Supporting Information

POTENT, METABOLICALLY STABLE PYRIMIDO-PYRROLO-OXAZINE-DIONE CFTR INHIBITORS FOR POLYCYSTIC KIDNEY DISEASE

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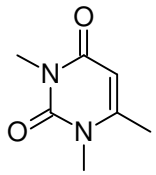
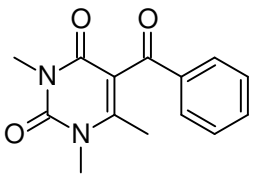
Contents

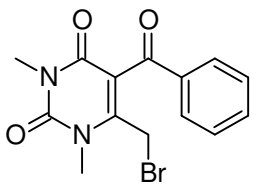
1,3,6-Trimethyl-1*H*,3*H*-pyrimidine-2,4-dione (2).[1] In a 250 mL round bottom flask, 6-methyluracil **1** (15.0 g, 119 mmol) and NaOH (9.55 g, 239 mmol) were dissolved in water (150 mL) under mild heat. The solution was maintained at 25 °C in an ice bath while dimethyl sulfate (23 mL, 30.59 g, 243 mmol) was added dropwise over 20 min with vigorous stirring. After 22 h, the reaction mixture contained a large quantity of white precipitate and had a pH of 9. NaOH (5.0 g, 125 mmol) was added to make the solution homogenous, and an ice bath was used to maintain a temperature of 25 °C while dimethyl sulfate (12 mL, 15.96 g, 127 mmol) was added dropwise over 10 min. The reaction was stirred for 72 h, then NaOH (2 g, 50 mmol) was added and the reaction extracted with $CHCl_3$ (5x50 mL). The chloroform extracts were pooled, dried over Na_2SO_4, and concentrated in vacuo to yield **2** (18 g, 98% yielded); m.p. 114-115 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 5.67 (s, 1H), 3.45 (s, 3H), 3.35 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.62, 152.53, 151.81, 101.16, 31.89, 28.11, 20.58. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_7H_{11}N_2O_2$, 155.17, found 155.14.



5-Benzoyl-1,3,6-trimethylpyrimidine-2,4(1*H*,3*H*)-dione (3).[2] In a 100 mL round bottom flask equipped with a condenser and an air lock was added compound **2** (5.00 g, 32.4 mmol), anhydrous zinc chloride [3] (4.45 g, 32.6 mmol), dry chlorobenzene (20 mL) and benzoyl chloride (freshly distilled, 4 mL, 4.84 g, 34.4 mmol). The reaction was refluxed in an oil bath and vigorously stirred for 3 h. After cooling, water (40 mL) was added through the condenser, dropwise at first and then with increasing speed. The condenser was then rearranged for distillation and the chlorobenzene was removed by azeotropic distillation. The solution was then cooled in an ice bath, and diethyl ether (30 mL) was added while stirring causing a precipitate to form. The precipitate was collected by filtration and recrystallized from 2-propanol (50 mL) to yield **3** (5.53 g, 66%); m.p. 143.2-143.7 °C. ^{1}H NMR (600 MHz, CD_3CN) δ 8.74 (d, J = 7.1, 2H), 8.46 (t, J = 6.0, 1H), 8.37 – 8.29 (m, 2H), 4.25 (s, 3H), 4.07 (s, 3H), 2.99 (s, 3H). ^{13}C NMR (151 MHz, CD_3CN) δ 195.15, 162.17, 153.72, 153.16, 139.21, 134.93, 130.49, 130.04, 113.43, 32.82, 28.61, 18.26. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{14}H_{15}N_2O_3$, 259.28, found 259.11.



5-Benzoyl-6-(bromomethyl)-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (4).[2] In a 50 mL round bottom flask **3** (1.00 g, 38.7 mmol) was dissolved in CCl_4 [4] (5 mL) and CH_2Cl_2 (4 mL) at 50 °C. Bromine (200 µL, 0.621 g, 38.8 mmol) was mixed with CCl_4 (5 mL) and CH_2Cl_2 (5 mL) in an addition funnel and added dropwise to the solution of **3** at such a rate as the



[1] Azas, N.; Rathelot, P.; Djekou, S.; Delmas, F.; Gellis, A.;Di Giorgio, C.; Vanelle, P.; Timon-David, P. Antiparasitic activity of highly conjugated pyrimidine-2,4-dione derivatives. *Farmaco* **2003**, 58, 1263–1270.

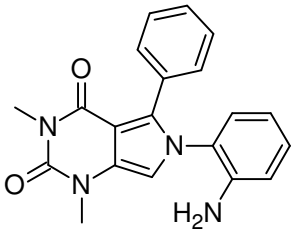
[2] Similarly carried out by: Tsupak, E. B.; Shevchenko, M. A.; Pozharskii, A. F.; Tkachenko, Yu. N. Pyrrolopyrimidines. 5. Reaction of 6-amino-1,3-dimethylpyrrolo[3,4-d]pyrimidine-2,4(1H,3H)-diones with 1,3-diketones. *Chemistry of Heterocyclic Compounds,* **2003***,* 39, 953-959

[3] A. P. Pray (1990). *Inorganic Syntheses*. **XXVIII**. New York: J. Wiley & Sons. pp. 321–322. Describes the preparation of anhydrous $ZnCl_2$, LiCl, $CuCl_2$, $CdCl_2$, $ThCl_4$, $CrCl_3$, $FeCl_3$, $CoCl_2$, and $NiCl_2$ from the corresponding hydrates.

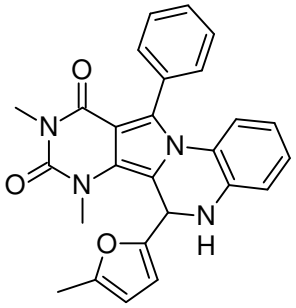
[4] The starting material was poorly soluble in CCl_4, CH_2Cl_2 can be substituted entirely. The reaction under anhydrous conditions was slow, though the addition of few drops of wet solvent resulted in quantitative yield in a few minutes.

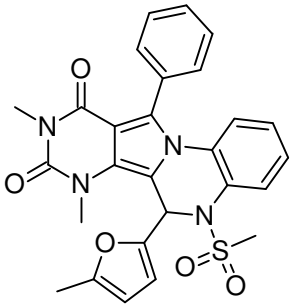
color was discharged between drops. The last few drops caused the reaction to stay brown. The solution was then brought to reflux for 10 min before the brown color was discharged by the addition of a few drops of acetone. The solution was refluxed for 30 min to remove HBr. The reaction was quantitative by TLC and the product crystallized when concentrated in vacuo to yield **4** (1.305 g, 100%). The product may be recrystallized from 2-propanol as colorless needles; m.p. 171.0-171.7 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.88 – 7.80 (m, 2H), 7.65 – 7.60 (m, 1H), 7.52 – 7.45 (m, 2H), 4.24 (s, 2H), 3.59 (s, 3H), 3.31 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 192.89, 160.94, 152.01, 149.58, 137.79, 134.46, 129.78, 129.15, 114.75, 31.96, 28.59, 23.67. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{14}H_{14}BrN_2O_3$, 338.18, found 338.81.

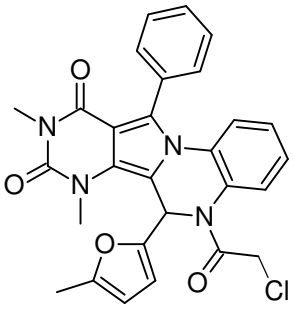
6-(2-Aminophenyl)-1,3-dimethyl-5-phenyl-1*H*-pyrrolo[3,4-*d*]pyrimidine-2,4(3*H*,6*H*)-dione (5). 1,2-Phenylenediamine (1.320 g, 12.2 mmol) in absolute EtOH (25 mL) was stirred in a 50 mL round bottom flask. The mixture was warmed on an oil bath until homogenous, and then **4** (2.055 g, 6.1 mmol) was added with the aid of a powder funnel and EtOH (5 mL). The solution was stirred vigorously at refluxed for 1 h, during which a white precipitate formed. The reaction was then cooled in an ice bath, filtered, and the precipitate washed with cold ethanol to yield **5** (2.0357 g, 96.5%) as a white powder. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.37 – 7.31 (m, 2H), 7.25 – 7.19 (m, 3H), 7.08 – 7.02 (m, 1H), 6.92 (s, 1H), 6.83 (dd, *J* = 1.3, 7.8, 1H), 6.75 (d, *J* = 8.1, 1H), 6.48 – 6.43 (m, 1H), 5.08 (s, 2H), 3.33 (s, 3H), 3.19 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 159.07, 150.89, 144.76, 133.51, 130.42, 129.49, 129.36, 129.05, 128.64, 127.89, 127.13, 123.10, 115.65, 115.46, 105.49, 102.23, 31.50, 27.40. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{20}H_{19}N_4O_2$, 347.39, found 347.05.



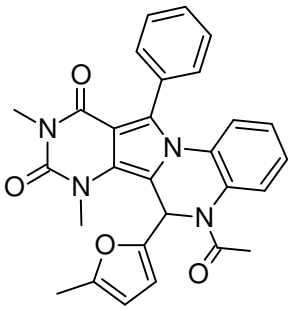
7,9-Dimethyl-6-(5-methylfuran-2-yl)-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (8, PPQ-102). In a 25 mL pear shaped flask was placed **5** (1.00 g, 2.89 mmol), 5-methylfurfural (332 mg, 0.30 mL, 3.02 mmol), a small crystal of *p*-toluene-sulfonic acid and 1,2-dichloroethane (10 mL). The mixture was stirred at reflux for 5 min until homogenous, and then concentrated in vacuo to yield a brown sold. The solid was then recrystallized from ethanol to yield **8** (PPQ-102) (1.05 g, 83%) as slightly yellow crystals. The product was recrystallized to give white crystals; m.p. 245-246 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.6, 1H), 6.95 – 6.90 (m, 1H), 6.83 (dd, *J* = 1.1, 7.9, 1H), 6.48 (d, *J* = 7.9, 1H), 6.45 – 6.40 (m, 1H), 6.01 (s, 1H), 5.75 (d, *J* = 2.1, 1H), 5.70 (d, *J* = 3.0, 1H), 4.93 (d, *J* = 2.0, 1H), 3.55 (s, 3H), 3.27 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.59, 152.98, 152.03, 151.67, 137.36, 132.01, 130.96, 130.17, 130.06, 129.08, 128.49, 128.27, 126.49, 124.82, 123.35, 121.10, 119.45, 117.42, 110.32, 109.74, 106.21, 105.24, 48.76, 32.04, 27.90, 13.70. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{23}N_4O_3$, 439.18, found 439.12.



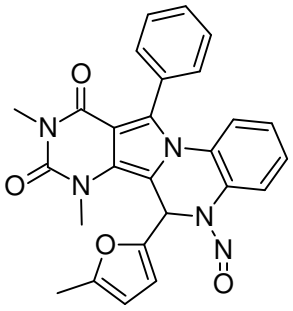
7,9-Dimethyl -6-(5-methylfuran-2-yl)-5-(methylsulfonyl)-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (9). 
In a 5 mL pear shaped flask **8** (21 mg 48.9 µmol) was dissolved in dry chloroform (1 mL). Methanesulfonyl chloride (5.5 µL, 7.7 mg, 67.2 µmol) was added followed by triethylamine (14 µL, 10.2 mg, 100 µmol) and the reaction was stirred for 30 min. TLC showed starting material so additional methanesulfonyl chloride (5.5 µL, 7.7 mg, 67.2 µmol) and triethylamine (14 µL, 10.2 mg, 100 µmol) were added. After 1 h TLC showed minimal starting material. The reaction was quenched and then purified by TLC-prep to give **9** (17.9 mg, 72.5%) as an amorphous solid. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.84 (d, *J* = 7.6, 1H), 7.60 (t, *J* = 7.3, 1H), 7.52 – 7.46 (m, 2H), 7.28 (t, *J* = 7.3, 1H), 7.17 – 7.12 (m, 1H), 6.98 – 6.93 (m, 1H), 6.87 – 6.79 (m, 2H), 6.62 (d, *J* = 8.3, 1H), 5.74 (d, *J* = 3.1, 1H), 5.72 (s, 1H), 3.56 (s, 3H), 3.27 (s, 3H), 2.63 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.36, 154.22, 151.76, 147.04, 132.08, 131.48, 130.59, 129.87, 129.78, 129.70, 129.63, 128.85, 128.40, 127.85, 127.73, 126.98, 124.94, 121.86, 111.93, 108.78, 106.40, 105.74, 52.08, 37.83, 32.39, 28.00, 13.77. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{27}H_{25}N_4O_5S$, 517.15, found 517.10.

5-(2-Chloroacetyl)-7,9-dimethyl -6-(5-methylfuran-2-yl)-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (10). 
In a 15 mL pear shaped flask **8** (163 mg, 371 µmol) was dissolved in dry CH_2Cl_2 (3 mL). Triethylamine (80 µL, 58 mg, 574 µmol) was added followed by chloroacetyl chloride (30 µL, 43 mg, 377 µmol) and the reaction was stirred for 1 h. The reaction was found to be incomplete by TLC so additional chloroacetyl chloride (10 µL, 14.2 mg, 126 µmol) was added. After 1 h TLC indicated no remaining starting material. The reaction was extracted with dilute citric acid, dried over $NaSO_4$, and diluted with ethanol (9 mL). The solution was placed on a rotary evaporator until a beige precipitate ceased to form. The mixture was then cooled in an ice bath and the precipitate was collected by filtration, washed with ethanol, and dried in vacuo to give **10** (170 mg, 89%) ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.86 (d, *J* = 7.1, 1H), 7.58 (t, *J* = 7.1, 1H), 7.55 (s, 1H), 7.47 (t, *J* = 7.5, 1H), 7.33 – 7.25 (m, *J* = 1.2, 7.9, 2H), 7.14 (td, *J* = 1.2, 7.8, 1H), 7.02 (d, *J* = 7.1, 1H), 6.97 – 6.92 (m, 1H), 6.64 (dd, *J* = 1.0, 8.3, 1H), 5.71 – 5.66 (m, 2H), 4.41 (dd, *J* = 13.3, 62.4, 2H), 3.58 (s, 3H), 3.27 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 165.09, 159.44, 153.82, 151.78, 147.81, 132.01, 131.13, 130.15, 129.80, 129.45, 129.01, 128.62, 128.39, 127.39, 126.73, 126.01, 124.66, 122.57, 111.58, 110.34, 106.22, 105.44, 47.66, 42.19, 32.24, 27.97, 13.71. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{28}H_{24}ClN_4O_4$, 515.15, found 515.07.

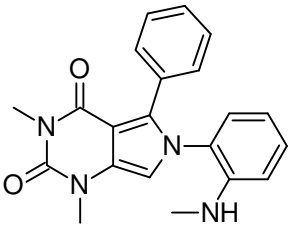
5-Acetyl-7,9-dimethyl -6-(5-methylfuran-2-yl)-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (11). In a 5 mL round bottom flask **8** (50 mg, 114 µmol) and DMAP (1.2 mg, 9.8 µmol) were stirred vigorously in acetic anhydride (2.16 g, 2.0 mL, 2.12 mmol) at 100 °C for 24 h. The reaction was then poured into water (20 mL) while stirring, alkalinized with sodium carbonate and stirred at room temperature for 30 min. The mixture was then extracted with CH_2Cl_2 (3x15 mL), the organic layers combined and dried over Na_2SO_4. The solvent was removed on a rotary evaporator and the residue purified by TLC prep to give **11** (49.0 mg, 89.4%) as a white solid after drying under high vacuum; m.p. 245-246 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.85 (d, *J* = 7.6, 1H), 7.62 (s, 1H), 7.57 (t, *J* = 7.5, 1H), 7.46 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.25 (d, *J* = 7.9, 1H), 7.12 (t, *J* = 7.7, 1H), 7.02 (d, *J* = 7.6, 1H), 6.88 (t, *J* = 7.9, 1H), 6.61 (d, *J* = 8.3, 1H), 5.68 (d, *J* = 2.8, 1H), 5.66 (d, *J* = 3.0, 1H), 3.59 (s, 3H), 3.26 (s, 3H), 2.32 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 168.72, 159.44, 153.42, 151.71, 148.56, 131.96, 130.53, 130.22, 130.08, 129.88, 129.48, 129.24, 128.51, 128.22, 126.79, 126.25, 126.22, 124.17, 122.13, 110.99, 110.93, 106.01, 105.15, 46.12, 32.13, 27.89, 22.59, 13.68. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{28}H_{25}N_4O_4$, 481.19, found 481.08.



7,9-Dimethyl-6-(5-methylfuran-2-yl)-5-nitroso-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (12). In a 5 mL pear shaped flask **8** (25 mg, 57 µmol) was dissolved in dichloromethane (2 mL), and 90% t-butyl nitrite (15.6 mg, 18 µL, 136 µmol) was added. The reaction was maintained at room temperature for 30 min, and then dried in vacuo. The residue was purified by TLC prep to give **12** (21 mg, 78.8%) as a foam after drying under high vacuum. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.89 (s, 1H), 7.83 (d, *J* = 7.7, 1H), 7.76 (d, *J* = 8.0, 1H), 7.60 (t, *J* = 7.6, 1H), 7.50 (t, *J* = 7.5, 1H), 7.32 (t, *J* = 7.5, 1H), 7.25 (t, *J* = 7.7, 1H), 7.04 – 6.99 (m, 2H), 6.72 (d, *J* = 8.4, 1H), 5.83 (d, *J* = 3.1, 1H), 5.74 (d, *J* = 2.6, 1H), 3.61 (s, 3H), 3.24 (s, 3H), 2.12 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.25, 154.07, 151.80, 147.00, 131.92, 131.57, 130.23, 129.99, 129.64, 129.02, 128.75, 128.59, 127.65, 127.09, 126.22, 125.56, 121.70, 120.79, 111.19, 106.94, 106.39, 106.02, 43.31, 32.13, 27.97, 13.68. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{22}N_5O_4$, 468.17, found 468.08.

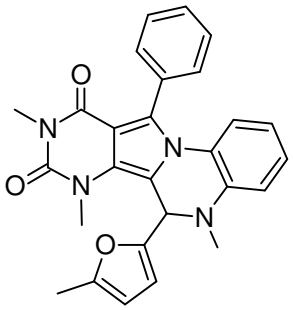


6-(N-methyl-2-aminophenyl)-1,3-dimethyl-5-phenyl-1*H*-pyrrolo[3,4-*d*]pyrimidine-2,4(3*H*,6*H*)-dione (7). In a 25 mL round bottom flask N-methyl-1,2-phenylenediamine (200 µl, 215 mg, 1.76 mmol) and EtOH (10 mL) were stirred. Ketone **4** (296 mg, 878 µmol) was added and the mixture was stirred vigorously at reflux for 30 min during which a precipitate formed. The reaction was then chilled in an ice bath. The precipitate was collected by filtration and washed with cold ethanol to yield **7** (0.263 g, 83%) as an off-white powder. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.30 – 7.26 (m, 2H), 7.24 – 7.16 (m, 4H), 6.93 (d, *J* = 1.0, 1H), 6.86 (d, *J* = 7.7, 1H), 6.62 (d, *J* = 8.3, 1H), 6.49 (t, *J* = 7.5, 1H), 5.07 (d, *J* = 4.8, 1H), 3.33 (s, 3H), 3.20 (s, 3H), 2.64 (d, *J* = 4.9, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 159.08, 150.91,

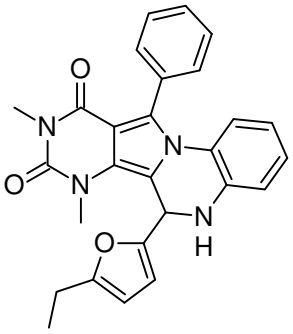


145.66, 133.75, 130.36, 129.99, 129.34, 129.10, 128.58, 127.95, 127.15, 123.52, 114.95, 110.52, 105.63, 102.41, 31.56, 29.65, 27.41. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{21}H_{21}N_4O_2$, 361.17, found 361.10.

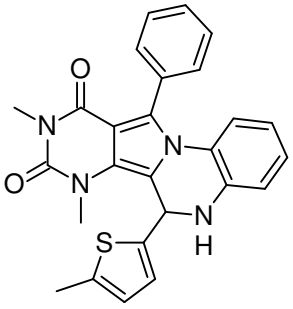
5,7,9-Trimethyl-6-(5-methylfuran-2-yl)-11-phenyl-5,6-dihydropyrimido [4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (13). In a 10 mL pear shaped flask was placed **7** (100 mg, 277 mmol), 5-methyl-2-furaldehyde (39µL, 43.1 mg, 392 µmol), a magnetic stir bar, a small crystal of *p*-toluene-sulfonic acid, and 1,2-dichloroethane (3 mL). The mixture was refluxed until homogenous, with no starting material remaining as determined by TLC. The reaction was then concentrated in vacuo and diluted with ethanol (7 mL) causing a precipitate to form. The precipitate was collected by filtration and washed with cold ethanol to yield **13** (98.6 mg, 78.5 %), as a white waxy solid; m.p. 174-175 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.83 (d, *J* = 7.5, 1H), 7.56 (t, *J* = 7.5, 1H), 7.44 (t, *J* = 7.5, 1H), 7.27 (t, *J* = 7.4, 1H), 7.07 – 7.01 (m, 1H), 6.96 (d, *J* = 7.5, 1H), 6.76 (d, *J* = 7.3, 1H), 6.60 – 6.53 (m, 1H), 6.51 – 6.44 (m, 1H), 5.82 (s, 1H), 5.72 (d, *J* = 2.2, 1H), 5.58 (d, *J* = 3.1, 1H), 3.55 (s, 3H), 3.25 (s, 3H), 3.10 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.63, 152.80, 151.97, 150.12, 139.23, 132.10, 130.94, 130.05, 129.59, 128.97, 128.47, 128.20, 126.71, 125.50, 122.36, 121.08, 118.70, 115.02, 112.17, 109.76, 106.14, 105.23, 55.89, 38.32, 32.37, 27.89, 13.73. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{27}H_{25}N_4O_3$, 453.19, found 453.17.



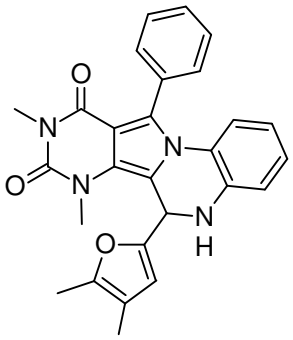
7,9-Dimethyl-6-(5-ethylfuran-2-yl)-11-phenyl-5,6-dihydropyrimido [4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (14). In a 5 mL pear shaped flask was placed **5** (50 mg, 144 µmol), 5-ethyl-2-furaldehyde (17.5µL, 18.4 mg, 149 µmol), a small crystal of *p*-toluene-sulfonic acid and 1,2-dichloroethane (1.5 mL). The mixture was refluxed for 34 min, concentrated in vacuo, and triturated with 2-butanone to give a white waxy precipitate. The precipitate was collected by filtration and washed with cold 2-butanone to yield **14** (37 mg, 57%); m.p. 224 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.35 (s, 0H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.94 – 6.89 (m, 1H), 6.82 (dd, *J* = 1.2, 7.9, 1H), 6.48 (d, *J* = 7.6, 1H), 6.46 – 6.40 (m, 1H), 6.01 (s, 1H), 5.75 (d, *J* = 3.1, 1H), 5.72 (d, *J* = 2.8, 1H), 4.91 (d, *J* = 2.1, 1H), 3.56 (s, 3H), 3.27 (s, 3H), 2.54 (q, *J* = 7.6, 2H), 1.12 (t, *J* = 7.6, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.59, 158.54, 152.03, 151.57, 137.43, 132.01, 130.96, 130.18, 130.06, 129.08, 128.55, 128.49, 128.27, 126.50, 124.87, 123.35, 121.11, 119.47, 117.38, 110.39, 109.39, 105.23, 104.50, 48.82, 32.05, 27.90, 21.51, 11.79. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{27}H_{25}N_4O_3$, 453.19, found 453.11.



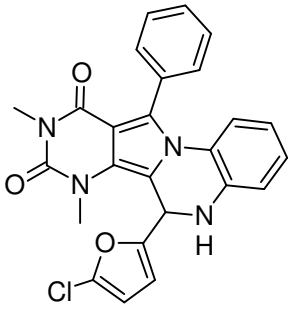
7,9-Dimethyl-6-(5-methylthiophene-2-yl)-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (15). In a 5 mL pear shaped flask was placed **5** (50 mg 144 µmol), 5-methyl-2-thiophenecarbaldehyde (16 µL, 18.7 mg, 148 µmol), a small crystal of *p*-toluene-sulfonic acid and 1,2-dichloroethane (3 mL). The mixture was refluxed for 30 min, concentrated in vacuo, and diluted with ethanol (6 mL) to slowly form a waxy white solid. The precipitate was collected by filtration and washed with cold ethanol to yield **15** (48.9 mg, 74.5%). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.95 – 6.90 (m, 1H), 6.78 (dd, *J* = 1.2, 7.9, 1H), 6.53 – 6.42 (m, 4H), 6.21 (d, *J* = 2.4, 1H), 4.61 (d, *J* = 2.4, 1H), 3.54 (s, 3H), 3.24 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.55, 152.00, 143.36, 140.95, 136.88, 132.05, 130.94, 130.05, 130.00, 129.12, 128.51, 128.29, 126.59, 125.75, 125.04, 124.96, 122.89, 121.20, 119.68, 117.81, 112.59, 105.26, 50.49, 32.22, 27.89, 15.52. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{23}N_4O_2S$, 455.15, found 455.08.



7,9-Dimethyl-6-(4,5-dimethylfuran-2-yl)-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (16). In a 5 mL pear shaped flask was placed **5** (100 mg, 289 µmol), 4,5-dimethyl-2-furaldehyde (37 µL, 37.6 mg, 303 µmol), a small crystal of *p*-toluene-sulfonic acid, and 1,2-dichloroethane (2 mL). The mixture was refluxed until homogenous, concentrated to dryness in vacuo and triturated with benzene and then ethanol to give **16** (89 mg, 68%) as a white waxy solid. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.92 (td, *J* = 1.3, 7.8, 1H), 6.83 (dd, *J* = 1.2, 7.9, 1H), 6.48 (d, *J* = 8.0, 1H), 6.45 – 6.39 (m, 1H), 5.97 (s, 1H), 5.61 (s, 1H), 4.91 (d, *J* = 2.1, 1H), 3.54 (s, 3H), 3.27 (s, 3H), 2.10 (s, 3H), 1.72 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.58, 152.03, 150.33, 148.13, 137.37, 131.99, 131.02, 130.10, 130.05, 129.07, 128.49, 128.28, 126.46, 124.78, 123.27, 121.07, 119.37, 117.37, 114.69, 112.22, 110.37, 105.25, 48.72, 31.97, 27.90, 11.48, 9.80. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{27}H_{25}N_4O_3$, 453.19, found 453.24.

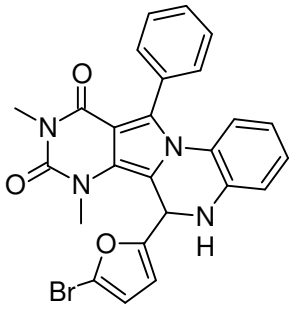


6-(5-Chlorofuran-2-yl)-7,9-dimethyl-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (17). In a 5 mL pear shaped flask was placed **5** (100 mg, 289 µmol), 5-chloro-2-furaldehyde (39.8 mg, 305 µmol), a small crystal of *p*-toluene-sulfonic acid, and 1,2-dichloroethane (1.5 mL). The mixture was refluxed for ~2 min until homogenous, concentrated in vacuo and then diluted with ethanol (5 mL). The solution was placed in a freezer overnight to give a light orange precipitate. The precipitate was collected by filtration and rinsed with cold ethanol to give **17** (107.6 mg, 81.2%). No m.p. (slow decomposition). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, 1H), 7.29 (t, *J* = 7.5, 1H), 7.01 (d, *J* = 7.7, 1H), 6.95 – 6.91 (m, 1H), 6.84 (dd, *J* = 1.1, 7.9, 1H), 6.50 – 6.42 (m, 2H), 6.03 (s, 1H), 5.98 (d, *J* = 3.3, 1H), 5.86 (d, *J* = 3.3, 1H), 4.89 (s, 1H), 3.53 (s, 3H), 3.26 (s, 3H). ^{13}C NMR

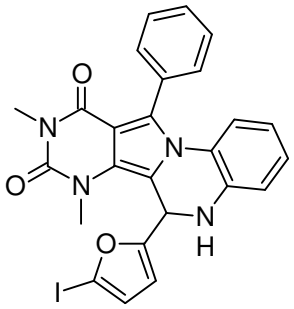


(151 MHz, CD_2Cl_2) δ 159.49, 153.07, 151.99, 136.79, 136.60, 131.97, 130.80, 130.57, 130.01, 129.19, 128.52, 128.32, 126.63, 124.79, 123.73, 121.12, 119.76, 117.49, 111.56, 109.12, 107.16, 105.29, 48.62, 32.06, 27.92. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{25}H_{20}ClN_4O_3$, 459.12, found 458.98.

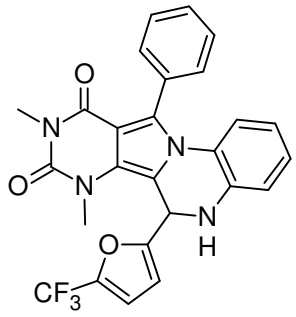
6-(5-Bromofuran-2-yl)-7,9-dimethyl-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (18). In a 5 mL pear shaped flask was placed **5** (100 mg, 289 µmol), 5-bromo-2-furaldehyde (53 mg, 303 µmol), a small crystal of *p*-toluene-sulfonic acid, and 1,2-dichloroethane (2 mL). The mixture was refluxed until homogenous, about 5 min, concentrated in vacuo and then diluted with ethanol (10 mL). An orange precipitate slowly formed which was aided by chilling the mixture in a freezer. The resulting solids were collected by filtration and rinsed with cold ethanol to give **18** (107.2 mg, 73.7%) as an orange powder. No m.p. (slow decomposition). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.96 – 6.90 (m, 1H), 6.84 (dd, *J* = 1.1, 7.9, 1H), 6.48 (d, *J* = 7.7, 1H), 6.47 – 6.41 (m, 1H), 6.12 (d, *J* = 3.3, 1H), 6.04 (d, *J* = 1.7, 1H), 5.85 (dd, *J* = 0.8, 3.3, 1H), 4.95 (d, *J* = 2.3, 1H), 3.53 (s, 3H), 3.27 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.49, 155.46, 151.98, 136.82, 131.97, 130.80, 130.56, 130.01, 129.18, 128.52, 128.31, 126.63, 124.76, 123.70, 122.37, 121.12, 119.72, 117.48, 112.20, 111.90, 109.18, 105.28, 48.62, 32.08, 27.93. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{25}H_{20}BrN_4O_3$, 503.07, found 503.00.



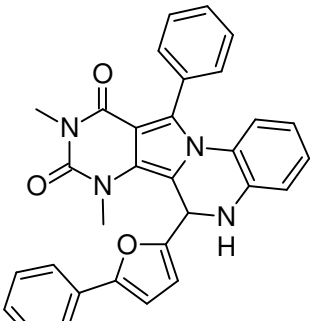
7,9-Dimethyl-6-(5-iodofuran-2-yl)-11-phenyl-5,6-dihydropyrimido[4',5'-3,4]pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (19). In a 5 mL pear shaped flask was placed **5** (150 mg, 433 µmol), 5-iodo-2-furaldehyde (106 mg, 478 µmol), a small crystal of *p*-toluene-sulfonic acid, a magnetic stir bar, and 1,2-dichloroethane (2 mL). The mixture was refluxed until homogenous, about 5 min, concentrated in vacuo and then diluted with ethanol (10 mL). A yellow precipitate slowly formed which was collected by filtration and rinsed with cold ethanol to give **19** (223 mg, 93.6%), as a light orange powder. No m.p. (slow decomposition). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.7, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.93 (td, *J* = 1.4, 7.9, 1H), 6.83 (dd, *J* = 1.2, 7.9, 1H), 6.48 (d, *J* = 7.3, 1H), 6.46 – 6.41 (m, 1H), 6.34 (d, *J* = 3.3, 1H), 6.09 (d, *J* = 2.0, 1H), 5.78 (d, *J* = 3.3, 1H), 4.95 (d, *J* = 2.4, 1H), 3.53 (s, 3H), 3.26 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.50, 158.97, 151.98, 136.86, 131.97, 130.80, 130.52, 130.01, 129.17, 128.51, 128.30, 126.62, 124.75, 123.64, 121.12, 120.97, 119.70, 117.47, 112.15, 109.34, 105.28, 88.96, 48.57, 32.10, 27.93. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{25}H_{20}IN_4O_3$, 551.06, found 551.01.



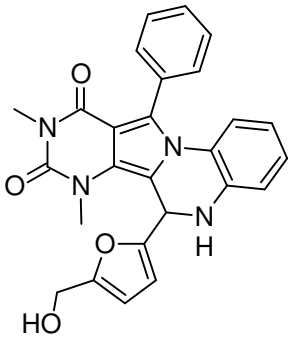
7,9-Dimethyl-11-phenyl-6-(5-trifluoromethylfuran-2-yl)-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (20). In a 5 mL pear shaped flask was placed **5** (100 mg, 289 µmol), 5-trifluoromethyl-2-furaldehyde (50 mg, 305 µmol), a small crystal of *p*-toluene-sulfonic acid, and 1,2-dichloroethane (2 mL). The mixture was refluxed for ~5 min until homogenous, concentrated in vacuo and diluted with ethanol (8 mL). The solution was placed in a freezer for 4 days during which yellow crystals formed. The crystals were filtered and rinsed with ethanol to give **20** (126 mg, 88.5%); m.p. 256-257 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.7, 1H), 7.56 (t, *J* = 7.4, 1H), 7.46 (tt, *J* = 1.2, 7.5, 1H), 7.30 (t, *J* = 7.4, 1H), 7.02 (d, *J* = 7.7, 1H), 6.93 (ddd, *J* = 1.6, 7.1, 8.0, 1H), 6.85 (dd, *J* = 1.2, 7.9, 1H), 6.61 (dd, *J* = 1.0, 3.4, 1H), 6.51 – 6.42 (m, *J* = 4.1, 7.1, 8.3, 2H), 6.10 (s, 1H), 5.95 (d, *J* = 3.5, 1H), 4.96 (d, *J* = 2.5, 1H), 3.55 (s, 3H), 3.26 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.47, 156.71, 151.99, 141.85, 141.57, 141.29, 141.01, 136.75, 131.97, 130.76, 130.72, 129.99, 129.24, 128.55, 128.34, 126.74, 124.80, 123.79, 121.71, 121.18, 119.94, 119.91, 118.17, 117.43, 112.80, 112.78, 110.02, 109.09, 105.31, 48.56, 32.14, 27.94. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{20}F_3N_4O_3$, 493.15, found 493.08.



7,9-Dimethyl-11-phenyl-6-(5-phenylfuran-2-yl)-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (21). In a 5 mL pear shaped flask was placed **5** (100 mg, 289 µmol), 5-phenyl-2-furaldehyde (52 mg, 302 µmol), a small crystal of *p*-toluene-sulfonic acid, and 1,2-dichloroethane (2 mL). The mixture was refluxed for ~5 min until homogenous, concentrated slightly in vacuo and diluted with ethanol (10 mL). A white waxy precipitate formed almost immediately, which was then chilled, filtered and washed with ethanol to give **21** (141.5 mg, 97.9%). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.57 (t, *J* = 7.6, 1H), 7.54 – 7.50 (m, 2H), 7.46 (t, *J* = 7.5, 1H), 7.35 (t, *J* = 7.8, 2H), 7.30 (t, *J* = 7.5, 1H), 7.24 (t, *J* = 7.4, 1H), 7.04 (d, *J* = 7.7, 1H), 6.92 (td, *J* = 1.3, 7.9, 1H), 6.85 (dd, *J* = 1.3, 7.9, 1H), 6.52 (d, *J* = 7.5, 1H), 6.48 – 6.44 (m, 2H), 6.14 (d, *J* = 1.3, 1H), 5.97 (d, *J* = 3.3, 1H), 4.94 (s, 1H), 3.62 (s, 3H), 3.26 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.55, 154.06, 153.27, 152.02, 137.34, 132.03, 130.90, 130.35, 130.27, 130.04, 129.13, 128.95, 128.51, 128.29, 127.88, 126.58, 124.92, 123.65, 123.48, 121.20, 119.63, 117.44, 110.72, 110.15, 105.71, 105.29, 48.85, 32.22, 27.91. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{31}H_{25}N_4O_3$, 501.19, found 501.13

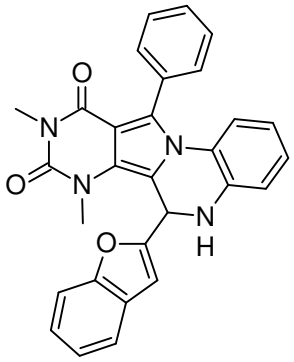


7,9-Dimethyl-11-phenyl-6-(5-hydroxymethylfuran-2-yl)-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (22). In a 5 mL pear shaped flask was placed **5** (50 mg, 144 µmol), 5-hydroxymethyl-2-furaldehyde (18.8 mg, 149 µmol), TFA (5 µL, 7.4 mg, 65 µmol) and 1,2-dichloroethane (1.5 mL). The mixture was refluxed for 10 min forming a precipitate. The reaction was continued for 5 min before chilling in an ice bath. The precipitate was filtered and washed with cold 1,2-dichloroethane to give **22** (44.9 mg, 68.4%), as a white waxy solid. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d,

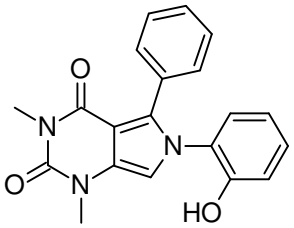


J = 7.5, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.4, 1H), 7.01 (d, *J* = 7.6, 1H), 6.93 – 6.90 (m, 1H), 6.83 (dd, *J* = 1.3, 7.9, 1H), 6.47 (dd, *J* = 1.2, 8.3, 1H), 6.45 – 6.40 (m, 1H), 6.07 – 6.03 (m, 2H), 5.79 (d, *J* = 3.1, 1H), 4.90 (s, 1H), 4.47 (s, 2H), 3.54 (s, 3H), 3.25 (s, 3H), 1.83 (s, 1H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.54, 154.73, 153.68, 152.02, 137.18, 131.99, 130.88, 130.36, 130.03, 129.14, 128.51, 128.30, 126.56, 124.86, 123.51, 121.13, 119.62, 117.40, 109.93, 109.77, 108.60, 105.27, 57.39, 48.78, 32.09, 27.90. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{23}N_4O_4$, 455.171931, found 455.15.

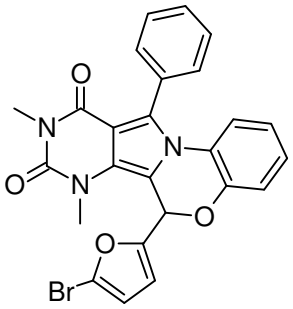
6-(Benzofuran-2-yl)-7,9-dimethyl-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (23). In a 5 mL pear shaped flask was placed **5** (100 mg, 289 µmol), 2-benzofurancarboxaldehyde (52 mg, 302 µmol), a small crystal of *p*-toluene-sulfonic acid, and 1,2-dichloroethane (2 mL). The mixture was refluxed for several min to give a white precipitate. The reaction was chilled in an ice bath, filtered, and the precipitate washed with cold 1,2-dichloroethane to give **23** (125 mg, 91.2%) as a white very waxy solid; m.p. 294-295 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.82 (d, *J* = 7.6, 1H), 7.57 (t, *J* = 7.6, 1H), 7.46 (t, *J* = 7.5, 1H), 7.41 (d, *J* = 8.3, 1H), 7.38 (d, *J* = 7.6, 1H), 7.30 (t, *J* = 7.5, 1H), 7.23 (t, *J* = 7.4, 1H), 7.13 (t, *J* = 7.4, 1H), 7.04 (d, *J* = 7.7, 1H), 6.89 (t, *J* = 7.5, 1H), 6.85 (d, *J* = 6.7, 1H), 6.49 (d, *J* = 8.2, 1H), 6.42 (t, *J* = 7.1, 1H), 6.27 (s, 1H), 6.20 (s, 1H), 5.03 (s, 1H), 3.58 (s, 3H), 3.27 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.53, 156.19, 155.16, 152.02, 136.95, 131.99, 130.88, 130.59, 130.00, 129.19, 128.55, 128.34, 127.75, 126.62, 124.85, 124.82, 123.83, 123.25, 121.35, 121.13, 119.76, 117.42, 111.32, 109.46, 106.07, 105.35, 49.10, 32.09, 27.93. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{29}H_{23}N_4O_3$, 475.18, found 475.01



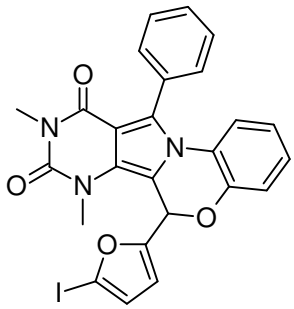
1,3-Dimethyl-6-(2-hydroxyphenyl)-5-phenyl-1*H*-pyrrolo[3,4-*d*]pyrimidine-2,4(3*H*,6*H*)-dione (27). In a 25 mL round bottom was placed o-aminophenol (163 mg, 1.5 mmol) and EtOH (10 mL). The mixture was warmed until homogenous and then compound **4** (250 mg, 741 µmol) was added. The mixture was stirred vigorously at reflux during which a precipitate formed. After 1 h the mixture was cooled in an ice bath, filtered, and the precipitate washed with cold EtOH to yield **27** (248 mg, 96.4%) as a white powder. ^{1}H NMR (600 MHz,) δ 10.02 (s, 1H), 7.29 – 7.26 (m, 2H), 7.24 – 7.17 (m, 4H), 7.10 (dd, *J* = 1.6, 7.8, 1H), 6.96 (s, 1H), 6.90 (dd, *J* = 1.1, 8.2, 1H), 6.77 (td, *J* = 1.2, 7.6, 1H), 3.34 (s, 3H), 3.21 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 159.11, 152.86, 150.91, 133.81, 130.35, 129.98, 129.67, 129.13, 128.58, 127.83, 127.18, 125.95, 118.99, 116.39, 106.16, 101.88, 31.50, 27.46. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{20}H_{18}N_3O_3$, 348.13, found 348.11.



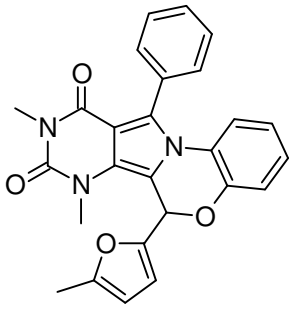
6-(5-Bromofuran-2-yl)-7,9-dimethyl-11-phenyl-6H-benzo[b]pyrimido[4',5'-3,4]pyrrolo[1,2-*d*]oxazine-8,10-(7*H*,9*H*)-dione (31). 5-Bromo-2-furaldehyde (186 mg, 1.06 mmol), **27** (300 mg, 864µmol), chloroform (6 mL) and TFA (10 µL, 14.9 mg, 130 µmol) were sealed in a Emrys 2-5 mL process vial [5] and submerged to the level of solvent in an oil bath at 150 °C for 19 min. The reaction was allowed to cool, filtered through a celite plug to remove impurities, and concentrated to dryness in vacuo. The residue was dissolved in a minimum volume of CH_2Cl_2 and then diluted with ethanol (15 mL). The solution was then placed on a rotary evaporator to remove CH_2Cl_2. Once the solution began to crystallize the mixture was allowed to stand. The mixture was then cooled, filtered, and the crystals rinsed with cold ethanol to give **31** (365 mg, 83.8%). No m.p. (slow decomposition). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d, *J* = 7.6, 1H), 7.58 (t, *J* = 7.5, 1H), 7.49 (t, *J* = 7.5, 1H), 7.33 (t, *J* = 7.5, 1H), 7.07 (d, *J* = 7.6, 1H), 7.05 – 6.98 (m, 2H), 6.79 (s, 1H), 6.64 (ddd, *J* = 2.2, 6.7, 8.6, 1H), 6.53 (d, *J* = 8.6, 1H), 6.14 (d, *J* = 3.4, 1H), 5.98 (dd, *J* = 0.8, 3.4, 1H), 3.47 (s, 3H), 3.26 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.35, 152.32, 151.83, 145.46, 131.86, 130.86, 130.19, 129.94, 129.53, 128.66, 128.49, 127.11, 125.85, 124.38, 124.11, 122.54, 120.39, 119.72, 114.75, 112.35, 106.50, 105.58, 68.13, 32.42, 27.94. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{25}H_{19}BrN_3O_4$, 504.06, found 504.03.

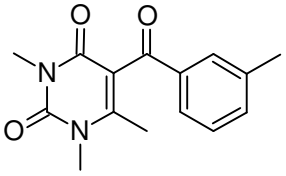


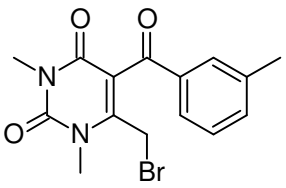
7,9-Dimethyl-6-(5-iodofuran-2-yl)-11-phenyl-6H-benzo[b]pyrimido[4',5'-3,4] pyrrolo[1,2-*d*]oxazine-8,10-(7*H*,9*H*)-dione (32). 5-Iodo-2-furaldehyde (84 mg, 378 µmol), **27** (100 mg, 288µmol), chloroform (1 mL), and TFA (10 µL, 14.9 mg, 130 µmol) were sealed in a Emrys 2-5 mL process vial and submerged to the level of solvent in an oil bath at 150 °C for 19 min. The reaction was cooled in an ice bath, filtered through a celite plug and dried in vacuo. The residue was then purified via flash chromatography to give **32** (68.4 mg, 43%). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d, *J* = 7.6, 1H), 7.58 (t, *J* = 7.6, 1H), 7.49 (t, *J* = 7.5, 1H), 7.33 (t, *J* = 7.5, 1H), 7.07 (d, *J* = 7.6, 1H), 7.05 – 6.98 (m, 2H), 6.84 (s, 0.7H), 6.80 (s, 0.3H), 6.67 – 6.61 (m, *J* = 2.3, 5.5, 6.7, 1H), 6.53 (d, *J* = 8.0, 1H), 6.36 (d, *J* = 3.3, 0.7H), 6.15 (d, *J* = 3.4, 0.3H), 5.99 (d, *J* = 3.3, 0.3H), 5.92 (d, *J* = 3.3, 0.7H), 3.47 (s, 0.74H), 3.47 (s, 2.27H), 3.26 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.34, 155.77, 152.32, 151.81, 145.49, 145.45, 131.85, 130.84, 130.80, 130.19, 129.94, 129.51, 128.65, 128.48, 127.09, 125.84, 124.37, 124.32, 124.10, 122.53, 122.50, 121.06, 120.37, 119.70, 114.89, 114.74, 112.34, 106.66, 106.49, 105.56, 91.02, 68.03, 32.42, 27.93. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{25}H_{19}IN_3O_4$, 552.04, found 552.07.



[5] An Emrys process vial is a commercially available thick walled vessel much like a test tube typically used for microwave reactions that may be sealed using a disposable plastic-lined metal cap. Precautions should be taken as the reaction vessel is under pressure when heated.

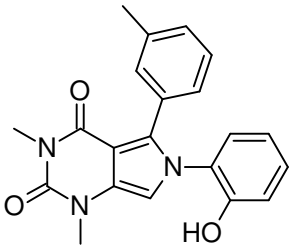
7,9-Dimethyl-6-(5-methylfuran-2-yl)-11-phenyl-6H-benzo[b]pyrimido[4',5'-3,4] pyrrolo[1,2-*d*]oxazine-8,10-(7*H*,9*H*)-dione (33).  5-Methylfurfural (8 µL, 8.9 mg, 80 µmol), **27** (25 mg, 72 µmol), chloroform (3 mL) and a small crystal of TsOH were sealed in a Emrys 2-5 mL process vial and submerged to the level of solvent in an oil bath at 150 °C for 35 min. Once the tube cooled, the contents were purified by TLC-prep to give **33** (15.6 mg, 49.4%) as a waxy white powder. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.6, 1H), 7.58 (t, *J* = 7.5, 1H), 7.48 (t, *J* = 7.5, 1H), 7.32 (t, *J* = 7.4, 1H), 7.07 (d, *J* = 7.6, 1H), 7.03 – 6.97 (m, 2H), 6.77 (s, 1H), 6.63 (ddd, *J* = 3.1, 5.7, 8.6, 1H), 6.53 (d, *J* = 8.0, 1H), 5.85 (d, *J* = 3.1, 1H), 5.77 (d, *J* = 2.2, 1H), 3.47 (s, 3H), 3.26 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.44, 154.52, 151.86, 148.60, 145.78, 131.90, 130.43, 130.36, 129.99, 129.42, 128.62, 128.44, 126.93, 126.01, 123.90, 122.25, 120.35, 119.67, 113.05, 107.72, 106.40, 105.51, 68.58, 32.37, 27.91, 13.81. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{22}N_3O_4$, 440.16, found 440.11.

5-*m*-Tolyl-1,3,6-trimethylpyrimidine-2,4(1*H*,3*H*)-dione (24).  In a 100 mL round bottom flask equipped with a condenser and an air lock was placed compound **2** (5.00 g, 32.4 mmol), anhydrous zinc chloride [3] (4.45 g, 32.6 mmol), dry chlorobenzene (20 mL) and *m*-tolyl chloride (4.6 mL, 5.38 g, 34.8 mmol). The reaction was brought to reflux in an oil bath and vigorously stirred for 3 h. After cooling, water (40 mL) was added through the condenser, dropwise at first and then with increasing speed. The condenser was then rearranged for distillation and the chlorobenzene was removed by azeotropic distillation. The solution was then cooled in an ice bath, and diethyl ether (30 mL) was added while stirring to give a precipitate. The precipitate was filtered and recrystallized from 2-propanol to yield **24** (1.11 g, 26.3%); m.p. 136.8-139 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.68 – 7.66 (m, 1H), 7.65 – 7.62 (m, 1H), 7.44 – 7.40 (m, 1H), 7.35 (t, *J* = 7.6, 1H), 3.46 (s, 3H), 3.30 (s, 3H), 2.40 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 194.00, 161.07, 152.22, 151.98, 139.22, 138.16, 134.94, 130.03, 129.01, 126.93, 113.36, 32.36, 28.32, 21.54, 17.99. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{15}H_{17}N_2O_3$, 273.12, found 237.10.

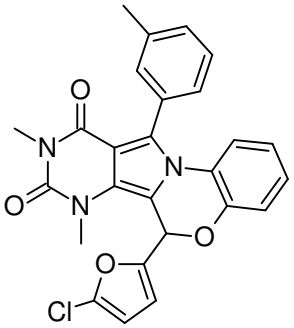
6-(Bromomethyl)- 5-*m*-tolyl-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione (25).  In a 25 mL 2-neck round bottom flask equipped with a condenser, addition funnel and air lock, compound **24** (1.00 g, 3.67 mmol) was dissolved in CH_2Cl_2 [4] (6 mL) and held at reflux. Bromine (200 µL, 0.624 g, 3.9 mmol) was mixed with CH_2Cl_2 (9 mL) in the addition funnel and added dropwise to the solution of **24** at such a rate that the color was discharged between drops. The last few drops caused the reaction to stay brown. The reaction continued for 10 min before the color was discharged by the addition of a few drops of acetone. TLC showed the reaction was quantitative. The reaction was dried in vacuo and the remaining solid crystallized from 2-propanol to yield **25** (1.20 g, 93%); m.p. 136.1-137 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.67 (s, 1H), 7.63 (d, *J* = 7.8, 1H), 7.45 (d, *J* = 7.5, 1H), 7.37 (t, *J* = 7.6, 1H), 4.22 (s, 2H), 3.60 (d, *J* = 6.6, 3H), 3.30 (d, *J* = 7.7, 3H), 2.41 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 193.00, 160.95, 152.09, 149.09, 139.30, 137.77, 135.37,

130.22, 129.04, 127.11, 115.04, 31.98, 28.62, 23.75, 21.55. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{15}H_{16}BrN_2O_3$, 351.03, found 350.99.

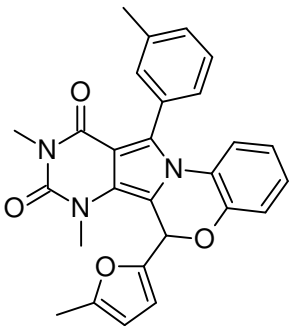
1,3-Dimethyl-6-(2-hydroxyphenyl)-5-*m*-tolyl-1*H*-pyrrolo[3,4-*d*]pyrimidine-2,4(3*H*,6*H*)-dione (26). In a 25 mL round bottom flask 2-aminophenol (683 mg, 6.26 mmol) was dissolved in warm EtOH (10 mL) and compound **25** (296 mg, 878 µmol) was added while stirring. The reaction was refluxed 20 min to give a white precipitate. The reaction was then cooled in an ice bath, filtered, and the precipitate washed with cold ethanol to yield **26** (1.08 g, 96.3%) as a off white powder. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.02 (s, 1H), 7.20 (td, *J* = 1.6, 8.2, 1H), 7.16 (s, 1H), 7.10 – 7.06 (m, 2H), 7.04 (d, *J* = 7.6, 1H), 7.01 (d, *J* = 7.5, 1H), 6.93 (s, 1H), 6.90 (dd, *J* = 0.8, 8.2, 1H), 6.77 (t, *J* = 7.6, 1H), 3.33 (s, 3H), 3.20 (s, 3H), 2.19 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 159.10, 152.91, 150.91, 136.04, 133.96, 131.15, 129.93, 129.59, 129.13, 128.54, 128.51, 127.28, 127.03, 126.03, 118.94, 116.34, 106.07, 101.81, 31.48, 27.47, 20.97. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{21}H_{19}N_3O_3$, 362.15, found 362.09.



6-(5-Chlorofuran-2-yl)-7,9-dimethyl-11-(*m*-tolyl)-6H-benzo[b]pyrimido[4',5'-3,4] pyrrolo[1,2-*d*]oxazine-8,10-(7*H*,9*H*)-dione (34). 5-Chlorofurfural (43 mg, 329 µmol), **26** (100 mg, 277 µmol), a small crystal of TsOH, and 1,2-dichloroethane (2.5 mL) were placed in an Emrys 2-5 mL process vial and submerged to the level of solvent in an oil bath at 150 °C for 20 min. Once the reaction had cooled the contents were purified by TLC prep to give **34** (88 mg, 67%) as an off white solid. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.59 (s, 0.5H), 7.56 (d, *J* = 7.6, 0.5H), 7.46 (t, *J* = 7.6, 0.5H), 7.30 (d, *J* = 7.7, 1H), 7.21 (t, *J* = 7.6, 0.5H), 7.06 – 6.98 (m, 2H), 6.89 (s, 0.5H), 6.85 (d, *J* = 7.6, 0.5H), 6.77 (s, 1H), 6.65 (qd, *J* = 2.3, 6.3, 1H), 6.54 (dd, *J* = 8.2, 12.6, 1H), 6.00 (s, 2H), 3.47 (s, 3H), 3.25 (d, *J* = 6.6, 3H), 2.47 (s, 1.5H), 2.23 (s, 1.5H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.33, 151.85, 150.01, 145.39, 145.34, 138.58, 138.43, 138.10, 132.23, 131.16, 131.13, 130.32, 130.29, 130.17, 130.14, 128.80, 128.52, 128.38, 127.07, 127.05, 126.92, 125.93, 124.30, 122.55, 122.50, 120.37, 120.33, 119.64, 114.40, 107.31, 106.26, 106.21, 105.55, 105.49, 68.10, 32.40, 32.37, 27.94, 27.92, 21.64, 21.35. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{21}ClN_3O_4$, 474.12, found 474.02.

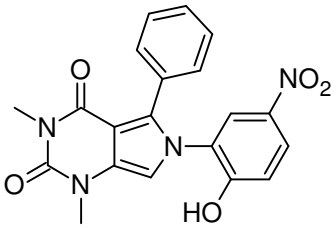


7,9-Dimethyl-6-(5-methylfuran-2-yl)-11-(*m*-tolyl)-6H-benzo[b]pyrimido[4',5'-3,4] pyrrolo[1,2-*d*]oxazine-8,10-(7*H*,9*H*)-dione (35). 5-Methylfurfural (33 µL, 37 mg, 332 µmol), **26** (100 mg, 277 µmol), TFA (5 µL, 7.4 mg, 65 µmol), and chloroform (3 mL) were sealed in a Emrys 2-5 mL process vial and submerged to the level of solvent in an oil bath at 150 °C for 24 min. Once the reaction had cooled, the contents were purified by flash chromatography to give **35** (92 mg, 74%) with a trace amount of impurity. The product was dissolved in a minimum volume of CH_2Cl_2 and then diluted with methanol (6 mL). The solution was placed on a rotary evaporator until a precipitate began to form. The mixture was then cooled, the precipitate filtered and washed

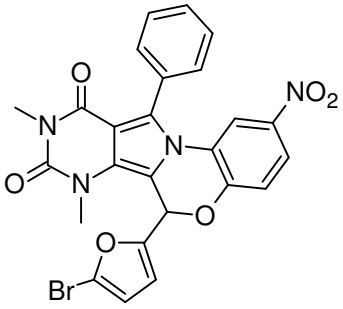


with cold methanol to give **35** (64 mg, 51%) as a pure ivory colored powder. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.60 (s, 0.5H), 7.57 (d, *J* = 7.6, 0.5H), 7.47 (t, *J* = 7.6, 0.5H), 7.30 (d, *J* = 7.7, 1H), 7.21 (t, *J* = 7.6, 0.5H), 7.05 – 6.97 (m, 2H), 6.91 (s, 0.5H), 6.86 (d, *J* = 7.6, 0.5H), 6.77 (s, 1H), 6.67 – 6.60 (m, 1H), 6.55 (dd, *J* = 8.3, 11.3, 1H), 5.85 (d, *J* = 2.8, 1H), 5.77 (d, *J* = 2.5, 1H), 3.47 (s, 3H), 3.26 (d, *J* = 6.2, 3H), 2.48 (s, 1.5H), 2.23 (s, 1.5H), 2.23 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.44, 159.43, 154.49, 151.89, 148.66, 145.72, 145.67, 138.52, 138.37, 132.28, 130.75, 130.72, 130.38, 130.33, 130.31, 130.19, 128.84, 128.48, 128.34, 126.98, 126.89, 126.87, 126.08, 123.82, 122.27, 122.22, 120.34, 120.30, 119.59, 113.01, 107.52, 107.47, 106.40, 105.49, 105.42, 68.53, 32.37, 32.34, 27.91, 27.89, 21.64, 21.35, 13.81. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{27}H_{24}N_3O_4$, 454.18, found 454.10.

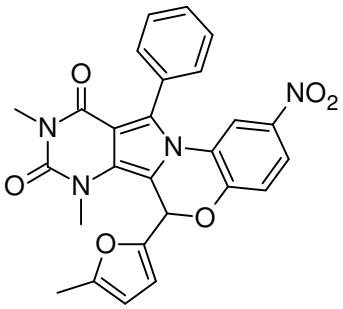
6-(2-hydroxy-5-nitrophenyl)-1,3-dimethyl-5-phenyl-1*H*-pyrrolo[3,4-*d*]pyrimidine-2,4(3*H*,6*H*)-dione (28). In a 25 mL round bottom flask was placed **4** (1.00 g, 2.97 mmol), 2-amino-4-nitrophenol (921 mg, 5.98 mmol), and methanol (12 mL). The reaction was stirred at reflux for 5 h, then cooled in an ice bath. The precipitate was filtered and rinsed with cold methanol to give **28** (1.32 g, 94%). ^{1}H NMR (600 MHz, DMSO-d_6) δ 11.72 (s, 1H), 8.19 (d, *J* = 2.8, 1H), 8.15 (dd, *J* = 2.9, 9.1, 1H), 7.31 – 7.21 (m, 5H), 7.08 (s, 1H), 7.01 (d, *J* = 9.1, 1H), 3.34 (s, 3H), 3.21 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 159.26, 159.03, 150.85, 138.89, 134.18, 130.34, 129.34, 128.85, 128.14, 127.36, 126.15, 126.09, 125.45, 116.60, 105.95, 102.41, 31.52, 27.48. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{20}H_{17}N_4O_5$, 393.12, found 393.02.



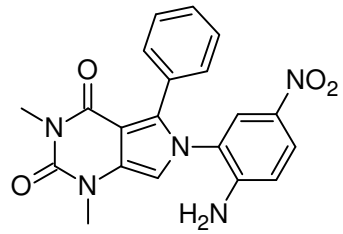
6-(5-bromofuran-2-yl)-7,9-Dimethyl-2-nitro-11-phenyl-6H-benzo[b]pyrimido[4',5'-3,4] pyrrolo[1,2-*d*]oxazine-8,10-(7*H*,9*H*)-dione (36). Pyrrole **28** (225 mg, 573 µmol), 5-bromofurfural (130 mg, 743 µmol), 1,2-dicholoroethane (4 mL), TFA (10 µL, 14.9 mg, 130 µmol) and 3 Å molecular sieve (500 mg, 8-12 mesh) were sealed in a Emrys 2-5 mL process vial and submerged to the level of solvent in an oil bath at 150 °C for 100 min. Upon cooling the reaction turned dark green and some impurities precipitated. The reaction was filtered through a celite plug and dried in vacuo. The residue was dissolved in CH_2Cl_2 (3 mL) and then diluted with ethanol (15 mL). The solution was then placed on a rotary evaporator until small crystals began to form. The mixture was cooled and the crystals were collected by filtration and rinsed with cold ethanol to give **36** (204 mg, 65%). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.91 (dd, *J* = 2.6, 8.9, 1H), 7.84 (d, *J* = 7.7, 1H), 7.69 (t, *J* = 7.6, 1H), 7.58 (t, *J* = 7.5, 1H), 7.39 (d, *J* = 2.6, 1H), 7.37 (t, *J* = 7.6, 1H), 7.18 (d, *J* = 8.9, 1H), 7.07 (d, *J* = 7.7, 1H), 6.92 (s, 1H), 6.17 (d, *J* = 3.4, 1H), 6.03 (d, *J* = 3.4, 1H), 3.48 (s, 4H), 3.27 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.10, 151.70, 151.31, 150.71, 142.06, 131.75, 131.63, 130.16, 129.53, 129.32, 129.18, 129.07, 125.55, 124.83, 124.74, 122.43, 120.23, 115.93, 115.22, 112.56, 106.48, 105.26, 68.75, 32.40, 28.01. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{25}H_{18}BrN_4O_6$, 549.04, found 549.05.



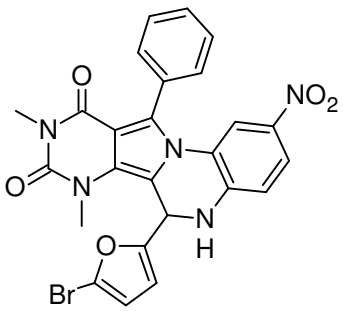
7,9-Dimethyl-6-(5-methylfuran-2-yl)-2-nitro-11-phenyl-6H-benzo[b]pyrimido[4',5'-3,4] pyrrolo[1,2-*d*]oxazine-8,10-(7*H*,9*H*)-dione (37). Pyrrole **28** (250 mg, 637 µmol), 5-methylfurfural (76 µl, 84 mg, 764 µmol), chloroform (8 mL), and TFA (10 µL, 14.9 mg, 130 µmol) were sealed in a Emrys 2-5 mL process vial and submerged to the level of solvent in an oil bath at 150 °C for 2.7 h. The reaction was then cooled and dried in vacuo. The residue was purified by flash chromatography to give **37** (245 mg, 79%) as a yellow foam after drying under high vacuum. To convert the foam to a powder, the foam was dissolved in CH_2Cl_2 (3 mL) and then diluted with methanol (15 mL). The volume of solvent was then reduced on a rotary evaporator. Once the solution began to precipitate the mixture was allowed to stand until precipitation ceased. The mixture was then cooled, filtered, and the precipitate rinsed with cold methanol to give **37** (179 mg). The mother liquor was reduced to yield additional **37** (38 mg). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.89 (dd, *J* = 2.6, 8.9, 1H), 7.84 (d, *J* = 7.7, 1H), 7.68 (t, *J* = 7.6, 1H), 7.57 (t, *J* = 7.5, 1H), 7.39 (d, *J* = 2.4, 1H), 7.36 (t, *J* = 7.6, 1H), 7.14 (d, *J* = 8.9, 1H), 7.07 (d, *J* = 7.7, 1H), 6.90 (s, 1H), 5.91 (d, *J* = 3.1, 1H), 5.79 (d, *J* = 2.9, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.20, 155.08, 151.75, 151.18, 147.73, 141.85, 131.80, 131.20, 130.05, 129.59, 129.51, 129.14, 129.02, 125.71, 124.23, 122.28, 120.11, 115.90, 113.51, 106.62, 106.51, 106.41, 69.32, 32.37, 27.98, 13.81. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{21}N_4O_6$, 485.15, found 485.03.



6-(2-Amino-5-nitrophenyl)-1,3-dimethyl-5-phenyl-1*H*-pyrrolo[3,4-*d*]pyrimidine-2,4(3*H*,6*H*)-dione (6). In a 25 mL round bottom flask 4-nitro-1,2-phenylenediamine (300 mg, 1.96 mmol), and **4** (330 mg, 979 µmol) were combined in ethanol (10 mL). The stirred mixture was brought to reflux for 3 h during which a yellow precipitate formed. The mixture was then chilled in an ice bath, filtered, and the precipitate washed with cold ethanol to give **6** (340 mg, 88.7%) as a waxy shiny yellow solid; mp > 300 °C. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.97 (dd, *J* = 2.7, 9.2, 1H), 7.86 (d, *J* = 2.6, 1H), 7.37 – 7.32 (m, 2H), 7.28 – 7.24 (m, 4H), 7.05 (s, 1H), 6.75 (d, *J* = 9.2, 1H), 6.65 (s, 2H), 3.35 (s, 3H), 3.21 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 159.06, 151.66, 150.89, 135.01, 133.84, 130.38, 129.34, 129.02, 128.32, 127.38, 126.19, 126.05, 121.34, 114.31, 105.49, 102.98, 31.59, 27.46. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{20}H_{18}N_5O_4$, 392.135880, found 392.03.

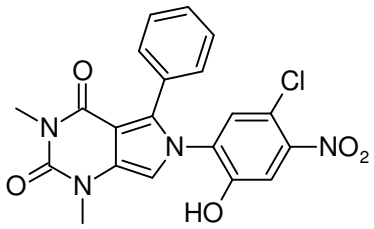


6-(5-Bromofuran-2-yl)-7,9-dimethyl-2-nitro-11-phenyl-5,6-dihydropyrimido[4',5'-3,4] pyrrolo[1,2-*a*]quinoxaline-8,10-(7*H*,9*H*)-dione (38). In a 5 mL pear shaped flask was placed **6** (100 mg, 256 *u*mol), 5-bromo-2-furaldehyde (50 mg, 286 µmol), TFA (10 µL, 14.9 mg, 130 µmol), and chloroform (2.5 mL). The mixture was refluxed for 1 h, dried in vacuo and purified by flash chromatography. The desired fractions were combined and dried in vacuo. The remaining solid was triturated in hot benzene and filtered to give **38** (103 mg, 73.6%) as a bright yellow solid. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.84 (d, *J* = 7.7, 1H), 7.82 (dd, *J* = 2.4,

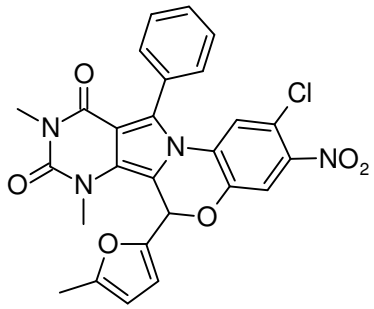


8.9, 1H), 7.66 (t, *J* = 7.3, 1H), 7.53 (t, *J* = 7.5, 1H), 7.37 (d, *J* = 2.3, 1H), 7.33 (t, *J* = 7.6, 1H), 7.02 (d, *J* = 7.7, 1H), 6.89 (d, *J* = 8.9, 1H), 6.16 (d, *J* = 2.3, 1H), 6.15 (d, *J* = 3.4, 1H), 5.90 (dd, *J* = 0.8, 3.4, 1H), 5.71 (d, *J* = 2.5, 1H), 3.54 (s, 3H), 3.28 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.31, 154.54, 151.89, 142.72, 139.43, 131.86, 131.25, 130.03, 129.79, 129.55, 129.05, 128.93, 123.95, 123.30, 122.99, 122.41, 116.84, 116.62, 112.38, 111.97, 107.73, 106.20, 48.22, 32.03, 28.02. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{25}H_{20}BrN_4O_3$, 548.06, found 547.96.

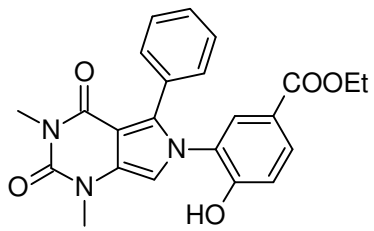
6-(5-Chloro-2-hydroxy-4-nitrophenyl)-1,3-dimethyl-5-phenyl-1*H*-pyrrolo[3,4-*d*]pyrimidine-2,4(3*H*,6*H*)-dione (29). In a 10 mL round bottom flask was placed **4** (200 mg, 595 µmol), 2-amino-4-chloro-5-nitrophenol (236 mg, 1.25 mmol), and ethanol (5 mL). The reaction was stirred at reflux for 5 h, then cooled and placed in a freezer. After several hours yellow crystals formed, which were filtered and rinsed with cold ethanol to give **29** (225 mg, 89%). ^{1}H NMR (600 MHz, DMSO-d_6) δ 11.33 (s, 1H), 7.79 (s, 1H), 7.44 (s, 1H), 7.30 (s, 5H), 7.10 (s, 1H), 3.33 (s, 3H), 3.20 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 158.98, 152.39, 150.82, 147.31, 134.14, 131.79, 130.50, 130.32, 129.23, 128.96, 128.33, 127.48, 113.90, 112.93, 105.91, 102.66, 31.55, 27.51. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{20}H_{16}ClN_4O_5$, 427.08, found 427.12



2-Chloro-7,9-Dimethyl-6-(5-methylfuran-2-yl)-3-nitro-11-phenyl-6H-benzo[b]pyrimido[4',5'-3,4] pyrrolo[1,2-*d*]oxazine-8,10-(7*H*,9*H*)-dione (39). Pyrrole **29** (97 mg, 227 µmol), 5-methylfurfural (25 µl, 27.7 mg, 252 µmol), TFA (5 µL, 7.4 mg, 65 µmol), 1,2-dichloroethane (2 mL) and a stir bar were sealed in a Emrys 2-5 mL process vial and submerged to the level of solvent in an oil bath at 150 °C for 2 h. The reaction was then cooled, diluted with ethanol (8 mL) and placed in a freezer. After several hours a precipitate formed which was filtered and rinsed with cold ethanol to give **39** (80 mg, 68%). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.7, 1H), 7.64 (dd, *J* = 6.1, 7.0, 2H), 7.58 (t, *J* = 7.5, 1H), 7.42 (t, *J* = 7.2, 1H), 7.08 (d, *J* = 7.7, 1H), 6.87 (s, 1H), 6.58 (s, 1H), 5.92 (d, *J* = 3.2, 1H), 5.82 (d, *J* = 2.3, 1H), 3.47 (s, 3H), 3.26 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.06, 155.28, 151.65, 147.36, 144.47, 144.05, 131.75, 131.54, 130.24, 130.02, 129.76, 129.15, 129.12, 128.96, 124.45, 122.71, 120.59, 117.46, 113.80, 107.06, 106.79, 106.71, 69.18, 32.36, 28.02, 13.84. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{20}ClN_4O_6$, 519.11, found 519.14.

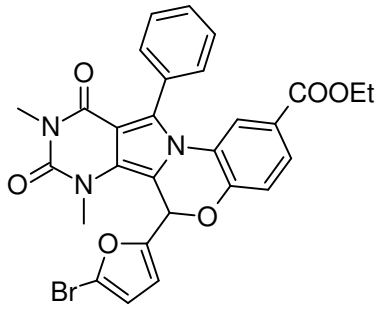


Ethyl 3-(1,3-dimethyl-2,4-dioxo-5-phenyl-3,4-dihydro-1*H*-pyrrolo[3,4-*d*]pyrimidin-6(2*H*)-yl)-4-hydroxybenzoate (30). In a 100 mL round bottom flask ethyl 3-amino-4-hydroxybenzoate (1.10 g, 6.07 mmol) and **4** (1.00 g, 2.98 mmol) were refluxed in ethanol (50 mL). After 2 h, the condenser was rearranged for distillation and ethanol (25 mL) was distilled off. The resulting solution was slowly poured into a vigorously stirred solution of ice cold water (200 mL) and citric acid (50 mg) to give a pink precipitate. The mixture was stirred for 10 min and then the solid was filtered and rinsed with cold water to give **30** (1.23 g, 98.5%)



after drying. The product was recrystallized from ethanol to give pale pink needles; m.p. 129.2-130 °C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 8.58 (s, 1H), 7.89 (dd, *J* = 2.1, 8.7, 1H), 7.67 (d, *J* = 2.1, 1H), 7.36 – 7.29 (m, 2H), 7.28 – 7.18 (m, 3H), 6.97 (d, *J* = 8.7, 1H), 4.25 (q, *J* = 7.1, 2H), 3.27 (s, 3H), 3.17 (s, 3H), 1.30 (t, *J* = 7.1, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 165.40, 159.72, 156.82, 151.91, 136.06, 132.09, 130.86, 130.65, 129.49, 128.99, 128.83, 127.84, 125.70, 122.92, 117.65, 104.70, 103.11, 61.23, 32.02, 28.08, 14.24. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{23}H_{22}N_3O_5$, 420.16, found 420.13.

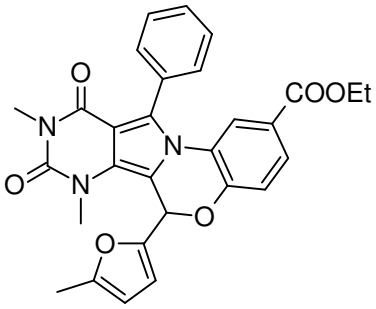
Ethyl 6-(5-Bromofuran-2-yl)-7,9-dimethyl-8,10-dioxo-11-phenyl-7,8,9,10-tetrahydro-6*H*-benzo[*b*]pyrimido [4',5':3,4]pyrrolo[1,2-*d*][1,4]oxazine-2-carboxylate (40).



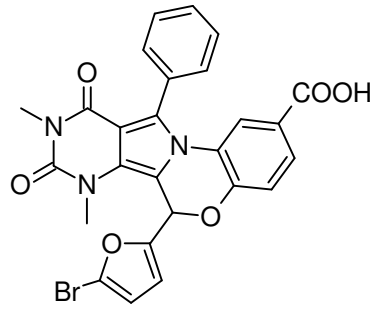
Pyrrole **30** (500 mg, 1.19 mmol), 5-bromofurfural (240 mg, 1.37 mmol), chloroform (7 mL), TFA (10 µL, 14.8 mg, 130 µmol), 3 Å molecular sieve[6] (2.0 g, 8-12 mesh beads) and a stir bar were sealed in a in a Emrys 10-20 mL process vial and submerged to the level of solvent in an oil bath at 150 °C. The reaction was stirred for 24 min then removed from the oil bath. Once the internal pressure had dropped the reaction vial was rapidly cooled in water. After cooling, the reaction was filtered through celite into a 50 mL recovery flask and the dried in vacuo. The residue was dissolved in a minimum volume of CH_2Cl_2 and rapidly diluted with warm ethanol (25 mL). Fine crystals began to form immediately. The mixture was then placed on a rotary evaporator and CH_2Cl_2 removed to increase the quantity of crystals. The mixture was then chilled, filtered, and the crystals rinsed with cold ethanol to give **40** (0.500 g, 76.4%) as fine white needle-like crystals. No m.p. (slow decomposition). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.68 (dd, *J* = 1.9, 8.4, 1H), 7.63 (t, *J* = 7.5, 1H), 7.52 (t, *J* = 7.5, 1H), 7.34 (t, *J* = 7.5, 1H), 7.23 (d, *J* = 1.8, 1H), 7.09 (d, *J* = 8.4, 1H), 7.06 (d, *J* = 7.7, 1H), 6.86 (s, 1H), 6.14 (d, *J* = 3.4, 1H), 5.98 (d, *J* = 2.9, 1H), 4.11 (dq, *J* = 7.2, 10.7, 1H), 4.00 (dq, *J* = 7.1, 10.7, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 1.14 (t, *J* = 7.1, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 165.03, 159.26, 151.87, 151.79, 149.08, 131.78, 131.27, 130.00, 129.80, 129.68, 128.84, 128.81, 128.29, 125.40, 124.69, 124.47, 124.42, 121.57, 119.64, 114.91, 112.43, 105.93, 105.67, 68.40, 61.28, 32.38, 27.95, 14.20. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{28}H_{23}BrN_3O_6$, 576.08, found 576.04.

[6] The formation of the oxazine ring produces water that collects as beads at or near the top of the tube during the reaction. If the reaction was scaled up such that the beads became large enough to drip back into to the reaction mixture the yield was diminished. The addition of molecular sieves reduced this problem for reactions containing <500 mg of the starting pyrrole.

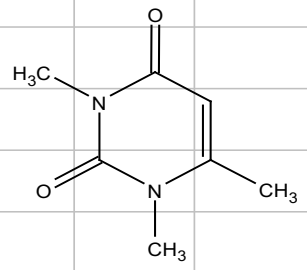
Ethyl 7,9-Dimethyl-8,10-dioxo- 6-(5-methylfuran-2-yl)-11-phenyl-7,8,9,10-tetrahydro-6*H*-benzo[*b*] pyrimido [4',5':3,4] pyrrolo[1,2-*d*][1,4]oxazine-2-carboxylate (41). Pyrrole **30** (138 mg, 329 µmol), 5-methylfurfural (36 µL, 39.9 mg, 362 µmol), chloroform (3 mL), and TFA (5 µL, 7.4 mg, 65 µmol) sealed in a Emrys 2-5 mL process vial and submerged in an oil bath at 150 °C for 2 h. After cooling the reaction was dried in vacuo. The residue was dissolved in a minimum volume of CH_2Cl_2 and then diluted with ethanol (10 mL). The solution was then placed on a rotary evaporator and solvent removed until the mixture ceased to precipitate. The mixture was then chilled, filtered, and the precipitate rinsed with cold ethanol to give **41** (168 mg, 82%). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.67 (dd, *J* = 1.9, 8.4, 1H), 7.63 (t, *J* = 7.5, 1H), 7.52 (t, *J* = 7.5, 1H), 7.34 (t, *J* = 7.5, 1H), 7.23 (d, *J* = 1.8, 1H), 7.09 – 7.02 (m, *J* = 4.5, 8.0, 2H), 6.83 (s, 1H), 5.85 (d, *J* = 3.2, 1H), 5.76 (d, *J* = 2.5, 1H), 4.10 (dq, *J* = 7.1, 10.7, 1H), 3.99 (dq, *J* = 7.1, 10.7, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 2.21 (s, 3H), 1.14 (t, *J* = 7.1, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 165.10, 159.37, 154.76, 151.83, 149.47, 148.20, 131.81, 130.84, 130.16, 129.72, 129.70, 128.80, 128.76, 128.13, 125.54, 124.38, 123.96, 121.54, 119.56, 113.22, 106.89, 106.49, 105.84, 68.89, 61.22, 32.34, 27.92, 14.20, 13.80. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{29}H_{26}N_3O_6$, 512.18, found 512.22.



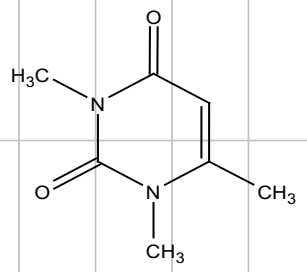
6-(5-Bromofuran-2-yl)-7,9-dimethyl-8,10-dioxo-11-phenyl-7,8,9,10-tetrahydro-6*H*-benzo[*b*]pyrimido [4',5':3,4]pyrrolo [1,2-*d*][1,4]oxazine-2-carboxylic acid (42). In a 500 mL round bottom flask **40** (1.00 g, 1.73 mmol) was dissolved in THF (100 mL) with gentle heating and then allowed to cool. A mixture of water (70 mL) and KOH (768 mg, 13.7 mmol) was quickly added to the vigorously stirred solution to give a white suspension. After 3 days the mixture was a homogenous yellow solution without **40** as determined by LC/MS. The THF was removed using a rotary evaporator leaving behind a viscous aqueous solution. The solution was made strongly acidic to litmus using 1% aq. HCl while stirring vigorously with a glass rod. The resulting gel was shaken with EtOAc (125 mL) and then quickly poured into a 1 liter separatory funnel where a precipitate formed in the organic layer. The 500 mL flask was rinsed by shaking with additional EtOAc (125 mL), and this was also added to separatory funnel. Further EtOAc (400 mL) was added to the funnel and the mixture vigorously shaken until all the solids dissolved. After settling, the lower yellow aqueous layer was discarded. The EtOAc layer was washed with brine, dried over Na_2SO_4 and dryed on a rotary evaporator. The resulting slightly yellow amorphous powder was loosened by swirling with CH_2Cl_2 (15 mL) and then diluted with diethyl ether (15 mL). The solids were collected by filtration and rinsed with a solution of CH_2Cl_2:Et_2O (1:1) to give **42** (791 mg, 83.2%) as a white solid. No m.p. (slow decomposition). Compound purity may be improved by recrystallizing from THF or triturating with CH_3CN. It is difficult, however, to remove **40** from the final product without utilizing silica column chromatography, so that every effort should be made to ensure that saponification is complete before workup. ^{1}H NMR (600 MHz, 91% CD_2Cl_2, 9% DMSO-d_6) δ 12.30 (s, 1H), 7.79 (d, *J* = 7.7, 1H), 7.63 (dd, *J* = 1.9, 8.4, 1H), 7.58 (t, *J* = 7.6, 1H), 7.46 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.17 (d, *J* = 1.7, 1H), 7.04 (d, *J* = 8.4, 1H), 7.01 (d, *J* = 7.7, 1H), 6.89 (s, 1H), 6.12 (d, *J* = 3.4, 1H), 5.96 (d, *J* = 3.3, 1H),



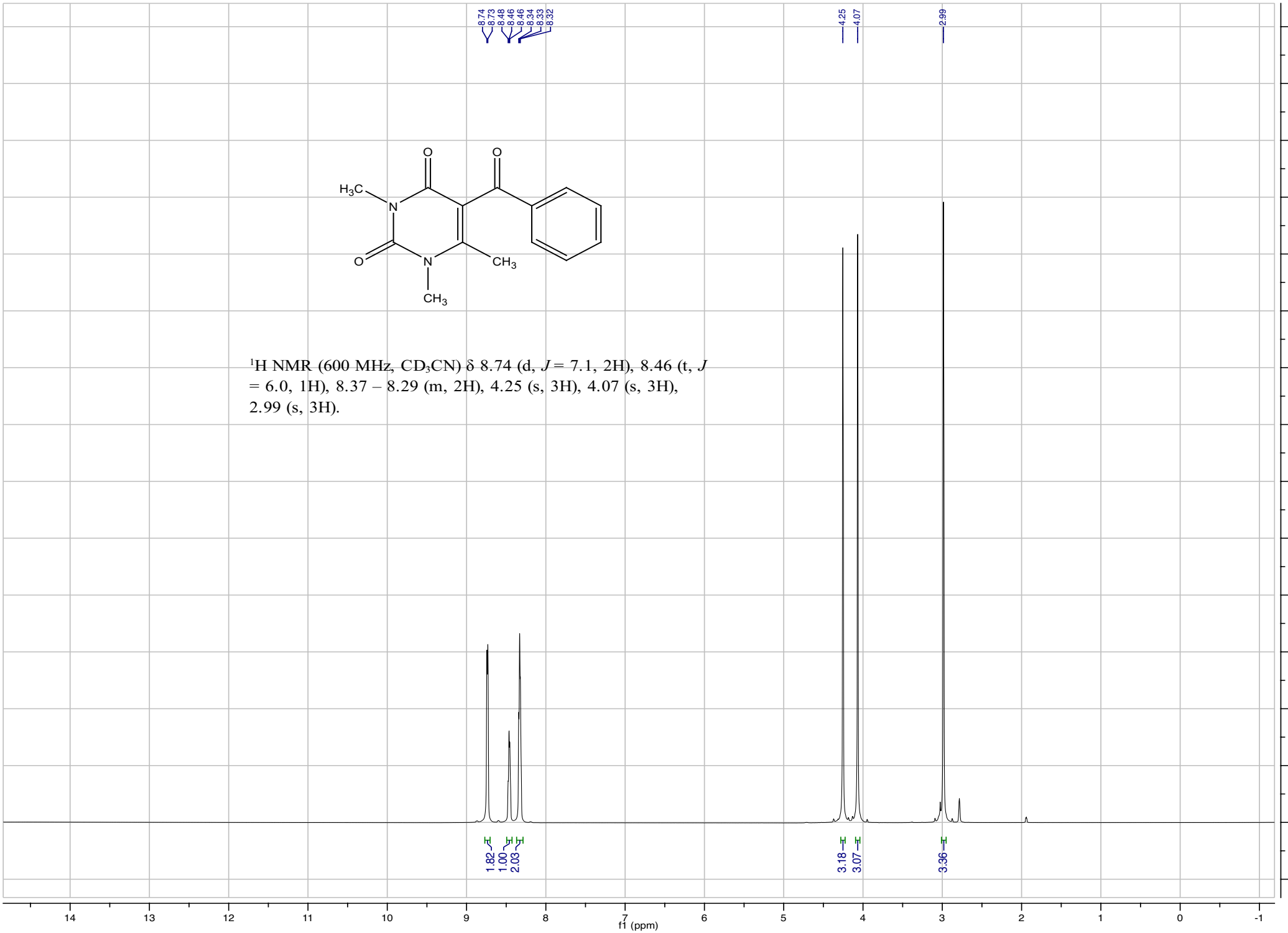
3.44 (s, 3H), 3.21 (s, 3H). ^{13}C NMR (151 MHz, 91% CD_2Cl_2, 9% DMSO-d_6) δ 166.69, 159.13, 151.86, 151.62, 148.96, 131.75, 131.00, 129.74, 129.65, 129.45, 128.59, 128.53, 128.45, 125.33, 125.23, 124.38, 124.20, 121.86, 119.42, 114.84, 112.34, 105.95, 105.66, 68.20, 32.28, 27.84. MS (ES+) (*m/z*): $[M+1]^+$ calculated for $C_{26}H_{19}BrN_3O_6$, 548.05, found 548.00.



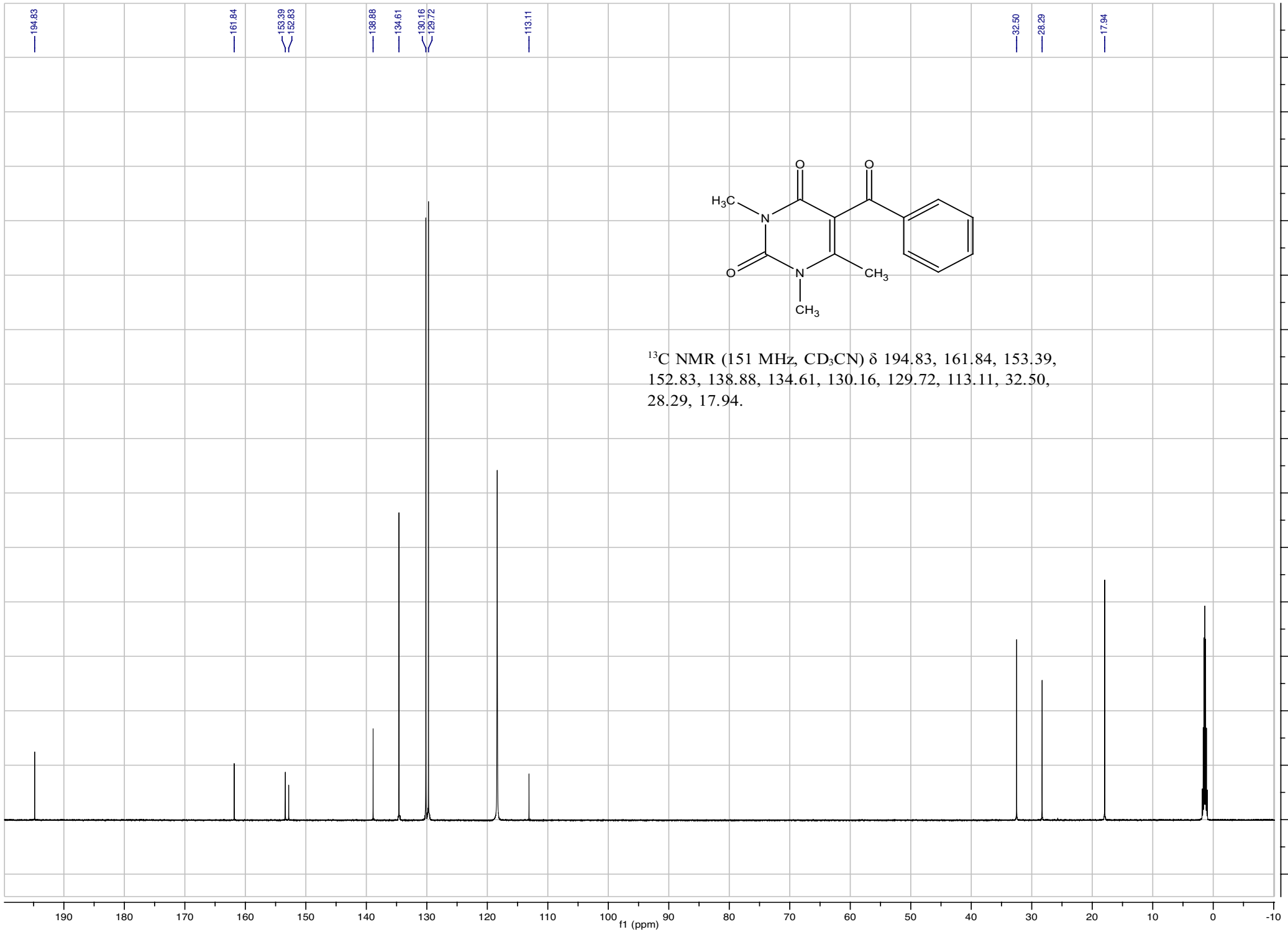
^{1}H NMR (600 MHz, $CDCl_3$) δ 5.67 (s, 1H), 3.45 (s, 3H), 3.35 (s, 3H), 2.29 (s, 3H).

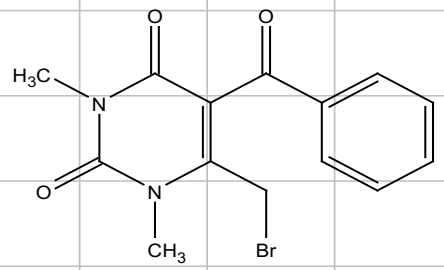


^{13}C NMR (151 MHz, $CDCl_3$) δ 162.62, 152.53, 151.81, 101.16, 31.89, 28.11, 20.58.

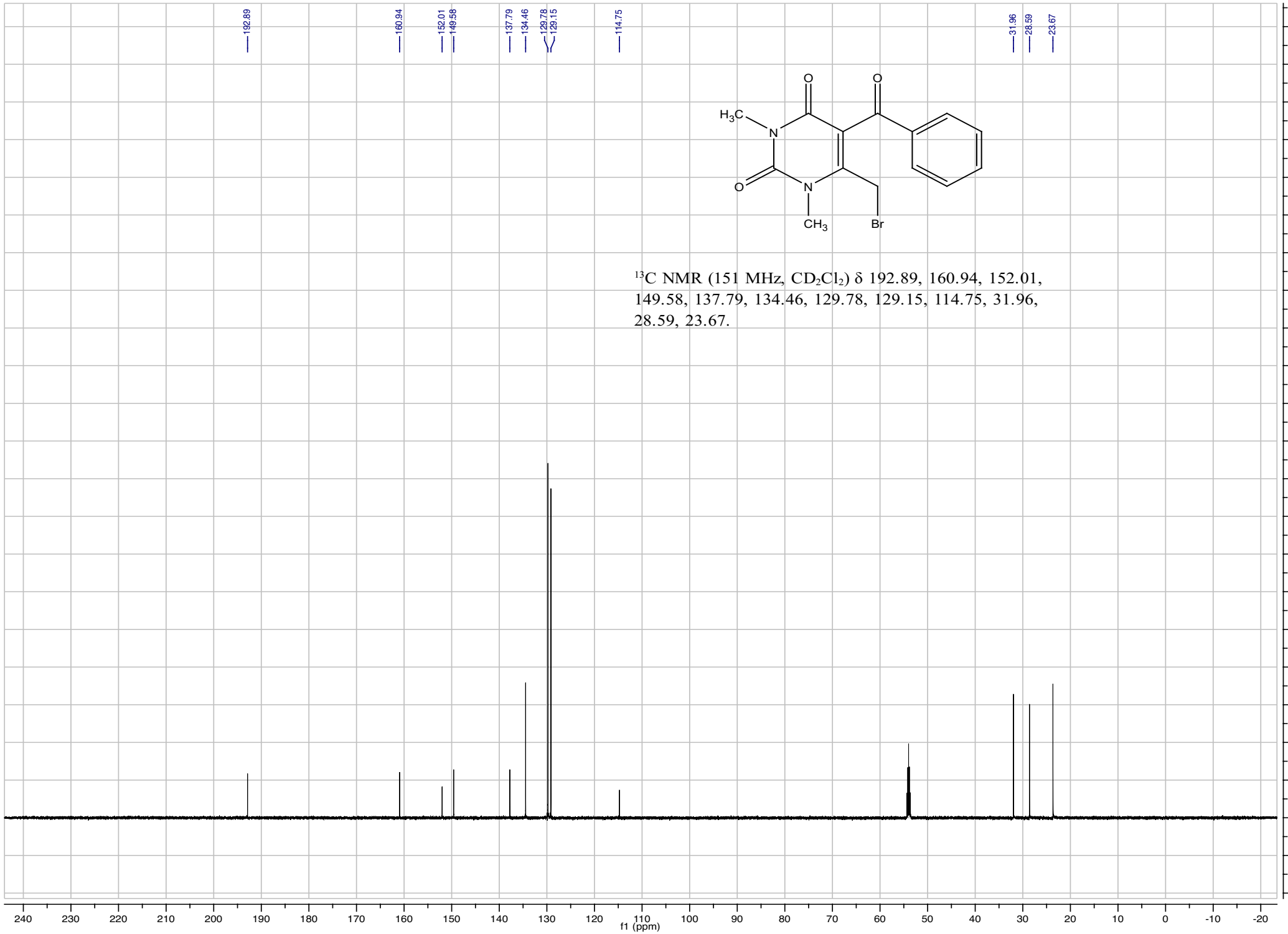


^{1}H NMR (600 MHz, CD_3CN) δ 8.74 (d, J = 7.1, 2H), 8.46 (t, J = 6.0, 1H), 8.37 – 8.29 (m, 2H), 4.25 (s, 3H), 4.07 (s, 3H), 2.99 (s, 3H).

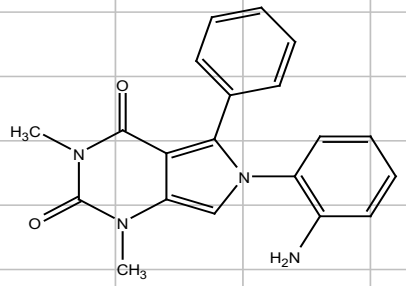

194.83
161.84
153.39
152.83
138.88
134.61
130.16
129.72
113.11
32.50
28.29
17.94
O
O
H3C
N
O
N
CH3
CH3
13C NMR (151 MHz, CD3CN) δ 194.83, 161.84, 153.39, 152.83, 138.88, 134.61, 130.16, 129.72, 113.11, 32.50, 28.29, 17.94.
f1 (ppm)



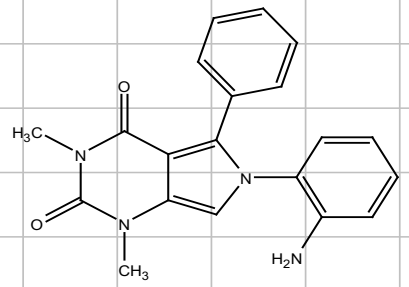
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.88 – 7.80 (m, 2H), 7.65 – 7.60 (m, 1H), 7.52 – 7.45 (m, 2H), 4.24 (s, 2H), 4.24 (s, 2H), 3.59 (s, 3H), 3.31 (s, 3H).



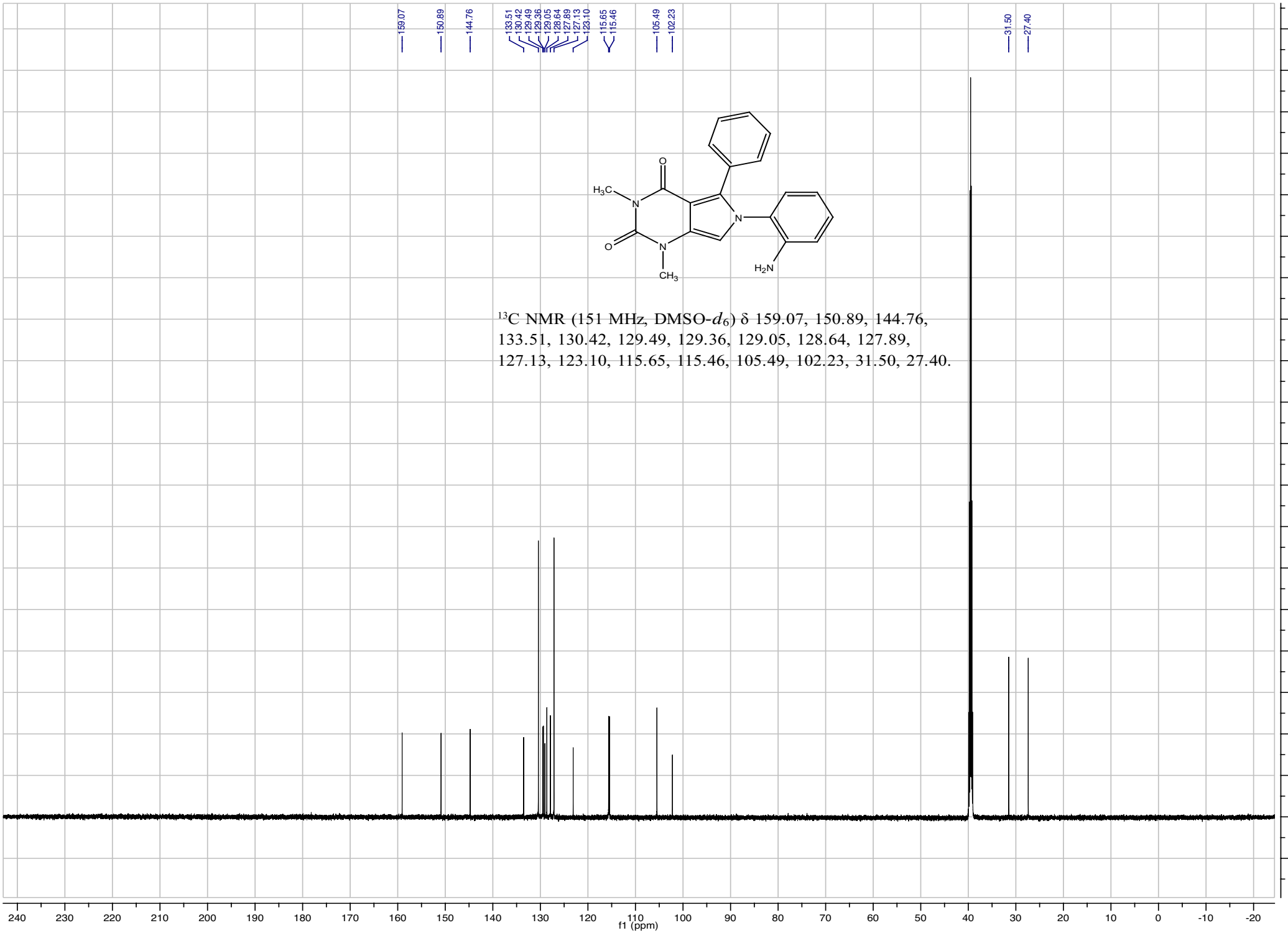
^{13}C NMR (151 MHz, CD_2Cl_2) δ 192.89, 160.94, 152.01, 149.58, 137.79, 134.46, 129.78, 129.15, 114.75, 31.96, 28.59, 23.67.

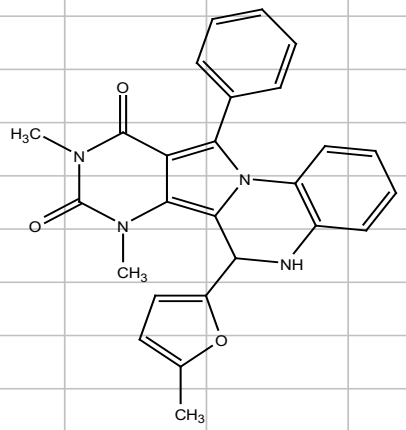


^{1}H NMR (600 MHz, DMSO-d_6) δ 7.37 – 7.31 (m, 2H), 7.25 – 7.19 (m, 3H), 7.08 – 7.02 (m, 1H), 6.92 (s, 1H), 6.83 (dd, J = 1.3, 7.8, 1H), 6.75 (d, J = 8.1, 1H), 6.48 – 6.43 (m, 1H), 5.08 (s, 2H), 3.33 (s, 3H), 3.19 (s, 3H).

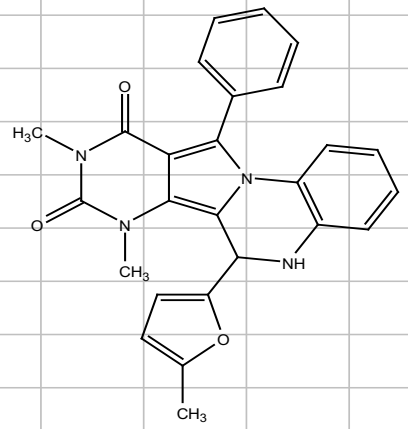


^{1}H NMR (600 MHz, DMSO-d_6) δ 7.37 – 7.31 (m, 2H), 7.25 – 7.19 (m, 3H), 7.08 – 7.02 (m, 1H), 6.92 (s, 1H), 6.83 (dd, J = 1.3, 7.8, 1H), 6.75 (d, J = 8.1, 1H), 6.48 – 6.43 (m, 1H), 5.08 (s, 2H), 3.33 (s, 3H), 3.19 (s, 3H).

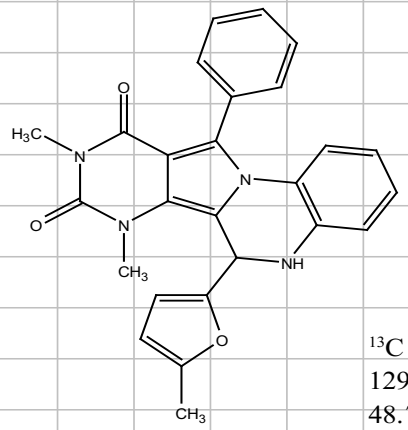

159.07
150.89
144.76
133.51
130.42
129.49
129.36
129.05
128.64
127.89
127.13
123.10
115.65
115.46
105.49
102.23
31.50
27.40
H3C
N
O
O
N
CH3
N
H2N
13C NMR (151 MHz, DMSO-d6) δ 159.07, 150.89, 144.76,
133.51, 130.42, 129.49, 129.36, 129.05, 128.64, 127.89,
127.13, 123.10, 115.65, 115.46, 105.49, 102.23, 31.50, 27.40.
f1 (ppm)



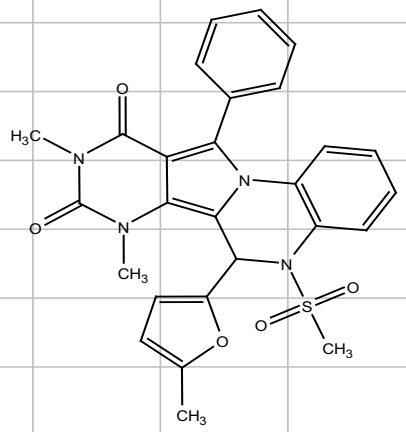
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.6, 1H), 6.95 – 6.90 (m, 1H), 6.83 (dd, *J* = 1.1, 7.9, 1H), 6.48 (d, *J* = 7.9, 1H), 6.45 – 6.40 (m, 1H), 6.01 (s, 1H), 5.75 (d, *J* = 2.1, 1H), 5.70 (d, *J* = 3.0, 1H), 4.93 (d, *J* = 2.0, 1H), 3.55 (s, 3H), 3.27 (s, 3H), 2.20 (s, 3H).



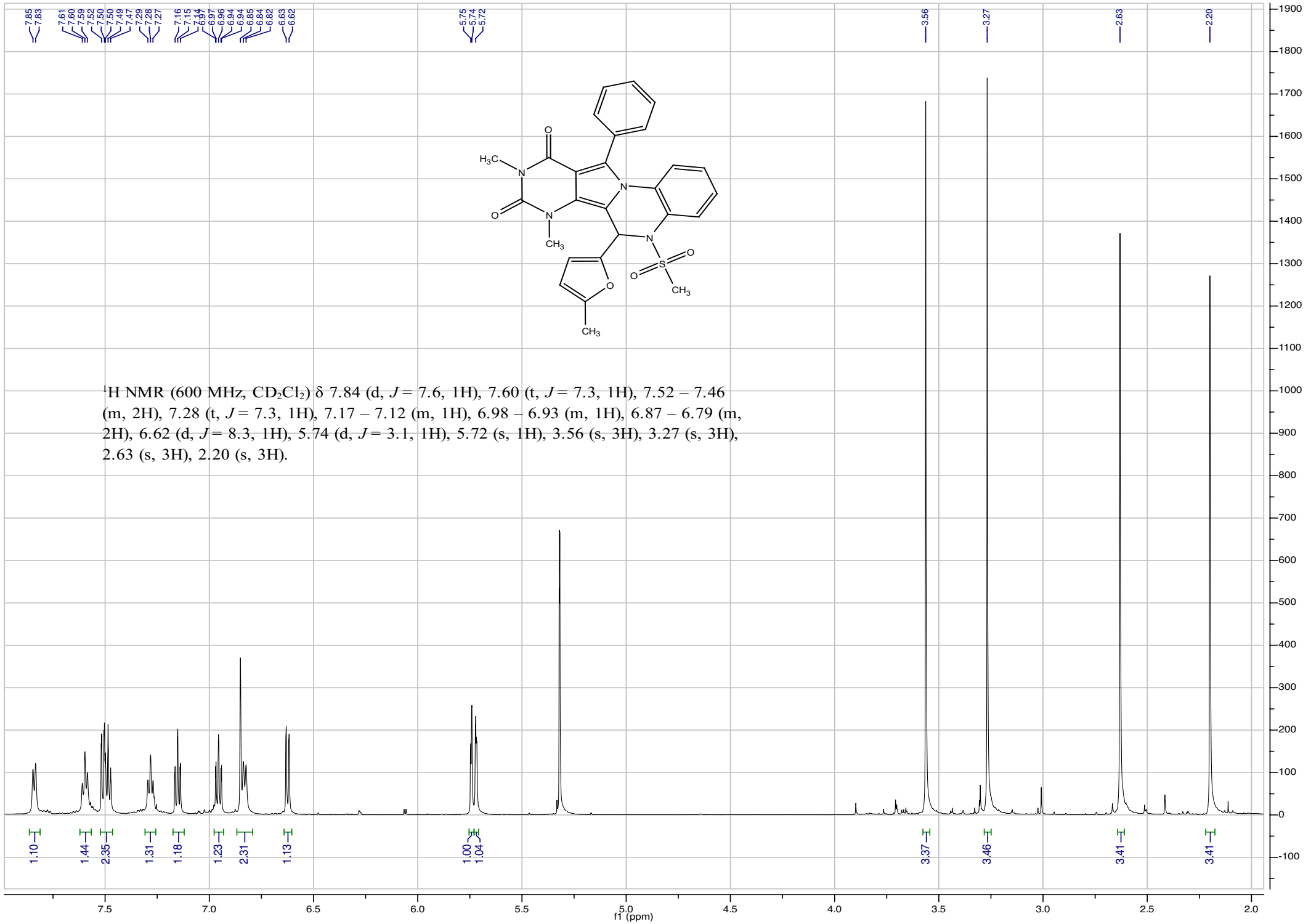
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.6, 1H), 6.95 – 6.90 (m, 1H), 6.83 (dd, *J* = 1.1, 7.9, 1H), 6.48 (d, *J* = 7.9, 1H), 6.45 – 6.40 (m, 1H), 6.01 (s, 1H), 5.75 (d, *J* = 2.1, 1H), 5.70 (d, *J* = 3.0, 1H), 4.93 (d, *J* = 2.0, 1H), 3.55 (s, 3H), 3.27 (s, 3H), 2.20 (s, 3H).



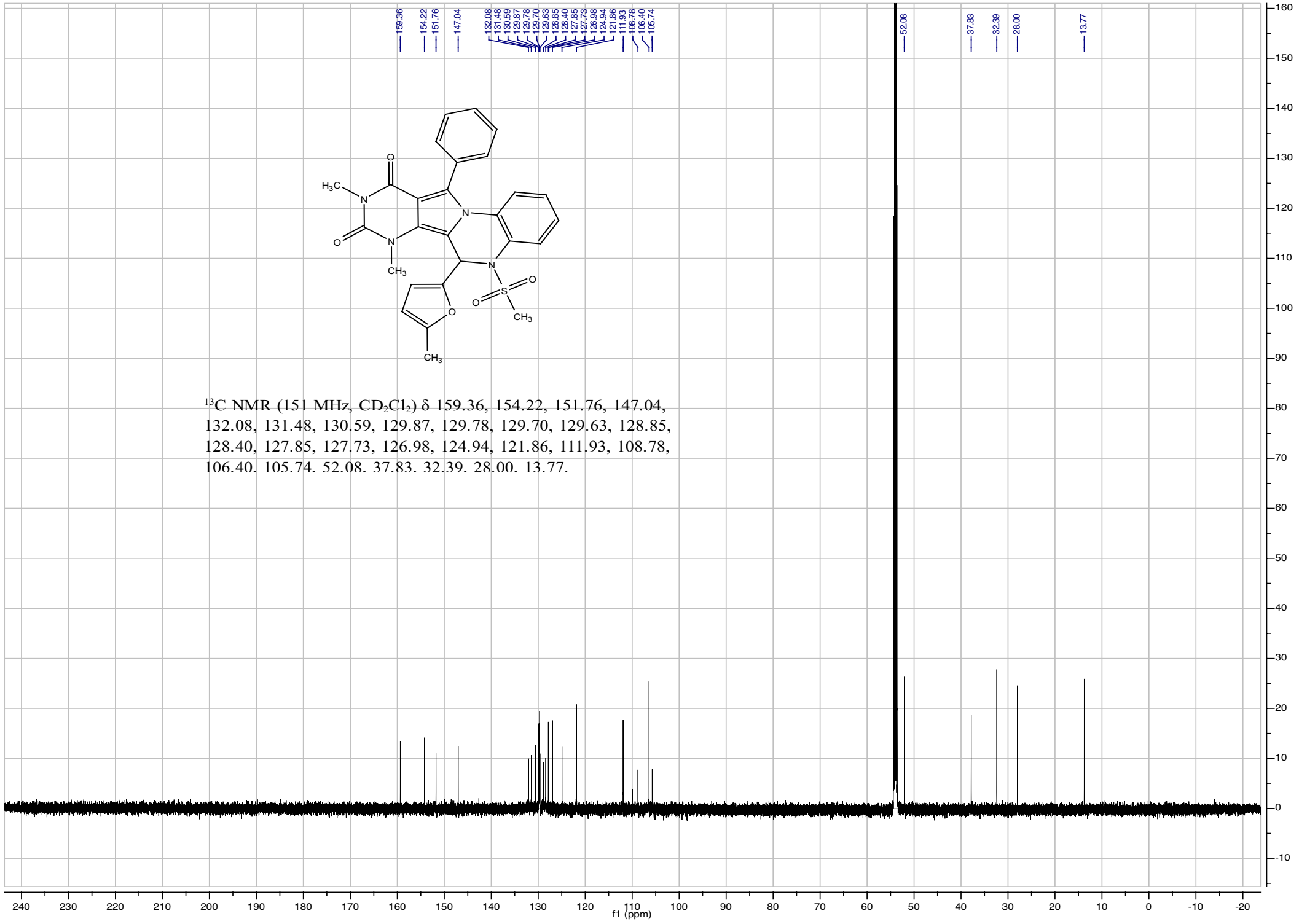
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.59, 152.98, 152.03, 151.67, 137.36, 132.01, 130.96, 130.17, 130.06, 129.08, 128.49, 128.27, 126.49, 124.82, 123.35, 121.10, 119.45, 117.42, 110.32, 109.74, 106.21, 105.24, 48.76, 32.04, 27.90, 13.70.



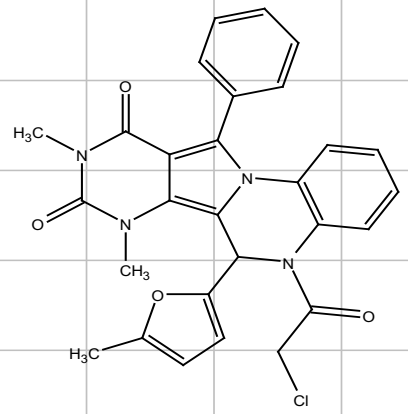
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.84 (d, *J* = 7.6, 1H), 7.60 (t, *J* = 7.3, 1H), 7.52 – 7.46 (m, 2H), 7.28 (t, *J* = 7.3, 1H), 7.17 – 7.12 (m, 1H), 6.98 – 6.93 (m, 1H), 6.87 – 6.79 (m, 2H), 6.62 (d, *J* = 8.3, 1H), 5.74 (d, *J* = 3.1, 1H), 5.72 (s, 1H), 3.56 (s, 3H), 3.27 (s, 3H), 2.63 (s, 3H), 2.20 (s, 3H).



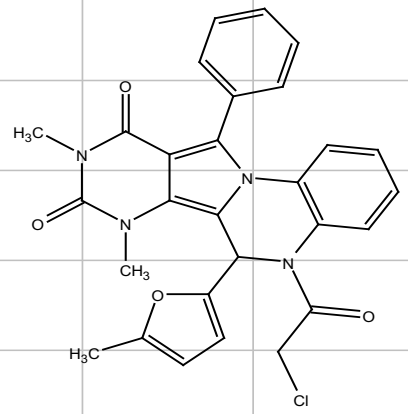
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.84 (d, J = 7.6, 1H), 7.60 (t, J = 7.3, 1H), 7.52 – 7.46 (m, 2H), 7.28 (t, J = 7.3, 1H), 7.17 – 7.12 (m, 1H), 6.98 – 6.93 (m, 1H), 6.87 – 6.79 (m, 2H), 6.62 (d, J = 8.3, 1H), 5.74 (d, J = 3.1, 1H), 5.72 (s, 1H), 3.56 (s, 3H), 3.27 (s, 3H), 2.63 (s, 3H), 2.20 (s, 3H).



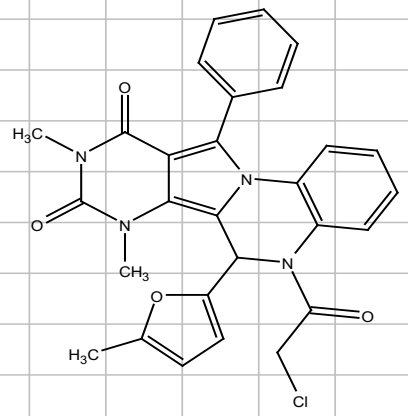
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.36, 154.22, 151.76, 147.04, 132.08, 131.48, 130.59, 129.87, 129.78, 129.70, 129.63, 128.85, 128.40, 127.85, 127.73, 126.98, 124.94, 121.86, 111.93, 108.78, 106.40. 105.74. 52.08. 37.83. 32.39. 28.00. 13.77.



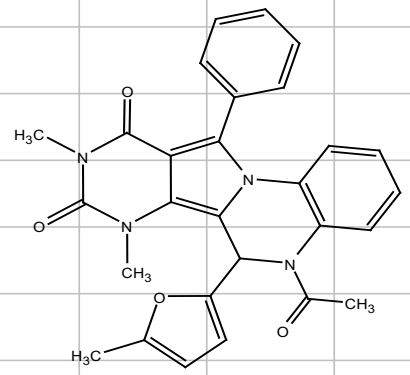
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.86 (d, J = 7.1, 1H), 7.58 (t, J = 7.1, 1H), 7.55 (s, 1H), 7.47 (t, J = 7.5, 1H), 7.33 – 7.25 (m, J = 1.2, 7.9, 2H), 7.14 (td, J = 1.2, 7.8, 1H), 7.02 (d, J = 7.1, 1H), 6.97 – 6.92 (m, 1H), 6.64 (dd, J = 1.0, 8.3, 1H), 5.71 – 5.66 (m, 2H), 4.41 (dd, J = 13.3, 62.4, 2H), 3.58 (s, 3H), 3.27 (s, 3H), 2.16 (s, 3H).



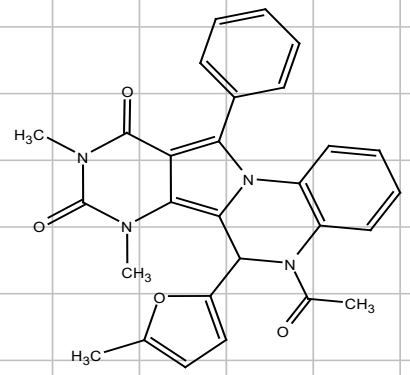
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.86 (d, *J* = 7.1, 1H), 7.58 (t, *J* = 7.1, 1H), 7.55 (s, 1H), 7.47 (t, *J* = 7.5, 1H), 7.33 – 7.25 (m, *J* = 1.2, 7.9, 2H), 7.14 (td, *J* = 1.2, 7.8, 1H), 7.02 (d, *J* = 7.1, 1H), 6.97 – 6.92 (m, 1H), 6.64 (dd, *J* = 1.0, 8.3, 1H), 5.71 – 5.66 (m, 2H), 4.41 (dd, *J* = 13.3, 62.4, 2H), 3.58 (s, 3H), 3.27 (s, 3H), 2.16 (s, 3H).



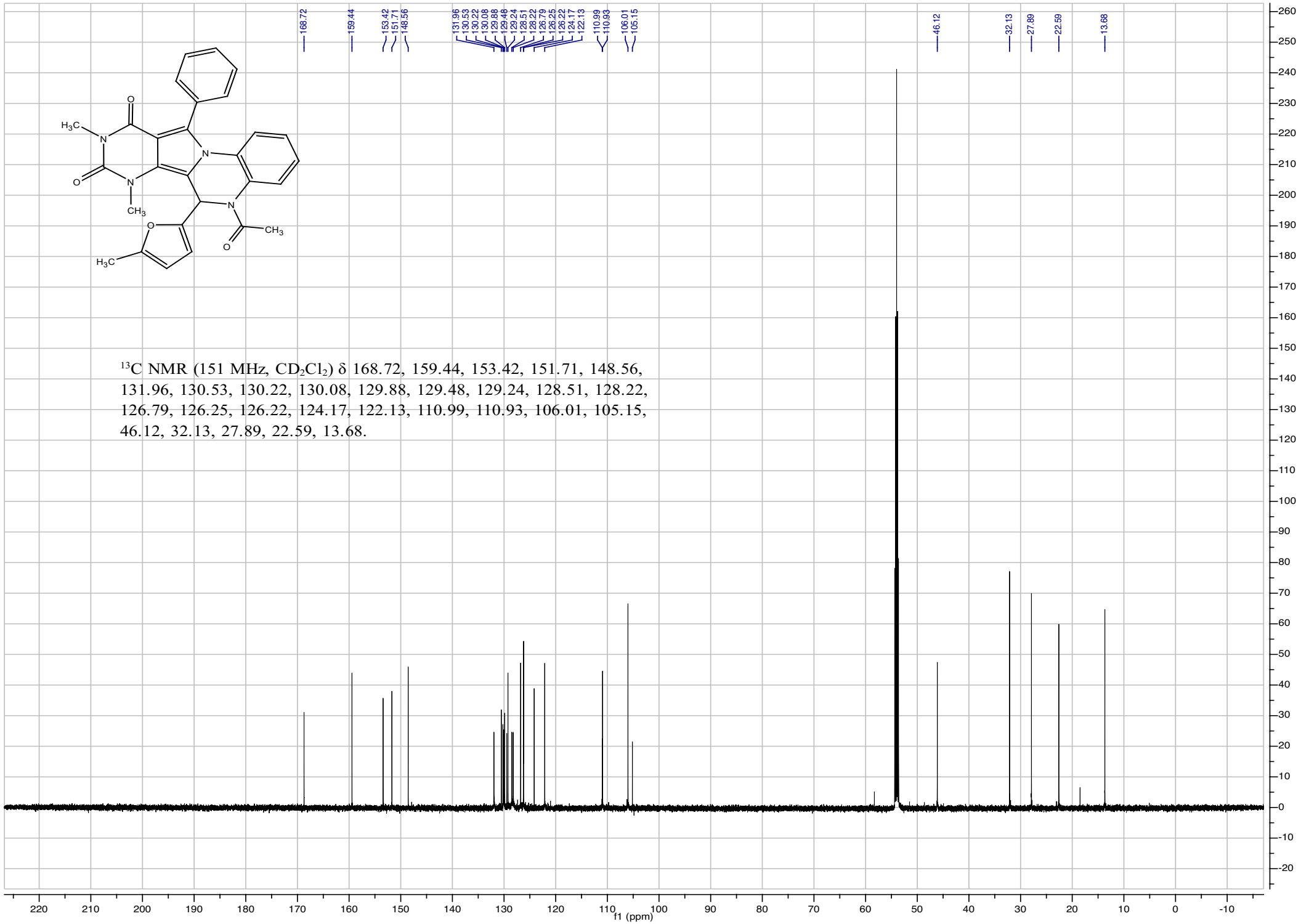
^{13}C NMR (151 MHz, CD_2Cl_2) δ 165.09, 159.44, 153.82, 151.78, 147.81, 132.01, 131.13, 130.15, 129.80, 129.45, 129.01, 128.62, 128.39, 127.39, 126.73, 126.01, 124.66, 122.57, 111.58, 110.34, 106.22, 105.44, 47.66, 42.19, 32.24, 27.97, 13.71.



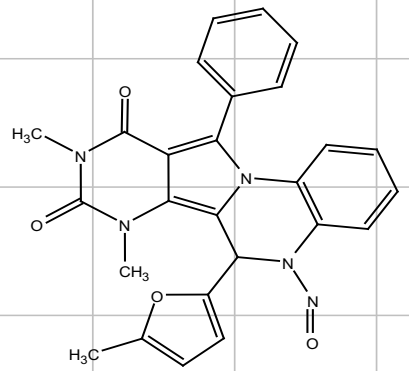
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.85 (d, *J* = 7.6, 1H), 7.62 (s, 1H), 7.57 (t, *J* = 7.5, 1H), 7.46 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.25 (d, *J* = 7.9, 1H), 7.12 (t, *J* = 7.7, 1H), 7.02 (d, *J* = 7.6, 1H), 6.88 (t, *J* = 7.9, 1H), 6.61 (d, *J* = 8.3, 1H), 5.68 (d, *J* = 2.8, 1H), 5.66 (d, *J* = 3.0, 1H), 3.59 (s, 3H), 3.26 (s, 3H), 2.32 (s, 3H), 2.16 (s, 3H).



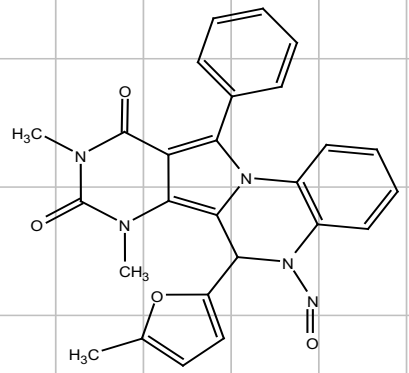
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.85 (d, *J* = 7.6, 1H), 7.62 (s, 1H), 7.57 (t, *J* = 7.5, 1H), 7.46 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.25 (d, *J* = 7.9, 1H), 7.12 (t, *J* = 7.7, 1H), 7.02 (d, *J* = 7.6, 1H), 6.88 (t, *J* = 7.9, 1H), 6.61 (d, *J* = 8.3, 1H), 5.68 (d, *J* = 2.8, 1H), 5.66 (d, *J* = 3.0, 1H), 3.59 (s, 3H), 3.26 (s, 3H), 2.32 (s, 3H), 2.16 (s, 3H).



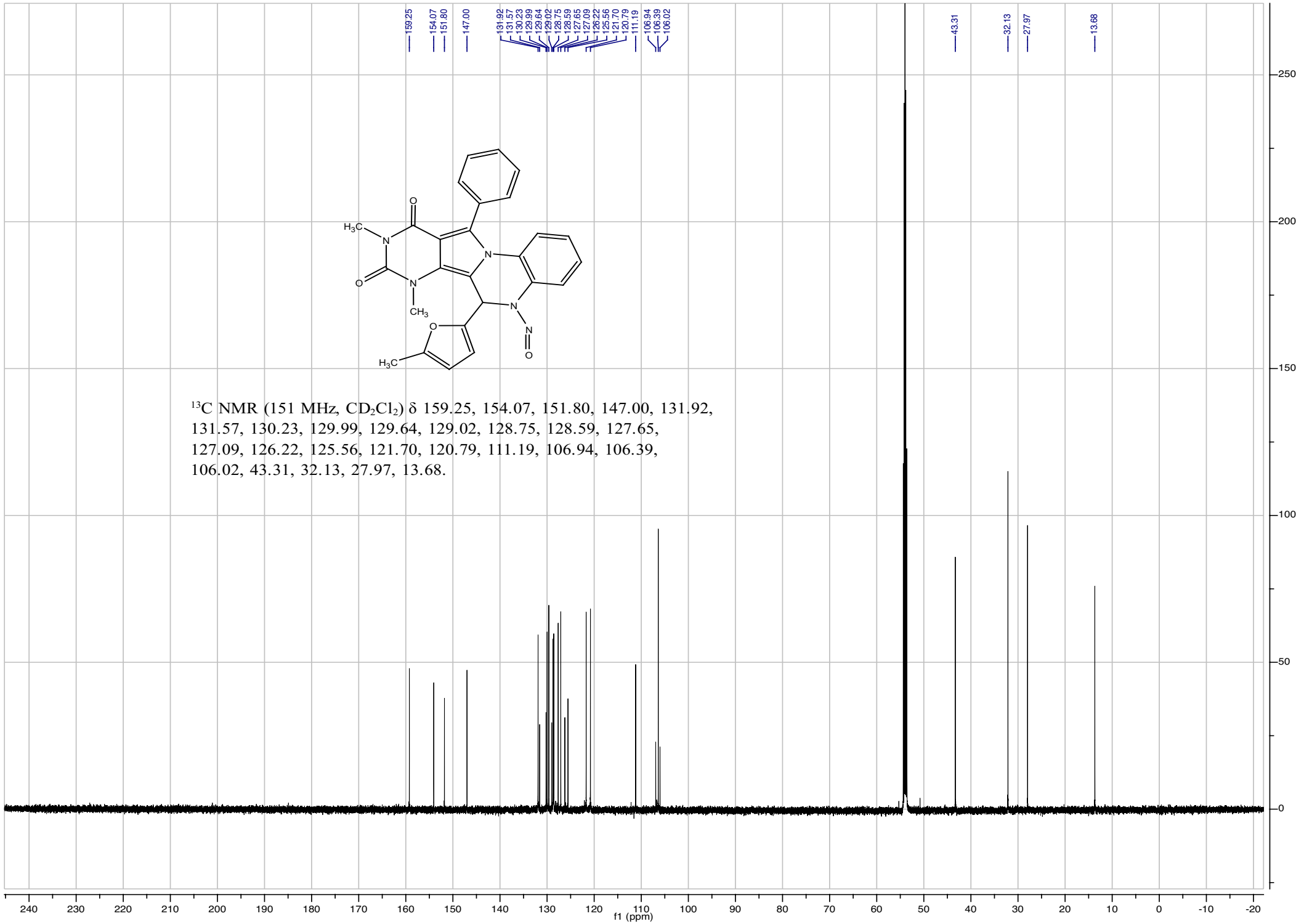
^{13}C NMR (151 MHz, CD_2Cl_2) δ 168.72, 159.44, 153.42, 151.71, 148.56, 131.96, 130.53, 130.22, 130.08, 129.88, 129.48, 129.24, 128.51, 128.22, 126.79, 126.25, 126.22, 124.17, 122.13, 110.99, 110.93, 106.01, 105.15, 46.12, 32.13, 27.89, 22.59, 13.68.



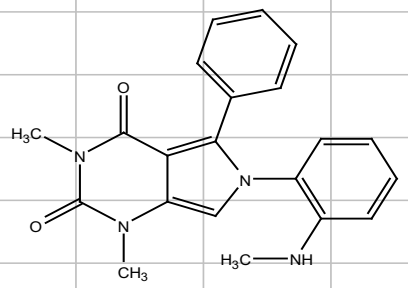
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.89 (s, 1H), 7.83 (d, *J* = 7.7, 1H), 7.76 (d, *J* = 8.0, 1H), 7.60 (t, *J* = 7.6, 1H), 7.50 (t, *J* = 7.5, 1H), 7.32 (t, *J* = 7.5, 1H), 7.25 (t, *J* = 7.7, 1H), 7.04 – 6.99 (m, 2H), 6.72 (d, *J* = 8.4, 1H), 5.83 (d, *J* = 3.1, 1H), 5.74 (d, *J* = 2.6, 1H), 3.61 (s, 3H), 3.24 (s, 3H), 2.12 (s, 3H).



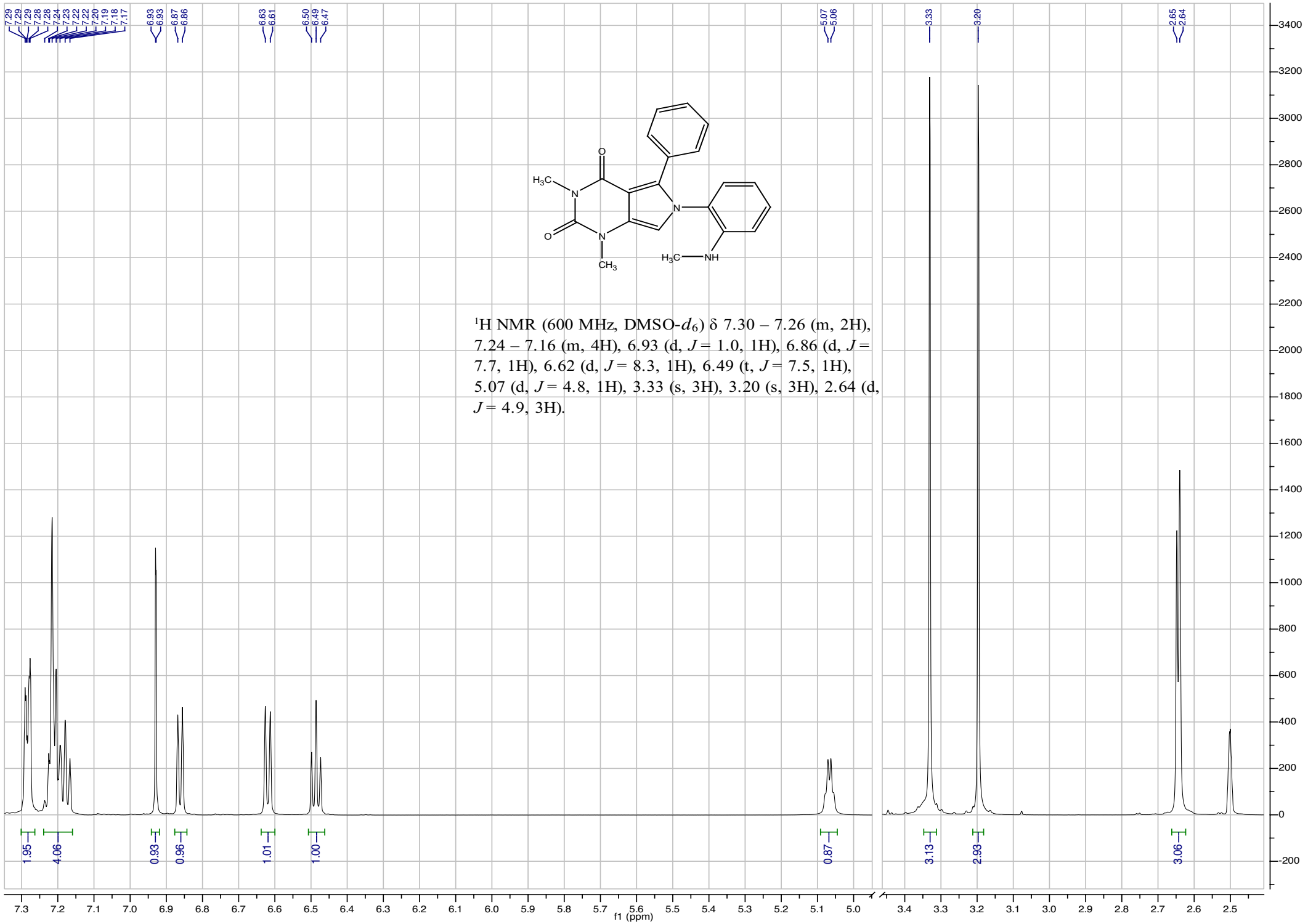
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.89 (s, 1H), 7.83 (d, J = 7.7, 1H), 7.76 (d, J = 8.0, 1H), 7.60 (t, J = 7.6, 1H), 7.50 (t, J = 7.5, 1H), 7.32 (t, J = 7.5, 1H), 7.25 (t, J = 7.7, 1H), 7.04 – 6.99 (m, 2H), 6.72 (d, J = 8.4, 1H), 5.83 (d, J = 3.1, 1H), 5.74 (d, J = 2.6, 1H), 3.61 (s, 3H), 3.24 (s, 3H), 2.12 (s, 3H).



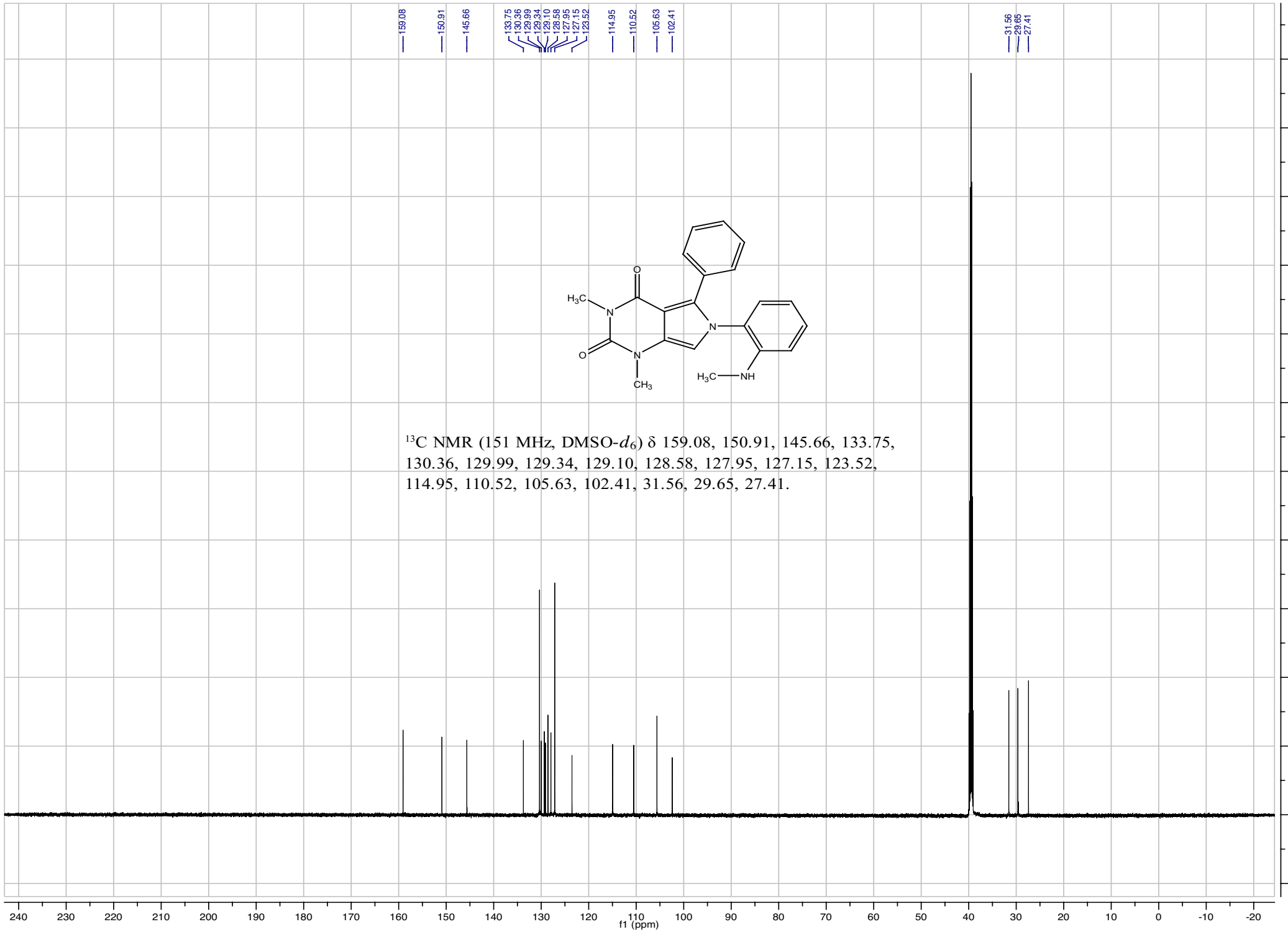
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.25, 154.07, 151.80, 147.00, 131.92, 131.57, 130.23, 129.99, 129.64, 129.02, 128.75, 128.59, 127.65, 127.09, 126.22, 125.56, 121.70, 120.79, 111.19, 106.94, 106.39, 106.02, 43.31, 32.13, 27.97, 13.68.



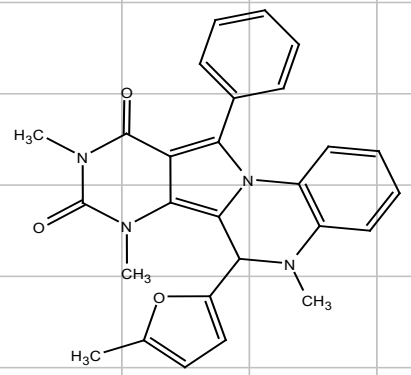
^{1}H NMR (600 MHz, DMSO-d_6) δ 7.30 – 7.26 (m, 2H), 7.24 – 7.16 (m, 4H), 6.93 (d, J = 1.0, 1H), 6.86 (d, J = 7.7, 1H), 6.62 (d, J = 8.3, 1H), 6.49 (t, J = 7.5, 1H), 5.07 (d, J = 4.8, 1H), 3.33 (s, 3H), 3.20 (s, 3H), 2.64 (d, J = 4.9, 3H).



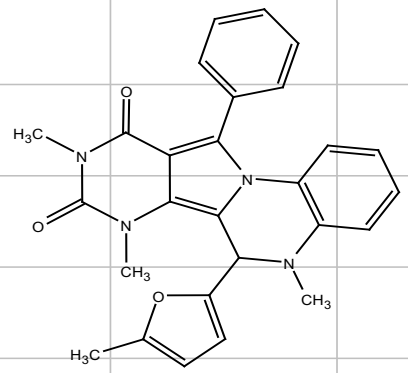
^{1}H NMR (600 MHz, DMSO-d_6) δ 7.30 – 7.26 (m, 2H), 7.24 – 7.16 (m, 4H), 6.93 (d, J = 1.0, 1H), 6.86 (d, J = 7.7, 1H), 6.62 (d, J = 8.3, 1H), 6.49 (t, J = 7.5, 1H), 5.07 (d, J = 4.8, 1H), 3.33 (s, 3H), 3.20 (s, 3H), 2.64 (d, J = 4.9, 3H).



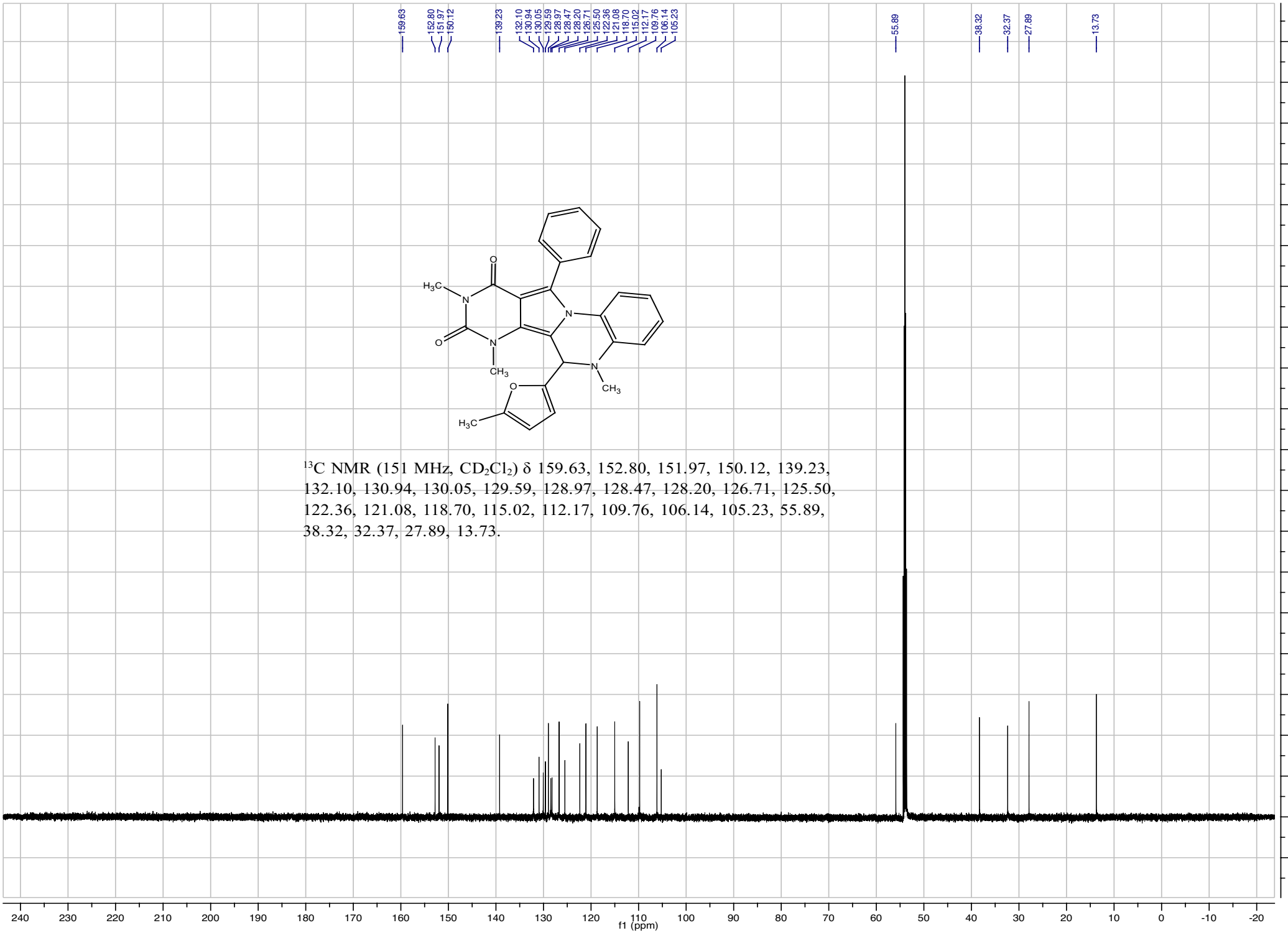
^{13}C NMR (151 MHz, DMSO-d_6) δ 159.08, 150.91, 145.66, 133.75, 130.36, 129.99, 129.34, 129.10, 128.58, 127.95, 127.15, 123.52, 114.95, 110.52, 105.63, 102.41, 31.56, 29.65, 27.41.



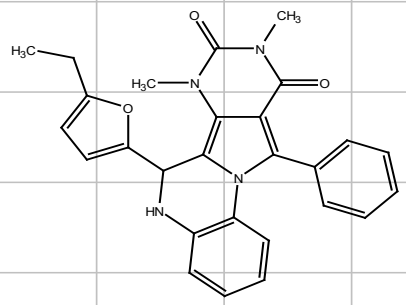
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.83 (d, *J* = 7.5, 1H), 7.56 (t, *J* = 7.5, 1H), 7.44 (t, *J* = 7.5, 1H), 7.27 (t, *J* = 7.4, 1H), 7.07 – 7.01 (m, 1H), 6.96 (d, *J* = 7.5, 1H), 6.76 (d, *J* = 7.3, 1H), 6.60 – 6.53 (m, 1H), 6.51 – 6.44 (m, 1H), 5.82 (s, 1H), 5.72 (d, *J* = 2.2, 1H), 5.58 (d, *J* = 3.1, 1H), 3.55 (s, 3H), 3.25 (s, 3H), 3.10 (s, 3H), 2.16 (s, 3H).



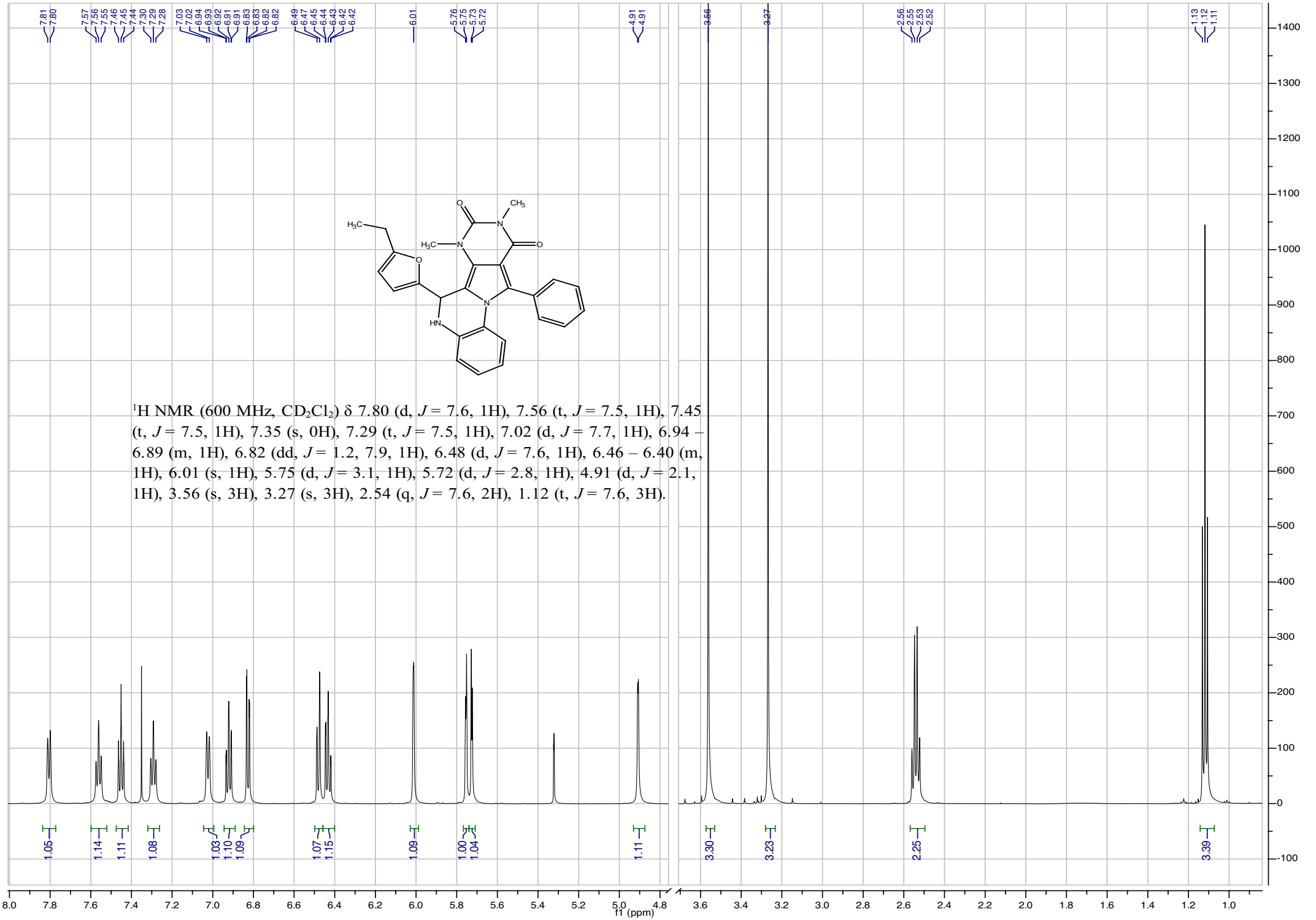
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.83 (d, *J* = 7.5, 1H), 7.56 (t, *J* = 7.5, 1H), 7.44 (t, *J* = 7.5, 1H), 7.27 (t, *J* = 7.4, 1H), 7.07 – 7.01 (m, 1H), 6.96 (d, *J* = 7.5, 1H), 6.76 (d, *J* = 7.3, 1H), 6.60 – 6.53 (m, 1H), 6.51 – 6.44 (m, 1H), 5.82 (s, 1H), 5.72 (d, *J* = 2.2, 1H), 5.58 (d, *J* = 3.1, 1H), 3.55 (s, 3H), 3.25 (s, 3H), 3.10 (s, 3H), 2.16 (s, 3H).



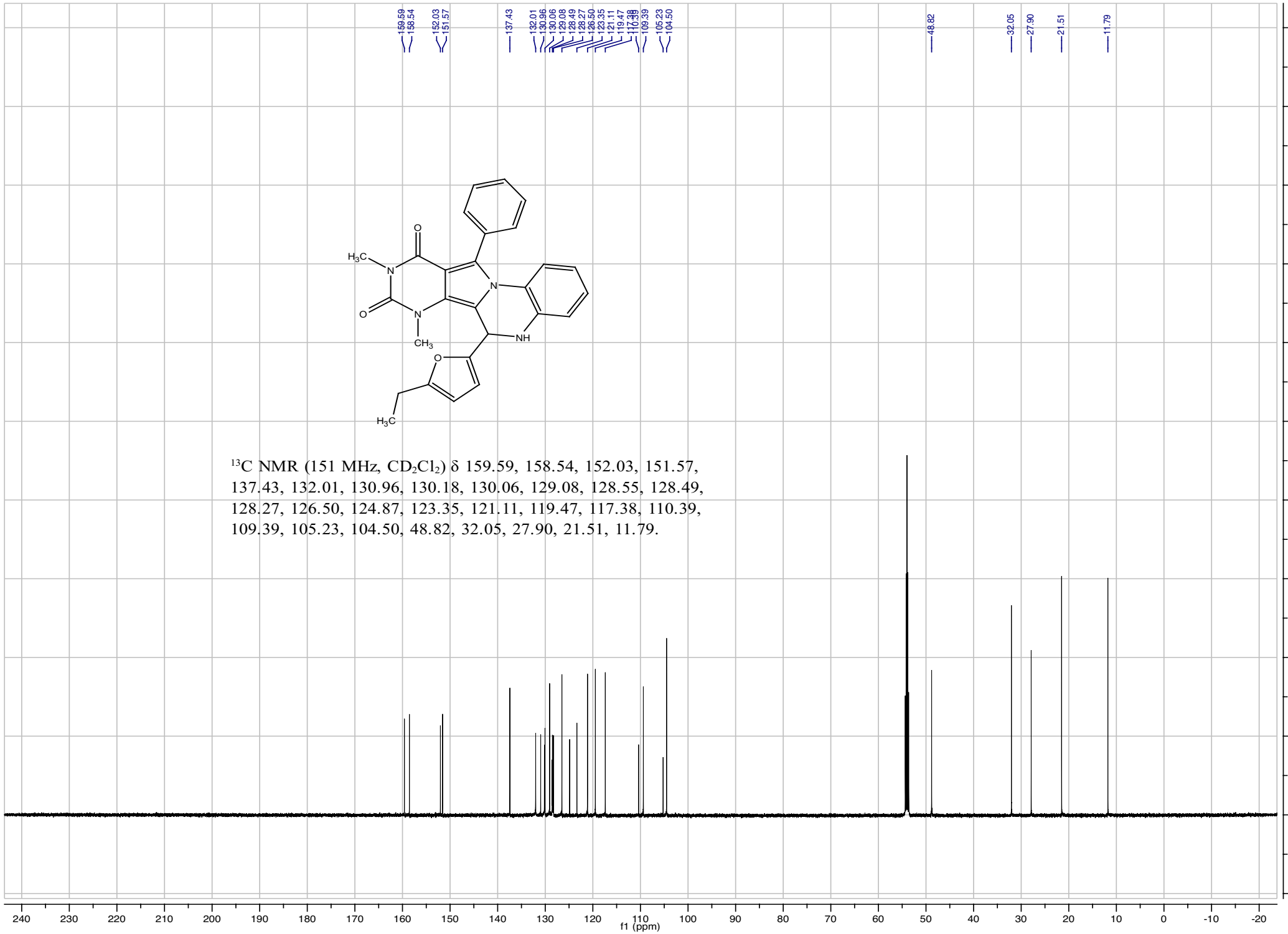
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.63, 152.80, 151.97, 150.12, 139.23, 132.10, 130.94, 130.05, 129.59, 128.97, 128.47, 128.20, 126.71, 125.50, 122.36, 121.08, 118.70, 115.02, 112.17, 109.76, 106.14, 105.23, 55.89, 38.32, 32.37, 27.89, 13.73.



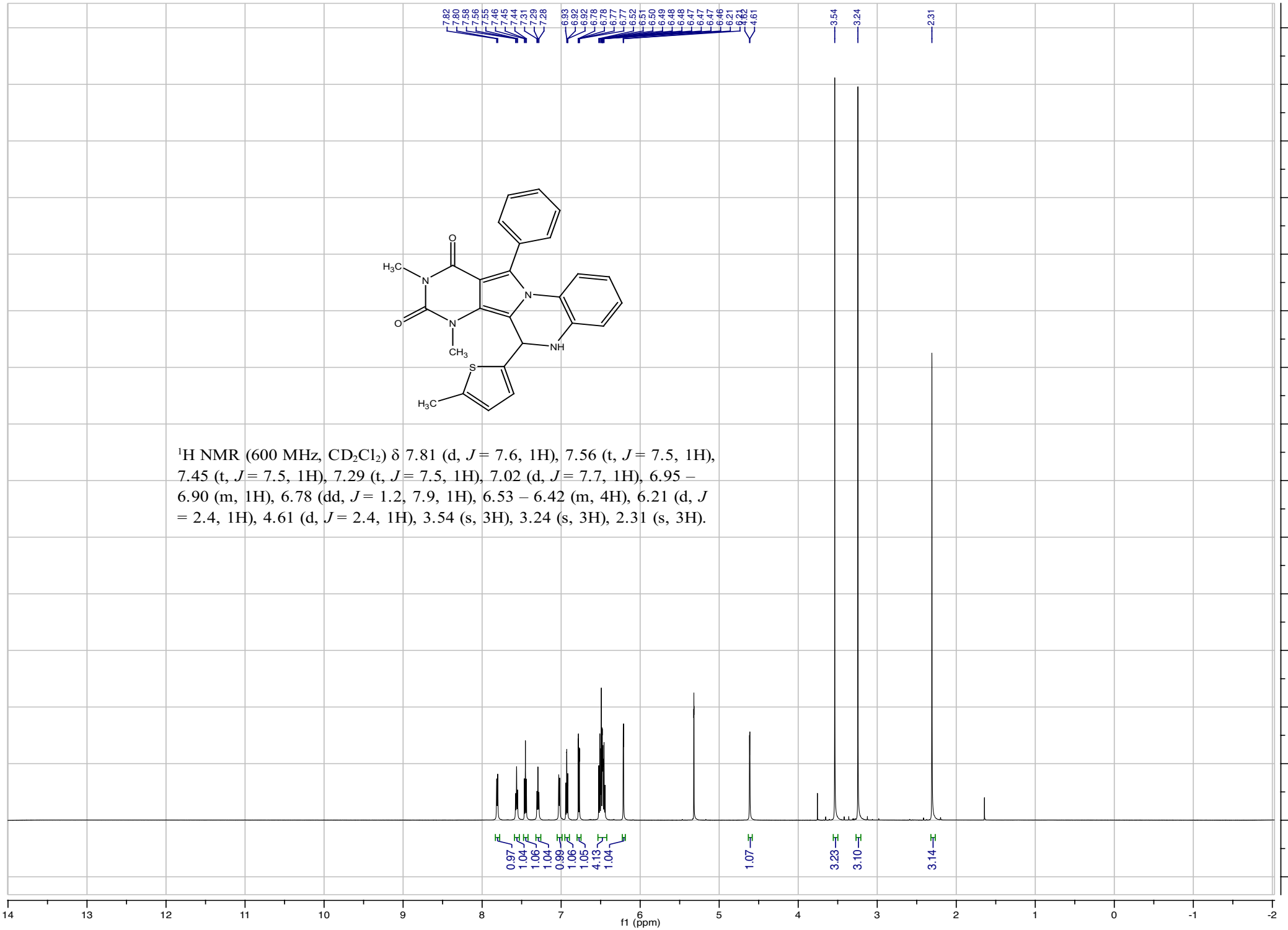
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, J = 7.6, 1H), 7.56 (t, J = 7.5, 1H), 7.45 (t, J = 7.5, 1H), 7.35 (s, 0H), 7.29 (t, J = 7.5, 1H), 7.02 (d, J = 7.7, 1H), 6.94 – 6.89 (m, 1H), 6.82 (dd, J = 1.2, 7.9, 1H), 6.48 (d, J = 7.6, 1H), 6.46 – 6.40 (m, 1H), 6.01 (s, 1H), 5.75 (d, J = 3.1, 1H), 5.72 (d, J = 2.8, 1H), 4.91 (d, J = 2.1, 1H), 3.56 (s, 3H), 3.27 (s, 3H), 2.54 (q, J = 7.6, 2H), 1.12 (t, J = 7.6, 3H).



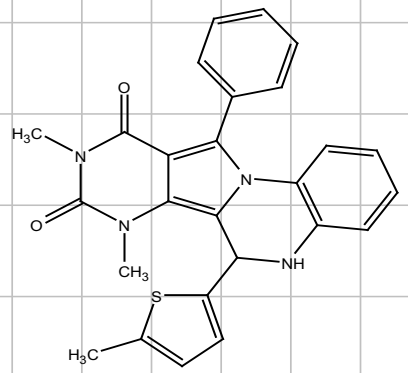
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, J = 7.6, 1H), 7.56 (t, J = 7.5, 1H), 7.45 (t, J = 7.5, 1H), 7.35 (s, 0H), 7.29 (t, J = 7.5, 1H), 7.02 (d, J = 7.7, 1H), 6.94 – 6.89 (m, 1H), 6.82 (dd, J = 1.2, 7.9, 1H), 6.48 (d, J = 7.6, 1H), 6.46 – 6.40 (m, 1H), 6.01 (s, 1H), 5.75 (d, J = 3.1, 1H), 5.72 (d, J = 2.8, 1H), 4.91 (d, J = 2.1, 1H), 3.56 (s, 3H), 3.27 (s, 3H), 2.54 (q, J = 7.6, 2H), 1.12 (t, J = 7.6, 3H).



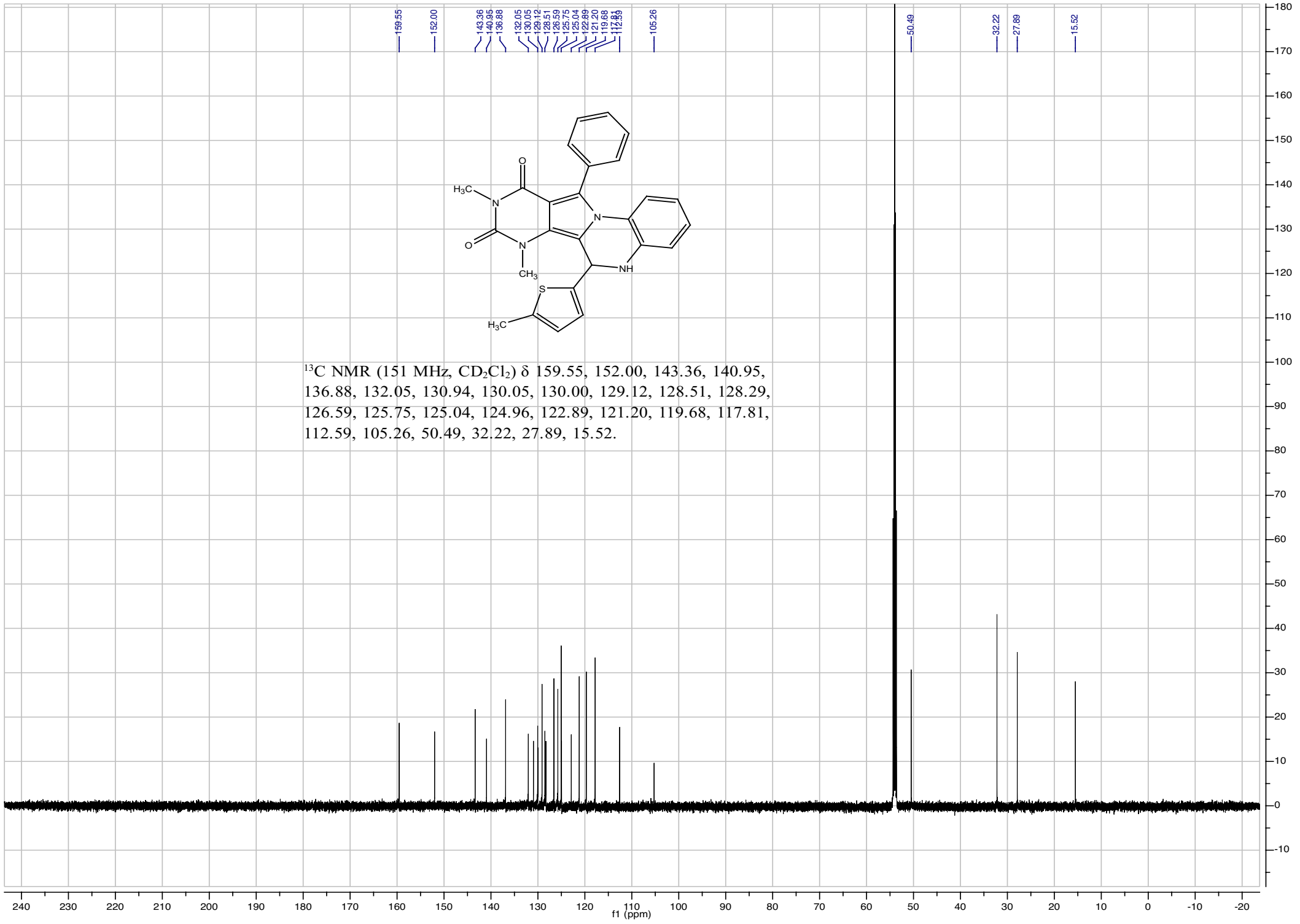
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.59, 158.54, 152.03, 151.57, 137.43, 132.01, 130.96, 130.18, 130.06, 129.08, 128.55, 128.49, 128.27, 126.50, 124.87, 123.35, 121.11, 119.47, 117.38, 110.39, 109.39, 105.23, 104.50, 48.82, 32.05, 27.90, 21.51, 11.79.



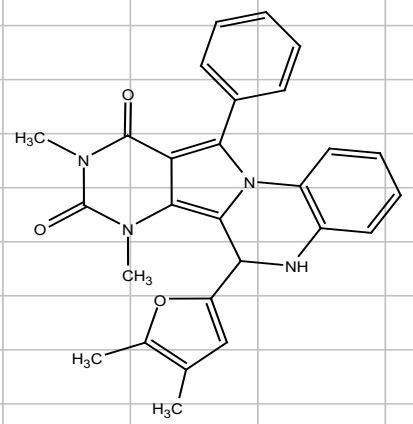
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, J = 7.6, 1H), 7.56 (t, J = 7.5, 1H), 7.45 (t, J = 7.5, 1H), 7.29 (t, J = 7.5, 1H), 7.02 (d, J = 7.7, 1H), 6.95 – 6.90 (m, 1H), 6.78 (dd, J = 1.2, 7.9, 1H), 6.53 – 6.42 (m, 4H), 6.21 (d, J = 2.4, 1H), 4.61 (d, J = 2.4, 1H), 3.54 (s, 3H), 3.24 (s, 3H), 2.31 (s, 3H).



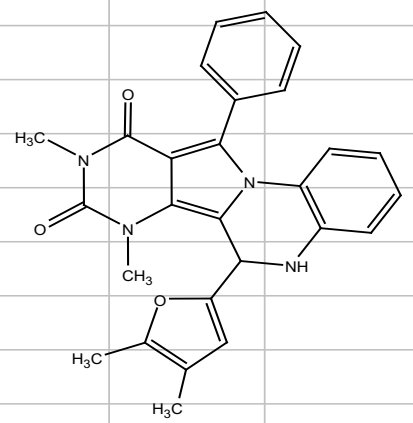
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.95 – 6.90 (m, 1H), 6.78 (dd, *J* = 1.2, 7.9, 1H), 6.53 – 6.42 (m, 4H), 6.21 (d, *J* = 2.4, 1H), 4.61 (d, *J* = 2.4, 1H), 3.54 (s, 3H), 3.24 (s, 3H), 2.31 (s, 3H).



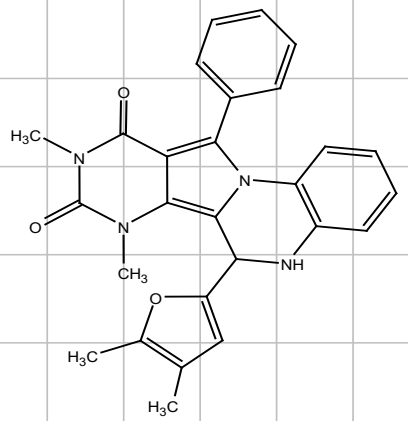
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.55, 152.00, 143.36, 140.95, 136.88, 132.05, 130.94, 130.05, 130.00, 129.12, 128.51, 128.29, 126.59, 125.75, 125.04, 124.96, 122.89, 121.20, 119.68, 117.81, 112.59, 105.26, 50.49, 32.22, 27.89, 15.52.



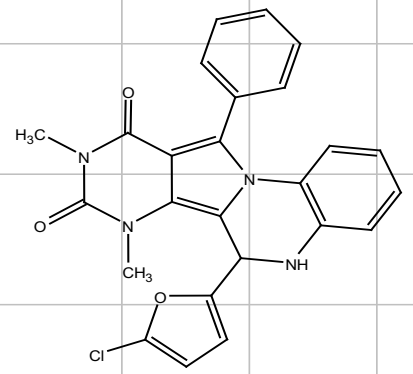
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.92 (td, *J* = 1.3, 7.8, 1H), 6.83 (dd, *J* = 1.2, 7.9, 1H), 6.48 (d, *J* = 8.0, 1H), 6.45 – 6.39 (m, 1H), 5.97 (s, 1H), 5.61 (s, 1H), 4.91 (d, *J* = 2.1, 1H), 3.54 (s, 3H), 3.27 (s, 3H), 2.10 (s, 3H), 1.72 (s, 3H).



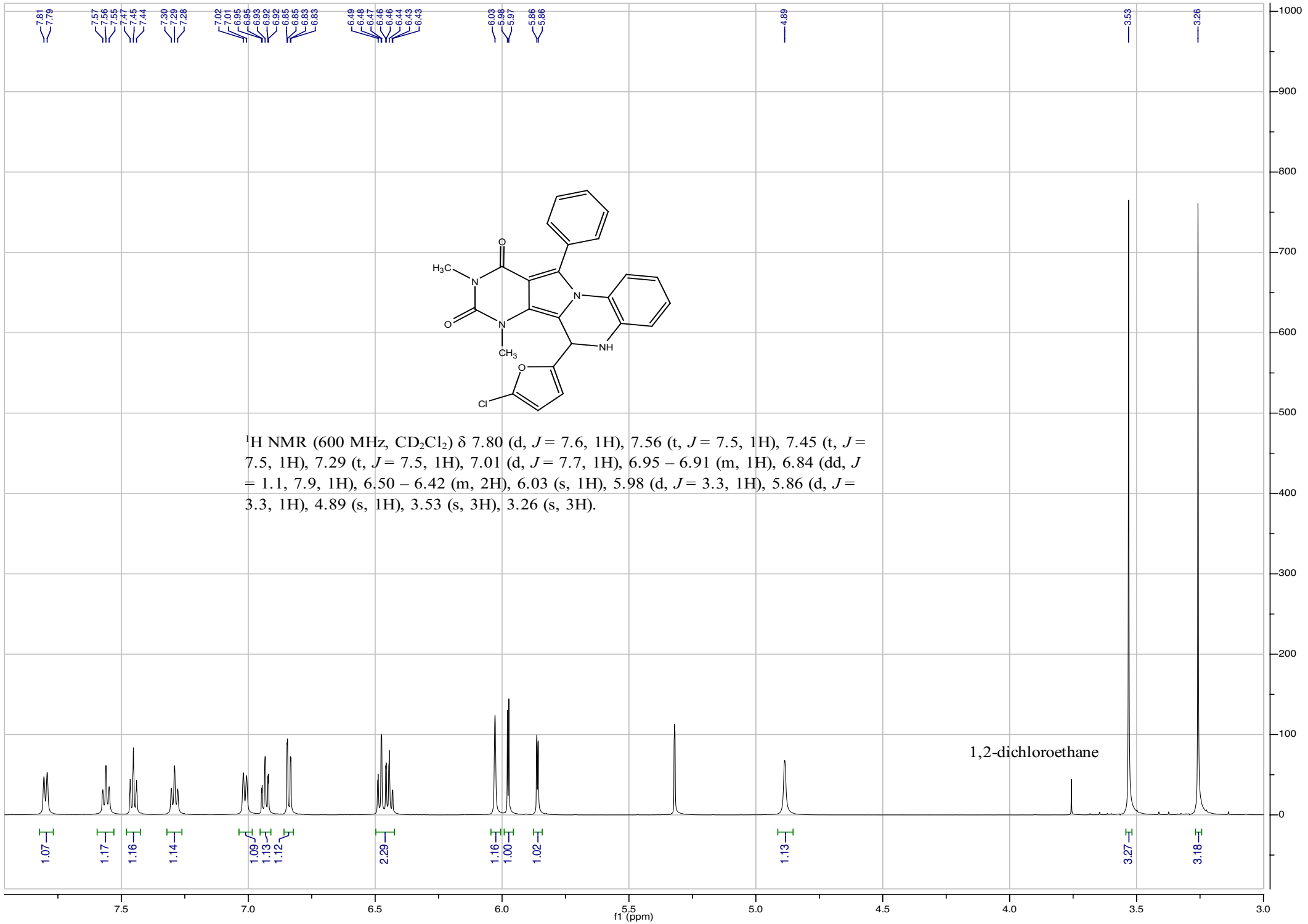
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.92 (td, *J* = 1.3, 7.8, 1H), 6.83 (dd, *J* = 1.2, 7.9, 1H), 6.48 (d, *J* = 8.0, 1H), 6.45 – 6.39 (m, 1H), 5.97 (s, 1H), 5.61 (s, 1H), 4.91 (d, *J* = 2.1, 1H), 3.54 (s, 3H), 3.27 (s, 3H), 2.10 (s, 3H), 1.72 (s, 3H).



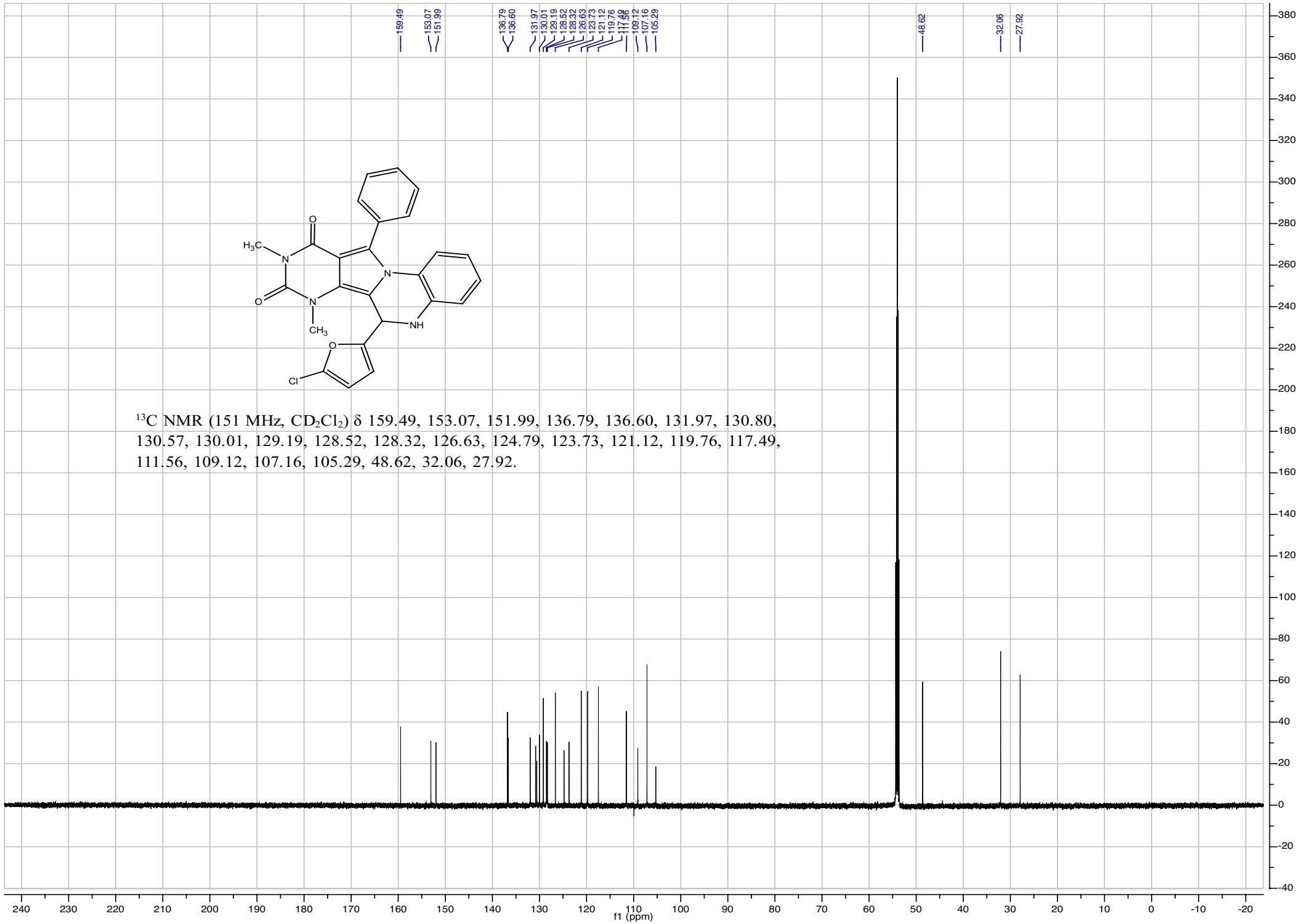
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.58, 152.03, 150.33, 148.13, 137.37, 131.99, 131.02, 130.10, 130.05, 129.07, 128.49, 128.28, 126.46, 124.78, 123.27, 121.07, 119.37, 117.37, 114.69, 112.22, 110.37, 105.25, 48.72, 31.97, 27.90, 11.48, 9.80.



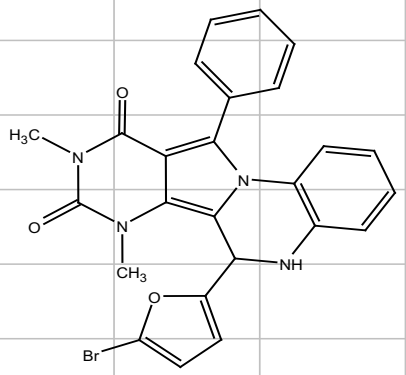
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.01 (d, *J* = 7.7, 1H), 6.95 – 6.91 (m, 1H), 6.84 (dd, *J* = 1.1, 7.9, 1H), 6.50 – 6.42 (m, 2H), 6.03 (s, 1H), 5.98 (d, *J* = 3.3, 1H), 5.86 (d, *J* = 3.3, 1H), 4.89 (s, 1H), 3.53 (s, 3H), 3.26 (s, 3H).



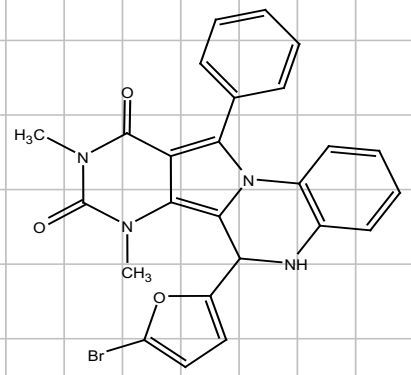
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.01 (d, *J* = 7.7, 1H), 6.95 – 6.91 (m, 1H), 6.84 (dd, *J* = 1.1, 7.9, 1H), 6.50 – 6.42 (m, 2H), 6.03 (s, 1H), 5.98 (d, *J* = 3.3, 1H), 5.86 (d, *J* = 3.3, 1H), 4.89 (s, 1H), 3.53 (s, 3H), 3.26 (s, 3H).



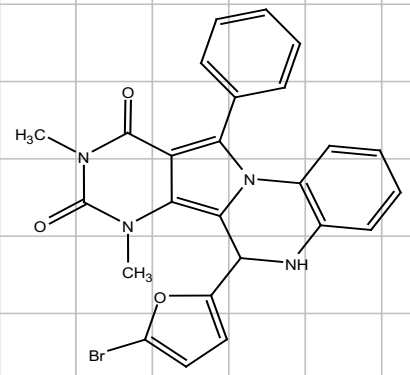
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.49, 153.07, 151.99, 136.79, 136.60, 131.97, 130.80, 130.57, 130.01, 129.19, 128.52, 128.32, 126.63, 124.79, 123.73, 121.12, 119.76, 117.49, 111.56, 109.12, 107.16, 105.29, 48.62, 32.06, 27.92.



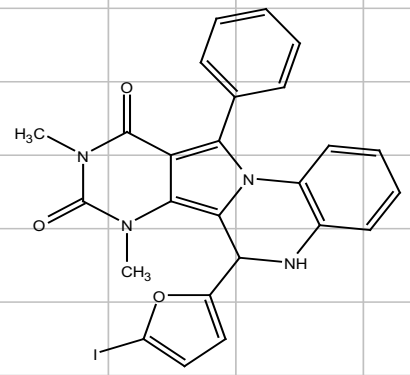
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.96 – 6.90 (m, 1H), 6.84 (dd, *J* = 1.1, 7.9, 1H), 6.48 (d, *J* = 7.7, 1H), 6.47 – 6.41 (m, 1H), 6.12 (d, *J* = 3.3, 1H), 6.04 (d, *J* = 1.7, 1H), 5.85 (dd, *J* = 0.8, 3.3, 1H), 4.95 (d, *J* = 2.3, 1H), 3.53 (s, 3H), 3.27 (s, 3H).



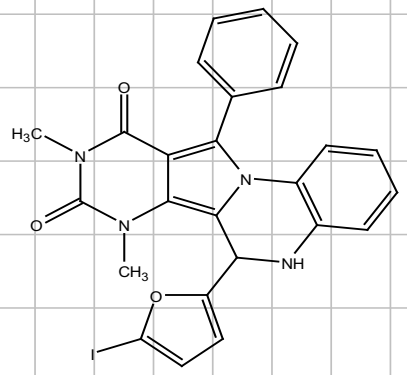
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.6, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.96 – 6.90 (m, 1H), 6.84 (dd, *J* = 1.1, 7.9, 1H), 6.48 (d, *J* = 7.7, 1H), 6.47 – 6.41 (m, 1H), 6.12 (d, *J* = 3.3, 1H), 6.04 (d, *J* = 1.7, 1H), 5.85 (dd, *J* = 0.8, 3.3, 1H), 4.95 (d, *J* = 2.3, 1H), 3.53 (s, 3H), 3.27 (s, 3H).



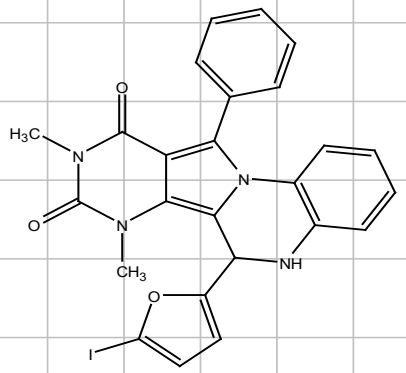
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.49, 155.46, 151.98, 136.82, 131.97, 130.80, 130.56, 130.01, 129.18, 128.52, 128.31, 126.63, 124.76, 123.70, 122.37, 121.12, 119.72, 117.48, 112.20, 111.90, 109.18, 105.28, 48.62, 32.08, 27.93.



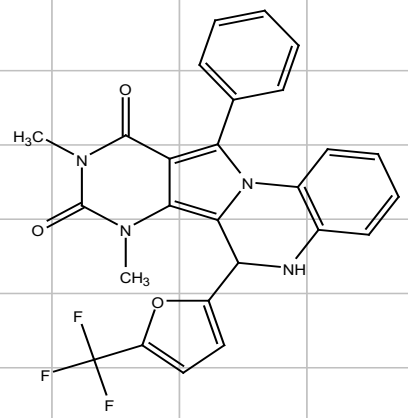
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, J = 7.7, 1H), 7.56 (t, J = 7.5, 1H), 7.45 (t, J = 7.5, 1H), 7.29 (t, J = 7.5, 1H), 7.02 (d, J = 7.7, 1H), 6.93 (td, J = 1.4, 7.9, 1H), 6.83 (dd, J = 1.2, 7.9, 1H), 6.48 (d, J = 7.3, 1H), 6.46 – 6.41 (m, 1H), 6.34 (d, J = 3.3, 1H), 6.09 (d, J = 2.0, 1H), 5.78 (d, J = 3.3, 1H), 4.95 (d, J = 2.4, 1H), 3.53 (s, 3H), 3.26 (s, 3H).



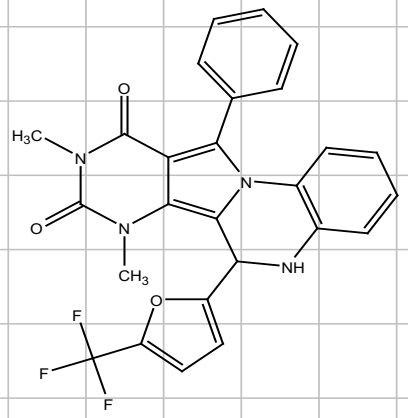
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.7, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.5, 1H), 7.02 (d, *J* = 7.7, 1H), 6.93 (td, *J* = 1.4, 7.9, 1H), 6.83 (dd, *J* = 1.2, 7.9, 1H), 6.48 (d, *J* = 7.3, 1H), 6.46 – 6.41 (m, 1H), 6.34 (d, *J* = 3.3, 1H), 6.09 (d, *J* = 2.0, 1H), 5.78 (d, *J* = 3.3, 1H), 4.95 (d, *J* = 2.4, 1H), 3.53 (s, 3H), 3.26 (s, 3H).



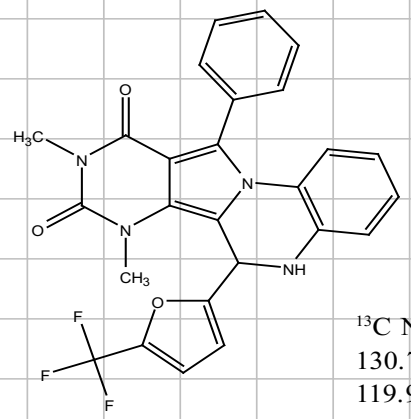
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.50, 158.97, 151.98, 136.86, 131.97, 130.80, 130.52, 130.01, 129.17, 128.51, 128.30, 126.62, 124.75, 123.64, 121.12, 120.97, 119.70, 117.47, 112.15, 109.34, 105.28, 88.96, 48.57, 32.10, 27.93.



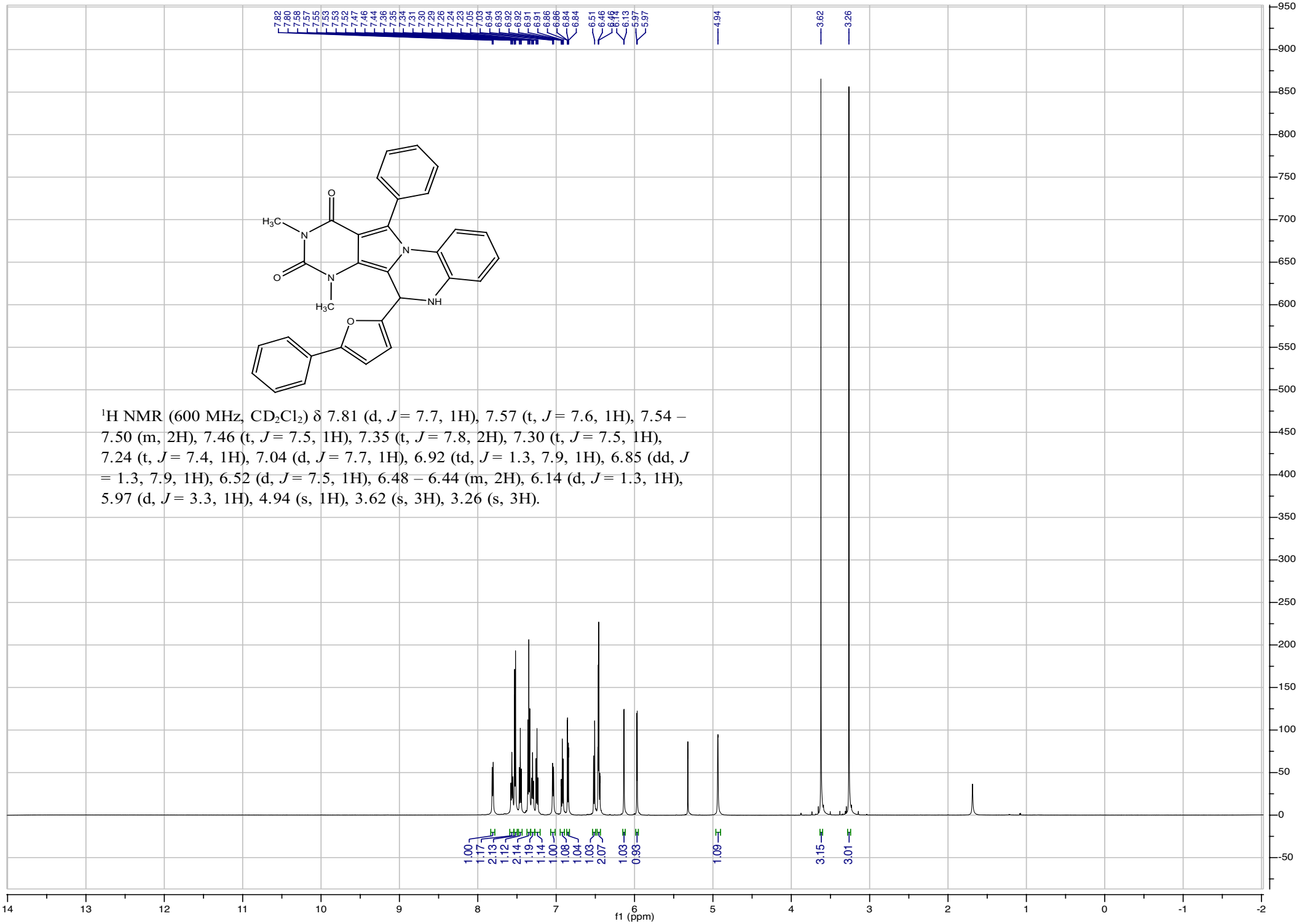
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, *J* = 7.7, 1H), 7.56 (t, *J* = 7.4, 1H), 7.46 (tt, *J* = 1.2, 7.5, 1H), 7.30 (t, *J* = 7.4, 1H), 7.02 (d, *J* = 7.7, 1H), 6.93 (ddd, *J* = 1.6, 7.1, 8.0, 1H), 6.85 (dd, *J* = 1.2, 7.9, 1H), 6.61 (dd, *J* = 1.0, 3.4, 1H), 6.51 – 6.42 (m, *J* = 4.1, 7.1, 8.3, 2H), 6.10 (s, 1H), 5.95 (d, *J* = 3.5, 1H), 4.96 (d, *J* = 2.5, 1H), 3.55 (s, 3H), 3.26 (s, 3H).



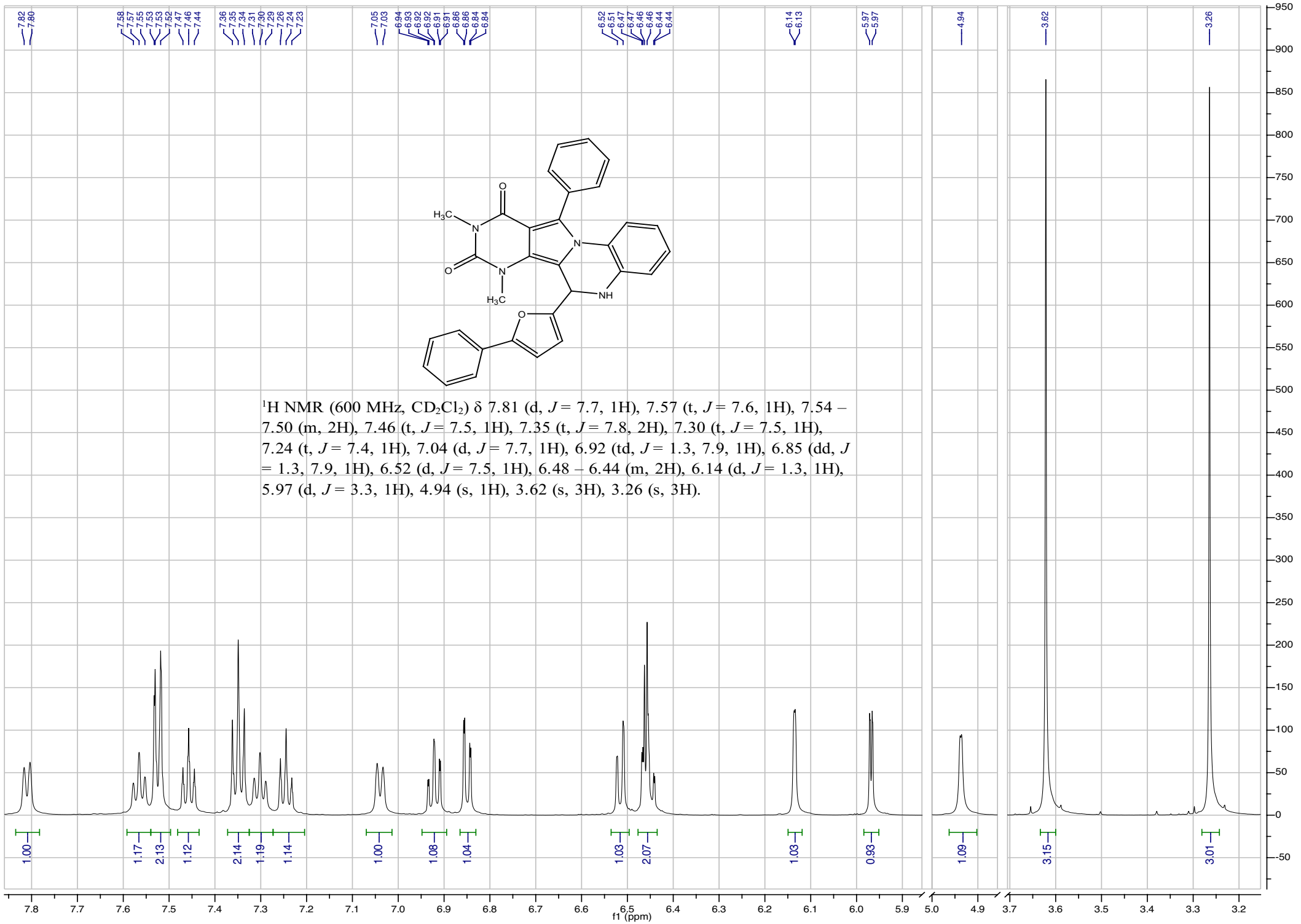
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, J = 7.7, 1H), 7.56 (t, J = 7.4, 1H), 7.46 (tt, J = 1.2, 7.5, 1H), 7.30 (t, J = 7.4, 1H), 7.02 (d, J = 7.7, 1H), 6.93 (ddd, J = 1.6, 7.1, 8.0, 1H), 6.85 (dd, J = 1.2, 7.9, 1H), 6.61 (dd, J = 1.0, 3.4, 1H), 6.51 – 6.42 (m, J = 4.1, 7.1, 8.3, 2H), 6.10 (s, 1H), 5.95 (d, J = 3.5, 1H), 4.96 (d, J = 2.5, 1H), 3.55 (s, 3H), 3.26 (s, 3H).



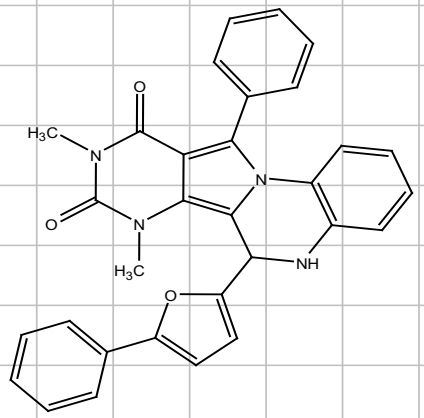
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.47, 156.71, 151.99, 141.85, 141.57, 141.29, 141.01, 136.75, 131.97, 130.76, 130.72, 129.99, 129.24, 128.55, 128.34, 126.74, 124.80, 123.79, 121.71, 121.18, 119.94, 119.91, 118.17, 117.43, 112.80, 112.78, 110.02, 109.09, 105.31, 48.56, 32.14, 27.94.



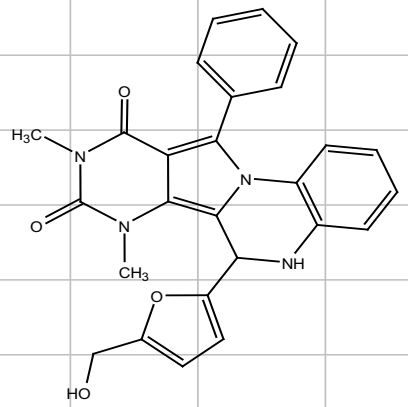
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, J = 7.7, 1H), 7.57 (t, J = 7.6, 1H), 7.54 – 7.50 (m, 2H), 7.46 (t, J = 7.5, 1H), 7.35 (t, J = 7.8, 2H), 7.30 (t, J = 7.5, 1H), 7.24 (t, J = 7.4, 1H), 7.04 (d, J = 7.7, 1H), 6.92 (td, J = 1.3, 7.9, 1H), 6.85 (dd, J = 1.3, 7.9, 1H), 6.52 (d, J = 7.5, 1H), 6.48 – 6.44 (m, 2H), 6.14 (d, J = 1.3, 1H), 5.97 (d, J = 3.3, 1H), 4.94 (s, 1H), 3.62 (s, 3H), 3.26 (s, 3H).



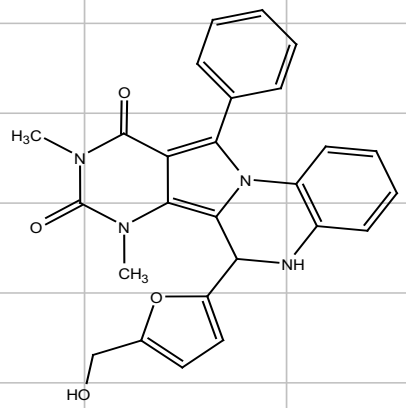
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.57 (t, *J* = 7.6, 1H), 7.54 – 7.50 (m, 2H), 7.46 (t, *J* = 7.5, 1H), 7.35 (t, *J* = 7.8, 2H), 7.30 (t, *J* = 7.5, 1H), 7.24 (t, *J* = 7.4, 1H), 7.04 (d, *J* = 7.7, 1H), 6.92 (td, *J* = 1.3, 7.9, 1H), 6.85 (dd, *J* = 1.3, 7.9, 1H), 6.52 (d, *J* = 7.5, 1H), 6.48 – 6.44 (m, 2H), 6.14 (d, *J* = 1.3, 1H), 5.97 (d, *J* = 3.3, 1H), 4.94 (s, 1H), 3.62 (s, 3H), 3.26 (s, 3H).



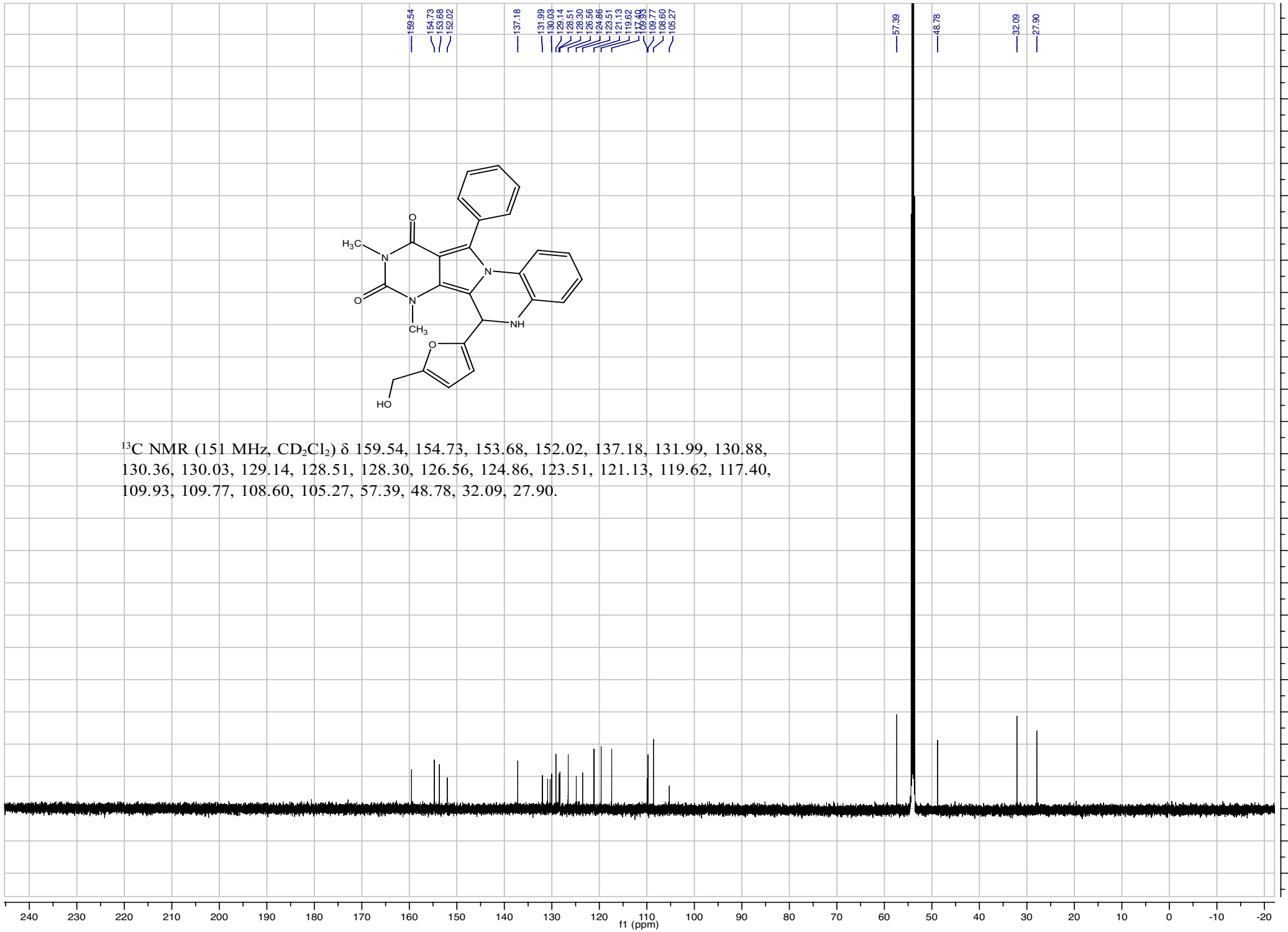
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.55, 154.06, 153.27, 152.02, 137.34, 132.03, 130.90, 130.35, 130.27, 130.04, 129.13, 128.95, 128.51, 128.29, 127.88, 126.58, 124.92, 123.65, 123.48, 121.20, 119.63, 117.44, 110.72, 110.15, 105.71, 105.29, 48.85, 32.22, 27.91.



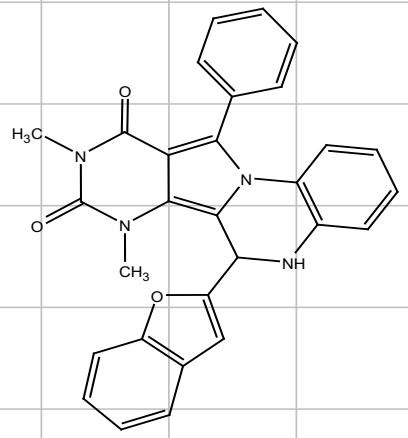
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d, *J* = 7.5, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.4, 1H), 7.01 (d, *J* = 7.6, 1H), 6.93 – 6.90 (m, 1H), 6.83 (dd, *J* = 1.3, 7.9, 1H), 6.47 (dd, *J* = 1.2, 8.3, 1H), 6.45 – 6.40 (m, 1H), 6.07 – 6.03 (m, 2H), 5.79 (d, *J* = 3.1, 1H), 4.90 (s, 1H), 4.47 (s, 2H), 3.54 (s, 3H), 3.25 (s, 3H), 1.83 (s, 1H).



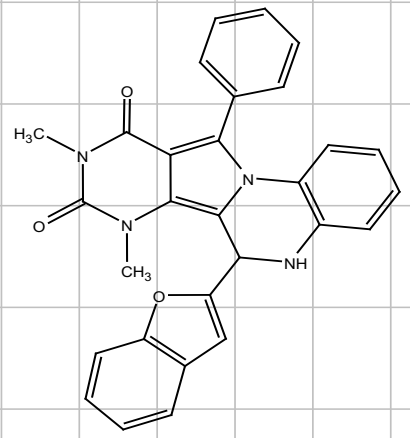
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d, *J* = 7.5, 1H), 7.56 (t, *J* = 7.5, 1H), 7.45 (t, *J* = 7.5, 1H), 7.29 (t, *J* = 7.4, 1H), 7.01 (d, *J* = 7.6, 1H), 6.93 – 6.90 (m, 1H), 6.83 (dd, *J* = 1.3, 7.9, 1H), 6.47 (dd, *J* = 1.2, 8.3, 1H), 6.45 – 6.40 (m, 1H), 6.07 – 6.03 (m, 2H), 5.79 (d, *J* = 3.1, 1H), 4.90 (s, 1H), 4.47 (s, 2H), 3.54 (s, 3H), 3.25 (s, 3H), 1.83 (s, 1H).



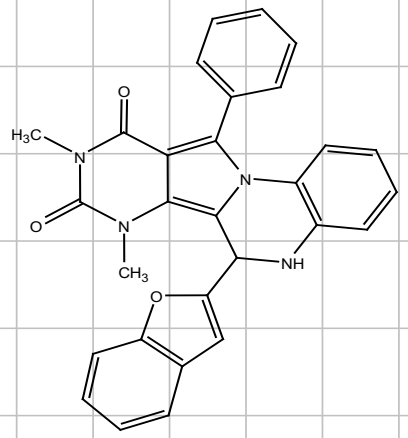
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.54, 154.73, 153.68, 152.02, 137.18, 131.99, 130.88, 130.36, 130.03, 129.14, 128.51, 128.30, 126.56, 124.86, 123.51, 121.13, 119.62, 117.40, 109.93, 109.77, 108.60, 105.27, 57.39, 48.78, 32.09, 27.90.



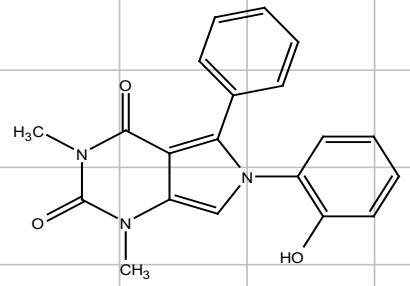
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.82 (d, *J* = 7.6, 1H), 7.57 (t, *J* = 7.6, 1H), 7.46 (t, *J* = 7.5, 1H), 7.41 (d, *J* = 8.3, 1H), 7.38 (d, *J* = 7.6, 1H), 7.30 (t, *J* = 7.5, 1H), 7.23 (t, *J* = 7.4, 1H), 7.13 (t, *J* = 7.4, 1H), 7.04 (d, *J* = 7.7, 1H), 6.89 (t, *J* = 7.5, 1H), 6.85 (d, *J* = 6.7, 1H), 6.49 (d, *J* = 8.2, 1H), 6.42 (t, *J* = 7.1, 1H), 6.27 (s, 1H), 6.20 (s, 1H), 5.03 (s, 1H), 3.58 (s, 3H), 3.27 (s, 3H).



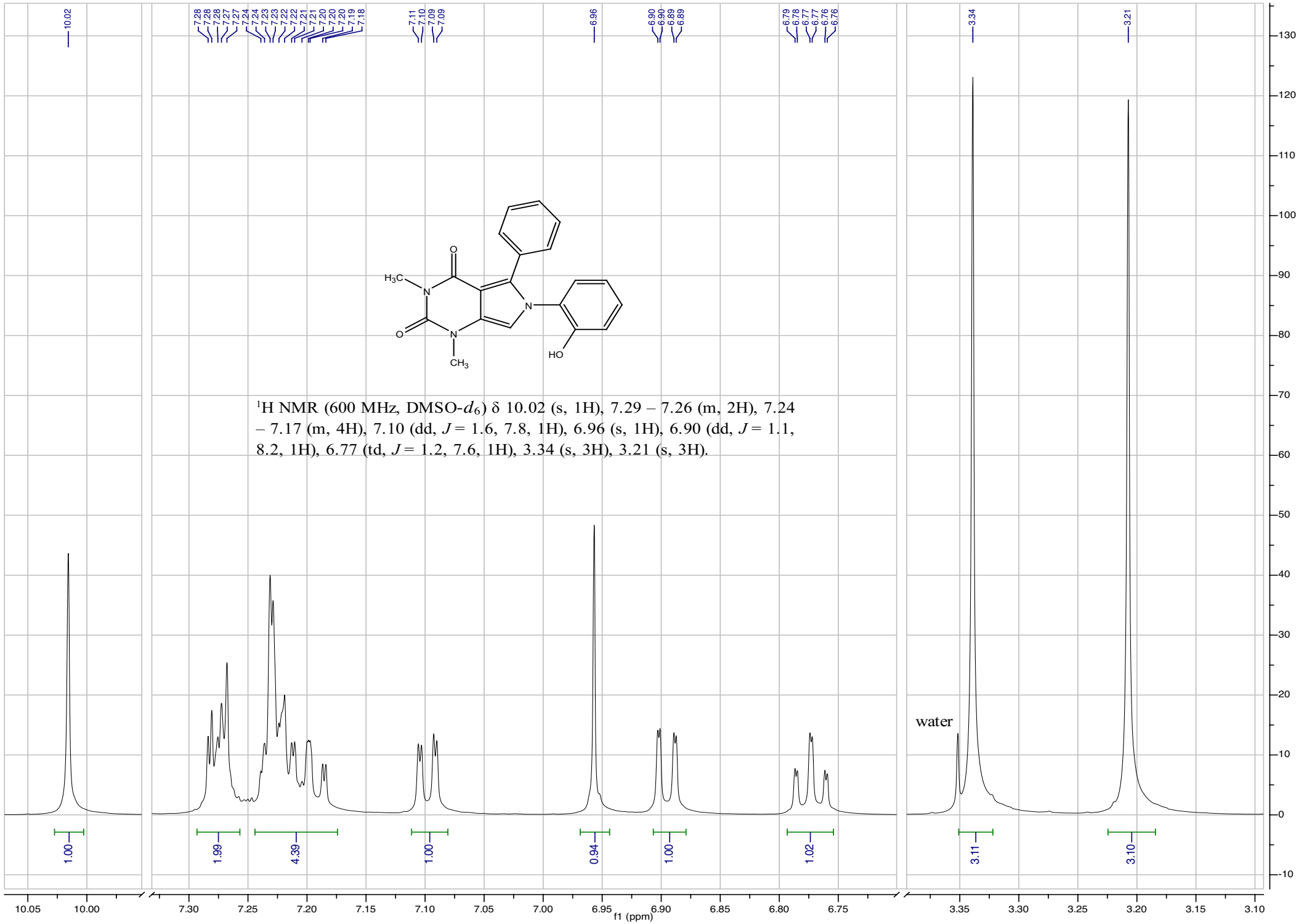
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.82 (d, J = 7.6, 1H), 7.57 (t, J = 7.6, 1H), 7.46 (t, J = 7.5, 1H), 7.41 (d, J = 8.3, 1H), 7.38 (d, J = 7.6, 1H), 7.30 (t, J = 7.5, 1H), 7.23 (t, J = 7.4, 1H), 7.13 (t, J = 7.4, 1H), 7.04 (d, J = 7.7, 1H), 6.89 (t, J = 7.5, 1H), 6.85 (d, J = 6.7, 1H), 6.49 (d, J = 8.2, 1H), 6.42 (t, J = 7.1, 1H), 6.27 (s, 1H), 6.20 (s, 1H), 5.03 (s, 1H), 3.58 (s, 3H), 3.27 (s, 3H).



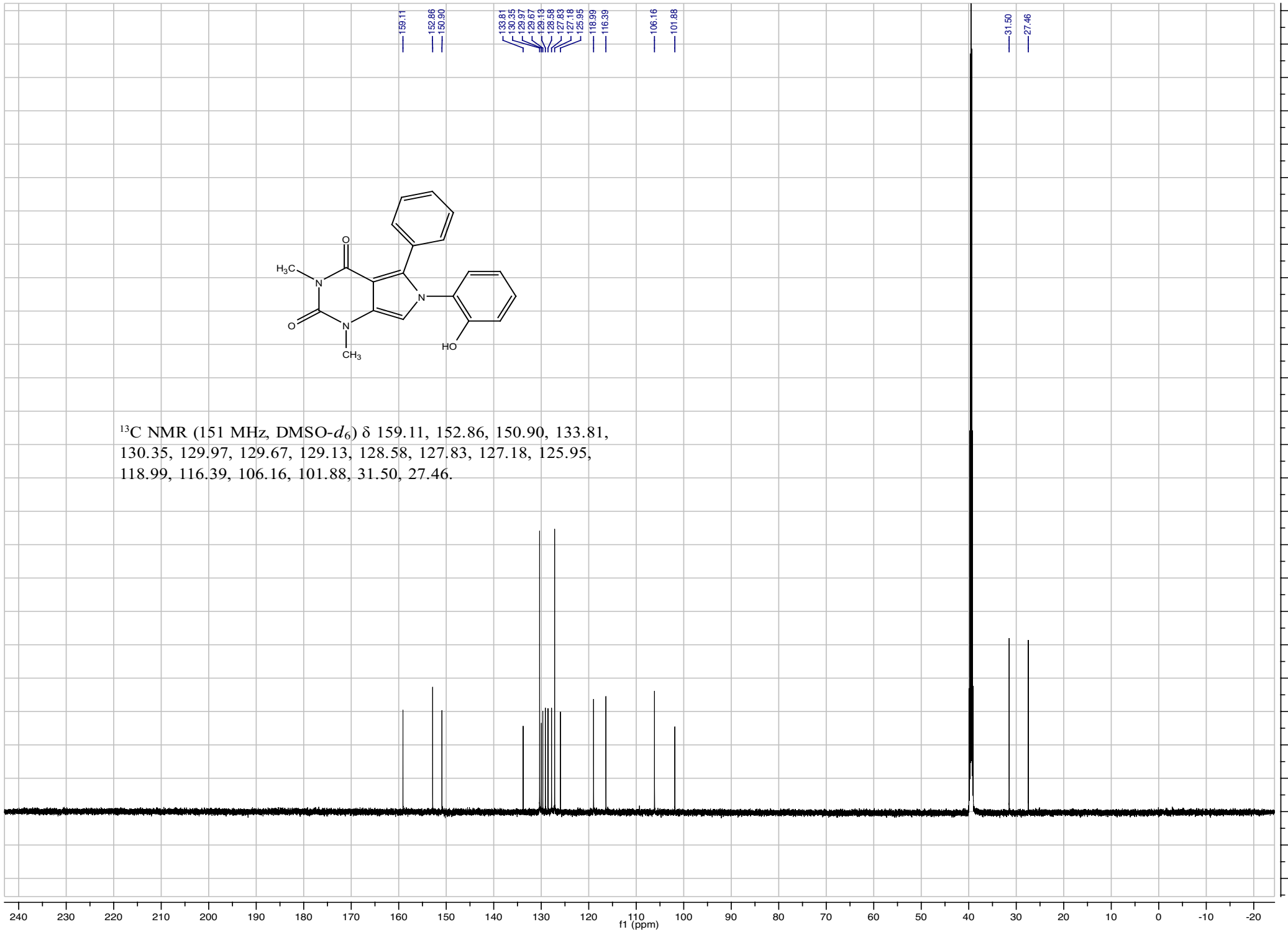
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.53, 156.19, 155.16, 152.02, 136.95, 131.99, 130.88, 130.59, 130.00, 129.19, 128.55, 128.34, 127.75, 126.62, 124.85, 124.82, 123.83, 123.25, 121.35, 121.13, 119.76, 117.42, 111.32, 109.46, 106.07, 105.35, 49.10, 32.09, 27.93.



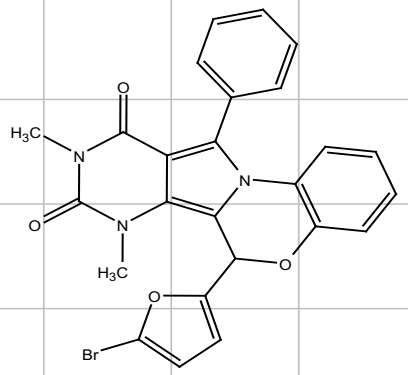
^{1}H NMR (600 MHz, DMSO-d_6) δ 10.02 (s, 1H), 7.29 – 7.26 (m, 2H), 7.24 – 7.17 (m, 4H), 7.10 (dd, J = 1.6, 7.8, 1H), 6.96 (s, 1H), 6.90 (dd, J = 1.1, 8.2, 1H), 6.77 (td, J = 1.2, 7.6, 1H), 3.34 (s, 3H), 3.21 (s, 3H).



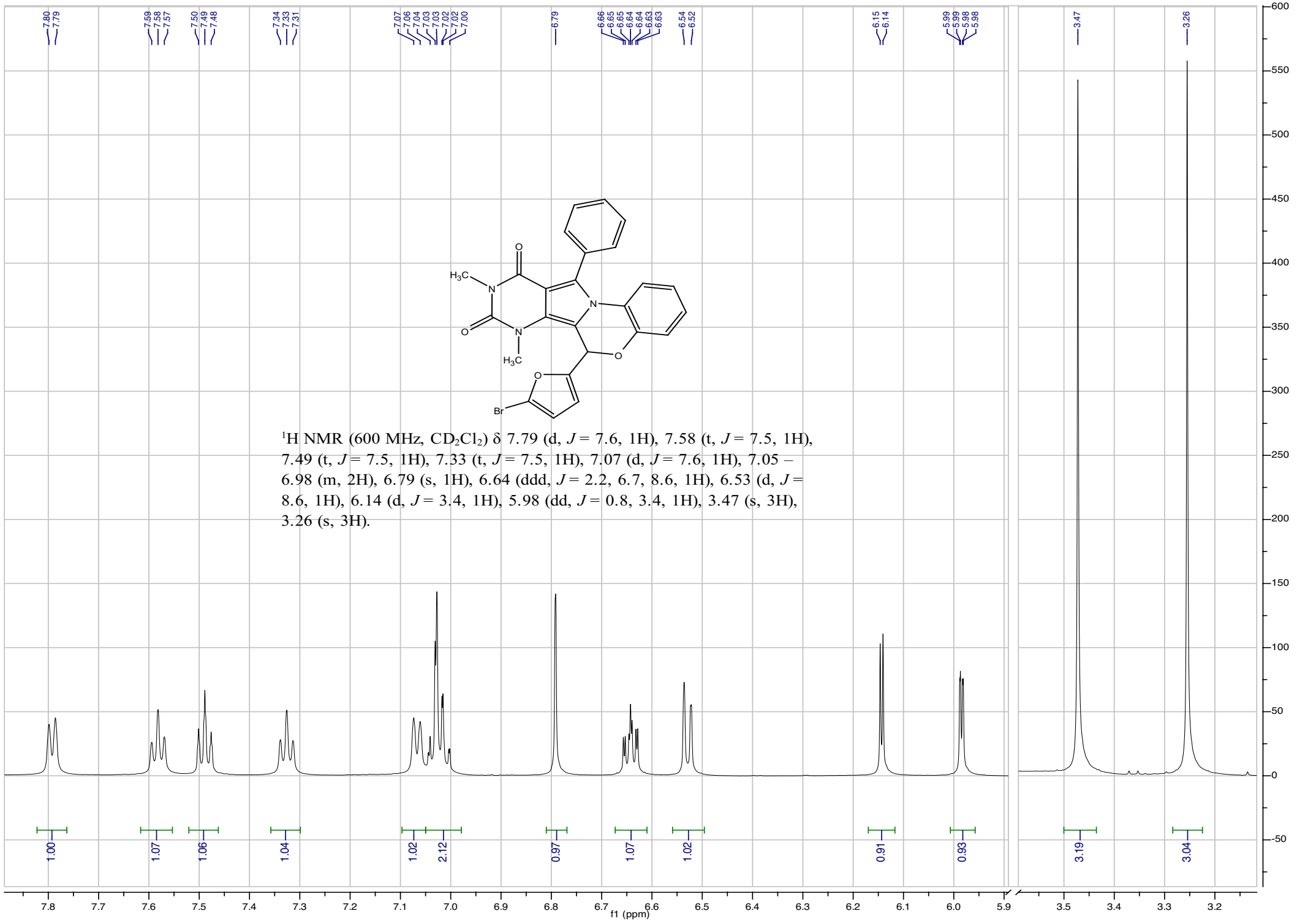
^{1}H NMR (600 MHz, DMSO-d_6) δ 10.02 (s, 1H), 7.29 – 7.26 (m, 2H), 7.24 – 7.17 (m, 4H), 7.10 (dd, J = 1.6, 7.8, 1H), 6.96 (s, 1H), 6.90 (dd, J = 1.1, 8.2, 1H), 6.77 (td, J = 1.2, 7.6, 1H), 3.34 (s, 3H), 3.21 (s, 3H).



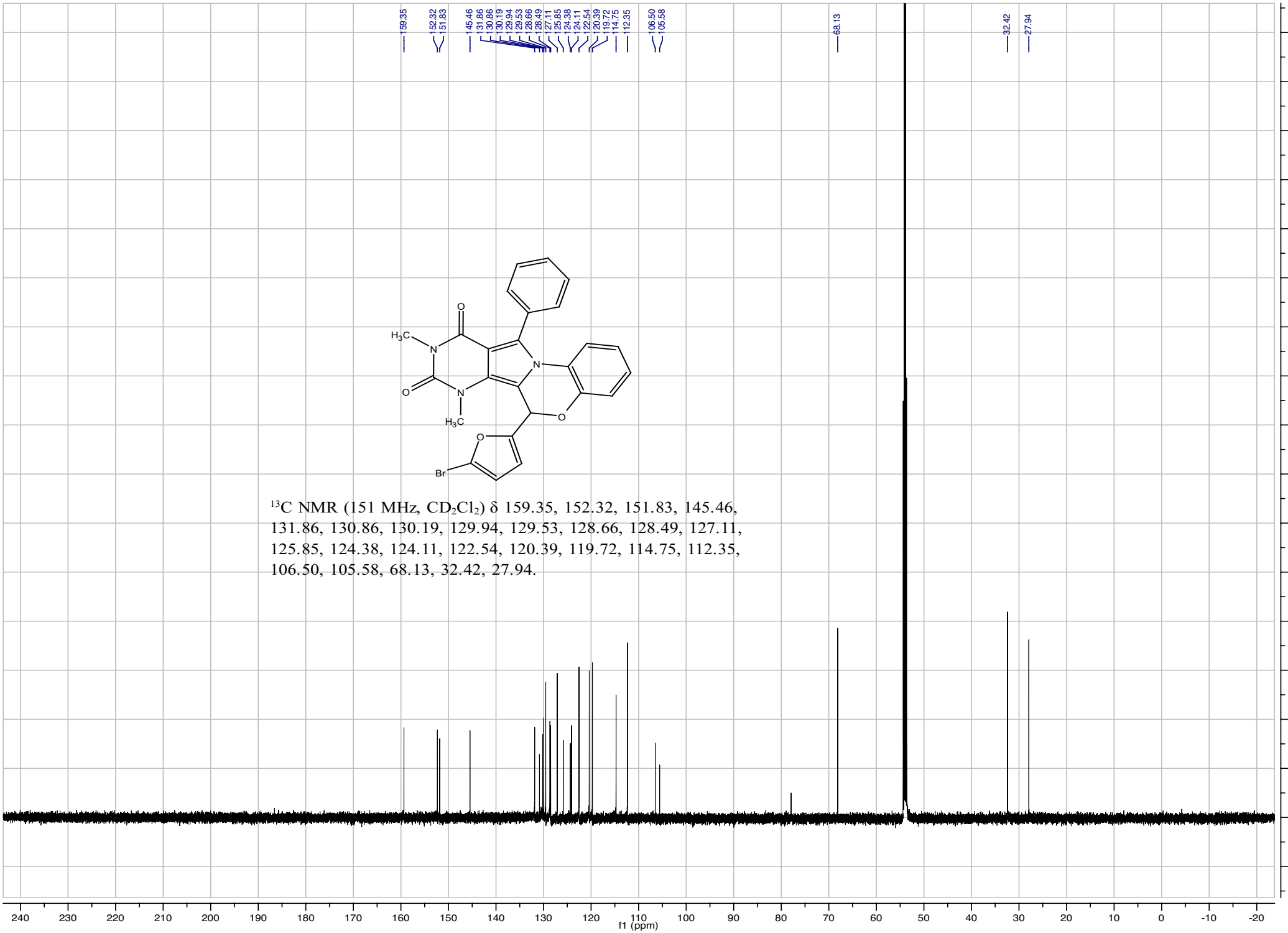
^{13}C NMR (151 MHz, DMSO-d_6) δ 159.11, 152.86, 150.90, 133.81, 130.35, 129.97, 129.67, 129.13, 128.58, 127.83, 127.18, 125.95, 118.99, 116.39, 106.16, 101.88, 31.50, 27.46.



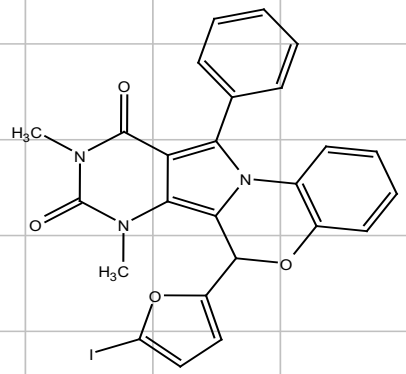
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d, *J* = 7.6, 1H), 7.58 (t, *J* = 7.5, 1H), 7.49 (t, *J* = 7.5, 1H), 7.33 (t, *J* = 7.5, 1H), 7.07 (d, *J* = 7.6, 1H), 7.05 – 6.98 (m, 2H), 6.79 (s, 1H), 6.64 (ddd, *J* = 2.2, 6.7, 8.6, 1H), 6.53 (d, *J* = 8.6, 1H), 6.14 (d, *J* = 3.4, 1H), 5.98 (dd, *J* = 0.8, 3.4, 1H), 3.47 (s, 3H), 3.26 (s, 3H).



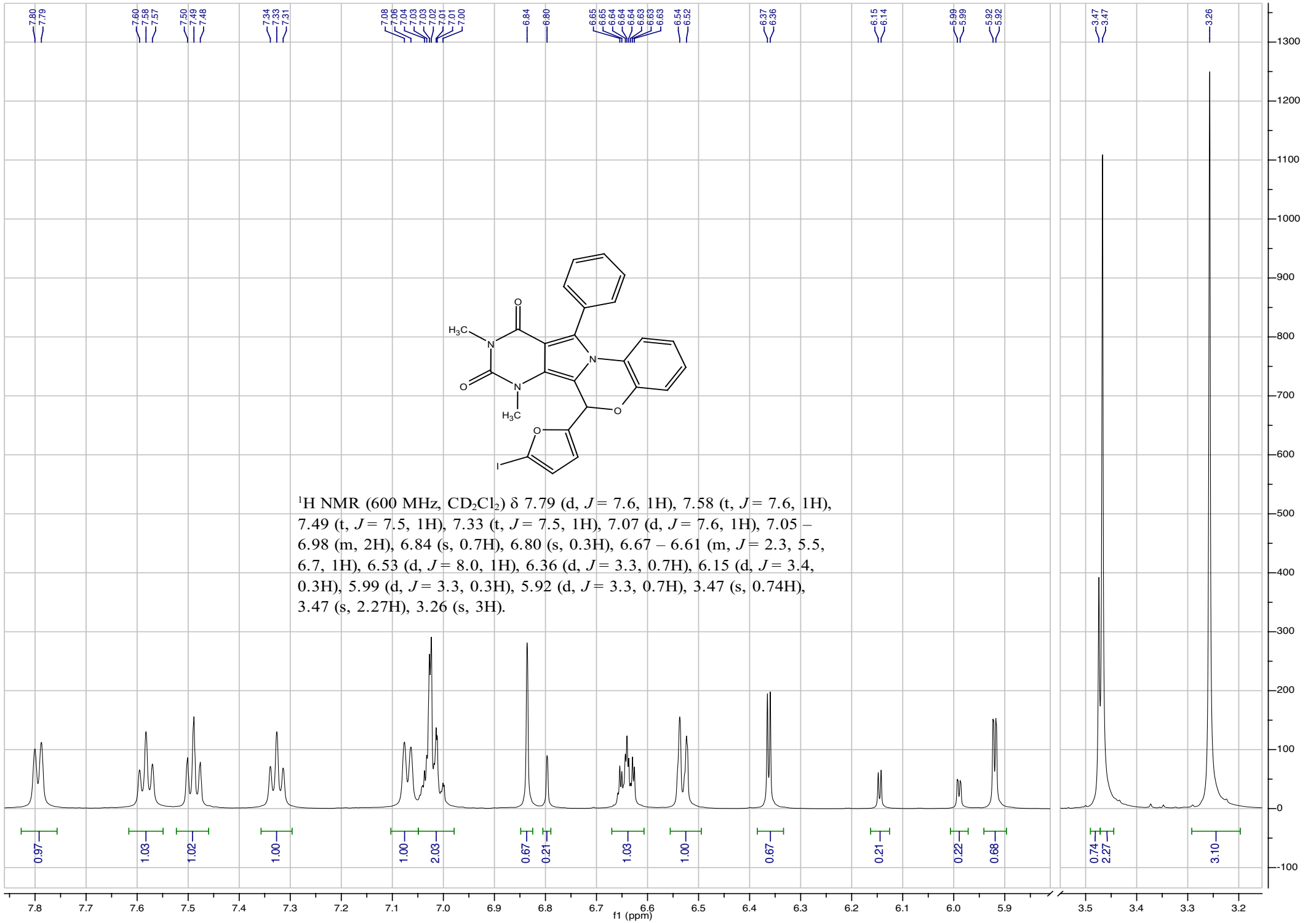
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d, *J* = 7.6, 1H), 7.58 (t, *J* = 7.5, 1H), 7.49 (t, *J* = 7.5, 1H), 7.33 (t, *J* = 7.5, 1H), 7.07 (d, *J* = 7.6, 1H), 7.05 – 6.98 (m, 2H), 6.79 (s, 1H), 6.64 (ddd, *J* = 2.2, 6.7, 8.6, 1H), 6.53 (d, *J* = 8.6, 1H), 6.14 (d, *J* = 3.4, 1H), 5.98 (dd, *J* = 0.8, 3.4, 1H), 3.47 (s, 3H), 3.26 (s, 3H).



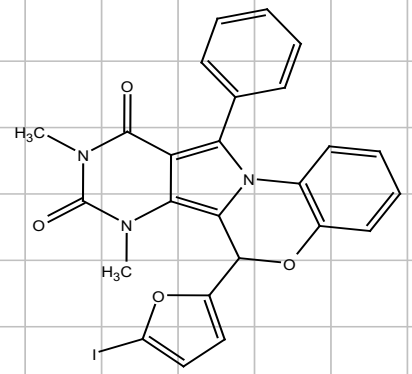
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.35, 152.32, 151.83, 145.46, 131.86, 130.86, 130.19, 129.94, 129.53, 128.66, 128.49, 127.11, 125.85, 124.38, 124.11, 122.54, 120.39, 119.72, 114.75, 112.35, 106.50, 105.58, 68.13, 32.42, 27.94.



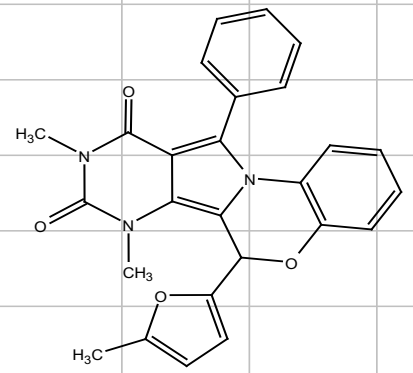
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d, *J* = 7.6, 1H), 7.58 (t, *J* = 7.6, 1H), 7.49 (t, *J* = 7.5, 1H), 7.33 (t, *J* = 7.5, 1H), 7.07 (d, *J* = 7.6, 1H), 7.05 – 6.98 (m, 2H), 6.84 (s, 0.7H), 6.80 (s, 0.3H), 6.67 – 6.61 (m, *J* = 2.3, 5.5, 6.7, 1H), 6.53 (d, *J* = 8.0, 1H), 6.36 (d, *J* = 3.3, 0.7H), 6.15 (d, *J* = 3.4, 0.3H), 5.99 (d, *J* = 3.3, 0.3H), 5.92 (d, *J* = 3.3, 0.7H), 3.47 (s, 0.74H), 3.47 (s, 2.27H), 3.26 (s, 3H).



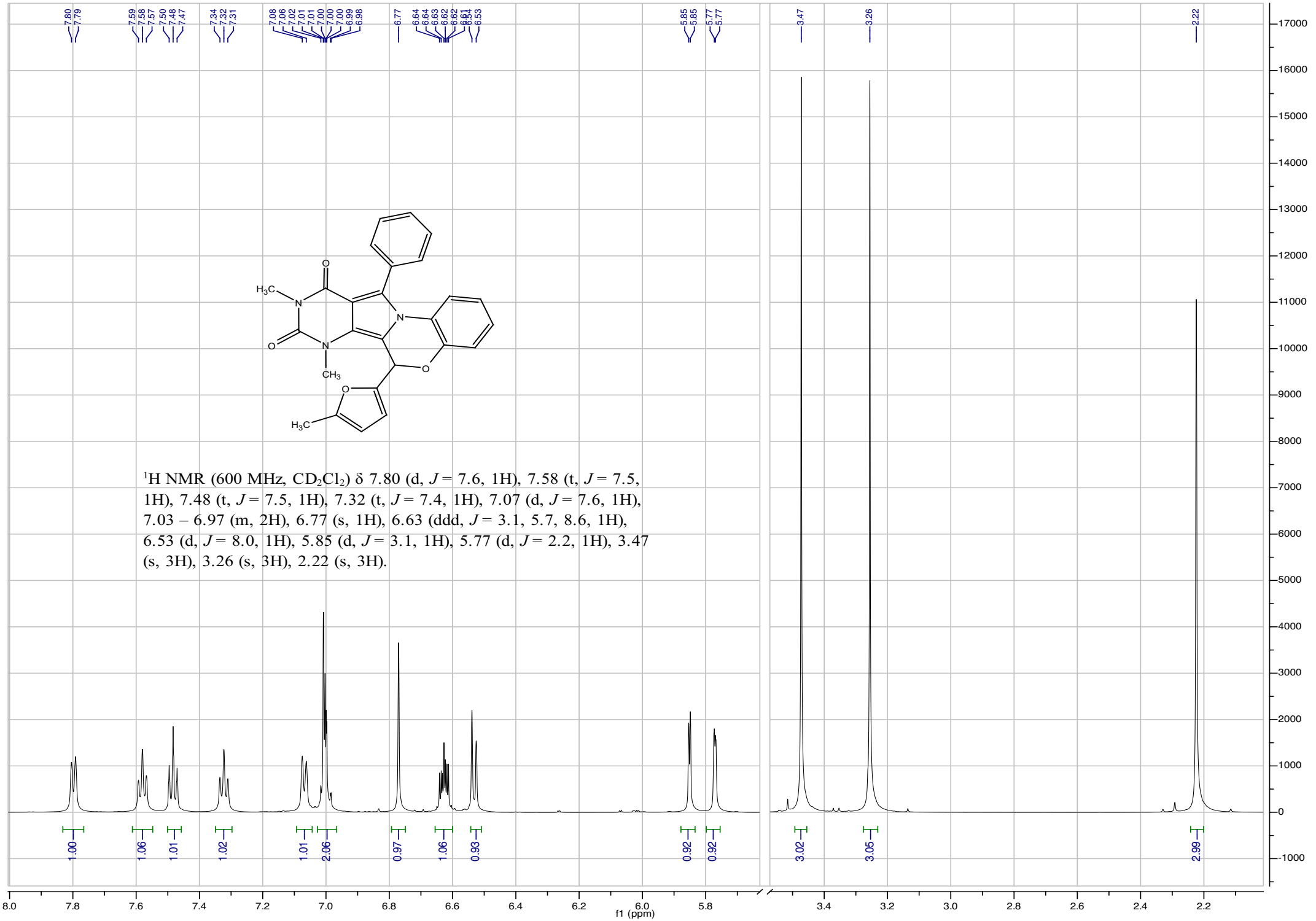
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.79 (d, J = 7.6, 1H), 7.58 (t, J = 7.6, 1H), 7.49 (t, J = 7.5, 1H), 7.33 (t, J = 7.5, 1H), 7.07 (d, J = 7.6, 1H), 7.05 – 6.98 (m, 2H), 6.84 (s, 0.7H), 6.80 (s, 0.3H), 6.67 – 6.61 (m, J = 2.3, 5.5, 6.7, 1H), 6.53 (d, J = 8.0, 1H), 6.36 (d, J = 3.3, 0.7H), 6.15 (d, J = 3.4, 0.3H), 5.99 (d, J = 3.3, 0.3H), 5.92 (d, J = 3.3, 0.7H), 3.47 (s, 0.74H), 3.47 (s, 2.27H), 3.26 (s, 3H).



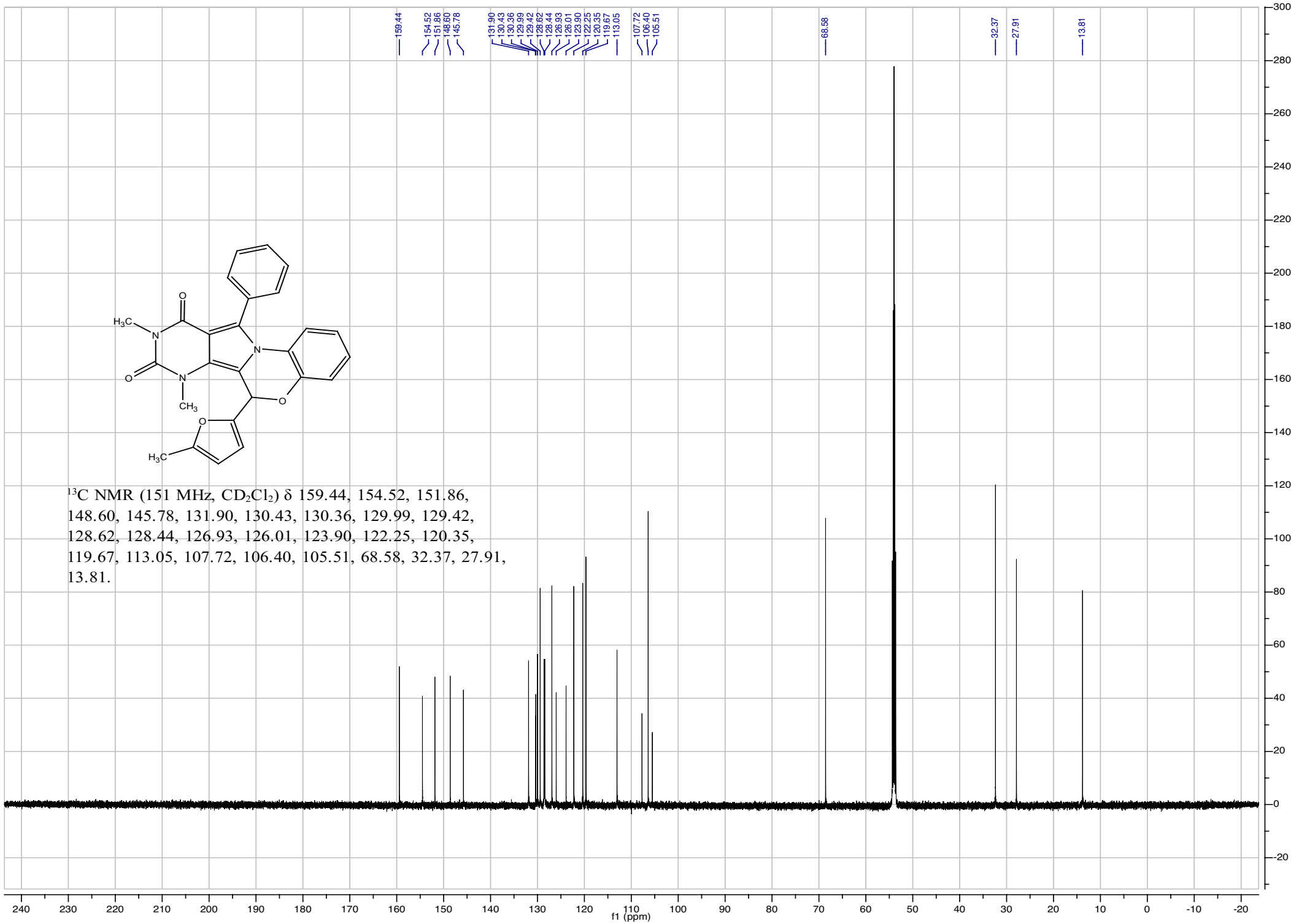
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.34, 155.77, 152.32, 151.81, 145.49, 145.45, 131.85, 130.84, 130.80, 130.19, 129.94, 129.51, 128.65, 128.48, 127.09, 125.84, 124.37, 124.32, 124.10, 122.53, 122.50, 121.06, 120.37, 119.70, 114.89, 114.74, 112.34, 106.66, 106.49, 105.56, 91.02, 68.03, 32.42, 27.93.



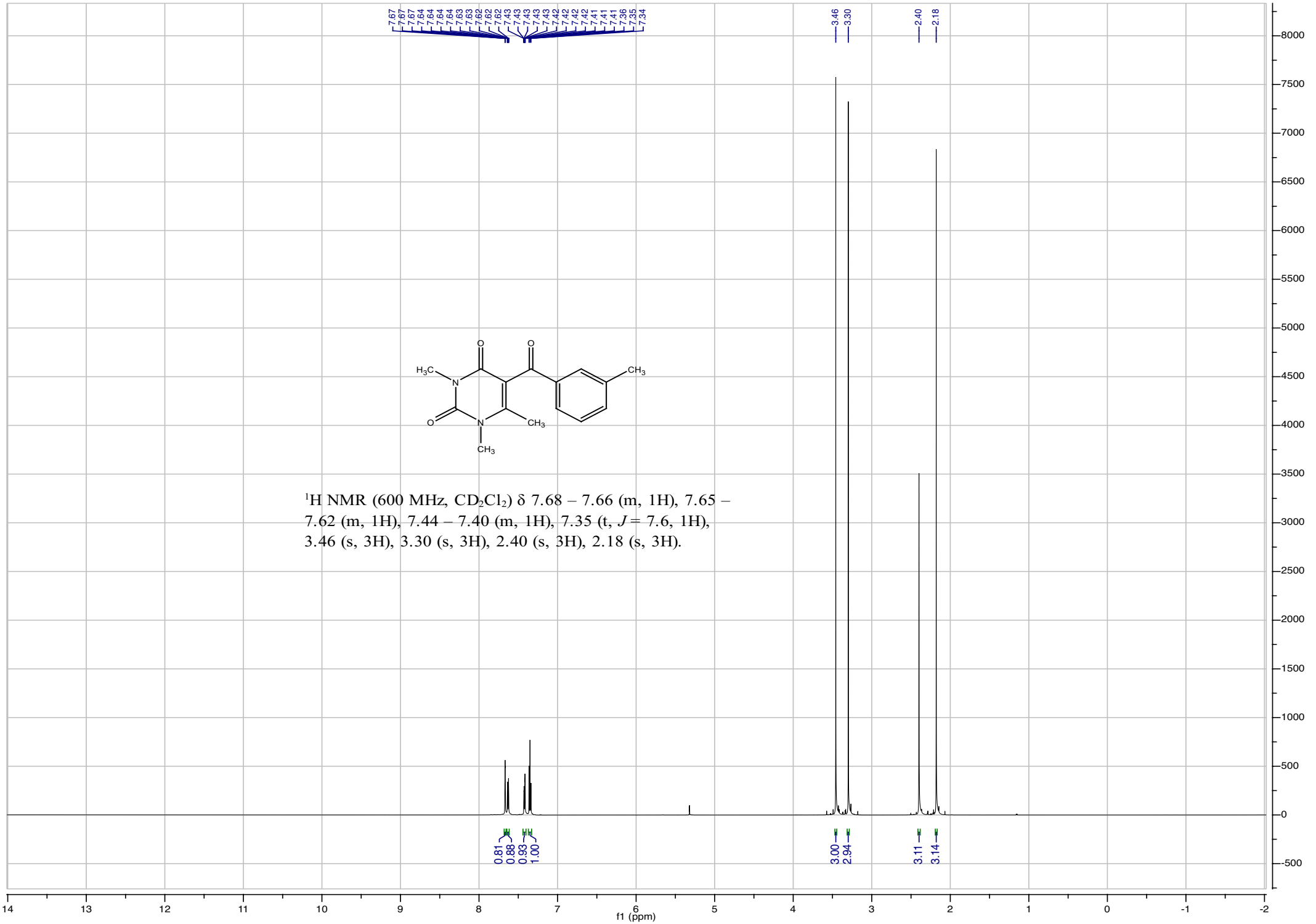
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, J = 7.6, 1H), 7.58 (t, J = 7.5, 1H), 7.48 (t, J = 7.5, 1H), 7.32 (t, J = 7.4, 1H), 7.07 (d, J = 7.6, 1H), 7.03 – 6.97 (m, 2H), 6.77 (s, 1H), 6.63 (ddd, J = 3.1, 5.7, 8.6, 1H), 6.53 (d, J = 8.0, 1H), 5.85 (d, J = 3.1, 1H), 5.77 (d, J = 2.2, 1H), 3.47 (s, 3H), 3.26 (s, 3H), 2.22 (s, 3H).



^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, J = 7.6, 1H), 7.58 (t, J = 7.5, 1H), 7.48 (t, J = 7.5, 1H), 7.32 (t, J = 7.4, 1H), 7.07 (d, J = 7.6, 1H), 7.03 – 6.97 (m, 2H), 6.77 (s, 1H), 6.63 (ddd, J = 3.1, 5.7, 8.6, 1H), 6.53 (d, J = 8.0, 1H), 5.85 (d, J = 3.1, 1H), 5.77 (d, J = 2.2, 1H), 3.47 (s, 3H), 3.26 (s, 3H), 2.22 (s, 3H).

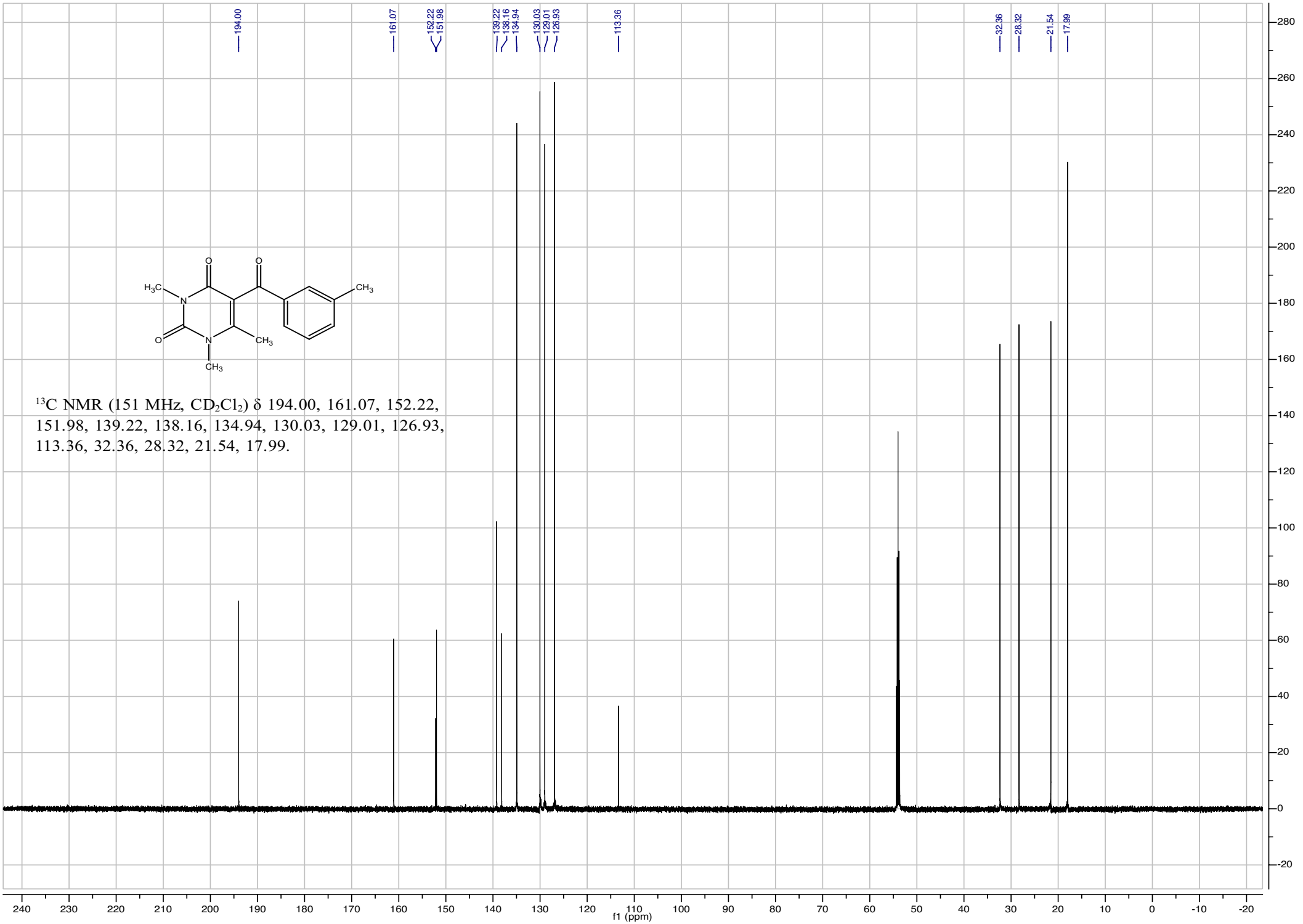


^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.44, 154.52, 151.86, 148.60, 145.78, 131.90, 130.43, 130.36, 129.99, 129.42, 128.62, 128.44, 126.93, 126.01, 123.90, 122.25, 120.35, 119.67, 113.05, 107.72, 106.40, 105.51, 68.58, 32.37, 27.91, 13.81.

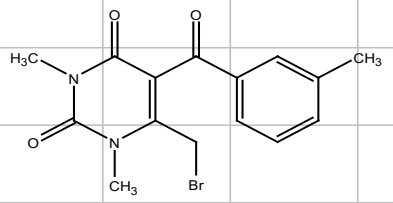


^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.68 – 7.66 (m, 1H), 7.65 – 7.62 (m, 1H), 7.44 – 7.40 (m, 1H), 7.35 (t, *J* = 7.6, 1H), 3.46 (s, 3H), 3.30 (s, 3H), 2.40 (s, 3H), 2.18 (s, 3H).

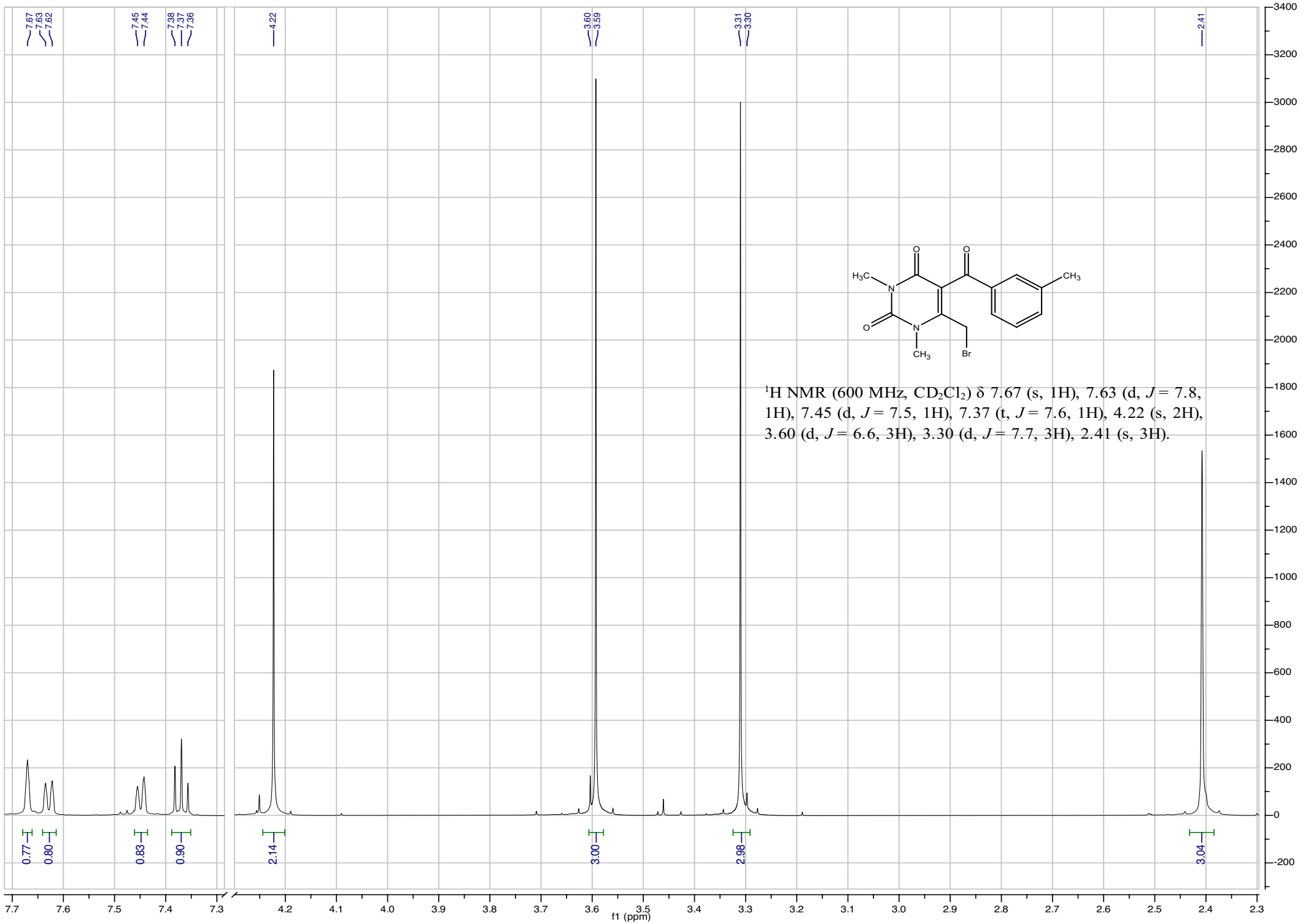
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.68 – 7.66 (m, 1H), 7.65 – 7.62 (m, 1H), 7.44 – 7.40 (m, 1H), 7.35 (t, J = 7.6, 1H), 3.46 (s, 3H), 3.30 (s, 3H), 2.40 (s, 3H), 2.18 (s, 3H).



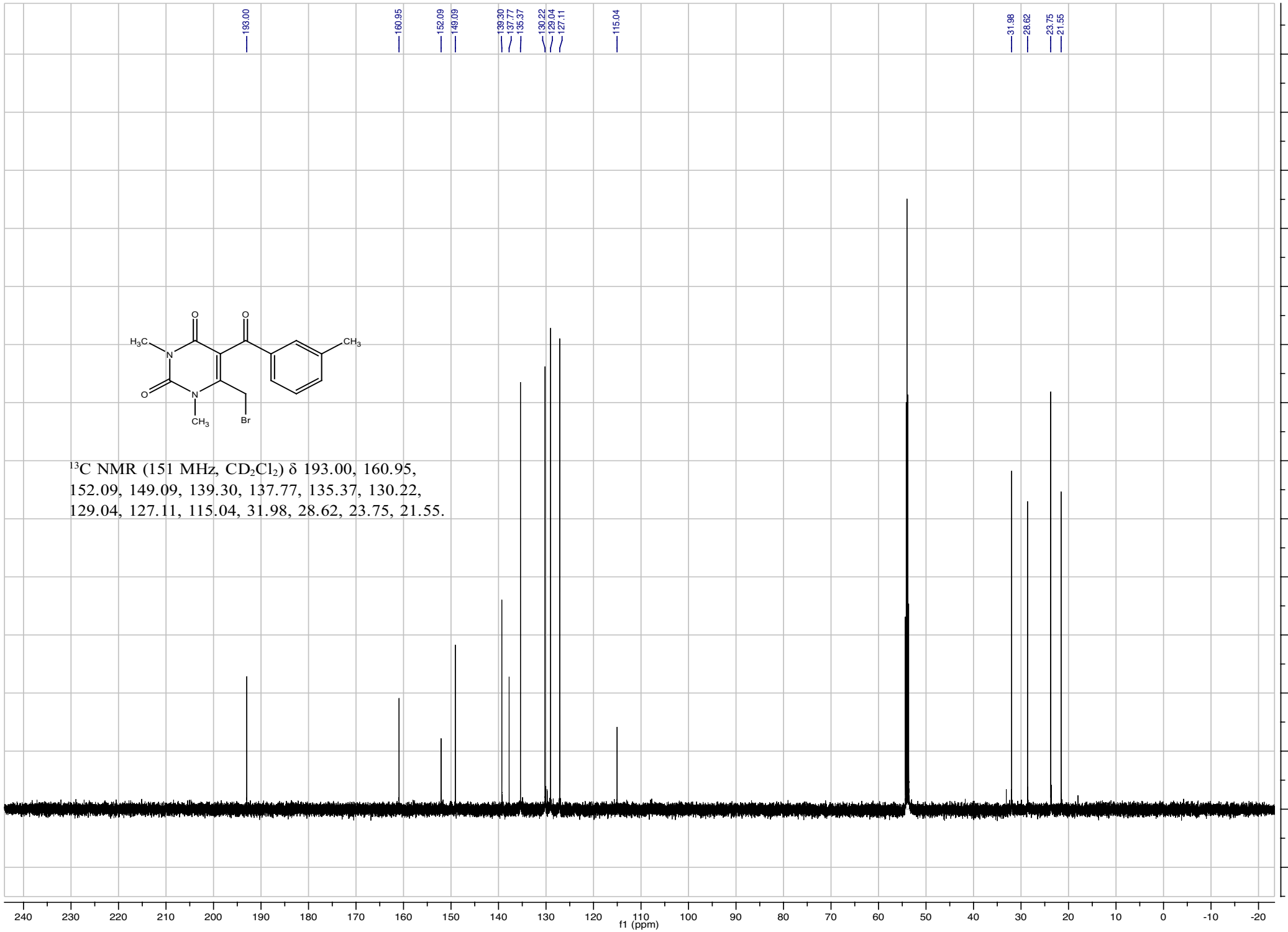
^{13}C NMR (151 MHz, CD_2Cl_2) δ 194.00, 161.07, 152.22, 151.98, 139.22, 138.16, 134.94, 130.03, 129.01, 126.93, 113.36, 32.36, 28.32, 21.54, 17.99.



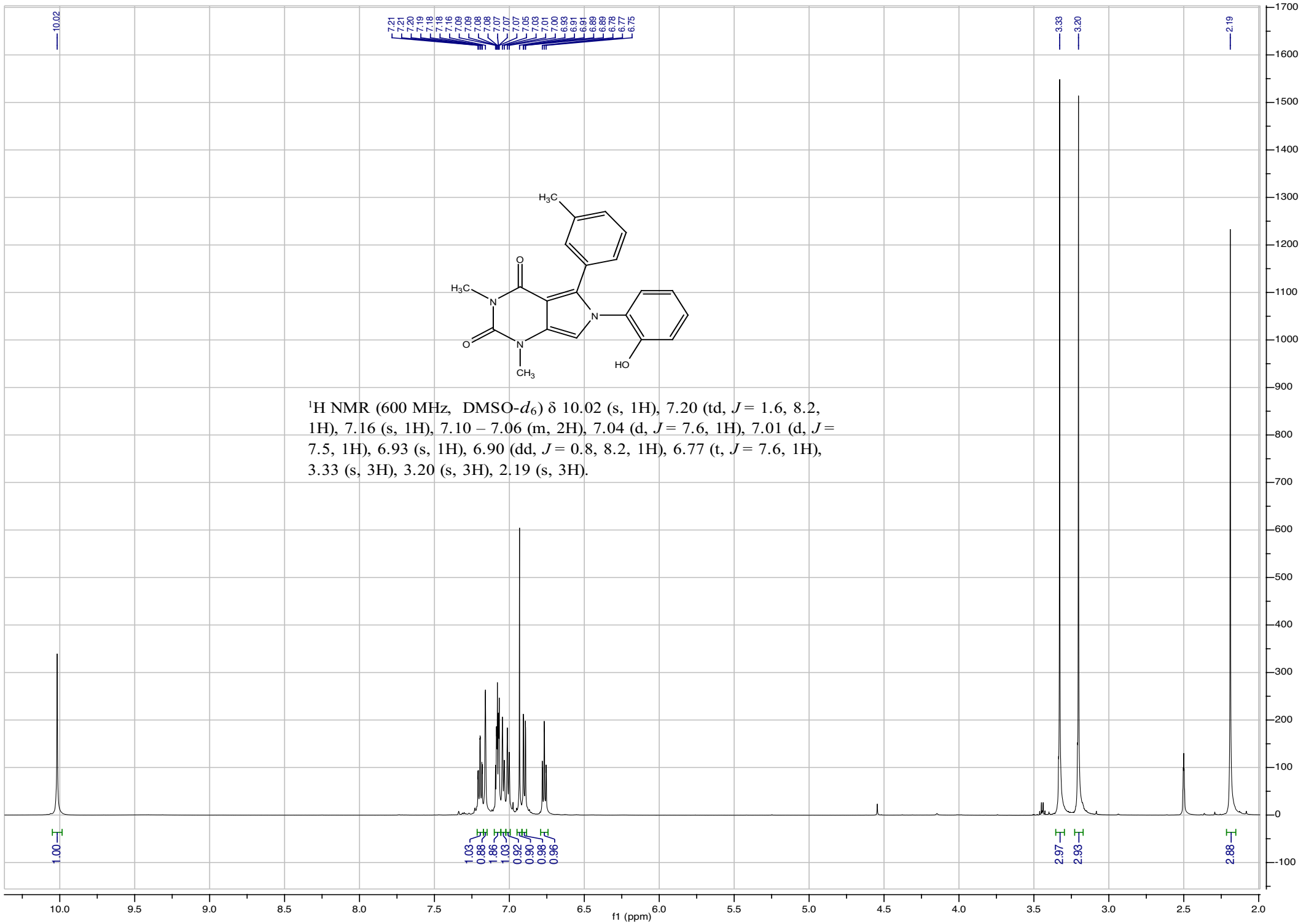
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.67 (s, 1H), 7.63 (d, J = 7.8, 1H), 7.45 (d, J = 7.5, 1H), 7.37 (t, J = 7.6, 1H), 4.22 (s, 2H), 3.60 (d, J = 6.6, 3H), 3.30 (d, J = 7.7, 3H), 2.41 (s, 3H).



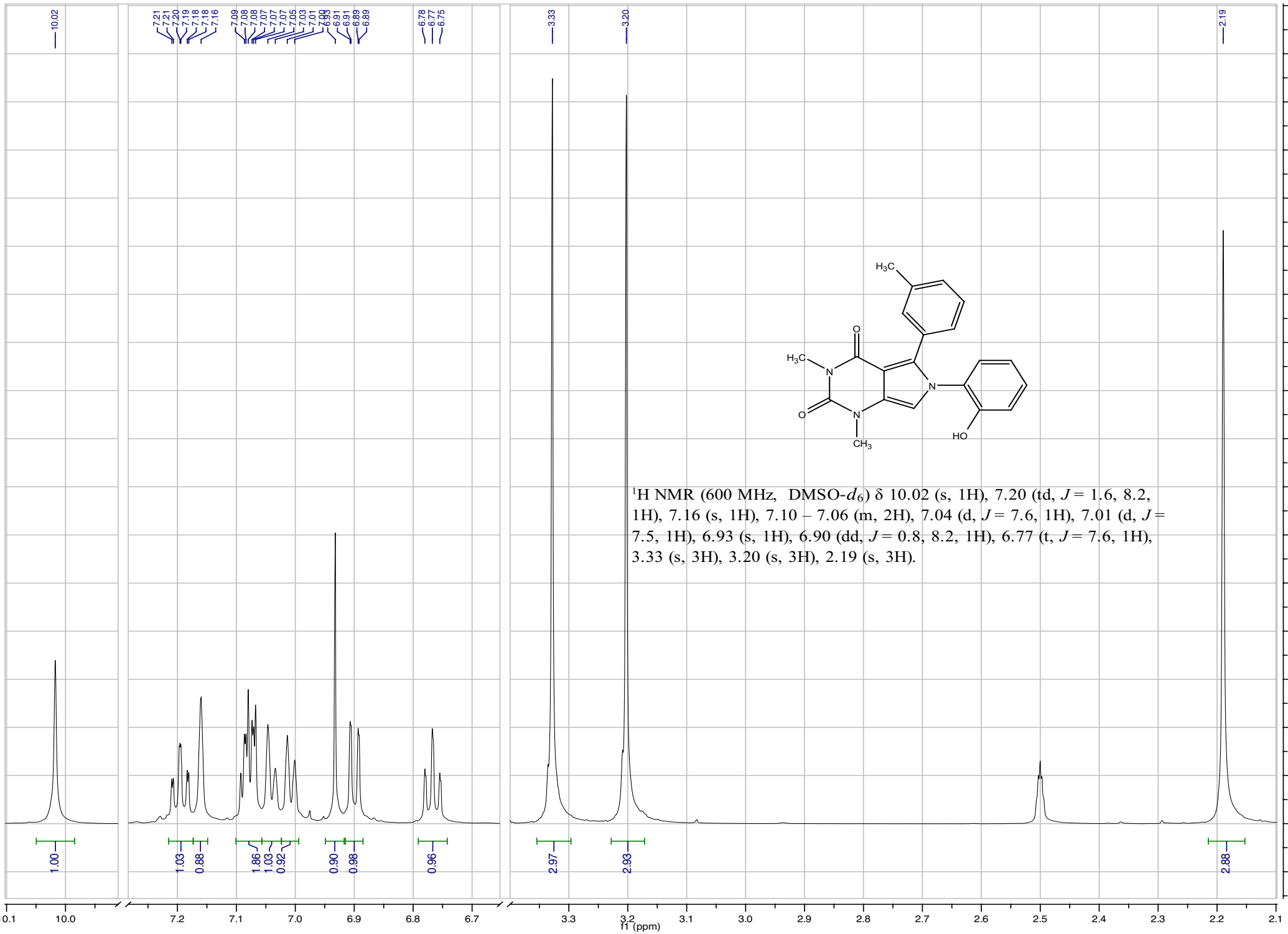
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.67 (s, 1H), 7.63 (d, J = 7.8, 1H), 7.45 (d, J = 7.5, 1H), 7.37 (t, J = 7.6, 1H), 4.22 (s, 2H), 3.60 (d, J = 6.6, 3H), 3.30 (d, J = 7.7, 3H), 2.41 (s, 3H).

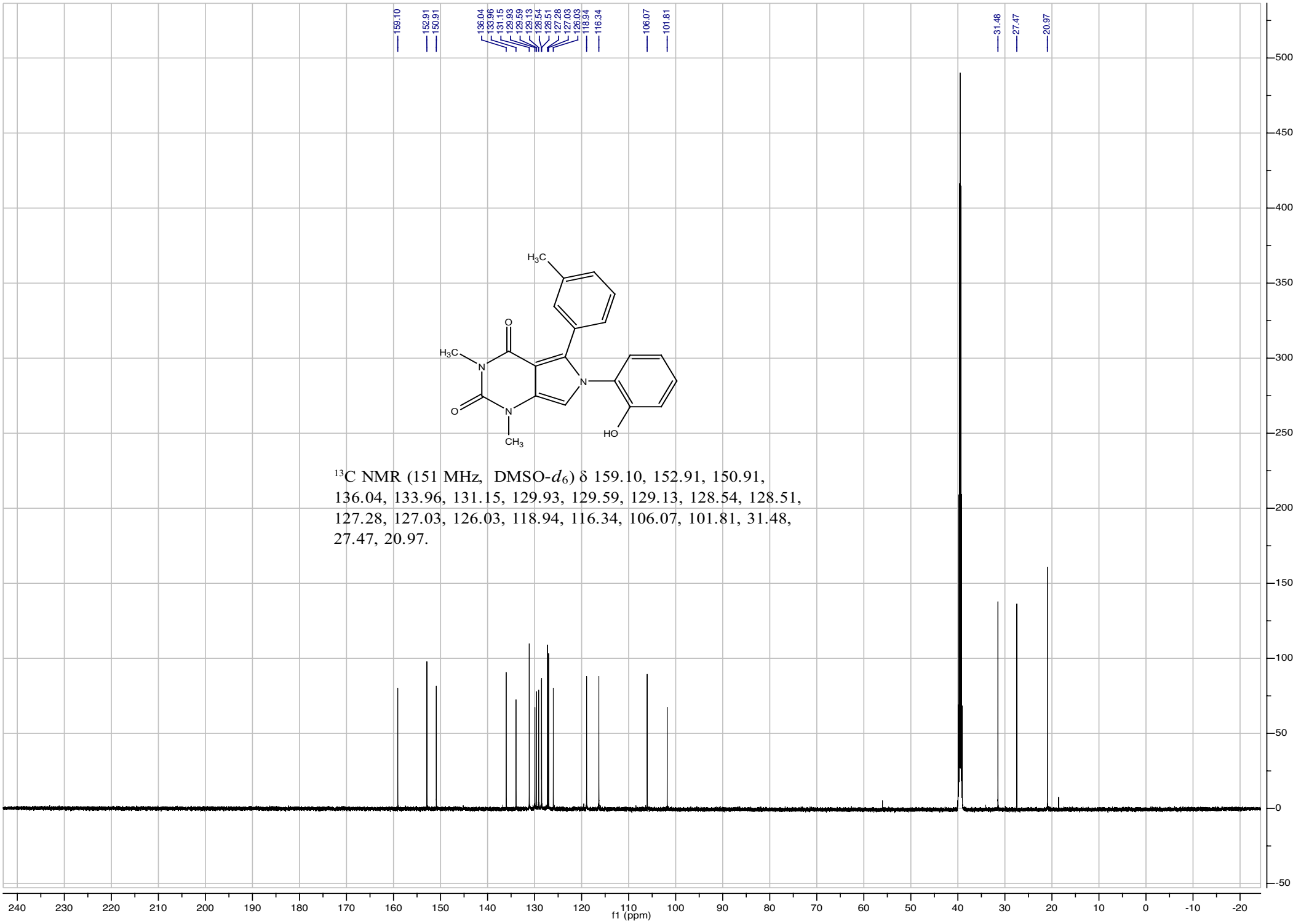


^{13}C NMR (151 MHz, CD_2Cl_2) δ 193.00, 160.95, 152.09, 149.09, 139.30, 137.77, 135.37, 130.22, 129.04, 127.11, 115.04, 31.98, 28.62, 23.75, 21.55.

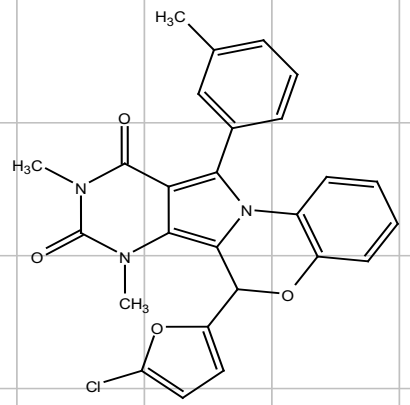


^{1}H NMR (600 MHz, DMSO-d_6) δ 10.02 (s, 1H), 7.20 (td, J = 1.6, 8.2, 1H), 7.16 (s, 1H), 7.10 – 7.06 (m, 2H), 7.04 (d, J = 7.6, 1H), 7.01 (d, J = 7.5, 1H), 6.93 (s, 1H), 6.90 (dd, J = 0.8, 8.2, 1H), 6.77 (t, J = 7.6, 1H), 3.33 (s, 3H), 3.20 (s, 3H), 2.19 (s, 3H).

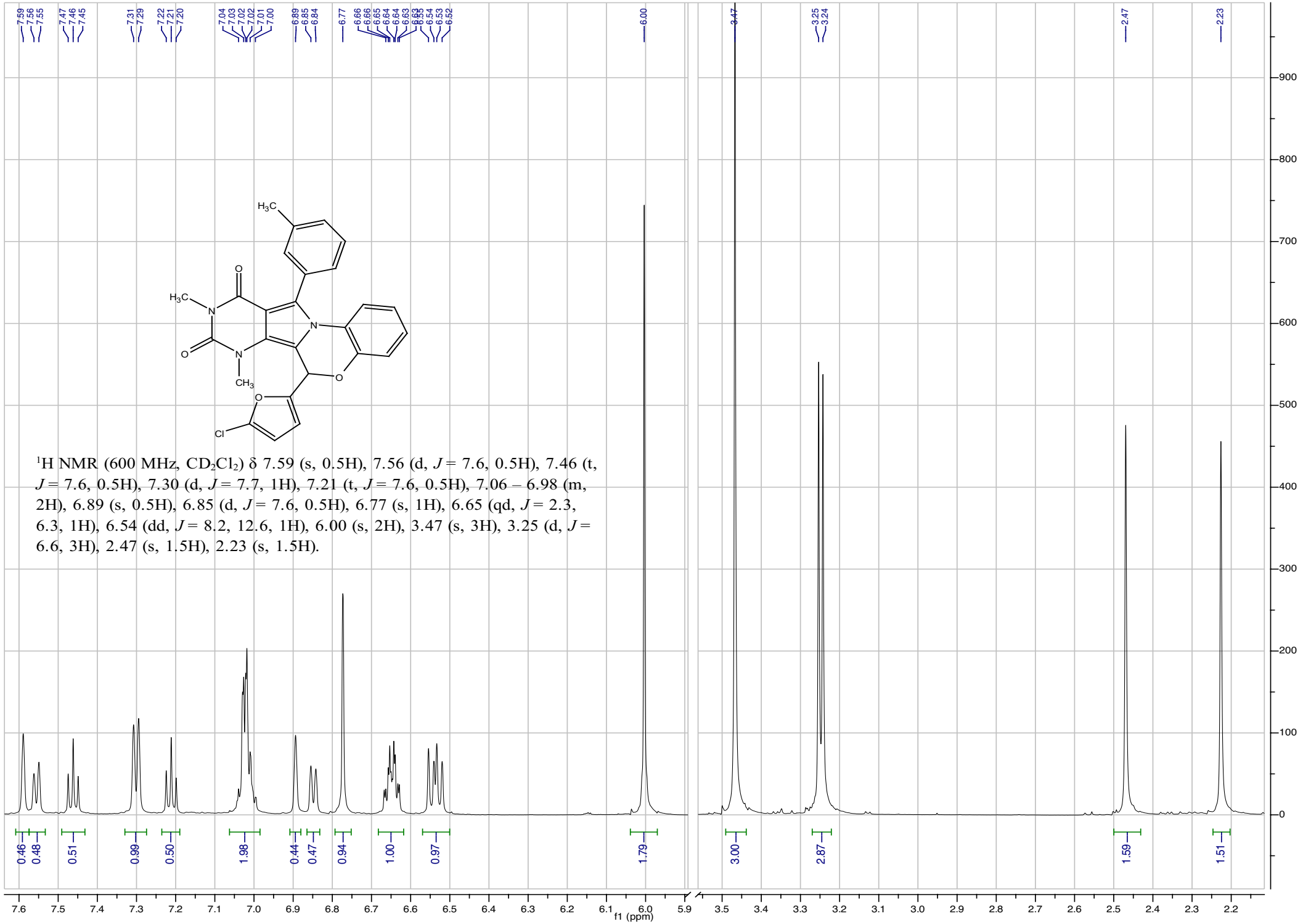

10.02
7.21
7.21
7.20
7.19
7.18
7.18
7.16
7.09
7.08
7.08
7.07
7.07
7.07
7.05
7.03
7.01
6.93
6.91
6.91
6.89
6.89
6.78
6.77
6.75
3.33
3.20
2.19
1.00
1.03
0.88
1.86
1.03
0.92
0.90
0.98
0.96
2.97
2.93
2.88
H3C
O
H3C
N
N
O
N
CH3
HO
[1]H NMR (600 MHz, DMSO-d6) δ 10.02 (s, 1H), 7.20 (td, J = 1.6, 8.2, 1H), 7.16 (s, 1H), 7.10 – 7.06 (m, 2H), 7.04 (d, J = 7.6, 1H), 7.01 (d, J = 7.5, 1H), 6.93 (s, 1H), 6.90 (dd, J = 0.8, 8.2, 1H), 6.77 (t, J = 7.6, 1H), 3.33 (s, 3H), 3.20 (s, 3H), 2.19 (s, 3H).
f1 (ppm)



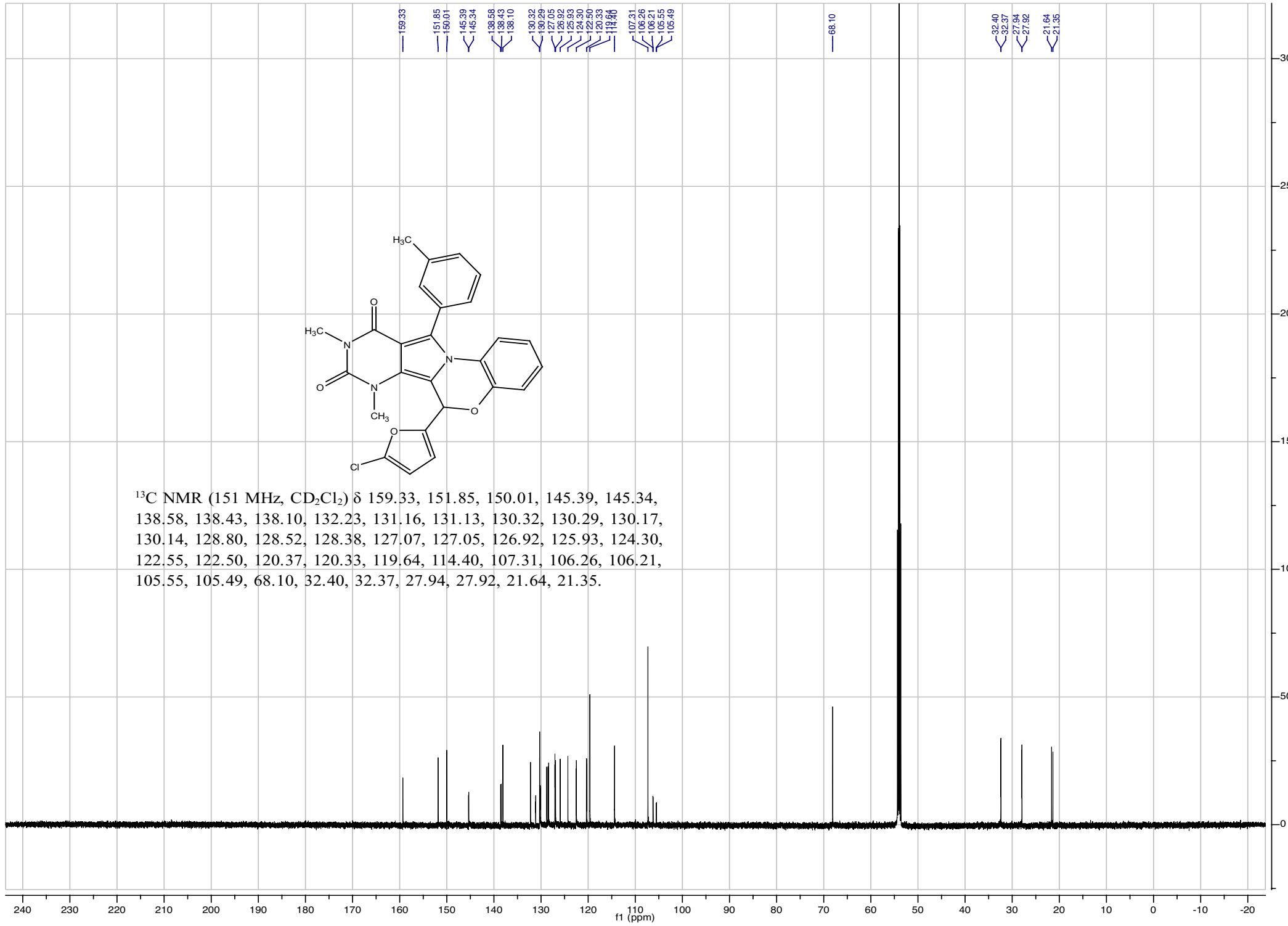
^{13}C NMR (151 MHz, DMSO-d_6) δ 159.10, 152.91, 150.91, 136.04, 133.96, 131.15, 129.93, 129.59, 129.13, 128.54, 128.51, 127.28, 127.03, 126.03, 118.94, 116.34, 106.07, 101.81, 31.48, 27.47, 20.97.



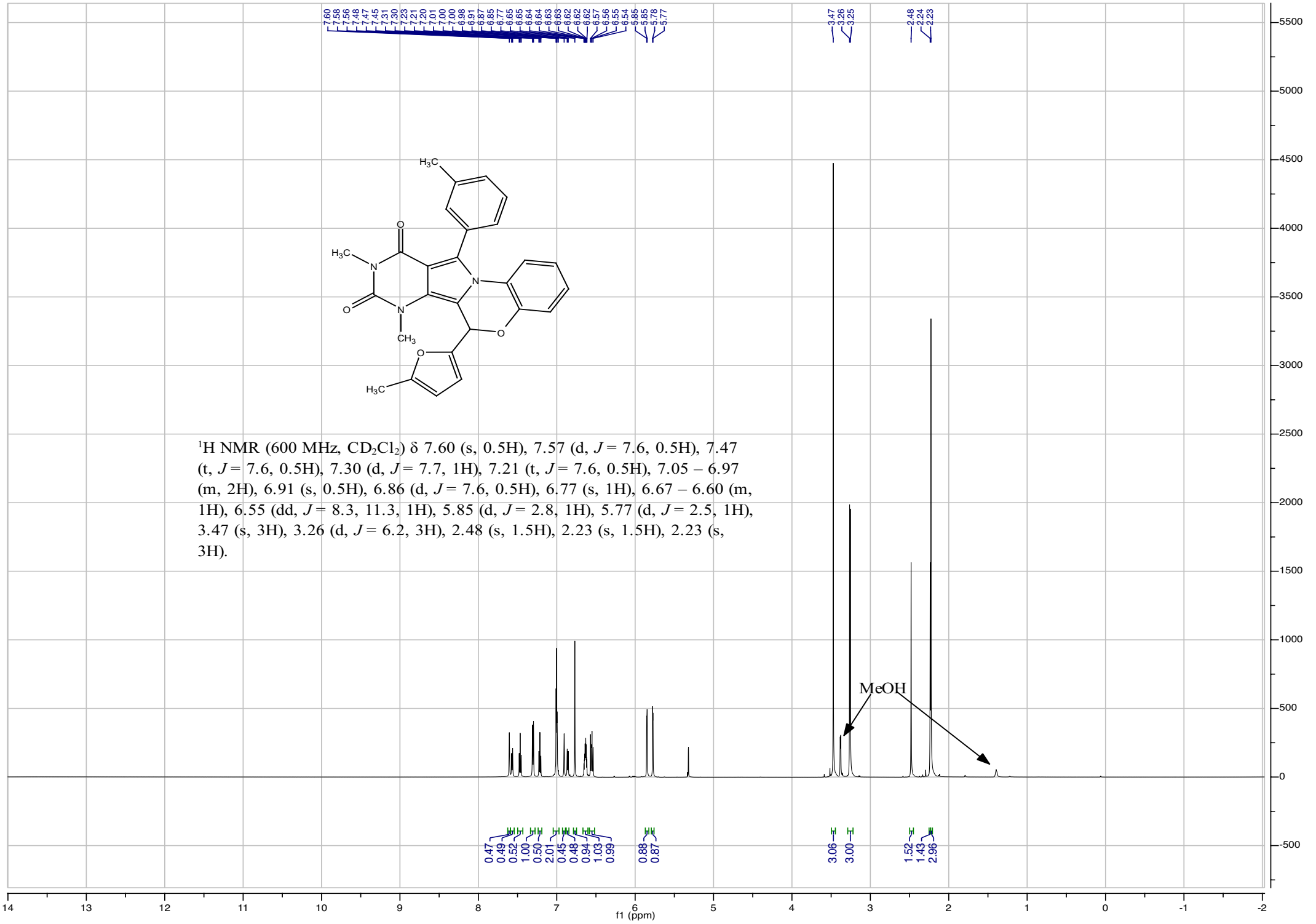
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.59 (s, 0.5H), 7.56 (d, *J* = 7.6, 0.5H), 7.46 (t, *J* = 7.6, 0.5H), 7.30 (d, *J* = 7.7, 1H), 7.21 (t, *J* = 7.6, 0.5H), 7.06 – 6.98 (m, 2H), 6.89 (s, 0.5H), 6.85 (d, *J* = 7.6, 0.5H), 6.77 (s, 1H), 6.65 (qd, *J* = 2.3, 6.3, 1H), 6.54 (dd, *J* = 8.2, 12.6, 1H), 6.00 (s, 2H), 3.47 (s, 3H), 3.25 (d, *J* = 6.6, 3H), 2.47 (s, 1.5H), 2.23 (s, 1.5H).



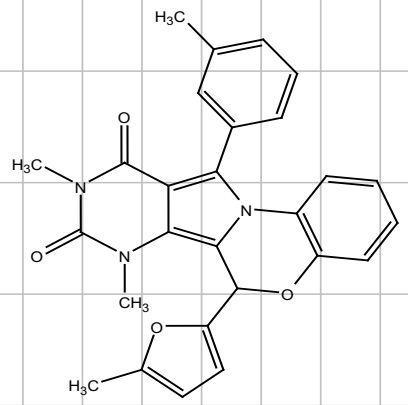
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.59 (s, 0.5H), 7.56 (d, J = 7.6, 0.5H), 7.46 (t, J = 7.6, 0.5H), 7.30 (d, J = 7.7, 1H), 7.21 (t, J = 7.6, 0.5H), 7.06 – 6.98 (m, 2H), 6.89 (s, 0.5H), 6.85 (d, J = 7.6, 0.5H), 6.77 (s, 1H), 6.65 (qd, J = 2.3, 6.3, 1H), 6.54 (dd, J = 8.2, 12.6, 1H), 6.00 (s, 2H), 3.47 (s, 3H), 3.25 (d, J = 6.6, 3H), 2.47 (s, 1.5H), 2.23 (s, 1.5H).



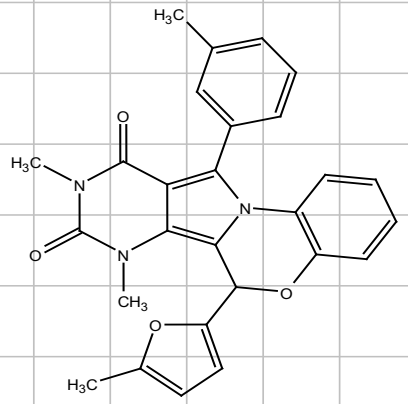
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.33, 151.85, 150.01, 145.39, 145.34, 138.58, 138.43, 138.10, 132.23, 131.16, 131.13, 130.32, 130.29, 130.17, 130.14, 128.80, 128.52, 128.38, 127.07, 127.05, 126.92, 125.93, 124.30, 122.55, 122.50, 120.37, 120.33, 119.64, 114.40, 107.31, 106.26, 106.21, 105.55, 105.49, 68.10, 32.40, 32.37, 27.94, 27.92, 21.64, 21.35.



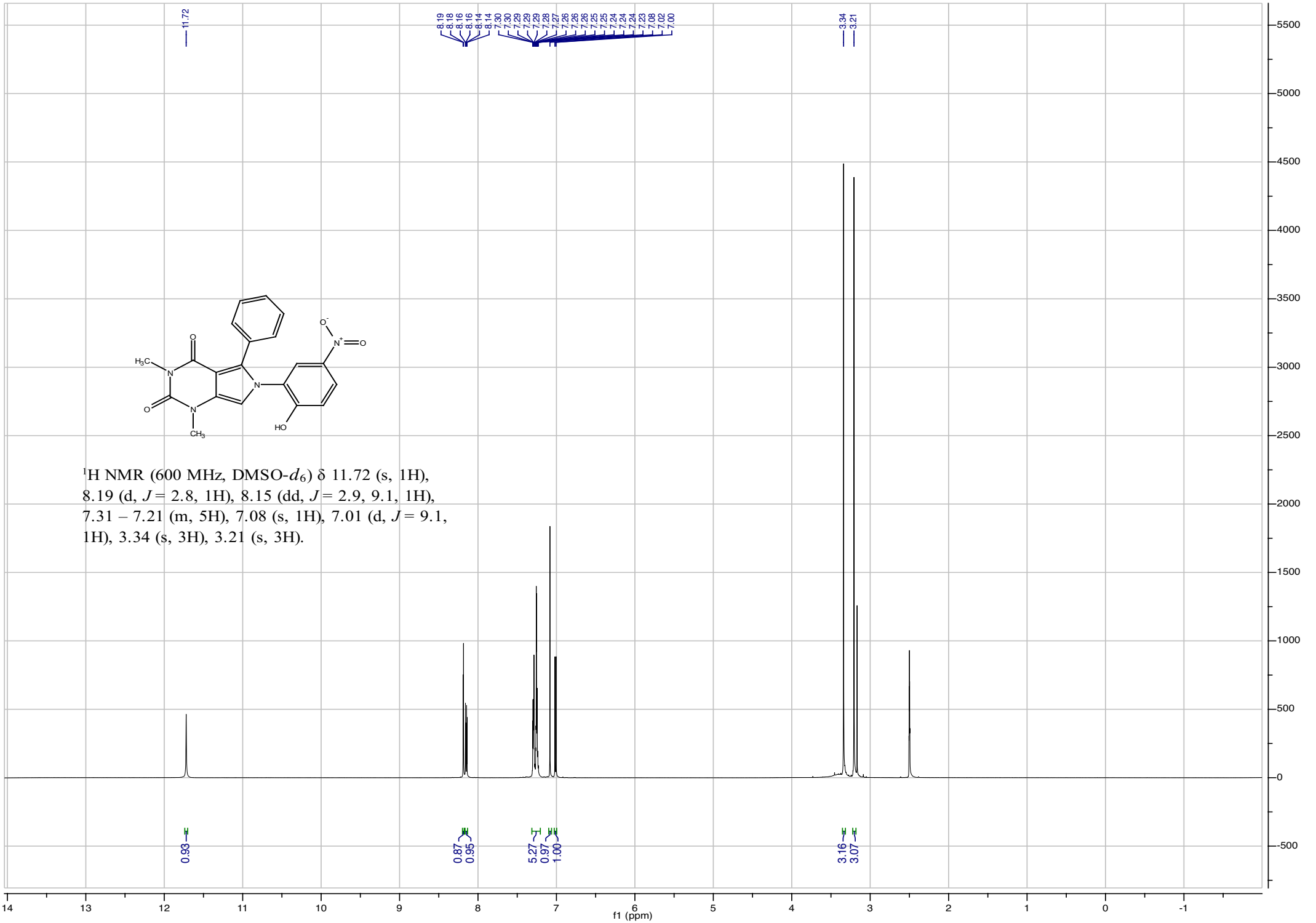
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.60 (s, 0.5H), 7.57 (d, J = 7.6, 0.5H), 7.47 (t, J = 7.6, 0.5H), 7.30 (d, J = 7.7, 1H), 7.21 (t, J = 7.6, 0.5H), 7.05 – 6.97 (m, 2H), 6.91 (s, 0.5H), 6.86 (d, J = 7.6, 0.5H), 6.77 (s, 1H), 6.67 – 6.60 (m, 1H), 6.55 (dd, J = 8.3, 11.3, 1H), 5.85 (d, J = 2.8, 1H), 5.77 (d, J = 2.5, 1H), 3.47 (s, 3H), 3.26 (d, J = 6.2, 3H), 2.48 (s, 1.5H), 2.23 (s, 1.5H), 2.23 (s, 3H).



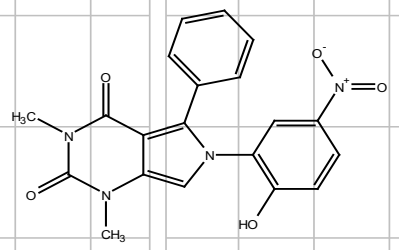
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.60 (s, 0.5H), 7.57 (d, J = 7.6, 0.5H), 7.47 (t, J = 7.6, 0.5H), 7.30 (d, J = 7.7, 1H), 7.21 (t, J = 7.6, 0.5H), 7.05 – 6.97 (m, 2H), 6.91 (s, 0.5H), 6.86 (d, J = 7.6, 0.5H), 6.77 (s, 1H), 6.67 – 6.60 (m, 1H), 6.55 (dd, J = 8.3, 11.3, 1H), 5.85 (d, J = 2.8, 1H), 5.77 (d, J = 2.5, 1H), 3.47 (s, 3H), 3.26 (d, J = 6.2, 3H), 2.48 (s, 1.5H), 2.23 (s, 1.5H), 2.23 (s, 3H).



^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.44, 159.43, 154.49, 151.89, 148.66, 145.72, 145.67, 138.52, 138.37, 132.28, 130.75, 130.72, 130.38, 130.33, 130.31, 130.19, 128.84, 128.48, 128.34, 126.98, 126.89, 126.87, 126.08, 123.82, 122.27, 122.22, 120.34, 120.30, 119.59, 113.01, 107.52, 107.47, 106.40, 105.49, 105.42, 68.53, 32.37, 32.34, 27.91, 27.89, 21.64, 21.35, 13.81.

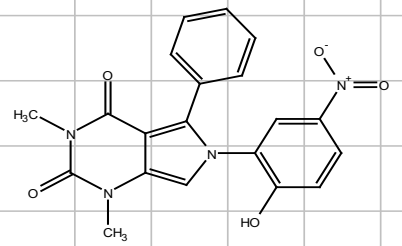


^{1}H NMR (600 MHz, DMSO-d_6) δ 11.72 (s, 1H), 8.19 (d, J = 2.8, 1H), 8.15 (dd, J = 2.9, 9.1, 1H), 7.31 – 7.21 (m, 5H), 7.08 (s, 1H), 7.01 (d, J = 9.1, 1H), 3.34 (s, 3H), 3.21 (s, 3H).

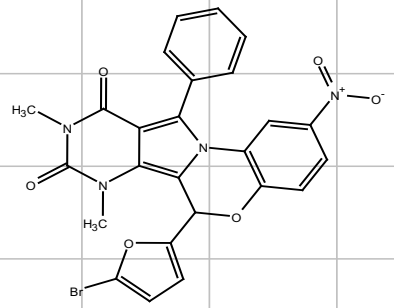


^{1}H NMR (600 MHz, DMSO-d_6) δ 11.72 (s, 1H), 8.19 (d, J = 2.8, 1H), 8.15 (dd, J = 2.9, 9.1, 1H), 7.31 – 7.21 (m, 5H), 7.08 (s, 1H), 7.01 (d, J = 9.1, 1H), 3.34 (s, 3H), 3.21 (s, 3H).

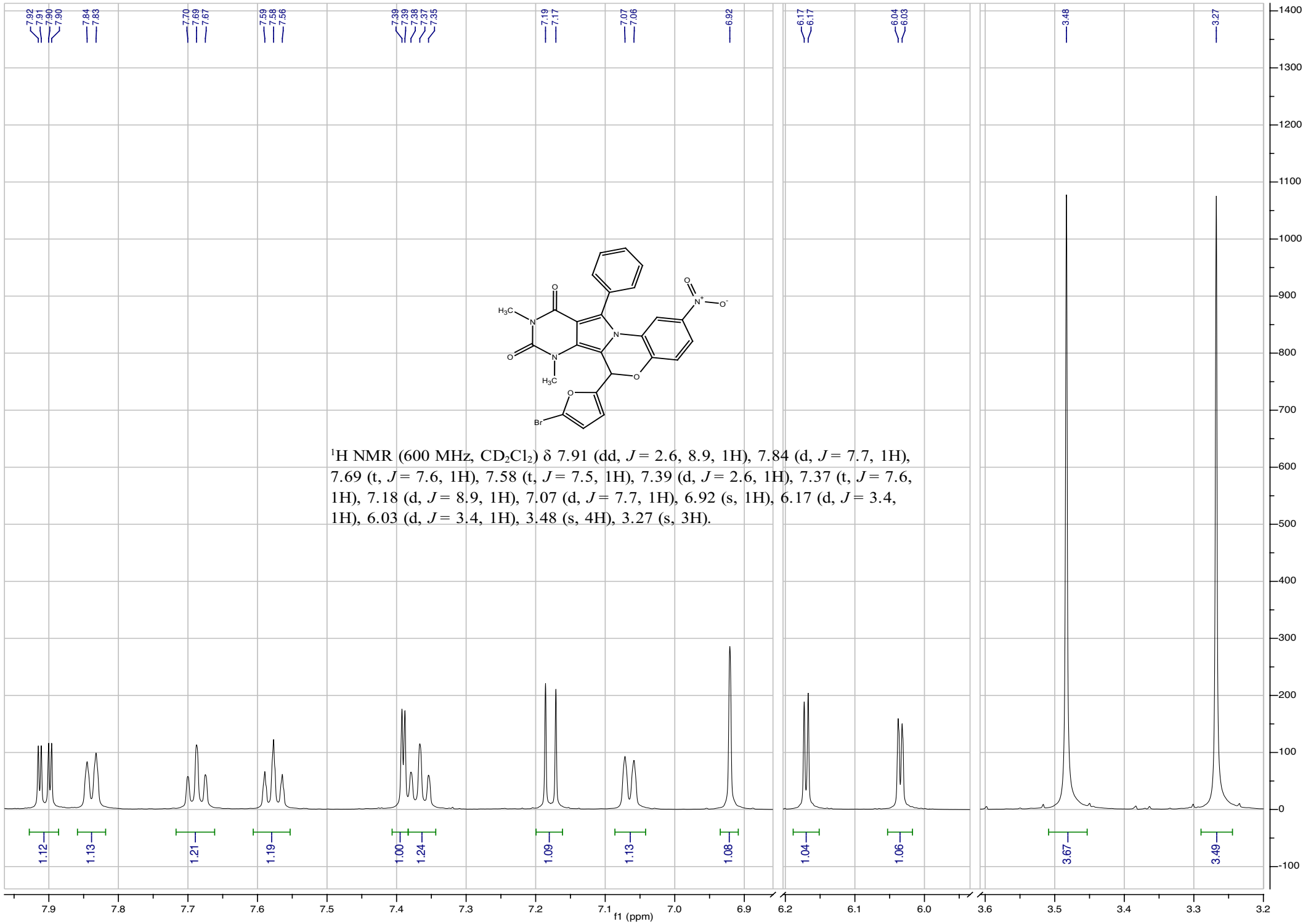
MeOH



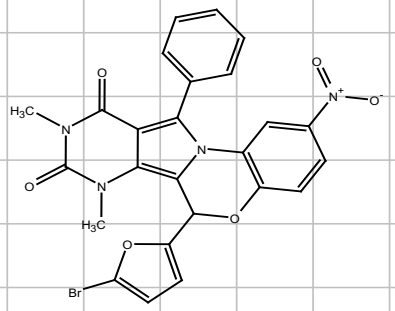
^{13}C NMR (151 MHz, DMSO-d_6) δ 159.26, 159.03, 150.85, 138.89, 134.18, 130.34, 129.34, 128.85, 128.14, 127.36, 126.15, 126.09, 125.45, 116.60, 105.95, 102.41, 31.52, 27.48.



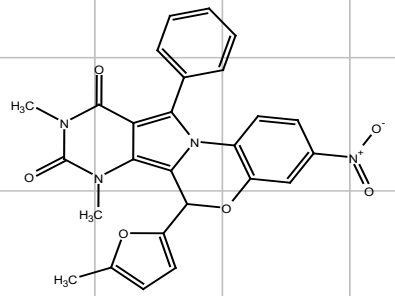
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.91 (dd, *J* = 2.6, 8.9, 1H), 7.84 (d, *J* = 7.7, 1H), 7.69 (t, *J* = 7.6, 1H), 7.58 (t, *J* = 7.5, 1H), 7.39 (d, *J* = 2.6, 1H), 7.37 (t, *J* = 7.6, 1H), 7.18 (d, *J* = 8.9, 1H), 7.07 (d, *J* = 7.7, 1H), 6.92 (s, 1H), 6.17 (d, *J* = 3.4, 1H), 6.03 (d, *J* = 3.4, 1H), 3.48 (s, 4H), 3.27 (s, 3H).



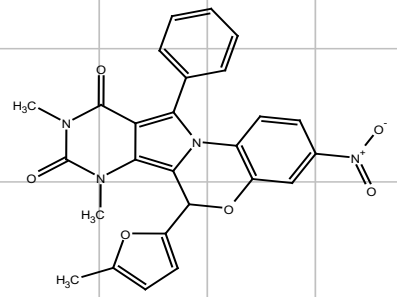
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.91 (dd, J = 2.6, 8.9, 1H), 7.84 (d, J = 7.7, 1H), 7.69 (t, J = 7.6, 1H), 7.58 (t, J = 7.5, 1H), 7.39 (d, J = 2.6, 1H), 7.37 (t, J = 7.6, 1H), 7.18 (d, J = 8.9, 1H), 7.07 (d, J = 7.7, 1H), 6.92 (s, 1H), 6.17 (d, J = 3.4, 1H), 6.03 (d, J = 3.4, 1H), 3.48 (s, 4H), 3.27 (s, 3H).



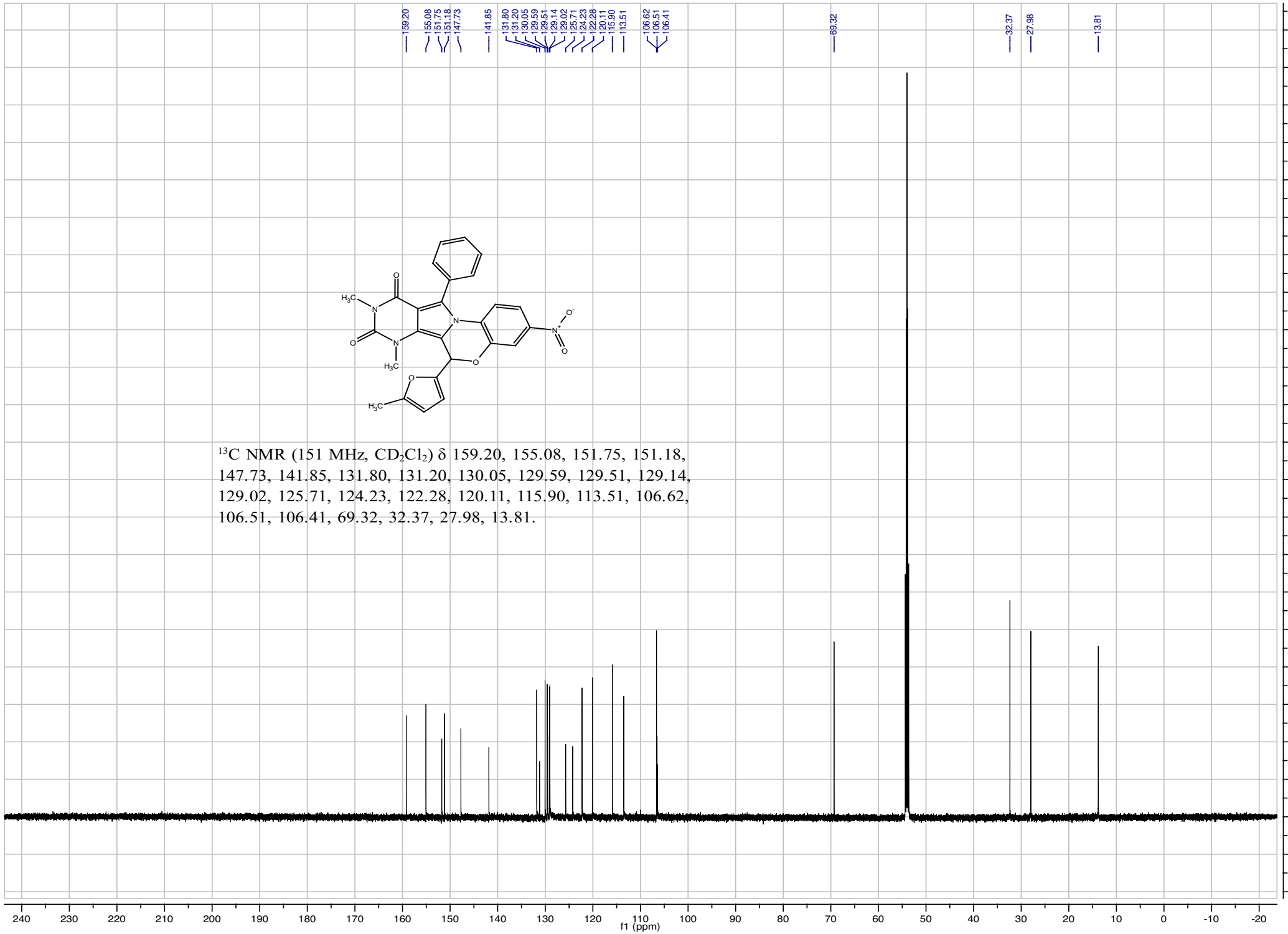
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.10, 151.70, 151.31, 150.71, 142.06, 131.75, 131.63, 130.16, 129.53, 129.32, 129.18, 129.07, 125.55, 124.83, 124.74, 122.43, 120.23, 115.93, 115.22, 112.56, 106.48, 105.26, 68.75, 32.40, 28.01.



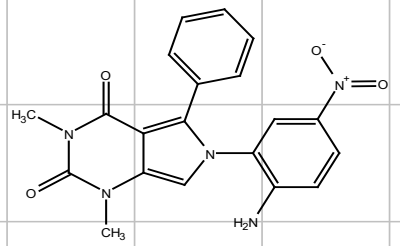
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.89 (dd, *J* = 2.6, 8.9, 1H), 7.84 (d, *J* = 7.7, 1H), 7.68 (t, *J* = 7.6, 1H), 7.57 (t, *J* = 7.5, 1H), 7.39 (d, *J* = 2.4, 1H), 7.36 (t, *J* = 7.6, 1H), 7.14 (d, *J* = 8.9, 1H), 7.07 (d, *J* = 7.7, 1H), 6.90 (s, 1H), 5.91 (d, *J* = 3.1, 1H), 5.79 (d, *J* = 2.9, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 2.20 (s, 3H).



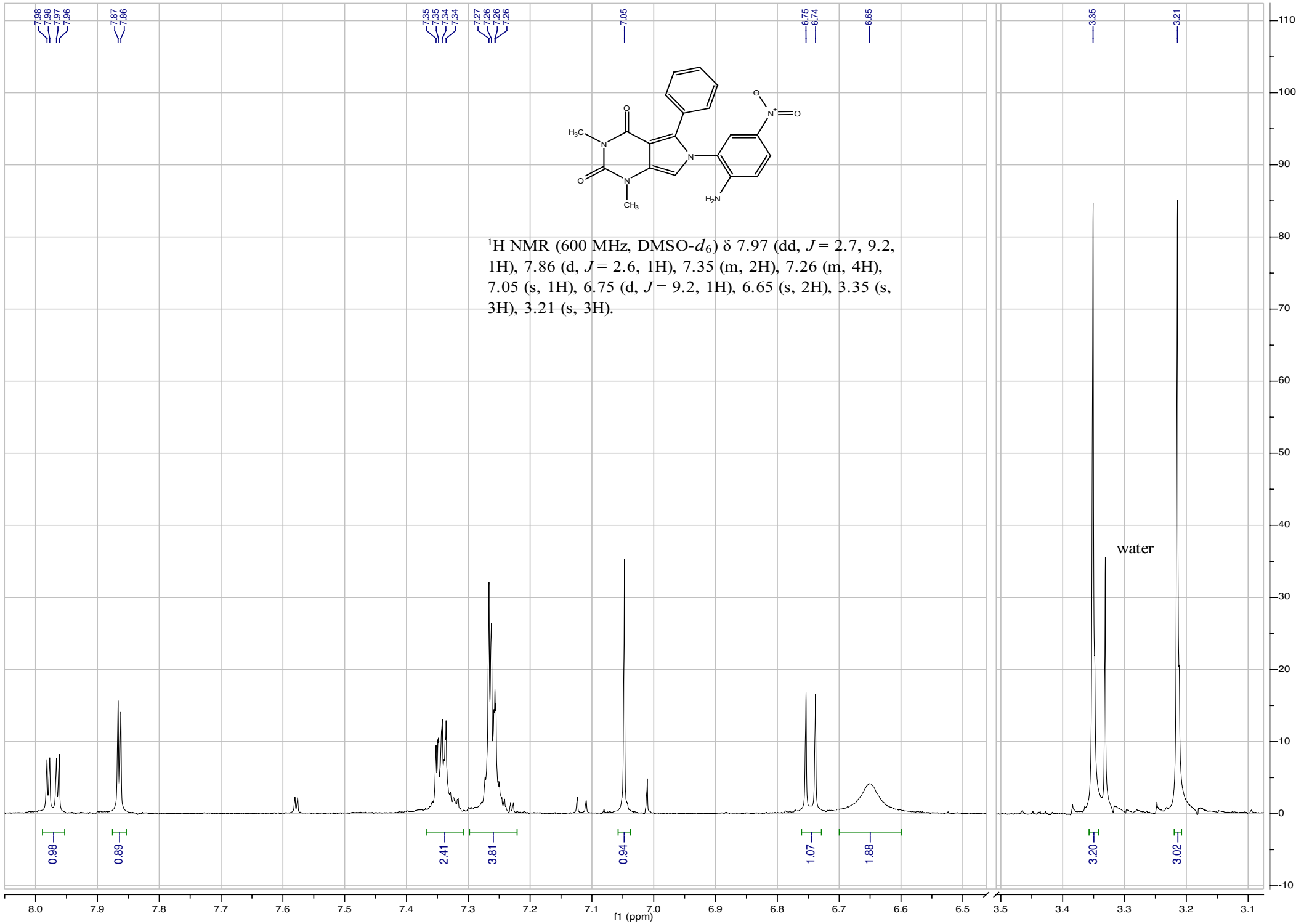
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.89 (dd, *J* = 2.6, 8.9, 1H), 7.84 (d, *J* = 7.7, 1H), 7.68 (t, *J* = 7.6, 1H), 7.57 (t, *J* = 7.5, 1H), 7.39 (d, *J* = 2.4, 1H), 7.36 (t, *J* = 7.6, 1H), 7.14 (d, *J* = 8.9, 1H), 7.07 (d, *J* = 7.7, 1H), 6.90 (s, 1H), 5.91 (d, *J* = 3.1, 1H), 5.79 (d, *J* = 2.9, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 2.20 (s, 3H).



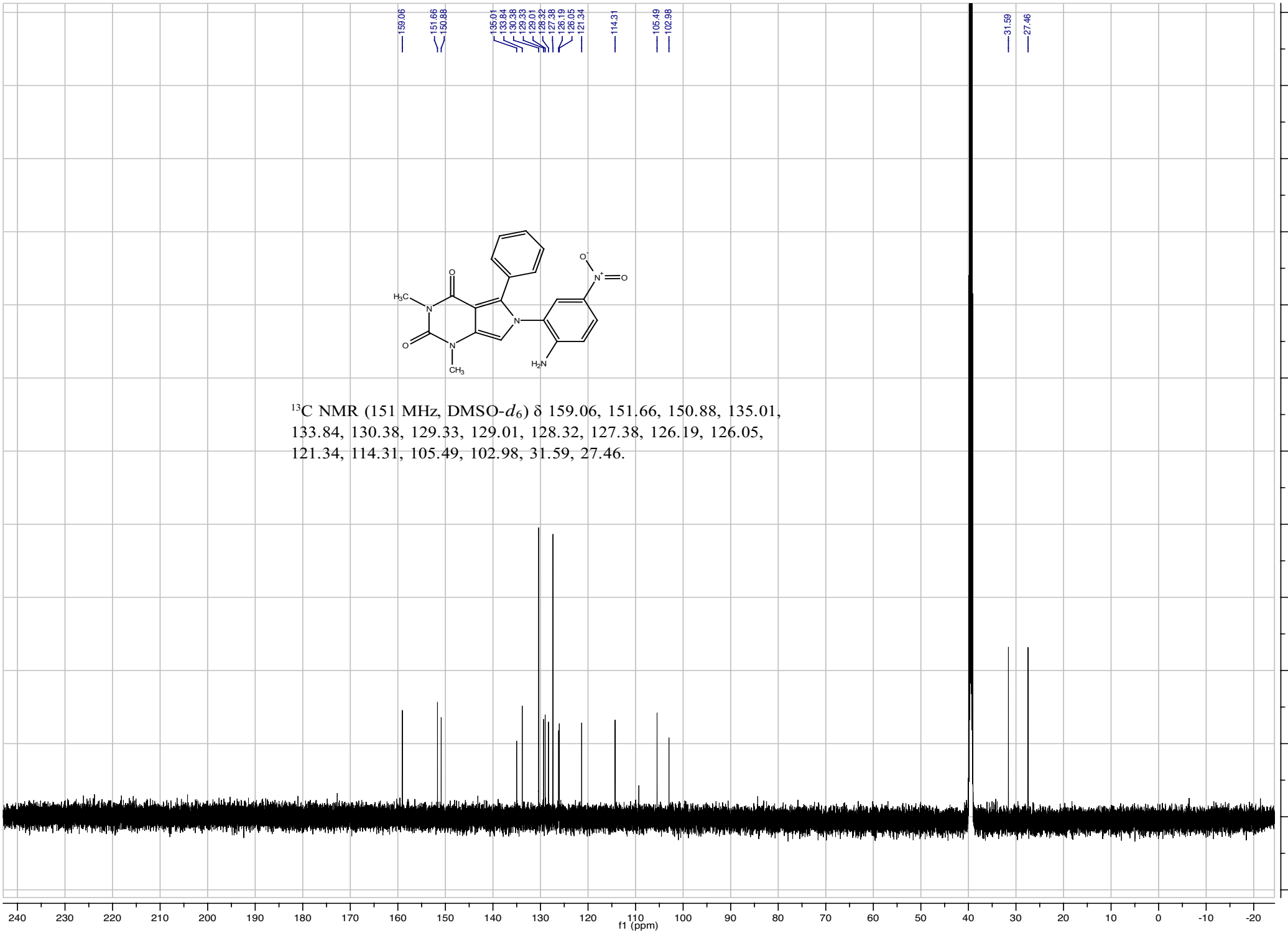
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.20, 155.08, 151.75, 151.18, 147.73, 141.85, 131.80, 131.20, 130.05, 129.59, 129.51, 129.14, 129.02, 125.71, 124.23, 122.28, 120.11, 115.90, 113.51, 106.62, 106.51, 106.41, 69.32, 32.37, 27.98, 13.81.



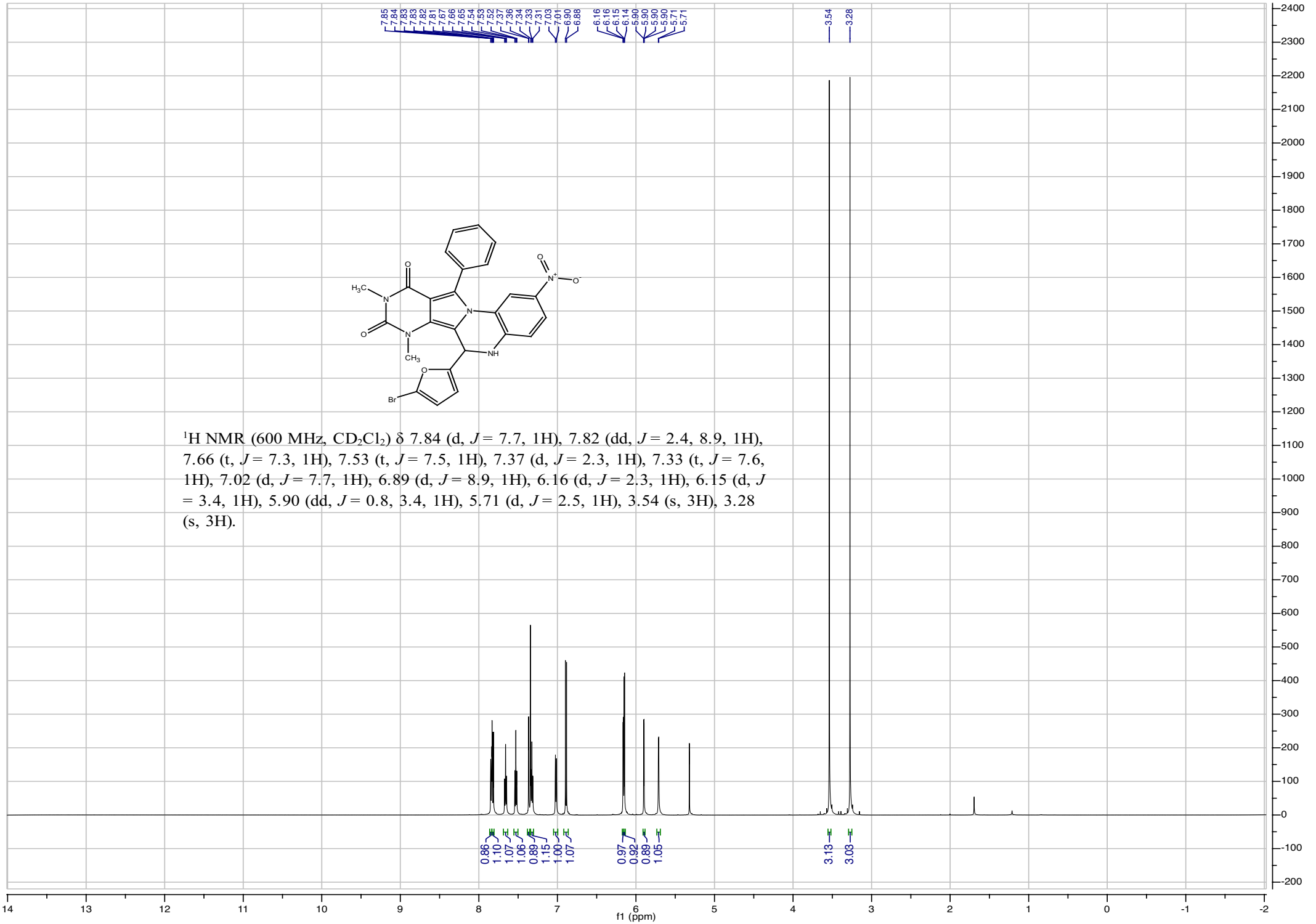
^{1}H NMR (600 MHz, DMSO-d_6) δ 7.97 (dd, J = 2.7, 9.2, 1H), 7.86 (d, J = 2.6, 1H), 7.35 (m, 2H), 7.26 (m, 4H), 7.05 (s, 1H), 6.75 (d, J = 9.2, 1H), 6.65 (s, 2H), 3.35 (s, 3H), 3.21 (s, 3H).



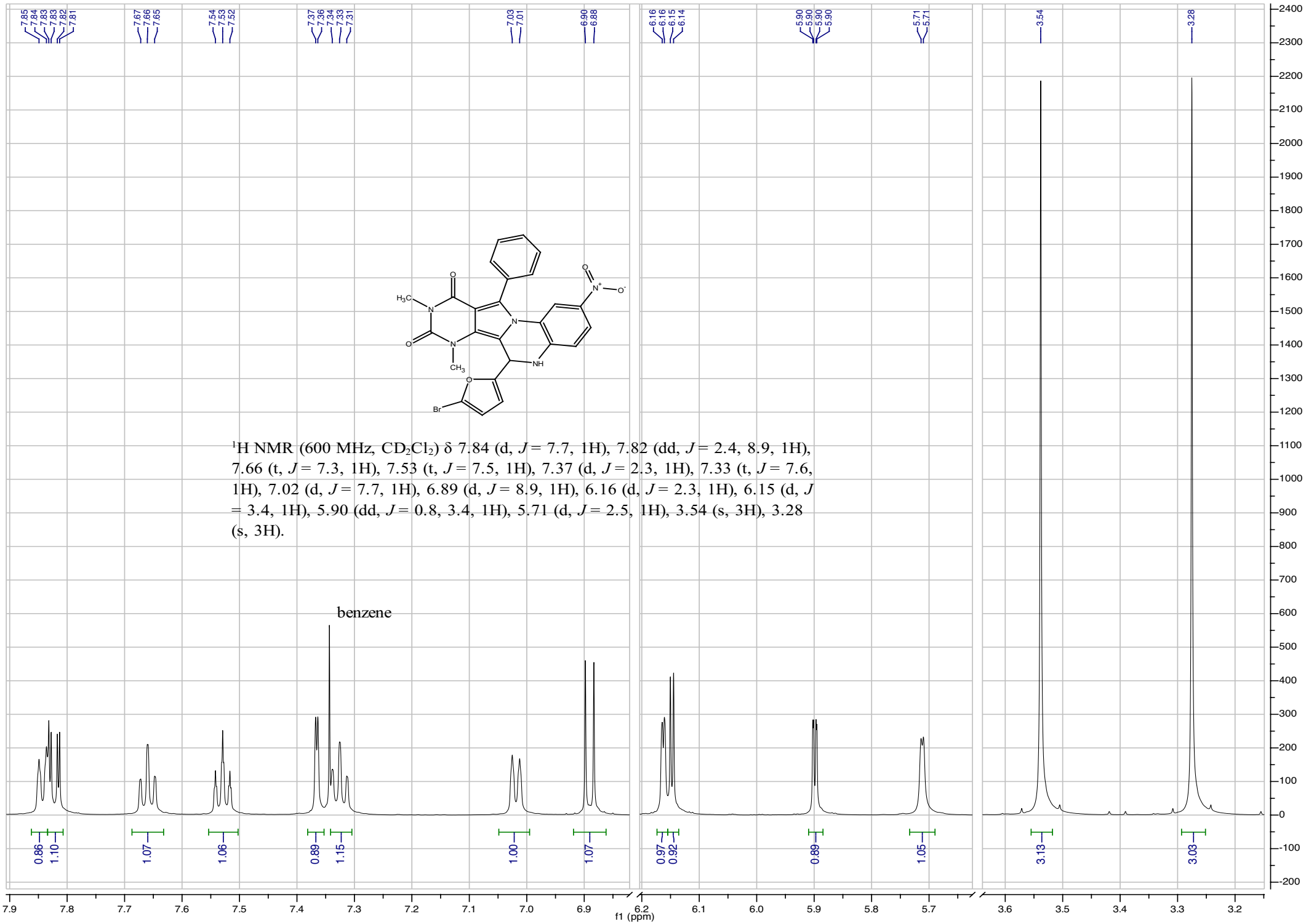
[1]H NMR (600 MHz, DMSO-d_6) δ 7.97 (dd, J = 2.7, 9.2, 1H), 7.86 (d, J = 2.6, 1H), 7.35 (m, 2H), 7.26 (m, 4H), 7.05 (s, 1H), 6.75 (d, J = 9.2, 1H), 6.65 (s, 2H), 3.35 (s, 3H), 3.21 (s, 3H).



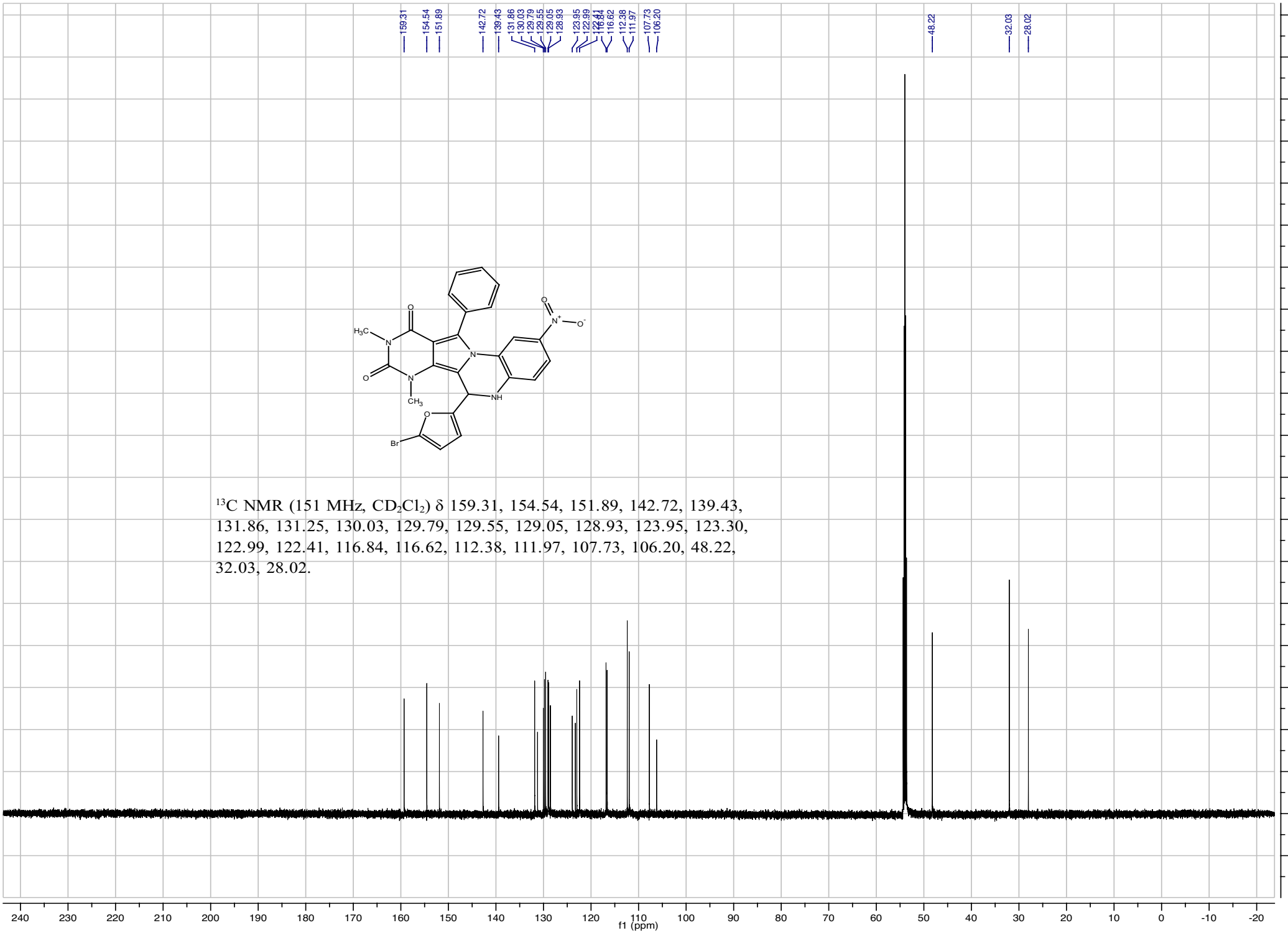
^{13}C NMR (151 MHz, DMSO-d_6) δ 159.06, 151.66, 150.88, 135.01, 133.84, 130.38, 129.33, 129.01, 128.32, 127.38, 126.19, 126.05, 121.34, 114.31, 105.49, 102.98, 31.59, 27.46.



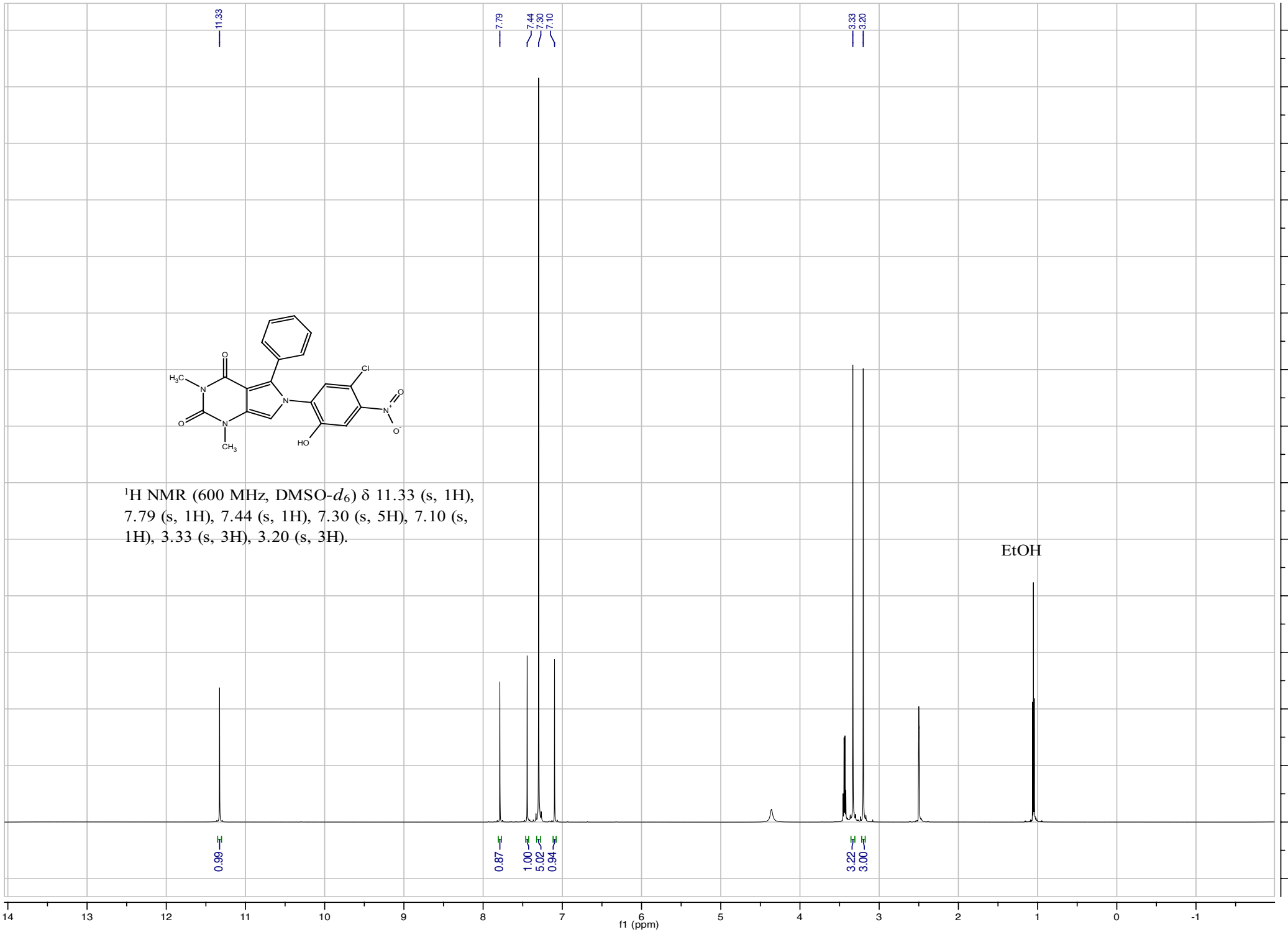
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.84 (d, J = 7.7, 1H), 7.82 (dd, J = 2.4, 8.9, 1H), 7.66 (t, J = 7.3, 1H), 7.53 (t, J = 7.5, 1H), 7.37 (d, J = 2.3, 1H), 7.33 (t, J = 7.6, 1H), 7.02 (d, J = 7.7, 1H), 6.89 (d, J = 8.9, 1H), 6.16 (d, J = 2.3, 1H), 6.15 (d, J = 3.4, 1H), 5.90 (dd, J = 0.8, 3.4, 1H), 5.71 (d, J = 2.5, 1H), 3.54 (s, 3H), 3.28 (s, 3H).



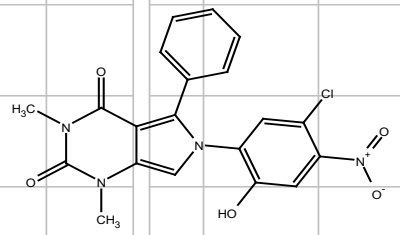
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.84 (d, *J* = 7.7, 1H), 7.82 (dd, *J* = 2.4, 8.9, 1H), 7.66 (t, *J* = 7.3, 1H), 7.53 (t, *J* = 7.5, 1H), 7.37 (d, *J* = 2.3, 1H), 7.33 (t, *J* = 7.6, 1H), 7.02 (d, *J* = 7.7, 1H), 6.89 (d, *J* = 8.9, 1H), 6.16 (d, *J* = 2.3, 1H), 6.15 (d, *J* = 3.4, 1H), 5.90 (dd, *J* = 0.8, 3.4, 1H), 5.71 (d, *J* = 2.5, 1H), 3.54 (s, 3H), 3.28 (s, 3H).



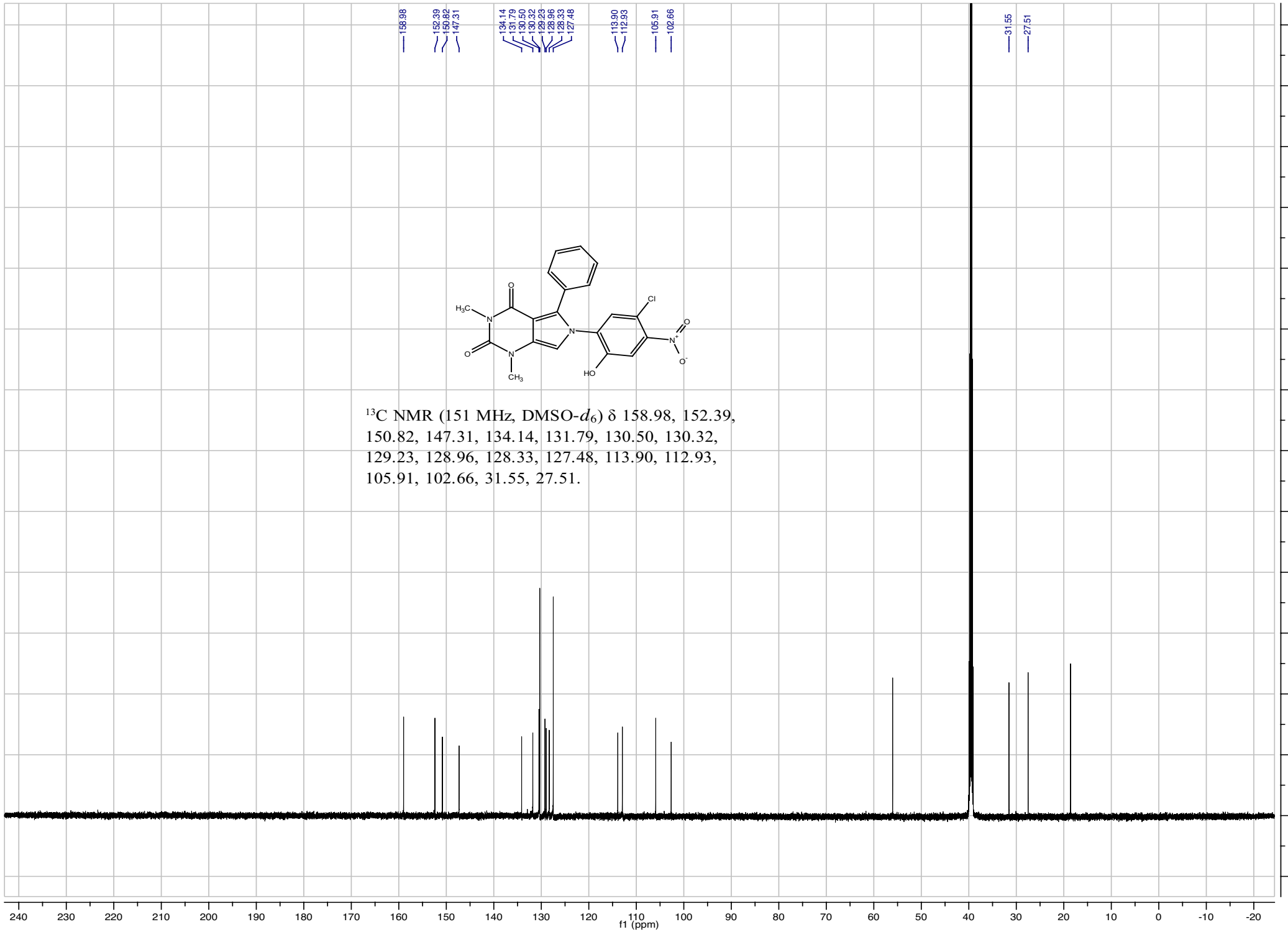
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.31, 154.54, 151.89, 142.72, 139.43, 131.86, 131.25, 130.03, 129.79, 129.55, 129.05, 128.93, 123.95, 123.30, 122.99, 122.41, 116.84, 116.62, 112.38, 111.97, 107.73, 106.20, 48.22, 32.03, 28.02.



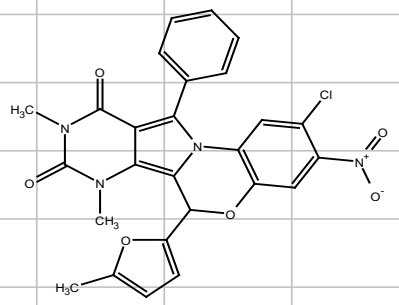
^{1}H NMR (600 MHz, DMSO-d_6) δ 11.33 (s, 1H), 7.79 (s, 1H), 7.44 (s, 1H), 7.30 (s, 5H), 7.10 (s, 1H), 3.33 (s, 3H), 3.20 (s, 3H).



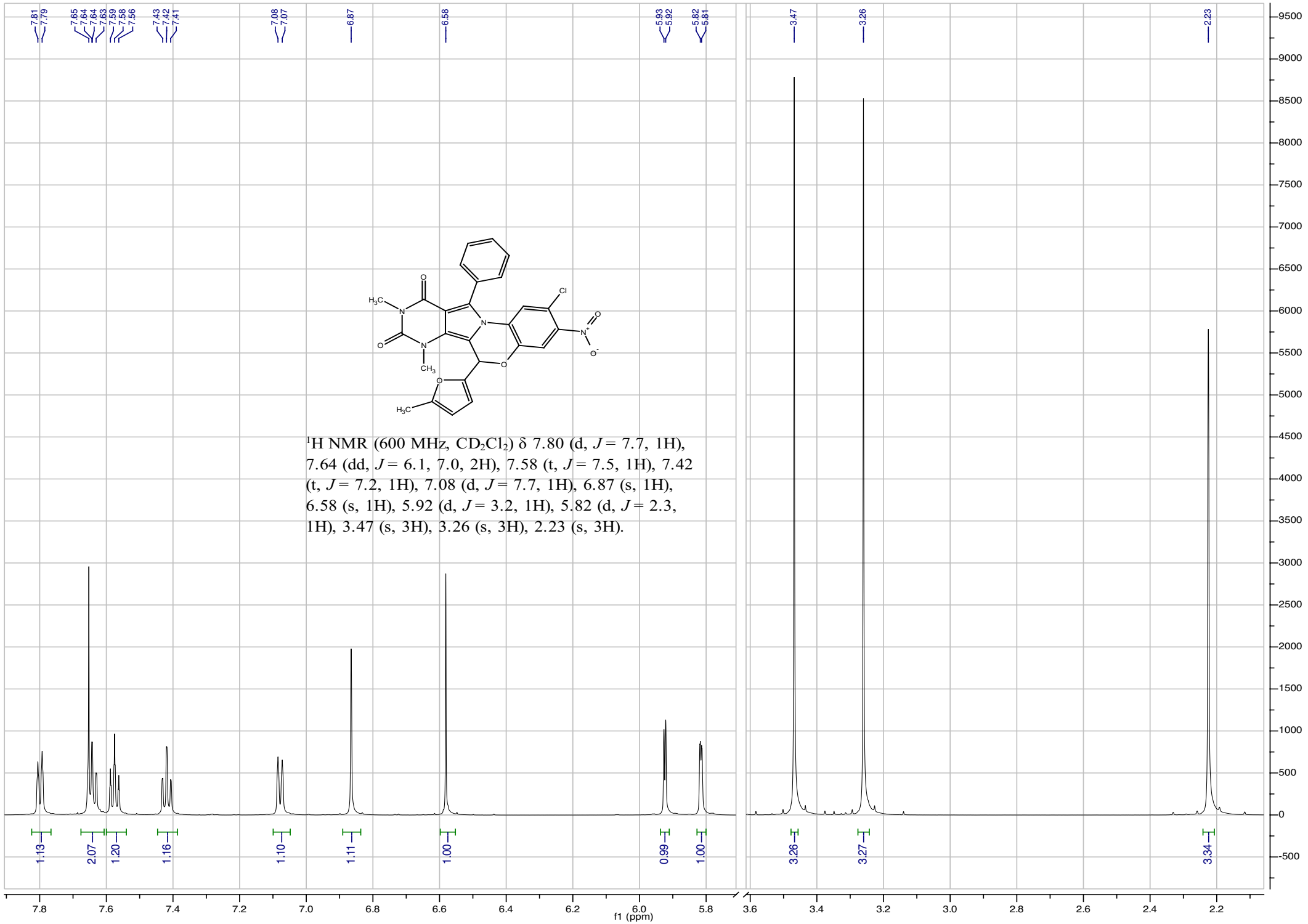
^{1}H NMR (600 MHz, DMSO-d_6) δ 11.33 (s, 1H), 7.79 (s, 1H), 7.44 (s, 1H), 7.30 (s, 5H), 7.10 (s, 1H), 3.33 (s, 3H), 3.20 (s, 3H).



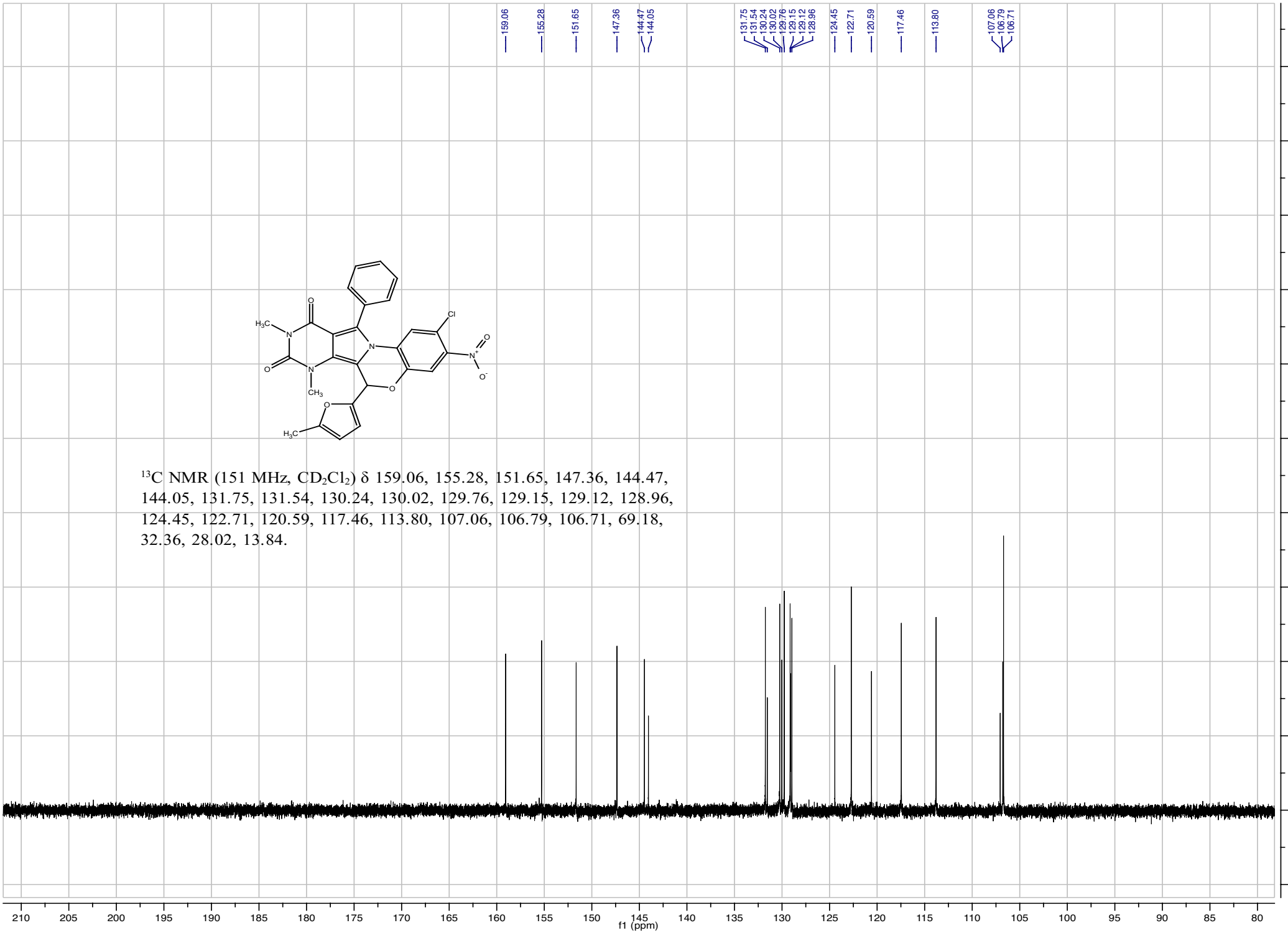
^{13}C NMR (151 MHz, DMSO-d_6) δ 158.98, 152.39, 150.82, 147.31, 134.14, 131.79, 130.50, 130.32, 129.23, 128.96, 128.33, 127.48, 113.90, 112.93, 105.91, 102.66, 31.55, 27.51.



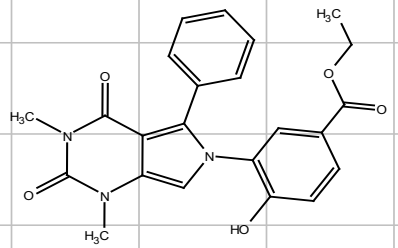
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, J = 7.7, 1H), 7.64 (dd, J = 6.1, 7.0, 2H), 7.58 (t, J = 7.5, 1H), 7.42 (t, J = 7.2, 1H), 7.08 (d, J = 7.7, 1H), 6.87 (s, 1H), 6.58 (s, 1H), 5.92 (d, J = 3.2, 1H), 5.82 (d, J = 2.3, 1H), 3.47 (s, 3H), 3.26 (s, 3H), 2.23 (s, 3H).



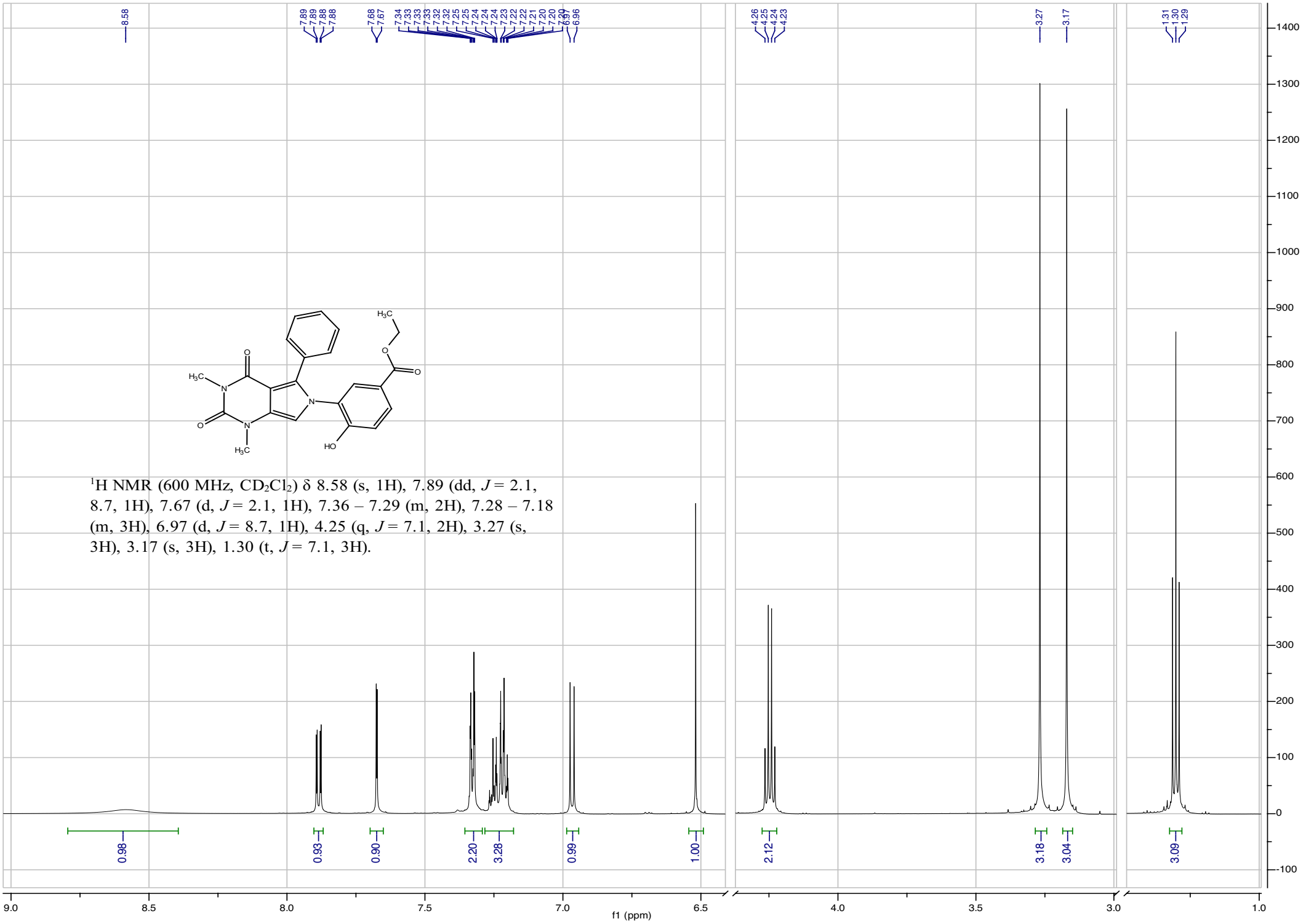
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.80 (d, J = 7.7, 1H), 7.64 (dd, J = 6.1, 7.0, 2H), 7.58 (t, J = 7.5, 1H), 7.42 (t, J = 7.2, 1H), 7.08 (d, J = 7.7, 1H), 6.87 (s, 1H), 6.58 (s, 1H), 5.92 (d, J = 3.2, 1H), 5.82 (d, J = 2.3, 1H), 3.47 (s, 3H), 3.26 (s, 3H), 2.23 (s, 3H).



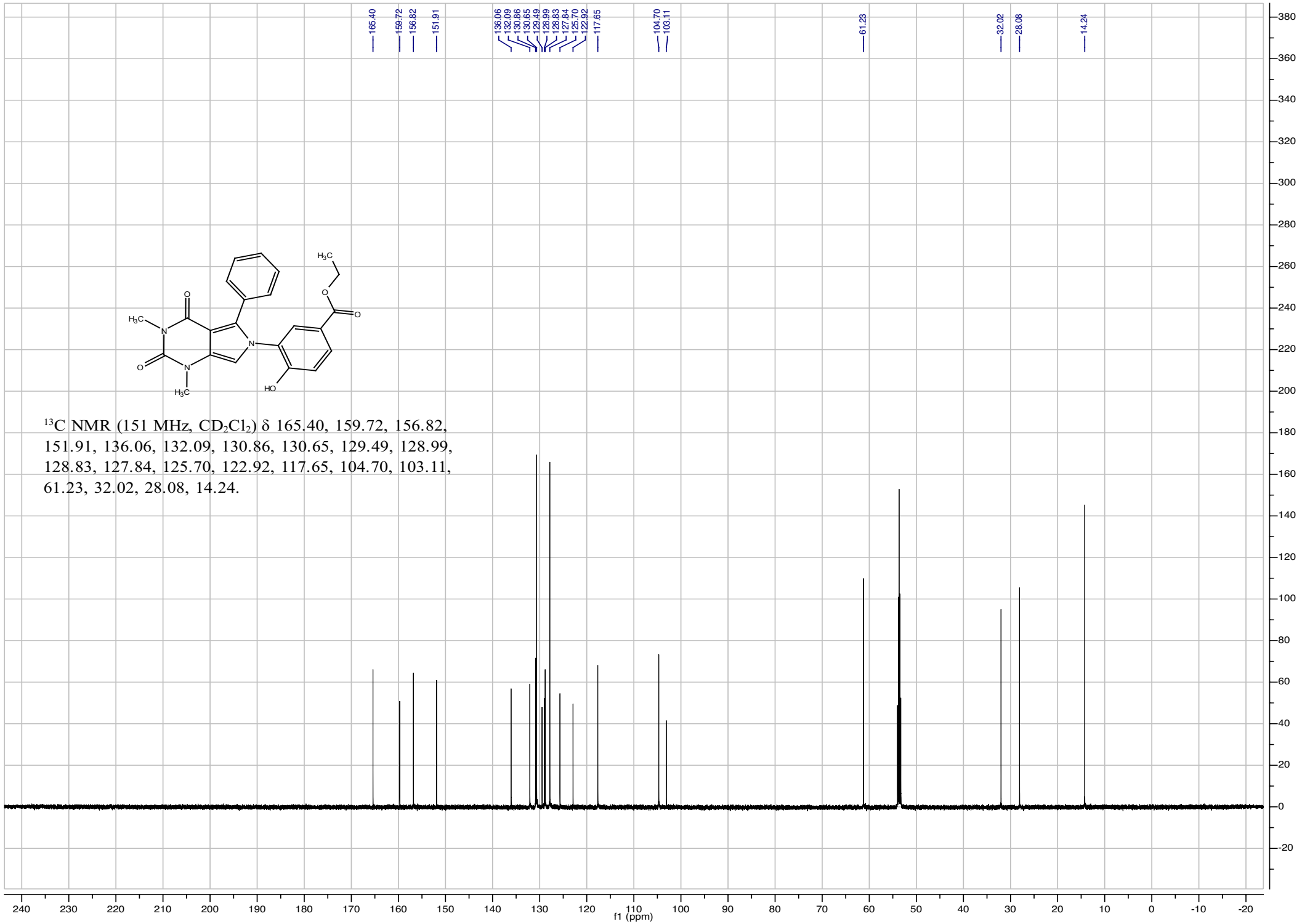
^{13}C NMR (151 MHz, CD_2Cl_2) δ 159.06, 155.28, 151.65, 147.36, 144.47, 144.05, 131.75, 131.54, 130.24, 130.02, 129.76, 129.15, 129.12, 128.96, 124.45, 122.71, 120.59, 117.46, 113.80, 107.06, 106.79, 106.71, 69.18, 32.36, 28.02, 13.84.



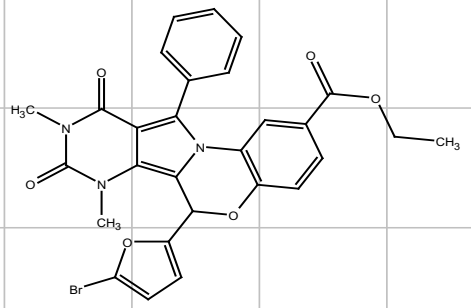
^{1}H NMR (600 MHz, CD_2Cl_2) δ 8.58 (s, 1H), 7.89 (dd, *J* = 2.1, 8.7, 1H), 7.67 (d, *J* = 2.1, 1H), 7.36 – 7.29 (m, 2H), 7.28 – 7.18 (m, 3H), 6.97 (d, *J* = 8.7, 1H), 4.25 (q, *J* = 7.1, 2H), 3.27 (s, 3H), 3.17 (s, 3H), 1.30 (t, *J* = 7.1, 3H).



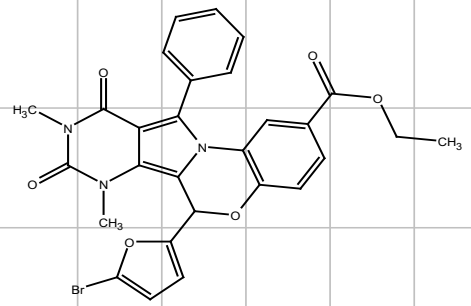
^{1}H NMR (600 MHz, CD_2Cl_2) δ 8.58 (s, 1H), 7.89 (dd, J = 2.1, 8.7, 1H), 7.67 (d, J = 2.1, 1H), 7.36 – 7.29 (m, 2H), 7.28 – 7.18 (m, 3H), 6.97 (d, J = 8.7, 1H), 4.25 (q, J = 7.1, 2H), 3.27 (s, 3H), 3.17 (s, 3H), 1.30 (t, J = 7.1, 3H).



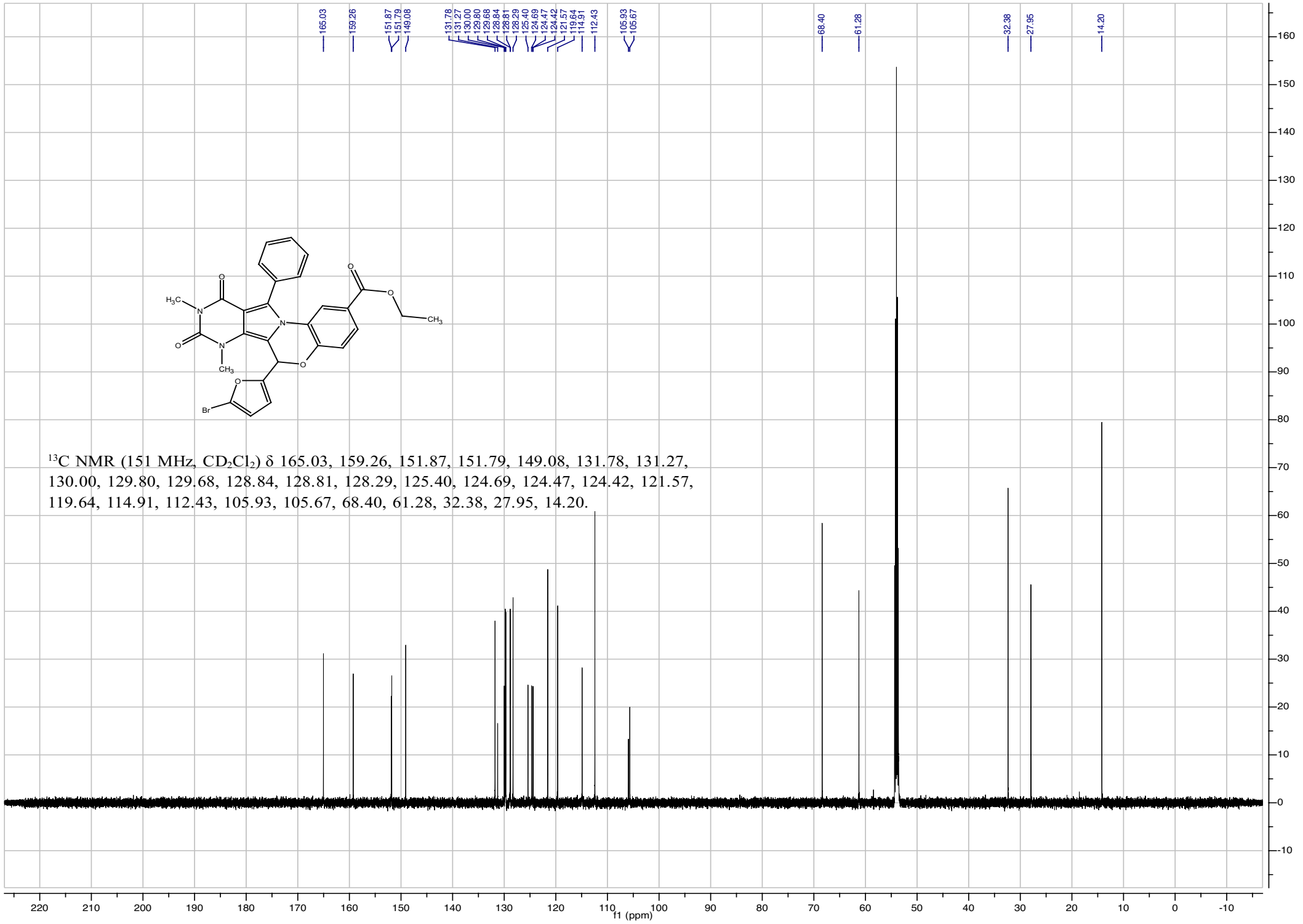
^{13}C NMR (151 MHz, CD_2Cl_2) δ 165.40, 159.72, 156.82, 151.91, 136.06, 132.09, 130.86, 130.65, 129.49, 128.99, 128.83, 127.84, 125.70, 122.92, 117.65, 104.70, 103.11, 61.23, 32.02, 28.08, 14.24.



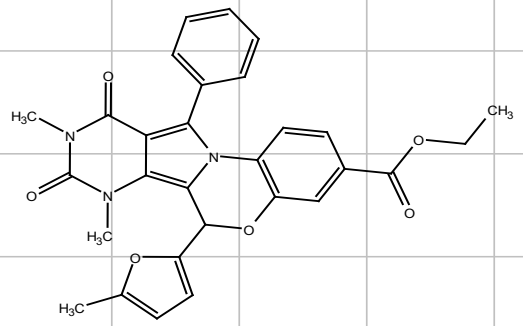
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.68 (dd, *J* = 1.9, 8.4, 1H), 7.63 (t, *J* = 7.5, 1H), 7.52 (t, *J* = 7.5, 1H), 7.34 (t, *J* = 7.5, 1H), 7.23 (d, *J* = 1.8, 1H), 7.09 (d, *J* = 8.4, 1H), 7.06 (d, *J* = 7.7, 1H), 6.86 (s, 1H), 6.14 (d, *J* = 3.4, 1H), 5.98 (d, *J* = 2.9, 1H), 4.11 (dq, *J* = 7.2, 10.7, 1H), 4.00 (dq, *J* = 7.1, 10.7, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 1.14 (t, *J* = 7.1, 3H).



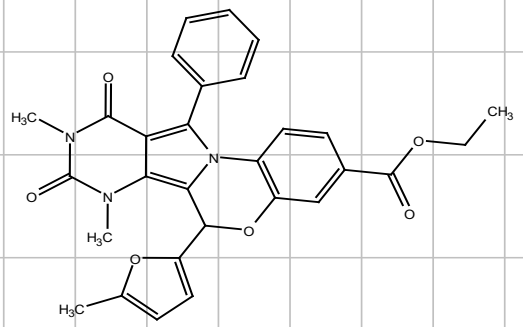
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, J = 7.7, 1H), 7.68 (dd, J = 1.9, 8.4, 1H), 7.63 (t, J = 7.5, 1H), 7.52 (t, J = 7.5, 1H), 7.34 (t, J = 7.5, 1H), 7.23 (d, J = 1.8, 1H), 7.09 (d, J = 8.4, 1H), 7.06 (d, J = 7.7, 1H), 6.86 (s, 1H), 6.14 (d, J = 3.4, 1H), 5.98 (d, J = 2.9, 1H), 4.11 (dq, J = 7.2, 10.7, 1H), 4.00 (dq, J = 7.1, 10.7, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 1.14 (t, J = 7.1, 3H).



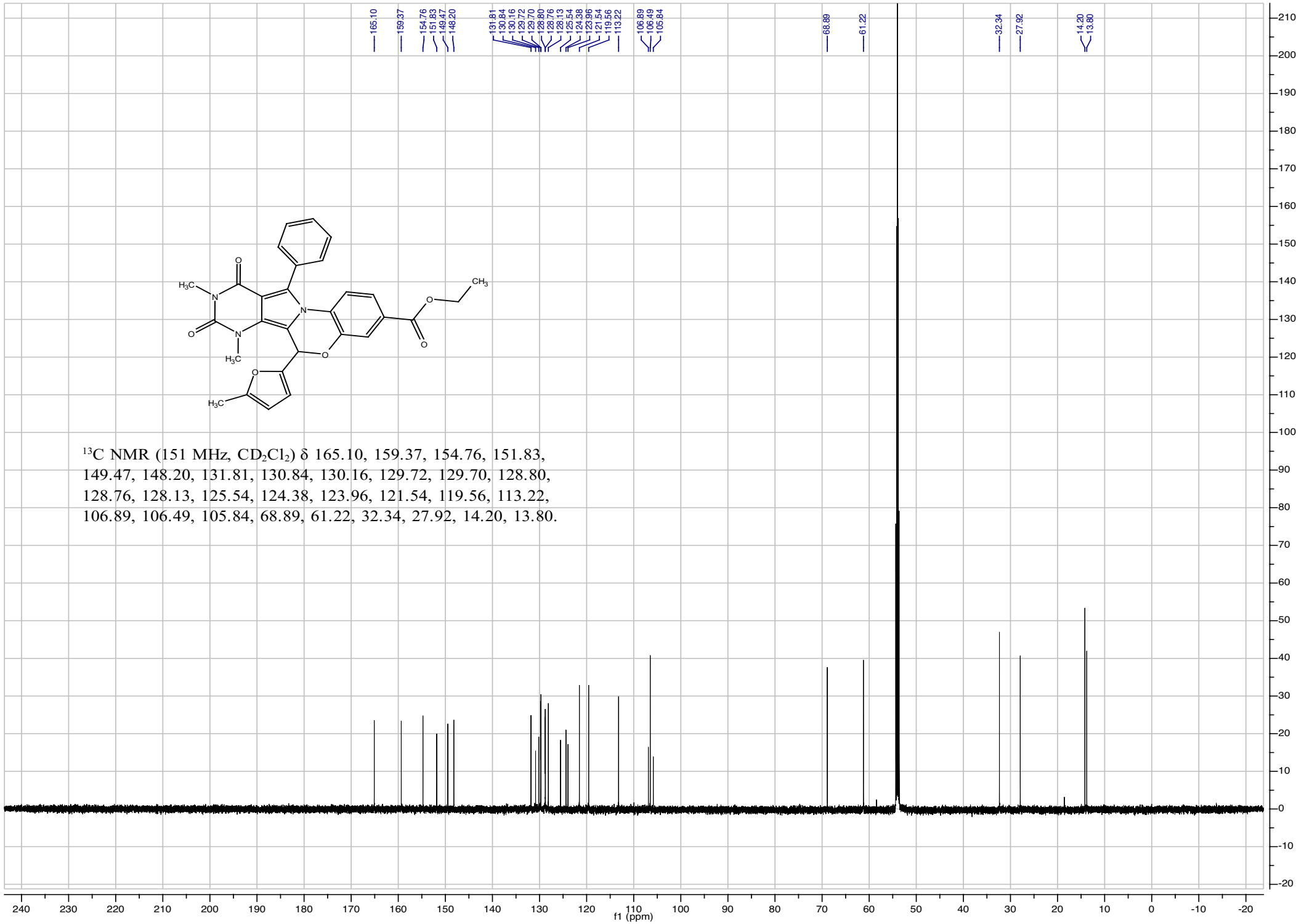
^{13}C NMR (151 MHz, CD_2Cl_2) δ 165.03, 159.26, 151.87, 151.79, 149.08, 131.78, 131.27, 130.00, 129.80, 129.68, 128.84, 128.81, 128.29, 125.40, 124.69, 124.47, 124.42, 121.57, 119.64, 114.91, 112.43, 105.93, 105.67, 68.40, 61.28, 32.38, 27.95, 14.20.



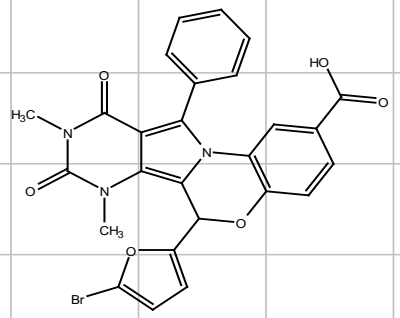
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, J = 7.7, 1H), 7.67 (dd, J = 1.9, 8.4, 1H), 7.63 (t, J = 7.5, 1H), 7.52 (t, J = 7.5, 1H), 7.34 (t, J = 7.5, 1H), 7.23 (d, J = 1.8, 1H), 7.09 – 7.02 (m, J = 4.5, 8.0, 2H), 6.83 (s, 1H), 5.85 (d, J = 3.2, 1H), 5.76 (d, J = 2.5, 1H), 4.10 (dq, J = 7.1, 10.7, 1H), 3.99 (dq, J = 7.1, 10.7, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 2.21 (s, 3H), 1.14 (t, J =



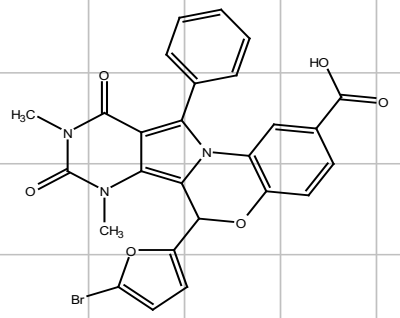
^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.81 (d, *J* = 7.7, 1H), 7.67 (dd, *J* = 1.9, 8.4, 1H), 7.63 (t, *J* = 7.5, 1H), 7.52 (t, *J* = 7.5, 1H), 7.34 (t, *J* = 7.5, 1H), 7.23 (d, *J* = 1.8, 1H), 7.09 – 7.02 (m, *J* = 4.5, 8.0, 2H), 6.83 (s, 1H), 5.85 (d, *J* = 3.2, 1H), 5.76 (d, *J* = 2.5, 1H), 4.10 (dq, *J* = 7.1, 10.7, 1H), 3.99 (dq, *J* = 7.1, 10.7, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 2.21 (s, 3H), 1.14 (t, *J* =



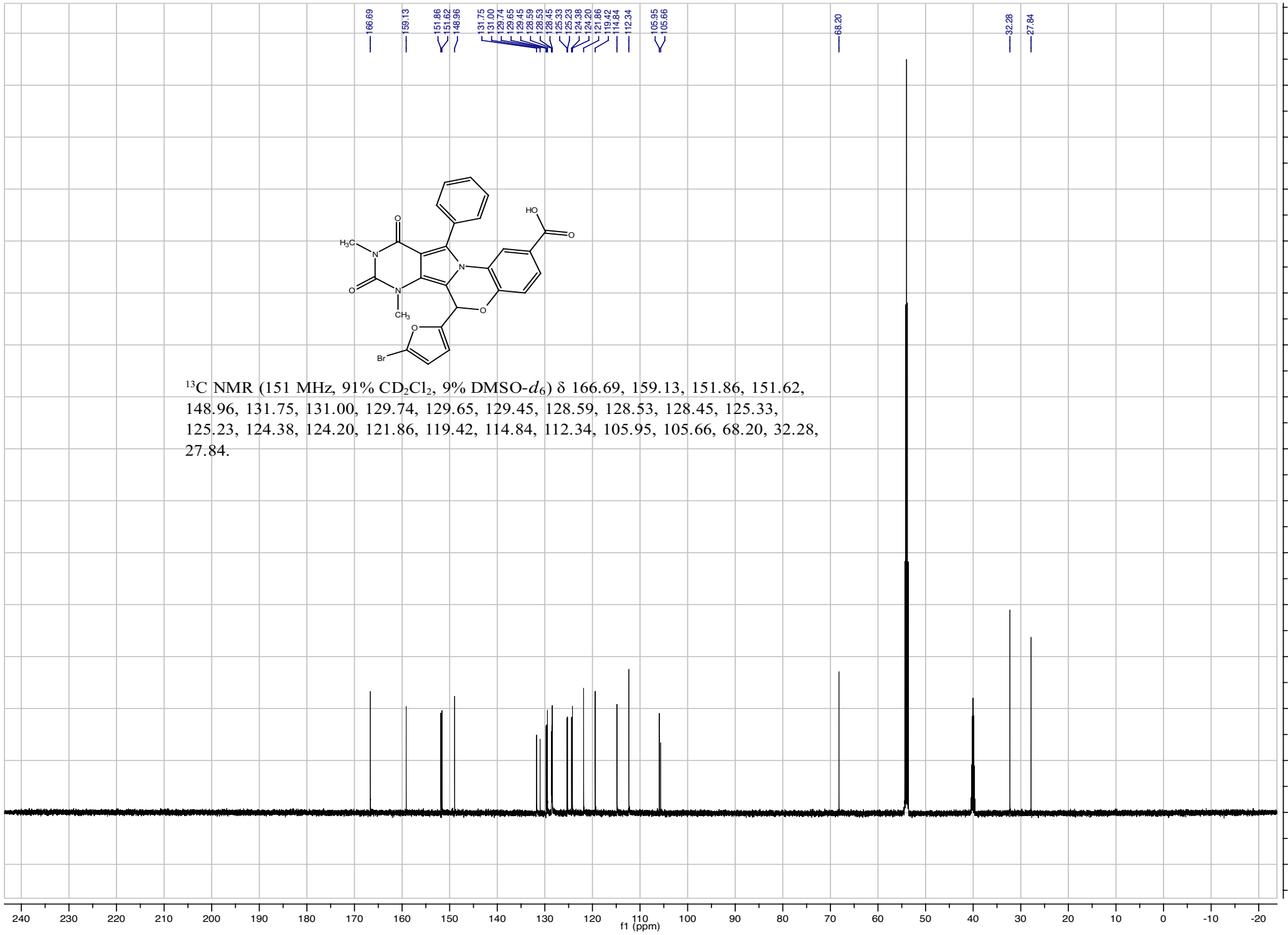
^{13}C NMR (151 MHz, CD_2Cl_2) δ 165.10, 159.37, 154.76, 151.83, 149.47, 148.20, 131.81, 130.84, 130.16, 129.72, 129.70, 128.80, 128.76, 128.13, 125.54, 124.38, 123.96, 121.54, 119.56, 113.22, 106.89, 106.49, 105.84, 68.89, 61.22, 32.34, 27.92, 14.20, 13.80.



^{1}H NMR (600 MHz, 91% CD_2Cl_2, 9% DMSO-d_6) δ 12.30 (s, 1H), 7.79 (d, J = 7.7, 1H), 7.63 (dd, J = 1.9, 8.4, 1H), 7.58 (t, J = 7.6, 1H), 7.46 (t, J = 7.5, 1H), 7.29 (t, J = 7.5, 1H), 7.17 (d, J = 1.7, 1H), 7.04 (d, J = 8.4, 1H), 7.01 (d, J = 7.7, 1H), 6.89 (s, 1H), 6.12 (d, J = 3.4, 1H), 5.96 (d, J = 3.3, 1H), 3.44 (s, 3H), 3.21 (s, 3H).



^{1}H NMR (600 MHz, 91% CD_2Cl_2, 9% DMSO-d_6) δ 12.30 (s, 1H), 7.79 (d, J = 7.7, 1H), 7.63 (dd, J = 1.9, 8.4, 1H), 7.58 (t, J = 7.6, 1H), 7.46 (t, J = 7.5, 1H), 7.29 (t, J = 7.5, 1H), 7.17 (d, J = 1.7, 1H), 7.04 (d, J = 8.4, 1H), 7.01 (d, J = 7.7, 1H), 6.89 (s, 1H), 6.12 (d, J = 3.4, 1H), 5.96 (d, J = 3.3, 1H), 3.44 (s, 3H), 3.21 (s, 3H).



^{13}C NMR (151 MHz, 91% CD_2Cl_2, 9% DMSO-d_6) δ 166.69, 159.13, 151.86, 151.62, 148.96, 131.75, 131.00, 129.74, 129.65, 129.45, 128.59, 128.53, 128.45, 125.33, 125.23, 124.38, 124.20, 121.86, 119.42, 114.84, 112.34, 105.95, 105.66, 68.20, 32.28, 27.84.