	-4.936328	2.187113	-1.112726
6	-4.996441	4.333419	-2.890408
1	-2.898204	3.946703	-3.185036
6	-6.130807	2.870183	-1.341105
1	-4.913347	1.355726	-0.415544
6	-6.164753	3.947625	-2.229610
1	-5.014969	5.163314	-3.591247
1	-7.033084	2.562988	-0.819892
1	-7.094799	4.479877	-2.407609
6	2.887775	4.441995	-0.556111
6	3.741617	4.586357	0.550304
6	2.741017	5.522423	-1.441042
6	4.426932	5.781906	0.767181
1	3.856134	3.754776	1.239351
6	3.429103	6.716774	-1.224614
1	2.089119	5.416134	-2.302920
6	4.273182	6.850282	-0.119656
1	5.078370	5.879545	1.631128
1	3.309667	7.540882	-1.922419
1	4.807882	7.780815	0.048922
6	4.789002	-2.250110	-0.738733
6	5.088125	-3.265664	-1.662525
6	5.733416	-1.948880	0.256234
6	6.295575	-3.960902	-1.591709
1	4.368619	-3.501489	-2.440776
6	6.939596	-2.645820	0.328361
1	5.507949	-1.169949	0.975723
6	7.224809	-3.654308	-0.594955
1	6.511809	-4.738948	-2.318483
1	7.654730	-2.403346	1.109559
1	8.164429	-4.196660	-0.538963
6	-1.856373	-4.153324	-1.502281
6	-3.089600	-4.407678	-0.876551
6	-1.311073	-5.152380	-2.328397
6	-3.745364	-5.625476	-1.054492
1	-3.528140	-3.646023	-0.243533
6	-1.967739	-6.370007	-2.507454
1	-0.372677	-4.963146	-2.840192
6	-3.185300	-6.613367	-1.867711
1	-4.692899	-5.800191	-0.552480

1	-1.530846	-7.125470	-3.154579
1	-3.695653	-7.562275	-2.006456
17	-5.044461	-2.910845	2.261756
6	-1.137422	0.494435	2.963547
1	-0.275061	0.535220	3.621847
6	-1.845274	1.737907	2.839853
6	-2.919858	1.963999	1.943983
6	-1.413748	2.834867	3.632159
6	-3.557885	3.199583	1.894264
1	-3.222612	1.174991	1.265886
6	-2.047894	4.067976	3.568969
1	-0.574348	2.693326	4.308536
6	-3.135533	4.256024	2.707461
1	-4.378287	3.347138	1.199673
1	-1.699471	4.885774	4.193968
1	-3.638056	5.217750	2.659371
1	0.881543	1.409824	1.311234

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^{5}(25a-8a)‡

Number of imaginary frequencies : 1
Electronic energy : HF=-3300.2208596
Zero-point correction= 0.860596 (Hartree/Particle)
Thermal correction to Energy= 0.914663
Thermal correction to Enthalpy= 0.915607
Thermal correction to Gibbs Free Energy= 0.770095
Sum of electronic and zero-point Energies= -3299.360264
Sum of electronic and thermal Energies= -3299.306197
Sum of electronic and thermal Enthalpies= -3299.305253
Sum of electronic and thermal Free Energies= -3299.450764

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Cartesian Coordinates

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6	-2.552853	0.042271	-1.645463
7	-1.420428	-0.663159	-1.309521
1	-4.484242	-0.560146	-2.626668
6	-1.660243	-1.979686	-1.633086
6	-2.968327	-2.097746	-2.232426
1	-3.397767	-3.007146	-2.625089
6	-3.521861	-0.851856	-2.233247
6	-0.774458	-3.048592	-1.393398
7	1.254655	-1.679210	-0.984614
6	2.574623	-1.981920	-0.707015
6	2.693585	-3.391369	-0.424005
1	3.602365	-3.895263	-0.130659
6	1.459432	-3.944422	-0.607127
1	1.178699	-4.980010	-0.485272
6	0.567429	-2.878593	-0.993399
6	-2.742304	1.425800	-1.447841
1	-0.367326	5.284811	-0.478703
6	-0.622017	4.261297	-0.710591
6	0.325648	3.198770	-0.952078
1	-2.815482	4.220431	-0.684850

7	-0.354305	2.015018	-1.164497
6	-1.699422	2.323192	-1.139160
6	-1.868655	3.721330	-0.822669
6	3.657414	-1.083472	-0.789034
1	4.603646	3.413253	-1.388663
6	4.087493	2.473304	-1.259476
6	4.629750	1.226626	-1.197372
1	5.673025	0.956023	-1.266086
6	3.527498	0.299642	-1.024005
7	2.340264	0.980290	-1.043326
6	2.651954	2.311243	-1.127653
6	1.723650	3.365521	-1.009063
6	3.607008	-0.270403	3.114157
6	3.296030	-1.510292	3.668222
6	2.008700	-2.011796	3.458897
6	1.094102	-1.301054	2.682409
6	1.542082	-0.078269	2.092128
1	4.578126	0.186545	3.298180
1	4.019593	-2.046039	4.273288
1	1.698993	-2.939935	3.931118
26	0.363363	0.144593	-0.638766
7	0.688422	0.633803	1.278716
6	-0.301393	-1.777846	2.521865
6	-0.531215	-3.124308	2.231913
6	-1.420799	-0.900962	2.697811
6	-1.819574	-3.646827	2.104180
1	0.318472	-3.779061	2.070610
6	-2.717960	-1.432822	2.546615
6	-2.897724	-2.778877	2.249424
1	-1.973899	-4.693728	1.873836
1	-3.583575	-0.807271	2.723064
7	2.768254	0.429425	2.342884
6	-4.121742	1.963448	-1.618005
6	-4.382804	3.035684	-2.489317
6	-5.202376	1.397600	-0.916498
6	-5.676196	3.535029	-2.641417
1	-3.564424	3.467866	-3.056240
6	-6.495266	1.898745	-1.066659
1	-5.019608	0.566655	-0.242795
6	-6.736634	2.971847	-1.927900
1	-5.856142	4.360450	-3.324454
1	-7.312486	1.452361	-0.507191
1	-7.743376	3.362495	-2.045492
6	2.261890	4.754963	-0.905911
6	3.102506	5.115399	0.160458
6	1.938389	5.726364	-1.867222
6	3.604047	6.413229	0.262781
1	3.353362	4.370625	0.909882
6	2.443993	7.022834	-1.766517
1	1.292868	5.454752	-2.697055
6	3.277301	7.370447	-0.700716
1	4.247411	6.677067	1.097567
1	2.189801	7.759969	-2.523084

1	3.669516	8.380474	-0.621643
6	5.035104	-1.635249	-0.623434
6	5.529241	-2.617860	-1.497705
6	5.868168	-1.175191	0.409705
6	6.817927	-3.128499	-1.340123
1	4.897702	-2.972157	-2.306705
6	7.155039	-1.689219	0.569480
1	5.492037	-0.416632	1.086841
6	7.634251	-2.667748	-0.304434
1	7.185860	-3.882594	-2.030314
1	7.782463	-1.326407	1.379001
1	8.637110	-3.066892	-0.181133
6	-1.281079	-4.435109	-1.600826
6	-2.465354	-4.869310	-0.977978
6	-0.597805	-5.338965	-2.434401
6	-2.938717	-6.167604	-1.165529
1	-3.010696	-4.183112	-0.341055
6	-1.073952	-6.635939	-2.625045
1	0.303932	-5.012464	-2.942722
6	-2.243406	-7.057286	-1.987551
1	-3.850797	-6.481643	-0.665648
1	-0.534161	-7.315303	-3.278829
1	-2.612367	-8.068388	-2.134791
17	-4.540397	-3.402904	2.060706
6	-1.204603	0.466699	3.119231
1	-0.322212	0.626598	3.730112
6	-2.055449	1.606888	2.980817
6	-3.124185	1.704310	2.051181
6	-1.788702	2.743905	3.792899
6	-3.904687	2.852584	1.981267
1	-3.301915	0.894694	1.354453
6	-2.571078	3.886456	3.715038
1	-0.958083	2.702660	4.492970
6	-3.643405	3.945160	2.815144
1	-4.710926	2.903035	1.256665
1	-2.349129	4.736641	4.354076
1	-4.257345	4.838940	2.752886
1	1.054213	1.585650	1.217080

8a

Number of imaginary frequencies : 0
Electronic energy : HF=-1263.5226351
Zero-point correction= 0.265811 (Hartree/Particle)
Thermal correction to Energy= 0.281589
Thermal correction to Enthalpy= 0.282533
Thermal correction to Gibbs Free Energy= 0.220946
Sum of electronic and zero-point Energies= -1263.256824
Sum of electronic and thermal Energies= -1263.241047
Sum of electronic and thermal Enthalpies= -1263.240102
Sum of electronic and thermal Free Energies= -1263.301689

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Cartesian Coordinates

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6	4.485911	-1.642877	0.099404
6	4.812683	-0.292805	-0.009175
6	3.768329	0.630916	-0.083634
6	2.443016	0.194820	-0.054867
6	2.236350	-1.209977	0.015327
1	5.268245	-2.396083	0.175852
1	5.848840	0.026702	-0.032508
1	3.990937	1.690101	-0.167774
7	0.949876	-1.698695	0.039261
6	1.262038	1.074155	-0.037922
6	1.351991	2.448451	0.240483
6	-0.014604	0.515898	-0.270452
6	0.224228	3.262819	0.261661
1	2.315554	2.894330	0.464029
6	-1.150092	1.326267	-0.244841
6	-1.020958	2.688441	0.014087
1	0.307957	4.322034	0.478264
1	-2.130320	0.900220	-0.423008
7	3.229277	-2.105421	0.103437
17	-2.463984	3.700555	0.039498
6	-0.125545	-0.967504	-0.632229
6	-1.465110	-1.583942	-0.264948
6	-1.774510	-1.859417	1.073955
6	-2.414591	-1.855349	-1.254786
6	-3.013699	-2.400445	1.413312
1	-1.035385	-1.649430	1.841165
6	-3.659383	-2.392191	-0.915325
1	-2.179180	-1.646762	-2.295567
6	-3.960551	-2.666426	0.419315
1	-3.243024	-2.612455	2.453870
1	-4.388292	-2.599399	-1.693654
1	-4.926295	-3.086898	0.685119
1	0.902693	-2.707287	-0.043390
1	-0.011103	-1.040713	-1.728952

[1a-1a']‡

Number of imaginary frequencies : 1
Electronic energy : HF=-642.9353269
Zero-point correction= 0.172339 (Hartree/Particle)
Thermal correction to Energy= 0.182842
Thermal correction to Enthalpy= 0.183786
Thermal correction to Gibbs Free Energy= 0.135182
Sum of electronic and zero-point Energies= -642.762988
Sum of electronic and thermal Energies= -642.752485
Sum of electronic and thermal Enthalpies= -642.751541
Sum of electronic and thermal Free Energies= -642.800145

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Cartesian Coordinates

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6	1.257163	-0.285602	-0.041963
6	2.867417	1.395093	0.165909
6	1.887677	2.365792	0.302585

6	0.543431	1.967858	0.268112
6	0.176880	0.631504	0.095285
1	3.929102	1.621002	0.189127
1	2.160481	3.405720	0.443856
1	-0.237048	2.711136	0.397444
6	-1.249114	0.225546	0.043543
6	-2.174286	1.024561	-0.651220
6	-1.717471	-0.923406	0.704139
6	-3.527424	0.689975	-0.680552
1	-1.826300	1.900529	-1.191157
6	-3.071316	-1.253701	0.675655
1	-1.018555	-1.555491	1.238858
6	-3.981551	-0.450138	-0.014876
1	-4.224420	1.315956	-1.230555
1	-3.415736	-2.142564	1.196569
1	-5.035185	-0.713410	-0.038348
7	2.521703	0.112938	-0.000892
7	1.032469	-1.667140	-0.247879
7	2.212021	-2.189066	-0.340328
7	3.319410	-1.809271	-0.297401

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^{3}[21-22]‡

Number of imaginary frequencies : 1
Electronic energy : HF=-2679.7092424
Zero-point correction= 0.772207 (Hartree/Particle)
Thermal correction to Energy= 0.820354
Thermal correction to Enthalpy= 0.821298
Thermal correction to Gibbs Free Energy= 0.686827
Sum of electronic and zero-point Energies= -2678.937036
Sum of electronic and thermal Energies= -2678.888889
Sum of electronic and thermal Enthalpies= -2678.887944
Sum of electronic and thermal Free Energies= -2679.022416

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Cartesian Coordinates

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6	1.040273	-2.858169	-0.894100
7	1.427152	-1.533957	-0.837678
1	2.168853	-4.798219	-0.963716
6	2.806910	-1.555046	-0.781411
6	3.290605	-2.916047	-0.844331
1	4.330835	-3.204375	-0.840868
6	2.200127	-3.720606	-0.904360
6	3.637315	-0.439681	-0.652261
7	1.843694	1.275153	-0.760876
6	1.851512	2.653974	-0.645663
6	3.190314	3.120843	-0.405676
1	3.471910	4.152085	-0.254567
6	4.000019	2.024616	-0.392204
1	5.066671	1.991942	-0.228442
6	3.162527	0.878522	-0.622804
6	-0.273977	-3.327483	-0.949703
1	-4.629794	-1.838120	-1.229317
6	-3.551574	-1.868026	-1.187019
6	-2.694133	-0.713750	-1.174607
1	-3.043501	-4.002127	-1.061279

7	-1.370001	-1.105721	-1.090710
6	-1.390915	-2.489566	-1.049953
6	-2.747721	-2.964540	-1.099698
6	0.731515	3.495234	-0.705318
1	-3.849518	3.371458	-1.224879
6	-2.816232	3.083948	-1.100258
6	-1.731720	3.890390	-0.975726
1	-1.701989	4.969633	-0.981367
6	-0.577101	3.028093	-0.855339
7	-0.961317	1.702602	-0.920289
6	-2.335157	1.721858	-1.060556
6	-3.166040	0.604245	-1.167986
6	2.156663	0.965871	2.498882
6	1.230552	1.996381	2.551034
6	-0.128308	1.667269	2.618267
6	-0.568954	0.339524	2.653759
6	0.461183	-0.642020	2.577607
1	3.224463	1.138360	2.420345
1	1.557149	3.028383	2.507830
1	-0.867801	2.460768	2.617346
7	1.312653	-2.616435	2.439998
7	2.438659	-2.307052	2.377191
26	0.233131	0.083542	-0.884401
7	0.167694	-2.029510	2.550025
6	-2.012713	0.021037	2.787403
6	-2.609738	-1.065738	2.125278
6	-2.830501	0.849372	3.579796
6	-3.978148	-1.303684	2.244257
1	-2.005305	-1.716841	1.509593
6	-4.198400	0.607890	3.697505
1	-2.387752	1.675052	4.129205
6	-4.779405	-0.470974	3.026965
1	-4.416681	-2.138557	1.707144
1	-4.806912	1.256998	4.321059
1	-5.845651	-0.659771	3.112732
7	1.742655	-0.305202	2.505455
6	-0.497262	-4.803517	-0.864640
6	-0.967970	-5.534406	-1.965546
6	-0.235552	-5.479908	0.337285
6	-1.172793	-6.911717	-1.867109
1	-1.168984	-5.016940	-2.899105
6	-0.441409	-6.856479	0.435041
1	0.123832	-4.915821	1.193053
6	-0.910301	-7.576017	-0.666779
1	-1.533529	-7.465642	-2.729382
1	-0.238736	-7.365778	1.373109
1	-1.070212	-8.647879	-0.590497
6	-4.644397	0.822835	-1.220489
6	-5.324187	1.293277	-0.086047
6	-5.376854	0.550174	-2.385275
6	-6.705828	1.485614	-0.117324
1	-4.764330	1.492083	0.821931
6	-6.758993	0.744372	-2.416036
1	-4.856330	0.186266	-3.266413
6	-7.427085	1.212249	-1.282117
1	-7.218813	1.843477	0.771200

1	-7.312545	0.532444	-3.326615
1	-8.502858	1.362175	-1.306090
6	0.951423	4.969667	-0.587092
6	1.651264	5.673200	-1.580184
6	0.466444	5.678971	0.523334
6	1.861994	7.047774	-1.464724
1	2.026761	5.133897	-2.444720
6	0.677443	7.053577	0.639678
1	-0.080727	5.145338	1.294884
6	1.376624	7.742106	-0.354129
1	2.401854	7.576683	-2.245198
1	0.297894	7.585447	1.507717
1	1.541113	8.812124	-0.264501
6	5.105527	-0.664111	-0.480555
6	5.590673	-1.294633	0.676827
6	6.021371	-0.242738	-1.456707
6	6.960333	-1.496877	0.851818
1	4.885311	-1.624224	1.433668
6	7.390872	-0.446801	-1.280822
1	5.652148	0.243121	-2.355169
6	7.864086	-1.073579	-0.125692
1	7.321027	-1.983660	1.753757
1	8.087114	-0.119305	-2.047927
1	8.930099	-1.232344	0.011109

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^{3}22 pyridine-N-Fe coordination

Number of imaginary frequencies : 0
Electronic energy : HF=-2679.7293314
Zero-point correction= 0.773091 (Hartree/Particle)
Thermal correction to Energy= 0.822885
Thermal correction to Enthalpy= 0.823829
Thermal correction to Gibbs Free Energy= 0.685212
Sum of electronic and zero-point Energies= -2678.956240
Sum of electronic and thermal Energies= -2678.906447
Sum of electronic and thermal Enthalpies= -2678.905502
Sum of electronic and thermal Free Energies= -2679.044119

.....

Cartesian Coordinates

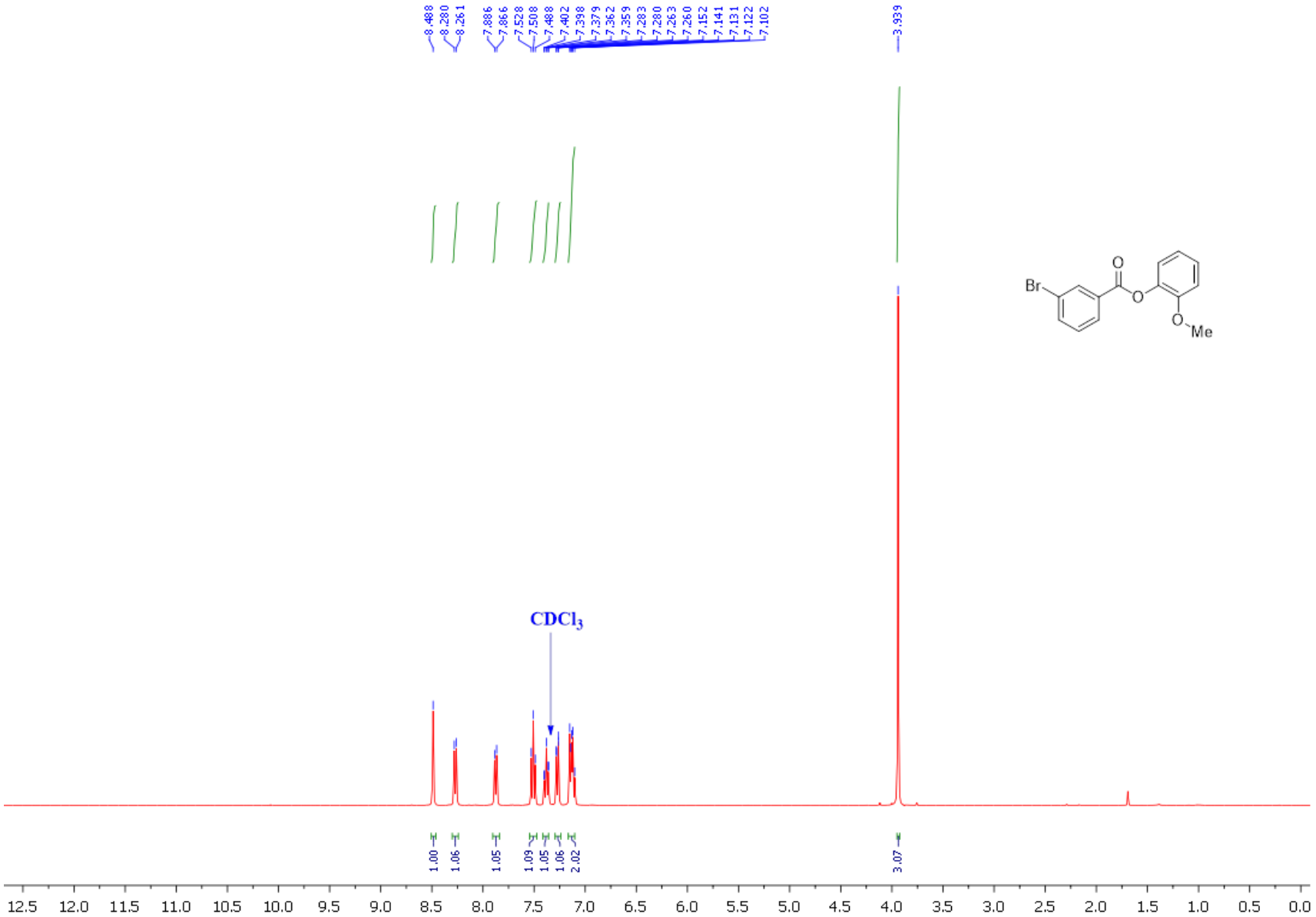
.....

6	0.217937	2.983703	-1.119741
7	-0.793847	2.123998	-0.741761
1	0.368032	5.221127	-1.246543
6	-1.839844	2.924714	-0.340343
6	-1.487134	4.317147	-0.497687
1	-2.137132	5.151060	-0.278159
6	-0.220687	4.353179	-0.989912
6	-3.089161	2.483461	0.118449
7	-2.736278	0.075552	-0.339550
6	-3.553341	-1.034842	-0.244833
6	-4.833696	-0.660529	0.305896
1	-5.647498	-1.341058	0.506925
6	-4.789021	0.679099	0.537469
1	-5.561374	1.302746	0.962122
6	-3.490377	1.140450	0.108665
6	1.504616	2.608902	-1.522553

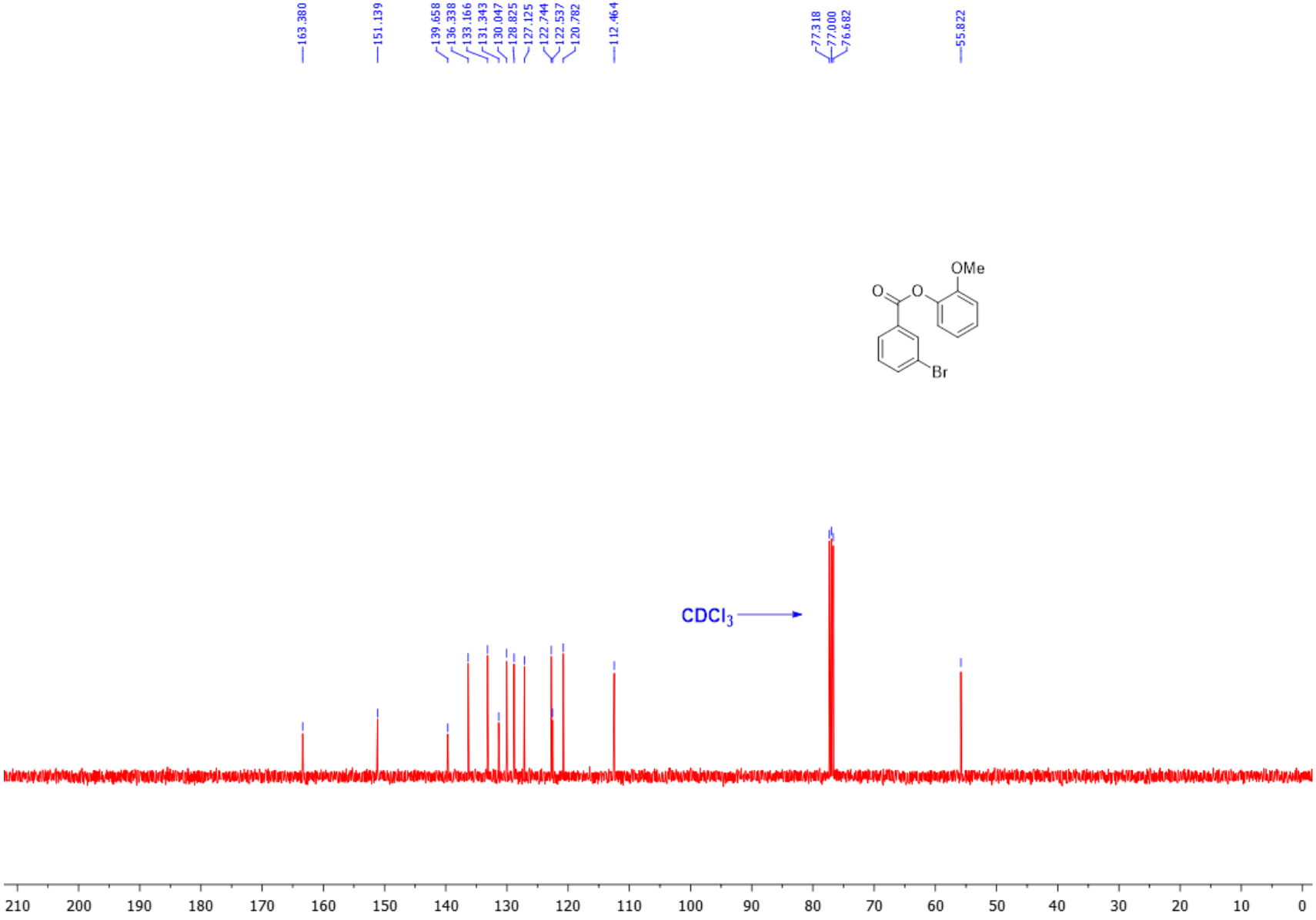
1	4.205225	-1.117445	-1.821410
6	3.343786	-0.472780	-1.728785
6	1.990578	-0.921977	-1.497369
1	4.125466	1.566004	-1.972309
7	1.143622	0.161735	-1.398598
6	1.930369	1.277028	-1.600333
6	3.303100	0.885603	-1.809106
6	-3.191859	-2.351978	-0.564525
1	0.522704	-4.900446	-1.573106
6	-0.132784	-4.068529	-1.360858
6	-1.481607	-4.088824	-1.185873
1	-2.142539	-4.941534	-1.224831
6	-1.891765	-2.728815	-0.927778
7	-0.801937	-1.883240	-1.004295
6	0.286982	-2.692446	-1.248453
6	1.612418	-2.267649	-1.409872
6	-0.765344	-1.342136	2.116778
6	-0.173609	-2.215145	3.024346
6	1.168518	-2.014371	3.340448
6	1.879417	-0.938089	2.796193
6	1.139768	-0.051468	1.975066
1	-1.779776	-1.488919	1.763026
1	-0.732670	-3.048852	3.434709
1	1.694322	-2.709687	3.988423
7	2.634802	1.727794	1.827696
7	3.517866	2.415484	2.044227
26	-0.779287	0.119698	-0.799146
7	1.622461	1.150063	1.423630
6	3.337252	-0.802566	3.042882
6	4.234209	-0.729443	1.963634
6	3.844220	-0.796644	4.351494
6	5.605894	-0.637886	2.192795
1	3.853778	-0.740362	0.946543
6	5.217595	-0.706835	4.577158
1	3.154776	-0.845386	5.189747
6	6.101583	-0.625015	3.498620
1	6.287153	-0.578930	1.348956
1	5.596789	-0.693344	5.594986
1	7.170670	-0.550559	3.675377
7	-0.124656	-0.287377	1.600774
6	2.507638	3.681523	-1.805801
6	3.010763	3.870026	-3.102162
6	2.981379	4.504977	-0.771907
6	3.960705	4.860079	-3.359042
1	2.651577	3.236303	-3.907685
6	3.932246	5.493371	-1.028333
1	2.605719	4.359876	0.236409
6	4.423429	5.674941	-2.323313
1	4.336447	4.996268	-4.369386
1	4.292210	6.117350	-0.215056
1	5.163561	6.444658	-2.523420
6	2.676786	-3.313858	-1.502955
6	3.003927	-4.080237	-0.372993
6	3.365982	-3.550407	-2.702047
6	4.000546	-5.054703	-0.439641
1	2.475448	-3.900196	0.558618

6	4.360873	-4.527119	-2.769363
1	3.113487	-2.965282	-3.581416
6	4.681897	-5.280857	-1.637886
1	4.246752	-5.634879	0.445441
1	4.882749	-4.700751	-3.706351
1	5.457214	-6.040132	-1.689894
6	-4.237429	-3.413364	-0.441947
6	-5.361592	-3.411795	-1.282783
6	-4.124653	-4.422839	0.527831
6	-6.345162	-4.394191	-1.158299
1	-5.457631	-2.633642	-2.034154
6	-5.107488	-5.405299	0.652552
1	-3.261370	-4.428321	1.186964
6	-6.220360	-5.394523	-0.191514
1	-7.206571	-4.380780	-1.820310
1	-5.005755	-6.175995	1.411667
1	-6.985791	-6.159429	-0.095119
6	-4.057180	3.513226	0.606277
6	-3.778658	4.256315	1.764578
6	-5.252009	3.768213	-0.085671
6	-4.672864	5.225532	2.220963
1	-2.855948	4.066182	2.304966
6	-6.145901	4.738064	0.370243
1	-5.471523	3.203511	-0.986924
6	-5.859176	5.469494	1.525175
1	-4.443419	5.788358	3.121634
1	-7.063549	4.925936	-0.180435
1	-6.554600	6.225016	1.879944

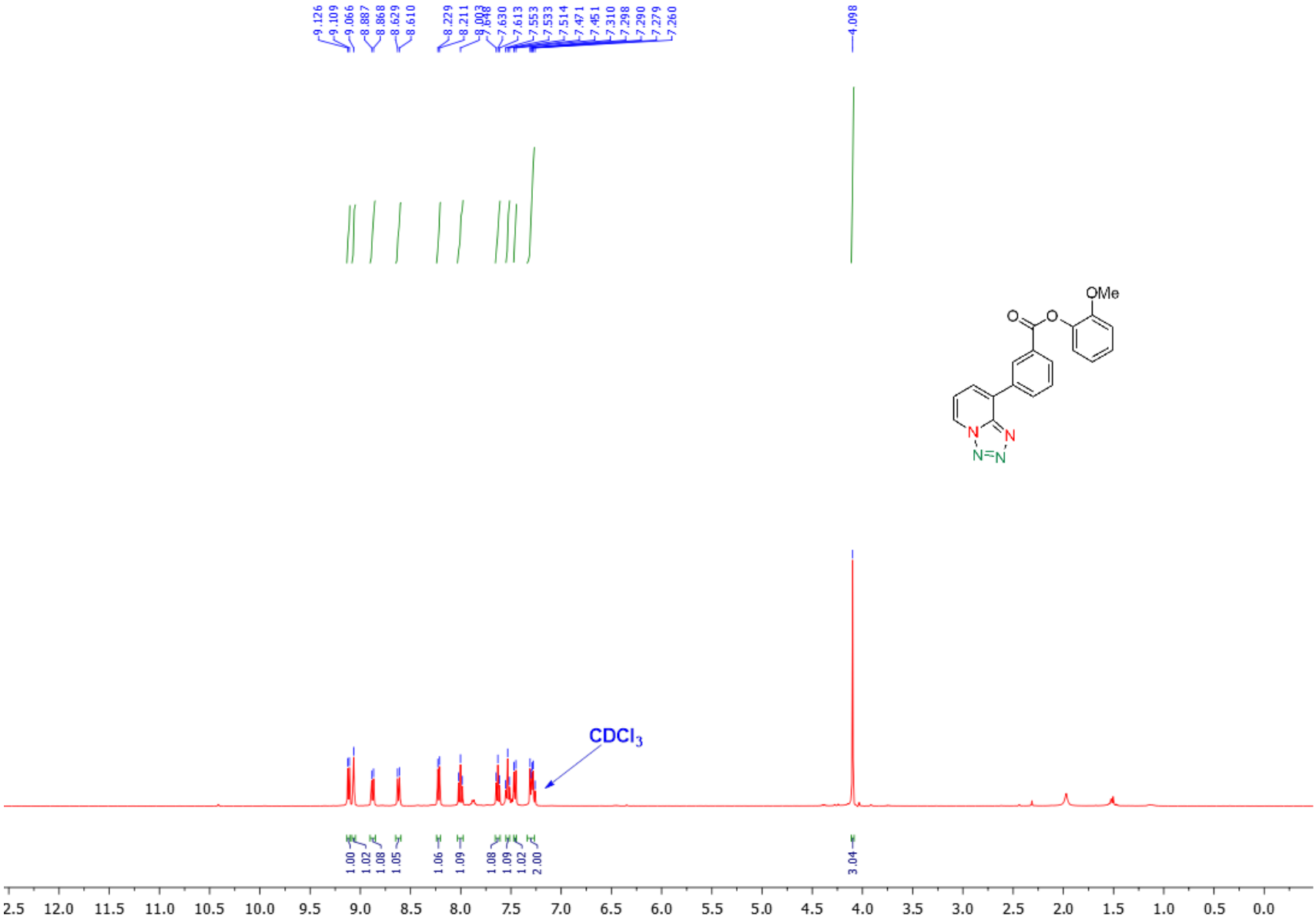
^{1}H-NMR of *2-methoxyphenyl 3-bromobenzoate* (25 °C, 400 MHz, $CDCl_3$):



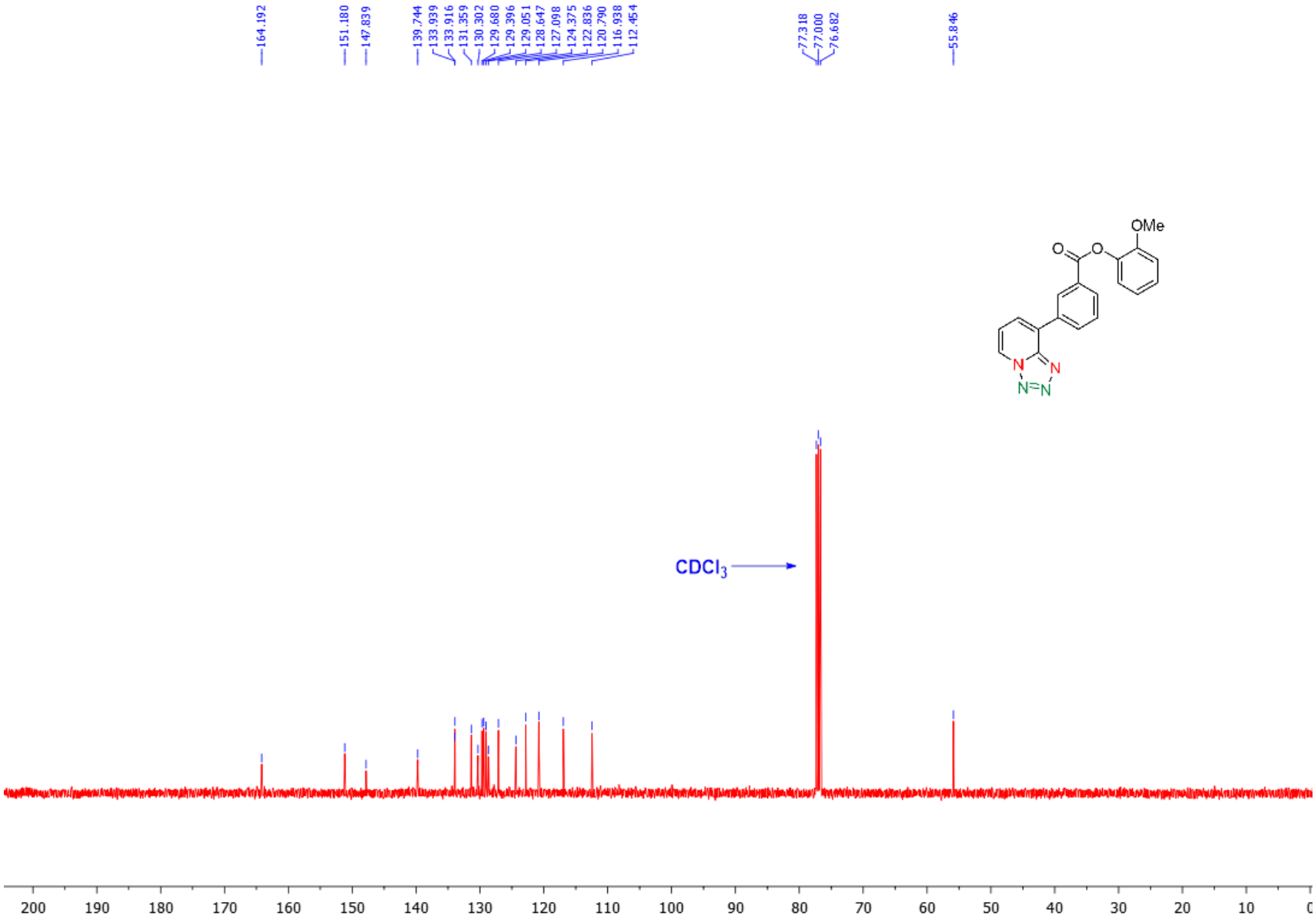
^{13}C-NMR of *2-methoxyphenyl 3-bromobenzoate* (25 ºC, 100 MHz, $CDCl_3$):



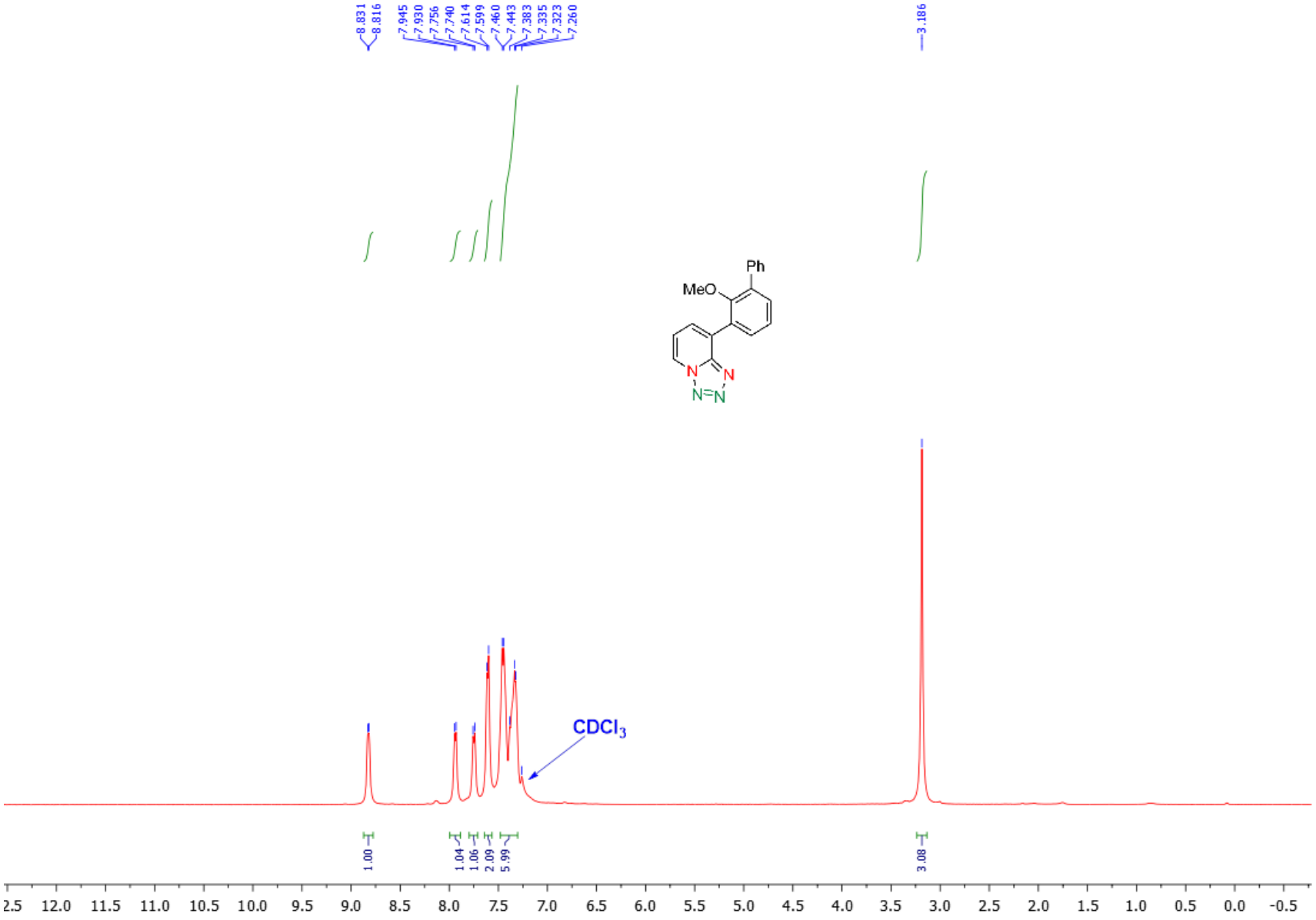
^{1}H-NMR of *2-methoxyphenyl 3-(tetrazolo[1,5-a]pyridin-8-yl)benzoate* (1b) (25 ^{o}C, 400 MHz, $CDCl_3$):



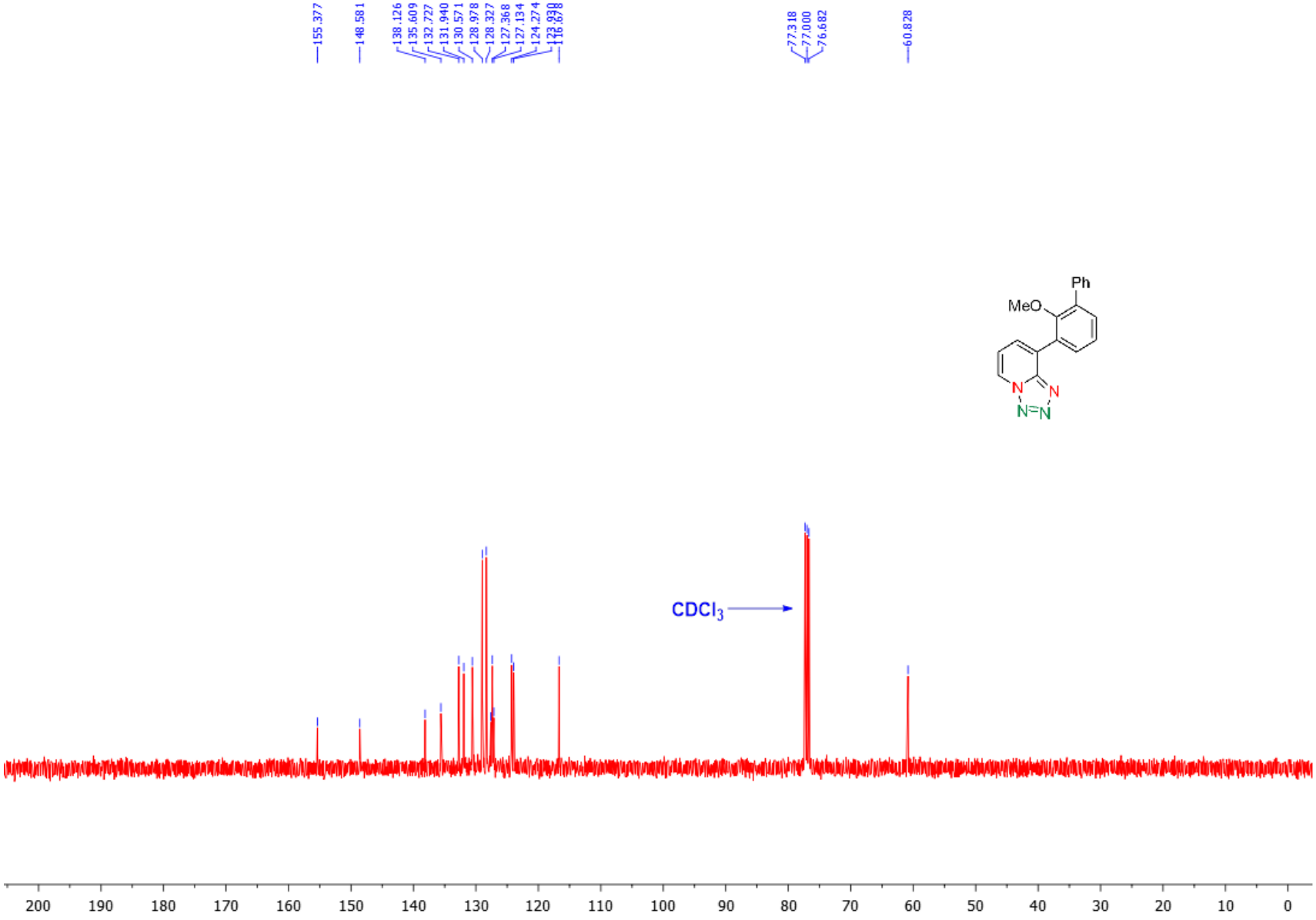
^{13}C-NMR of *3-(tetrazolo[1,5-a]pyridin-8-yl)benzoate (1b)* (25 °C, 100 MHz, $CDCl_3$):



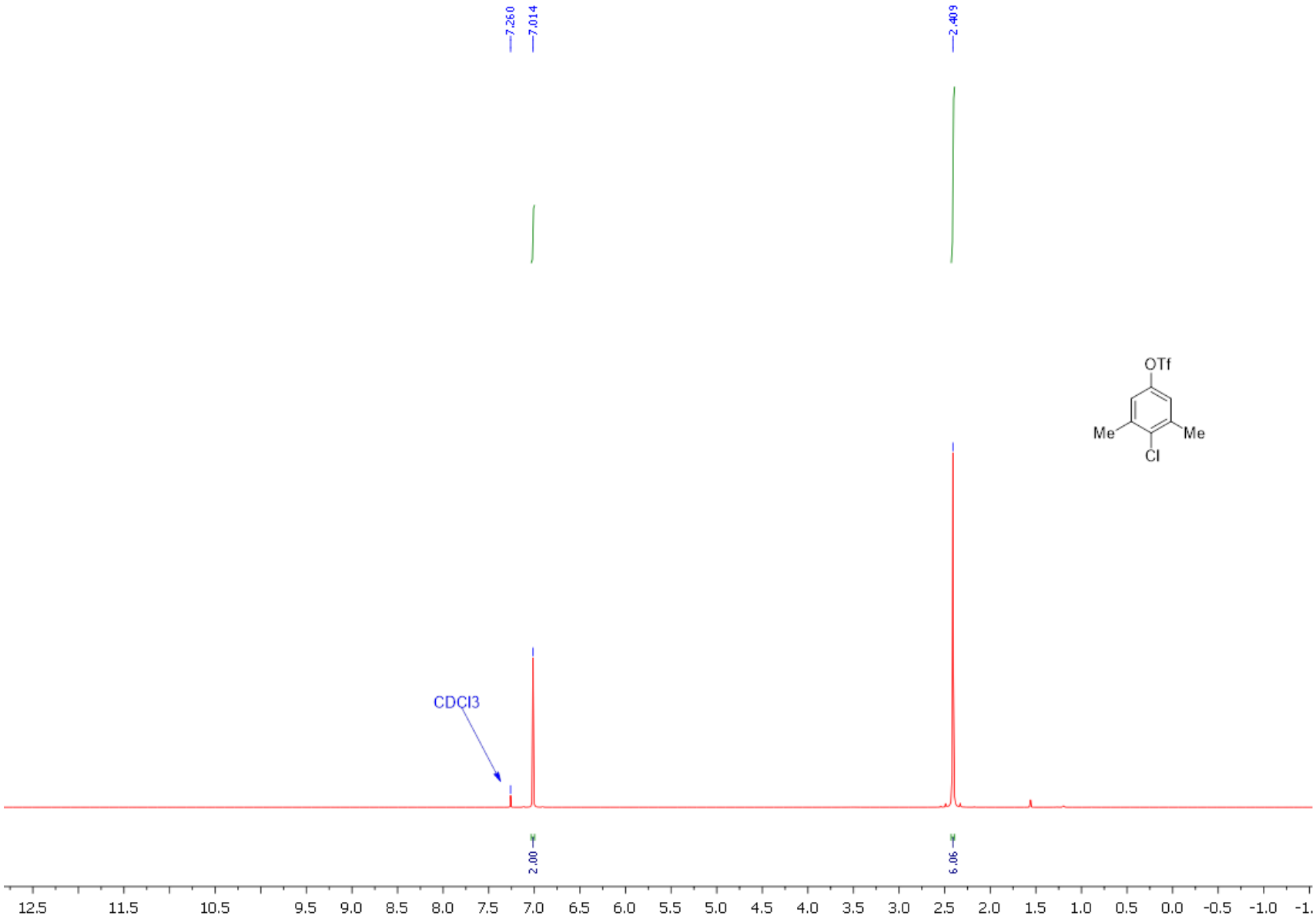
^{1}H-NMR of *8-(2-methoxy-[1,1'-biphenyl]-3-yl)tetrazolo[1,5-a]pyridine (1c)* (25 °C, 400 MHz, $CDCl_3$):



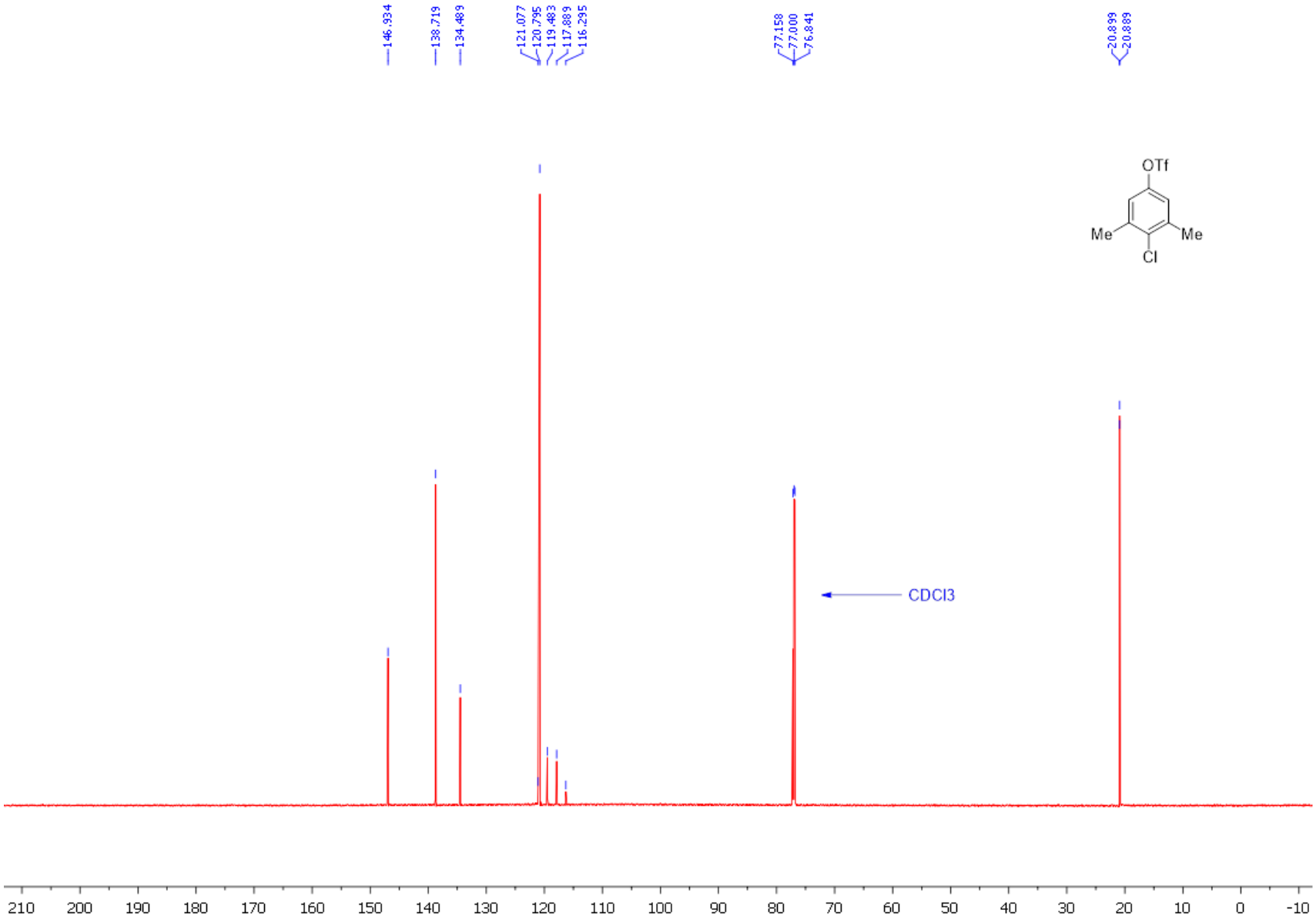
^{13}C-NMR of *8-(2-methoxy-[1,1'-biphenyl]-3-yl)tetrazolo[1,5-a]pyridine (1c))* (25 ºC, 100 MHz, $CDCl_3$):



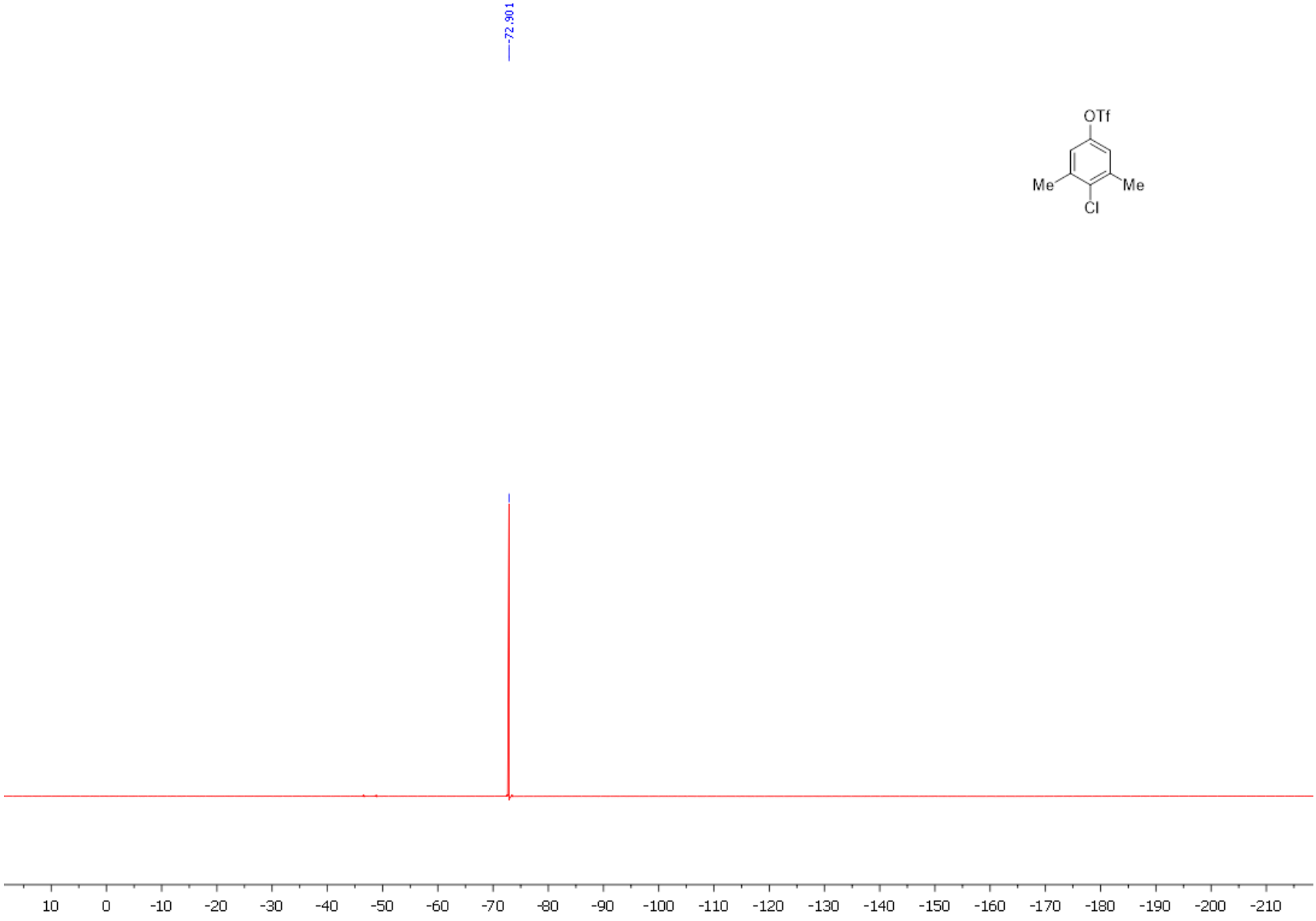
^{1}H-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ^{o}C, 800 MHz, $CDCl_3$):



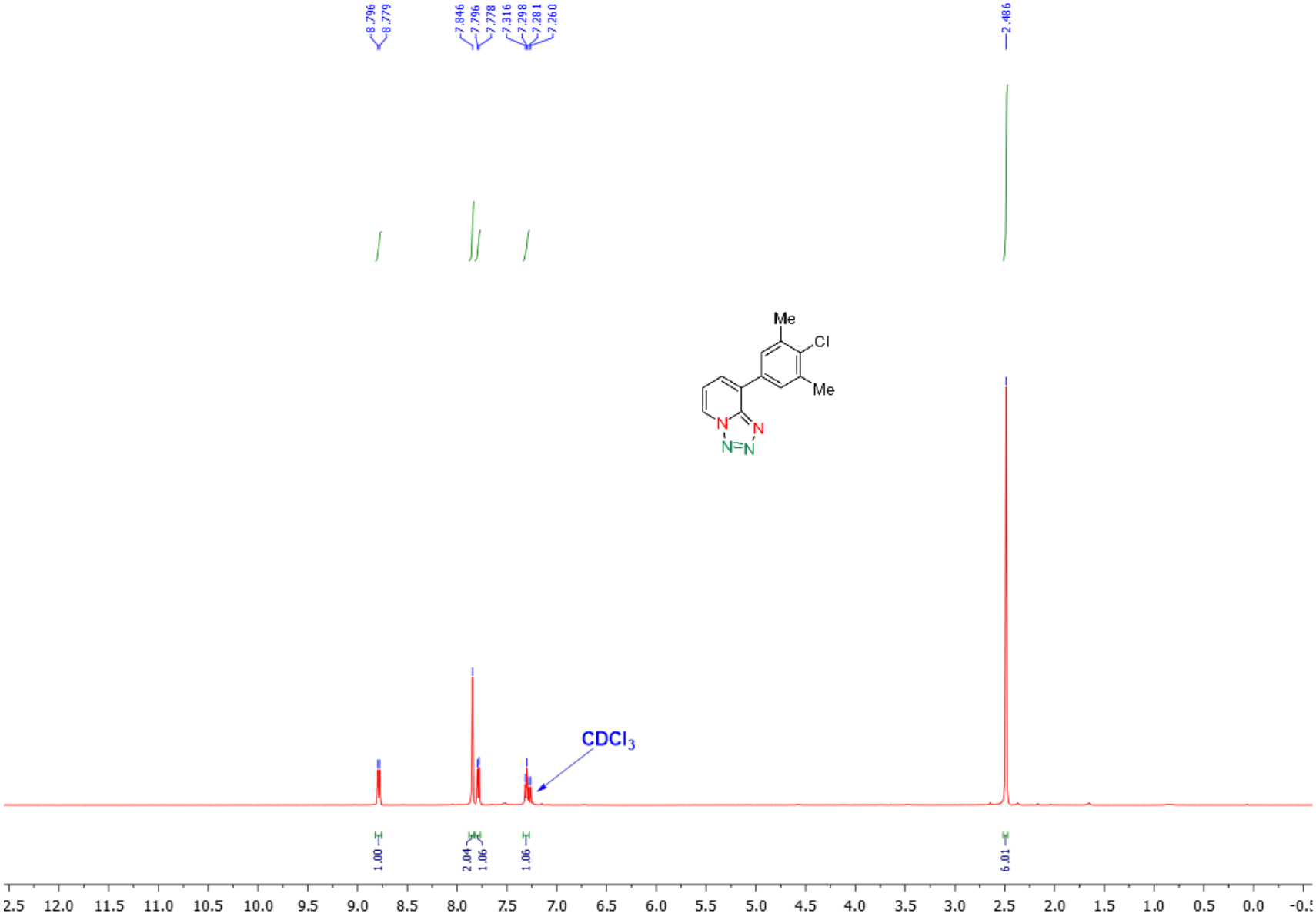
^{13}C-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ºC, 200 MHz, $CDCl_3$):



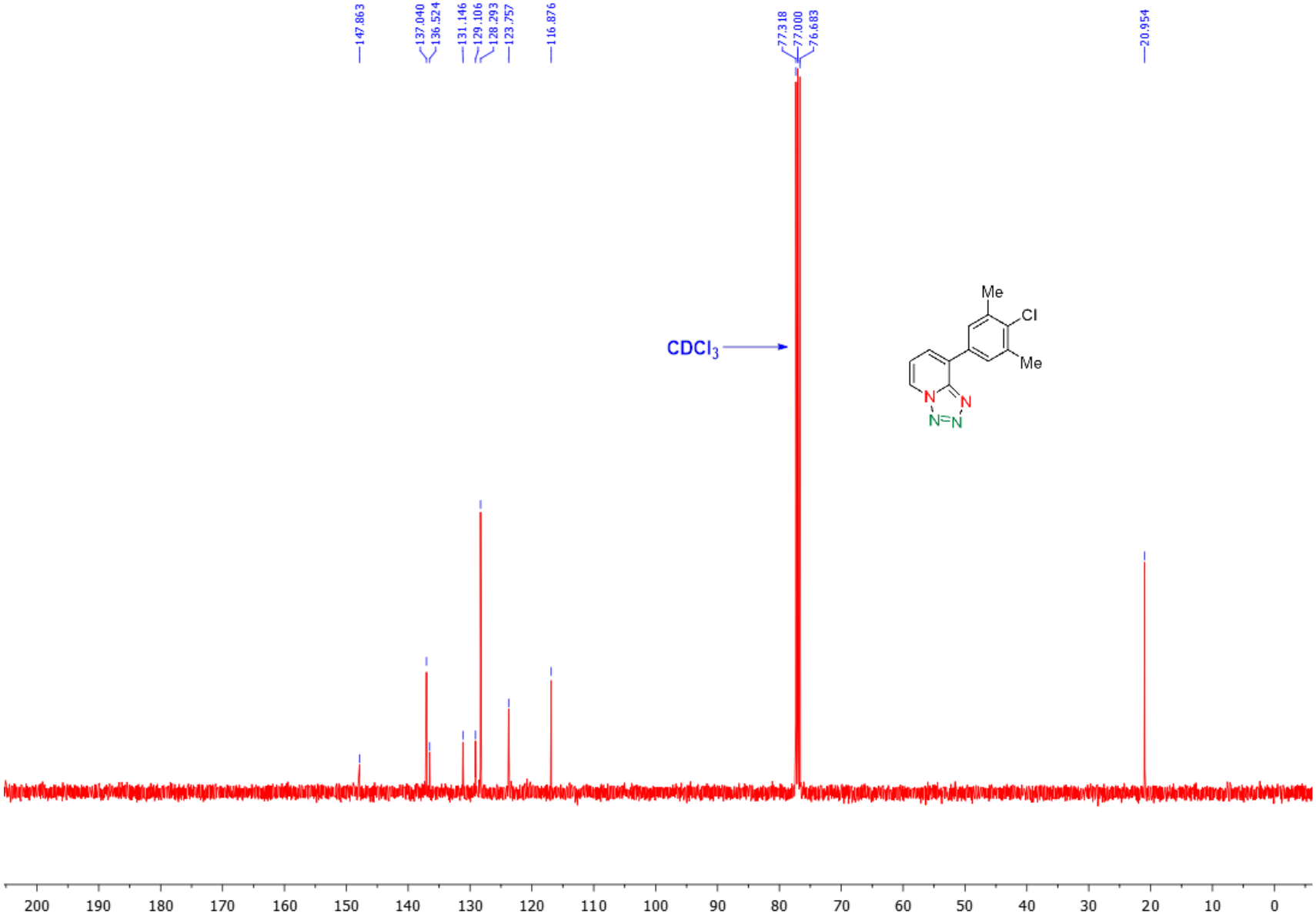
^{19}F-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 °C, 376 MHz, $CDCl_3$):



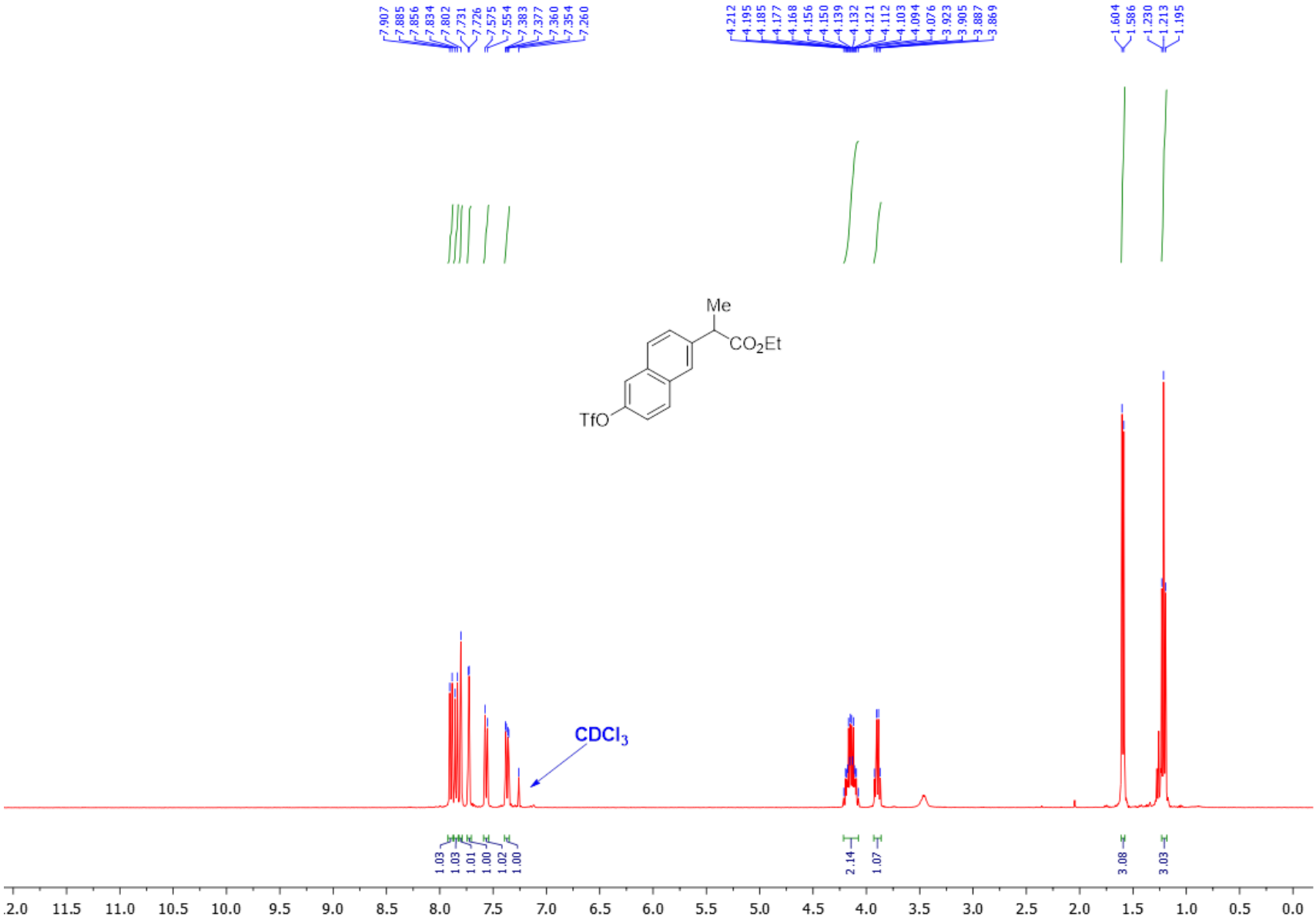
^{1}H-NMR of *8-(4-chloro-3,5-dimethylphenyl)tetrazolo[1,5-a]pyridine (1d)* (25 ºC, 400 MHz, $CDCl_3$):



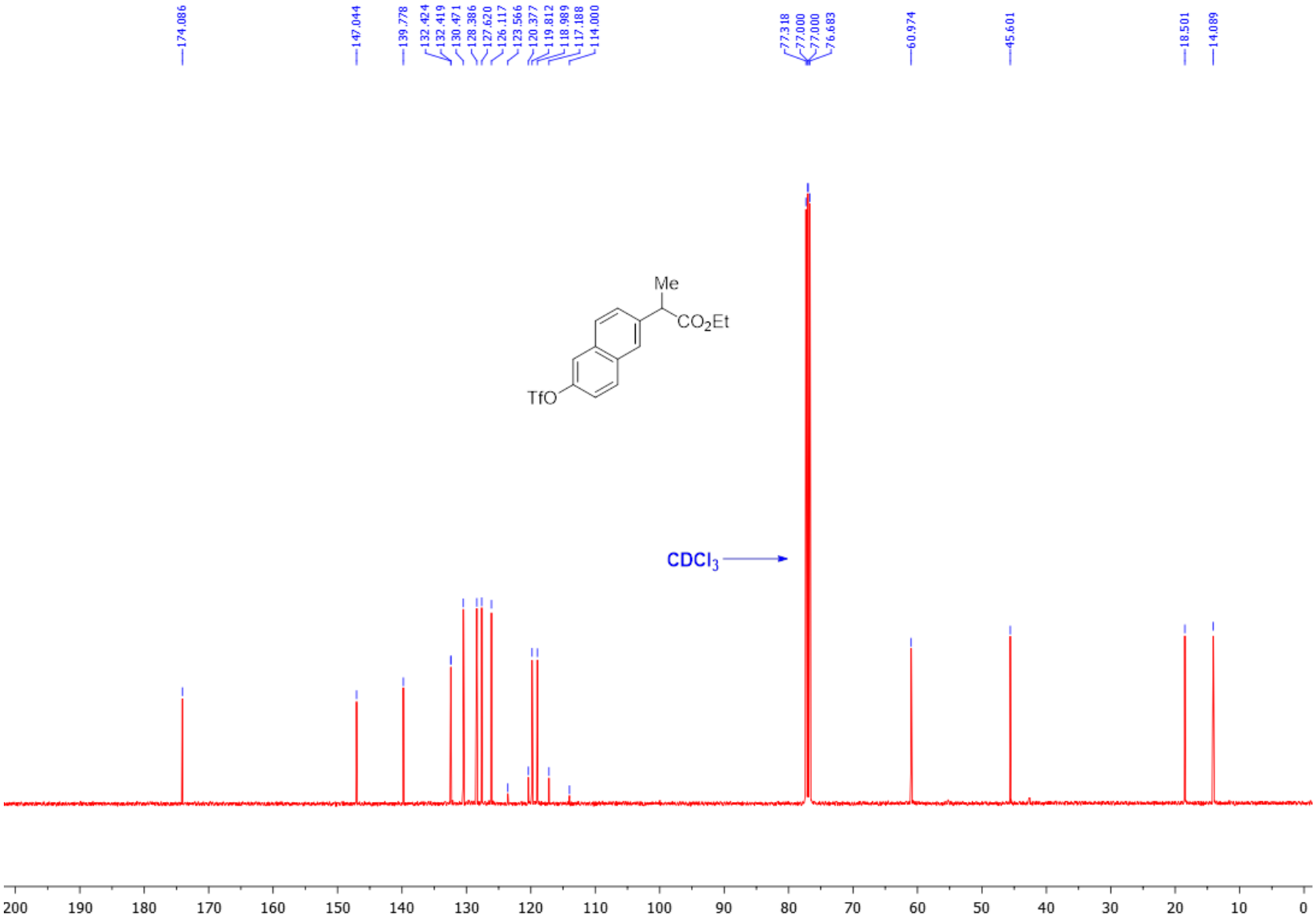
^{13}C-NMR of *8-(4-chloro-3,5-dimethylphenyl)tetrazolo[1,5-a]pyridine (1d))* (25 °C, 100 MHz, $CDCl_3$):



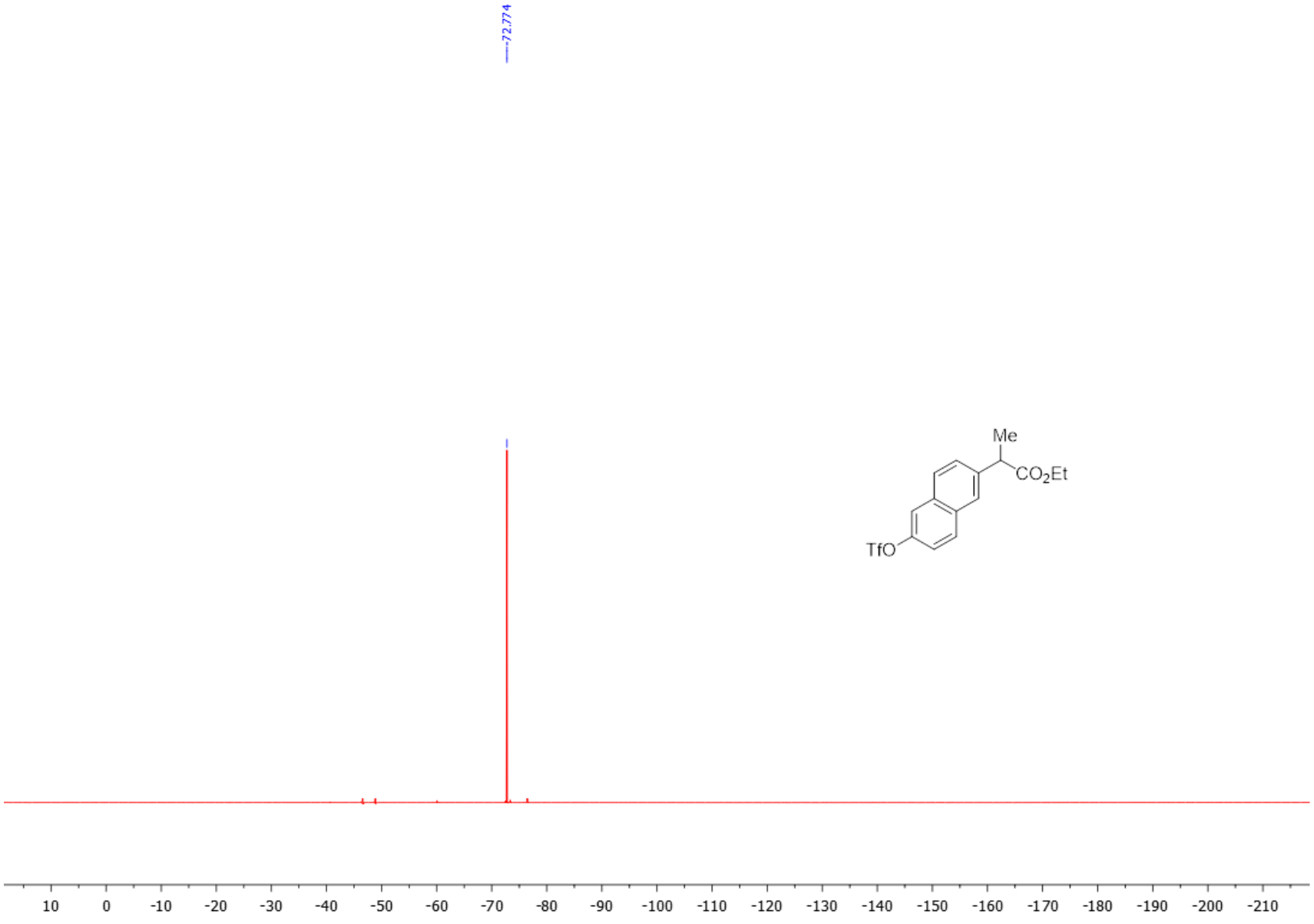
^{1}H-NMR of *ethyl 2-(6-(((trifluoromethyl)sulfonyl)oxy)naphthalen-2-yl)propanoate* (25 °C, 400 MHz, $CDCl_3$):



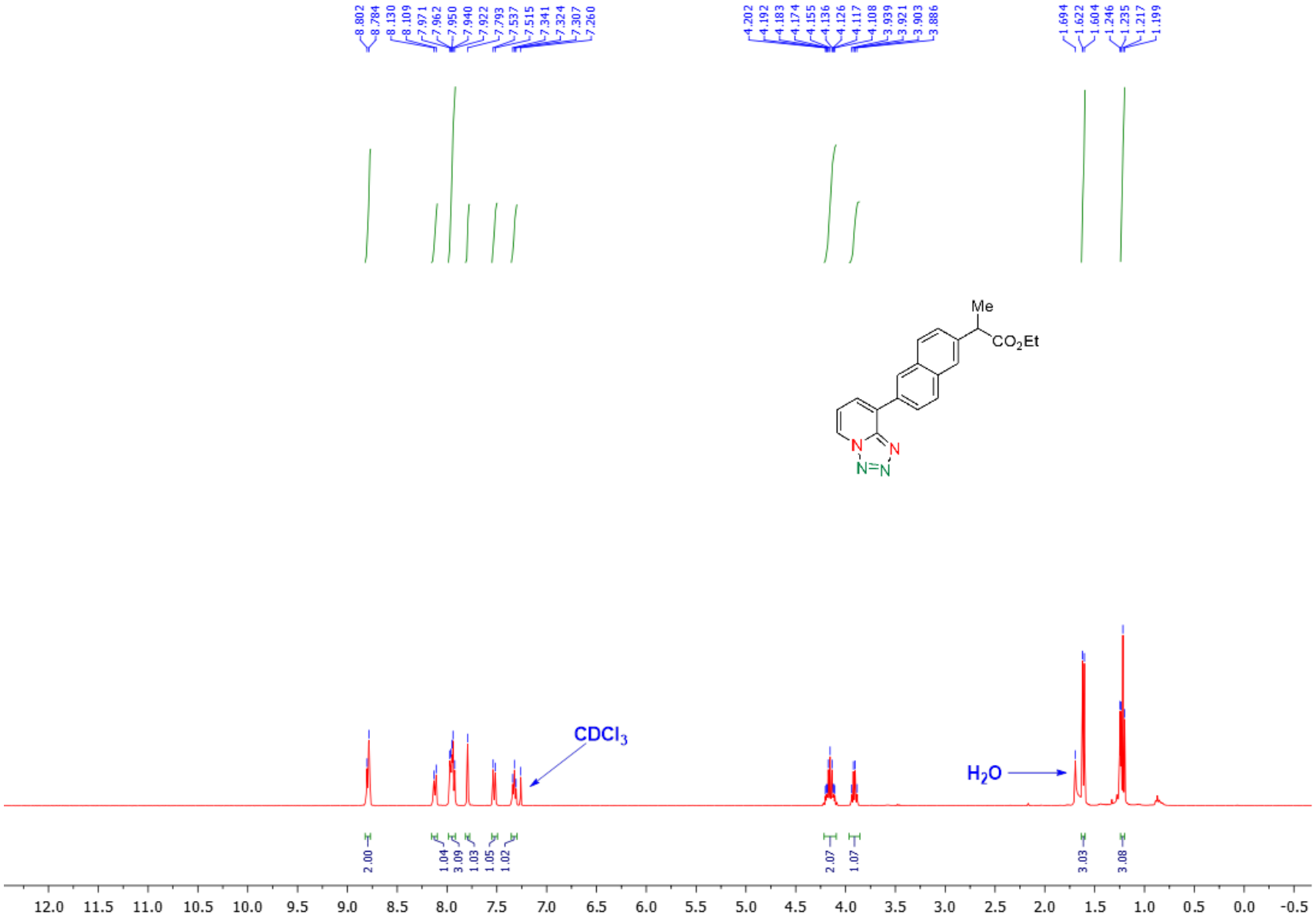
^{13}C-NMR of *ethyl 2-(6-(((trifluoromethyl)sulfonyl)oxy)naphthalen-2-yl)propanoate* (25 ºC, 100 MHz, $CDCl_3$):



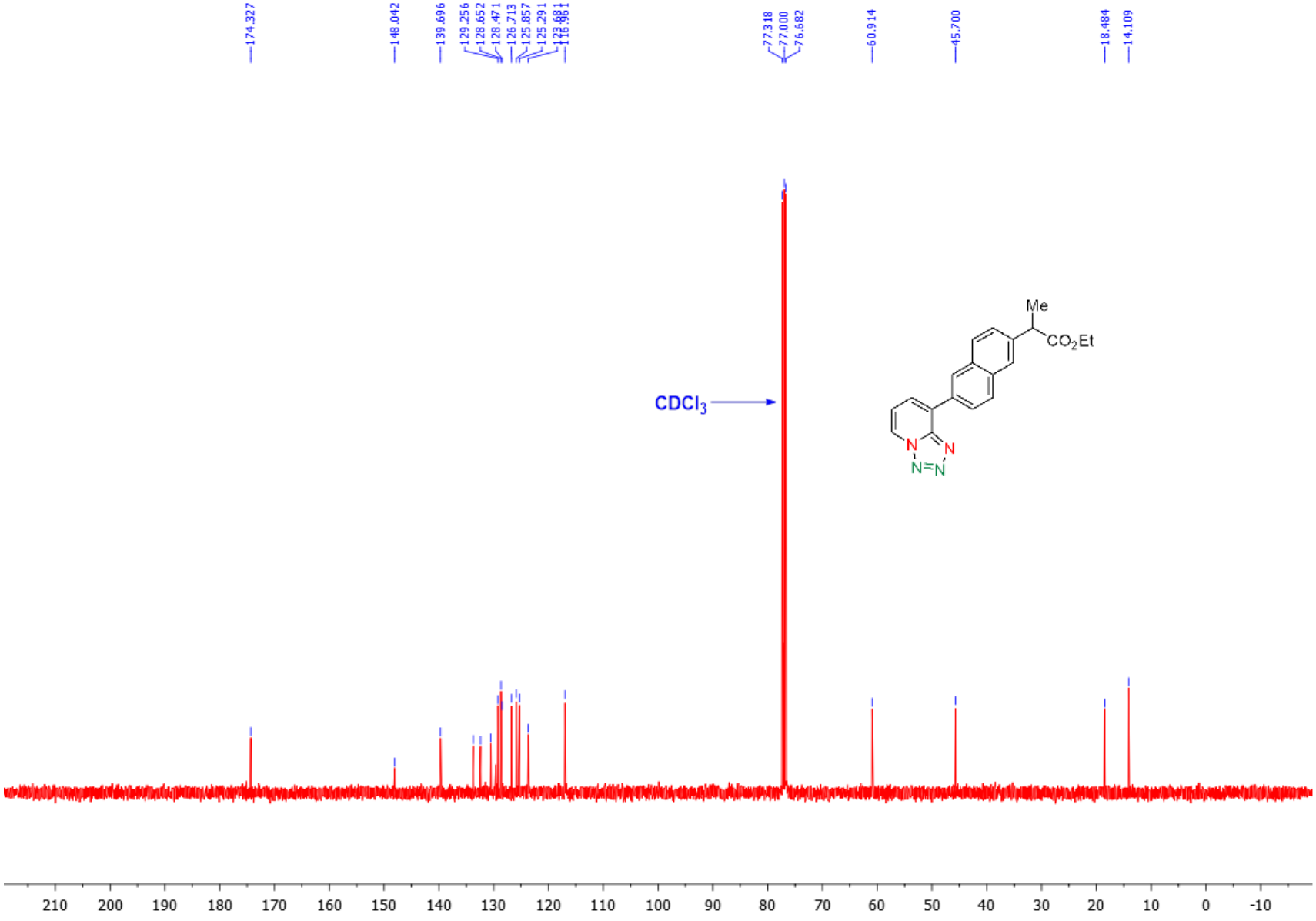
^{19}F-NMR of *ethyl 2-(6-(((trifluoromethyl)sulfonyl)oxy)naphthalen-2-yl)propanoate* (25 °C, 376 MHz, $CDCl_3$):



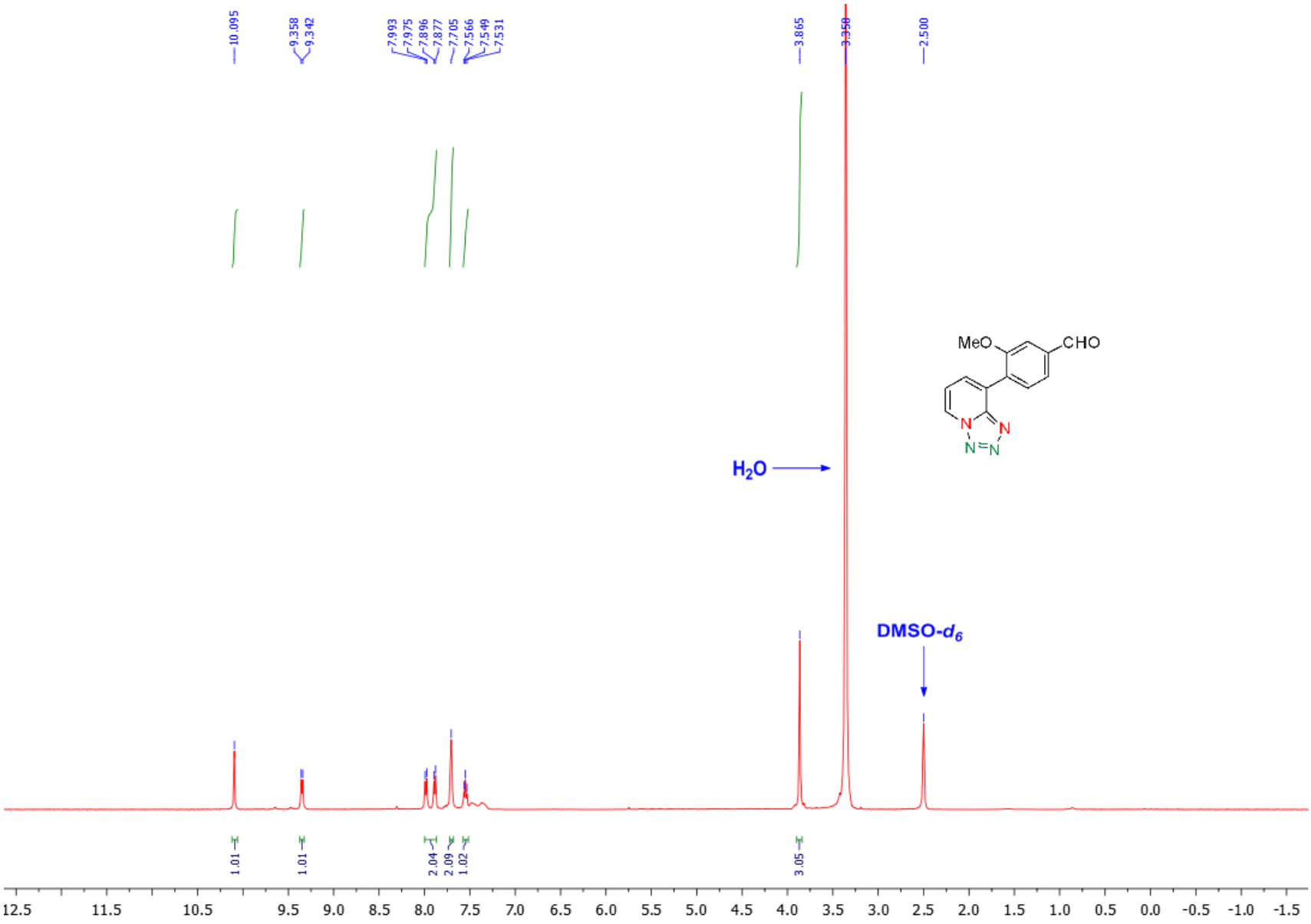
^{1}H-NMR of *ethyl 2-(6-(tetrazolo[1,5-a]pyridin-8-yl)naphthalen-2-yl)propanoate (1e)* (25 °C, 400 MHz, $CDCl_3$):



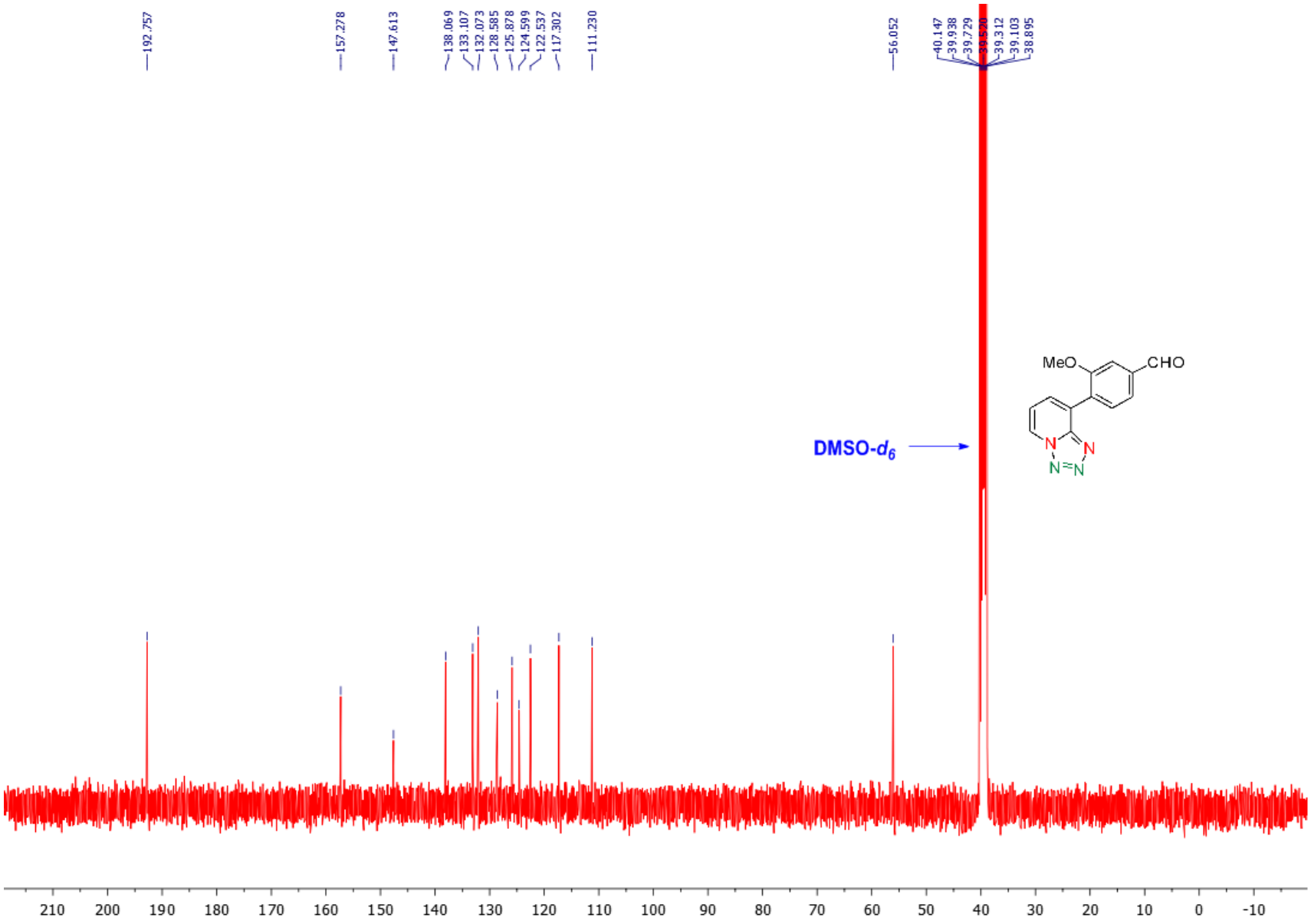
^{13}C-NMR of *ethyl 2-(6-(tetrazolo[1,5-a]pyridin-8-yl)naphthalen-2-yl)propanoate (1e)* (25 °C, 100 MHz, $CDCl_3$):



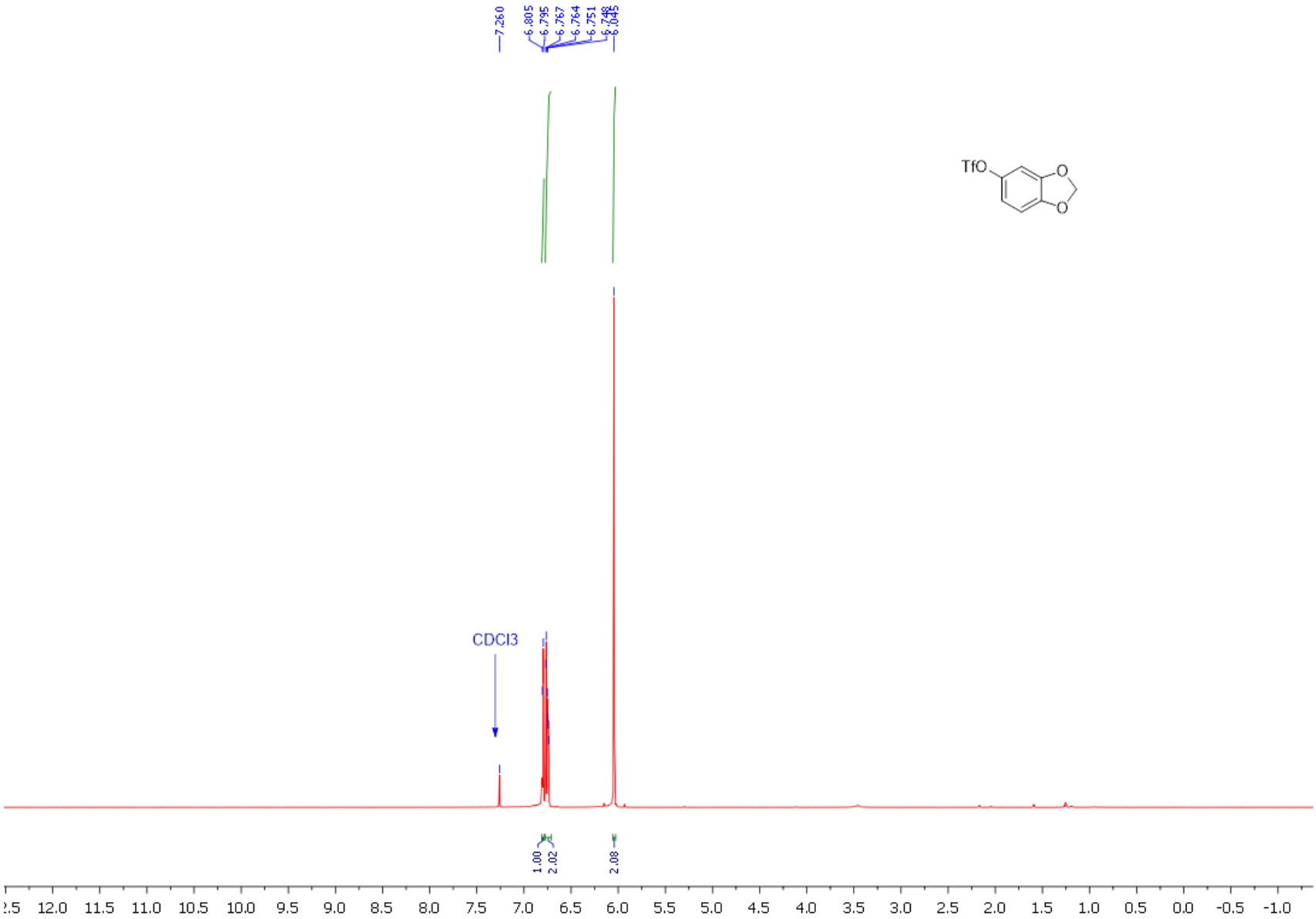
^{1}H-NMR of *3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)benzaldehyde (1f)* (25 ^{o}C, 400 MHz, DMSO-d_6):



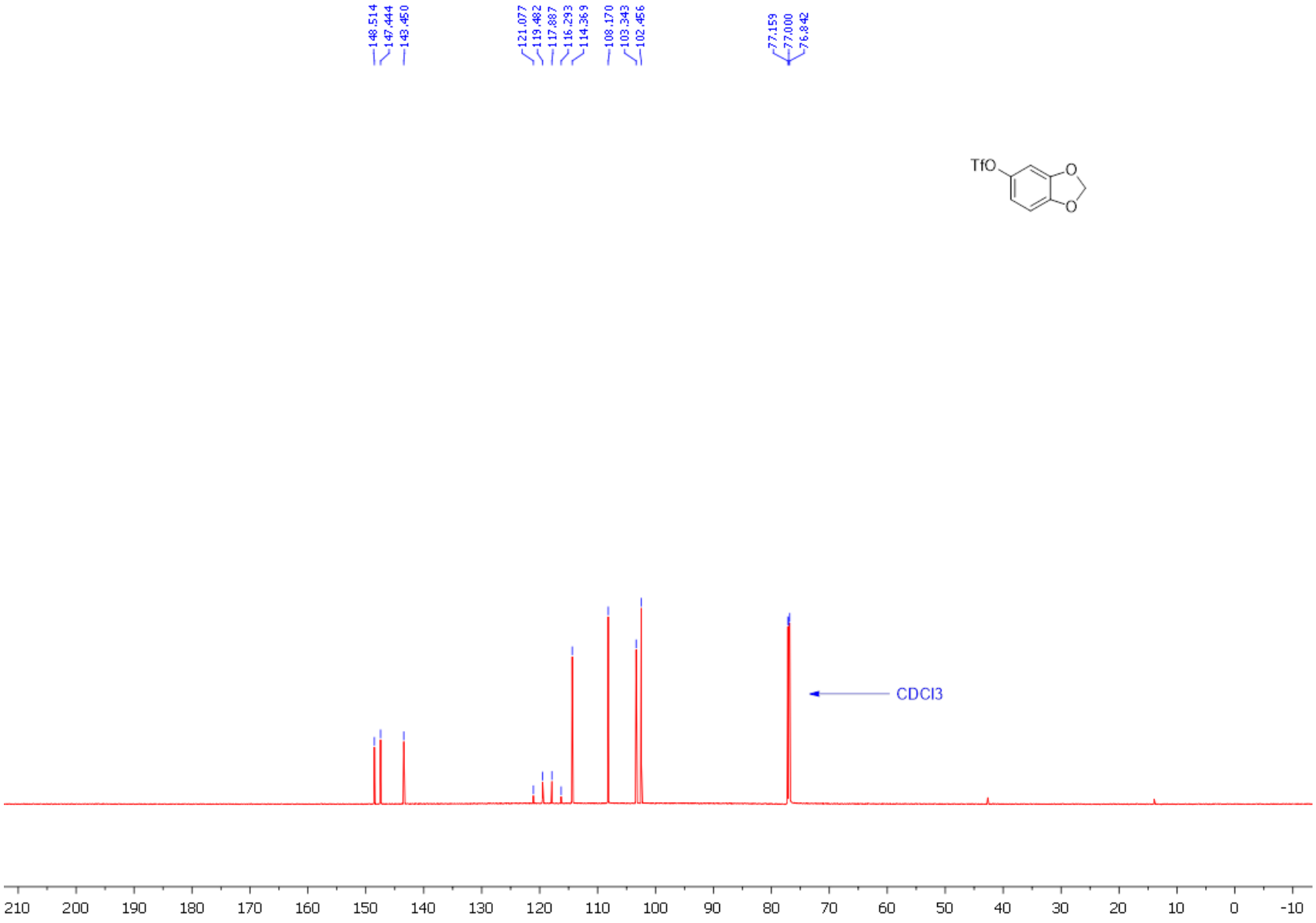
^{13}C-NMR of *3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)benzaldehyde (1f)* (25 ºC, 100 MHz, DMSO-d_6):



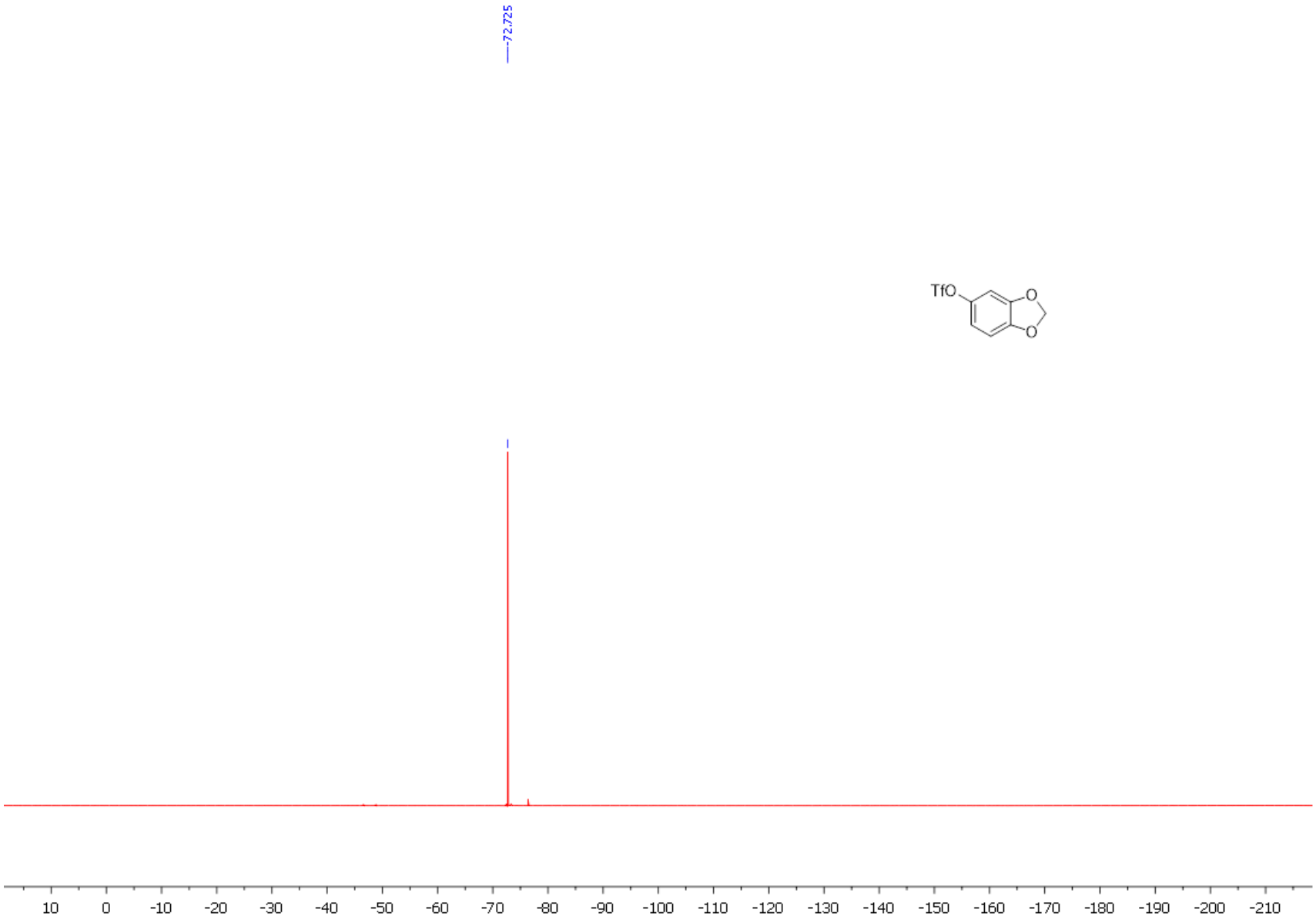
^{1}H-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ^{o}C, 800 MHz, $CDCl_3$):



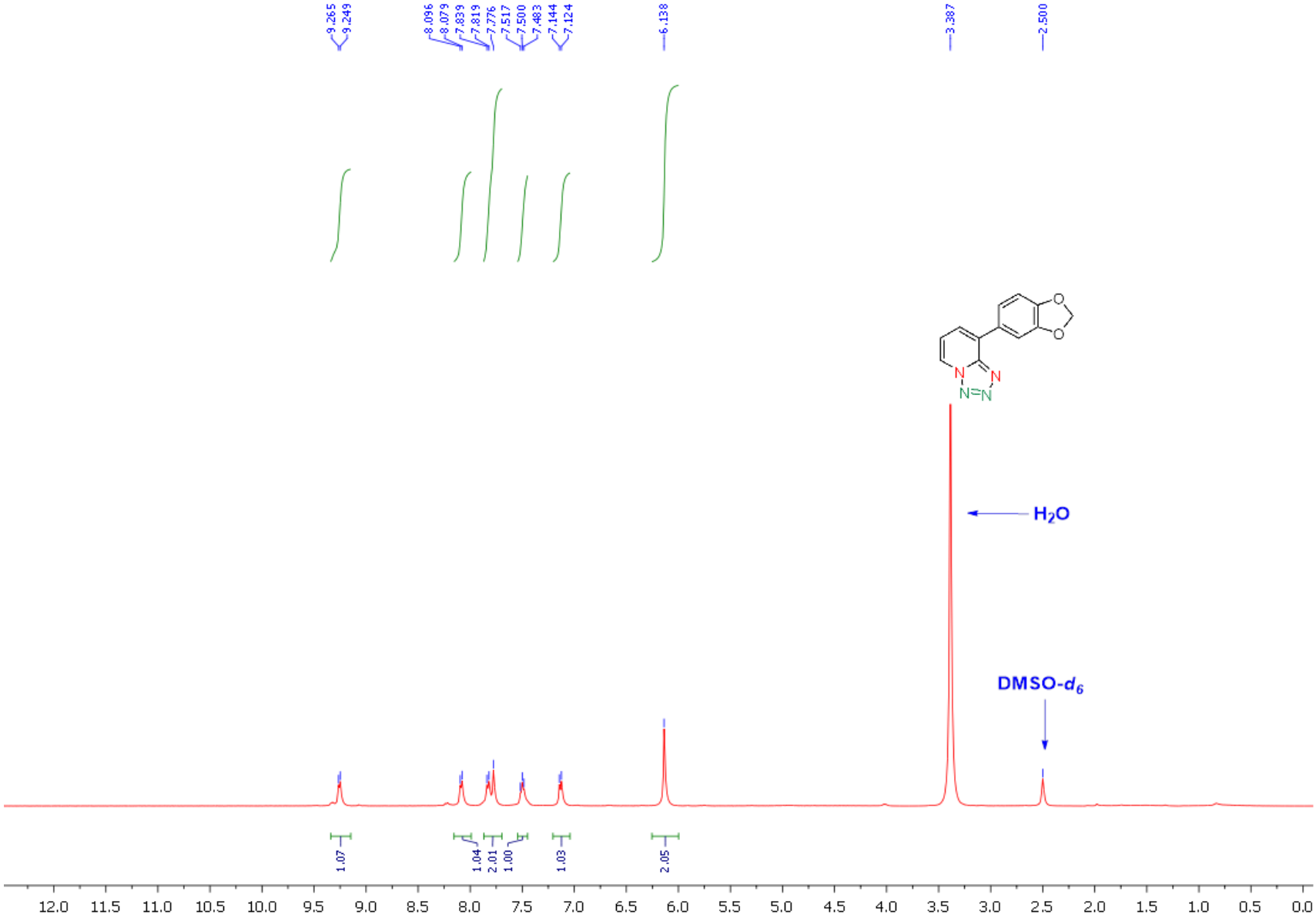
^{13}C-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ºC, 200 MHz, $CDCl_3$):



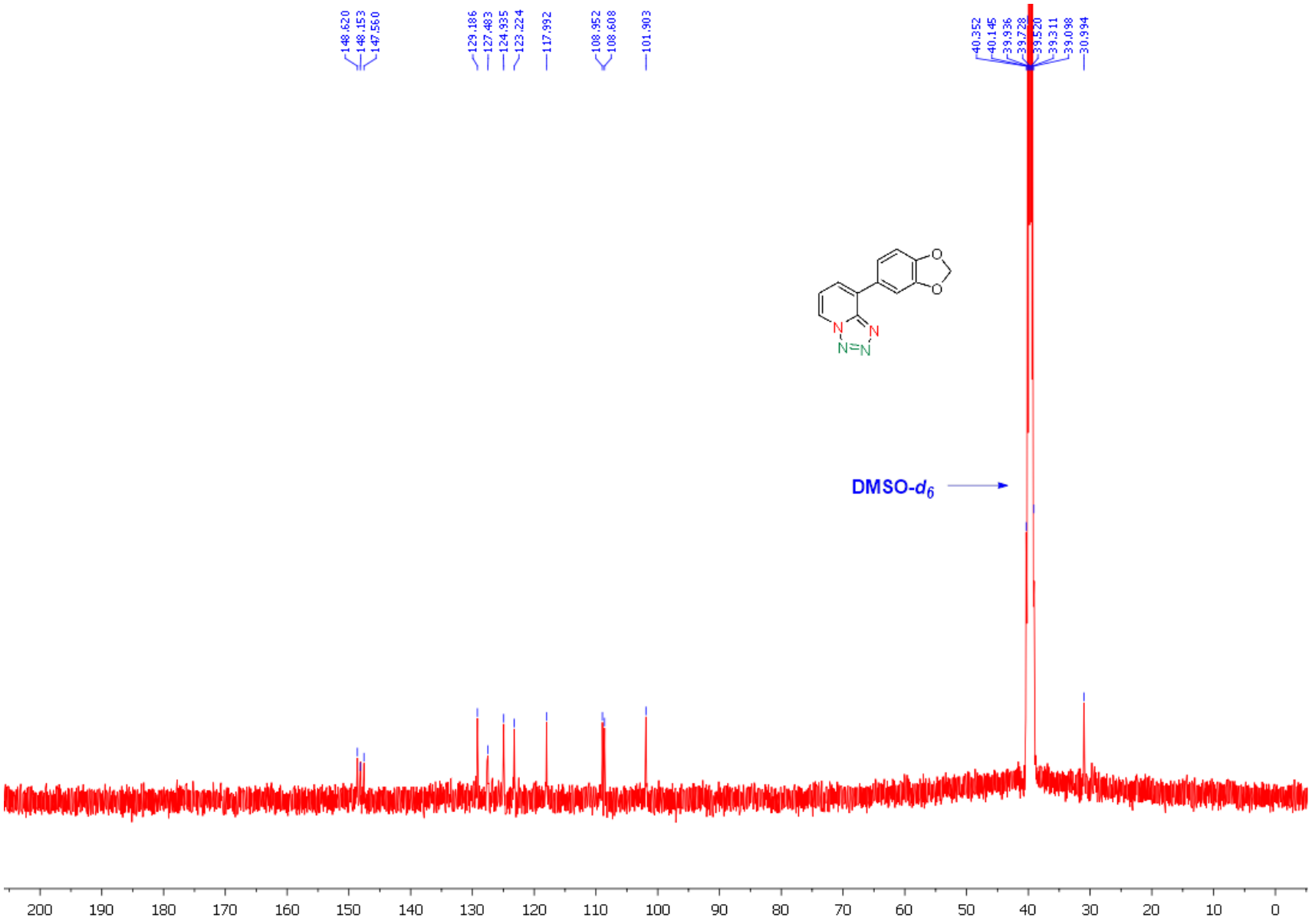
^{19}F-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 °C, 376 MHz, $CDCl_3$):



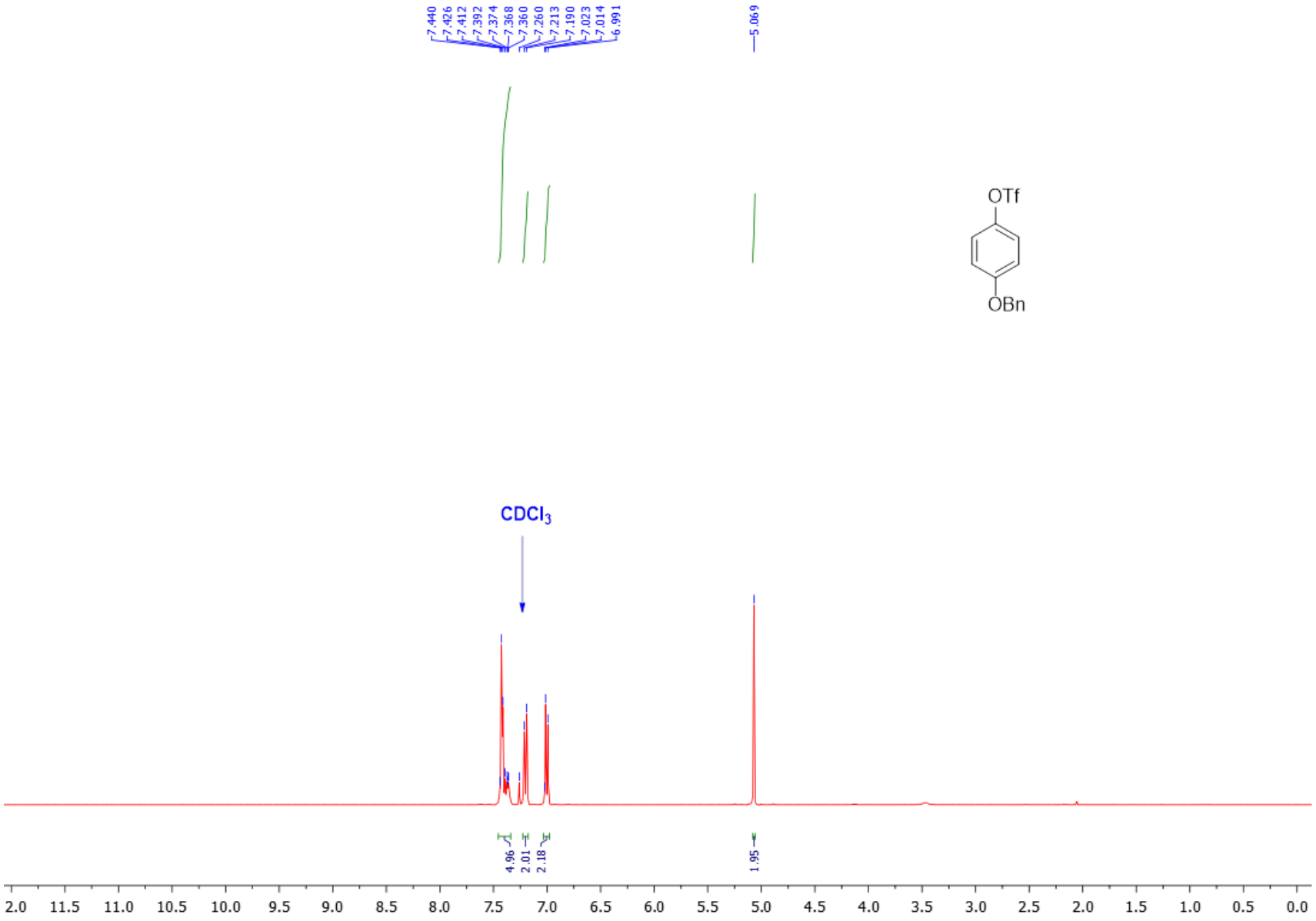
^{1}H-NMR of *8-(benzo[d][1,3]dioxol-5-yl)tetrazolo[1,5-a]pyridine (1g)* (25 ºC, 400 MHz, DMSO-d_6):



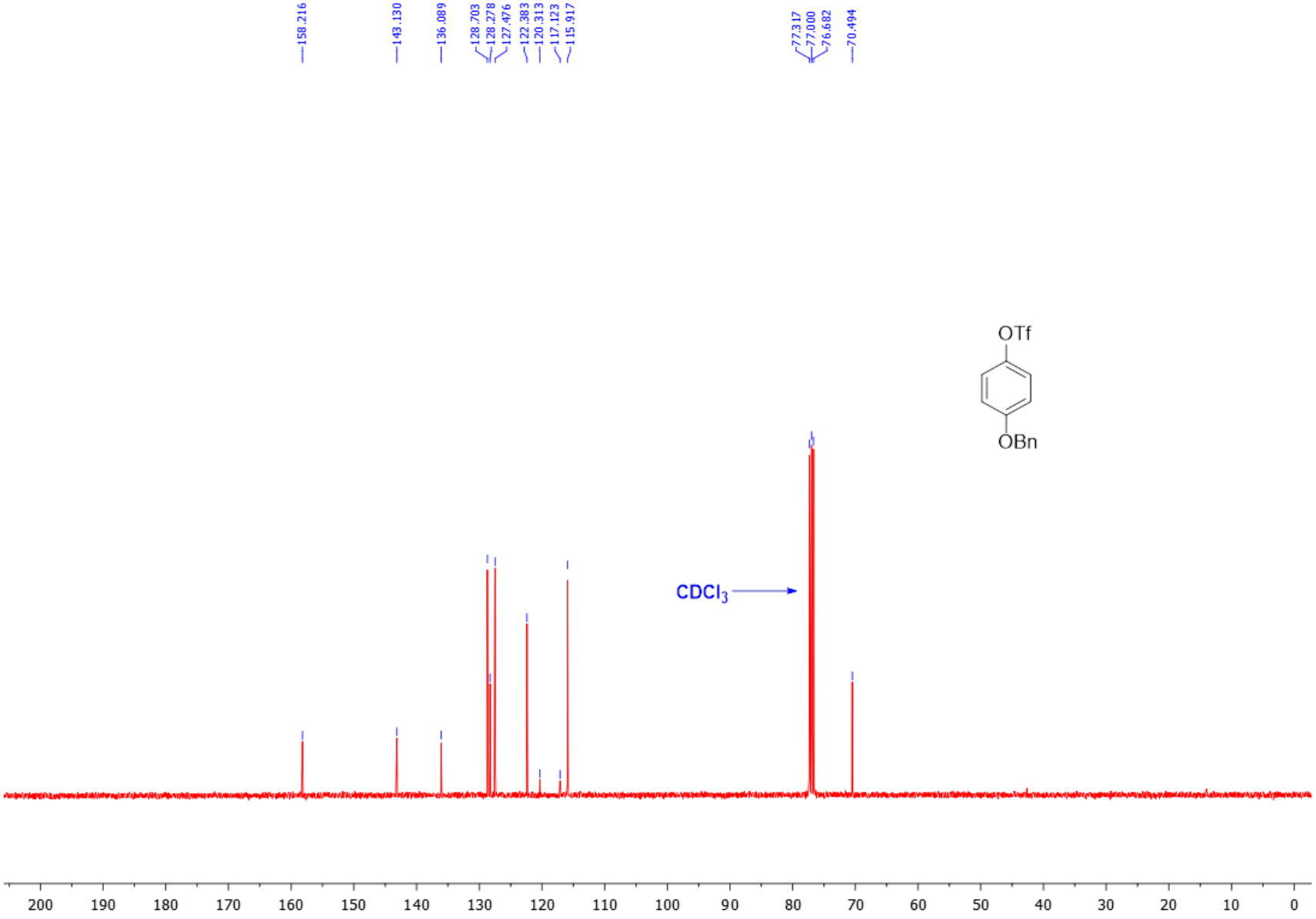
^{13}C-NMR of *8-(benzo[d][1,3]dioxol-5-yl)tetrazolo[1,5-a]pyridine (1g)* (25 ºC, 100 MHz, DMSO-d_6):



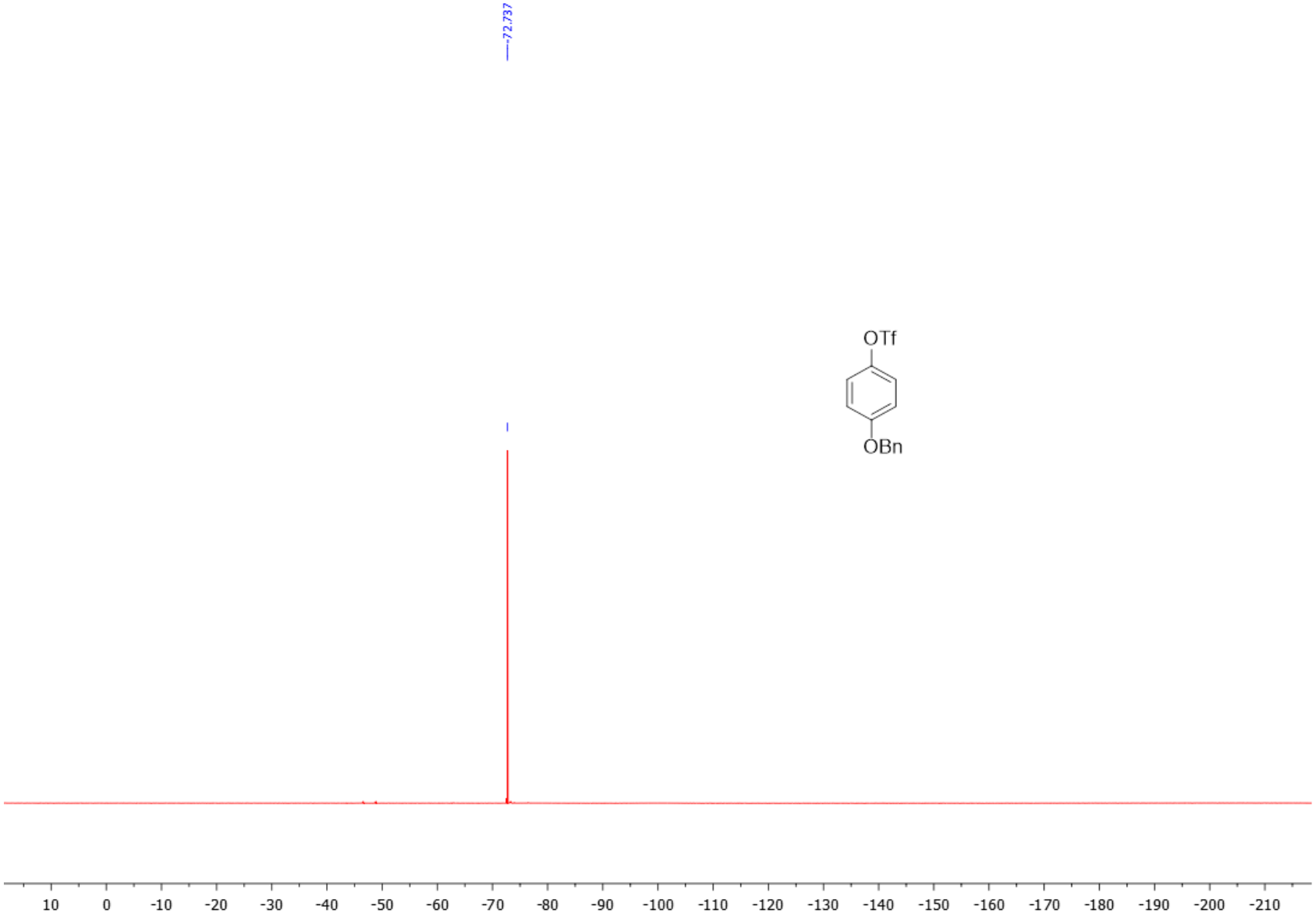
^{1}H-NMR of *4-(benzyloxy)phenyl trifluoromethanesulfonate* (25 ^{o}C, 400 MHz, $CDCl_3$):



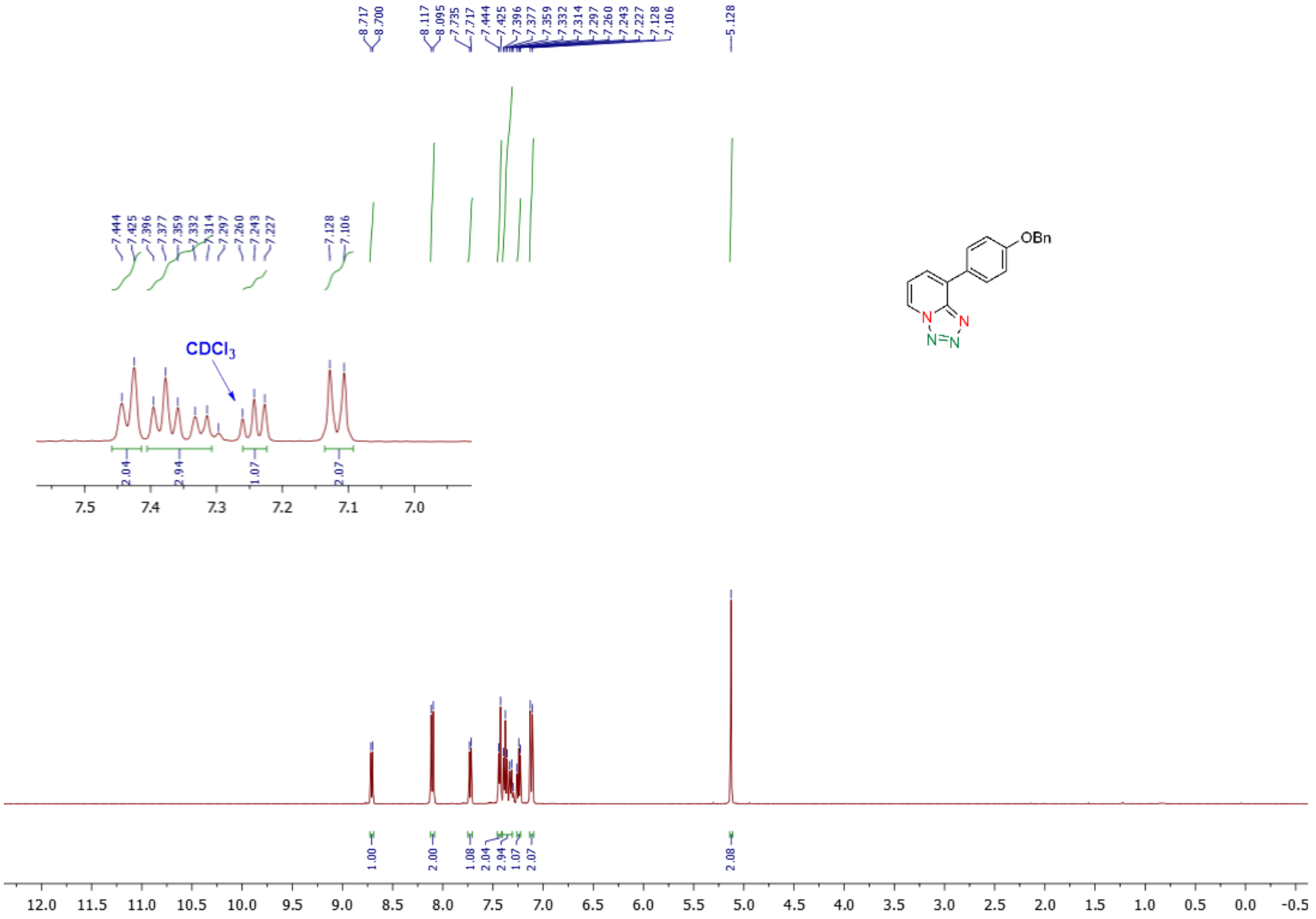
^{13}C-NMR of *4-(benzyloxy)phenyl trifluoromethanesulfonate)* (25 ^{o}C, 100 MHz, $CDCl_3$):



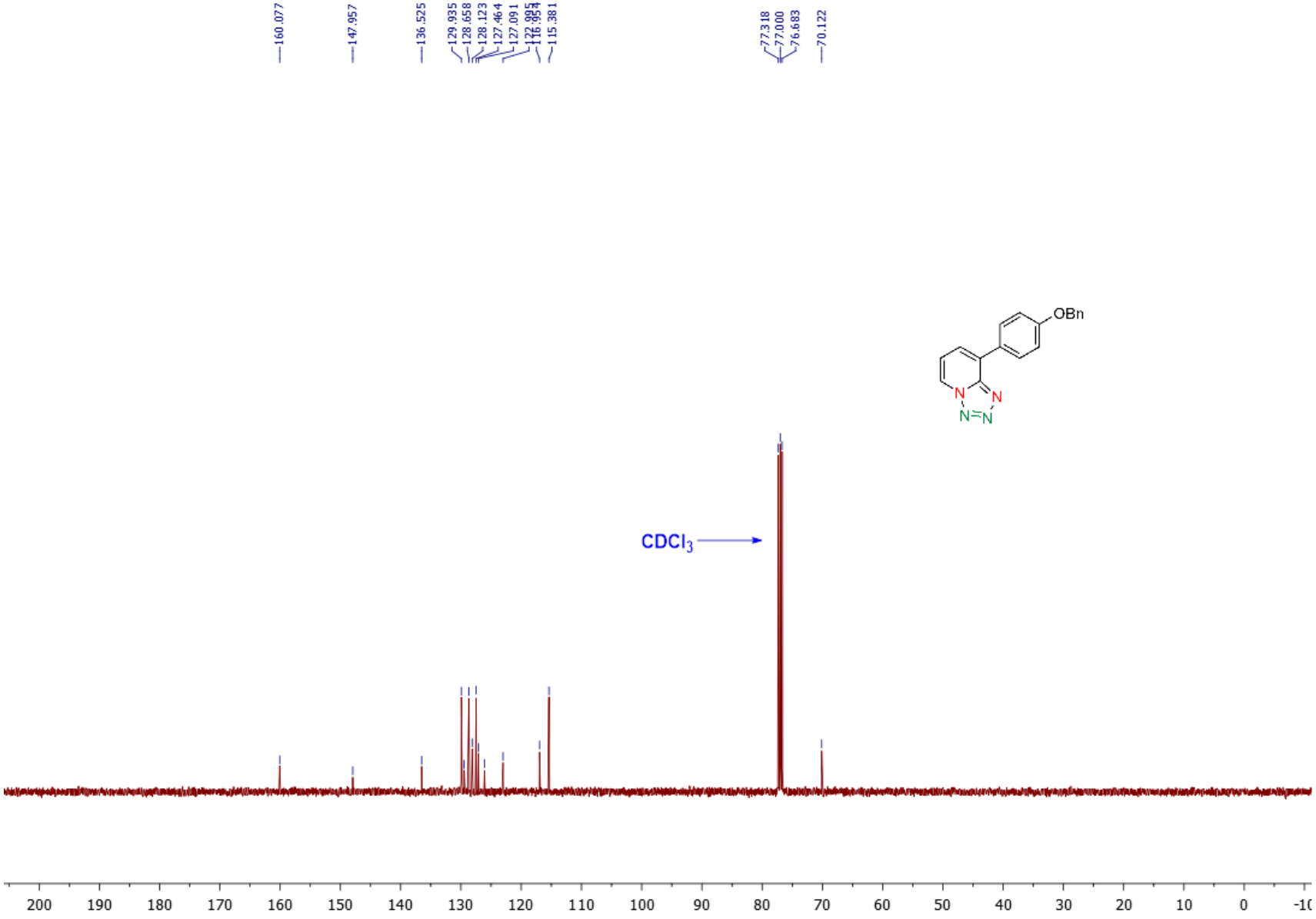
^{19}F-NMR of *4-(benzyloxy)phenyl trifluoromethanesulfonate* (25 °C, 376 MHz, $CDCl_3$):



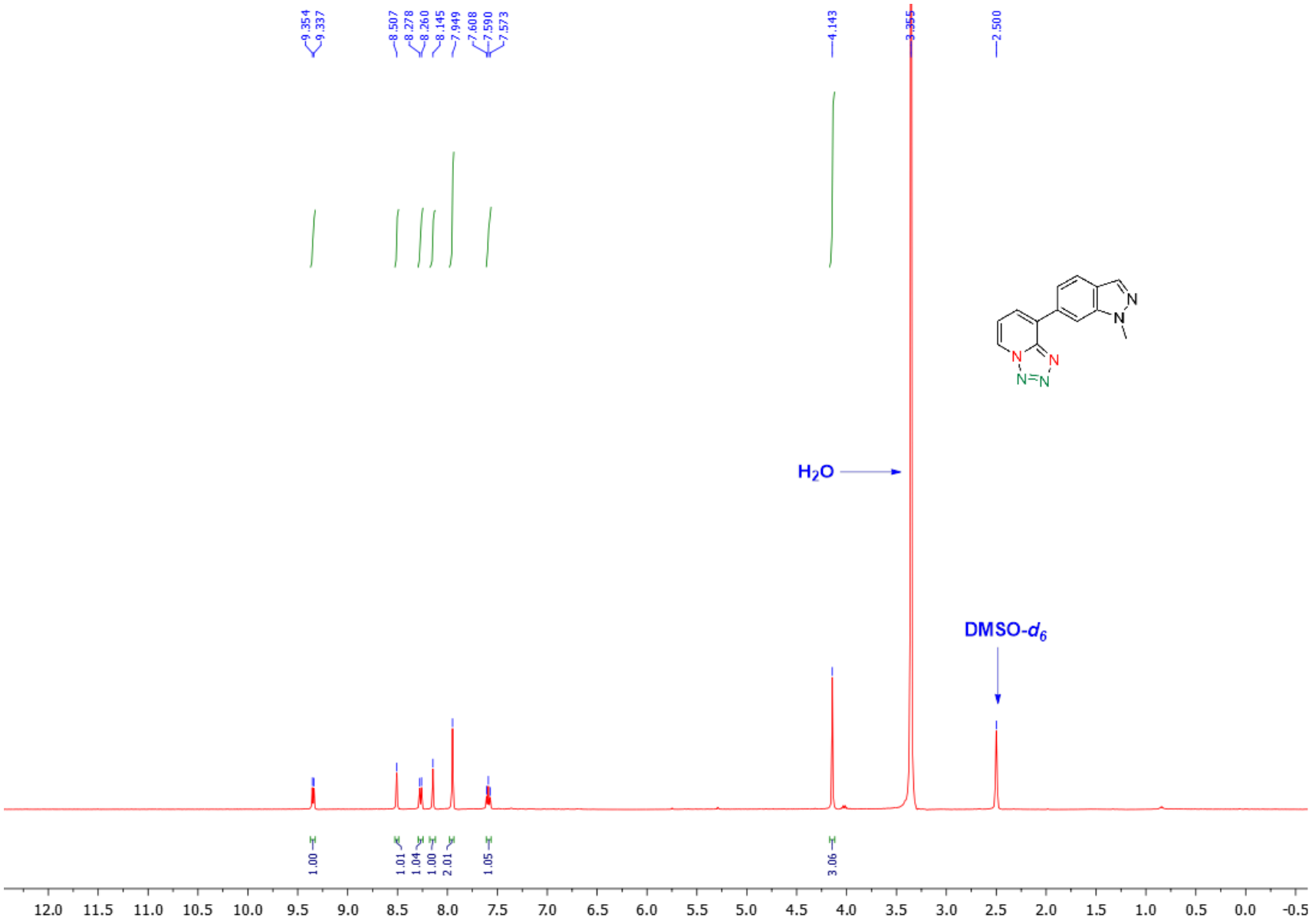
^{1}H-NMR of *8-(4-(benzyloxy)phenyl)tetrazolo[1,5-a]pyridine (1h)* (25 ºC, 400 MHz, $CDCl_3$):



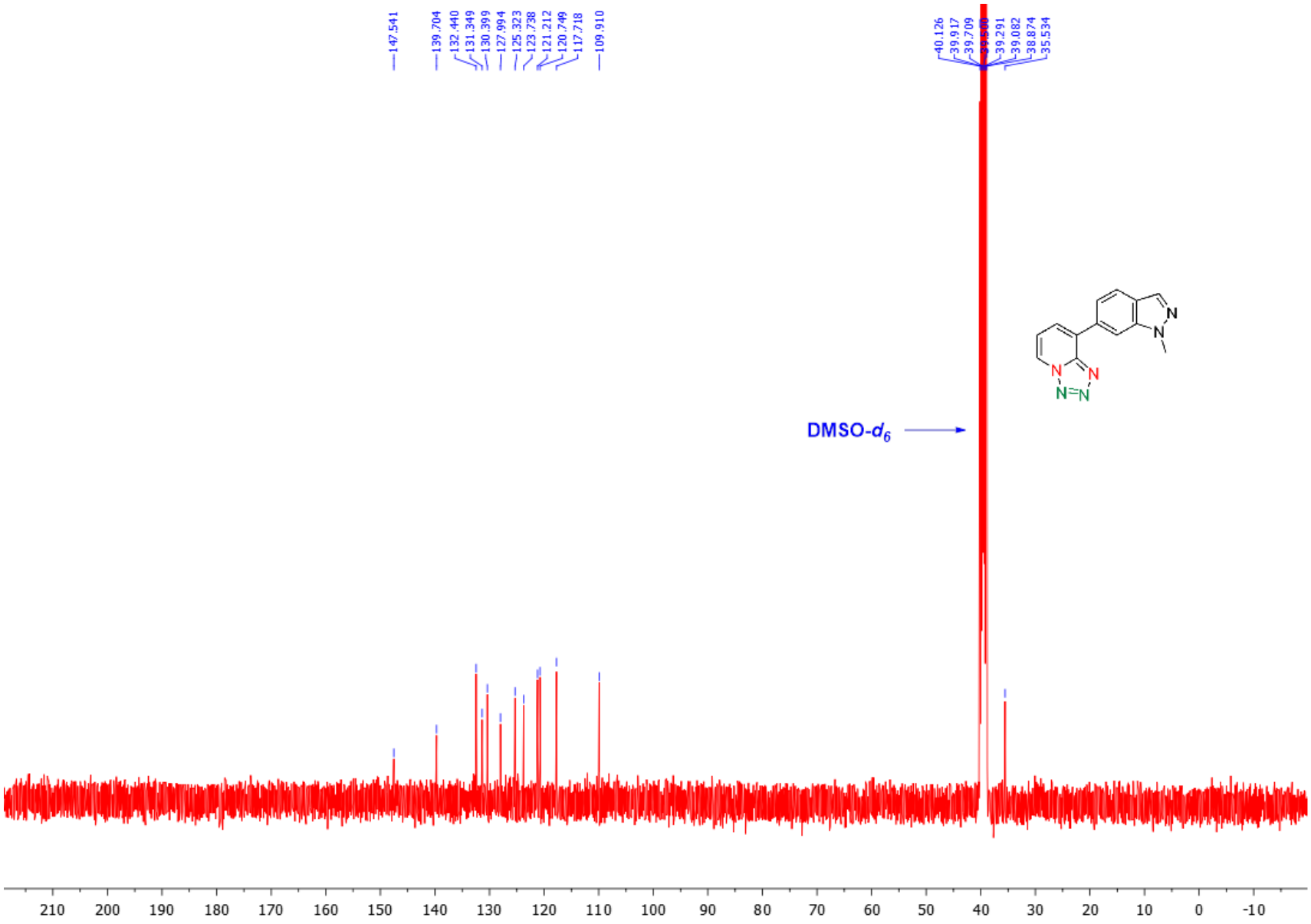
^{13}C-NMR of *8-(4-(benzyloxy)phenyl)tetrazolo[1,5-a]pyridine (1h)* (25 °C, 100 MHz, $CDCl_3$):



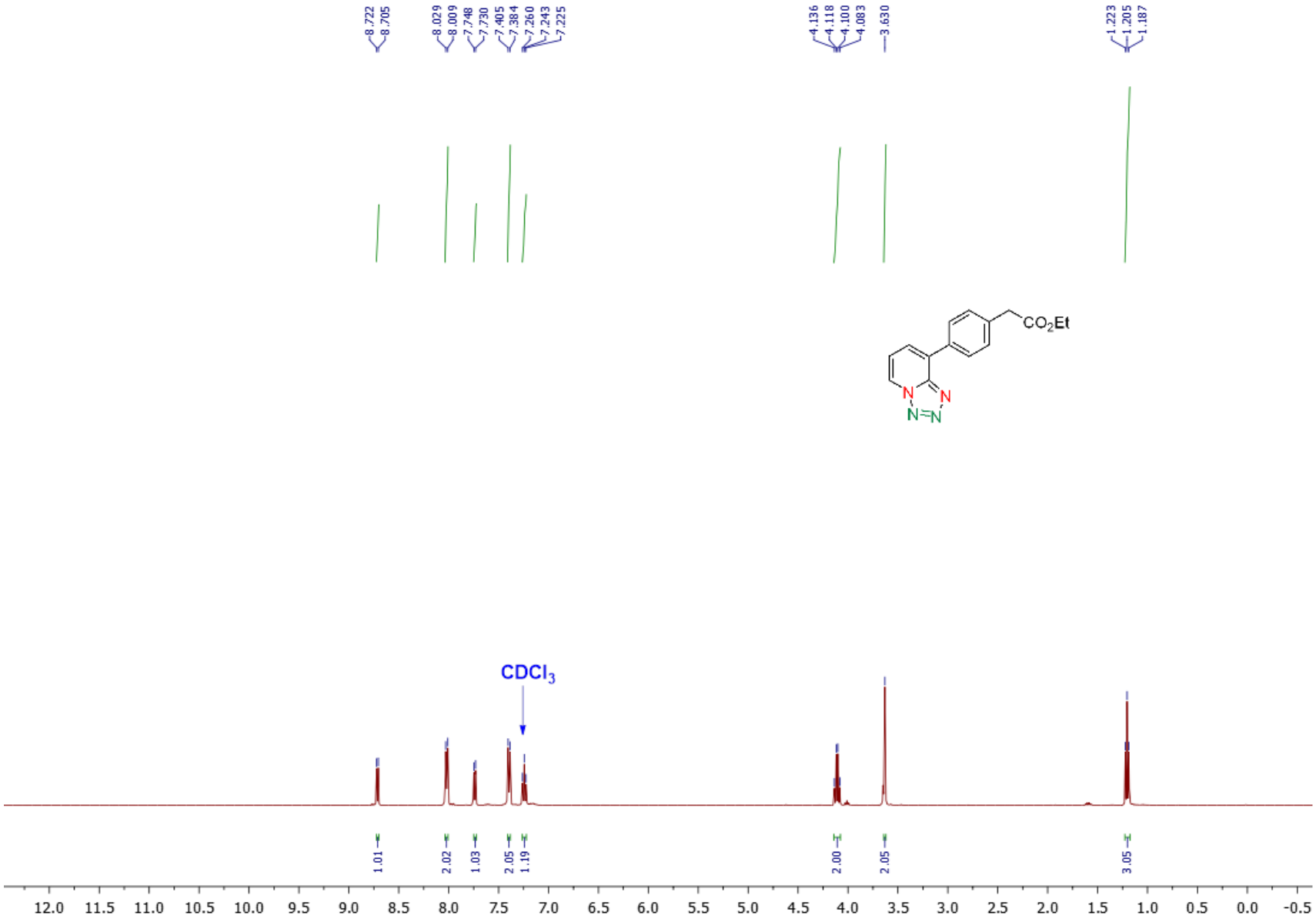
^{1}H-NMR of *8-(1-methyl-1H-indazol-6-yl)tetrazolo[1,5-a]pyridine (1i) (25 °C, 400 MHz, DMSO-d_6):*



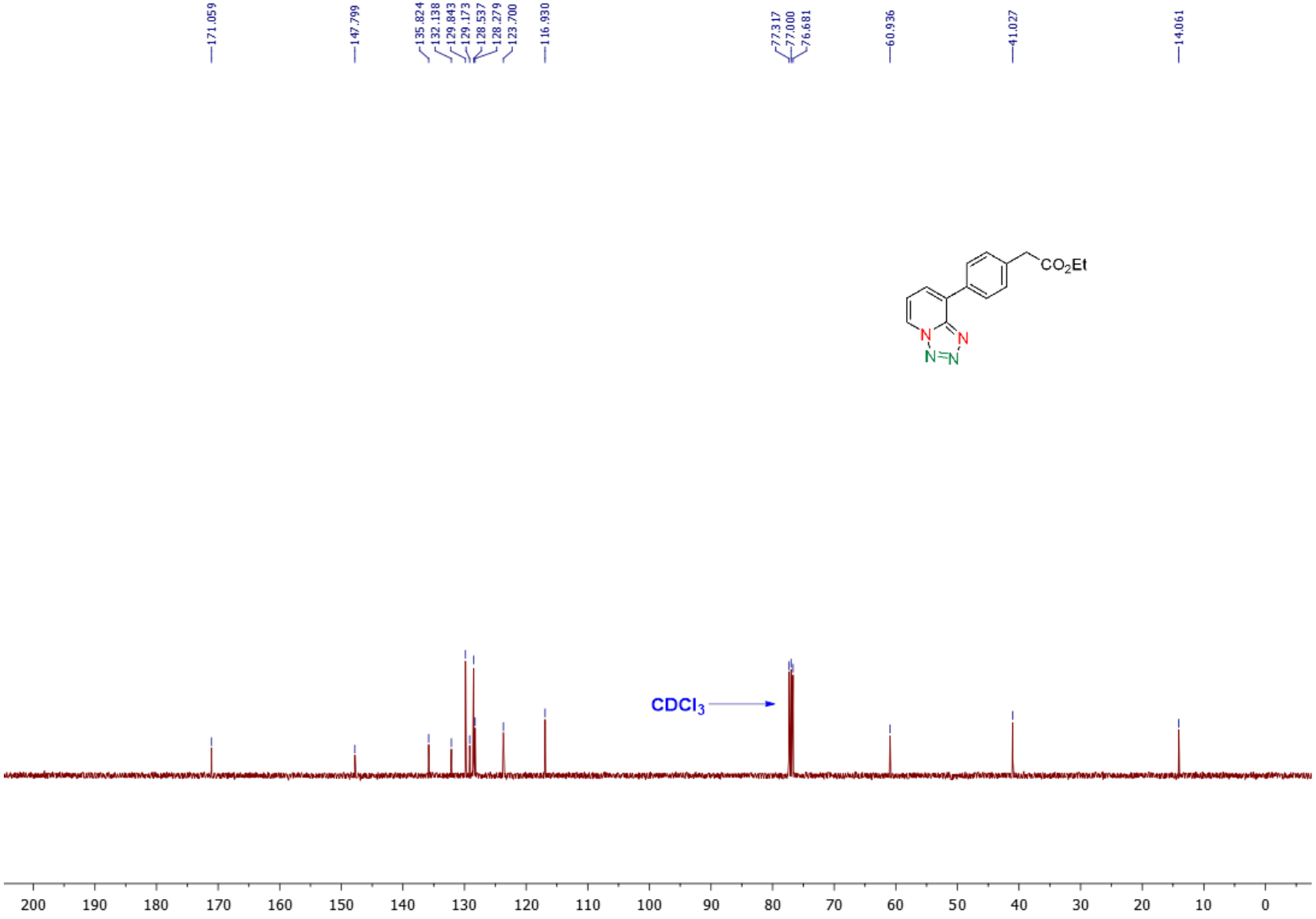
^{13}C-NMR of *8-(1-methyl-1H-indazol-6-yl)tetrazolo[1,5-a]pyridine (1i))* (25 ºC, 100 MHz, DMSO-d_6):



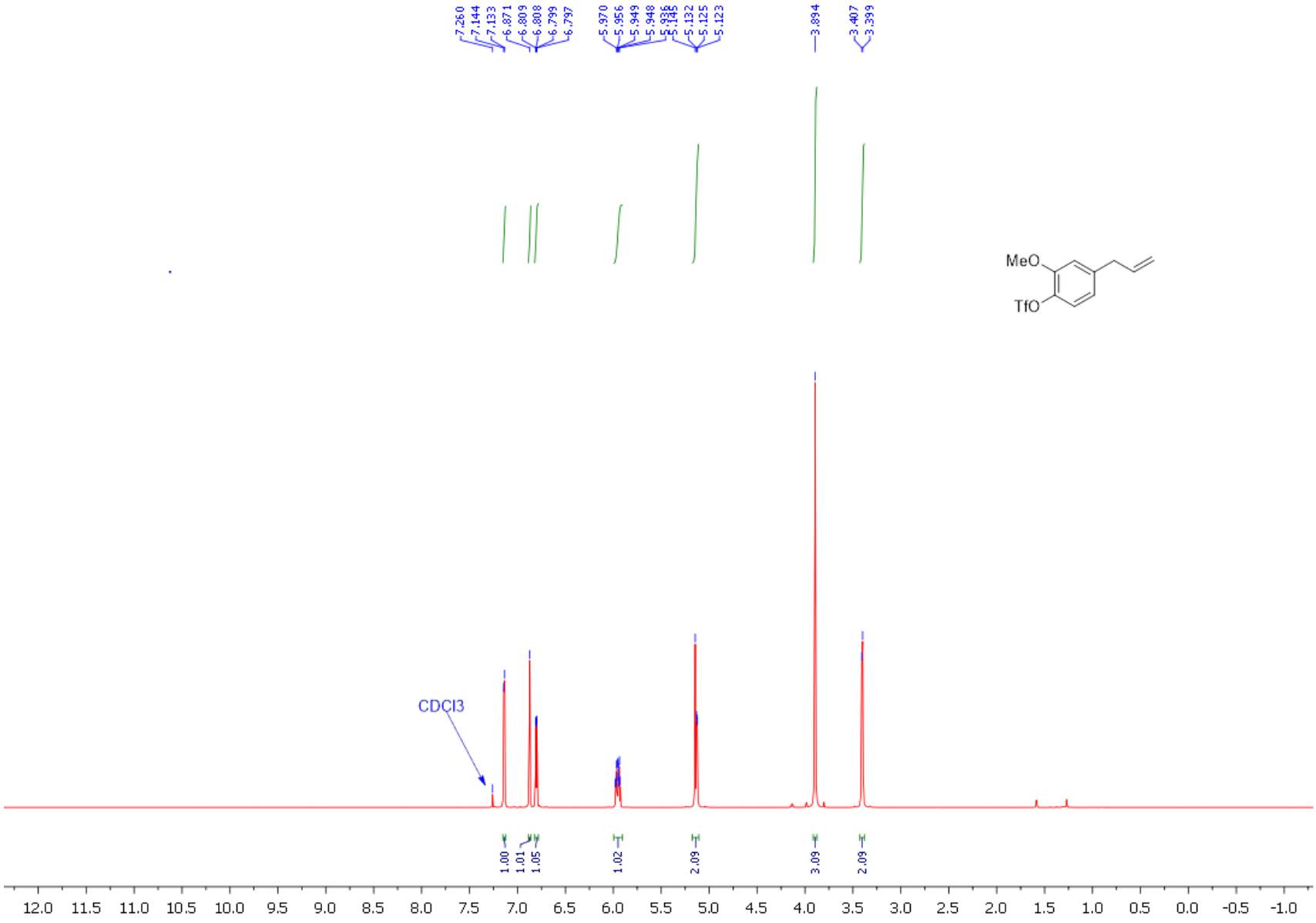
^{1}H-NMR of *ethyl 2-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetate (1j)* (25 ^{o}C, 400 MHz, $CDCl_3$):



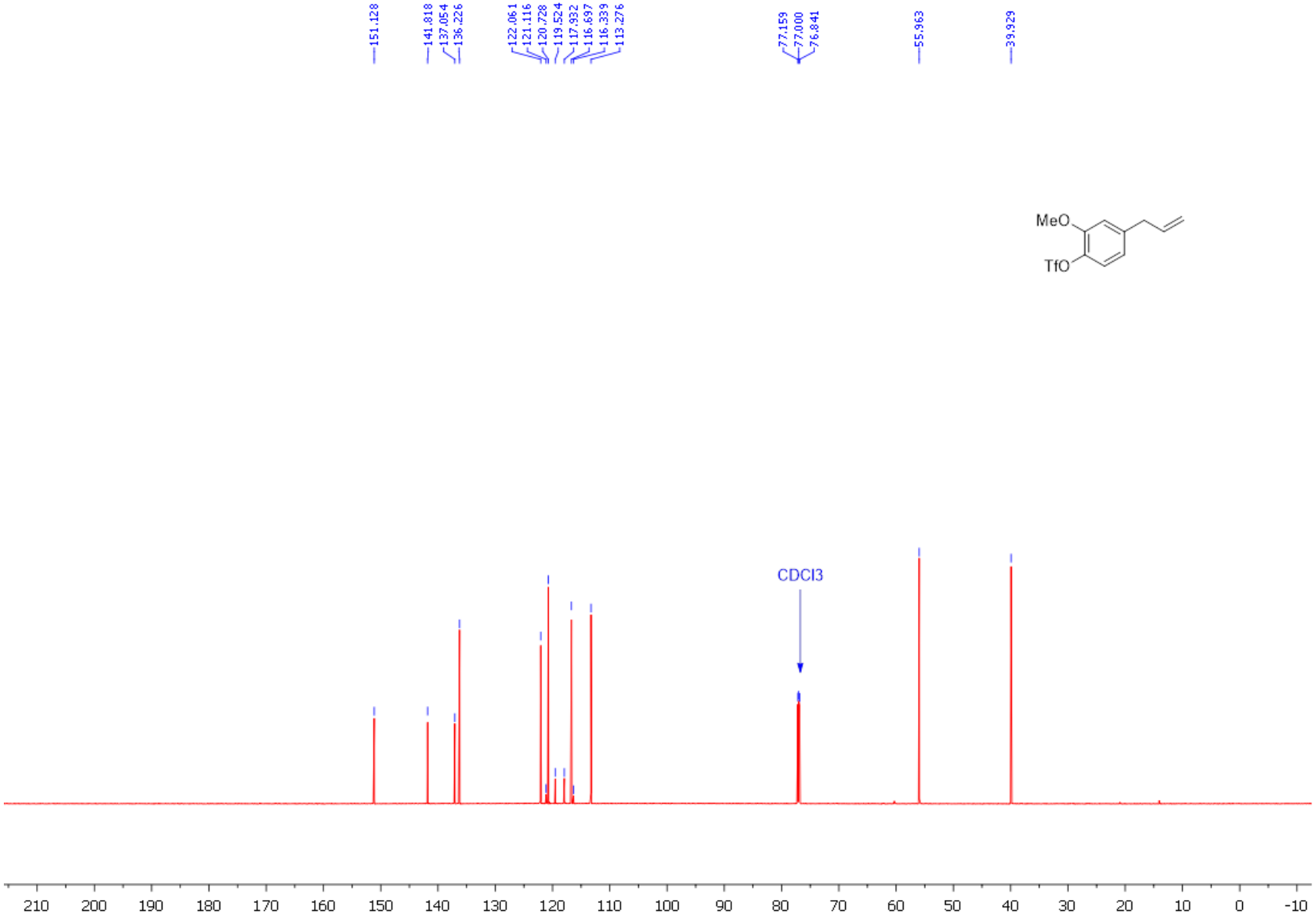
^{13}C-NMR of *ethyl 2-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetate (1j)* (25 ºC, 100 MHz, $CDCl_3$):



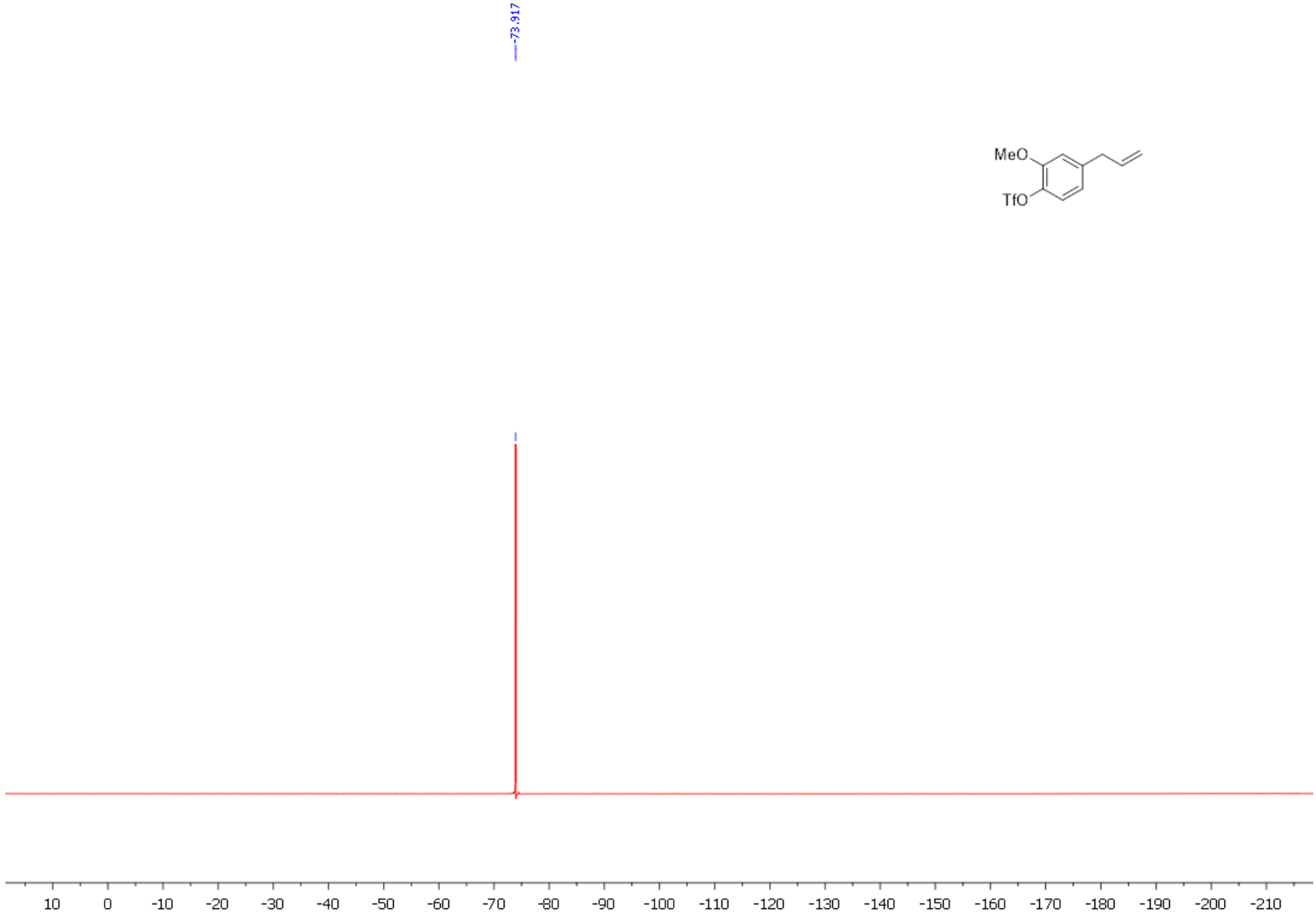
^{1}H-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ^{o}C, 800 MHz, $CDCl_3$):



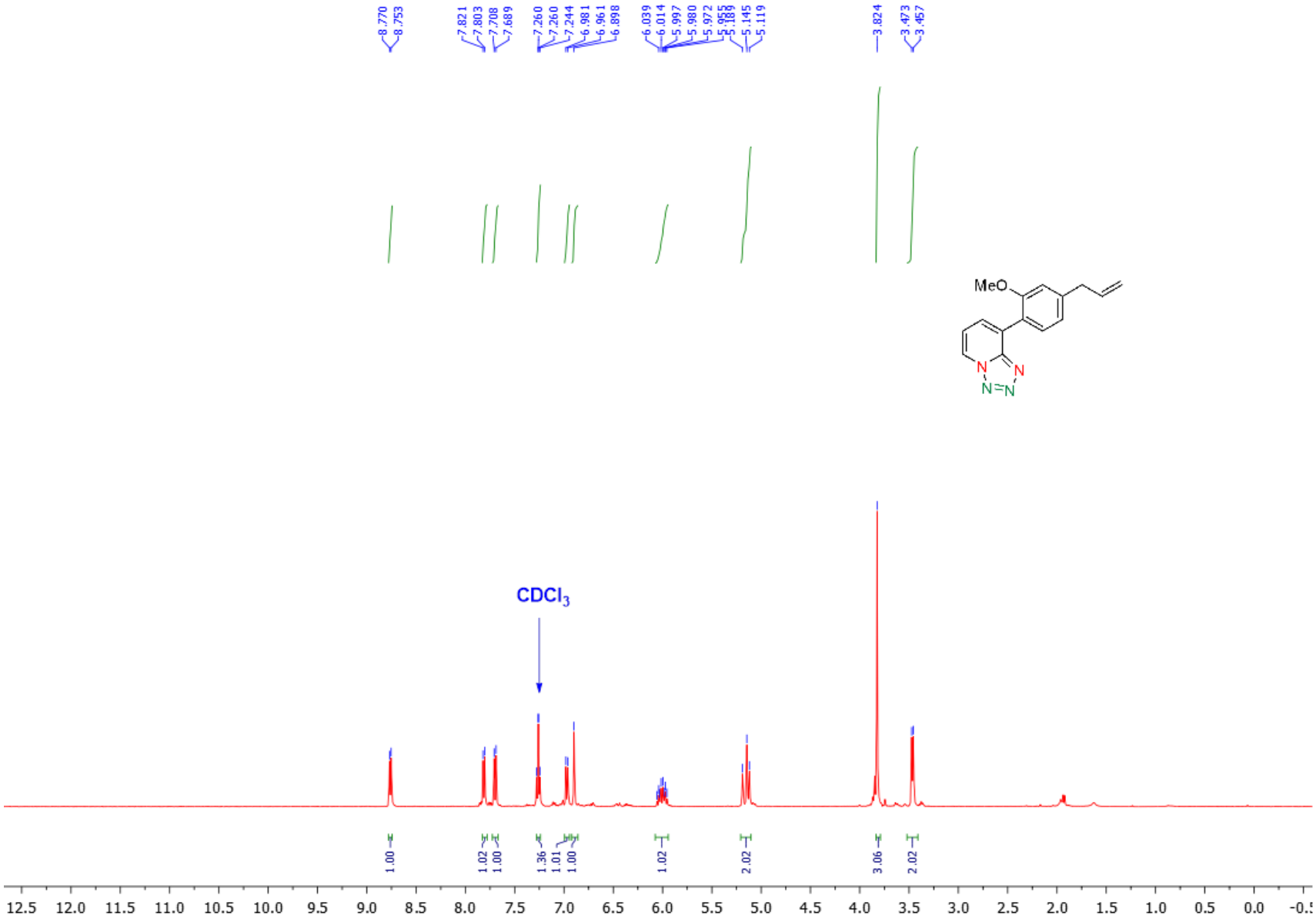
^{13}C-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 °C, 200 MHz, $CDCl_3$):



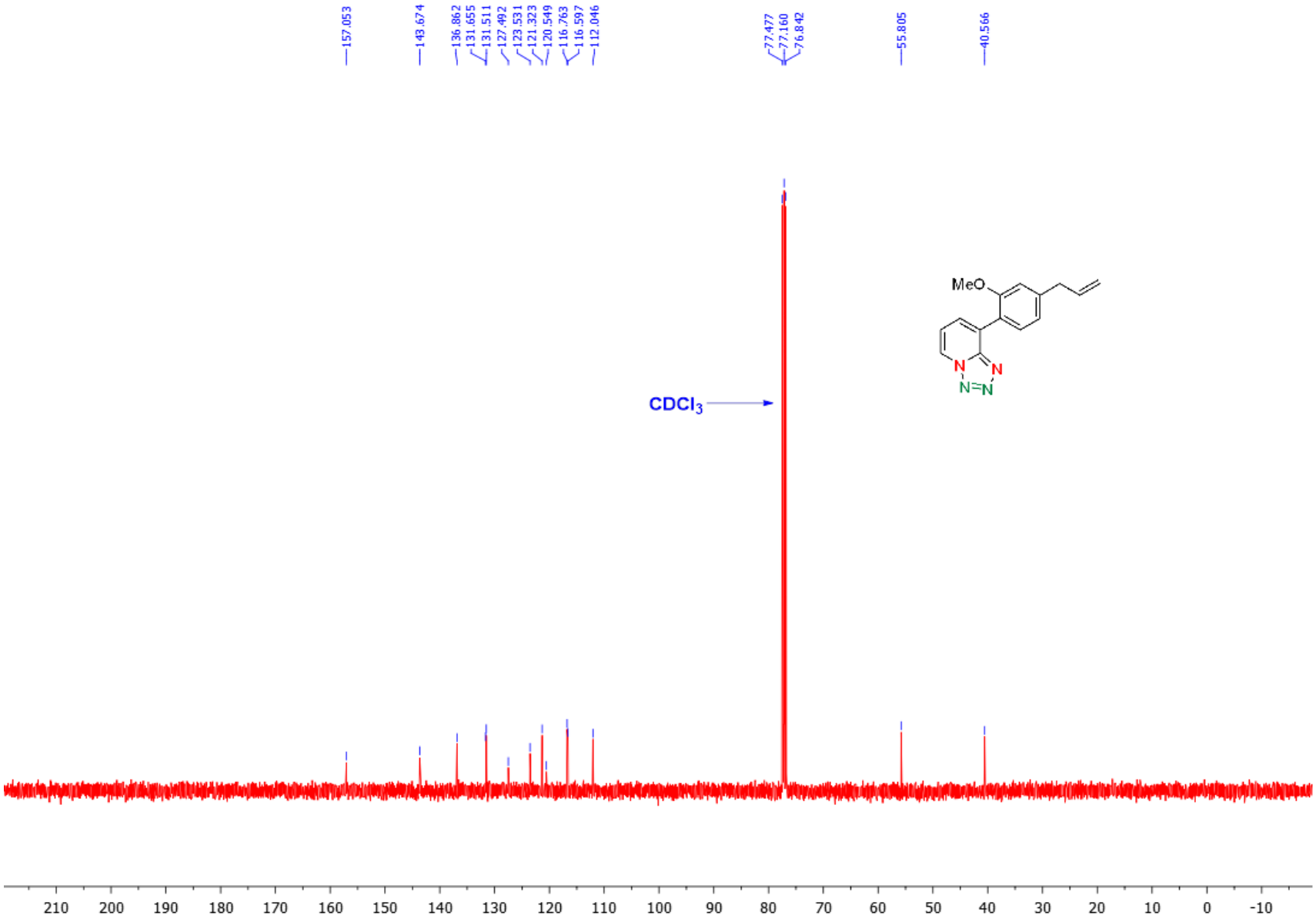
^{19}F-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ºC, 376 MHz, $CDCl_3$):



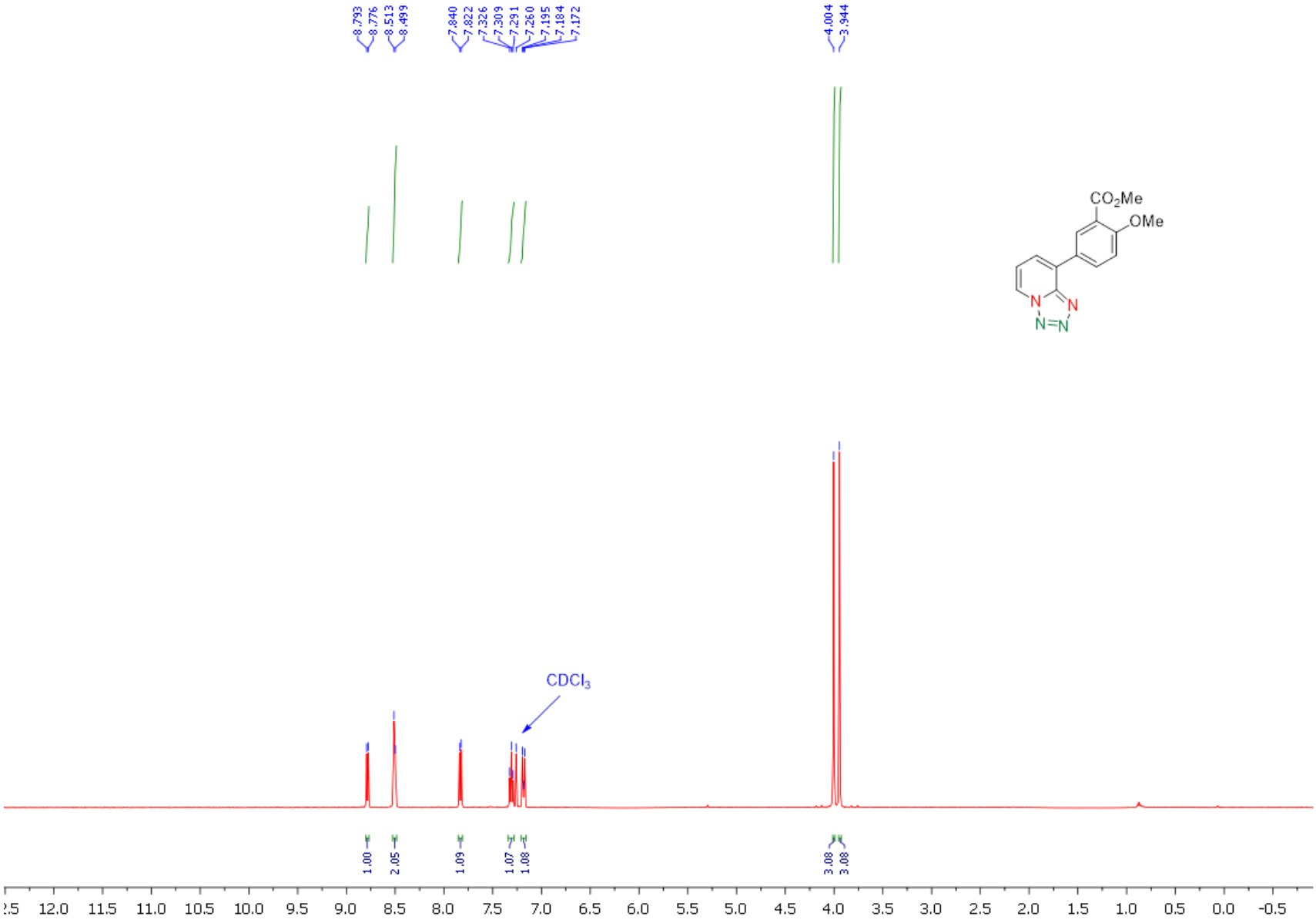
^{1}H-NMR of *8-(4-allyl-2-methoxyphenyl)tetrazolo[1,5-a]pyridine (1k)* (25 ^{o}C, 400 MHz, $CDCl_3$):



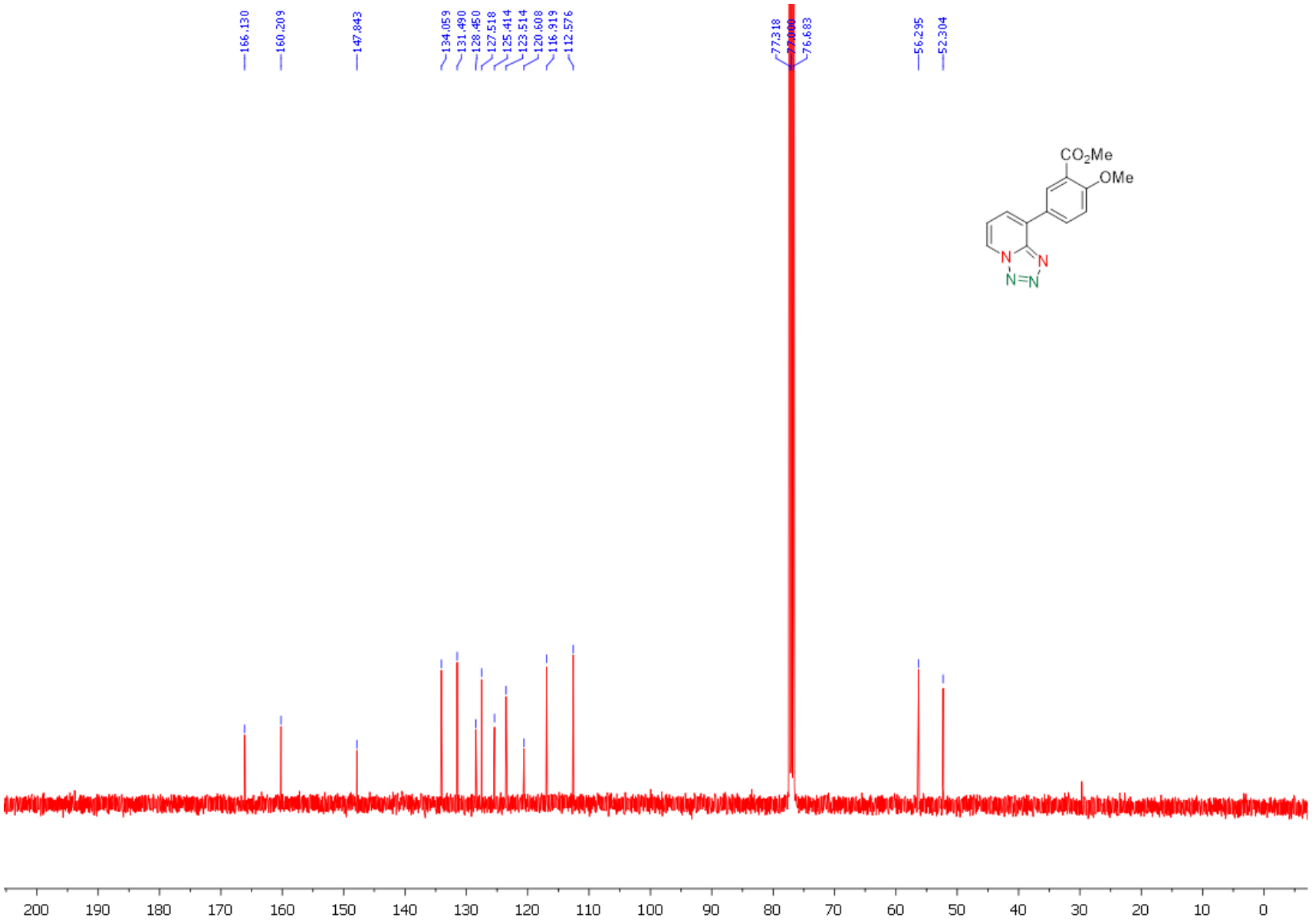
^{13}C-NMR of *8-(4-allyl-2-methoxyphenyl)tetrazolo[1,5-a]pyridine (1k)* (25 °C, 100 MHz, $CDCl_3$):



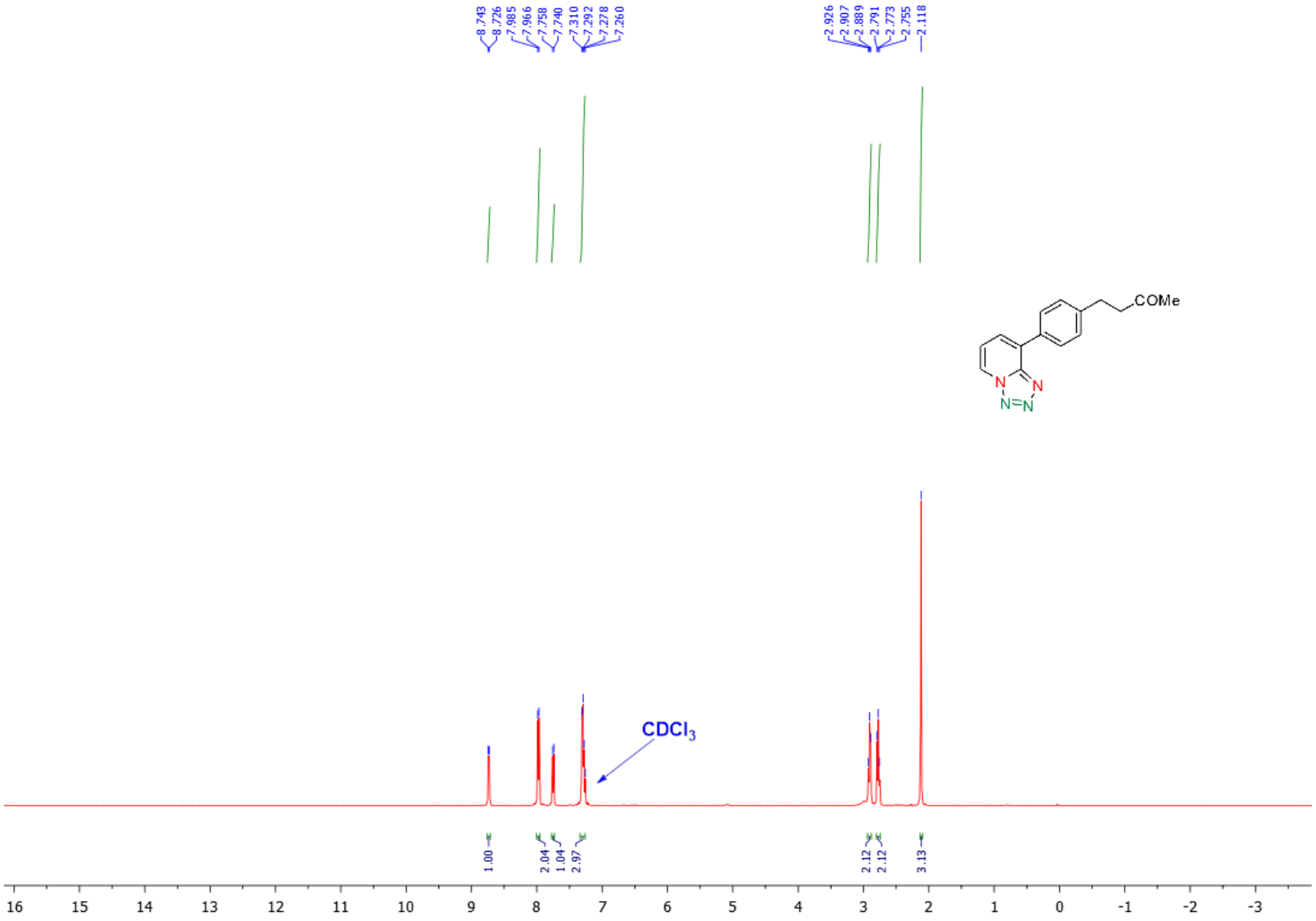
^{1}H-NMR of *methyl 2-methoxy-5-(tetrazolo[1,5-a]pyridin-8-yl)benzoate((1l)* (25 ^{o}C, 400 MHz, $CDCl_3$):



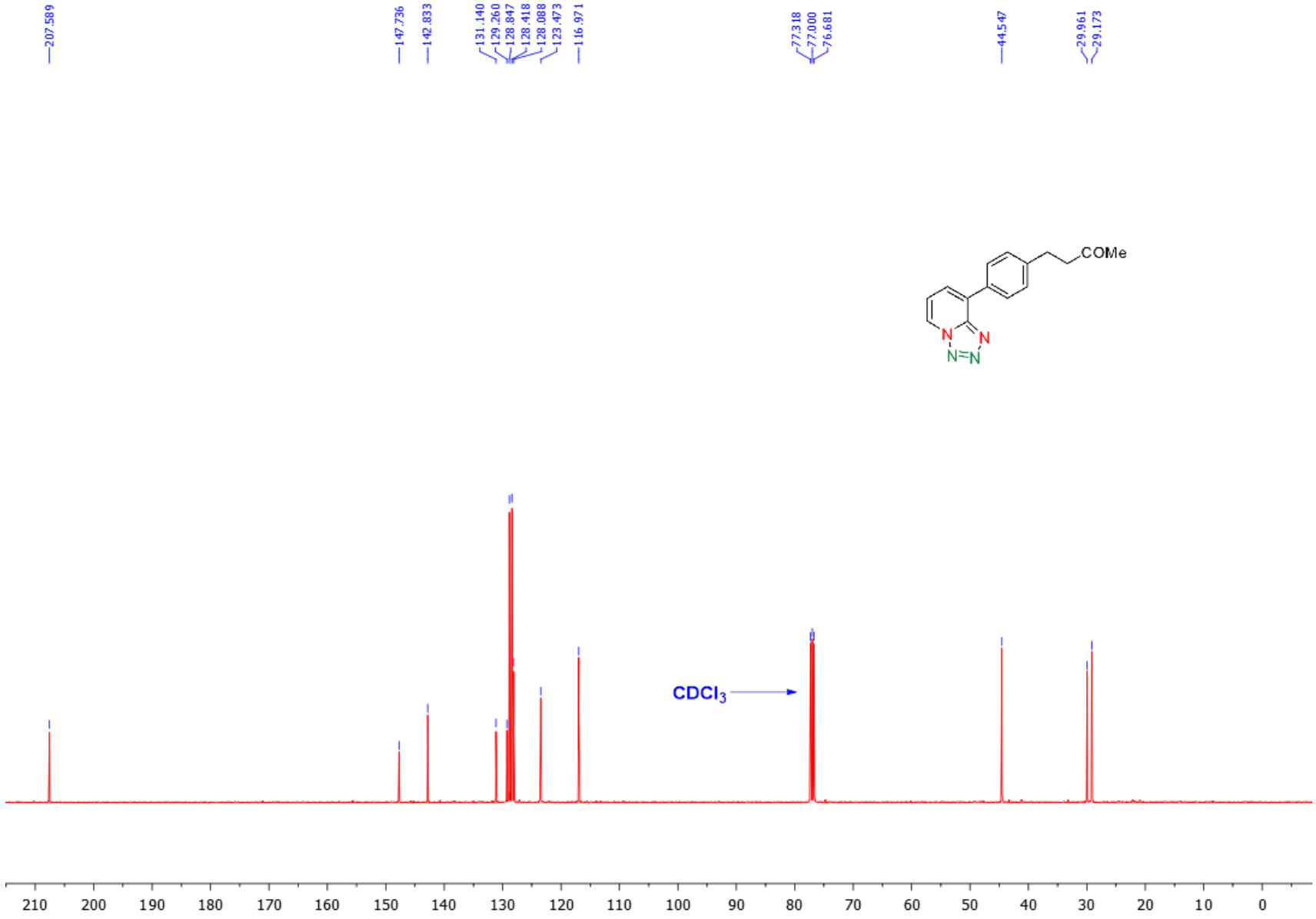
^{13}C-NMR of *methyl 2-methoxy-5-(tetrazolo[1,5-a]pyridin-8-yl)benzoate((1l)* (25 ºC, 100 MHz, $CDCl_3$):



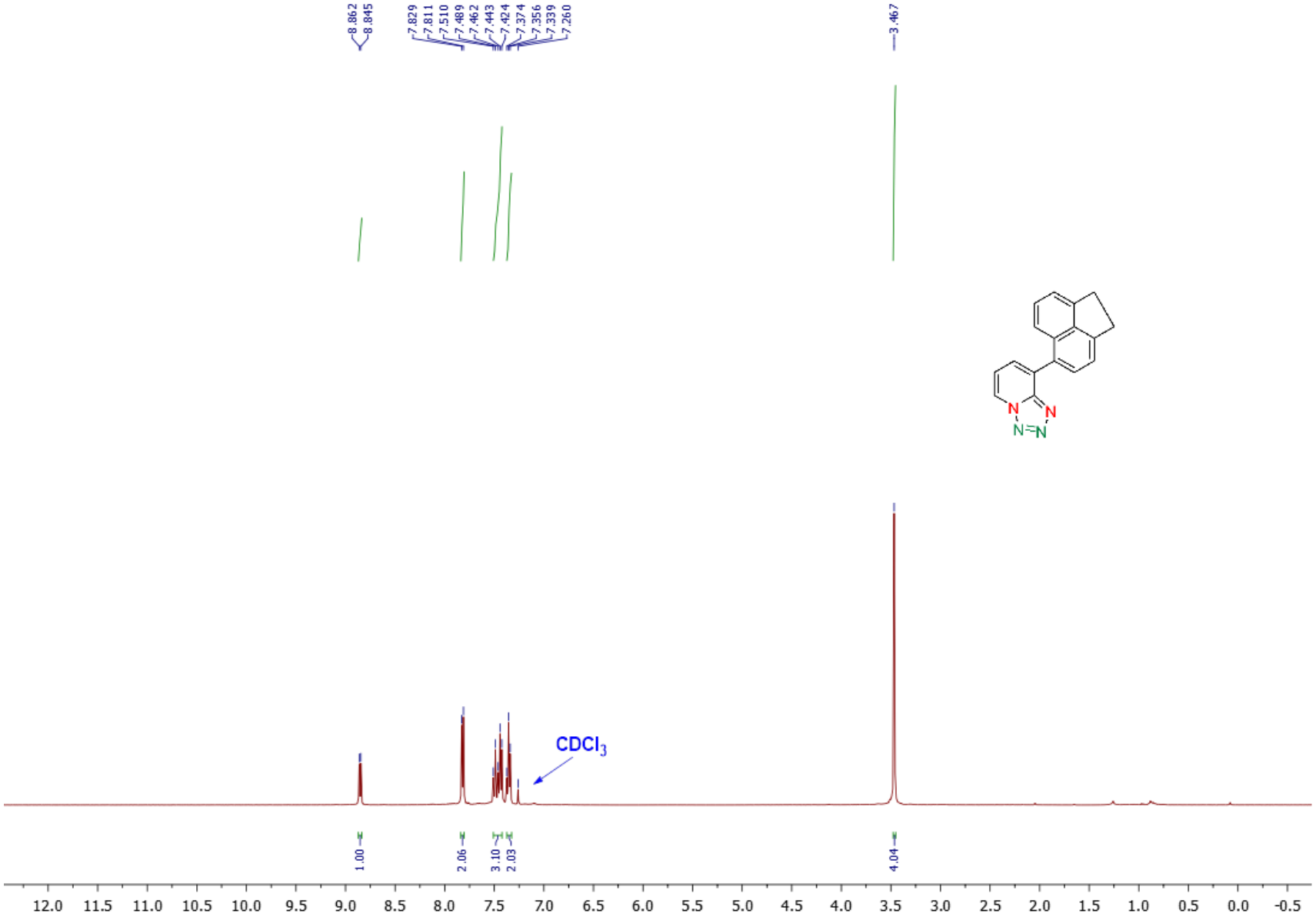
^{1}H-NMR of *4-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)butan-2-one (1m)* (25 °C, 400 MHz, $CDCl_3$):



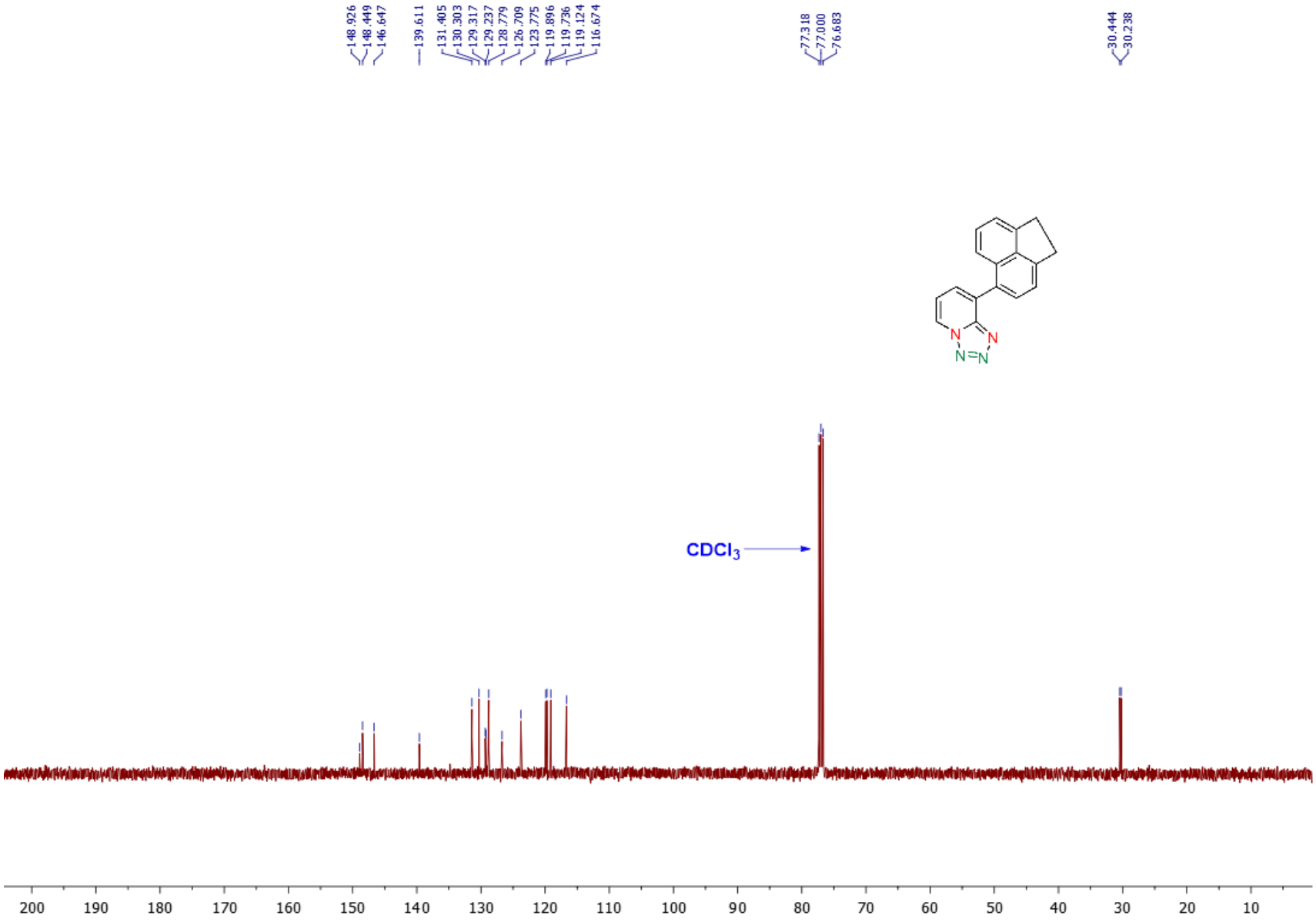
^{13}C-NMR of *4-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)butan-2-one (1m)* (25 ºC, 100 MHz, $CDCl_3$):



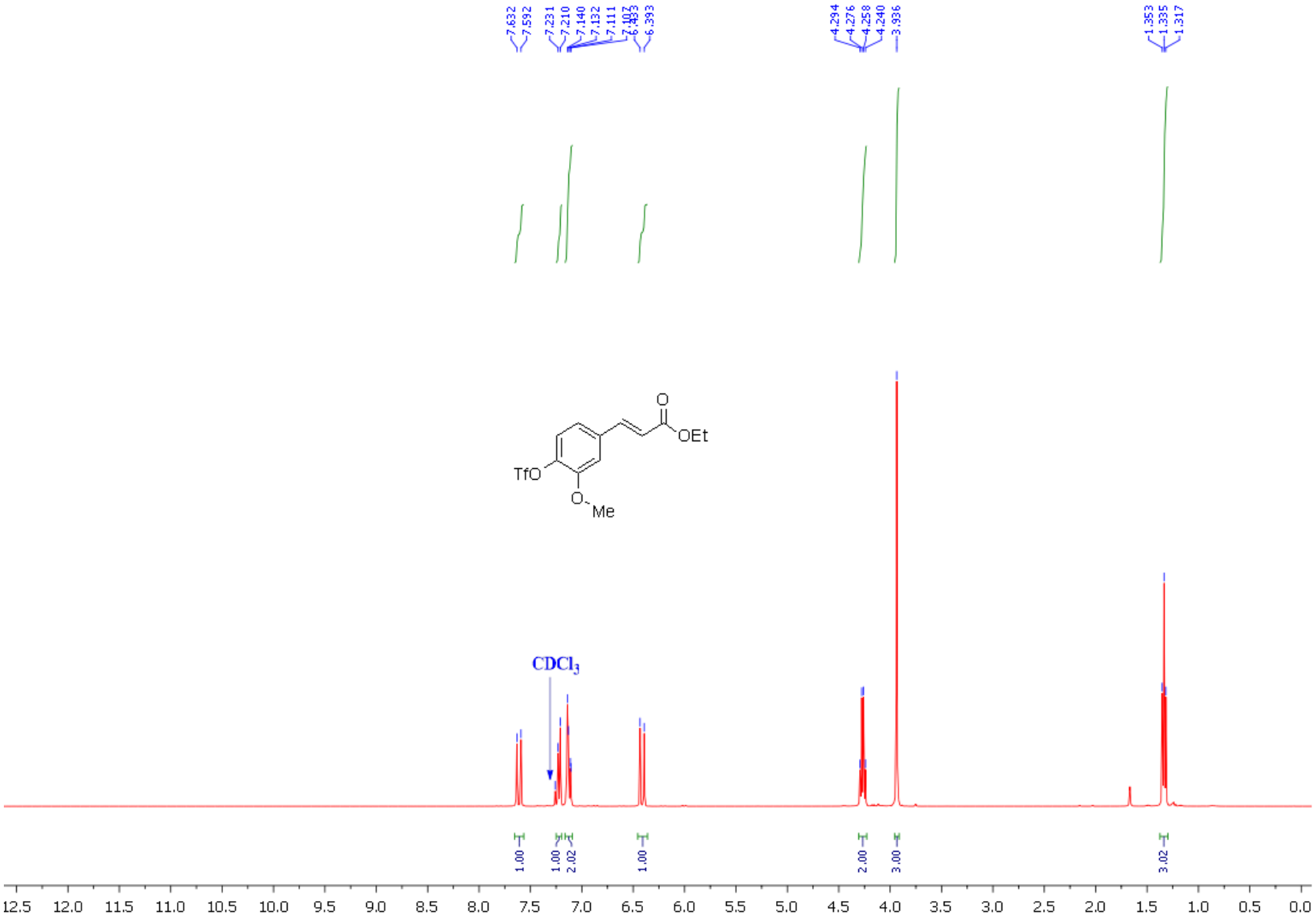
^{1}H-NMR of *(8-(1,2-dihydroacenaphthylen-5-yl)tetrazolo[1,5-a]pyridine (1n)* (25 ^{o}C, 400 MHz, $CDCl_3$):



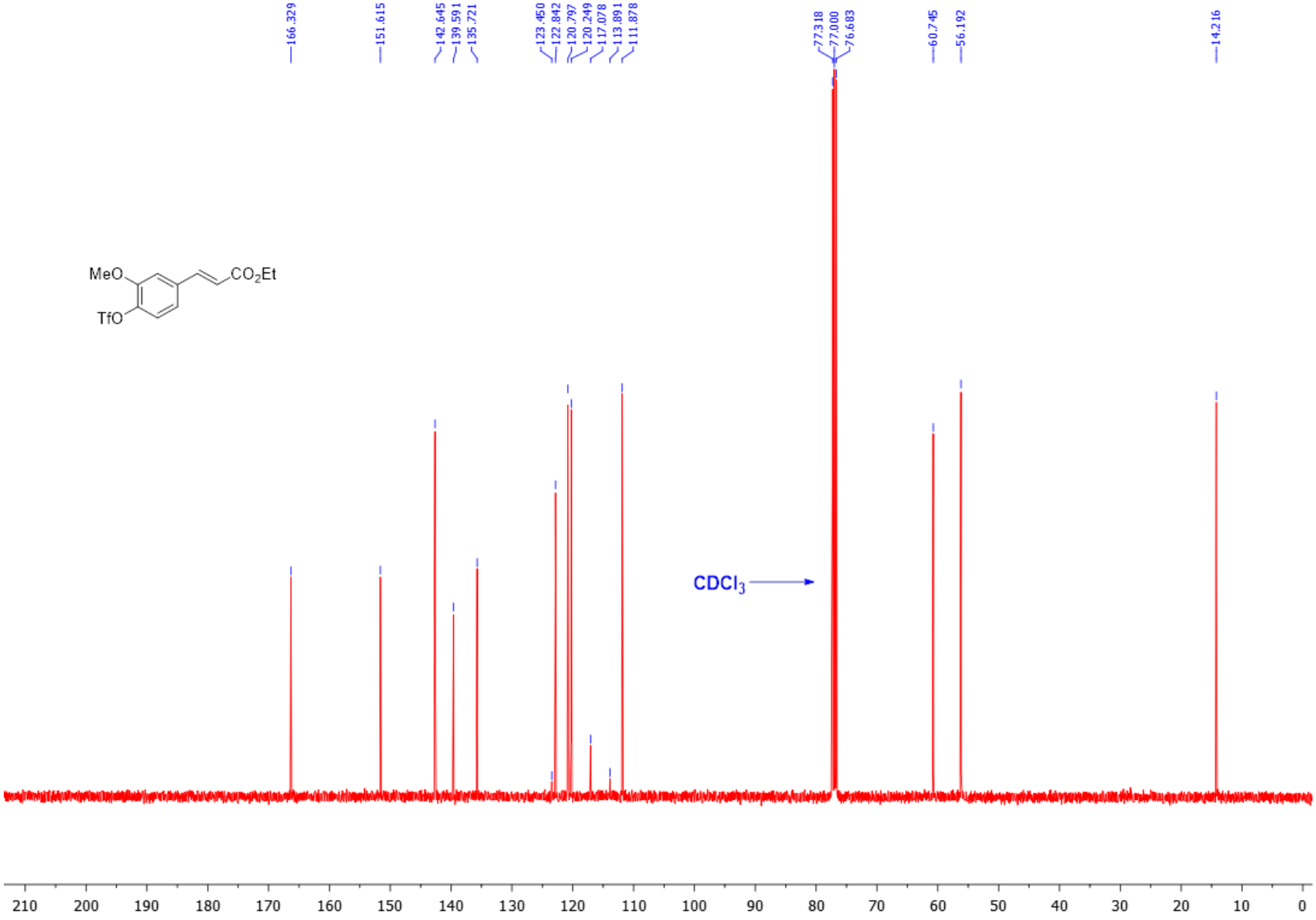
^{13}C-NMR of *(8-(1,2-dihydroacenaphthylen-5-yl)tetrazolo[1,5-a]pyridine (1n)* (25 °C, 100 MHz, $CDCl_3$):



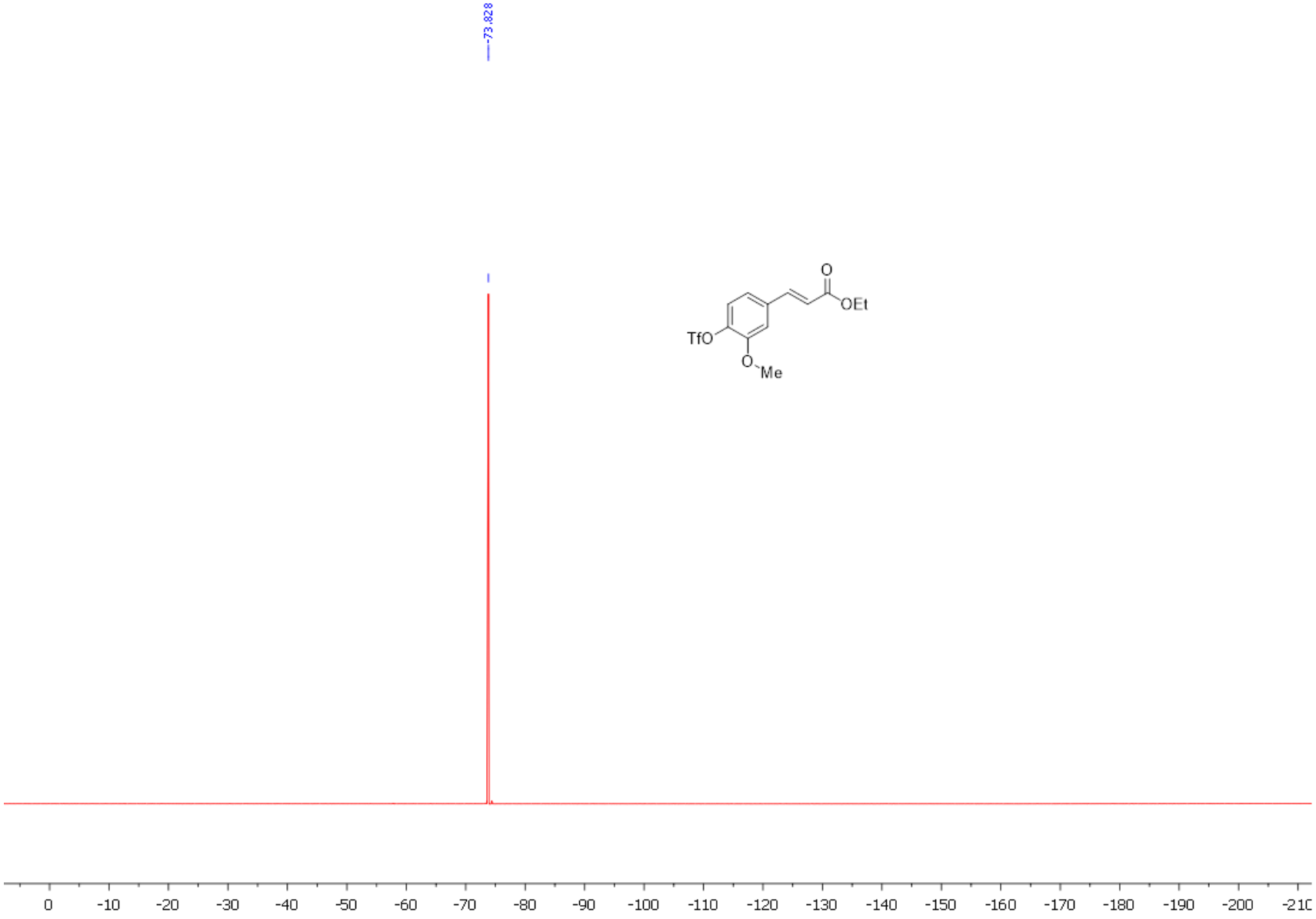
^{1}H-NMR of *ethyl (E)-3-(3-methoxy-4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acrylate* (25 °C, 400 MHz, $CDCl_3$):



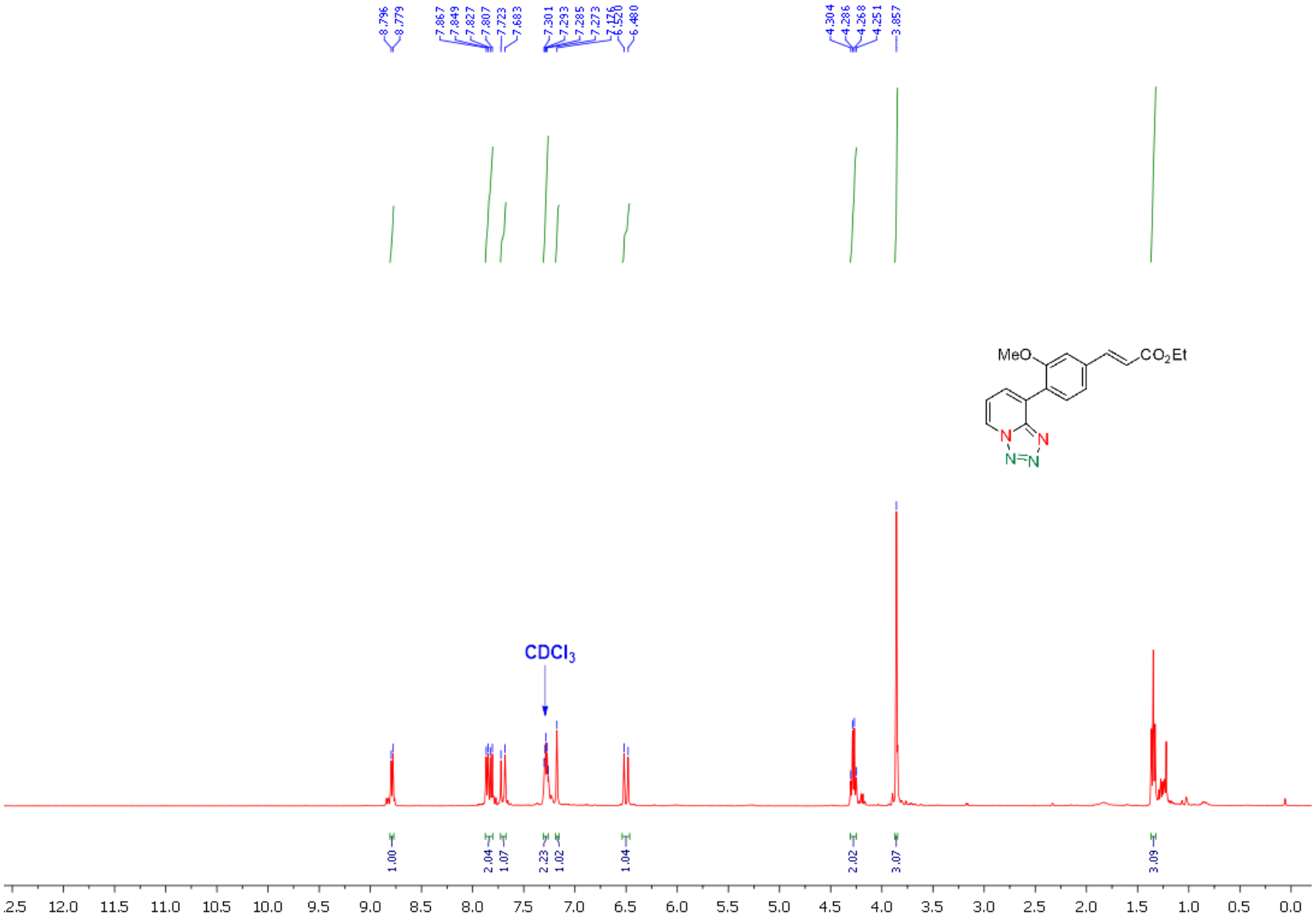
^{13}C-NMR of *ethyl (E)-3-(3-methoxy-4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acrylate* (25 °C, 100 MHz, $CDCl_3$):



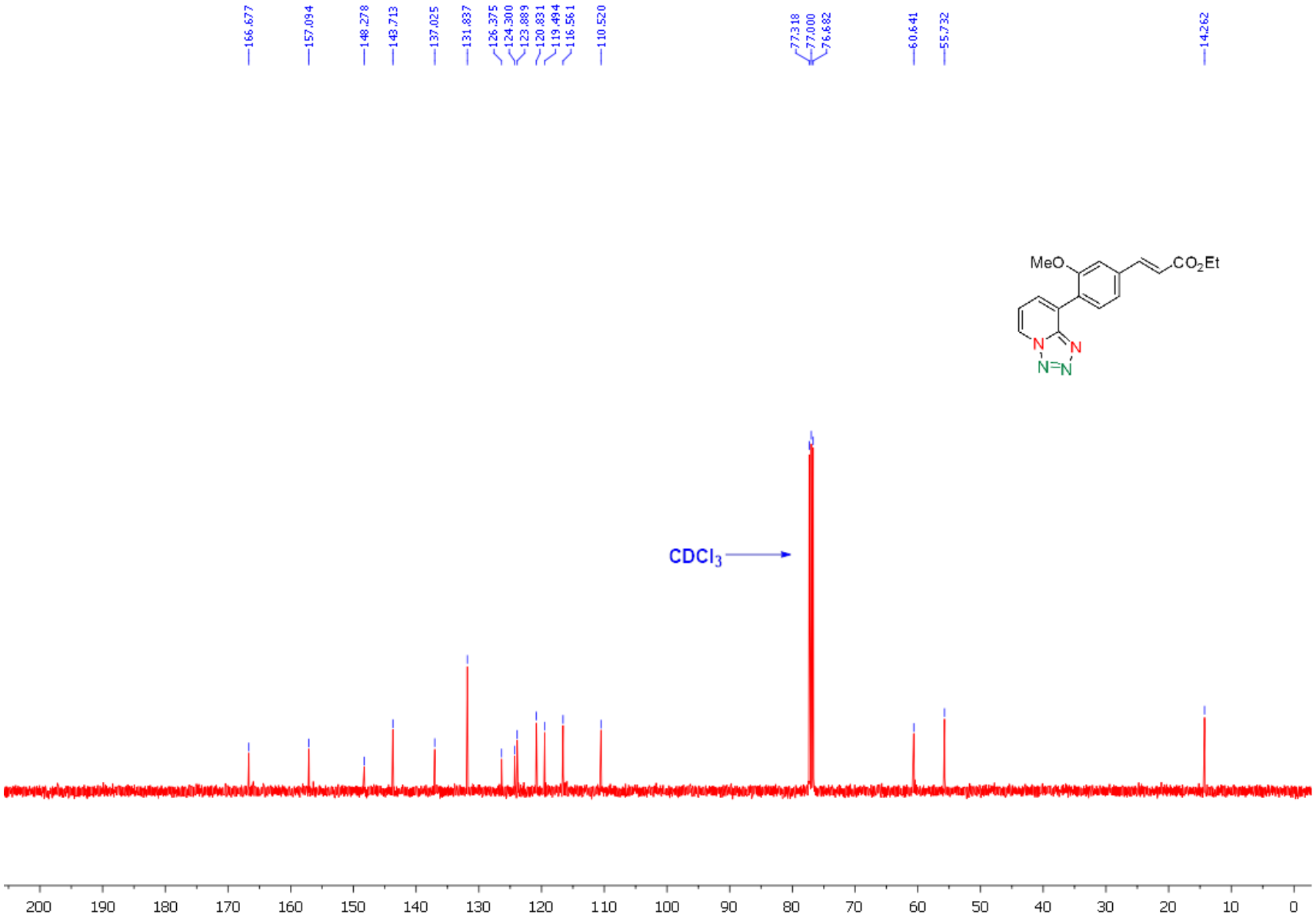
^{19}F-NMR of *ethyl (E)-3-(3-methoxy-4-(((trifluoromethyl)sulfonyl)oxy)phenyl)acrylate* (25 °C, 376 MHz, $CDCl_3$):



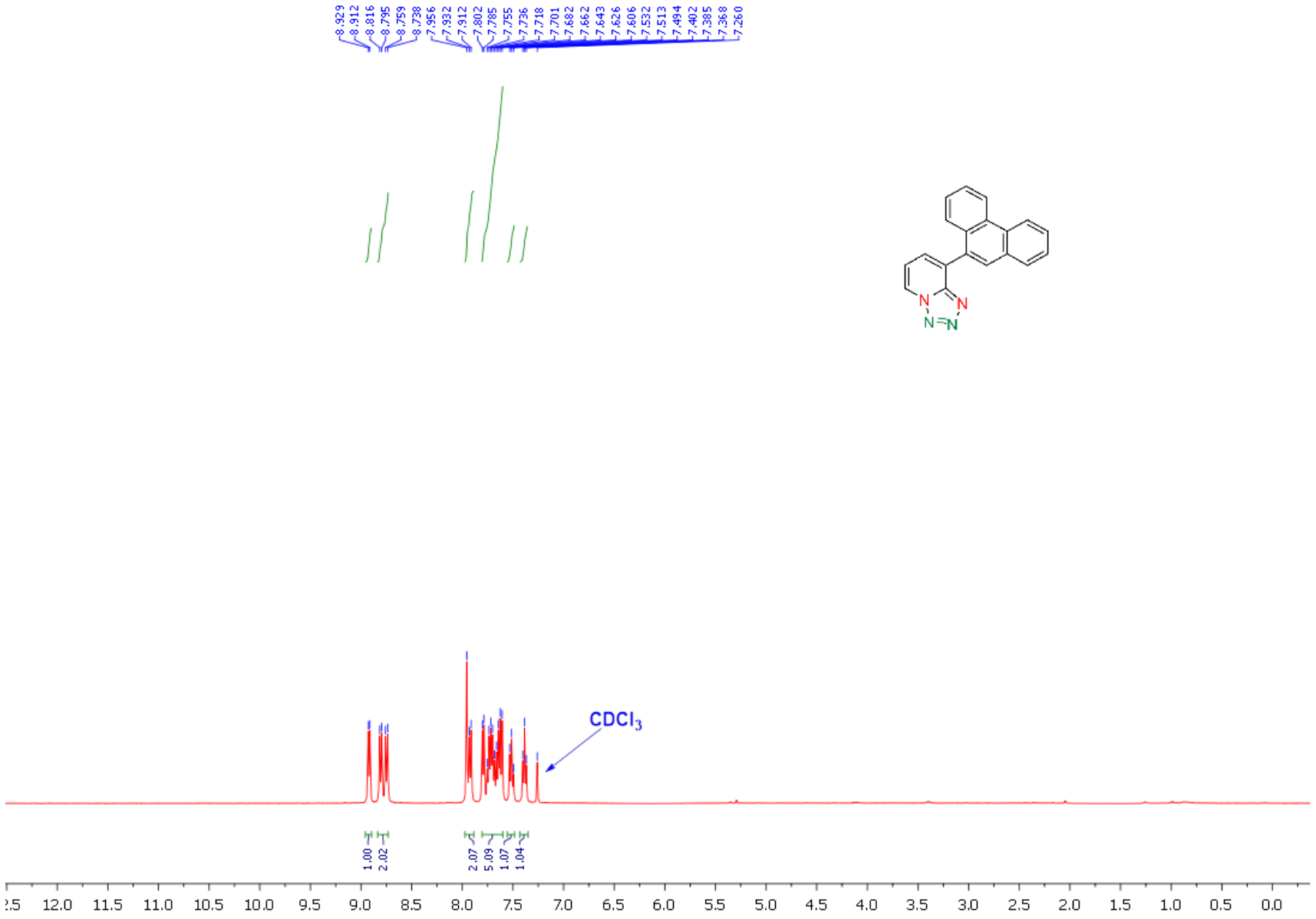
^{1}H-NMR of *ethyl (E)-3-(3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acrylate (1o)* (25 °C, 400 MHz, $CDCl_3$):



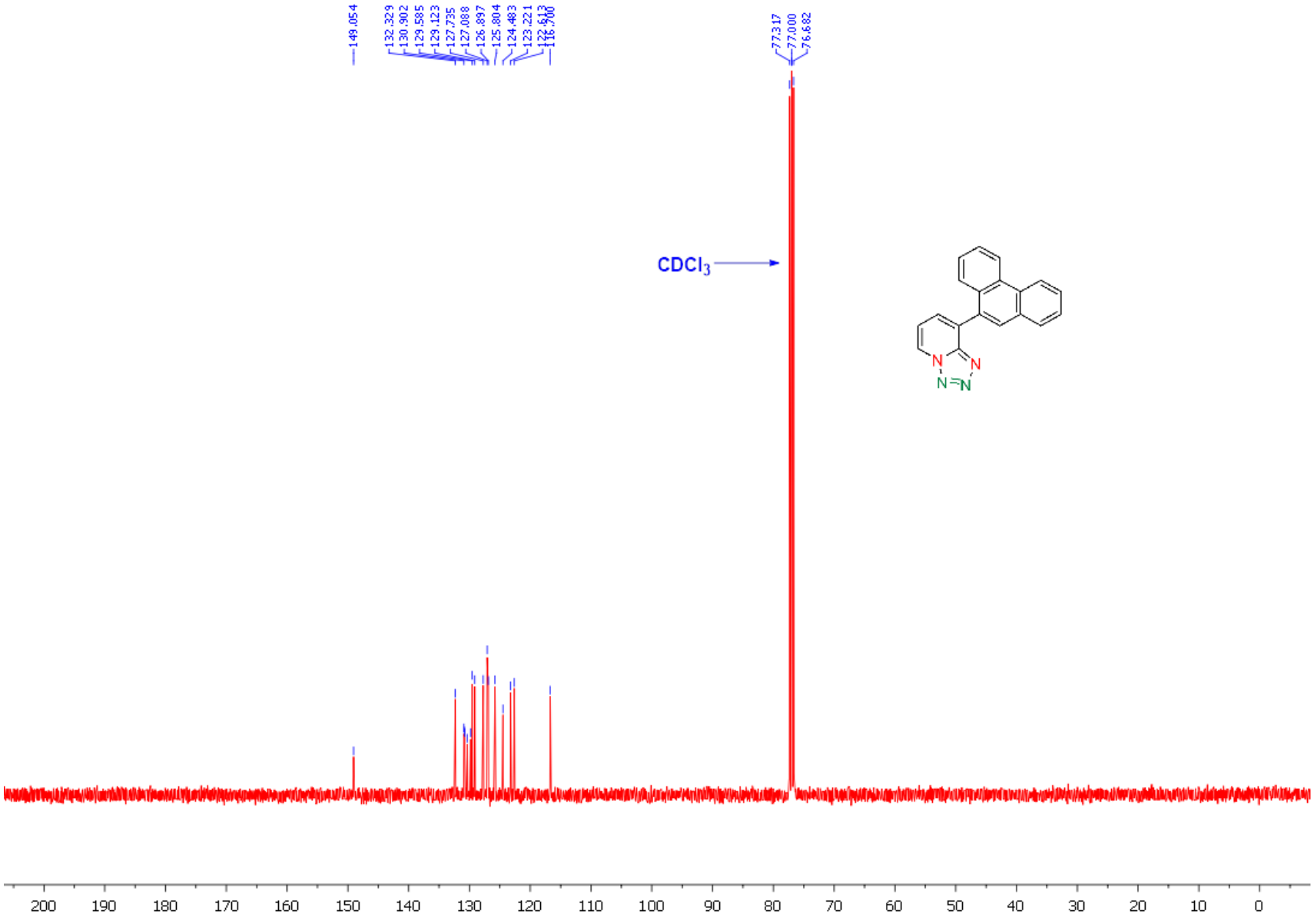
^{13}C-NMR of *ethyl (E)-3-(3-methoxy-4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acrylate (1o)* (25 °C, 100 MHz, $CDCl_3$):



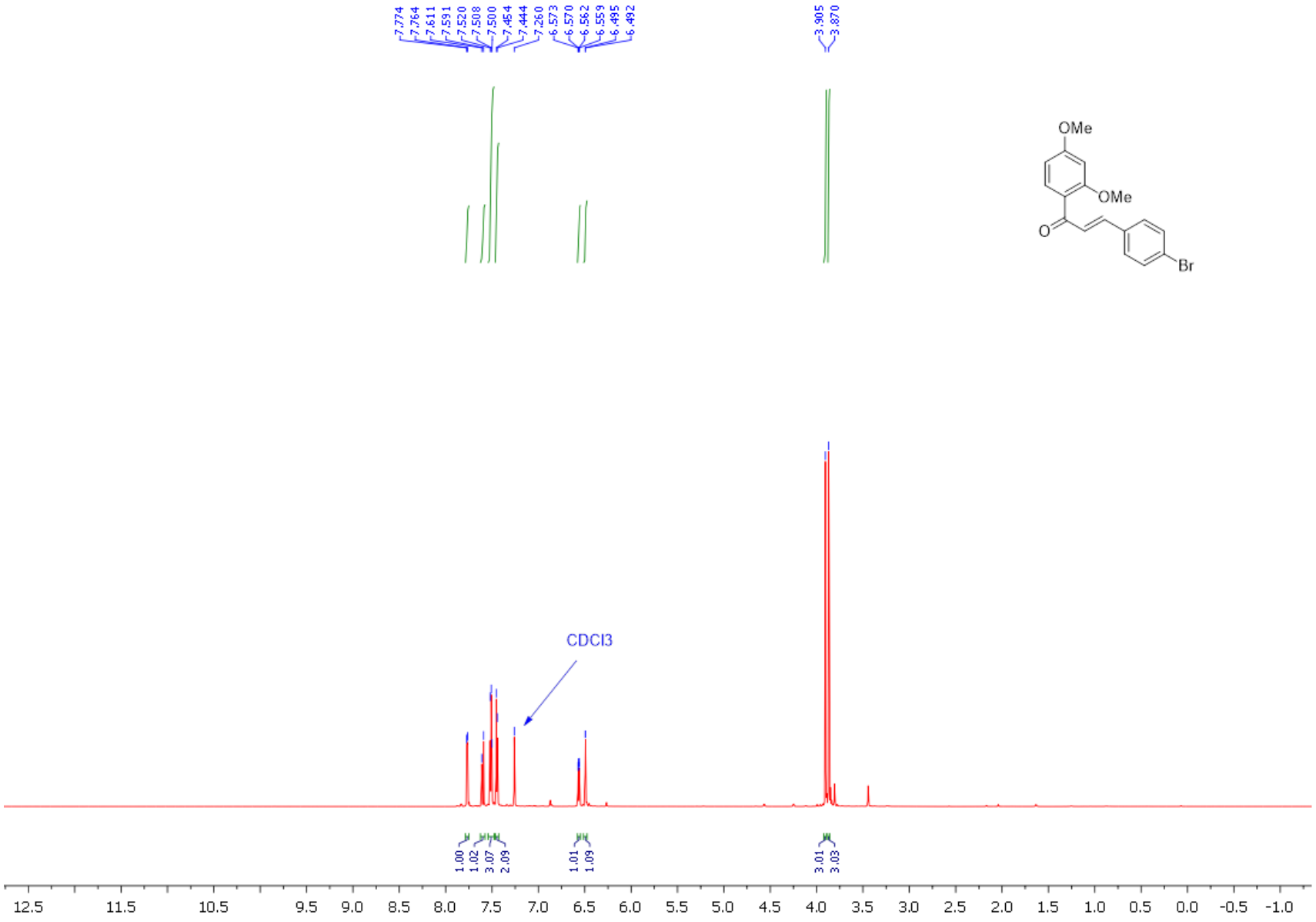
^{1}H-NMR of *8-(phenanthren-9-yl)tetrazolo[1,5-a]pyridine (1p)* (25 °C, 400 MHz, $CDCl_3$):



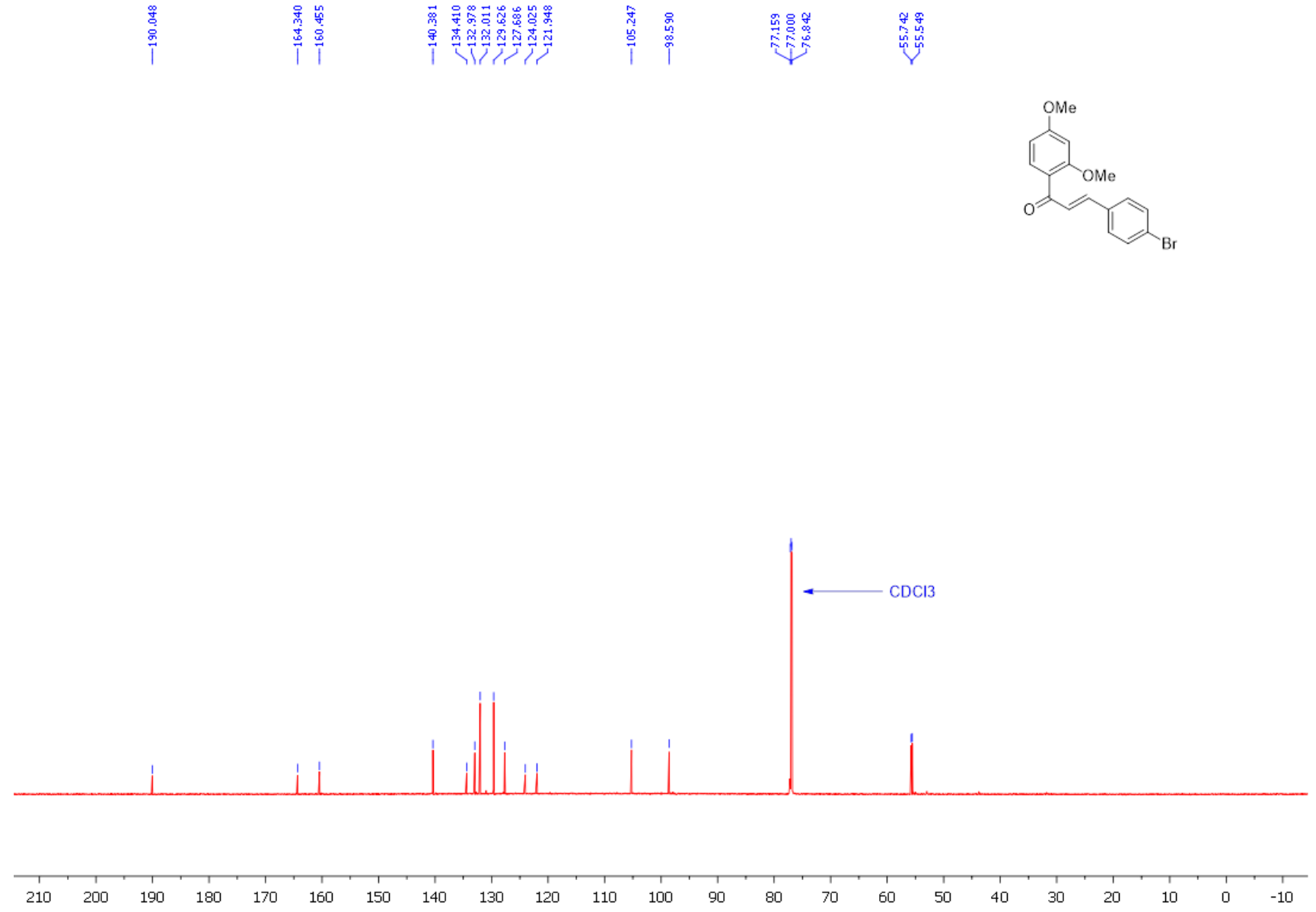
^{13}C-NMR of *8-(phenanthren-9-yl)tetrazolo[1,5-a]pyridine (1p)* (25 °C, 100 MHz, $CDCl_3$):



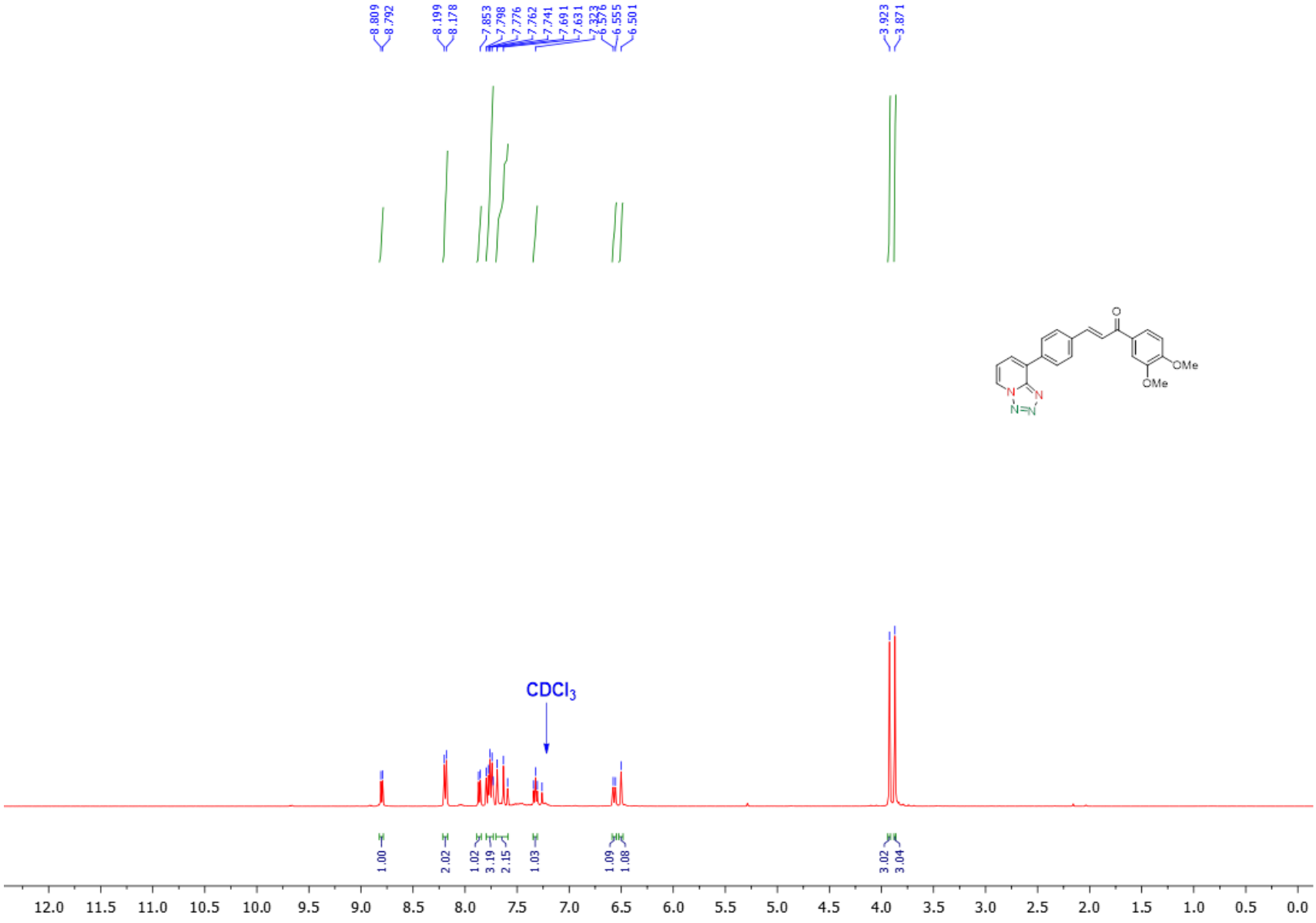
^{1}H-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ^{o}C, 800 MHz, $CDCl_3$):



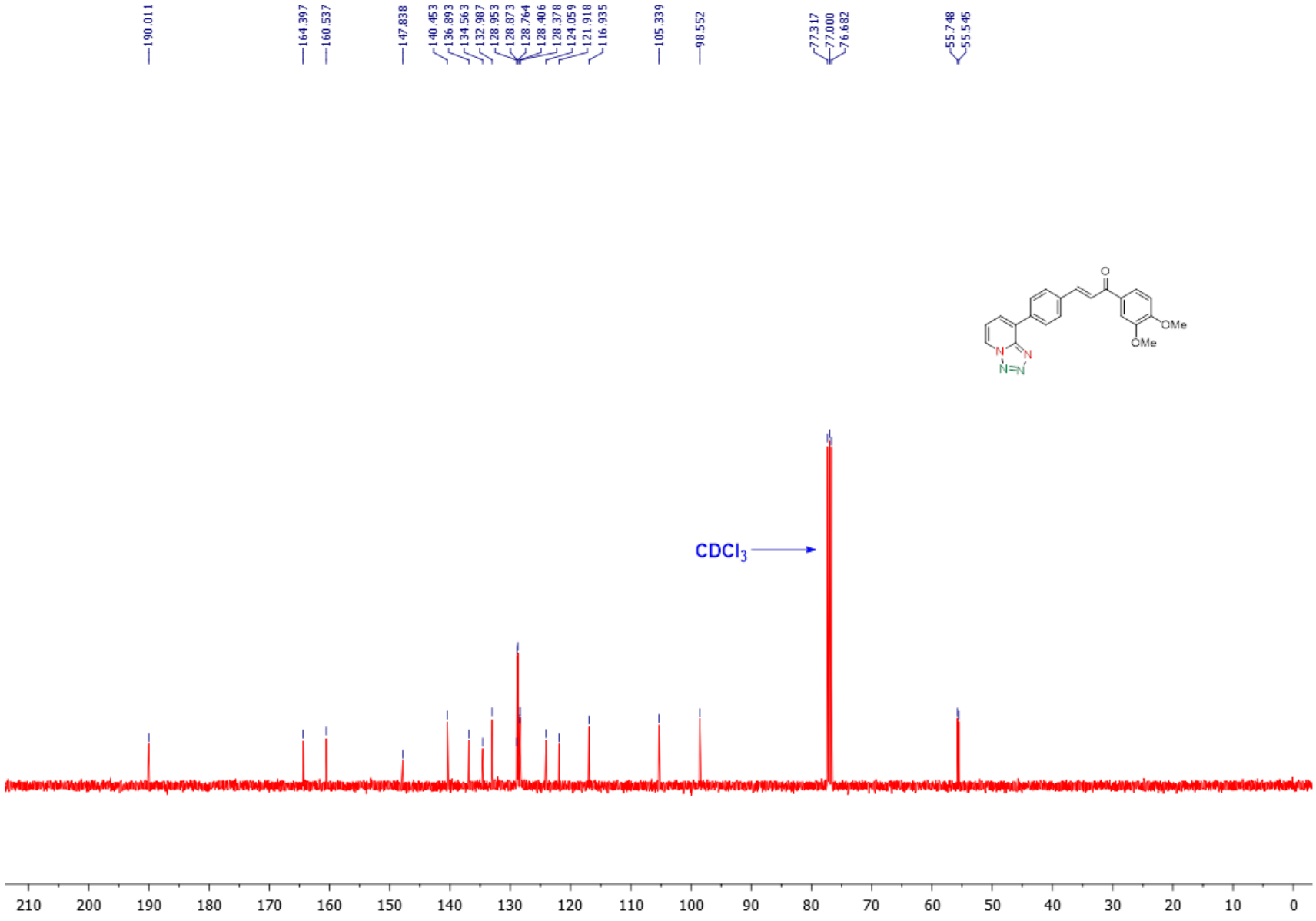
^{13}C-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ºC, 200 MHz, $CDCl_3$):



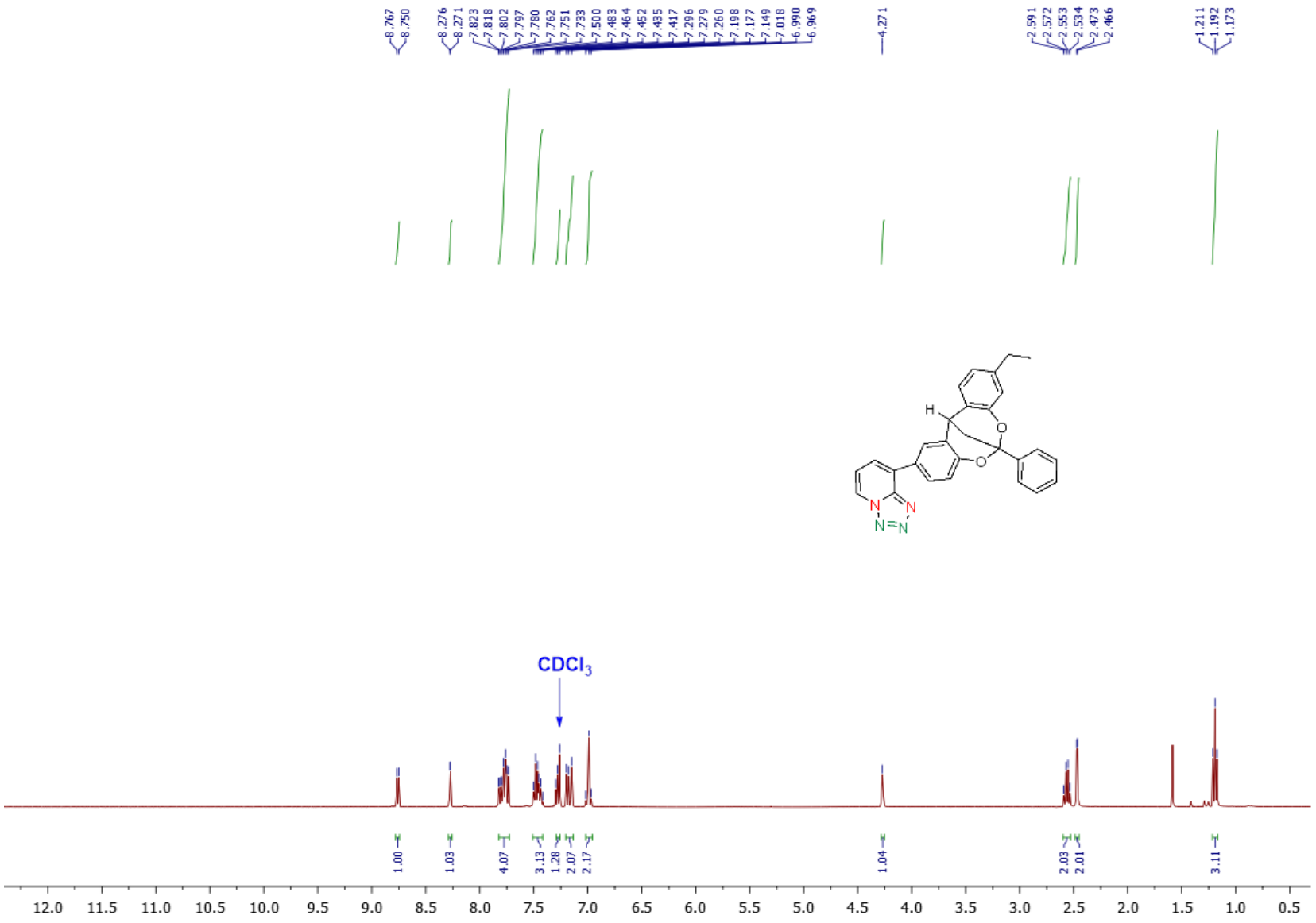
^{1}H-NMR of *(E)-1-(2,4-dimethoxyphenyl)-3-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)prop-2- en-1-one (1q)* (25 ^{o}C, 400 MHz, $CDCl_3$):



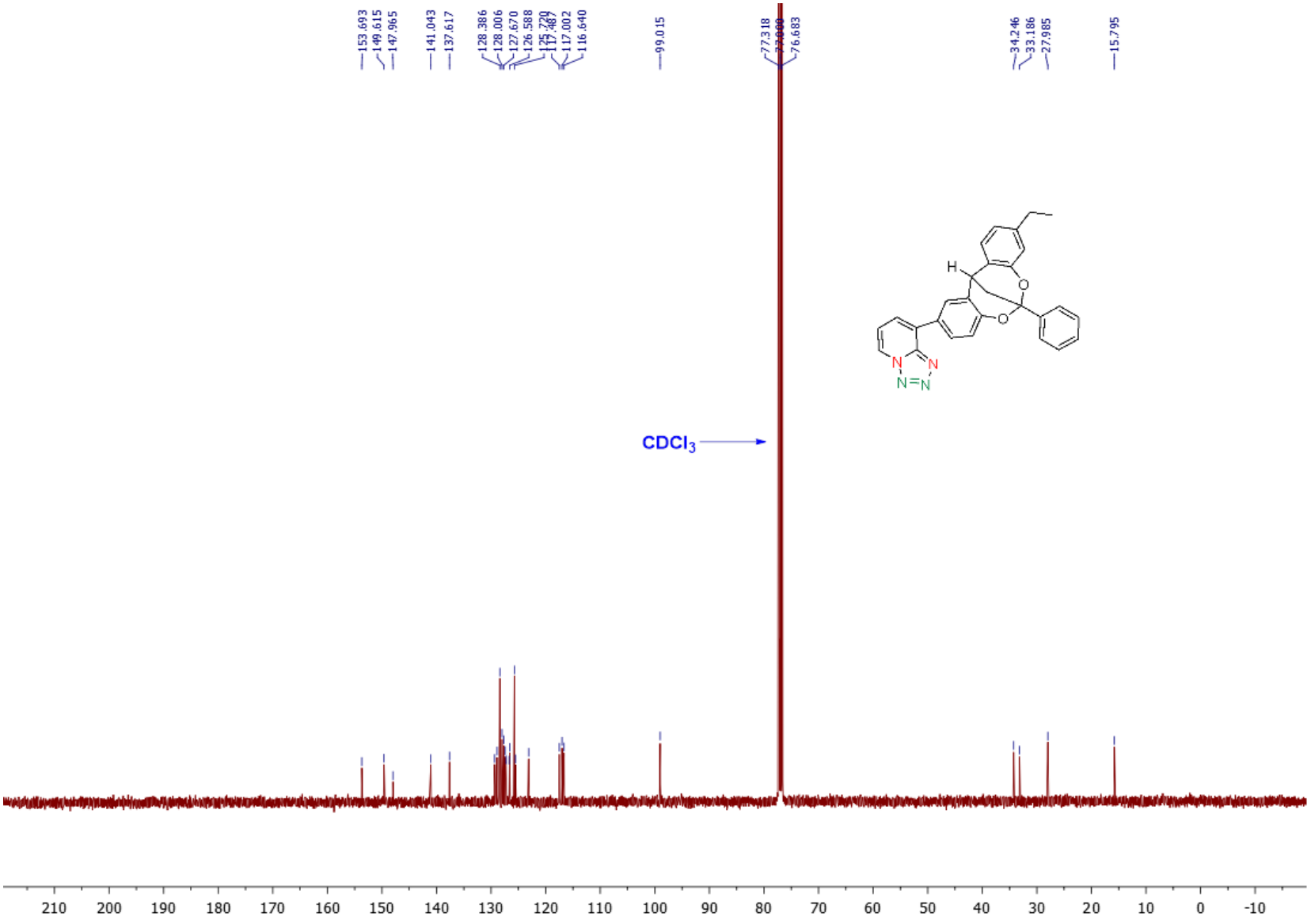
^{13}C-NMR of *(E)-1-(2,4-dimethoxyphenyl)-3-(4-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)prop-2- en-1-one (1q)* (25 ºC, 100 MHz, $CDCl_3$):



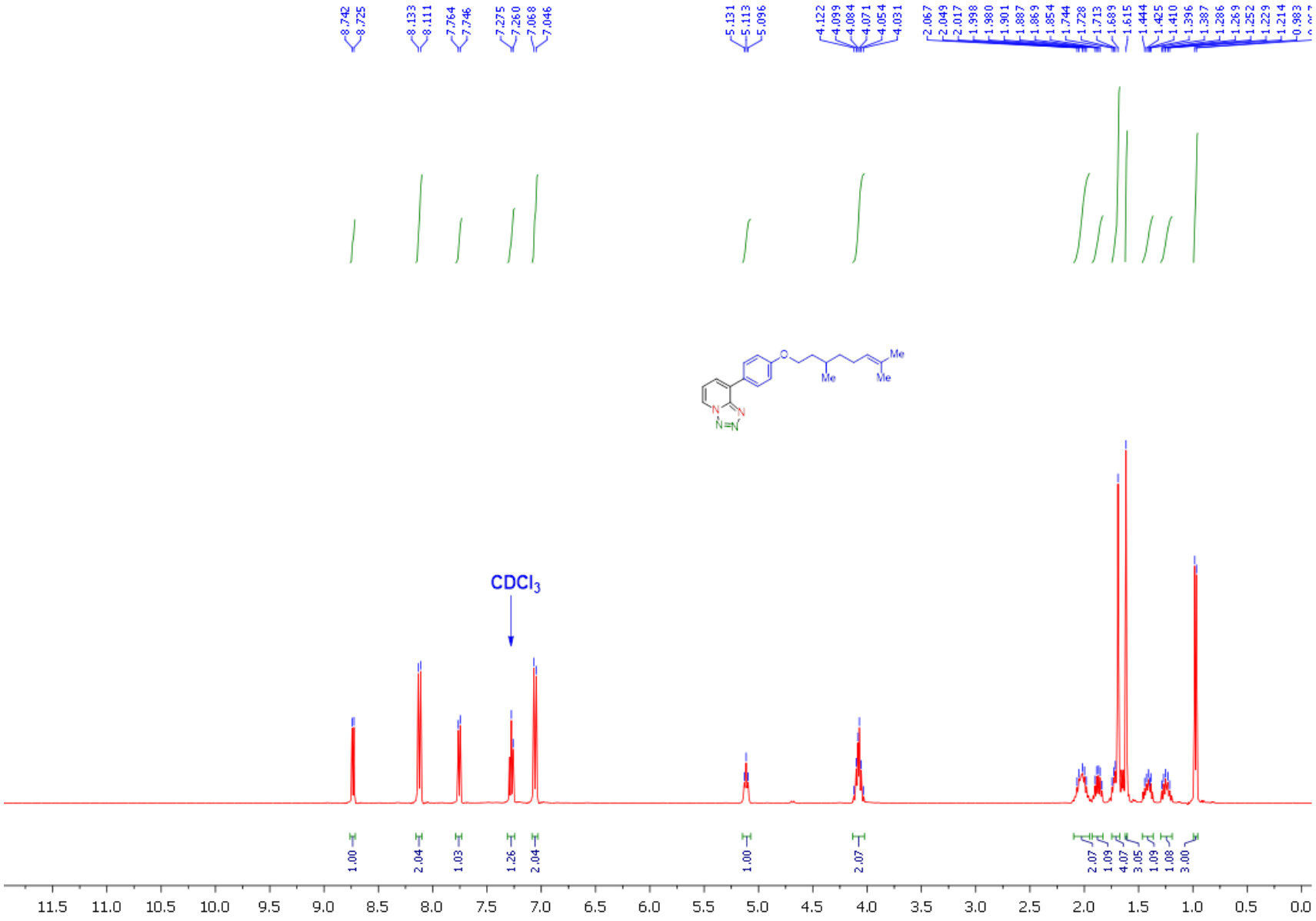
^{1}H-NMR of *8-((6R,12R)-10-ethyl-6-phenyl-12H-6,12-methanodibenzo[d,g][1,3]dioxocin-2- yl)tetrazolo[1,5-a]pyridine (1r)* (25 ^{o}C, 400 MHz, $CDCl_3$):



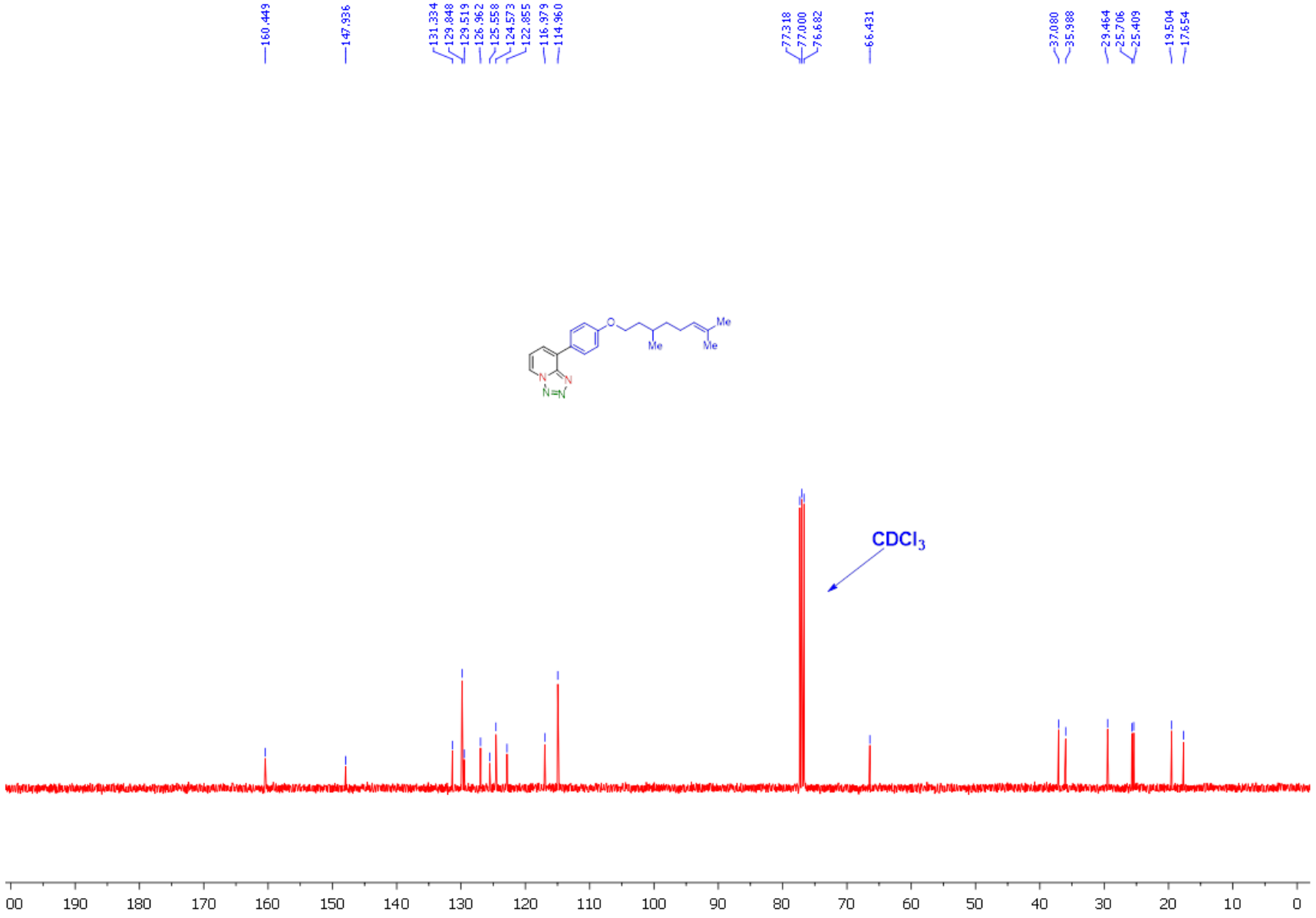
^{13}C-NMR 8-*((6R,12R)-10-ethyl-6-phenyl-12H-6,12-methanodibenzo[d,g][1,3]dioxocin-2- yl)tetrazolo[1,5-a]pyridine (1r)* (25 ºC, 100 MHz, $CDCl_3$):



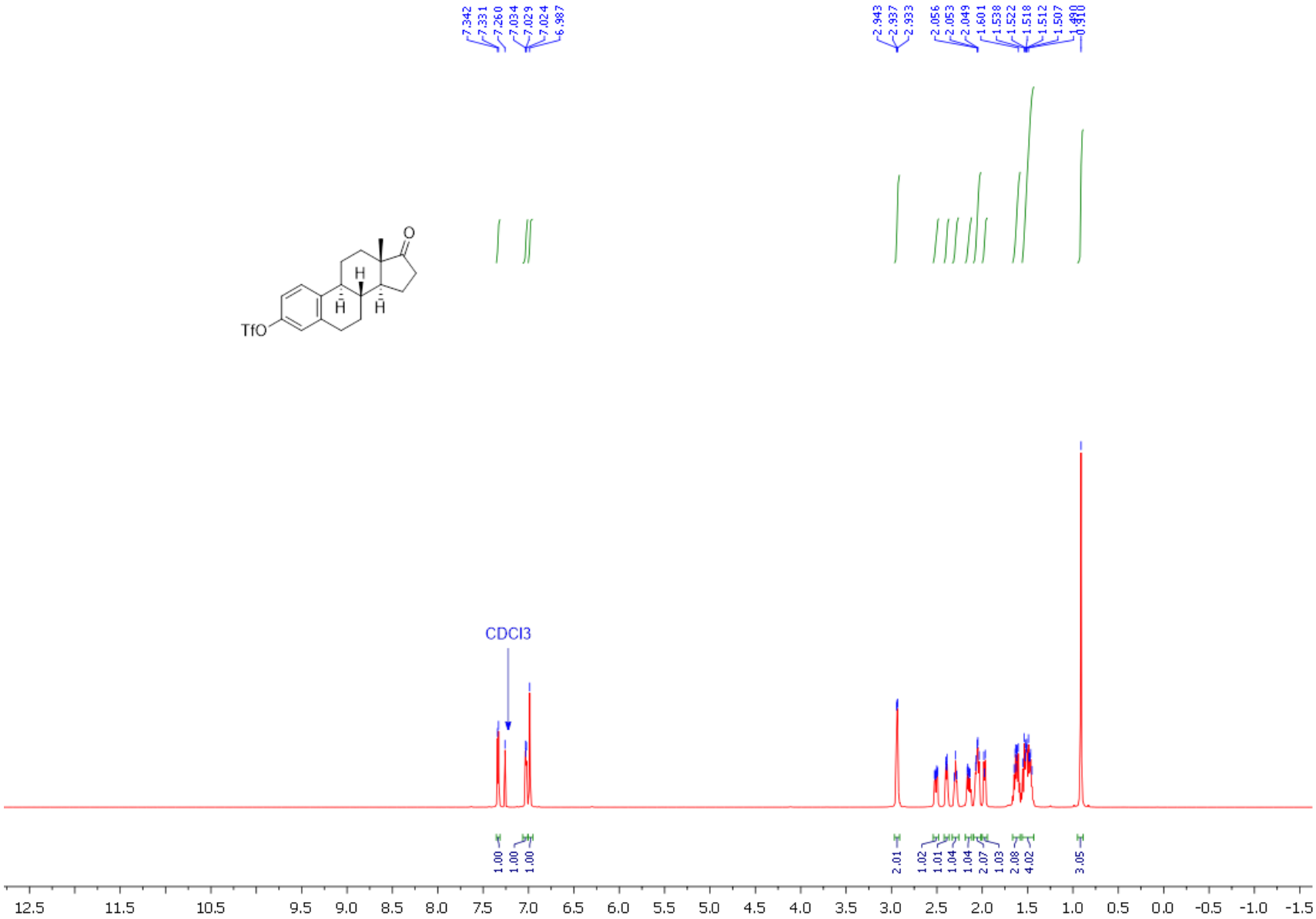
^{1}H-NMR of *8-(4-((3,7-dimethyloct-6-en-1-yl)oxy)phenyl)tetrazolo[1,5-a]pyridine (1s)* (25 °C, 400 MHz, $CDCl_3$):



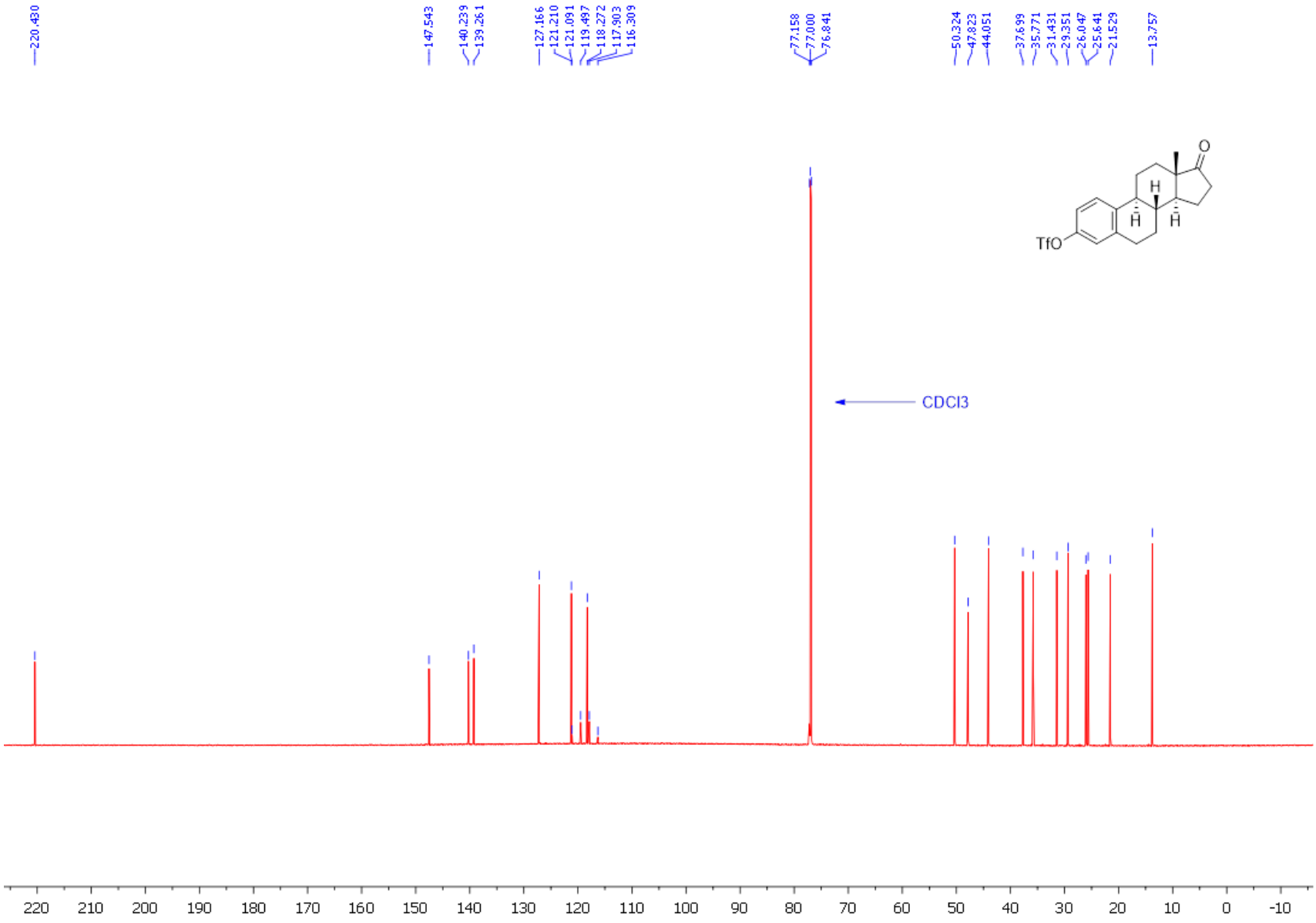
^{13}C-NMR of *8-(4-((3,7-dimethyloct-6-en-1-yl)oxy)phenyl)tetrazolo[1,5-a]pyridine (1s)* (25 ºC, 100 MHz, $CDCl_3$):



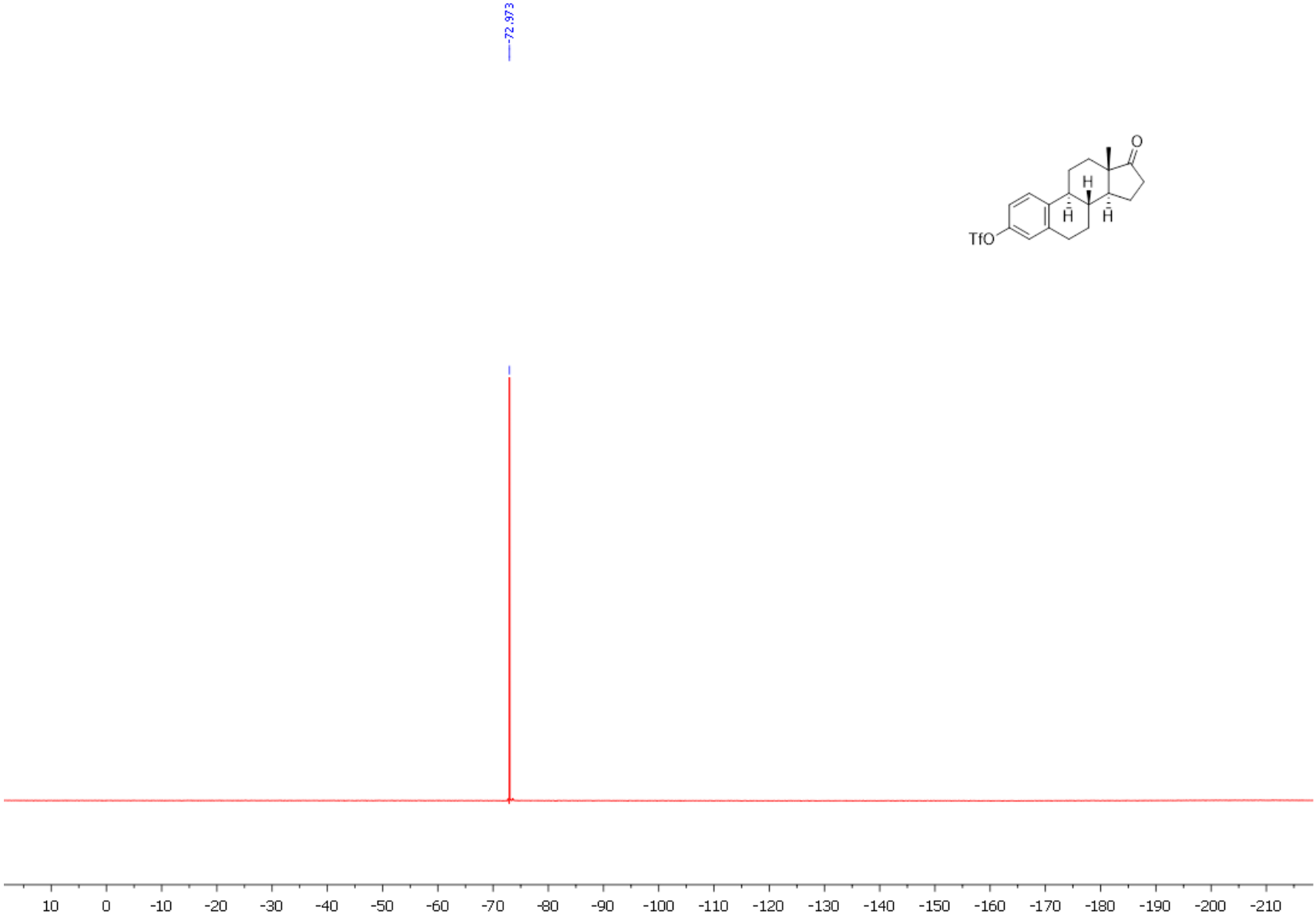
^{1}H-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ^{o}C, 800 MHz, $CDCl_3$):



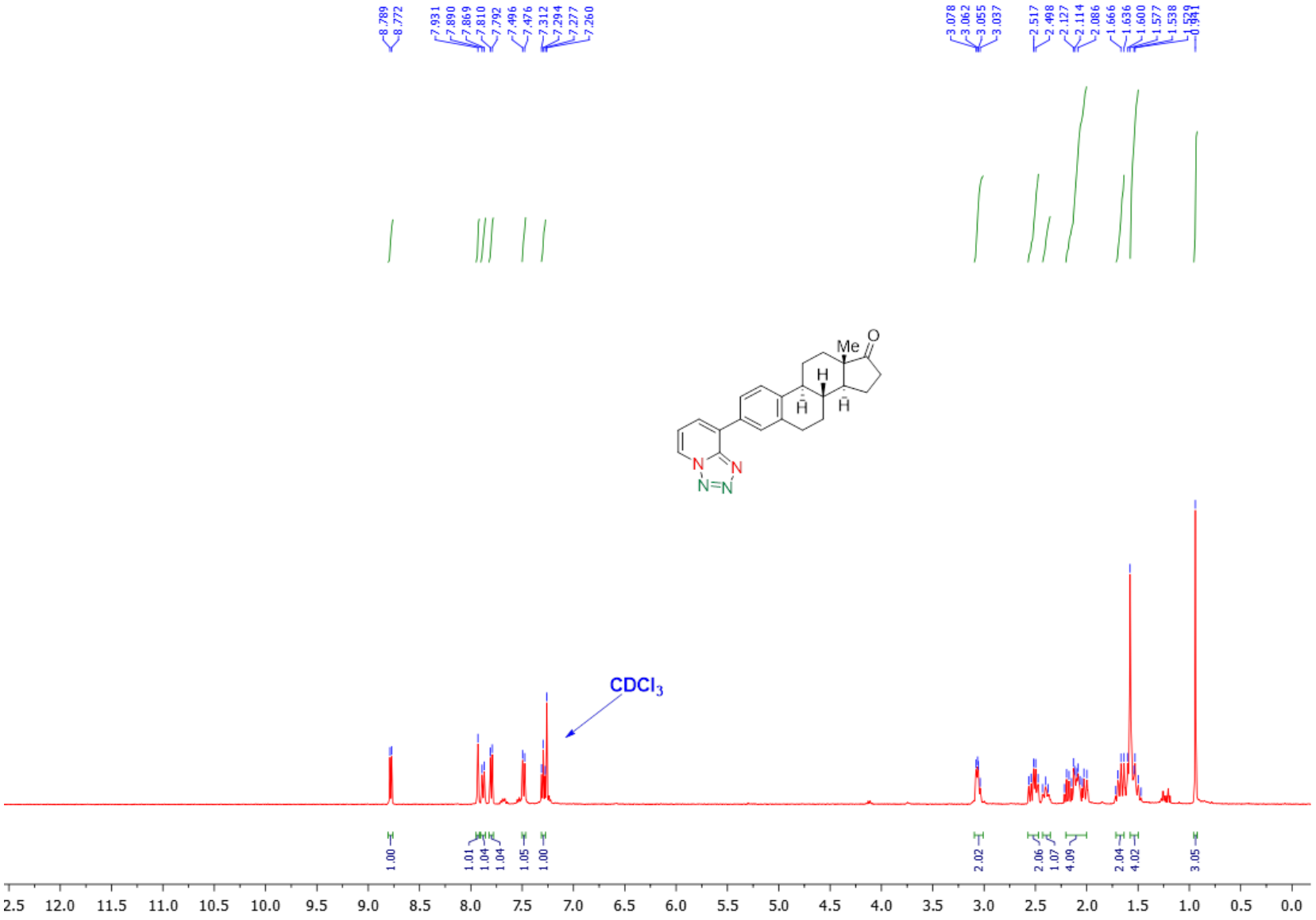
^{13}C-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ^{o}C, 200 MHz, $CDCl_3$):



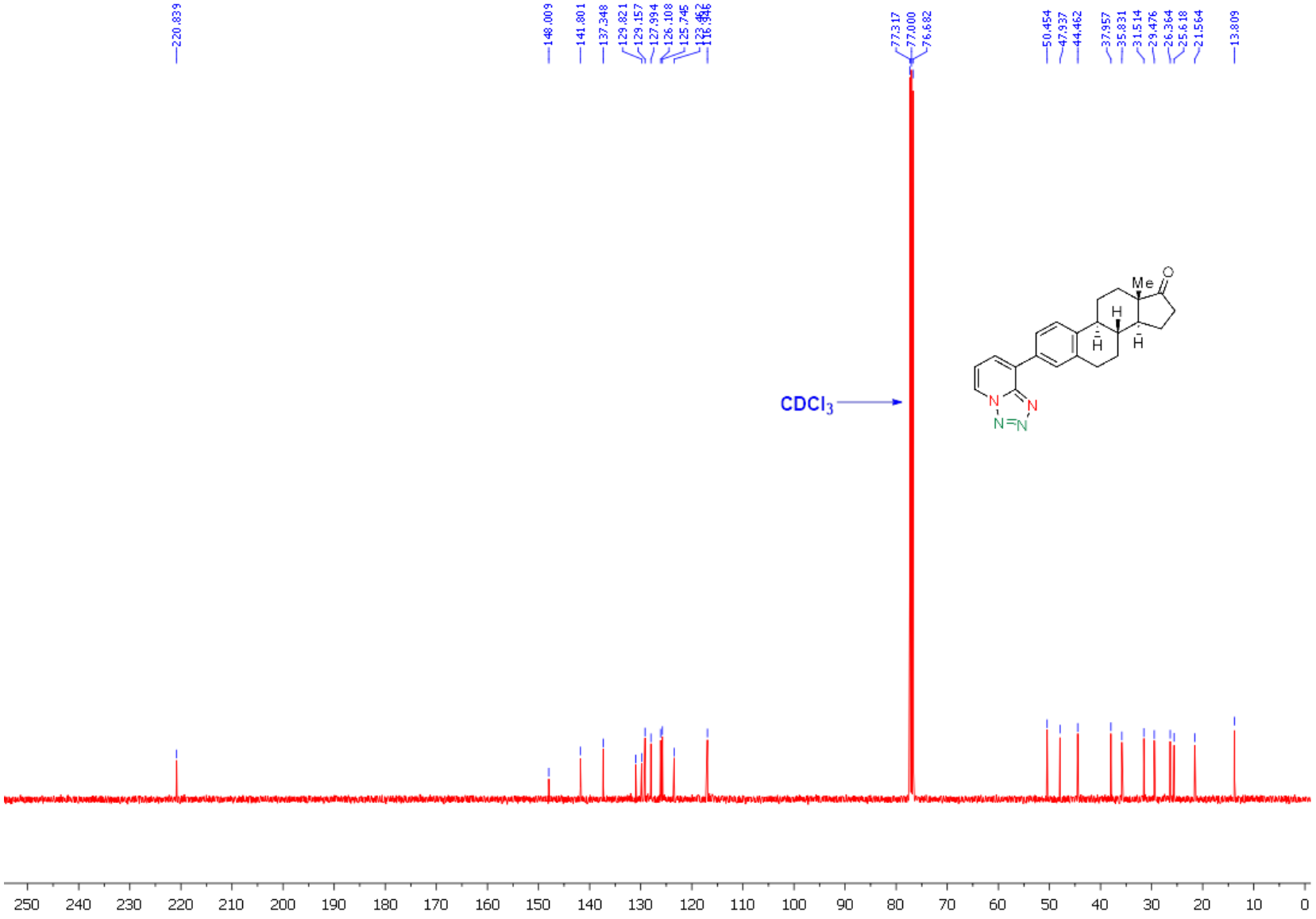
^{19}F-NMR of *4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate* (25 ºC, 376 MHz, $CDCl_3$):



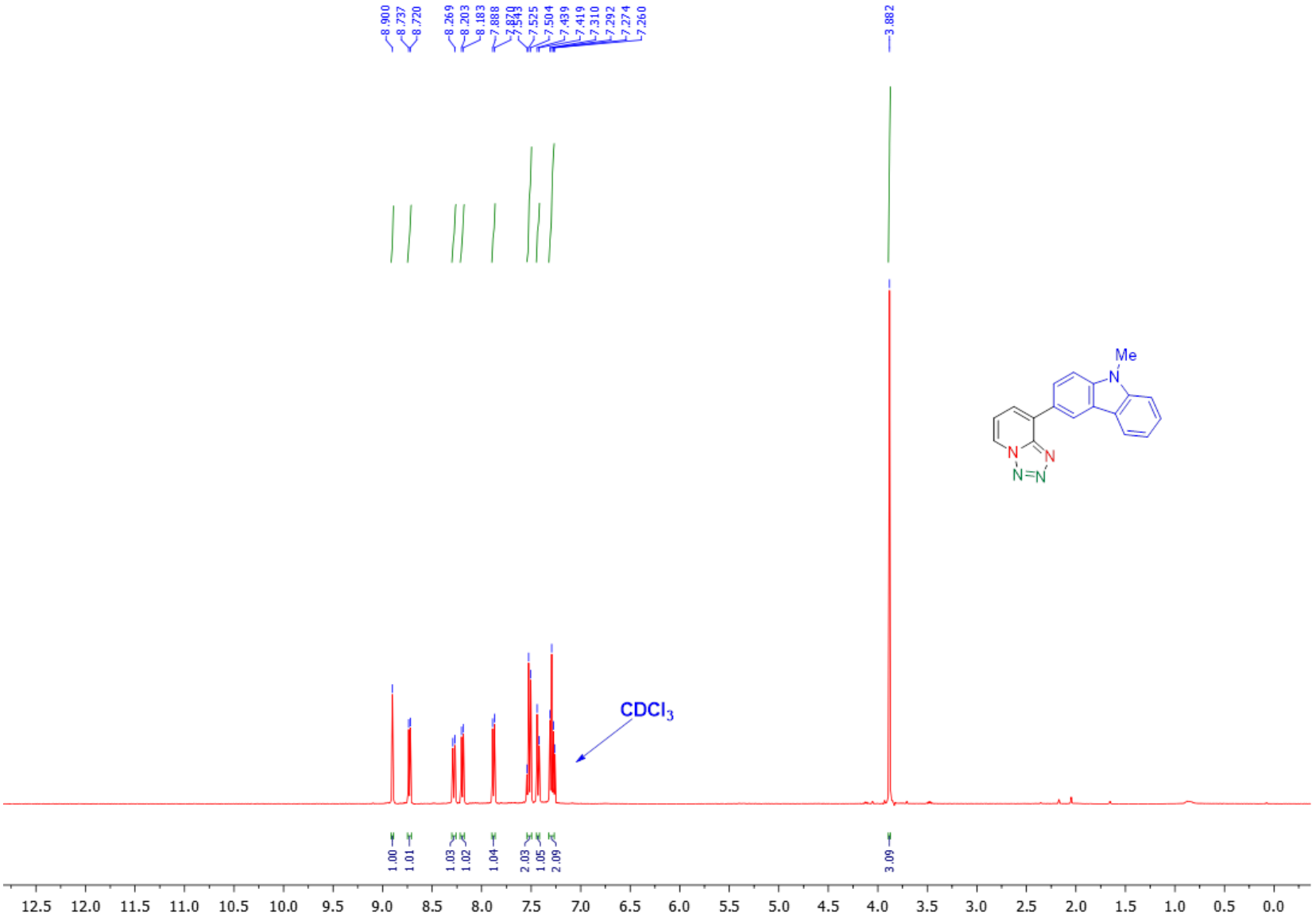
^{1}H-NMR of *8R,9S,13S,14S)-13-methyl-2-(tetrazolo[1,5-a]pyridin-8 yl)6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one((1t)* (25 ºC, 400 MHz, $CDCl_3$):



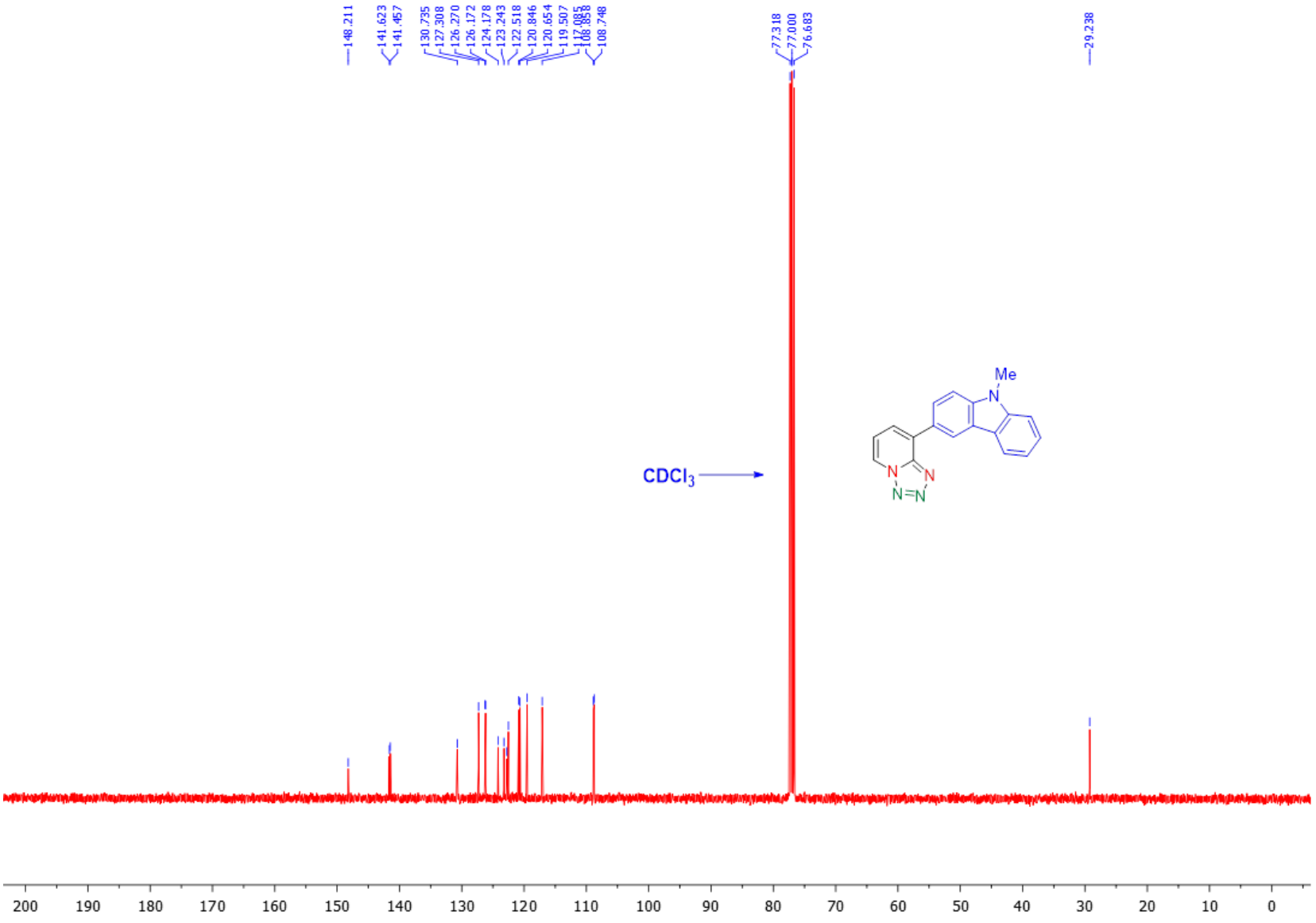
^{13}C-NMR of *8R,9S,13S,14S)-13-methyl-2-(tetrazolo[1,5-a]pyridin-8 yl)6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one((1t)* (25 ºC, 100 MHz, $CDCl_3$):



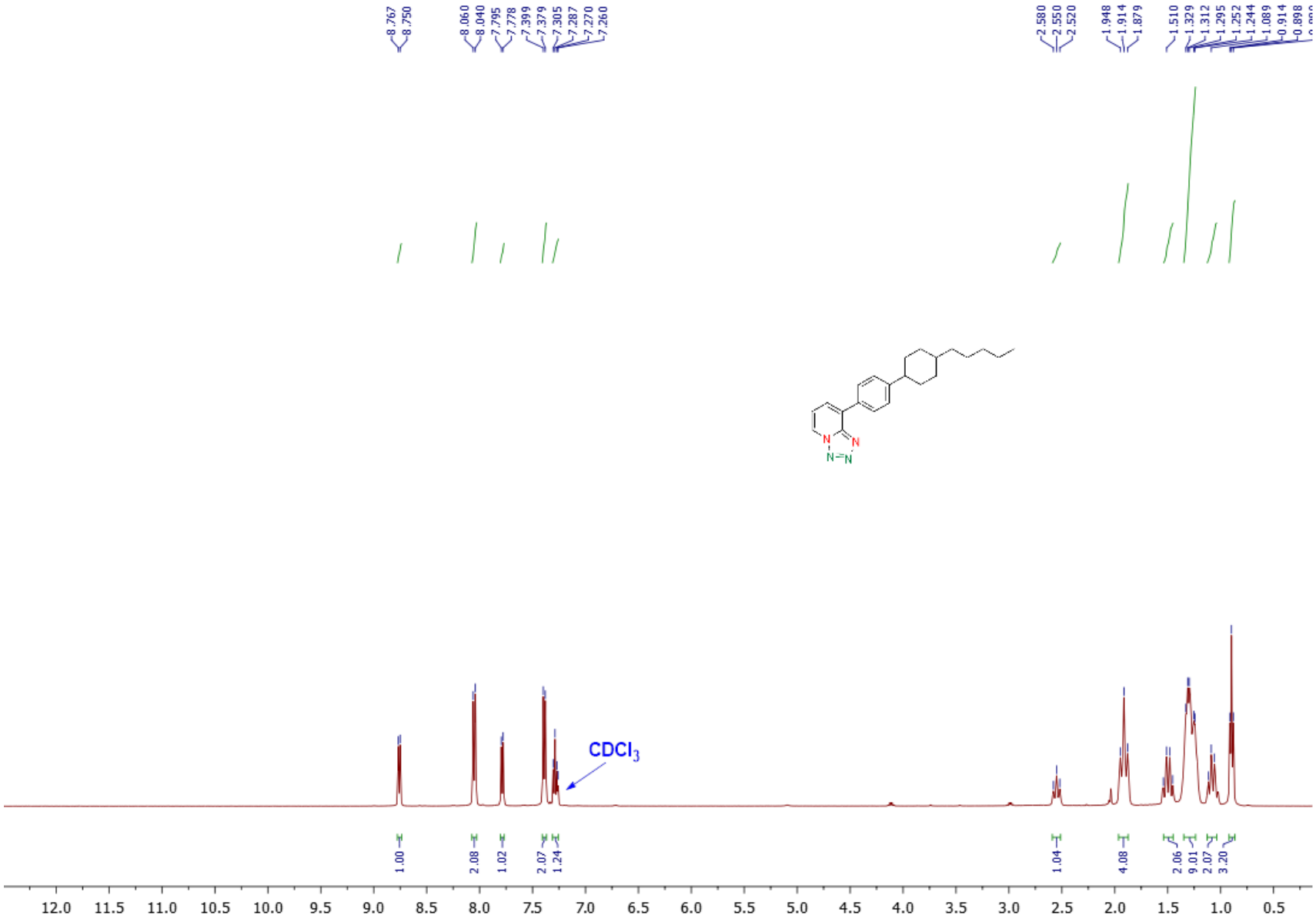
^{1}H-NMR of *9-methyl-3-(tetrazolo[1,5-a]pyridin-8-yl)-9H-carbazole (1u)* (25 °C, 400 MHz, $CDCl_3$):



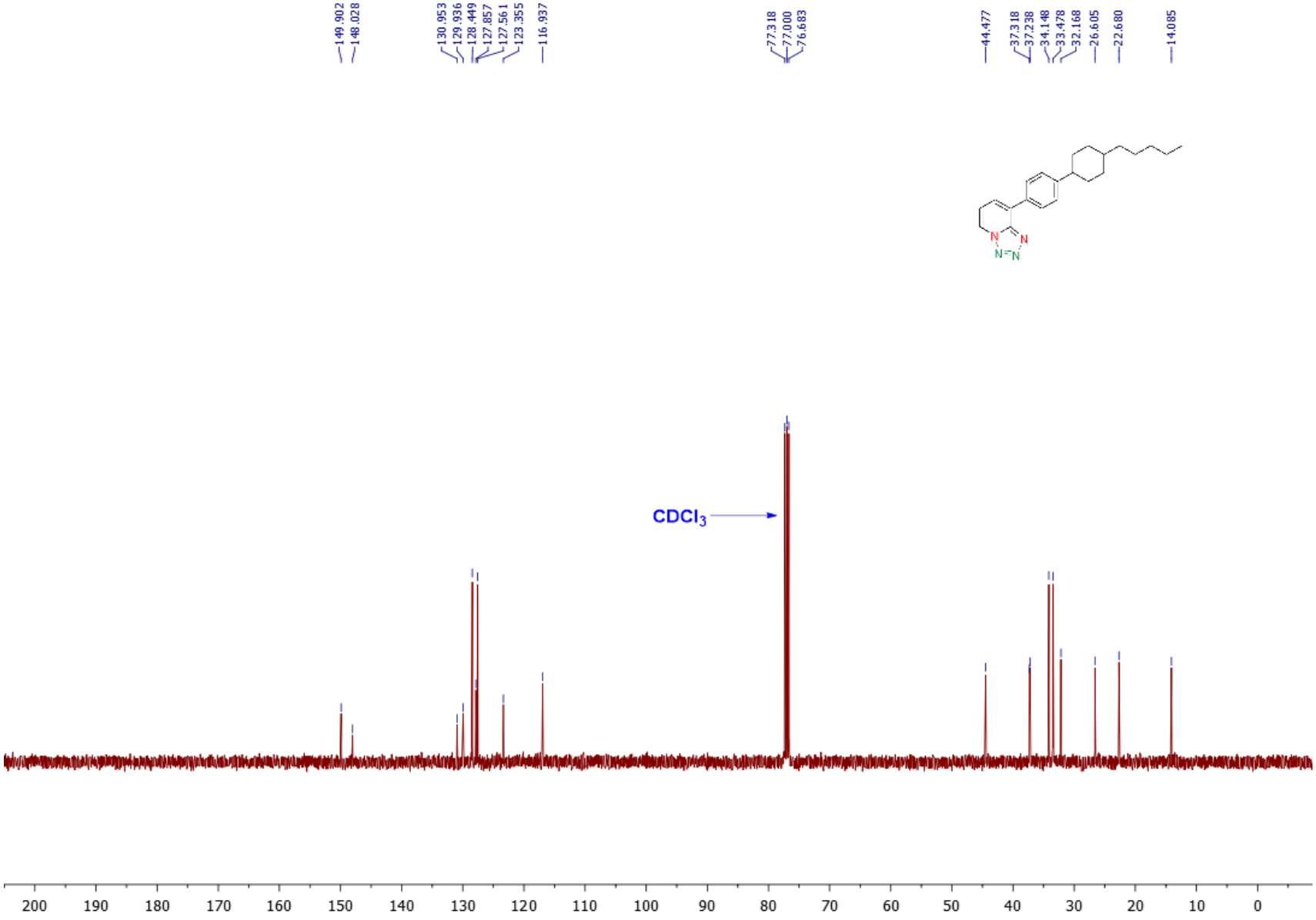
^{13}C-NMR of *9-methyl-3-(tetrazolo[1,5-a]pyridin-8-yl)-9H-carbazole (1u)* (25 °C, 100 MHz, $CDCl_3$):



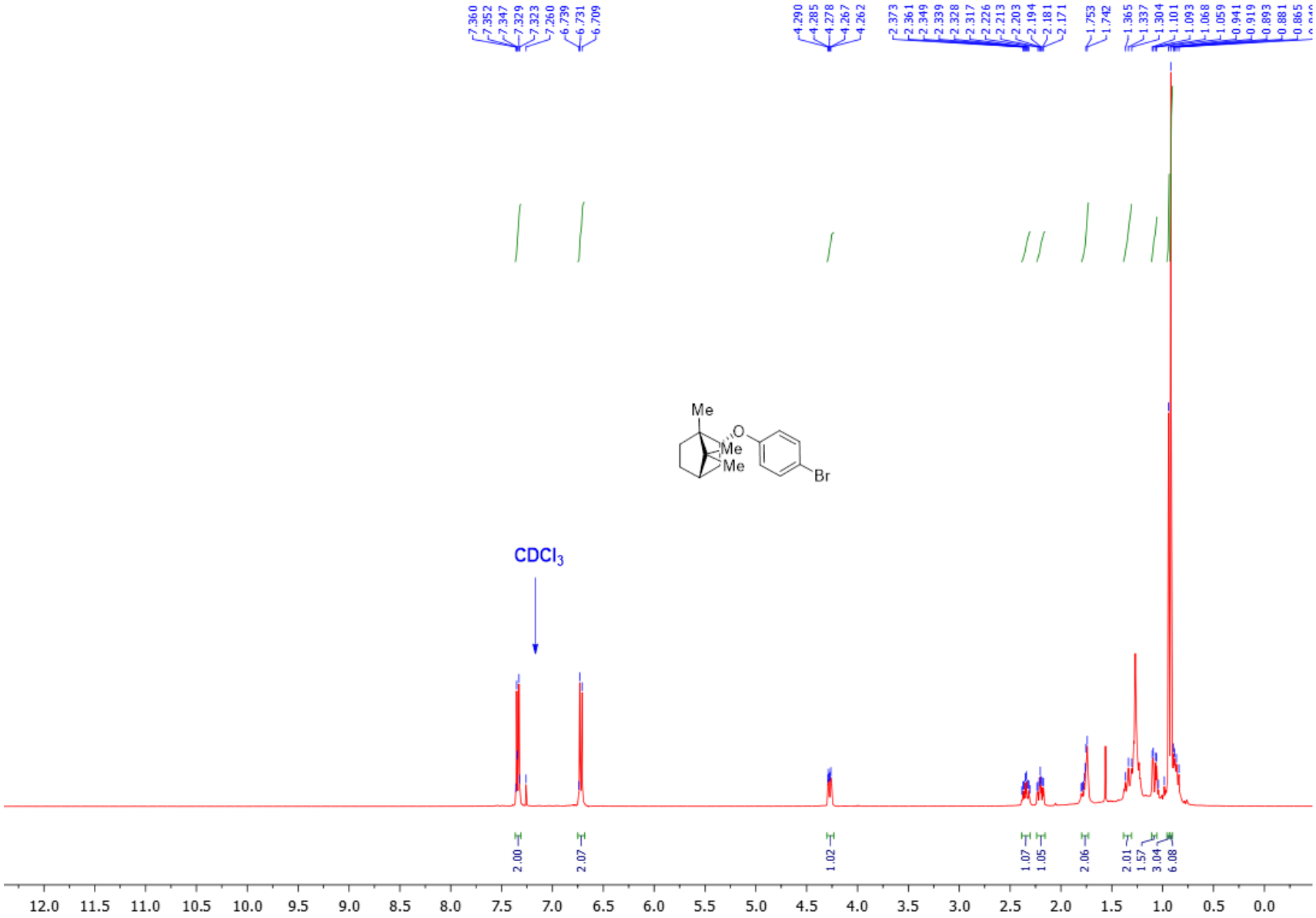
^{1}H-NMR of *8-(4-(4-(2λ5,5λ3-pentan-2-yl)cyclohexyl)phenyl)tetrazolo[1,5-a]pyridine (1v)* (25 ºC, 400 MHz, $CDCl_3$):



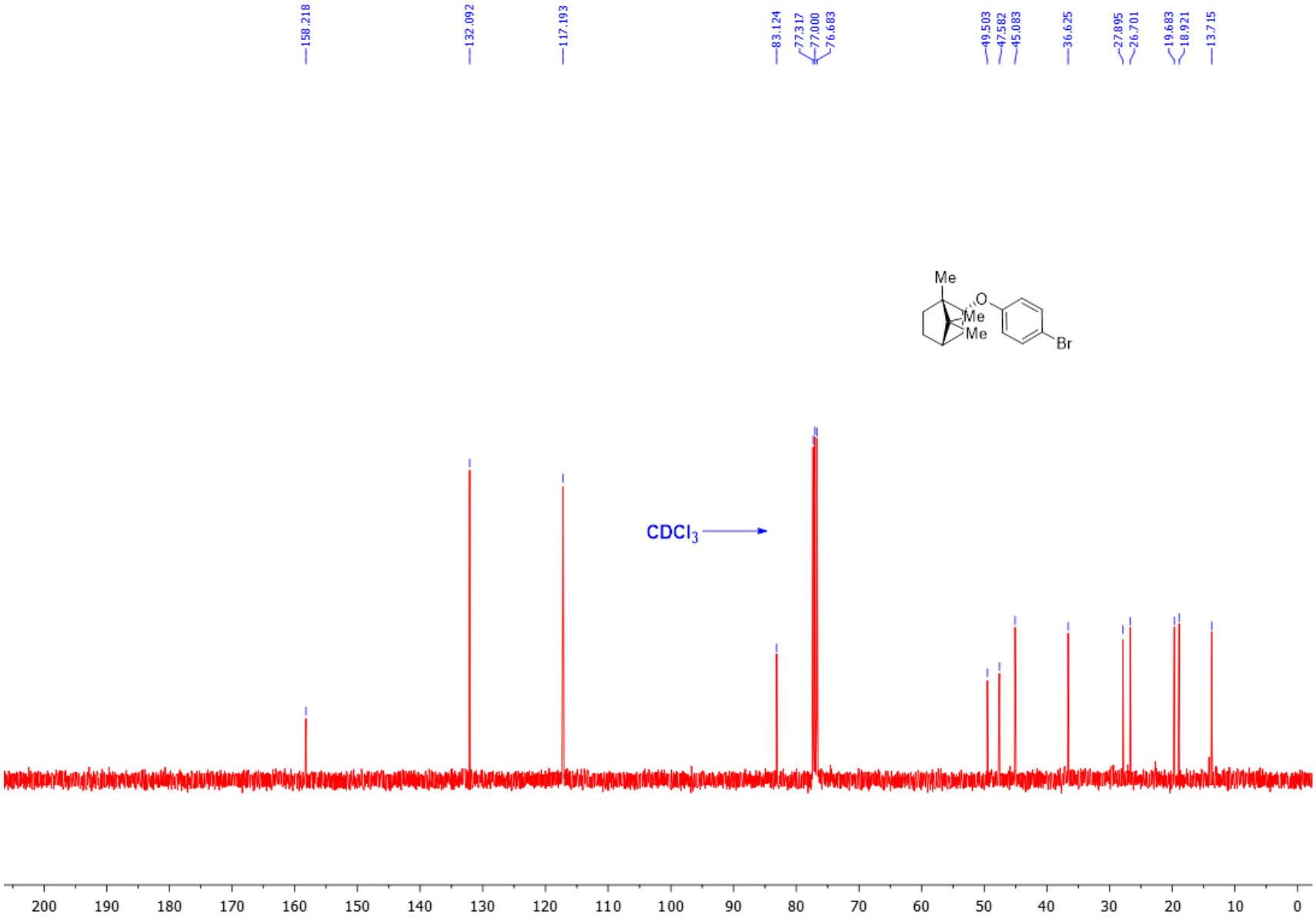
^{13}C-NMR of *8-(4-(4-(2λ5,5λ3-pentan-2-yl)cyclohexyl)phenyl)tetrazolo[1,5-a]pyridine(1v)* (25 ºC, 100 MHz, $CDCl_3$):



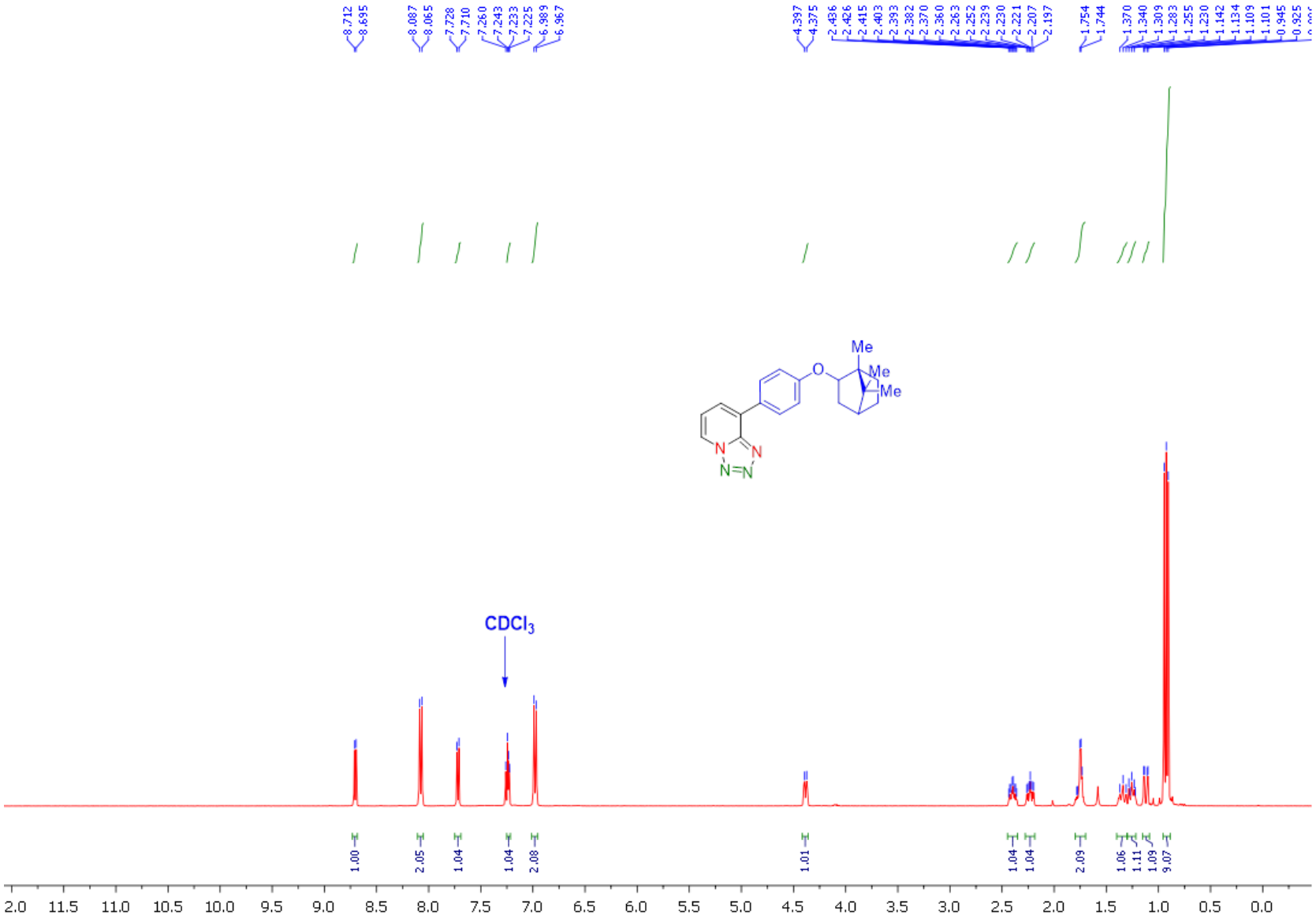
^{1}H-NMR of *(1S,2R,4S)-2-(4-bromophenoxy)-1,7,7-trimethylbicyclo[2.2.1]heptane* (25 ºC, 400 MHz, $CDCl_3$):



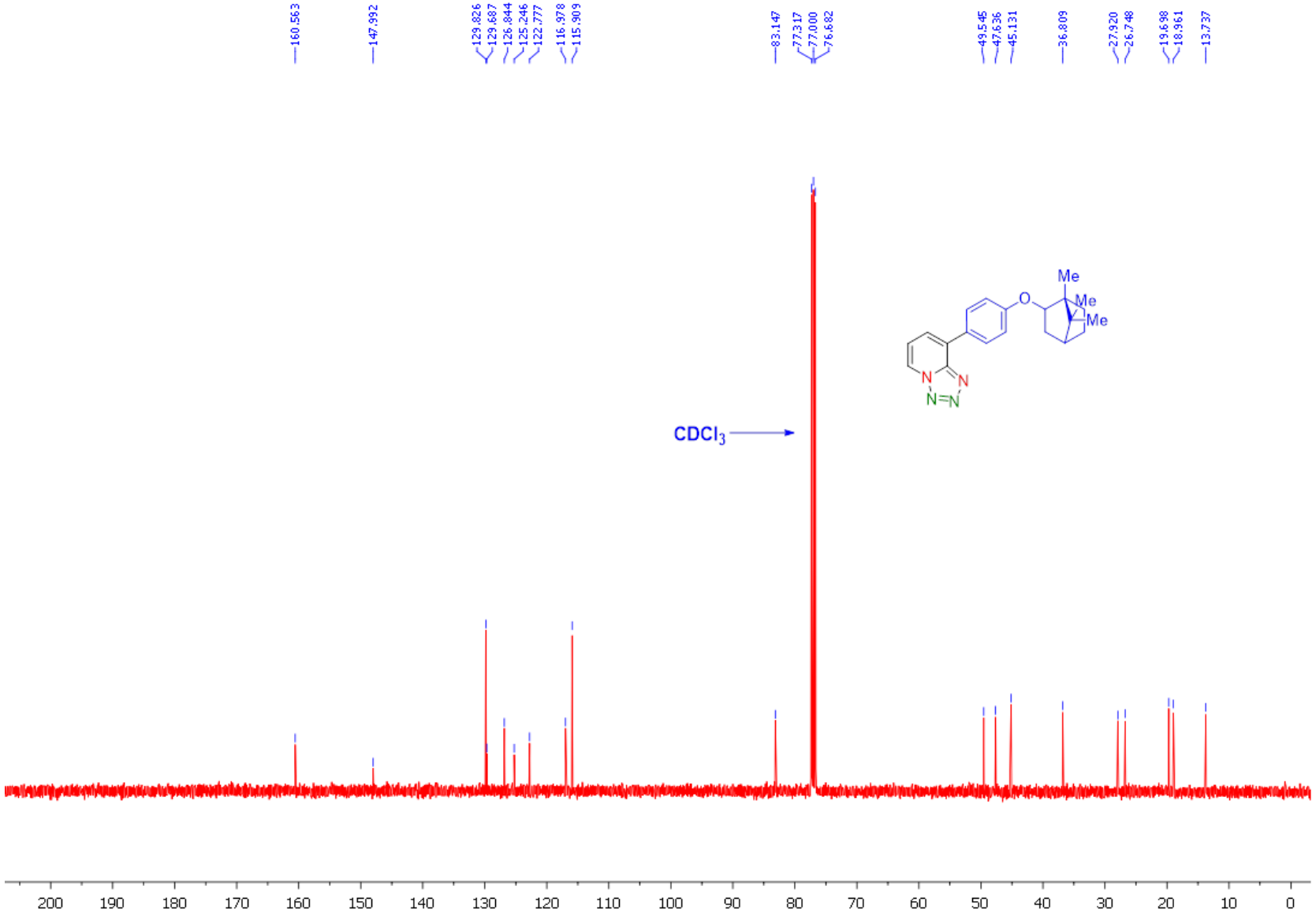
^{13}C-NMR of *(1S,2R,4S)-2-(4-bromophenoxy)-1,7,7-trimethylbicyclo[2.2.1]heptane* (25 °C, 100 MHz, $CDCl_3$):



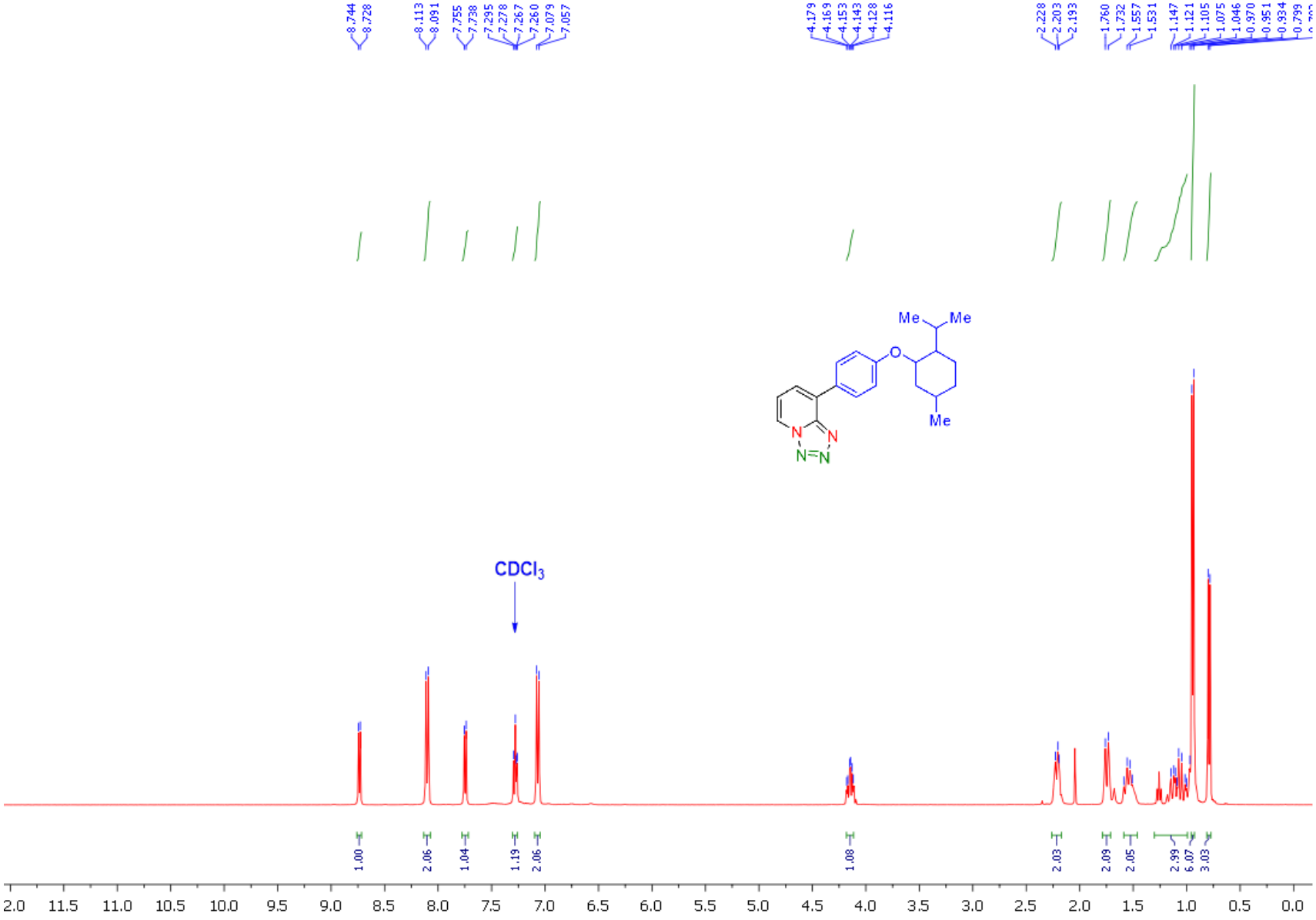
^{1}H-NMR of *-(4-(((1R,2S,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2- yl)oxy)phenyl)tetrazolo[1,5-a]pyridine (1w)* (25 ºC, 400 MHz, $CDCl_3$):



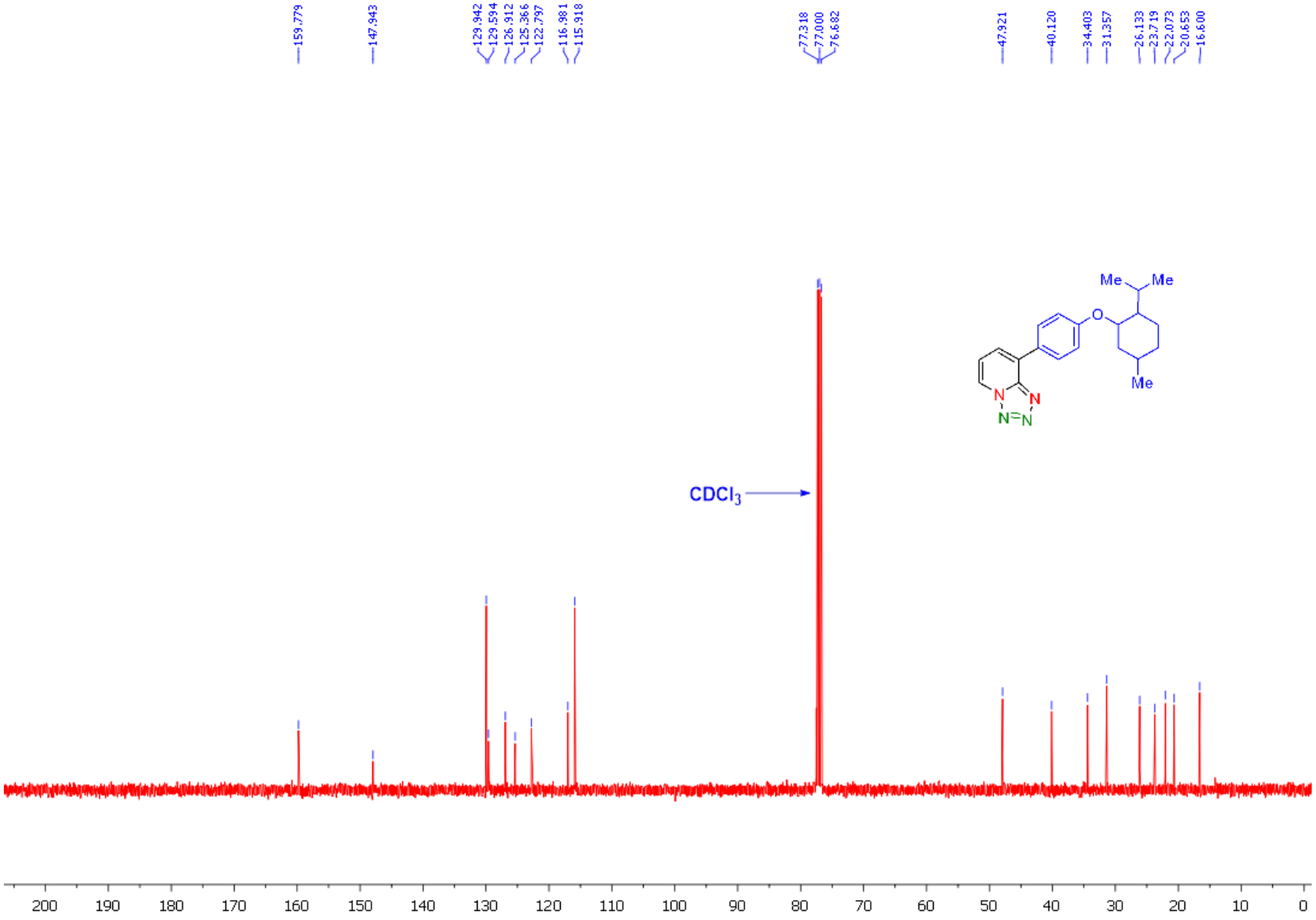
^{13}C-NMR of *-(4-(((1R,2S,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2- yl)oxy)phenyl)tetrazolo[1,5-a]pyridine (1w)* (25 ºC, 100 MHz, $CDCl_3$):



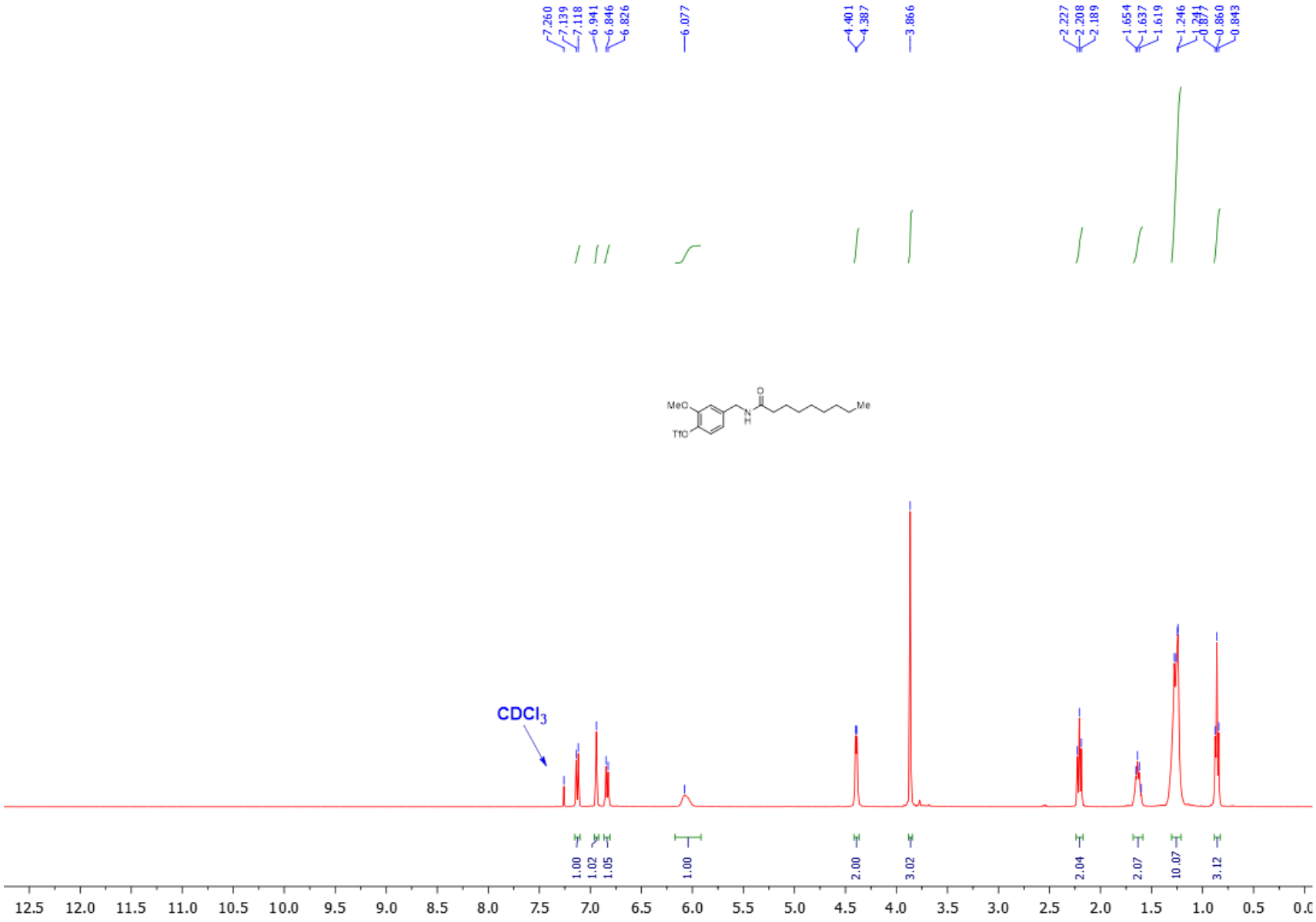
^{1}H-NMR of *8-(4-(((2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)phenyl)tetrazolo[1,5- a]pyridine (1x)* (25 °C, 400 MHz, $CDCl_3$):



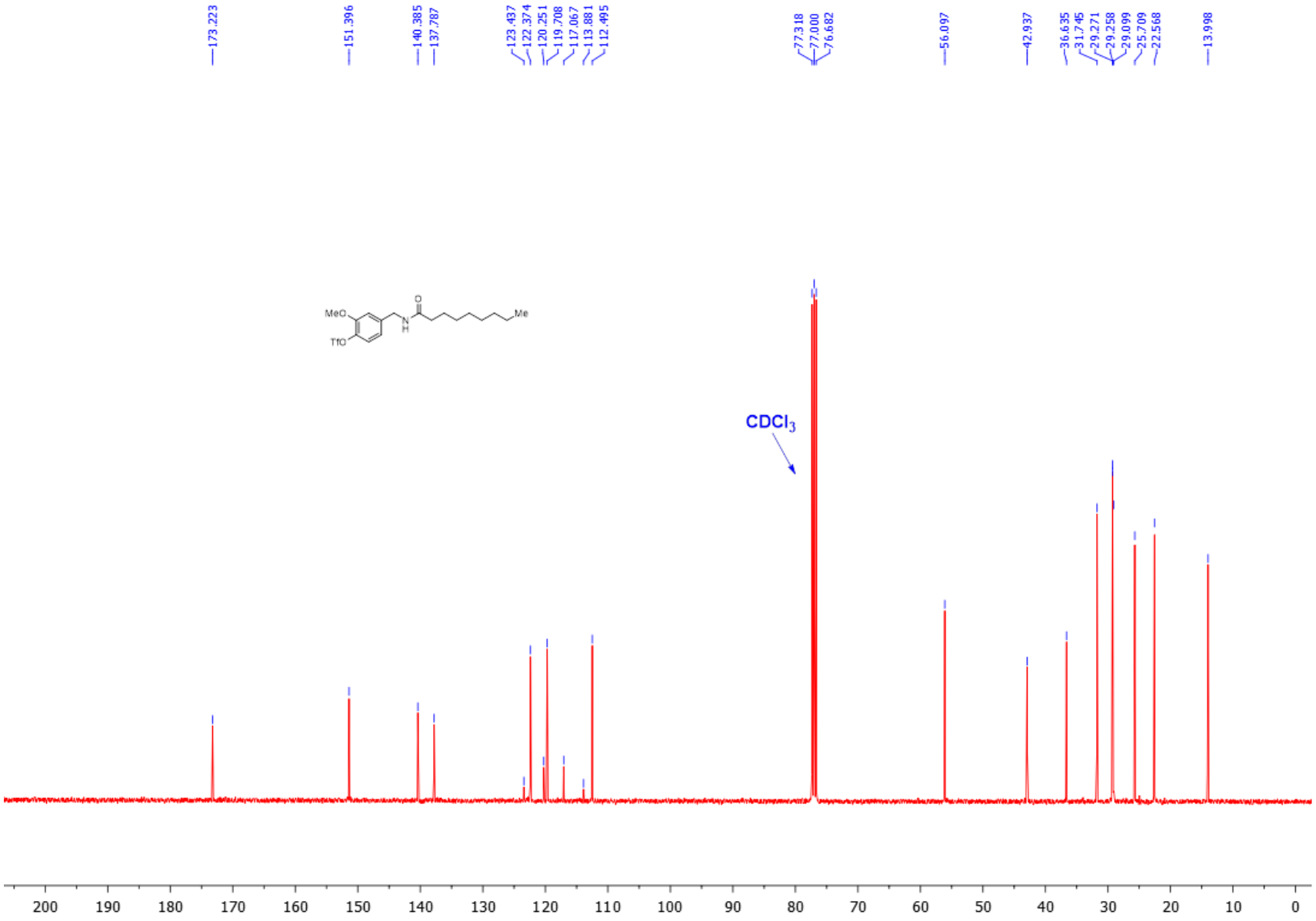
^{13}C-NMR of *8-(4-(((2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)phenyl)tetrazolo[1,5- a]pyridine (1x)* (25 °C, 100 MHz, $CDCl_3$):



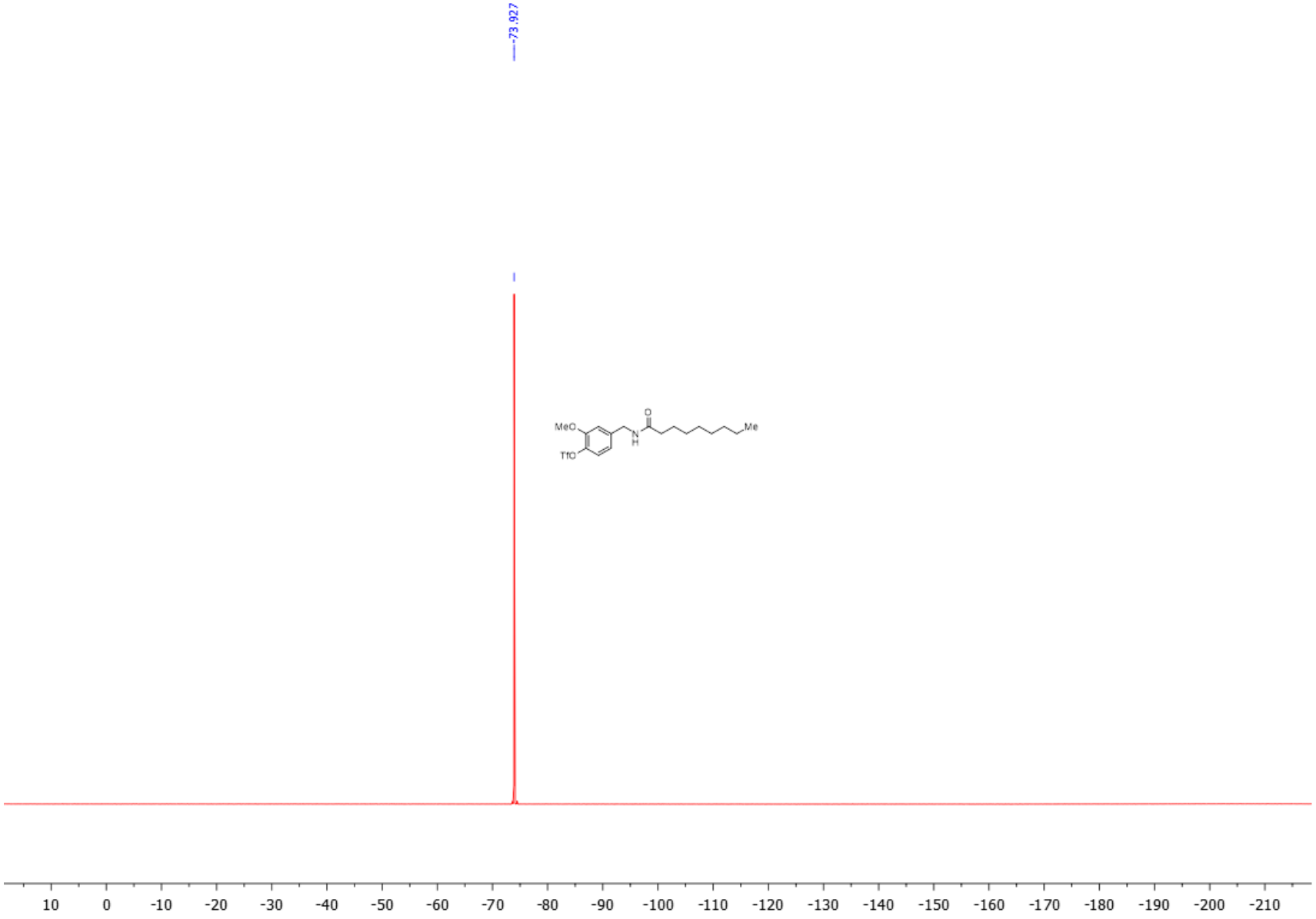
^{1}H-NMR of *2-methoxy-4-(nonanamidomethyl)phenyl trifluoromethanesulfonate:* (25 ^{o}C, 400 MHz, $CDCl_3$):



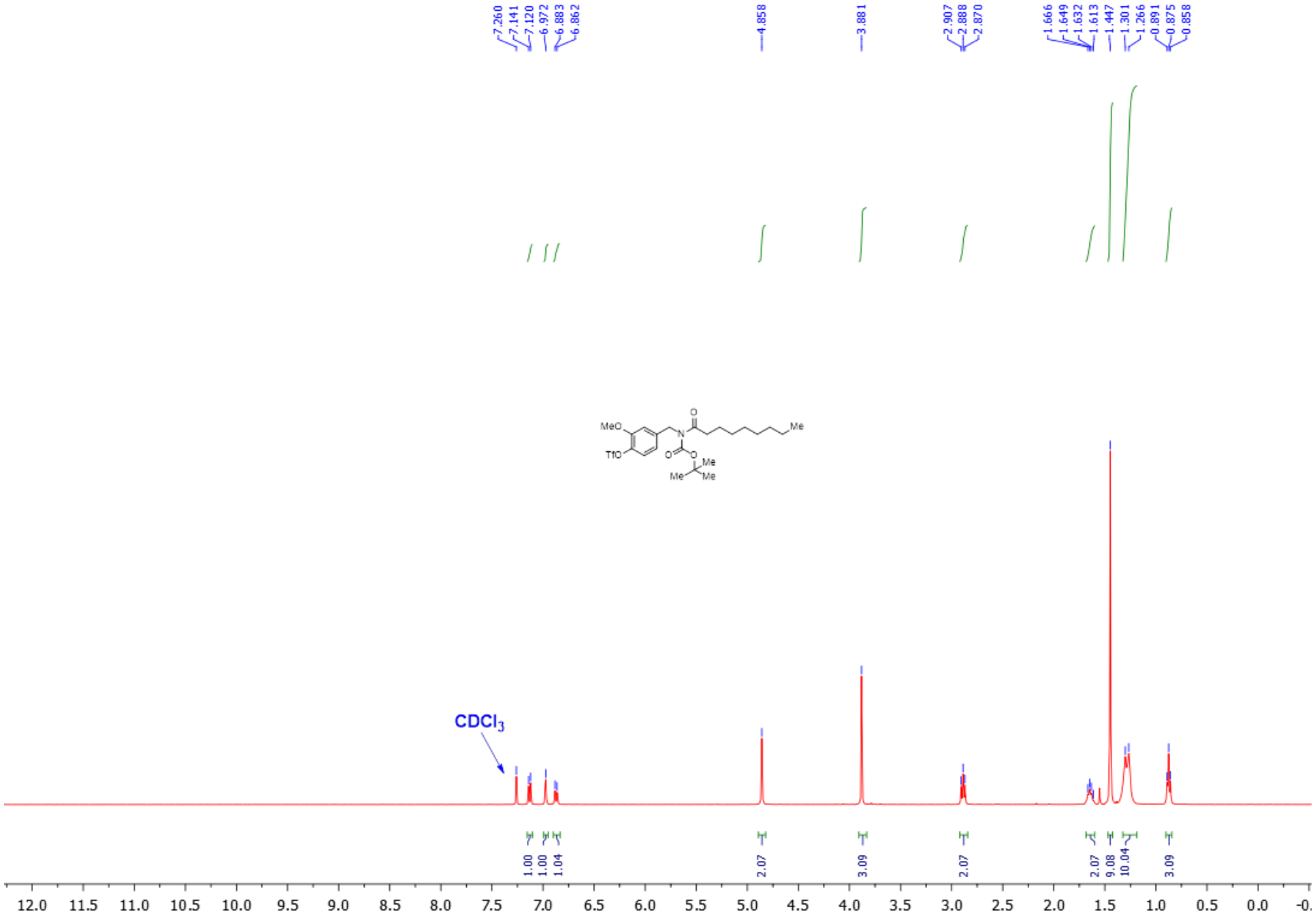
^{13}C-NMR of *2-methoxy-4-(nonanamidomethyl)phenyl trifluoromethanesulfonate* (25 ºC, 100 MHz, $CDCl_3$):



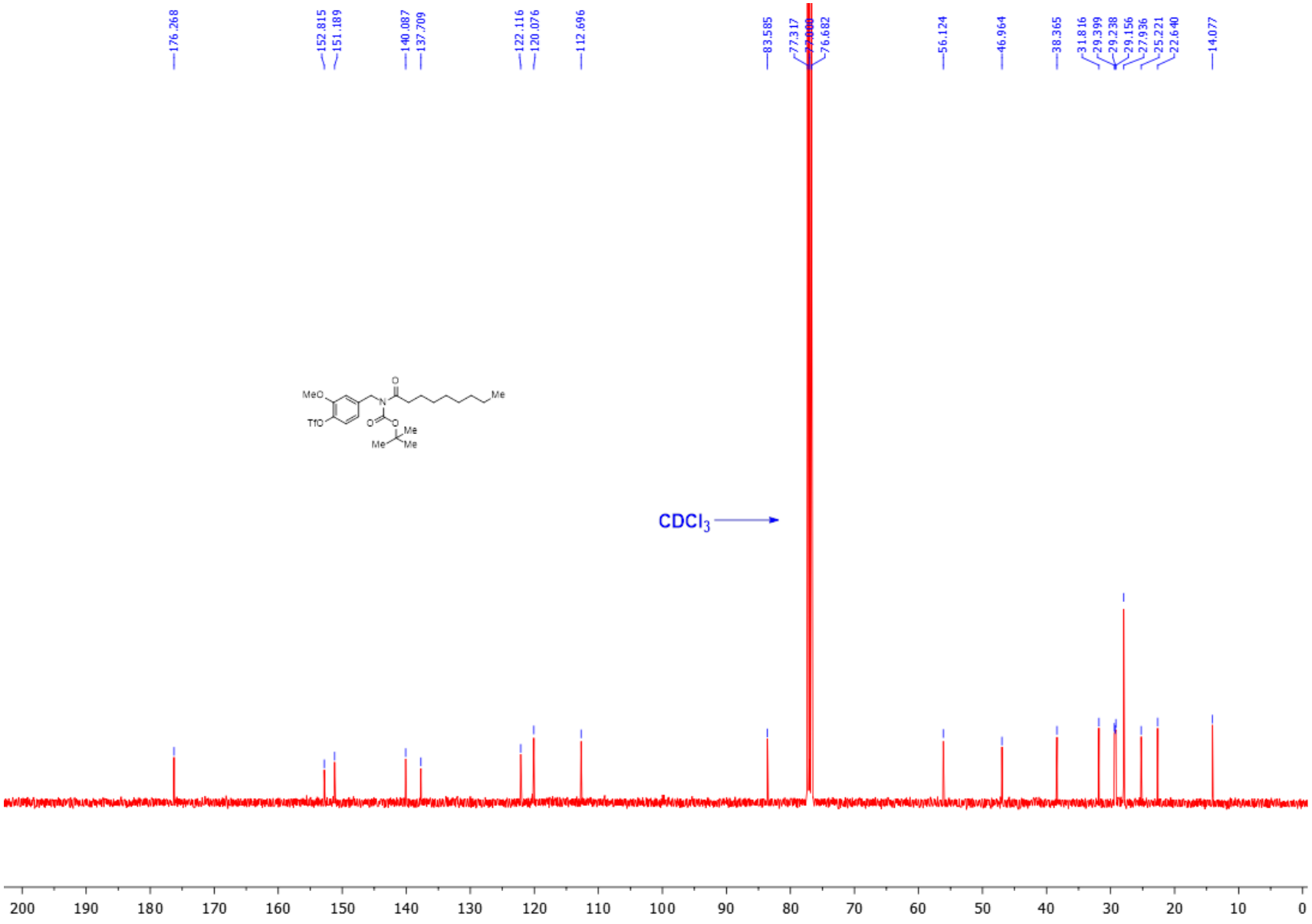
^{19}F-NMR of *2-methoxy-4-(nonanamidomethyl)phenyl trifluoromethanesulfonate)* (25 ^{o}C, 376 MHz, $CDCl_3$):



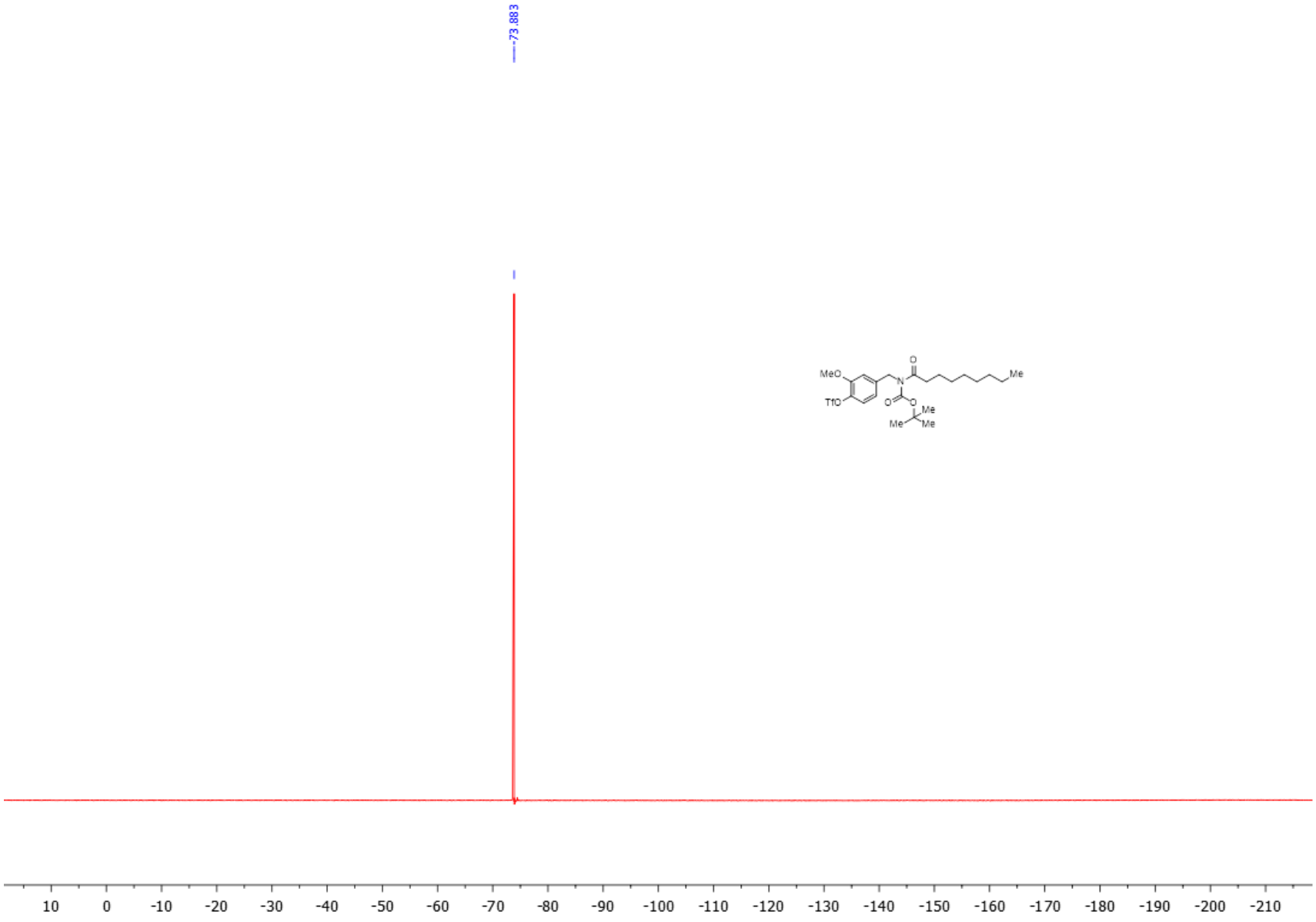
^{1}H-NMR of *4-((N-(tert-butoxycarbonyl)nonanamido)methyl)-2-methoxyphenyl trifluoromethanesulfonate* (25 ºC, 400 MHz, $CDCl_3$):



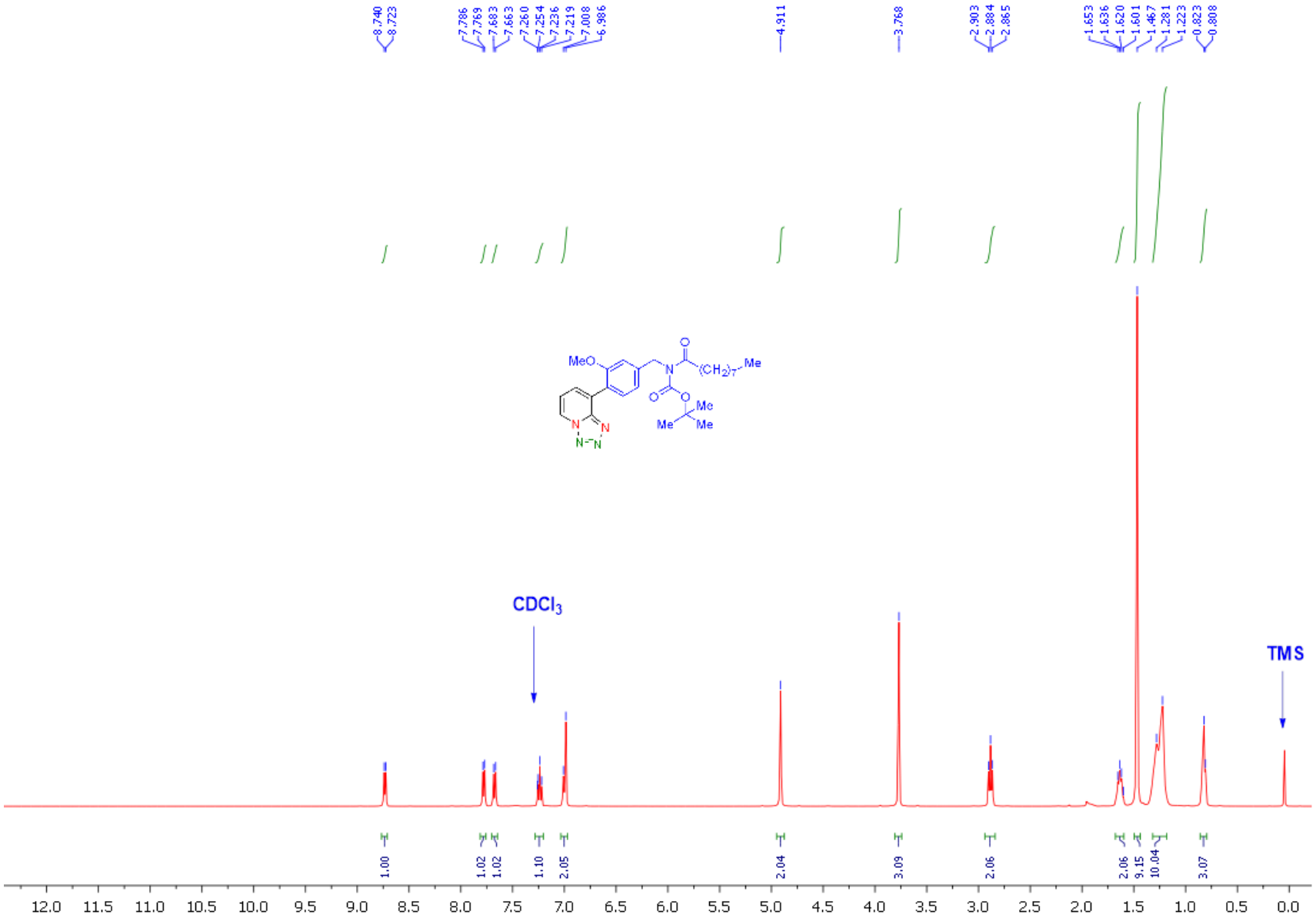
^{13}C-NMR of *4-((N-(tert-butoxycarbonyl)nonanamido)methyl)-2-methoxyphenyl trifluoromethanesulfonate* (25 °C, 100 MHz, $CDCl_3$):



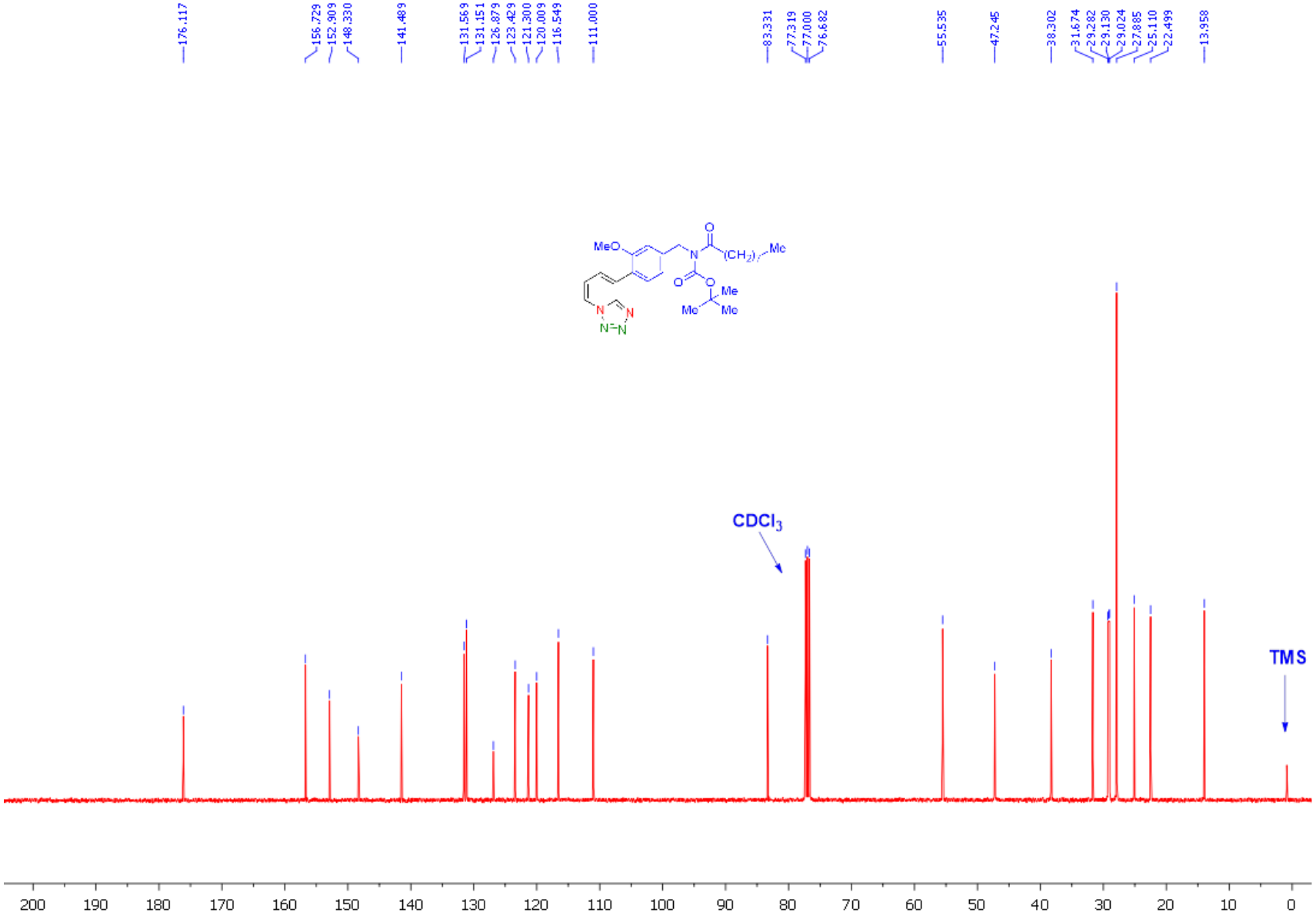
^{19}F-NMR of *4-((N-(tert-butoxycarbonyl)nonanamido)methyl)-2-methoxyphenyl trifluoromethanesulfonate* (25 °C, 376 MHz, $CDCl_3$):



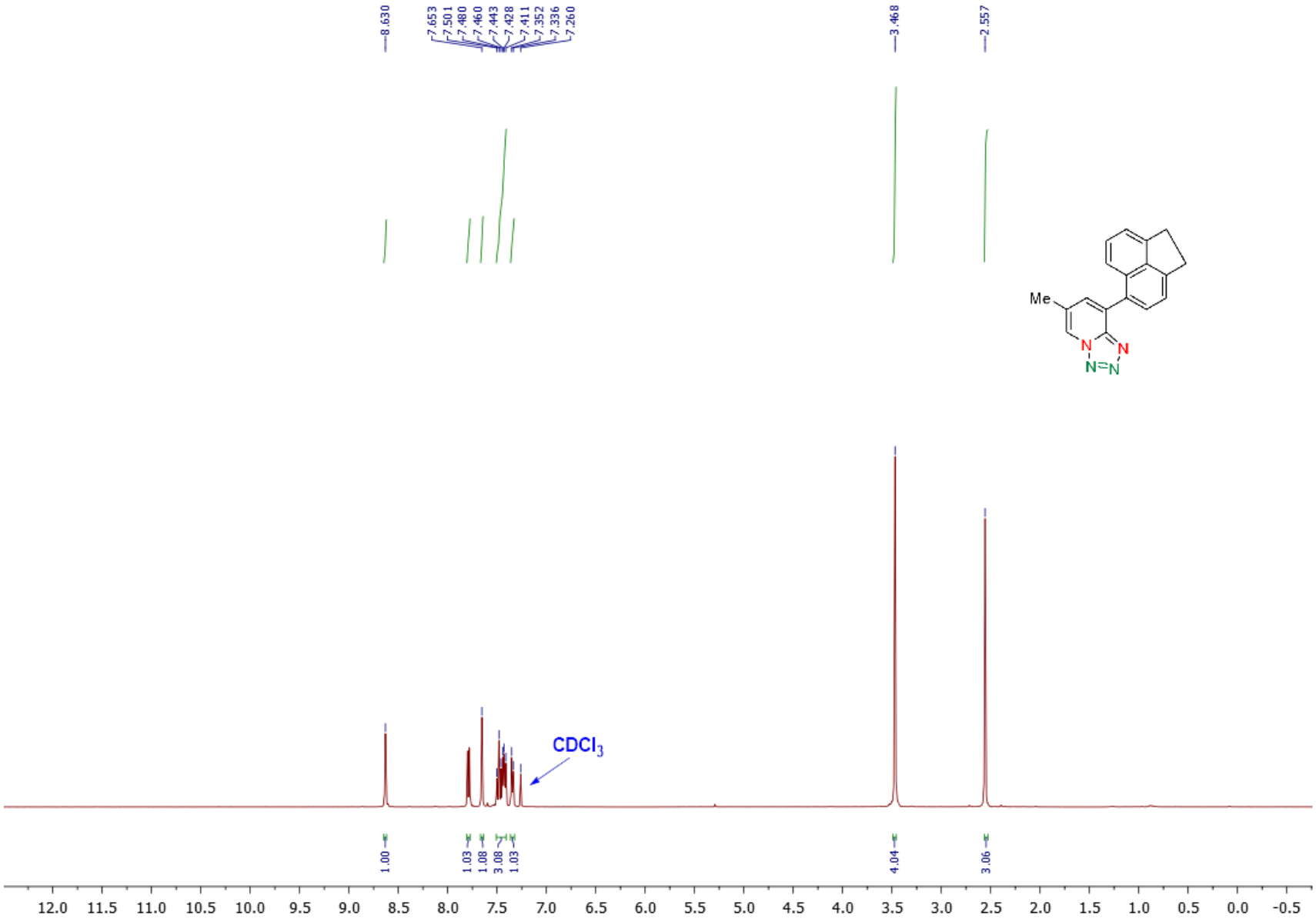
^{1}H-NMR of *tert-butyl (3-methoxy-4-(tetrazolo[1,5-a]pyridin-8- yl)benzyl)(propionyl)carbamate (1y)* (25 ^{o}C, 400 MHz, $CDCl_3$):



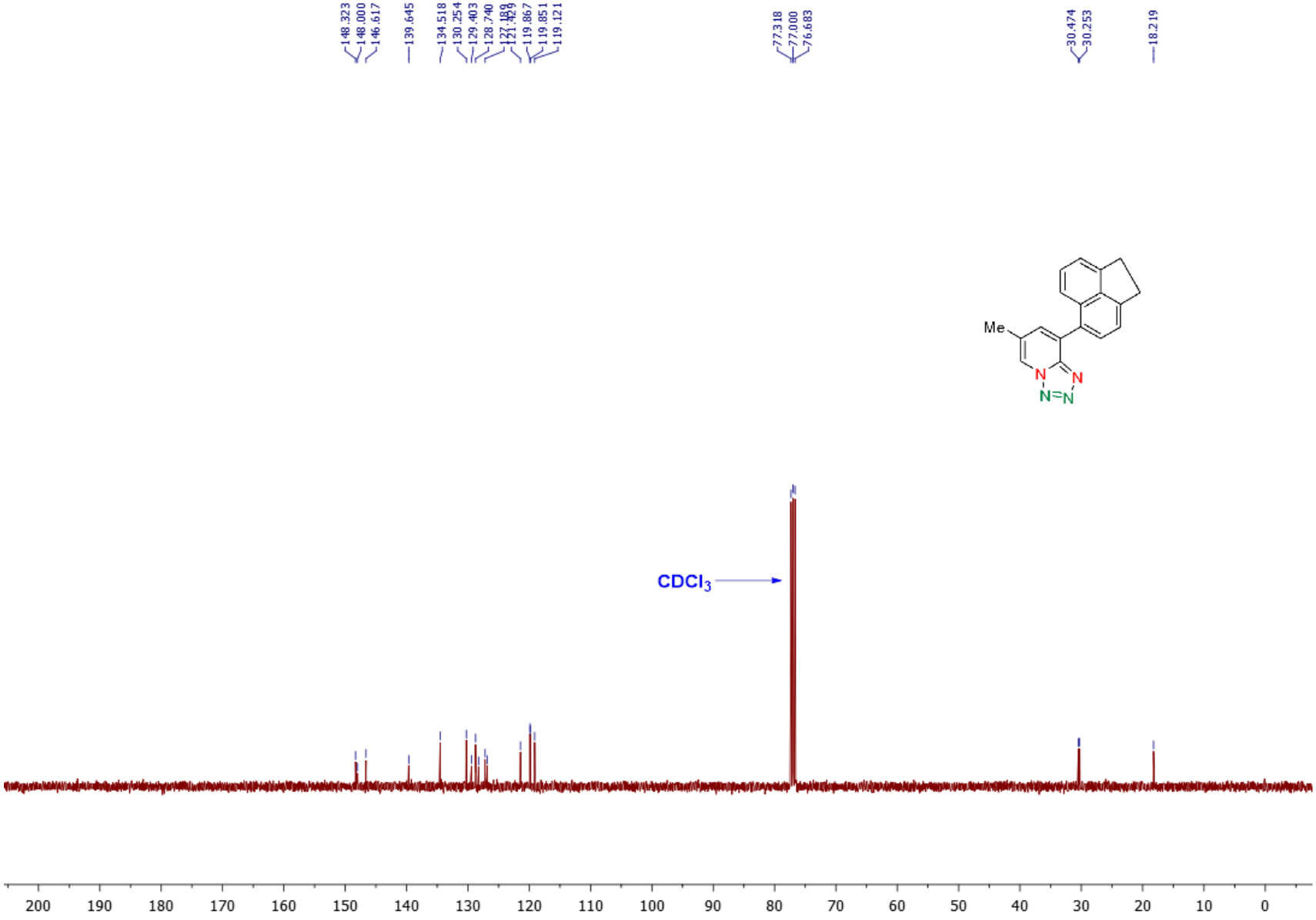
^{13}C-NMR of *tert-butyl (3-methoxy-4-(tetrazolo[1,5-a]pyridin-8- yl)benzyl)(propionyl)carbamate (1y* (25 °C, 100 MHz, $CDCl_3$):



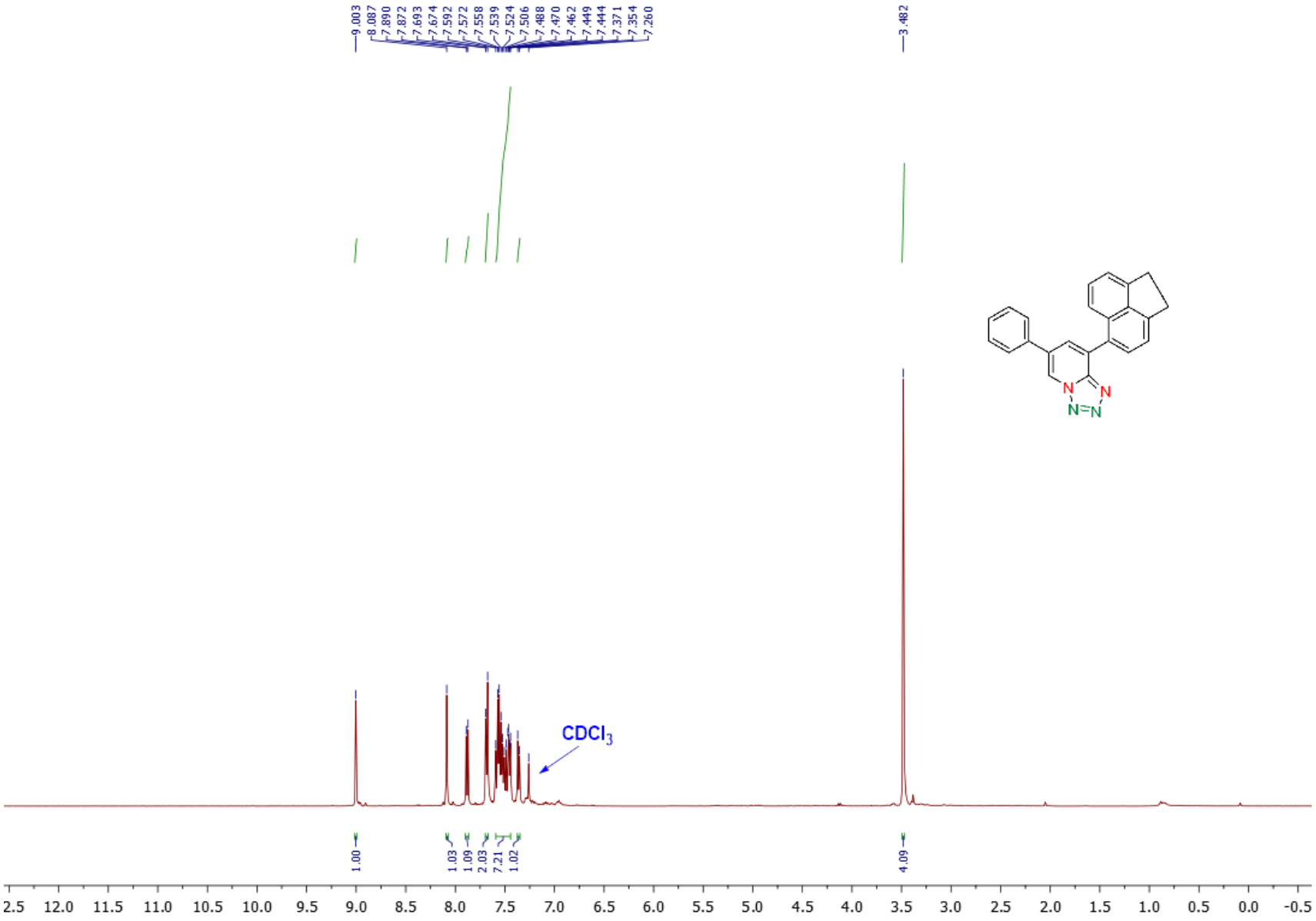
^{1}H-NMR of *8-(1,2-dihydroacenaphthylen-5-yl)-6-methyltetrazolo[1,5-a]pyridine (3a)* (25 ^{o}C, 400 MHz, $CDCl_3$):



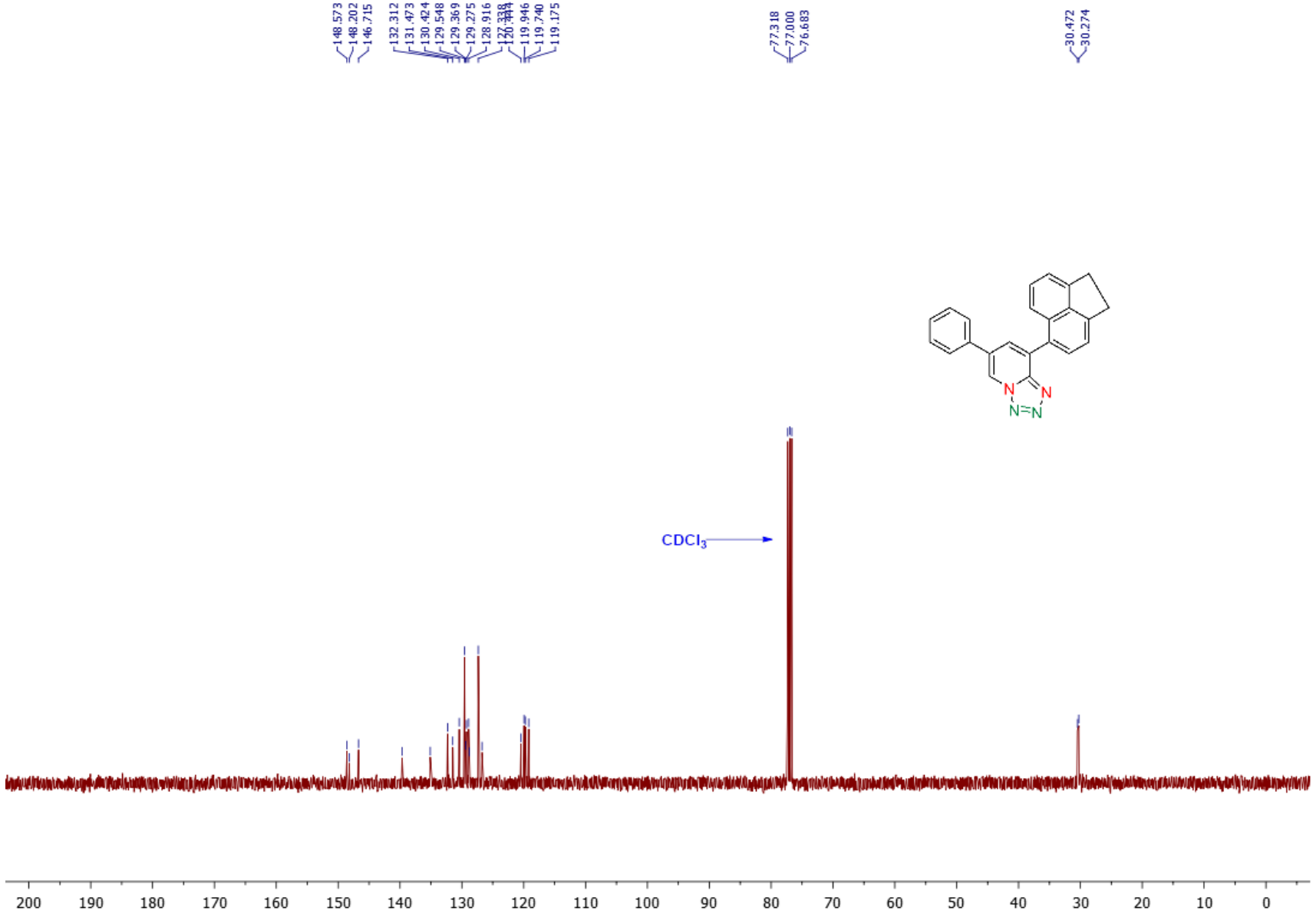
^{13}C-NMR of *8-(1,2-dihydroacenaphthylen-5-yl)-6-methyltetrazolo[1,5-a]pyridine (3a)* (25 ºC, 100 MHz, $CDCl_3$):



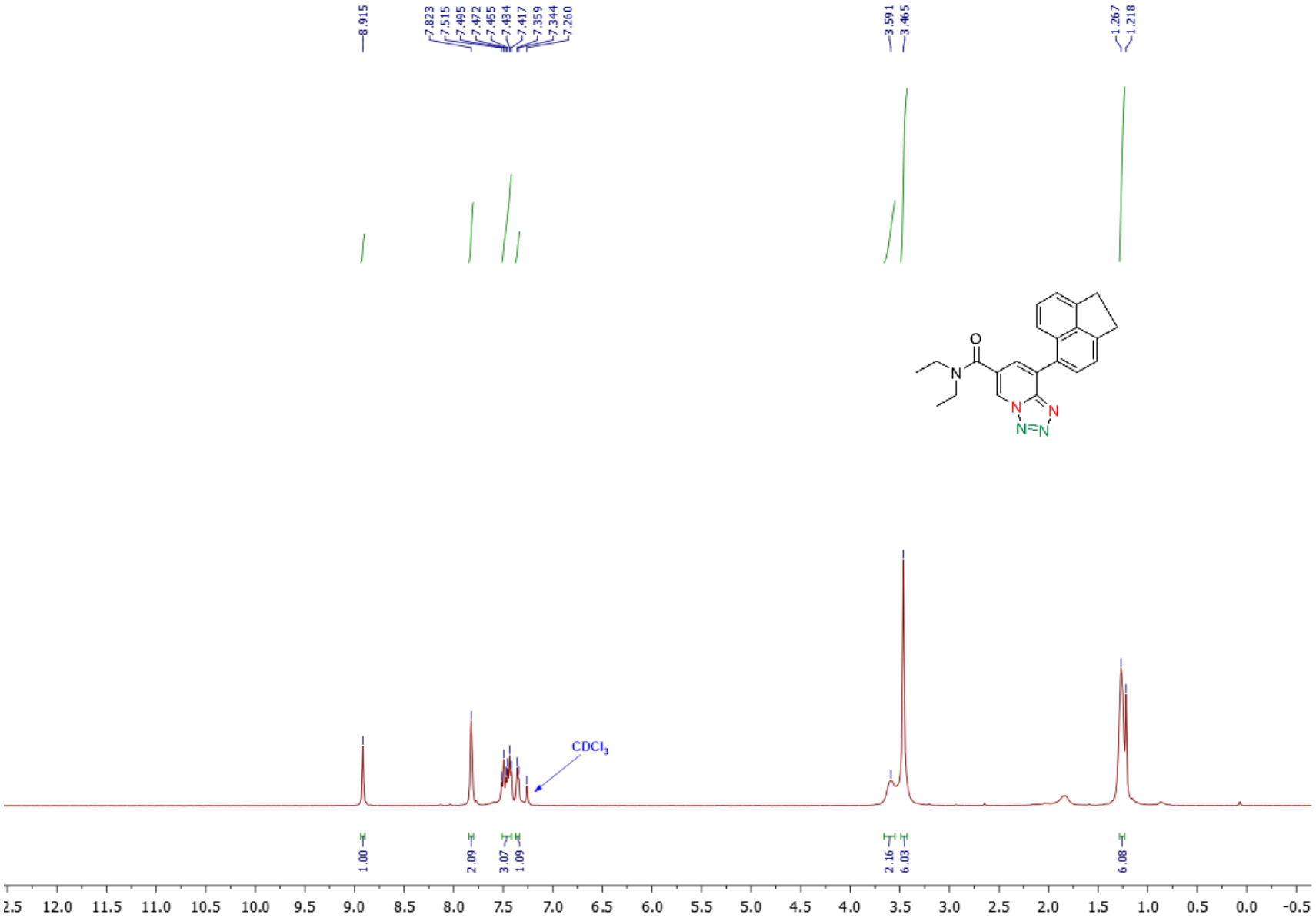
^{1}H-NMR of *8-(1,2-dihydroacenaphthylen-5-yl)-6-phenyltetrazolo[1,5-a]pyridine (3b)* (25 ^{o}C, 400 MHz, $CDCl_3$):



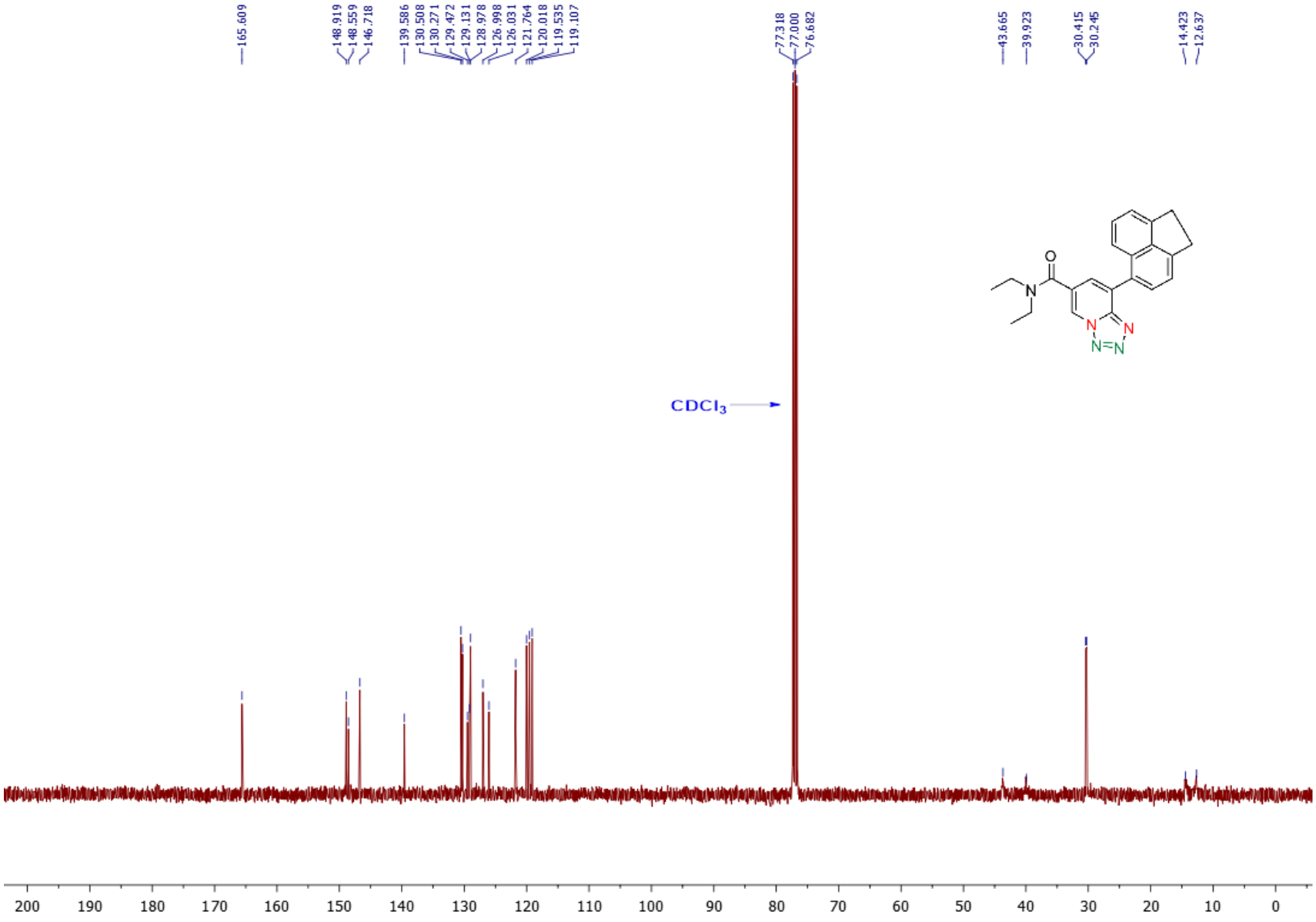
^{13}C-NMR of *8-(1,2-dihydroacenaphthylen-5-yl)-6-phenyltetrazolo[1,5-a]pyridine (3b)* (25 ºC, 100 MHz, $CDCl_3$):



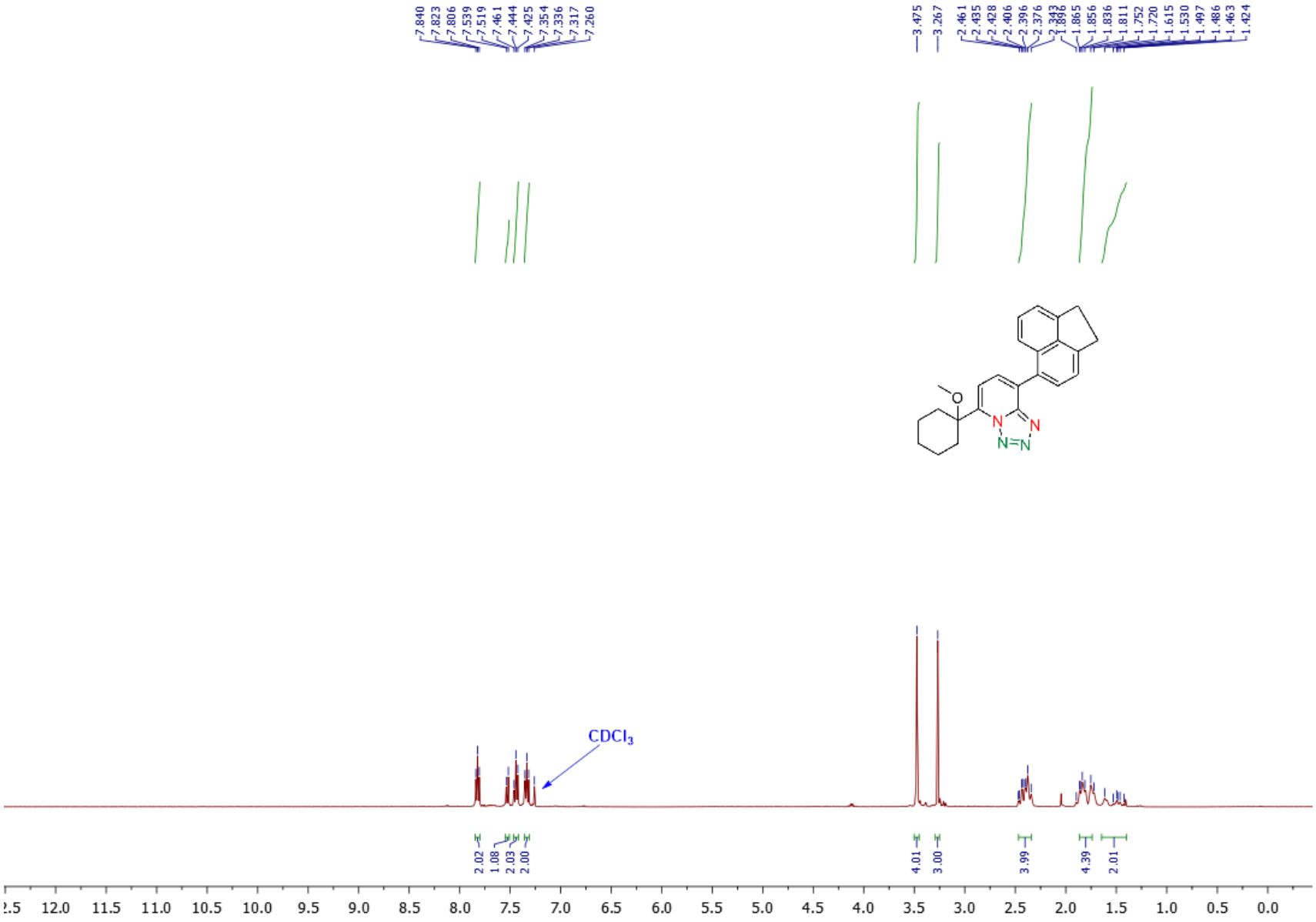
^{1}H-NMR of *8-(1,2-dihydroacenaphthylen-5-yl)-N,N-diethyltetrazolo[1,5-a]pyridine-6- carboxamide (3c)*(25 ºC, 400 MHz, $CDCl_3$):



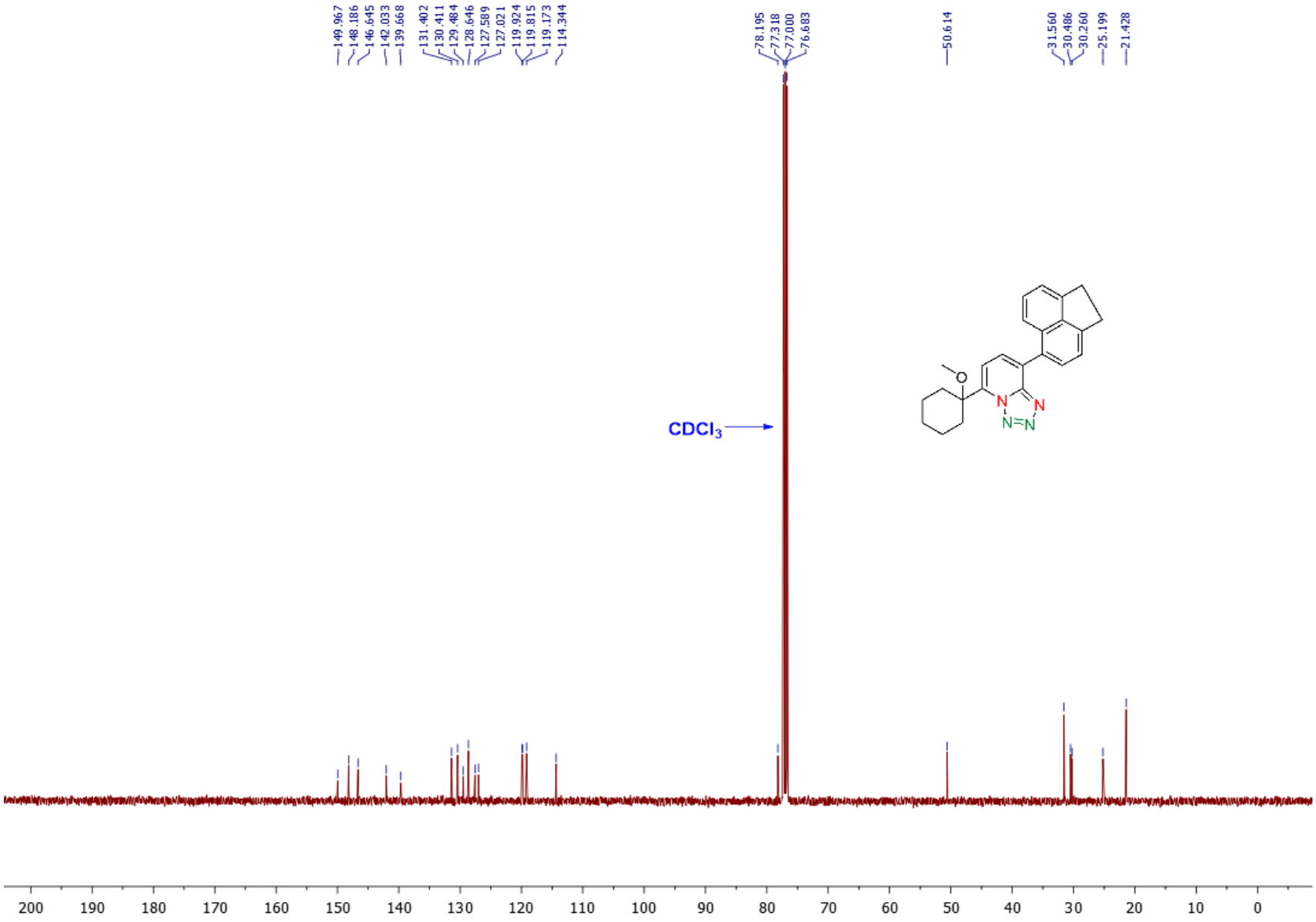
^{13}C-NMR of *8-(1,2-dihydroacenaphthylen-5-yl)-N,N-diethyltetrazolo[1,5-a]pyridine-6- carboxamide (3c)* (25 °C, 100 MHz, $CDCl_3$):



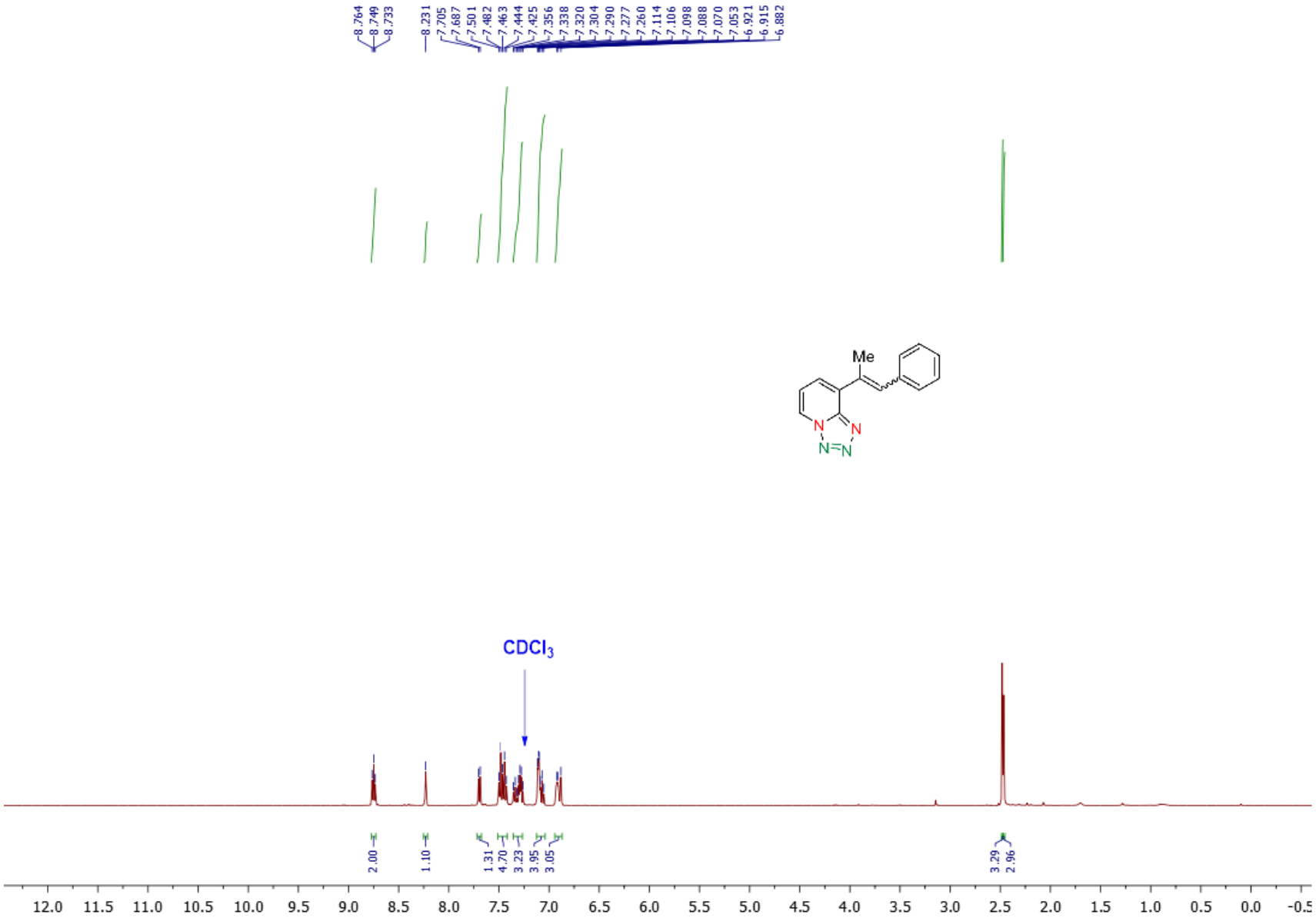
^{1}H-NMR of *8-(1,2-dihydroacenaphthylen-5-yl)-5-(1-methoxycyclohexyl)tetrazolo[1,5- a]pyridine (3d)* (25 °C, 400 MHz, $CDCl_3$):



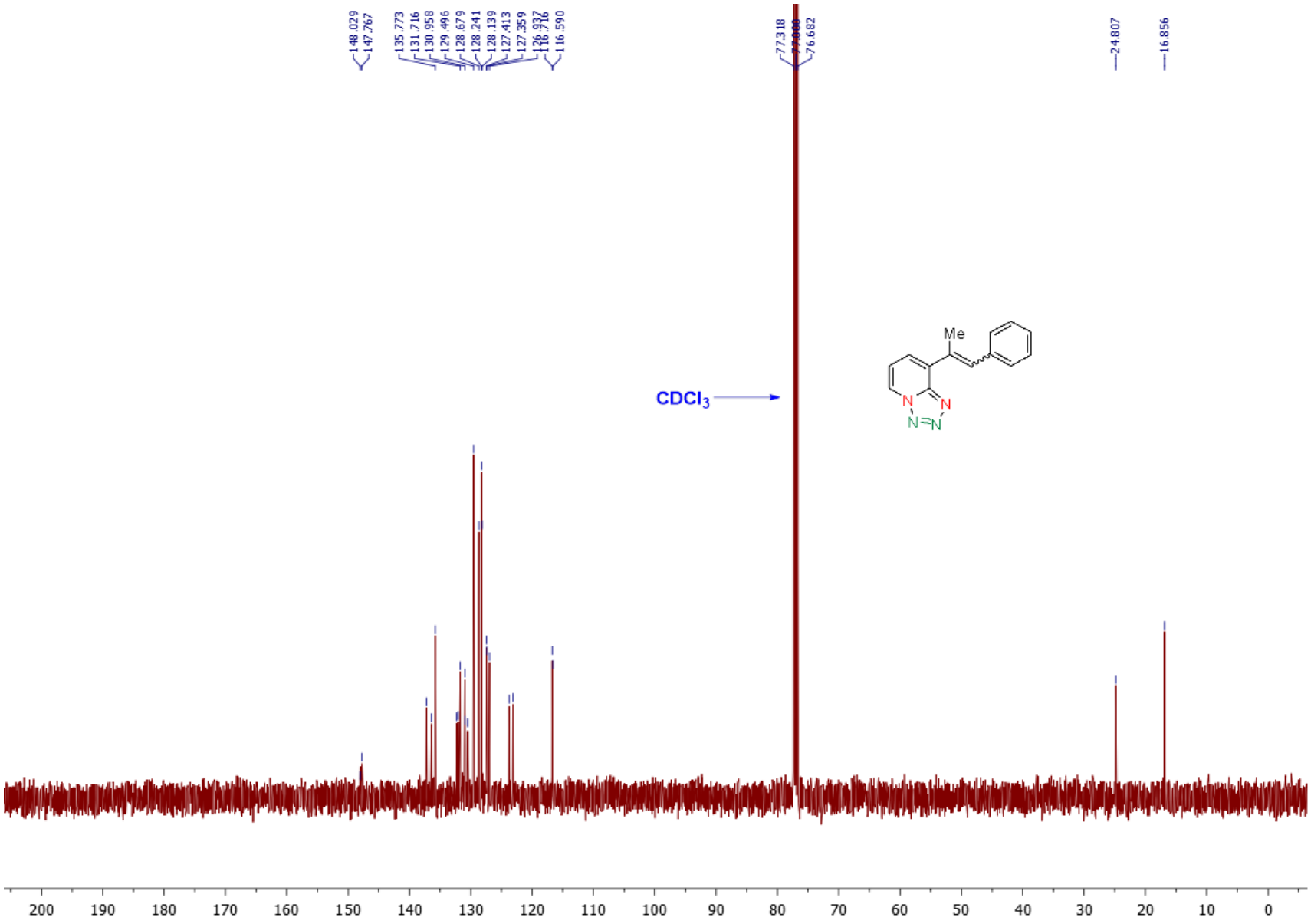
^{13}C-NMR of *8-(1,2-dihydroacenaphthylen-5-yl)-5-(1-methoxycyclohexyl)tetrazolo[1,5- a]pyridine (3d)* (25 °C, 100 MHz, $CDCl_3$):



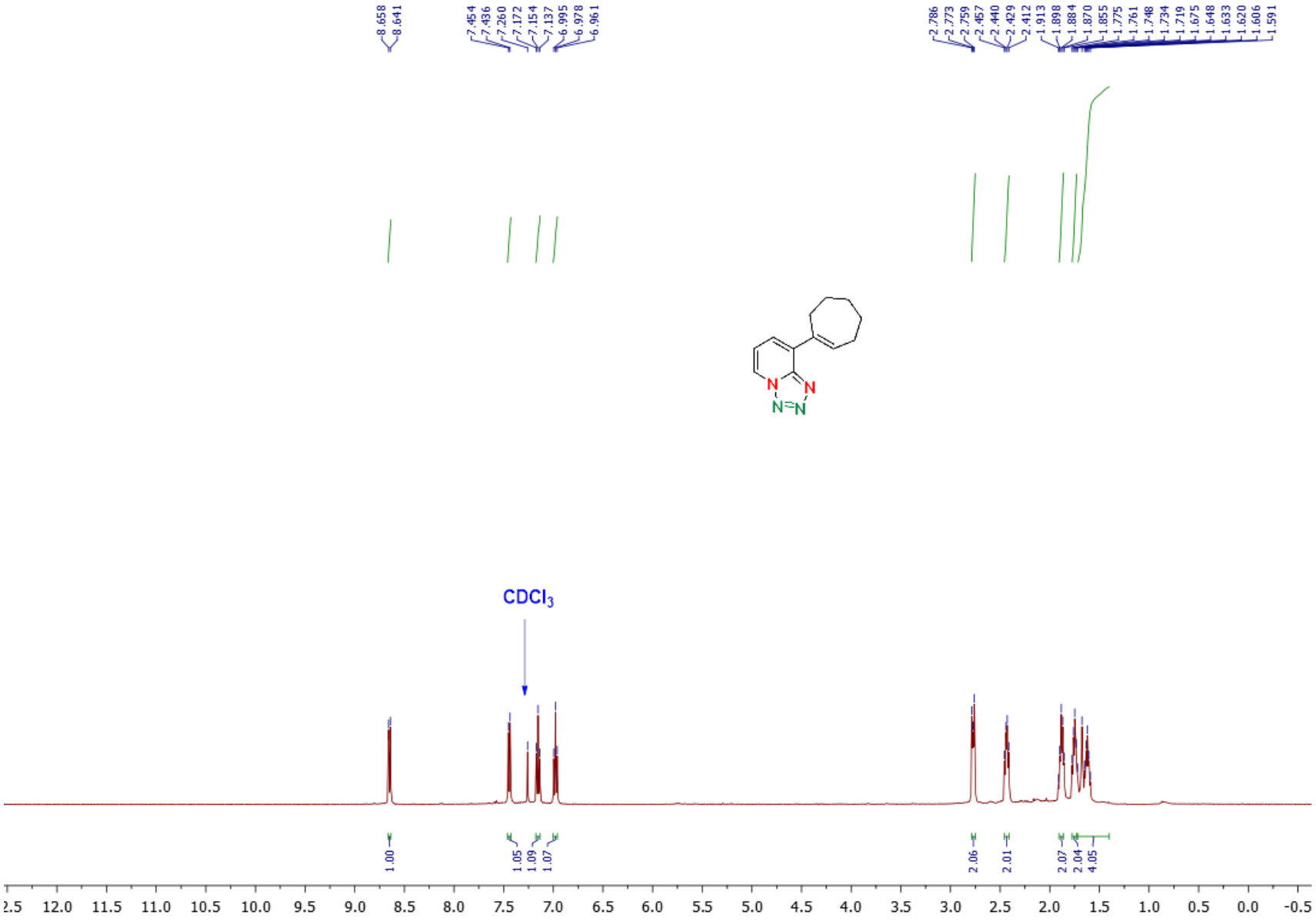
^{1}H-NMR of *8-(1-phenylprop-1-en-2-yl)tetrazolo[1,5-a]pyridine (5a)* (25 °C, 400 MHz, $CDCl_3$):



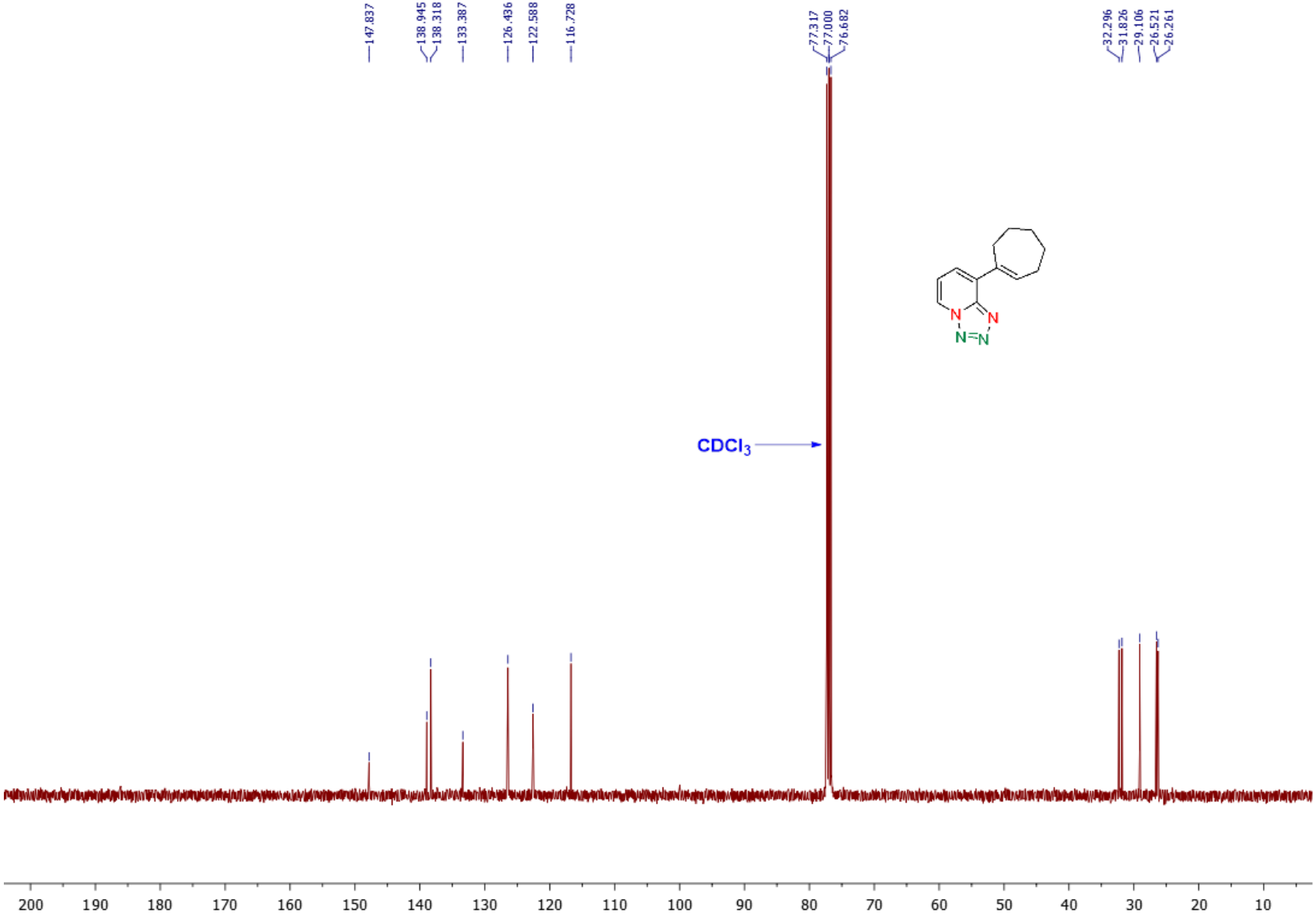
^{13}C-NMR of *8-(1-phenylprop-1-en-2-yl)tetrazolo[1,5-a]pyridine (5a))* (25 °C, 100 MHz, $CDCl_3$):



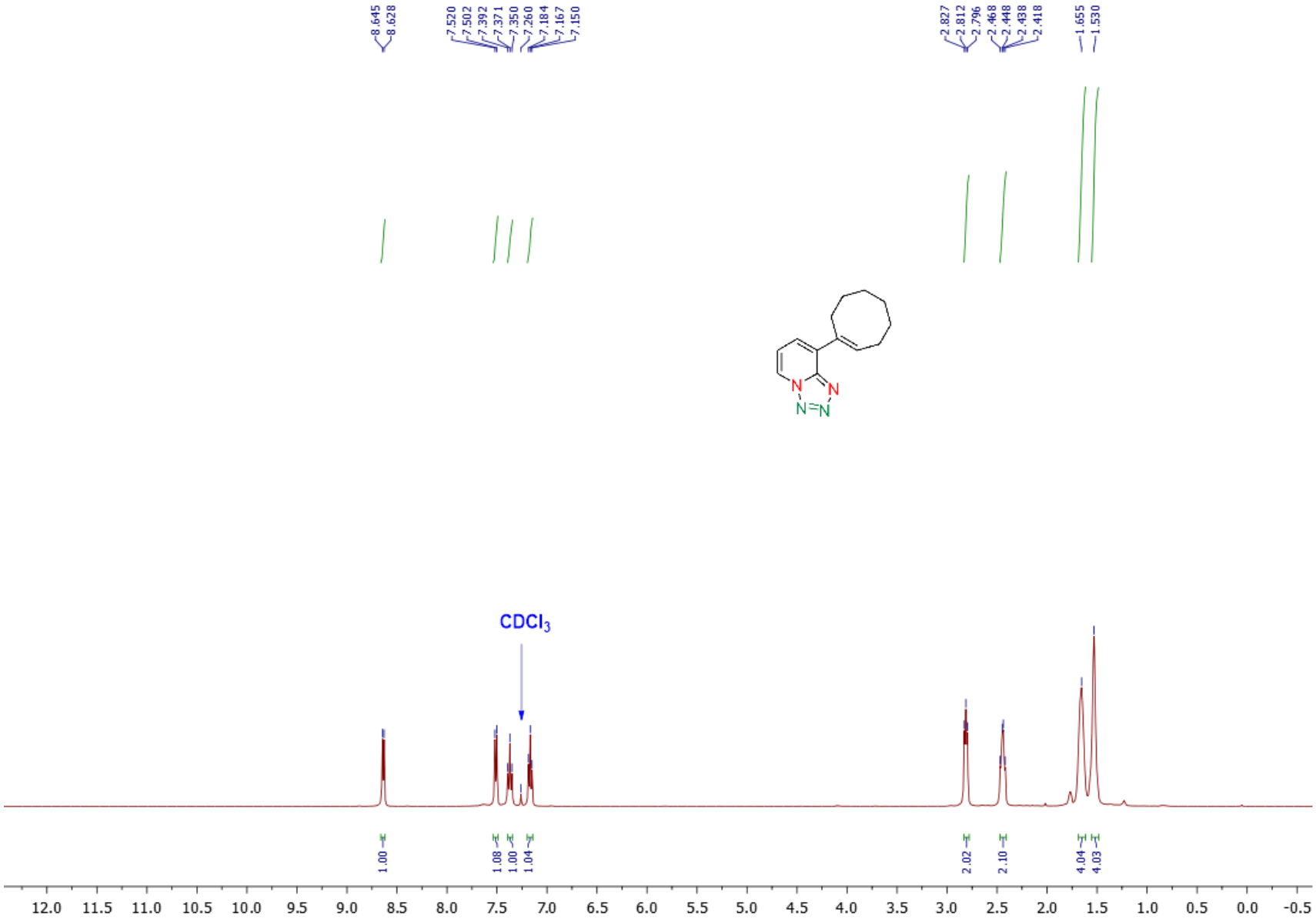
^{1}H-NMR of *8-(cyclohept-1-en-1-yl)tetrazolo[1,5-a]pyridine (5b)* (25 ^{o}C, 400 MHz, $CDCl_3$):



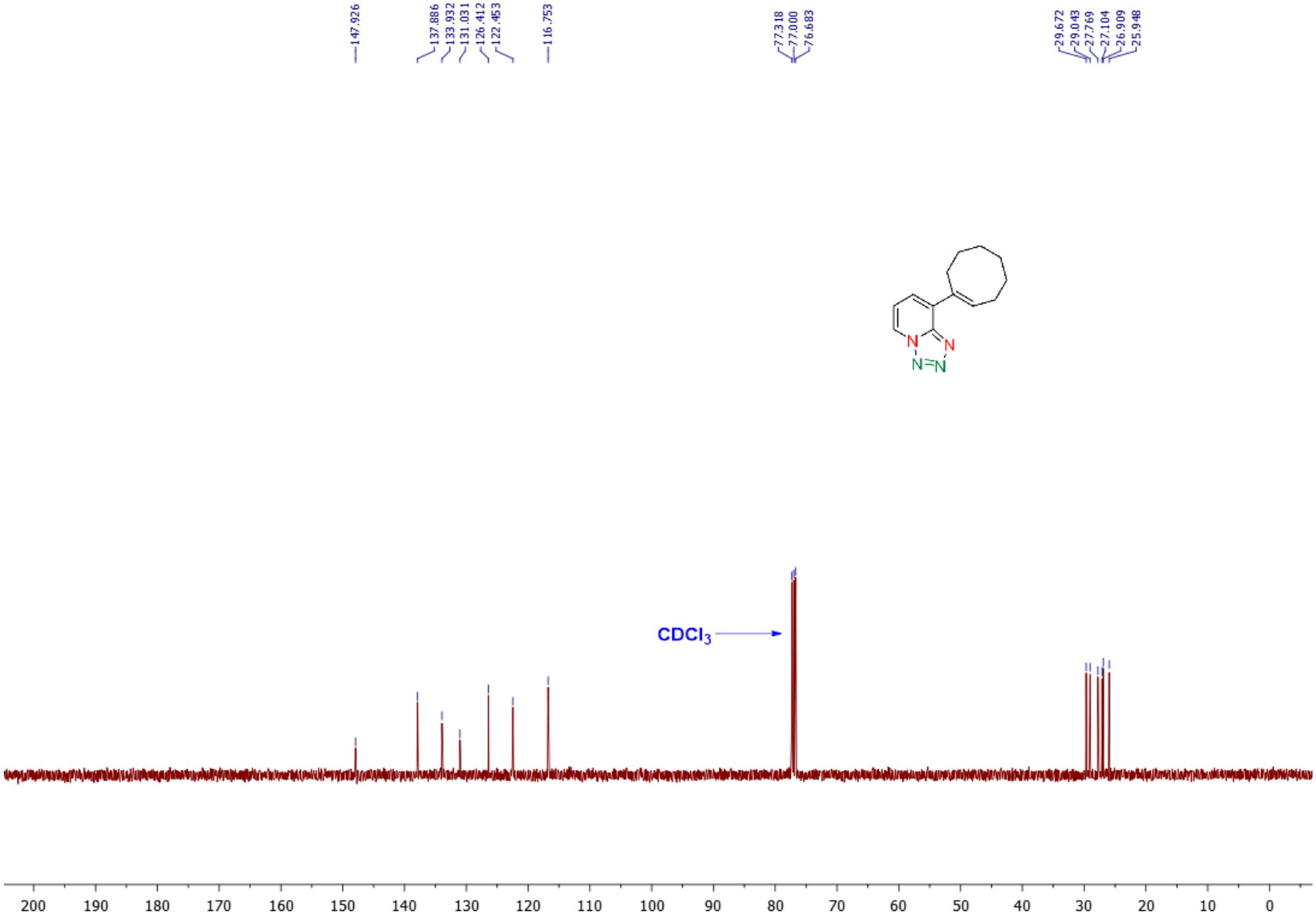
^{13}C-NMR of *8-(cyclohept-1-en-1-yl)tetrazolo[1,5-a]pyridine (5b)* (25 ºC, 100 MHz, $CDCl_3$):



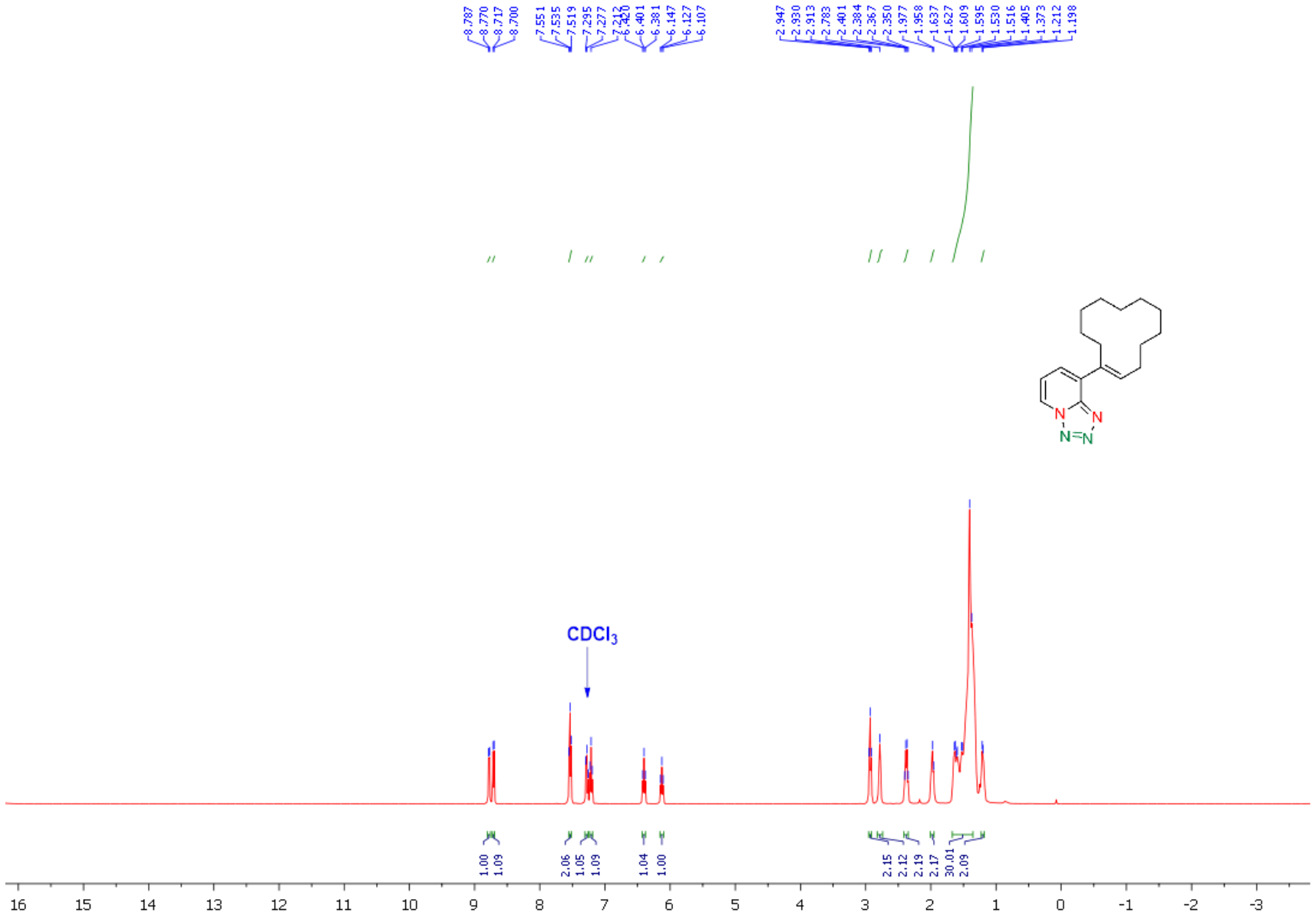
^{1}H-NMR of *(E)-8-(cyclooct-1-en-1-yl)tetrazolo[1,5-a]pyridine (5c)* (25 ^{o}C, 400 MHz, $CDCl_3$):



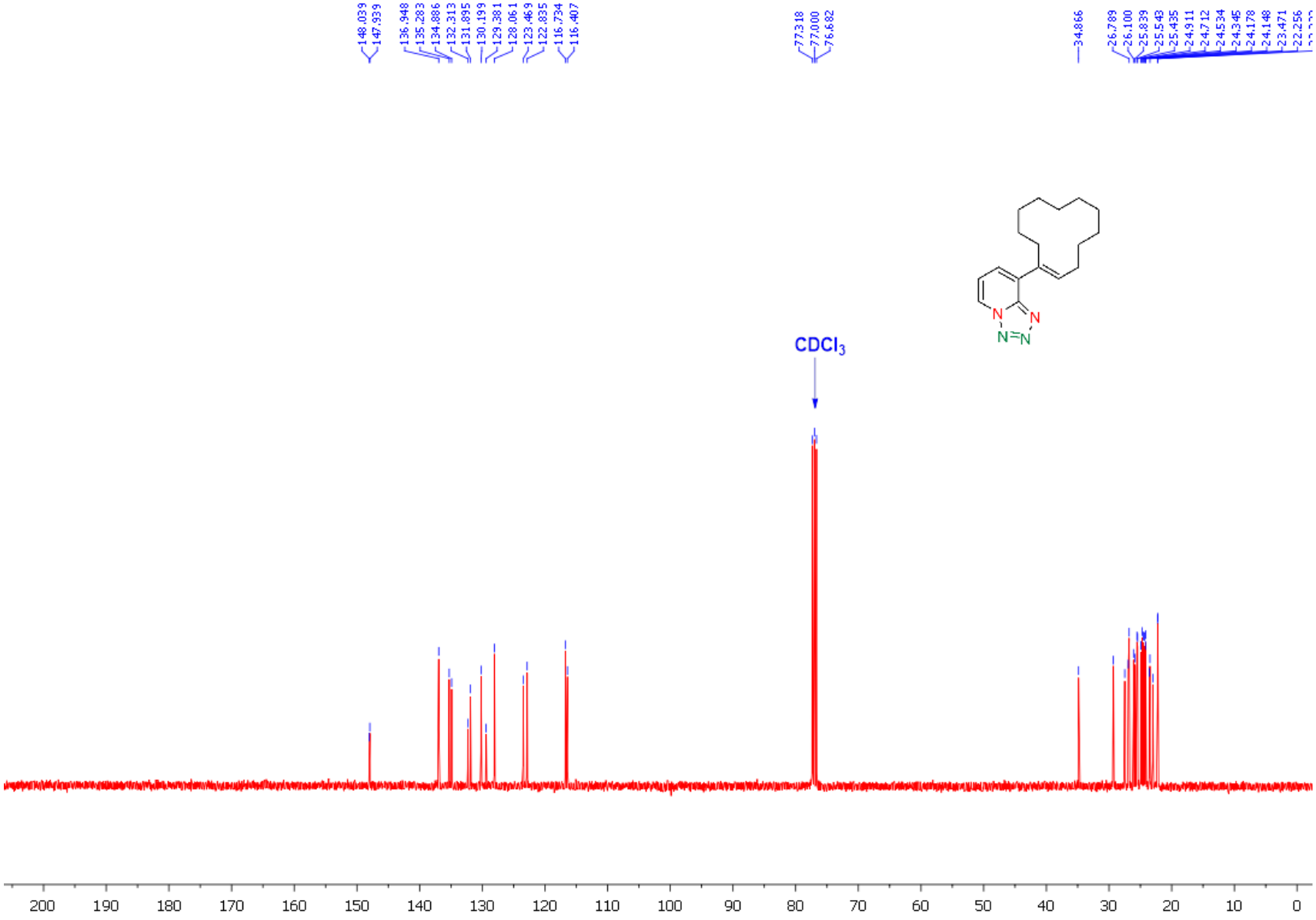
^{13}C-NMR of *(E)-8-(cyclooct-1-en-1-yl)tetrazolo[1,5-a]pyridine (5c)* (25 ºC, 100 MHz, $CDCl_3$):



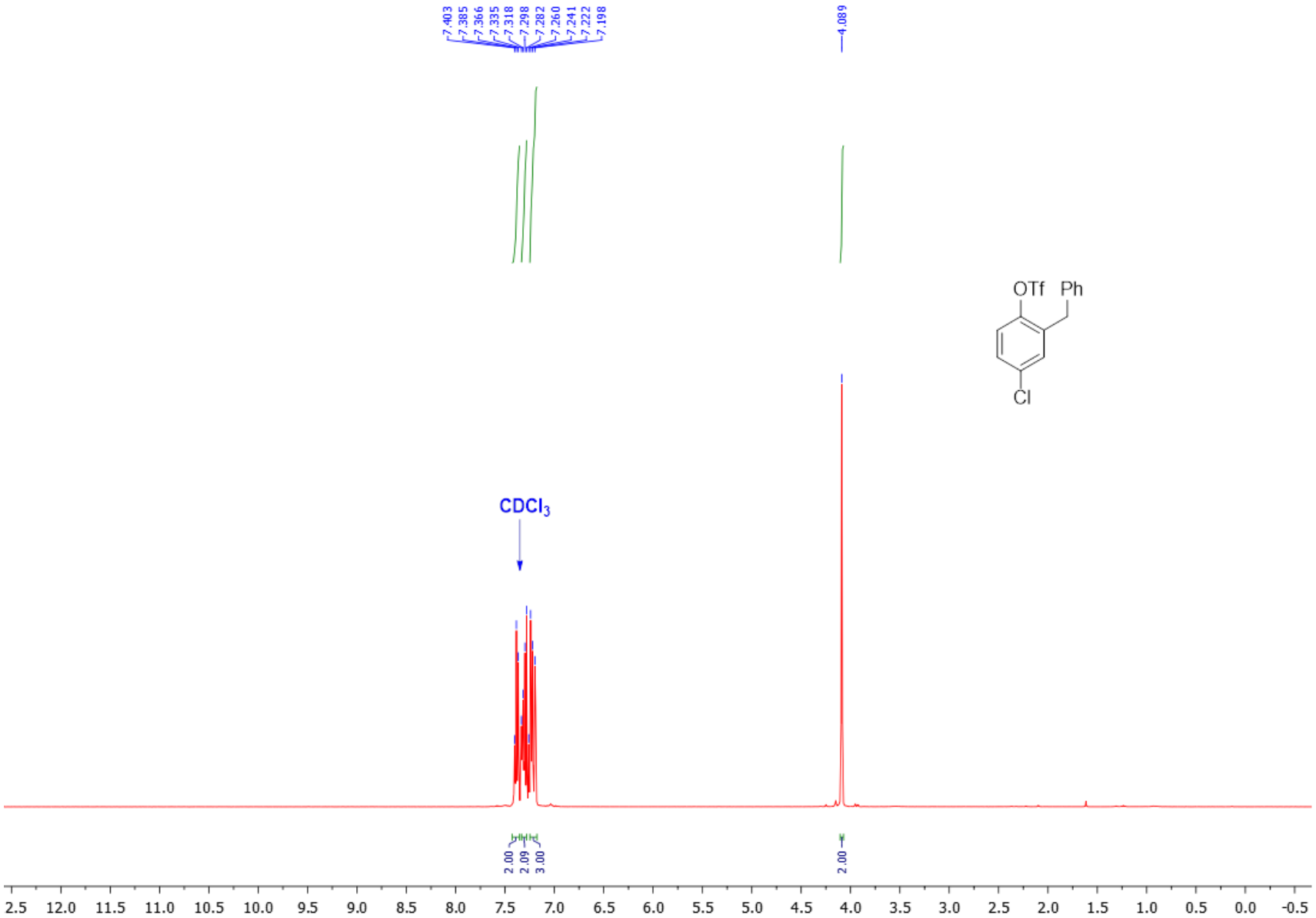
^{1}H-NMR of *(E)-8-(cyclododec-1-en-1-yl)tetrazolo[1,5-a]pyridine (5d)* (25 ^{o}C, 400 MHz, $CDCl_3$):



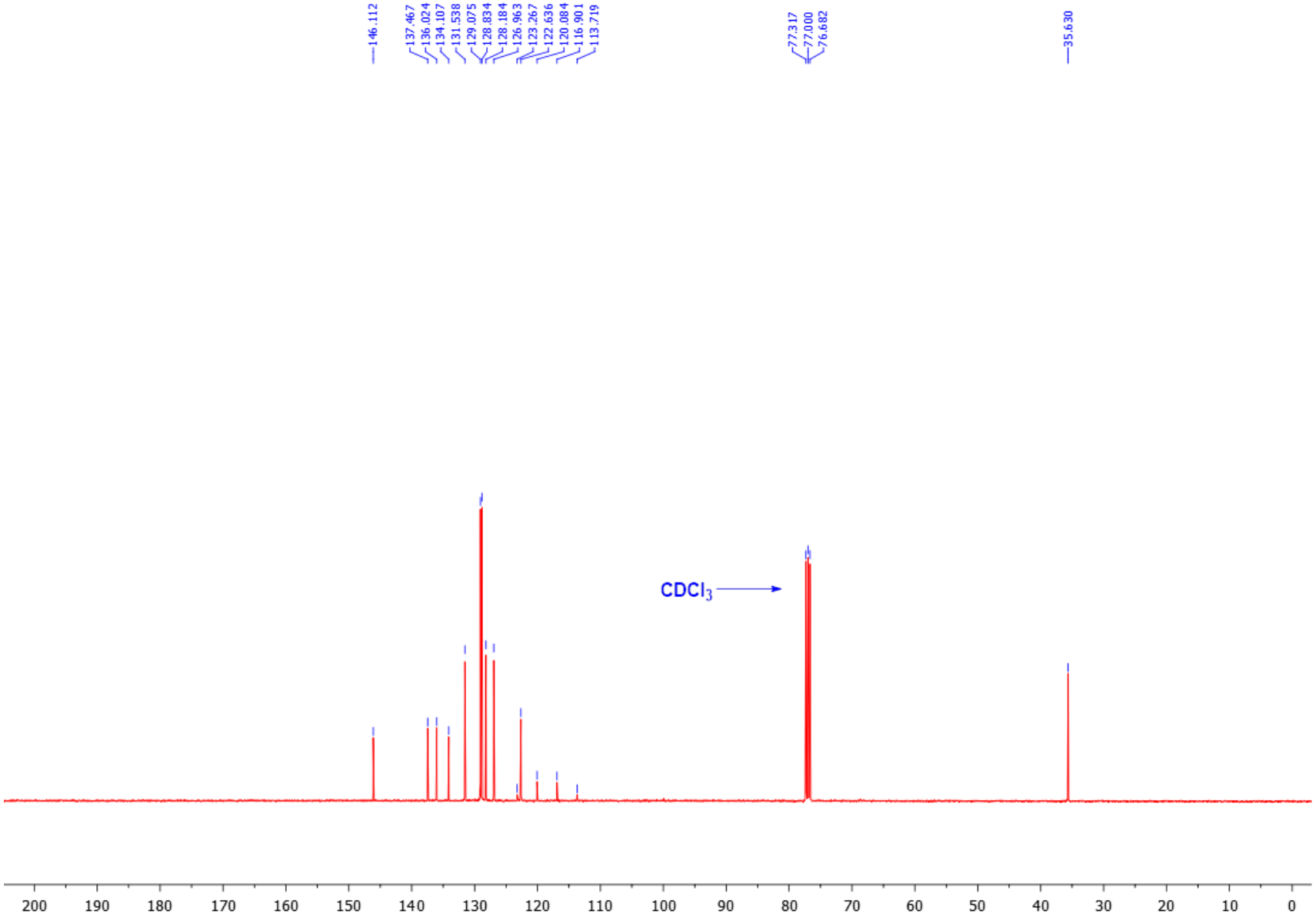
^{13}C-NMR of *(E)-8-(cyclododec-1-en-1-yl)tetrazolo[1,5-a]pyridine (5d)* (25 °C, 100 MHz, $CDCl_3$):



^{1}H-NMR of *2-benzyl-4-chlorophenyl trifluoromethanesulfonate* (25 ^{o}C, 400 MHz, $CDCl_3$):

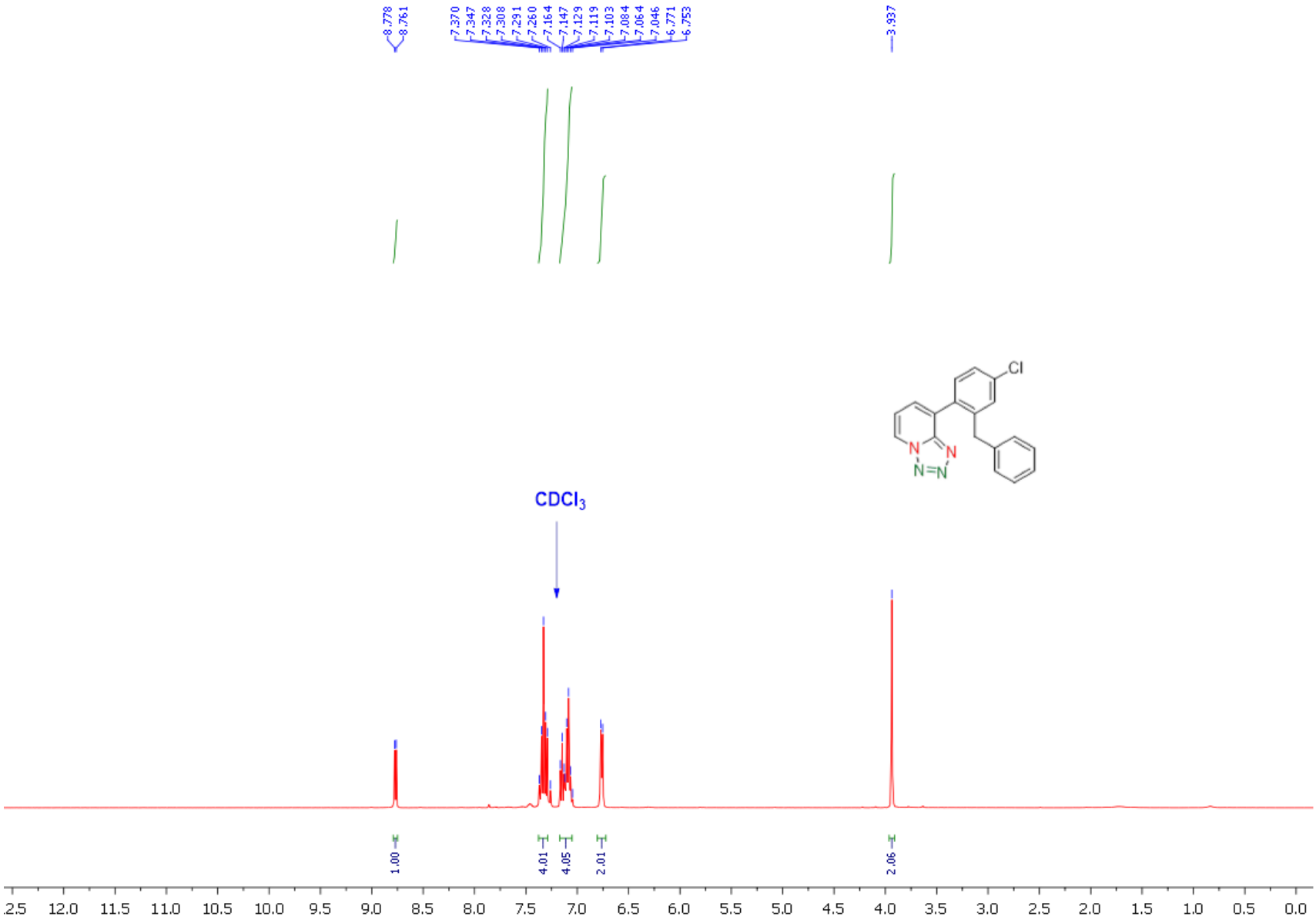


^{13}C-NMR *2-benzyl-4-chlorophenyl trifluoromethanesulfonate* (25 ºC, 100 MHz, $CDCl_3$):

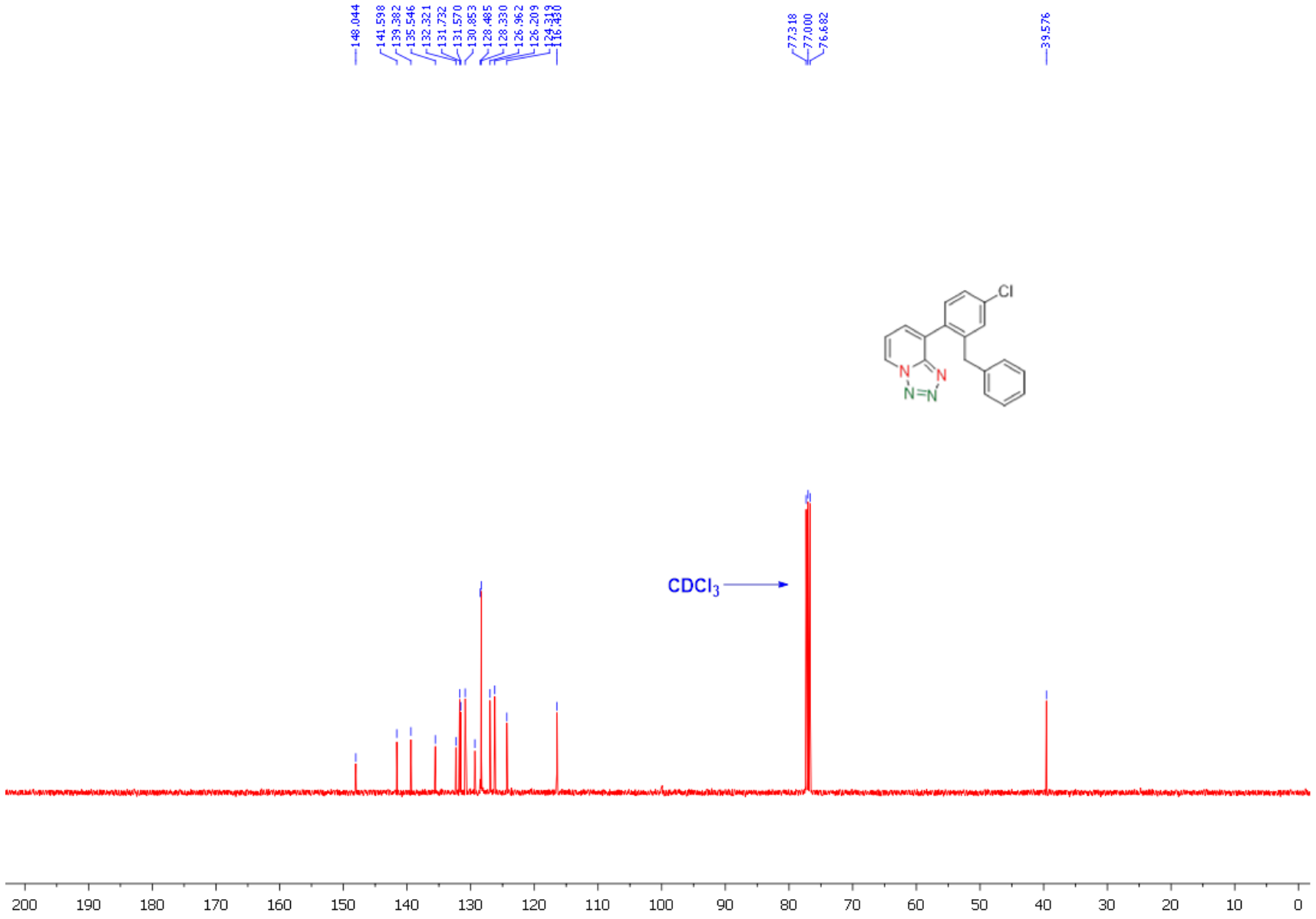


^{19}F-NMR of *2-benzyl-4-chlorophenyl trifluoromethanesulfonate* (25 ºC, 376 MHz, $CDCl_3$):

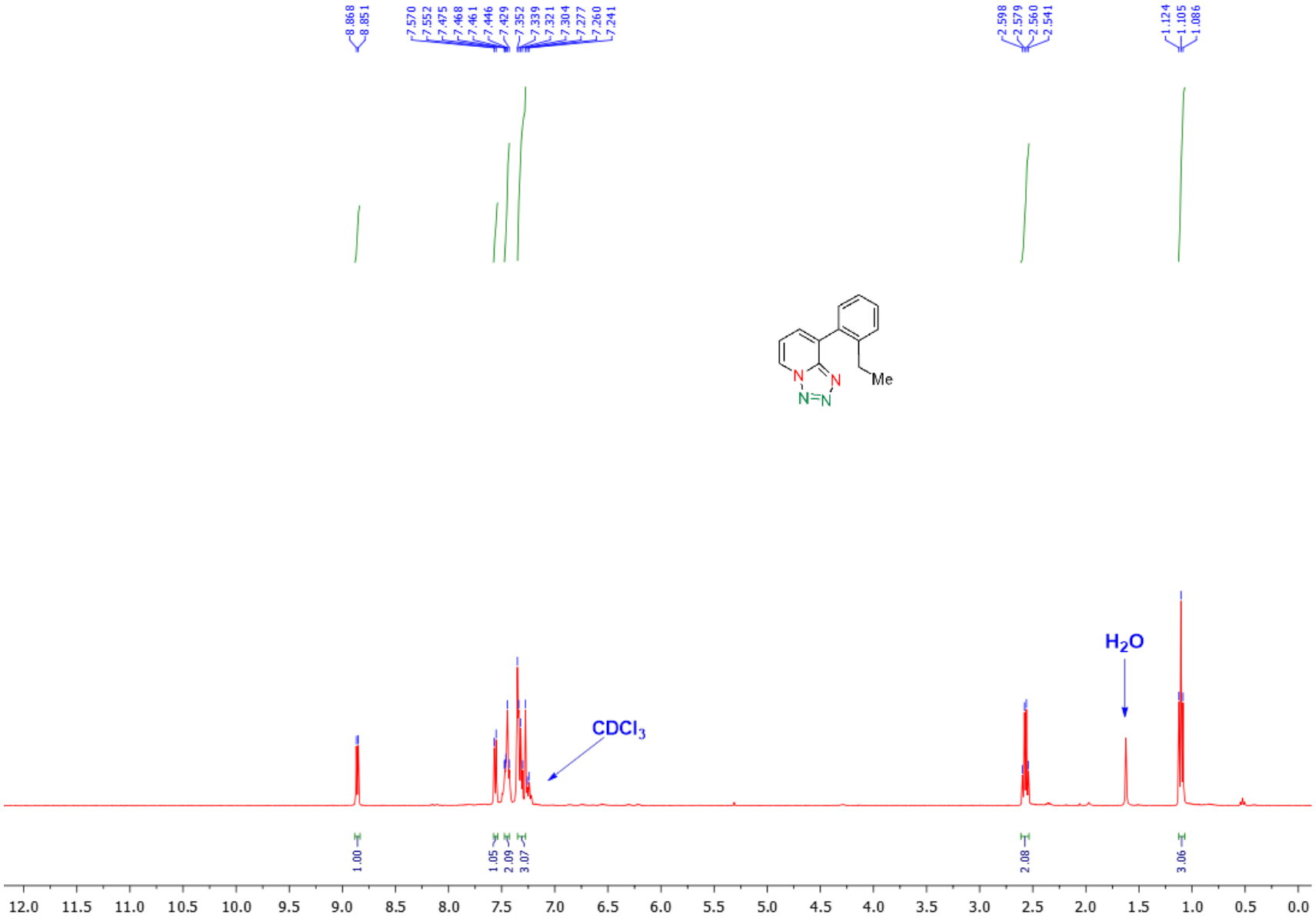
^{1}H-NMR of *8-(2-benzyl-4-chlorophenyl)tetrazolo[1,5-a]pyridine (7a)* (25 ^{o}C, 400 MHz, $CDCl_3$):



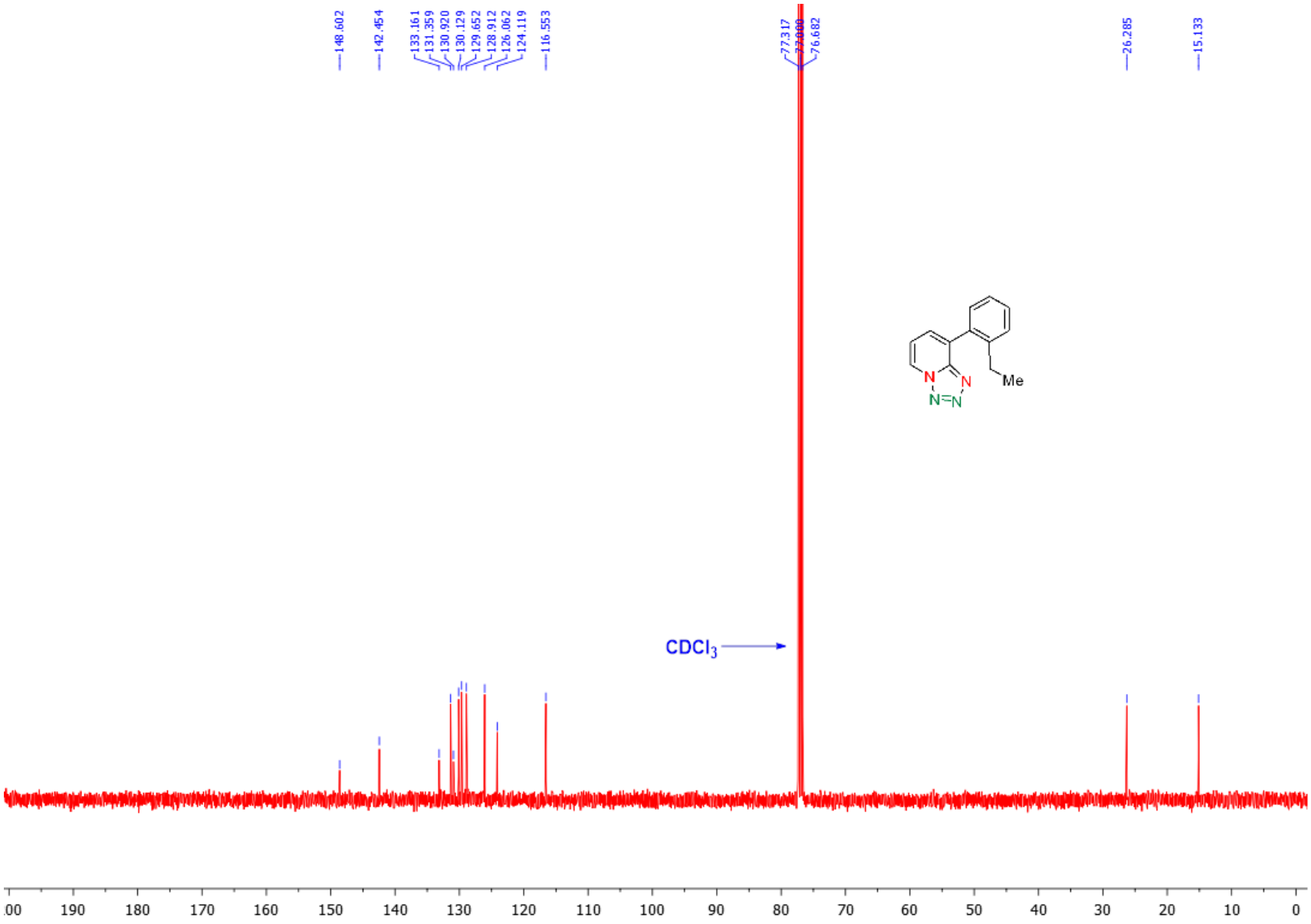
^{13}C-NMR of *8-(2-benzyl-4-chlorophenyl)tetrazolo[1,5-a]pyridine (7a)* (25 ºC, 100 MHz, $CDCl_3$):



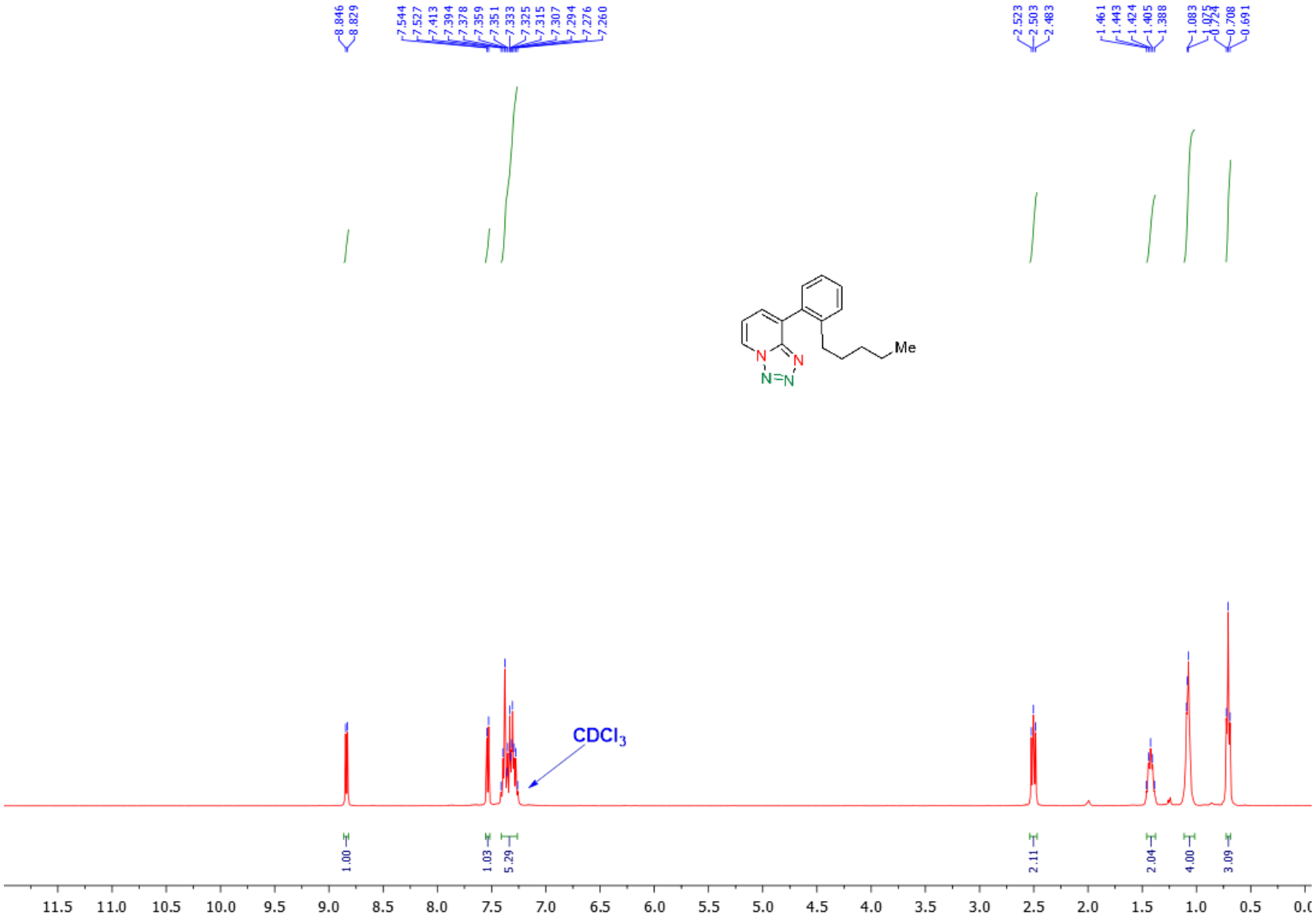
^{1}H-NMR of *8-(2-ethylphenyl)tetrazolo[1,5-a]pyridine (7b)* (25 °C, 400 MHz, $CDCl_3$):



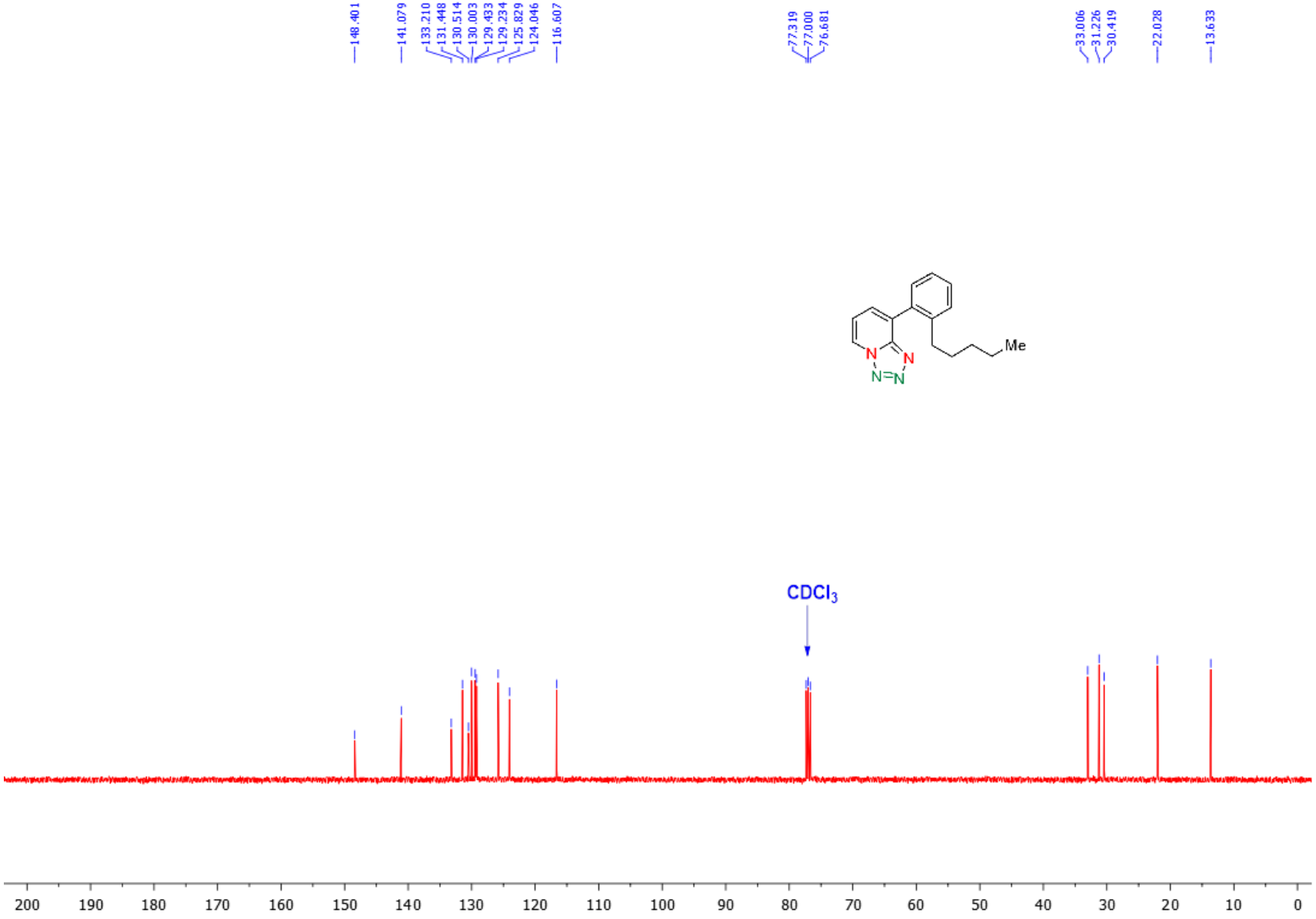
^{13}C-NMR of *8-(2-ethylphenyl)tetrazolo[1,5-a]pyridine (7b)* (25 °C, 100 MHz, $CDCl_3$):



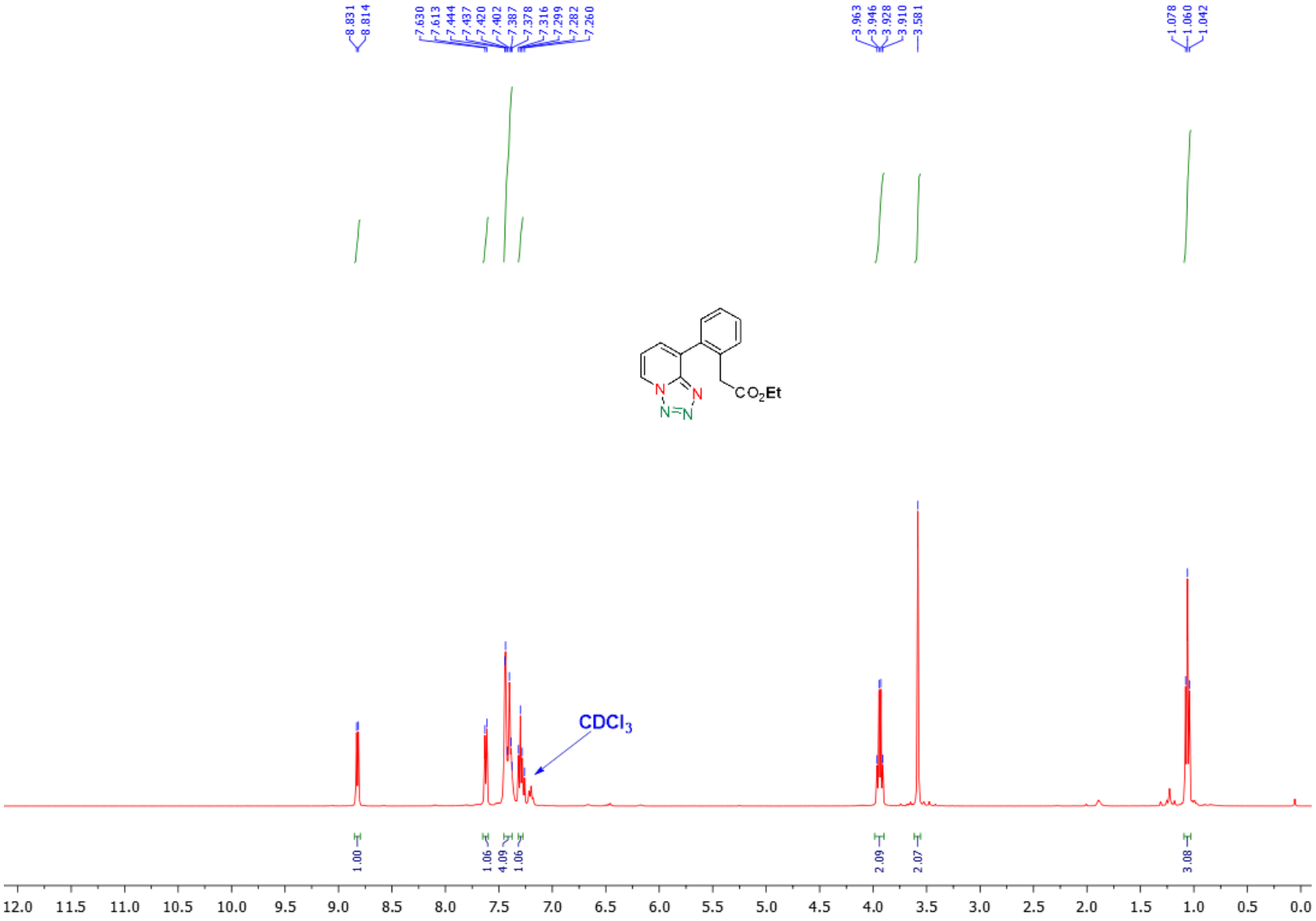
^{1}H-NMR of *8-(2-pentylphenyl)tetrazolo[1,5-a]pyridine (7c)* (25 ºC, 400 MHz, $CDCl_3$):



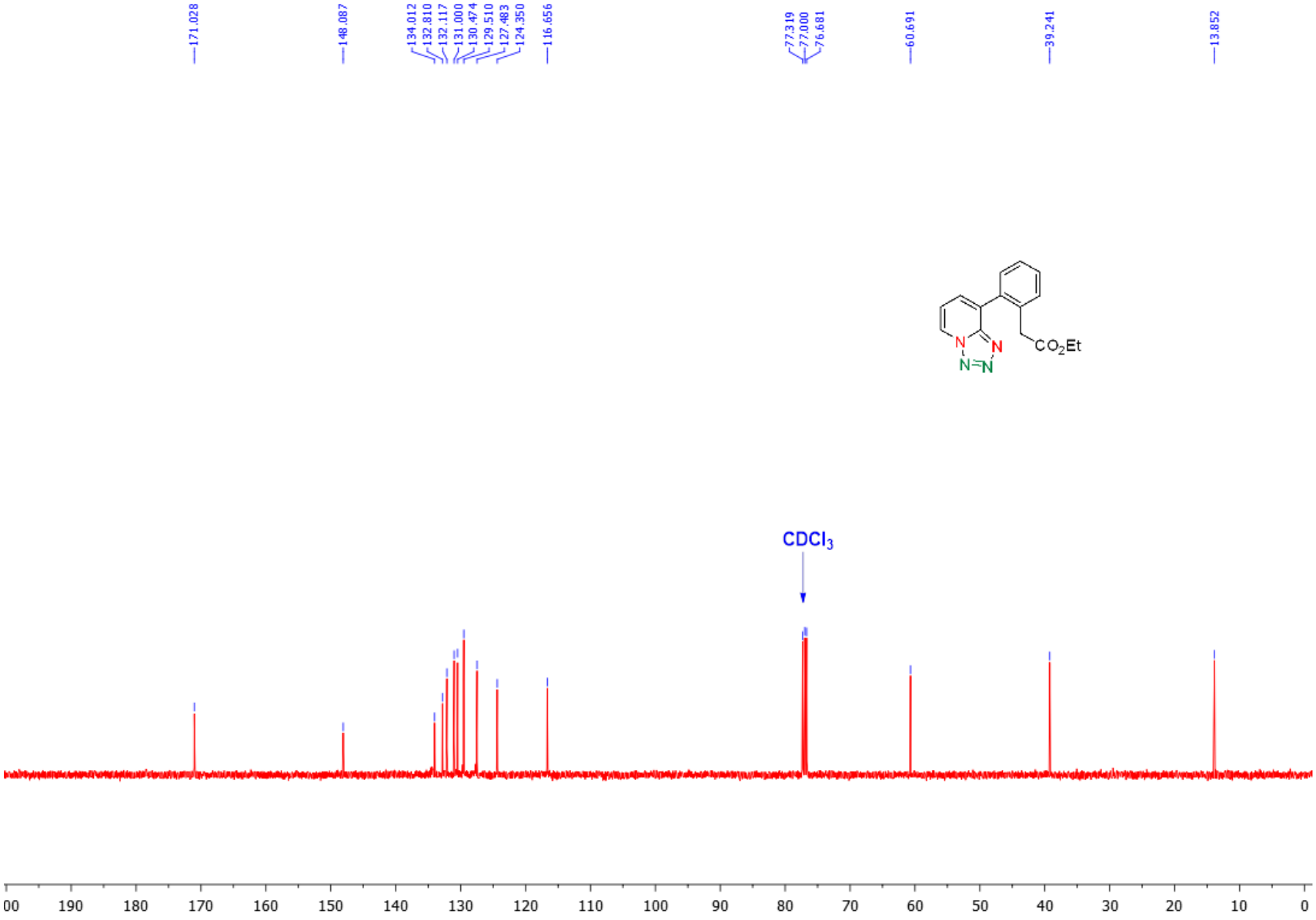
^{13}C-NMR of *8-(2-pentylphenyl)tetrazolo[1,5-a]pyridine (7c* (25 ºC, 100 MHz, $CDCl_3$):



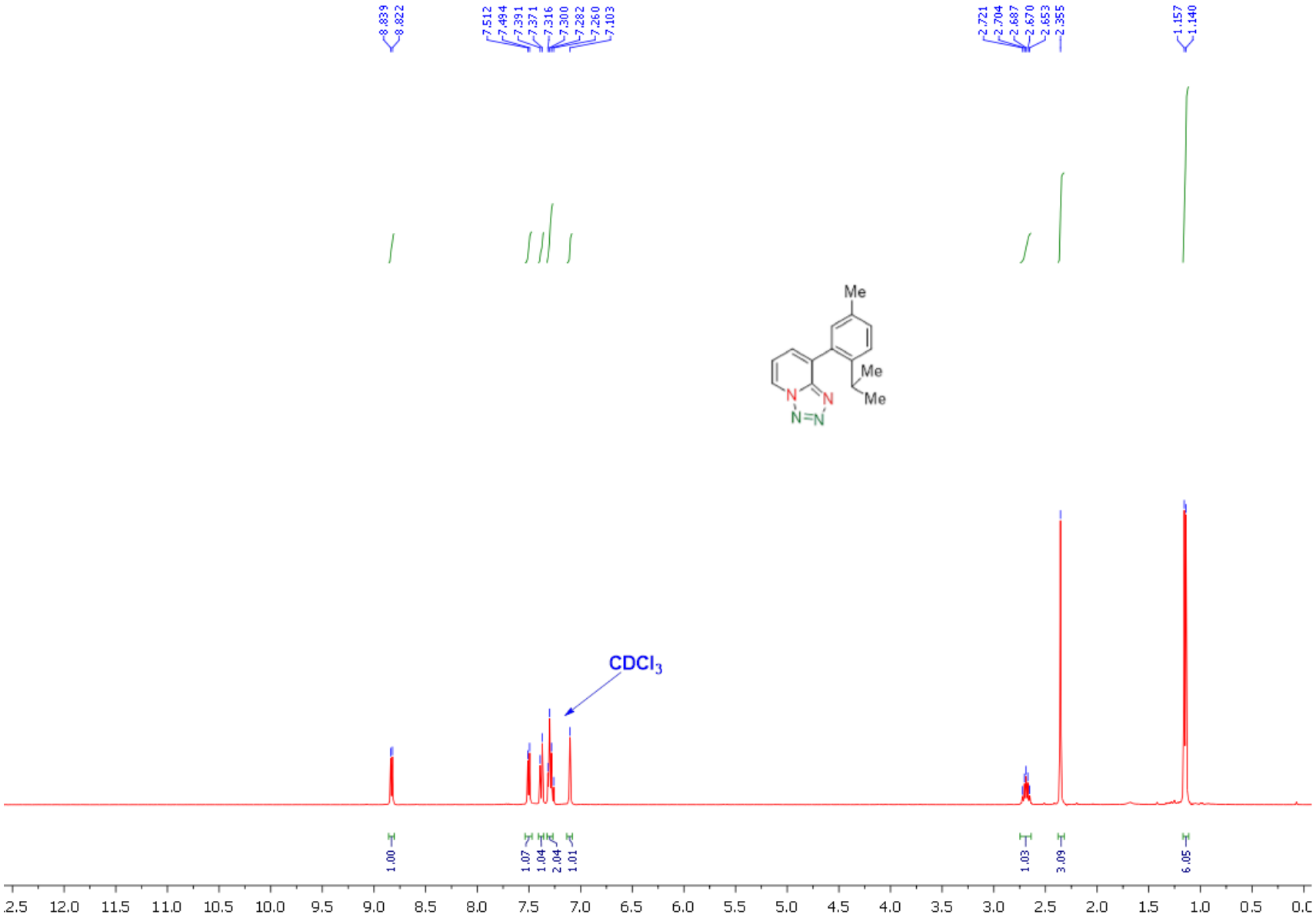
^{1}H-NMR of *ethyl 2-(2-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetate (7d)* (25 ^{o}C, 400 MHz, $CDCl_3$):



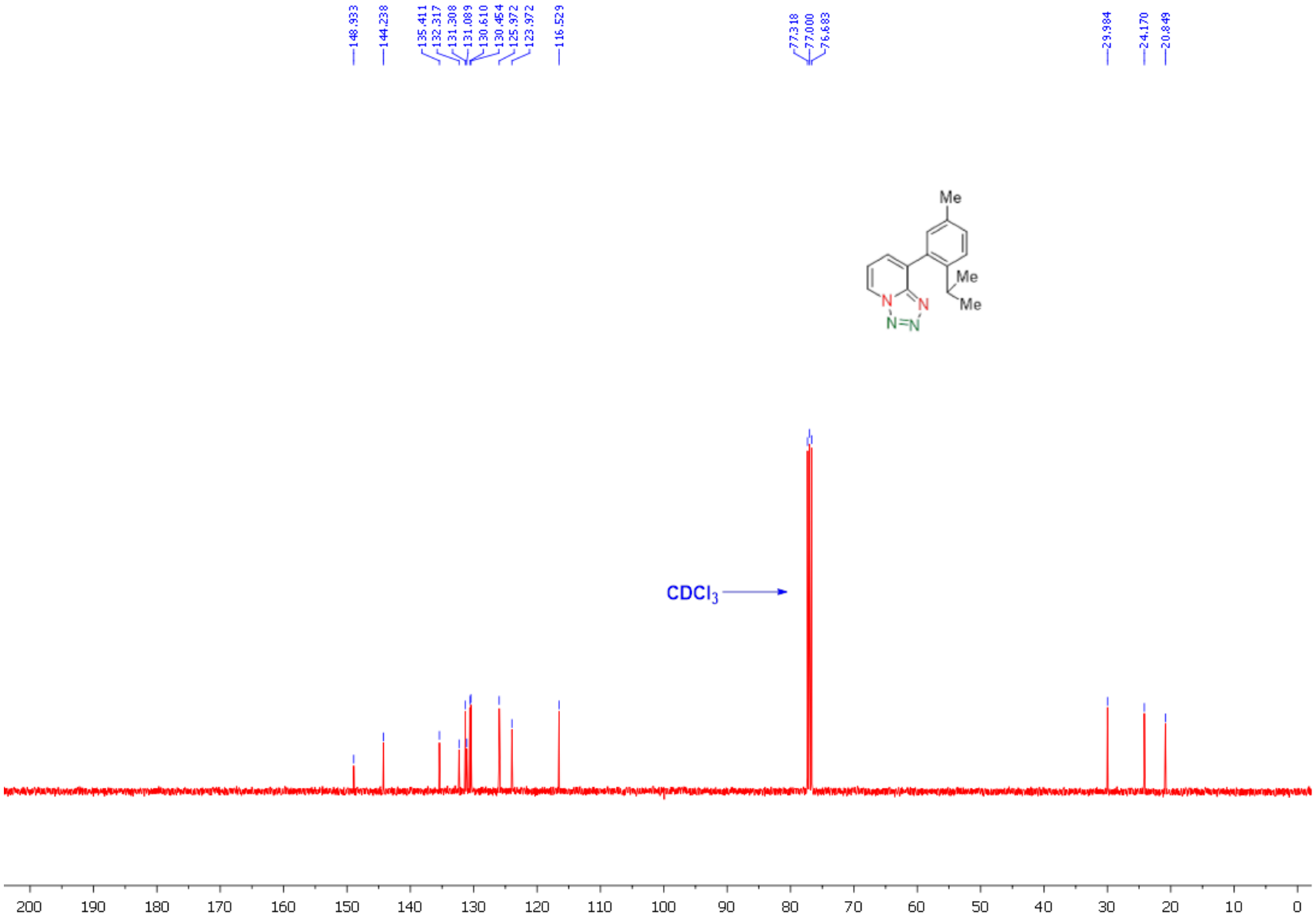
^{13}C-NMR of *ethyl 2-(2-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetate (7d)* (25 °C, 100 MHz, $CDCl_3$):



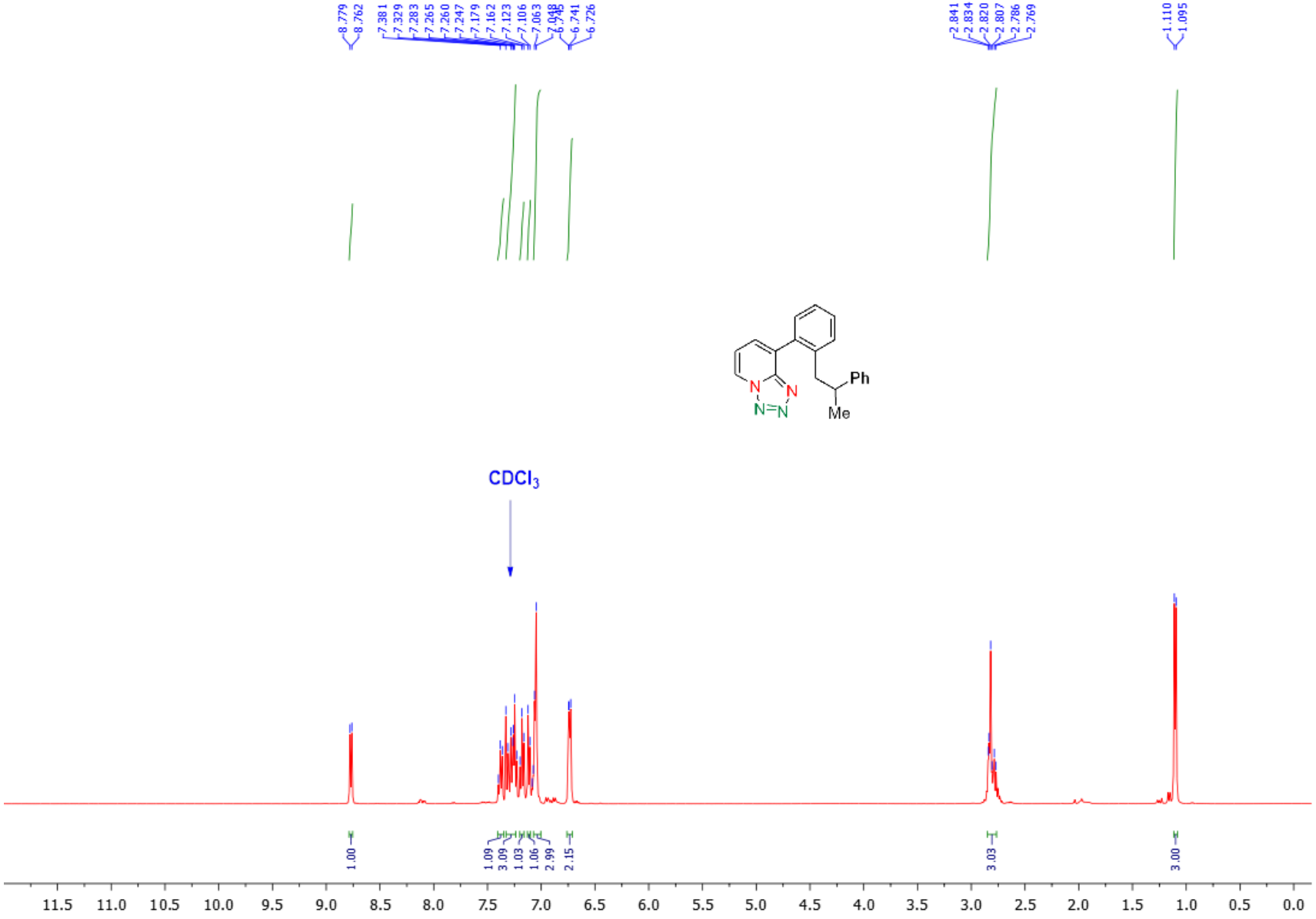
^{1}H-NMR of *8-(2-isopropyl-5-methylphenyl)tetrazolo[1,5-a]pyridine (7e)* (25 ^{o}C, 400 MHz, $CDCl_3$):



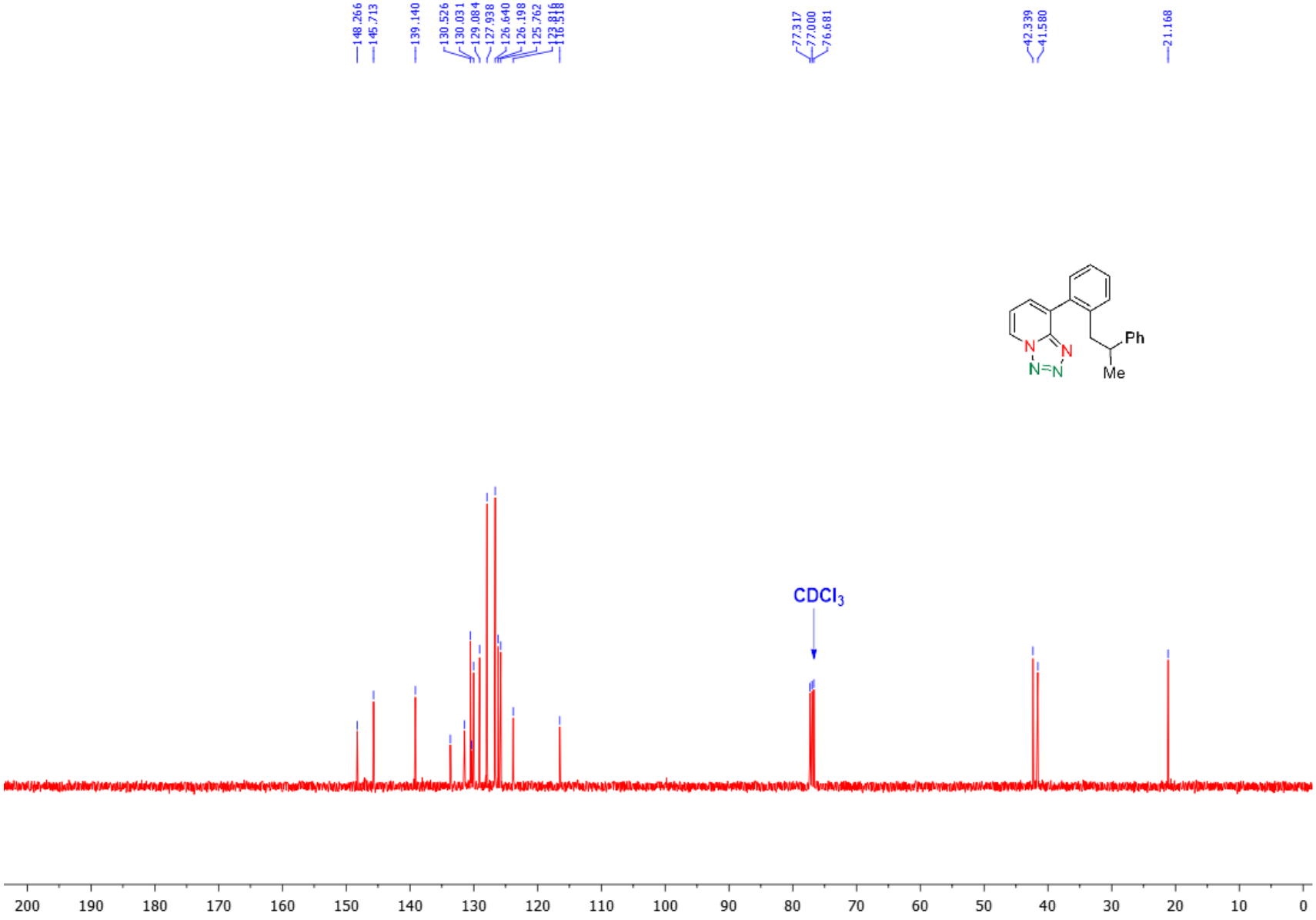
^{13}C-NMR of *8-(2-isopropyl-5-methylphenyl)tetrazolo[1,5-a]pyridine (7e)* (25 °C, 100 MHz, $CDCl_3$):



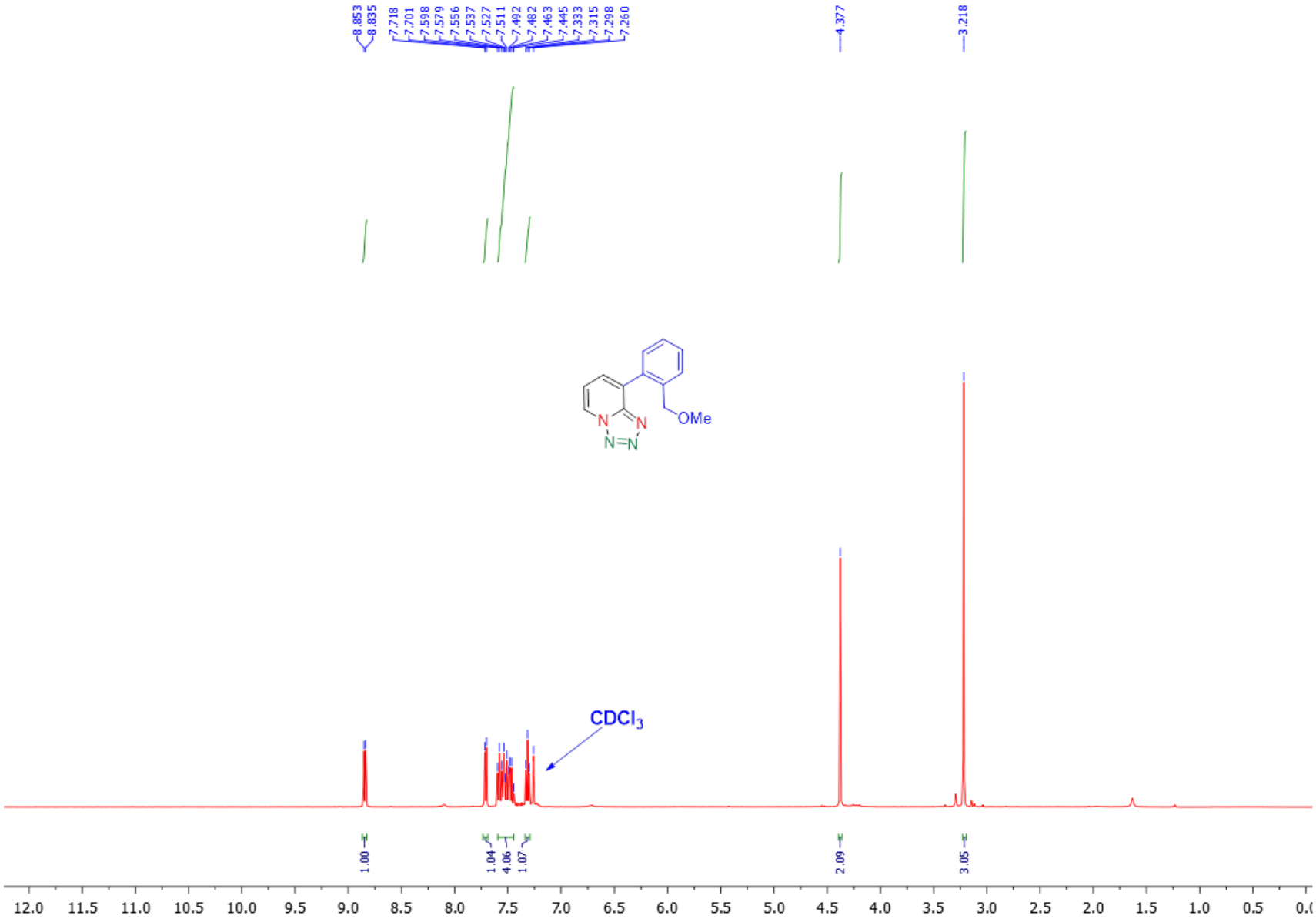
^{1}H-NMR of *8-(2-(2-phenylpropyl)phenyl)tetrazolo[1,5-a]pyridine (7f)* (25 °C, 400 MHz, $CDCl_3$):



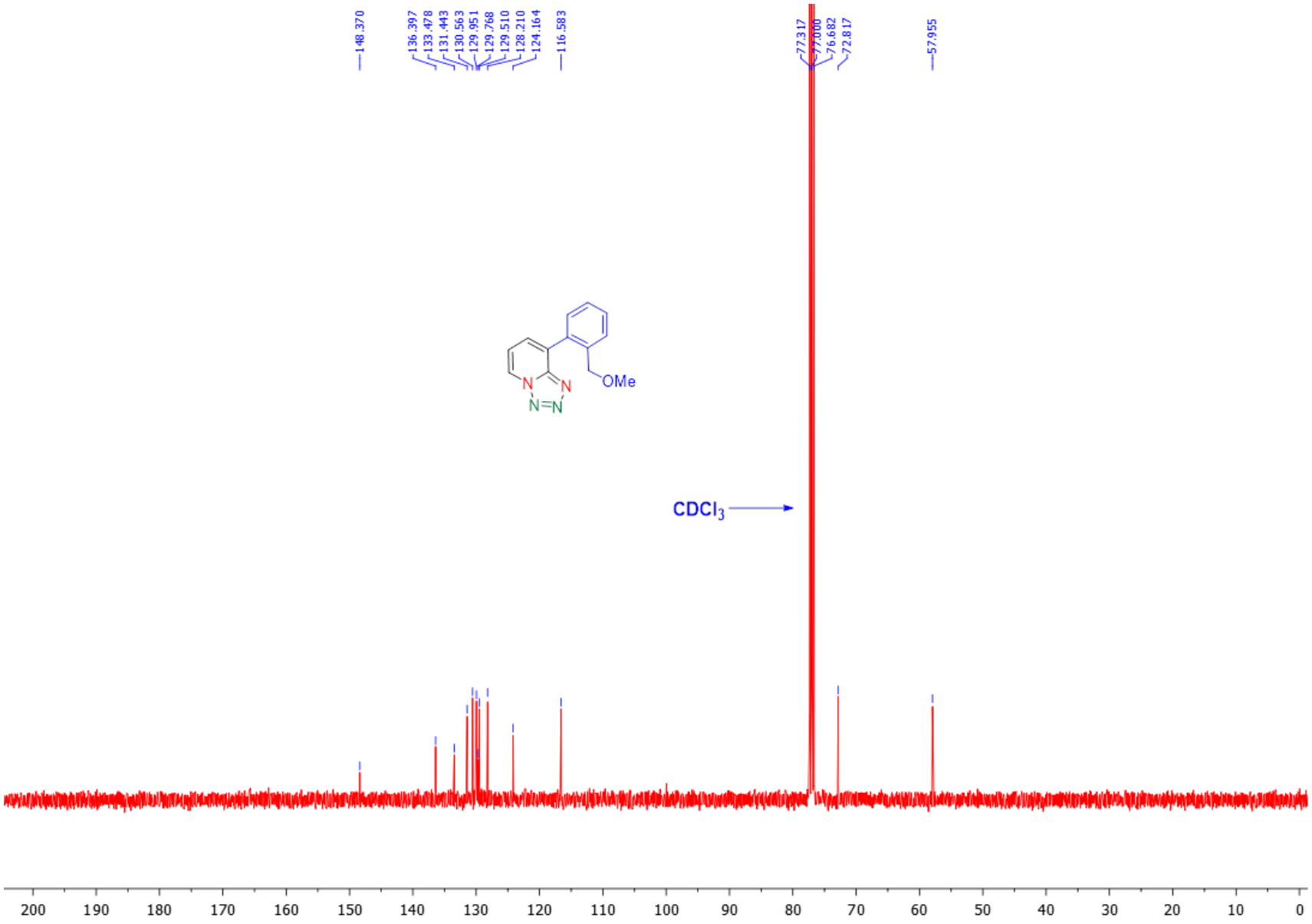
^{13}C-NMR of *8-(2-(2-phenylpropyl)phenyl)tetrazolo[1,5-a]pyridine (7f)* (25 °C, 100 MHz, $CDCl_3$):



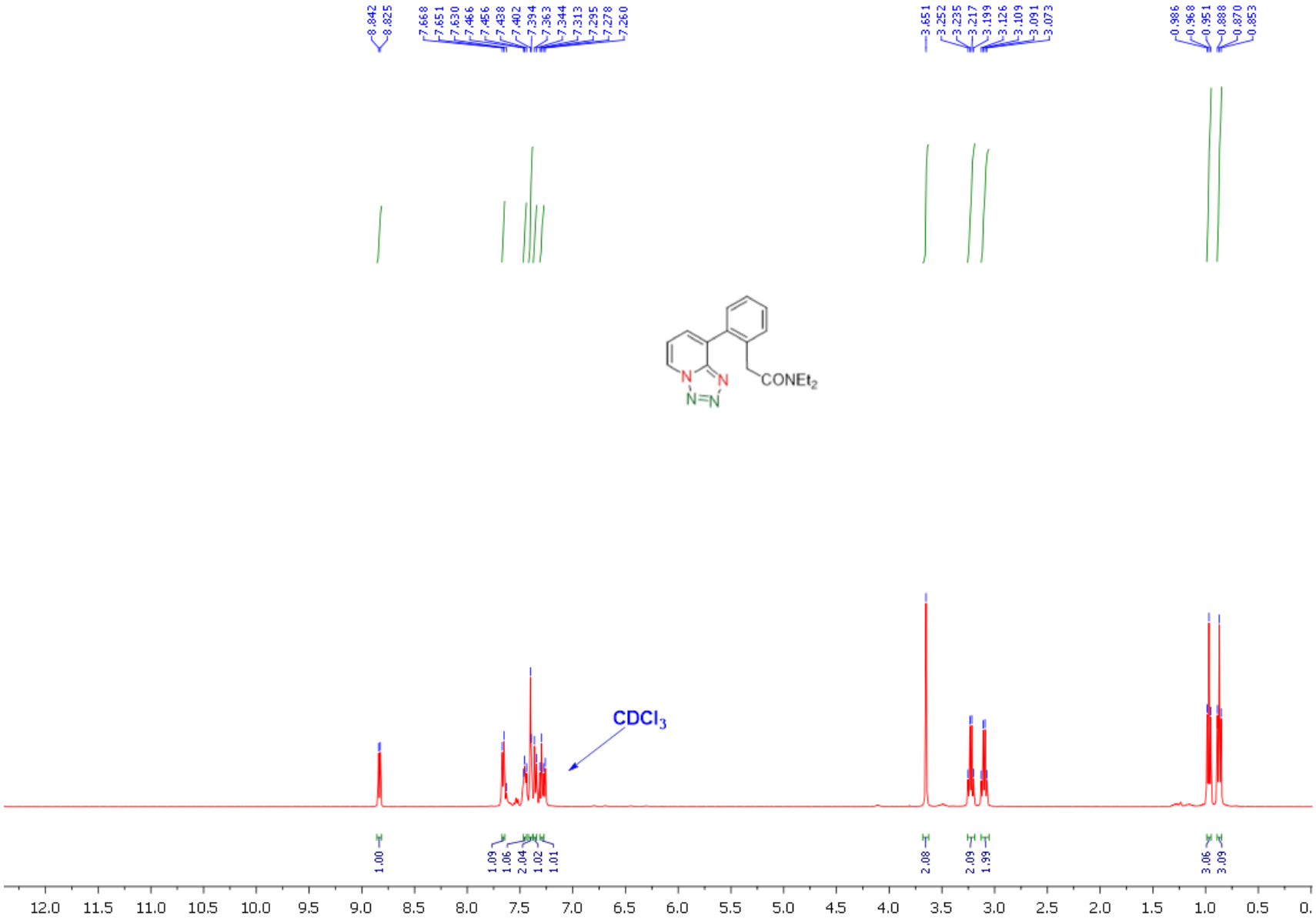
^{1}H-NMR of *8-(2-(methoxymethyl)phenyl)tetrazolo[1,5-a]pyridine (7g)* (25 °C, 400 MHz, $CDCl_3$):



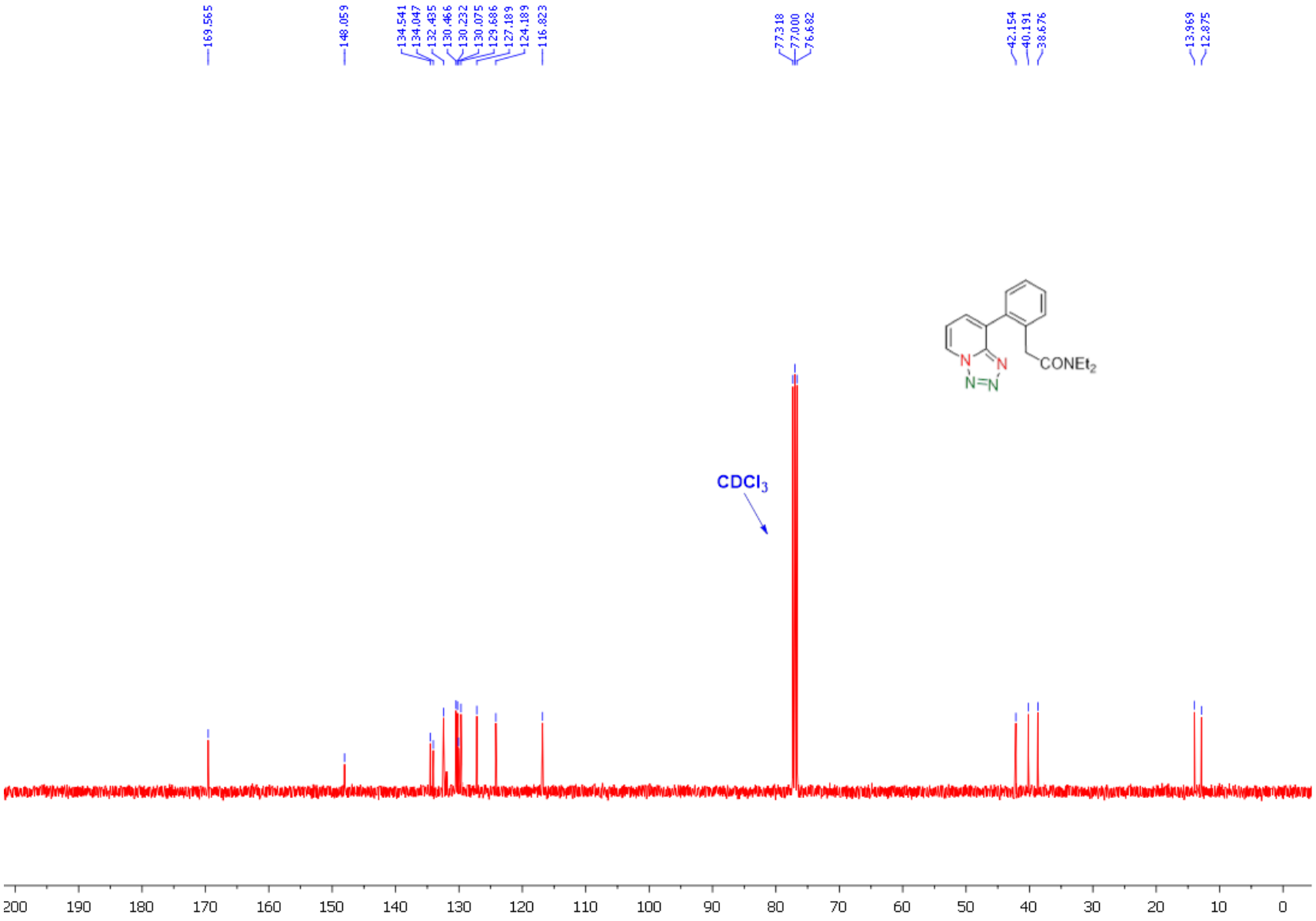
^{13}C-NMR of *8-(2-(methoxymethyl)phenyl)tetrazolo[1,5-a]pyridine (7g)* (25 ºC, 100 MHz, $CDCl_3$):



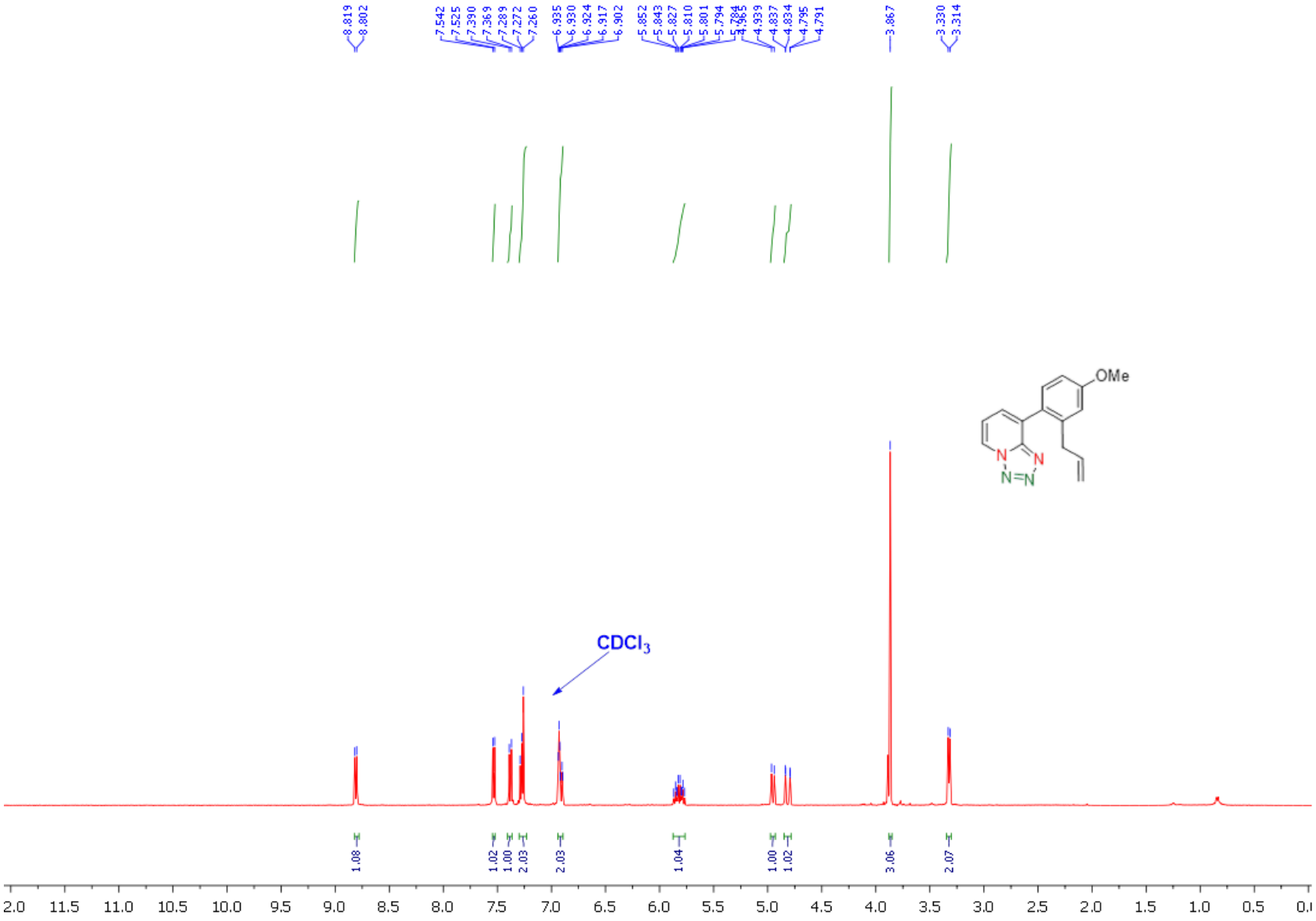
^{1}H-NMR of *N,N-diethyl-2-(2-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetamide (7h)* (25 ^{o}C, 400 MHz, $CDCl_3$):



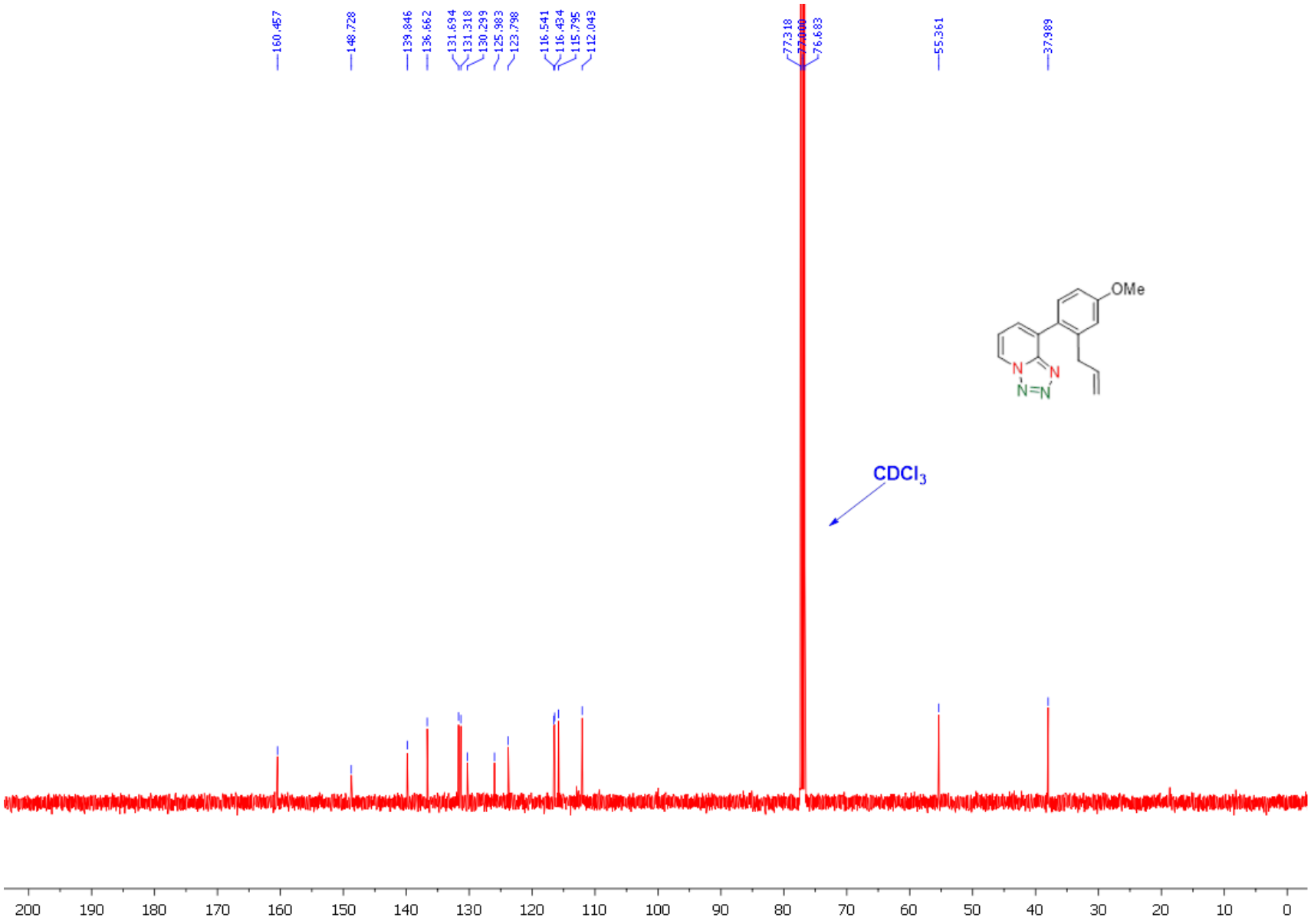
^{13}C-NMR of *N,N-diethyl-2-(2-(tetrazolo[1,5-a]pyridin-8-yl)phenyl)acetamide (7h)* (25 °C, 100 MHz, $CDCl_3$):



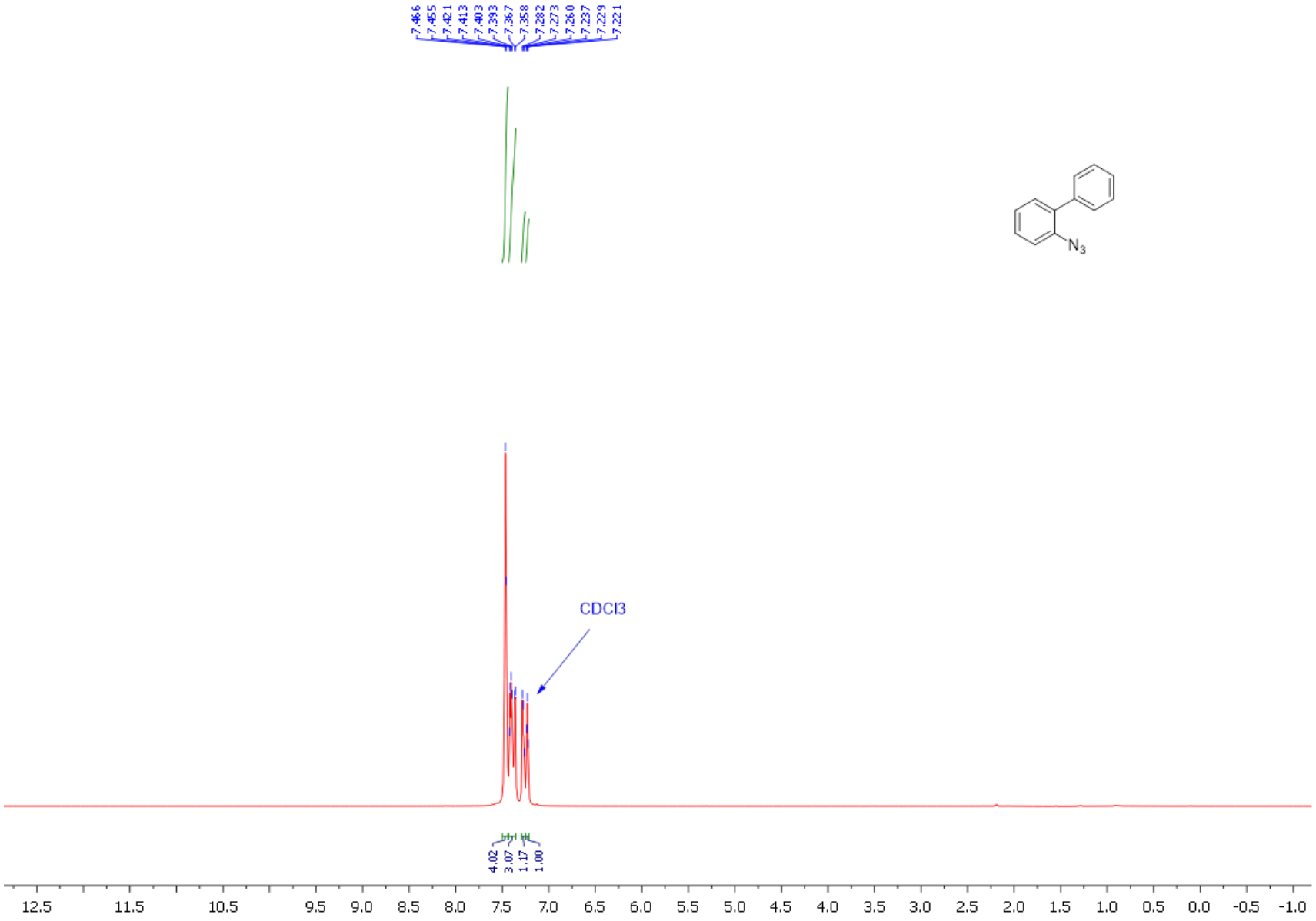
^{1}H-NMR of *8-(2-allyl-4-methoxyphenyl)tetrazolo[1,5-a]pyridine (7i)* (25 ^{o}C, 400 MHz, $CDCl_3$):



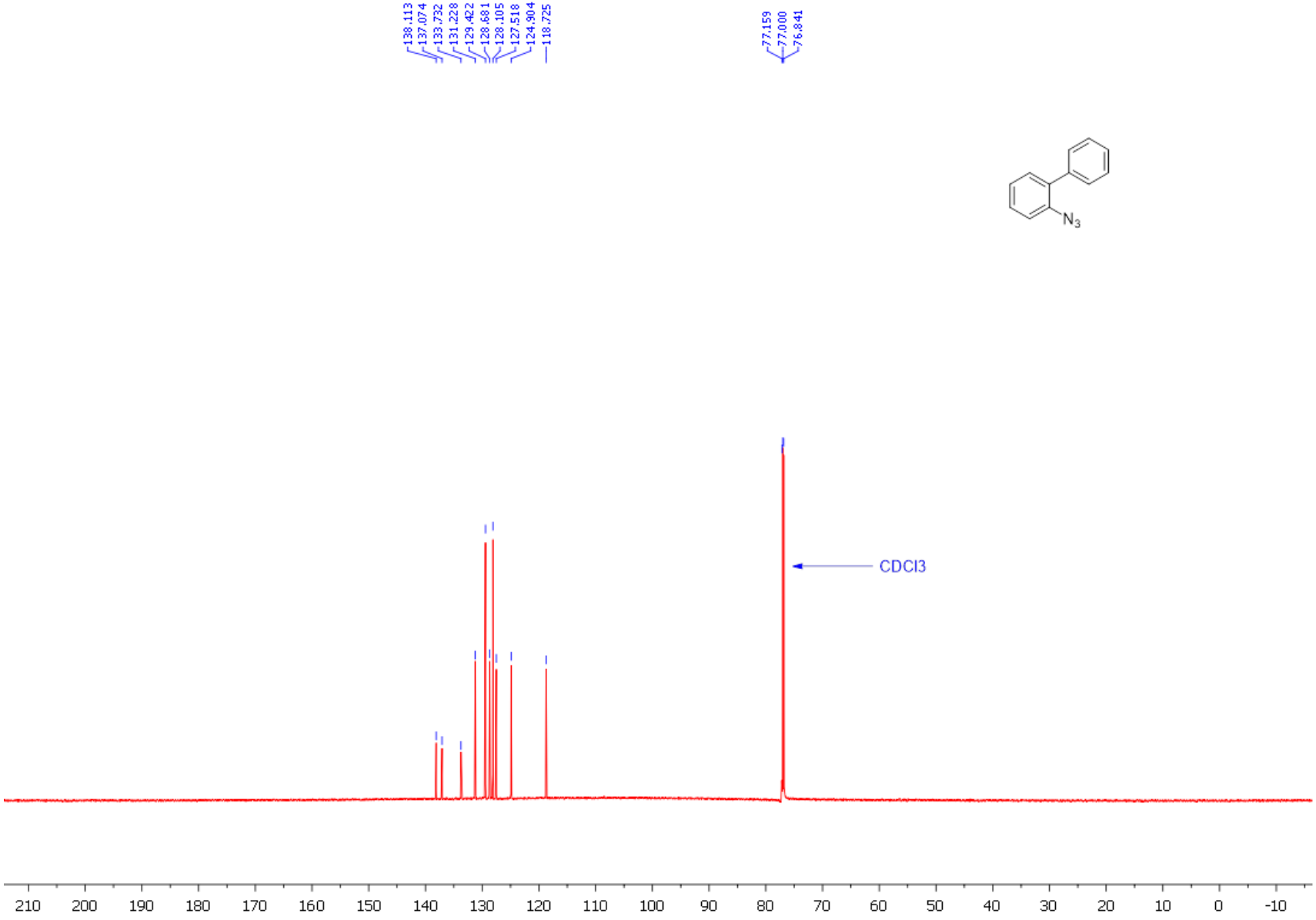
^{13}C-NMR of *8-(2-allyl-4-methoxyphenyl)tetrazolo[1,5-a]pyridine (7i)* (25 °C, 100 MHz, $CDCl_3$):



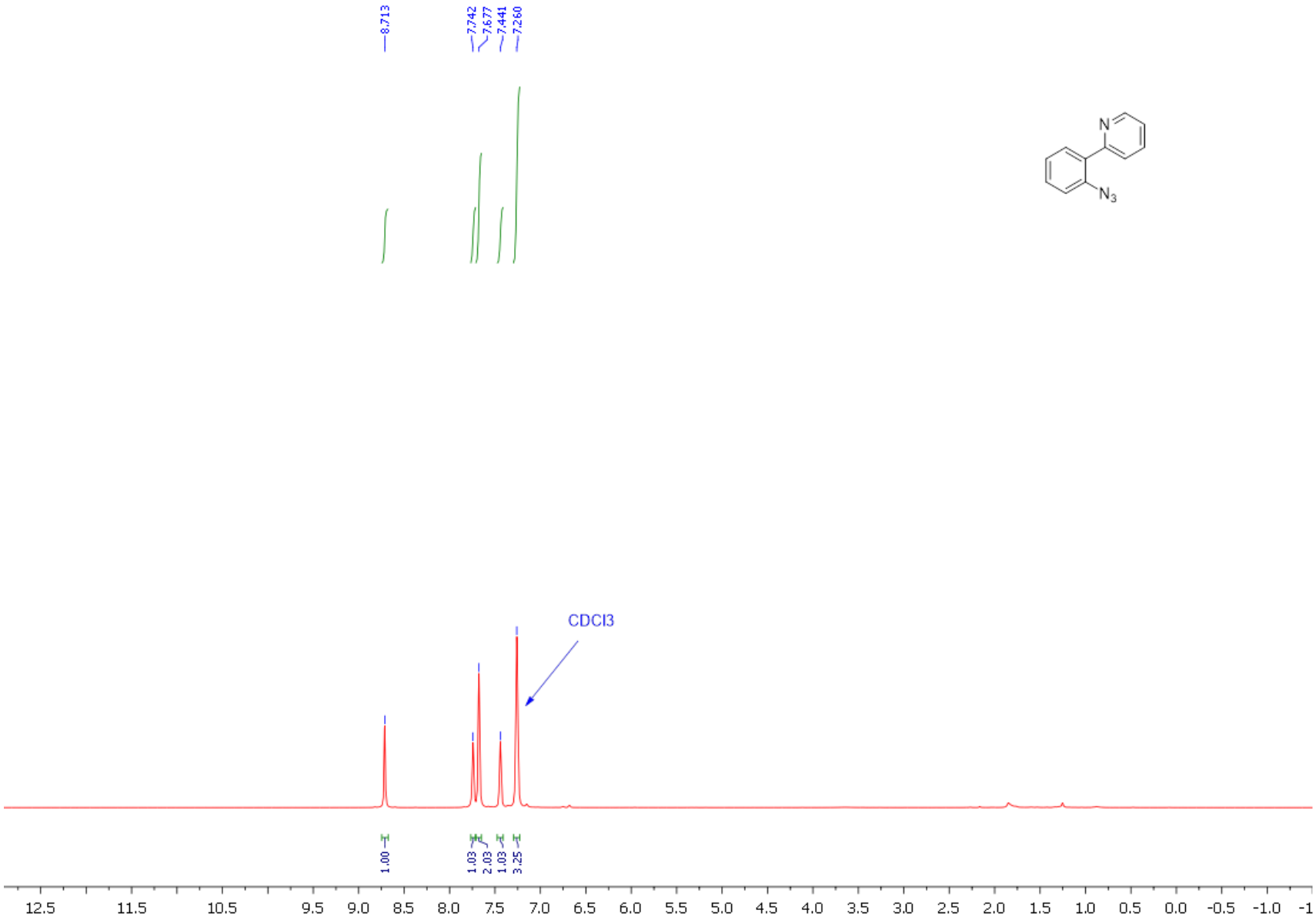
^{1}H-NMR of *2-azido-1,1'-biphenyl (9a)* (25 ^{o}C, 800 MHz, $CDCl_3$):



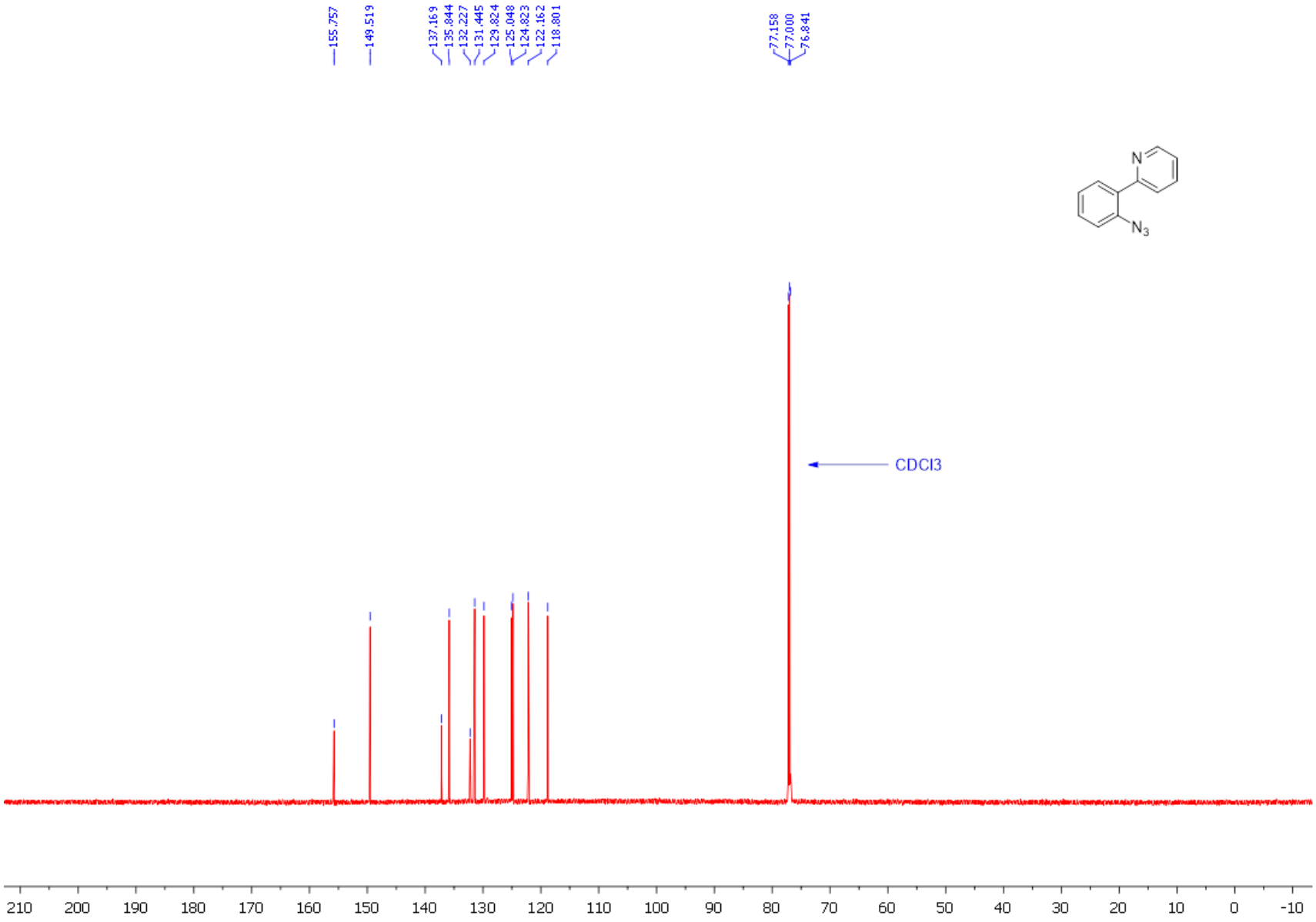
^{13}C-NMR of *2-azido-1,1'-biphenyl (9a)* (25 °C, 200 MHz, $CDCl_3$):



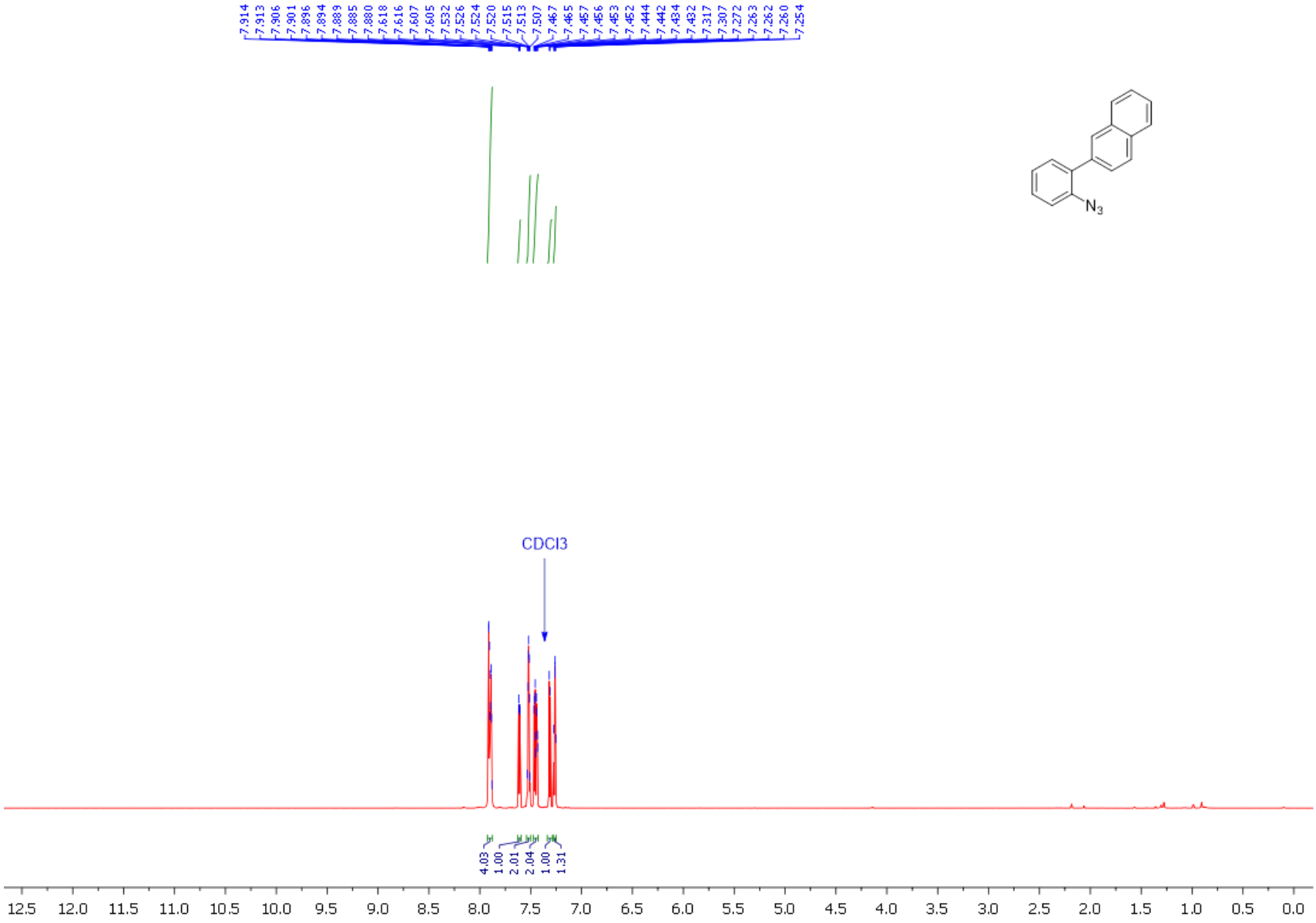
^{1}H-NMR of *2-(2-azidophenyl)pyridine (9c)* (25 ^{o}C, 800 MHz, $CDCl_3$):



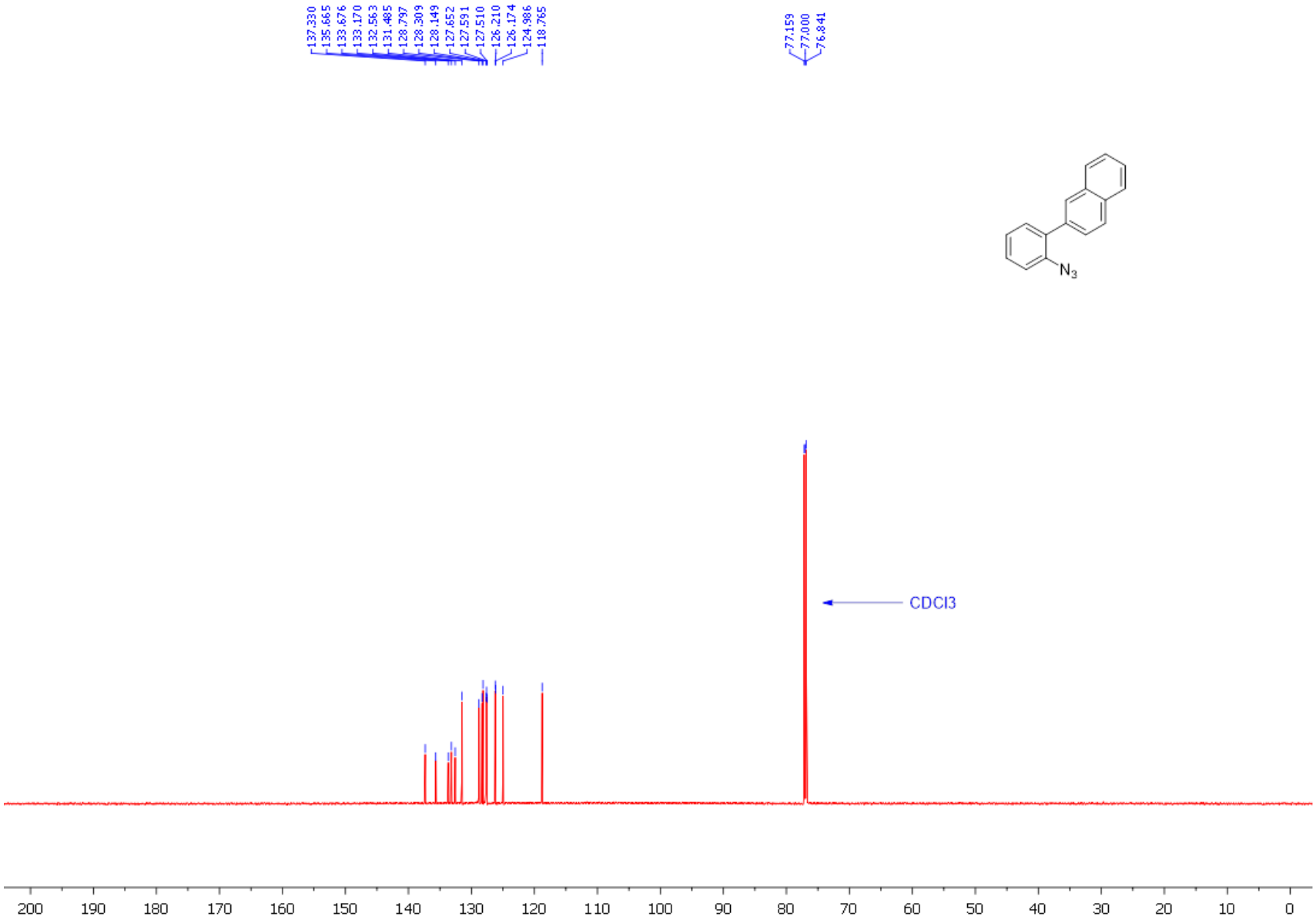
^{13}C-NMR of *2-(2-azidophenyl)pyridine (9c)* (25 °C, 200 MHz, $CDCl_3$):



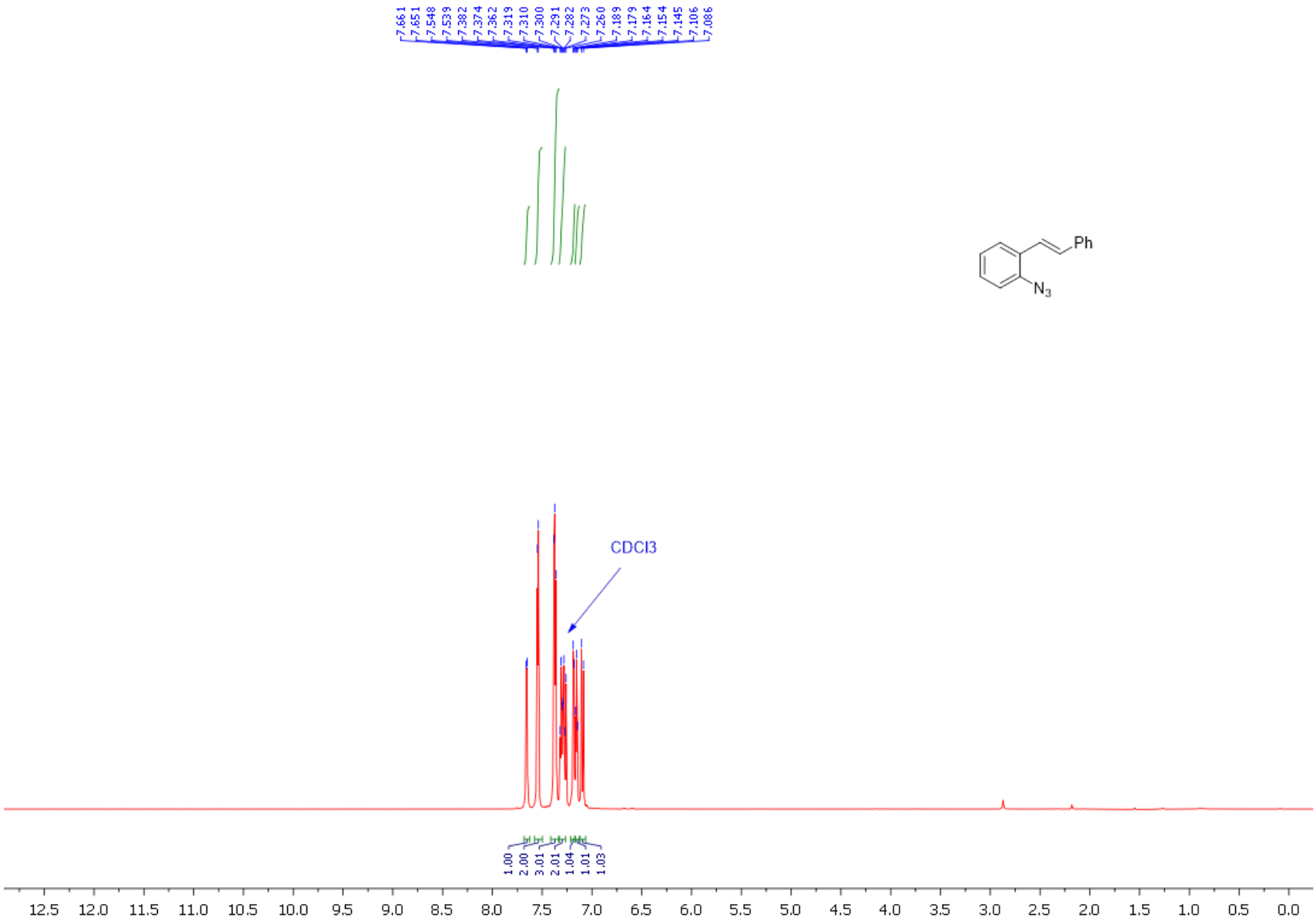
^{1}H-NMR of *2-(2-azidophenyl)naphthalene (9b)* (25 ºC, 800 MHz, $CDCl_3$):



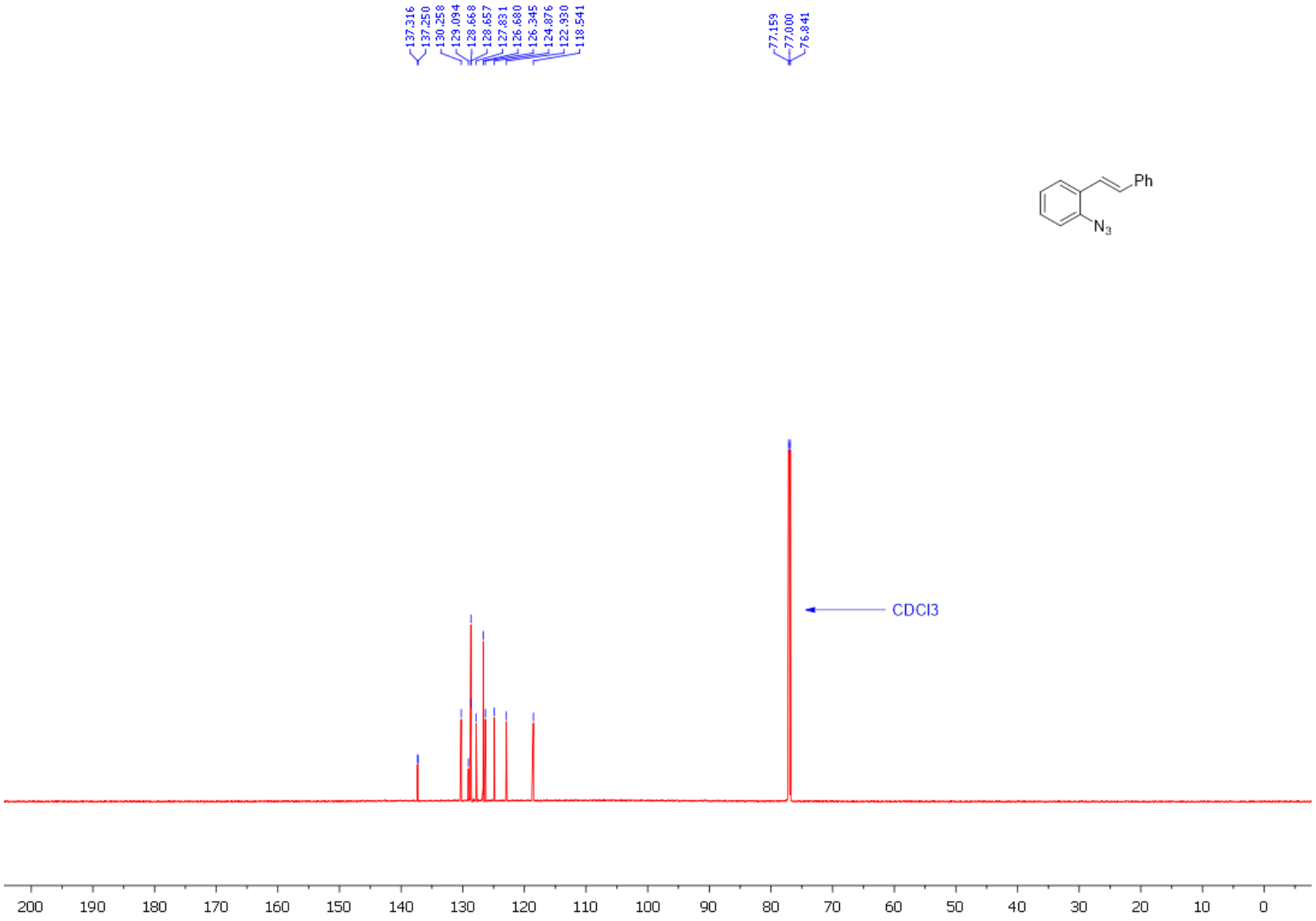
^{13}C-NMR of *2-(2-azidophenyl)naphthalene (9b)* (25 °C, 200 MHz, $CDCl_3$):



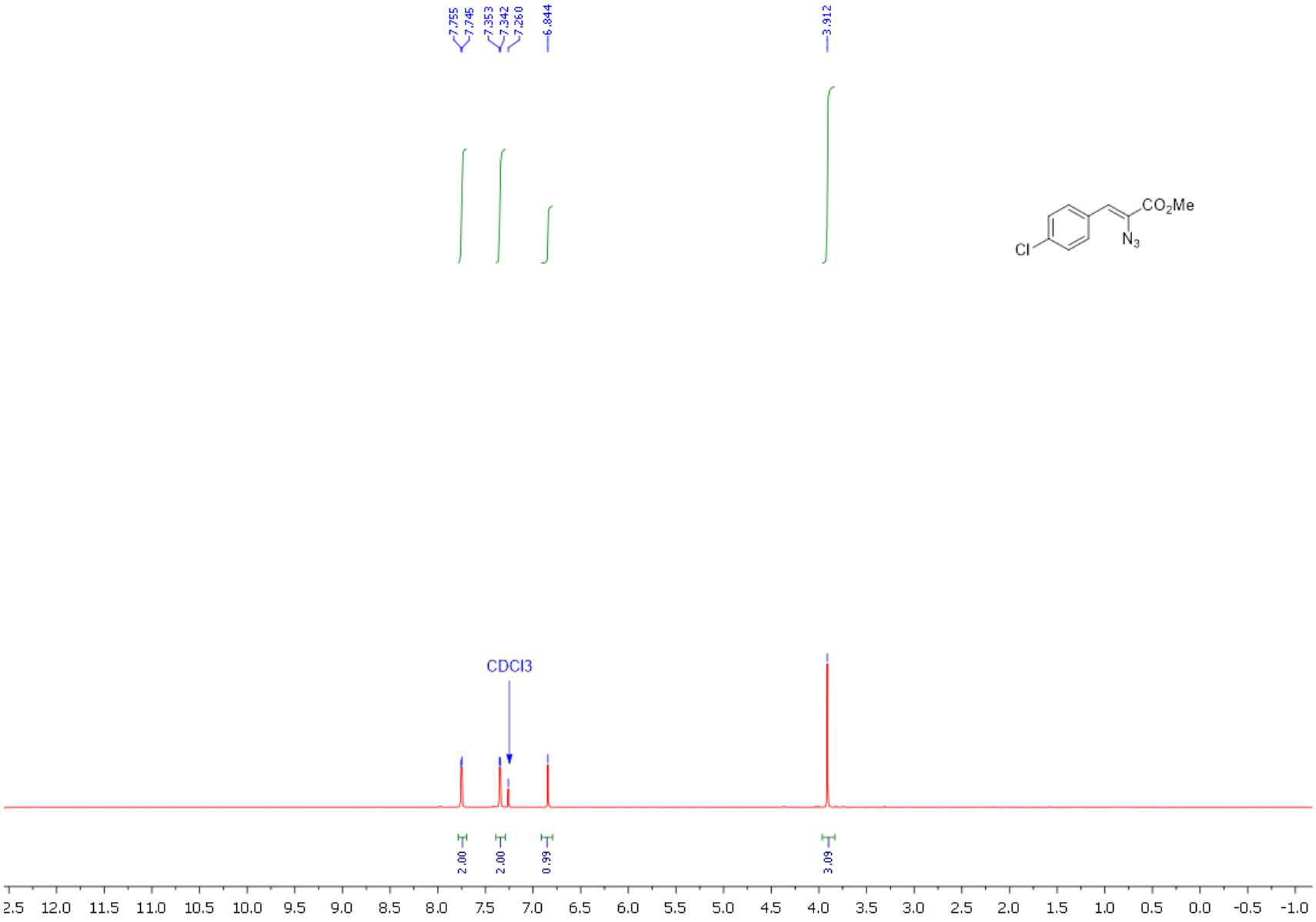
^{1}H-NMR of *(E)-1-azido-2-styrylbenzene (9d)* (25 ^{o}C, 800 MHz, $CDCl_3$):



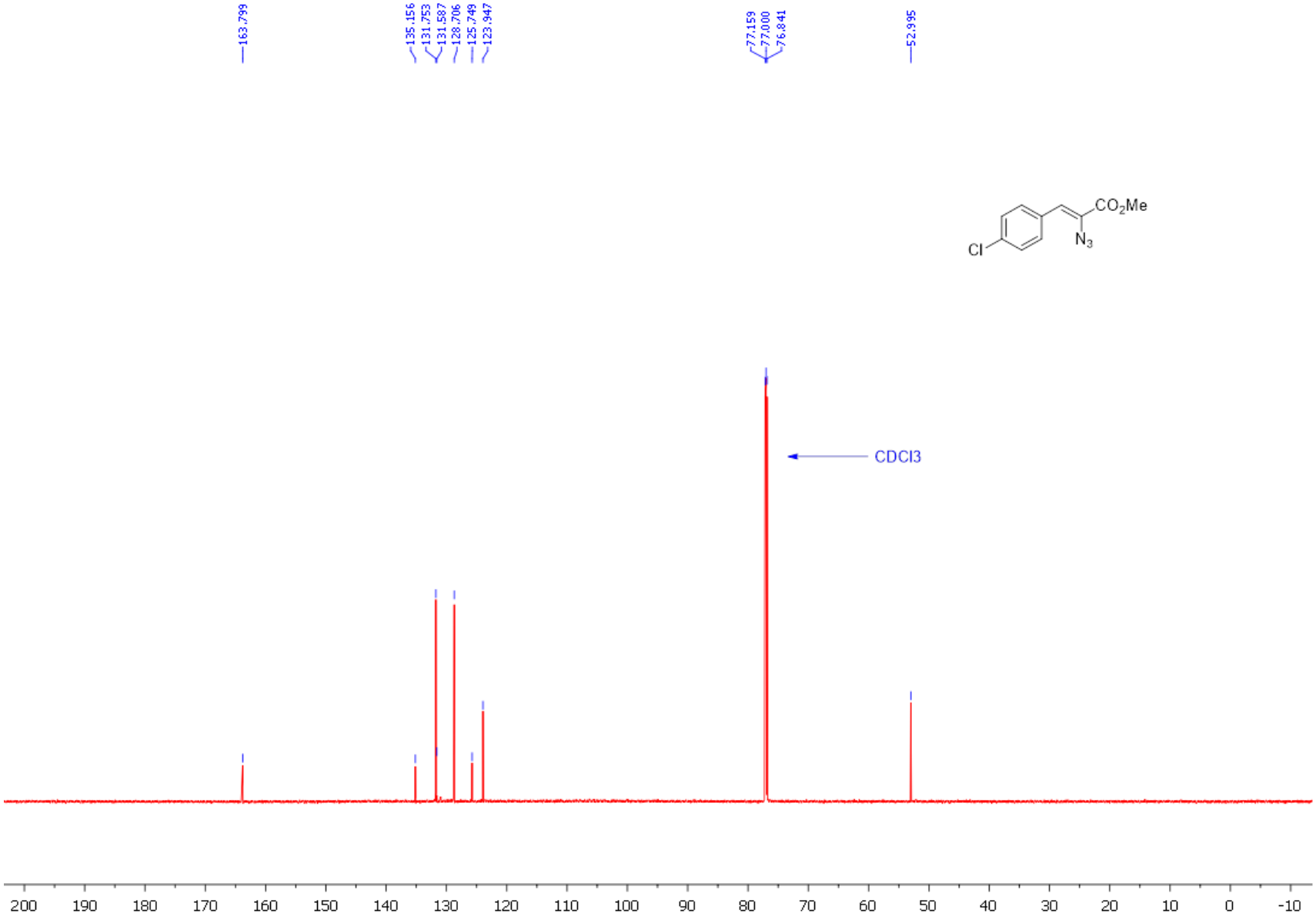
^{13}C-NMR of *(E)-1-azido-2-styrylbenzene (9d)* (25 °C, 200 MHz, $CDCl_3$):



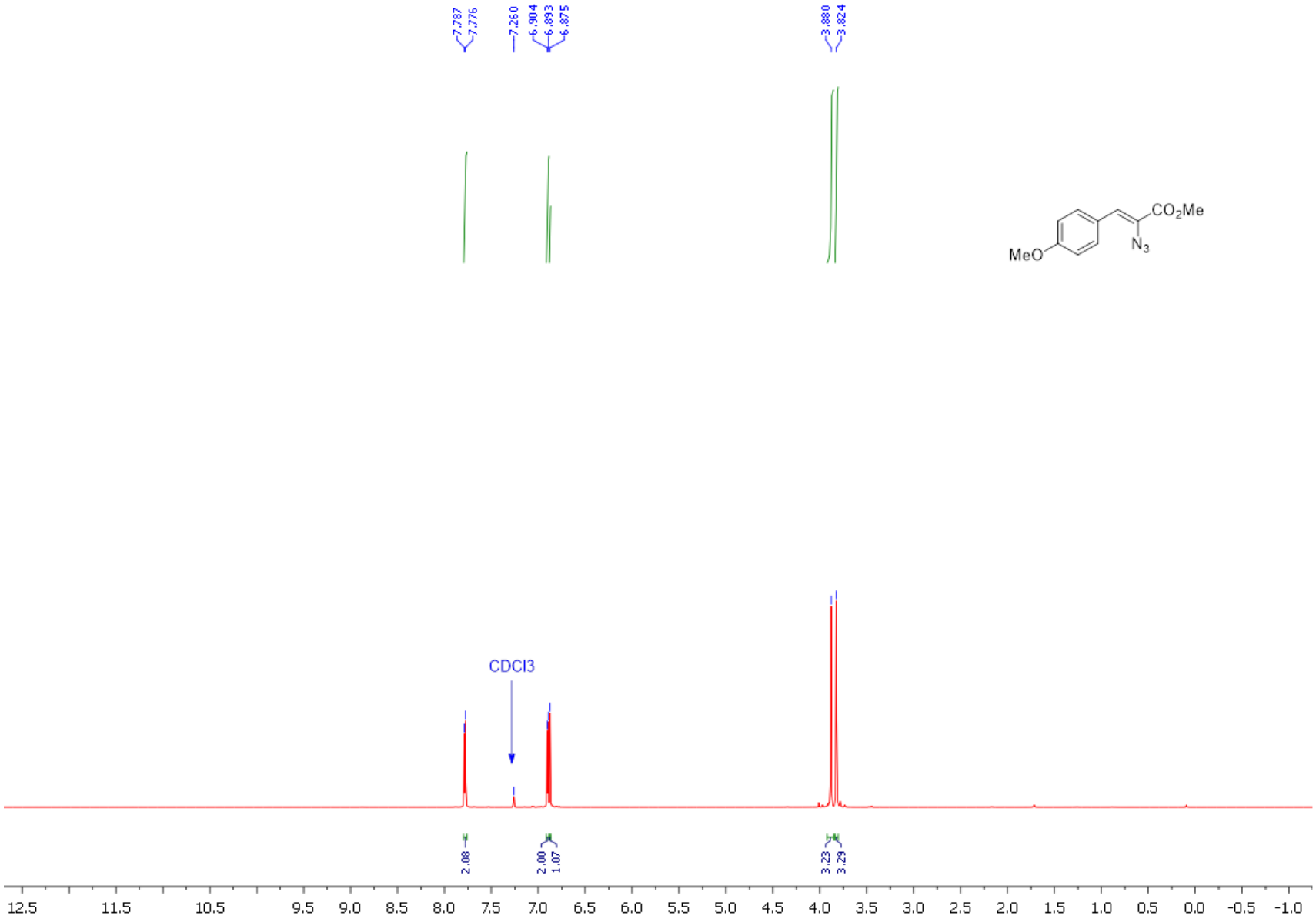
^{1}H-NMR of *methyl (Z)-2-azido-3-(4-chlorophenyl)acrylate (9e)* (25 °C, 800 MHz, $CDCl_3$):



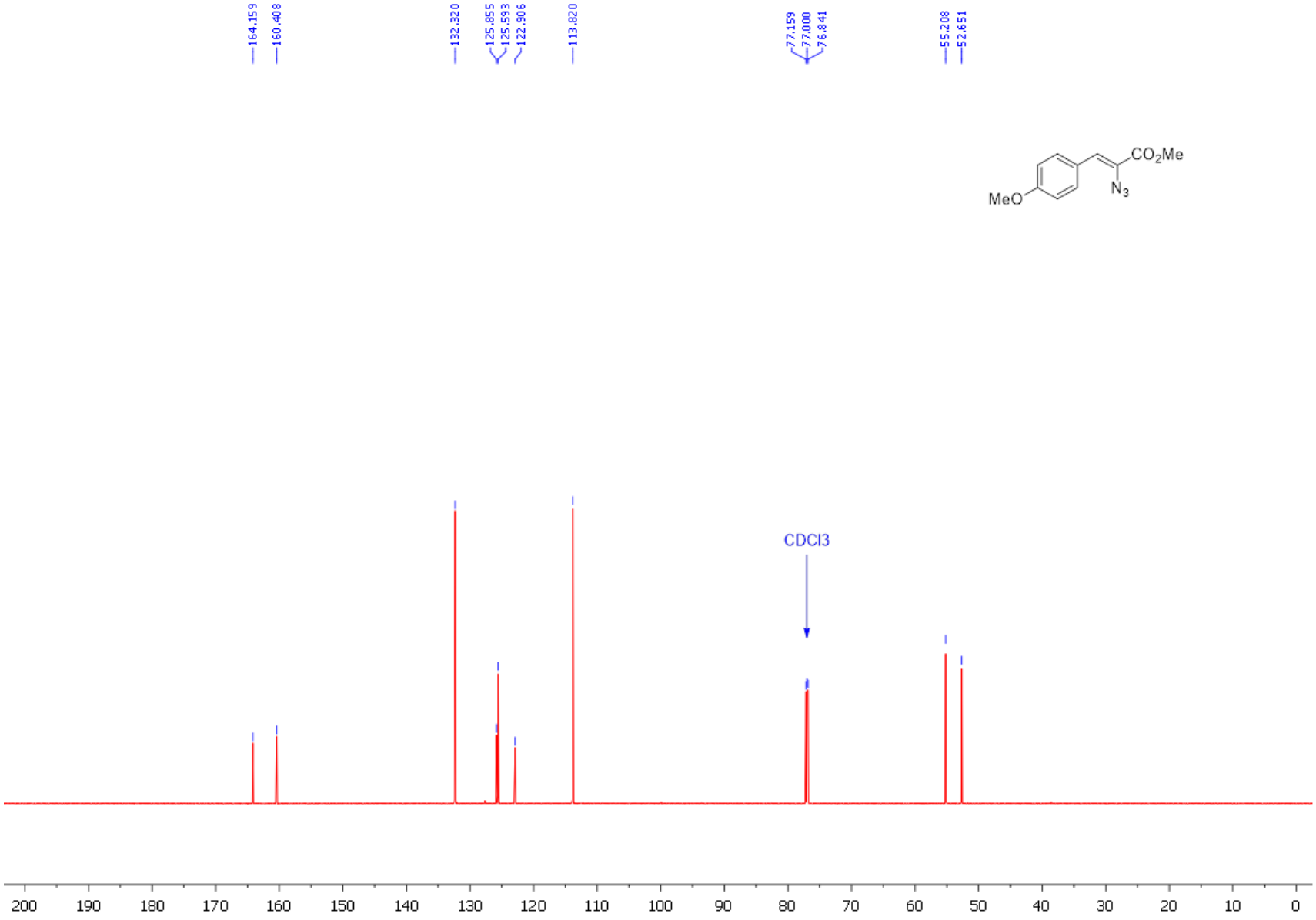
^{13}C-NMR of *methyl (Z)-2-azido-3-(4-chlorophenyl)acrylate (9e)* (25 °C, 200 MHz, $CDCl_3$):



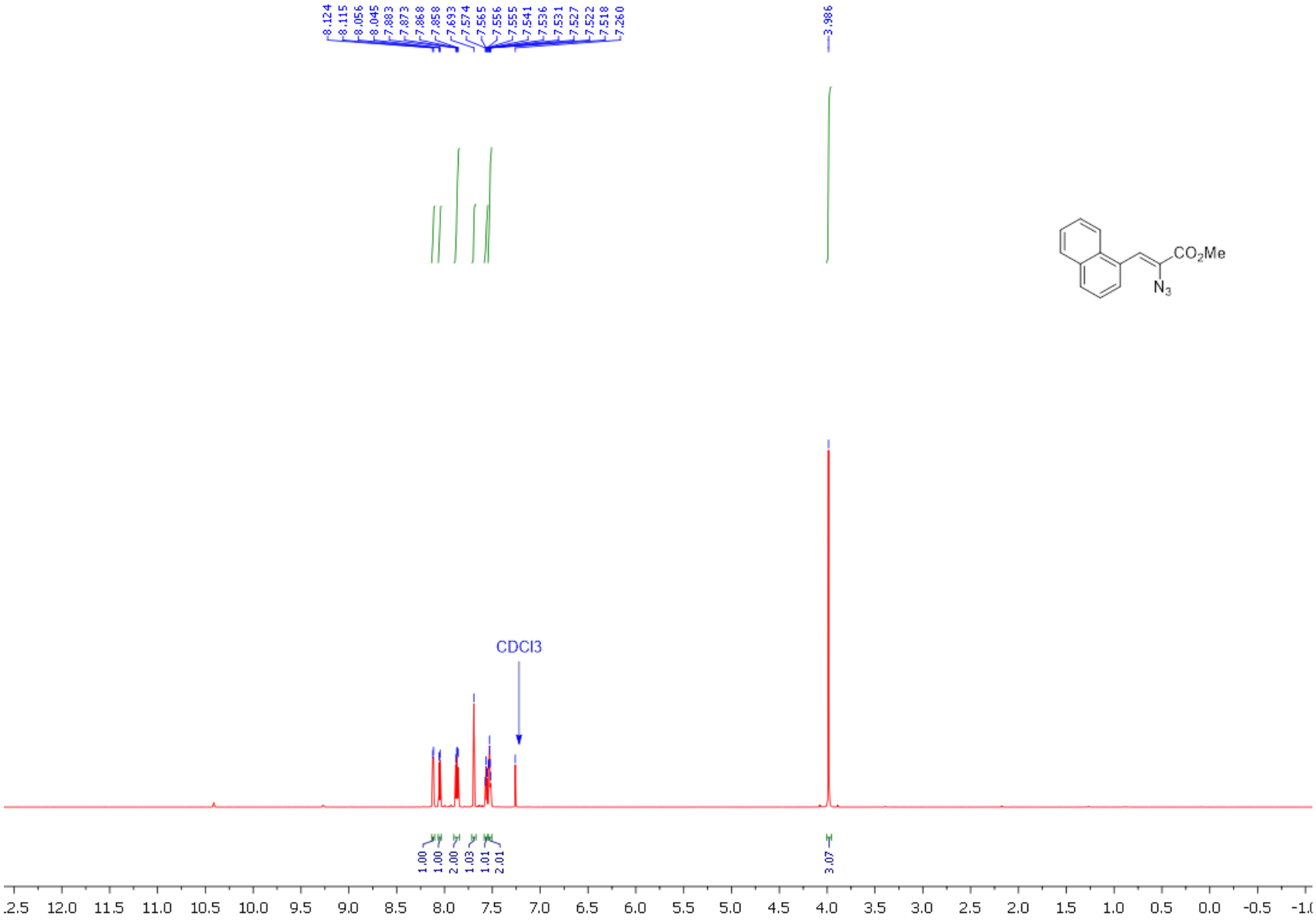
^{1}H-NMR of *methyl (Z)-2-azido-3-(4-methoxyphenyl)acrylate (9f)* (25 ^{o}C, 800 MHz, $CDCl_3$):



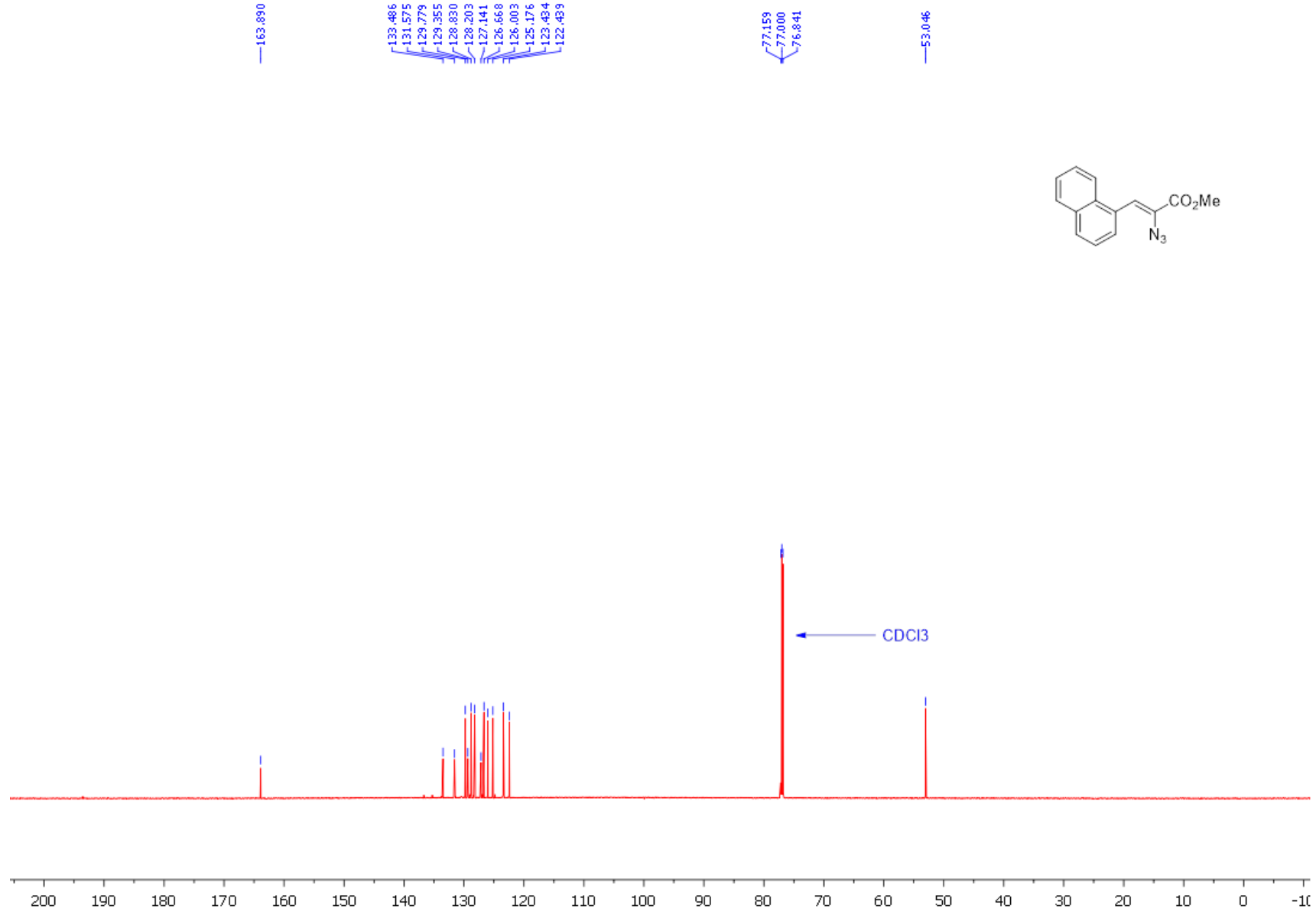
^{13}C-NMR of *methyl (Z)-2-azido-3-(4-methoxyphenyl)acrylate (9f)* (25 °C, 200 MHz, $CDCl_3$):



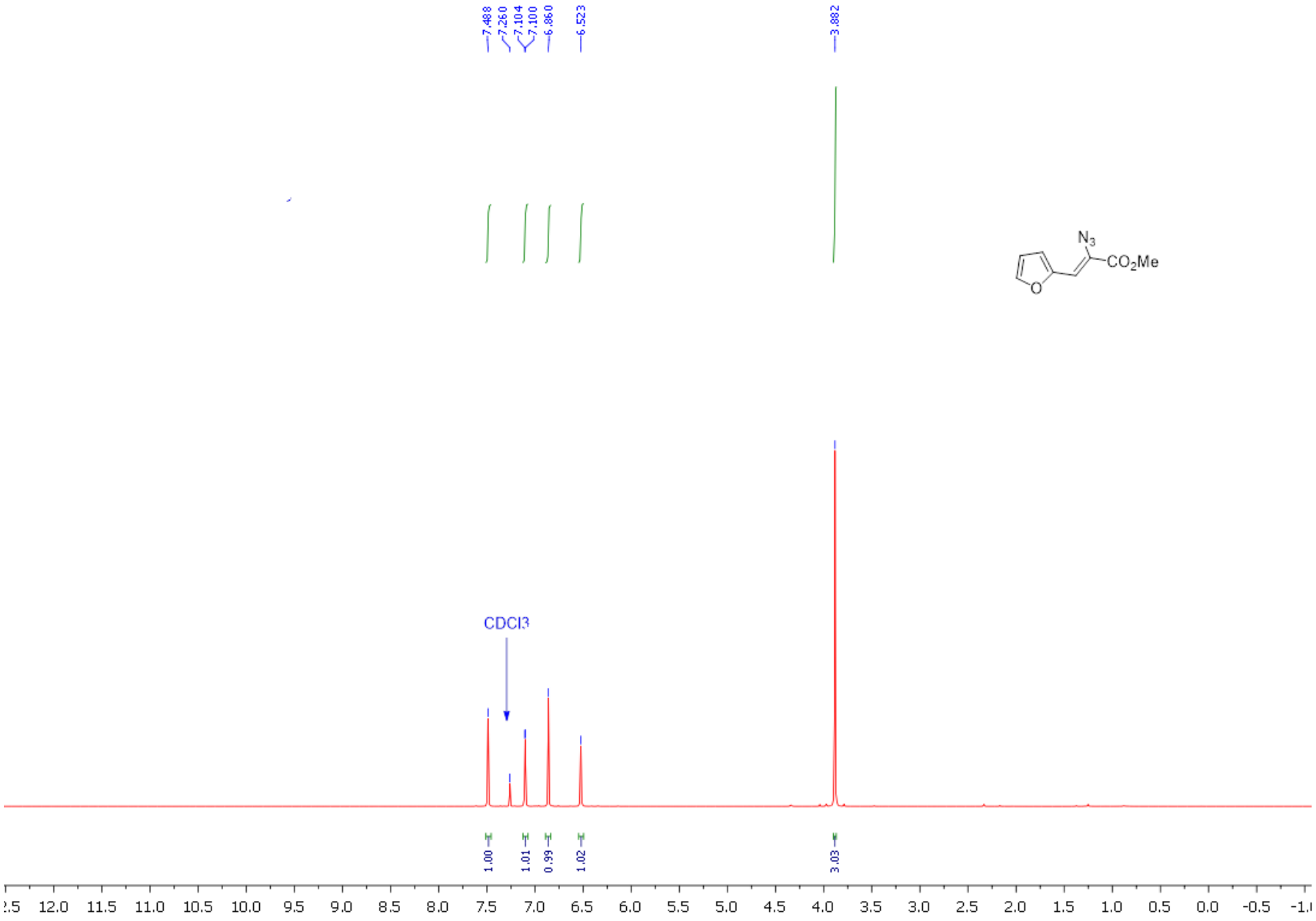
^{1}H-NMR of *methyl (Z)-2-azido-3-(naphthalen-1-yl)acrylate (9g)* (25 ^{o}C, 800 MHz, $CDCl_3$):



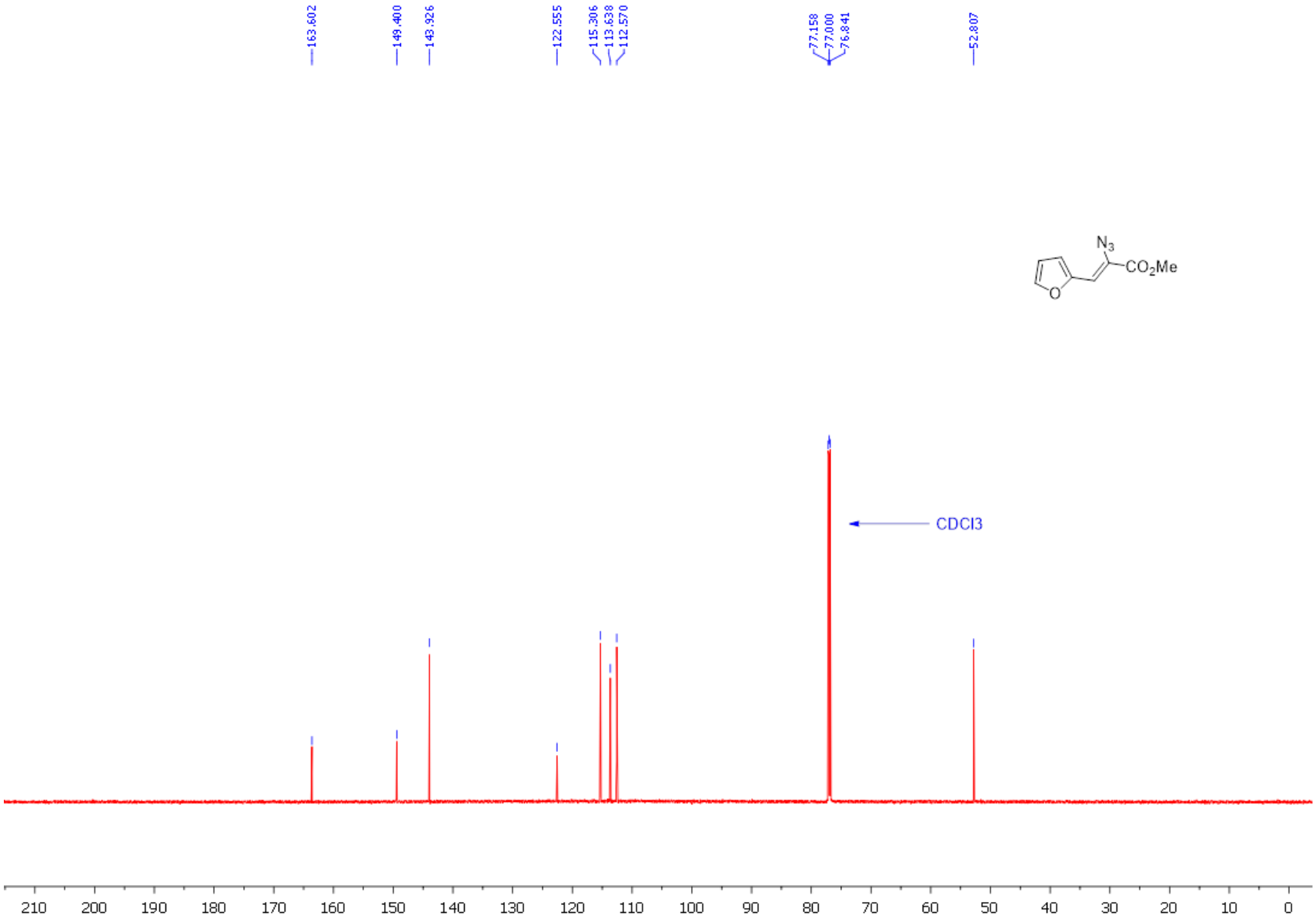
^{13}C-NMR of *methyl (Z)-2-azido-3-(naphthalen-1-yl)acrylate (9g)* (25 °C, 200 MHz, $CDCl_3$):



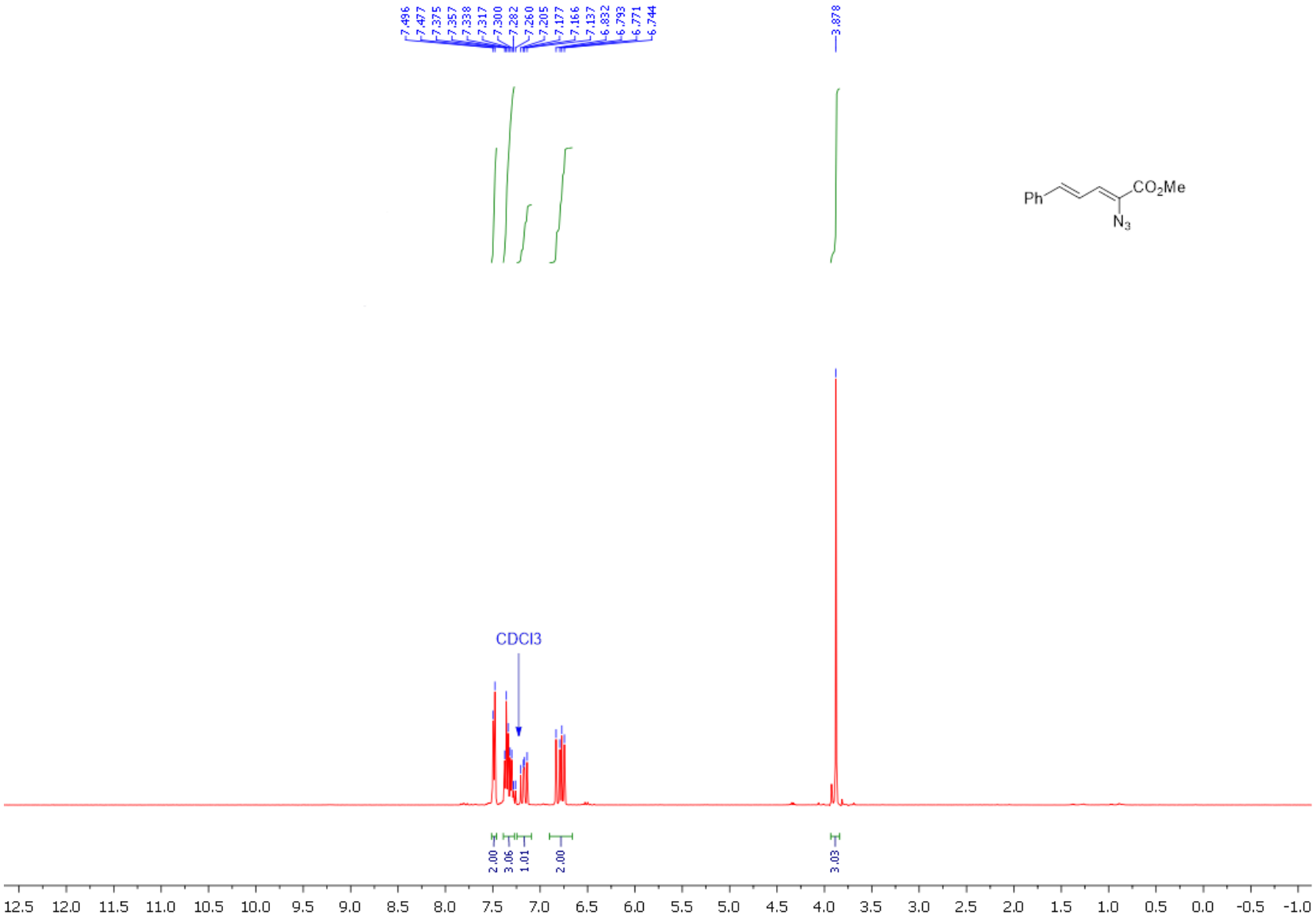
^{1}H-NMR of *methyl (Z)-2-azido-3-(furan-2-yl)acrylate (9h)* (25 ^{o}C, 800 MHz, $CDCl_3$):



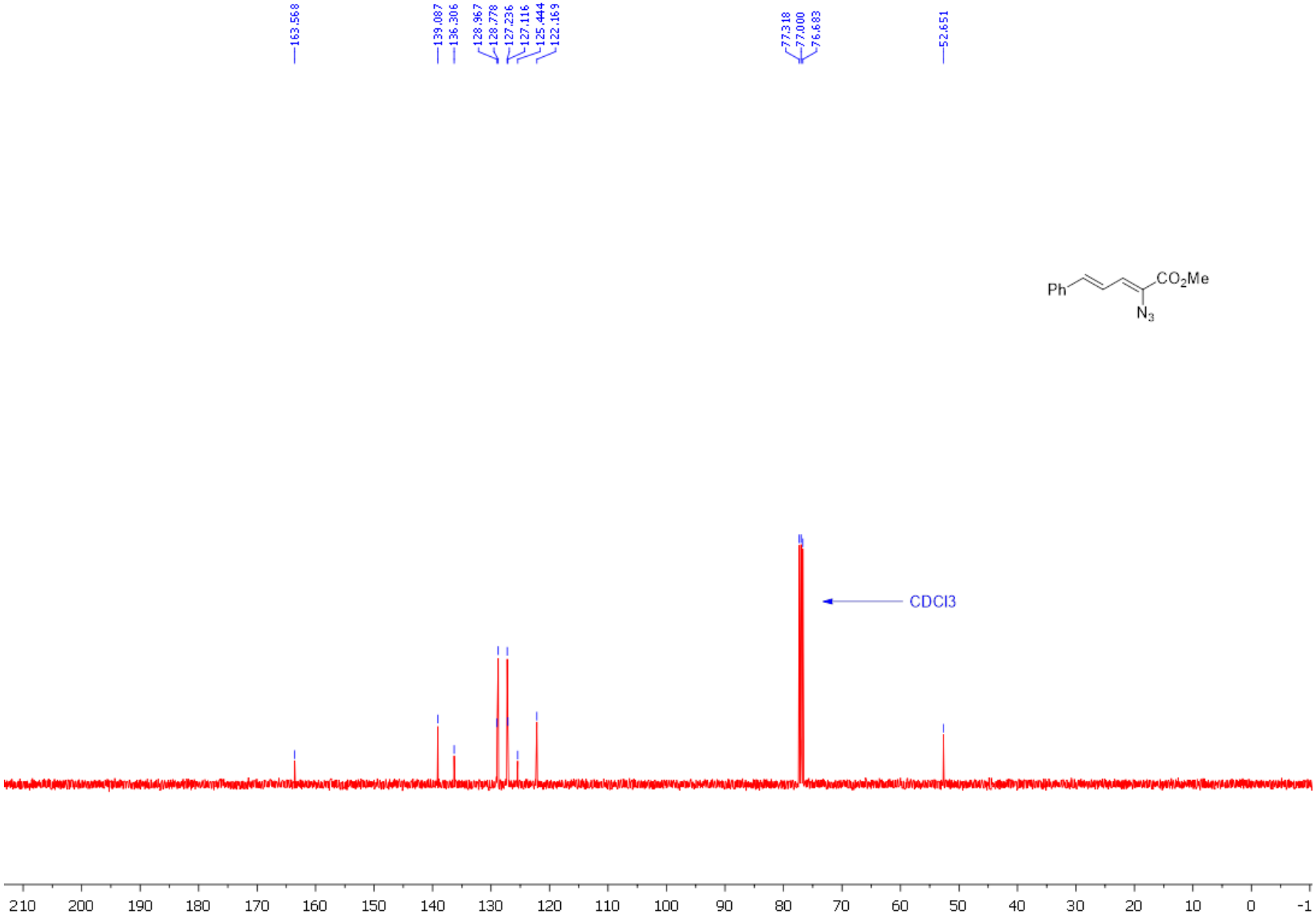
^{13}C-NMR of *methyl (Z)-2-azido-3-(furan-2-yl)acrylate (9h)* (25 ^{o}C, 200 MHz, $CDCl_3$):



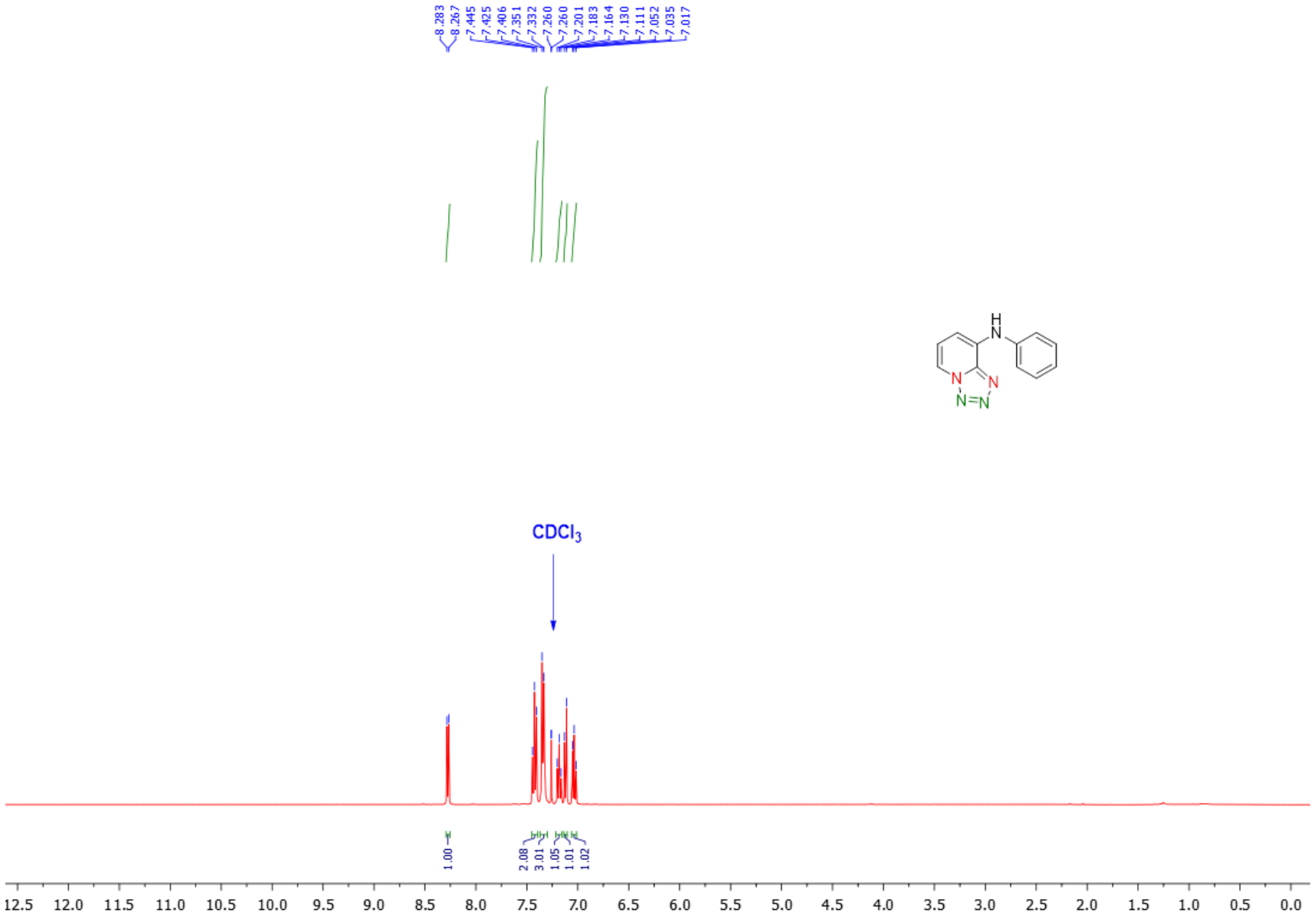
^{1}H-NMR of *methyl (2Z,4E)-2-azido-5-phenylpenta-2,4-dienoate (9i)* (25 ^{o}C, 400 MHz, $CDCl_3$):



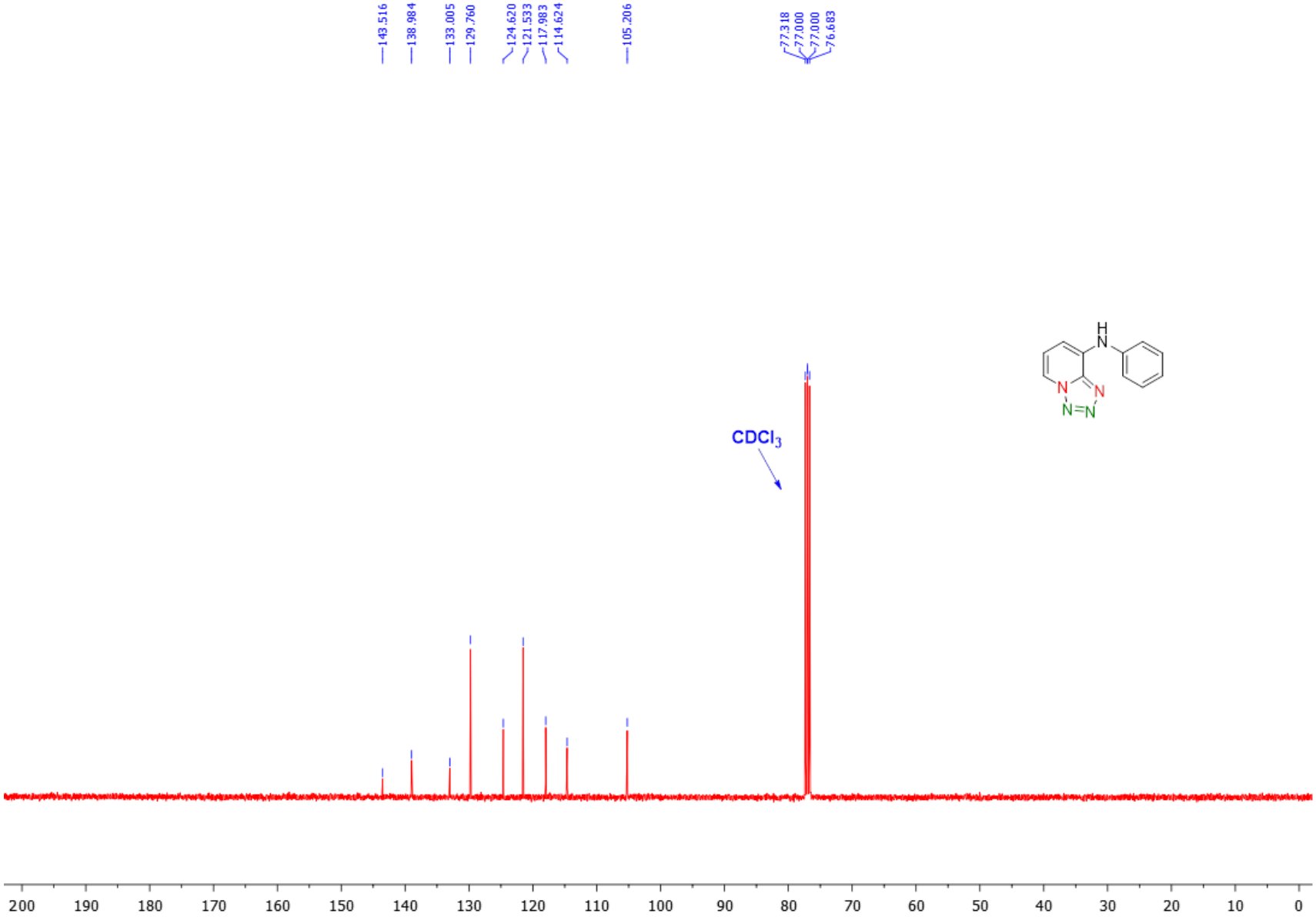
^{13}C-NMR of *methyl (2Z,4E)-2-azido-5-phenylpenta-2,4-dienoate (9i)* (25 ºC, 100 MHz, $CDCl_3$):



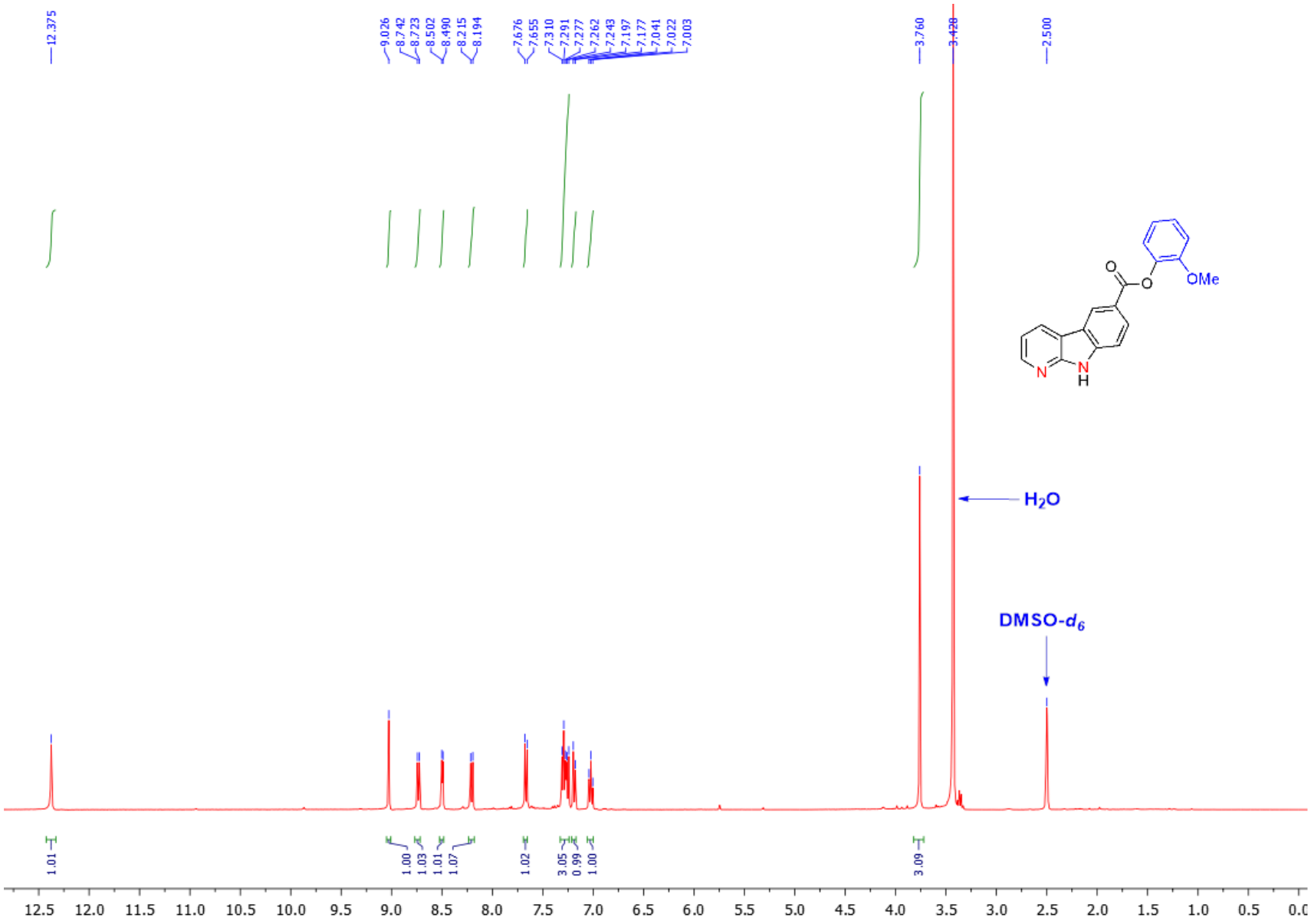
^{1}H-NMR of *N-phenyltetrazolo[1,5-a]pyridin-8-amine (15)* (25 ºC, 400 MHz, $CDCl_3$):



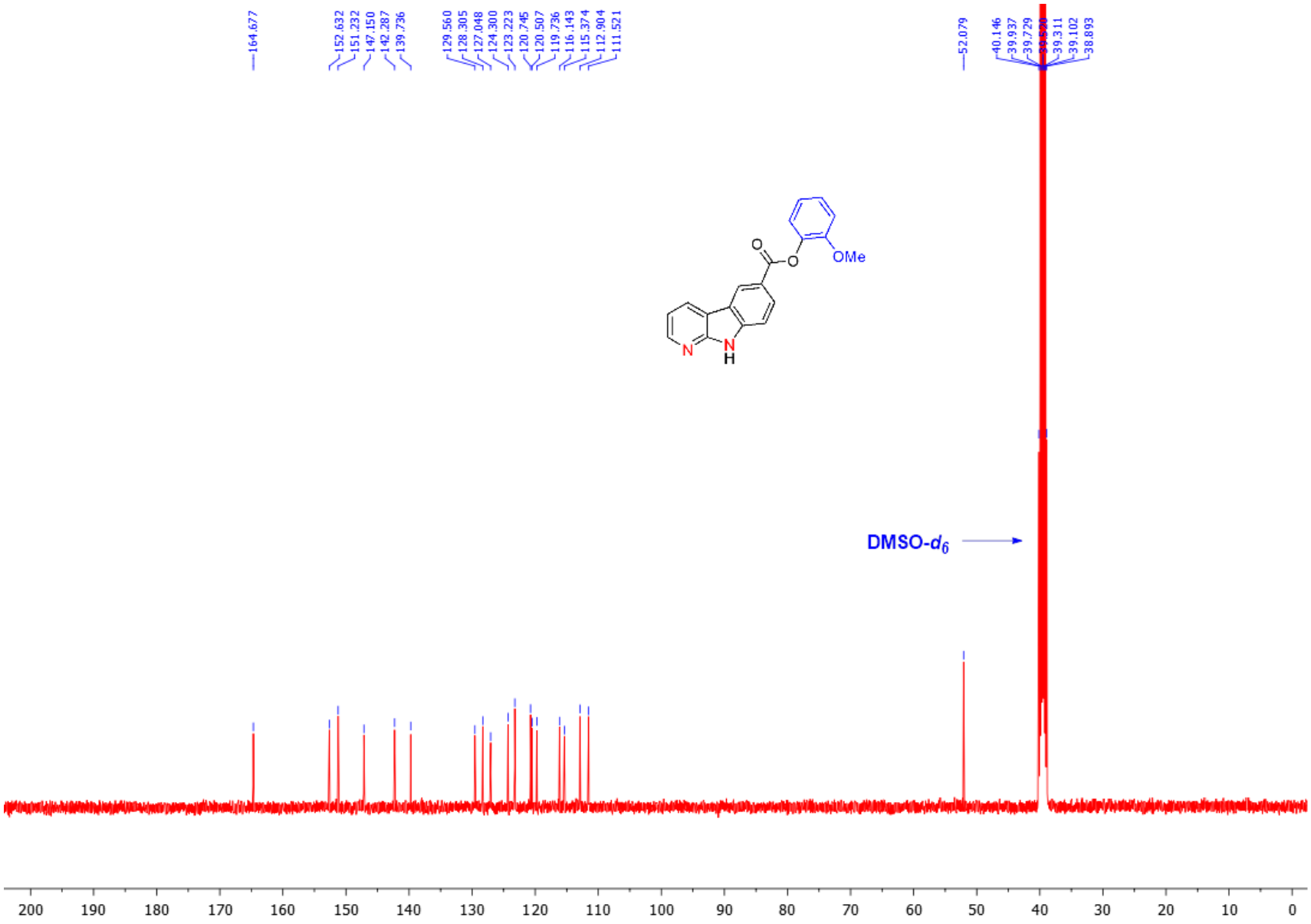
^{13}C-NMR of *N-phenyltetrazolo[1,5-a]pyridin-8-amine (15)* (25 °C, 100 MHz, $CDCl_3$):



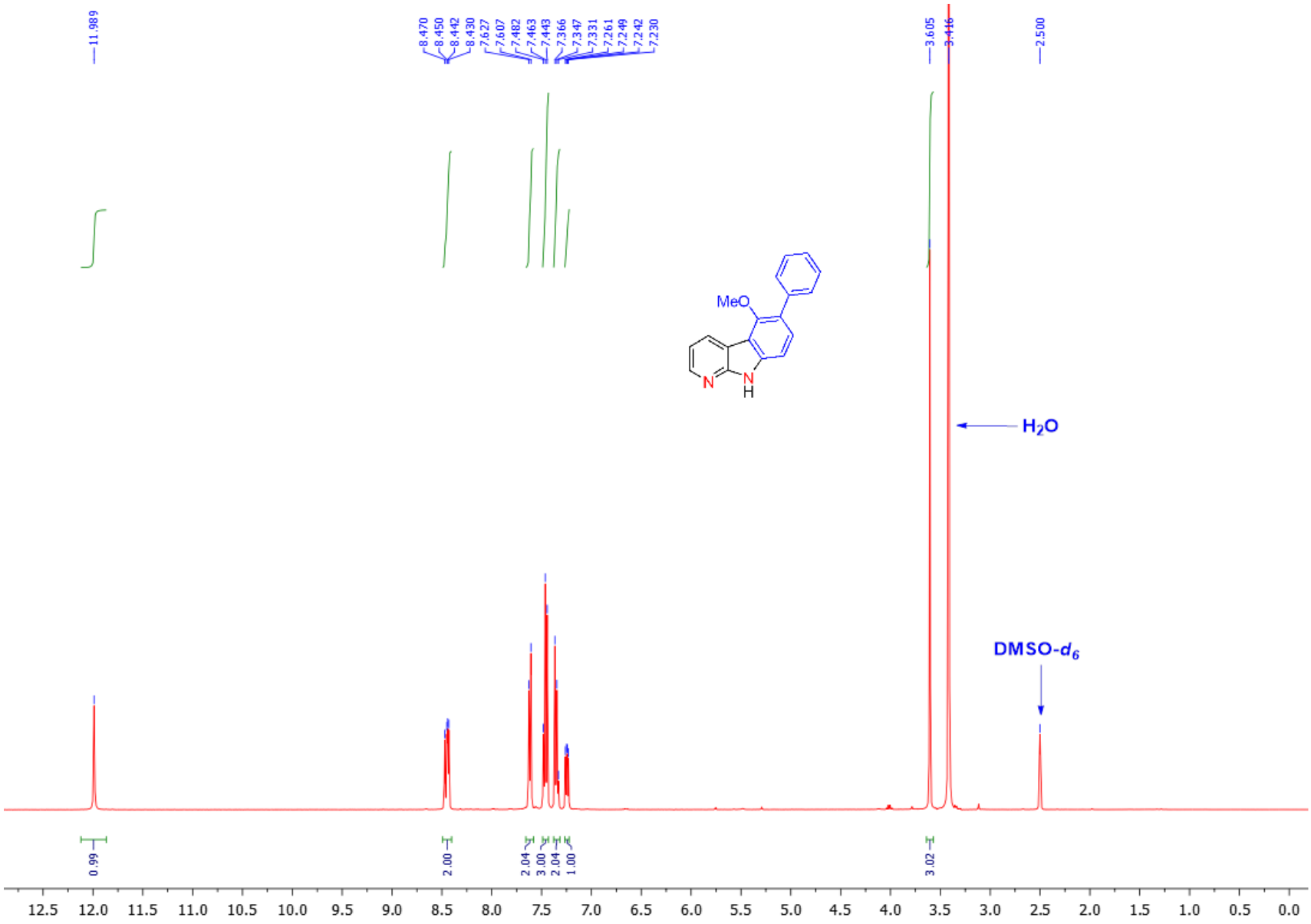
^{1}H-NMR of *2-methoxyphenyl 9H-pyrido[2,3-b]indole-6-carboxylate (2b)* (25 ºC, 400 MHz, DMSO-d_6):



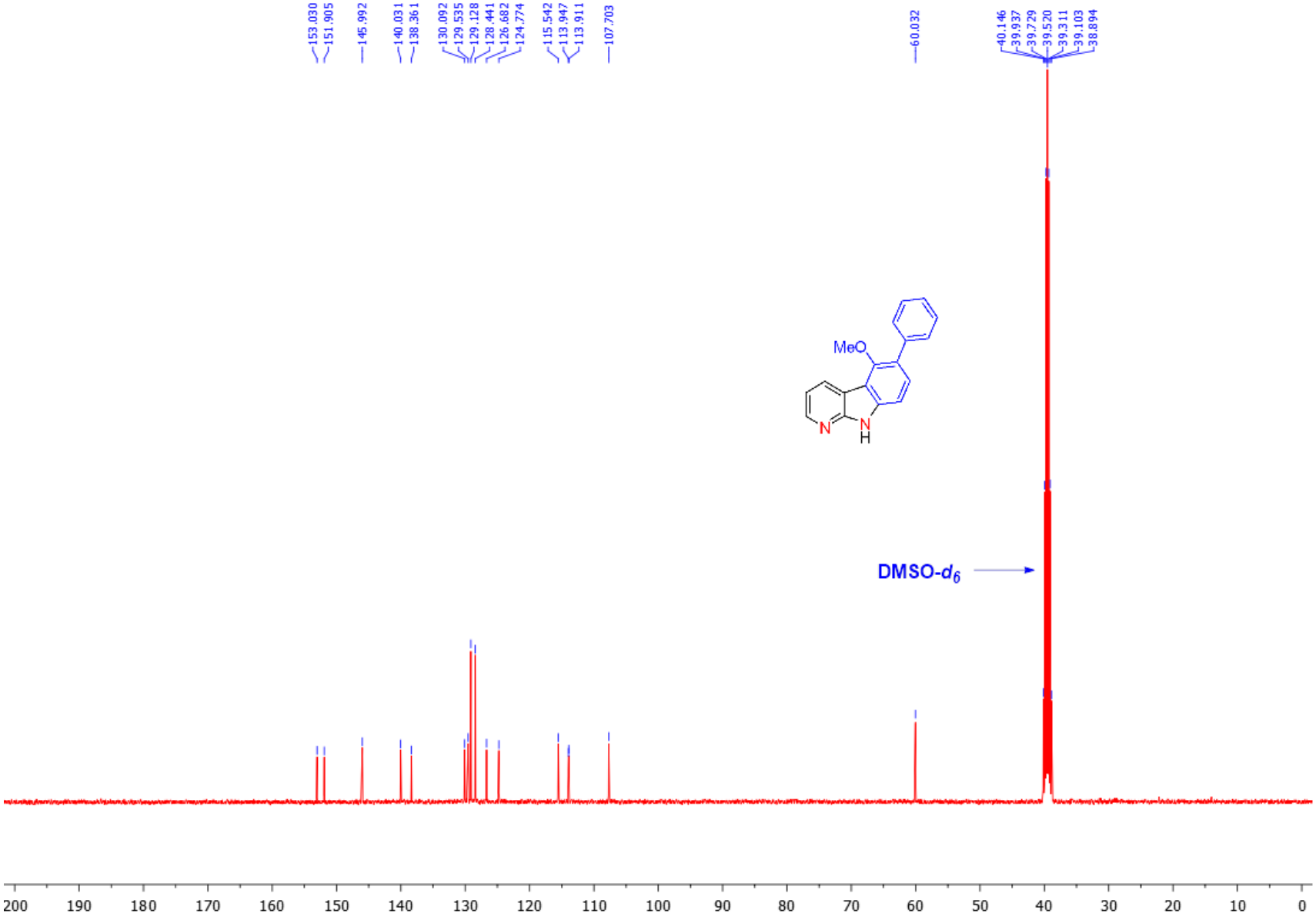
^{13}C-NMR of *2-methoxyphenyl 9H-pyrido[2,3-b]indole-6-carboxylate (2b)* (25 °C, 100 MHz, DMSO-d_6):



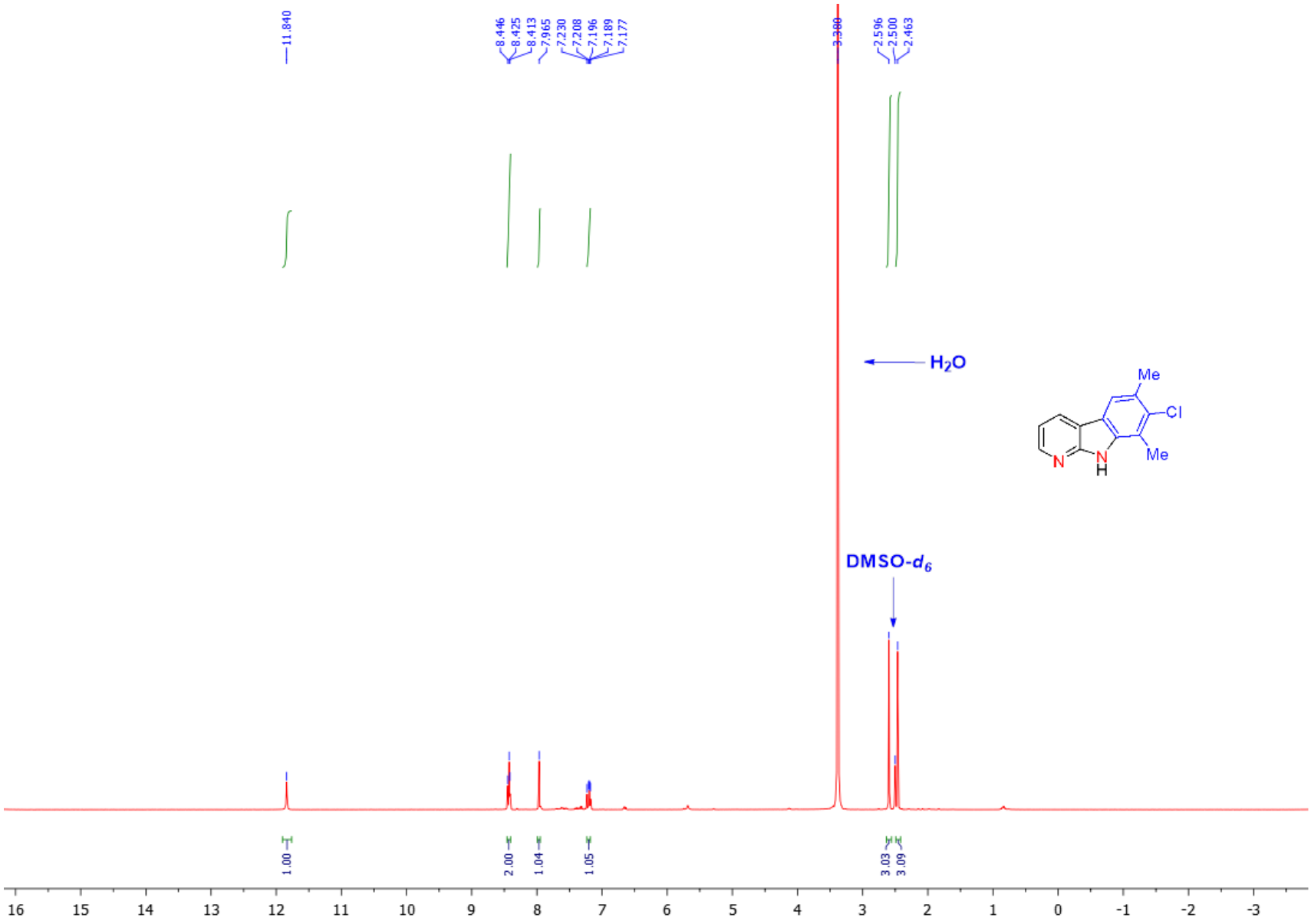
^{1}H-NMR of *5-methoxy-6-phenyl-9H-pyrido[2,3-b]indole (2c)* (25 ºC, 400 MHz, DMSO-d_6):



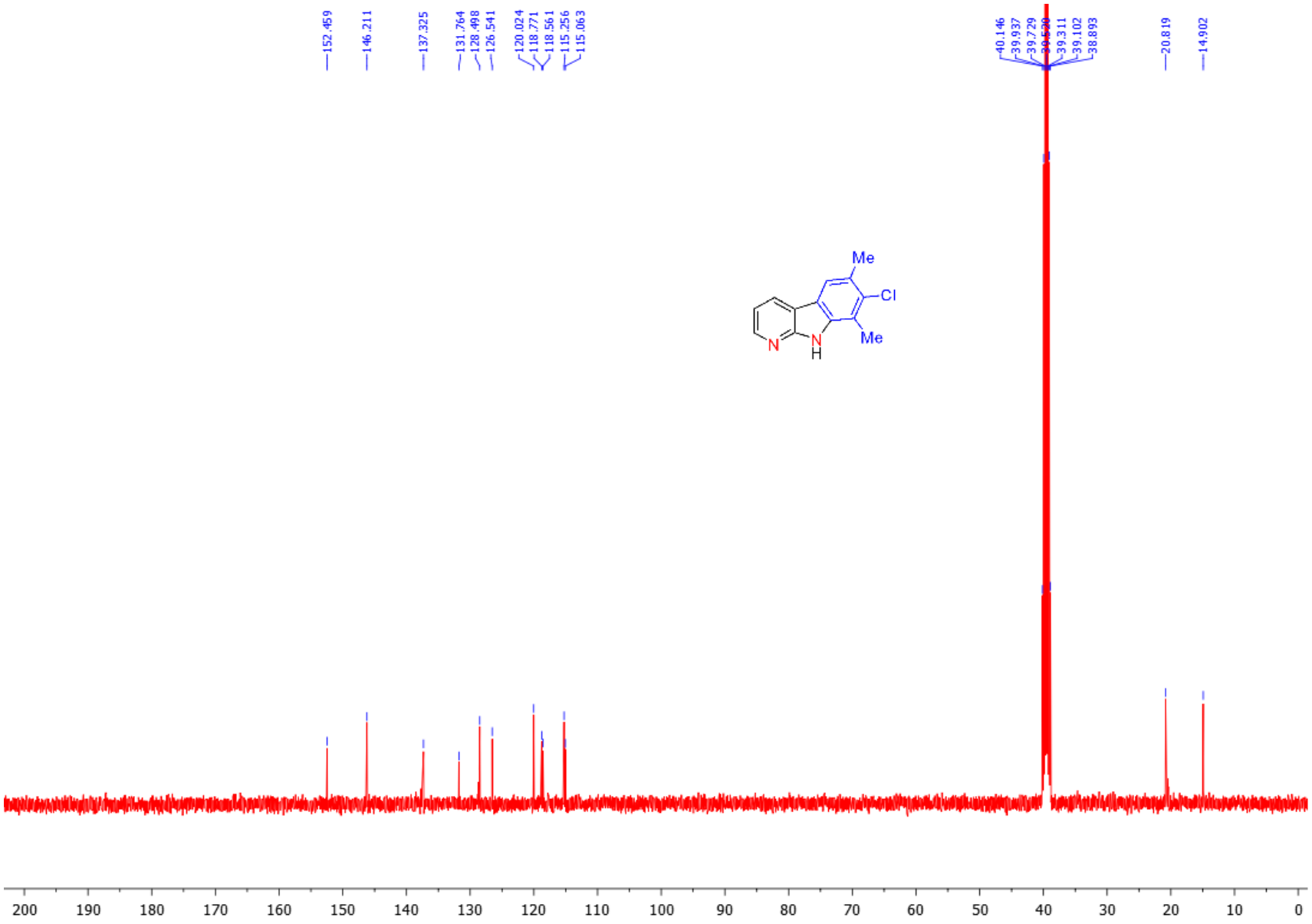
^{13}C-NMR of *5-methoxy-6-phenyl-9H-pyrido[2,3-b]indole (2c)* (25 °C, 100 MHz, DMSO-d_6):



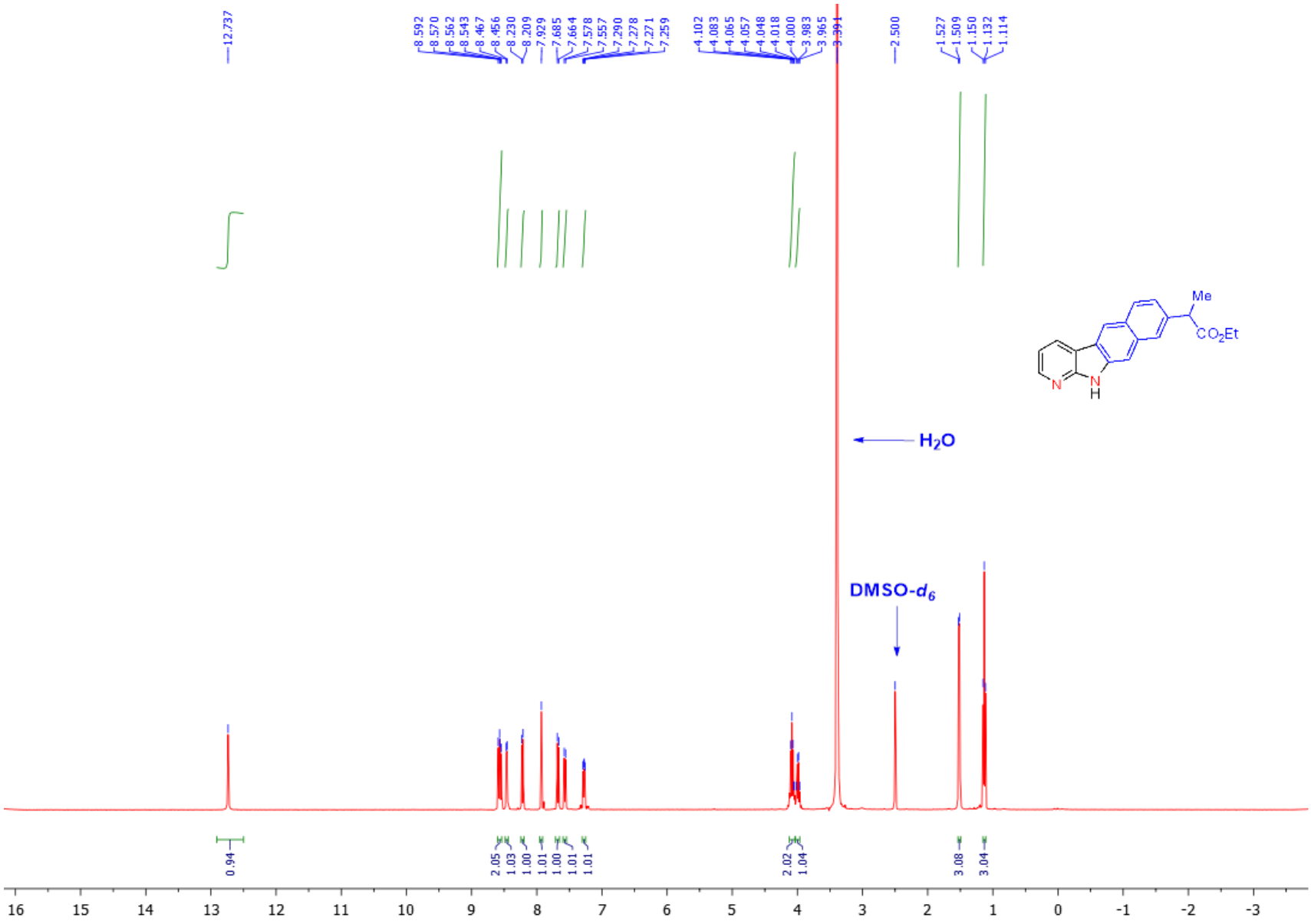
^{1}H-NMR of *7-chloro-6,8-dimethyl-9H-pyrido[2,3-b]indole (2d)*(25 ºC, 400 MHz, DMSO-d_6):



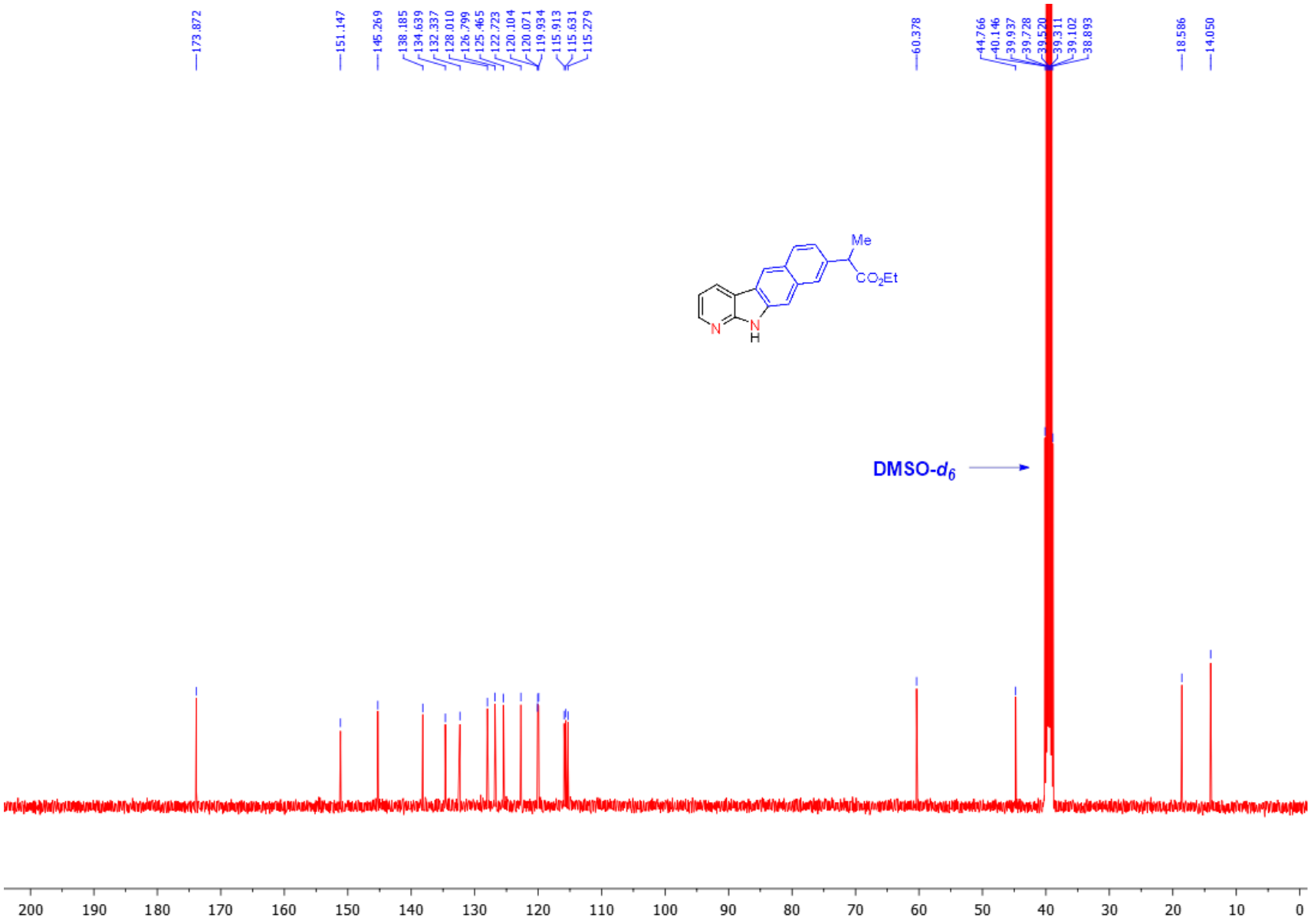
^{13}C-NMR of *7-chloro-6,8-dimethyl-9H-pyrido[2,3-b]indole (2d)(* (25 ºC, 100 MHz, DMSO-d_6):



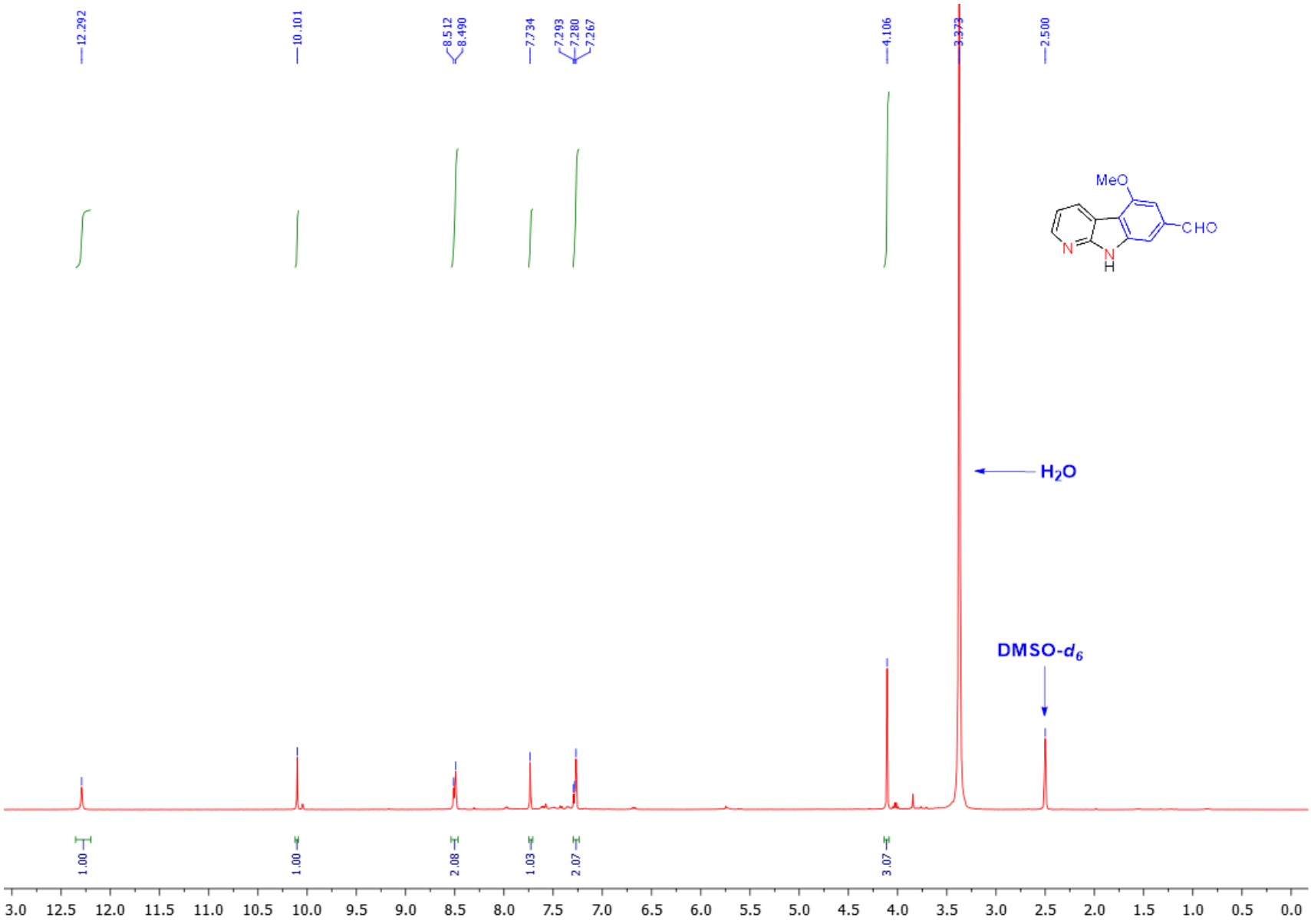
[1]H-NMR of *ethyl 2-(11H-benzo[f]pyrido[2,3-b]indol-8-yl)propanoate (2e)* (25 °C, 400 MHz, DMSO-d_6):



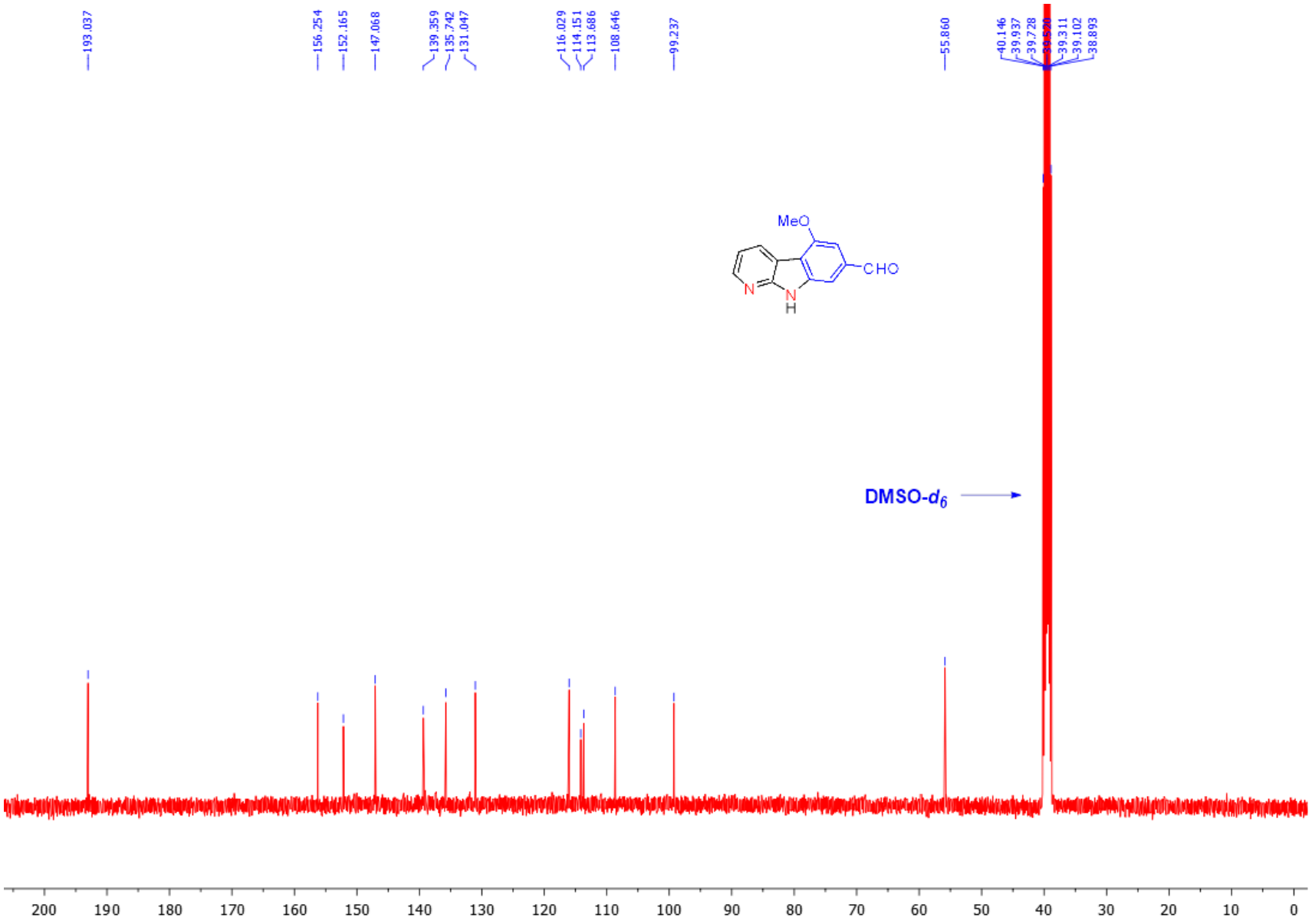
^{13}C-NMR of *ethyl 2-(11H-benzo[f]pyrido[2,3-b]indol-8-yl)propanoate (2e)* (25 ºC, 100 MHz, DMSO-d_6):



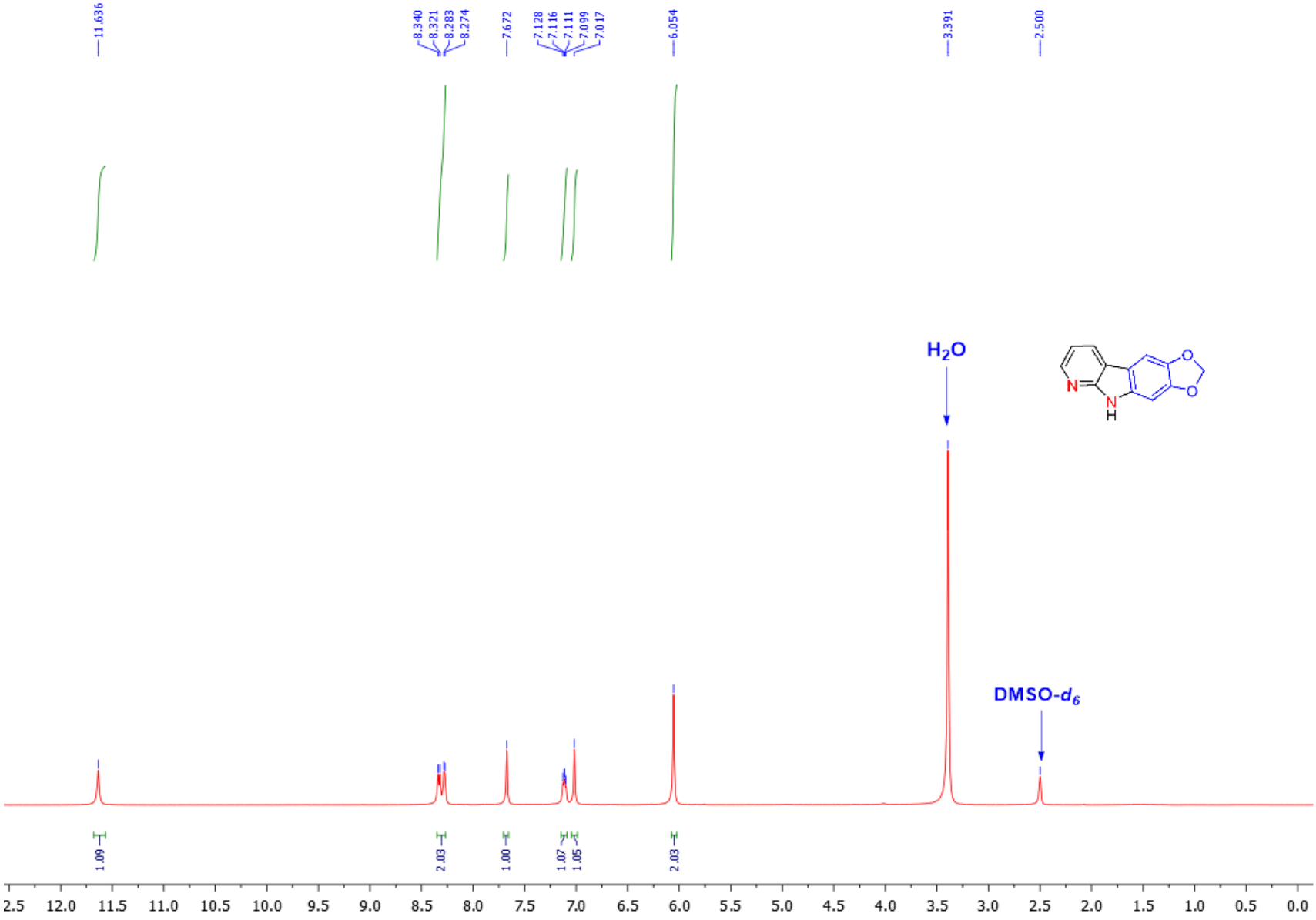
^{1}H-NMR of *5-methoxy-9H-pyrido[2,3-b]indole-7-carbaldehyde (2f)* (25 ºC, 400 MHz, DMSO-d_6):



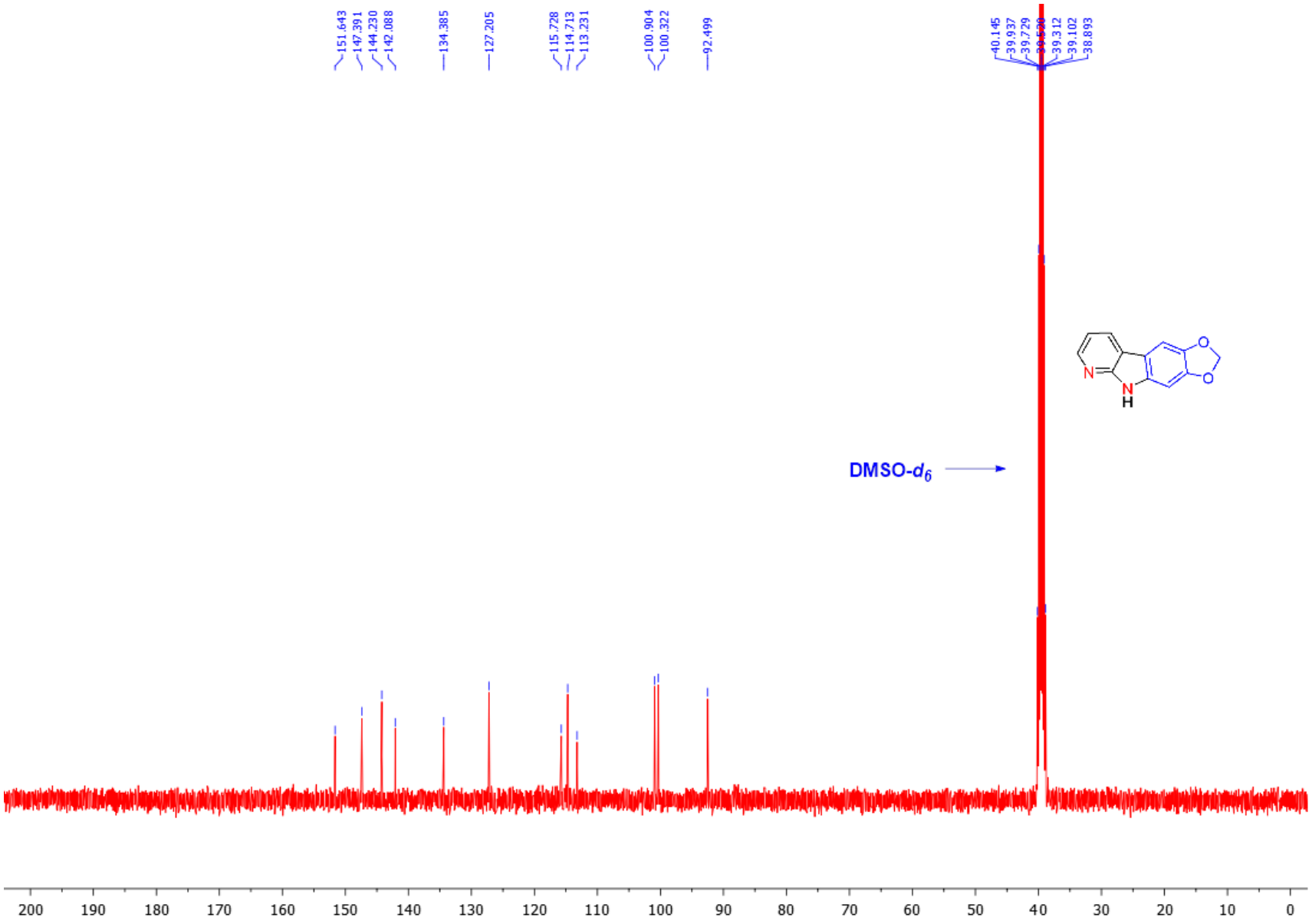
^{13}C-NMR of *5-methoxy-9H-pyrido[2,3-b]indole-7-carbaldehyde (2f)* (25 °C, 100 MHz, DMSO-d_6):



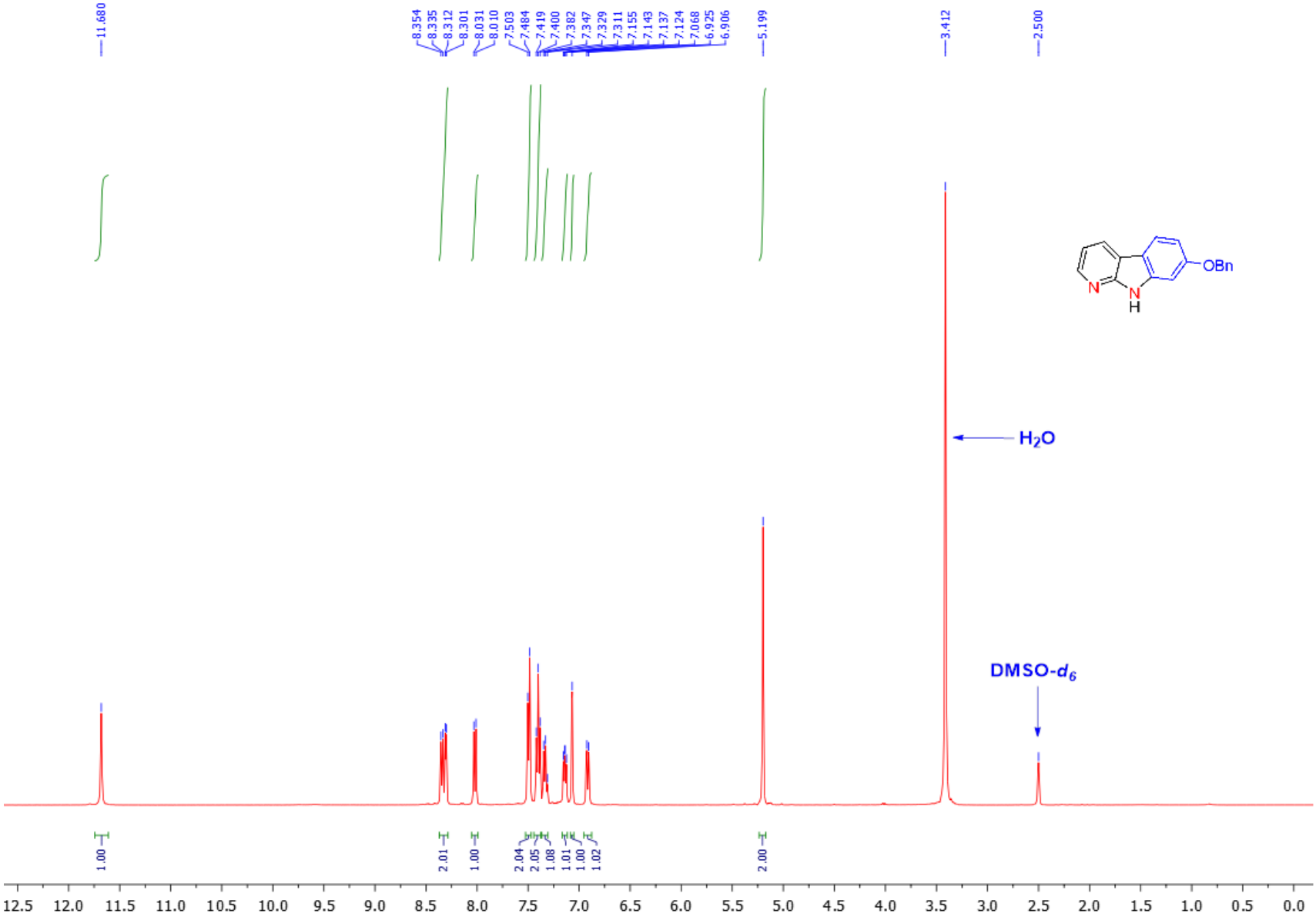
^{1}H-NMR of *5H-[1,3]dioxolo[4,5-f]pyrido[2,3-b]indole (2g)* (25 °C, 400 MHz, DMSO-d_6):



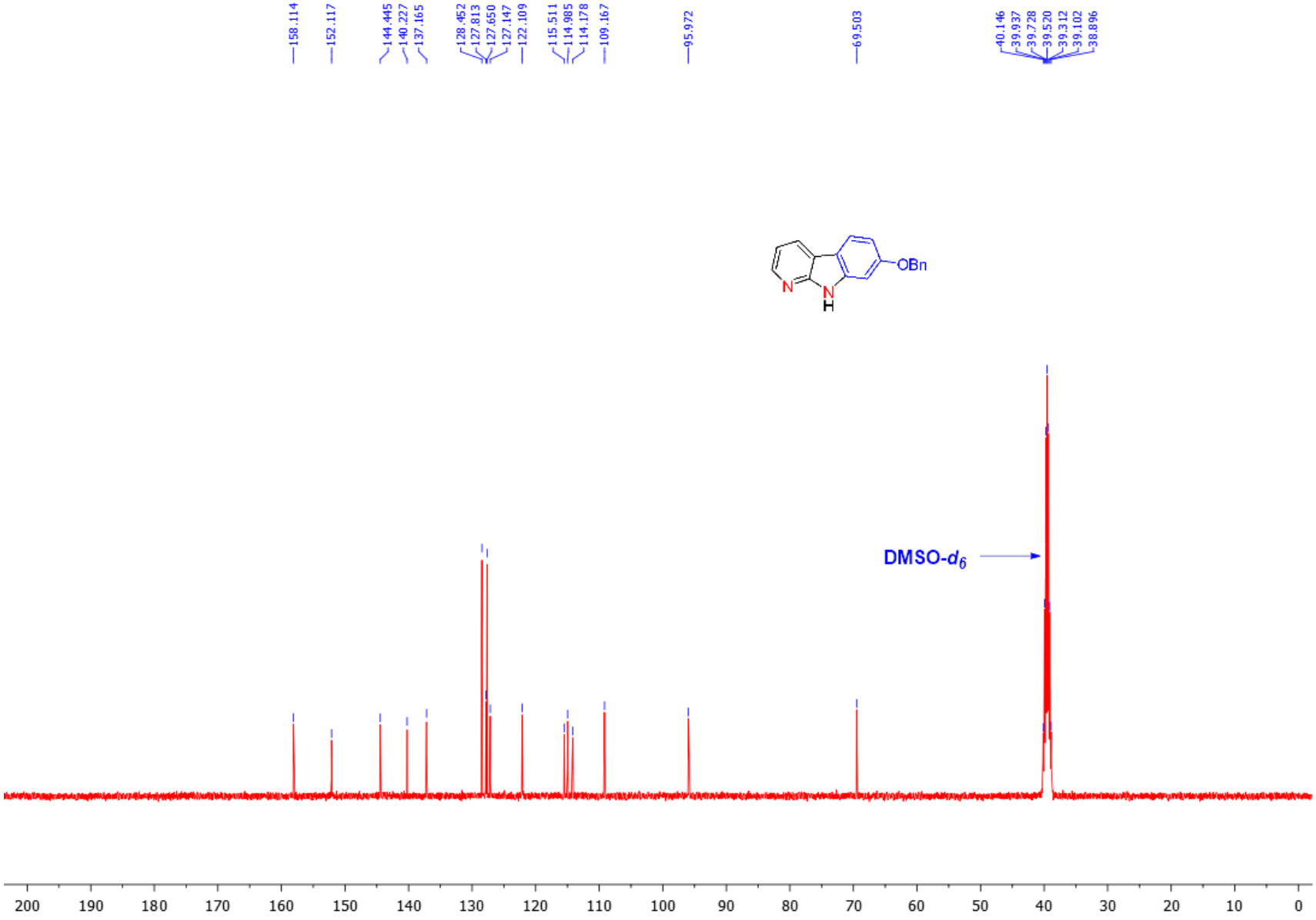
^{13}C-NMR of *5H-[1,3]dioxolo[4,5-f]pyrido[2,3-b]indole (2g)* (25 ºC, 100 MHz, DMSO-d_6):



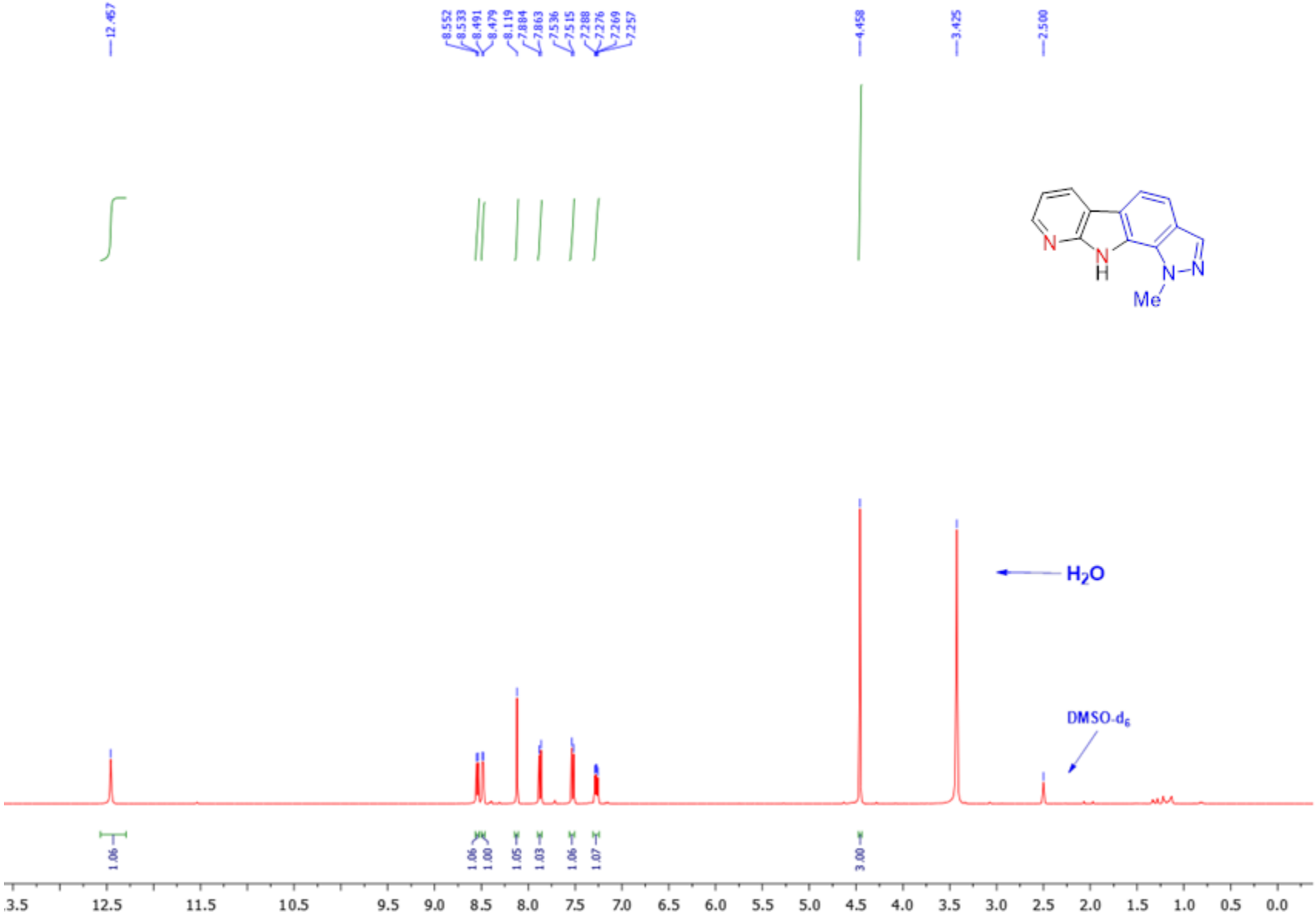
^{1}H-NMR of *7-(benzyloxy)-9H-pyrido[2,3-b]indole (2h)* (25 °C, 400 MHz, DMSO-d_6):



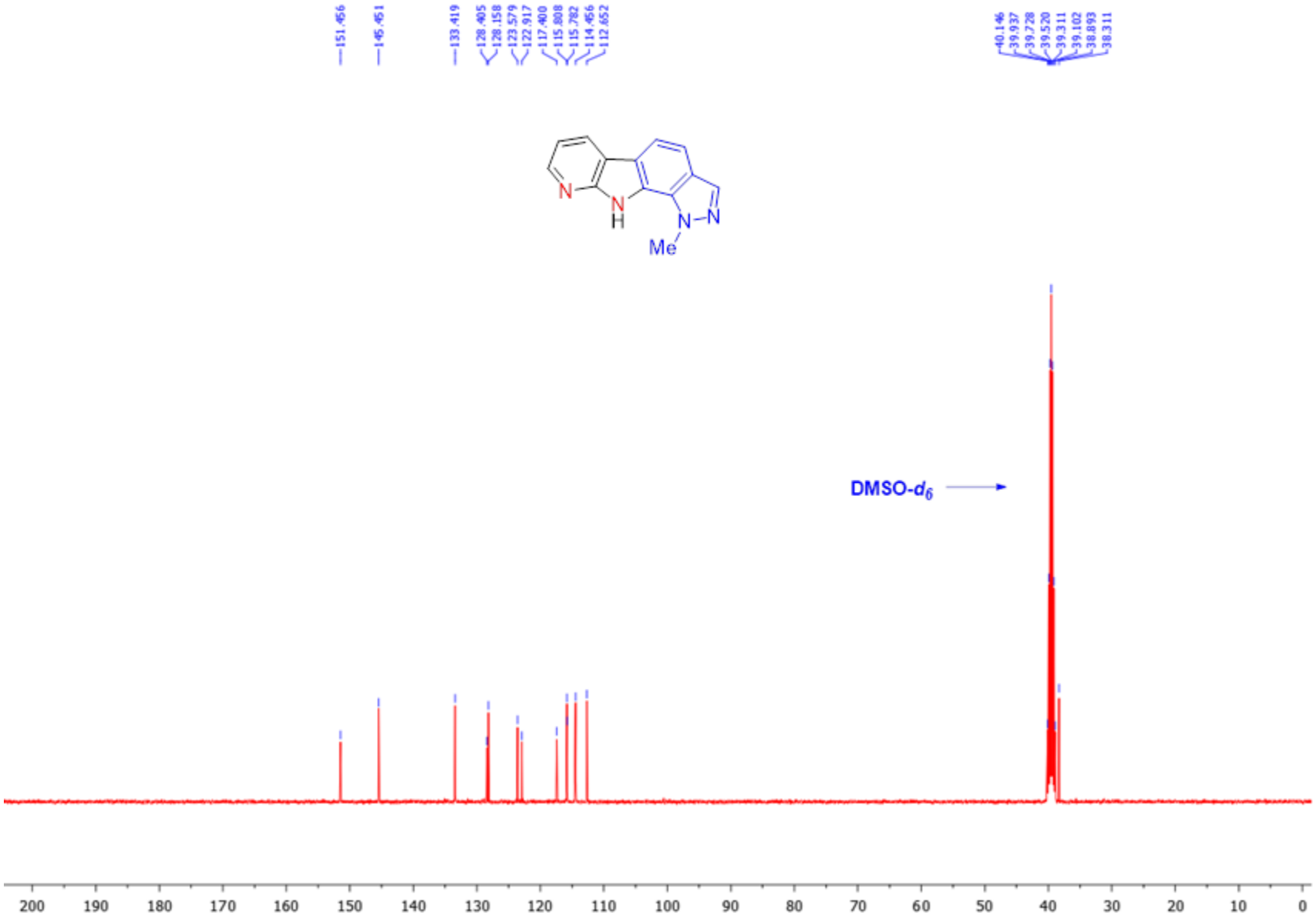
^{13}C-NMR of *7-(benzyloxy)-9H-pyrido[2,3-b]indole (2h)* (25 ºC, 100 MHz, DMSO-d_6):



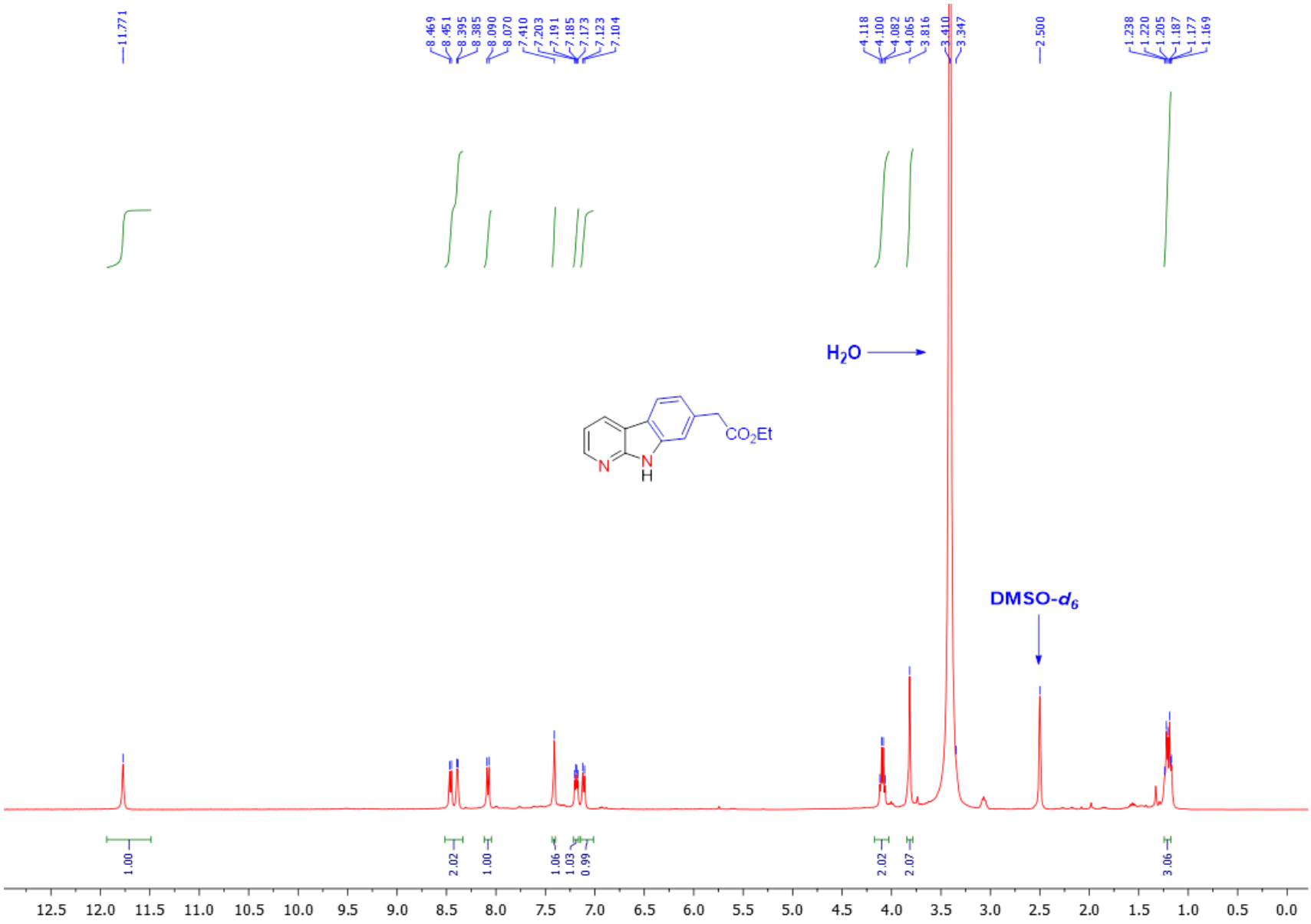
^{1}H-NMR of *1-methyl-1,10-dihydropyrido[3',2':4,5]pyrrolo[3,2-g]indazole (2i)* (25 ºC, 400 MHz DMSO-d_6):



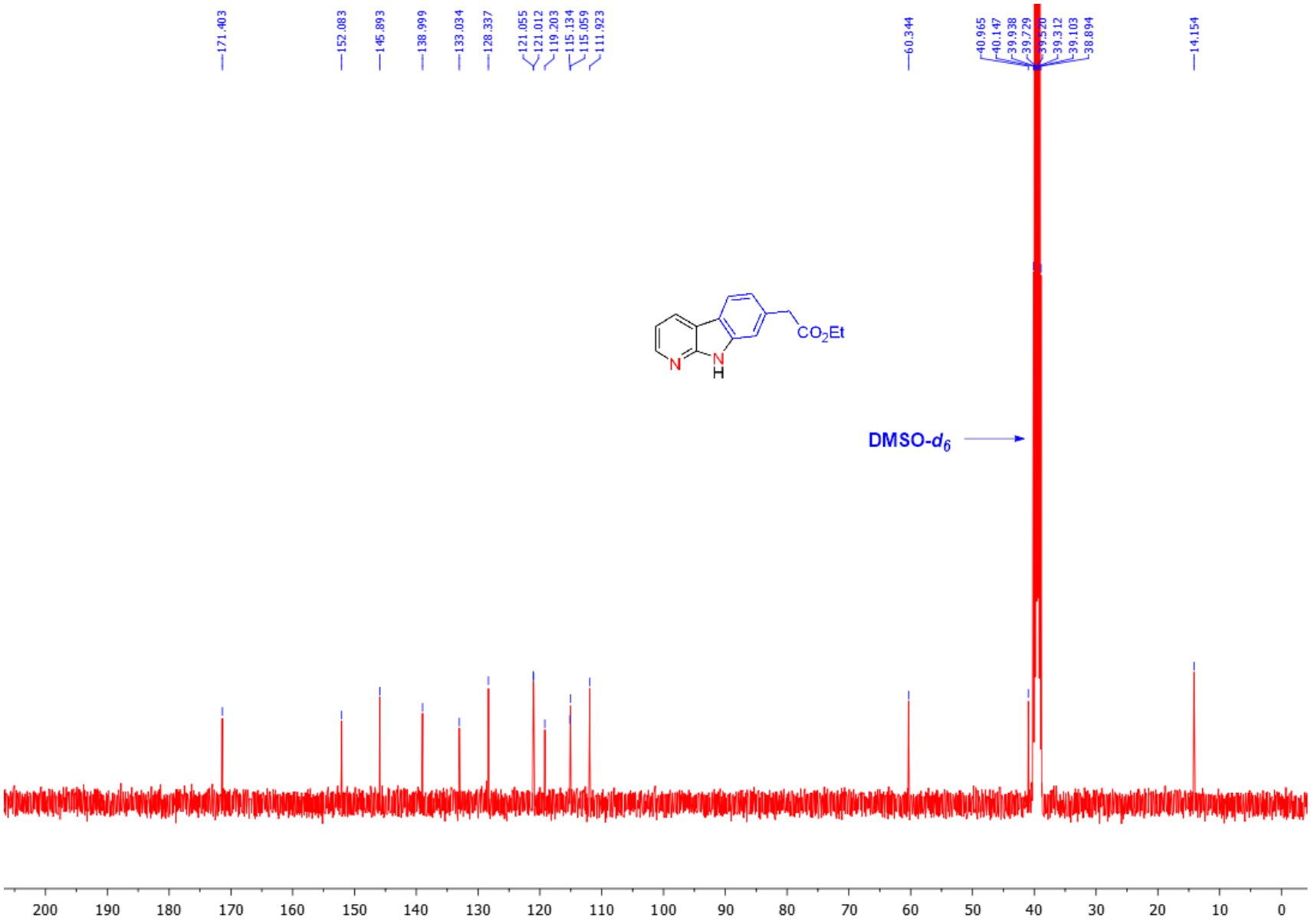
^{13}C-NMR of *1-methyl-1,10-dihydropyrido[3',2':4,5]pyrrolo[3,2-g]indazole (2i)* (25 ºC, 100 MHz, DMSO-d_6):



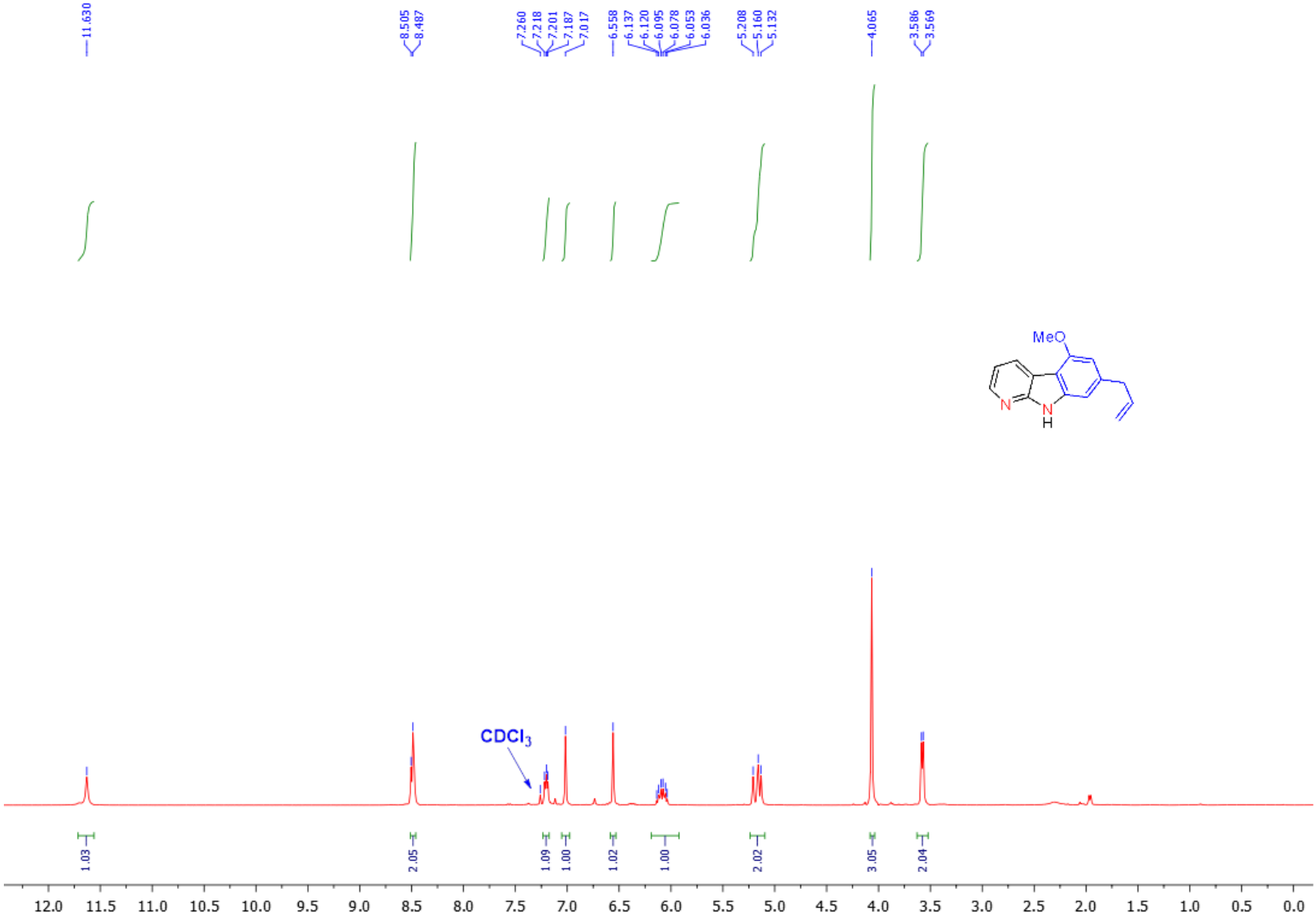
^{1}H-NMR of *ethyl 2-(9H-pyrido[2,3-b]indol-7-yl)acetate (2j)* (25 ºC, 400 MHz, DMSO-d_6):



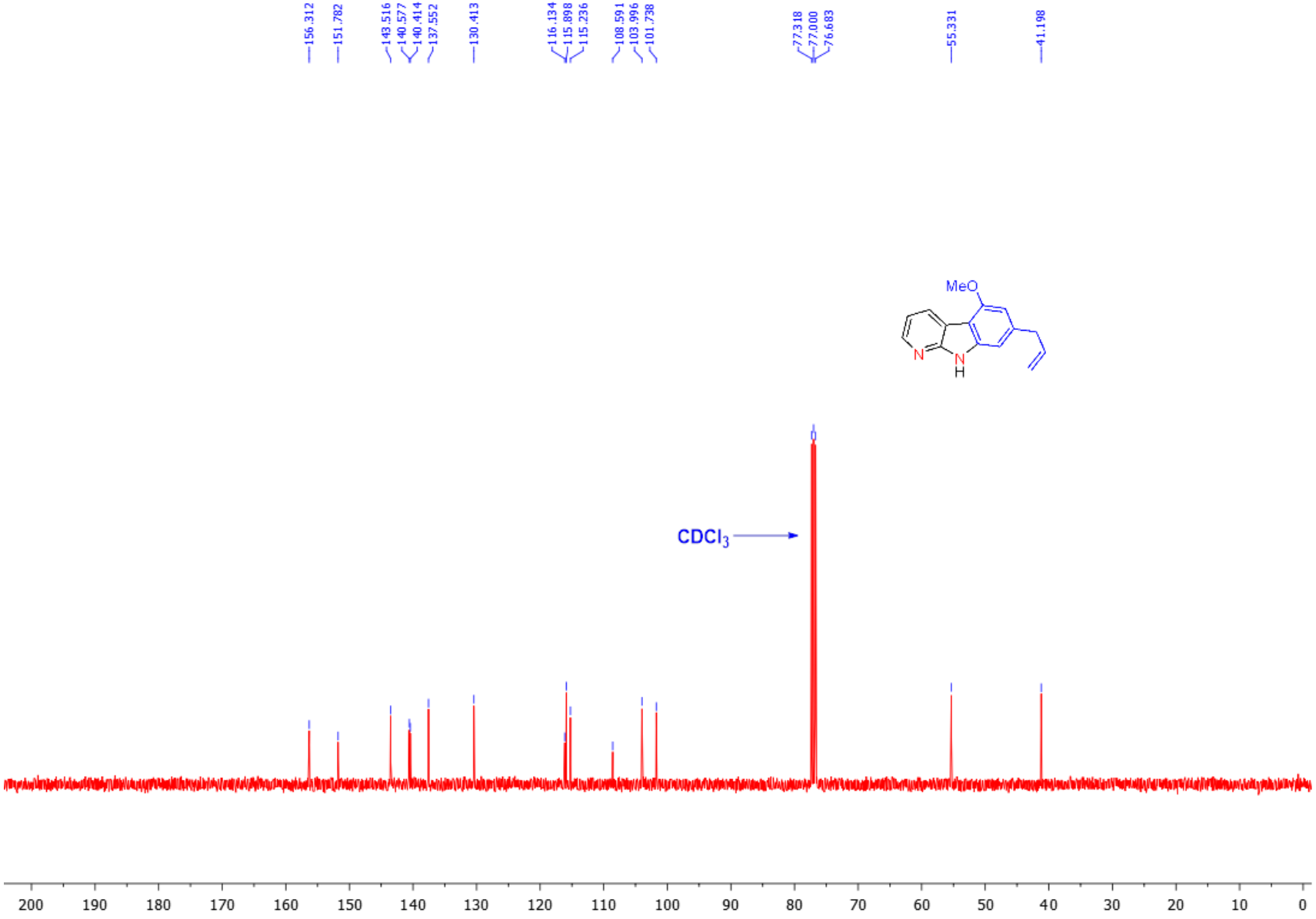
^{13}C-NMR of *ethyl 2-(9H-pyrido[2,3-b]indol-7-yl)acetate (2j)* (25 ºC, 100 MHz, DMSO-d_6):



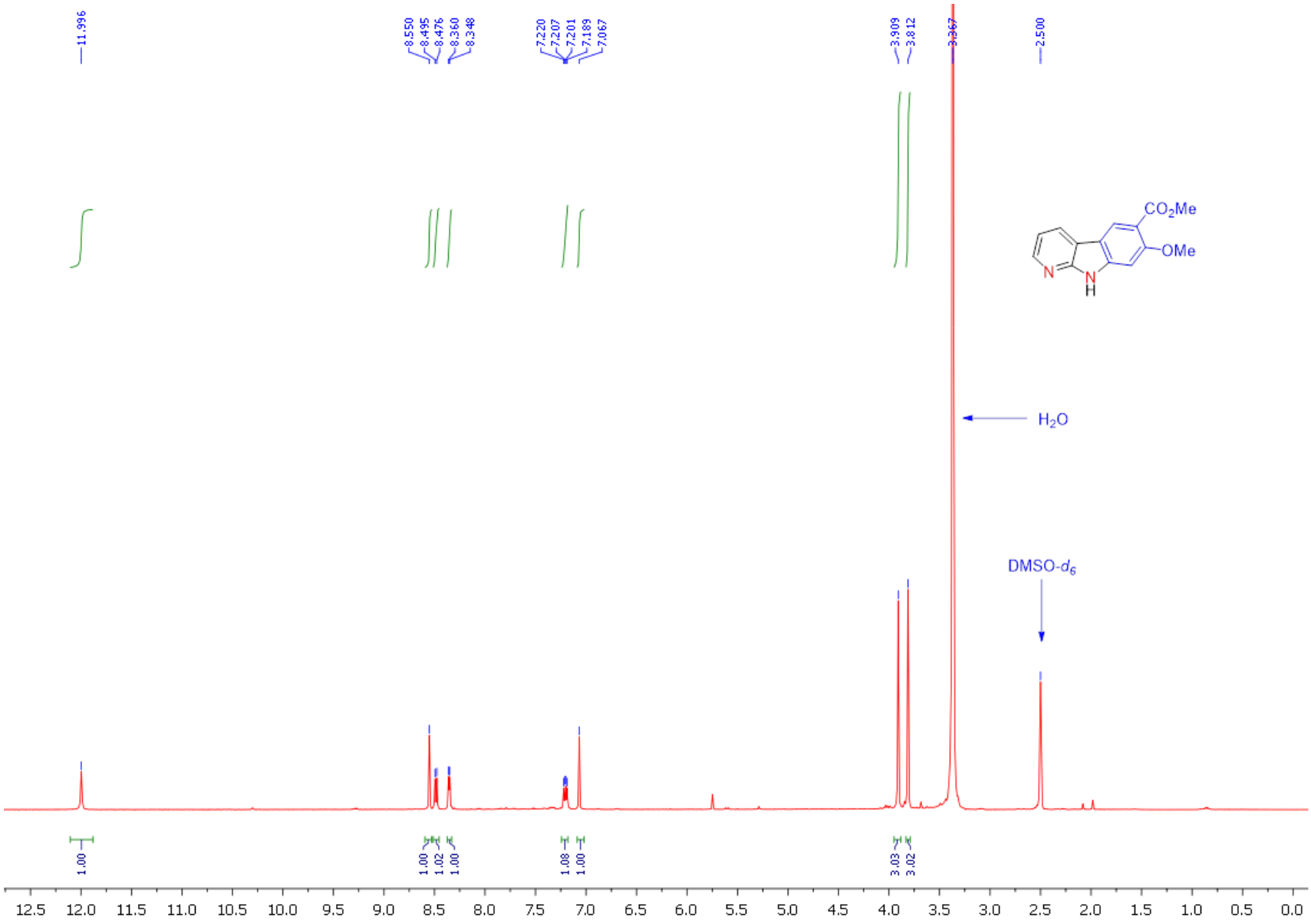
^{1}H-NMR of *7-allyl-5-methoxy-9H-pyrido[2,3-b]indole (2k)* (25 °C, 400 MHz, $CDCl_3$):



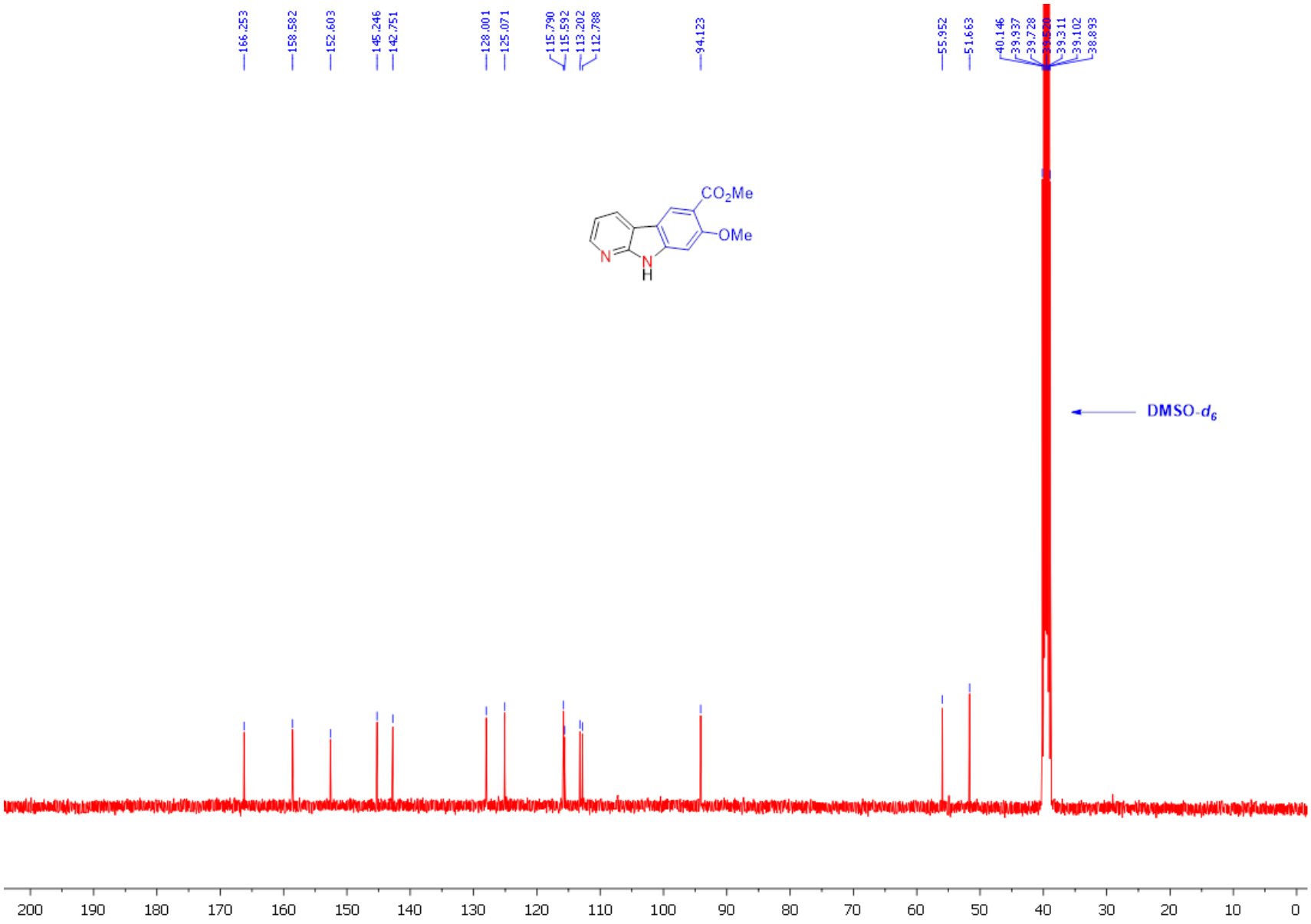
^{13}C-NMR of *7-allyl-5-methoxy-9H-pyrido[2,3-b]indole (2k*) (25 ºC, 100 MHz, $CDCl_3$):



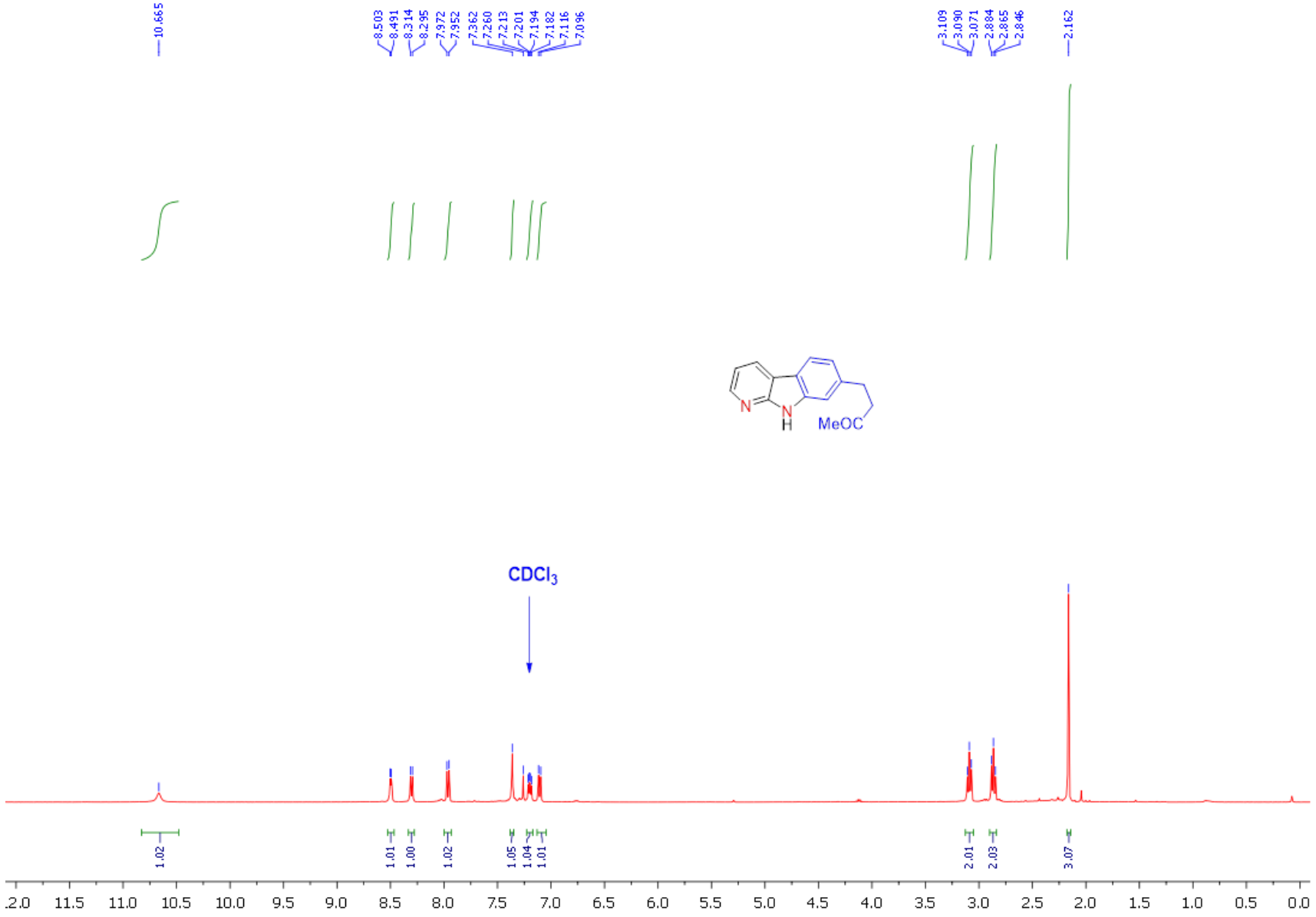
^{1}H-NMR of *methyl 6-methoxy-9H-pyrido[2,3-b]indole-7-carboxylate (2l)* (25 ºC, 400 MHz, DMSO-d_6):



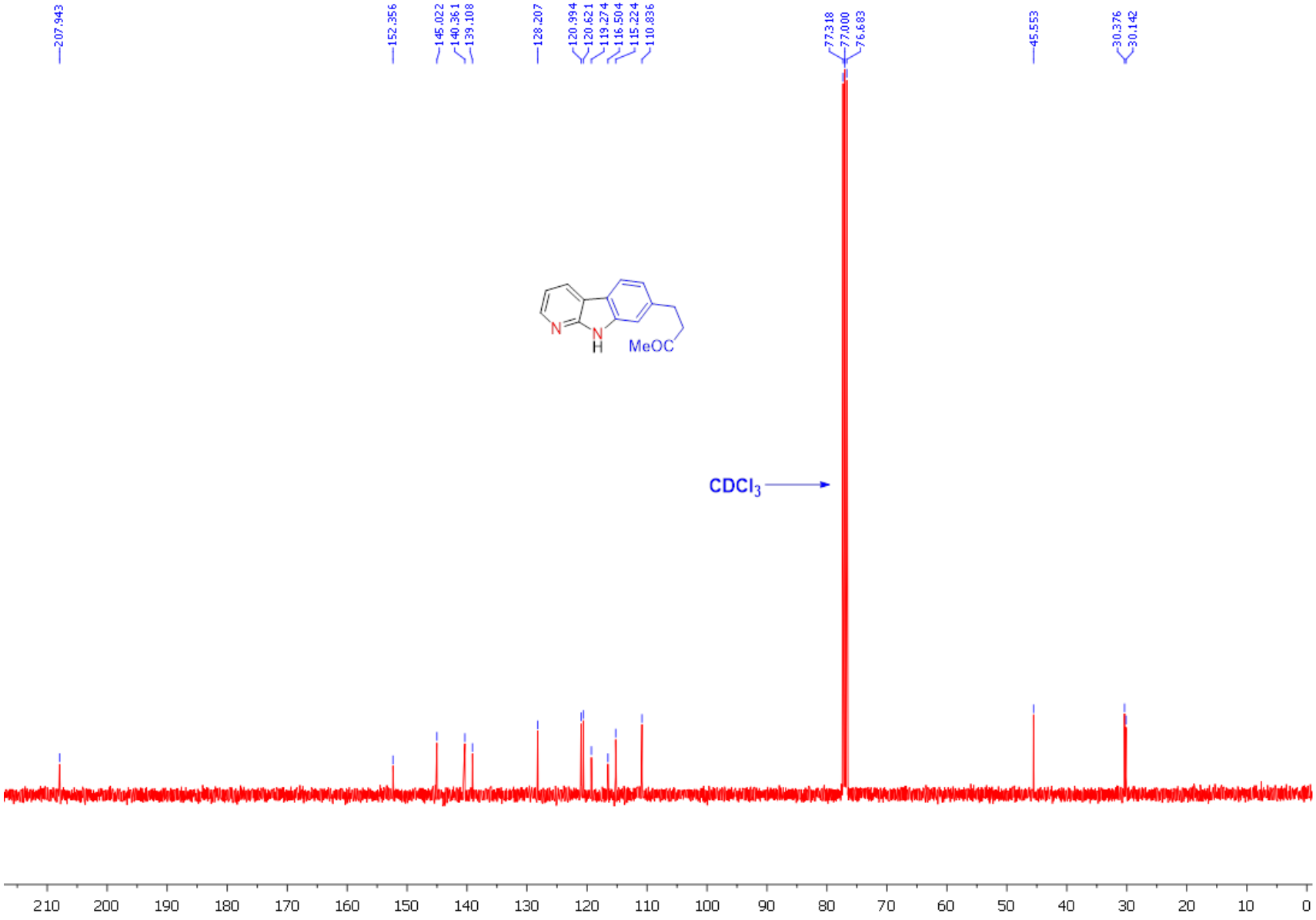
^{13}C-NMR of *methyl 6-methoxy-9H-pyrido[2,3-b]indole-7-carboxylate (2l)* (25 ºC, 100 MHz, DMSO-d_6):



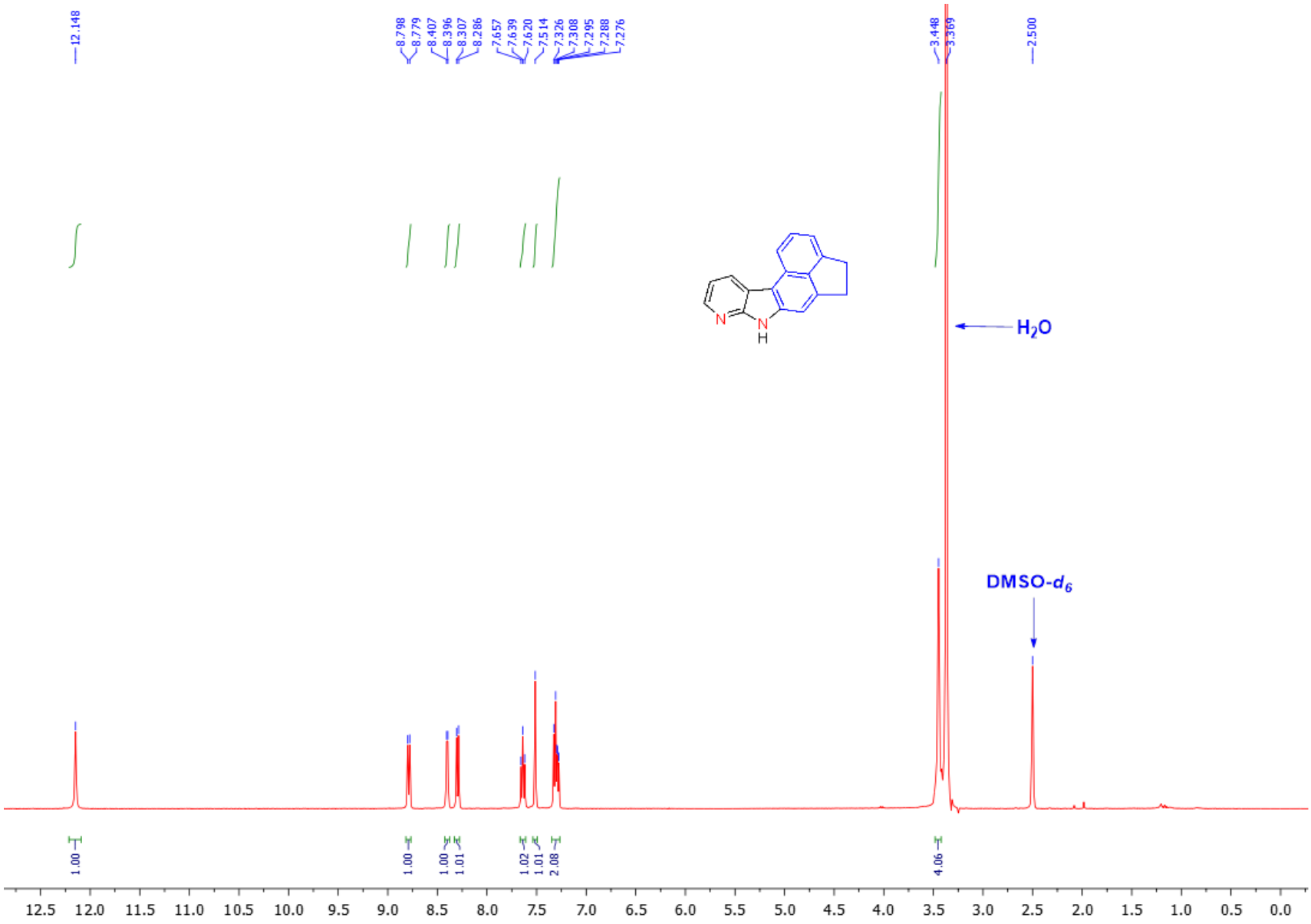
^{1}H-NMR of *4-(9H-pyrido[2,3-b]indol-7-yl)butan-2-one (2m)* (25 °C, 400 MHz, $CDCl_3$):



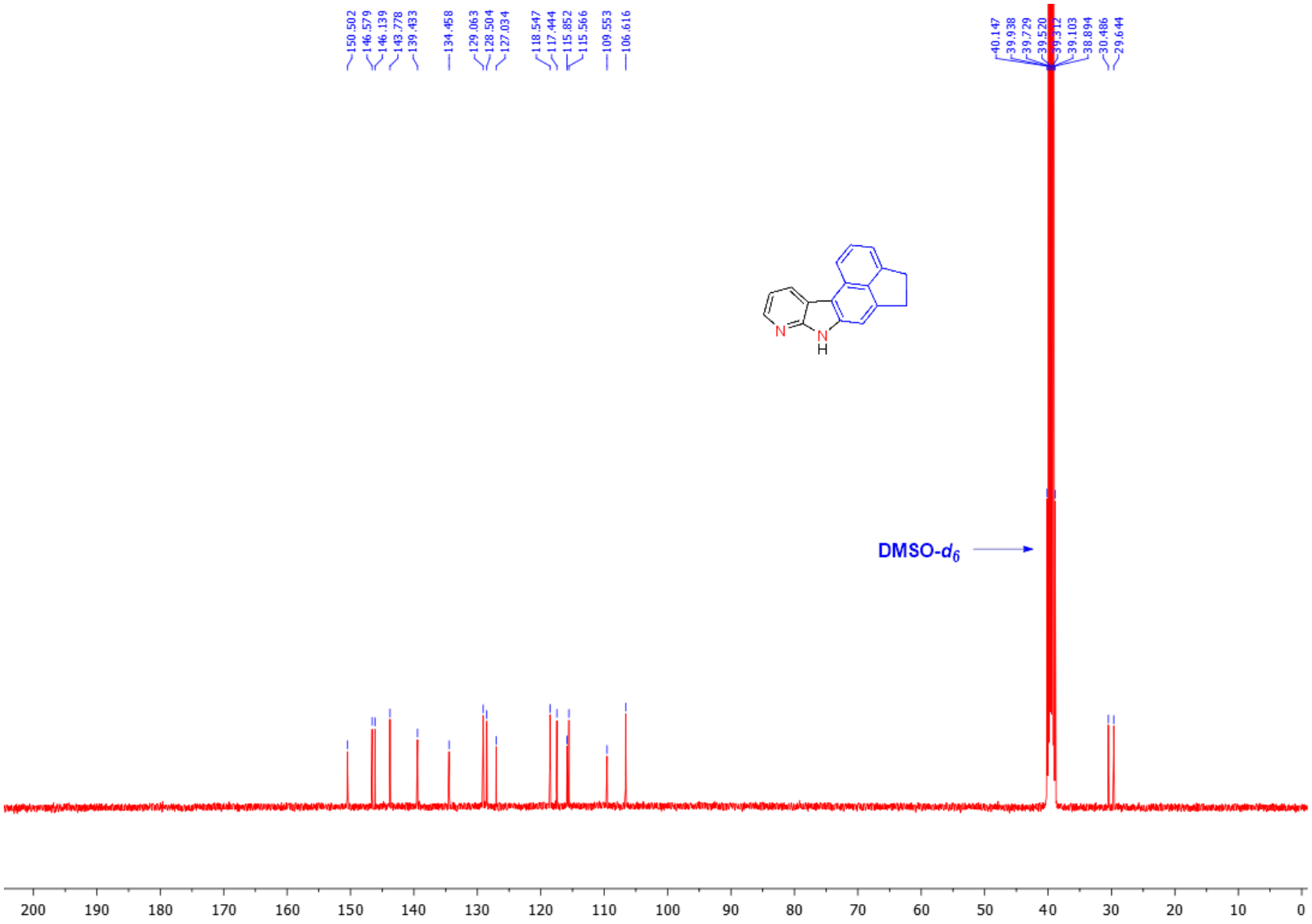
^{13}C-NMR of *4-(9H-pyrido[2,3-b]indol-7-yl)butan-2-one (2m)* (25 °C, 100 MHz, $CDCl_3$):



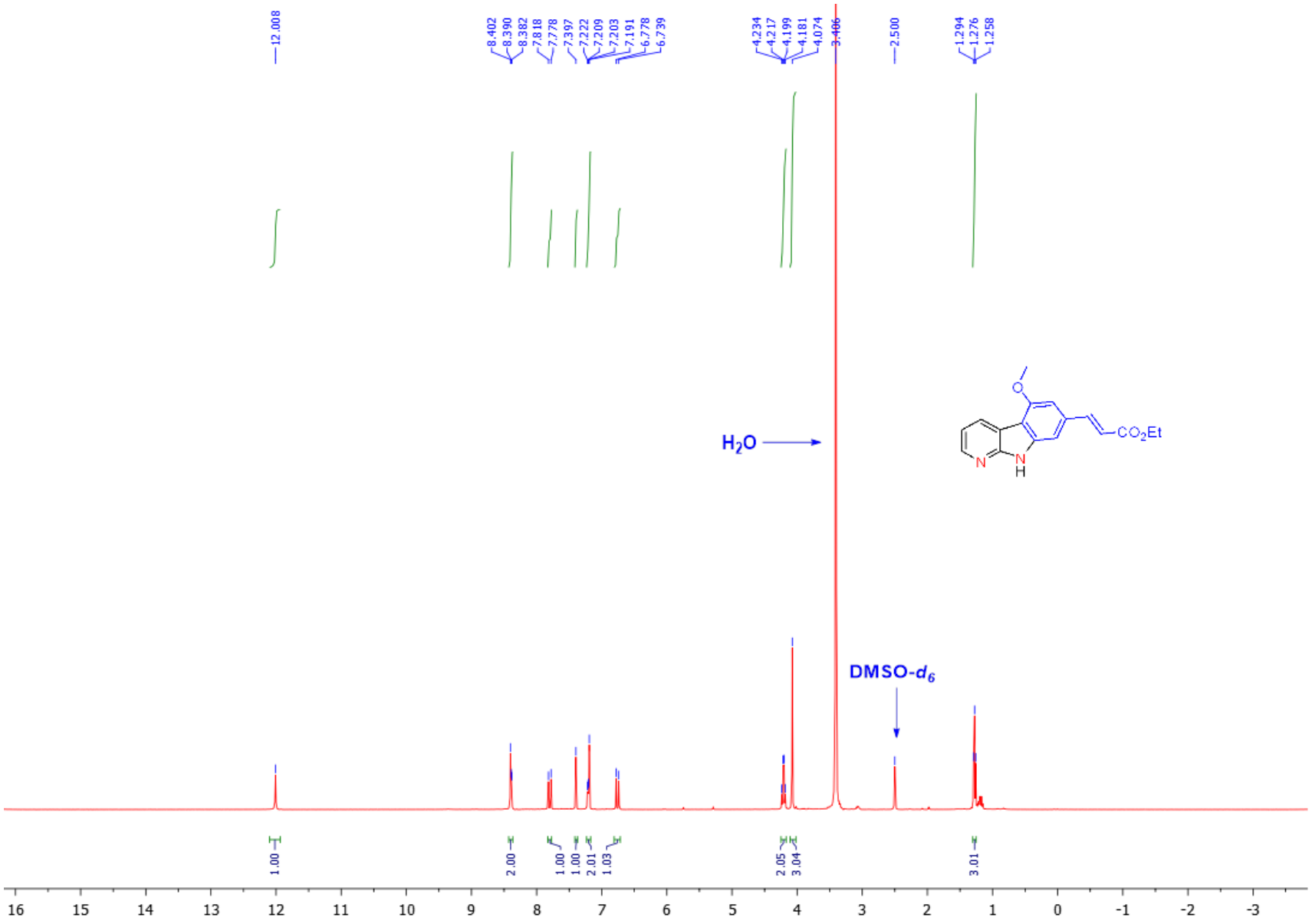
^{1}H-NMR of *5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole (2n)* (25 ^{o}C, 400 MHz, , DMSO-d_6):



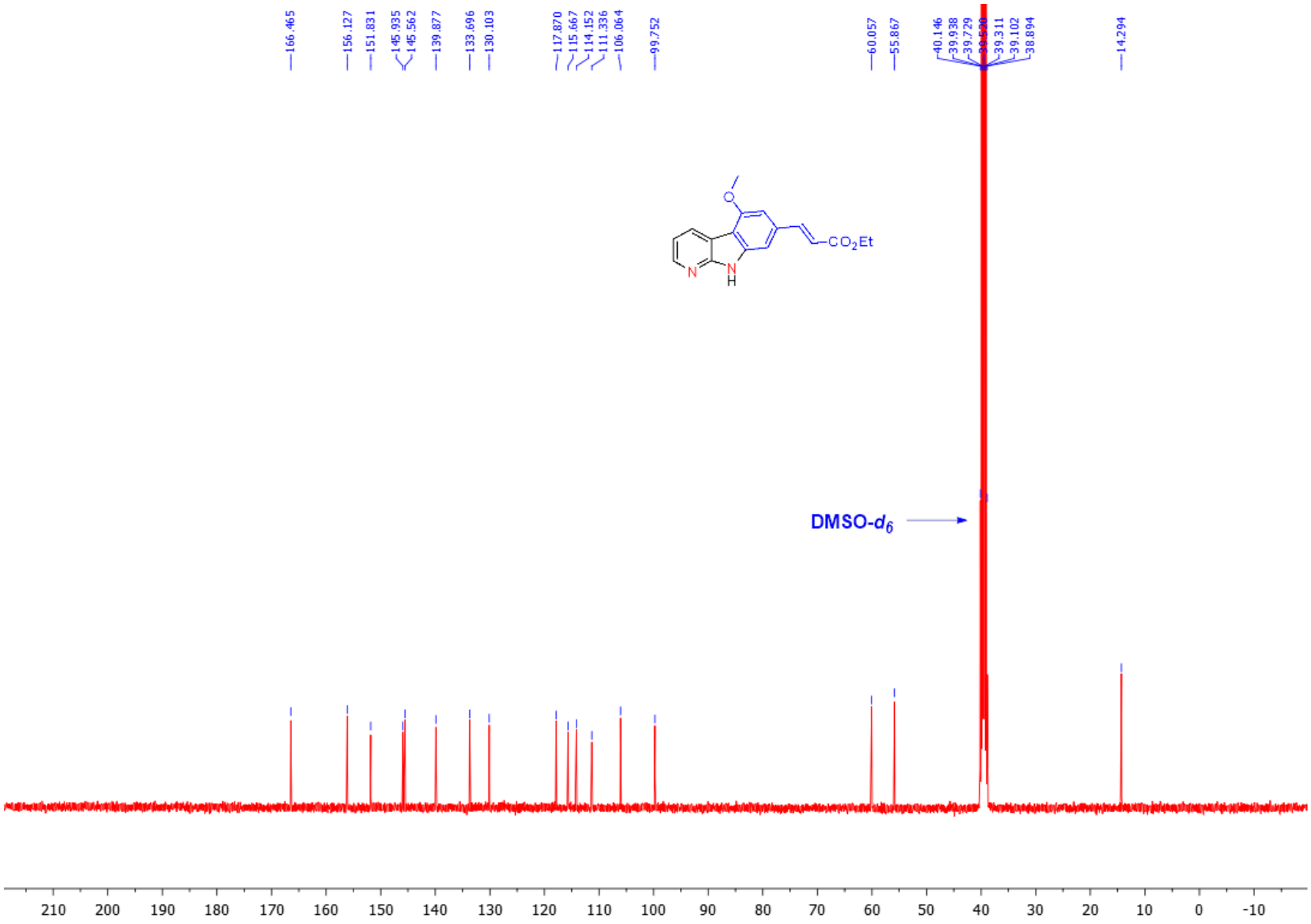
^{13}C-NMR of *5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole (2n)* (25 ºC, 100 MHz, DMSO-d_6):



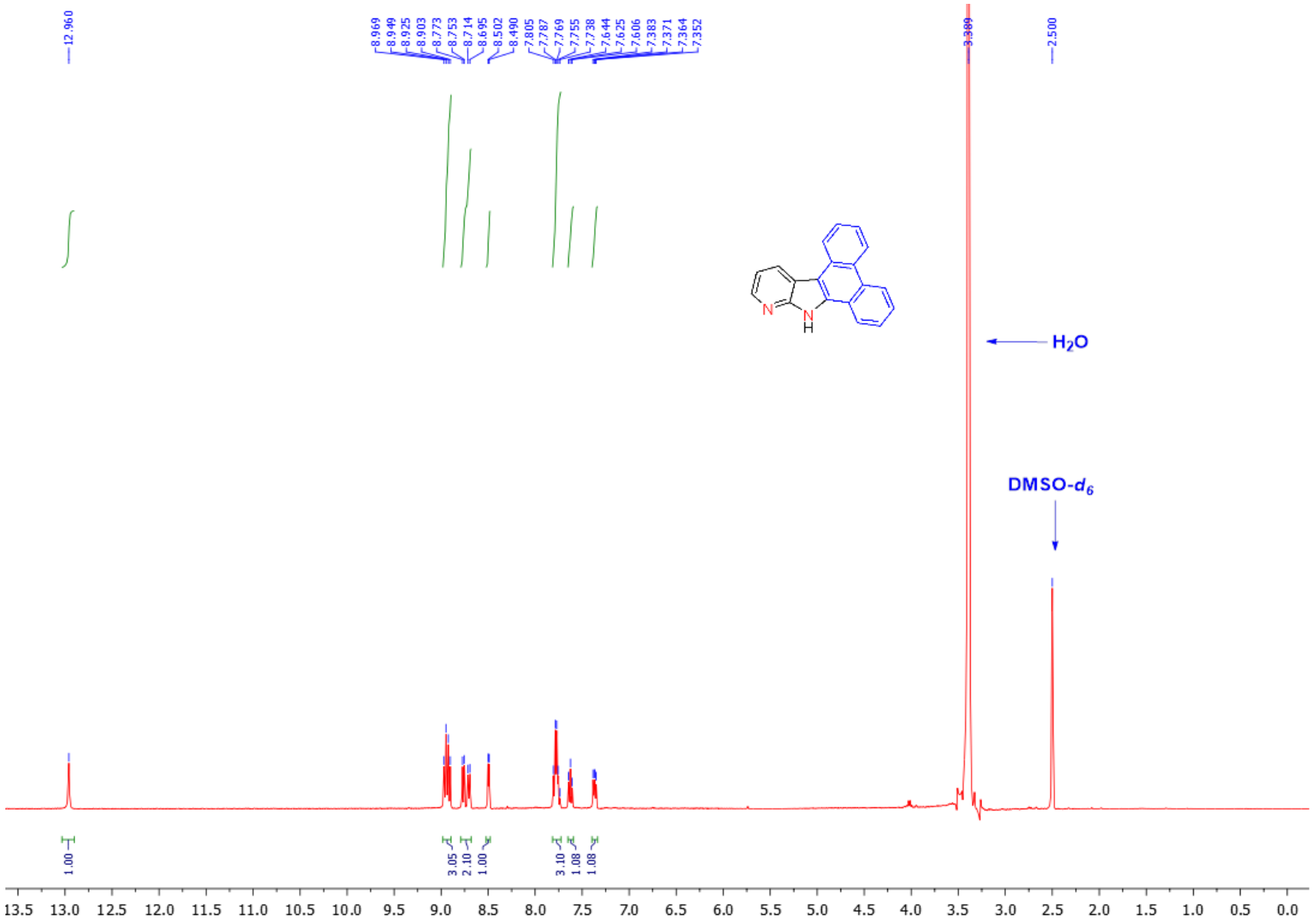
^{1}H-NMR of *ethyl (E)-3-(5-methoxy-9H-pyrido[2,3-b]indol-7-yl)acrylate (2o)* (25 ^{o}C, 400 MHz, DMSO-d_6):



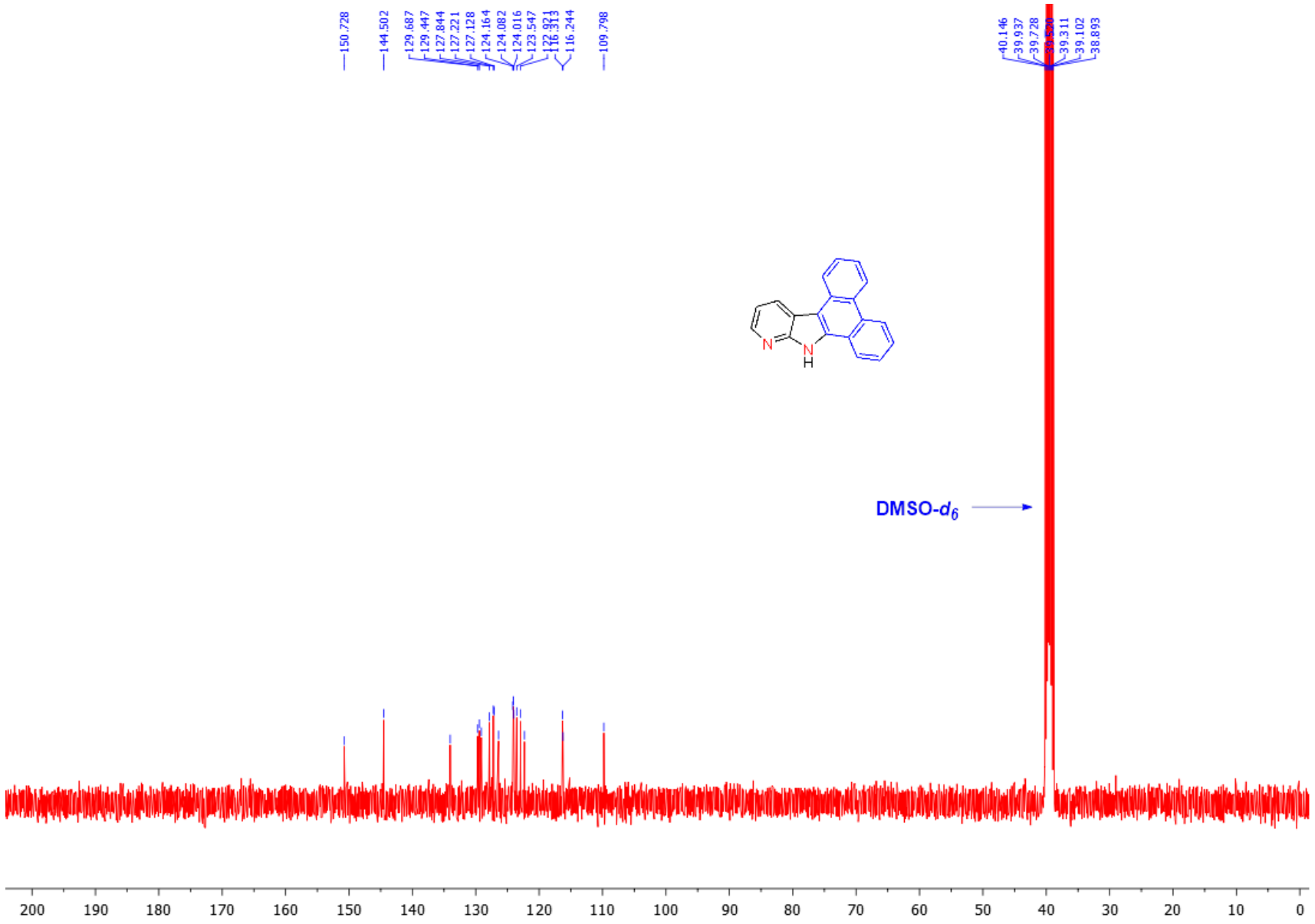
^{13}C-NMR of *ethyl (E)-3-(5-methoxy-9H-pyrido[2,3-b]indol-7-yl)acrylate (2o)* (25 ºC, 100 MHz, DMSO-d_6):



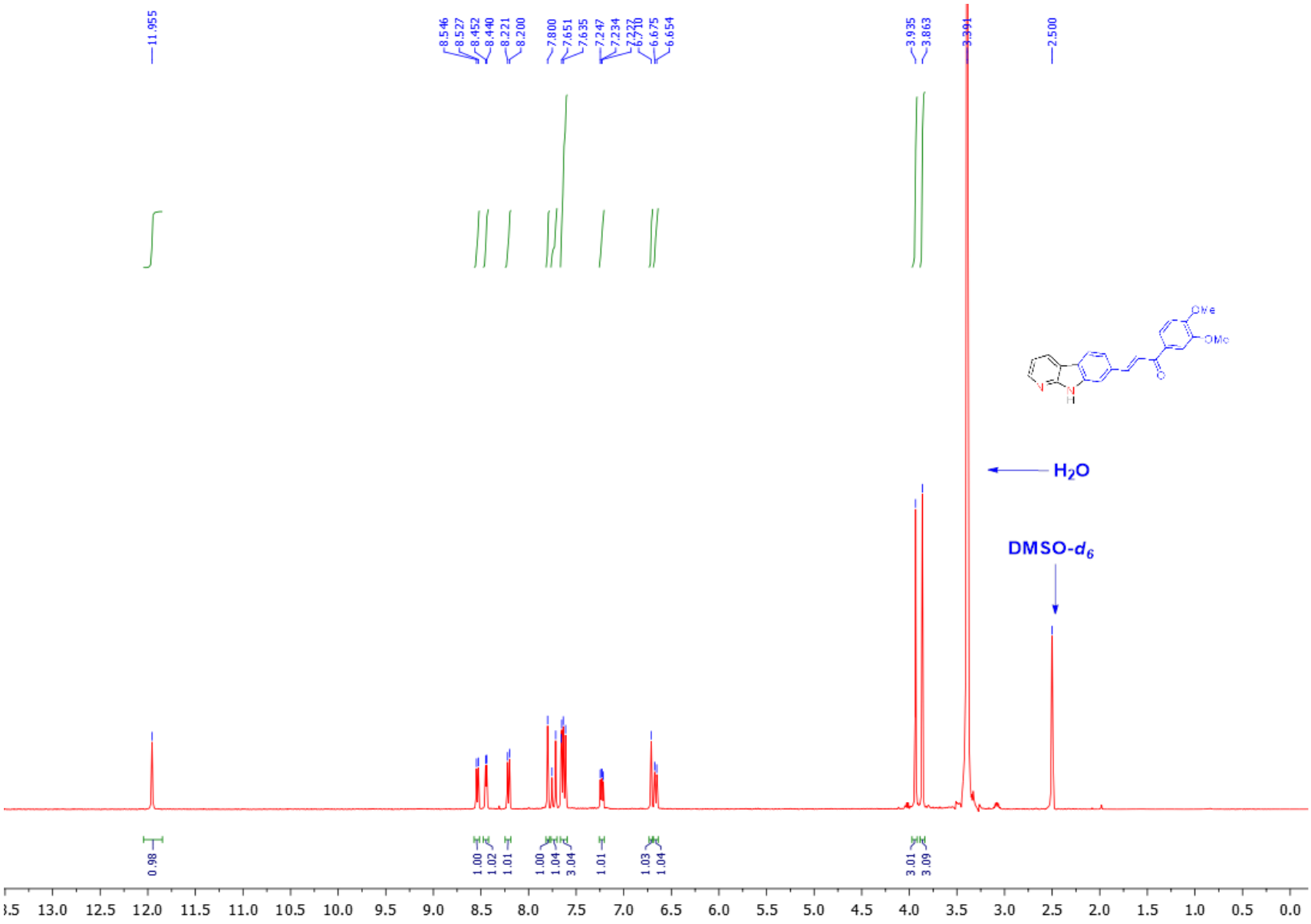
^{1}H-NMR of *9H-dibenzo[e,g]pyrido[2,3-b]indole (2p)* (25 °C, 400 MHz, DMSO-d_6):



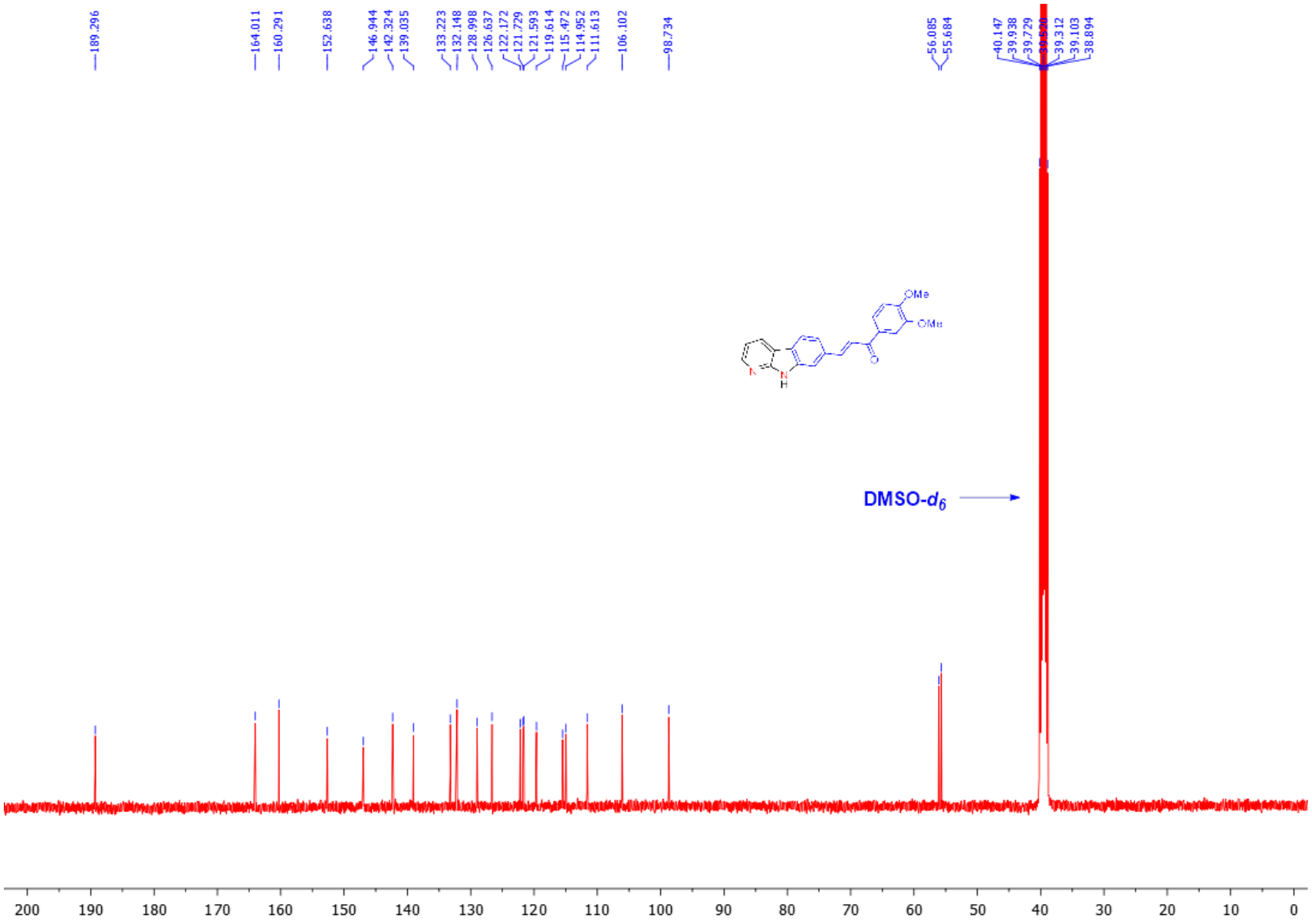
^{13}C-NMR of *9H-dibenzo[e,g]pyrido[2,3-b]indole (2p)* (25 °C, 100 MHz, DMSO-d_6):



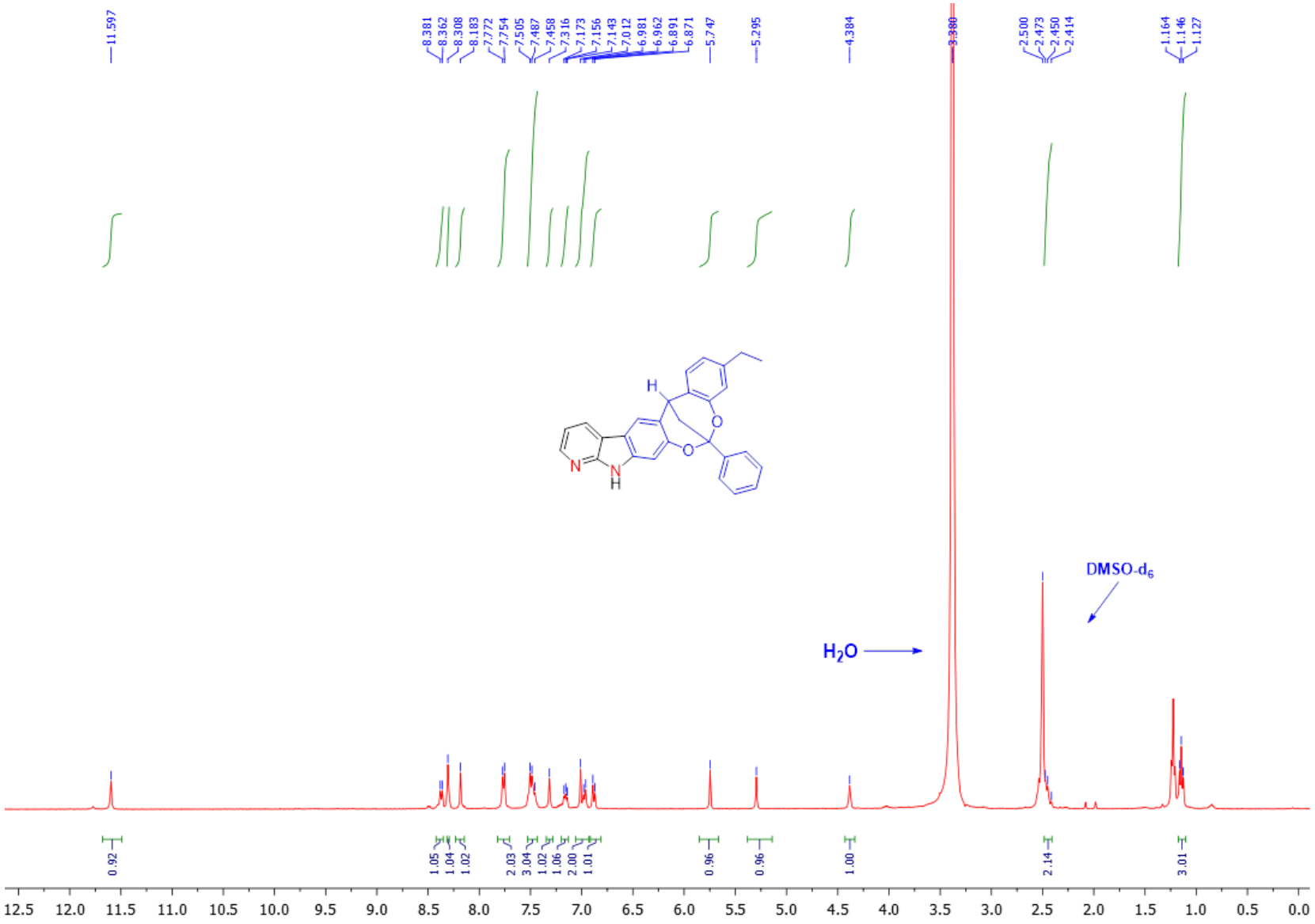
^{1}H-NMR of *(E)-1-(3,4-dimethoxyphenyl)-3-(9H-pyrido[2,3-b]indol-7-yl)prop-2-en-1-one (2q)* (25 ^{o}C, 400 MHz, $CDCl_3$):



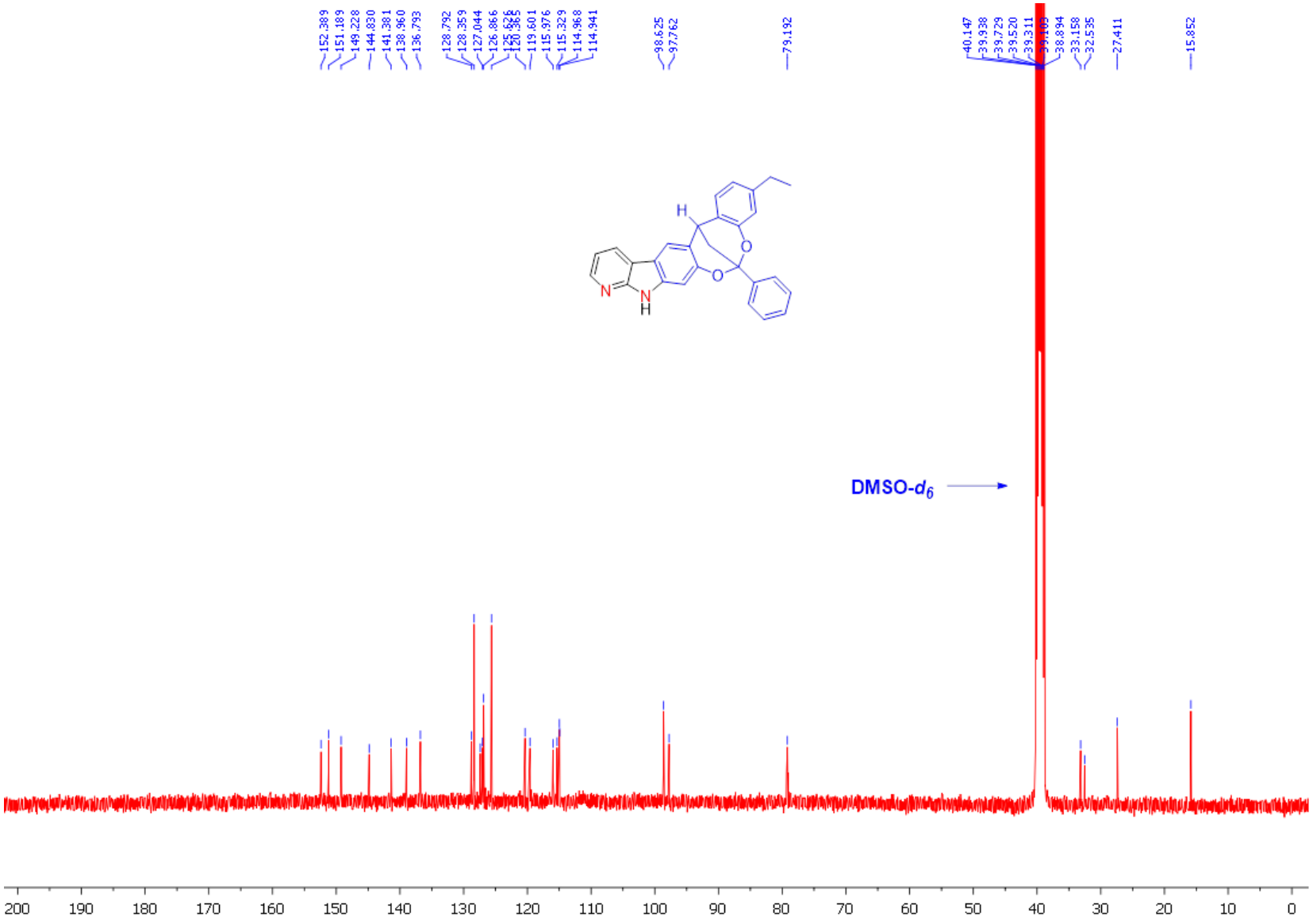
^{13}C-NMR of *(E)-1-(3,4-dimethoxyphenyl)-3-(9H-pyrido[2,3-b]indol-7-yl)prop-2-en-1-one (2q)* (25 ºC, 100 MHz, $CDCl_3$):



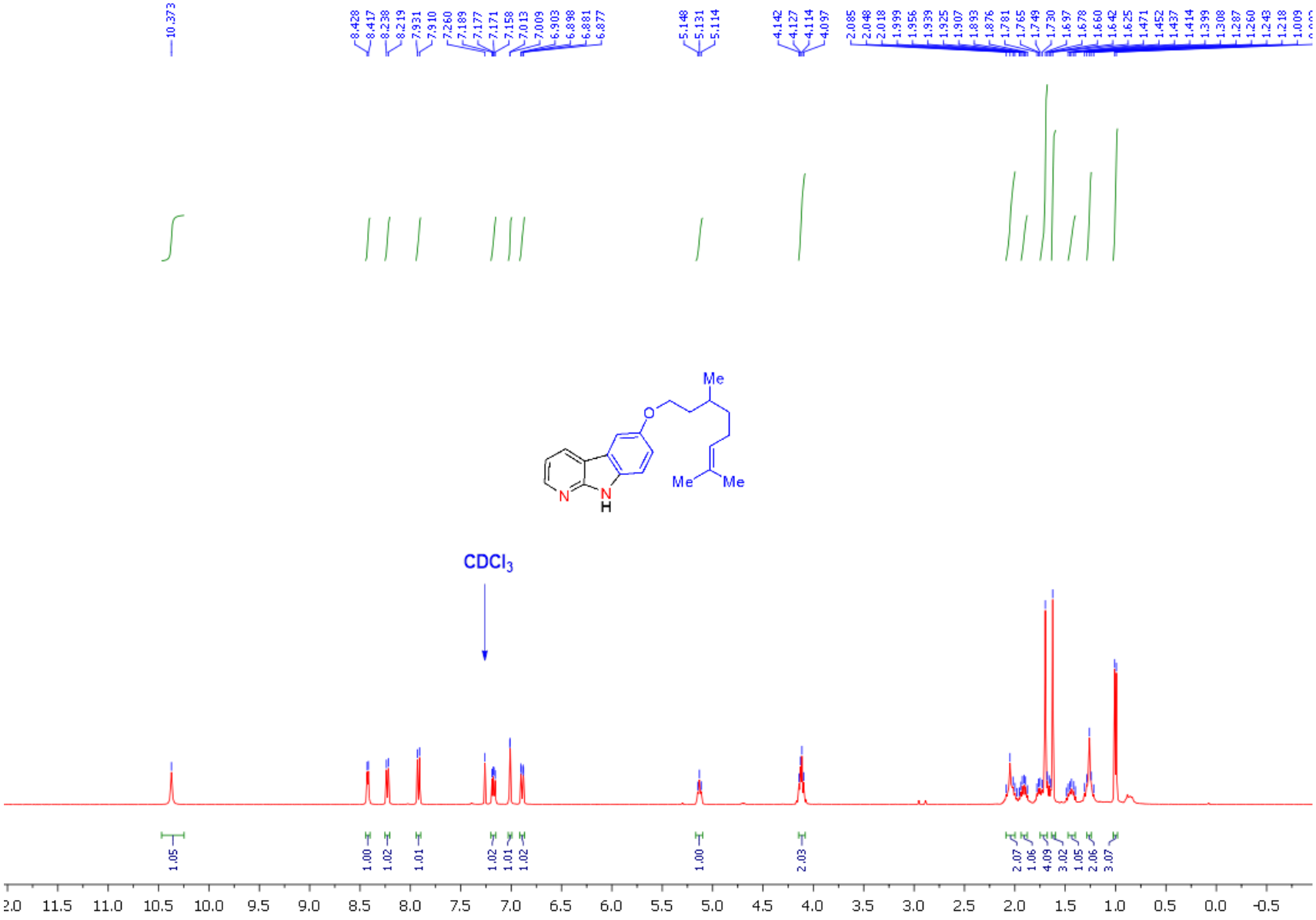
[1]H-NMR of *3-ethyl-6-phenyl-9,15-dihydro-6,15-methanobenzo[7,8][1,3]dioxocino[5,4-f]pyrido[2,3-b]indole (2r)* (25 °C, 400 MHz, DMSO-d_6):



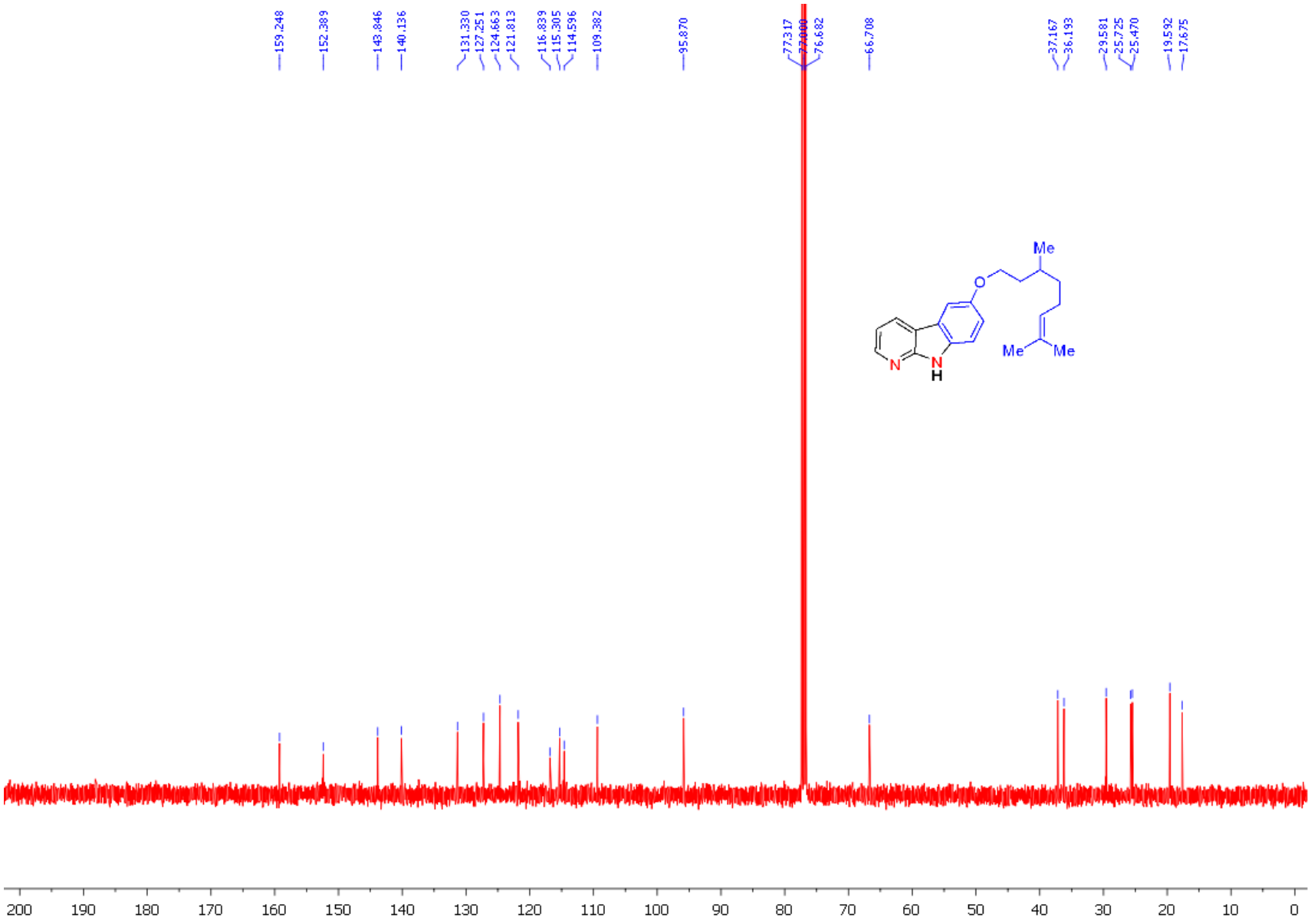
^{13}C-NMR of *3-ethyl-6-phenyl-9,15-dihydro-6,15-methanobenzo[7,8][1,3]dioxocino[5,4-f]pyrido[2,3-b]indole (2r)* (25 °C, 100 MHz, DMSO-d_6):



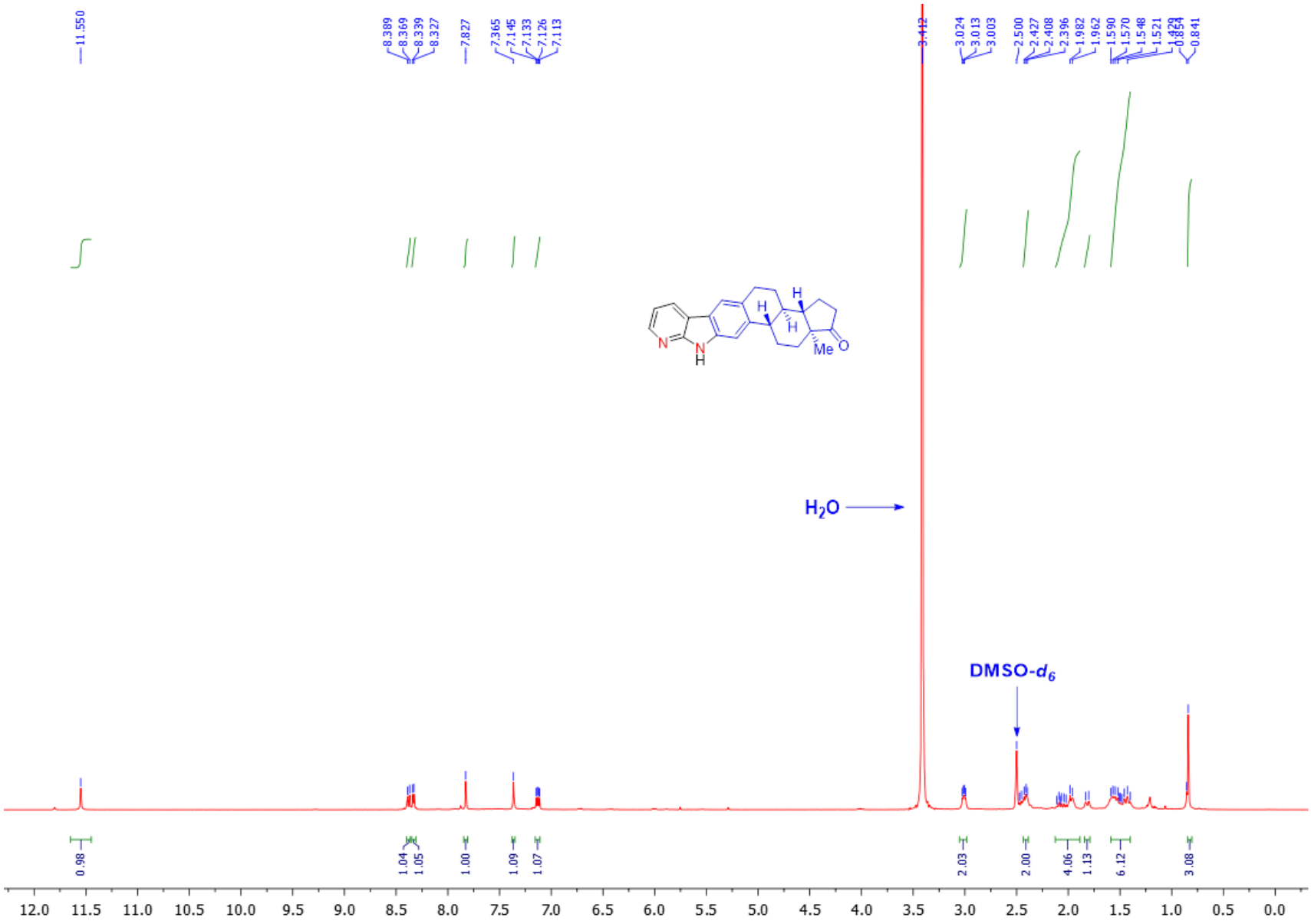
^{1}H-NMR of *6-((3,7-dimethyloct-6-en-1-yl)oxy)-9H-pyrido[2,3-b]indole (2s)* (25 °C, 400 MHz, $CDCl_3$):



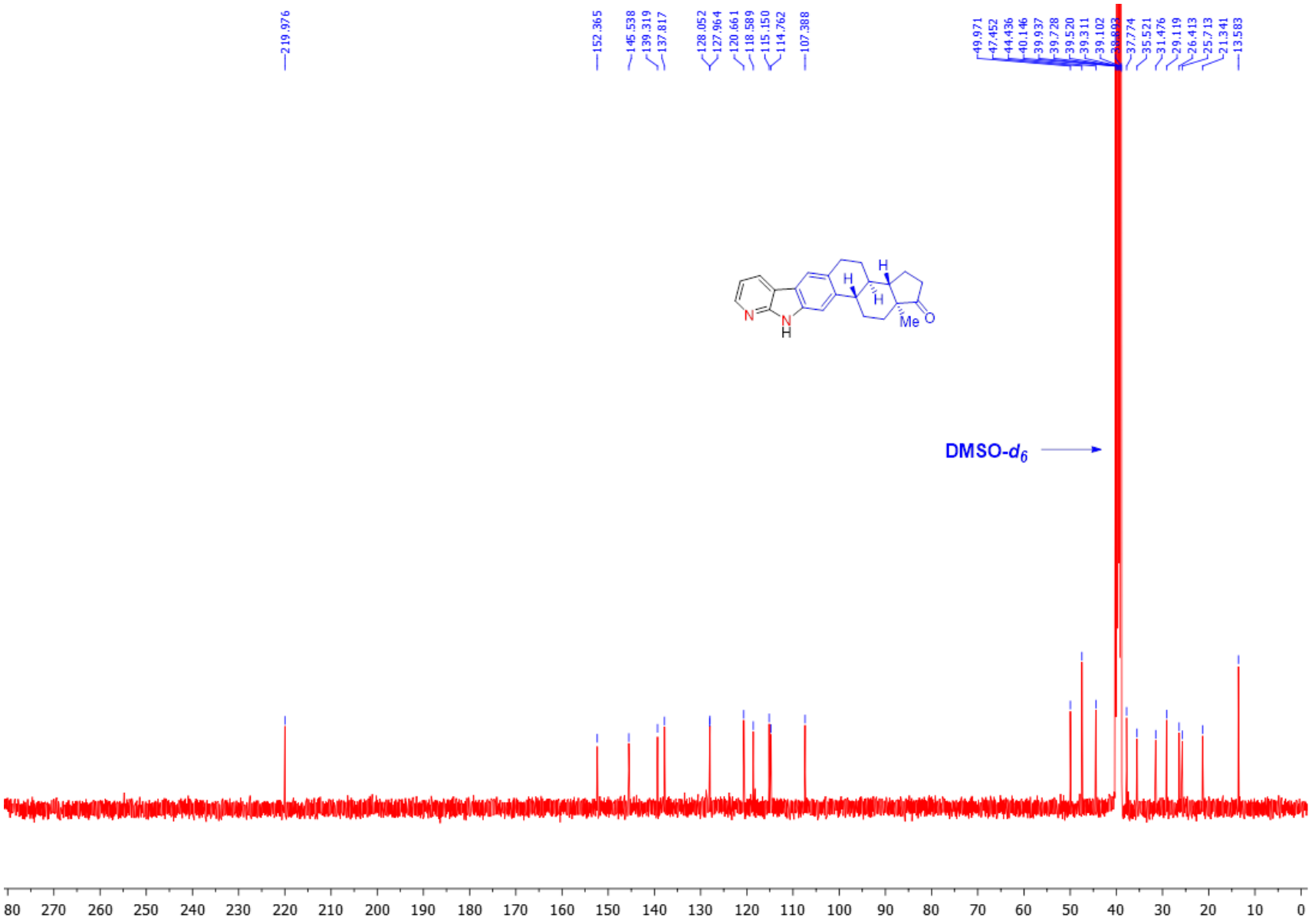
^{13}C-NMR of *6-((3,7-dimethyloct-6-en-1-yl)oxy)-9H-pyrido[2,3-b]indole (2s)* (25 °C, 100 MHz, $CDCl_3$):



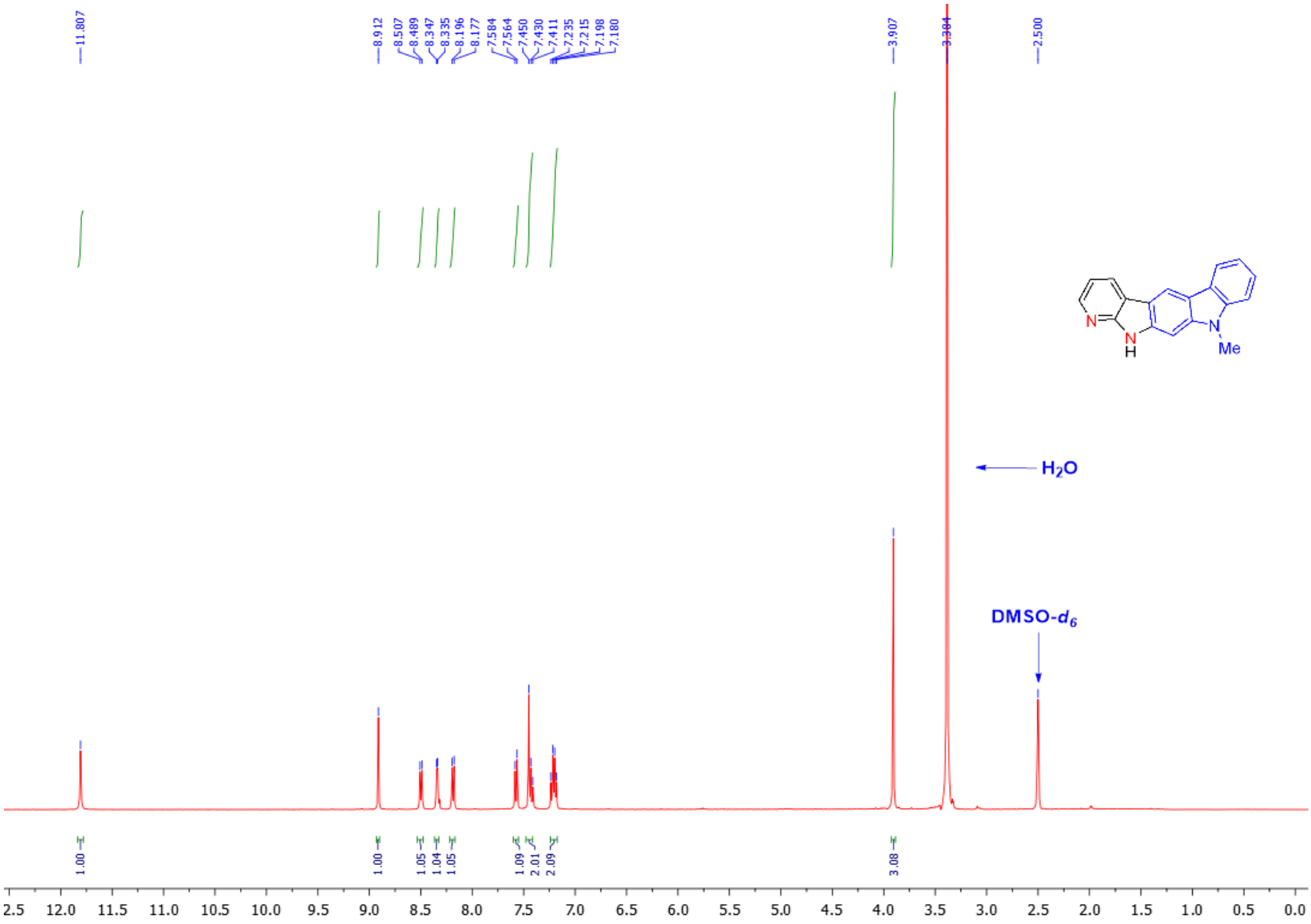
^{1}H-NMR of *2t* (25 °C, 400 MHz, $CDCl_3$):



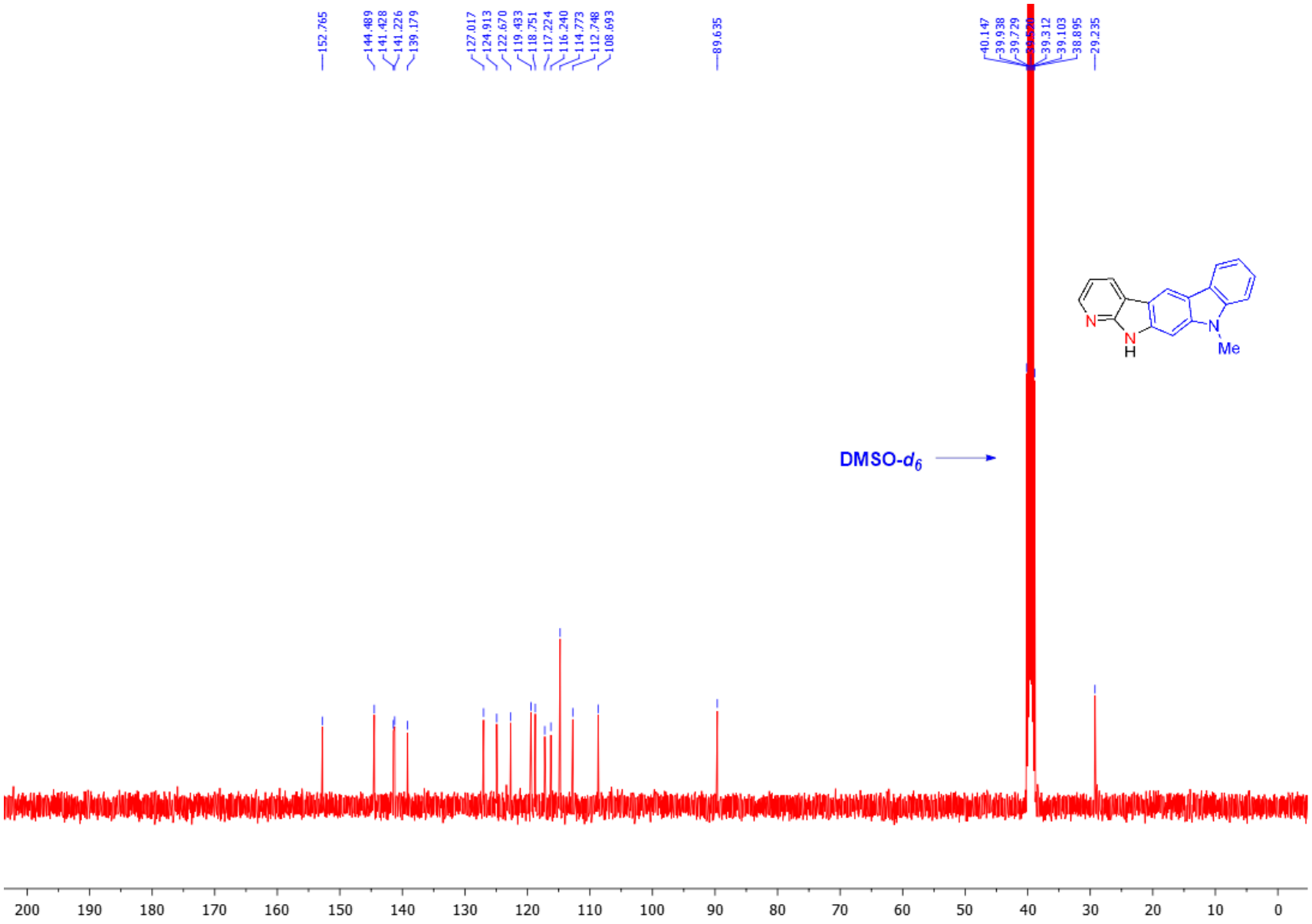
^{13}C-NMR of *2t* (25 °C, 100 MHz, $CDCl_3$):



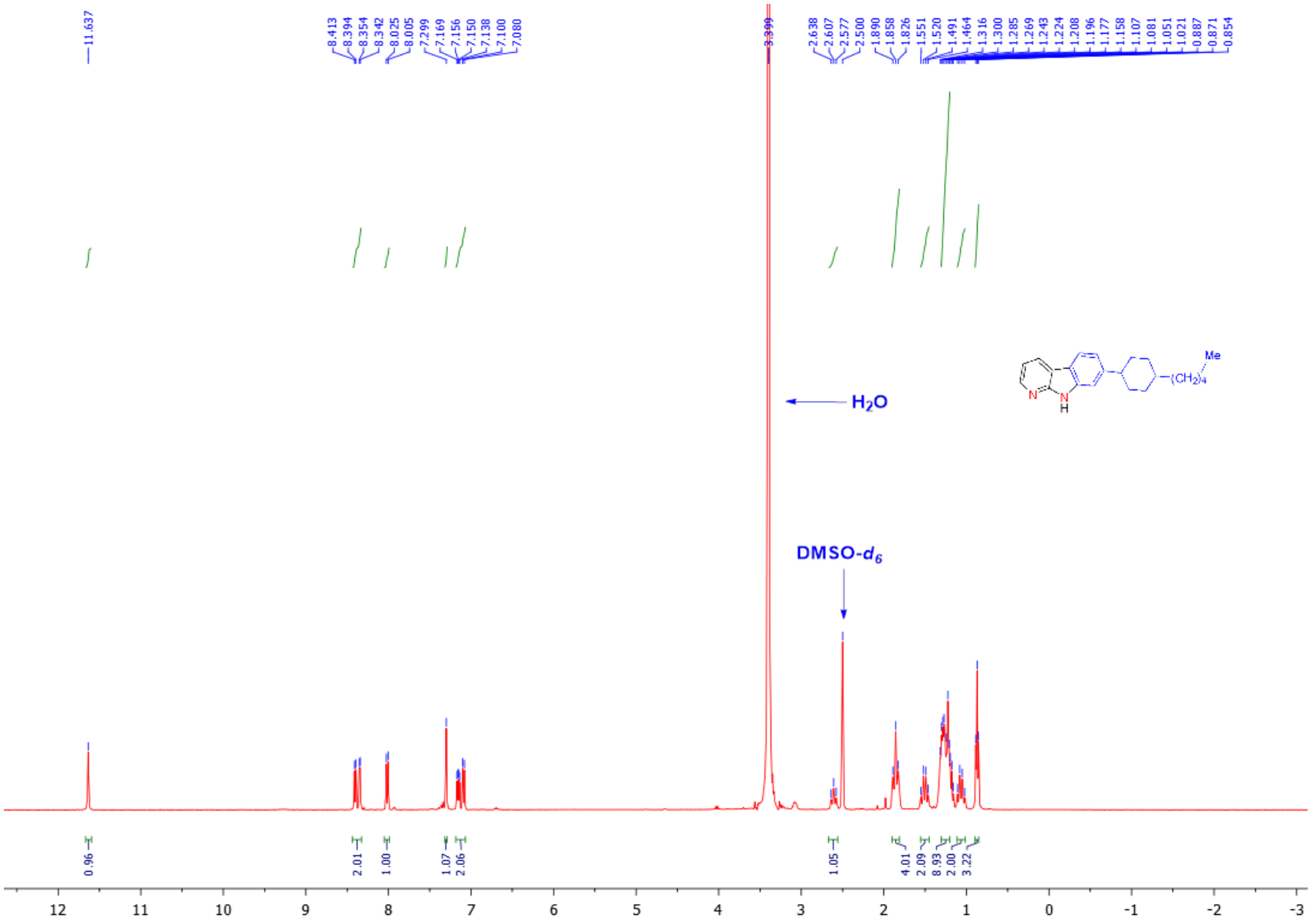
[1]H-NMR of *10-methyl-10,12-dihydropyrido[3',2':4,5]pyrrolo[2,3-b]carbazole (2u)* (25 °C, 400 MHz, DMSO-d_6):



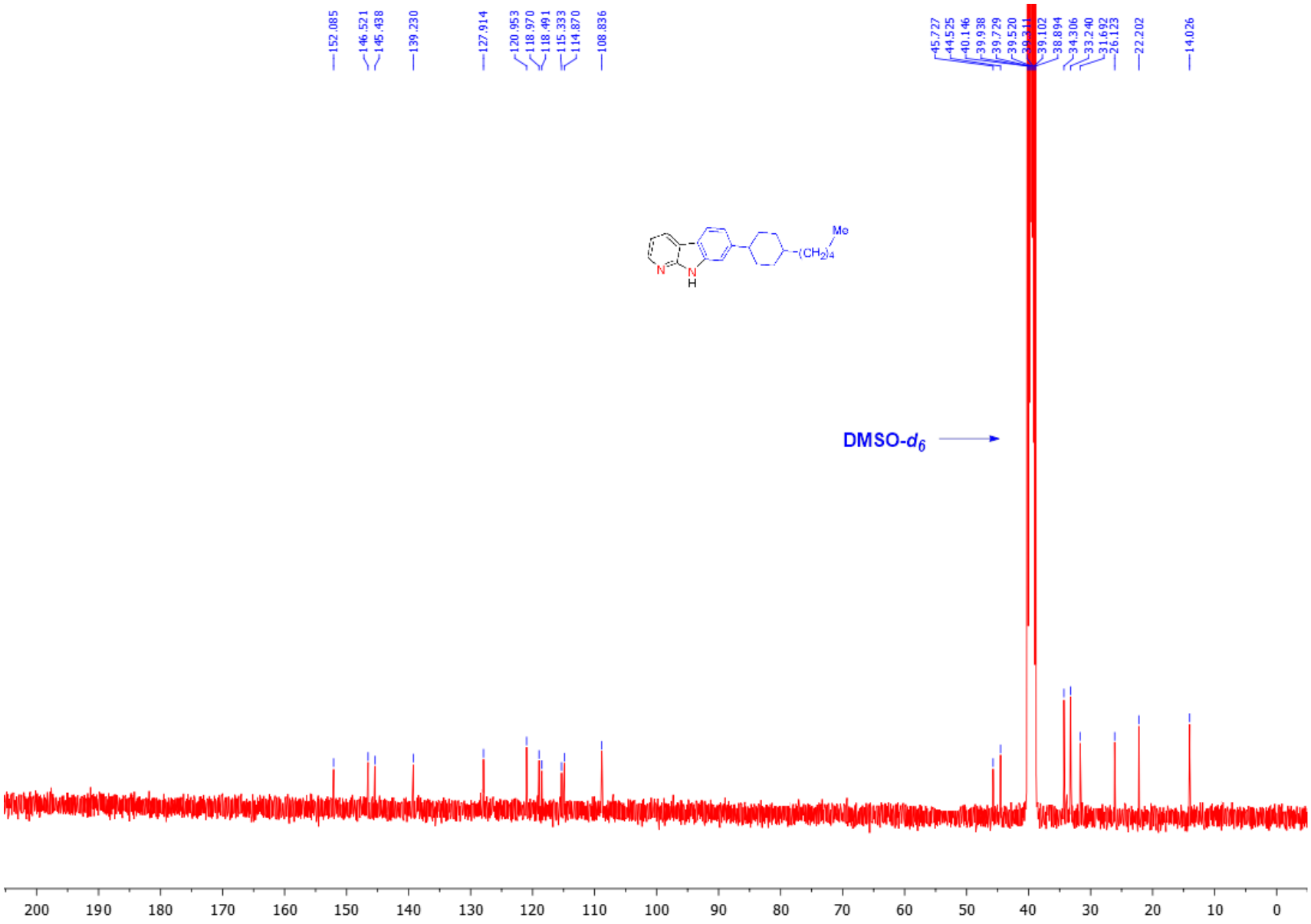
^{13}C-NMR of *10-methyl-10,12-dihydropyrido[3',2':4,5]pyrrolo[2,3-b]carbazole (2u)* (25 ºC, 100 MHz, DMSO-d_6):



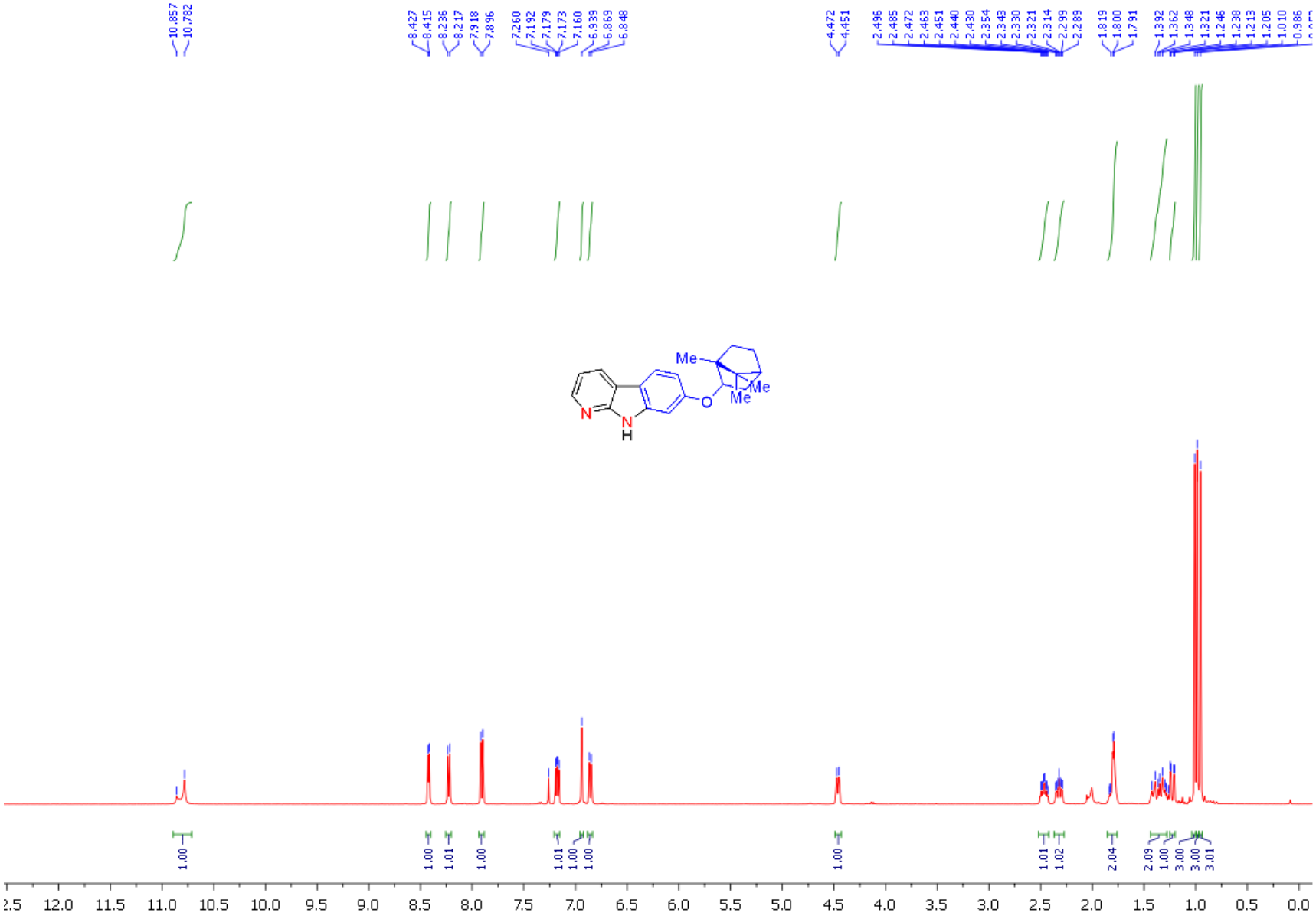
^{1}H-NMR of *7-(4-pentylcyclohexyl)-9H-pyrido[2,3-b]indole (2v)* (25 °C, 400 MHz, DMSO-d_6):



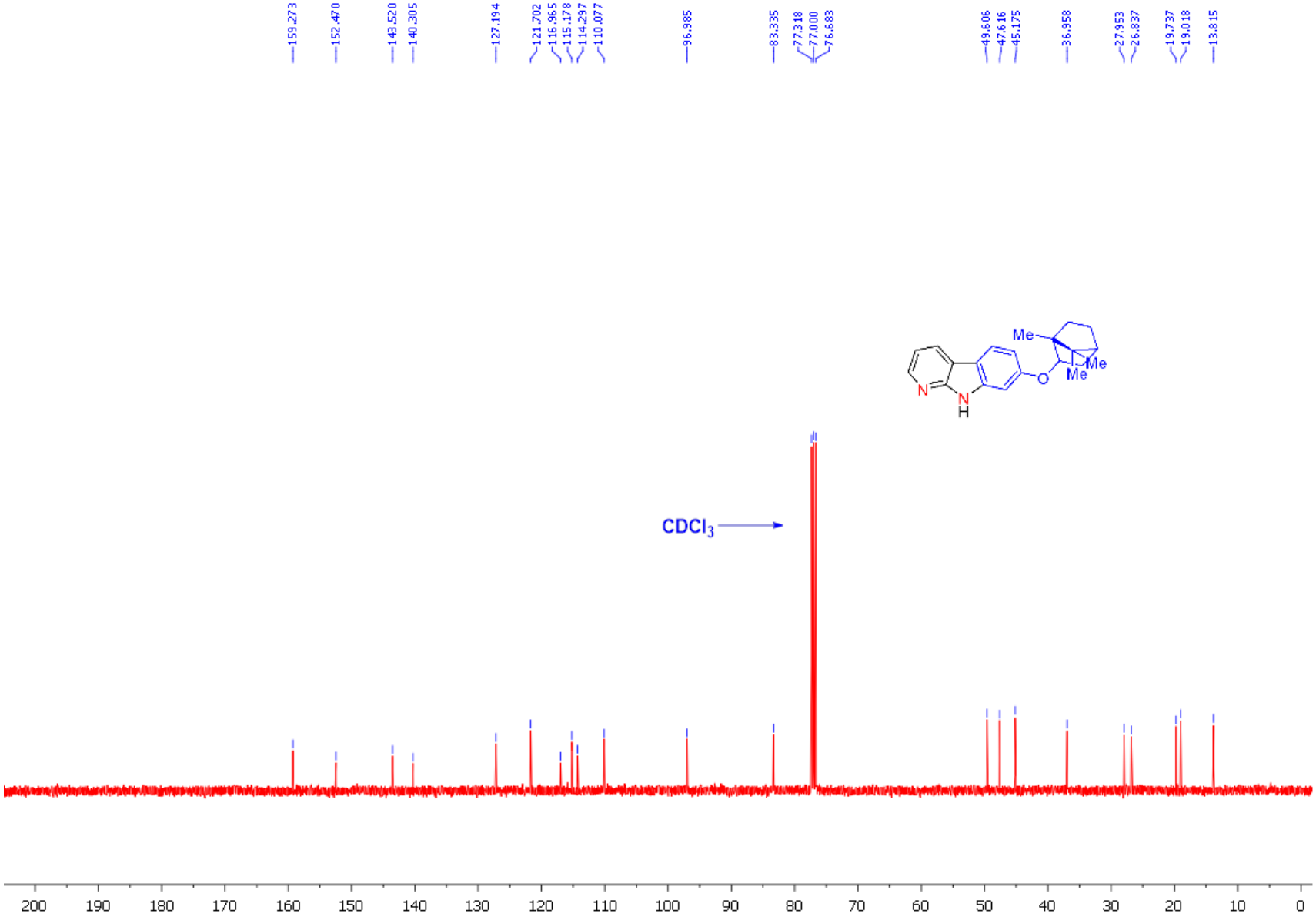
^{13}C-NMR of *7-(4-pentylcyclohexyl)-9H-pyrido[2,3-b]indole (2v)* (25 °C, 100 MHz, DMSO-d_6):



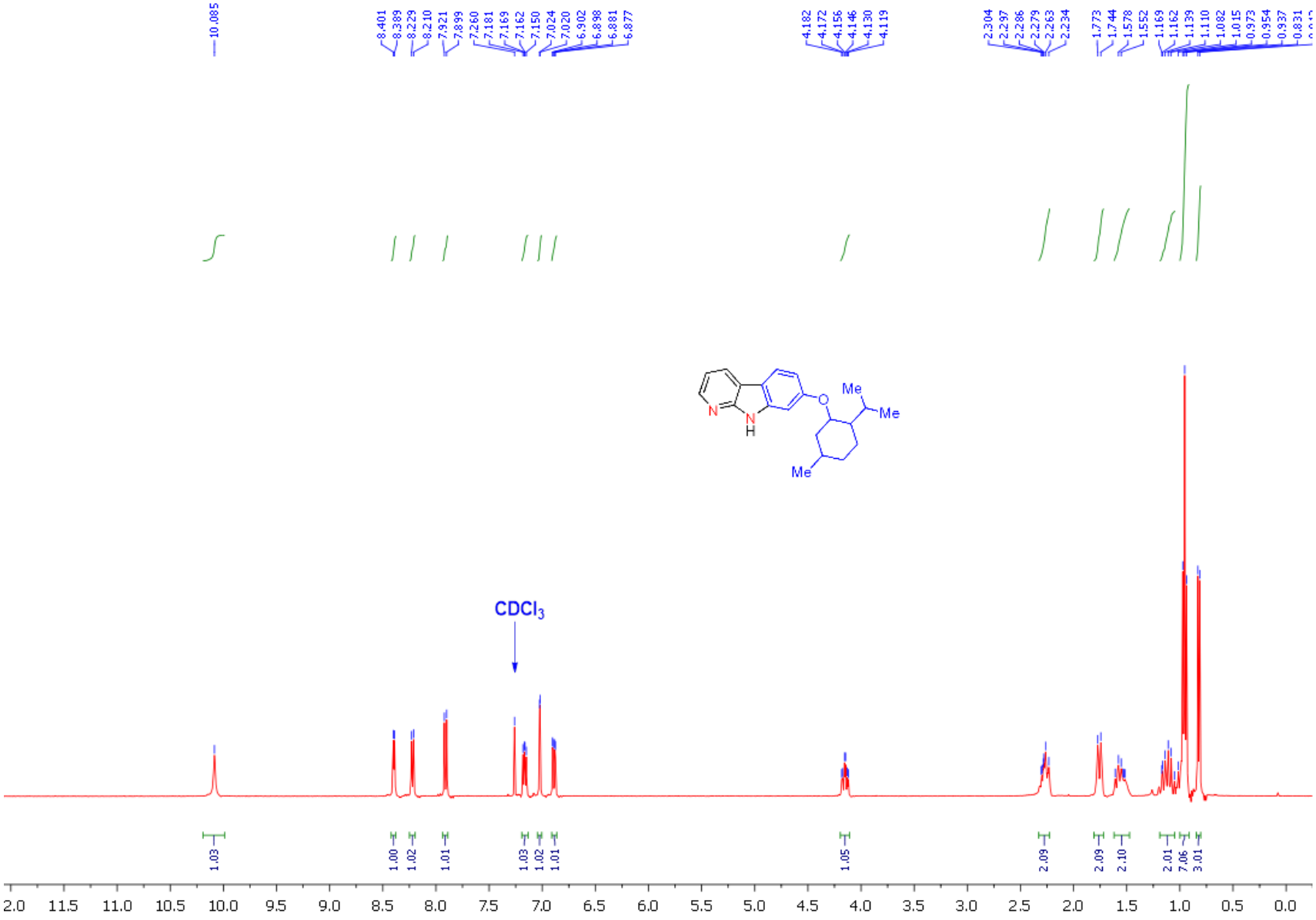
^{1}H-NMR of *7-(((1S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)-9H-pyrido[2,3-b]indole (2w)* (25 °C, 400 MHz, $CDCl_3$):



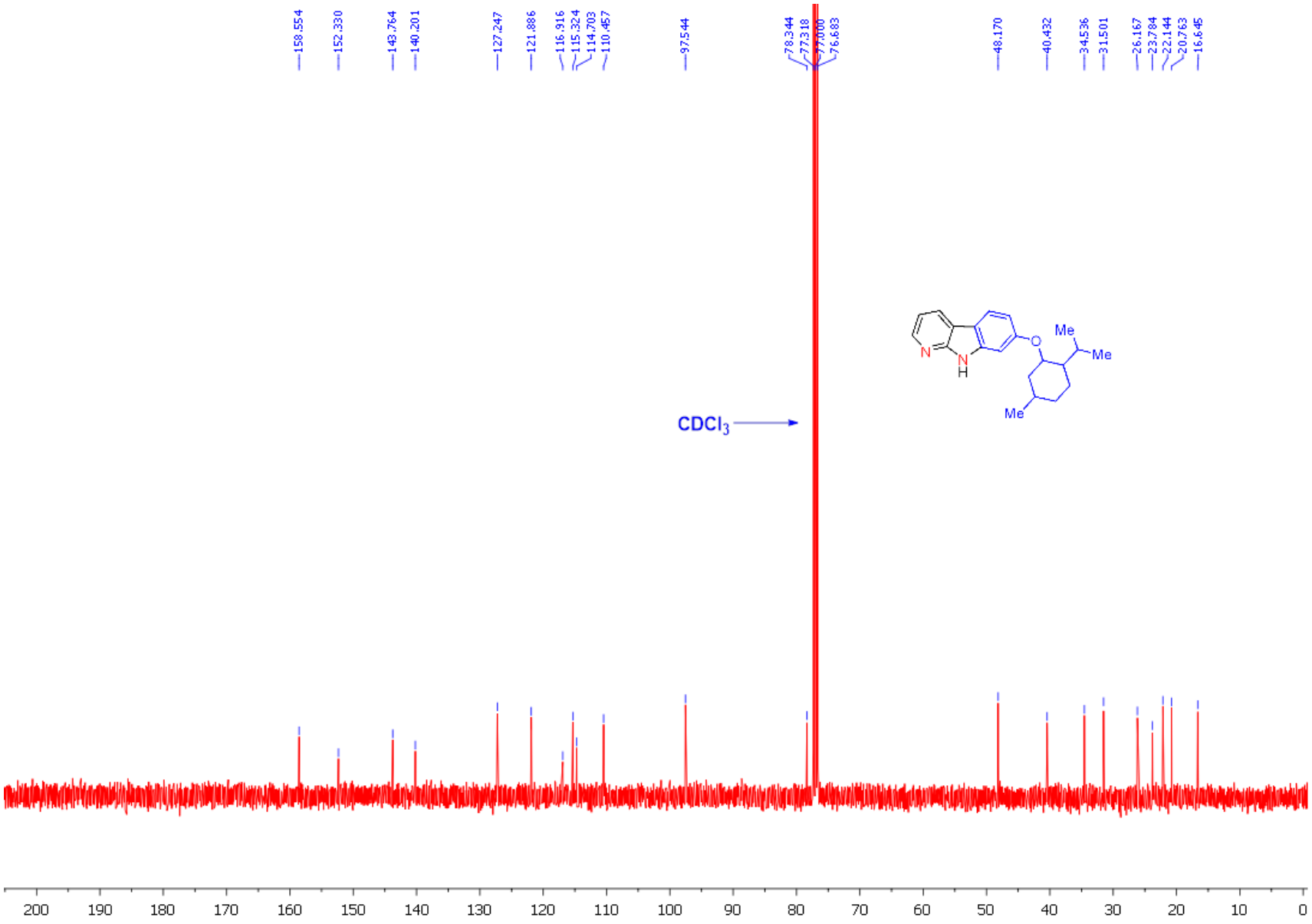
^{13}C-NMR of *7-(((1S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)-9H-pyrido[2,3-b]indole (2w)* (25 °C, 100 MHz, $CDCl_3$):



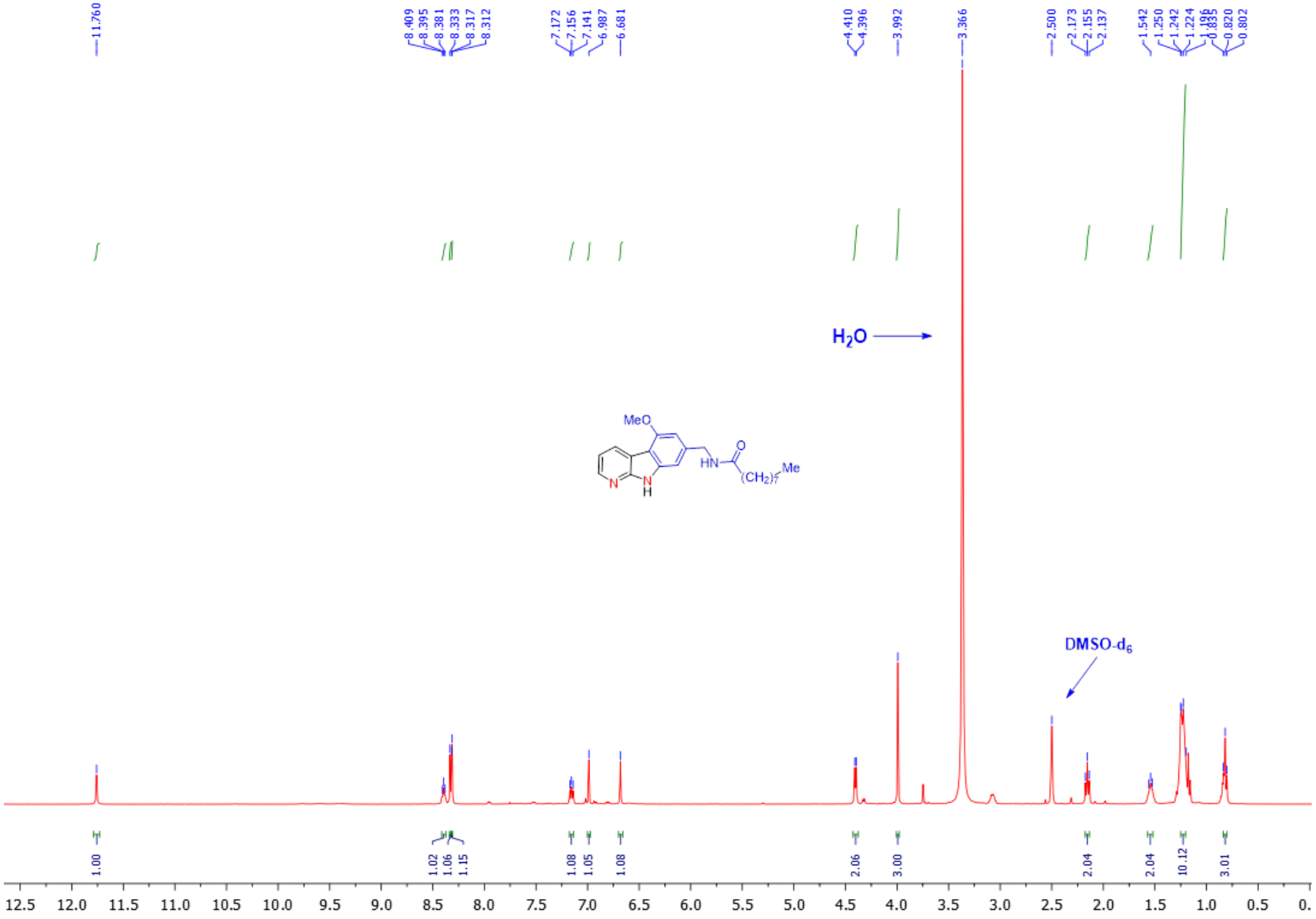
^{1}H-NMR of *7-((2-isopropyl-5-methylcyclohexyl)oxy)-9H-pyrido[2,3-b]indole (2x)* (25 °C, 400 MHz, $CDCl_3$):



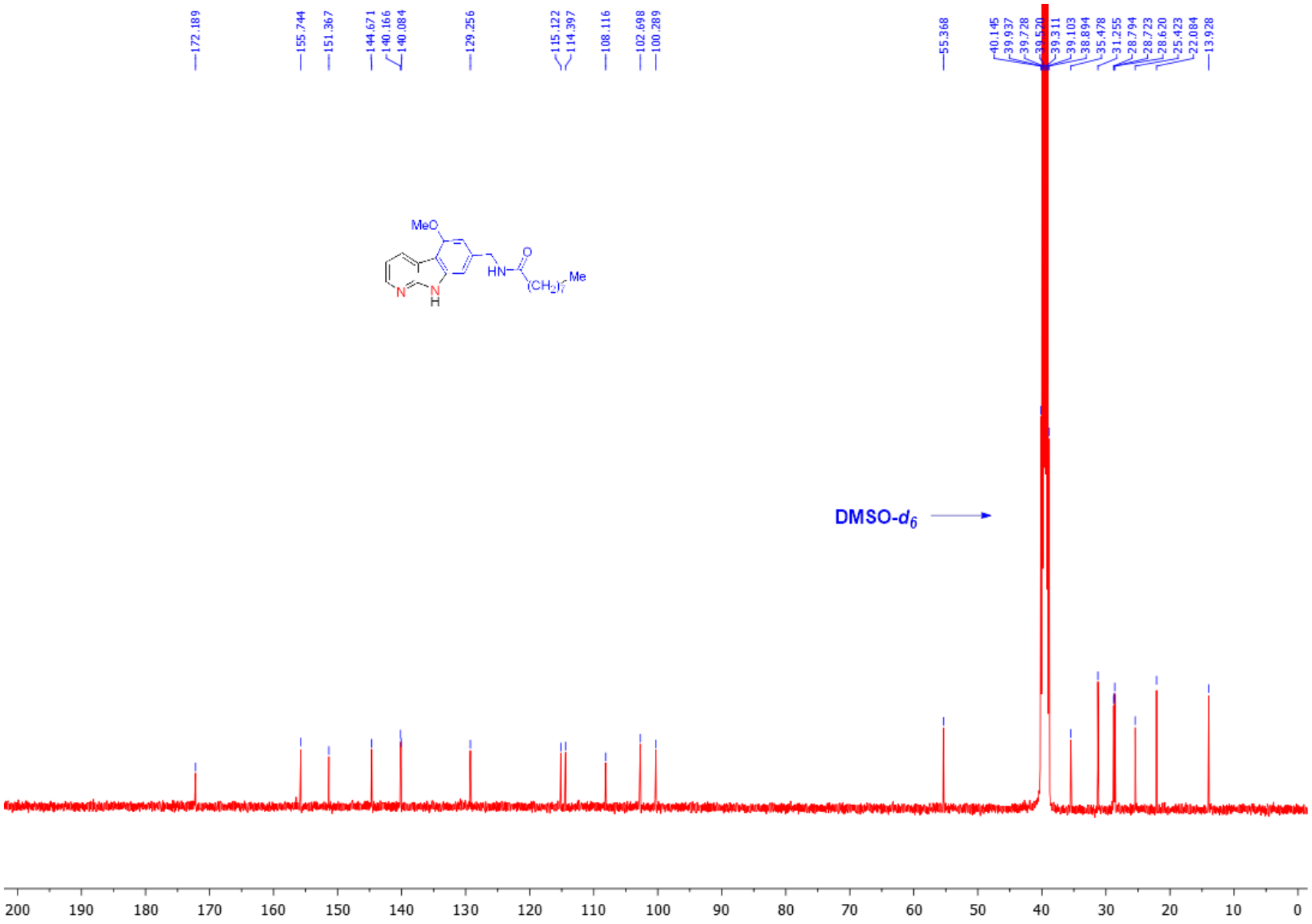
^{13}C-NMR of *7-((2-isopropyl-5-methylcyclohexyl)oxy)-9H-pyrido[2,3-b]indole (2x))* (25 °C, 100 MHz, $CDCl_3$):



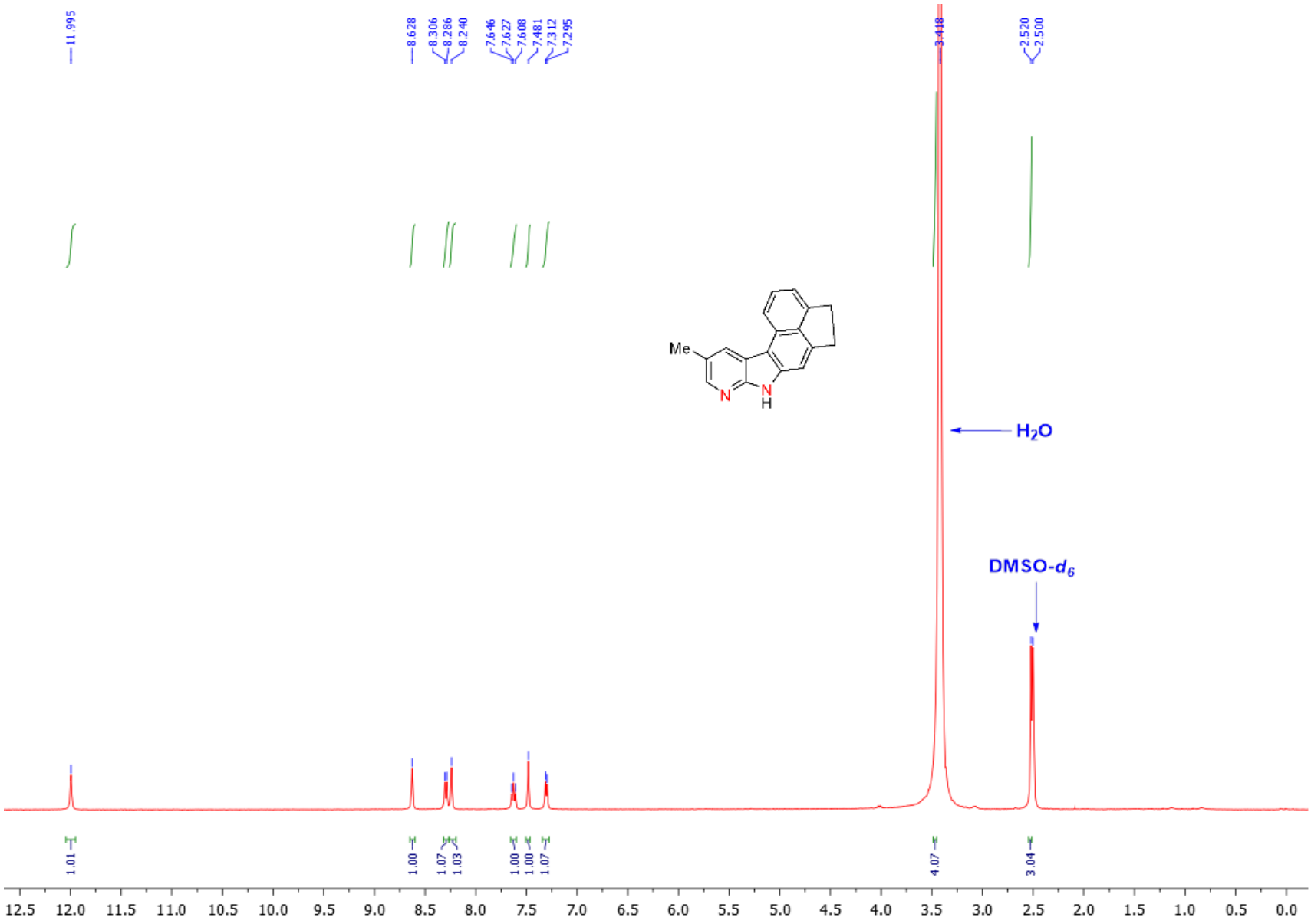
^{1}H-NMR of *N-((5-methoxy-9H-pyrido[2,3-b]indol-7-yl)methyl)nonanamide (2y)* (25 ^{o}C, 400 MHz, $CDCl_3$):



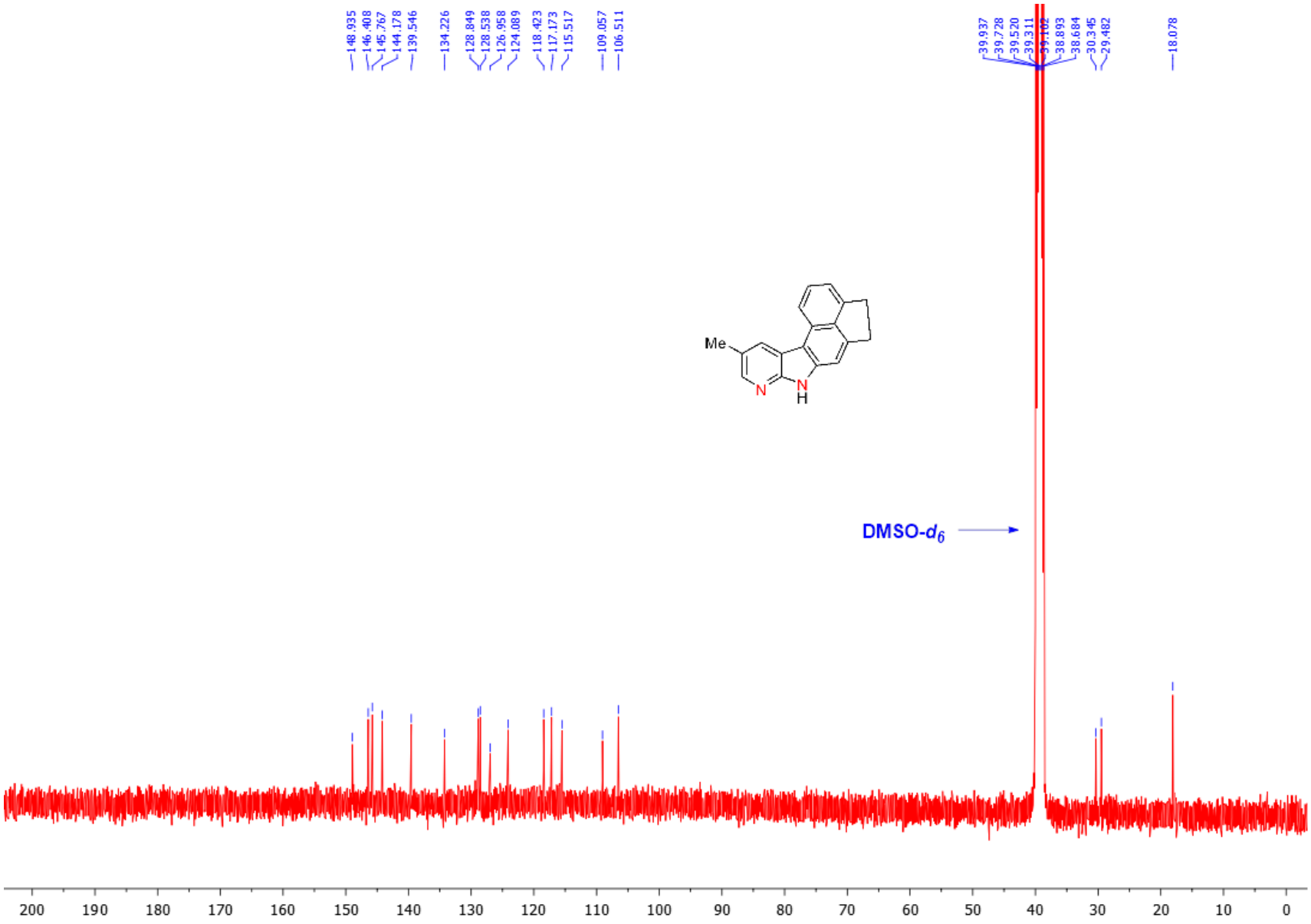
^{13}C-NMR of *N-((5-methoxy-9H-pyrido[2,3-b]indol-7-yl)methyl)nonanamide (2y)* (25 °C, 100 MHz, $CDCl_3$):



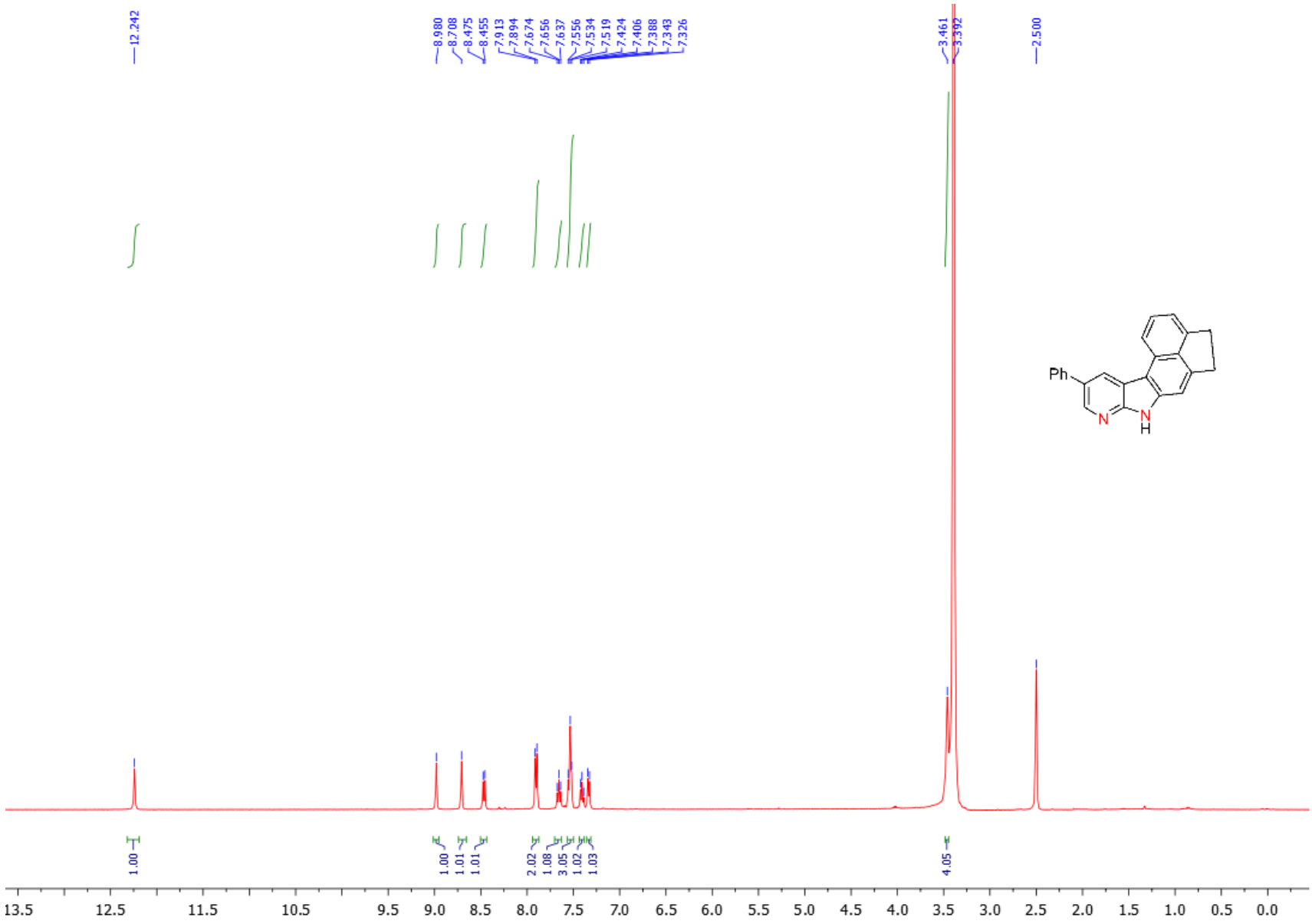
^{1}H-NMR of *10-methyl-5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole (4a)* (25 ^{o}C, 400 MHz, DMSO-d_6):



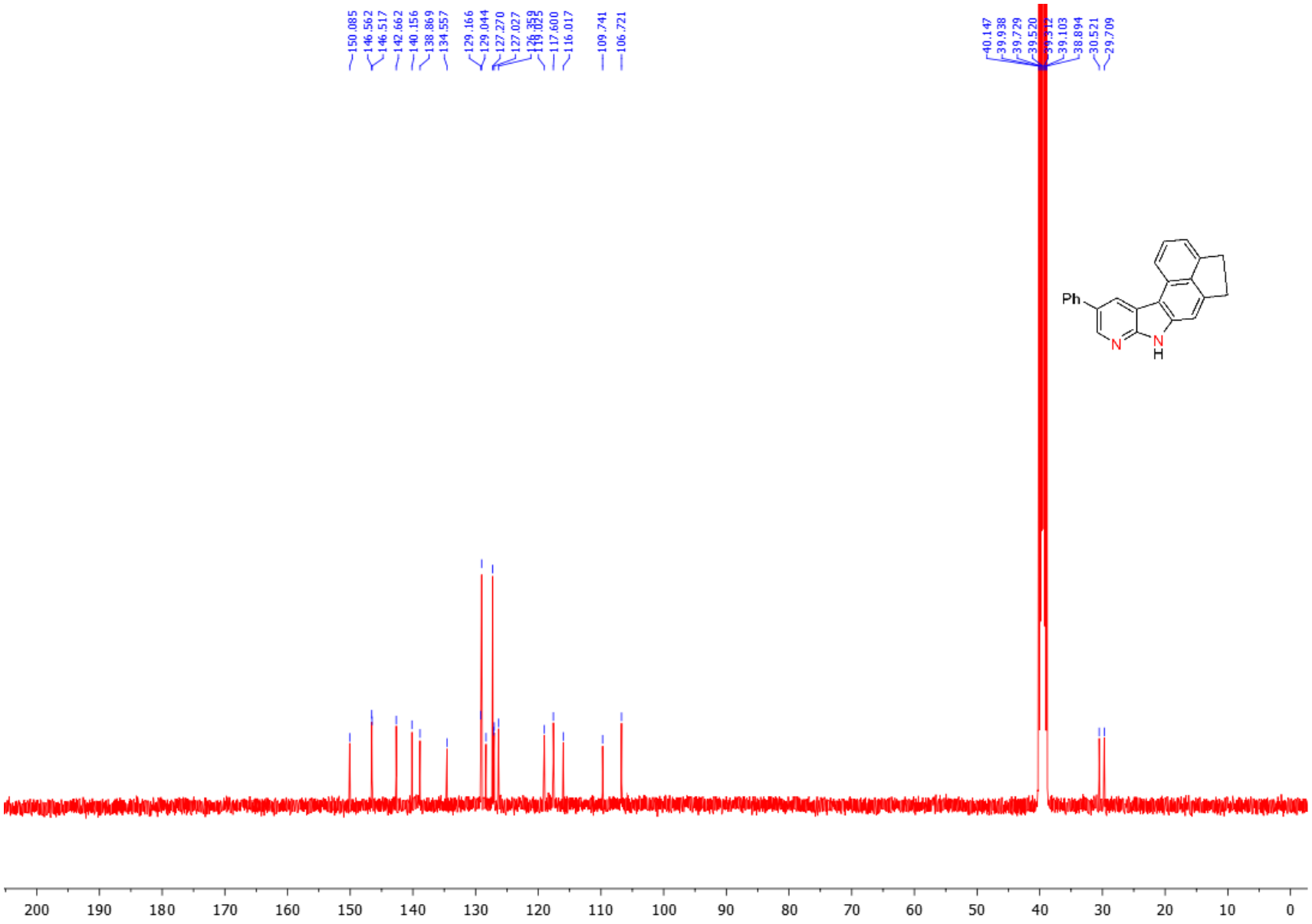
^{13}C-NMR of *10-methyl-5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole (4a)* (25 ºC, 100 MHz, DMSO-d_6):



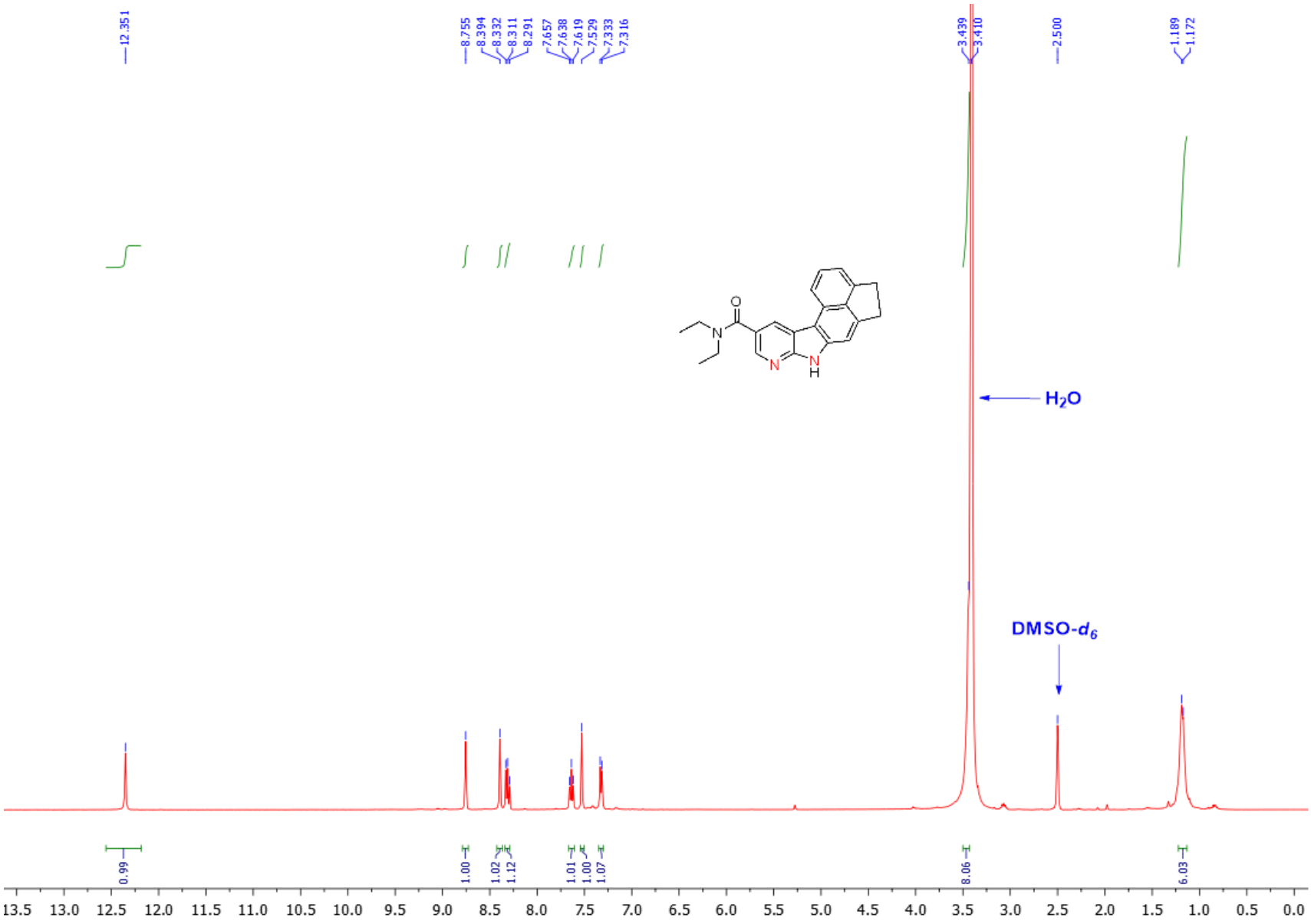
^{1}H-NMR of *10-phenyl-5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole (4b)* (25 ^{o}C, 400 MHz, DMSO-d_6):



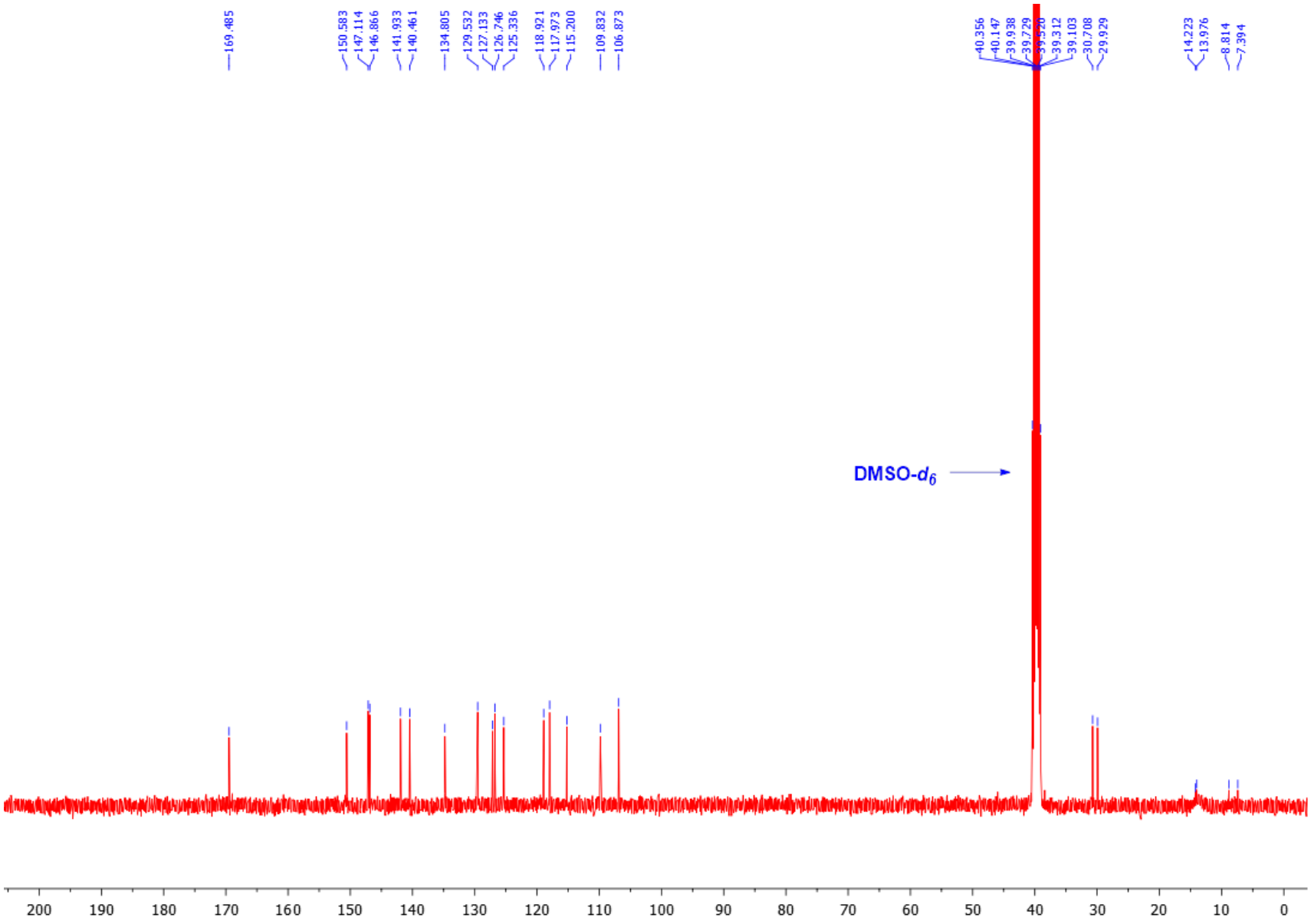
^{13}C-NMR of *10-phenyl-5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole (4b)* (25 ºC, 100 MHz, DMSO-d_6):



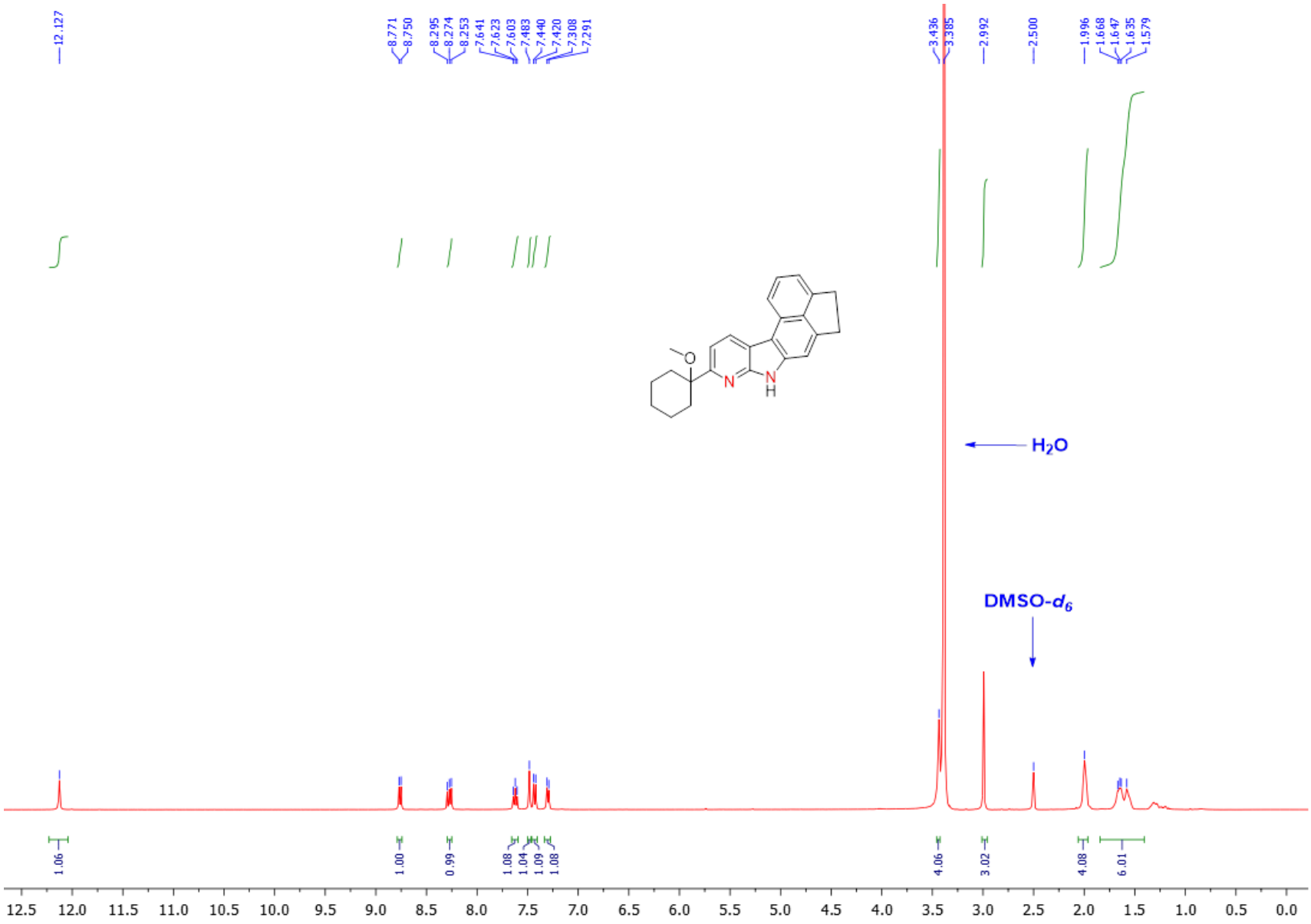
^{1}H-NMR of *N,N-diethyl-5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole-10-carboxamide (4c)* (25 ºC, 400 MHz, DMSO-*d*$_6$):



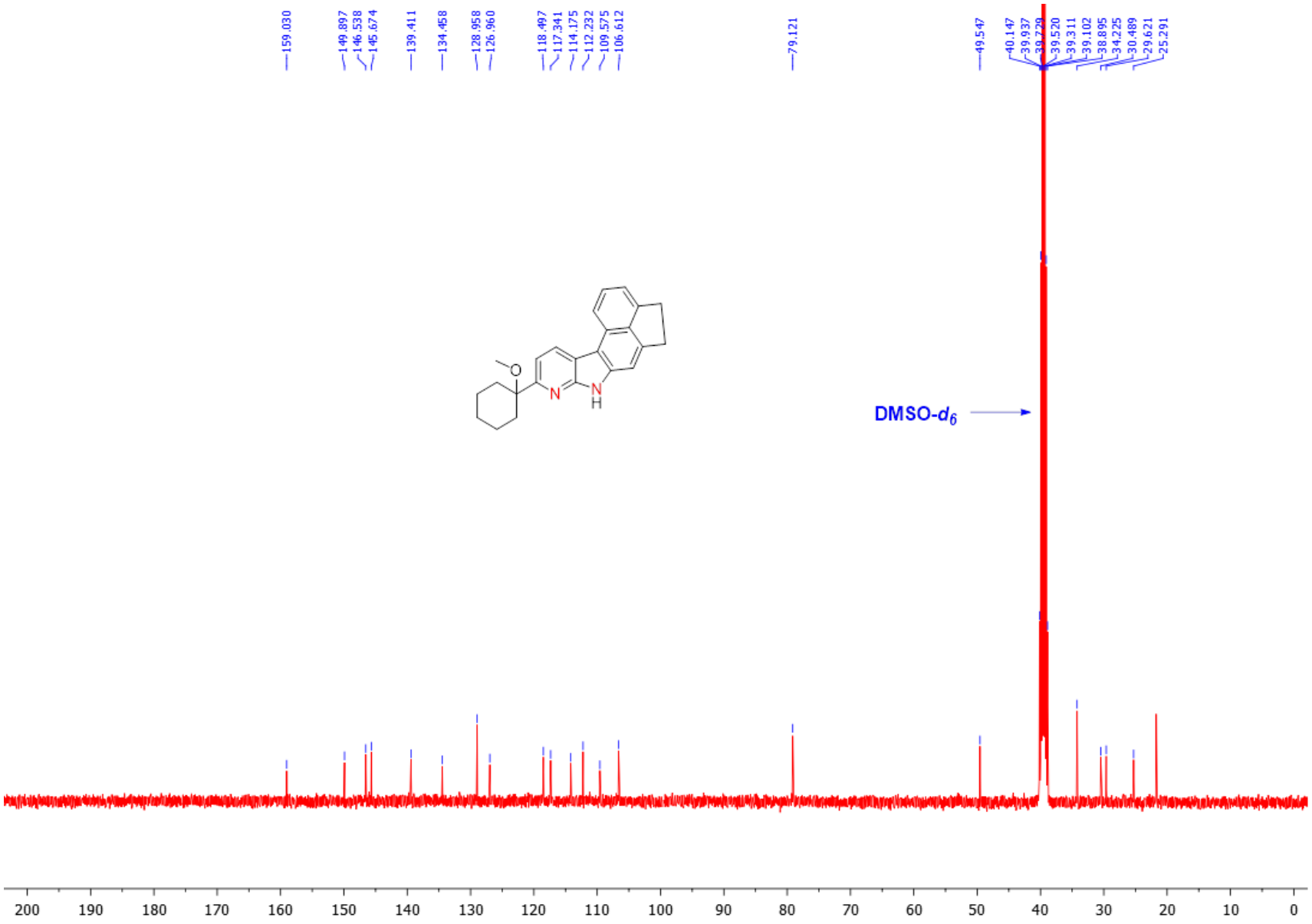
^{13}C-NMR of *N,N-diethyl-5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole-10-carboxamide (4c)* (25 ºC, 100 MHz, DMSO-d_6):



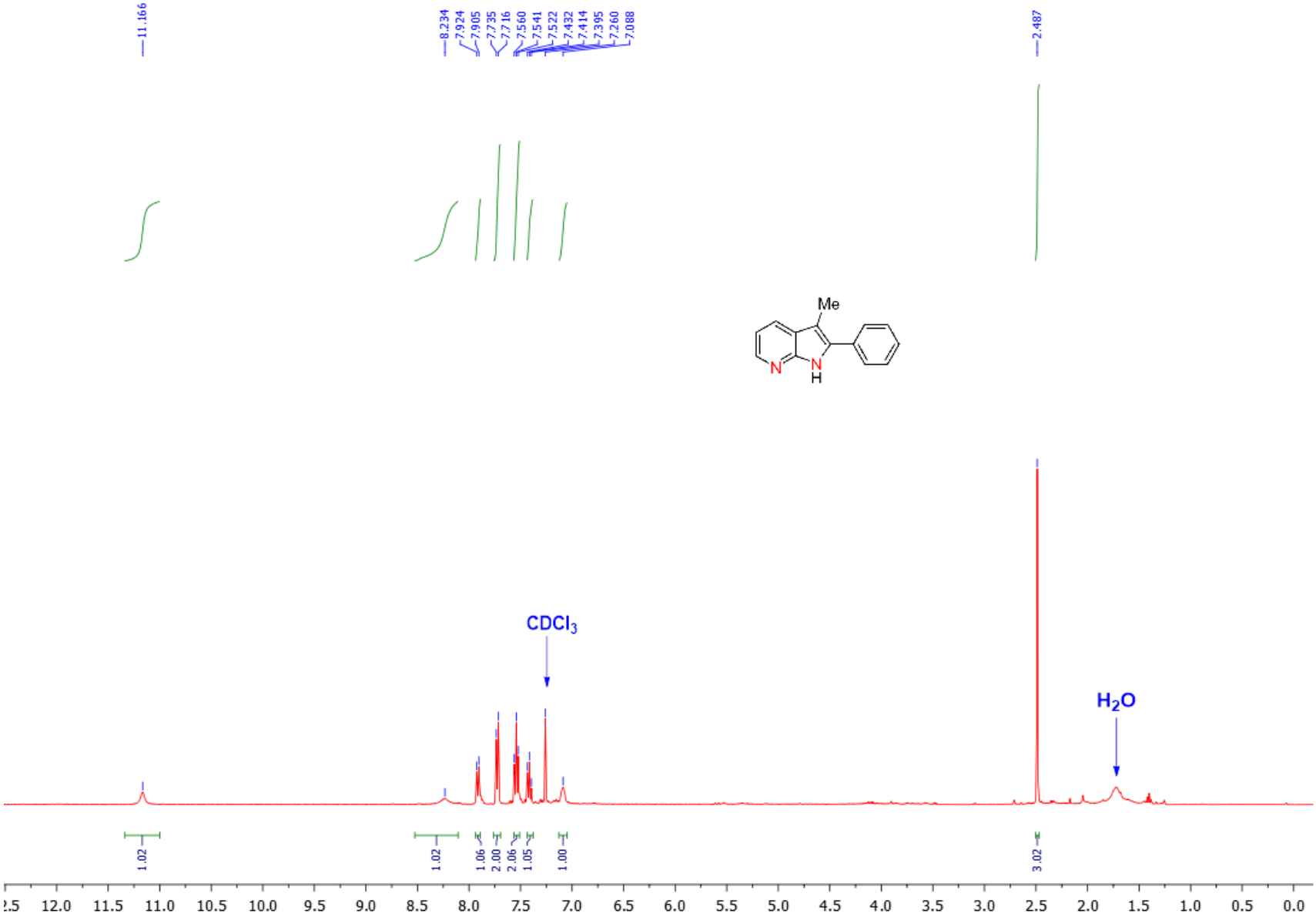
^{1}H-NMR of *9-(1-methoxycyclohexyl)-5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole (4d)* (25 ºC, 400 MHz, DMSO-d_6):



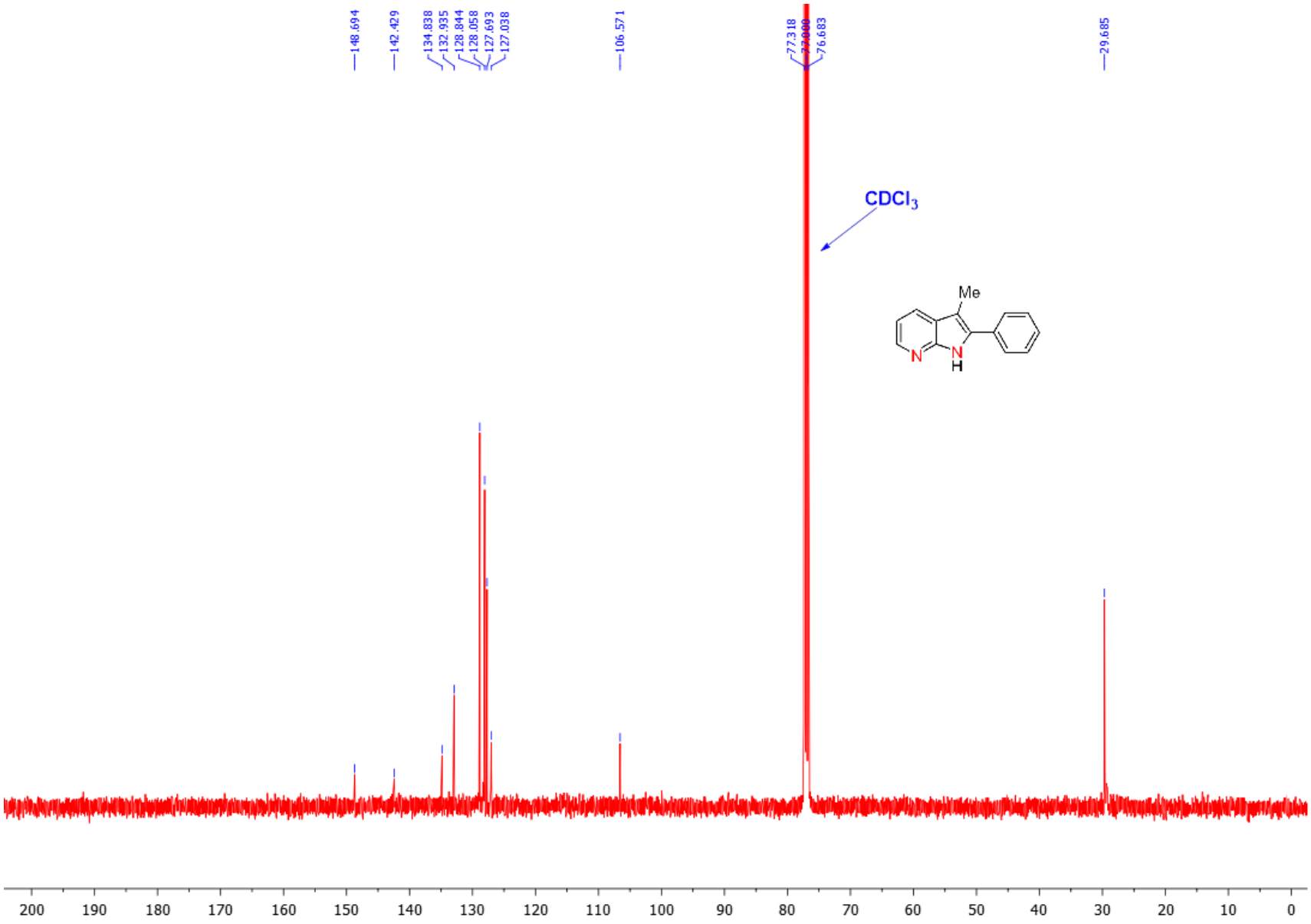
^{13}C-NMR of *9-(1-methoxycyclohexyl)-5,7-dihydro-4H-indeno[7,1-ef]pyrido[2,3-b]indole (4d)* (25 ºC, 100 MHz, DMSO-d_6):



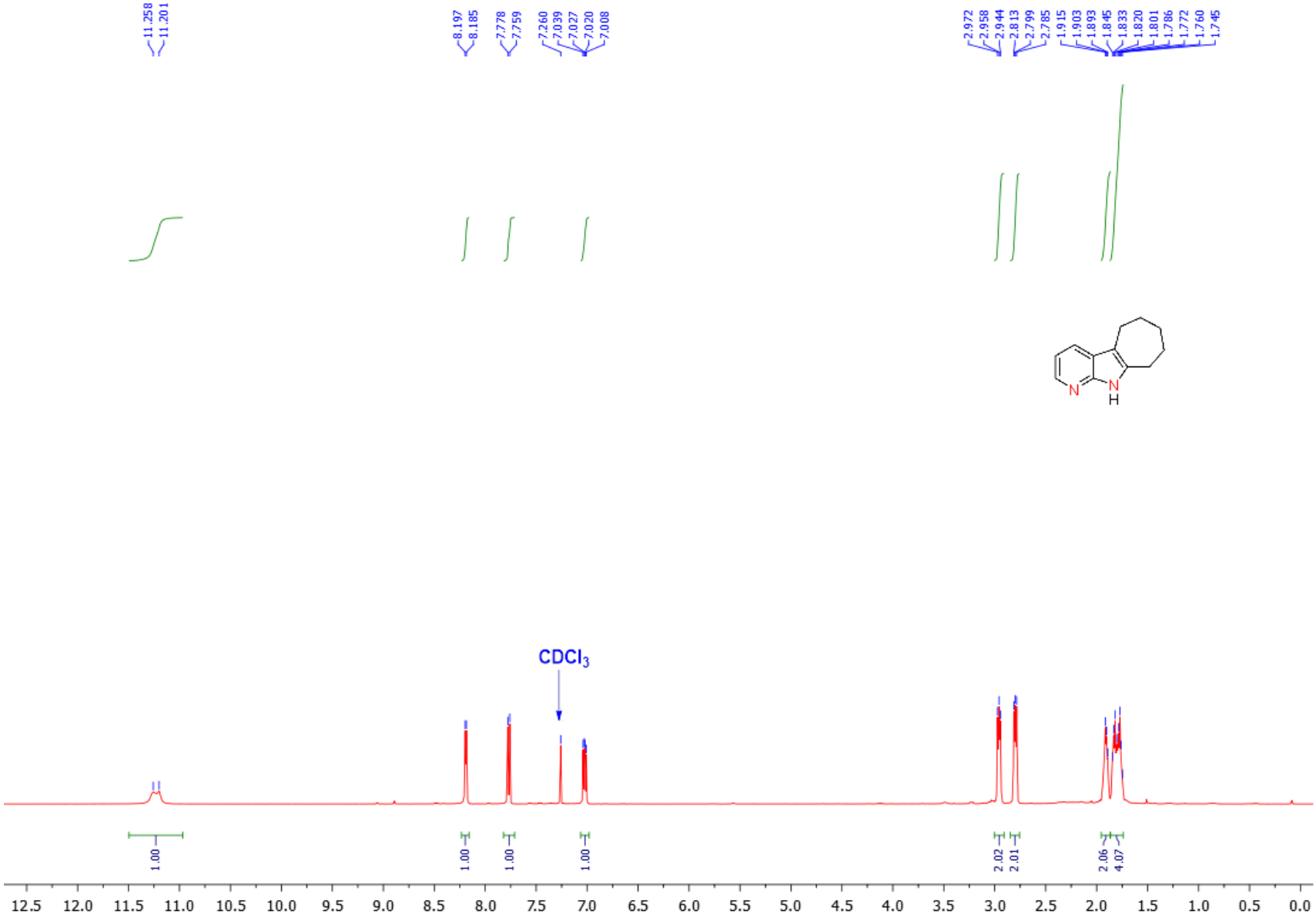
^{1}H-NMR of *3-methyl-2-phenyl-1H-pyrrolo[2,3-b]pyridine (6a)* (25 ^{o}C, 400 MHz, $CDCl_3$):



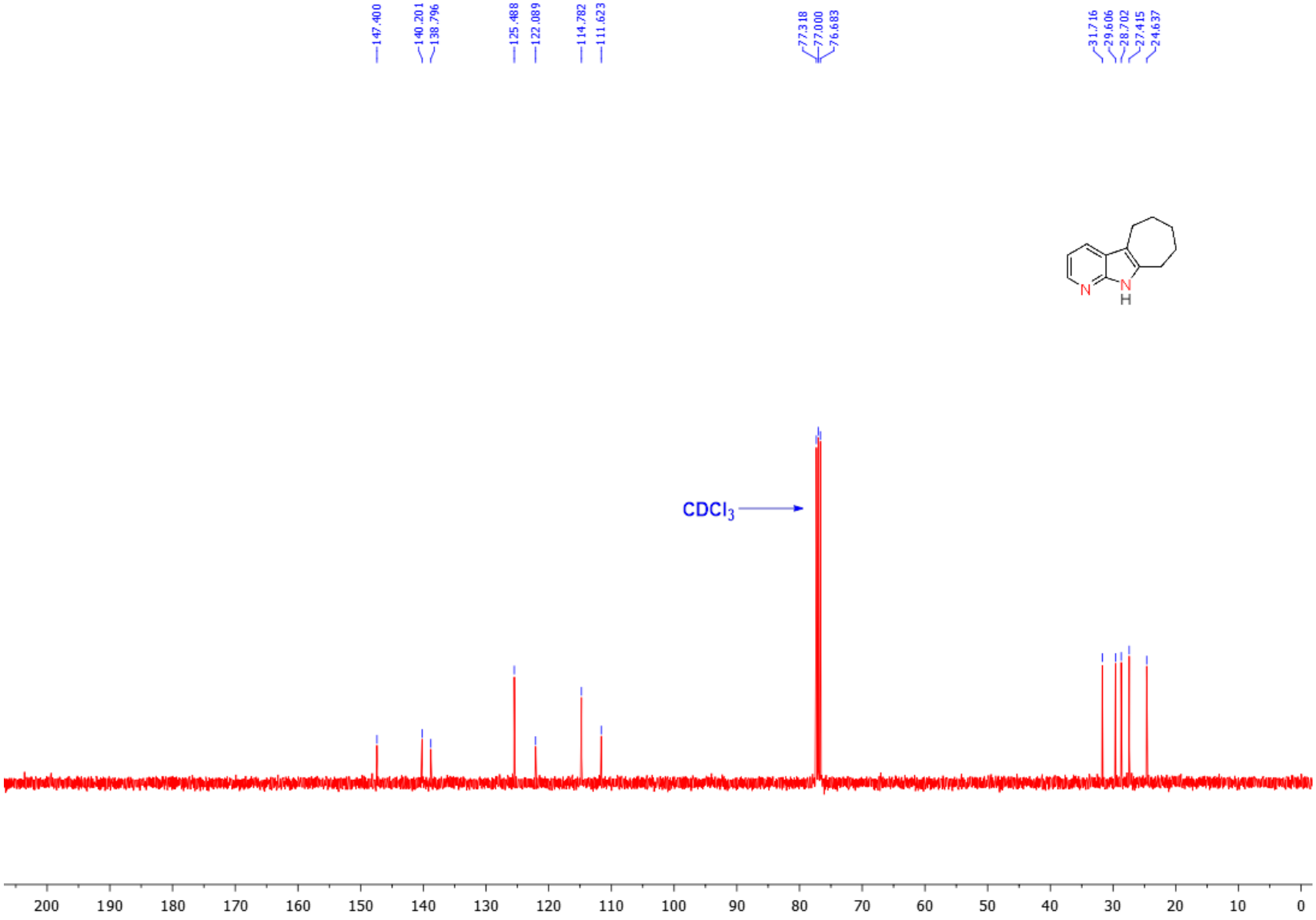
^{13}C-NMR of *3-methyl-2-phenyl-1H-pyrrolo[2,3-b]pyridine (6a)* (25 °C, 100 MHz, $CDCl_3$):



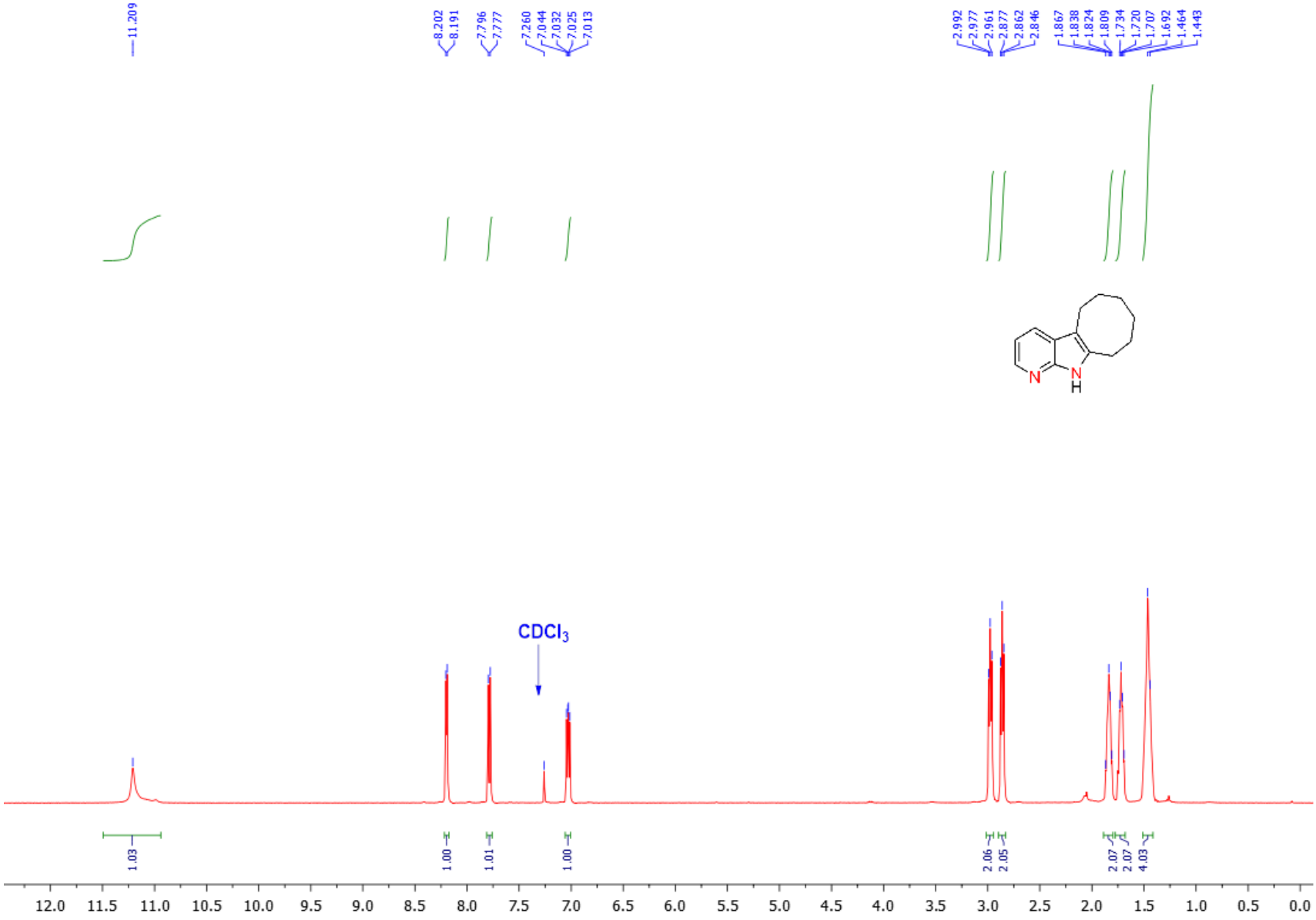
^{1}H-NMR of *5,6,7,8,9,10-hexahydrocyclohepta[4,5]pyrrolo[2,3-b]pyridine (6b)* (25 ^{o}C, 400 MHz, $CDCl_3$):



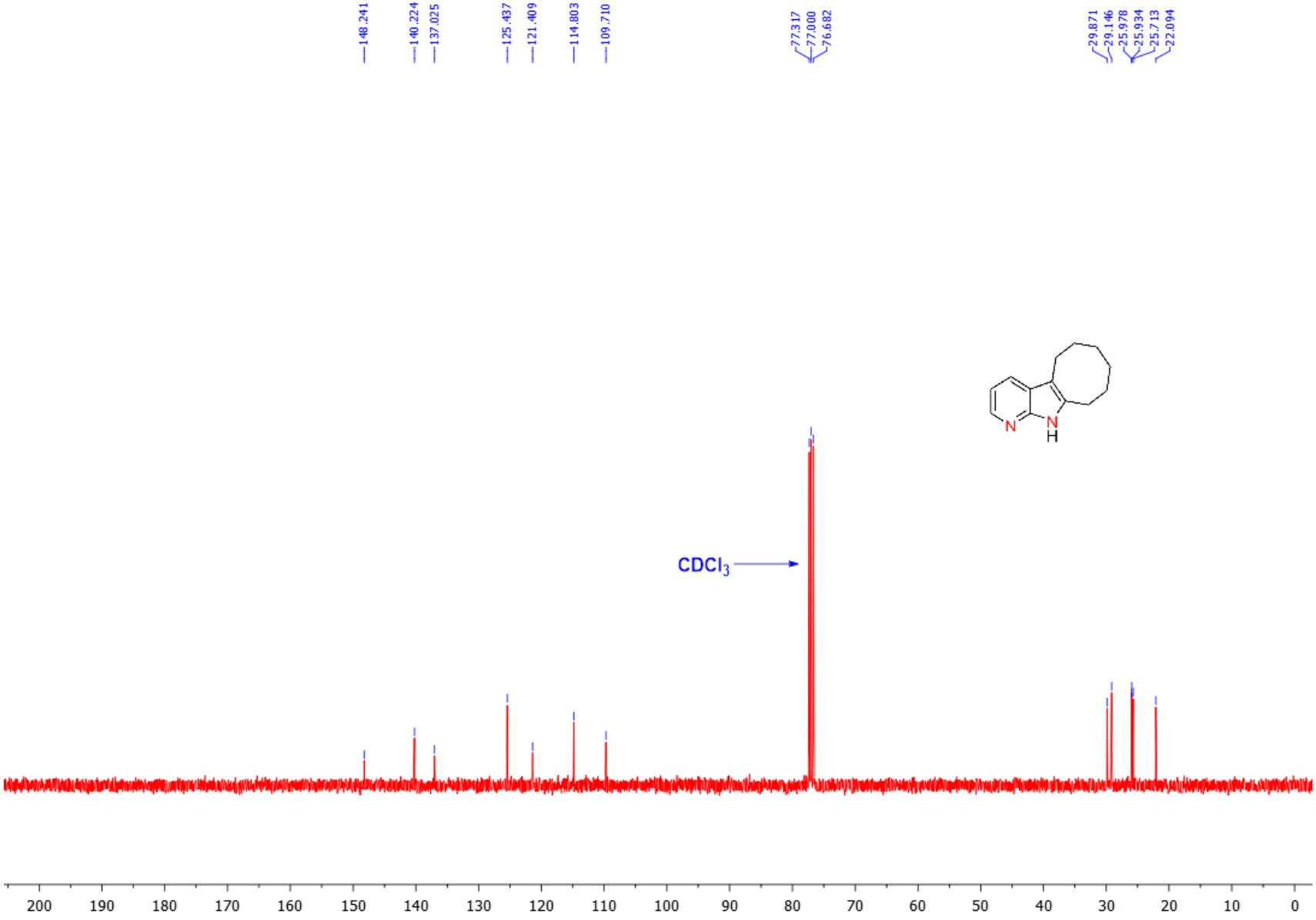
^{13}C-NMR of *5,6,7,8,9,10-hexahydrocyclohepta[4,5]pyrrolo[2,3-b]pyridine (6b)* (25 ºC, 100 MHz, $CDCl_3$):



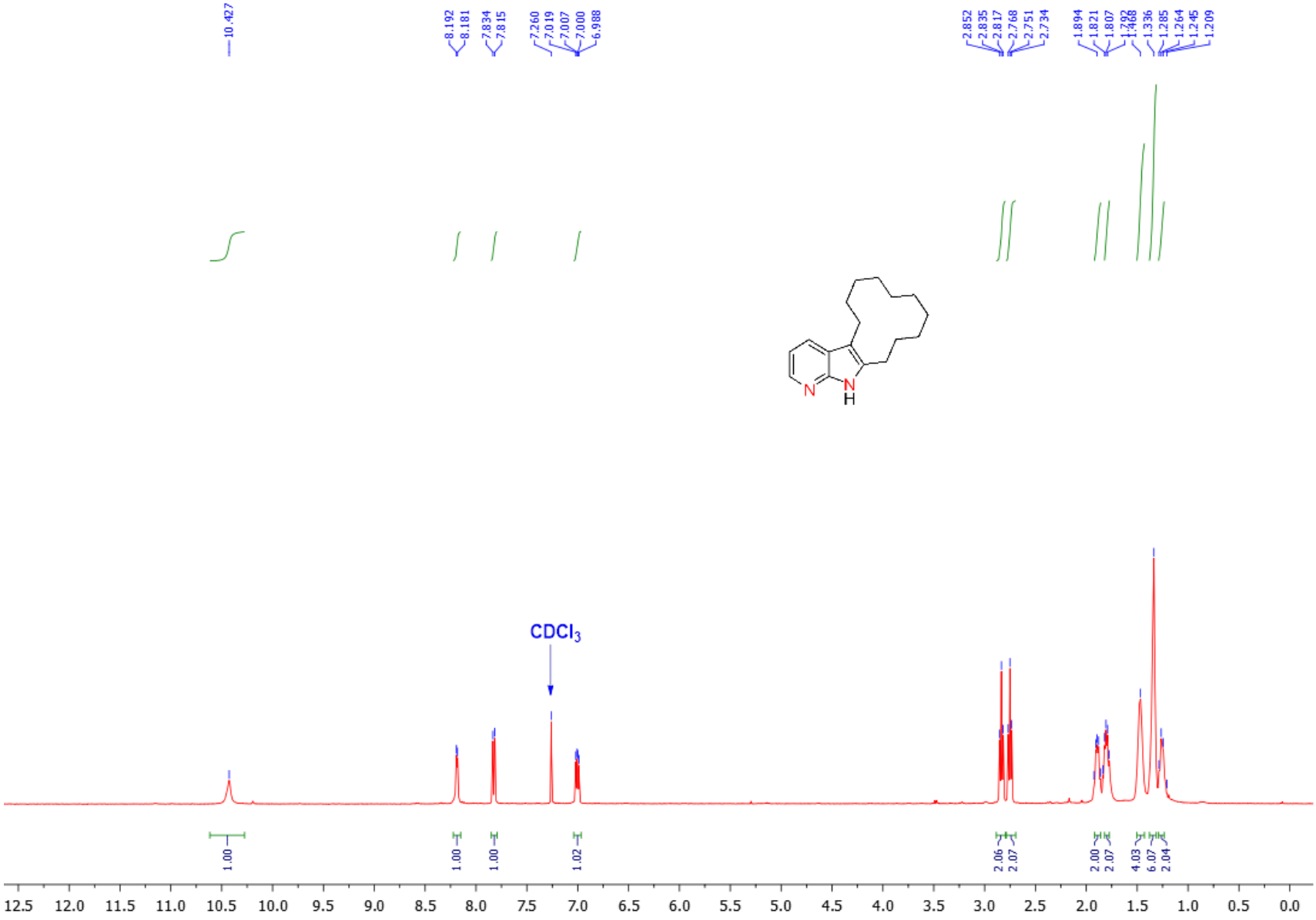
^{1}H-NMR of *6,7,8,9,10,11-hexahydro-5H-cycloocta[4,5]pyrrolo[2,3-b]pyridine (6c)* (25 °C, 400 MHz, $CDCl_3$):



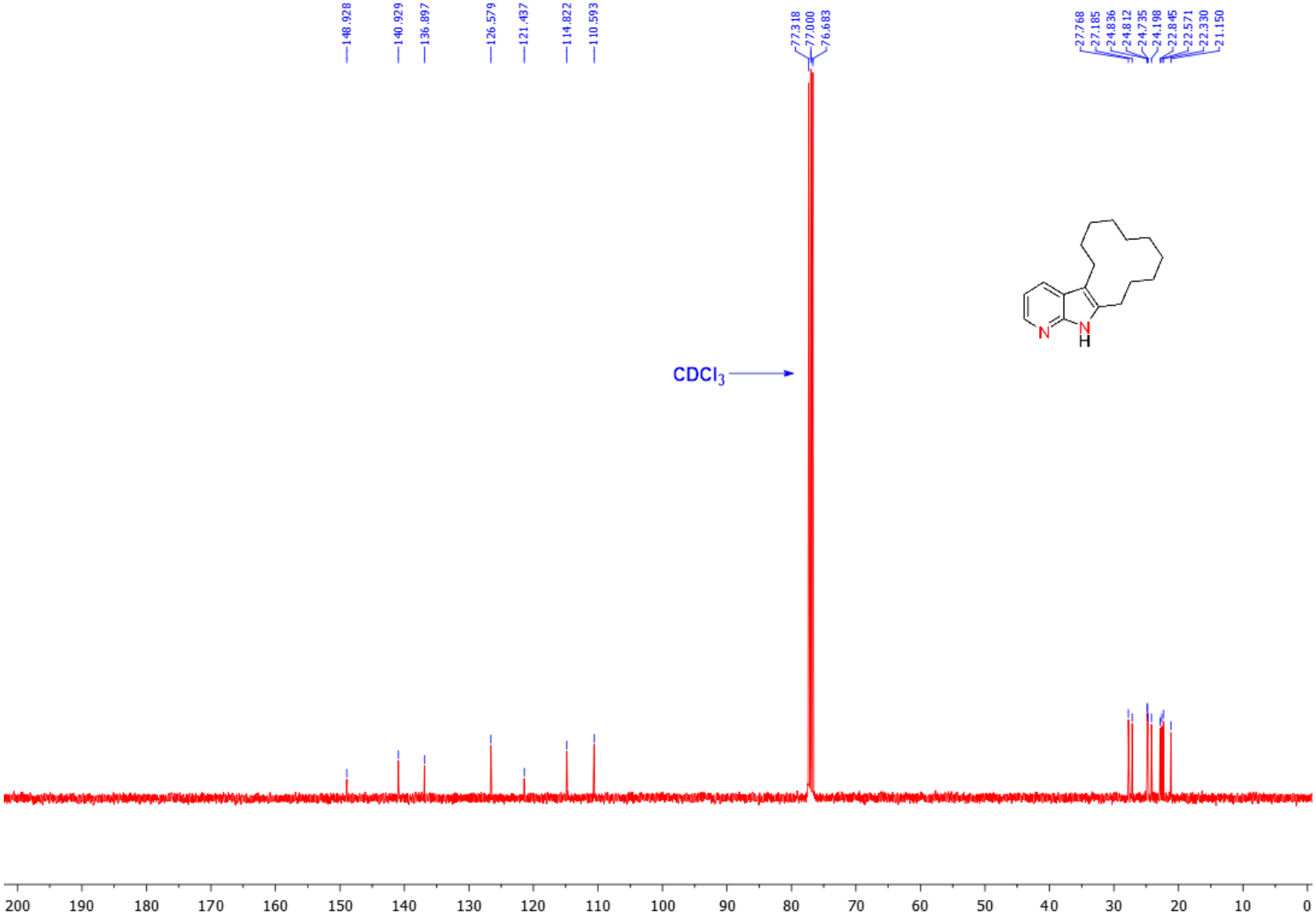
^{13}C-NMR of *6,7,8,9,10,11-hexahydro-5H-cycloocta[4,5]pyrrolo[2,3-b]pyridine (6c)* (25 ºC, 100 MHz, $CDCl_3$):



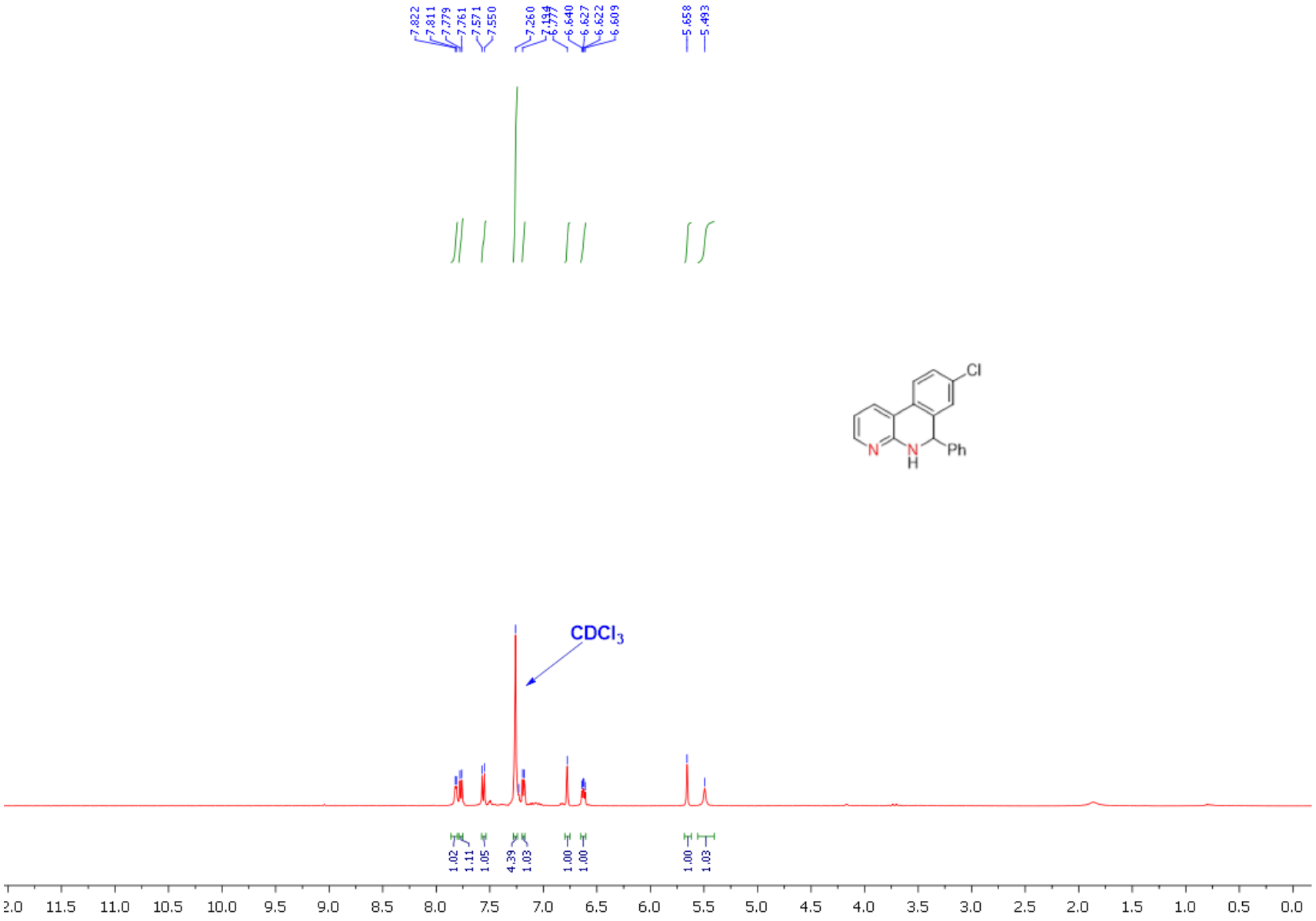
^{1}H-NMR of *2-(1-phenylethyl)-2,3-dihydro-1H-pyrrolo[2,3-b]pyridine (6d)* (25 °C, 400 MHz, $CDCl_3$):



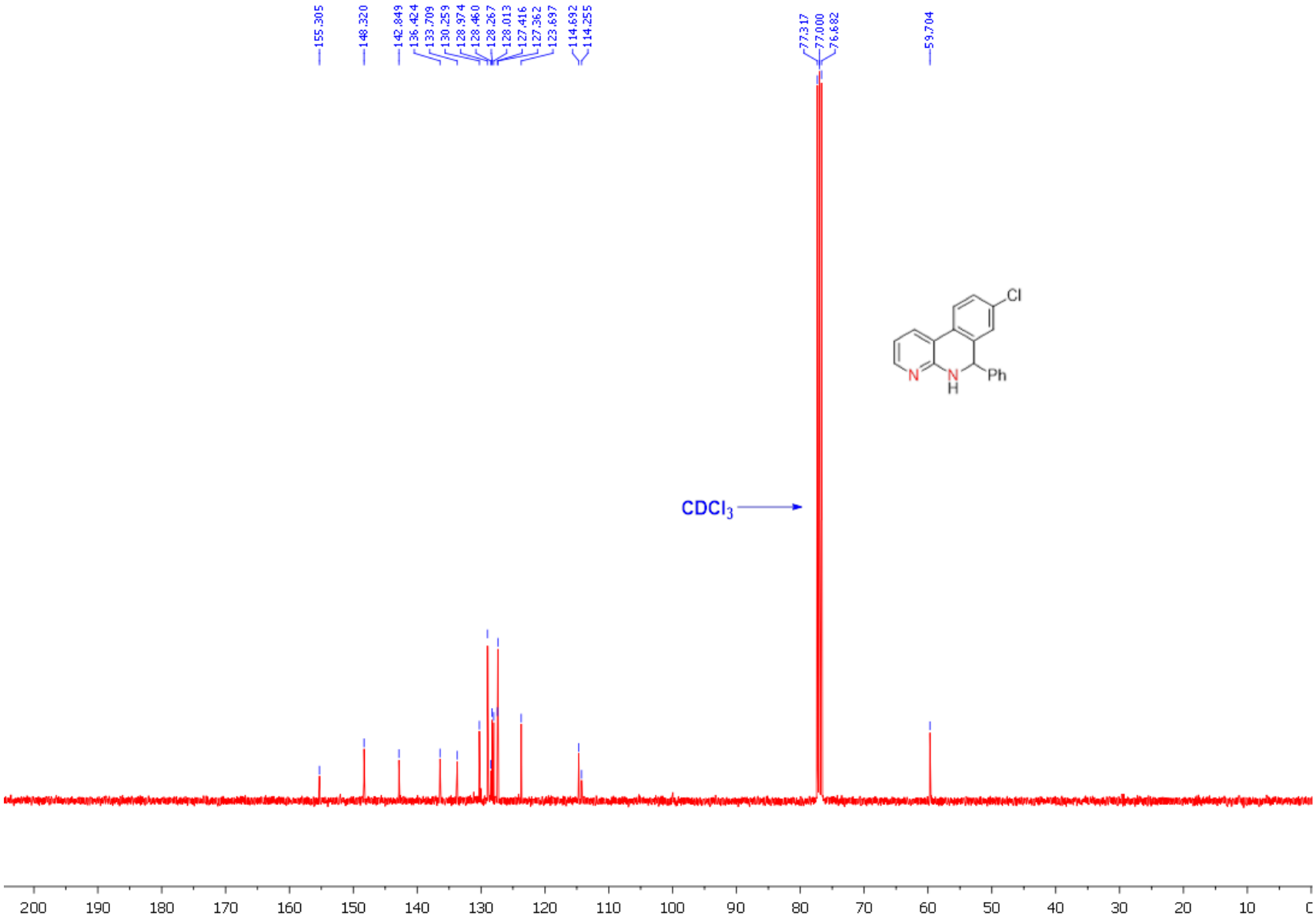
^{13}C-NMR of *2-(1-phenylethyl)-2,3-dihydro-1H-pyrrolo[2,3-b]pyridine (6d)* (25 °C, 100 MHz, $CDCl_3$):



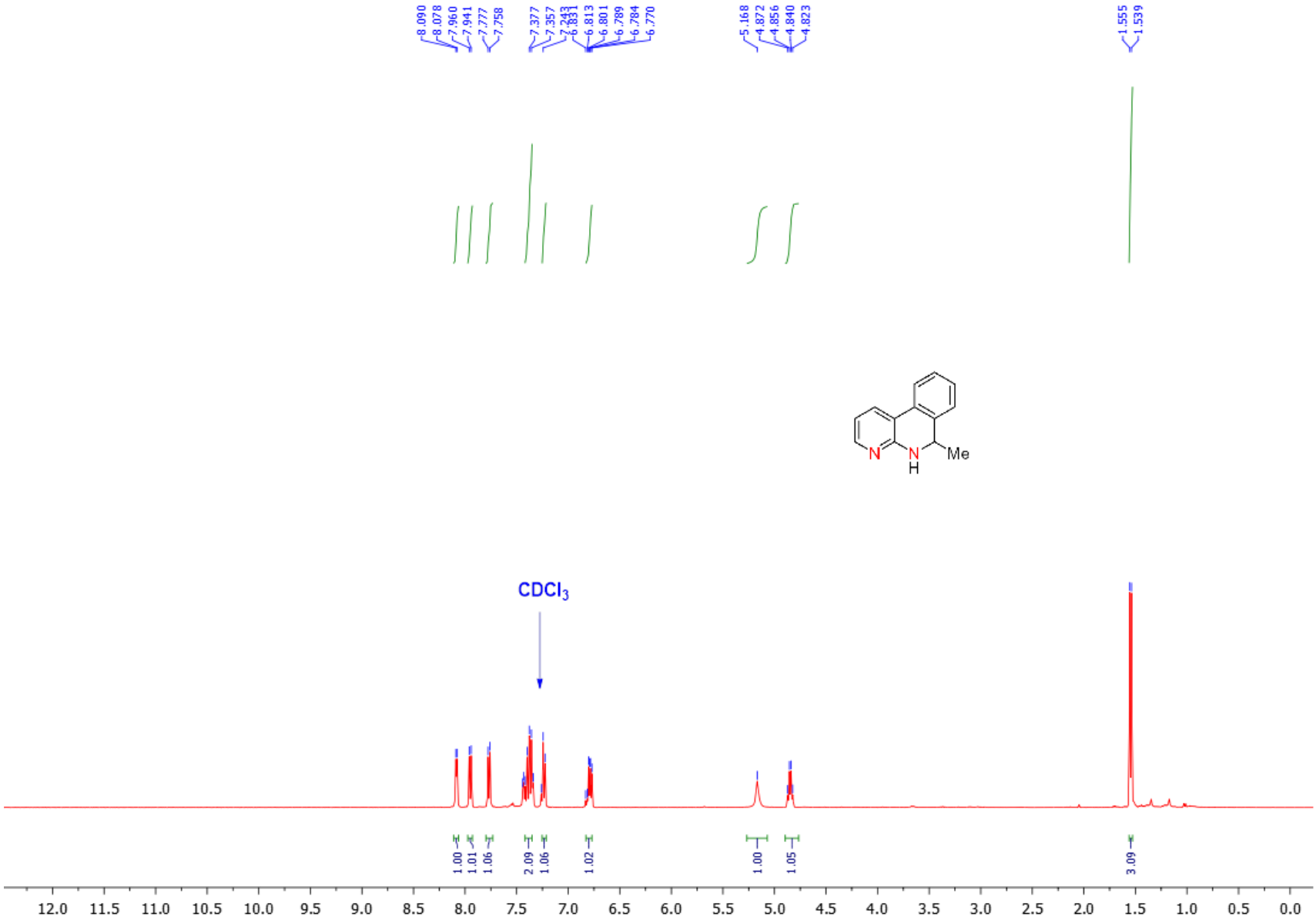
^{1}H-NMR of *8-chloro-6-phenyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8a)* (25 °C, 400 MHz, $CDCl_3$):



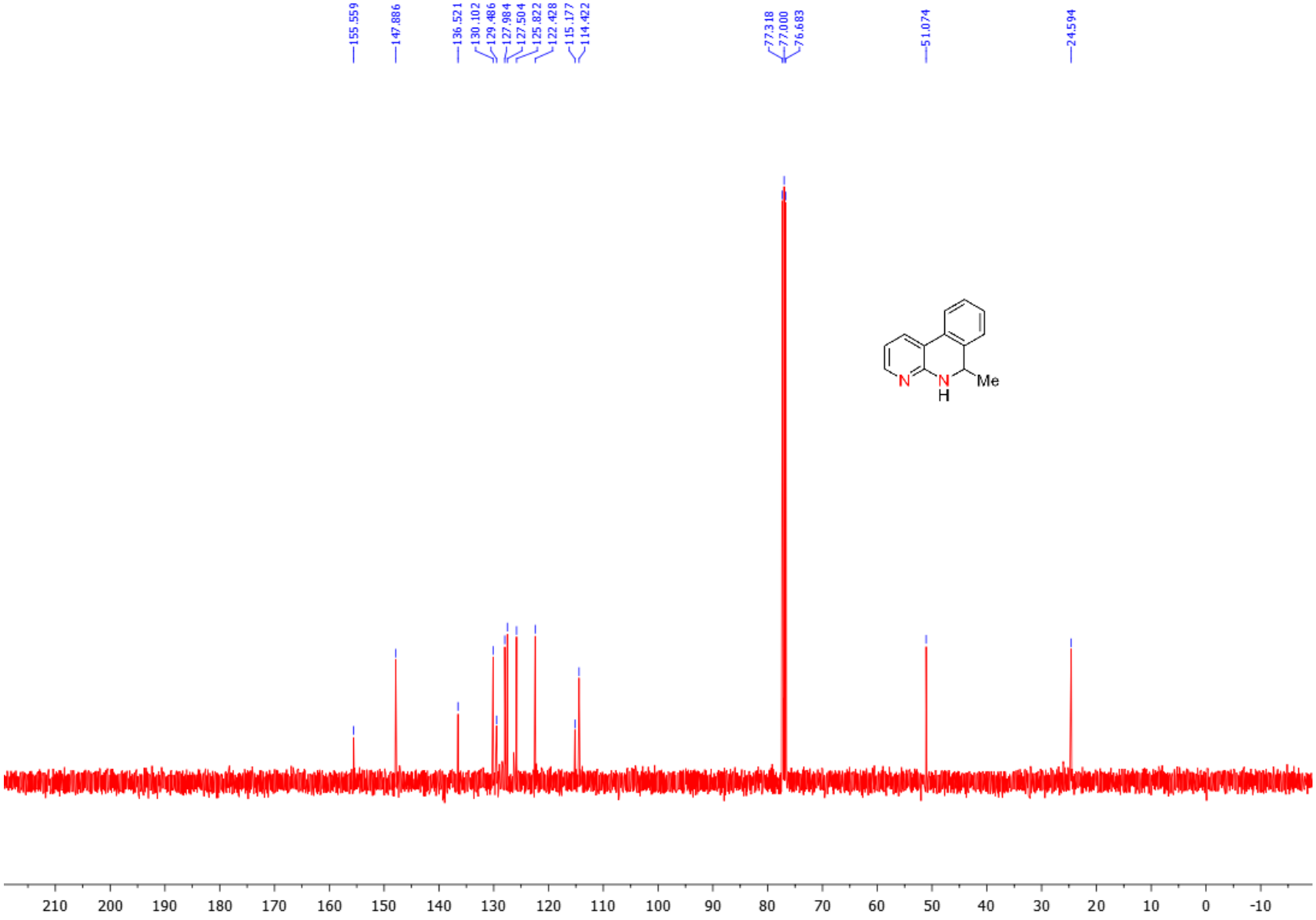
^{13}C-NMR of *8-chloro-6-phenyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8a)* (25 °C, 100 MHz, $CDCl_3$):



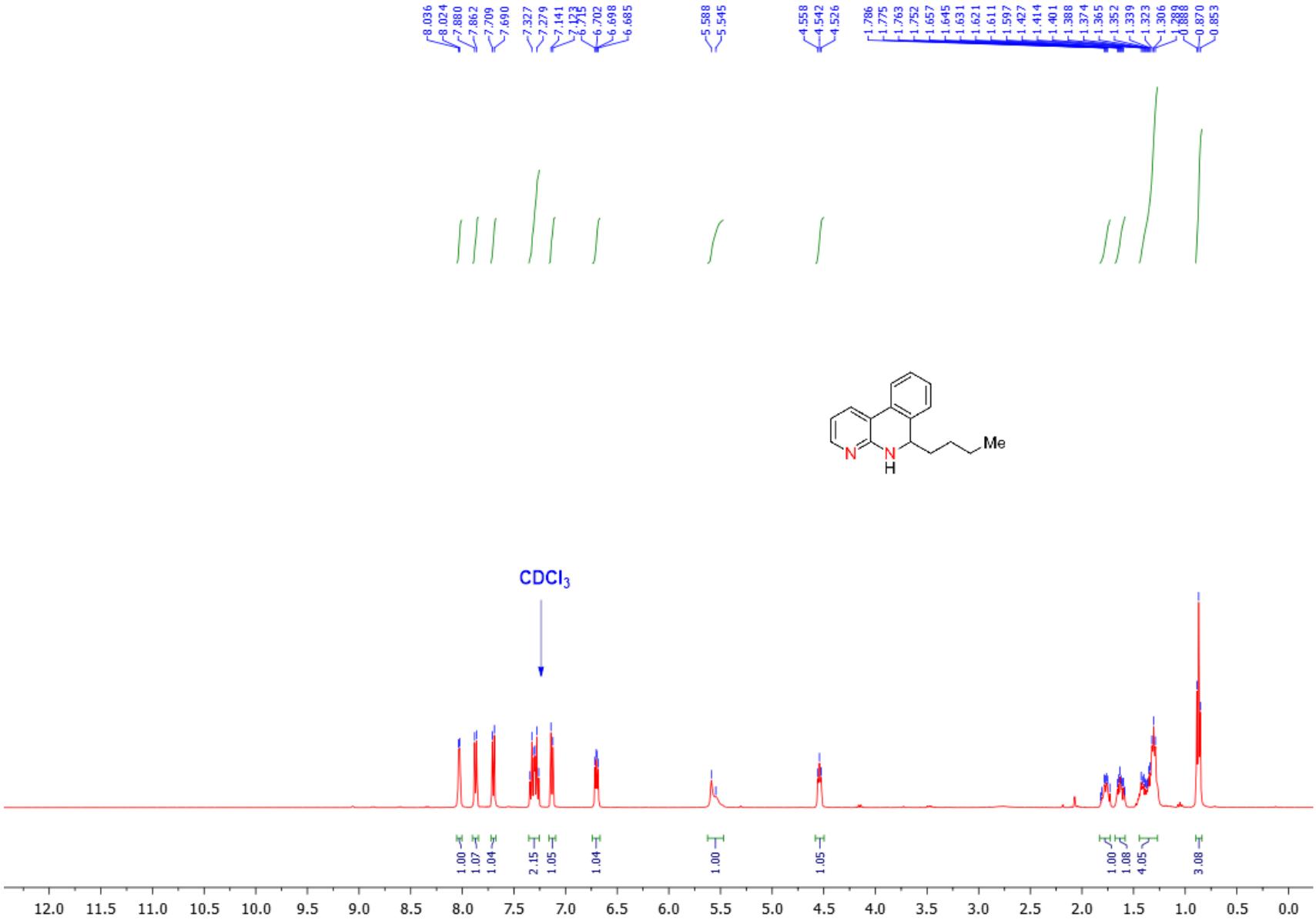
^{1}H-NMR of *6-methyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8b)* (25 ^{o}C, 400 MHz, $CDCl_3$):



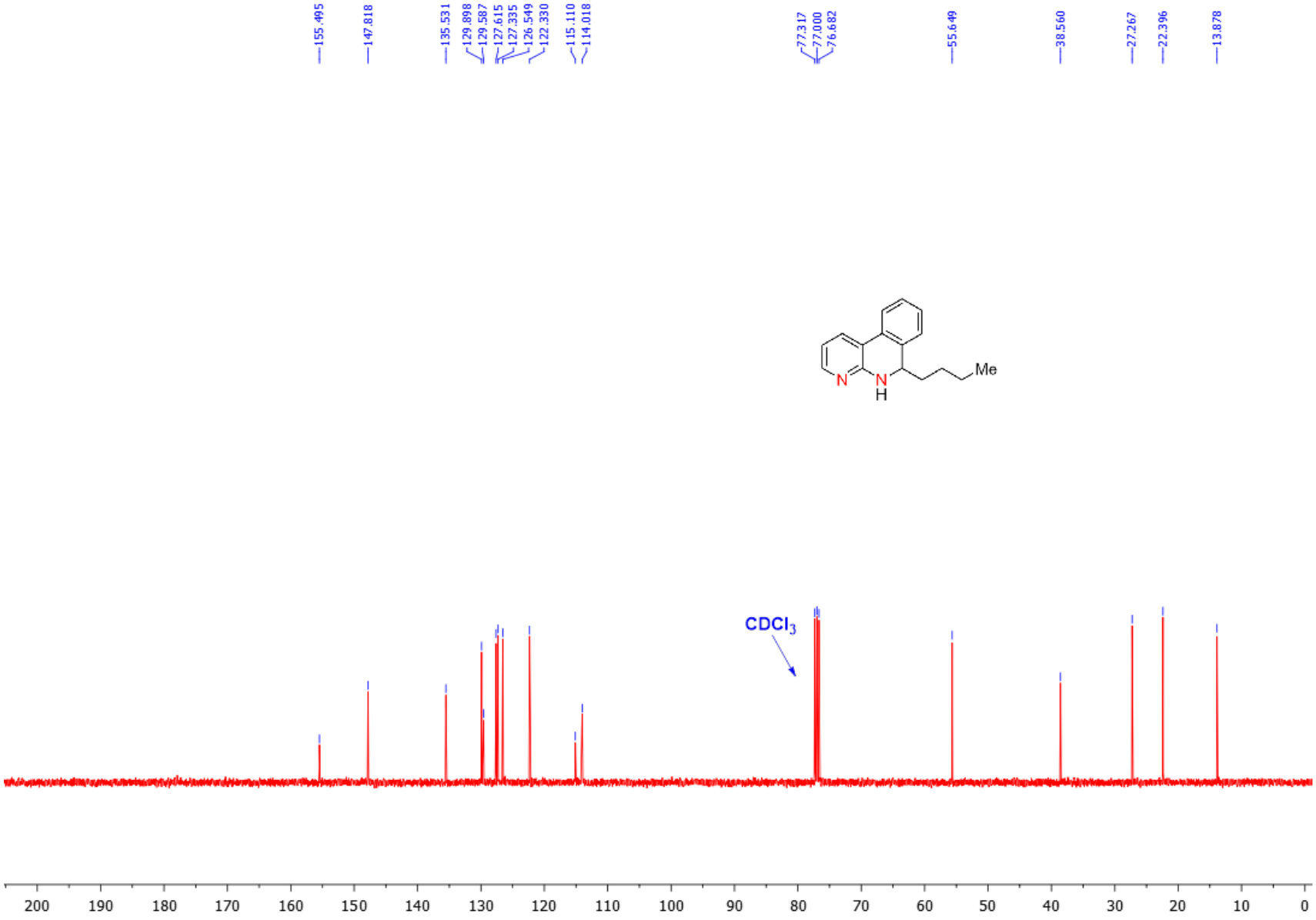
^{13}C-NMR of *6-methyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8b)* (25 °C, 100 MHz, $CDCl_3$):



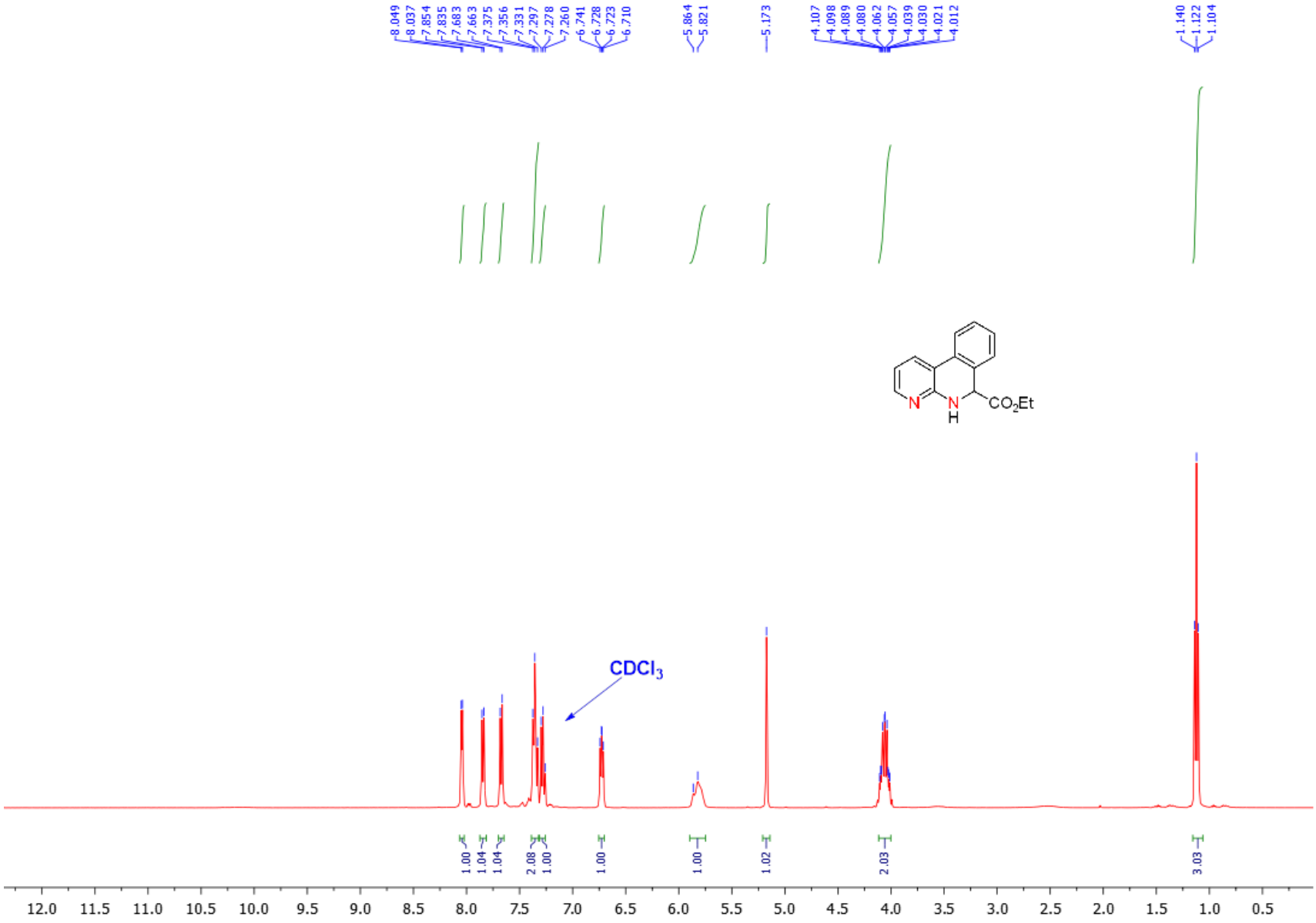
^{1}H-NMR of *6-butyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8c)* (25 ^{o}C, 400 MHz, $CDCl_3$):



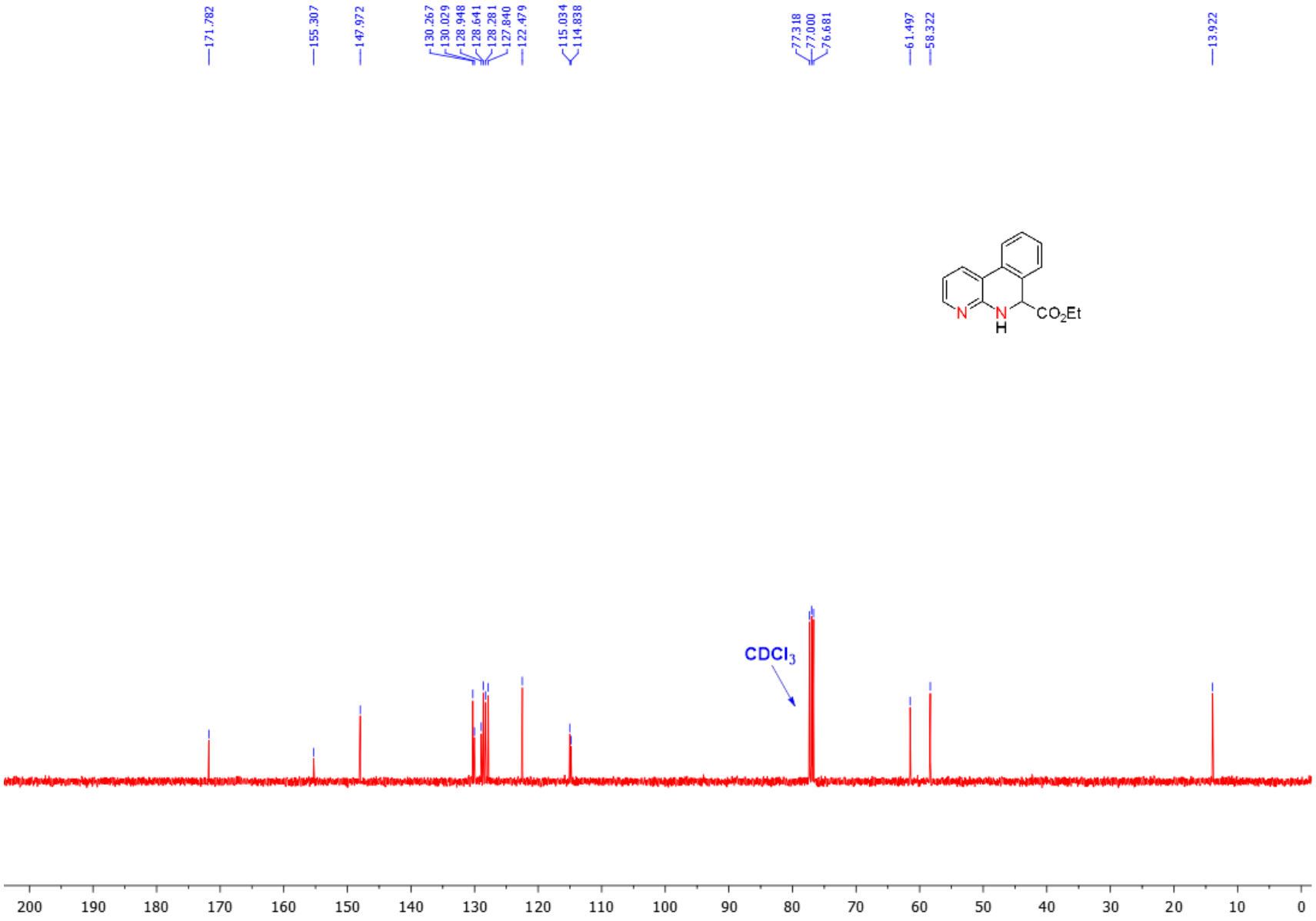
^{13}C-NMR of *6-butyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8c)* (25 ºC, 100 MHz, $CDCl_3$):



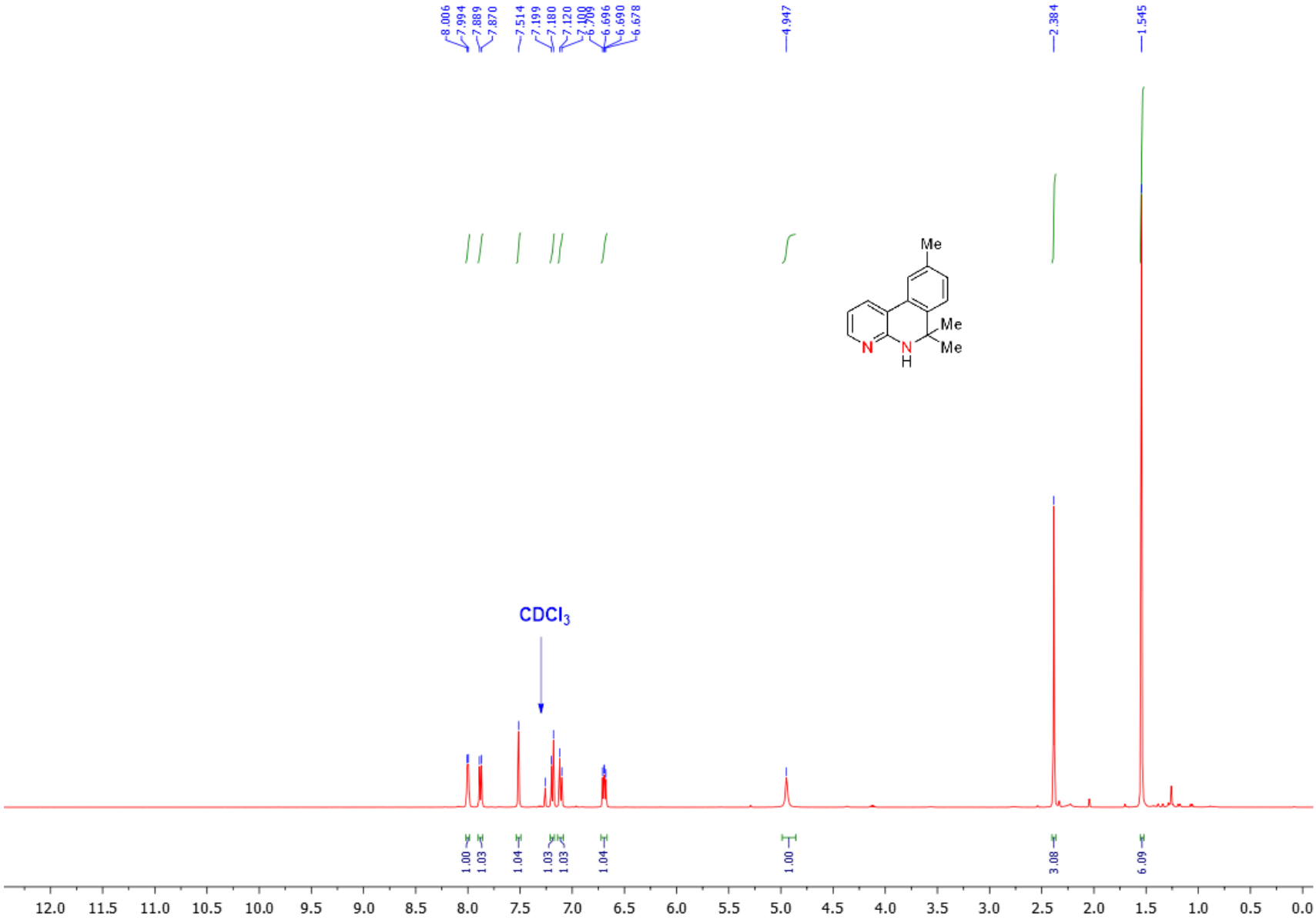
^{1}H-NMR of *ethyl 5,6-dihydrobenzo[c][1,8]naphthyridine-6-carboxylate (8d)* (25 °C, 400 MHz, $CDCl_3$):



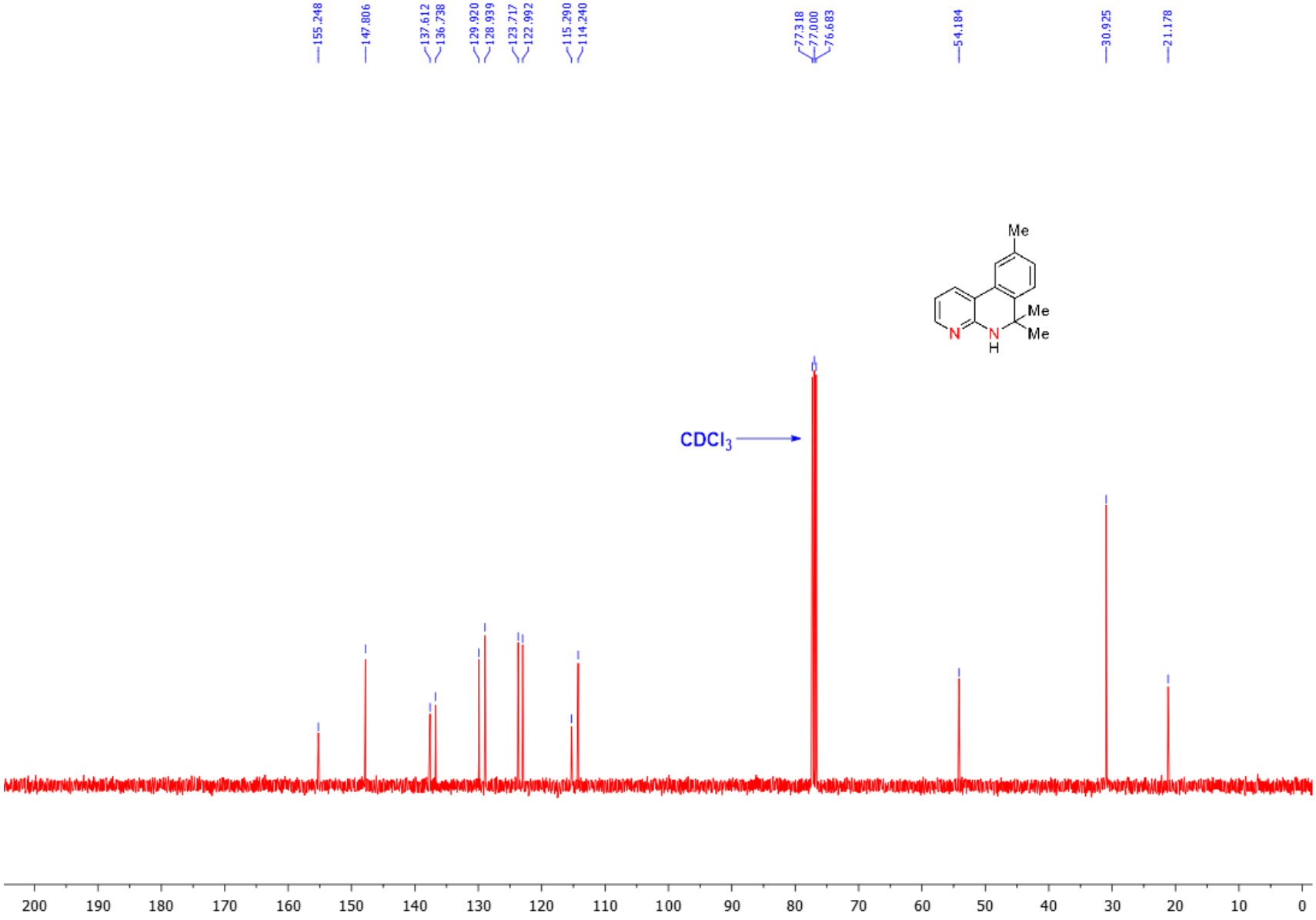
^{13}C-NMR of *ethyl 5,6-dihydrobenzo[c][1,8]naphthyridine-6-carboxylate (8d)* (25 °C, 100 MHz, $CDCl_3$):



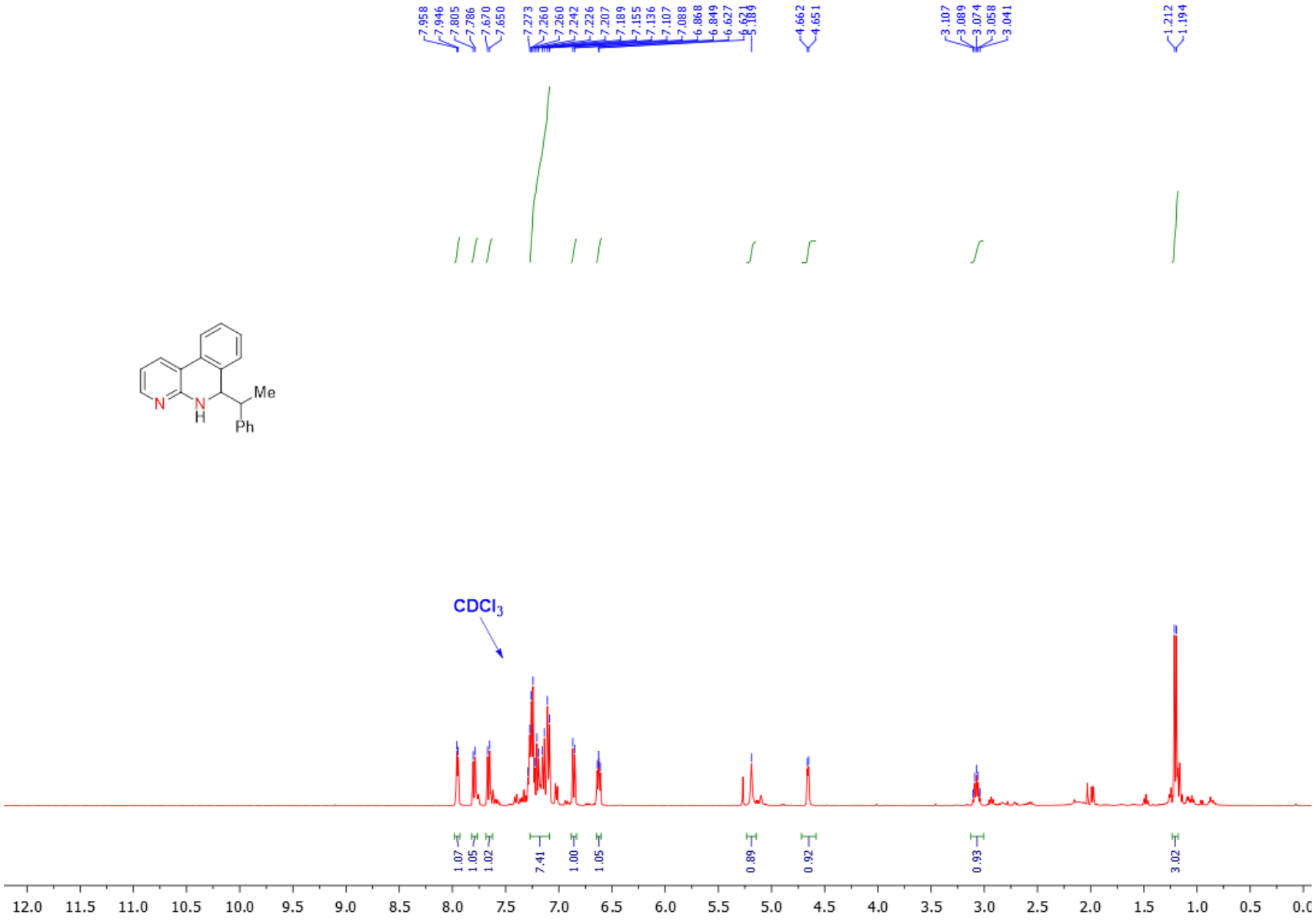
^{1}H-NMR of *6,6,9-trimethyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8e)* (25 ^{o}C, 400 MHz, $CDCl_3$):



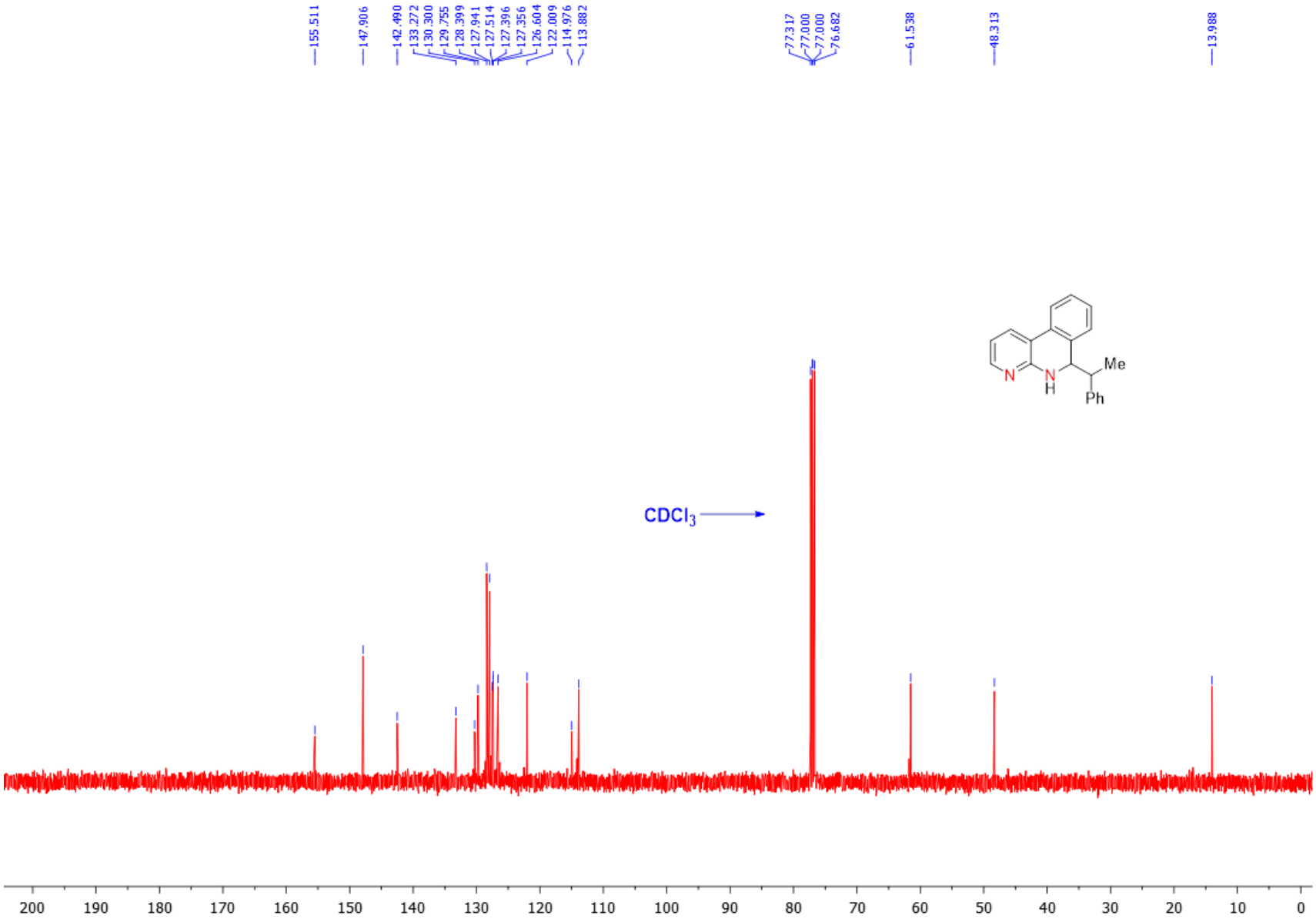
^{13}C-NMR of *6,6,9-trimethyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8e)* (25 °C, 100 MHz, $CDCl_3$):



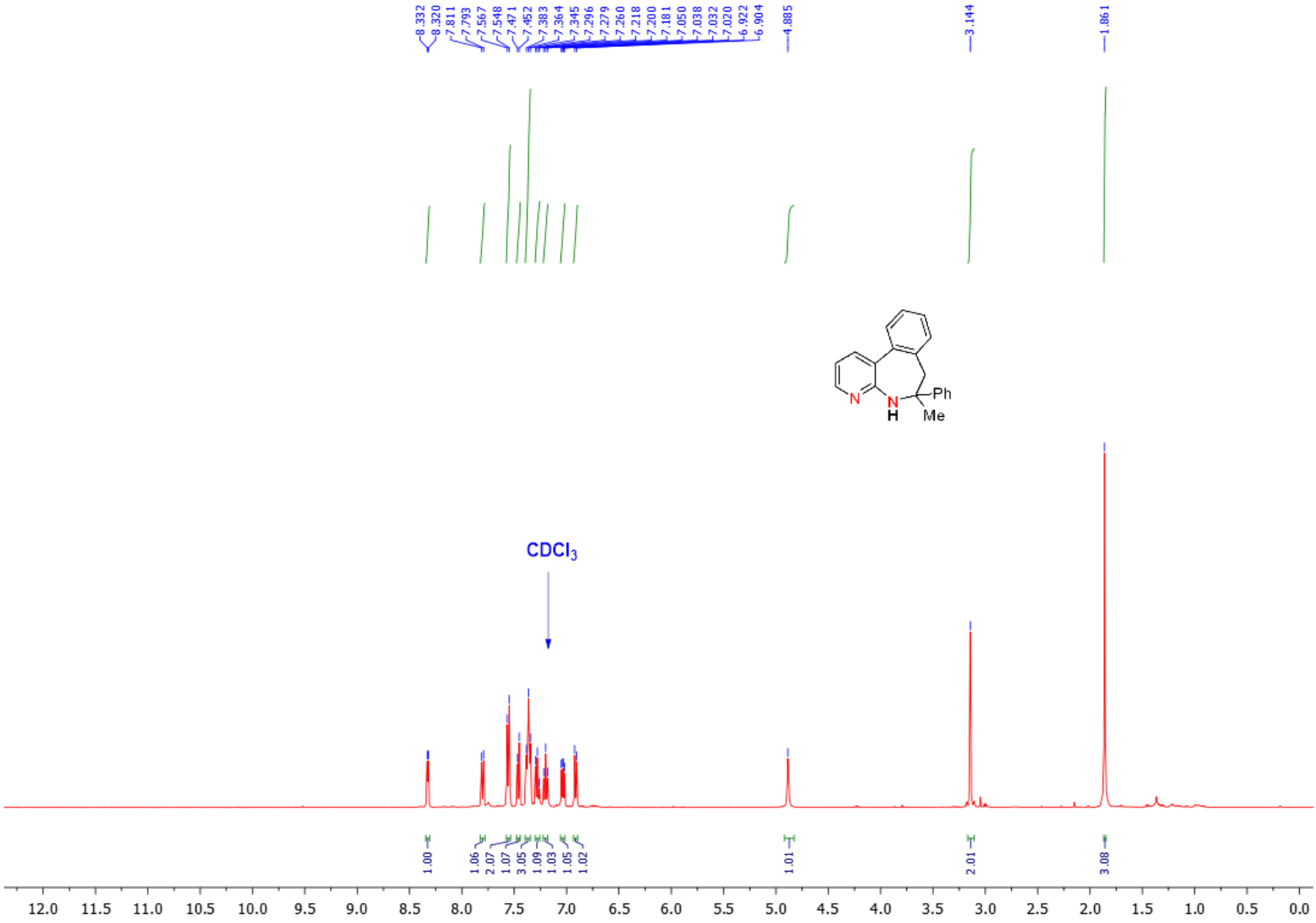
^{1}H-NMR of *6-(1-phenylethyl)-5,6-dihydrobenzo[c][1,8]naphthyridine (8f)* (25 ^{o}C, 400 MHz, $CDCl_3$):



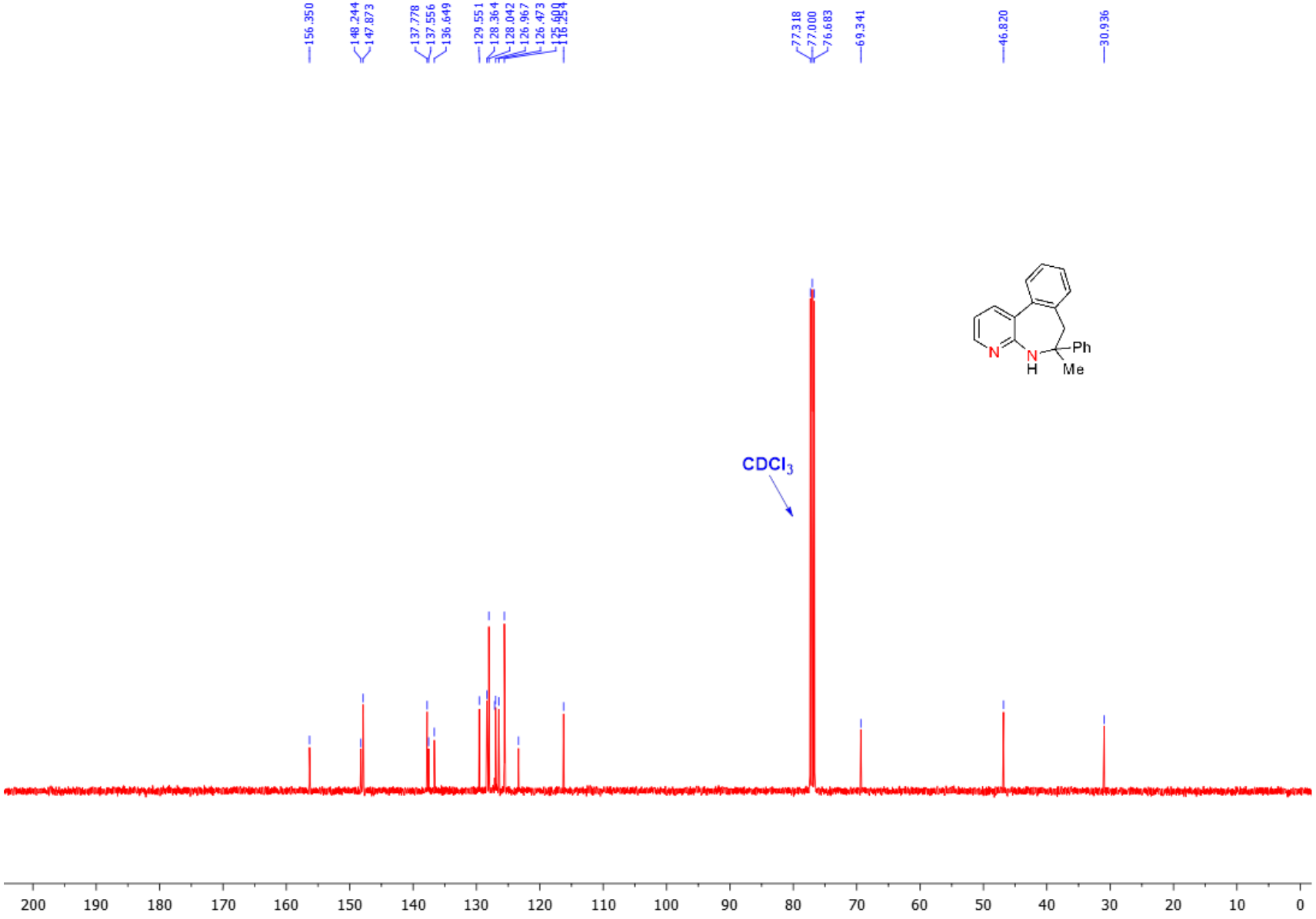
^{13}C-NMR of *6-(1-phenylethyl)-5,6-dihydrobenzo[c][1,8]naphthyridine (8f)* (25 °C, 100 MHz, $CDCl_3$):



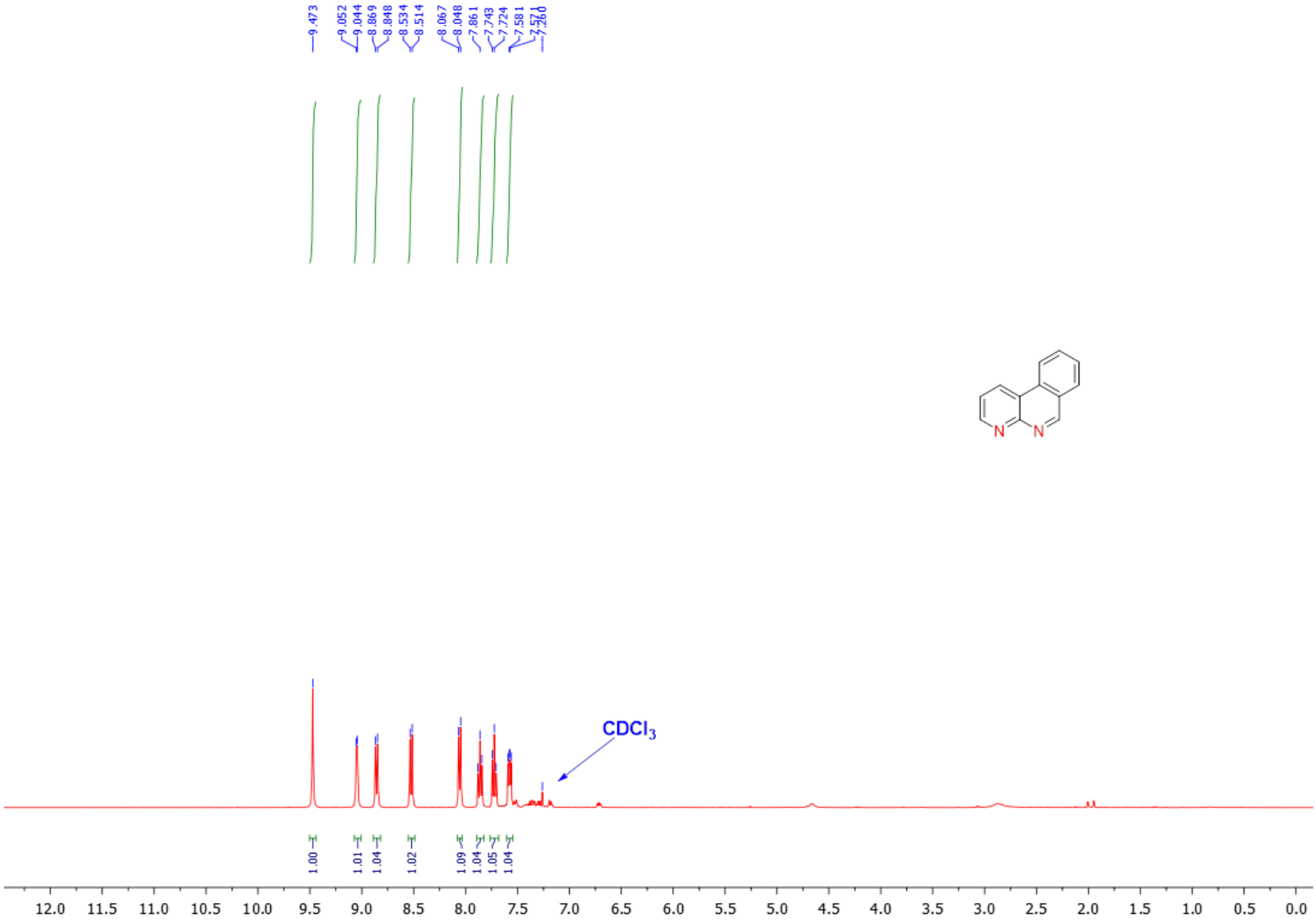
^{1}H-NMR of *6-methyl-6-phenyl-6,7-dihydro-5H-benzo[d]pyrido[2,3-b]azepine (8f')* (25 °C, 400 MHz, $CDCl_3$):



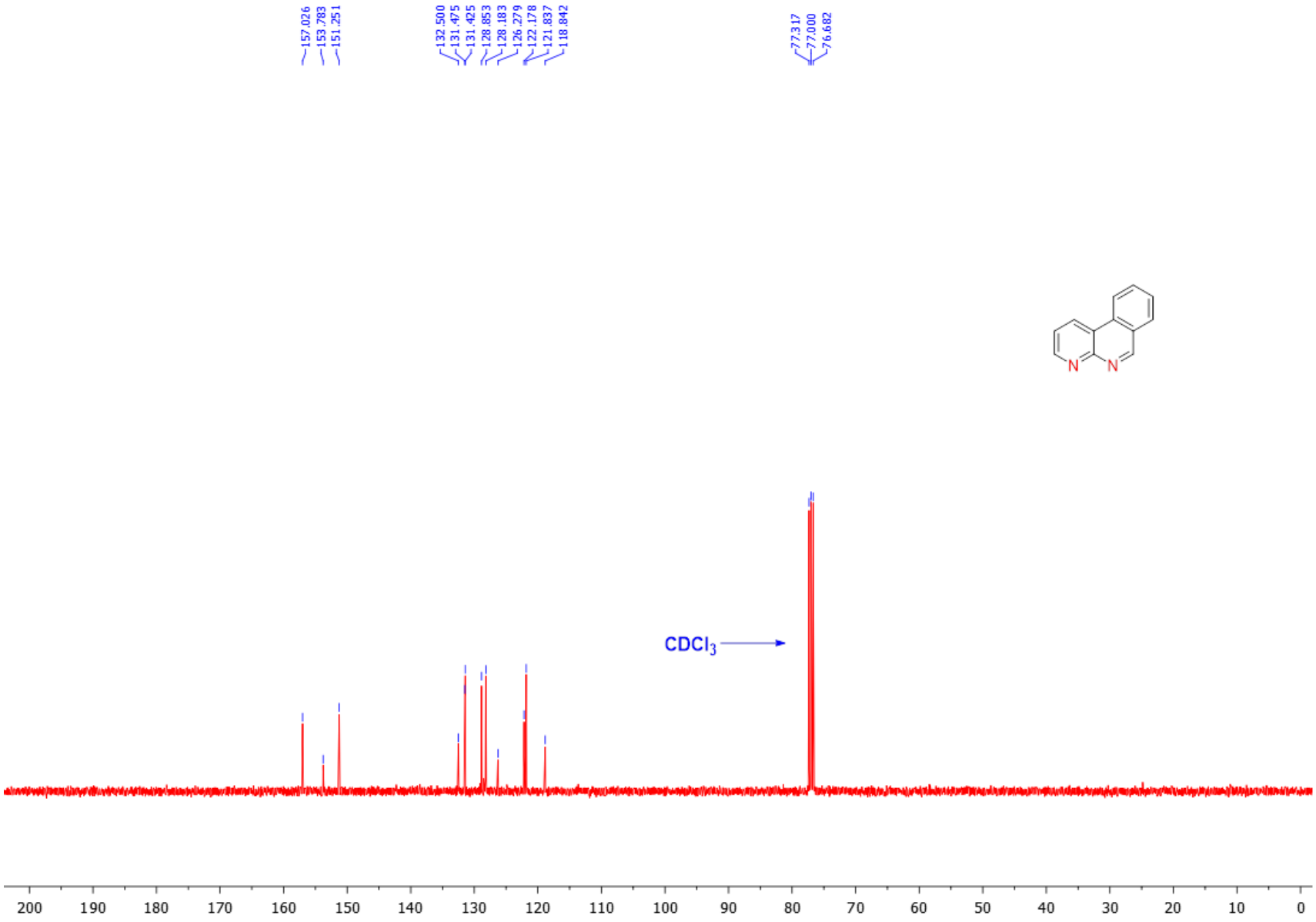
^{13}C-NMR of *6-methyl-6-phenyl-6,7-dihydro-5H-benzo[d]pyrido[2,3-b]azepine (8f')* (25 °C, 100 MHz, $CDCl_3$):



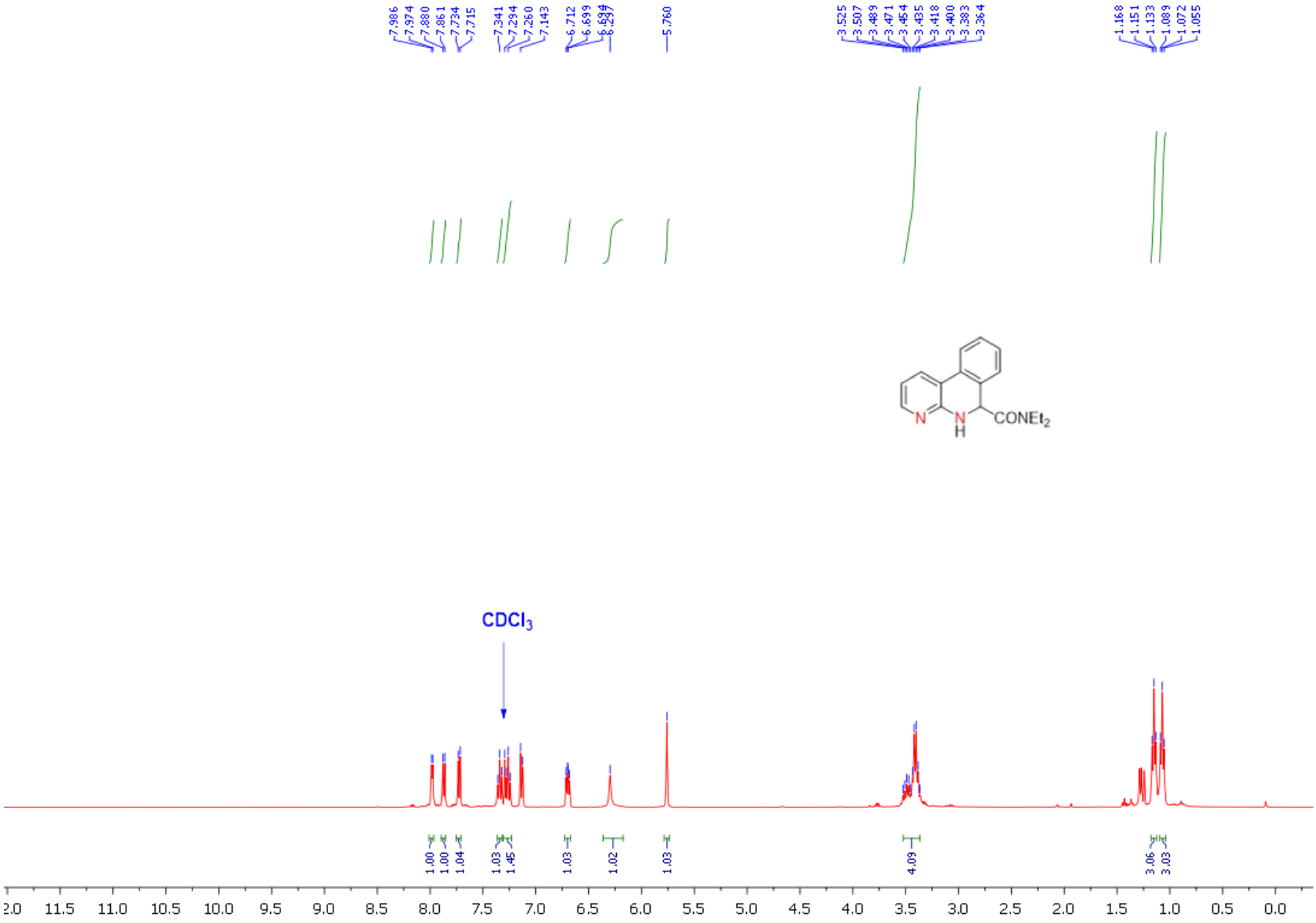
^{1}H-NMR of *benzo[c][1,8]naphthyridine (8g)* (25 ^{o}C, 400 MHz, $CDCl_3$):



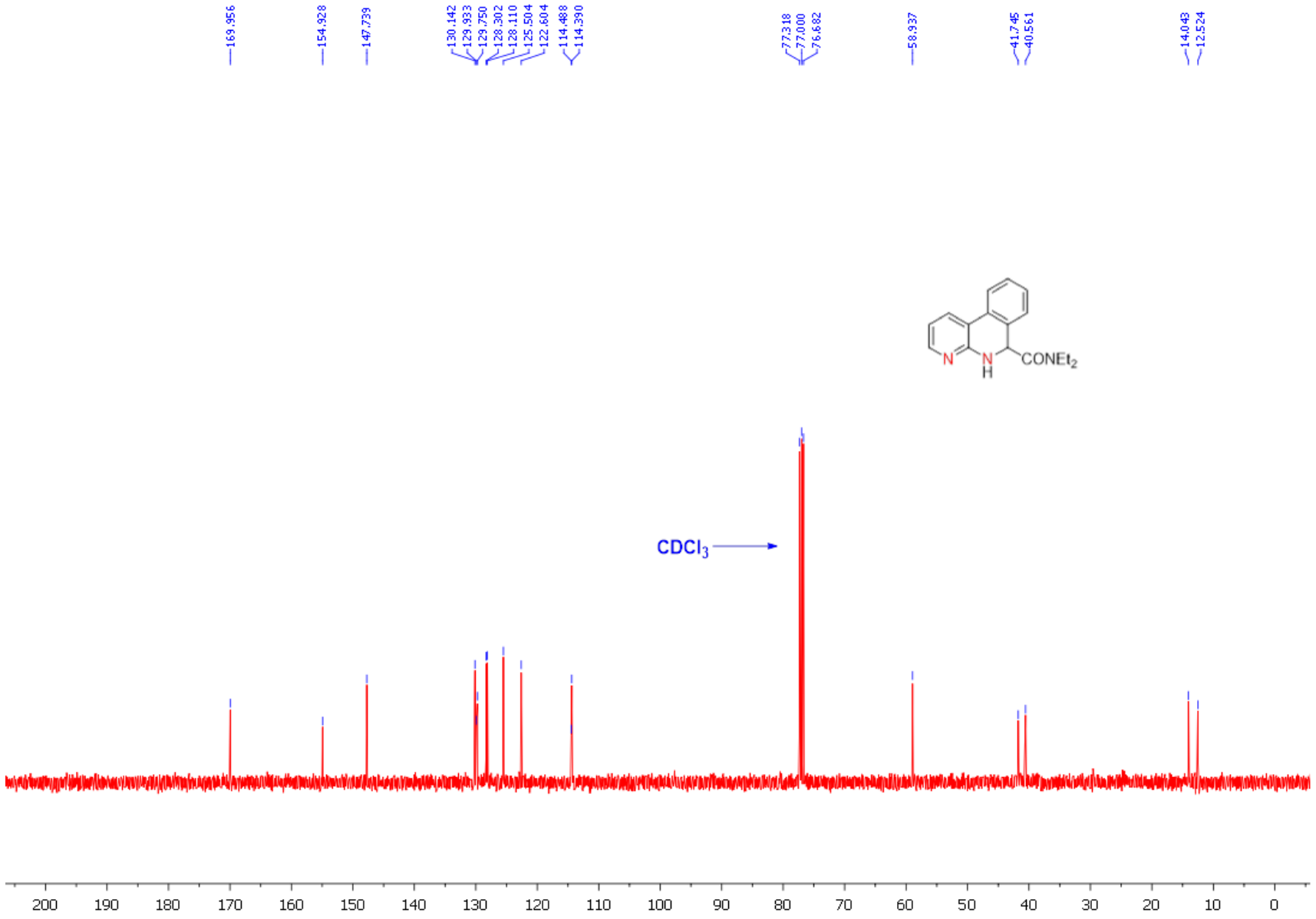
^{13}C-NMR of *benzo[c][1,8]naphthyridine (8g))* (25 ^{o}C, 100 MHz, $CDCl_3$):



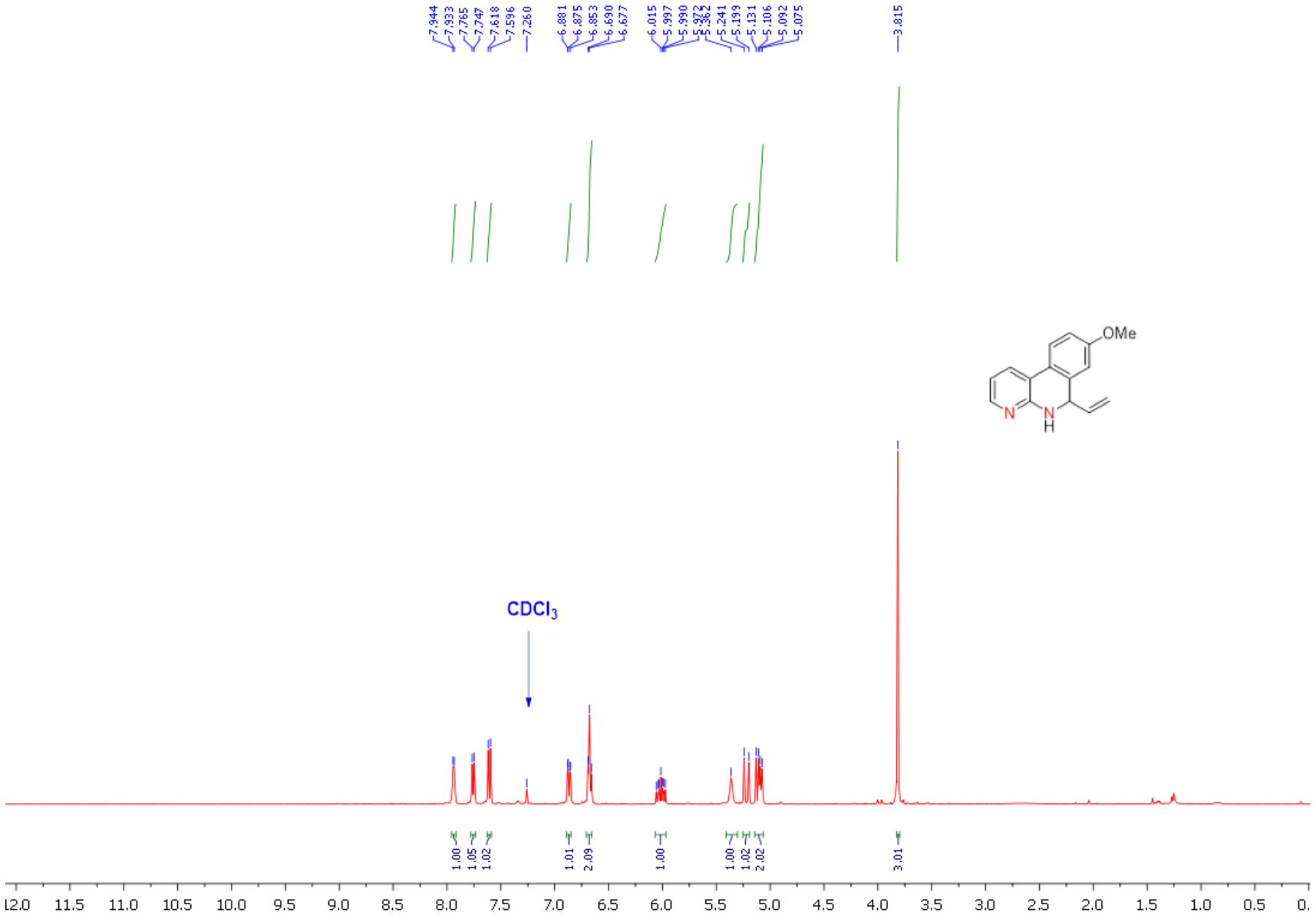
^{1}H-NMR of *N,N-diethyl-5,6-dihydrobenzo[c][1,8]naphthyridine-6-carboxamide (8h)* (25 ºC, 400 MHz, $CDCl_3$):



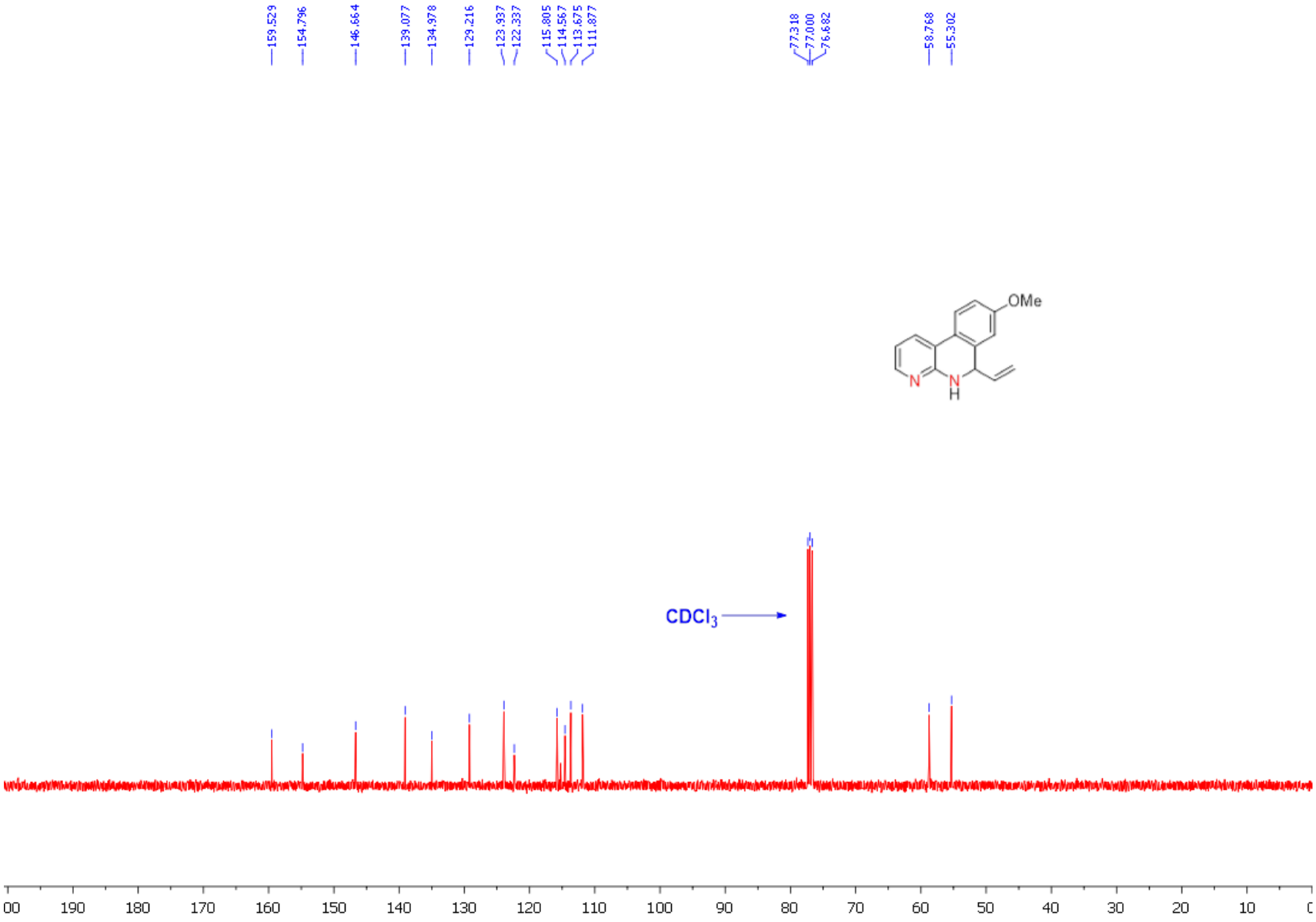
^{13}C-NMR of *N,N-diethyl-5,6-dihydrobenzo[c][1,8]naphthyridine-6-carboxamide(8h)* (25 ºC, 100 MHz, $CDCl_3$):



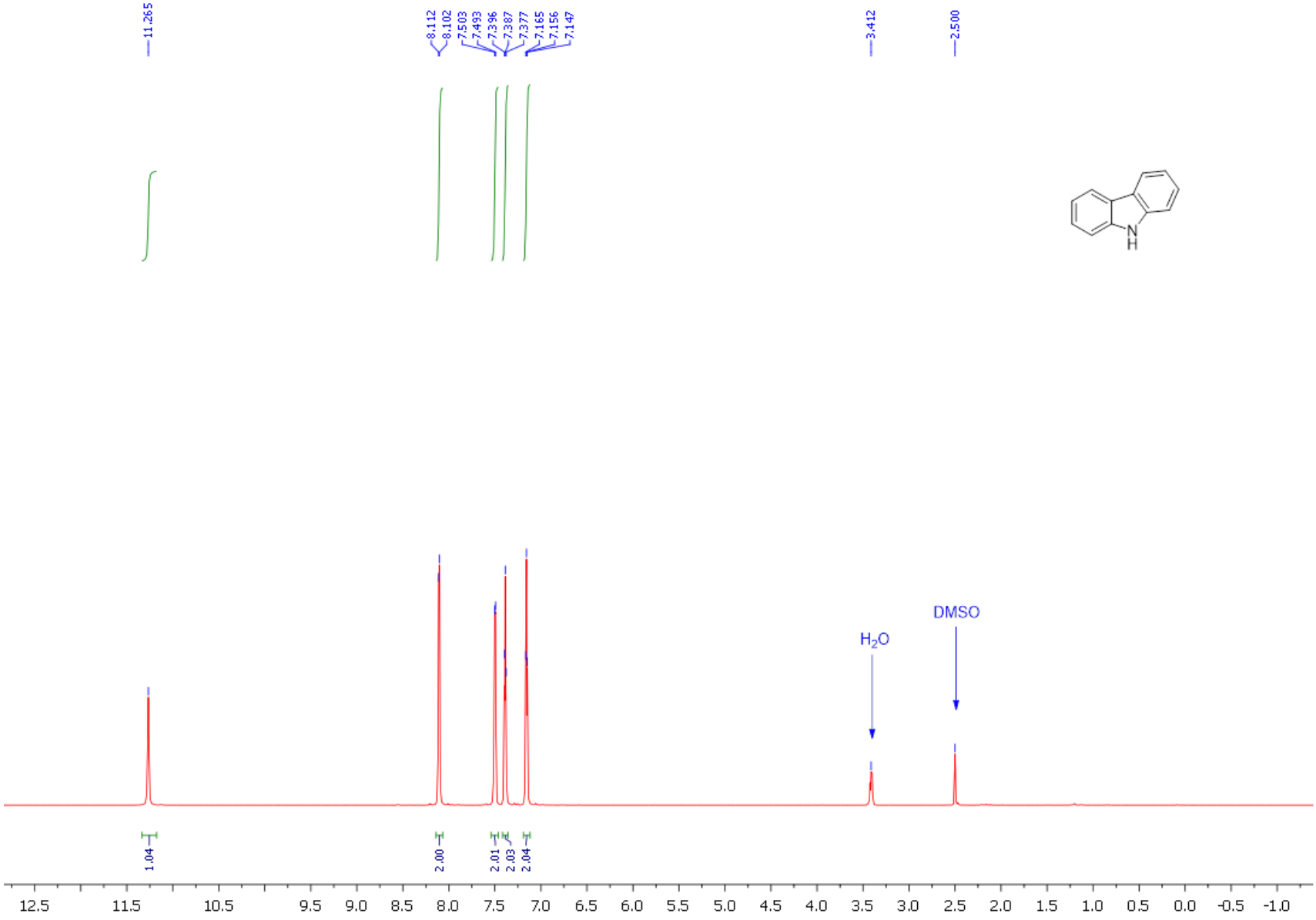
^{1}H-NMR of *8-methoxy-6-vinyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8i)* (25 ^{o}C, 400 MHz, $CDCl_3$):



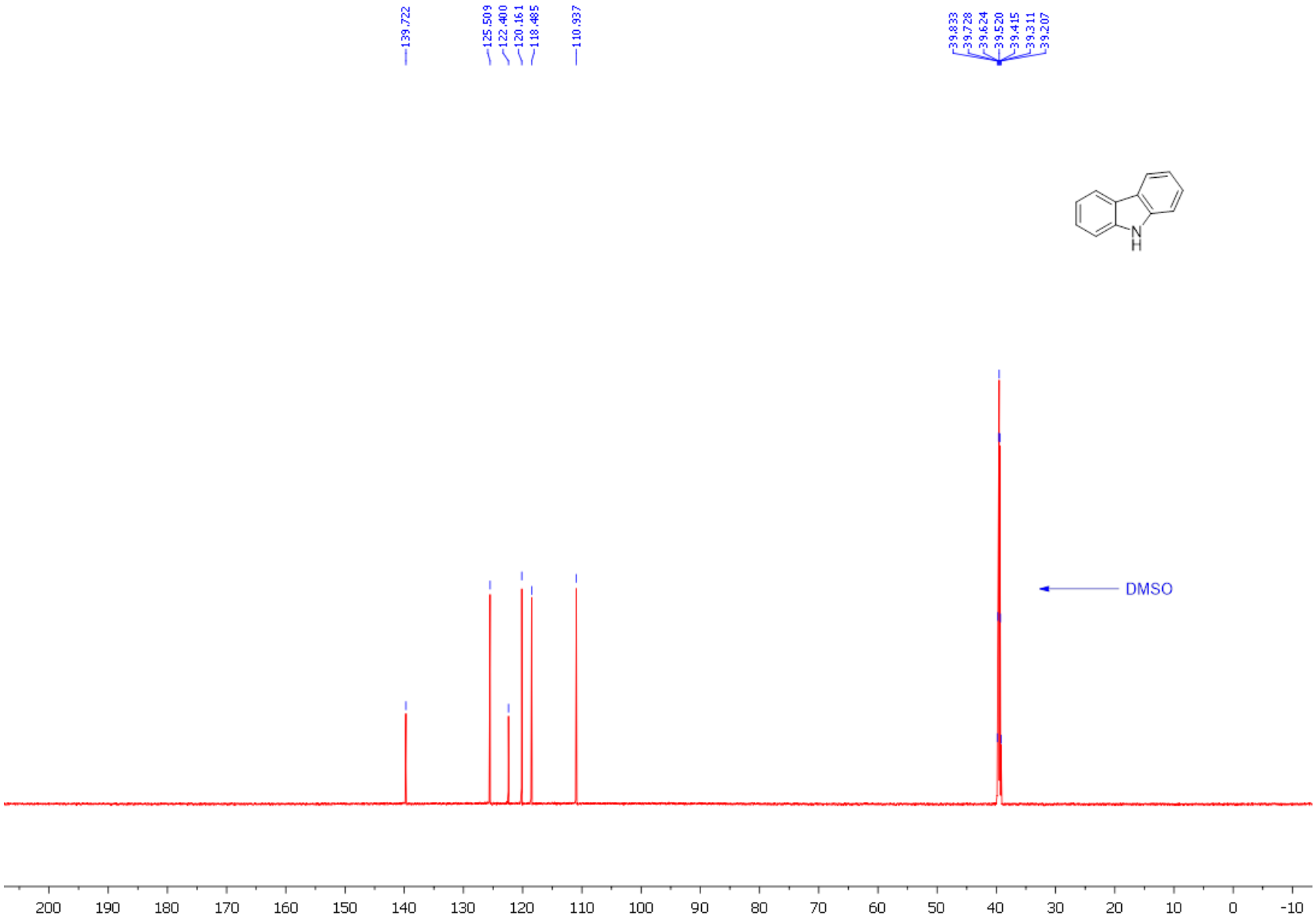
^{13}C-NMR of *8-methoxy-6-vinyl-5,6-dihydrobenzo[c][1,8]naphthyridine (8i)* (25 °C, 100 MHz, $CDCl_3$):



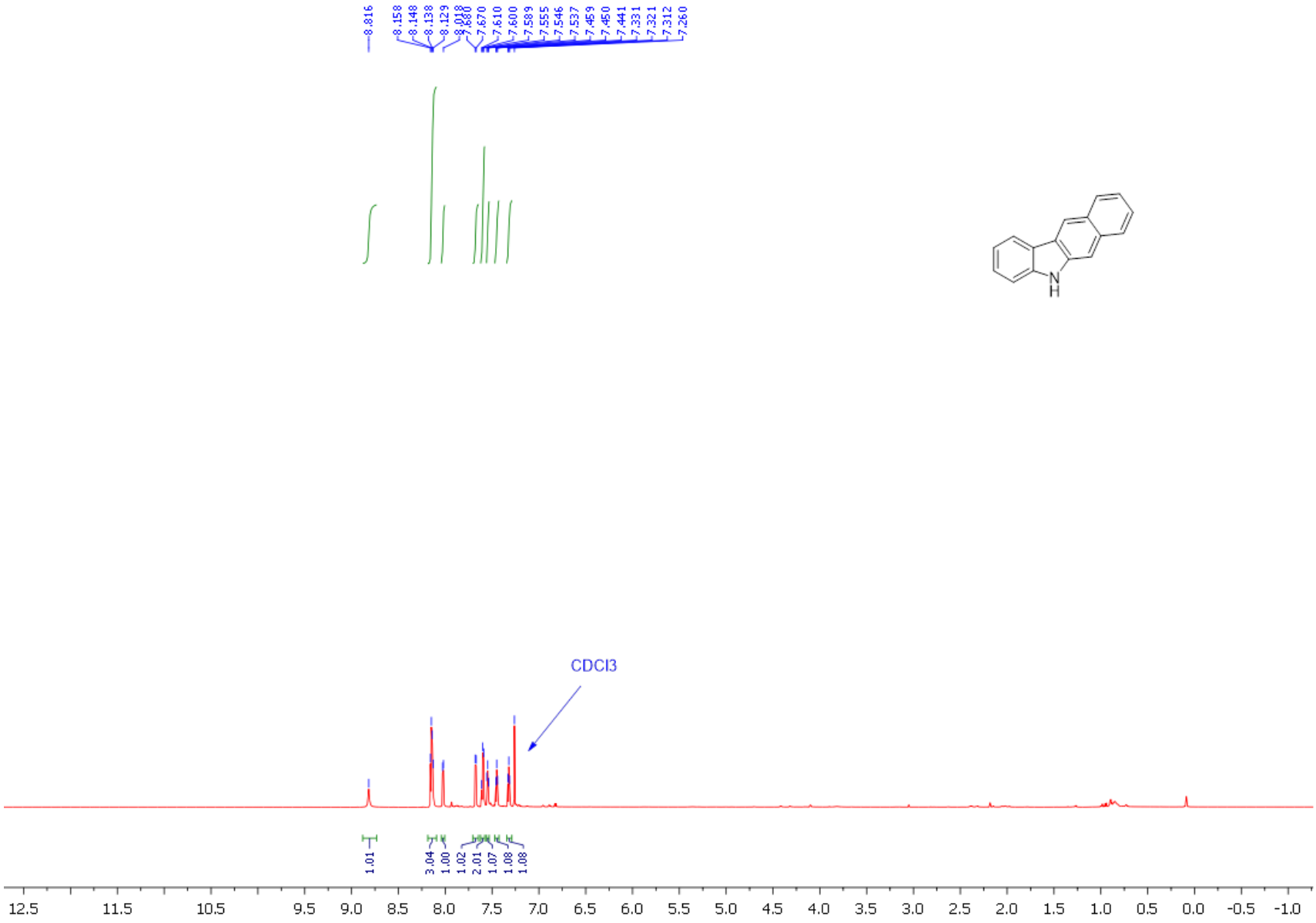
^{1}H-NMR of *9H-carbazole (10a)* (25 ^{o}C, 800 MHz, DMSO-d_6):



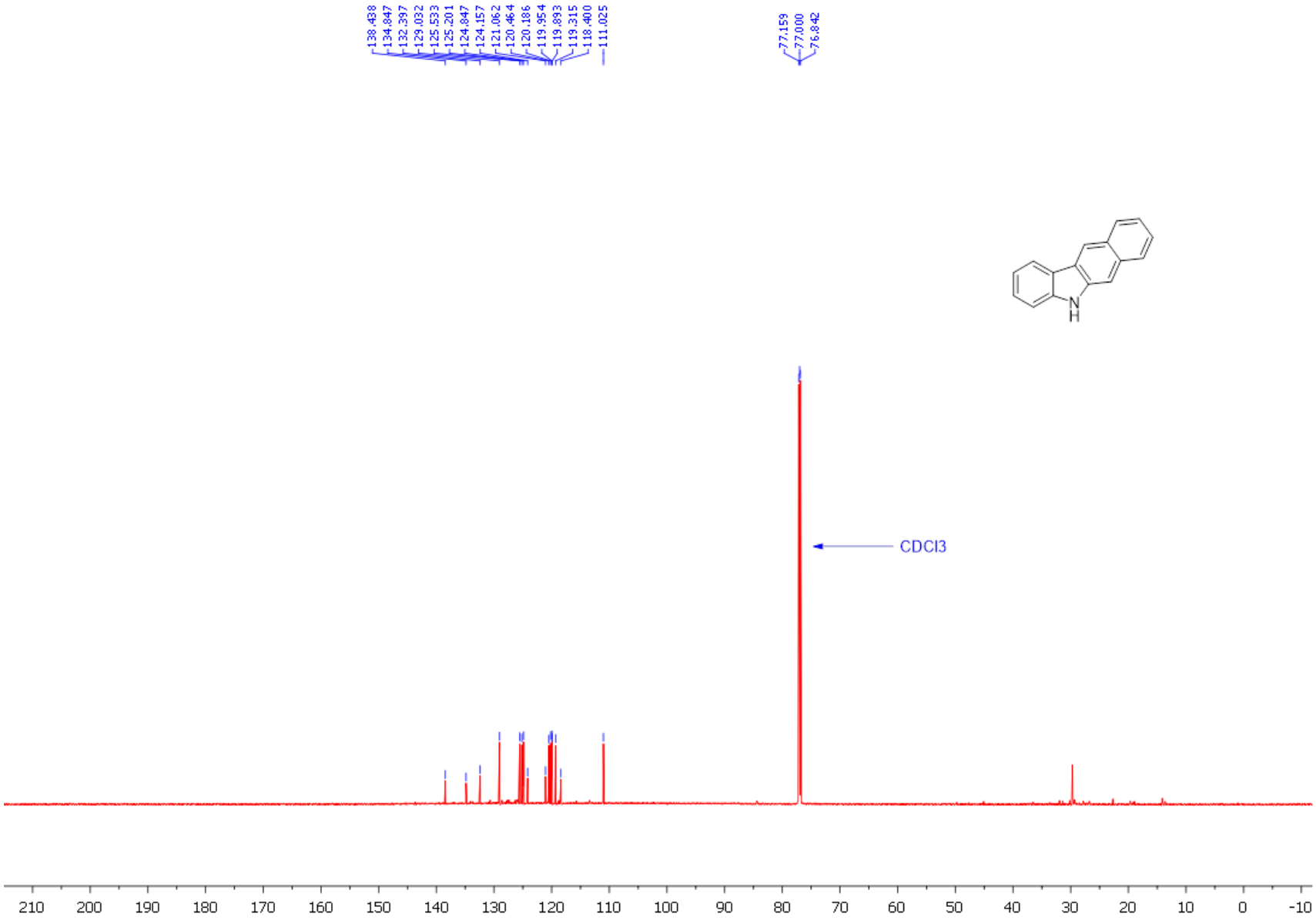
^{13}C-NMR of *9H-carbazole (10a)* (25 ºC, 200 MHz, DMSO-d_6):



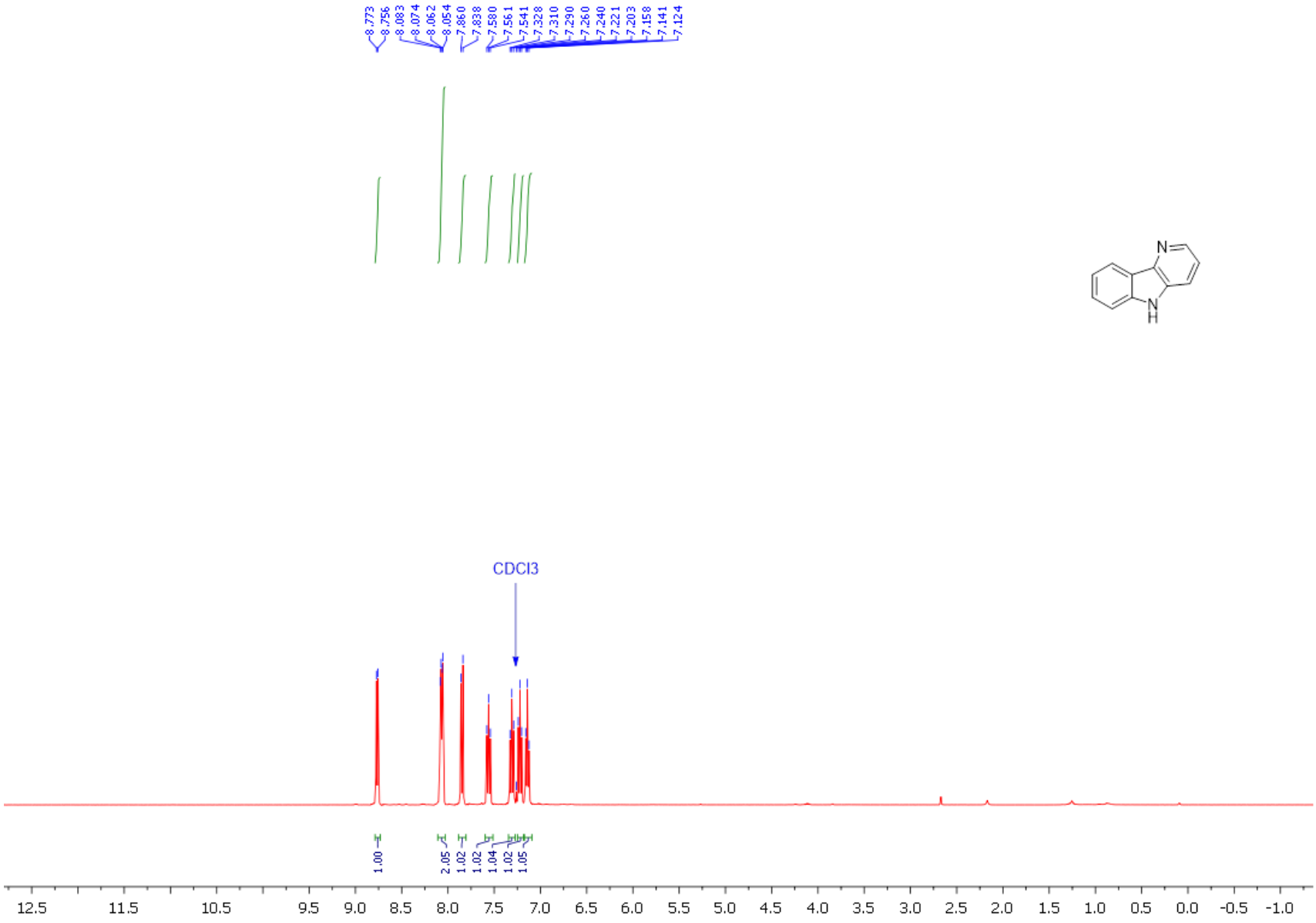
^{1}H-NMR of *5H-benzo[b]carbazole (10b)* (25 ^{o}C, 800 MHz, $CDCl_3$):



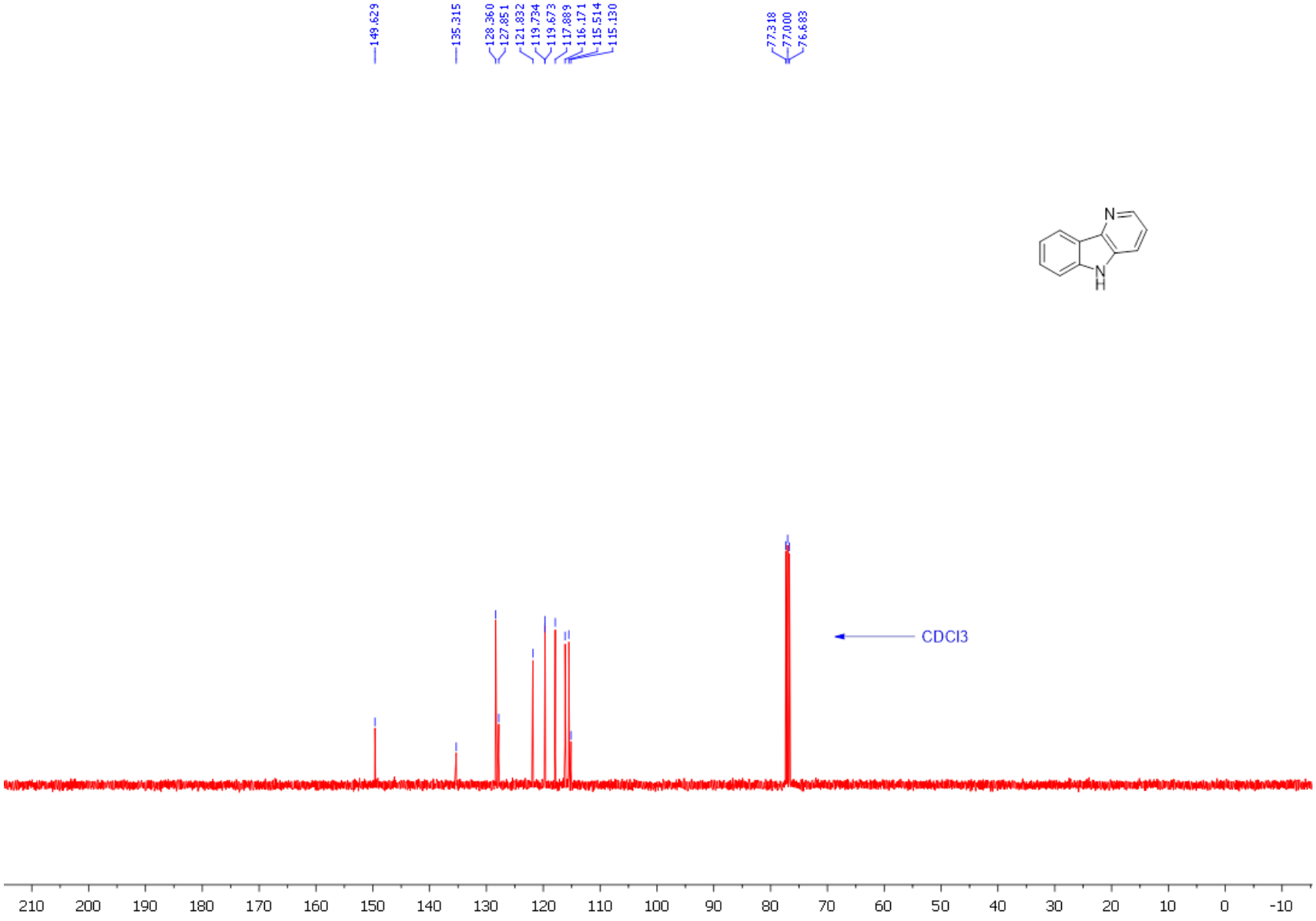
^{13}C-NMR of *pyrido[2,3-b]quinoxaline (16)* (25 ºC, 200 MHz, $CDCl_3$):



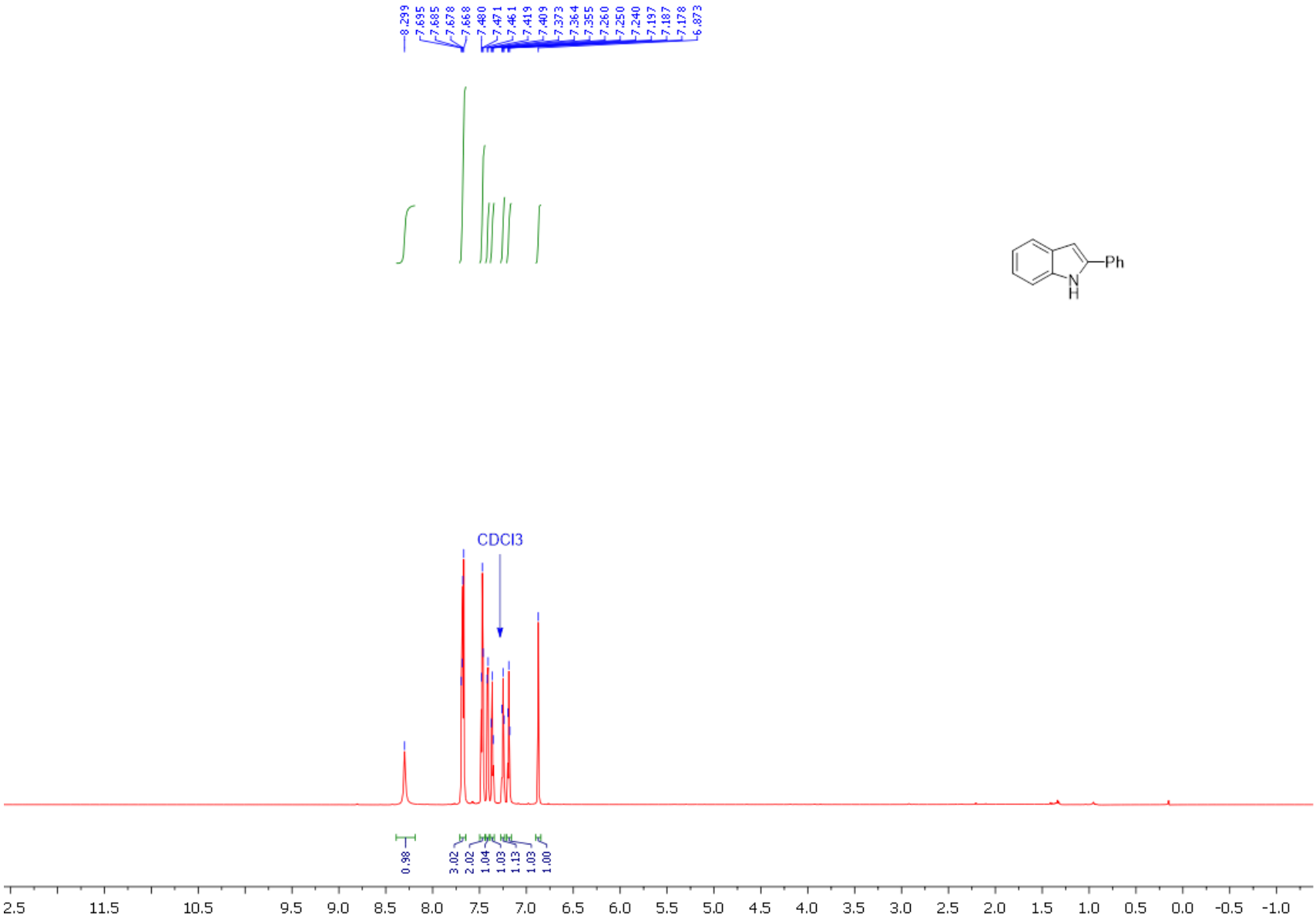
^{1}H-NMR of *5H-pyrido[3,2-b]indole (10c)* (25 °C, 400 MHz, $CDCl_3$):



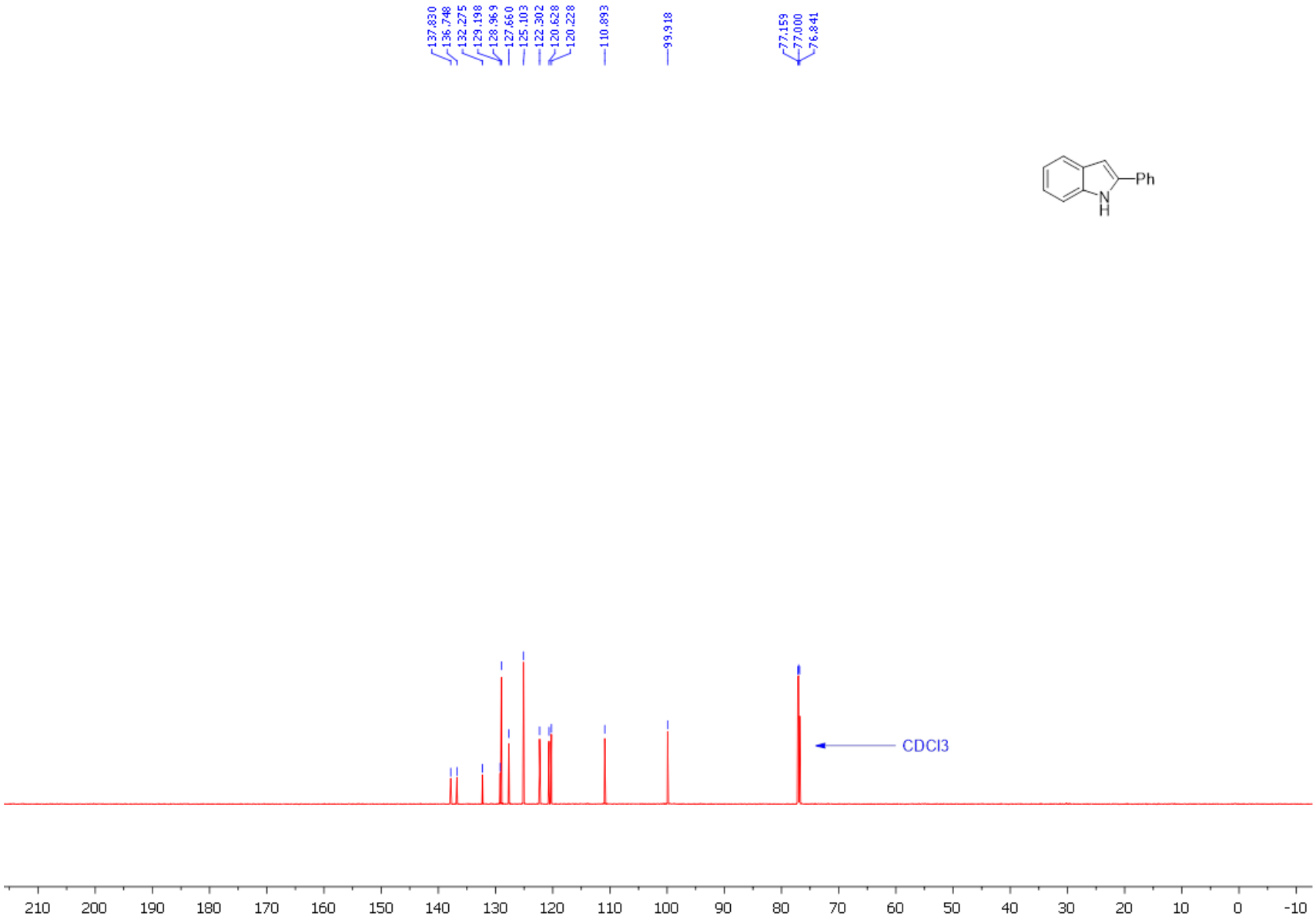
^{13}C-NMR of *5H-pyrido[3,2-b]indole (10c)* (25 ºC, 100 MHz, $CDCl_3$):



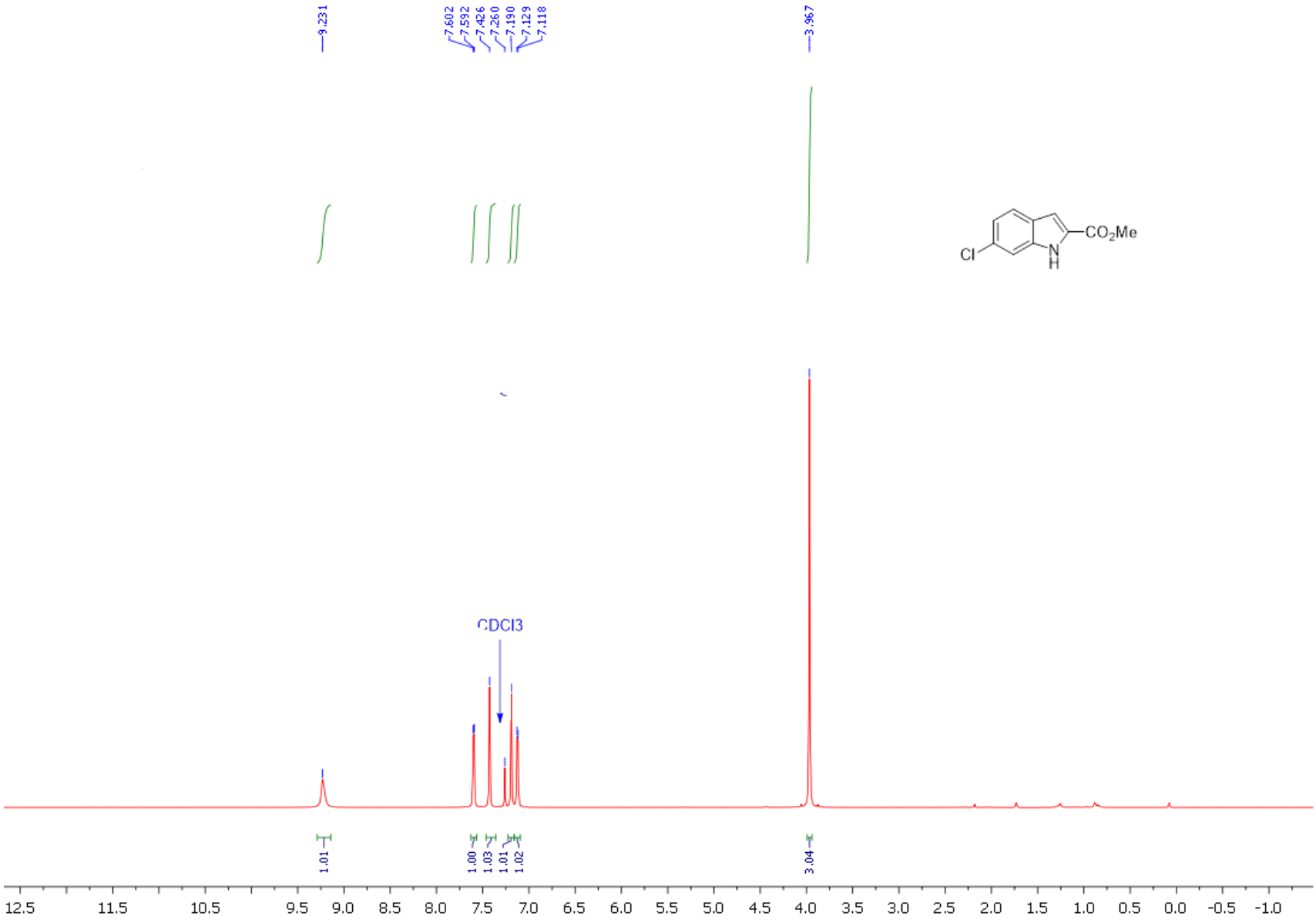
^{1}H-NMR of *2-phenyl-1H-indole (10d)* (25 ^{o}C, 800 MHz, $CDCl_3$):



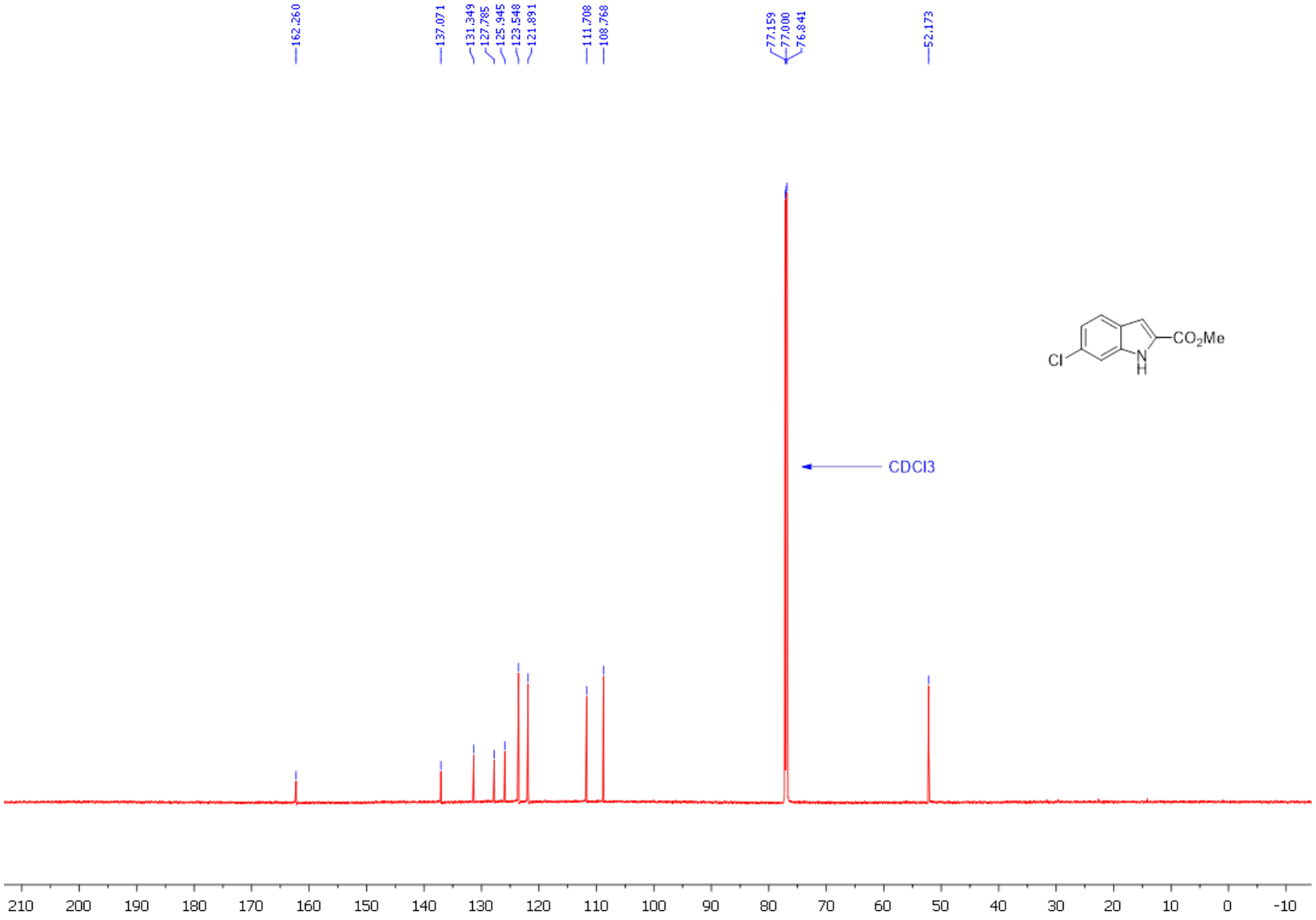
^{13}C-NMR of *2-phenyl-1H-indole (10d)* (25 ºC, 200 MHz, $CDCl_3$):



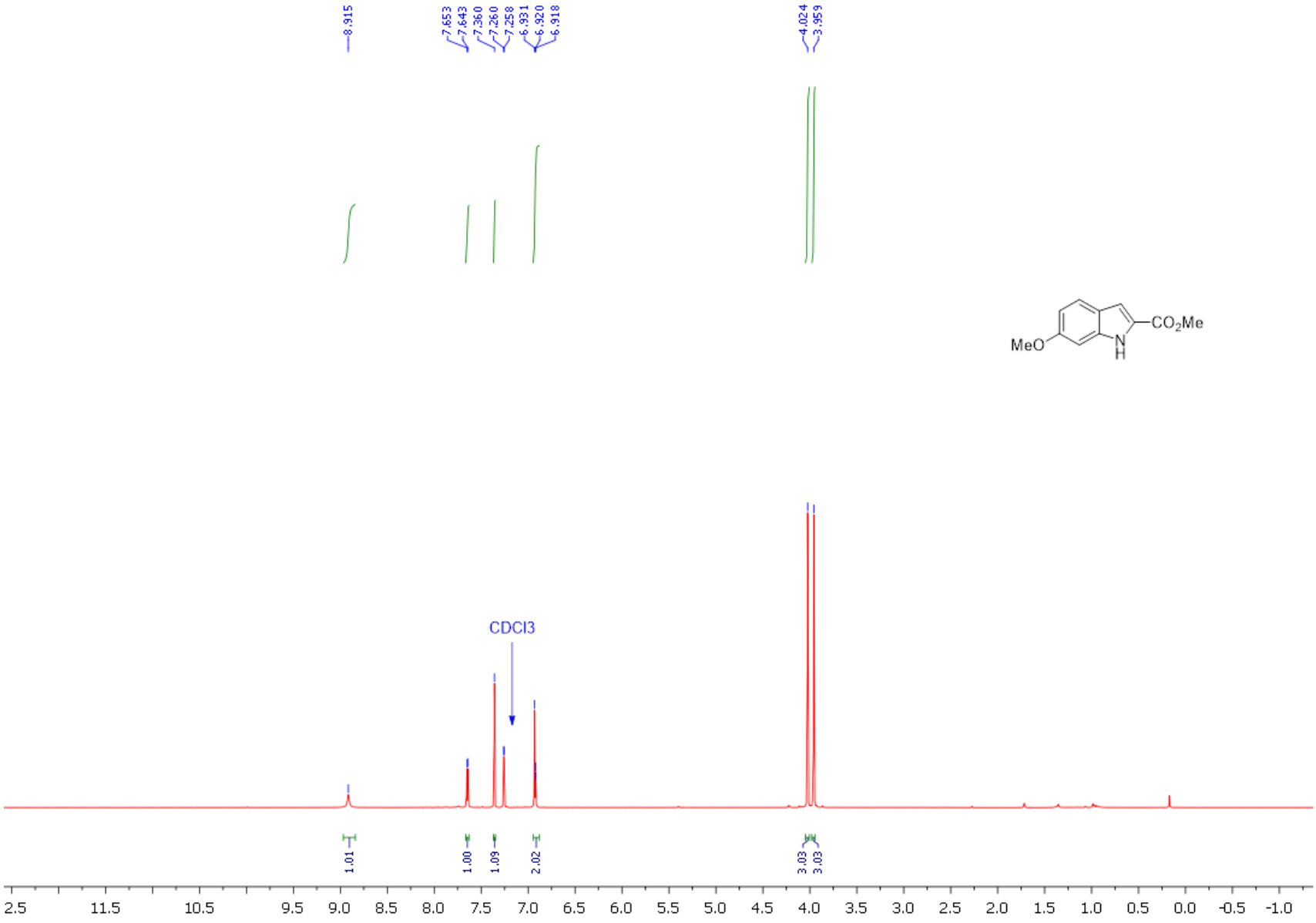
^{1}H-NMR of *methyl 6-chloro-1H-indole-2-carboxylate (10e)* (25 ºC, 800 MHz, $CDCl_3$):



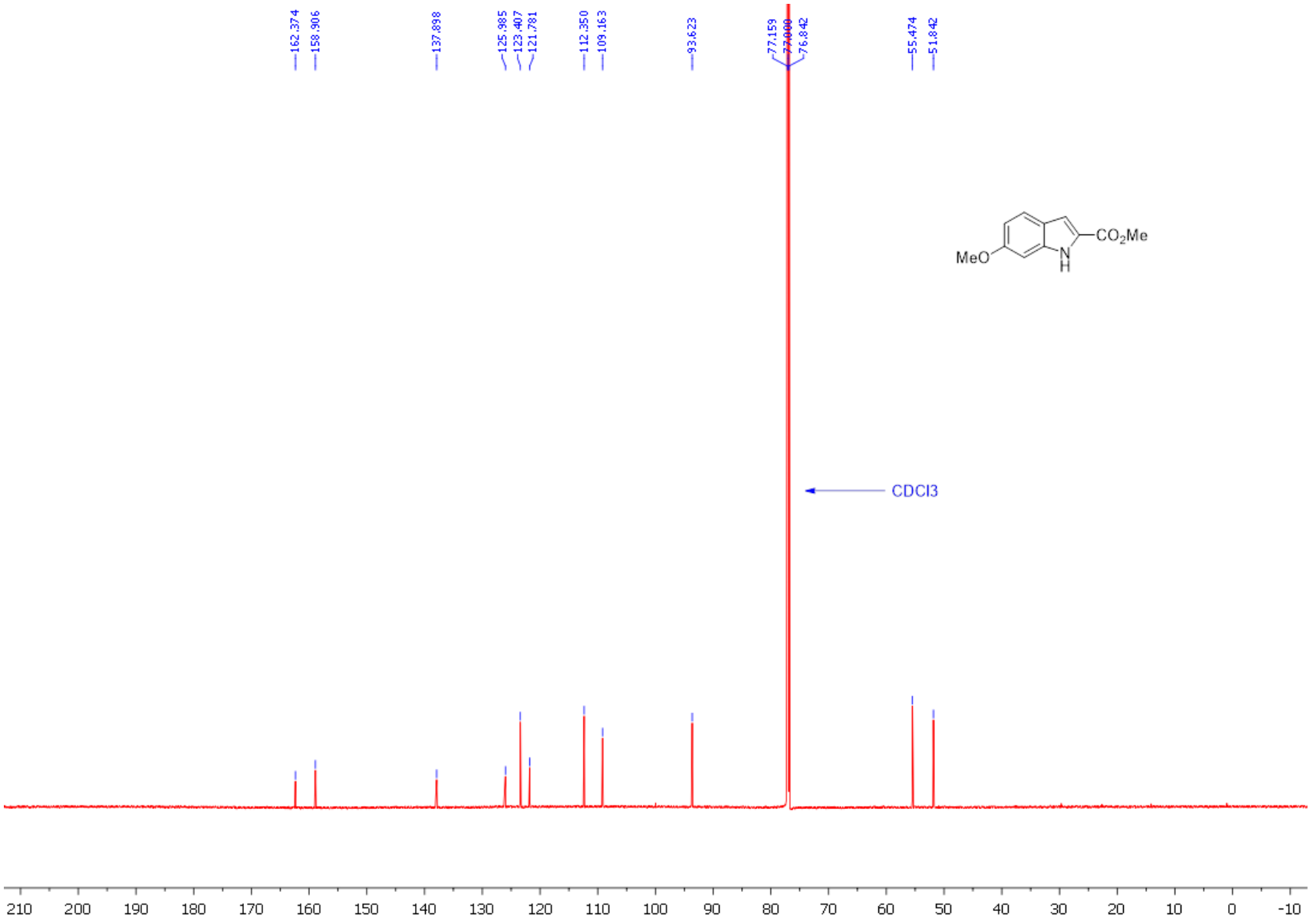
^{13}C-NMR of *methyl 6-chloro-1H-indole-2-carboxylate (10e)* (25 ºC, 200 MHz, $CDCl_3$):



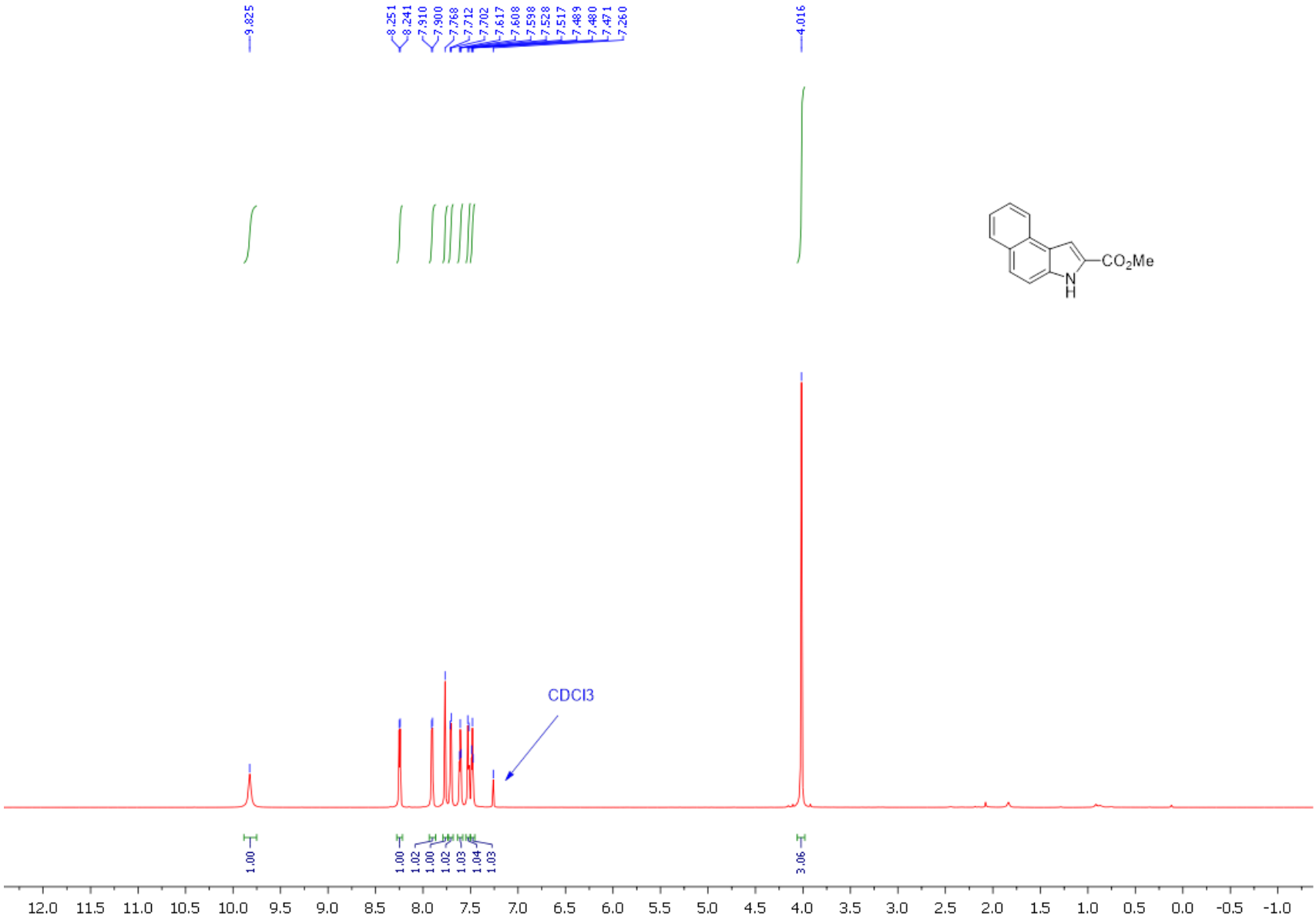
^{1}H-NMR of *methyl 6-methoxy-1H-indole-2-carboxylate (10f)* (25 ^{o}C, 800 MHz, $CDCl_3$):



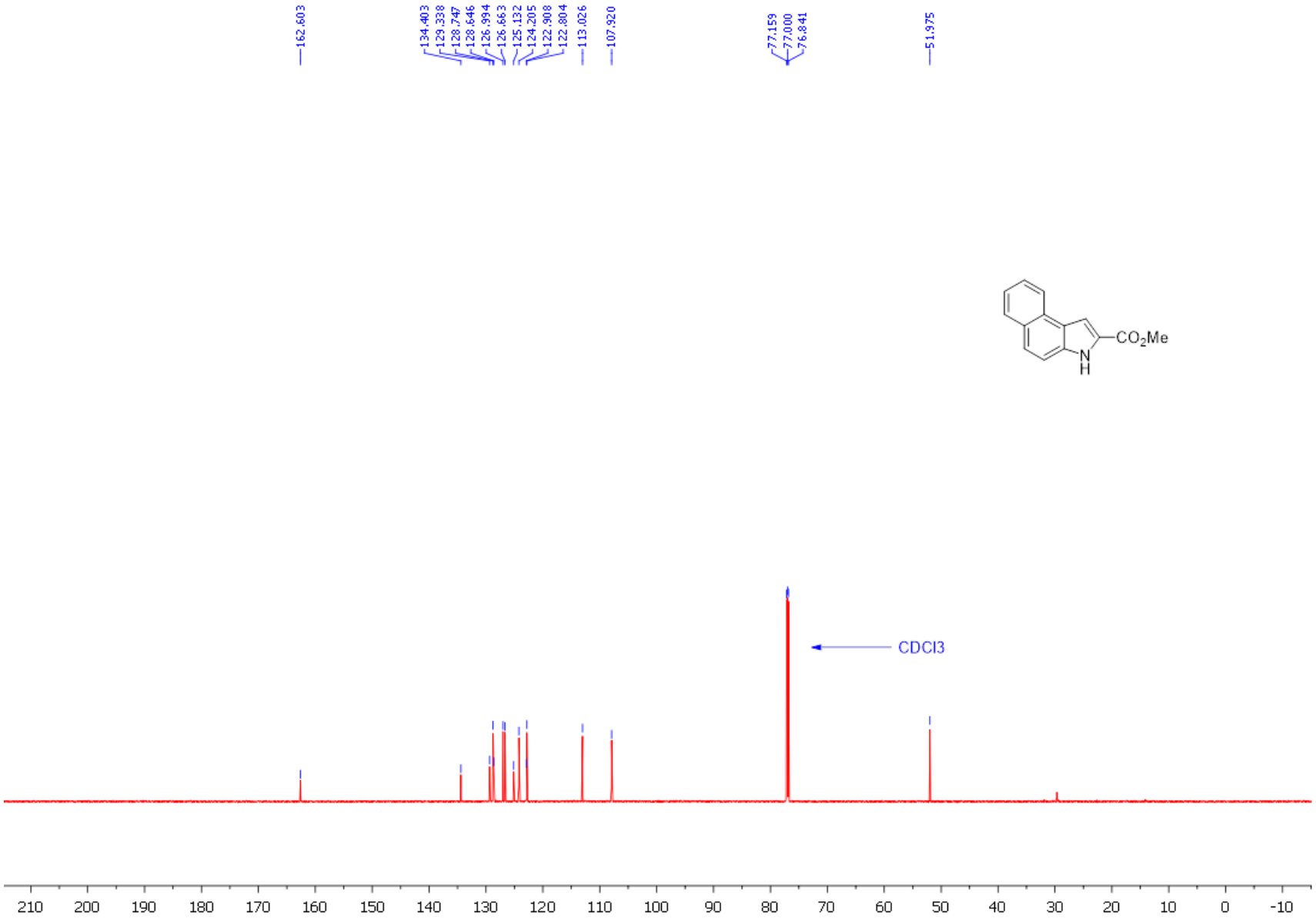
^{13}C-NMR of *methyl 6-methoxy-1H-indole-2-carboxylate (10f)* (25 ºC, 200 MHz, $CDCl_3$):



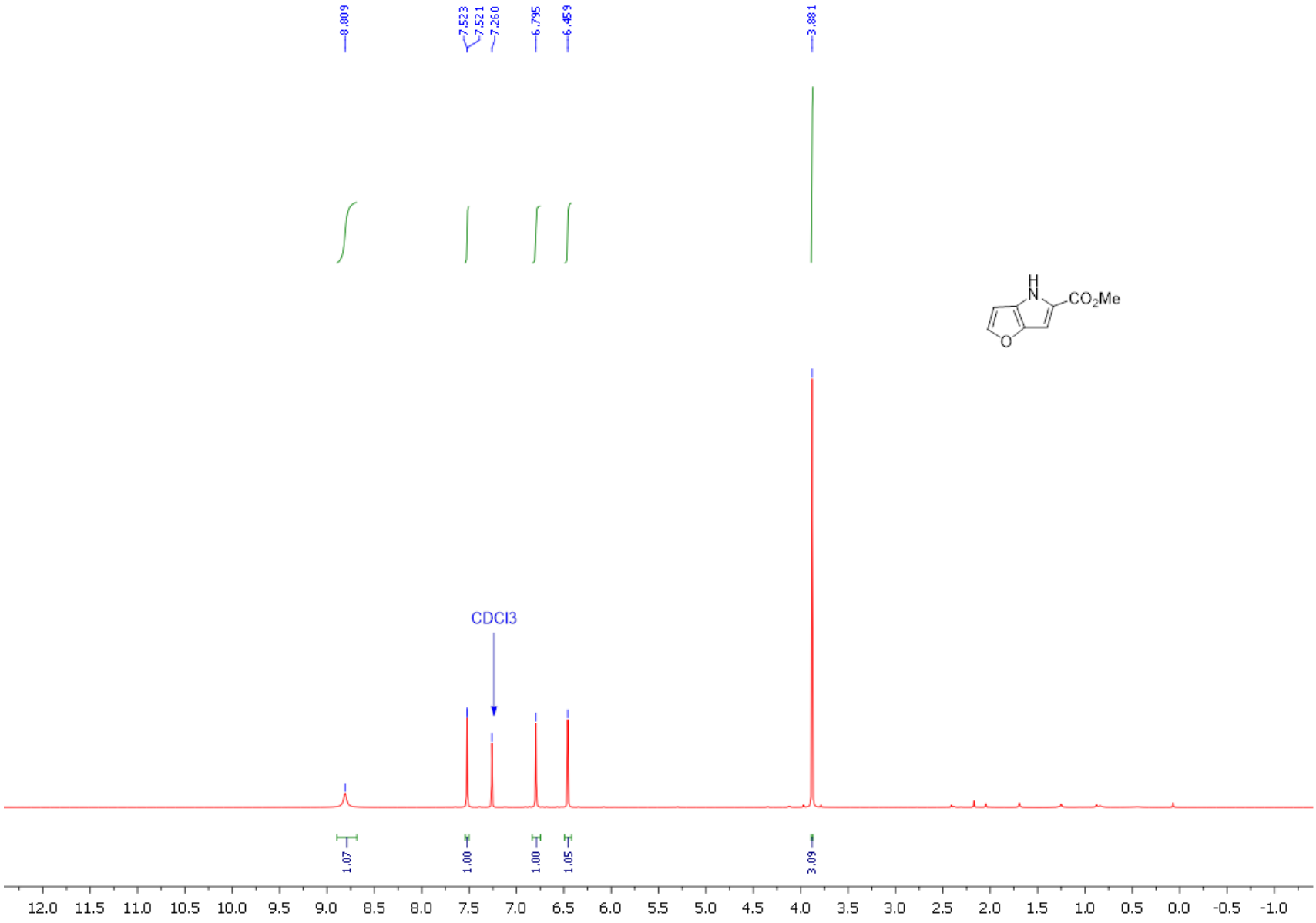
^{1}H-NMR of *methyl 3H-benzo[e]indole-2-carboxylate (10g)* (25 ^{o}C, 800 MHz, $CDCl_3$):



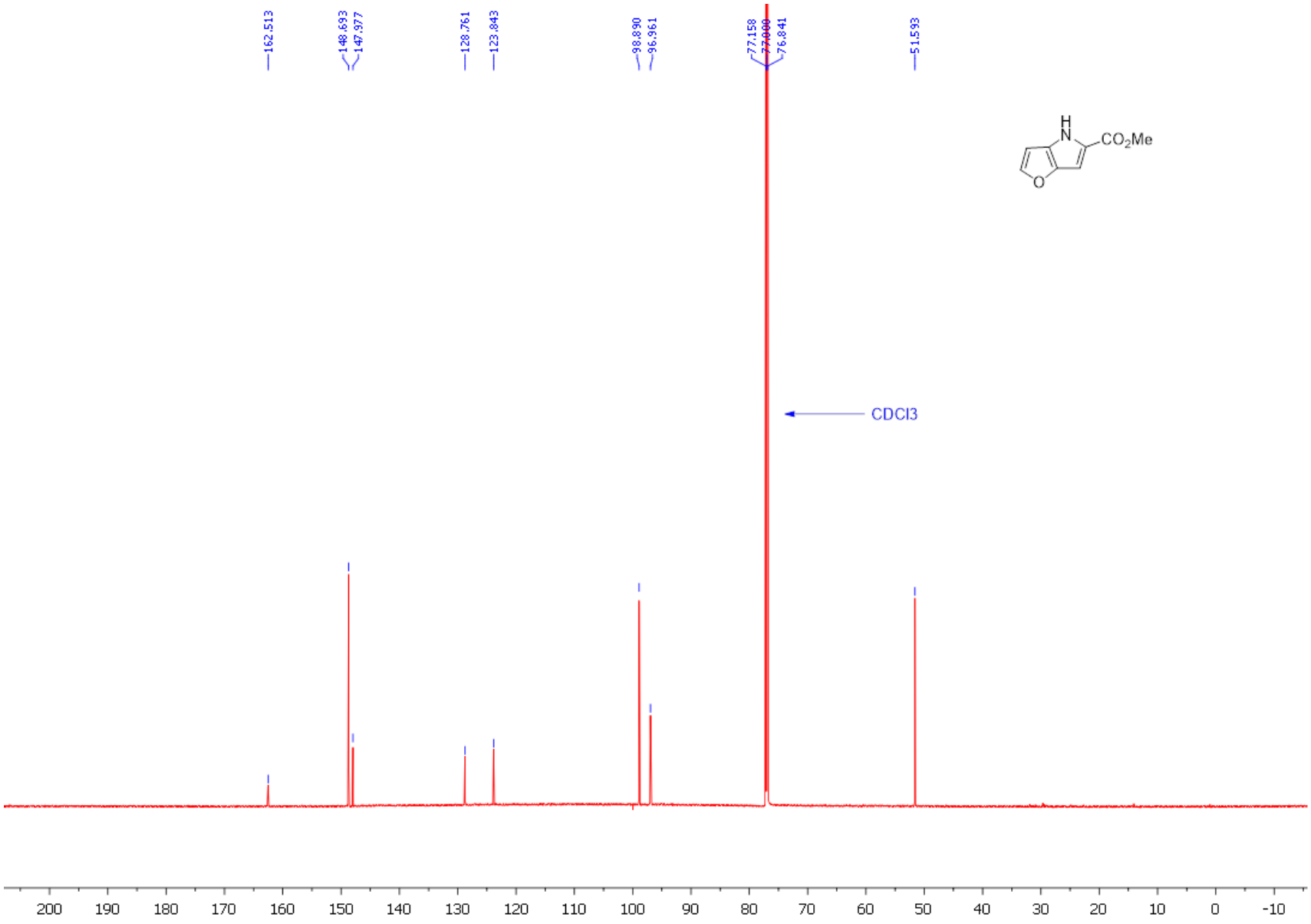
^{13}C-NMR of *methyl 3H-benzo[e]indole-2-carboxylate (10g)* (25 ºC, 200 MHz, $CDCl_3$):



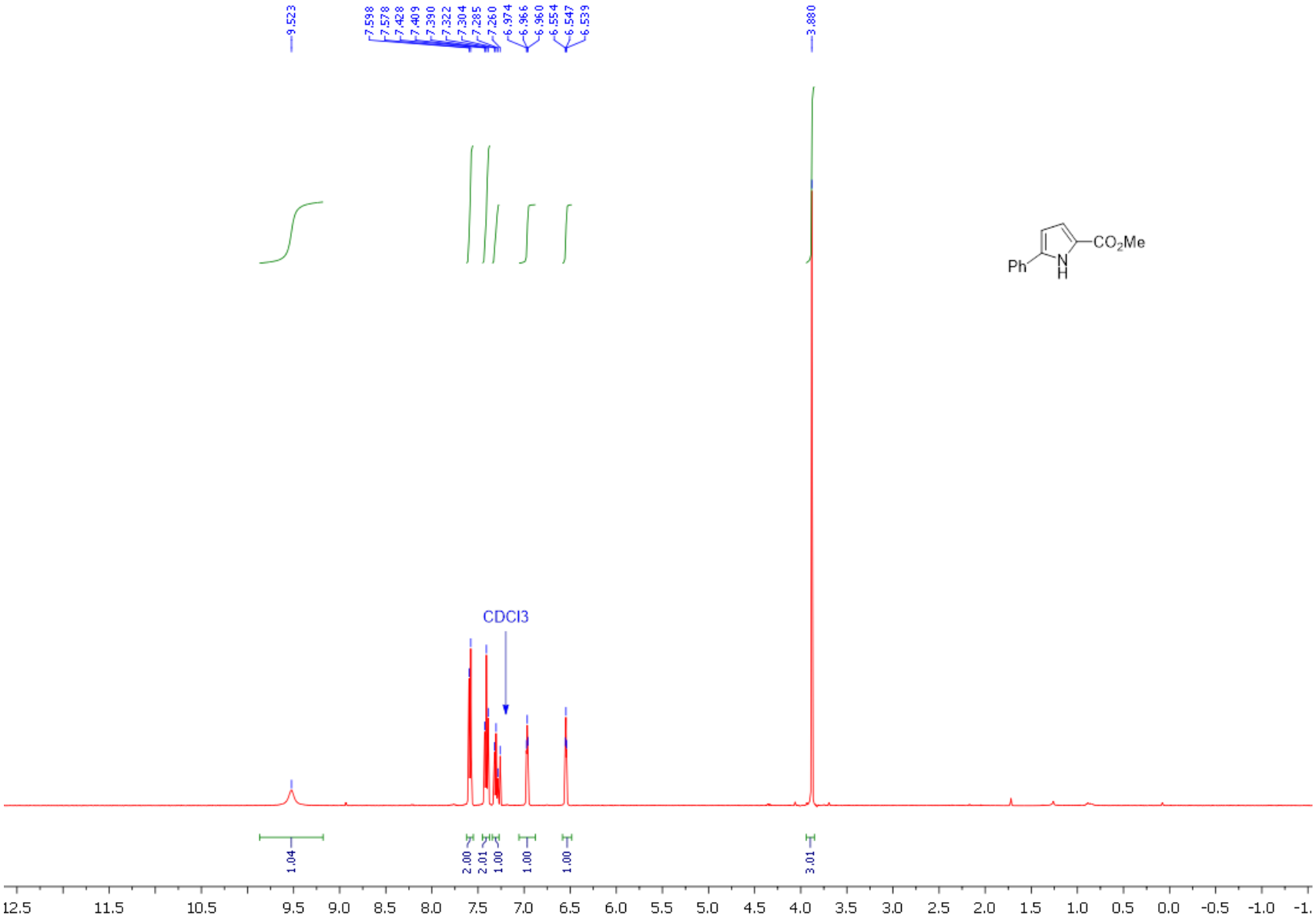
^{1}H-NMR of *methyl 4H-furo[3,2-b]pyrrole-5-carboxylate (10h)* (25 ^{o}C, 800 MHz, $CDCl_3$):



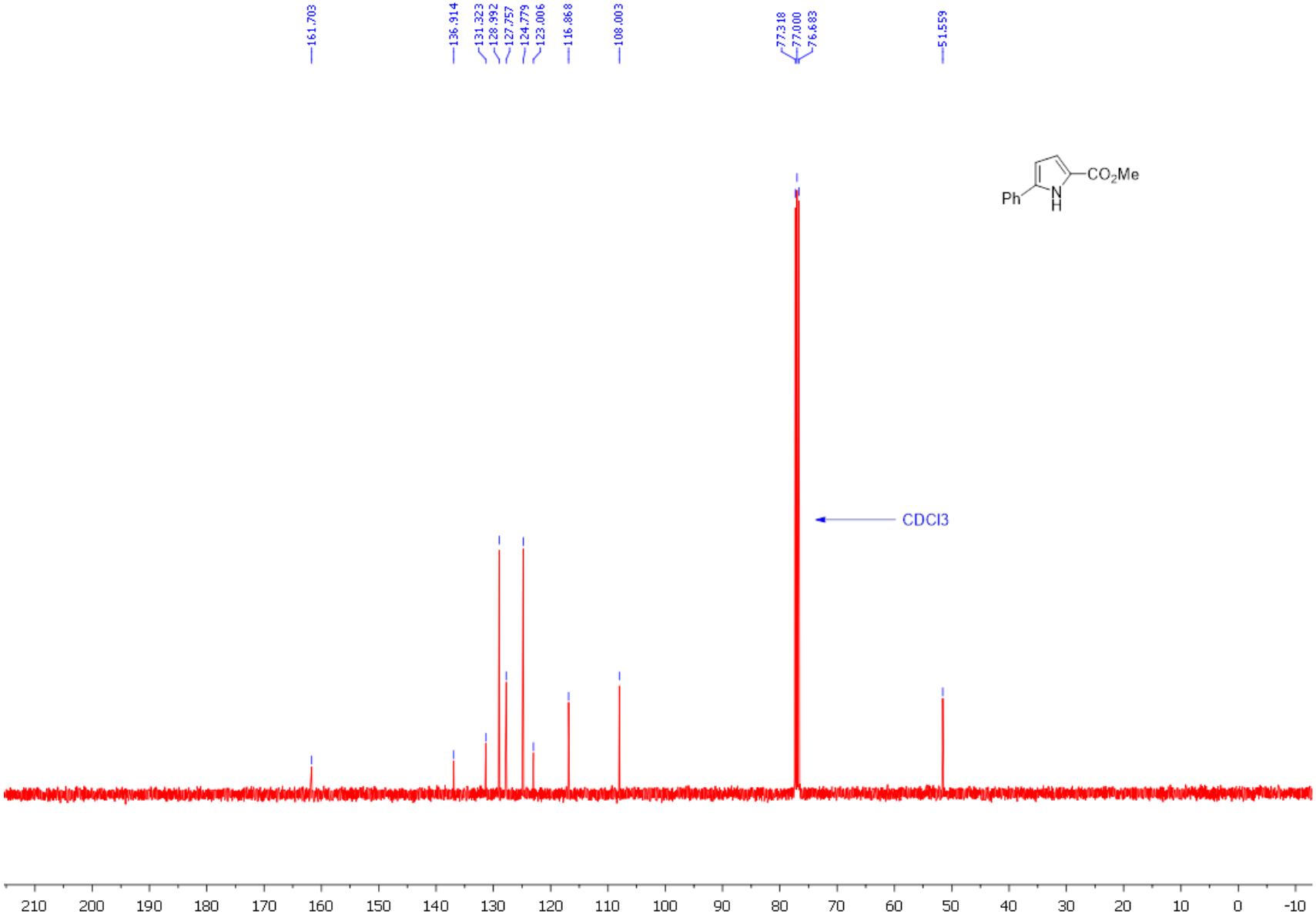
^{13}C-NMR of *methyl 4H-furo[3,2-b]pyrrole-5-carboxylate (10h)* (25 °C, 200 MHz, $CDCl_3$):



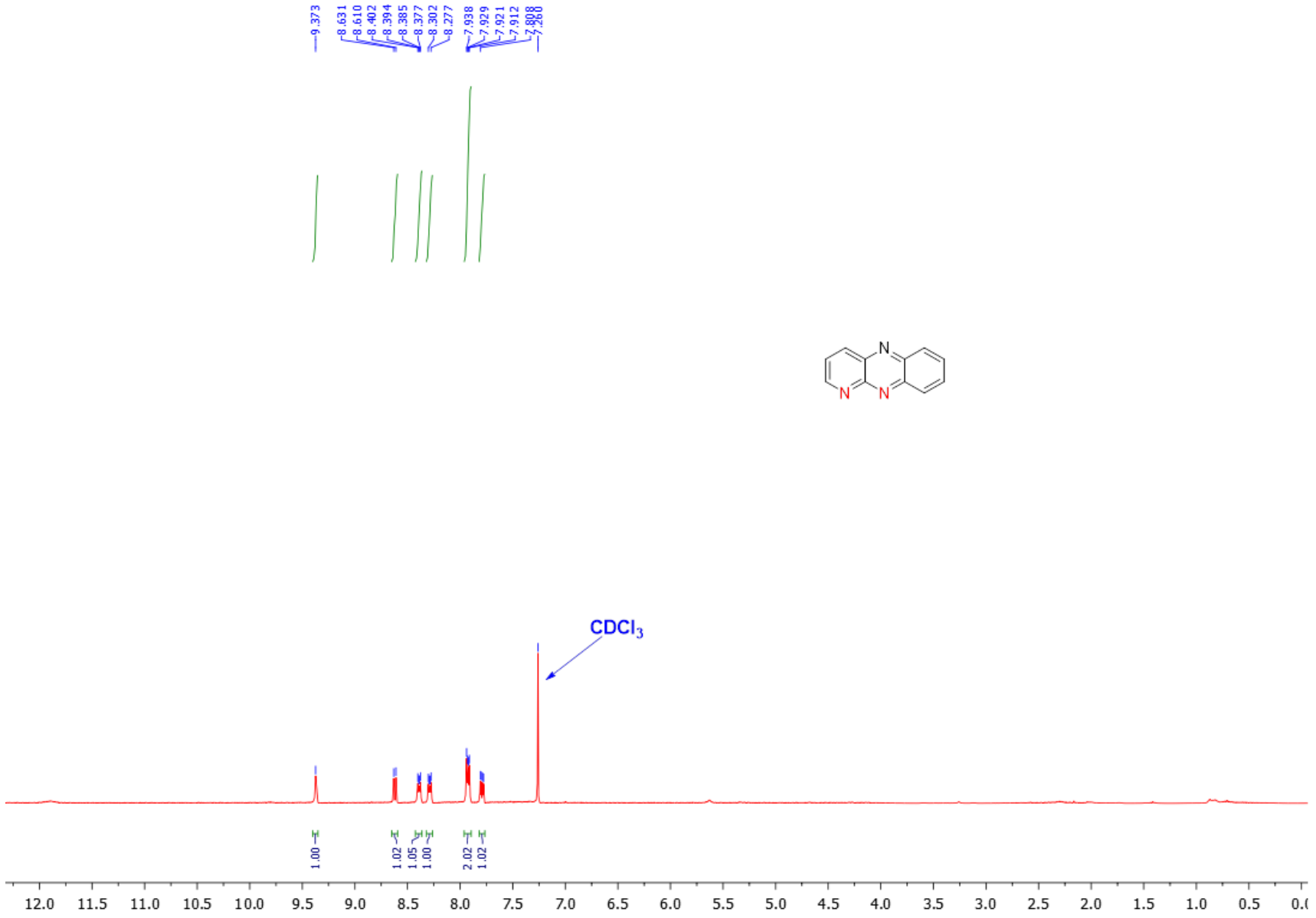
^{1}H-NMR of *methyl 5-phenyl-1H-pyrrole-2-carboxylate (10i)* (25 ^{o}C, 400 MHz, $CDCl_3$):



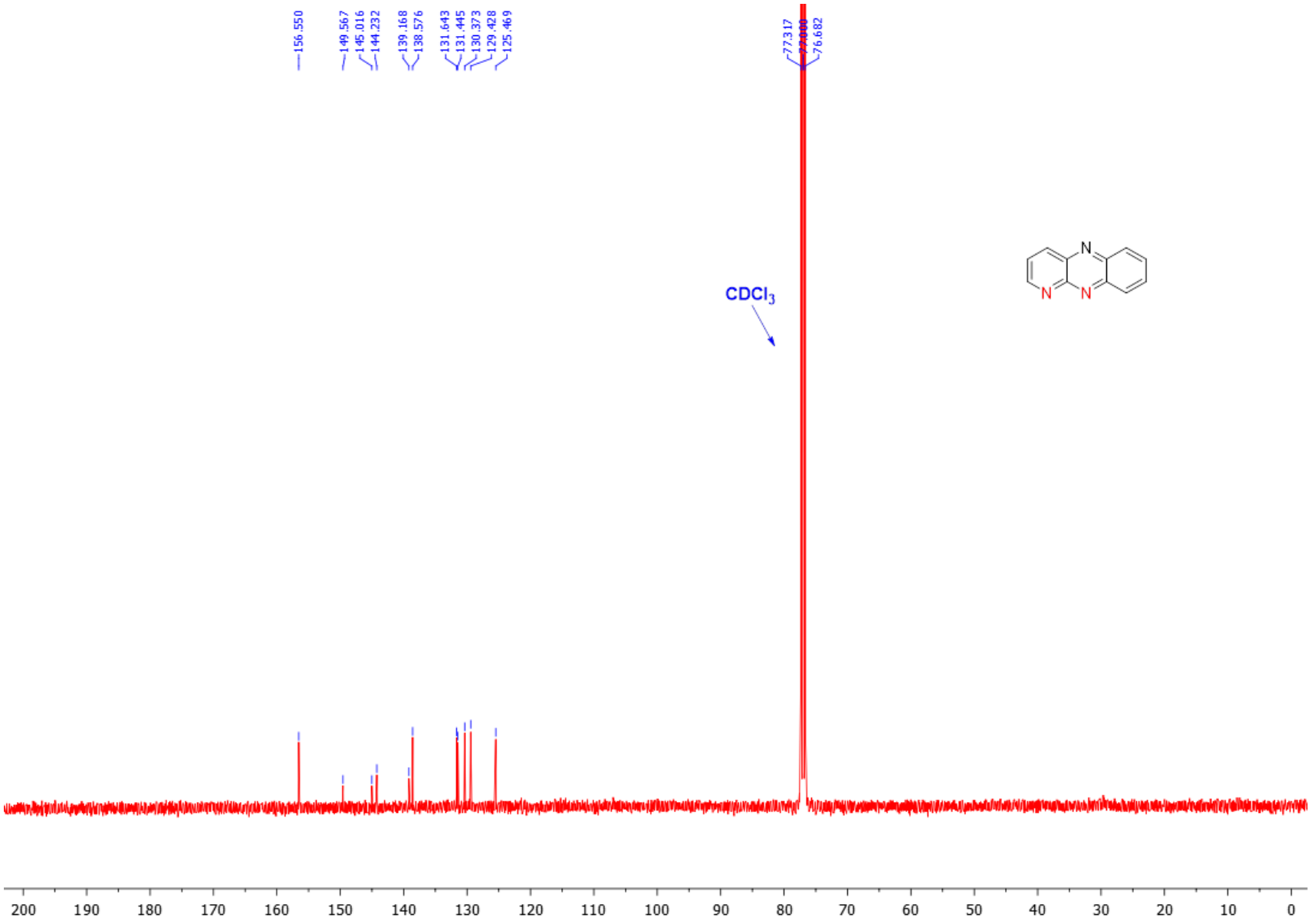
^{13}C-NMR of *methyl 5-phenyl-1H-pyrrole-2-carboxylate (10i)* (25 °C, 100 MHz, $CDCl_3$):



^{1}H-NMR of *pyrido[2,3-b]quinoxaline (16)* (25 ^{o}C, 400 MHz, $CDCl_3$):



^{13}C-NMR of *pyrido[2,3-b]quinoxaline (16)* (25 ºC, 100 MHz, $CDCl_3$):



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