Photoinitiated Cascade for Rapid Access to Pyrroloquinazolinone Core of Vasicinone, Luotonins and Related Alkaloids

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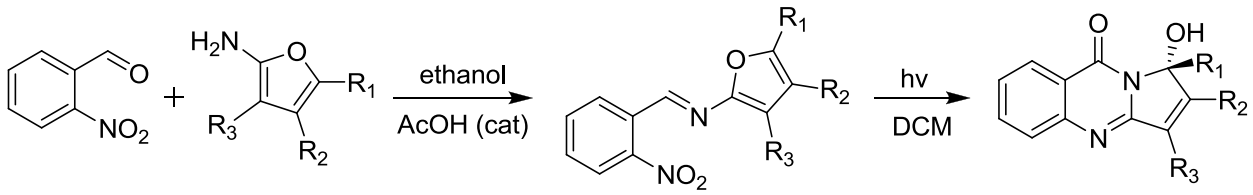
SUPPORTING INFORMATION

Contents

1. Experimental Procedures and Characterization Data

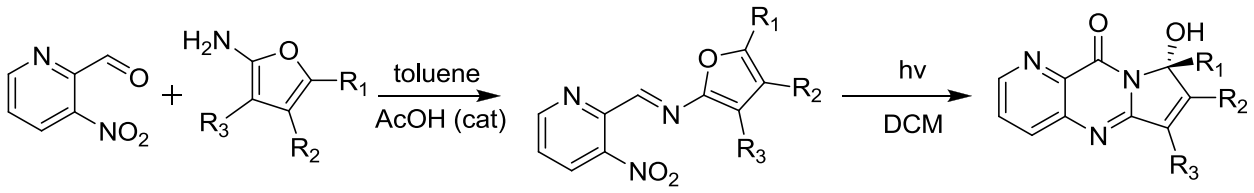
Common solvents were purchased from Fisher Scientific and used as is. Common reagents, aldehydes and aminofurans, were purchased from Sigma-Aldrich, TCI America, AK Scientific, Oakwood Chemical or AstaTech and used without additional purification. NMR spectra were recorded at 25 °C on a Bruker Avance III 500 MHz instrument in $CDCl_3$ with TMS as an internal standard (unless noted otherwise). X-Ray structures were obtained with a Bruker APEX II instrument. High resolution mass spectra were obtained on a Waters Synapt G2 HDMS Quadrupole/ToF mass spectrometer with electrospray ionization (Central Analytical Laboratory, University of Colorado Boulder) by Dr. D. Sai Reddy and Dmitry Kuznetsov. Flash column chromatography was performed using Teledyne Ultra-Pure Silica Gel (230 – 400 mesh) on a Teledyne Isco Combiflash Rf.

General procedure A:



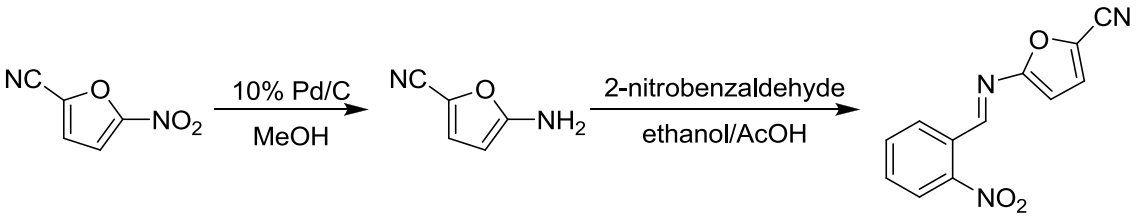
To a stirred solution of nitro aldehyde (0.95 mmol) in ethanol (10 mL), primary aniline (0.95 mmol) and 6-8 drops of acetic acid was added at 20 °C and the mixture was stirred at 50 °C for 3-5 hrs. After that another 0.5 eq (0.475 mmol) of primary aniline was added and the reaction was stirred at 50 °C for 3-5 hrs (imine formation was monitored by ^{1}H NMR). After completion of the reaction, the solvent was removed under vacuum and dissolved in CH_2Cl_2 (50 ml). The CH_2Cl_2 layer was washed with saturated $NaHCO_3$ solution (10 mL) followed by brine solution (10 mL). The CH_2Cl_2 layer was dried over anhydrous Na_2SO_4, filtered and diluted with CH_2Cl_2 to 0.01M. This solution was then irradiated with UV LED-based illuminator, seven 2.9 W @ 365 nm LED Engin chips (or two for **1f**); the reaction progress was monitored by ^{1}H NMR. After completion of the reaction, the solvent was removed under vacuum and the residue was subjected to purification by flash chromatography on silica gel.

General procedure B:



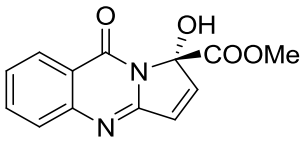
To a stirred solution of nitro aldehyde (1.05 mmol) in toluene (10 mL), primary aniline (1.05 mmol) and 6-8 drops of acetic acid was added at 20 °C and the mixture was stirred at 70 °C for 3-5 hrs. After that another 0.5 eq (0.525 mmol) of primary aniline was added to the reaction mixture and stirring was continued at 70 °C for 3-5 hrs (imine formation was monitored by ^{1}H NMR). After completion of the reaction, the solvent was removed under vacuum and the residue was dissolved in CH_2Cl_2 (50 ml). The CH_2Cl_2 layer was washed saturated $NaHCO_3$ solution (10 mL) followed by brine solution (10 mL). The CH_2Cl_2 layer was dried over anhydrous Na_2SO_4, filtered and diluted with CH_2Cl_2 to 0.01M. This solution was then irradiated with UV LED-based illuminator, seven 2.9 W @ 365 nm LED Engin chips (or two for 1f), the reaction progress was monitored by ^{1}H NMR. After completion of the reaction, the solvent was removed under vacuum and the residue was subjected to purification by flash chromatography on silica gel.

(E)-5-(2-nitrobenzylideneamino)furan-2-carbonitrile (3ae)

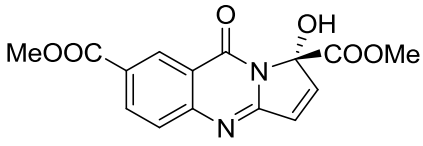


10% Pd/C (25 mg, 0.1 w/w) was added to a stirred solution of 5-nitrofuran-2-carbonitrile (0.25 g, 1.8 mmol) in MeOH (10 mL) at 20 °C and hydrogen pressure was applied using a small balloon. The reaction was stirred for 15 hrs at 20 °C, while the progress was monitored by ^{1}H NMR. The solids were filtered through Celite pad and washed with an additional 10 mL MeOH. The solvent was removed under vacuum to yield a crude product as brown oil. The crude product was redissolved in ethanol (15 mL) and to this solution was added 2-ntrobenzaldehyde (0.273 g, 1.8 mmol) and 6-8 drops of acetic acid. The resulting mixture was stirred at 50 °C for 6 h. After completion of the reaction, the solvent was removed under vacuum and the residue was dissolved in CH_2Cl_2 (100 ml). The CH_2Cl_2 layer was washed saturated $NaHCO_3$ solution (20 mL) followed

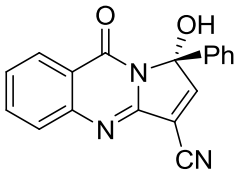
by brine solution (20 mL) and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the crude product was purified by flash chromatography on neutral alumina with a gradient of 5%→35% ethyl acetate in hexanes to afford 277 mg (64%) of **3ae**. Also 65 mg (24%) of 2-ntrobenzaldehyde was recovered. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.55 (d, *J* = 3.7 Hz, 1H), 7.17 (d, *J* = 3.7 Hz, 1H), 7.67 (ddd, *J* = 8.9, 7.4, 1.5 Hz, 1H), 7.75 (tt, *J* = 7.6, 1.1 Hz, 1H), 8.09 (dd, *J* = 8.2, 1.3 Hz, 1H), 8.30 (dd, *J* = 7.8, 1.5 Hz, 1H), 9.23 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.1, 155.2, 149.7, 133.6, 132.3, 129.9, 129.3, 124.9, 124.5, 123.3, 111.5, 107.0.



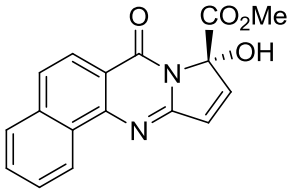
Methyl 1-hydroxy-9-oxo-1,9-dihydropyrrolo[2,1-b]quinazoline-1-carboxylate (4aa): General procedure A was followed on a 0.175 g (1.1 mmol) scale of 2-nitro aldehyde (**1a**). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 5%→30% of ethyl acetate in hexanes to afford 0.23 g (77%) of **4aa** as an off-white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 – 8.22 (m, 1H), 7.82 – 7.71 (m, 2H), 7.50 (ddd, *J* = 8.2, 6.7, 1.7 Hz, 1H), 6.83 – 6.76 (m, 2H), 5.25 (s, 1H), 3.81 (s, 3H).; ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.9, 159.4, 155.7, 149.1, 141.2, 134.8, 129.8, 128.1, 127.5, 126.7, 121.0, 91.3, 54.4; HRMS (ESI) calcd for $C_{13}H_{11}N_2O_4^+$ (MH+) 259.0714, found 259.0725



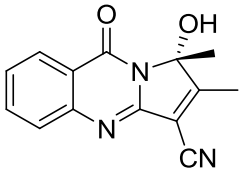
Dimethyl 1-hydroxy-9-oxo-1,9-dihydropyrrolo[2,1-b]quinazoline-1,7-dicarboxylate (4ba): General procedure A was followed on a 0.2 g (0.95 mmol) scale of methyl 3-formyl-4-nitrobenzoate (**4b**). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 5%→25% of ethyl acetate in hexanes to afford 0.21 g (69%) of **4ba** as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.92 (d, *J* = 2.0 Hz, 1H), 8.39 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.79 (d, *J* = 8.5 Hz, 1H), 6.87 (d, *J* = 6.0 Hz, 1H), 6.81 (d, *J* = 6.0 Hz, 1H), 5.04 (br s, 1H), 3.96 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.6, 165.7, 158.8, 157.3, 152.2, 142.2, 135.2, 129.7, 129.1, 129.0, 128.3, 120.9, 91.4, 54.5, 52.5; HRMS (ESI) calcd for $C_{15}H_{13}N_2O_6^+$ (MH+) 317.0769, found 317.0771.



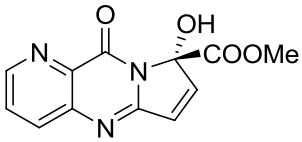
1-Hydroxy-9-oxo-1-phenyl-1,9-dihydropyrrolo[2,1-b]quinazoline-3-carbonitrile (4ab): General procedure A was followed on a 0.15 g (1.3 mmol) scale of 2-nitro aldehyde (**1a**) (Note; during the imine formation observed brown color impurities, after the imine formation, the brown color impurities were removed by filtration of neutral alumina slurry). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 5%→35% of ethyl acetate in hexanes to afford 0.195 g (65%) of **4ab** as a brown solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 7.9 Hz, 1H), 7.89 (d, *J* = 8.1 Hz, 1H), 7.84 (t, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.40 (s, 1H), 7.39 – 7.34 (m, 5H), 5.64 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.7, 155.3, 151.0, 148.7, 135.3, 134.4, 130.1, 129.5, 128.7, 128.4, 126.8, 125.2, 121.3, 111.6, 110.3, 95.9; HRMS (ESI) calcd for $C_{18}H_{12}N_3O_2^+$ (MH+) 302.0925, found 302.0933.



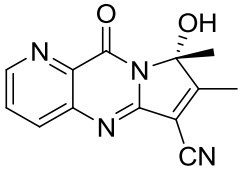
M**ethyl 9-hydroxy-7-oxo-7,9-dihydrobenzo[h]pyrrolo[2,1-b]quinazoline-9-carboxylate (4ca):** General procedure A was followed on a 0.13 g (0.64 mmol) scale of 1-nitro-2-naphthaldehyde (**1c**) (Note; during the imine formation observed brown color impurities, after the imine formation, the brown color impurities were removed by filtration of neutral alumina slurry). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 5%→45% ethyl acetate in hexanes to afford 82 g (41%) of **4ca** as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.05 – 8.98 (m, 1H), 8.19 (d, *J* = 8.7 Hz, 1H), 7.93 (dd, *J* = 6.8, 2.2 Hz, 1H), 7.88 (d, *J* = 8.7 Hz, 1H), 7.72 (tt, *J* = 7.0, 5.2 Hz, 2H), 6.92 (d, *J* = 5.9 Hz, 1H), 6.86 (d, *J* = 5.9 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.9, 159.7, 155.8, 148.1, 141.1, 136.4, 130.3, 130.1, 129.4, 128.0, 127.8, 127.2, 125.2, 121.4, 117.4, 91.6, 54.4; HRMS (ESI) calcd for $C_{17}H_{13}N_2O_4^+$ (MH+) 309.0870, found 309.0878



1-Hydroxy-1,2-dimethyl-9-oxo-1,9-dihydropyrrolo[2,1-b]quinazoline-3-carbonitrile (4ac): General procedure A was followed on a 0.222 g (1.47 mmol) scale of 2-nitro aldehyde (**1a**) (Note; during the imine formation observed brown color impurities, after the imine formation, the brown color impurities were removed by filtration of neutral alumina slurry). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 5%→35% of ethyl acetate in hexanes to afford 0.275 g (74%) of **4ac** as an off-white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.79 – 7.72 (m, 2H), 7.51 – 7.46 (m, 1H), 2.40 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.9, 160.2, 150.2, 148.5, 135.0, 128.1, 127.7, 126.4, 120.9, 110.7, 108.3, 94.4, 22.3, 12.8; HRMS (ESI) calcd for $C_{14}H_{12}N_3O_2^+$ (MH+) 254.0925, found 254.0926.

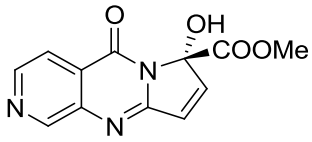


Methyl 8-hydroxy-10-oxo-8,10-dihydropyrido[3,2-d]pyrrolo[1,2-a]pyrimidine-8-carboxylate (4da): General procedure B was followed on a 65 mg (0.42 mmol) scale of 3-nitropicolinaldehyde (**1d**). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 5%→80% of ethyl acetate in hexanes to afford 76 mg (69%) of **4da** as a brown thick oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.88 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.11 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.73 (dd, *J* = 8.3, 4.4 Hz, 1H), 6.91 (d, *J* = 6.0 Hz, 1H), 6.81 (d, *J* = 6.0 Hz, 1H), 3.85 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.3, 157.9, 156.4, 149.9, 146.1, 142.5, 138.2, 136.2, 129.3, 128.7, 91.7, 54.6; HRMS (ESI) calcd for $C_{12}H_{10}N_3O_4^+$ (MH+) 260.0666, found 260.0675

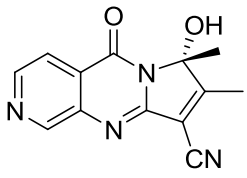


8-Hydroxy-7,8-dimethyl-10-oxo-8,10-dihydropyrido[3,2-d]pyrrolo[1,2-a]pyrimidine-6-carbonitrile (4dc): General procedure B was followed on a 0.16 g (1.05 mmol) scale of 3-nitropicolinaldehyde (**1d**). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 0%→3% of methanol in chloroform to afford 195 mg (73%) of **4dc** as a brown solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.87

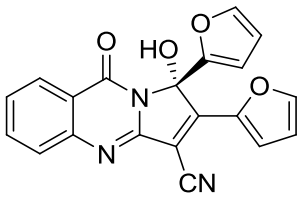
(dd, *J* = 4.4, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.73 (dd, *J* = 8.3, 4.4 Hz, 1H), 5.29 (s, 1H), 2.45 (s, 3H), 2.09 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.3, 158.6, 150.9, 150.1, 145.6, 137.9, 136.4, 128.9, 110.4, 108.0, 95.0, 22.2, 12.9; HRMS (ESI) calcd for $C_{13}H_{11}N_4O_2^+$ (MH+) 255.0877, found 255.0882.



Methyl 7-hydroxy-5-oxo-5,7-dihydropyrido[3,4-d]pyrrolo[1,2-a]pyrimidine-7-carboxylate (4ea): General procedure B was followed on a 128 mg (0.84 mmol) scale of 3-nitropicolinaldehyde X (**1e**). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 0%→10% of methanol in chloroform to afford 165 mg (76%) of **4ea** as a brown solid.^{1}H NMR (500 MHz, $CDCl_3$) δ 9.21 – 9.12 (d, *J* = 0.9 Hz, 1H), 8.79 – 8.63 (d, *J* = 5.1 Hz, 1H), 8.11 – 7.94 (dd, *J* = 5.2, 0.9 Hz, 1H), 6.92 – 6.85 (d, *J* = 6.0 Hz, 1H), 6.84 – 6.77 (d, *J* = 6.0 Hz, 1H), 5.72 – 5.54 (s, 1H), 3.84 – 3.81 (s, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.4, 158.1, 157.3, 151.3, 147.2, 143.7, 142.1, 129.4, 126.4, 118.7, 91.6, 54.6; HRMS (ESI) calcd for $C_{12}H_{10}N_3O_4^+$ (MH+) 260.0666, found 260.0671.



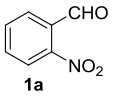
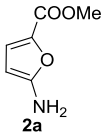
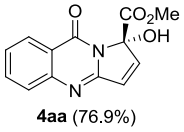
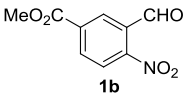
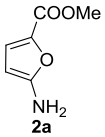
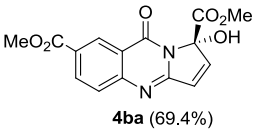
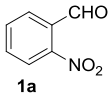
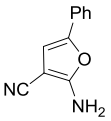
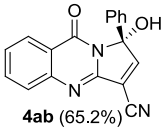
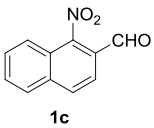
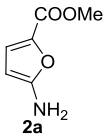
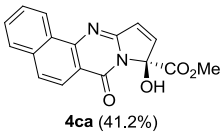
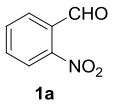
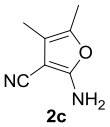
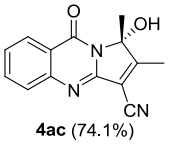
7-Hydroxy-7,8-dimethyl-5-oxo-5,7-dihydropyrido[3,4-d]pyrrolo[1,2-a]pyrimidine-9-carbonitrile (4ec): General procedure B was followed on a 0.12 g (0.79 mmol) scale of 3-nitroisonicotinaldehyde (**1e**). After the photochemical reaction the crude product was purified by flash chromatography on silica gel with a gradient of 0%→7% of methanol in chloroform to afford 124 mg (62%) of **4ec** as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.17 – 8.99 (d, *J* = 0.8 Hz, 1H), 8.78 – 8.65 (d, *J* = 5.2 Hz, 1H), 8.04 – 7.92 (dd, *J* = 5.2, 0.9 Hz, 1H), 7.54 – 7.48 (s, 1H), 2.40 – 2.25 (s, 3H), 2.01 – 1.85 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 174.2, 157.6, 153.3, 150.7, 147.3, 143.0, 127.2, 119.0, 111.9, 106.1, 95.9, 20.3, 13.1; HRMS (ESI) calcd for $C_{13}H_{11}N_4O_2^+$ (MH+) 255.0877, found 255.0888.

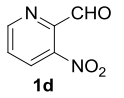
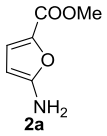
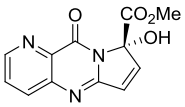
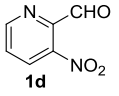
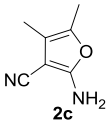
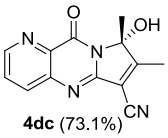
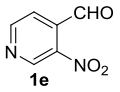
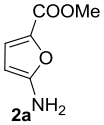
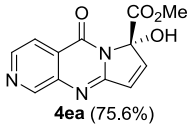
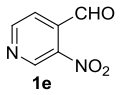
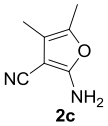
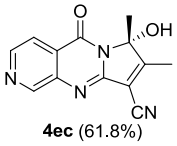
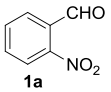
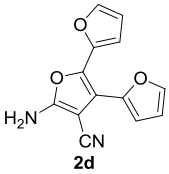
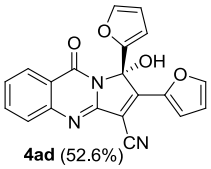


1,2-Di(furan-2-yl)-1-hydroxy-9-oxo-1,9-dihydropyrrolo[2,1-b]quinazoline-3-carbonitrile (4ad): General procedure B was followed on a 50 mg (0.33 mmol) scale of 2-nitro aldehyde (**1a**). After the photochemical reaction, the crude product was purified

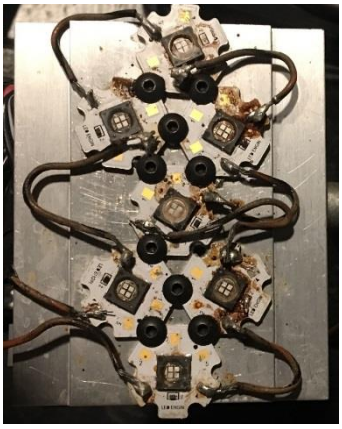
by flash chromatography on silica gel with a gradient of 5%→65 % of ethyl acetate in hexanes to afford 62 mg (53%) of **4ad** as a pale-yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 – 8.17 (d, *J* = 7.8 Hz, 1H), 7.90 – 7.85 (d, *J* = 8.0 Hz, 1H), 7.83 – 7.80 (d, *J* = 7.7 Hz, 1H), 7.80 – 7.79 (d, *J* = 1.8 Hz, 1H), 7.53 – 7.48 (t, *J* = 7.6 Hz, 1H), 7.32 – 7.30 (d, *J* = 1.7 Hz, 1H), 7.30 – 7.28 (d, *J* = 3.7 Hz, 1H), 6.80 – 6.75 (d, *J* = 3.6 Hz, 1H), 6.66 – 6.59 (dd, *J* = 3.7, 1.7 Hz, 1H), 6.43 – 6.39 (dd, *J* = 3.4, 1.8 Hz, 1H), 5.84 – 5.78 (s, 1H); ^{13}C NMR (126 MHz, DMSO) δ 157.4, 152.0, 151.4, 150.5, 148.5, 148.4, 144.9, 144.0, 135.7, 128.2, 128.0, 126.8, 121.5, 121.4, 114.8, 112.7, 111.7, 110.8, 97.2, 91.6; HRMS (ESI) calcd for $C_{20}H_{12}N_3O_4^+$ (MH+) 358.0823, found 358.0822.

Table S1. Irradiation times with 20.3 W 365 nm UV LEDs

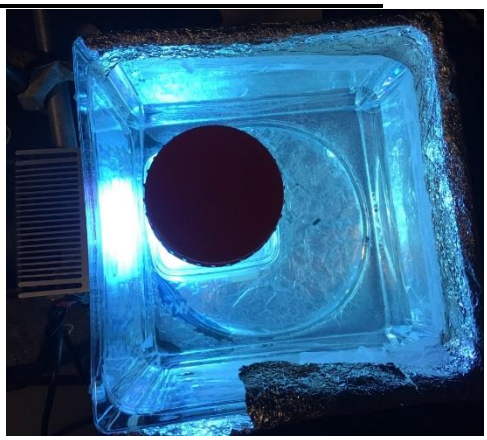
Aldehyde	Aminofuran	product	Irradiation Time (h)
 **1a**	 **2a**	 **4aa** (76.9%)	3.5
 **1b**	 **2a**	 **4ba** (69.4%)	3
 **1a**	 **2b**	 **4ab** (65.2%)	6
 **1c**	 **2a**	 **4ca** (41.2%)	6.5
 **1a**	 **2c**	 **4ac** (74.1%)	4

 **1d**	 **2a**	 **4da** (68.9%)	4.5
 **1d**	 **2c**	 **4dc** (73.1%)	9
 **1e**	 **2a**	 **4ea** (75.6%)	5.5
 **1e**	 **2c**	 **4ec** (61.8%)	12
 **1a**	 **2d**	 **4ad** (52.6%)	7.5

Photochemical setup

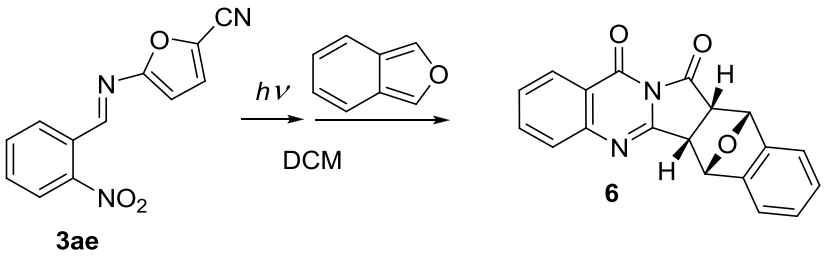


In-house fabricated irradiator with seven 2.9W UV LEDs mounted on a CPU heat sink



A preparative scale experiment with square bottle being irradiated in a temperature-controlled water bath, wrapped in aluminum foil to prevent light loss (the seven UV LED 20.3W 365 nm irradiator is located on the left side of the bath). Square bottles are used to minimize light scattering

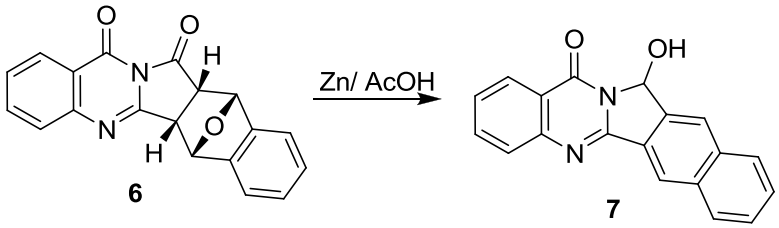
22-Oxa-4,12-diazahexacyclo[13.6.1.$0^{2,14}$.$0^{3,12}$.$0^{5,10}$.$0^{16,21}$]docosa-3,5,7,9,16(21),17,19-heptaene-11,13-dione (6):



3ae

Photoprecursor **3ae** (100 mg, 0.41 mmol) was dissolved in DCM (diluted to 0.01M) and the solution was irradiated with a UV LED illuminator (seven 2.9 W @ 365 nm LED Engin chips) for 1h 30 min. After completion of the reaction (progress of the reaction was monitored by ^{1}H NMR), 0.241 mg (2.05 mmol) of isobenzofuran was added and the reaction was allowed to stir at 20 ^{o}C for 1 hr. The solvent was removed under vacuum and the crude product was purification by flash chromatography on silica gel using 65% ethyl acetate in hexanes to afford compound **6** (85 mg, 66%) as a thick brown oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.74 (ddd, *J* = 8.6, 7.2, 1.6 Hz, 1H), 7.61 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.44 – 7.38 (m, 1H), 7.35 (d, *J* = 7.4 Hz, 1H), 7.15 (td, *J* = 7.5, 1.1 Hz, 1H), 7.04 (d, *J* = 7.4 Hz, 1H), 6.94 (td, *J* = 7.5, 1.0 Hz, 1H), 5.93 (d, *J* = 5.8 Hz, 1H), 5.87 (d, *J* = 5.8 Hz, 1H), 4.23 (dd, *J* = 8.8, 5.7 Hz, 1H), 3.93 (dd, *J* = 8.8, 5.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.3, 157.7, 154.8, 146.5, 140.7, 140.3, 135.8, 128.6, 128.3, 127.9, 127.8, 127.3, 121.3, 121.0, 120.9, 82.2, 81.1, 48.5, 45.7; HRMS (ESI) calcd for $C_{19}H_{13}N_2O_3^+$ (MH+) 317.0921, found 317.0922.

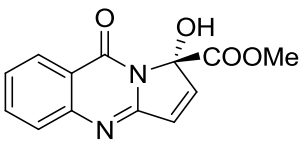
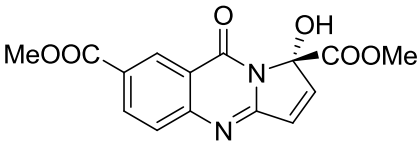
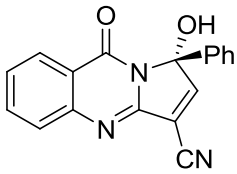
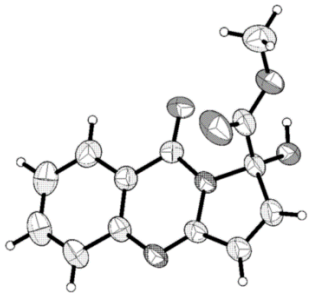
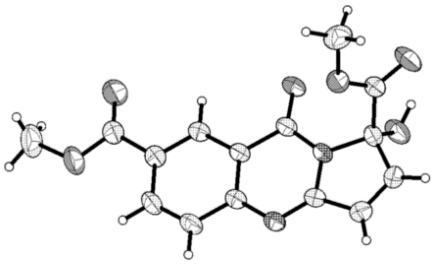
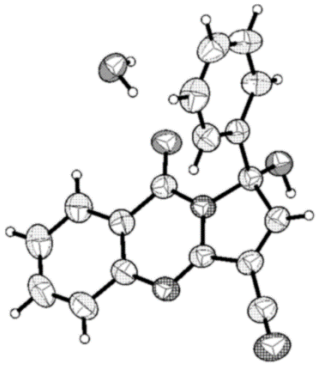
12-Hydroxy-3,11- diazapentacyclo[11.8.0.0^{2,11}.0^{4,9}.0^{15,20}]henicosa-1(21),2,4,6,8,13,15(20),16, 18-nonaen-10-one (7) (carbaluotonin B):



Zn powder (51 mg, 0.79 mmol) was added to a stirred solution of **6** (50 mg, 1.58 mmol) in acetic acid (2 mL) at 20 ^{o}C. The resultant suspension was heated to 100 ^{o}C and stirred for 2 h. The reaction was cooled to 20 ^{o}C, 10 mL of water and 10 mL of ethyl acetate was added, the solids were filtered off by passing the mixture through Celite pad (the pad was washed with additional

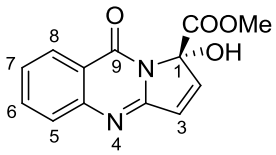
10 mL of ethyl acetate). The layers were separated and the aqueous layer was re-extracted with ethyl acetate (2 x 10 mL). The combined organic layers were evaporated under vacuum and the crude product was purified by flash chromatography on silica gel using 25% ethyl acetate in hexanes to afford carbaluotonin B (**7**) as a white solid (34 mg, 72%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.72 (s, 1H), 8.26 (dd, J = 13.7, 6.7 Hz, 3H), 8.16 (d, J = 8.0 Hz, 1H), 7.89 (t, J = 7.4 Hz, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.69 (dt, J = 16.0, 7.1 Hz, 2H), 7.59 (dd, J = 8.1, 4.8 Hz, 2H), 6.96 (d, J = 8.4 Hz, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.0, 153.6, 149.5, 139.2, 135.7, 135.1, 134.0, 129.9, 129.5, 129.1, 128.7, 127.8, 127.7, 127.3, 126.7, 124.4, 123.4, 122.2, 82.8; HRMS (ESI) calcd for $C_{19}H_{13}N_2O_2^+$ (MH+) 301.0972, found 301.0981.

3. X-Ray Structures

4aa	**4ba**	**4ab**
		
		
CCDC deposit #1894985	CCDC deposit #1894984	CCDC deposit #1894983

4. Computations of NMR spectra

Methyl 1-hydroxy-9-oxo-pyrrolo[2,1-b]quinazoline-1-carboxylate



4aa

	Conf 1	Conf 2
Rel energy (kcal/mol):	0.0	1.0

iGau	jGau	Jexp	Jcalc	diff	1	2		
21	22	7.80	7.84	0.04	[7.84	7.85]	H7	H8
24	25	6.00	6.08	0.08	[6.06	6.16]	H1	H2

For Js: rmsd=0.06Hz N=2 {0.04 0.08}

H-nom	iGau	Exp	Calc	diff	1	2
H8	22	8.28	8.41	0.13	[8.41	8.41]
H7	21	7.53	7.51	-0.02	[7.51	7.53]
H6	20	7.80	7.79	-0.01	[7.78	7.82]
H5	23	7.80	7.74	-0.06	[7.73	7.79]
H1	24	6.87	6.69	-0.18	[6.67	6.80]
H2	25	6.85	6.63	-0.22	[6.62	6.66]
H-OMe	28	3.83	3.88	0.05	[3.86	3.97]

1H chem shifts: rmsd=0.12ppm N=7 {-0.22 0.13}

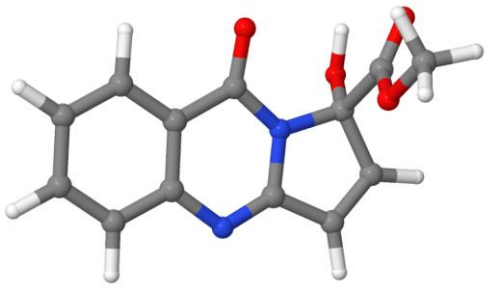
m=1.000 b=0.00

C-nom	iGau	Exp	Calc	diff	1	2
C-COO	15	167.80	168.50	0.70	[168.32	169.50]
C10	10	159.40	158.68	-0.72	[158.59	159.19]
C3b	8	155.80	154.52	-1.28	[154.55	154.33]
C4b	5	148.90	150.50	1.60	[150.39	151.09]
C2	12	141.50	143.07	1.57	[143.04	143.24]
C6	1	134.90	133.27	-1.63	[133.21	133.57]
C3	13	129.50	129.35	-0.15	[129.28	129.72]
C8	3	127.90	128.46	0.56	[128.51	128.20]
C5	6	127.60	128.07	0.47	[128.01	128.38]
C7	2	126.70	124.84	-1.86	[124.84	124.85]
C8b	4	120.90	121.92	1.02	[122.01	121.40]
C1	11	91.50	91.42	-0.08	[90.80	94.87]
C-OMe	18	54.40	53.44	-0.96	[53.50	53.13]

13C chem shifts: RMSD=1.12ppm (MAE=0.97) N=13 {-1.86 1.60}

Fractions: 0.847 0.153

Conformer 1

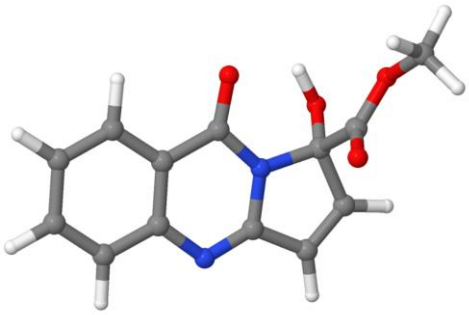


Energy: -911.80118 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	4.49664	-0.18344	0.41331
C	4.05267	-1.40109	-0.13164
C	2.71486	-1.56243	-0.46315
C	1.80810	-0.51183	-0.25892

C	2.24916	0.72051	0.29314
C	3.61029	0.86261	0.62535
N	-0.35273	0.46269	-0.38845
C	0.16260	1.61839	0.18046
N	1.39397	1.79374	0.52944
C	0.38978	-0.69137	-0.60785
C	-1.79656	0.58494	-0.67824
C	-2.07055	1.98703	-0.15689
C	-0.95385	2.56038	0.30846
O	-2.10295	0.49642	-2.02914
C	-2.57761	-0.52287	0.08186
O	-3.36885	-1.24599	-0.48094
O	-2.28645	-0.55080	1.38181
C	-2.93870	-1.59015	2.14054
O	-0.13720	-1.71391	-1.03573
H	5.54477	-0.06003	0.67262
H	4.75602	-2.21313	-0.29162
H	2.34002	-2.49001	-0.88421
H	3.93607	1.80811	1.04710
H	-3.06050	2.41876	-0.23206
H	-0.83176	3.55459	0.71757
H	-2.42395	-0.41369	-2.18116
H	-2.58055	-1.46949	3.16239
H	-2.66236	-2.56976	1.74392
H	-4.02374	-1.47023	2.09189

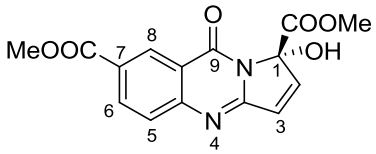
Conformer 2



Energy: -911.79957 Hartree (Rel: 1.0 kcal/mol)
XYZ coordinates for conf 2:

C	-4.56606	-0.36019	-0.42671
C	-4.04744	-1.60061	-0.01406
C	-2.69865	-1.71897	0.28730
C	-1.85376	-0.60407	0.17863
C	-2.37078	0.65478	-0.23680
C	-3.74365	0.75128	-0.53660
N	0.25044	0.46436	0.32713
C	-0.33634	1.65422	-0.06784
N	-1.58745	1.80017	-0.35477
C	-0.42628	-0.72856	0.49580
C	1.69482	0.60552	0.57222
C	1.88056	2.09261	0.32069
C	0.72972	2.66302	-0.06107
O	2.06088	0.26395	1.86875
C	2.43187	-0.22486	-0.52595
O	2.11561	-0.20656	-1.69223
O	3.45760	-0.91384	-0.01307
C	4.18342	-1.72165	-0.96008
O	0.17084	-1.73776	0.87870
H	-5.62327	-0.27069	-0.66185
H	-4.70252	-2.46303	0.06769
H	-2.26731	-2.66183	0.60842
H	-4.12914	1.71557	-0.85175
H	2.84683	2.56379	0.44753
H	0.55344	3.69864	-0.32016
H	1.88055	-0.69237	1.95347
H	4.97235	-2.20437	-0.38379
H	4.60568	-1.09439	-1.74911
H	3.51861	-2.46446	-1.40746

Dimethyl 1-hydroxy-9-oxo-pyrrolo[2,1-b]quinazoline-1,7-dicarboxylate



4ba

	Conf 1	Conf 2
Rel energy (kcal/mol):	0.0	0.4

iGau	jGau	Jexp	Jcalc	diff		1	2			
22	24	8.50	8.64	0.14	[	8.63	8.65	]	H6	H5
25	26	5.95	6.06	0.11	[	6.06	6.06	]	H2	H3

For Js: rmsd=0.12Hz N=2 {0.11 0.14}

H-nom	iGau	Exp	Calc	diff		1	2	
H8	23	8.96	9.04	0.08	[	8.96	9.20	]
H6	22	8.62	8.55	-0.07	[	8.62	8.40	]
H5	24	7.81	7.67	-0.14	[	7.70	7.62	]
H2	25	6.89	6.76	-0.13	[	6.76	6.75	]
H3	26	6.83	6.63	-0.20	[	6.64	6.62	]
H-MeO2C-C7	35	3.99	4.03	0.04	[	4.04	4.02	]
H-MeO2C-C1	29	3.85	3.87	0.02	[	3.87	3.87	]

1H chem shifts: rmsd=0.11ppm N=7 {-0.20 0.08}

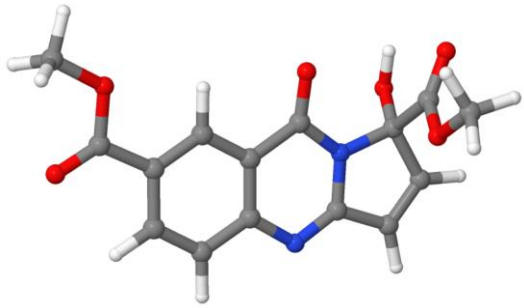
m=1.000 b=0.00

C-nom	iGau	Exp	Calc	diff		1	2	
C	15	167.60	167.88	0.28	[	167.89	167.85	]
C	20	165.70	166.77	1.07	[	166.99	166.33	]
C	10	158.80	158.24	-0.56	[	158.29	158.14	]
C	8	157.30	156.44	-0.86	[	156.42	156.47	]
C	5	152.20	153.80	1.60	[	153.82	153.77	]
C	12	142.20	144.08	1.88	[	144.00	144.25	]
C	1	135.20	136.11	0.91	[	136.81	134.70	]
C	3	129.70	132.40	2.70	[	131.59	134.05	]
C	13	129.10	128.73	-0.37	[	128.74	128.71	]
C	2	129.00	127.37	-1.63	[	127.39	127.32	]
C	6	128.30	127.43	-0.87	[	127.52	127.26	]
C	4	120.90	121.72	0.82	[	121.56	122.04	]
C	11	91.40	90.99	-0.41	[	91.00	90.97	]
C	18	54.50	53.56	-0.94	[	53.54	53.61	]
C	32	52.50	51.74	-0.76	[	51.83	51.56	]

13C chem shifts: RMSD=1.22ppm (MAE=1.04) N=15 {-1.63 2.70}

Fractions: 0.670 0.330

Conformer 1

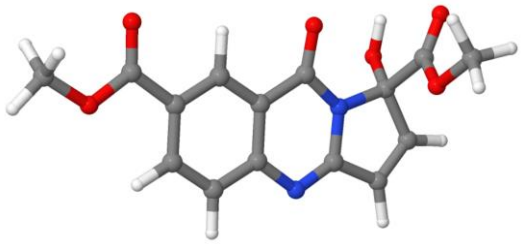


Energy: -1139.67692 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	3.07814	1.76086	0.49998
C	3.13844	0.40254	0.12225
C	1.96453	-0.27535	-0.19853
C	0.73451	0.39056	-0.14953
C	0.66909	1.75846	0.23250
C	1.86757	2.42701	0.55635
N	-1.62075	0.48851	-0.43753

C	-1.58873	1.81092	-0.02552
N	-0.52455	2.46511	0.31049
C	-0.50168	-0.33625	-0.48513
C	-2.99411	0.04189	-0.75590
C	-3.78111	1.30209	-0.43160
C	-2.97284	2.29384	-0.03735
O	-3.16772	-0.31666	-2.08468
C	-3.37006	-1.17135	0.13987
O	-3.81539	-2.19422	-0.33028
O	-3.16562	-0.93221	1.43379
C	-3.44780	-2.03503	2.32124
O	-0.60005	-1.52466	-0.76972
C	4.47685	-0.25037	0.08534
O	5.52027	0.31081	0.36051
H	4.00608	2.26673	0.74572
H	1.98158	-1.31881	-0.49059
H	1.80722	3.47058	0.84749
H	-4.85380	1.33322	-0.57464
H	-3.23748	3.30703	0.23468
H	-3.15579	-1.29349	-2.11231
H	-3.22010	-1.66615	3.32070
H	-2.81480	-2.88820	2.06709
H	-4.49865	-2.32385	2.24285
O	4.40940	-1.54663	-0.29025
C	5.66755	-2.23486	-0.34850
H	5.42956	-3.25099	-0.66422
H	6.14888	-2.23878	0.63321
H	6.33518	-1.75388	-1.06844

Conformer 2

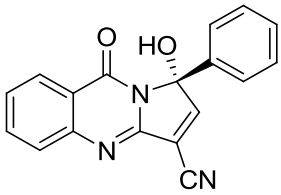


Energy: -1139.67625 Hartree (Rel: 0.4 kcal/mol)
XYZ coordinates for conf 2:

C	3.12831	1.42390	0.47169
C	3.09054	0.08702	0.02057
C	1.86716	-0.49394	-0.30654
C	0.68394	0.24235	-0.19312
C	0.71643	1.58867	0.26396
C	1.96229	2.15973	0.59313
N	-1.66569	0.50958	-0.41693
C	-1.53771	1.80143	0.06595
N	-0.42574	2.36593	0.41034
C	-0.60509	-0.38337	-0.53624
C	-3.07251	0.16931	-0.71981
C	-3.76741	1.45825	-0.30959
C	-2.88704	2.37266	0.11605
O	-3.30178	-0.10645	-2.05966
C	-3.50504	-1.06258	0.12385
O	-4.03056	-2.02755	-0.38403
O	-3.24992	-0.90584	1.42147
C	-3.57839	-2.03417	2.25971
O	-0.78932	-1.54469	-0.88093
C	4.31936	-0.74329	-0.12130
O	4.33089	-1.89923	-0.49605
H	4.08338	1.87012	0.72483
H	1.82782	-1.52111	-0.65265
H	1.97556	3.18744	0.94119
H	-4.83869	1.56609	-0.42293
H	-3.07837	3.38432	0.44850
H	-3.34999	-1.07929	-2.13897
H	-3.29912	-1.73414	3.26909
H	-3.00966	-2.91103	1.94225
H	-4.64763	-2.25092	2.19971

O	5.44037	-0.06373	0.21655
C	6.66310	-0.80630	0.10011
H	7.45315	-0.11744	0.40085
H	6.81349	-1.13914	-0.93036
H	6.64500	-1.68141	0.75535

1-Hydroxy-9-oxo-1-phenyl-1,9-dihydropyrrolo[2,1-b]quinazoline-3-carbonitrile



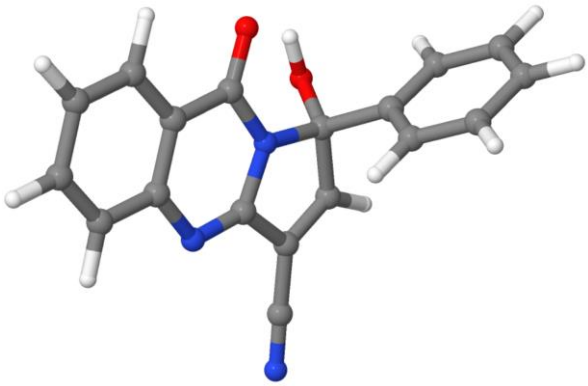
4ab

Conf 1
Rel energy (kcal/mol): 0.0

C-nom	iGau	Exp	Calc	diff	1
C-C	22	159.70	159.12	-0.58	[159.12]
C-C	14	151.00	151.57	0.57	[151.57]
C-C	16	148.70	150.31	1.61	[150.31]
C-C	7	134.40	136.04	1.64	[136.04]
C-C	21	121.30	121.60	0.30	[121.60]
C-C	3	111.60	112.51	0.91	[112.51]
C-C	2	110.30	111.33	1.03	[111.33]
C-C	5	95.90	97.19	1.29	[97.19]
C-CH	4	155.30	155.00	-0.30	[155.00]
C-CH	18	135.30	134.31	-0.99	[134.31]
C-CH	10	130.10	129.04	-1.06	[129.04]
C-CH	17	129.50	128.74	-0.76	[128.74]
C-CH	9	129.50	128.53	-0.97	[128.53]
C-CH	11	128.70	128.53	-0.17	[128.53]
C-CH	20	128.40	128.30	-0.10	[128.30]
C-CH	19	126.80	125.88	-0.92	[125.88]
C-CH	8	125.20	125.34	0.14	[125.34]
C-CH	12	125.20	125.34	0.14	[125.34]

13C chem shifts: RMSD=0.89ppm (MAE=0.75) N=18 {-1.06 1.64}

Conformer 1

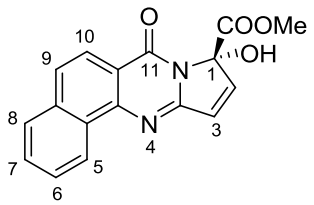


Energy: -1007.21803 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

N	0.16245	4.82032	0.57593
C	-0.02803	3.72124	0.24907
C	-0.27288	2.37710	-0.15226
C	-1.39864	1.88222	-0.70494
C	-1.28896	0.38582	-0.93653
O	-1.44026	0.09842	-2.29870

C	-2.30368	-0.35915	-0.05492
C	-3.51776	-0.76636	-0.61936
C	-4.48100	-1.39915	0.16797
C	-4.24320	-1.62234	1.52481
C	-3.03670	-1.20751	2.09331
C	-2.07305	-0.57406	1.30944
N	0.10600	0.14731	-0.49618
C	0.72590	1.29357	-0.03154
N	1.94015	1.37359	0.39000
C	2.67817	0.19337	0.32688
C	4.00229	0.20547	0.80372
C	4.77865	-0.94260	0.73878
C	4.26145	-2.13044	0.19210
C	2.96041	-2.16194	-0.28885
C	2.15927	-1.01215	-0.21990
C	0.78175	-1.04459	-0.72827
O	0.22750	-1.98094	-1.30450
H	-2.30548	2.42508	-0.93672
H	-1.19219	-0.84633	-2.38375
H	-3.69691	-0.59448	-1.67537
H	-5.41658	-1.71914	-0.28243
H	-4.99271	-2.11647	2.13675
H	-2.84308	-1.37812	3.14865
H	-1.13794	-0.25763	1.76228
H	4.38862	1.13261	1.21448
H	5.79912	-0.92162	1.11133
H	4.88118	-3.02098	0.14503
H	2.53410	-3.06216	-0.71994

Methyl 1-hydroxy-11-oxo-naphtho[1,2-e]pyrimidino[2,3-a]pyrrol-1-carboxylate



4ca

Conf 1

Rel energy (kcal/mol): 0.0

iGau	jGau	Jexp	Jcalc	diff		1		
28	29	8.65	8.65	0.00	[	8.65]	H9	H10
25	26	7.60	8.06	0.46	[	8.06]	H7	H8
30	31	5.95	6.05	0.10	[	6.05]	H2	H3

For Js: rmsd=0.27Hz N=3 {0.00 0.46}

H-nom	iGau	Exp	Calc	diff		1	
H5	27	9.04	9.16	0.12	[	9.16]	
H10	29	8.22	8.37	0.15	[	8.37]	
H8	26	7.96	7.86	-0.10	[	7.86]	
H9	28	7.91	7.78	-0.13	[	7.78]	
H7	25	7.76	7.83	0.07	[	7.83]	
H6	24	7.73	7.79	0.06	[	7.79]	
H2	30	6.95	6.75	-0.20	[	6.75]	
H3	31	6.88	6.75	-0.13	[	6.75]	
H-OMe	34	3.85	3.87	0.02	[	3.87]	

1H chem shifts: rmsd=0.12ppm N=9 {-0.20 0.15}

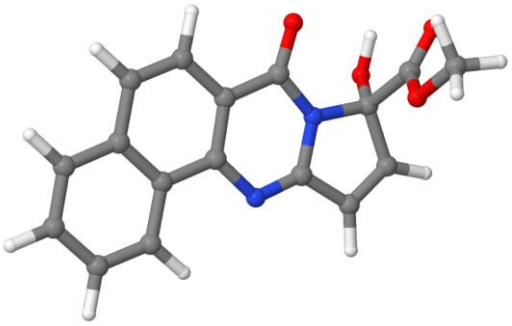
m=1.000 b=0.00

C-nom	iGau	Exp	Calc	diff		1	
C-COO	20	167.90	168.17	0.27	[	168.17]	
C11	11	159.70	158.67	-1.03	[	158.67]	
C3a	13	155.80	154.73	-1.07	[	154.73]	
C4a	10	148.10	150.10	2.00	[	150.10]	
C2	16	141.10	143.41	2.31	[	143.41]	
C8b	4	136.40	135.49	-0.91	[	135.49]	

C4b	5	130.30	130.06	-0.24	[130.06]
C3	17	130.10	129.18	-0.92	[129.18]
C7	2	129.40	128.16	-1.24	[128.16]
C5	6	128.00	127.19	-0.81	[127.19]
C8	3	127.80	126.97	-0.83	[126.97]
C9	7	127.20	126.18	-1.02	[126.18]
C6	1	125.20	125.39	0.19	[125.39]
C10	8	121.40	124.05	2.65	[124.05]
C10a	9	117.40	118.66	1.26	[118.66]
C1	15	91.60	91.24	-0.36	[91.24]
C-OMe	23	54.40	53.50	-0.90	[53.50]

13C chem shifts: RMSD=1.26ppm (MAE=1.06) N=17 {-1.24 2.65}

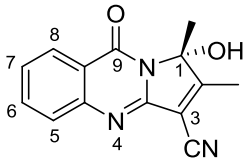
Conformer 1



Energy: -1065.44429 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

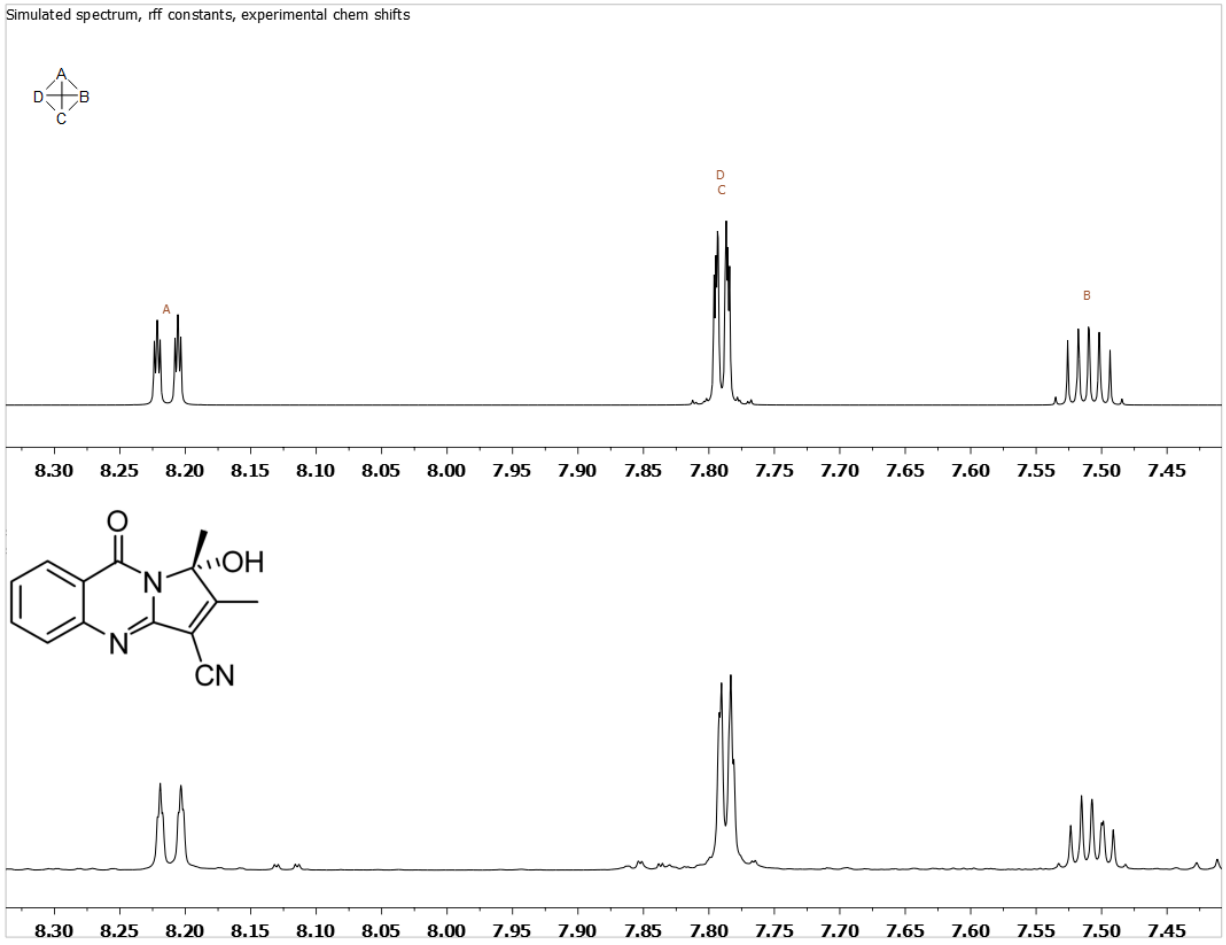
C	4.88160	1.49998	0.54592
C	5.60310	0.28829	0.44805
C	4.94498	-0.89125	0.17036
C	3.53974	-0.91218	-0.02157
C	2.81417	0.31603	0.07768
C	3.51410	1.51380	0.36427
C	2.84003	-2.12338	-0.30794
C	1.48273	-2.12564	-0.48949
C	0.74487	-0.91606	-0.39959
C	1.38742	0.30302	-0.11728
C	-0.70971	-0.95225	-0.59179
N	-1.28046	0.31499	-0.52278
C	-0.57129	1.45898	-0.21314
N	0.70534	1.50547	-0.00621
C	-2.72263	0.58721	-0.69729
C	-2.76262	2.08110	-0.41459
C	-1.53856	2.55932	-0.15682
O	-1.40311	-1.94766	-0.78487
O	-3.19052	0.31691	-1.97497
C	-3.53744	-0.25763	0.32208
O	-4.46996	-0.94792	-0.02269
O	-3.10066	-0.10644	1.57190
C	-3.77504	-0.90657	2.56513
H	5.40916	2.42426	0.76507
H	6.68020	0.28877	0.59242
H	5.49622	-1.82535	0.09417
H	2.94662	2.43467	0.43572
H	3.40656	-3.04842	-0.37905
H	0.93612	-3.03756	-0.70593
H	-3.69363	2.62976	-0.47896
H	-1.24966	3.57964	0.05817
H	-3.61795	-0.56050	-1.93404
H	-3.28627	-0.66713	3.50895
H	-3.66364	-1.96676	2.32671
H	-4.83669	-0.65032	2.60082

1-Hydroxy-1,2-dimethyl-9-oxo-pyrrolo[2,1-b]quinazoline-3-carbonitrile



4ac

The aromatic part of the proton spectrum looks unusual because of the second order effects due to the overlap of Hc and Hd. Shown below is a simulation of ^{1}H NMR for **4ac** using the calculated proton spin-spin coupling constants and experimental chemical shifts (experimental spectrum is shown below simulated).



Conf 1
Rel energy (kcal/mol): 0.0

H-nom	iGau	Exp	Calc	diff		1	
H8	23	8.21	8.46	0.25	[	8.46	]
H7	20	7.51	7.60	0.09	[	7.60	]
H6	21	7.79	7.93	0.14	[	7.93	]
H5	22	7.79	7.87	0.08	[	7.87	]
H-Me-C2	24	2.43	2.46	0.03	[	2.46	]
H-Me-C2	25	2.43	2.46	0.03	[	2.46	]
H-Me-C2	26	2.43	2.46	0.03	[	2.46	]
H-Me-C1	27	2.07	1.91	-0.16	[	1.91	]

H-Me-C1	28	2.07	1.91	-0.16	[1.91]
H-Me-C1	29	2.07	1.91	-0.16	[1.91]

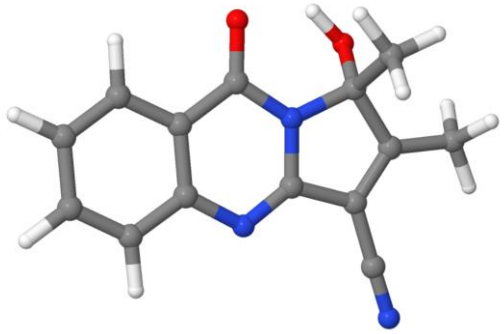
1H chem shifts: RMSD=0.13ppm (MAE=0.11) N=10 {-0.16 0.25}

m=1.000 b=0.00

C-nom	iGau	Exp	Calc	diff	1
C2	12	169.90	169.54	-0.36	[169.54]
C9	10	160.20	159.80	-0.40	[159.80]
C4b	4	150.20	150.47	0.27	[150.47]
C3a	8	148.50	150.18	1.68	[150.18]
C6	2	135.00	134.19	-0.81	[134.19]
C5	3	128.10	128.45	0.35	[128.45]
C8	6	127.70	128.11	0.41	[128.11]
C7	1	126.40	125.43	-0.97	[125.43]
C8a	5	120.90	120.81	-0.09	[120.81]
C-CN	18	110.70	111.49	0.79	[111.49]
C3	11	108.30	110.18	1.88	[110.18]
C1	13	94.40	95.11	0.71	[95.11]
C-Me-C1	16	22.30	23.05	0.75	[23.05]
C-Me-C2	15	12.80	12.76	-0.04	[12.76]

13C chem shifts: RMSD=0.86ppm (MAE=0.68) N=14 {-0.97 1.88}

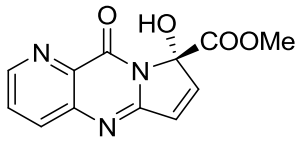
Conformer 1



Energy: -854.81450 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	4.42044	-0.23337	-0.04911
C	4.27999	1.16352	0.03834
C	3.02351	1.74920	0.08418
C	1.86550	0.94886	0.04933
C	2.01469	-0.46299	-0.03256
C	3.29309	-1.04022	-0.08787
N	0.62423	1.57848	0.07117
C	-0.39830	0.79281	0.06040
N	-0.35227	-0.58864	0.06622
C	0.82127	-1.31511	-0.06880
C	-1.82576	1.15385	-0.00238
C	-2.58794	0.03482	-0.05963
C	-1.70148	-1.20254	0.05142
O	0.79140	-2.54230	-0.20214
C	-4.06314	-0.07741	-0.21166
C	-1.94568	-1.97904	1.35640
O	-1.87812	-2.01374	-1.07881
C	-2.29589	2.49729	-0.03735
N	-2.70587	3.58514	-0.06265
H	5.41057	-0.67787	-0.08729
H	5.16588	1.79215	0.06638
H	2.89792	2.82546	0.14293
H	3.36850	-2.12077	-0.15702
H	-4.52806	0.90344	-0.33766
H	-4.51334	-0.56691	0.66174
H	-4.29539	-0.70361	-1.08169
H	-1.21435	-2.78763	1.43624
H	-2.94945	-2.41292	1.33601
H	-1.85269	-1.32810	2.23163
H	-1.16019	-2.67782	-1.03105

Methyl 8-hydroxy-10-oxo-8,10-dihydropyrido[3,2-d]pyrrolo[1,2-a]pyrimidine-8-carboxylate



4da

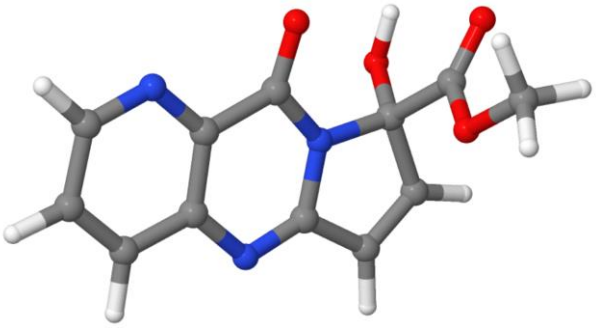
	Conf 1	Conf 2
Rel energy (kcal/mol):	0.0	0.9

C-nom	iGau	Exp	Calc	diff	1	2
C-C	16	167.33	168.16	0.83	[167.93	169.19]
C-C	10	157.84	156.49	-1.35	[156.36	157.08]
C-C	8	156.34	155.31	-1.03	[155.36	155.09]
C-C	4	146.05	148.33	2.28	[148.18	148.98]
C-C	5	138.15	141.83	3.68	[141.95	141.32]
C-C	14	91.73	91.92	0.19	[91.18	95.18]
C-CH	1	149.93	148.66	-1.27	[148.64	148.75]
C-CH	13	142.50	144.40	1.90	[144.36	144.57]
C-CH	3	136.23	135.71	-0.52	[135.64	136.00]
C-CH	12	129.30	128.70	-0.60	[128.62	129.07]
C-CH	2	128.69	126.11	-2.58	[126.07	126.31]
C-CH3	19	54.56	53.57	-0.99	[53.64	53.28]

13C chem shifts: RMSD=1.73ppm (MAE=1.43) N=12 {-2.58 3.68}

Fractions: 0.814 0.186

Conformer 1

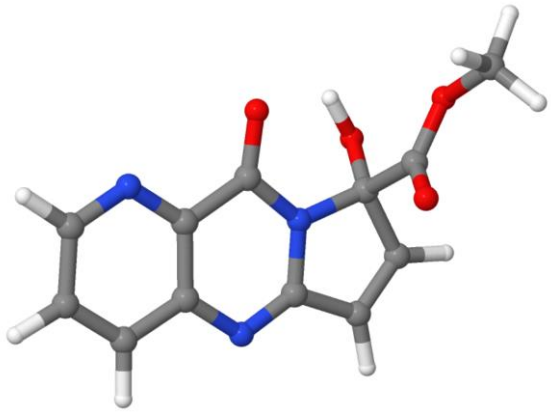


Energy: -927.82996 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	3.92497	-1.41555	-0.18157
C	4.46077	-0.24460	0.38607
C	3.61756	0.82369	0.63241
C	2.25220	0.70760	0.30460
C	1.82254	-0.52042	-0.26541
N	2.64341	-1.55770	-0.49874
N	1.40734	1.78052	0.56071
C	0.17467	1.61332	0.20584
N	-0.33860	0.47150	-0.38296
C	0.39008	-0.69523	-0.61848
O	-0.15287	-1.69913	-1.05137
C	-0.93834	2.55708	0.35090
C	-2.05581	1.99412	-0.12487
C	-1.78427	0.60063	-0.66930
O	-2.09108	0.53566	-2.02036
C	-2.56556	-0.51846	0.07470
O	-3.36967	-1.22005	-0.49621
O	-2.25882	-0.57840	1.36969
C	-2.90429	-1.63563	2.11051
H	4.56812	-2.27029	-0.38398
H	5.51901	-0.19023	0.62453
H	3.96876	1.75297	1.07018
H	-0.81320	3.54331	0.77796
H	-3.04480	2.42923	-0.19335
H	-2.41390	-0.37093	-2.18897

H	-2.53113	-1.54282	3.12986
H	-3.98938	-1.51065	2.08034
H	-2.63619	-2.60479	1.68398

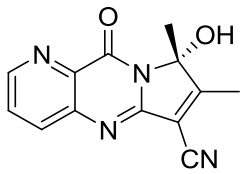
Conformer 2



Energy: -927.82856 Hartree (Rel: 0.9 kcal/mol)
XYZ coordinates for conf 2:

C	-3.91454	-1.61866	0.01623
C	-4.52425	-0.42462	-0.41322
C	-3.74868	0.71270	-0.54241
C	-2.37333	0.64238	-0.24256
C	-1.86610	-0.61744	0.18035
N	-2.62353	-1.71982	0.30739
N	-1.60243	1.79165	-0.36871
C	-0.34998	1.65121	-0.07718
N	0.23670	0.46851	0.32685
C	-0.42522	-0.73814	0.50401
O	0.18560	-1.72971	0.88906
C	0.71062	2.66578	-0.07846
C	1.86325	2.10258	0.30775
C	1.68317	0.61713	0.57025
O	2.05162	0.28762	1.86775
C	2.41847	-0.21946	-0.52498
O	2.10706	-0.19524	-1.69247
O	3.43229	-0.91996	-0.00681
C	4.14925	-1.74359	-0.94780
H	-4.50510	-2.52651	0.12624
H	-5.58707	-0.40632	-0.63612
H	-4.16000	1.66344	-0.86691
H	0.52929	3.69822	-0.34641
H	2.82768	2.57847	0.43136
H	1.88542	-0.67084	1.95828
H	4.93022	-2.23323	-0.36668
H	3.47460	-2.47995	-1.39087
H	4.58119	-1.12654	-1.73953

8-Hydroxy-7,8-dimethyl-10-oxo-8,10-dihydropyrido[3,2-d]pyrrolo[1,2-a]pyrimidine-6-carbonitrile



4dc

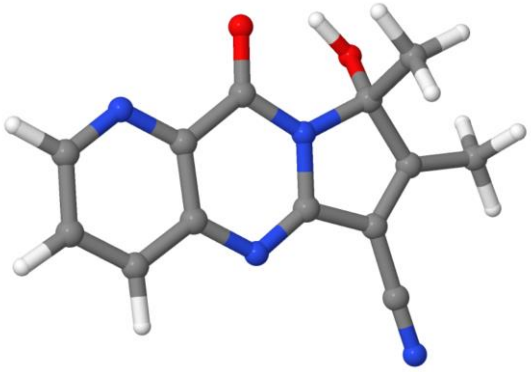
	Conf 1
Rel energy (kcal/mol):	0.0

C-nom	**iGau**	**Exp**	**Calc**	**diff**	**1**
C-C	13	171.30	170.98	-0.32	[170.98]
C-C	10	158.60	157.54	-1.06	[157.54]
C-C	8	150.90	150.91	0.01	[150.91]

C-C	4	145.60	148.46	2.86	[148.46]
C-C	5	137.90	140.69	2.79	[140.69]
C-C	18	110.40	111.34	0.94	[111.34]
C-C	12	108.00	109.60	1.60	[109.60]
C-C	14	95.00	95.48	0.48	[95.48]
C-CH	1	150.10	149.17	-0.93	[149.17]
C-CH	3	136.40	136.09	-0.31	[136.09]
C-CH	2	128.90	126.87	-2.03	[126.87]
C-CH3	16	22.20	22.78	0.58	[22.78]
C-CH3	17	12.90	12.89	-0.01	[12.89]

13C chem shifts: RMSD=1.42ppm (MAE=1.07) N=13 {-2.03 2.86}

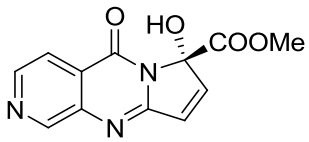
Conformer 1



Energy: -870.84336 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	4.31559	-0.28971	-0.04061
C	4.26729	1.11568	0.03751
C	3.03513	1.74159	0.07741
C	1.86757	0.95305	0.04349
C	2.03643	-0.45580	-0.03253
N	3.23576	-1.06031	-0.07802
N	0.63044	1.58399	0.06386
C	-0.39002	0.79272	0.05607
N	-0.33724	-0.58519	0.06295
C	0.83607	-1.32260	-0.07581
O	0.79684	-2.54148	-0.21595
C	-1.81766	1.15226	-0.00132
C	-2.57726	0.03139	-0.05508
C	-1.68685	-1.20341	0.05050
O	-1.86526	-2.00963	-1.08167
C	-1.92355	-1.98291	1.35499
C	-4.05243	-0.08479	-0.20093
C	-2.28843	2.49554	-0.03385
N	-2.69735	3.58379	-0.05702
H	5.27458	-0.80353	-0.07490
H	5.18833	1.69053	0.06207
H	2.93101	2.82072	0.13128
H	-1.14958	-2.67660	-1.03731
H	-1.83108	-1.33307	2.23109
H	-2.92567	-2.42054	1.33610
H	-1.18910	-2.78888	1.43169
H	-4.52104	0.89454	-0.32447
H	-4.49692	-0.57659	0.67408
H	-4.28575	-0.71182	-1.07008

Methyl 7-hydroxy-5-oxo-5,7-dihydropyrido[3,4-d]pyrrolo[1,2-a]pyrimidine-7-carboxylate



4ea

```
                                    Conf 1 Conf 2
              Rel energy (kcal/mol):    0.0    1.2
```

C-nom	iGau	Exp	Calc	diff	1	2
C-C	16	167.40	167.93	0.53	[167.80	168.95]
C-C	10	158.10	158.06	-0.04	[157.98	158.66]
C-C	8	157.30	155.64	-1.66	[155.67	155.45]
C-C	4	143.70	144.45	0.75	[144.38	144.95]
C-C	5	126.40	127.21	0.81	[127.28	126.67]
C-C	13	91.60	91.41	-0.19	[90.92	95.11]
C-CH	3	151.30	152.89	1.59	[152.85	153.17]
C-CH	1	147.20	147.39	0.19	[147.39	147.41]
C-CH	12	142.10	143.60	1.50	[143.59	143.64]
C-CH	11	129.40	129.01	-0.39	[128.95	129.48]
C-CH	6	118.70	119.51	0.81	[119.56	119.17]
C-CH3	19	54.60	53.70	-0.90	[53.75	53.34]

13C chem shifts: RMSD=0.94ppm (MAE=0.78) N=12 {-1.66 1.59}

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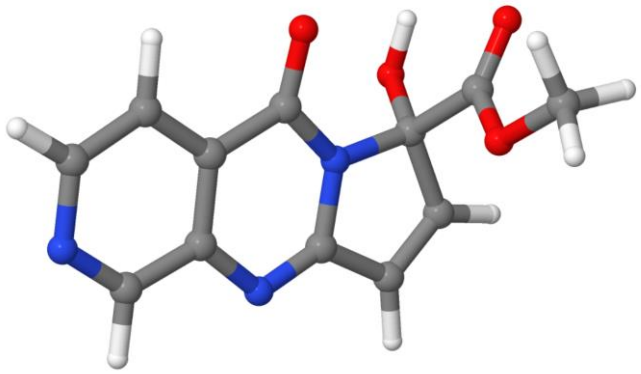
                        Fractions:  0.884  0.116
```

Conformer 1



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Energy: -927.83344 Hartree (Rel:  0.0 kcal/mol)
XYZ coordinates for conf 1:
C          4.06227       -1.32821       -0.09958
N          4.50269       -0.16940        0.43306
C          3.62093        0.80388        0.62183
C          2.25081        0.69728        0.29545
C          1.81184       -0.52557       -0.26249
C          2.74053       -1.55413       -0.45866
N          1.41134        1.77603        0.54055
C          0.17859        1.60896        0.18974
N         -0.34290        0.45637       -0.38569
C          0.38967       -0.70112       -0.61382
C         -0.93170        2.55672        0.32009
C         -2.05113        1.99290       -0.15007
C         -1.78753        0.59152       -0.67789
O         -0.13366       -1.72149       -1.04500
O         -2.08826        0.50907       -2.02920
C         -2.57830       -0.51416        0.07590
O         -3.37170       -1.22781       -0.49594
O         -2.29144       -0.55070        1.37535
C         -2.95710       -1.58629        2.12972
H          4.81345       -2.10262       -0.23835
H          3.98037        1.73644        1.05287
H          2.41451       -2.49777       -0.88367
H         -0.80305        3.54817        0.73370
H         -3.03781        2.43213       -0.22485
H         -2.44771       -0.38738       -2.17926
H         -2.59916       -1.47304        3.15235
H         -2.69098       -2.56716        1.72952
H         -4.04036       -1.45298        2.07924
```
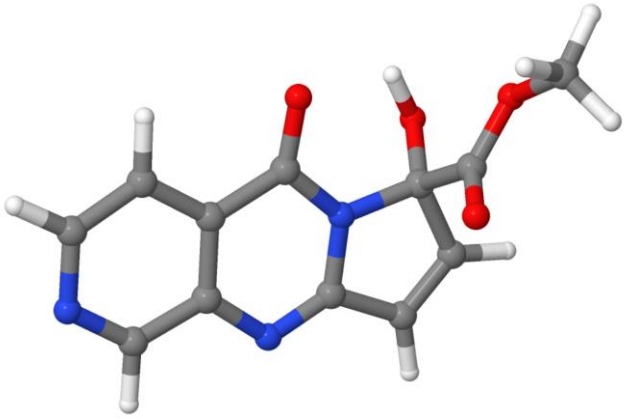
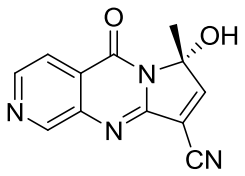

Conformer 2



Energy: -927.83153 Hartree (Rel: 1.2 kcal/mol)
XYZ coordinates for conf 2:

C	-4.05767	-1.52804	-0.03456
N	-4.57225	-0.34592	-0.43353
C	-3.75142	0.69158	-0.52792
C	-2.37028	0.63162	-0.23531
C	-1.85298	-0.61902	0.18113
C	-2.71941	-1.71402	0.28166
N	-1.60453	1.78324	-0.36283
C	-0.35187	1.64659	-0.07476
N	0.24264	0.46084	0.32914
C	-0.42080	-0.73859	0.49865
C	0.70734	2.66145	-0.07791
C	1.86272	2.10116	0.30445
C	1.68923	0.61526	0.56976
O	0.17535	-1.74643	0.87772
O	2.06149	0.29232	1.86817
C	2.42711	-0.22151	-0.52302
O	2.10830	-0.21161	-1.68839
O	3.45240	-0.90536	-0.00428
C	4.18081	-1.72109	-0.94402
H	-4.76176	-2.35458	0.02986
H	-4.17168	1.64274	-0.84910
H	-2.33373	-2.67689	0.60021
H	0.52306	3.69372	-0.34441
H	2.82606	2.57977	0.42540
H	1.93095	-0.67070	1.95895
H	4.96854	-2.19867	-0.36208
H	4.60411	-1.09908	-1.73645
H	3.51659	-2.46724	-1.38641

7-Hydroxy-7,8-dimethyl-5-oxo-5,7-dihydropyrido[3,4-d]pyrrolo[1,2-a]pyrimidine-9-carbonitrile



4ec

(NMR is in DMSO)

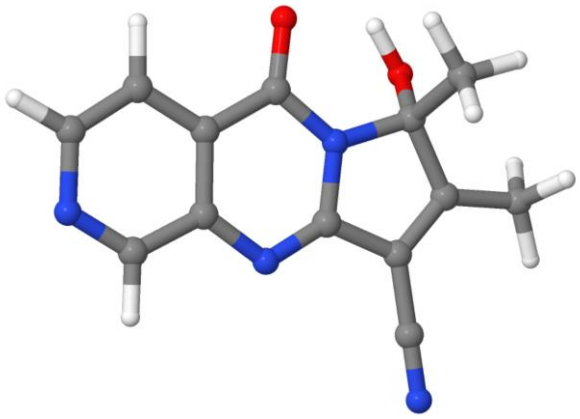
	Conf 1
Rel energy (kcal/mol):	0.0

C-nom	iGau	Exp	Calc	diff	1
C	12	174.20	174.75	0.55	[176.30]
C	10	157.60	158.29	0.69	[159.69]
C	3	153.30	150.97	-2.33	[152.30]
C	8	150.70	151.56	0.86	[152.89]
C	1	147.30	146.46	-0.84	[147.75]

C	4	143.00	143.44	0.44	[144.70]
C	5	127.20	126.08	-1.12	[127.18]
C	6	119.00	119.35	0.35	[120.39]
C	18	111.90	113.17	1.27	[114.15]
C	11	106.10	106.36	0.26	[107.28]
C	13	95.90	96.46	0.56	[97.29]
C	15	20.30	22.01	1.71	[22.16]
C	16	13.10	13.58	0.48	[13.65]

13C chem shifts: CRMSD=1.05ppm (CMAE=0.88) N=13 {-2.33 1.71}

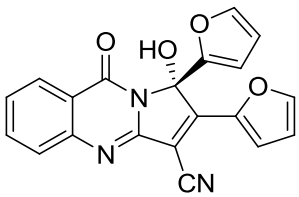
Conformer 1



Energy: -870.85983 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	4.39131	-0.16051	-0.03001
N	4.27133	1.18342	0.04098
C	3.04927	1.70146	0.07254
C	1.86860	0.92716	0.03991
C	2.01678	-0.47765	-0.03101
C	3.30562	-1.02345	-0.07077
N	0.63768	1.56848	0.05908
C	-0.38877	0.78273	0.04601
N	-0.35032	-0.59786	0.04479
C	0.81796	-1.33183	-0.06802
C	-1.81033	1.15618	-0.00419
C	-2.58857	0.04776	-0.05390
C	-1.71260	-1.20021	0.03873
O	0.80029	-2.55835	-0.18549
C	-1.95551	-1.98502	1.33593
C	-4.06558	-0.04852	-0.17409
O	-1.90834	-1.98643	-1.10562
C	-2.24949	2.50922	-0.02965
N	-2.60710	3.61570	-0.04934
H	5.40610	-0.54959	-0.05525
H	2.95938	2.78482	0.12547
H	3.43863	-2.09825	-0.12890
H	-1.23964	-2.80823	1.40169
H	-2.96758	-2.39777	1.32128
H	-1.84146	-1.34391	2.21474
H	-4.32568	-0.68057	-1.03143
H	-4.52469	0.93462	-0.29795
H	-4.49614	-0.52593	0.71515
H	-1.27787	-2.72915	-1.03359

1,2-Di(furan-2-yl)-1-hydroxy-9-oxo-1,9-dihydropyrrolo[2,1-b]quinazoline-3-carbonitrile



4ad

(NMR is in DMSO)

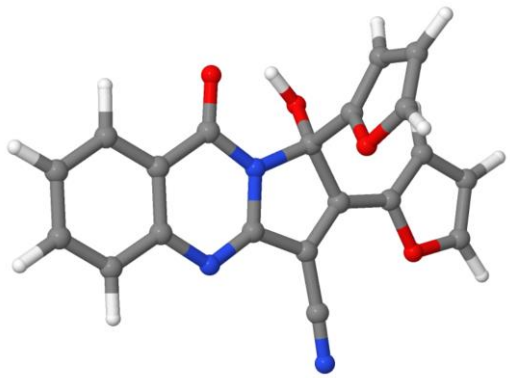
	Conf 1	Conf 2	Conf 3	Conf 4
Rel energy (kcal/mol):	0.0	0.8	1.2	2.6

C-nom	iGau	Exp	Calc	diff	1	2	3	4
C	10	157.40	158.91	1.51	[159.89	160.32	159.96	160.02]
C	24	152.00	151.97	-0.03	[152.90	153.20	152.28	152.32]
C	8	151.40	151.26	-0.14	[152.07	152.59	152.04	152.15]
C	13	150.50	150.30	-0.20	[150.84	151.97	152.07	152.61]
C	4	148.50	149.58	1.08	[150.45	150.48	150.47	150.42]
C	16	148.40	147.18	-1.22	[148.43	146.84	147.16	147.29]
C	20	144.90	144.01	-0.89	[144.72	145.11	144.37	144.28]
C	17	144.00	142.66	-1.34	[143.36	143.46	143.38	143.39]
C	2	135.70	135.33	-0.37	[135.90	135.94	135.81	135.78]
C	6	128.20	127.80	-0.40	[128.17	128.34	128.24	128.30]
C	3	128.00	127.20	-0.80	[127.59	127.62	127.51	127.52]
C	22	126.80	126.43	-0.37	[126.58	127.45	127.16	127.15]
C	1	121.50	126.00	4.50	[126.35	126.41	126.35	126.43]
C	5	121.40	120.16	-1.24	[120.30	120.67	120.58	120.89]
C	26	114.80	115.80	1.00	[115.91	116.00	116.12	116.16]
C	23	112.70	112.97	0.27	[113.06	113.00	113.18	113.26]
C	18	111.70	111.24	-0.46	[111.62	109.35	113.12	108.49]
C	19	110.80	110.49	-0.31	[110.37	111.02	110.63	111.14]
C	12	97.20	94.56	-2.64	[94.71	92.79	93.89	92.95]
C	14	91.60	93.57	1.97	[93.11	93.37	93.93	94.06]

13C chem shifts: CRMSD=1.46ppm (CMAE=1.04) N=20 {-2.64 4.50}

Fractions: 0.708 0.195 0.089 0.009

Conformer 1

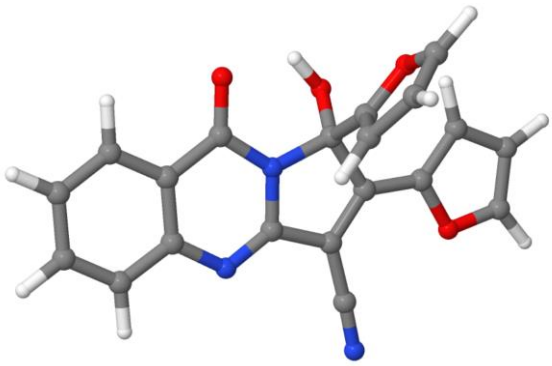


Energy: -1233.84815 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	-5.49465	0.23398	-0.31876
C	-5.46660	-1.04509	0.26631
C	-4.26097	-1.68700	0.51194
C	-3.04203	-1.06283	0.18267
C	-3.07750	0.23235	-0.40518
C	-4.30573	0.86535	-0.65458
N	-1.85625	-1.74914	0.42843
C	-0.76874	-1.11833	0.12776
N	-0.70702	0.16168	-0.38680
C	-1.82040	0.89873	-0.75590
O	-1.69183	1.98948	-1.32259
C	0.60951	-1.60325	0.21933
C	1.47434	-0.64351	-0.24548
C	0.68265	0.63072	-0.59579
O	0.90807	1.00616	-1.92275
C	0.99471	1.76930	0.34477
C	2.88282	-0.69759	-0.40344
C	1.55060	2.99864	0.15095
C	1.60920	3.61620	1.44474
C	1.08936	2.71478	2.32229
O	0.70906	1.57759	1.66701
C	3.80710	0.19309	-0.91916
C	5.07323	-0.43897	-0.83443

C	4.84724	-1.66934	-0.27543
O	3.53302	-1.84523	-0.00925
C	0.90849	-2.90365	0.69728
N	1.10940	-3.97811	1.09829
H	-6.44463	0.72431	-0.50729
H	-6.39886	-1.53791	0.52671
H	-4.22892	-2.67632	0.95707
H	-4.30037	1.85132	-1.10790
H	0.23579	1.69602	-2.10882
H	1.87514	3.41777	-0.79027
H	1.98659	4.60130	1.68019
H	0.92103	2.71804	3.38827
H	3.58767	1.17289	-1.31503
H	6.02766	-0.03982	-1.14552
H	5.49380	-2.49390	-0.01538

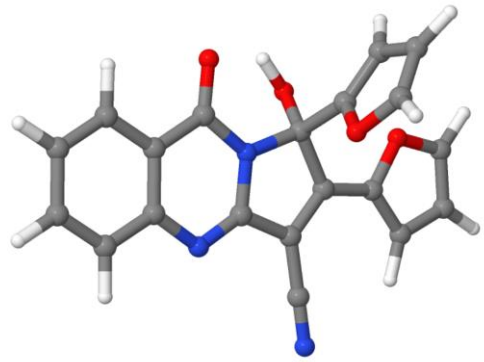
Conformer 2



Energy: -1233.84693 Hartree (Rel: 0.8 kcal/mol)
XYZ coordinates for conf 2:

C	-5.52163	0.35148	-0.30977
C	-5.53041	-0.94118	0.24488
C	-4.34297	-1.61716	0.48805
C	-3.10603	-1.01450	0.18732
C	-3.10404	0.29482	-0.36917
C	-4.31422	0.96214	-0.61724
N	-1.94000	-1.73611	0.42729
C	-0.83384	-1.12474	0.15693
N	-0.73530	0.17187	-0.31393
C	-1.82770	0.94084	-0.68976
O	-1.66829	2.03764	-1.23351
C	0.53042	-1.64612	0.24626
C	1.42198	-0.69988	-0.19873
C	0.66141	0.59820	-0.53276
O	0.89779	0.95582	-1.86306
C	0.98841	1.71488	0.43642
C	2.82862	-0.79239	-0.35815
C	0.54009	2.03549	1.68542
C	1.29840	3.17760	2.10242
C	2.15224	3.46150	1.08060
O	1.97813	2.57587	0.05576
C	3.77992	0.07481	-0.86549
C	5.02521	-0.59881	-0.79144
C	4.76122	-1.82854	-0.24811
O	3.44280	-1.96580	0.01944
C	0.79321	-2.96138	0.70344
N	0.96288	-4.04782	1.08658
H	-6.45750	0.86869	-0.49700
H	-6.47689	-1.41783	0.48316
H	-4.33926	-2.61752	0.90901
H	-4.28055	1.95832	-1.04643
H	0.30009	1.71191	-2.03784
H	-0.23634	1.53049	2.24224
H	1.20966	3.71392	3.03666
H	2.90072	4.22177	0.91821
H	3.58873	1.06750	-1.24279
H	5.99140	-0.22655	-1.09966
H	5.38164	-2.67682	-0.00081

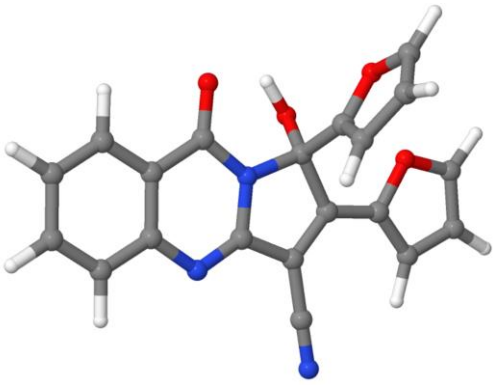
Conformer 3



Energy: -1233.84620 Hartree (Rel: 1.2 kcal/mol)
XYZ coordinates for conf 3:

C	5.48237	-0.38813	-0.34223
C	5.50857	0.89498	0.23390
C	4.33067	1.58508	0.48324
C	3.08598	1.00672	0.16677
C	3.06636	-0.29265	-0.41229
C	4.26720	-0.97478	-0.66537
N	1.92963	1.73976	0.41702
C	0.81675	1.14809	0.12877
N	0.69995	-0.13055	-0.37721
C	1.78142	-0.91283	-0.74874
O	1.60800	-2.00229	-1.30511
C	-0.53946	1.68323	0.23416
C	-1.45131	0.75722	-0.21302
C	-0.70913	-0.54497	-0.57962
O	-0.95359	-0.89557	-1.90851
C	-1.05279	-1.67863	0.35590
C	-2.86261	0.88960	-0.32673
C	-1.77197	-2.82360	0.18576
C	-1.76628	-3.48861	1.45643
C	-1.05161	-2.69432	2.30048
O	-0.60826	-1.58073	1.64463
C	-3.74421	1.92233	-0.05136
C	-5.03884	1.45376	-0.38274
C	-4.87341	0.17081	-0.83703
O	-3.57213	-0.18623	-0.81163
C	-0.79888	2.98969	0.71320
N	-1.01565	4.06462	1.10640
H	6.41103	-0.91667	-0.53376
H	6.46121	1.35271	0.48447
H	4.34042	2.57782	0.92179
H	4.22018	-1.96305	-1.11127
H	-0.32459	-1.62391	-2.09581
H	-2.24915	-3.15060	-0.72610
H	-2.23202	-4.43303	1.70057
H	-0.77187	-2.76625	3.34032
H	-3.48538	2.89535	0.33940
H	-5.97208	1.99113	-0.29715
H	-5.56040	-0.57981	-1.19786

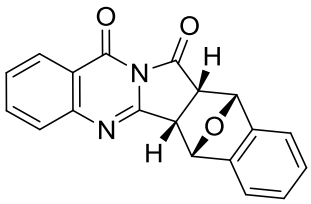
Conformer 4



Energy: -1233.84398 Hartree (Rel: 2.6 kcal/mol)
XYZ coordinates for conf 4:

C	5.50374	-0.52534	-0.27755
C	5.57080	0.78408	0.23194
C	4.41487	1.52044	0.45034
C	3.15219	0.96350	0.16916
C	3.09102	-0.36275	-0.34193
C	4.27002	-1.09161	-0.56535
N	2.01922	1.74321	0.38497
C	0.88774	1.17027	0.13477
N	0.72999	-0.13287	-0.29434
C	1.78654	-0.96063	-0.64369
O	1.57796	-2.06573	-1.15288
C	-0.45208	1.74853	0.22070
C	-1.39177	0.82898	-0.17970
C	-0.68779	-0.50334	-0.51427
O	-0.92438	-0.83981	-1.84749
C	-1.06540	-1.61420	0.44464
C	-2.79994	0.99175	-0.28719
C	-0.79036	-1.83768	1.76326
C	-1.46833	-3.05045	2.11261
C	-2.10330	-3.46880	0.98246
O	-1.87048	-2.60051	-0.04405
C	-3.65329	2.06157	-0.07265
C	-4.96294	1.60152	-0.35405
C	-4.83349	0.28635	-0.71898
O	-3.54012	-0.09840	-0.68634
C	-0.67366	3.07986	0.64704
N	-0.85922	4.17574	0.99600
H	6.41542	-1.09016	-0.44569
H	6.53783	1.22574	0.45463
H	4.45602	2.53370	0.83712
H	4.19165	-2.09941	-0.96022
H	-0.37583	-1.63254	-2.01653
H	-0.17756	-1.22365	2.40825
H	-1.47412	-3.54123	3.07570
H	-2.72344	-4.31900	0.74299
H	-3.36645	3.05306	0.24541
H	-5.88234	2.16567	-0.29502
H	-5.54256	-0.47147	-1.01644

DA product of pyrrolo[2,1-b]quinazoline-1,9-dione and isobenzofuran



6

Conf 1
Rel energy (kcal/mol): 0.0

iGau	jGau	Jexp	Jcalc	diff		1		
25	28	7.90	7.86	-0.04	[	7.86]	H	H
26	28	1.50	1.56	0.06	[	1.56]	H	H
26	27	8.10	8.07	-0.03	[	8.07]	H	H
25	26	7.20	7.13	-0.07	[	7.13]	H	H
25	27	1.05	1.20	0.15	[	1.20]	H	H
35	36	7.40	7.41	0.01	[	7.41]	H	H
34	35	7.50	7.49	-0.01	[	7.49]	H	H
33	35	1.15	1.06	-0.09	[	1.06]	H	H
33	34	7.35	7.37	0.02	[	7.37]	H	H
34	36	1.00	1.04	0.04	[	1.04]	H	H
29	31	5.75	5.64	-0.11	[	5.64]	H	H
30	32	5.80	5.75	-0.05	[	5.75]	H	H
29	30	8.75	8.56	-0.19	[	8.56]	H	H

For Js: rmsd=0.09Hz N=13 {-0.19 0.15}

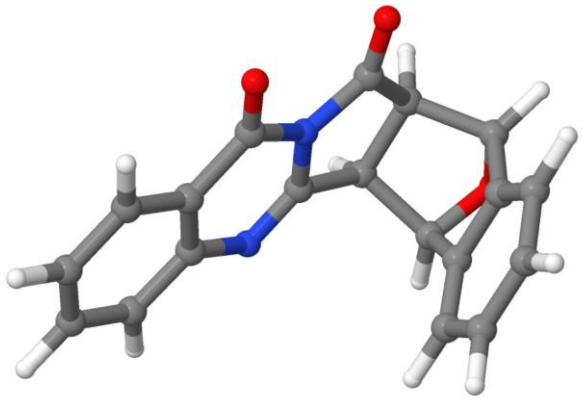
H-nom	iGau	Exp	Calc	diff		1
H	28	8.12	8.31	0.19	[	8.31]
H	26	7.77	7.71	-0.06	[	7.71]
H	27	7.64	7.57	-0.07	[	7.57]
H	25	7.44	7.42	-0.02	[	7.42]
H	36	7.37	7.46	0.09	[	7.46]
H	35	7.17	7.31	0.14	[	7.31]
H	33	7.06	7.19	0.13	[	7.19]
H	34	6.97	7.13	0.16	[	7.13]
H	31	5.95	5.55	-0.40	[	5.55]
H	32	5.90	5.51	-0.39	[	5.51]
H	29	4.26	3.96	-0.30	[	3.96]
H	30	3.95	3.65	-0.30	[	3.65]

1H chem shifts: RMSD=0.22ppm (MAE=0.19) N=12 {-0.40 0.19}
m=1.000 b=0.00

C-nom	iGau	Exp	Calc	diff		1
C-C	13	170.20	172.19	1.99	[	172.19]
C-C	10	157.50	157.04	-0.46	[	157.04]
C-C	8	154.70	155.37	0.67	[	155.37]
C-C	4	146.30	147.50	1.20	[	147.50]
C-C	15	140.60	142.04	1.44	[	142.04]
C-C	16	140.20	141.62	1.42	[	141.62]
C-C	5	120.80	122.41	1.61	[	122.41]
C-CH	2	135.60	133.60	-2.00	[	133.60]
C-CH	6	128.50	129.66	1.16	[	129.66]
C-CH	20	128.10	127.46	-0.64	[	127.46]
C-CH	19	127.80	127.14	-0.66	[	127.14]
C-CH	1	127.60	125.18	-2.42	[	125.18]
C-CH	3	127.20	126.91	-0.29	[	126.91]
C-CH	21	121.20	121.27	0.07	[	121.27]
C-CH	18	120.80	120.75	-0.05	[	120.75]
C-CH	14	82.10	82.78	0.68	[	82.78]
C-CH	17	80.90	81.82	0.92	[	81.82]
C-CH	12	48.40	50.32	1.92	[	50.32]
C-CH	11	45.50	47.71	2.21	[	47.71]

13C chem shifts: RMSD=1.35ppm (MAE=1.15) N=19 {-2.42 2.21}

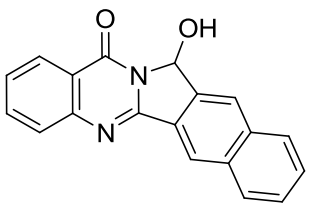
Conformer 1



Energy: -1066.41564 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	-4.81518	-0.36756	0.59545
C	-4.65596	-1.24034	-0.49387
C	-3.46010	-1.28038	-1.19875
C	-2.39301	-0.44410	-0.82811
C	-2.55706	0.43370	0.26847
C	-3.77018	0.46432	0.97321
N	-1.20642	-0.51325	-1.55986
C	-0.25509	0.27071	-1.20236
N	-0.30693	1.19205	-0.14809
C	-1.46220	1.32989	0.68370
C	1.09950	0.32638	-1.85621
C	1.86360	1.42935	-1.09110
C	0.91152	1.94092	-0.01914
C	2.04968	-0.91441	-1.63308
C	1.97705	-1.33620	-0.17801
C	2.67129	-0.33113	0.51381
C	3.12025	0.63287	-0.56886
C	1.36779	-2.38322	0.49693
C	1.49246	-2.42146	1.89455
C	2.18147	-1.41945	2.58282
C	2.77101	-0.34625	1.89682
O	-1.50502	2.11146	1.61199
O	1.12334	2.80751	0.78773
O	3.33063	-0.25484	-1.68426
H	-5.75439	-0.34410	1.14029
H	-5.47547	-1.89030	-0.78855
H	-3.31858	-1.94749	-2.04309
H	-3.86142	1.14986	1.80952
H	1.00343	0.51957	-2.92692
H	2.18928	2.26204	-1.71893
H	1.98134	-1.68768	-2.39635
H	4.00530	1.23879	-0.38243
H	0.81546	-3.15489	-0.03206
H	1.04593	-3.24208	2.44923
H	2.26172	-1.47075	3.66500
H	3.28809	0.44057	2.43866

Carbaluotonin B



7

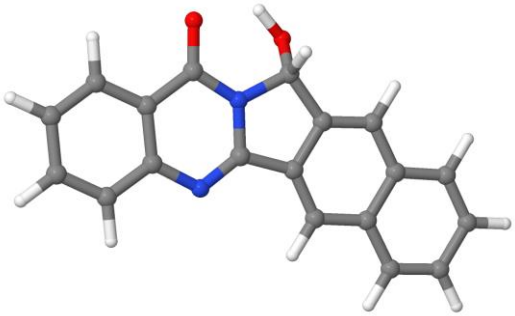
Conf 1

Rel energy (kcal/mol): 0.0

C-nom	iGau	Exp	Calc	diff	1
C-C	10	160.00	160.84	0.84	[161.41]
C-C	8	153.60	152.88	-0.72	[153.35]
C-C	4	149.50	150.58	1.08	[151.02]
C-C	12	139.20	137.50	-1.70	[137.77]
C-C	16	135.70	134.52	-1.18	[134.76]
C-C	15	134.00	132.69	-1.31	[132.90]
C-C	11	129.50	128.94	-0.56	[129.11]
C-C	5	122.20	121.25	-0.95	[121.32]
C-CH	2	135.10	134.96	-0.14	[135.20]
C-CH	18	129.90	130.01	0.11	[130.19]
C-CH	21	129.10	128.94	-0.16	[129.11]
C-CH	6	128.70	128.00	-0.70	[128.15]
C-CH	3	127.80	127.46	-0.34	[127.61]
C-CH	20	127.70	128.86	1.16	[129.02]
C-CH	19	127.30	127.64	0.34	[127.79]
C-CH	14	126.70	125.97	-0.73	[126.10]
C-CH	17	124.40	125.47	1.07	[125.59]
C-CH	1	123.40	125.64	2.24	[125.76]
C-CH	13	82.80	84.95	2.15	[84.56]

13C chem shifts: CRMSD=1.10ppm (CMAE=0.92) N=19 {-1.70 2.24}

Conformer 1



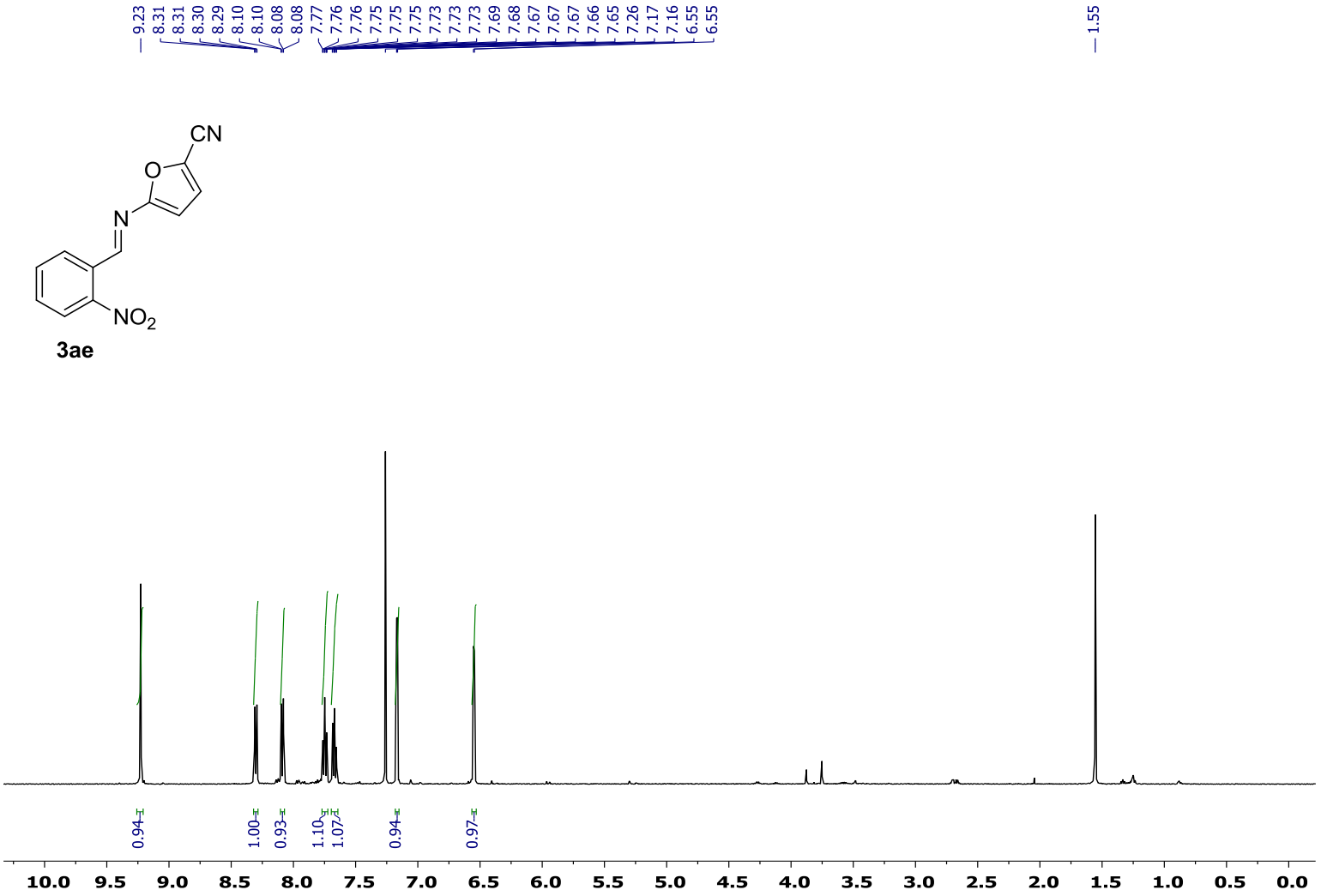
Energy: -991.24565 Hartree (Rel: 0.0 kcal/mol)
XYZ coordinates for conf 1:

C	5.53892	-0.79363	0.03164
C	4.99430	-2.09023	0.09259
C	3.62095	-2.28384	0.08257
C	2.74459	-1.18165	0.00895
C	3.30234	0.12570	-0.05341
C	4.69557	0.30497	-0.03903
N	1.37520	-1.42096	0.00734
C	0.61459	-0.37460	-0.06791
N	1.07335	0.93083	-0.15696
C	2.40936	1.28548	-0.12682
C	-0.84891	-0.30801	-0.07226
C	-1.23639	1.05750	-0.15649
C	-0.01108	1.93880	-0.24322
C	-1.77856	-1.31900	0.00276
C	-3.15916	-0.98379	0.00458
C	-3.55428	0.39936	-0.06984
C	-2.55782	1.41601	-0.15300
C	-4.16855	-1.98340	0.08186
C	-5.50228	-1.64004	0.08695
C	-5.89067	-0.27863	0.01501
C	-4.93928	0.71560	-0.06135
O	2.74504	2.47588	-0.15883
O	0.04809	2.87042	0.80135
H	-2.86188	2.45762	-0.21023
H	6.61580	-0.65597	0.04101
H	5.65663	-2.94943	0.14925
H	3.19135	-3.27950	0.13150
H	5.08844	1.31561	-0.08528
H	-1.47009	-2.35859	0.06477
H	0.07973	2.43821	-1.21679
H	0.88615	3.35362	0.66496
H	-3.86671	-3.02604	0.13749
H	-6.26316	-2.41285	0.14639

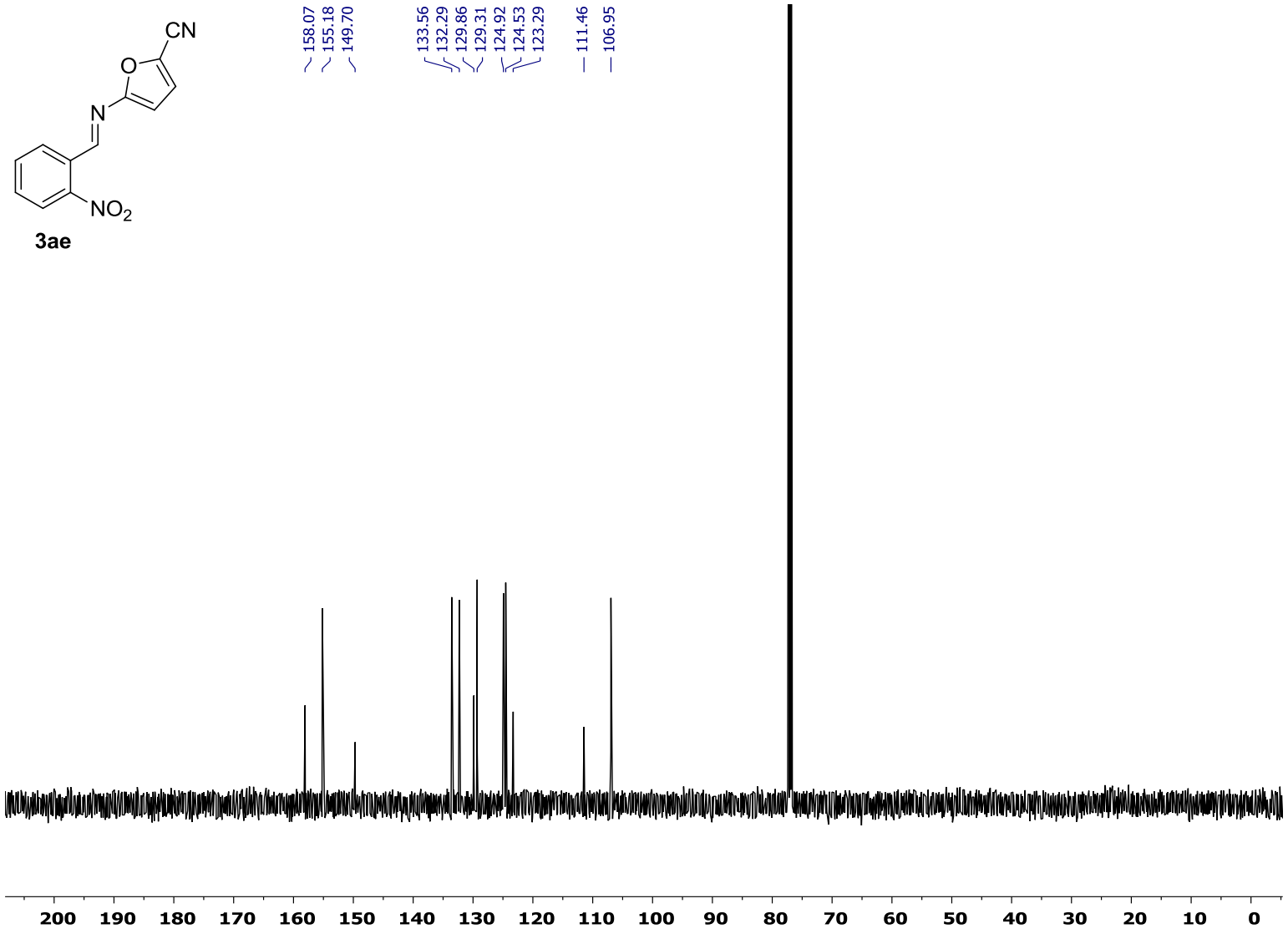
H	-6.94593	-0.02115	0.01999
H	-5.23712	1.75938	-0.11729

4. NMR Spectra

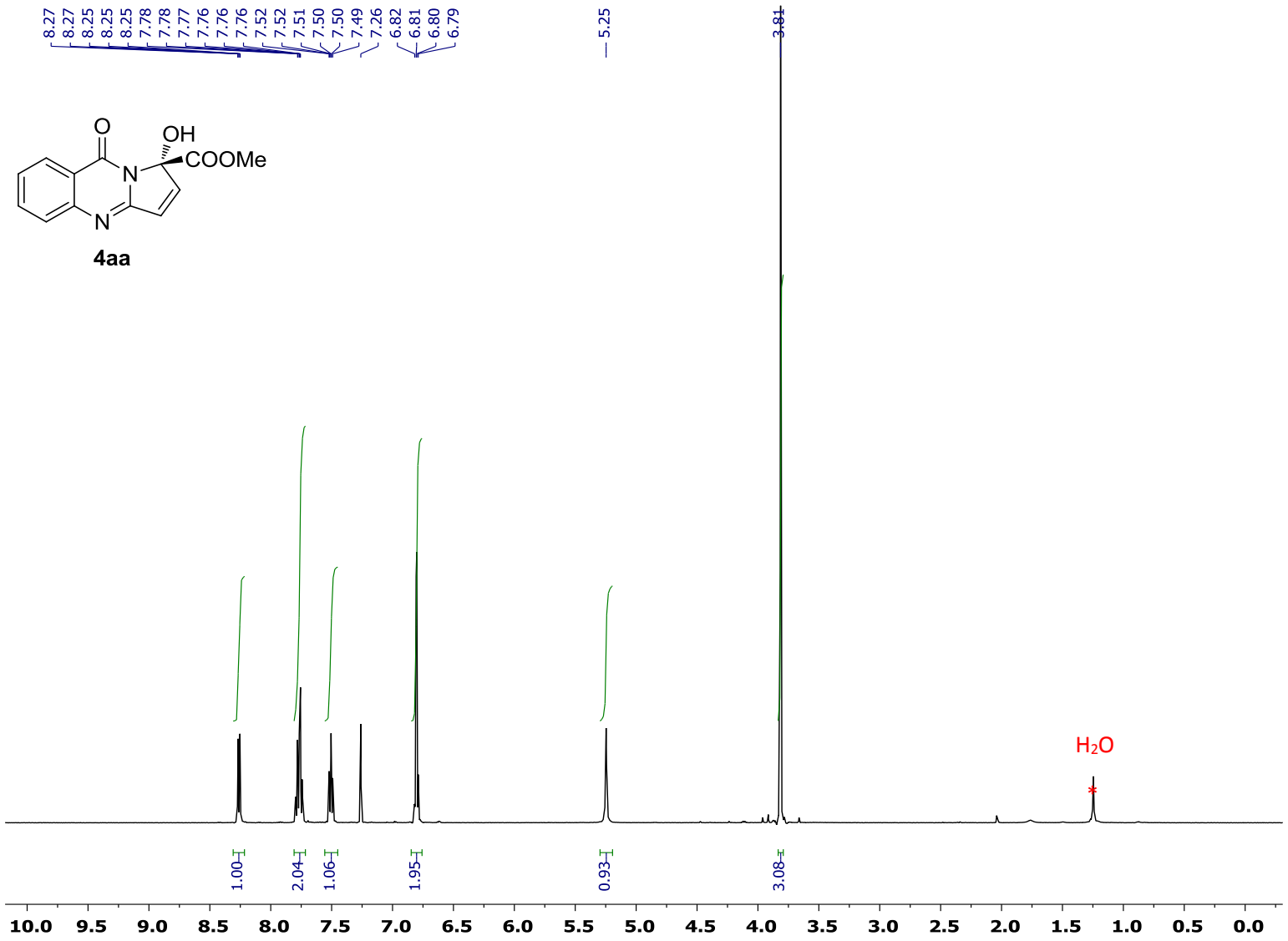
^{1}H NMR (500 MHz, $CDCl_3$)



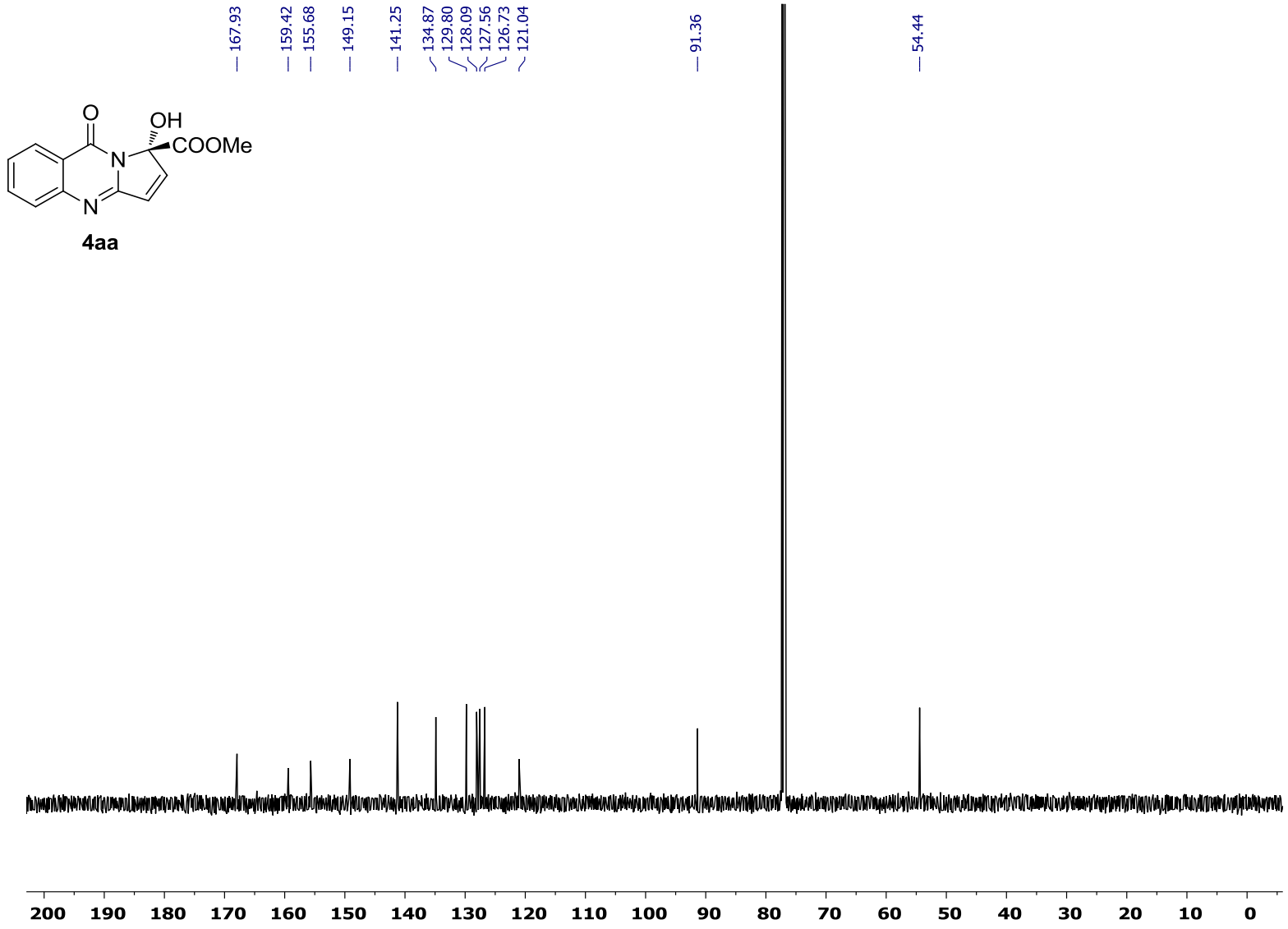
^{13}C NMR (126 MHz, $CDCl_3$)



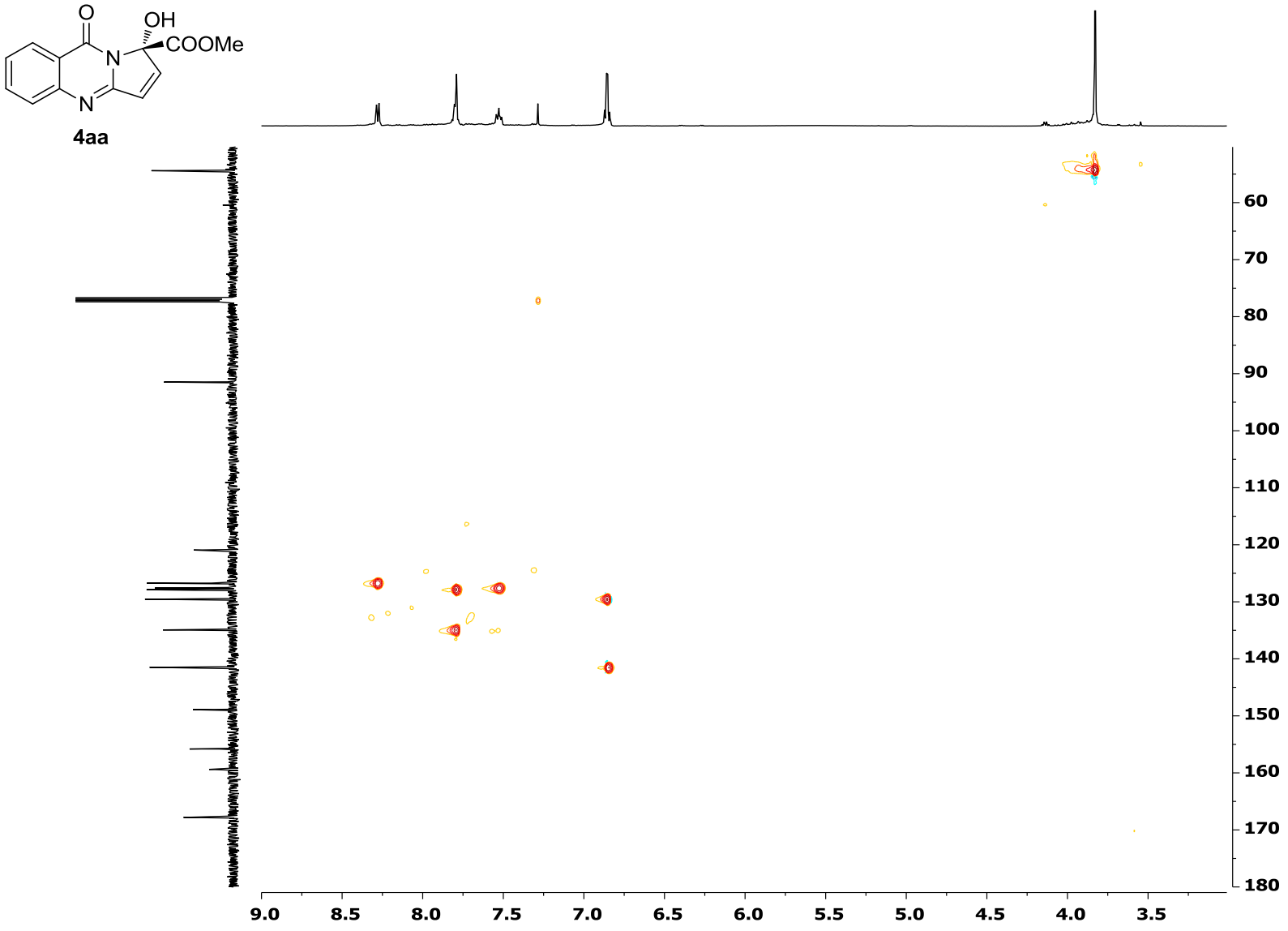
^{1}H NMR (500 MHz, $CDCl_3$)



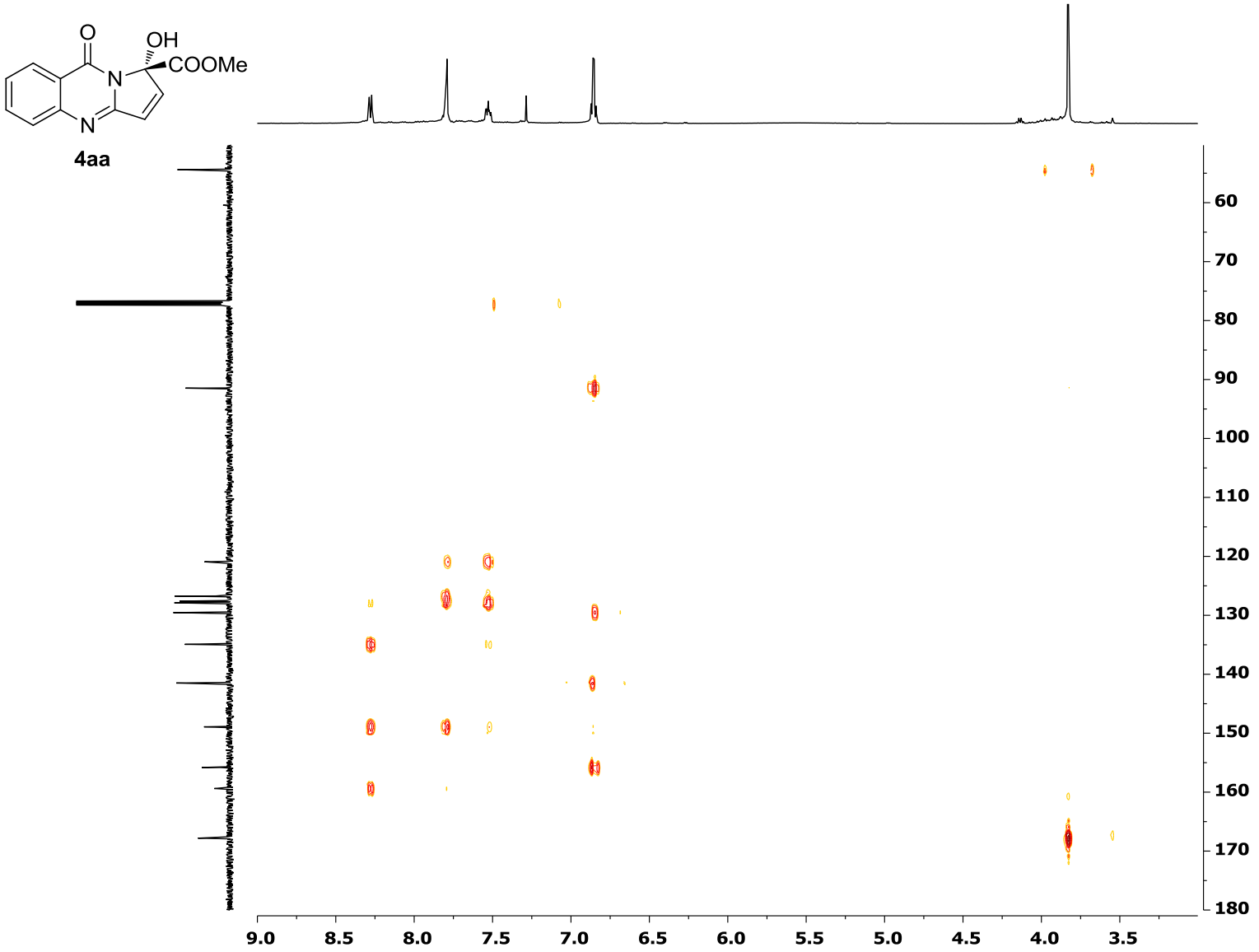
^{13}C NMR (126 MHz, $CDCl_3$)



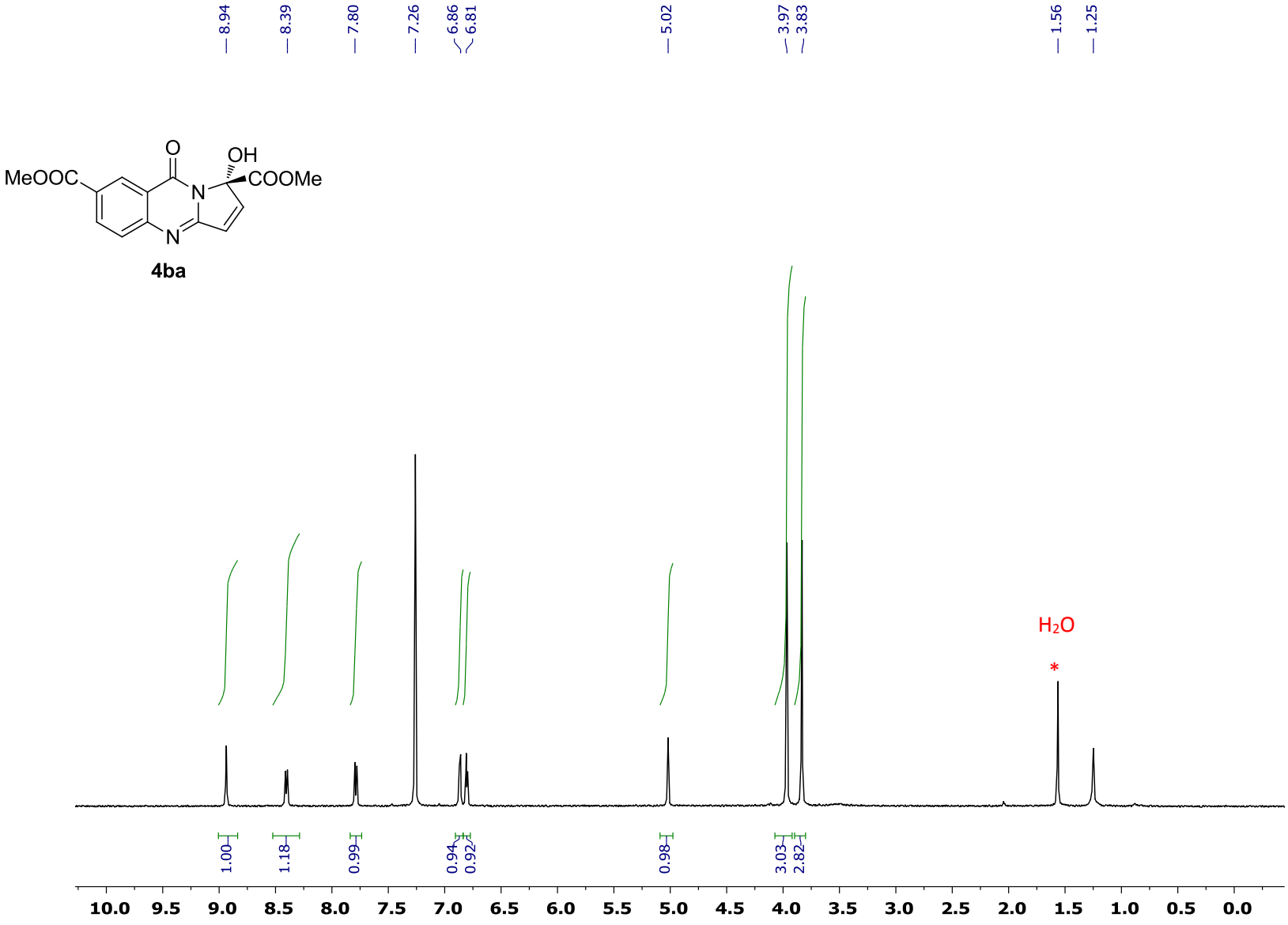
HSQC NMR (500 MHz, $CDCl_3$)



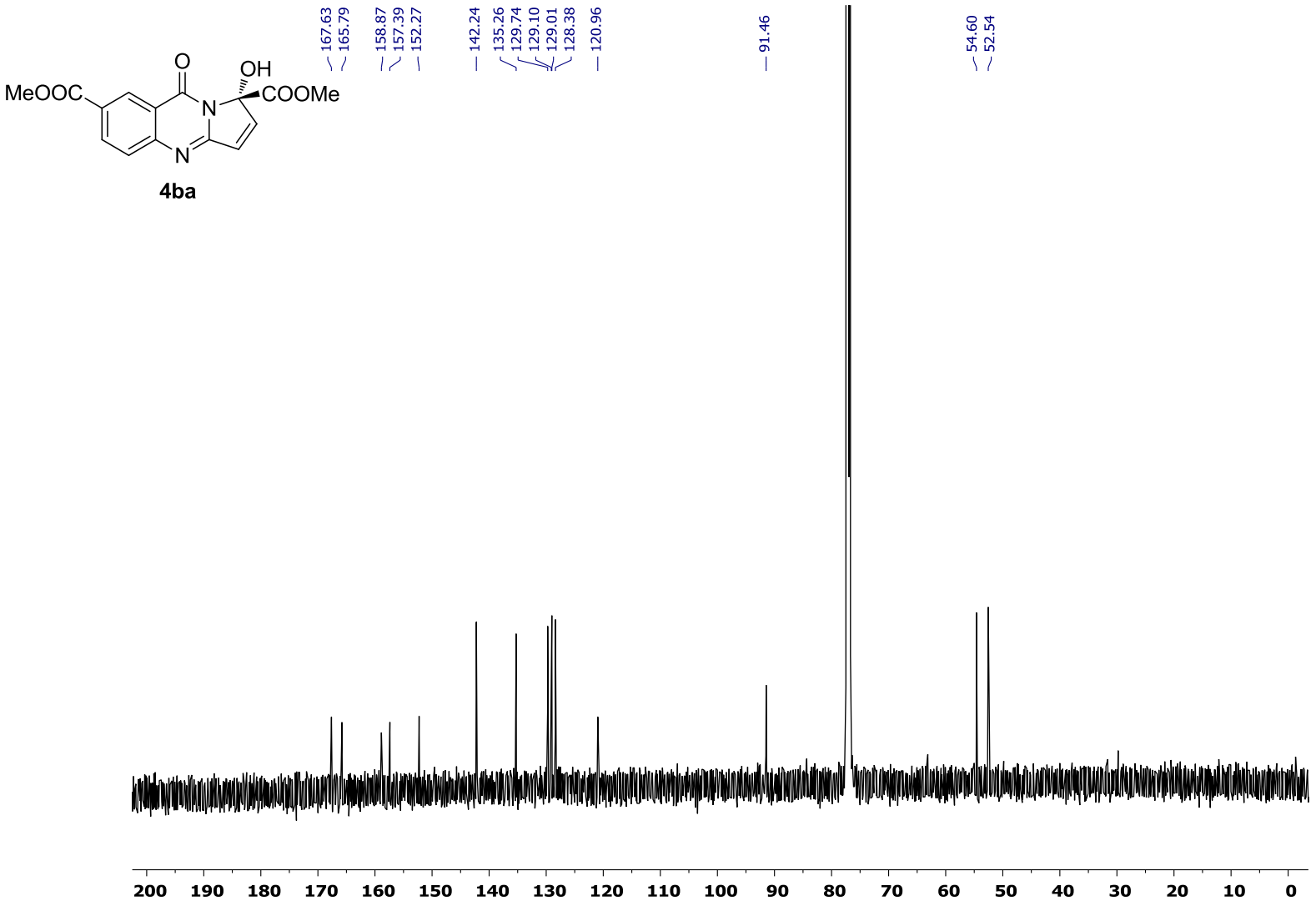
HMBC NMR (500 MHz, $CDCl_3$)



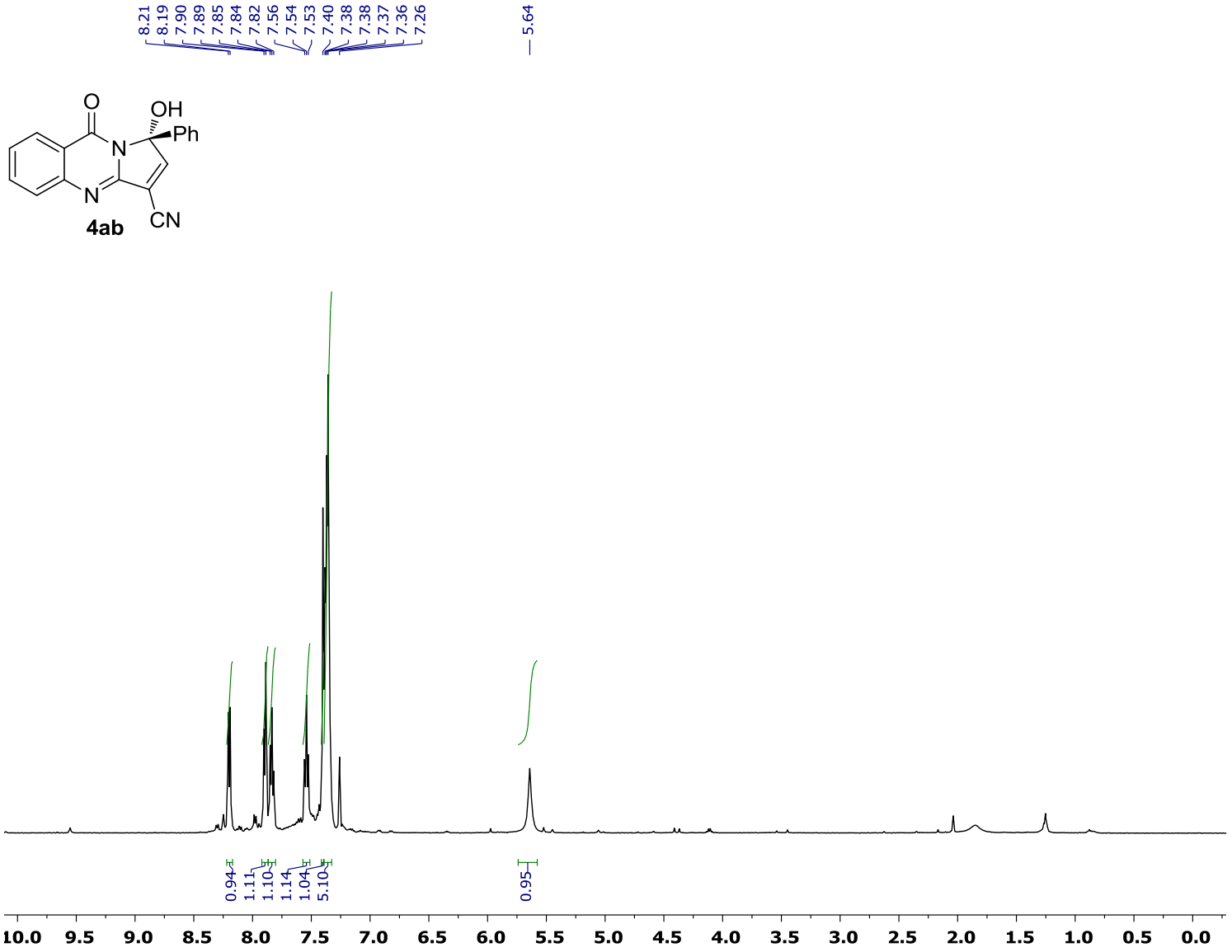
^{1}H NMR (500 MHz, $CDCl_3$)



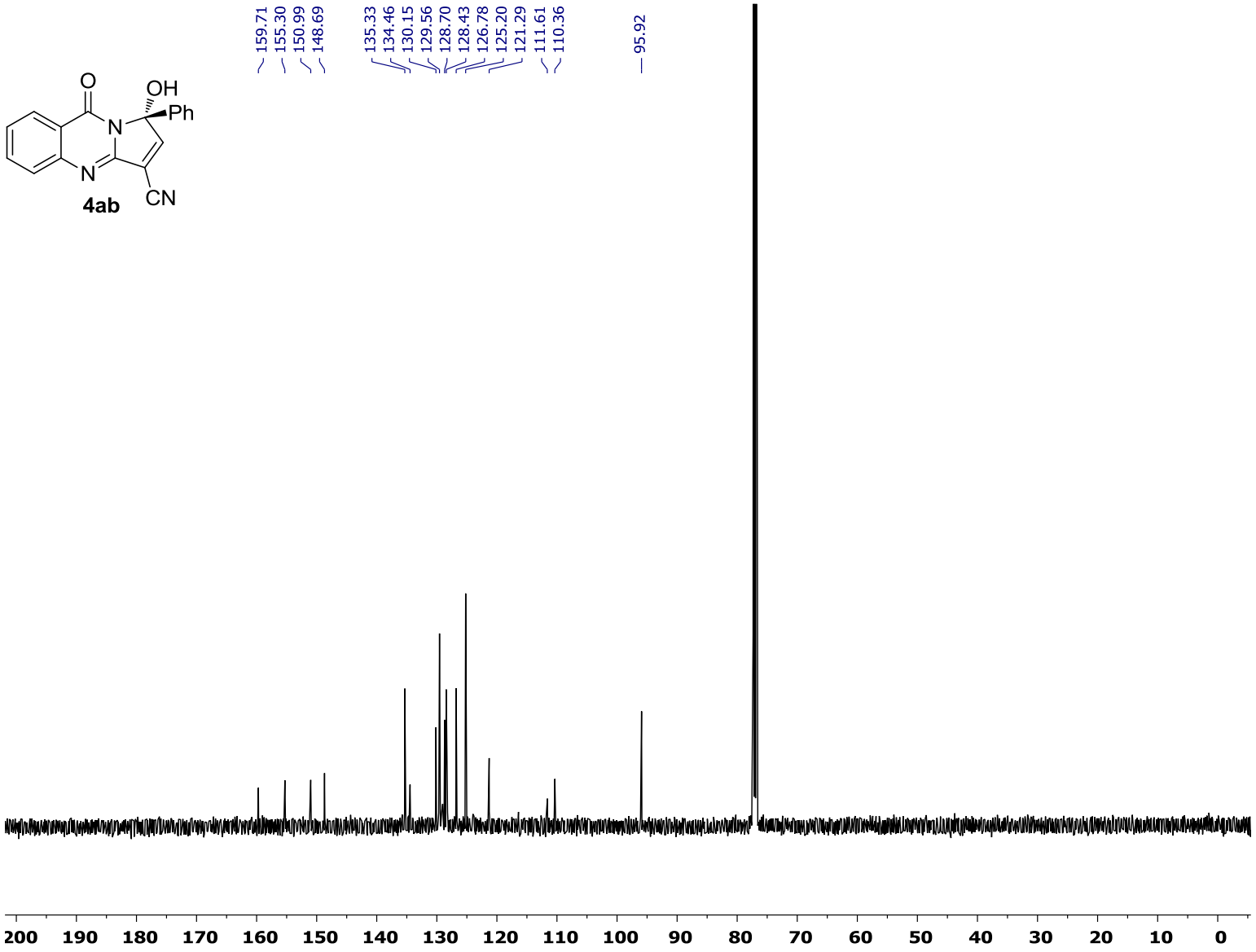
^{13}C NMR (126 MHz, $CDCl_3$)



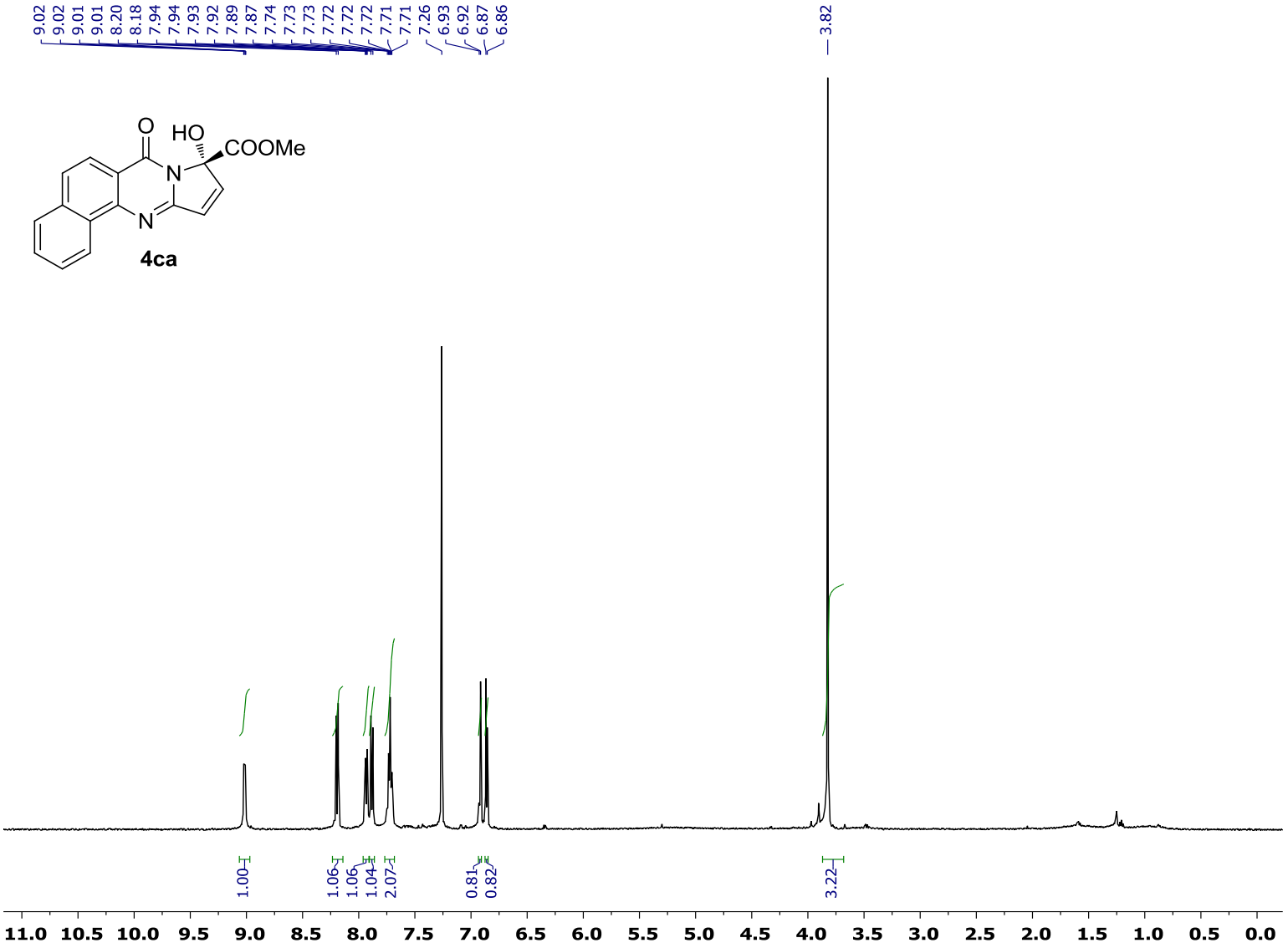
^{1}H NMR (500 MHz, $CDCl_3$)



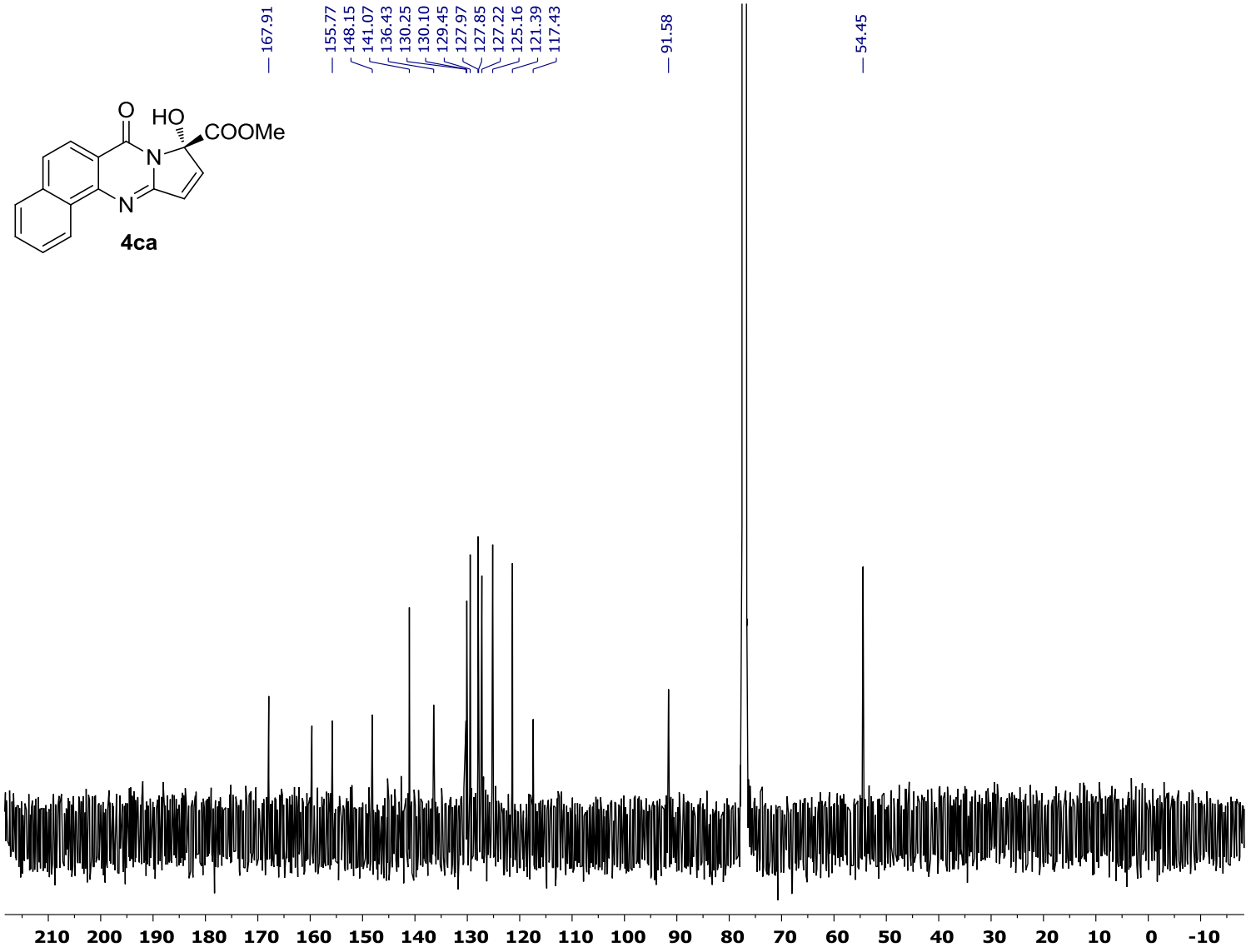
^{13}C NMR (126 MHz, $CDCl_3$)



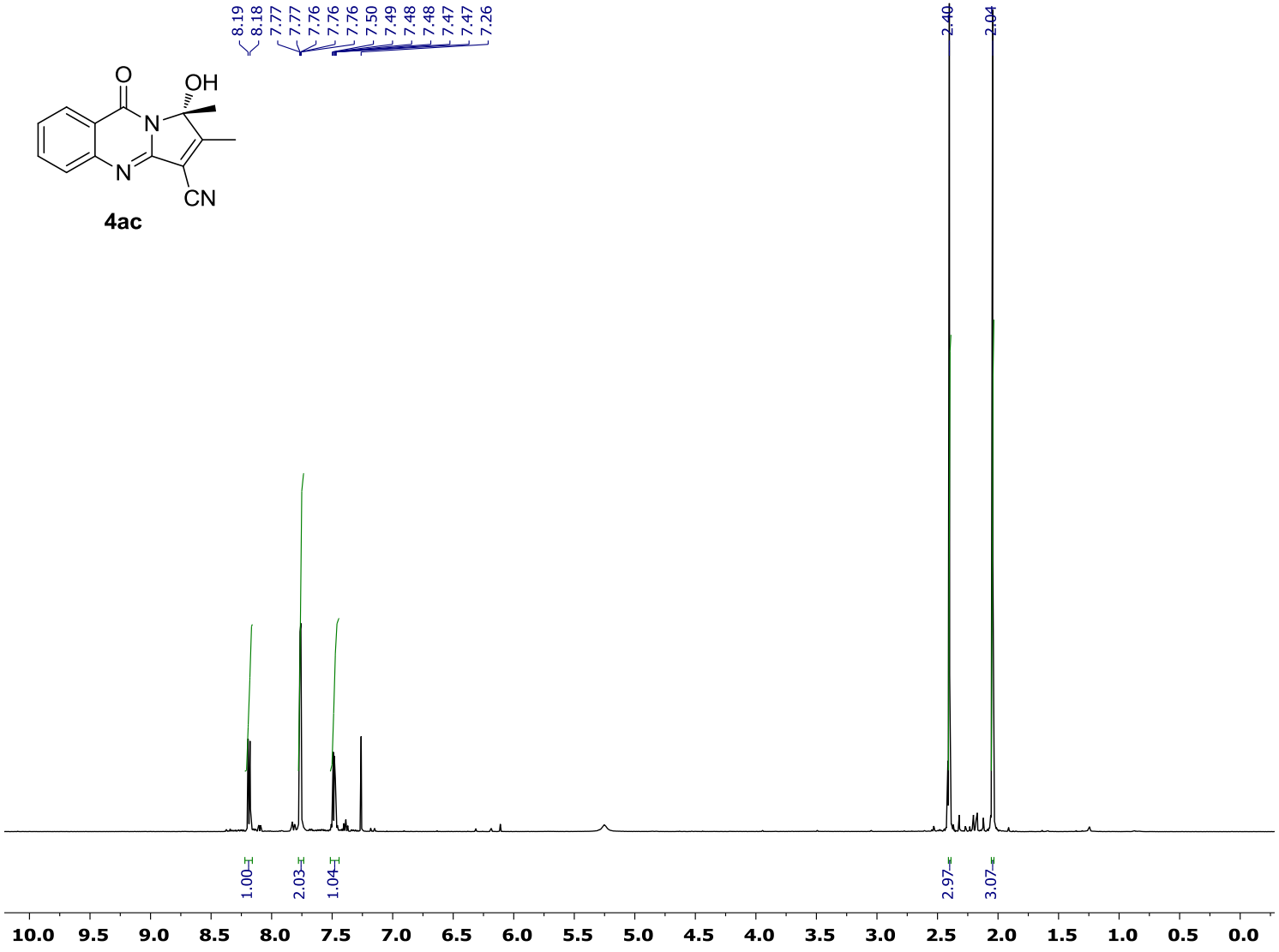
^{1}H NMR (500 MHz, $CDCl_3$)



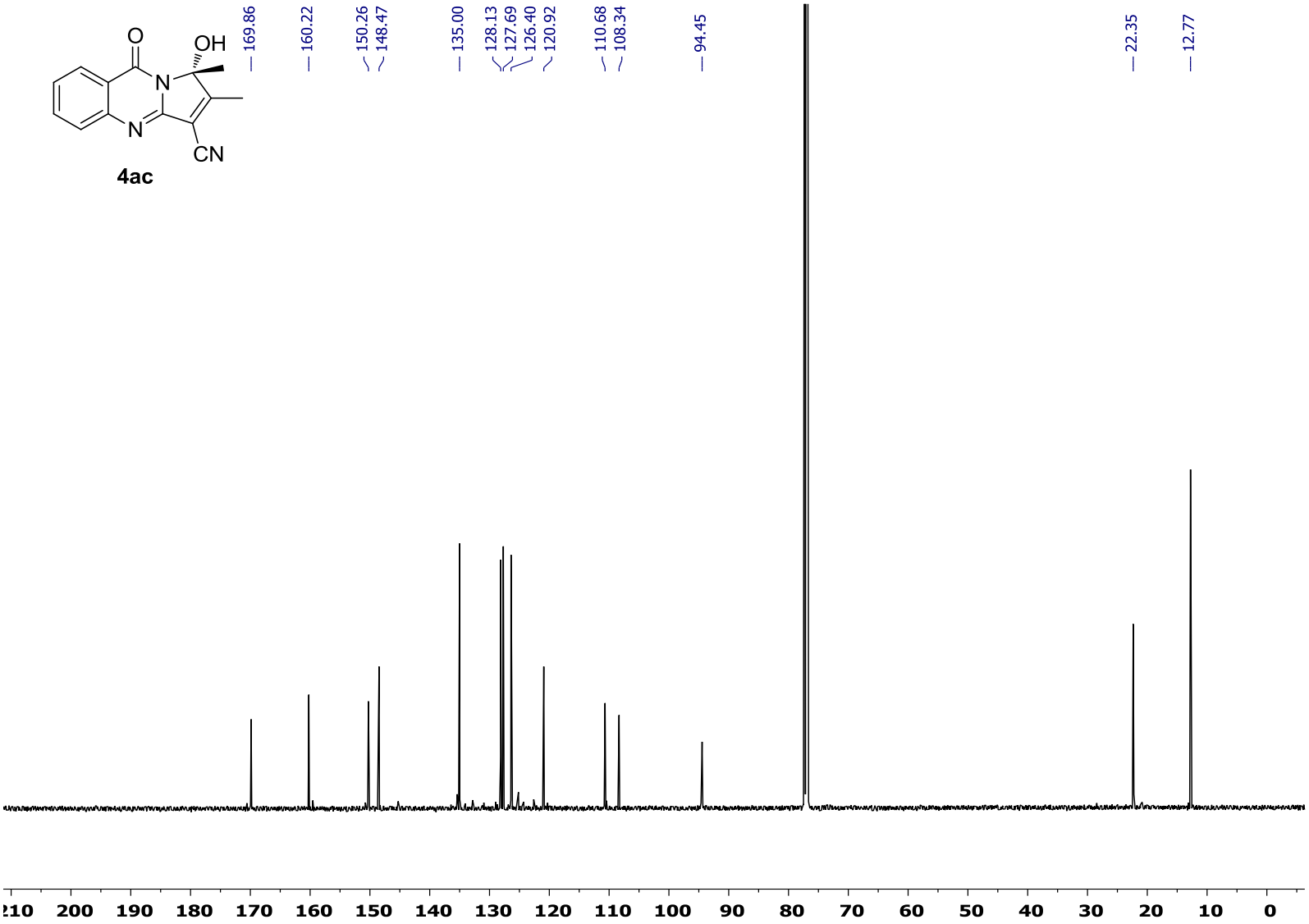
^{13}C NMR (126 MHz, $CDCl_3$)



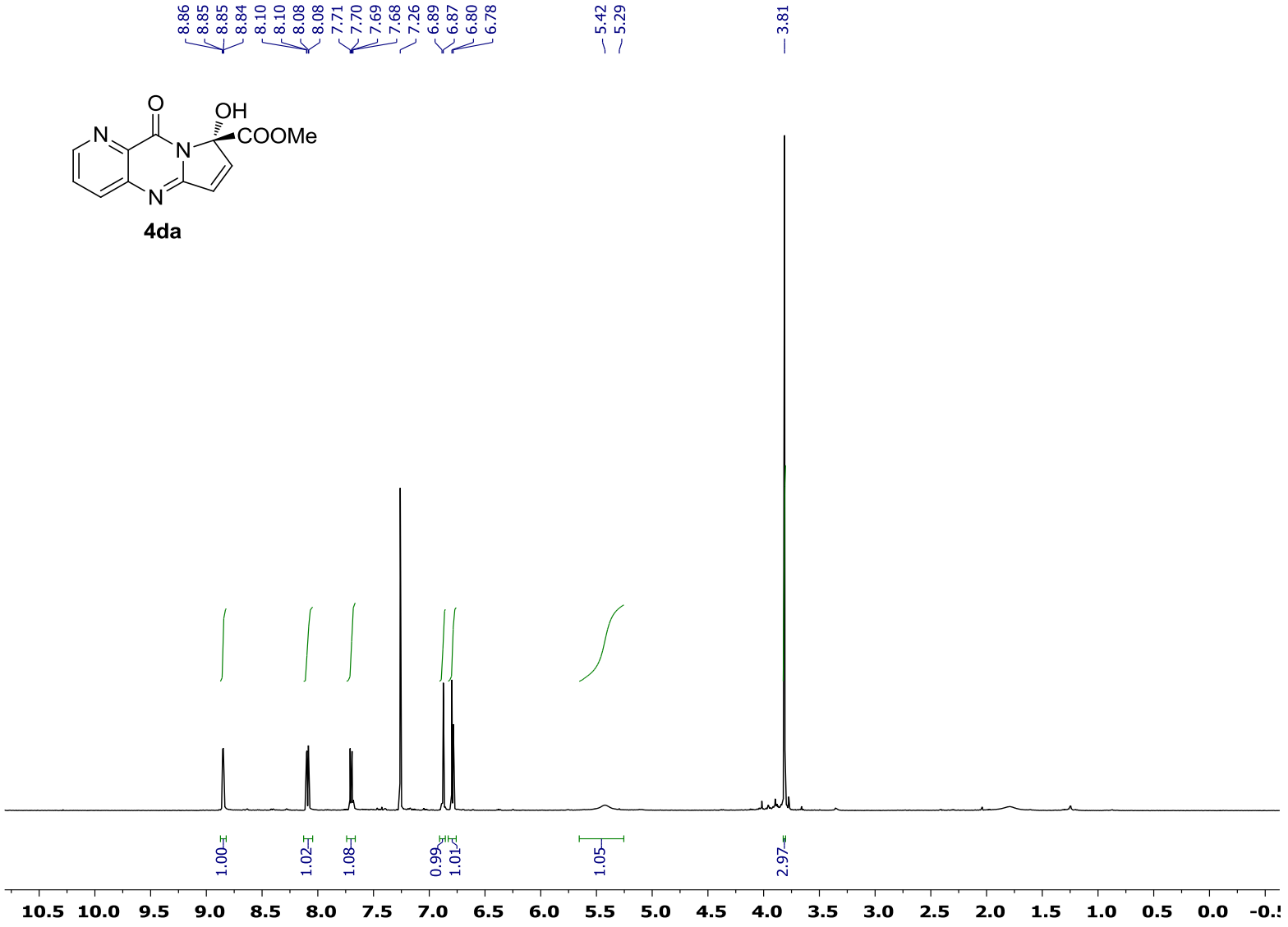
^{1}H NMR (500 MHz, $CDCl_3$)



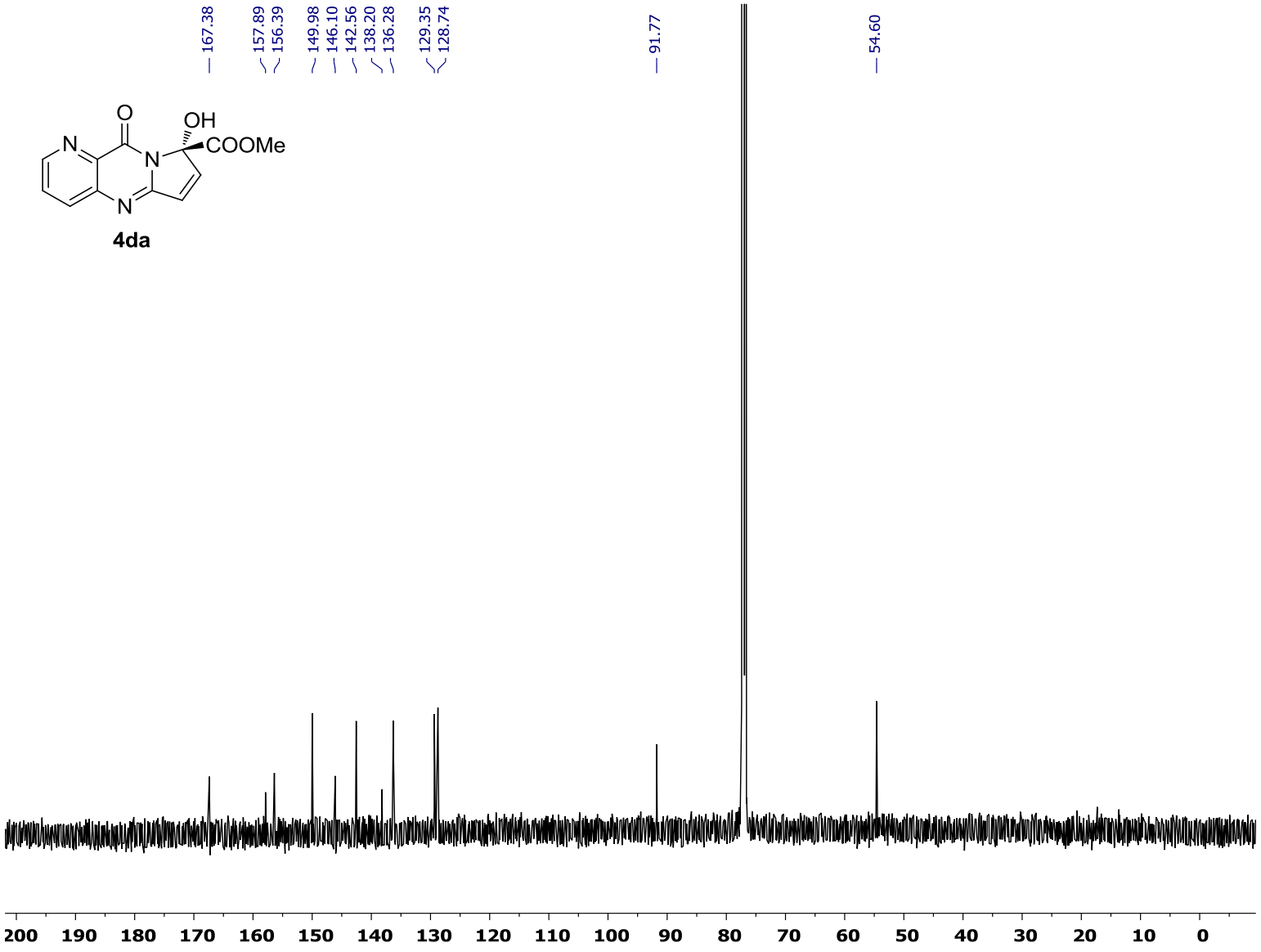
^{13}C NMR (126 MHz, $CDCl_3$)



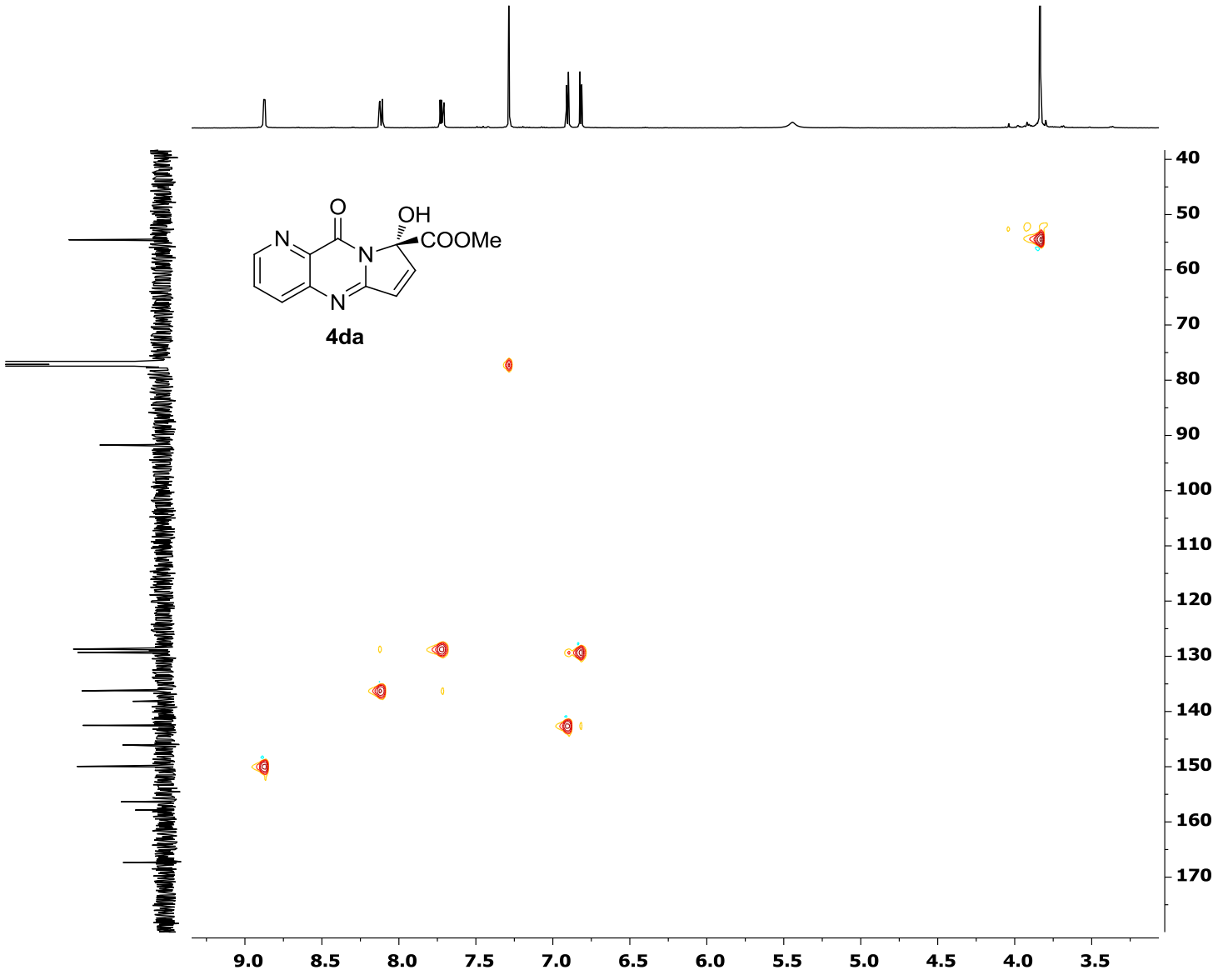
^{1}H NMR (500 MHz, $CDCl_3$)



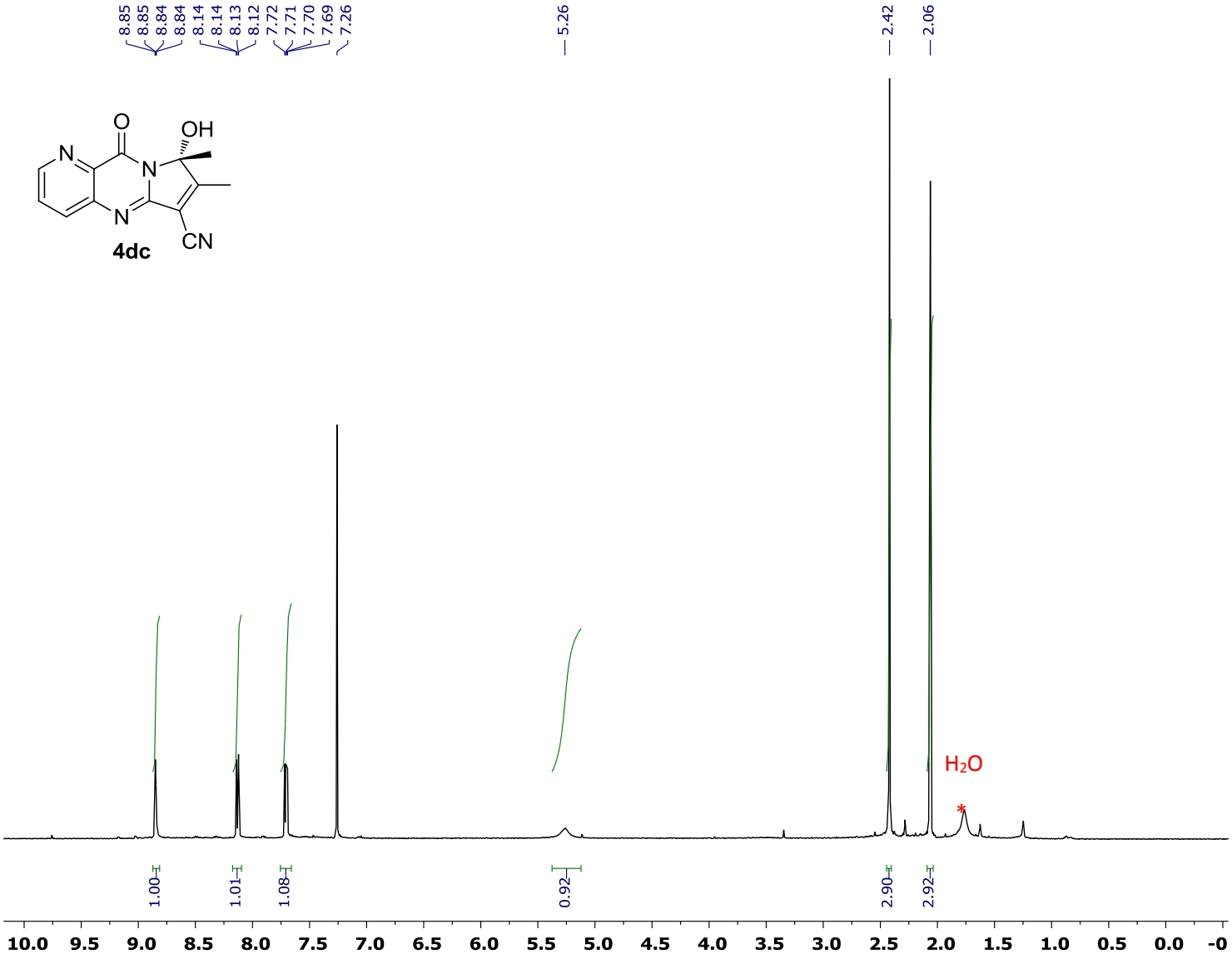
^{13}C NMR (126 MHz, $CDCl_3$)



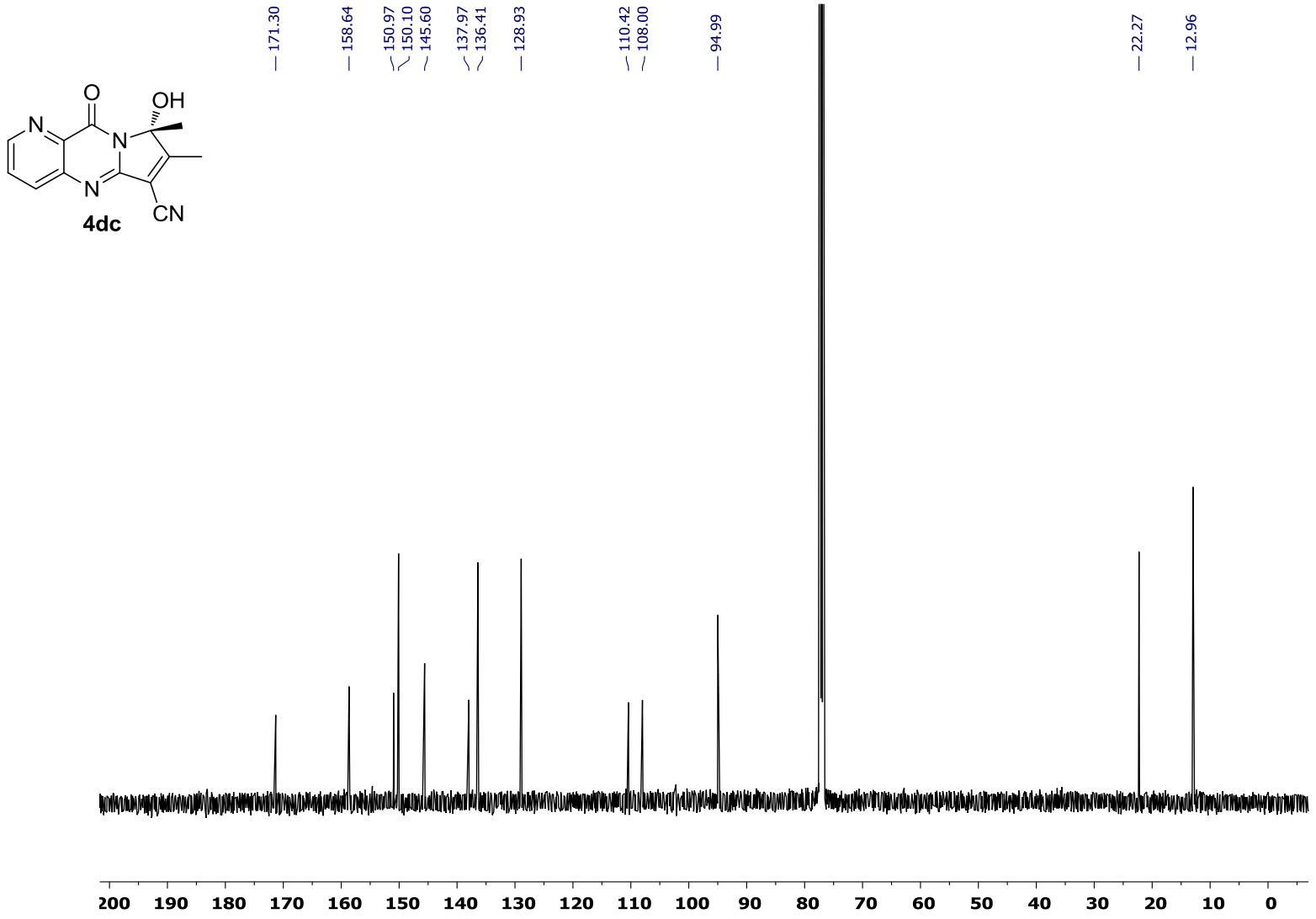
HSQC NMR (500 MHz, $CDCl_3$)



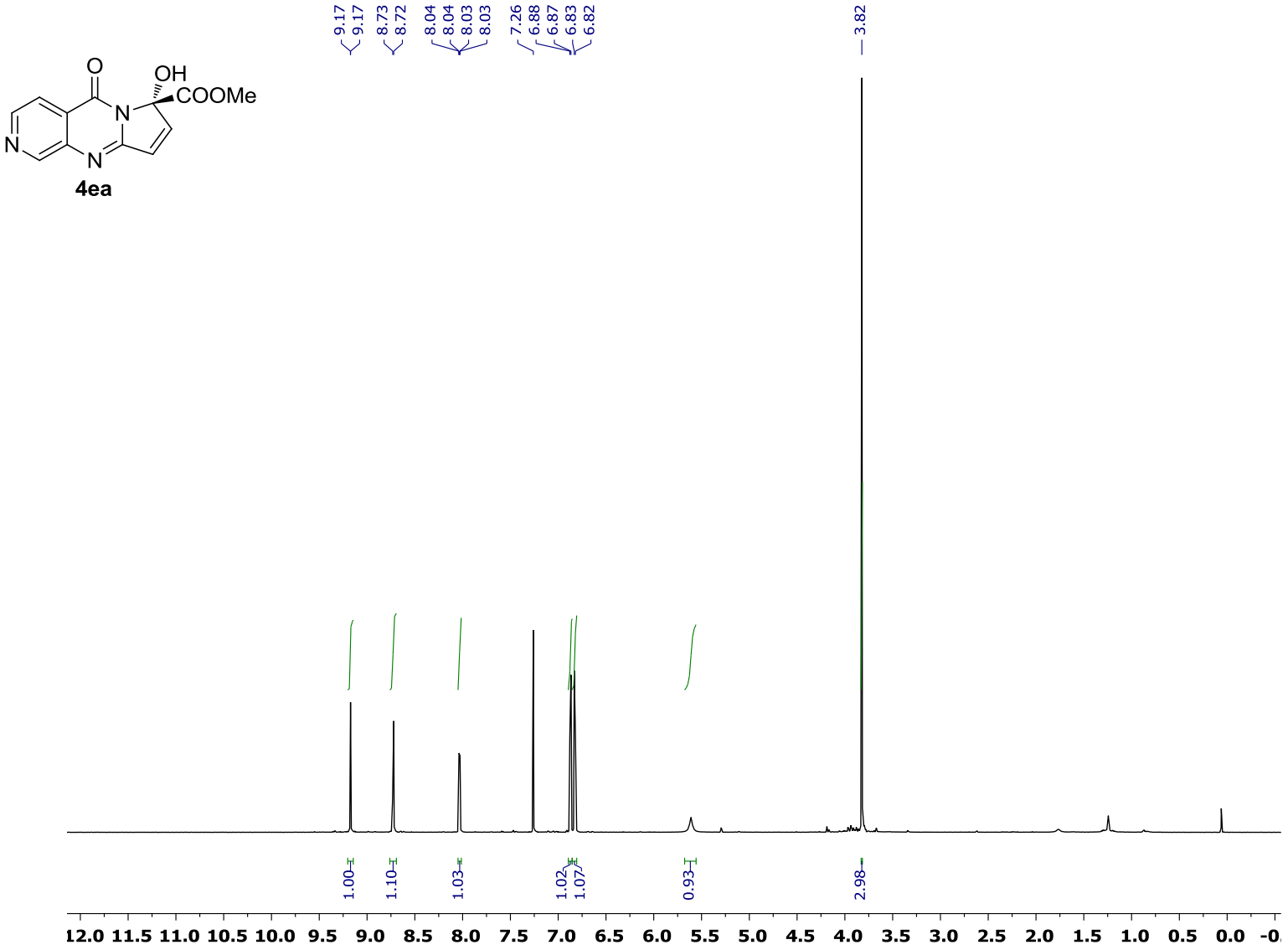
^{1}H NMR (500 MHz, $CDCl_3$)



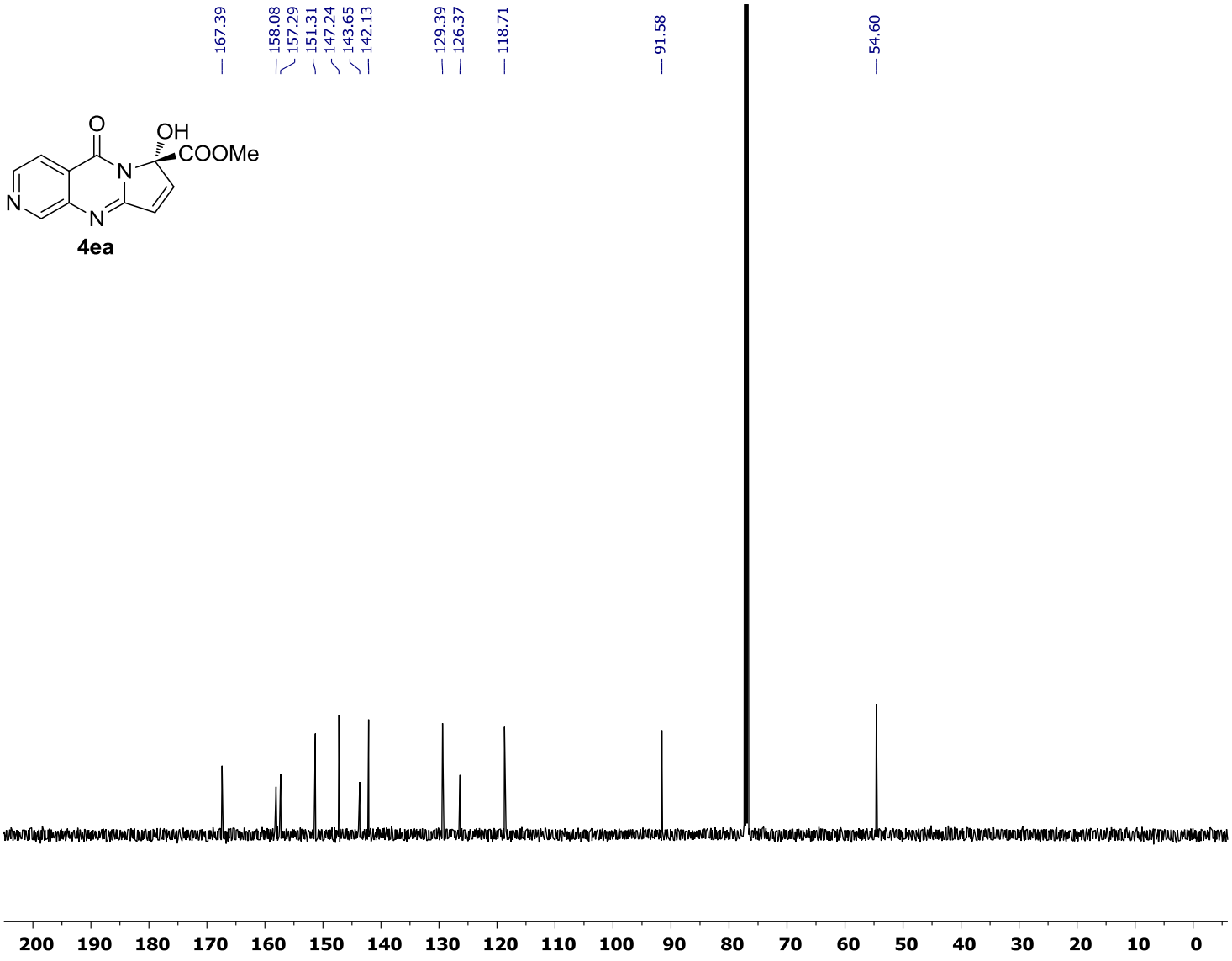
^{13}C NMR (126 MHz, $CDCl_3$)



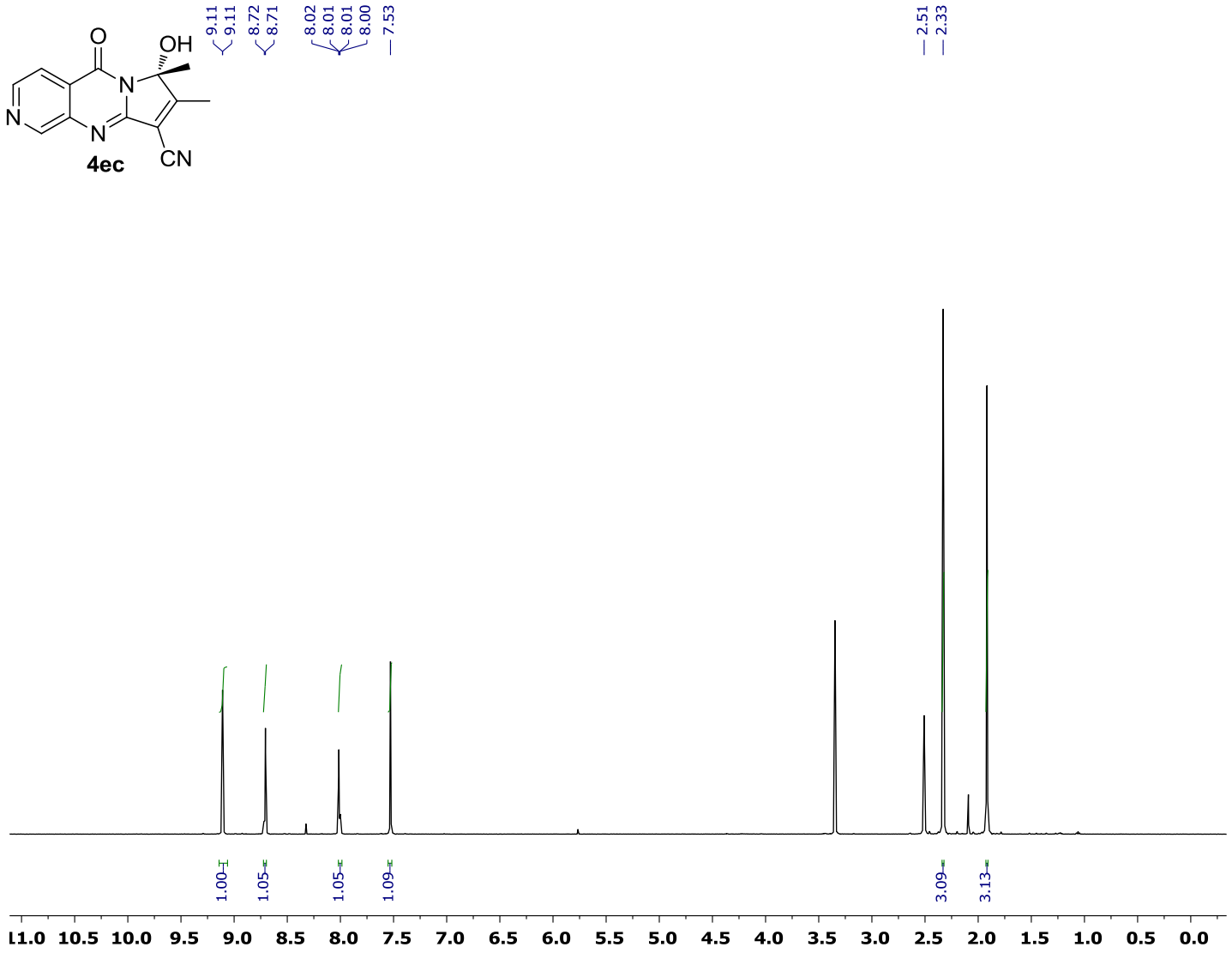
^{1}H NMR (500 MHz, $CDCl_3$)



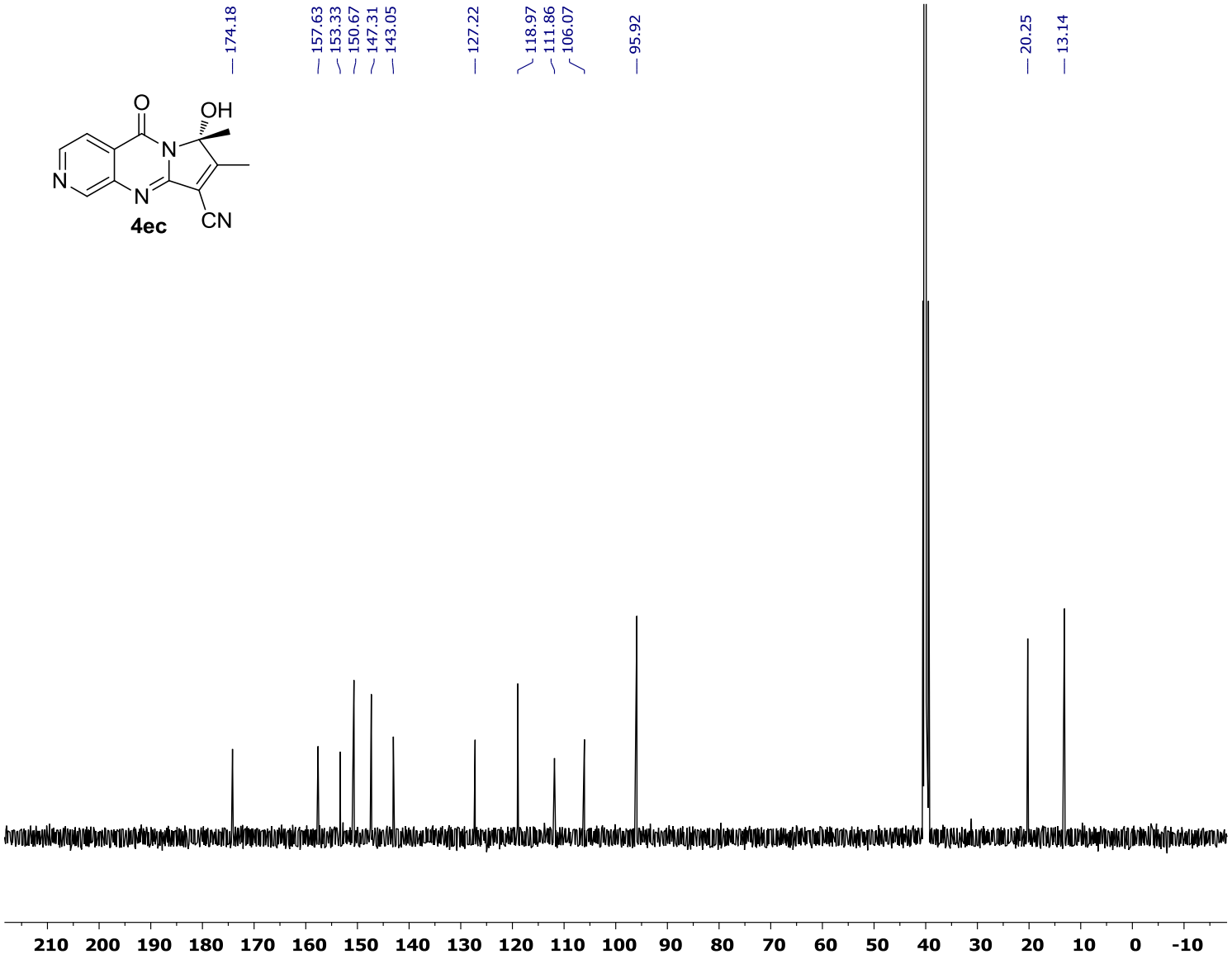
^{13}C NMR (126 MHz, $CDCl_3$)



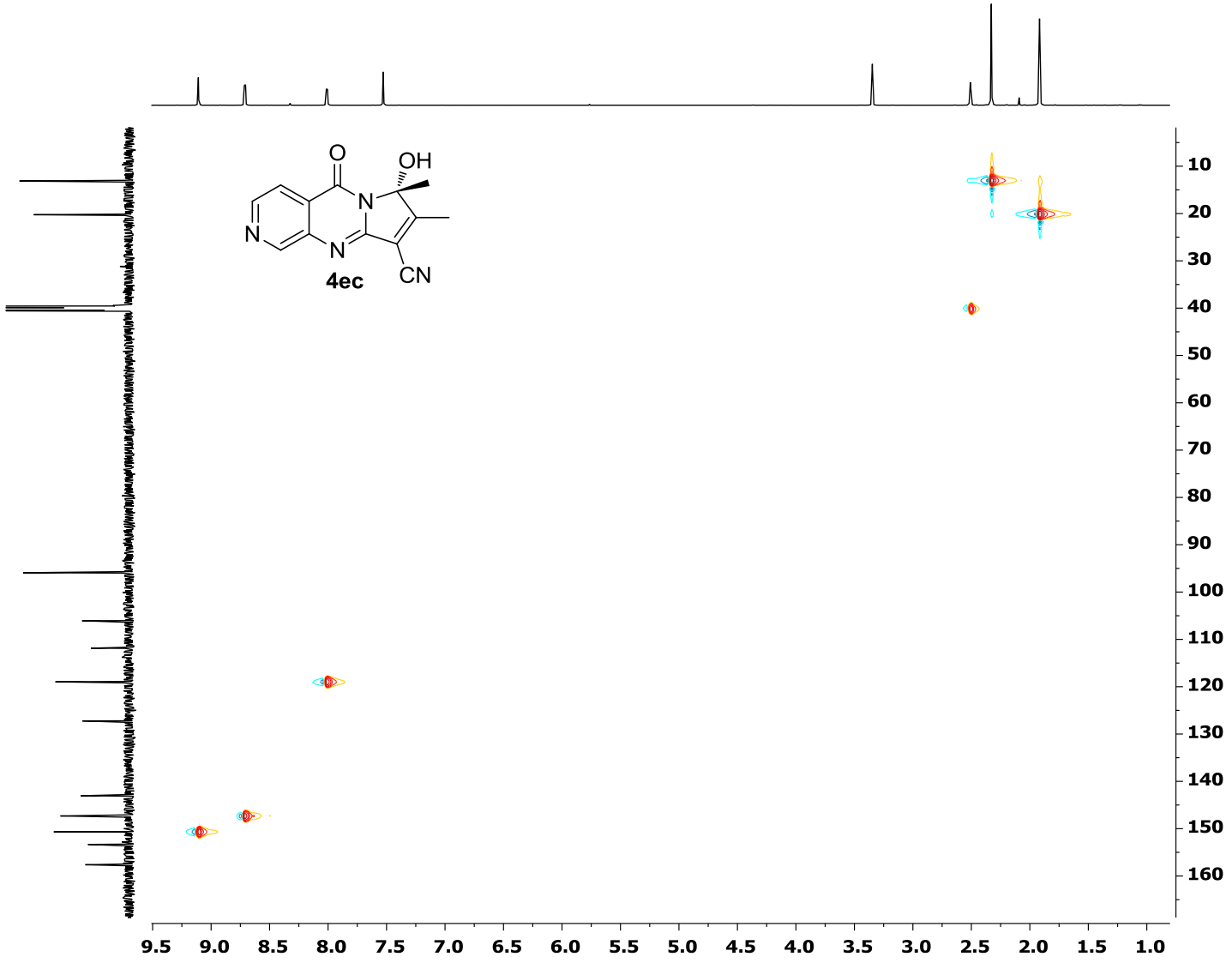
^{1}H NMR (500 MHz, DMSO)



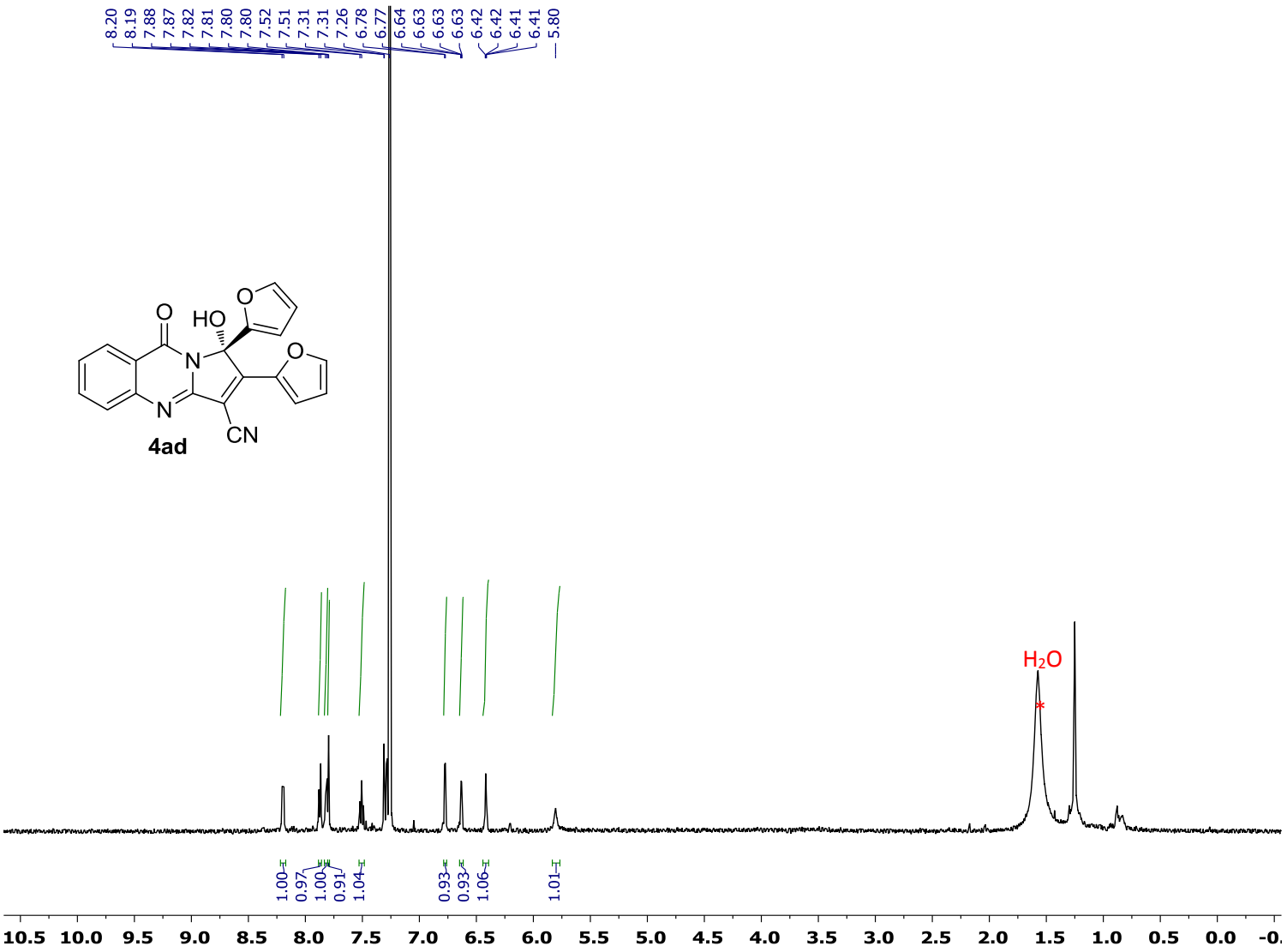
^{13}C NMR (126 MHz, DMSO)



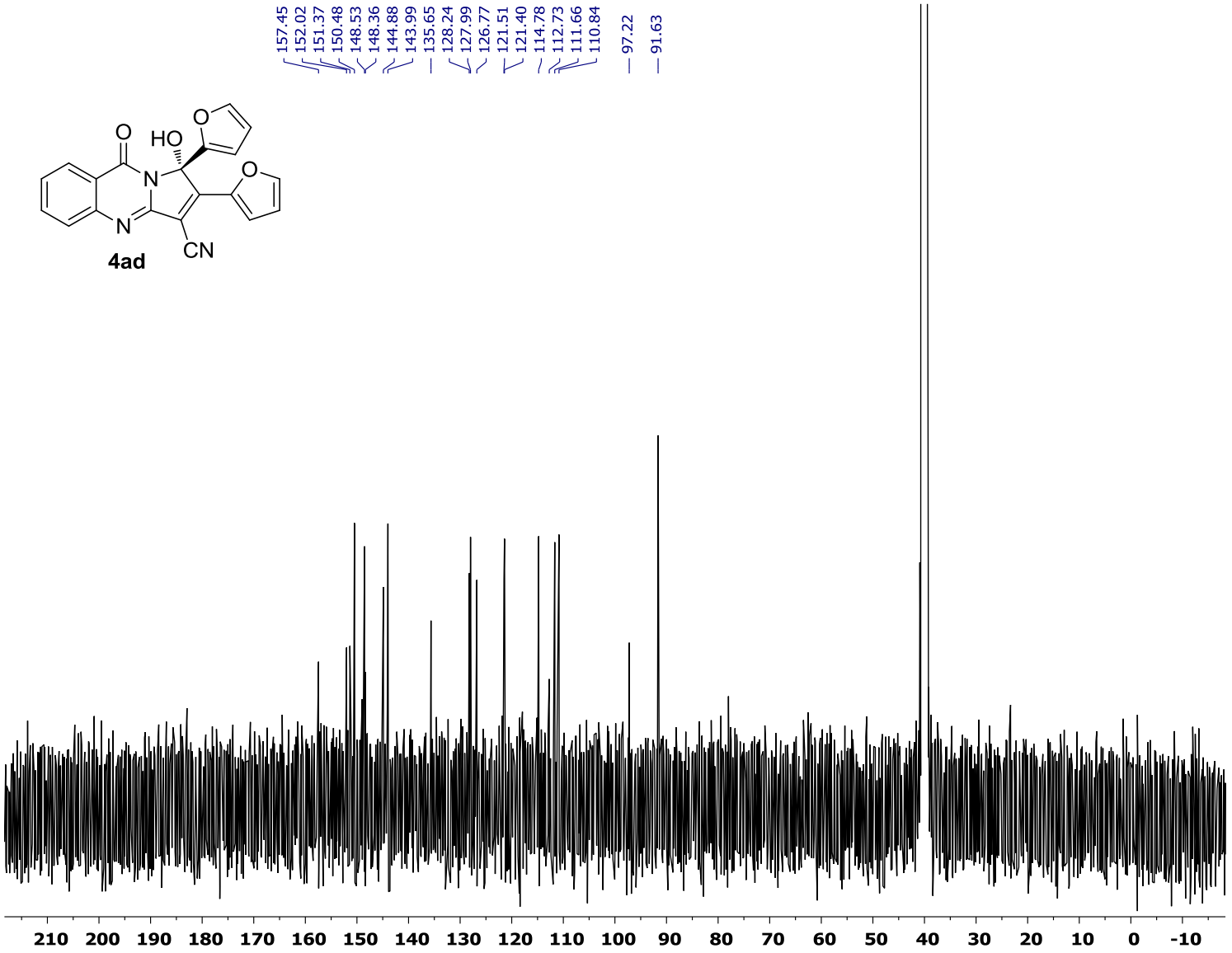
HSQC NMR (500 MHz, DMSO)



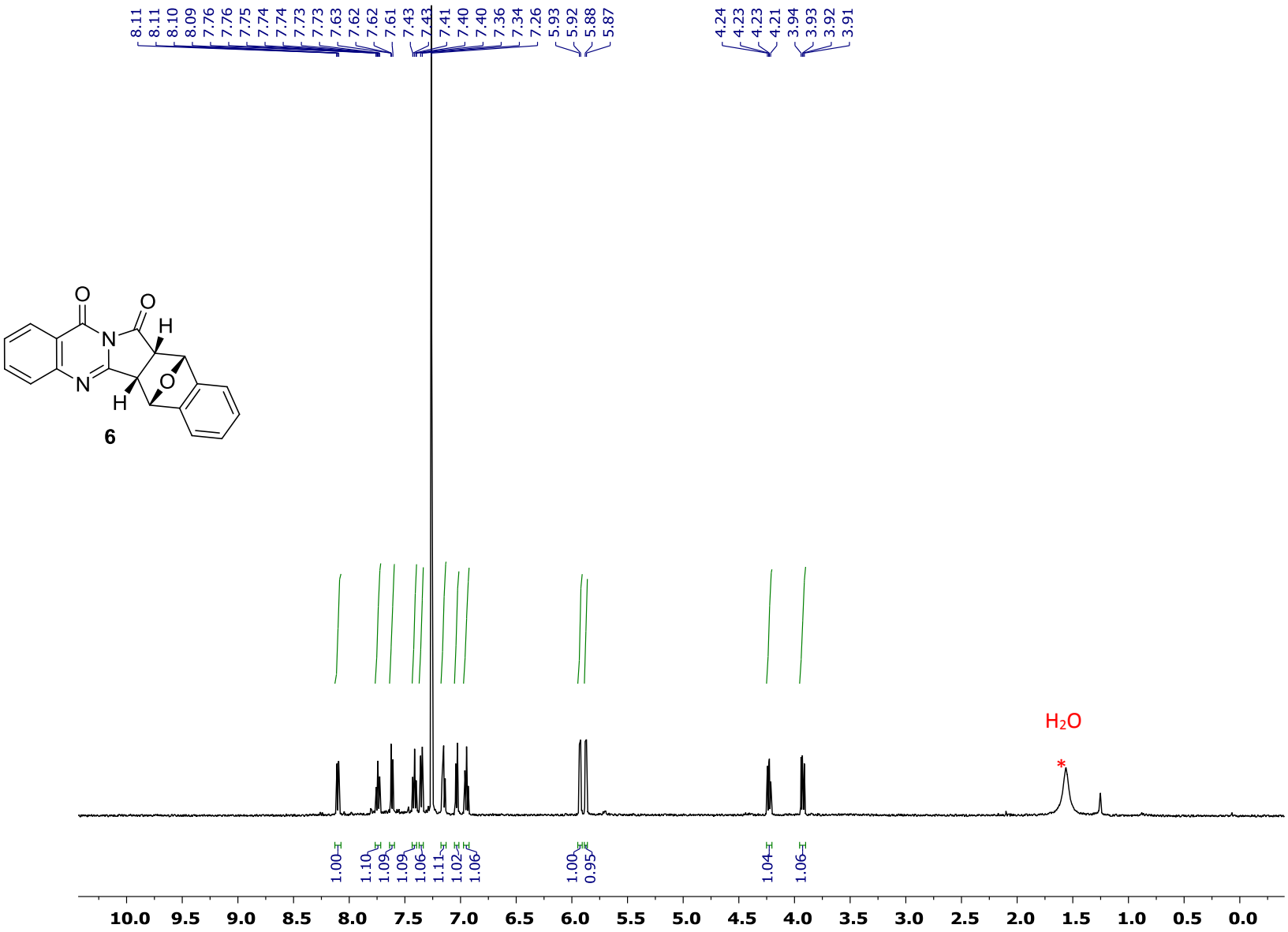
^{1}H NMR (500 MHz, $CDCl_3$)



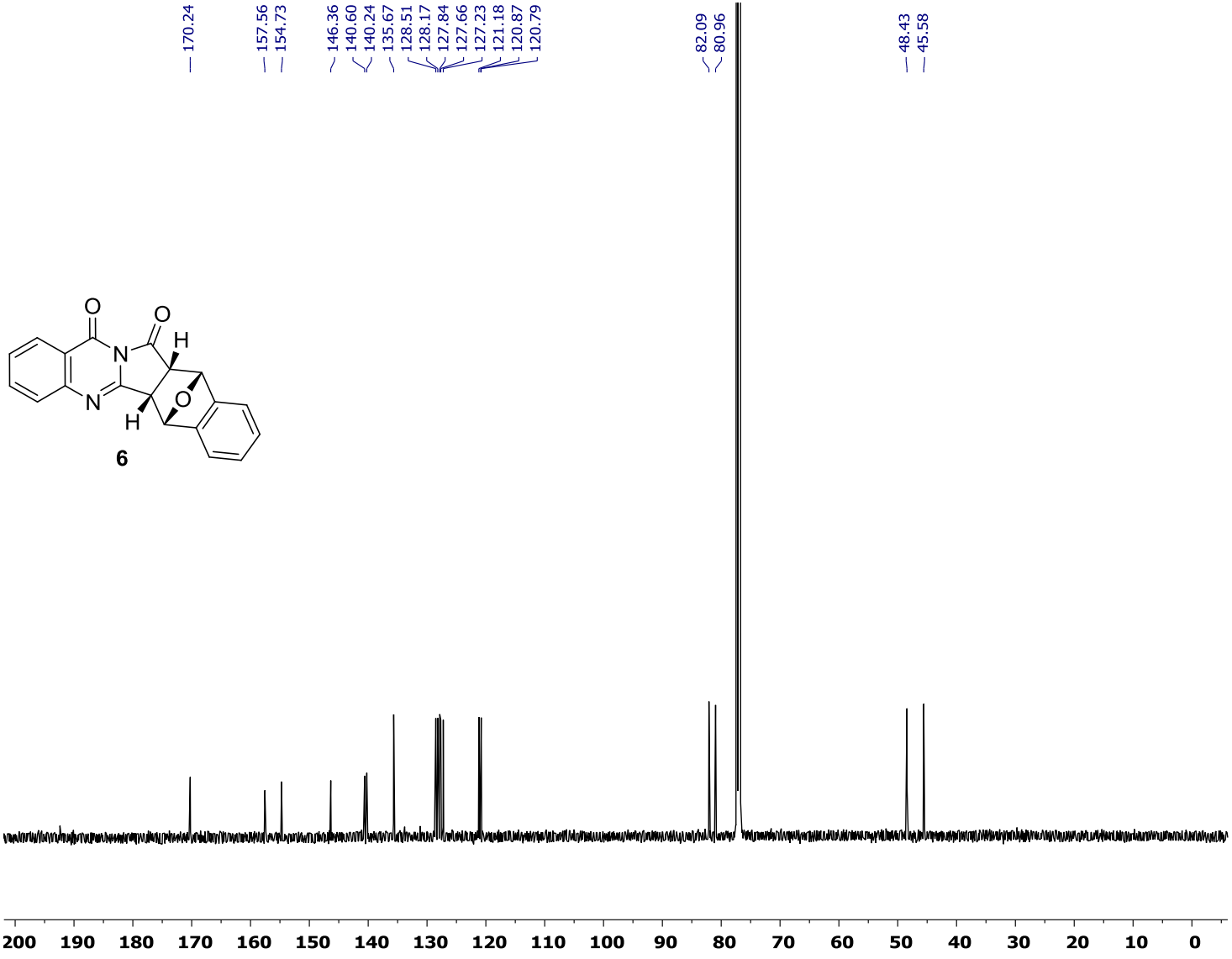
^{13}C NMR (126 MHz, DMSO-d_6)



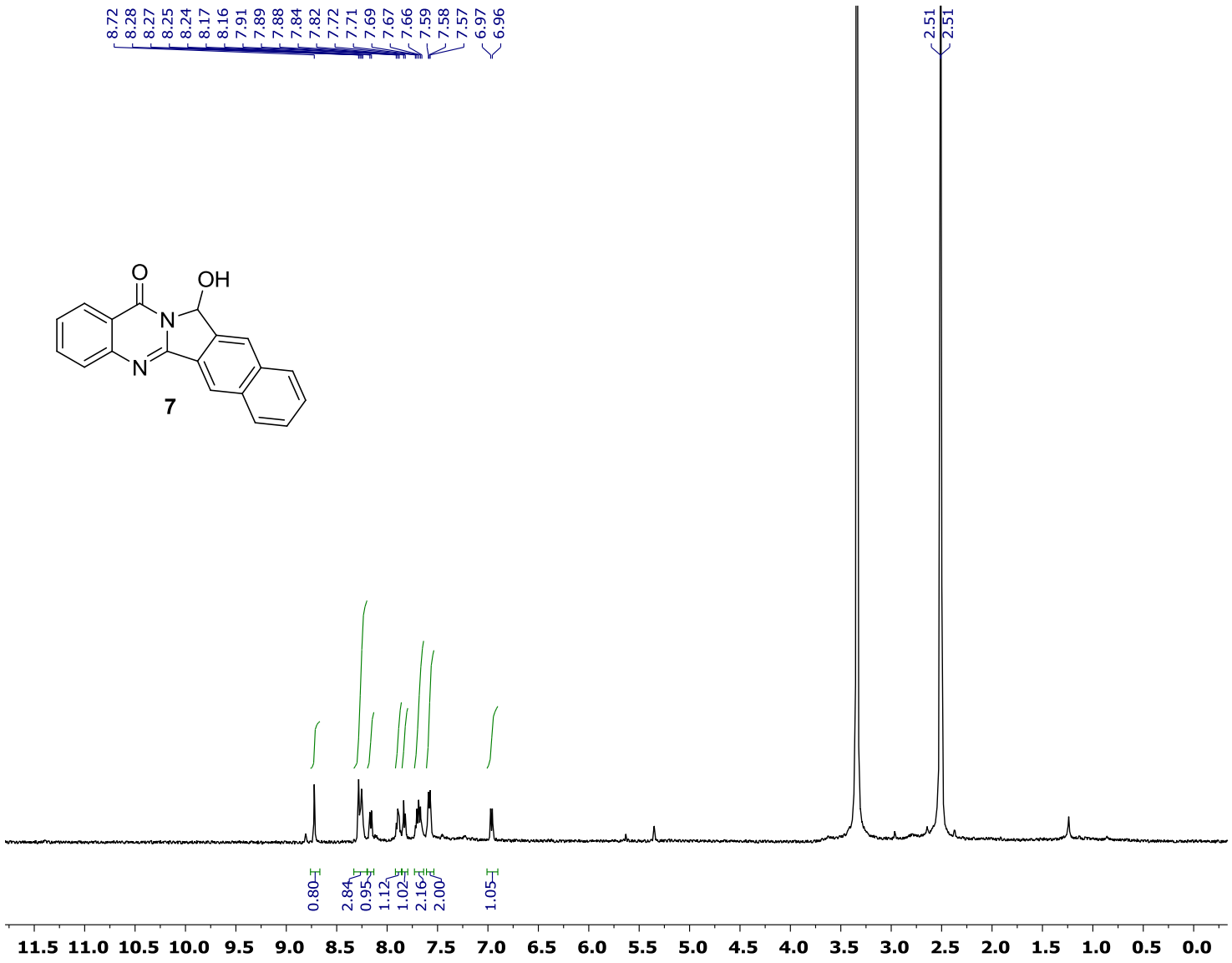
^{1}H NMR (500 MHz, $CDCl_3$)



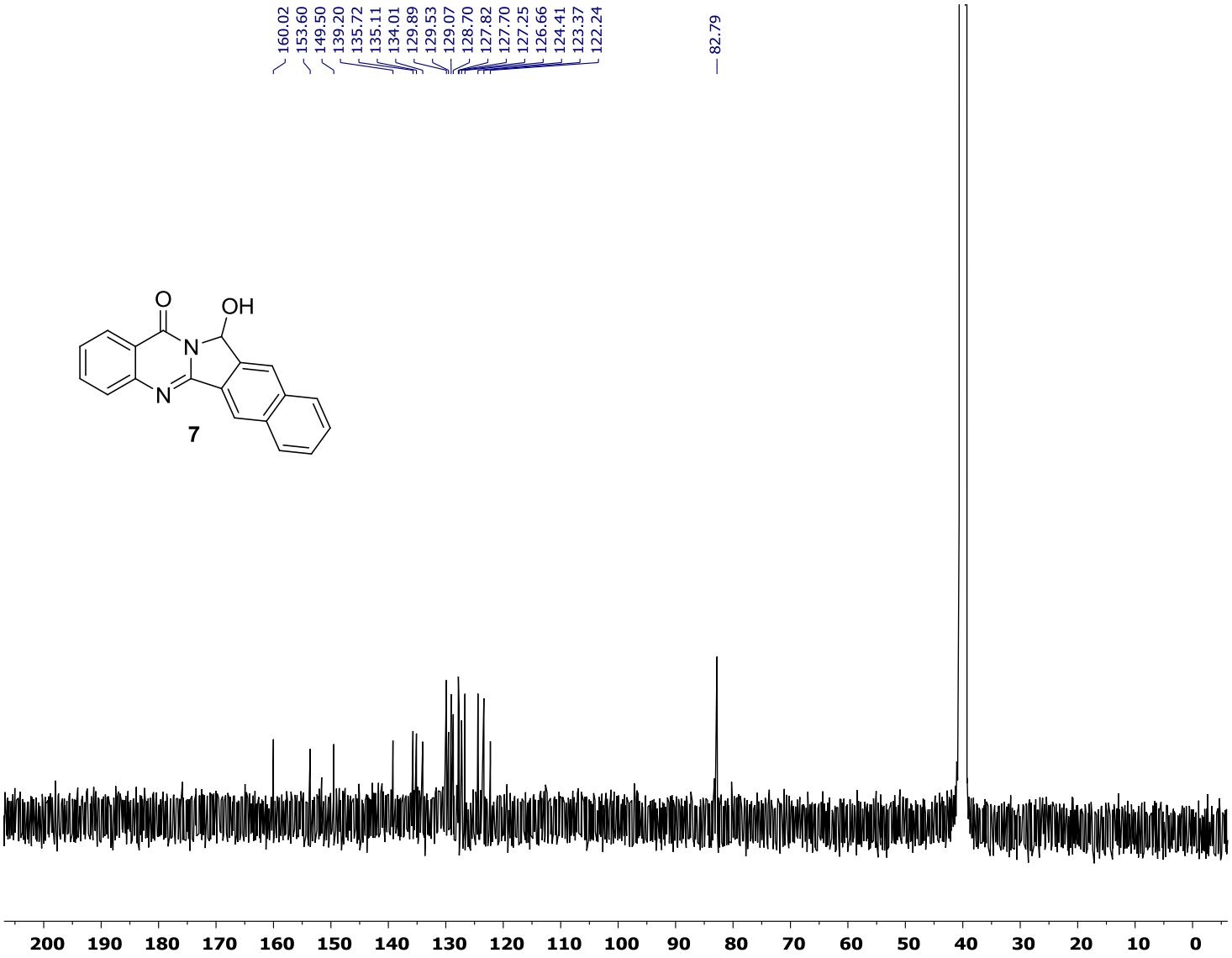
^{13}C NMR (126 MHz, $CDCl_3$)



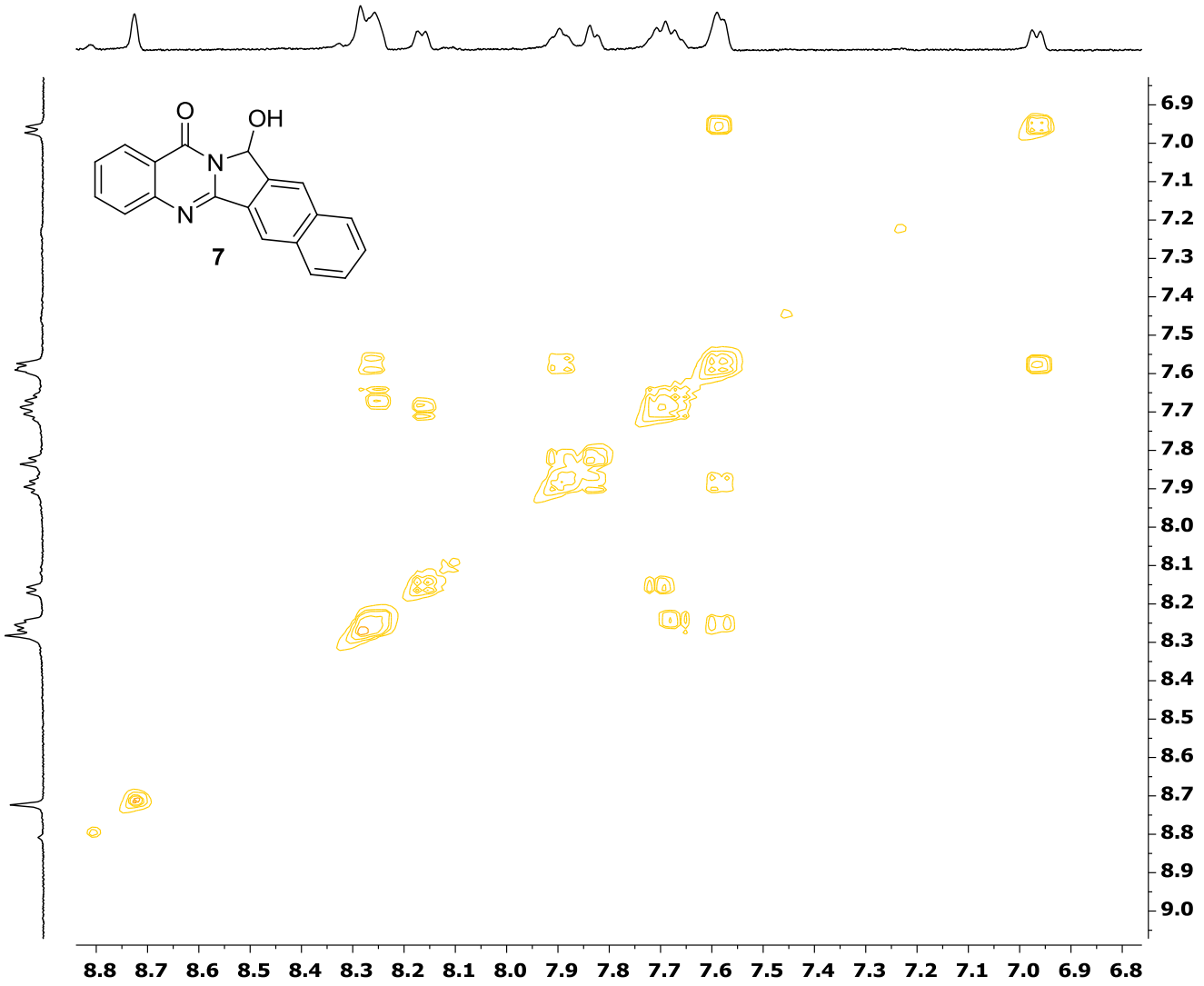
^{1}H NMR (500 MHz, DMSO-d6)



^{13}C NMR (126 MHz, DMSO-d6)



COSY NMR (500 MHz, DMSO-d6)



HSQC NMR (500 MHz, DMSO-d6)