Supporting Information

Construction of Unsymmetrical Heterobiaryls *via* Cp*Rh(III) Catalysed C-H/C-H Coupling of Heteroarenes

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1. Experimental Section

1.1 Reagent Information

All the reactions were performed in screw-cap reaction vials under air atmosphere, unless an inert atmosphere is stated. All solvents were bought from Aldrich in sure seal bottles and used as such. All chemicals were bought from Sigma-Aldrich, Alfa Aesar, and TCI. For column chromatography, silica gel (230-400 mesh) from Merck was used. A gradient elution using EtOAc/*n*-hexane was performed based on Merck aluminum TLC sheets (silica gel 60F254).

1.2 Analytical Information

For heating screw cap vials, IKA dry blocks were used and gram scale synthesis was carried out on preheated oil bath. The melting points were recorded on a Bronsted Electrothermal 9100. All isolated compounds were characterized by ^{1}H NMR, ^{13}C NMR, ESI-MS, Fourier transform infrared (FTIR), and high-resolution mass spectrometry (HRMS). Mass spectrometry was recorded on Q-TOF-Micromass and maXis Impact mass spectrometers. Copies of ^{1}H and ^{13}C NMR are attached in the Supporting Information. IR was -Avance 600 MHz analyzed by Shimadzu IR Prestige-21 with ZnSe single-reflection ATR accessory. Nuclear magnetic resonance was performed on Bruker instrument. All ^{1}H NMR experiments are reported in units, parts per million (ppm), and measured relative to the deuterated chloroform signal (7.260). All proton decoupled ^{13}C NMR spectra are reported in ppm relative to deuterated chloroform (77.16).

1.3 General procedure for heteroarylation of quinoline *N*-oxides with benzoxazoles

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide (0.2 mmol), benzoxazole (1.5 equiv.), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP (1.0 mL) were added. The subsequent mixture was stirred at 100 ˚C for 24 hours. After completion, the solvent was evaporated under reduced pressure, and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and EtOAc/*n*-hexane as the eluent.

1.4 General procedure for the preparation of quinolines-*N*-oxides

Quinoline *N*-oxides **1a**-**1g**, **1o**, **1p** and **1t** are already reported and synthesized from the reported method.[1] Quinoline *N*-oxides **1h**, **1k**-**1l**, **1n** and **1s** are also already reported and were prepared from the literature report.[2] The quinoline *N*-oxides **1i**,[3] **1j**[4] and **1m**[5] were prepared from the reported methodologies. The quinoline *N*-oxide **1r** is already known and synthesized by following the reported procedure.[6]

1.5 General procedure for the synthesis of benzoxazoles

The benzoxazoles **2b**-**2l** were prepared by following the literature procedure through the condensation of 2-aminophenols with triethyl orthoformate method.[7]

1.6 General procedure for the synthesis of *N*-pyridyl/pyrimidyl indolines

N-pyridyl indolines **4a**-**4b** are already known and prepared by following the reported protocol.[8] The *N*-pyrimidyl indolines **4c**-**4d** are also already reported and synthesized from the known protocol.[9]

1.7 General procedure for the synthesis of *N*-pyridyl/pyrimidyl indoles

N-pyridyl indole **4e** and **4g** are already known and synthesized from the literature method.[8] The *N*-pyrimidyl indole **4f** is commercially available and used as such.

1.8 General procedure for the synthesi of *N*-pivaloyl indolines

The *N*-pivaloyl indoline **4h** and **4i** are already known and synthesized from the reported literature protocol.[10]

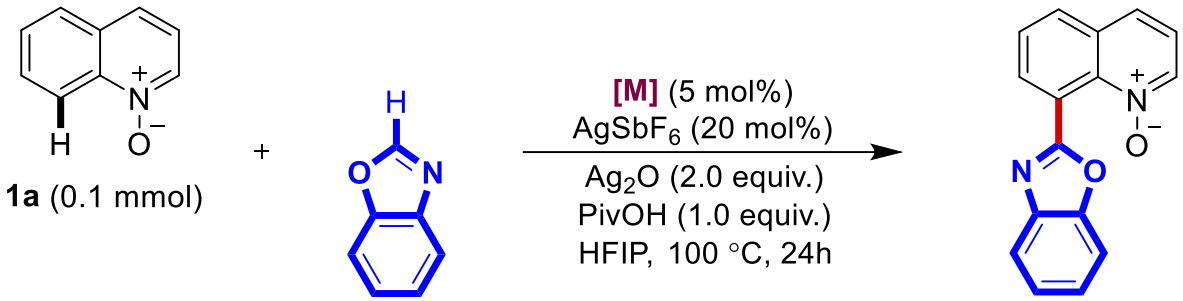
1.9 General procedure for the synthesis of (Z)-1-phenylethan-1-one O-methyl oxime (4n).

The oxime of acetophenone is already reported and synthesized by following the literature method.[11]

All other starting material including **4j**, **4k**, **4l**, **4m**, **4o**, **4p** and **5a**-**5h** were commercial available and used as such.

2. Optimization details for heteroarylation

2.1 Catalyst Screening (Table S1)

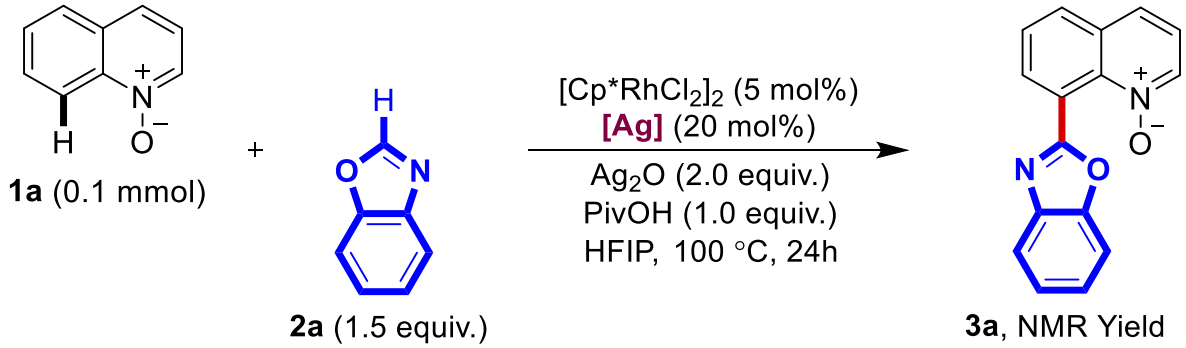


Entry	[M]	NMR yield (%)
1.	**$[Cp^*RhCl_2]_2$**	**63**
2.	$RhCl_3.xH_2O$	Nd
3.	$[RhCl(PPh_3)_3]$	Nd
4.	$[Rh_2(OAc)_4]$	Nd
5.	$[Rh(cod)Cl]_2$	Nd
6.	$[Cl_2Ru(p\text{-cymene})]_2$	Nd

7.	$[Cp^*IrCl_2]_2$	Nd
8.	$[Cp^*Co(CO)I_2]$	Nd
9.	$[Cp^*Co(MeCN)_3][SbF_6]_2$	Nd

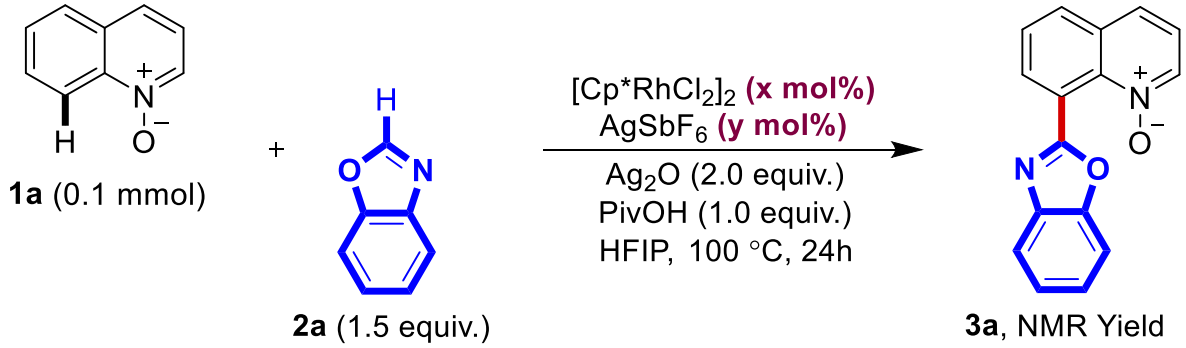
Nd: Not detected

2.2 Silver salt screening (Table S2)



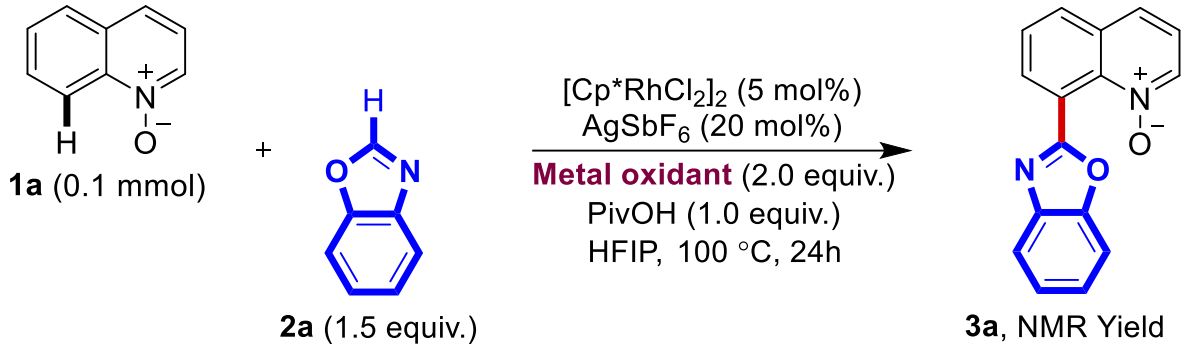
Entry	[Ag]	NMR yield (%)
1.	**$AgSbF_6$**	**63**
2.	AgOTf	25
3.	$AgNTf_2$	30
4.	$AgBF_4$	42

2.3 Quantity variation of $[Cp^*RhCl_2]_2$ and $AgSbF_6$ (Table S3)



Entry	$[Cp^*RhCl_2]_2$ (x mol%)	$AgSbF_6$ (y mol%)	NMR yield (%)
1.	**5**	**20**	**63**
2.	5	10	30
3.	2.5	10	10
4.	2.5	5	5

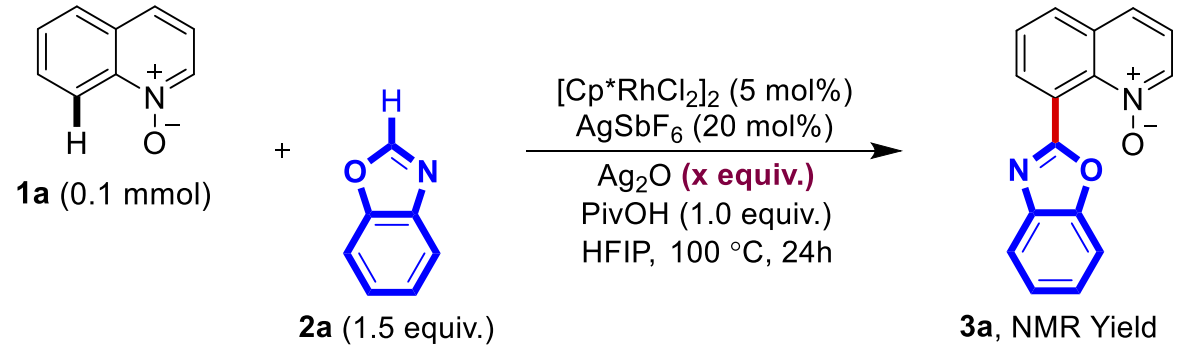
2.4 Metal oxidant screening (Table S4)



Entry	Metal oxide	NMR yield (%)
1.	**Ag_2O**	**63**
2.	CuO	Nd
3.	Cu_2O	Nd
4.	Ag_2SO_4	Nd
5.	AgOAc	Nd
6.	Ag_2CO_3	Nd
7.	$AgOCF_3$	Nd
8.	AgBr	Nd
9.	$AgNTf_2$	Nd
10.	$AgNO_3$	Nd

Nd: Not detected

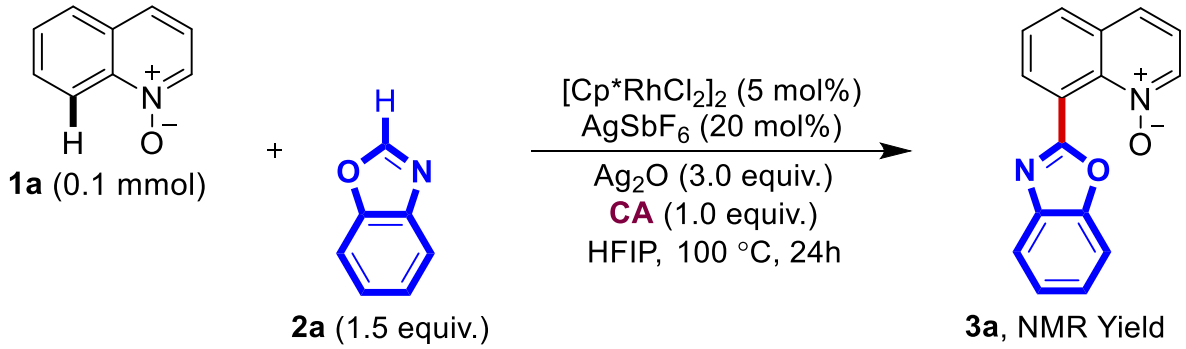
2.5 Quantity variation of Ag_2O (Table S5)



Entry	Ag_2O (x equiv.)	NMR yield (%)
1.	0.5	<5
2.	1.0	12
3.	1.5	25
4.	2.0	63
5.	2.5	68

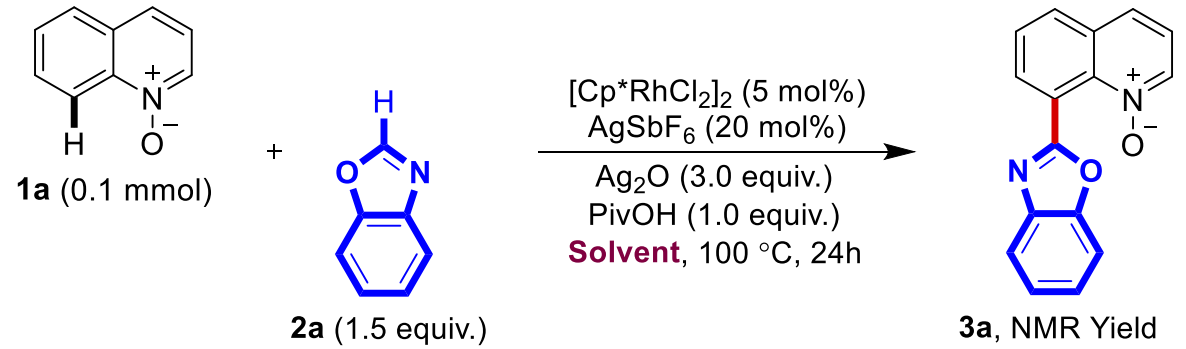
6.	**3.0**	**80**
7.	4.0	78

2.6 Carboxylic acid screening (Table S6)



Entry	Carboxylic acid (CA)	NMR yield (%)
1.	**PivOH**	**80**
2.	AcOH	20
3.	AdCOOH	16
4.	TFA	10

2.7 *Solvent screening (Table S7)*

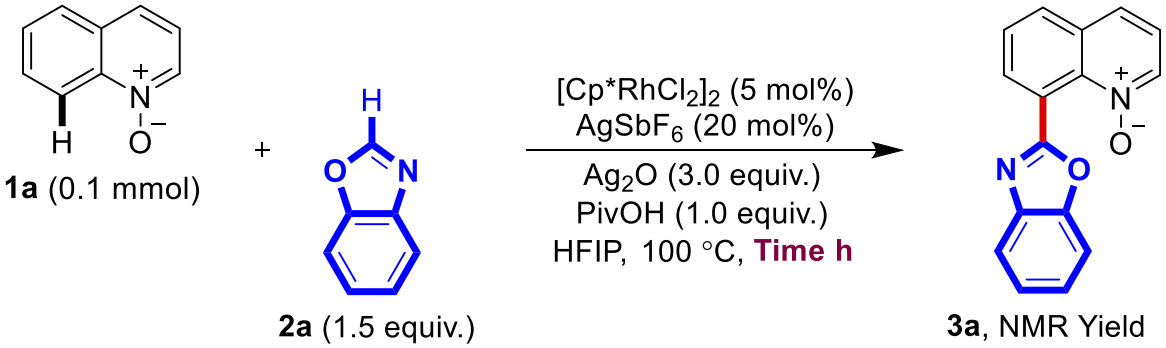


Entry	Solvent (0.5 mL)	NMR yield (%)
1.	**HFIP**	**80**
2.	TFE	22
3.	MeOH	Nd
4.	EtOH	Nd
5.	*n*-BuOH	Nd
6.	2-Propanol	Nd
7.	Ethanediol	Nd
8.	*tert*-Am-OH	Nd

9.	*iso*-Am-OH	Nd
10.	*tert*-Bu-OH	Nd
11.	DCE	Nd

Nd: Not detected

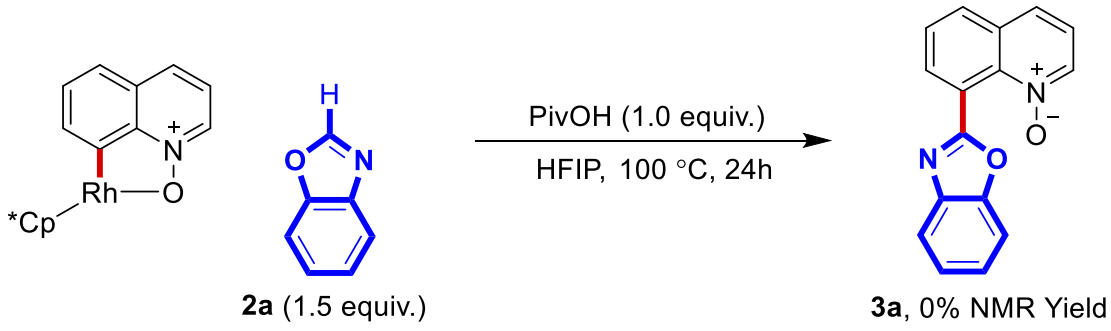
2.8 ***Time screening (Table S8)***



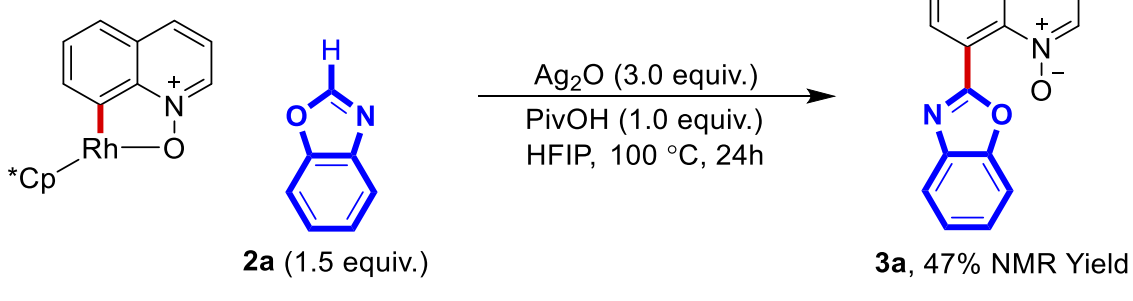
Entry	Time (hours)	NMR yield (%)
1.	6	21
2.	12	55
3.	18	62
4.	**24**	**80**
5.	**36**	**85**

3. Intermediate studies

3.1 Stochiometric reaction of species I without Ag_2O (Scheme S1)



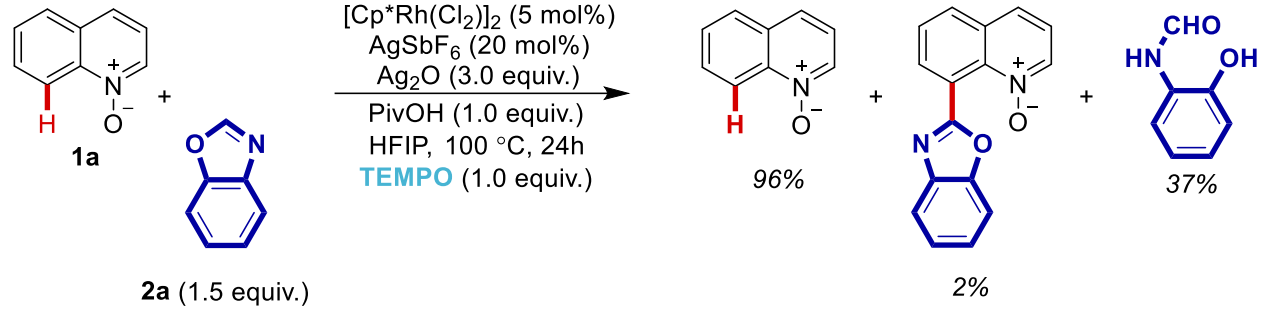
3.2 Stochiometric reaction of species I with Ag_2O (Scheme S2)



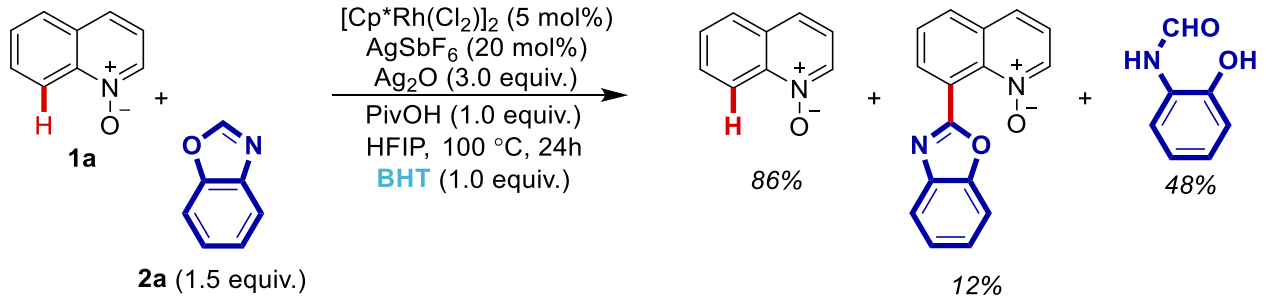
4. Mechanistic studies

4.1 Radical Quenching experiments

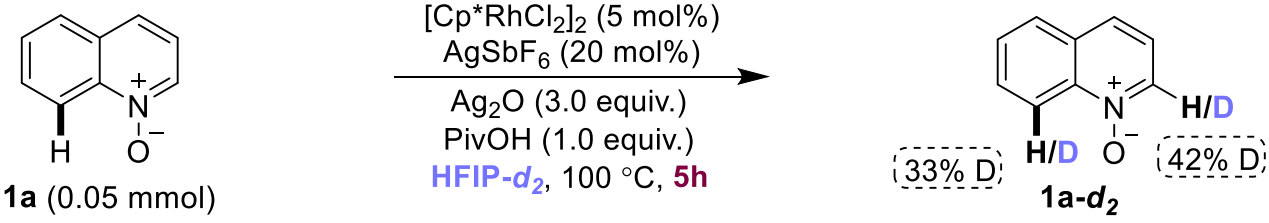
4.1.1 In TEMPO (Scheme S3)



4.1.2 In BHT (Scheme S4)



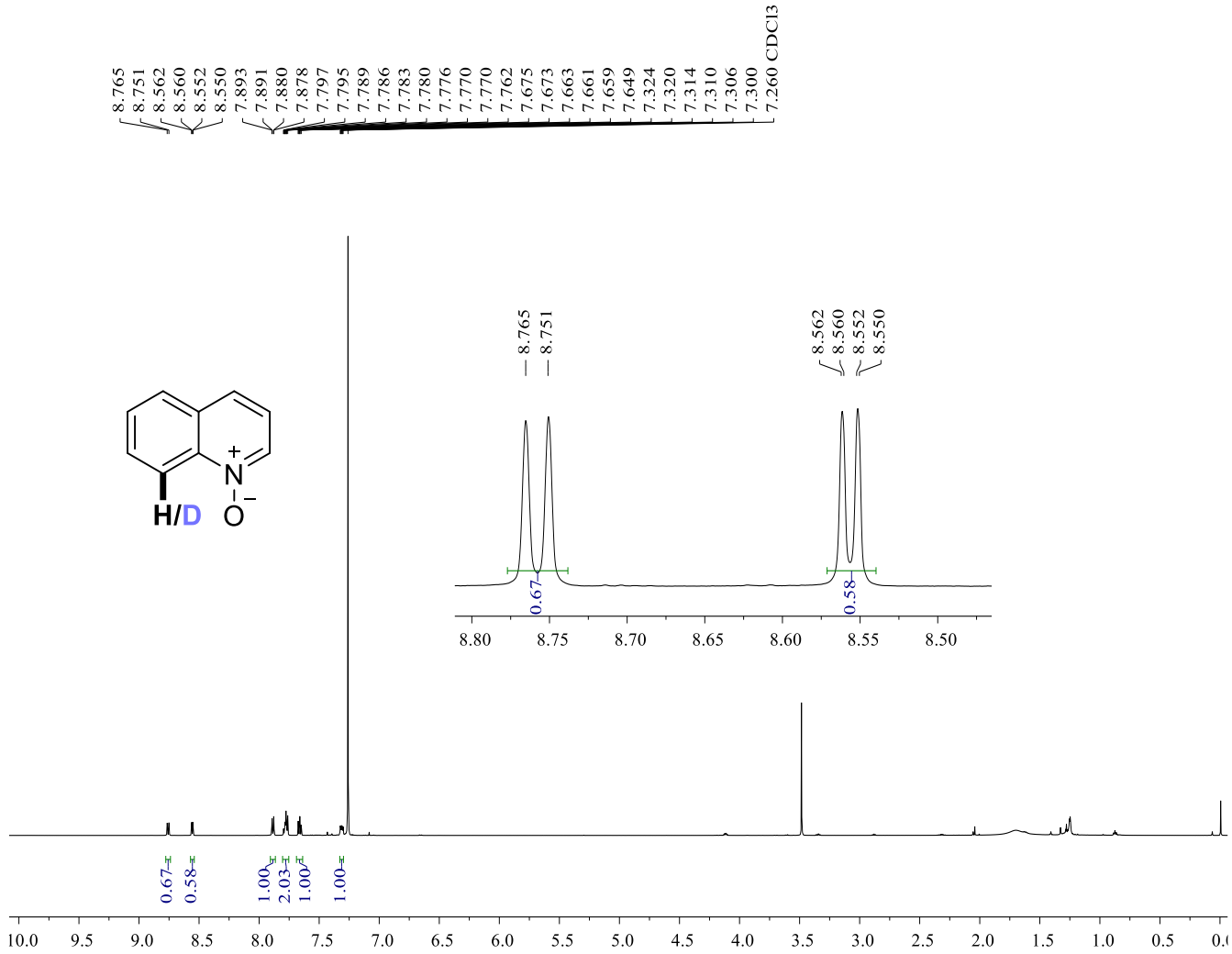
4.2 Deuterium labelling experiment without 2a (Scheme S5)



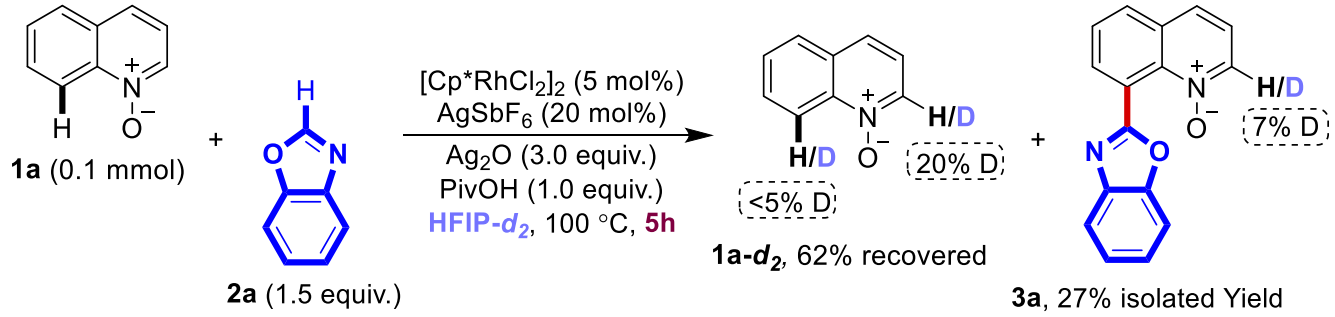
Deuterium Labelling Experiment without 2a

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide (0.05 mmol), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP-d_2 (0.25 mL) were added. The subsequent mixture was stirred at 100 ˚C for 5 h. After completion, the solvent was evaporated under reduced pressure and crude mixture was isolated from column chromatography (100% EtOAc/*n*-hexane). The obtained reactant was analysed by 1H NMR.

^{1}H NMR



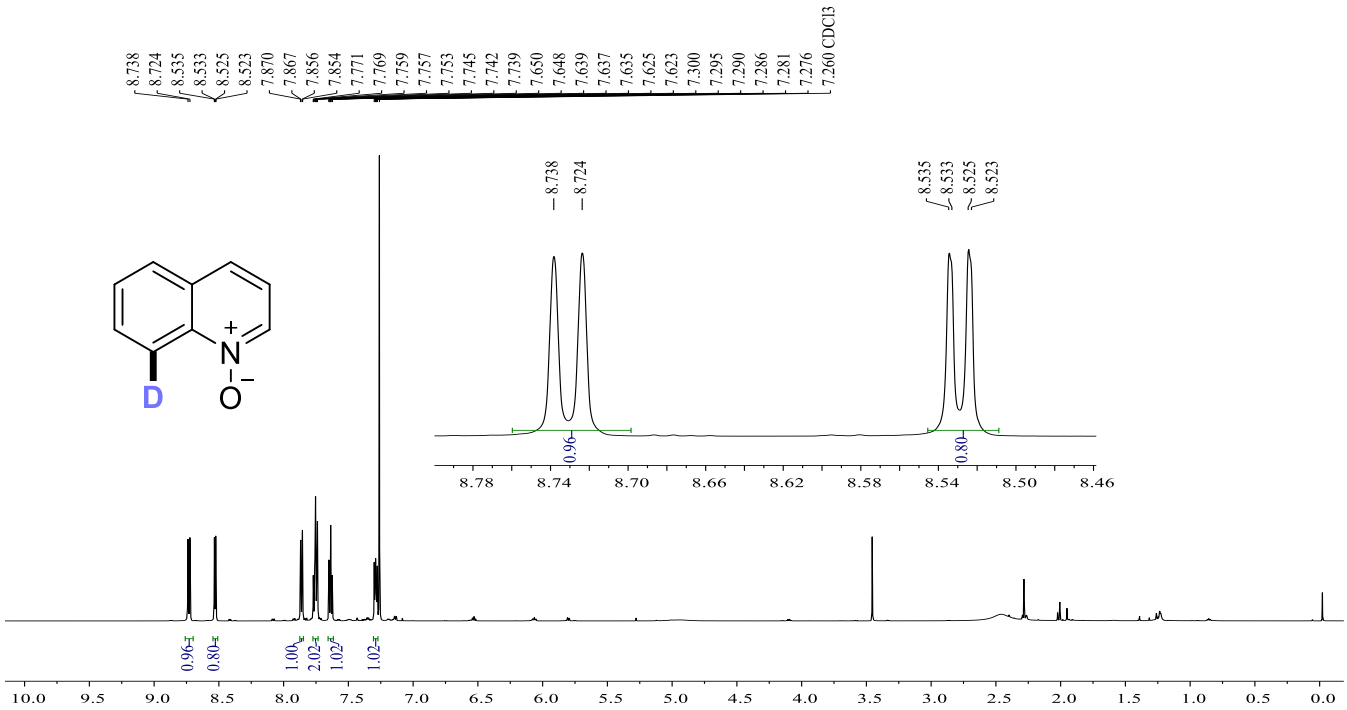
4.3 Deuterium labelling experiment with 2a (Scheme S6)



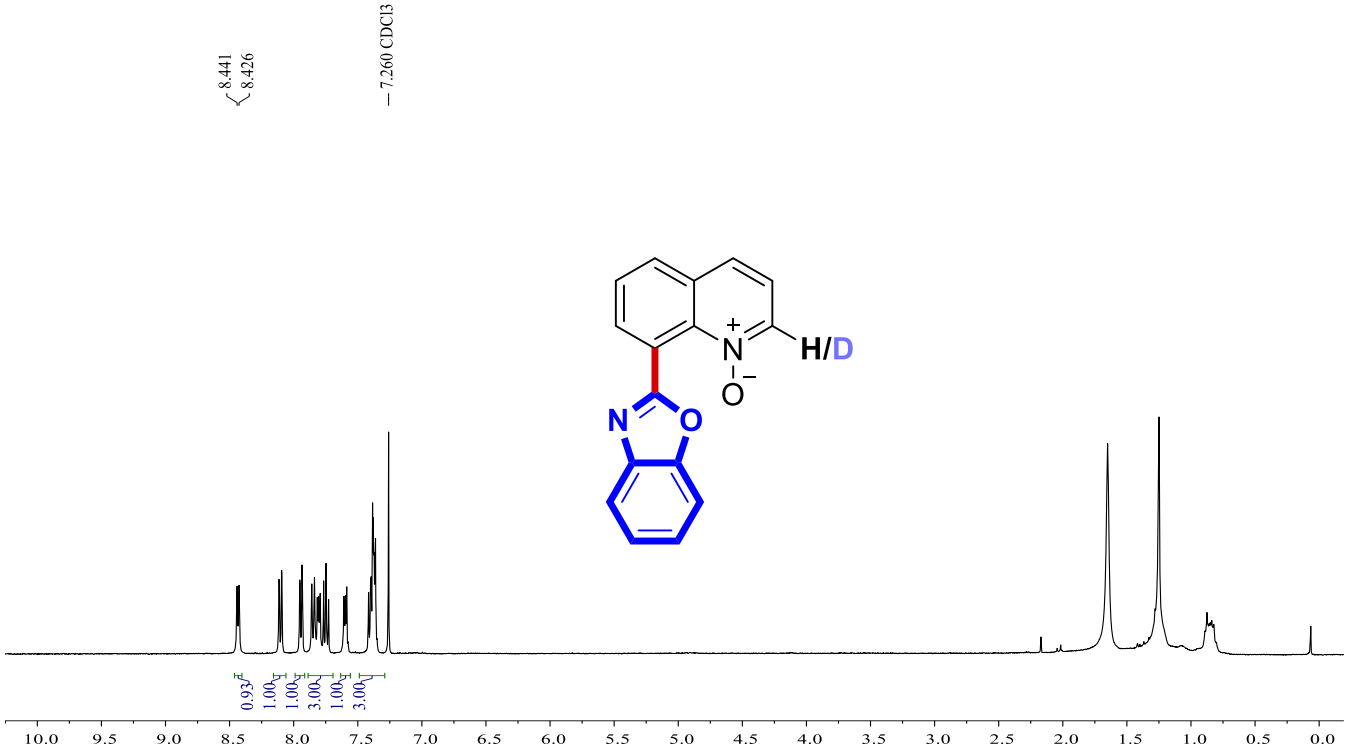
Deuterium Labelling Experiment with 2a

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide (**1a**) (0.1 mmol), benzoxazole (**2a**) (1.5 equiv.), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP-d_2 (0.5 mL) were added. The subsequent mixture was stirred at 100 ˚C for 5 h. After completion, the solvent was evaporated under reduced pressure, and column chromatrogphy was performed to recover **1a** and isolate **3a** which were analysed by 1H NMR.

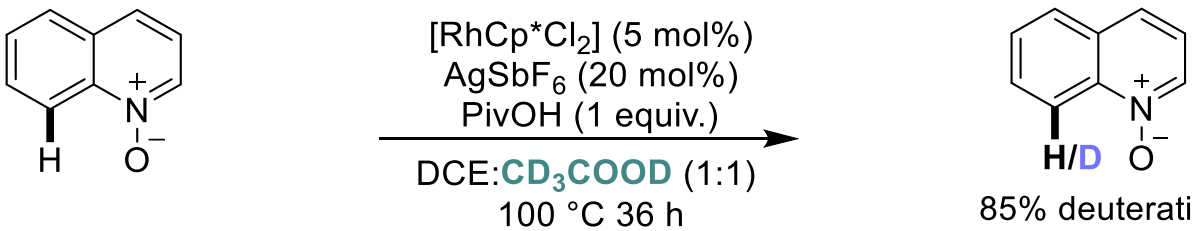
^{1}H NMR



^{1}H NMR



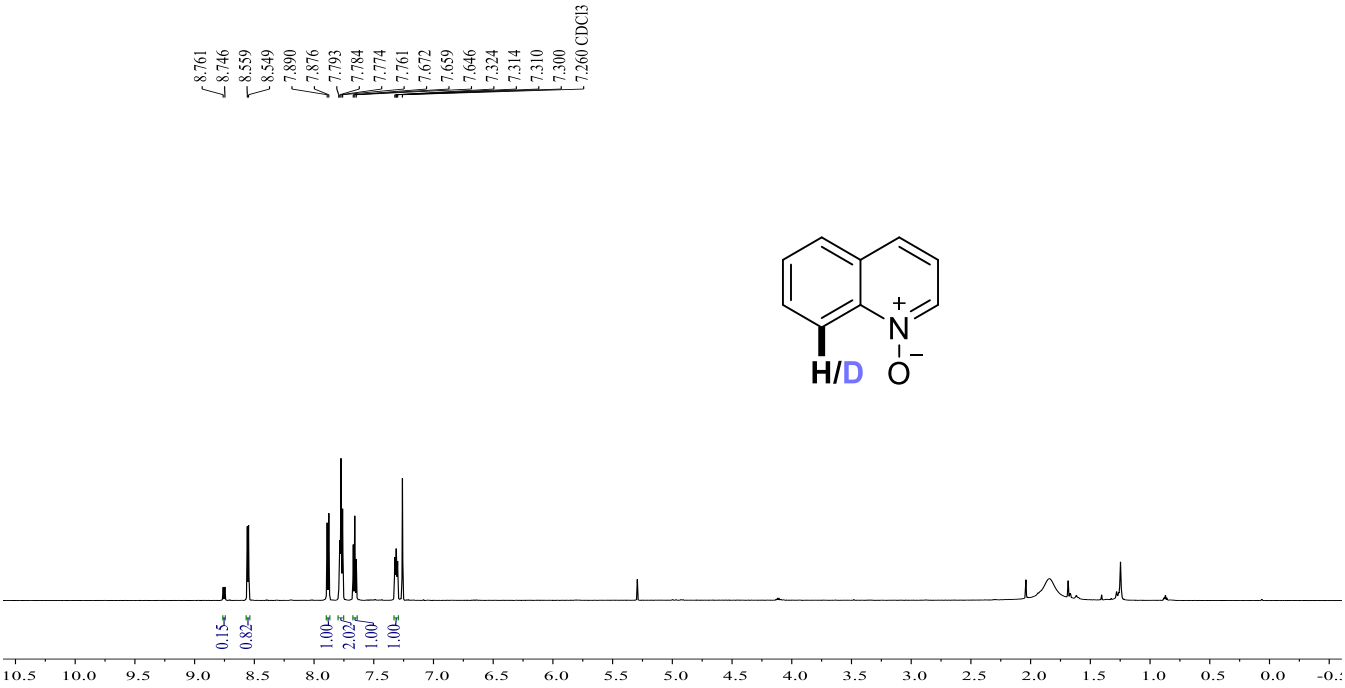
4.4 Synthesis of quinoline N-oxide-d$_1$ (Scheme S7)



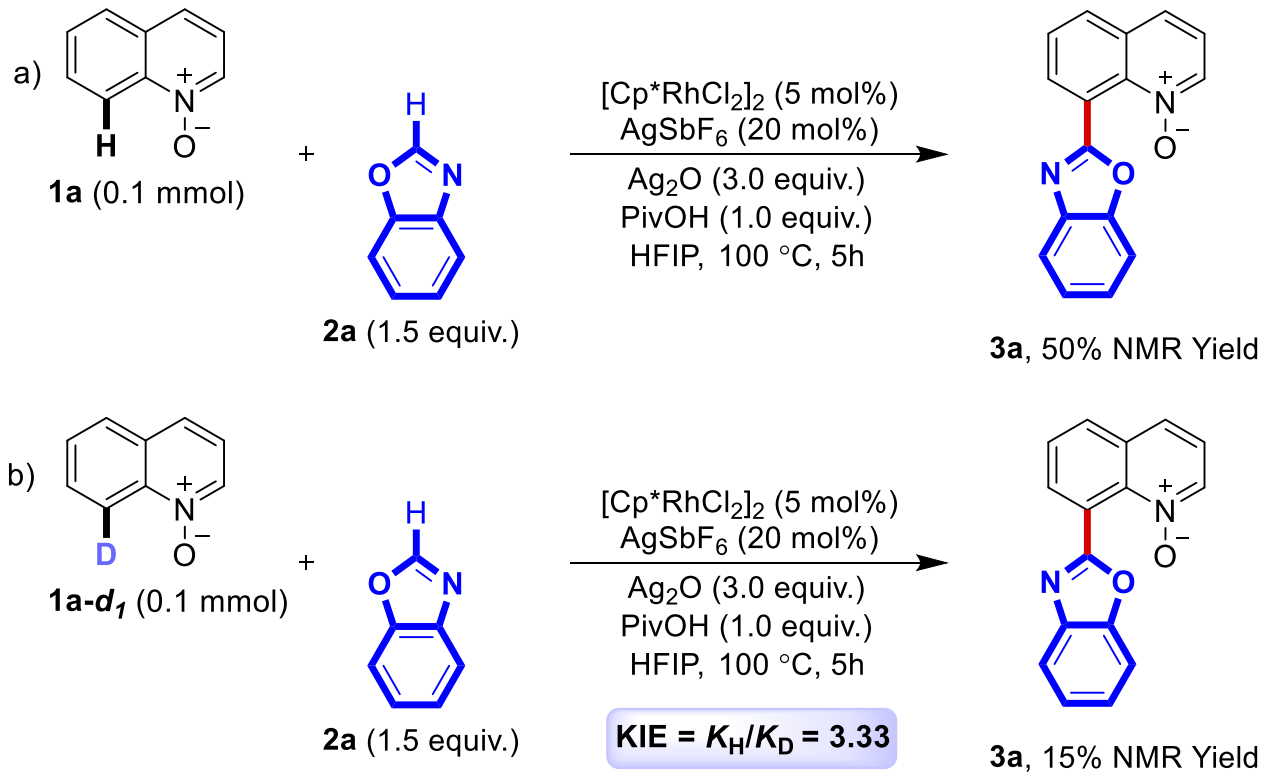
General procedure for the synthesis of d1-quinoline N-oxide

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, $[Cl_2RhCp^*]_2$ (5 mol%), $AgSbF_6$ (20 mol%), PivOH (1.0 equiv.), quinoline *N*-oxide (0.5 mmol) and DCE:CD_3COOD (1:1) as solvnet were added and stirred at 100 °C for 36 h. After completion, the solvent was evaporated under reduced pressure and **1a-*d*$_1$** was isolated by performing column chromatography.

^{1}H NMR



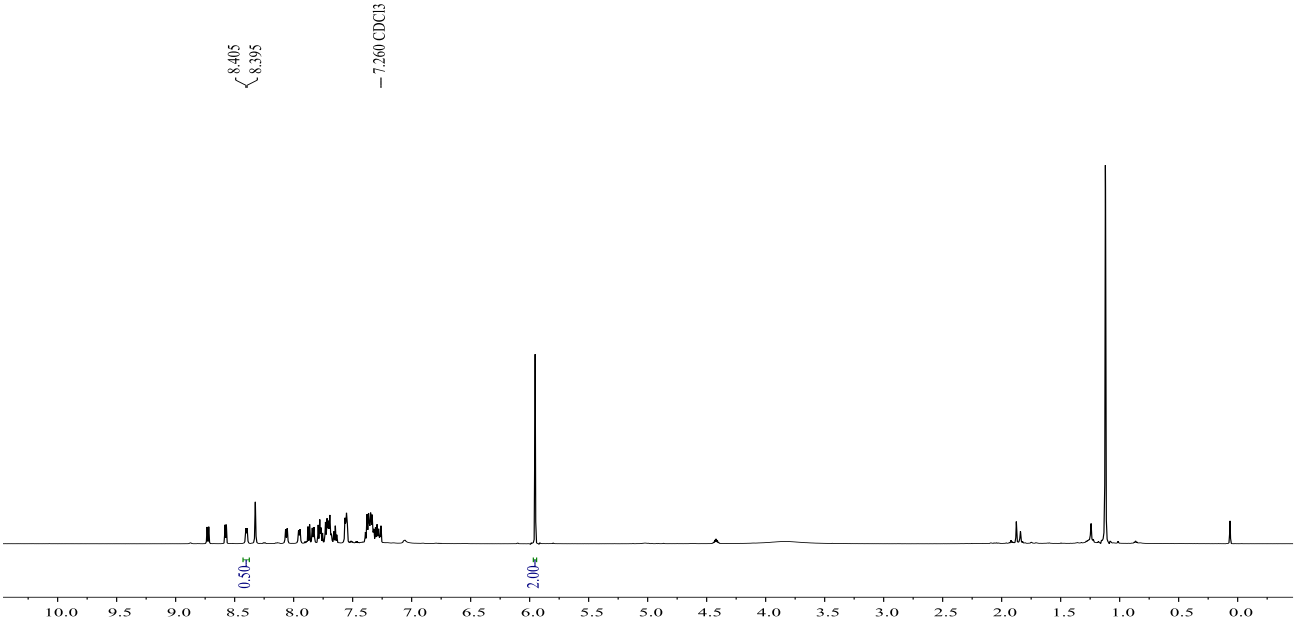
4.5 Parallell experiment between 1a and 1a-d$_1$ (Scheme S8)



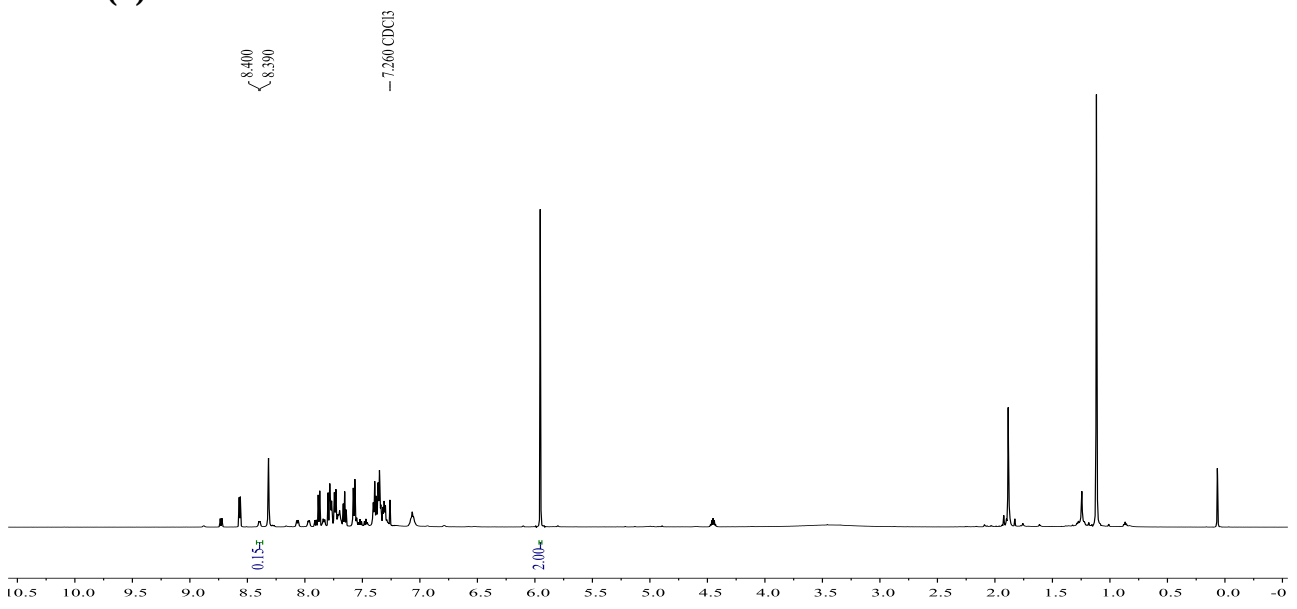
Parallel reaction between 1a and 1a-d_1

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide (**1a**) (0.1 mmol), benzoxazole (**2a**) (1.5 equiv.), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP (0.5 mL) were added. The subsequent mixture was stirred at 100 ˚C for 5h. Simultaneously in another oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide-d_1 (**1a-*d*$_1$**) (0.1 mmol), benzoxazole (**2a**) (1.5 equiv.), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP (0.5 mL) were added. The subsequent mixture was stirred at 100 ˚C for 5 h. After completion, the solvent was evaporated under reduced pressure from both the reaction mixtures, and ^{1}H NMR analysis was performed for both.

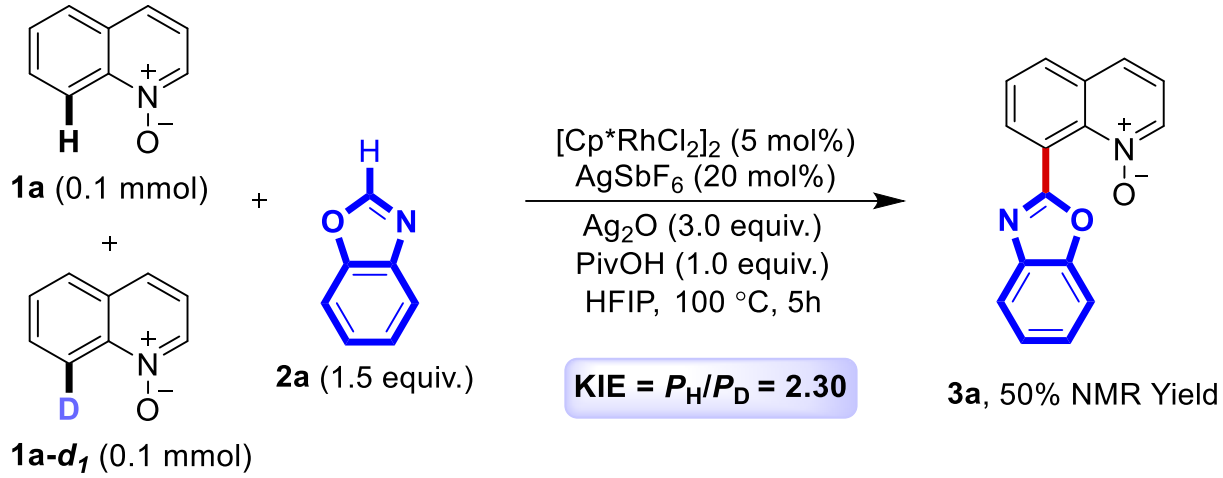
^{1}H NMR (a)



^{1}H NMR (b)



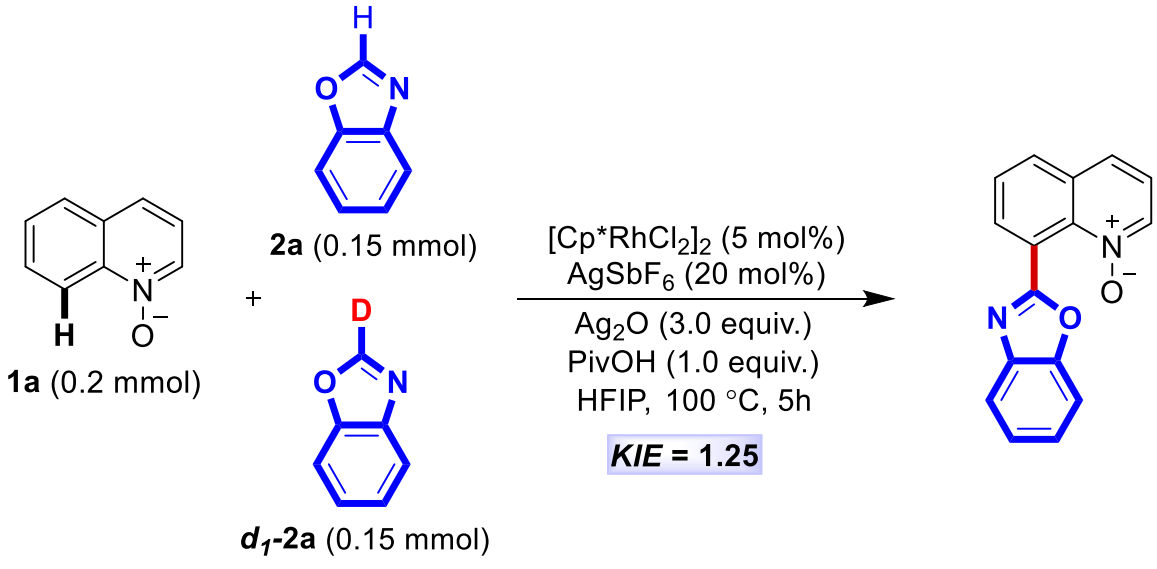
4.6 Competitive experiment between 1a and 1a-d_1 (Scheme S9)



Competitive reaction between 1a and 1a-d_1

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide (**1a**) (0.1 mmol), d_1-quinoline *N*-oxide (**1a-*d*$_1$**) (0.1 mmol), benzoxazole (**2a**) (1.5 equiv.), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP (0.5 mL) were added. The subsequent mixture was stirred at 100 ˚C for 5 h. The subsequent mixture was stirred at 100 ˚C for 5h. After completion, the solvent was evaporated under reduced pressure and ^{1}H NMR analysis was peformed.

4.7 Parallel experiment between 2a and 2a- d_1 (Scheme S10)

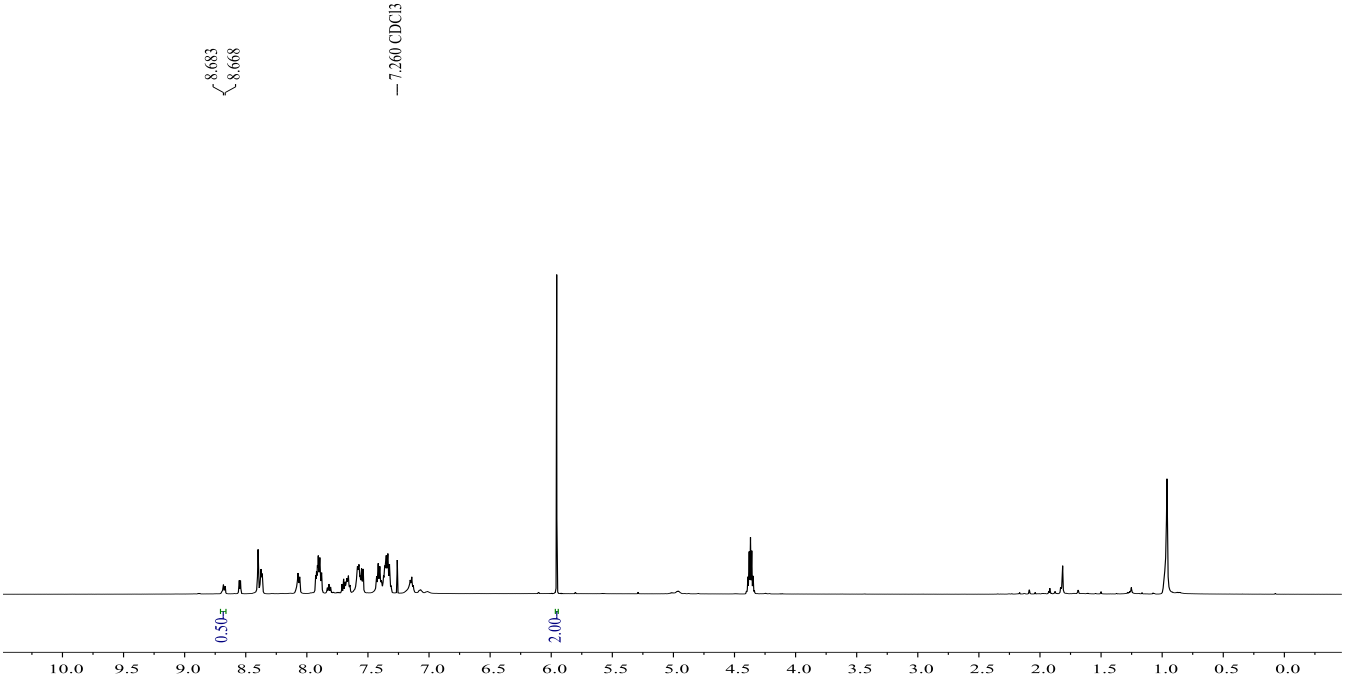


Parallel reaction between 2a and 2a-d_1

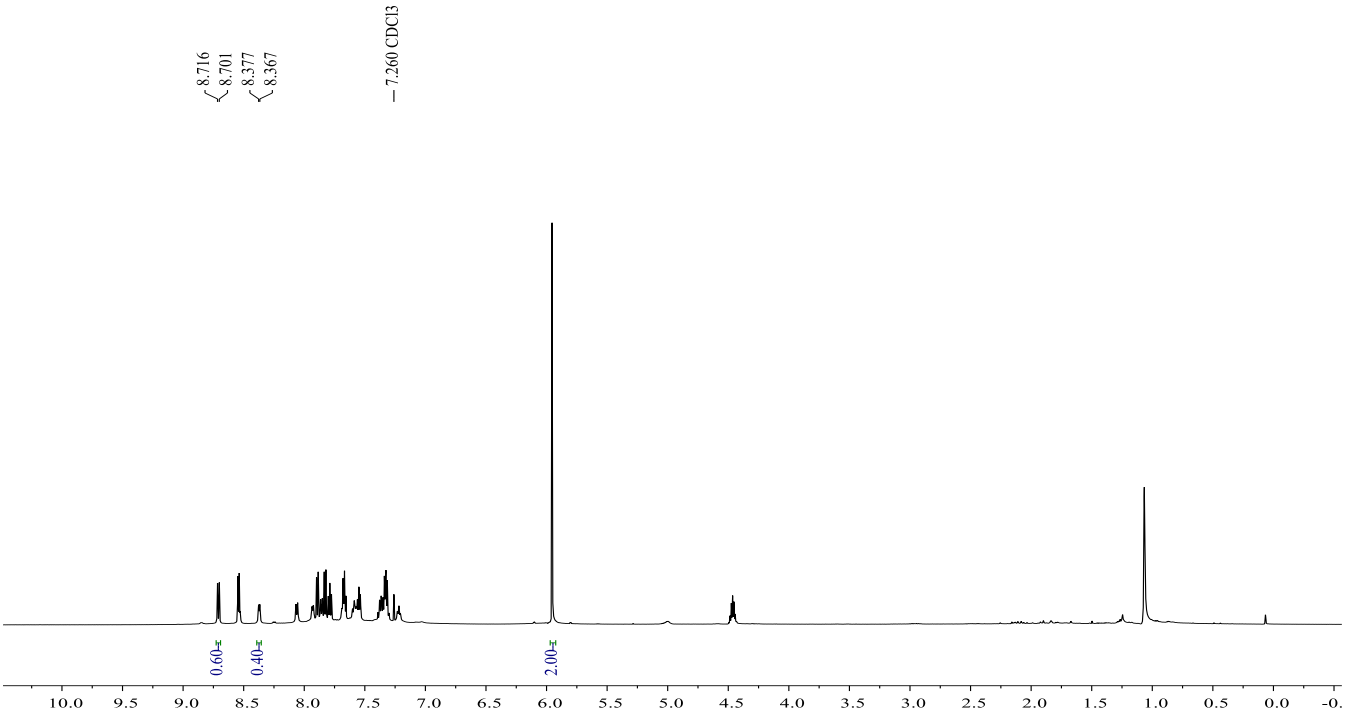
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide (**1a**) (0.1 mmol), benzoxazole (**2a**) (1.5 equiv.), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP (0.5 mL) were added. The subsequent mixture was stirred at 100 ˚C

for 5h. Simultaneously in another oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide (**1a**) (0.1 mmol), d_1-benzoxazole (**2a-*d*$_1$**) (1.5 equiv.), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP (0.5 mL) were added. The subsequent mixture was stirred at 100 ˚C for 5 h. After completion, the solvent was evaporated under reduced pressure from both the reaction mixtures, and ^{1}H NMR analysis was peformed for both.

^{1}H NMR (with benzoxazole)

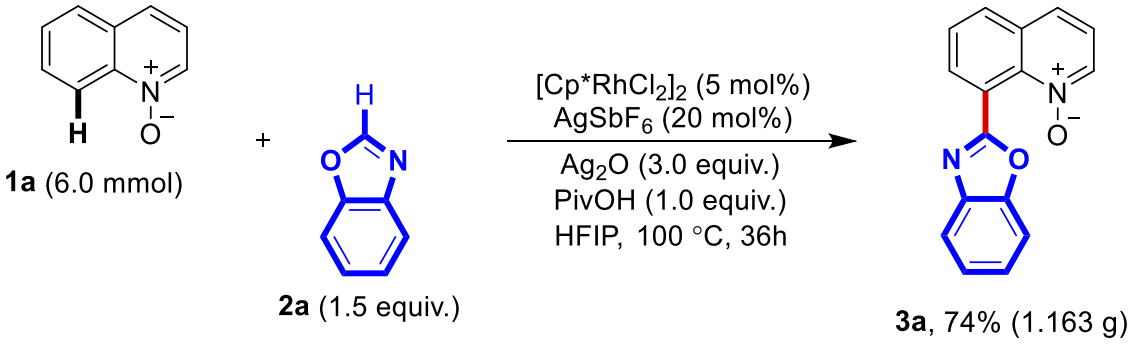


^{1}H NMR (with benzoxazole-*d*$_1$)



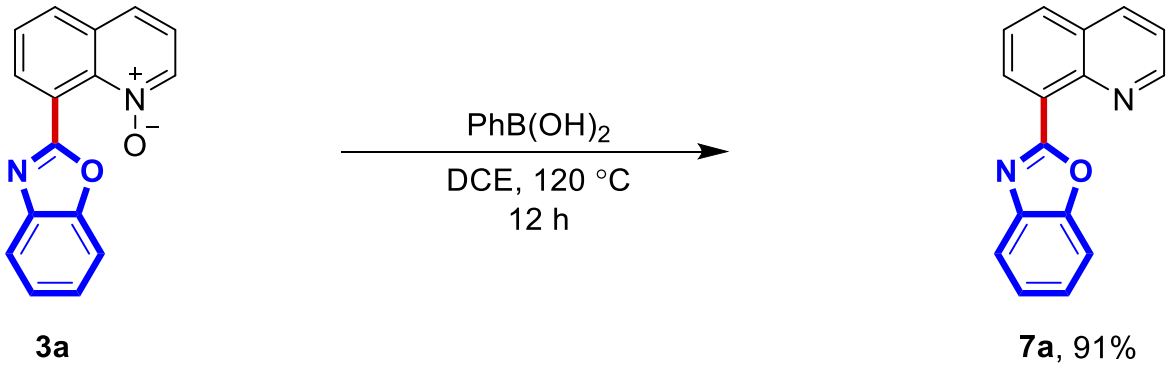
5. *General procedure for the gram scale synthesis (Scheme 2a, main manuscript)*

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, quinoline *N*-oxide (**1a**) (6.0 mmol), benzoxazole (**2a**) (1.5 equiv.), $[RhCp^*Cl_2]_2$ (5 mol%), $AgSbF_6$ (20 mol%), Ag_2O (3.0 equiv.), PivOH (1.0 equiv.) and HFIP (15.0 mL) were added. The subsequent mixture was stirred at 100 ˚C for 36 h. After completion, the solvent was evaporated under reduced pressure and **3a** was isolated in 74% (1.163 g) yield by performing column chromatography.



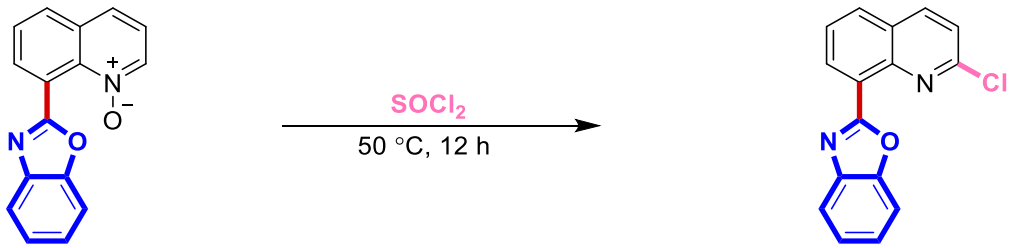
6. *General procedure for the synthesis of 7a (Scheme 2b, main manuscript)*

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 8-(benzo[d]oxazol-2-yl)quinoline 1-oxide (**3a**) (0.1 mmol), phenyl boronic acid (1.5 equiv.) and DCE (0.5 mL) were added. The subsequent mixture was stirred at 120 ˚C for 12 h. After completion, the solvent was evaporated under reduced pressure and **7a** was isolated from column chromatography (30% EtOAc/*n*-hexane) as brown viscous, yield = 22.4 mg (91%).



7. *General procedure for the synthesis of 7b (Scheme 2b, main manuscript)*

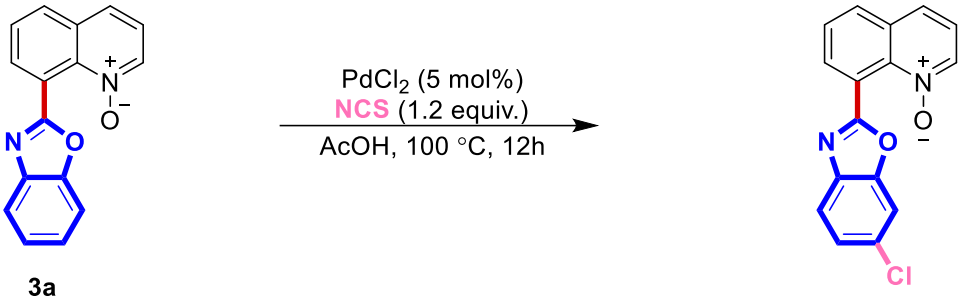
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 8-(benzo[d]oxazol-2-yl)quinoline 1-oxide (**3a**) (0.1 mmol), thionyl chloride (0.5 mL) were added. The subsequent mixture was stirred at 50 ˚C for 12h. After completion, the solvent was evaporated under reduced pressure and **7b** was isolated from column chromatography (12% EtOAc/*n*-hexane) as off white solid, yield = 21.3 mg (76%).



3a **7b**, 76%

8. *General procedure for the synthesis of 3zc (Scheme 2b, main manuscript)*

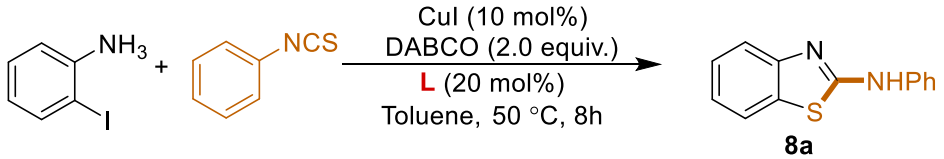
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 8-(benzo[d]oxazol-2-yl)quinoline 1-oxide (**3a**) (0.1 mmol), *N*-chlorosuccinimide (1.2 equiv.), $PdCl_2$ (5 mol%) and AcOH (0.5 mL) were added. The subsequent mixture was stirred at 100 ˚C for 12h. After completion, the solvent was evaporated under reduced pressure and **3zc** was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 24.9 mg (84%).



3a **3zc**, 84%

9. *General procedure for 7a mediated Copper catalysed synthesis of 8a (Scheme 2c, main manuscript)*

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, a solution of isothiocyanate (1.1 equiv) in toluene (1.0 mL) was added to a mixture of 2-iodoaniline (0.3 mmol), DABCO (2.0 equiv.), CuI (10 mol%) and **7a** (20 mol%) in toluene (1 mL) at room temperature. The mixture was then allowed to stir at 50 °C for 8 h. After completion, mixture was cooled to room temperature. The solvent was evaporated and the residue was diluted with EtOAc (20 mL), washed with H_2O (20 mL) and brine (20 mL) and dried by anhydrous $MgSO_4$. Evaporation of the solvent followed by purification on silica gel provided the product **8a** in 80% isolated yield.

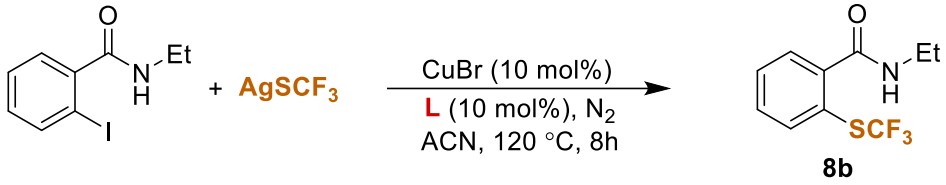


8a

Entry	Ligand (L)	Yield
1.	1,10-phenanthroline	88%
2.	7a	80%

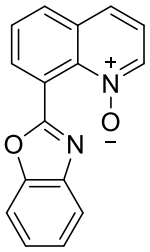
10. *General procedure for 7a mediated Copper catalysed synthesis of 8b (Scheme 2c, main manuscript)*

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, CuBr (0.02 mmol), **7a** (0.02 mmol), $AgSCF_3$ (0.3 mmol) and *N*-ethyl-2-iodobenzamide (0.2 mmol) were dissolved in dry DMF (1 mL) under N_2 atmosphere. The tube was sealed and the mixture was stirred at the corresponding temperature for 8 h. After completion of the reaction, the mixture was directly subjected to flash column chromatography on silica gel with a gradient eluent of petroleum ether and ethyl acetate (range from 20:1 to 5:1) to provide the product **8b** in 97% isolated yield.

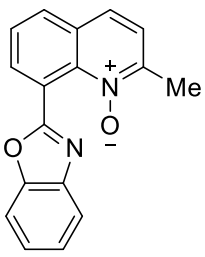


Entry	Ligand (L)	Yield
1.	1,10-phenanthroline	95%
2.	7a	97%

11. Characterization Data



*8-(benzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3a**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 40.3 mg (77%). Mp = 192-194 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.42 (d, J = 6.0 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 7.2 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.78-7.76 (m, 1H), 7.73 (t, J = 7.8 Hz, 1H), 7.59-7.57 (m, 1H), 7.40-7.35 (m, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 163.52, 151.11, 141.65, 139.73, 137.18, 134.99, 131.79, 131.51, 127.99, 126.35, 124.98, 124.37, 122.21, 122.01, 120.21, 110.83. IR (ZnSe) ν_{max} (cm^{-1}): 2758, 2357, 2249, 2202, 2025, 2202, 1234, 972, 825, 756. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{11}N_2O_2$ 263.0815; found, 263.0816.



*8-(benzo[d]oxazol-2-yl)-2-methylquinoline 1-oxide (Table 2, Entry **3b**):* Following the general procedure for heteroarylation, 2-methylquinoline *N*-oxide (**1b**) (31.8 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 52.4 mg (95%). Mp = 192-194 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.06 (dd, J = 8.4, 1.2 Hz, 1H), 7.90-7.88 (m, 1H), 7.78-7.77 (m, 2H), 7.69-7.66 (m, 1H), 7.61-7.58 (m, 1H), 7.42 (d, J = 9.0 Hz, 1H), 7.3-7.34 (m, 2H), 2.61 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.2, 151.0, 147.8, 141.6, 139.7, 135.0, 131.8, 130.2, 127.0, 125.9, 124.9, 124.3, 124.2, 121.6, 120.2, 110.9, 19.0. IR (ZnSe) ν_{max} (cm^{-1}) 3116, 2152, 2133, 2068, 2002, 1550, 1454, 1234, 980, 744. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_2$ 277.0972; found, 277.0976.

*8-(benzo[d]oxazol-2-yl)-2-phenylquinoline 1-oxide (Table 2, Entry **3c**):* Following the general procedure for heteroarylation, 2-phenylquinoline *N*-oxide (**1c**) (44.2 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 66.2 mg (98%). Mp = 182-184 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.07 (d, J = 7.8 Hz, 1H), 7.89 (d, J = 6.6 Hz, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.83-7.82 (m, 2H), 7.69-7.65 (m, 2H), 7.57 (d, J = 9.0 Hz, 1H), 7.52-7.51 (m, 1H), 7.40-7.35 (m, 3H), 7.31-7.28 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.4, 151.1, 146.5, 141.6, 140.4, 135.4, 132.8, 131.7, 130.6, 129.9, 129.6, 128.4, 127.6, 126.0, 124.7, 124.6, 124.2, 122.2, 120.0, 110.8. IR (ZnSe) ν_{max} (cm^{-1}): 3695, 2179, 1705, 1550, 1446, 1361, 1192, 1091, 752, 474. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{22}H_{15}N_2O_2$ 339.1128; found, 339.1126

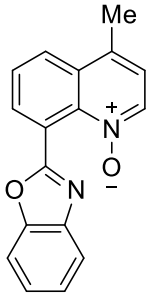
*8-(benzo[d]oxazol-2-yl)-2-(4-nitrophenyl)quinoline 1-oxide (Table 2, Entry **3d**):* Following the general procedure for heteroarylation, 2-(4-nitrophenyl)quinoline *N*-oxide (**1d**) (53.2 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 34.5 mg (45%). Mp = 196-198 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.24 (d, J = 8.4 Hz, 2H), 8.11 (d, J = 7.8 Hz, 1H), 8.05 (d, J = 8.4 Hz, 2H), 7.94 (d, J = 7.2 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.75 (t, J = 7.8 Hz, 1H), 7.72-7.70 (m, 1H), 7.59 (d, J = 9.0 Hz, 1H), 7.55-7.52 (m, 1H), 7.35-7.32 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 163.9, 151.0, 148.1, 144.0, 141.5, 140.5, 139.1, 135.7, 131.8, 131.0, 130.8, 128.3, 125.7, 124.9, 124.4, 123.9, 123.5, 122.4, 120.1, 110.9. IR (ZnSe) ν_{max} (cm^{-1}): 3788, 3109, 2295, 2013, 1720, 1512, 1346, 1222, 952, 466. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{22}H_{14}N_3O_4$ 384.0979; found, 384.0978.

*8-(benzo[d]oxazol-2-yl)-2-(4-methoxyphenyl)quinoline 1-oxide (Table 2, Entry **3e**):* Following the general procedure for heteroarylation, 2-(4-methoxyphenyl)quinoline *N*-oxide (**1e**) (50.2 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as yellow solid, yield = 71.4 mg (97%). Mp = 165-167 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.05 (d, J = 8.4 Hz, 1H), 7.91-7.89 (m, 3H), 7.80 (d, J = 8.4 Hz, 1H), 7.78-7.76 (m, 1H), 7.70-7.67 (m, 1H), 7.59 (d, J = 8.4 Hz, 1H), 7.55 (dd, J = 6.0, 1.8 Hz, 1H), 7.36-7.31 (m, 2H), 6.94-6.93 (m, 2H), 3.81 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.5, 160.8, 151.2, 145.9, 141.9, 140.7, 135.2, 131.6, 131.3, 130.3, 127.3, 125.2, 124.6, 124.3, 124.1, 122.4, 120.1, 113.8, 110.9, 55.5. IR (ZnSe) ν_{max} (cm^{-1}): 3707, 2225, 2059, 1928, 1712, 1608, 1442, 1242, 1026, 740. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{23}H_{17}N_2O_3$ 369.1234; found, 369.1234.

*8-(benzo[d]oxazol-2-yl)-3-methylquinoline 1-oxide (Table 2, Entry **3f**):* Following the general procedure for heteroarylation, 3-methylquinoline *N*-oxide (**1f**) (31.8 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 38.6 mg (70%). Mp = 60-62°C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.34 (s, 1H), 8.01 (dd, J = 8.4, 1.8 Hz, 1H), 7.87 (dd, J = 7.2, 1.2 Hz, 1H), 7.76-7.75 (m, 1H), 7.71-7.68 (m, 2H), 7.57-7.55 (m, 1H), 7.36-7.33 (m, 2H), 2.46 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 163.6, 151.1, 141.4, 138.9, 137.5, 134.3, 132.9, 131.3, 131.2, 128.1, 127.2, 125.1, 124.4, 121.5, 120.1, 110.8, 18.7. IR (ZnSe): ν_{max} (cm^{-1}): 2922, 2853,

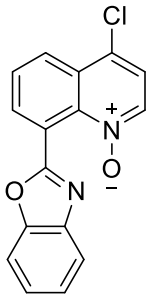
2357, 1752, 1557, 1455, 1371, 1234, 1191, 756. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_2$ 277.0972; found, 277.0974.

*8-(benzo[d]oxazol-2-yl)-4-methylquinoline 1-oxide (Table 2, Entry **3g**):* Following the general procedure



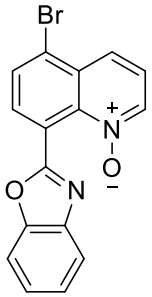
for heteroarylation, 4-methylquinoline *N*-oxide (**1g**) (31.8 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (100% EtOAc/*n*-hexane) as brown solid, yield = 52.4 mg (95%). Mp = 202-204 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.31 (d, J = 6.6 Hz, 1H), 8.22 (dd, J = 8.4, 1.2 Hz, 1H), 7.94 (dd, J = 7.2, 1.2 Hz, 1H), 7.79-7.77 (m, 1H), 7.76-7.74 (m, 1H), 7.56-7.54 (m, 1H), 7.35-7.32 (m, 2H), 7.23 (d, J = 6.6 Hz, 1H), 2.73 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 163.8, 151.1, 141.6, 139.1, 136.7, 135.8, 134.9, 130.8, 128.3, 127.8, 124.9, 124.3, 122.8, 122.3, 120.1, 110.8, 18.9. IR (ZnSe): ν_{max} (cm^{-1}): 2357, 1846, 1549, 1450, 1391, 1301, 1253, 994, 837, 750. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_2$ 277.0972; found, 277.0975.

*8-(benzo[d]oxazol-2-yl)-4-chloroquinoline 1-oxide (Table 2, Entry **3h**):* Following the general procedure



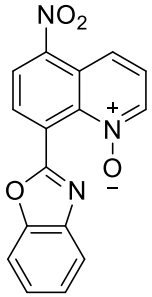
for heteroarylation, 4-chloroquinoline *N*-oxide (**1h**) (35.8 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 28.4 mg (48%). Mp = 158-160 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.48 (d, J = 8.4 Hz, 1H), 8.34 (d, J = 6.6 Hz, 1H), 8.00 (dd, J = 7.2, 1.2 Hz, 1H), 7.87-7.84 (m, 1H), 7.79-7.78 (m, 1H), 7.59-7.57 (m, 1H), 7.47 (d, J = 6.6 Hz, 1H), 7.37-7.36 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 163.0, 151.1, 141.6, 140.4, 136.7, 135.8, 130.4, 129.0, 128.9, 128.8, 125.1, 124.5, 122.6, 122.3, 120.3, 110.8. IR (ZnSe): ν_{max} (cm^{-1}): 2357, 1706, 1544, 1453, 1373, 1294, 1228, 1007, 818, 748. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{10}ClN_2O_2$ 297.0425; found, 297.0428.

*8-(benzo[d]oxazol-2-yl)-5-bromoquinoline 1-oxide (Table 2, Entry **3i**):* Following the general procedure



for heteroarylation, 5-bromoquinoline *N*-oxide (**1i**) (44.6 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 51.7 mg (76%). Mp = 205-207 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.43 (d, J = 6.0 Hz, 1H), 8.20 (d, J = 8.4 Hz, 1H), 8.01 (d, J = 7.8 Hz, 1H), 7.7-7.74 (m, 2H), 7.56-7.55 (m, 1H), 7.48-7.45 (m, 1H), 7.35-7.33 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 162.9, 151.0, 141.5, 140.4, 137.5, 134.6, 132.0, 130.9, 126.3, 125.8, 125.1, 124.5, 123.0, 121.8, 120.2, 110.8. IR (ZnSe): ν_{max} (cm^{-1}): 3070, 2926, 2357, 1899, 1764, 1605, 1549, 1447, 1386, 976. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{10}BrN_2O_2$ 340.9920; found, 340.9932.

*8-(benzo[d]oxazol-2-yl)-5-nitroquinoline 1-oxide (Table 2, Entry **3j**):* Following the general procedure



for heteroarylation, 5-nitroquinoline *N*-oxide (**1j**) (38.1 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 38.7 mg (63%). Mp = 184-186 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.50-8.46 (m, 2H), 8.41 (d, J = 7.8 Hz, 1H), 8.01 (d, J = 7.8 Hz, 1H), 7.79-7.78 (m, 1H), 7.59-7.56 (m, 2H), 7.40-7.36 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 161.6, 151.1, 148.1, 141.4, 140.7, 137.8, 133.1, 127.8, 125.5, 125.1, 124.9, 124.8, 120.9, 120.4, 110.9. IR (ZnSe): ν_{max} (cm^{-1}): 3088,

2357, 1706, 1528, 1454, 1346, 1236, 1196, 1112, 978. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{10}N_3O_4$ 308.0666; found, 308.0664.

*8-(benzo[d]oxazol-2-yl)-6-methoxyquinoline 1-oxide (Table 2, Entry **3k**):* Following the general procedure for heteroarylation, 6-methoxyquinoline *N*-oxide (**1k**) (35.0 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as off white solid, yield = 29.2 mg (50%). Mp = 192-194 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.26 (d, J = 6.0 Hz, 1H), 7.80-7.79 (m, 1H), 7.69 (d, J = 8.4 Hz, 1H), 7.59-7.58 (m, 1H), 7.56 (d, J = 3.0 Hz, 1H), 7.38-7.35 (m, 2H), 7.31-7.29 (m, 2H), 3.96 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 163.0, 158.2, 151.1, 141.7, 135.5, 135.0, 133.0, 127.0, 125.0, 124.3, 123.6, 122.5, 120.3, 110.8, 109.4, 56.2. IR (ZnSe): ν_{max} (cm^{-1}): 3080, 2965, 2848, 2357, 1697, 1606, 1554, 1452, 1371, 1323. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_3$ 293.0921; found, 293.0923.

*8-(benzo[d]oxazol-2-yl)-6-methylquinoline 1-oxide (Table 2, Entry **3l**):* Following the general procedure for heteroarylation, 6-methylquinoline *N*-oxide (**1l**) (31.8 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 27.6 mg (50%). Mp = 117-119 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.35 (d, J = 6.0 Hz, 1H), 7.84 (s, 1H), 7.77-7.76 (m, 3H), 7.57-7.56 (m, 1H), 7.36-7.32 (m, 3H), 2.56 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 163.6, 151.1, 141.5, 138.5, 138.0, 137.2, 136.5, 131.6, 130.6, 126.3, 125.0, 124.4, 122.1, 121.5, 120.1, 110.8, 21.2. IR (ZnSe): ν_{max} (cm^{-1}) 2962, 2918, 2848, 2310, 1716, 1558, 1456, 1232, 864, 746. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_2$ 277.0972; found, 277.0971.

*8-(benzo[d]oxazol-2-yl)-6-isopropylquinoline 1-oxide (Table 2, Entry **3m**):* Following the general procedure for heteroarylation, 6-isoropylquinoline *N*-oxide (**1m**) (37.5 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 35.3 mg (58%). Mp = 192-194 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.37 (d, J = 6.0 Hz, 1H), 7.87 (d, J = 2.4 Hz, 1H), 7.85 (d, J = 1.8 Hz, 1H), 7.81 (d, J = 9.0 Hz, 1H), 7.79-7.78 (m, 1H), 7.58-7.57 (m, 1H), 7.37-7.34 (m, 3H), 3.17-3.01 (m, 1H), 1.36 (s, 3H), 1.35 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 163.7, 151.1, 149.1, 141.6, 138.3, 136.6, 135.0, 131.7, 128.0, 126.5, 125.0, 124.3, 122.1, 121.8, 120.2, 110.8, 34.0, 23.6. IR (ZnSe): ν_{max} (cm^{-1}): 3055, 2961, 2357, 1934, 1771, 1609, 1555, 1451, 1235, 748. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{19}H_{17}N_2O_2$ 305.1285; found, 305.1287.

*8-(benzo[d]oxazol-2-yl)-6-(tert-butyl)quinoline 1-oxide (Table 2, Entry **3n**):* Following the general procedure for heteroarylation, 6-(*tert*-butyl)quinoline *N*-oxide (**1n**) (40.2 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 45.2 mg (71%). Mp = 224-226 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): ^{1}H NMR (600 MHz, Chloroform-d) δ 8.37 (d, J = 6.0 Hz, 1H), 7.99 (dd, J = 8.4, 1.8 Hz, 2H), 7.82-7.80 (m, 2H), 7.60-7.58 (m, 1H), 7.39-7.34 (m, 3H), 1.43 (s, 9H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 163.9, 151.4,

151.1, 141.7, 138.2, 136.5, 134.0, 131.5, 126.9, 126.3, 124.9, 124.3, 122.0, 121.7, 120.2, 110.8, 35.3, 31.1. IR (ZnSe): ν_{max} (cm^{-1}): 3055, 2955, 2357, 1928, 1772, 1612, 1557, 1450, 1365, 1236. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{19}N_2O_2$ 319.1441; found, 319.1441.

*8-(benzo[d]oxazol-2-yl)-6-(methoxycarbonyl)quinoline 1-oxide (Table 2, Entry **3o**):* Following the general procedure for heteroarylation, 6-(methoxycarbonyl)quinoline *N*-oxide (**1o**) (40.6 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as light brown solid, yield = 39.7 mg (62%). Mp = 188-190 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.81 (d, J = 2.4 Hz, 1H), 8.51 (d, J = 2.4 Hz, 1H), 8.48 (d, J = 6.0 Hz, 1H), 7.93 (d, J, 8.4 Hz, 1H), 7.82 – 7.79 (m, 1H), 7.60 – 7.58 (m, 1H), 7.46 – 7.44 (m, 1H), 7.39 – 7.36 (m, 2H), 4.00 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 163.8, 156.9, 151.0, 145.2, 141.5, 135.1, 131.6, 127.06, 125.07, 124.9, 124.4, 124.4, 122.9, 120.2, 111.0, 110.5, 64.6, 18.6, 14.7. IR (ZnSe): ν_{max} (cm^{-1}) 3093, 3080, 2351, 2310, 1622, 1562, 1440, 1423, 1240, 732. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{18}H_{13}N_2O_4$ 321.0870; found, 321.0870.

*8-(benzo[d]oxazol-2-yl)-6-ethoxy-2-methylquinoline 1-oxide (Table 2, Entry **3p**):* Following the general procedure for heteroarylation, 6-ethoxy-2-methylquinoline *N*-oxide (**1p**) (40.6 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as light brown solid, yield = 39.7 mg (62%). Mp = 169-171 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 7.73 (s, 1H), 7.62 (d, J = 9.0 Hz, 1H), 7.58-7.57 (m, 1H), 7.49 (d, J = 3.0 Hz, 1H), 7.36-7.32 (m, 2H), 7.30-7.27 (m, 2H), 4.15 (q, J = 14.4, 7.2 Hz, 2H), 2.53 (s, 3H), 1.46 (t, J = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.7, 162.5, 151.0, 141.5, 141.2, 138.5, 134.3, 134.0, 131.1, 129.7, 126.7, 125.0, 124.4, 122.9, 122.7, 120.2, 110.7, 52.9. IR (ZnSe): ν_{max} (cm^{-1}) 2978, 2929, 2326, 1614, 1558, 1454, 1328, 1234, 1219, 860. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{19}H_{17}N_2O_3$ 321.1234; found, 321.1238.

*8-(benzo[d]oxazol-2-yl)-6-(tert-butyl)-2-methylquinoline 1-oxide (Table 2, Entry **3q**):* Following the general procedure for heteroarylation, 6-(*tert*-butyl)-2-methylquinoline *N*-oxide (**1q**) (43.0 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 65.1 mg (98%). Mp = 200-202 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 7.95 – 7.93 (m, 2H), 7.79 – 7.77 (m, 1H), 7.72 (d, J = 9.0 Hz, 1H), 7.60 – 7.58 (m, 1H), 7.37 – 7.33 (m, 3H), 2.58 (s, 3H), 1.41 (s, 9H). 13C{1H} NMR (150 MHz, CDCl3, δ): 164.5, 151.0, 150.2, 146.7, 141.7, 138.1, 133.8, 130.2, 126.9, 125.8, 124.8, 124.2, 123.9, 121.3, 120.2, 110.9, 35.1, 31.1, 18.8. IR (ZnSe): ν_{max} (cm^{-1}) 2958, 2351, 2310, 1716, 1556, 1456, 1332, 1240, 769, 752. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{21}H_{21}N_2O_2$ 333.1598; found, 333.1592.

*8-(benzo[d]oxazol-2-yl)-4,6-dichloroquinoline 1-oxide (Table 2, Entry **3r**):* Following the general procedure for heteroarylation, 4,6-dichloroquinoline *N*-oxide (**1r**) (42.6 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 30.3 mg (46%). Mp = 201-203 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.44 (d, J = 2.4 Hz, 1H), 8.30 (d, J = 6.6 Hz, 1H), 7.94 (d, J = 1.8 Hz, 1H), 7.76-7.71 (m, 1H), 7.57-7.55 (m, 1H), 7.49 (d, J = 6.6 Hz, 1H), 7.38-7.34 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 161.5, 151.0, 141.2, 138.7, 137.0, 136.5, 135.7, 129.9, 127.6, 125.5, 124.8, 124.3, 123.4, 120.3, 110.9. IR (ZnSe): ν_{max} (cm^{-1}) 3101, 2351, 2318, 1683, 1544, 1454, 1307, 856, 827, 744. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_9Cl_2N_2O_2$ 331.0036; found, 331.0034.

*4-(benzo[d]oxazol-2-yl)phenanthridine 5-oxide (Table 2, Entry **3s**):* Following the general procedure for heteroarylation, phenanthridine *N*-oxide (**1s**) (39.0 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 31.2 mg (50%). Mp = 232-234 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.80 (d, J = 8.4 Hz, 1H), 8.75 (s, 1H), 8.54 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 7.2 Hz, 1H), 7.89 (t, J = 7.8 Hz, 1H), 7.80-7.77 (m, 3H), 7.71-7.69 (m, 1H), 7.58-7.57 (m, 1H), 7.37-7.33 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.1, 151.0, 141.7, 137.8, 136.0, 134.0, 130.2, 129.8, 128.6, 127.8, 126.9, 126.4, 126.3, 126.2, 124.9, 124.3, 122.8, 122.6, 120.1, 110.8. IR (ZnSe): ν_{max} (cm^{-1}) 2927, 2850, 2267, 2351, 2310, 1668, 1556, 1452, 1226, 1190, 738. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{13}N_2O_2$ 313.0972; found, 313.0969.

*5-(benzo[d]oxazol-2-yl)benzo[f]quinoline 4-oxide (Table 2, Entry **3t**):* Following the general procedure for heteroarylation, benzo[f]quinoline *N*-oxide (**1t**) (39.0 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 49.9 mg (80%). Mp = 218-220 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.63 (d, J = 8.4 Hz, 1H), 8.59 (d, J = 8.4 Hz, 1H), 8.48 (d, J = 6.0 Hz, 1H), 8.28 (s, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.86-7.84 (m, 1H), 7.82-7.80 (m, 1H), 7.78-7.76 (m, 1H), 7.60-7.58 (m, 1H), 7.55-7.52 (m, 1H), 7.39-7.35 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.0, 151.2, 141.7, 138.8, 137.4, 137.3, 130.7, 130.0, 129.9, 129.8, 129.7, 129.4, 124.9, 124.3, 123.6, 122.6, 120.9, 120.2, 119.4, 110.8. IR (ZnSe): ν_{max} (cm^{-1}) 2970, 2931, 2353, 1652, 1558, 1456, 1381, 1126, 948, 815. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{13}N_2O_2$ 313.0972; found, 313.0972.

*8-(4-methylbenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3u**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 4-methylbenzoxazole (**2b**) (39.9 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 54.1 mg (98%). Mp = 187-189 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.42 (d, J = 6.0 Hz, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 6.6 Hz, 1H), 7.83 (d, J = 8.4 Hz, 1H), 7.73-7.71 (m, 1H), 7.40 (d, J = 7.8 Hz, 1H), 7.38-7.35 (m, 1H), 7.25-7.23 (m, 1H), 7.16 (d, J = 7.8 Hz, 1H), 2.64 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 162.7, 150.8, 140.8, 139.7, 137.2, 135.1, 131.7, 131.5, 130.5, 128.0, 126.4, 125.0, 124.7, 122.1, 122.1, 108.1, 16.7. IR (ZnSe): ν_{max} (cm^{-1}) 2920, 2351,

2310, 2156, 1716, 1556, 1232, 975, 819, 748. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_2$ 277.0972; found, 277.0972.

*8-(5-methylbenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3v**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 5-methylbenzoxazole (**2c**) (39.9 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (100% EtOAc/*n*-hexane) as brown solid, yield = 52.4 mg (95%). Mp = 156-158 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.41 (d, J = 6.0 Hz, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.90 (d, J = 6.6 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.71-7.68 (m, 1H), 7.56 (s, 1H), 7.44 (d, J = 8.4 Hz, 1H), 7.36-7.33 (m, 1H), 7.15 (d, J = 8.4 Hz, 1H), 2.48 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 163.5, 149.3, 141.8, 139.6, 137.1, 134.9, 134.1, 131.7, 131.4, 127.9, 126.3, 126.0, 122.1, 122.0, 120.0, 110.1, 21.6. IR (ZnSe): ν_{max} (cm^{-1}) 2920, 2856, 2351, 2310, 1652, 1556, 1180, 975, 819, 758. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_2$ 277.0972; found, 277.0974.

*8-(5-(tert-butyl)benzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3w**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 5-(*tert*-butyl)benzoxazole (**2d**) (52.5 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 56.0 mg (88%). Mp = 153-155 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.42 (d, J = 6.6 Hz, 1H), 8.08 (d, J = 7.8 Hz, 1H), 7.91 (d, J = 7.2 Hz, 1H), 7.84 (J = 8.4 Hz, 1H), 7.82 (s, 1H), 7.74-7.71 (m, 1H), 7.50 (d, J = 8.4 Hz, 1H), 7.43-7.41 (m, 1H), 7.39-7.36 (m, 1H), 1.41 (s, 9H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 162.7, 150.8, 140.8, 139.7, 137.2, 135.1, 131.7, 131.5, 130.5, 128.0, 126.4, 125.0, 124.7, 122.1, 122.1, 108.1, 16.7. IR (ZnSe): ν_{max} (cm^{-1}) 2960, 2868, 2308, 1716, 1558, 1246, 975, 819, 748, 651. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{19}N_2O_2$ 319.1441; found, 319.1441.

*8-(5-nitrobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3x**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 5-nitrobenzoxazole (**2e**) (49.2 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 60.2 mg (98%). Mp = 218-220 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.66 (s, 1H), 8.44 (d, J = 6.0 Hz, 1H), 8.32 (dd, J = 9.0, 2.4 Hz, 1H), 8.16 (d, J = 8.4 Hz, 1H), 7.96 (dd, J = 7.2, 1.2 Hz, 1H), 7.91 (d, J = 8.4 Hz, 1H), 7.79 (t, J = 7.8 Hz, 1H), 7.66 (dd, J = 9.0, 1.2 Hz, 1H), 7.46-7.43 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 166.7, 154.6, 145.3, 142.1, 139.5, 137.1, 135.0, 132.4, 131.5, 128.1, 126.7, 122.5, 121.1, 120.7, 116.6, 111.0. IR (ZnSe): ν_{max} (cm^{-1}) 3113, 2351, 2310, 1550, 1517, 1344, 1246, 977, 815, 750. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{10}N_3O_4$ 308.0666; found, 308.0666.

*8-(5-bromobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3y**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 5-bromobenzoxazole (**2f**) (59.1 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 42.8 mg (63%). Mp = 228-230 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.42 (dd, J = 6.0, 1.2 Hz, 1H), 8.11 (dd, J = 8.4, 1.2 Hz, 1H), 7.93 – 7.90 (m, 2H), 7.85 (d, J = 9.0 Hz, 1H), 7.74 (t, J = 7.8 Hz, 1H), 7.47 – 7.44 (m, 2H), 7.41 – 7.38 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.7, 150.1, 143.3, 139.6, 137.1, 134.9, 132.0, 131.5, 128.0, 128.0, 126.4,

123.2, 122.3, 121.4, 117.0, 112.1. IR (ZnSe): ν_{max} (cm^{-1}) 2351, 2310, 2150, 1992, 1716, 1541, 1506, 1456, 974, 756. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{10}BrN_2O_2$ 340.9920; found, 340.9922.

*8-(5-chloro-6-nitrobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3z**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 5-chloro-6-nitrobenzoxazole (**2g**) (59.4 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 35.5 mg (52%). Mp = 236-238 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): δ 8.45 – 8.43 (m, 1H), 8.18 – 8.16 (m, 1H), 8.13 – 8.12 (m, 1H), 7.95 – 7.93 (m, 1H), 7.92 – 7.89 (m, 2H), 7.80 – 7.77 (m, 1H), 7.47 – 7.43 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 168.8, 148.5, 145.5, 144.7, 139.4, 137.1, 134.8, 132.5, 131.5, 128.1, 126.7, 123.5, 122.6, 120.3, 109.0. IR (ZnSe): ν_{max} (cm^{-1}) 3099, 2351, 1548, 1533, 1448, 1247, 979, 875, 823, 750. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_9ClN_3O_4$ 342.0276; found, 342.0275.

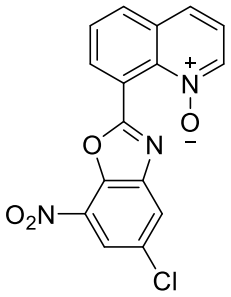
*8-(6-methylbenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3za**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 6-methylbenzoxazole (**2h**) (39.9 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 28.7 mg (52%). Mp = 186-188 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.42 (d, J = 6.0 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.94-7.93 (m, 1H), 7.84 (d, J = 8.4, 1.8 Hz, 1H), 7.73 (t, J = 7.8 Hz, 1H), 7.66 (d, J = 7.8 Hz, 1H), 7.40-7.37 (m, 2H), 7.18 (d, J = 8.4 Hz, 1H), 2.50 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 162.9, 151.4, 139.8, 139.5, 137.2, 135.3, 135.0, 131.7, 131.5, 128.0, 126.3, 125.6, 122.2, 119.6, 111.0, 21.9. IR (ZnSe): ν_{max} (cm^{-1}) 3057, 2976, 2918, 2353, 1622, 1554, 974, 812, 750. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{13}N_2O_2$ 277.0972; found, 277.0972.

*8-(6-nitrobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3zb**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 6-nitrobenzoxazole (**2i**) (49.2 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 58.9 mg (96%). Mp = 213-215 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.47 (s, 1H), 8.44 (d, J = 6.0 Hz, 1H), 8.33 (dd, J = 8.4, 1.8 Hz, 1H), 8.16 (d, J = 7.8 Hz, 1H), 7.96 (d, J = 7.2 Hz, 1H), 7.90 (d, J = 8.4 Hz, 1H), 7.88-7.86 (m, 1H), 7.80-7.77 (m, 1H), 7.4-7.43 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 168.3, 150.2, 147.0, 145.2, 139.5, 137.0, 134.7, 132.4, 131.5, 128.1, 126.5, 122.5, 120.8, 120.5, 120.1, 107.5. IR (ZnSe): ν_{max} (cm^{-1}) 3057, 2351, 2310, 1716, 1521, 1338, 979, 823, 754, 549. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{10}N_3O_4$ 308.0666; found, 308.0666.

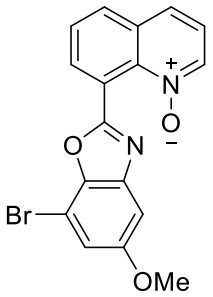
*8-(6-chlorobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3zc**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 6-chlorobenzoxazole (**2j**) (45.9 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown solid, yield = 58.0 mg (98%). Mp = 190-192 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.43 (d, J = 6.0 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 6.6 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.74 (t, J = 7.8 Hz, 1H), 7.69 (d, J = 8.4 Hz, 1H), 7.58 (s, 1H), 7.40-7.38 (m, 1H), 7.35 (d, J = 8.4 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.2, 151.3, 140.5, 139.7, 137.1, 134.9,

131.9, 131.5, 130.5, 128.0, 126.2, 125.0, 122.3, 121.5, 120.7, 111.5. IR (ZnSe): ν_{max} (cm^{-1}) 3057, 2351, 2310, 1716, 1558, 1228, 1188, 819, 804, 752. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{10}ClN_2O_2$ 297.0425; found, 297.0430.

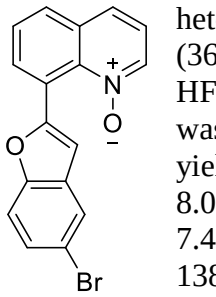
*8-(5-chloro-7-nitrobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3zd**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 5-chloro-7-nitrobenzoxazole (**2k**) (59.4 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as yellow solid, yield = 56.6 mg (83%). Mp = 280-282 °C. ^1H NMR (600 MHz, $CDCl_3$, δ): 8.40 (d, J = 6.0 Hz, 1H), 8.20 (s, 1H), 8.17 (d, J = 7.8 Hz, 1H), 8.08 (s, 1H), 7.96 (d, J = 7.2 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.80-7.77 (m, 1H), 7.45-7.43 (m, 1H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 167.2, 146.0, 142.9, 139.6, 136.9, 134.8, 133.1, 132.5, 131.5, 129.8, 128.0, 126.7, 126.3, 122.6, 121.0, 120.1. IR (ZnSe): ν_{max} (cm^{-1}) 3109, 3010, 2351, 2310, 1716, 1558, 1533, 1215, 819, 752. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_9ClN_3O_4$ 342.0276; found, 342.0278.



*8-(5-methoxy-7-bromobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3ze**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 5-methoxy-7-bromobenzoxazole (**2l**) (68.1 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (95% EtOAc/*n*-hexane) as brown, yield = 45.1 mg (61%). Mp = 220-222 °C. ^1H NMR (600 MHz, $CDCl_3$, δ): 8.44 (d, J = 6.0 Hz, 1H), 8.11 (dd, J = 8.4, 1.8 Hz, 1H), 7.93 – 7.91 (m, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.74 (dd, J = 8.4, 7.2 Hz, 1H), 7.41 (dd, J = 8.4, 6.0 Hz, 1H), 7.22 (d, J = 2.4 Hz, 1H), 7.13 (d, J = 2.4 Hz, 1H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 164.4, 157.8, 144.3, 142.7, 137.1, 134.9, 131.9, 131.5, 127.9, 126.3, 122.3, 121.4, 116.5, 103.1, 102.3, 56.4. IR (ZnSe): ν_{max} (cm^{-1}) 3080, 2933, 2351, 2310, 1595, 1556, 1209, 993, 817, 750. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{12}BrN_2O_3$ 371.0026; found, 371.0028.



*8-(benzofuran-2-yl)quinoline 1-oxide (Table 3, Entry **6a**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 2,3-Benzofuran (**5a**) (22.6 µL, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 38.1 mg (73%). Mp = 74-76 °C. ^1H NMR (600 MHz, $CDCl_3$, δ): 8.47 (d, J = 6.6 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.82 – 7.8 (m, 2H), 7.68 – 7.66 (m, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.34 (dd, J = 8.4, 6.0 Hz, 1H), 7.29 – 7.23 (m, 2H), 6.76 (s, 1H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 156.3, 155.1, 140.0, 137.9, 135.8, 132.0, 130.8, 129.1, 127.9, 126.5, 124.7, 123.9, 122.7, 121.8, 120.9, 111.3, 104.4. IR (ZnSe): ν_{max} (cm^{-1}) 2318, 2156, 1716, 1558, 1506, 1456, 1234, 974, 827, 758. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{12}NO_2$ 262.0863; found, 262.0867.



*8-(5-bromobenzofuran-2-yl)quinoline 1-oxide (Table 3, Entry **6b**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 5-Bromobenzofuran (**5b**) (36.8 µL, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown semi solid, yield = 36.6 mg (57%). ^1H NMR (600 MHz, $CDCl_3$, δ): 8.53 (d, J = 6.0 Hz, 1H), 8.04 – 8.02 (m, 1H), 7.87 (d, J = 9.0 Hz, 1H), 7.82 (dd, J = 7.2, 1.2 Hz, 1H), 7.72 – 7.68 (m, 2H), 7.41 – 7.35 (m, 3H), 6.71 (s, 1H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 157.5, 153.8, 139.7, 138.2, 136.0, 131.9, 131.1, 131.0, 128.0, 127.4, 126.8, 124.1, 123.5, 121.9, 115.8, 112.8,

103.9. IR (ZnSe): ν_{max} (cm^{-1}) 3091, 2922, 2852, 2355, 1556, 1440, 1375, 974, 804, 756. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{11}BrNO_2$ 339.9968; found, 339.9972.

*8-(5-phenylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6c**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 2-phenylthiophene (**5c**) (48.1 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown viscous, yield = 47.9 mg (79%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.43 (d, J = 6.0 Hz, 1H), 7.91 (dd, J = 7.8, 12. Hz, 1H), 7.84 (d, J = 8.4 Hz, 1H), 7.75 (dd, J = 7.2, 1.2 Hz, 1H), 7.63 – 7.59 (m, 3H), 7.37 – 7.31 (m, 3H), 7.27 – 7.24 (m, 1H), 7.21 (d, J = 3.6 Hz, 1H), 6.93 (d, J = 3.6 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 144.4, 142.7, 139.1, 138.1, 136.6, 134.5, 132.2, 129.8, 128.9, 128.5, 128.3, 127.9, 127.8, 127.4, 125.7, 122.0, 121.5. IR (ZnSe): ν_{max} (cm^{-1}) 2351, 2310, 1716, 1541, 1456, 1276, 1101, 754, 694, 634. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{19}H_{14}NOS$ 304.0791; found, 304.0798.

*8-(5-methylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6d**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 2-methylthiophene (**5d**) (19.4 µL, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (60% EtOAc/*n*-hexane) as dark brown viscous, yield = 25.5 mg (53%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.41 (d, J = 6.0 Hz, 1H), 7.91 (d, J = 8.4 Hz, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.70 (d, J = 7.2 Hz, 1H), 7.61 (t, J = 7.8 Hz, 1H), 7.36 – 7.34 (m, 1H), 6.74 (d, J = 3.6 Hz, 1H), 6.65 (d, J = 3.5 Hz, 1H), 2.51 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 141.0, 140.3, 139.3, 138.1, 136.5, 132.2, 129.5, 129.2, 128.1, 127.9, 126.4, 124.1, 121.4, 15.3. IR (ZnSe): ν_{max} (cm^{-1}) 2920, 2850, 2351, 2310, 1716, 1419, 1184, 1101, 750, 522. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{14}H_{12}NOS$ 242.0634; found, 242.0634.

*8-(5-ethylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6e**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 2-ethylthiophene (**5e**) (22.2 µL, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (60% EtOAc/*n*-hexane) as dark brown viscous, yield = 31.6 mg (62%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.51 (d, J = 6.0 Hz, 1H), 7.89 (dd, J = 8.4, 1.8 Hz, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.72 (dd, J = 7.2, 1.2 Hz, 1H), 7.60 (t, J = 7.8 Hz, 1H), 7.35 – 7.33 (m, 1H), 6.80 (d, J = 3.0 Hz, 1H), 6.71 (d, J = 3.6 Hz, 1H), 2.91 – 2.87 (m, 2H), 1.36 – 1.34 (m, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 147.9, 140.5, 139.4, 138.1, 136.4, 132.2, 129.4, 129.4, 127.8, 127.7, 126.3, 122.2, 121.3, 23.5, 15.9. IR (ZnSe): ν_{max} (cm^{-1}) 2978, 2308, 1616, 1558, 1454, 1328, 1219, 962, 860, 763. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{15}H_{14}NOS$ 256.0791; found, 256.0791.

*8-(5-proplthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6f**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 2-propylthiophene (**5f**) (25.1 µL, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as dark brown viscous, yield = 34.4 mg (64%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.42 (dd, J = 6.0, 1.2 Hz, 1H), 7.92 – 7.89 (m, 2H), 7.72 (dd, J = 7.2, 1.2 Hz, 1H), 7.62 – 7.60 (m, 1H), 7.36 (dd, J = 8.4, 6.0 Hz, 1H), 6.75 (d, J = 3.0 Hz, 1H), 6.66 (d, J = 3.0 Hz, 1H 1H), 2.81 – 2.78 (m, 2H), 1.76 – 1.69 (m, 2H), 1.00 (t, J = 7.8 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 146.1, 140.6, 139.3, 138.1, 136.5, 132.2, 129.4, 129.3, 128.0, 127.9, 126.3, 122.9, 121.4,

32.3, 24.9, 14.0. IR (ZnSe): ν_{max} (cm^{-1}) 2962, 2924, 2850, 2353, 1622, 1558, 1454, 1234, 1188, 744. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{16}NOS$ 270.0947; found, 270.0948.

*8-(5-pentylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6g**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 2-pentylthiophene (**5g**) (49.0 µL, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as dark brown viscous, yield = 38.6 mg (65%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.43 (d, J = 7.8, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.94 (dd, J = 8.4, 1.8 Hz, 1H), 7.75 (dd, J = 7.2, 1.2 Hz, 1H), 7.65 – 7.62 (m, 1H), 7.41 (dd, J = 8.4, 6.0 Hz, 1H), 6.72 (d, J = 3.6 Hz, 1H), 6.63 (d, J = 3.6 Hz, 1H), 2.79 (t, J = 7.8 Hz, 2H), 1.71 – 1.66 (m, 2H), 1.40 – 1.32 (m, 4H), 0.90 (t, J = 7.2 Hz, 4H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 146.5, 140.3, 139.0, 138.4, 136.9, 132.2, 129.5, 129.2, 128.0, 126.4, 122.8, 121.4, 31.6, 31.4, 30.2, 22.6, 14.1. IR (ZnSe): ν_{max} (cm^{-1}) 2962, 2351, 2308, 1558, 1456, 1240, 887, 769, 752, 571. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{18}H_{20}NOS$ 298.1260; found, 298.1256.

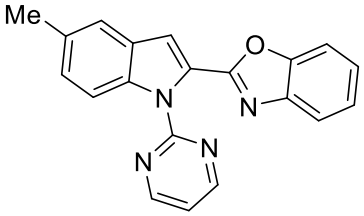
*8-(5-hexylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6h**):* Following the general procedure for heteroarylation, quinoline *N*-oxide (**1a**) (29.0 mg, 0.2 mmol), 2-hexylthiophene (**5h**) (33.7 µL, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as dark brown viscous, yield = 33.0 mg (53%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.38 (dd, J = 6.0, 1.2 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.95 – 7.94 (m, 1H), 7.75 (dd, J = 7.2, 1.2 Hz, 1H), 7.64 (t, J = 7.8 Hz, 1H), 7.41 (dd, J = 8.4, 6.0 Hz, 1H), 6.71 (d, J = 3.6 Hz, 1H), 6.63 (d, J = 3.6 Hz, 1H), 2.79 (t, J = 7.8 Hz, 2H), 1.71 – 1.66 (m, 2H), 1.42 – 1.37 (m, 2H), 1.32 – 1.29 (m, 4H), 0.90 – 0.88 (m, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 146.6, 140.1, 138.7, 138.7, 137.2, 132.2, 129.6, 129.0, 128.2, 126.5, 122.8, 121.5, 31.75, 31.74, 30.2, 29.1, 22.7, 14.2. IR (ZnSe): ν_{max} (cm^{-1}) 2960, 2870, 2167, 1556, 1246, 1213, 975, 819, 748, 651. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{19}H_{22}NOS$ 312.1417; found, 312.1410.

*2-(1-(pyridin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6i**):* Following the general procedure for heteroarylation, *N*-pyridyl indoline (**4a**) (39.2 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as off white solid, yield = 61.0 mg (98%). Mp = 134-136 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.65 (d, J = 4.8 Hz, 1H), 7.92-7.89 (m, 1H), 7.77 (d, J = 8.4 Hz, 1H), 7.61-7.60(m, 2H), 7.47-7.45 (m, 2H), 7.44-7.40 (m, 2H), 7.34-7.31 (m, 1H), 7.30-7.24 (m, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, δ): 157.2, 151.5, 150.3, 149.5, 142.0, 139.9, 138.3, 127.8, 126.6, 125.5, 125.1, 124.6, 123.0, 122.3, 122.2, 122.0, 120.3, 111.6, 111.0, 110.5. IR (ZnSe): ν_{max} (cm^{-1}) 3059, 2351, 2310, 1716, 1622, 1577, 1436, 1215, 788, 738. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{14}N_3O$ 312.1131; found, 312.1131.

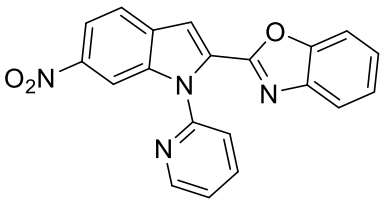
*2-(5-methyl-1-(pyridin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6j**):* Following the general procedure for heteroarylation, 5-methyl-*N*-pyridyl indoline (**4b**) (42.0 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as off white solid, yield = 63.7 mg (98%). Mp = 115-117 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ):

8.63 (d, *J* = 4.8 Hz, 1H), 7.90 – 7.87 (m, 1H), 7.61 – 7.60 (m, 1H), 7.55 (s, 1H), 7.53 (s, 1H), 7.43 – 7.41 (m, 2H), 7.39 – 7.37 (m, 2H), 7.29 – 7.27 (m, 2H), 7.15 (d, *J* = 8.4 Hz, 1H), 2.48 (s, 3H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$, *δ*): 157.3, 151.6, 150.3, 149.4, 142.0, 138.4, 138.2, 131.4, 128.0, 127.3, 126.4, 125.0, 124.5, 122.8, 122.1, 121.6, 120.2, 111.3, 110.7, 110.4, 21.5. IR (ZnSe): ν_{max} (cm^{-1}) 2927, 2856, 2353, 2320, 1622, 1581, 1242, 1145, 790, 738. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{21}H_{16}N_3O$ 326.1288; found, 326.1288.

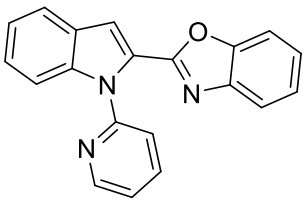
*2-(5-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6k**):* Following the general procedure for heteroarylation, 5-methyl-*N*-pyrimidyl indoline (**4c**) (42.2 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as off white solid, yield = 63.9 mg (98%). Mp = 113-115 °C. ^{1}H NMR (600 MHz, $CDCl_3$, *δ*): 8.65 (d, *J* = 4.8 Hz, 2H), 8.24 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.52 (s, 1H), 7.44 – 7.42 (m, 2H), 7.35 – 7.30 (m, 2H), 7.24 (d, *J* = 9.0 Hz, 1H), 7.12 (t, *J* = 4.2 Hz, 0H), 2.49 (s, 3H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$, *δ*): 158.24, 158.21, 157.7, 150.7, 142.0, 137.1, 132.4, 128.8, 127.7, 126.7, 125.0, 124.5, 121.7, 120.2, 117.8, 113.8, 113.8, 110.5, 21.4. IR (ZnSe): ν_{max} (cm^{-1}) 2954, 2376, 2310, 1622, 1558, 1417, 1145, 827, 740, 630. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{15}N_4O$ 327.1240; found, 327.1240.



*2-(6-nitro-1-(pyrimidin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6l**):* Following the general procedure for heteroarylation, 6-nitro-*N*-pyrimidyl indoline (**4d**) (48.4 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as yellow solid, yield = 59.3 mg (83%). Mp = 190-192 °C. ^{1}H NMR (600 MHz, $CDCl_3$, *δ*): 9.23 (s, 1H), 8.75 (dd, *J* = 4.8, 1.8 Hz, 2H), 8.18 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.76 – 7.75 (m, 1H), 7.51 (s, 1H), 7.48 – 7.46 (m, 1H), 7.39 – 7.35 (m, 2H), 7.29 (t, *J* = 4.8 Hz, 1H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$, *δ*): 158.7, 156.9, 156.6, 150.7, 146.0, 141.7, 137.2, 133.0, 131.5, 125.8, 124.9, 122.2, 120.7, 119.1, 118.1, 112.7, 111.1, 110.8. IR (ZnSe): ν_{max} (cm^{-1}) 2962, 2353, 2310, 1558, 1506, 1417, 1338, 1166, 835, 750. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{13}N_4O_3$ 357.0982; found, 357.1191.



*2-(1-(pyridin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6i**):* Following the general procedure for heteroarylation, *N*-pyridyl indole (**4e**) (38.8 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as off white solid, yield = 57.2 mg (92%). Mp = 134-136 °C. ^{1}H NMR (600 MHz, $CDCl_3$, *δ*): 8.65 (d, *J* = 4.8 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.61 -7.60 (m, 2H), 7.47 – 7.45 (m, 2H), 7.44 – 7.40 (m, 2H), 7.33 – 7.31 (m, 1H), 7.29 – 7.24 (m, 3H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$, *δ*): 157.2, 151.5, 150.3, 149.5, 142.0, 139.9, 138.3, 127.8, 126.5, 125.5, 125.1, 124.6, 123.0, 122.3, 122.2, 122.0, 120.3, 111.6, 111.0, 110.5. IR (ZnSe): ν_{max} (cm^{-1}) 2962, 2353, 2310, 1558, 1506, 1417, 1338, 1166, 788, 740. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{14}N_3O$ 312.1131; found, 312.1131.



*2-(1-(pyrimidin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6m**):* Following the general procedure for heteroarylation, *N*-pyrimidyl indole (**4f**) (39.0 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as off white solid, yield = 58.7 mg (94%). Mp = 156-158 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.69 (d, J = 5.4 Hz, 2H), 8.34 (d, J = 8.4 Hz, 1H), 7.76 – 7.74 (m, 2H), 7.50 (s, 1H), 7.45 – 7.41 (m, 2H), 7.36 – 7.30 (m, 3H), 7.17 (t, J = 4.8 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 158.3, 158.1, 157.7, 150.7, 142.0, 138.8, 128.6, 126.7, 126.1, 125.1, 124.6, 122.9, 122.1, 120.3, 118.1, 114.0, 114.0, 110.6. IR (ZnSe): ν_{max} (cm^{-1}) 2353, 2310, 1992, 1716, 1652, 1558, 1506, 1338, 1136, 744. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{19}H_{13}N_4O$ 313.1084; found, 313.1083.

*1-(2-(benzo[d]oxazol-2-yl)-1-(pyridin-2-yl)-1H-indol-3-yl)ethan-1-one (Table 3, Entry **6n**):* Following the general procedure for heteroarylation, 1-(1-(*pyridin*-2-yl)-1H-indol-3-yl)ethan-1-one (**4g**) (47.2 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as off white solid, yield = 45.9 mg (65%). Mp = 185-187 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.45-8.43 (m, 1H), 8.39-8.38 (m, 1H), 7.83-7.80 (m, 1H), 7.73 (d, J = 7.8 Hz, 1H), 7.56-7.54 (m, 2H), 7.45 (d, J = 7.8 Hz, 1H), 7.43-7.36 (m, 4H), 7.27-7.25 (m, 1H), 2.41 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 194.8, 155.4, 150.8, 150.1, 149.7, 141.3, 138.7, 137.1, 129.1, 126.3, 126.3, 125.9, 125.0, 124.0, 123.2, 123.2, 121.7, 120.9, 120.8, 111.5, 111.1, 30.3. IR (ZnSe): ν_{max} (cm^{-1}) 2351, 2154, 1992, 1716, 1652, 1506, 1473, 1136, 921, 742. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{22}H_{16}N_3O_2$ 354.1237; found, 354.1242.

*1-(7-(benzo[d]oxazol-2-yl)indolin-1-yl)-2,2-dimethylpropan-1-one (Table 3, Entry **6o**):* Following the general procedure for heteroarylation, *N*-pivaloyl indoline (**4h**) (40.6 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as brown solid, yield = 57.0 mg (89%). Mp = 180-182 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 7.90 (d, J = 7.8 Hz, 1H), 7.75 (dd, J = 6.6, 2.4 Hz, 1H), 7.48 – 7.46 (m, 1H), 7.37 (d, J = 7.8 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.18 (t, J = 7.8 Hz, 1H), 4.31 (t, J = 7.8 Hz, 2H), 3.17 – 3.14 (m, 2H), 1.33 (s, 9H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 178.9, 162.9, 150.6, 143.1, 142.0, 135.0, 128.6, 127.1, 124.7, 124.5, 124.3, 120.2, 119.0, 110.3, 50.7, 40.2, 30.7, 28.3. IR (ZnSe): ν_{max} (cm^{-1}) 2972, 2351, 2310, 1647, 1558, 1506, 1195, 956, 885, 746. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{21}N_2O_2$ 321.1598; found, 321.1602.

*1-(7-(benzo[d]oxazol-2-yl)-5-methylindolin-1-yl)-2,2-dimethylpropan-1-one (Table 3, Entry **6p**):* Following the general procedure for heteroarylation, 5-methyl-*N*-pivaloyl indoline (**4i**) (43.4 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as light brown solid, yield = 48.8 mg (73%). Mp = 199-201 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 7.75 – 7.73 (m, 2H), 7.46 (d, J = 7.8 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.20 (s, 1H), 4.30 (t, J = 7.8 Hz, 2H), 3.13 – 3.10 (m, 2H), 2.38 (s, 3H), 1.32 (s, 9H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 178.8, 163.2, 150.6, 141.9, 140.7, 135.1, 134.5, 128.9, 128.0, 124.7, 124.3, 120.1, 118.4, 110.2, 50.9, 40.2, 30.7, 28.3, 21.0. IR (ZnSe): ν_{max} (cm^{-1}) 2972, 2351, 2310, 1647, 1558,

1448, 1317, 1165, 862, 746. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{21}H_{23}N_2O_2$ 335.1754; found, 335.1761.

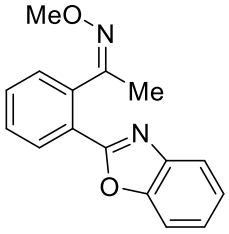
*2-(2-(1H-pyrazol-1-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6q**):* Following the general procedure for heteroarylation, 1-phenyl pyrazole (**4j**) (18.0 µL, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as transparent liquid, yield = 31.3 mg (60%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.17 (d, J = 7.8 Hz, 1H), 7.75-7.73 (dd, 6.6, 1.8 Hz, 1H), 7.68-7.62 (m, 3H), 7.60 (d, J = 2.4 Hz, 1H), 7.58-7.55 (m, 1H), 7.38-7.36 (m, 1H), 7.34-7.30 (m, 2H), 6.42-6.41 (m, 1H).^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 161.3, 150.9, 141.7, 141.2, 139.8, 132.0, 131.6, 130.9, 128.6, 127.1, 125.5, 124.6, 123.5, 120.5, 110.8, 107.1. IR (ZnSe): ν_{max} (cm^{-1}) 2920, 2850, 2310, 1622, 1519, 1454, 1392, 1236, 1029, 744. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{12}N_3O$ 262.0975; found, 262.0975.

*2-(2-(3-methyl-1H-pyrazol-1-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6r**):* Following the general procedure for heteroarylation, 3-methyl-1-phenyl-1H-pyrazole (**4k**) (31.6 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as transparent liquid, yield = 33.1 mg (60%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.14 (dd, J = 7.8, 1.8 Hz, 1H), 7.76 – 7.74 (m, 1H), 7.66 – 7.61 (m, 2H), 7.54 – 7.51 (m, 1H), 7.43 (d, J = 2.4 Hz, 1H), 7.42 – 7.39 (m, 1H), 7.35 – 7.30 (m, 2H), 6.18 (d, J = 2.4 Hz, 1H), 2.30 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 161.4, 150.9, 150.5, 141.7, 139.8, 132.0, 131.8, 131.6, 128.1, 126.9, 125.5, 124.6, 122.9, 120.4, 110.8, 107.1, 13.7. IR (ZnSe): ν_{max} (cm^{-1}) 2920, 2850, 2310, 1732, 1527, 1454, 1236, 1028 744, 700. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{14}N_3O$ 276.1131; found, 276.1132.

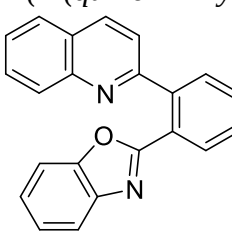
*2-(2-(pyridin-2-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6s**):* Following the general procedure for heteroarylation, 2-phenyl pyridine (**4l**) (28.5 µL, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as brown viscous, yield = 53.3mg (98%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.66 (d, J = 4.8 Hz, 2H), 8.08 – 8.07 (m, 1H), 8.02 (dd, J = 7.8, 1.2 Hz, 1H), 7.72 – 7.70 (m, 1H), 7.67 – 7.64 (m, 1H), 7.62 – 7.59 (m, 1H), 7.32 – 7.24 (m, 3H), 7.17 – 7.16 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 166.3, 163.8, 157.0, 150.8, 142.0, 139.3, 131.1, 131.0, 130.7, 129.7, 127.2, 124.9, 124.3, 120.3, 119.1, 110.4. IR (ZnSe): ν_{max} (cm^{-1}) 2954, 2351, 2318, 1716, 1558, 1452, 1415, 1236, 1028, 744. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{18}H_{13}N_2O$ 273.1022; found, 273.1022.

*2-(2-(pyrimidin-2-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6t**):* Following the general procedure for heteroarylation, 2-phenyl pyrimdine (**4m**) (31.2 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as brown viscous, yield = 44.8 mg (82%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.57 (d, J = 4.8 Hz, 1H), 8.14 (d, J = 7.8 Hz, 1H), 7.71-7.66 (m, 3H), 7.65-7.62 (m, 1H), 7.59-7.56 (m, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.32-7.23 (m, 4H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 163.7, 158.7, 150.9, 149.3, 141.9, 136.4, 131.2, 131.0, 130.8, 128.8, 126.5, 125.0, 124.4, 123.9, 122.3, 120.3, 110.6. IR (ZnSe): ν_{max} (cm^{-1}) 3074, 2162, 1571, 1556, 1452, 1413, 1236, 1029, 744, 632. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{17}H_{12}N_3O$ 274.0975; found, 274.0979.

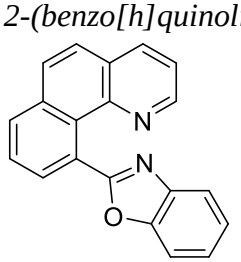
*2-(benzo[d]oxazol-2-yl)phenyl)ethan-1-one O-methyl oxime (Table 3, Entry **6u**):* Following the general procedure for heteroarylation, 1-phenylethan-1-one O-methyl oxime (**4n**) (29.8 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (10% EtOAc/*n*-hexane) as transparent liquid, yield = 34.6 mg (65%). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.26 (d, J = 7.8 Hz, 0.2H), 8.17 (d, J = 7.8 Hz, 1H), 7.81 – 7.78 (m, 1.2H), 7.59 – 7.48 (m, 4.2H), 7.38 – 7.35 (m, 2.4H), 3.92 (s, 3H), 3.61 (s, 0.6H), 2.32 (s, 0.6H), 2.13 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 162.6, 162.2, 157.2, 150.9, 150.9, 142.2, 142.1, 138.2, 131.3, 130.3, 130.0, 129.6, 129.0, 128.7, 128.0, 125.9, 125.3, 125.3, 124.7, 124.6, 120.5, 110.7, 110.7, 62.0, 61.7, 22.0, 16.8. IR (ZnSe): ν_{max} (cm^{-1}) 2937, 2818, 2351, 2312, 1454, 1242, 1043, 869, 746, 704. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{15}N_2O_2$ 267.1128; found, 267.1133.



*2-(2-(quinolin-2-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6v**):* Following the general procedure for heteroarylation, 2-phenylquinoline (**4o**) (41.0 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (5% EtOAc/*n*-hexane) as off white solid, yield = 23.2 mg (36%). Mp = 118-120 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.21 (d, J = 7.8 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 8.04 (t J = 4.8 Hz, 1H), 7.86 – 7.83 (m, 2H), 7.71 – 7.66 (m, 3H), 7.63 (t, J = 7.8 Hz, 1H), 7.57 – 7.55 (m, 1H), 7.40 (d, J = 8.4 Hz, 1H), 7.29 – 7.27 (m, 1H), 7.23 – 7.21 (m, 1H), 7.19 (d, J = 8.4 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 150.9, 141.9, 131.4, 131.2, 131.0, 129.1, 127.6, 127.1, 126.8, 126.6, 125.1, 124.5, 122.2, 122.2, 120.3, 110.6. IR (ZnSe): ν_{max} (cm^{-1}) 3041, 2351, 2320, 1456, 1234, 1029, 810, 740, 702, 619. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{22}H_{15}N_2O$ 323.1179; found, 323.1179.

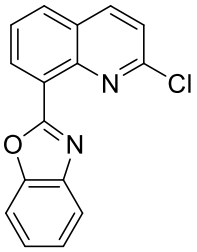


*2-(benzo[h]quinolin-10-yl)benzo[d]oxazole (Table 3, Entry **6w**):* Following the general procedure for heteroarylation, benzo[h]quinoline (**4p**) (35.8 mg, 0.2 mmol), benzoxazole (**2a**) (35.8 mg, 0.3 mmol), $[Cp^*RhCl_2]_2$ (6.0 mg, 5 mol %), PivOH (20.5 mg, 0.2 mmol), and HFIP (1.0 mL) were used, and the reaction was run at 100 °C for 24 h. The title compound was isolated from column chromatography (20% EtOAc/*n*-hexane) as off white solid, yield = 58.0 mg (98%). Mp = 182-184 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.36 (d, J = 4.2 Hz, 1H), 8.15 - 8.12 (m, 2H), 7.97 (d, J = 7.2 Hz, 1H), 7.91-7.89 (m, 2H), 7.81-7.76 (m, 2H), 7.55 (d, J = 7.8 Hz, 1H), 7.44-7.39 (m, 2H), 7.36-7.34 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 166.8, 151.2, 148.2, 145.2, 142.5, 135.8, 134.5, 132.1, 131.3, 131.2, 127.9, 127.5, 127.3, 126.6, 126.2, 124.6, 124.1, 122.0, 120.3, 110.7. IR (ZnSe): ν_{max} (cm^{-1}) 2357, 1994, 1622, 1558, 1454, 1419, 1234, 958, 837, 727. HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{20}H_{13}N_2O$ 297.1022; found, 297.1022.

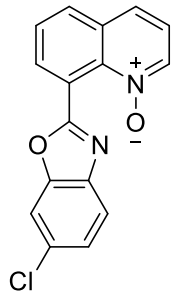


*8-(6-chlorobenzo[d]oxazol-2-yl)quinoline 1-oxide (Scheme S14, **7a**):* ^{1}H NMR (600 MHz, $CDCl_3$, δ): 9.15 (dd, J = 4.2, 1.8 Hz, 1H), 8.48 (dd, J = 7.2, 1.2 Hz, 1H), 8.21 (dd, J = 8.4, 1.8 Hz, 1H), 7.98 – 7.96 (m, 1H), 7.92 – 7.91 (m, 1H), 7.66 – 7.63 (m, 2H), 7.48 (dd, J = 8.4, 4.2 Hz, 1H), 7.37 – 7.36 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 162.2, 151.8, 150.9, 145.7, 142.2, 136.8, 132.8, 131.8, 128.8, 126.0, 125.4, 124.5, 121.8, 120.7, 110.8. IR (ZnSe): ν_{max} (cm^{-1}) 2918, 2351, 1556, 1452, 1226, 1190, 1124, 756, 738, 559.

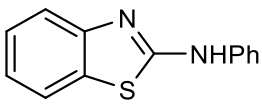
*8-(6-chlorobenzo[d]oxazol-2-yl)quinoline 1-oxide (Scheme S15, **7b**):* Mp = 105-107 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.53 (dd, J = 7.2, 1.2 Hz, 1H), 8.19 (d, J = 8.4 Hz, 1H), 8.02 – 8.00 (m, 1H), 7.90 – 7.89 (m, 1H), 7.72 – 7.69 (m, 2H), 7.50 (d, J = 9.0 Hz, 1H), 7.43 – 7.38 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 162.0, 152.3, 151.4, 145.4, 142.1, 139.3, 133.7, 131.4, 127.5, 126.6, 125.9, 125.5, 124.6, 123.5, 120.7, 111.1. IR (ZnSe): ν_{max} (cm^{-1}). HRMS (ESI-TOF) (m/z): $[M + H]^+$ calcd for $C_{16}H_{10}ClN_2O$ 281.0476; found, 281.0483. IR (ZnSe): ν_{max} (cm^{-1}) 2924, 2856, 2351, 2310, 1585, 1450, 1238, 1097, 839, 750.



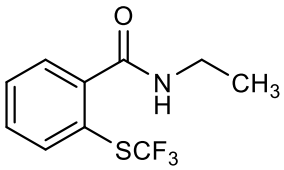
*8-(6-chlorobenzo[d]oxazol-2-yl)quinoline 1-oxide (Scheme S16, **3zc**):* %). ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.43 – 8.42 (m, 1H), 8.10 (dd, J = 8.4, 1.2 Hz, 1H), 7.93 – 7.92 (m, 1H), 7.85 – 7.84 m, 1H), 7.75 – 7.73 (m, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.59 (d, J = 1.8 Hz, 1H), 7.39 (dd, J = 8.4, 6.0 Hz, 1H), 7.36 – 7.34 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.2, 151.3, 140.5, 139.7, 137.1, 134.9, 131.9, 131.5, 130.5, 128.0, 126.1, 125.0, 122.3, 121.5, 120.7, 111.5. IR (ZnSe): ν_{max} (cm^{-1}) 2353, 2164, 1716, 1558, 1506, 1228, 819, 804, 752, 530.



*2-(benzo[h]quinolin-10-yl)benzo[d]oxazole (Scheme S17, **8a**):* ^{1}H NMR (600 MHz, $CDCl_3$, δ): 7.64 (dd, J = 7.8, 1.2 Hz, 1H), 7.59 (dd, J = 8.4, 1.2 Hz, 1H), 7.52 – 7.50 (m, 2H), 7.41 (dd, J = 8.4, 7.2 Hz, 2H), 7.35 – 7.32 (m, 1H), 7.19 – 7.15 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 164.6, 151.6, 140.0, 130.1, 129.7, 126.3, 124.5, 122.6, 121.0, 120.3, 119.6.



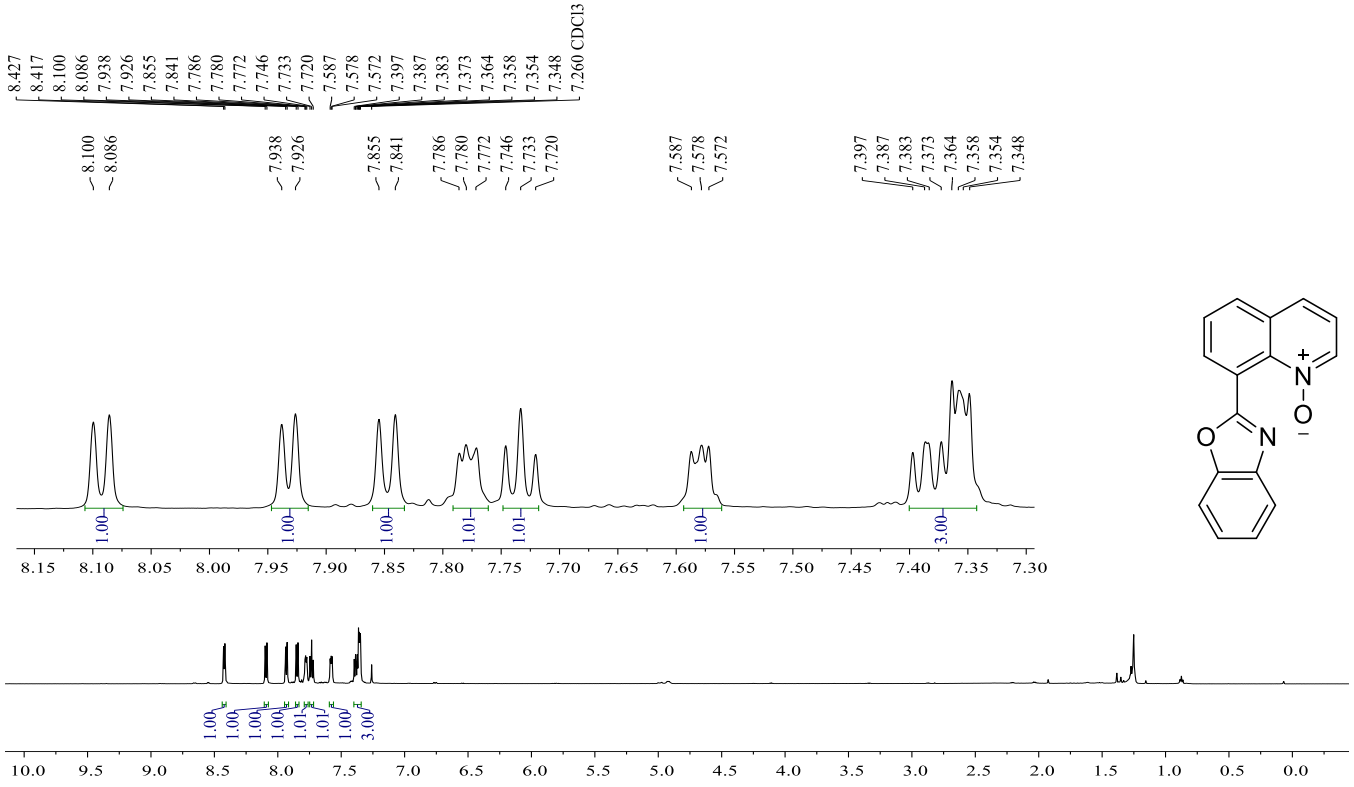
*2-(benzo[h]quinolin-10-yl)benzo[d]oxazole (Scheme S18, **8b**):* ^{1}H NMR (600 MHz, $CDCl_3$, δ): 7.73 (d, J = 7.2 Hz, 1H), 7.55 – 7.54 (m, 1H), 7.50 – 7.45 (m, 2H), 5.99 (s, 1H), 3.52 – 3.47 (m, 2H), 1.26 – 1.24 (m, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 167.6, 142.4, 136.9, 132.7, 130.8, 130.7, 129.64 (m,) 128.45, 35.20, 14.79.



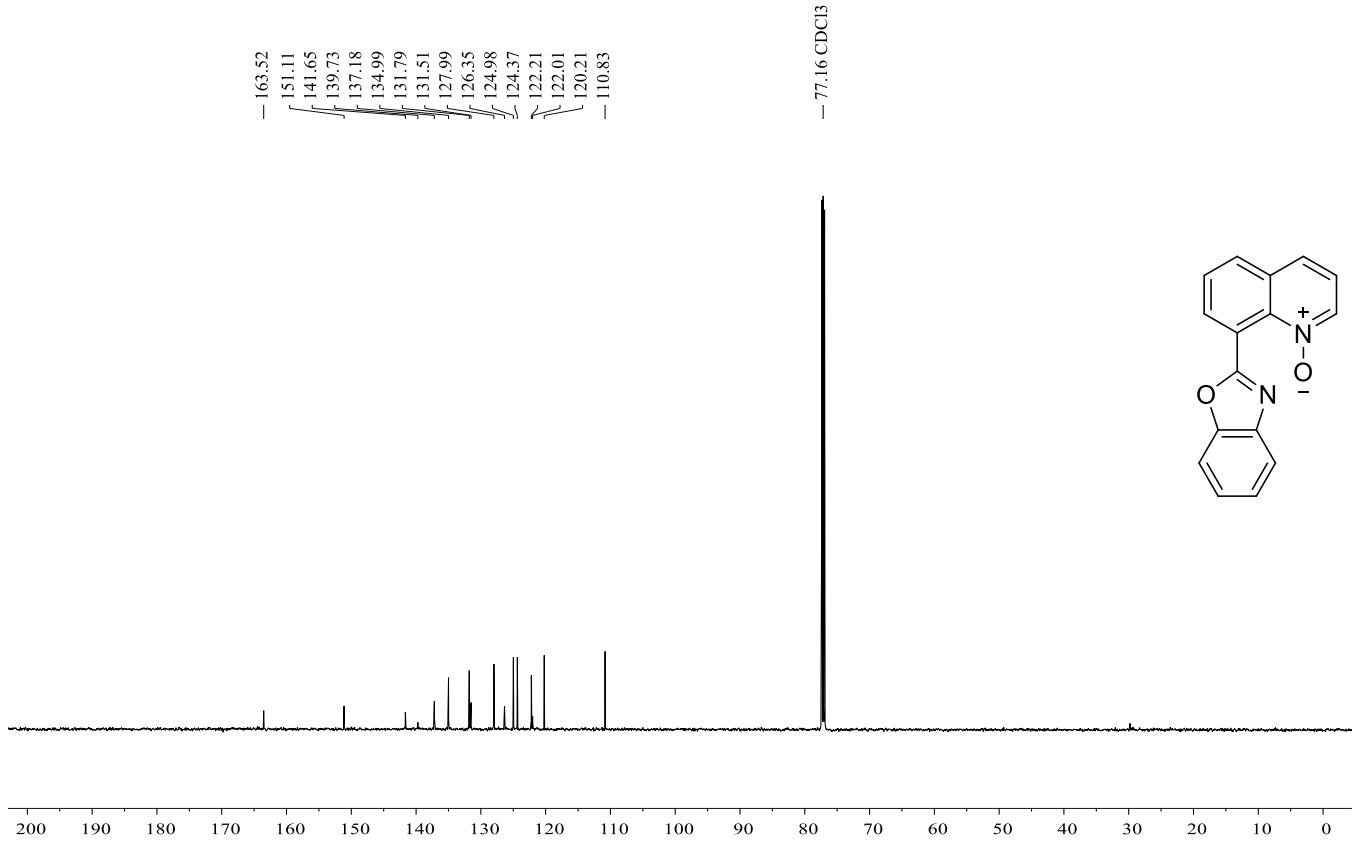
12. ^{1}H and ^{13}C Spectral data

*8-(benzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3a**)*

^{1}H NMR (600 MHz)

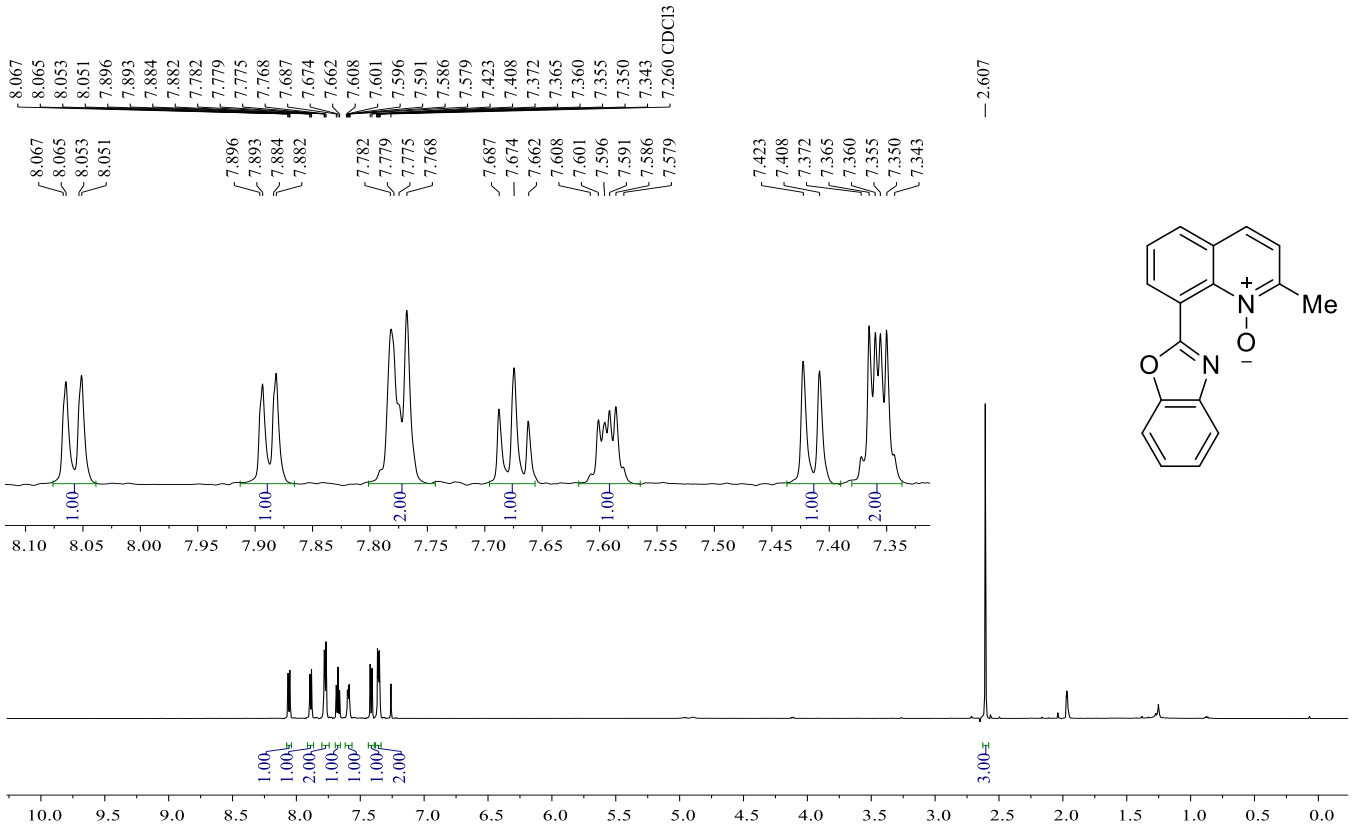


^{13}C{^{1}H} NMR (150 MHz)

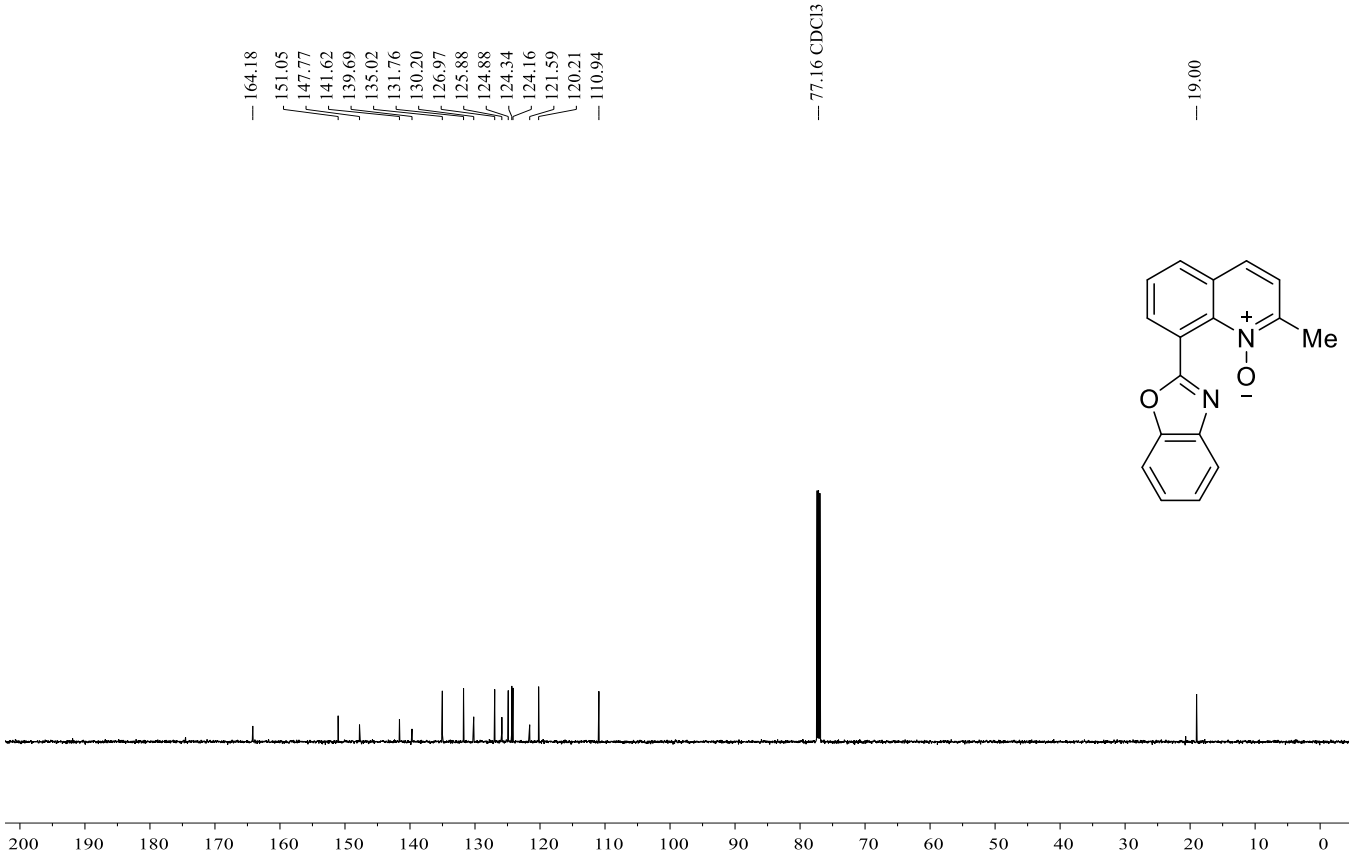


*8-(benzo[d]oxazol-2-yl)-2-methylquinoline 1-oxide (Table 2, Entry **3b**)*

^{1}H NMR (600 MHz)

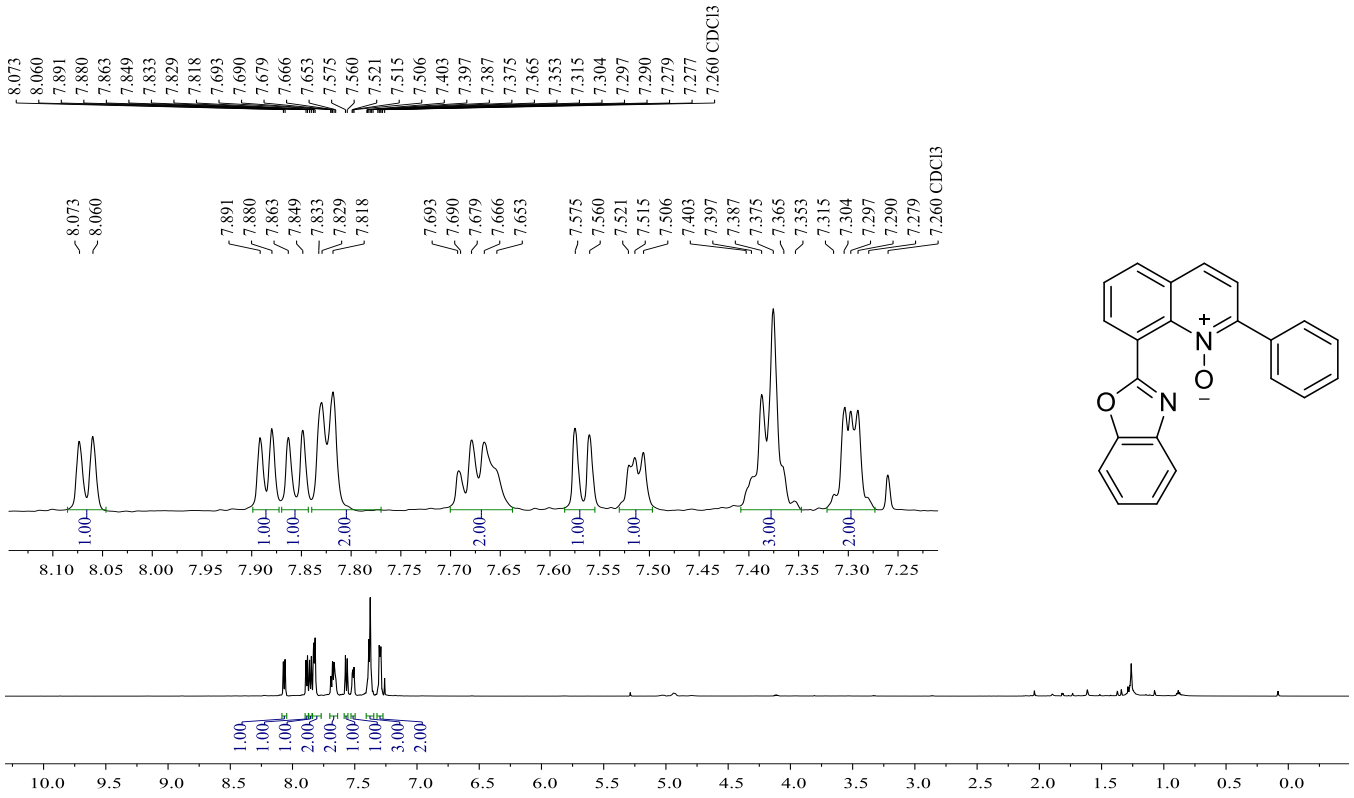


^{13}C{^{1}H} NMR (150 MHz)

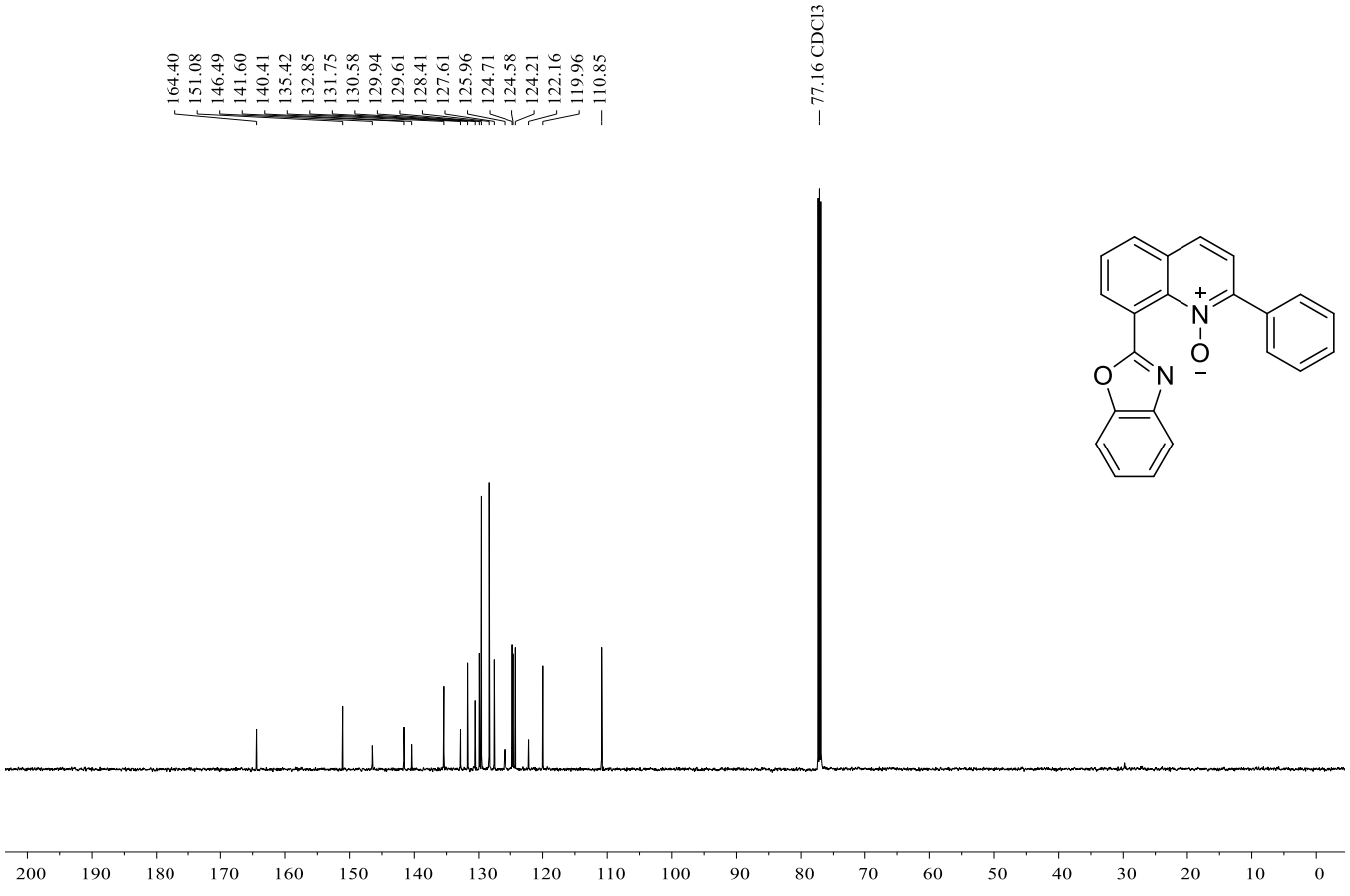


*8-(benzo[d]oxazol-2-yl)-2-phenylquinoline 1-oxide (Table 2, Entry **3c**)*

^{1}H NMR (600 MHz)

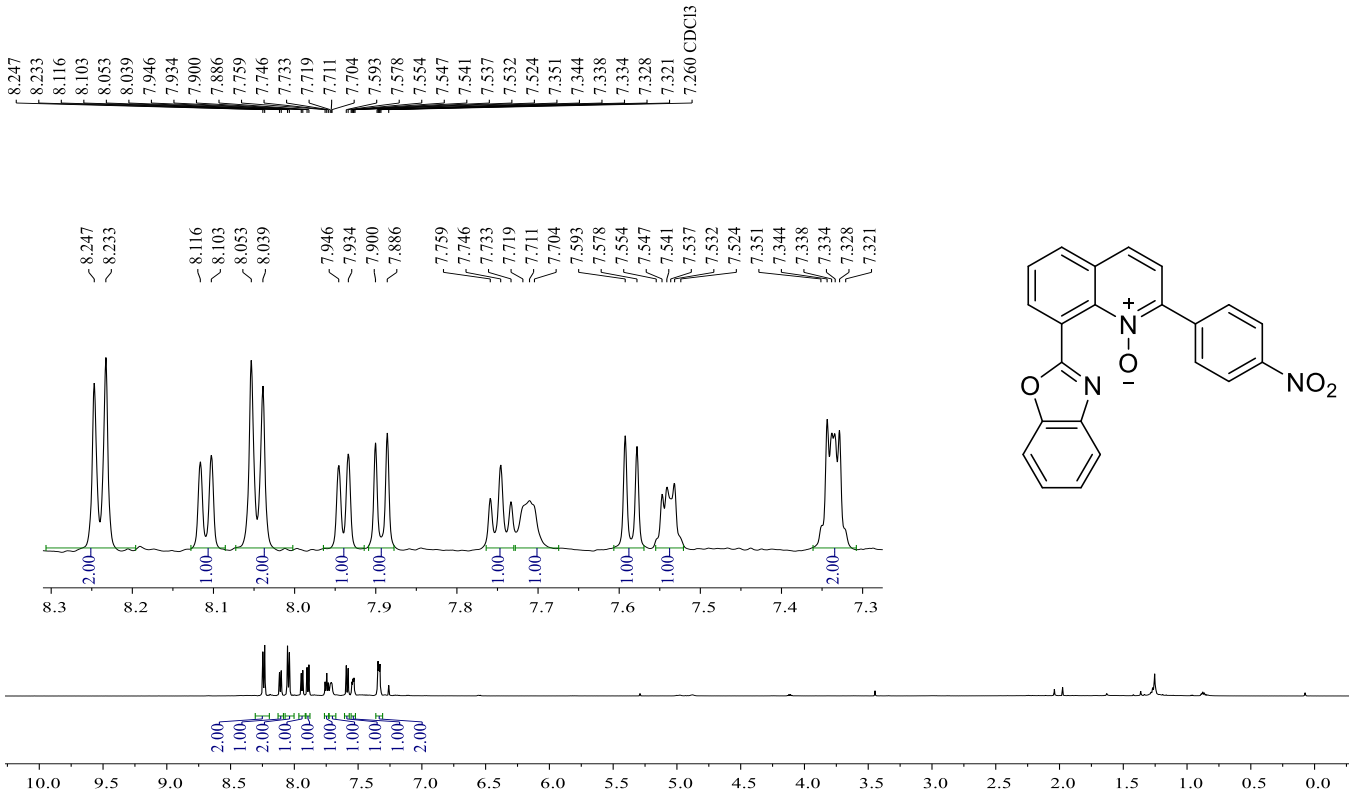


^{13}C{^{1}H} NMR (150 MHz)

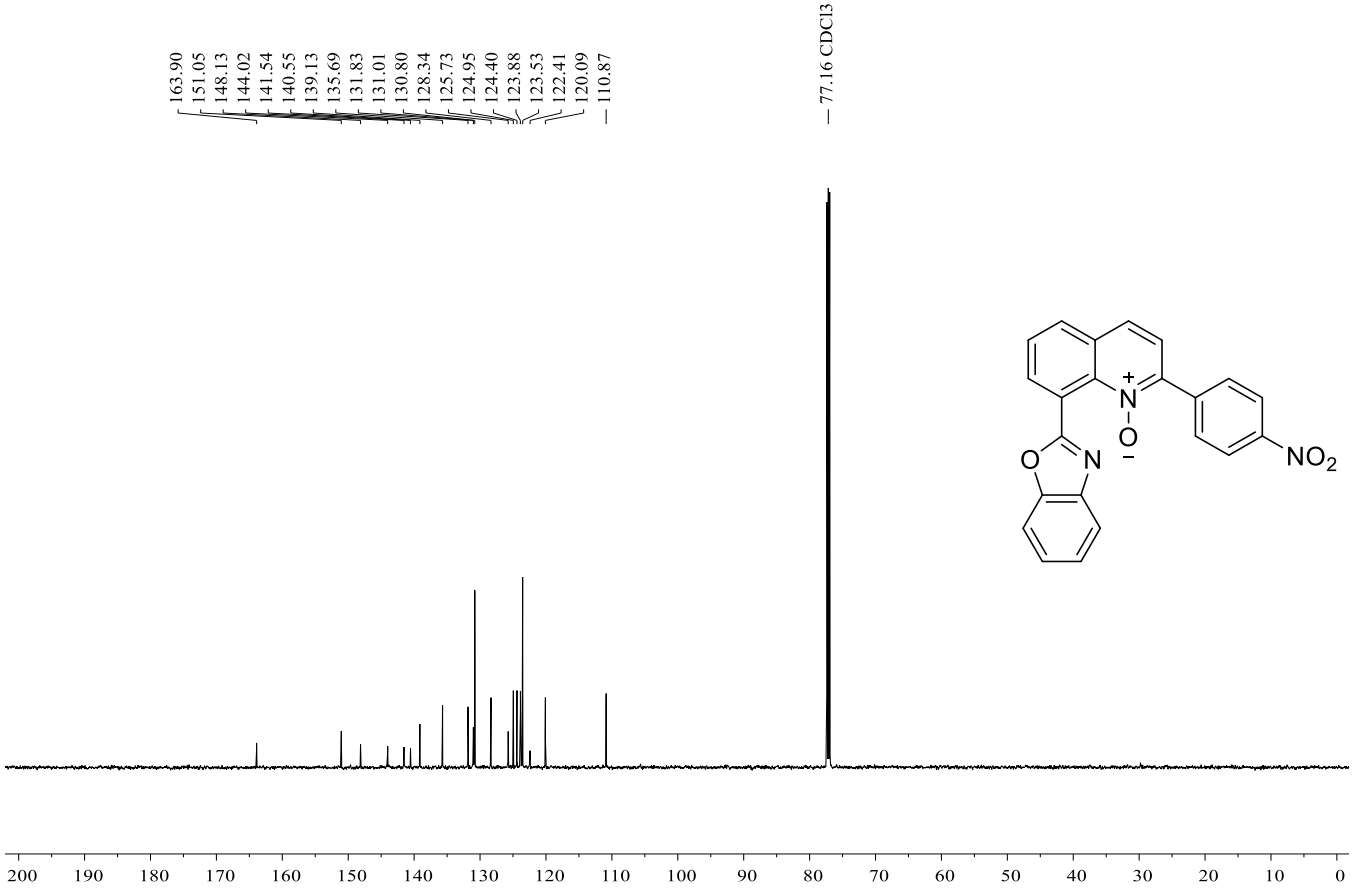


*8-(benzo[d]oxazol-2-yl)-2-(4-nitrophenyl)quinoline 1-oxide (Table 2, Entry **3d**)*

^{1}H NMR (600 MHz)

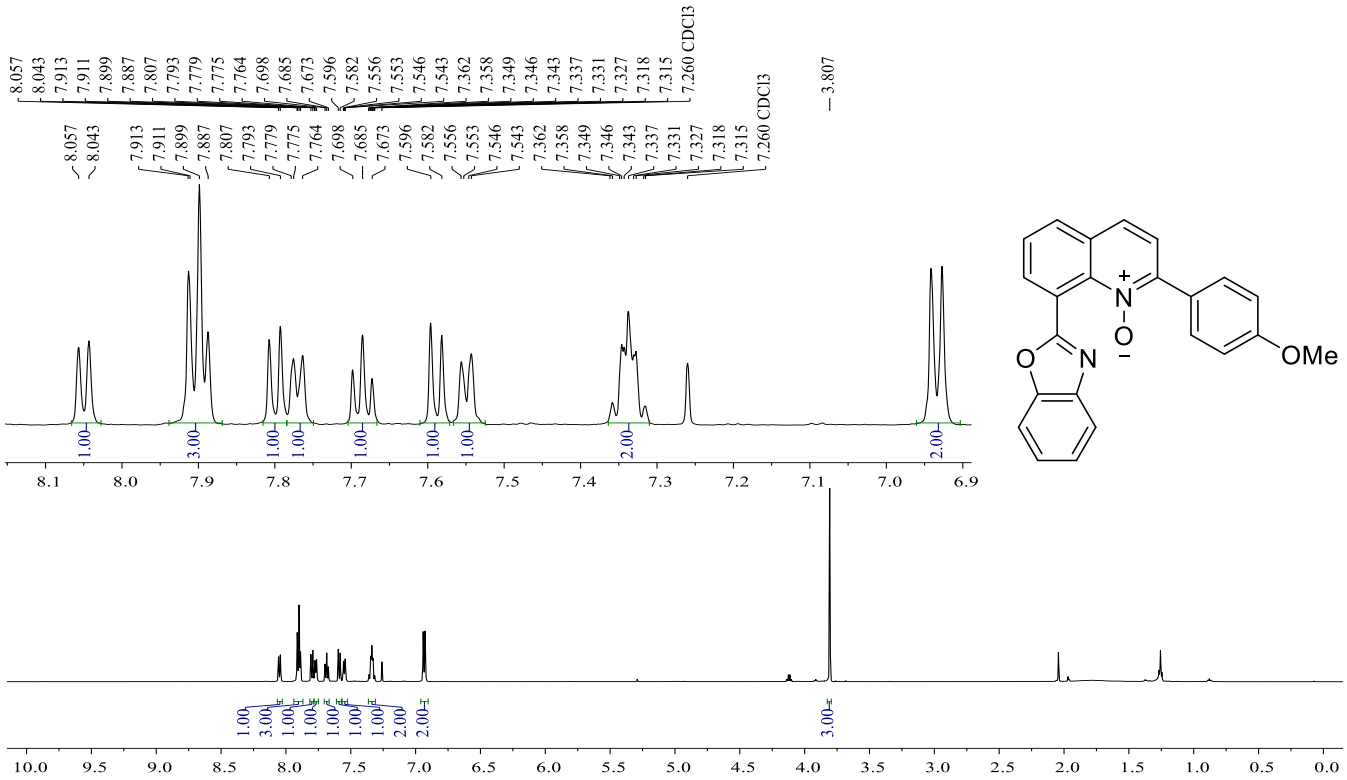


^{13}C{^{1}H} NMR (150 MHz)

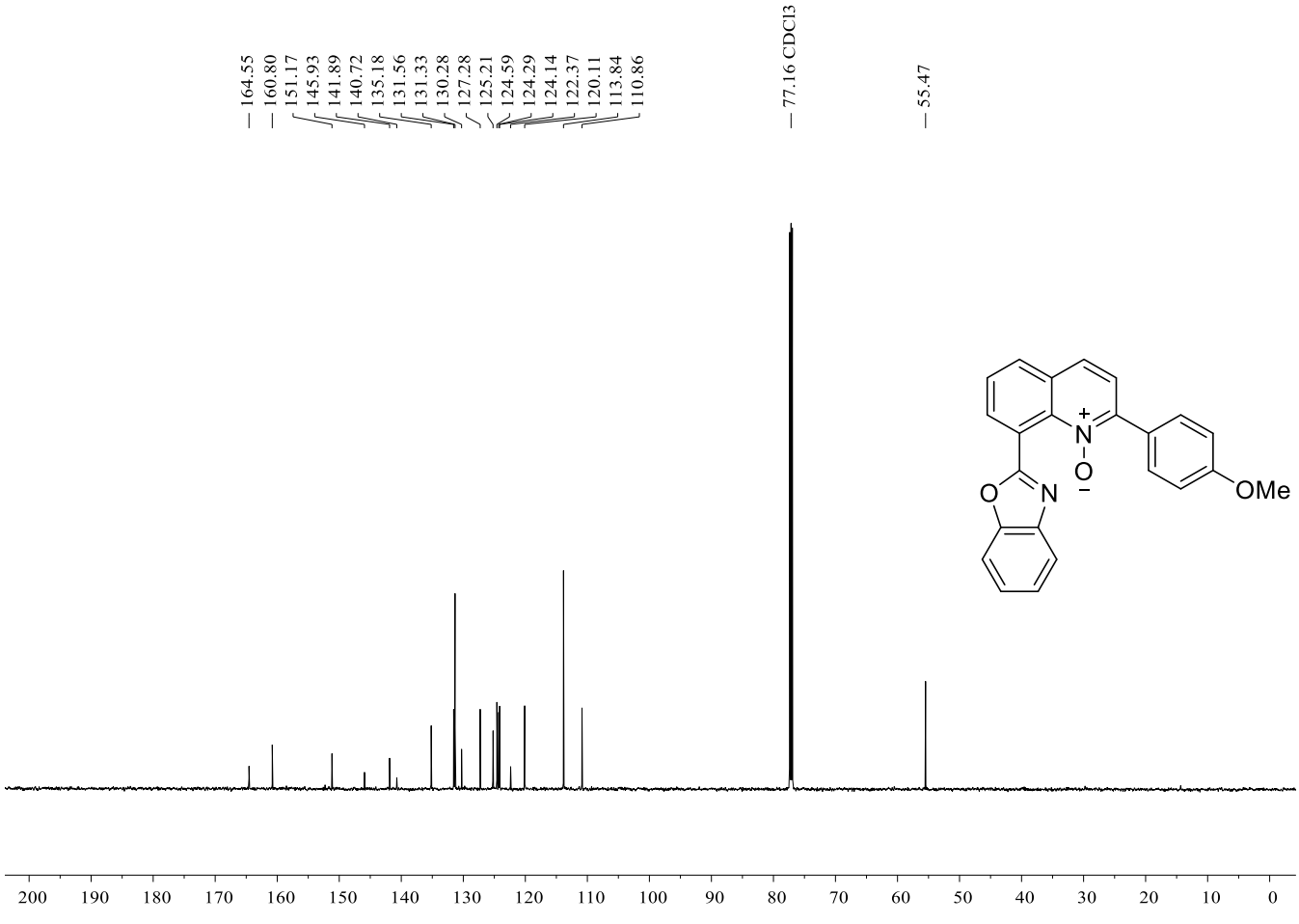


*8-(benzo[d]oxazol-2-yl)-2-(4-methoxyphenyl)quinoline 1-oxide (Table 2, Entry **3e**)*

^{1}H NMR (600 MHz)

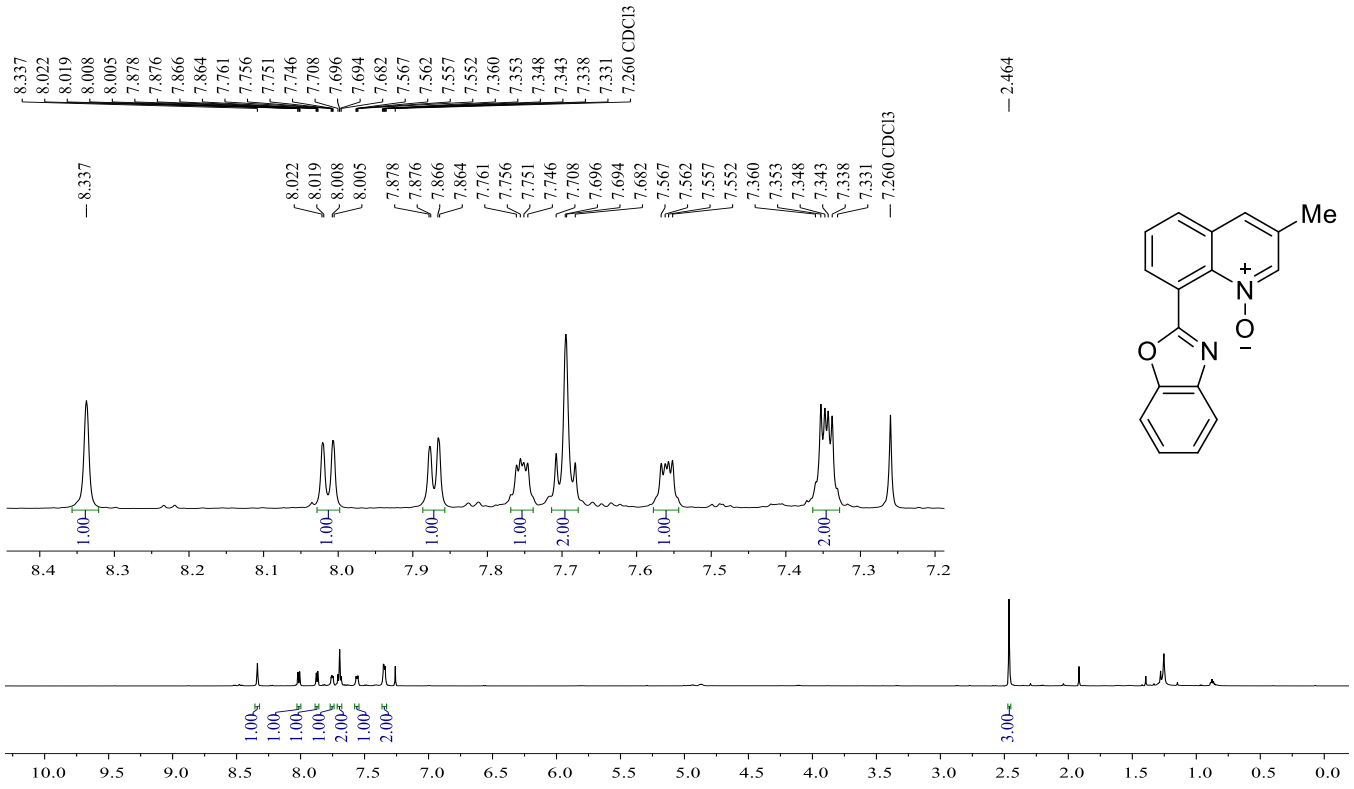


^{13}C{^{1}H} NMR (150 MHz)

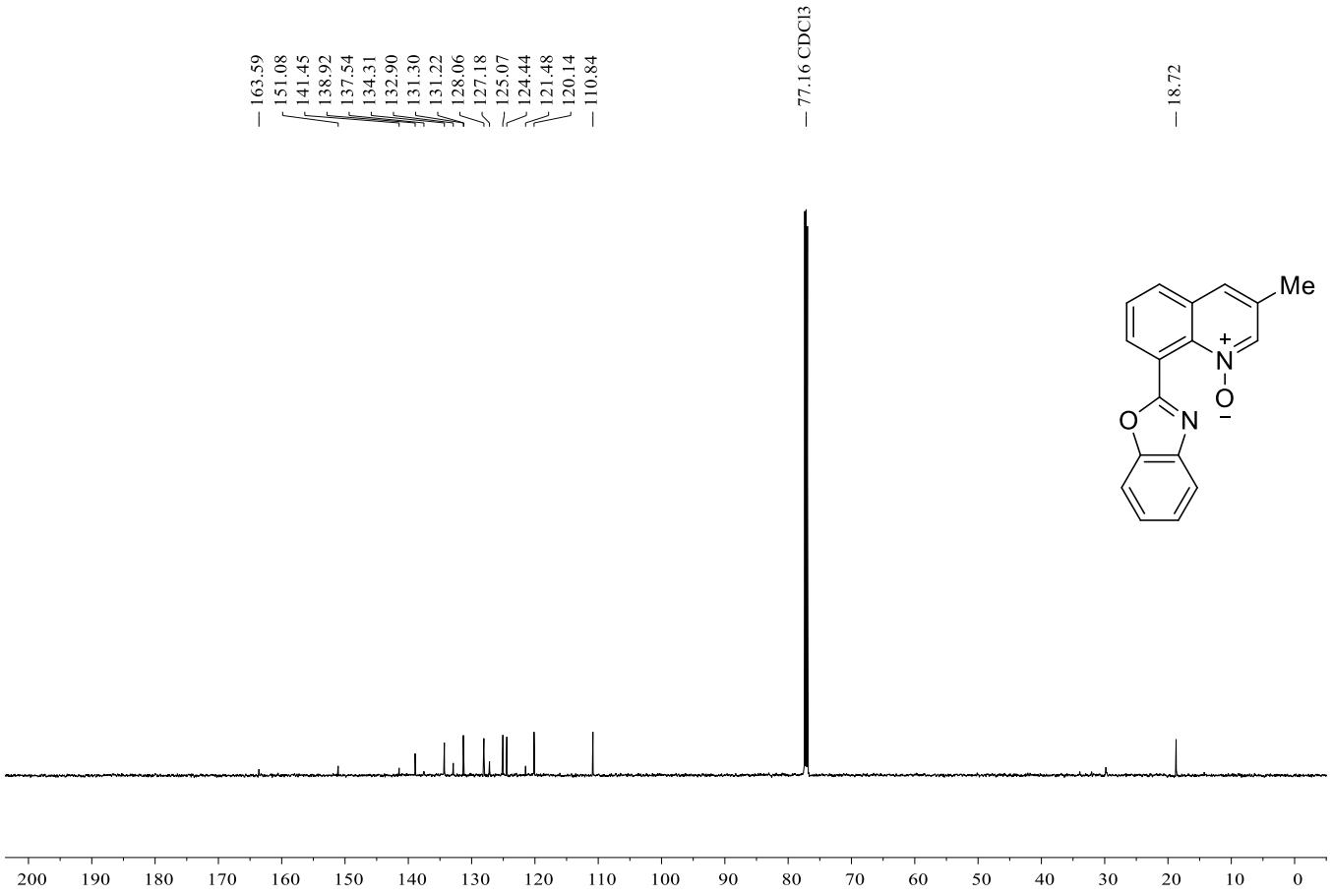


*8-(benzo[d]oxazol-2-yl)-3-methylquinoline 1-oxide (Table 2, Entry **3f**)*

^{1}H NMR (600 MHz)

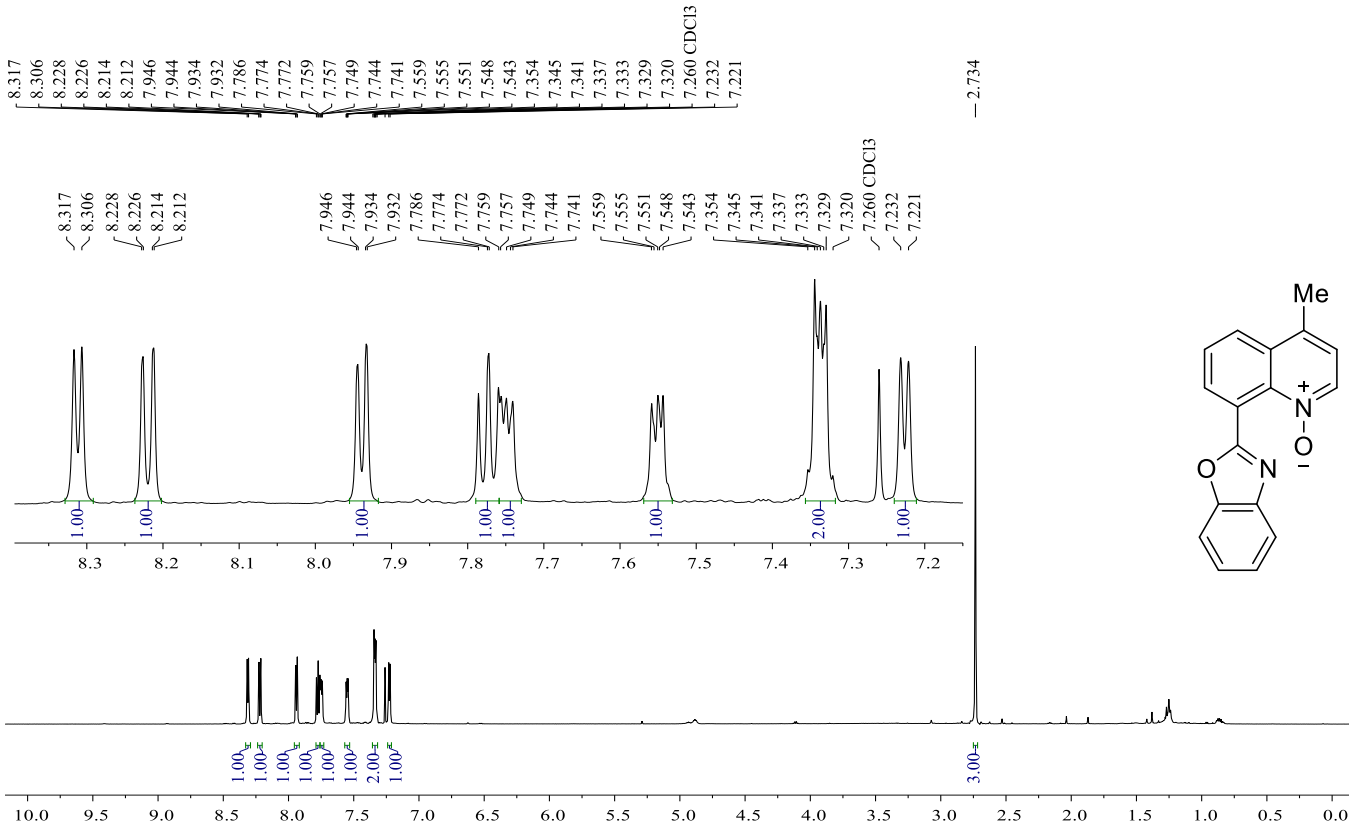


^{13}C{^{1}H} NMR (150 MHz)

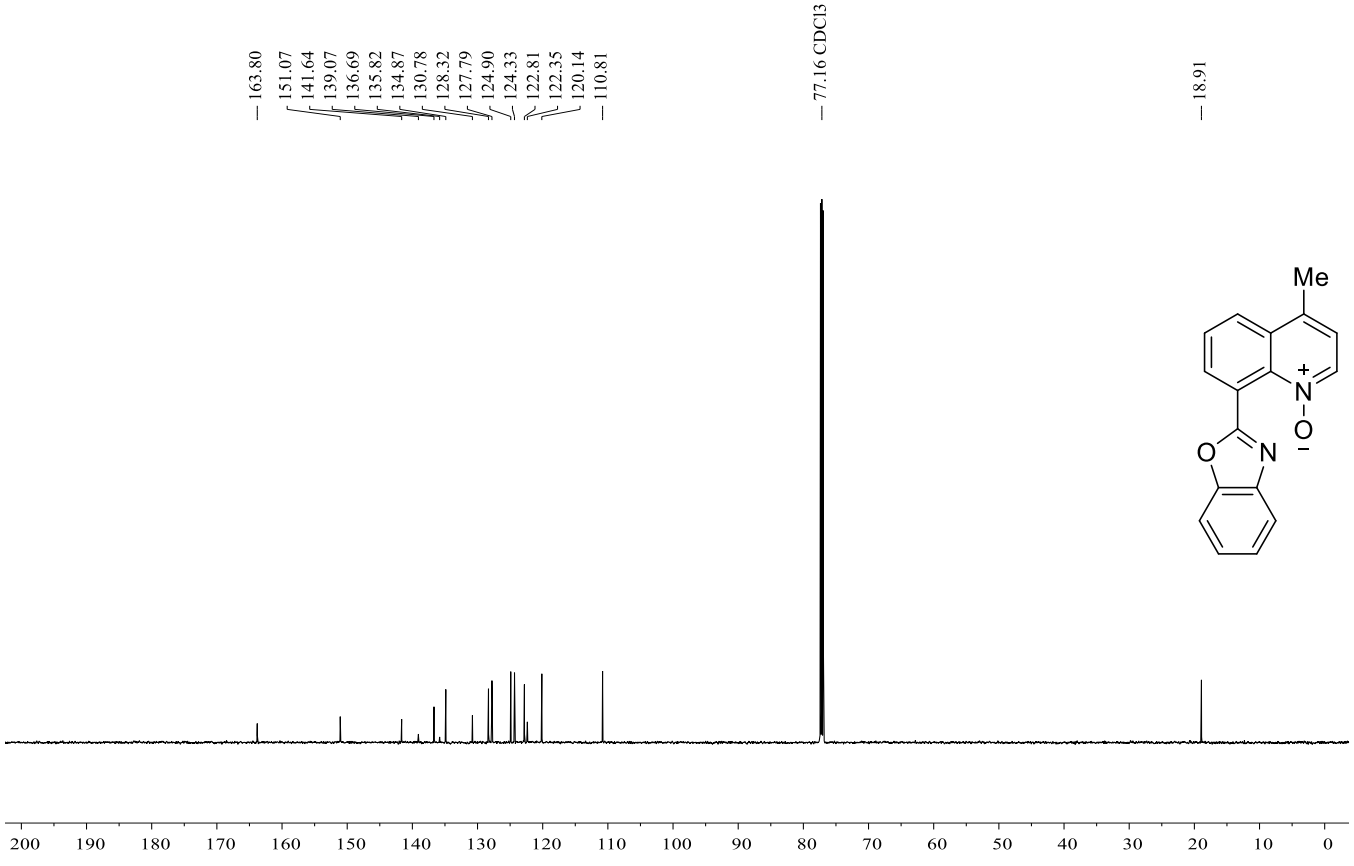


*8-(benzo[d]oxazol-2-yl)-4-methylquinoline 1-oxide (Table 2, Entry **3g**)*

^{1}H NMR (600 MHz)

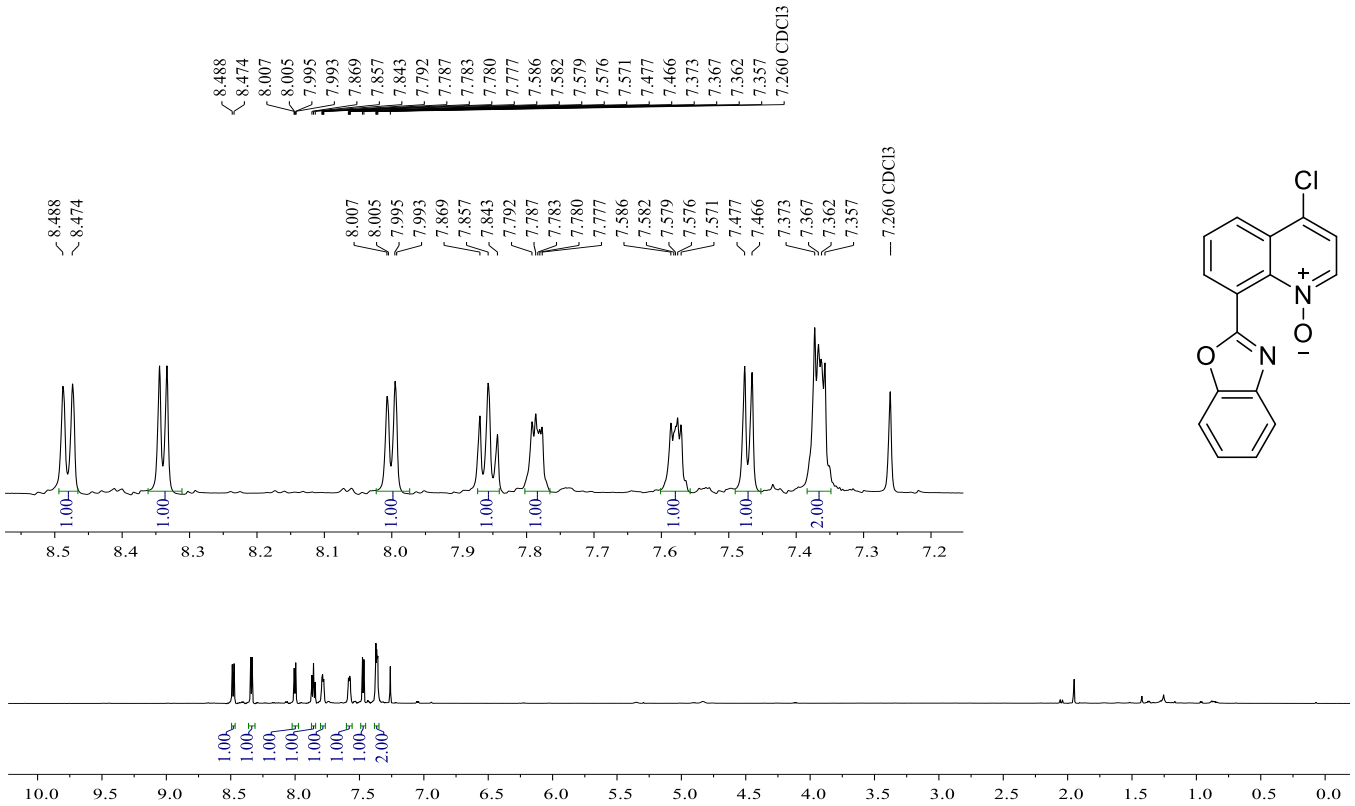


^{13}C{^{1}H} NMR (150 MHz)

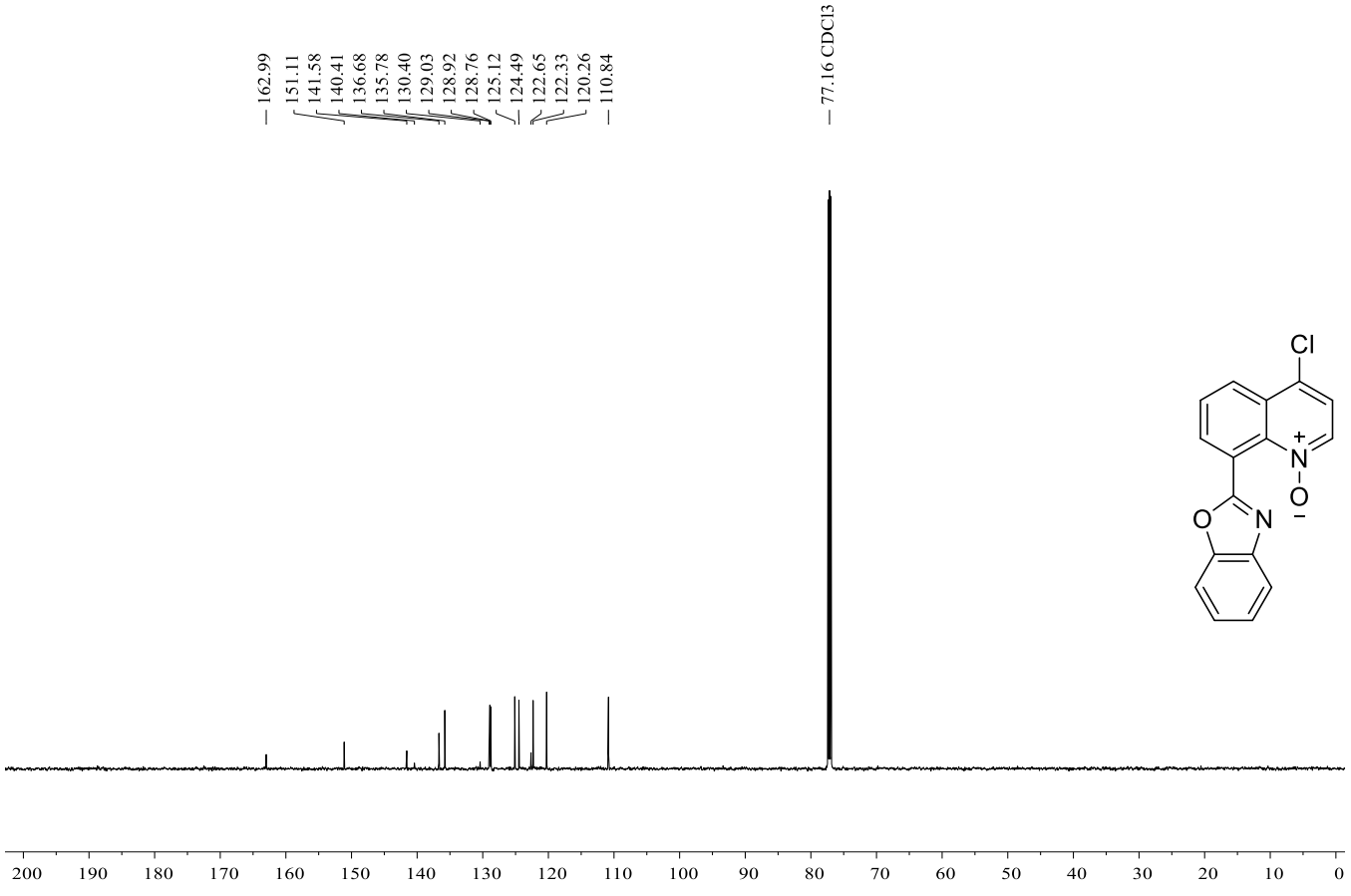


*8-(benzo[d]oxazol-2-yl)-4-chloroquinoline 1-oxide (Table 2, Entry **3h**)*

^{1}H NMR (600 MHz)

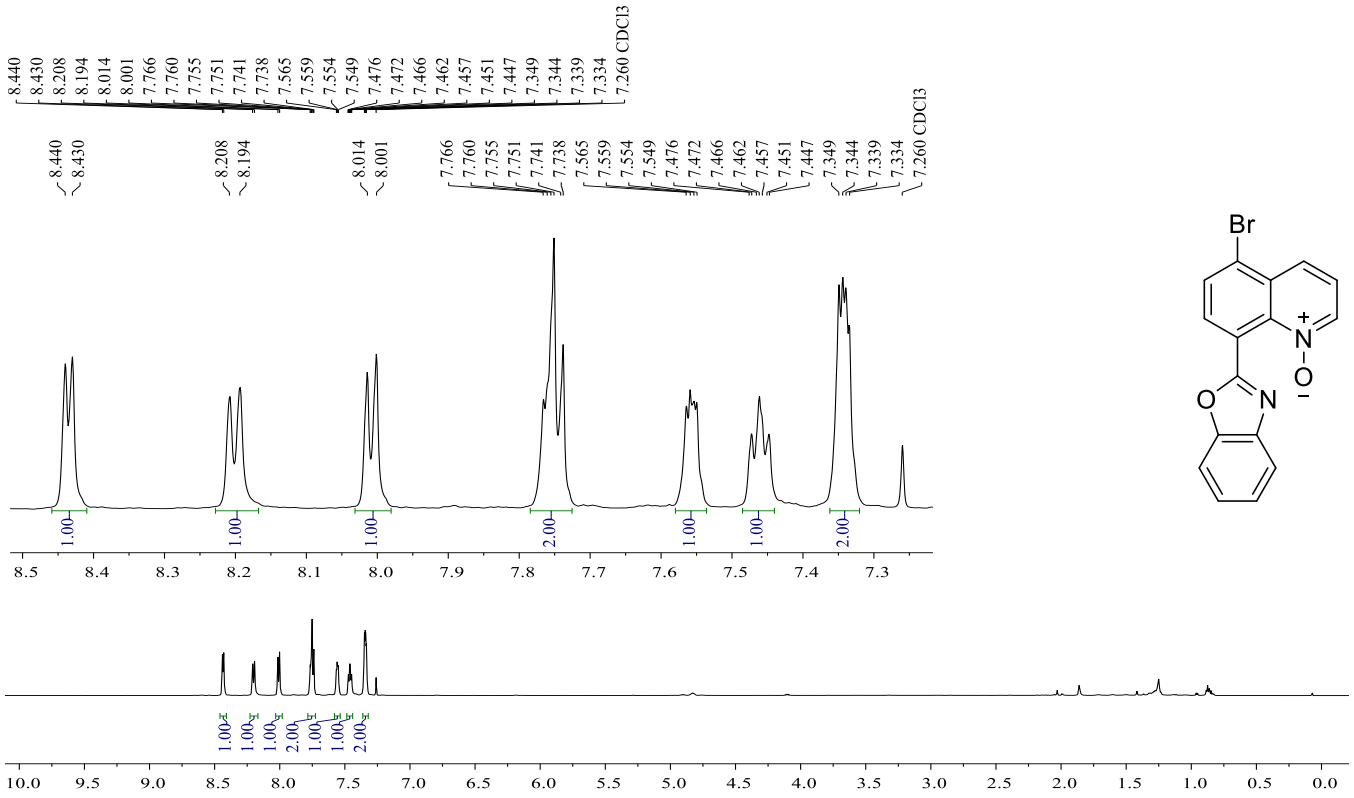


^{13}C{^{1}H} NMR (150 MHz)

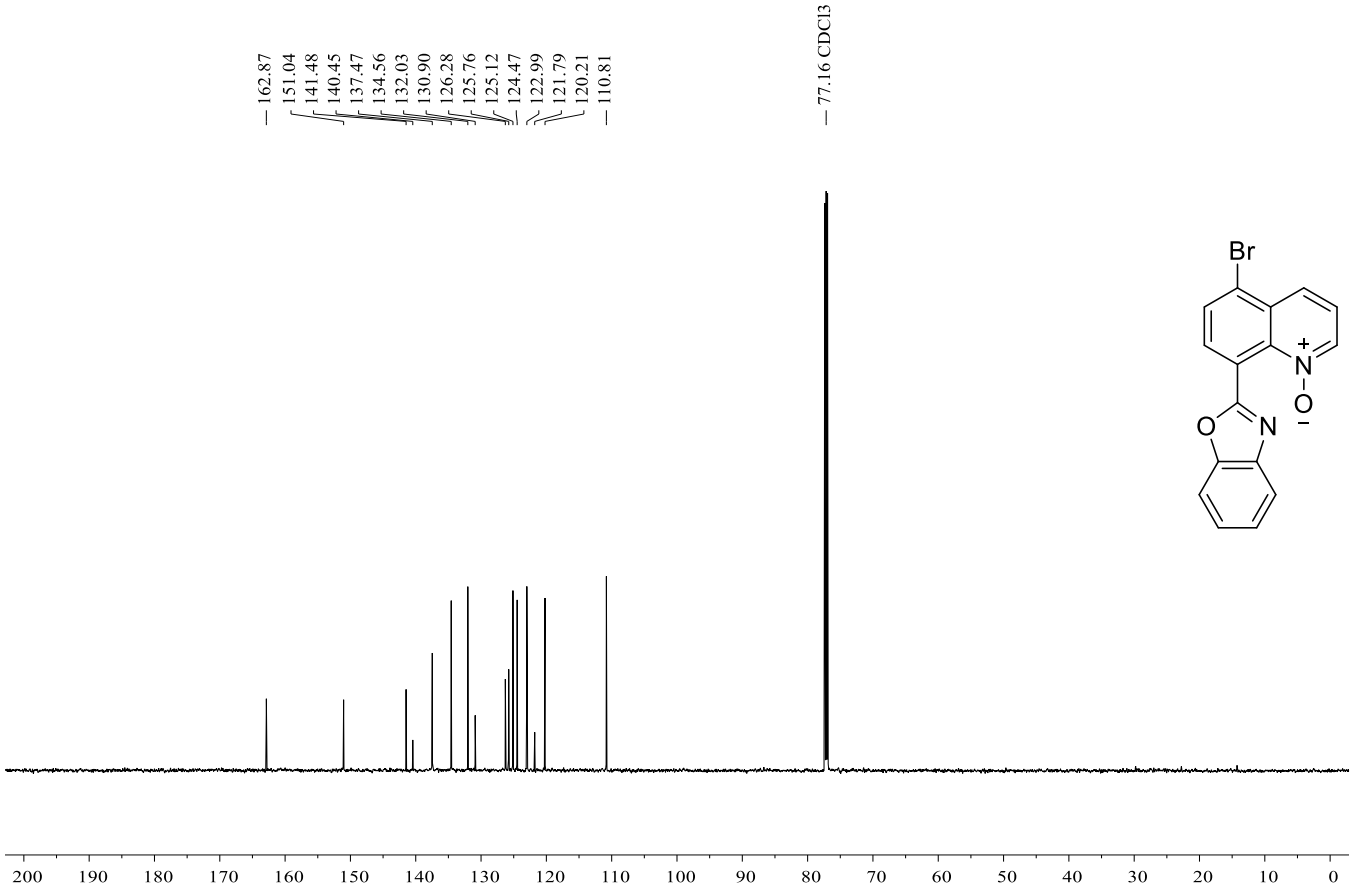


*8-(benzo[d]oxazol-2-yl)-5-bromoquinoline 1-oxide (Table 2, Entry **3i**)*

^{1}H NMR (600 MHz)

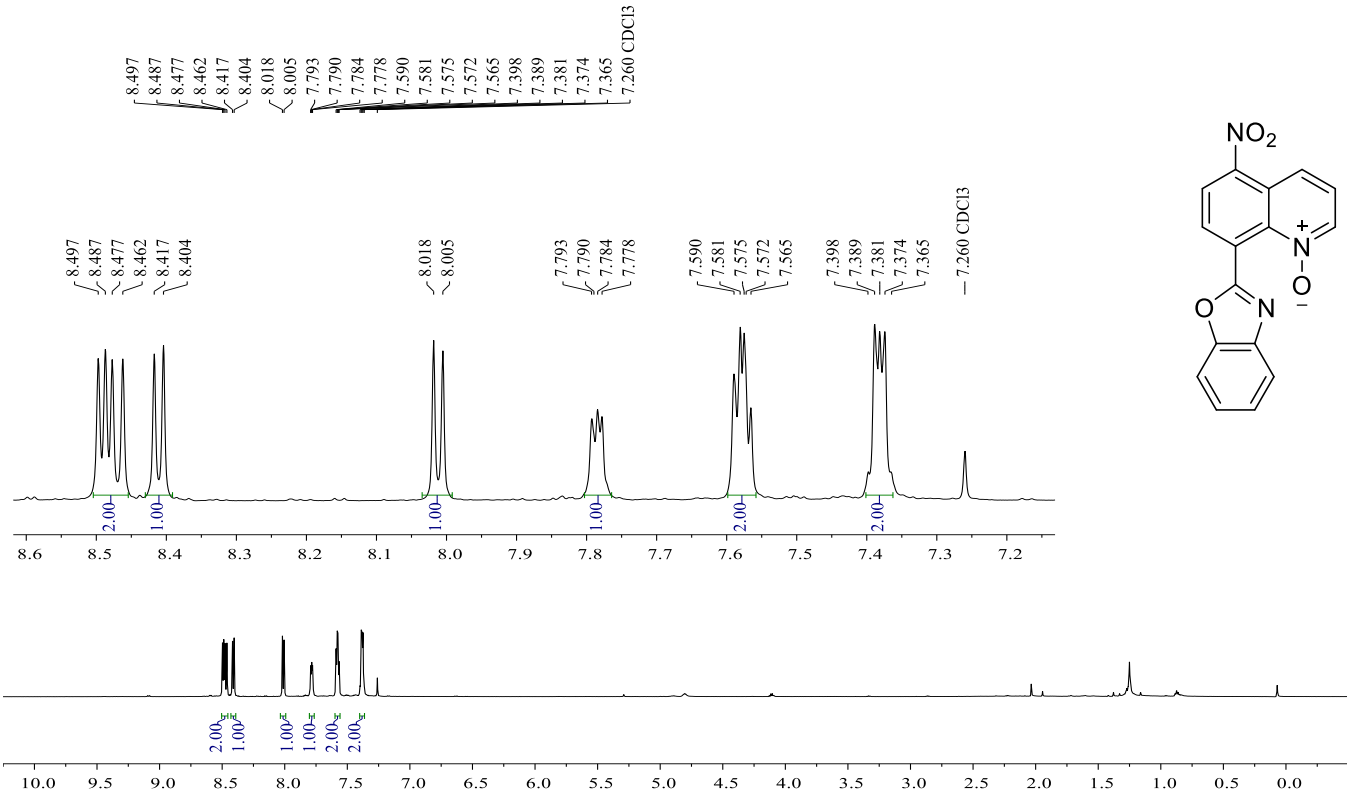


^{13}C{^{1}H} NMR (150 MHz)

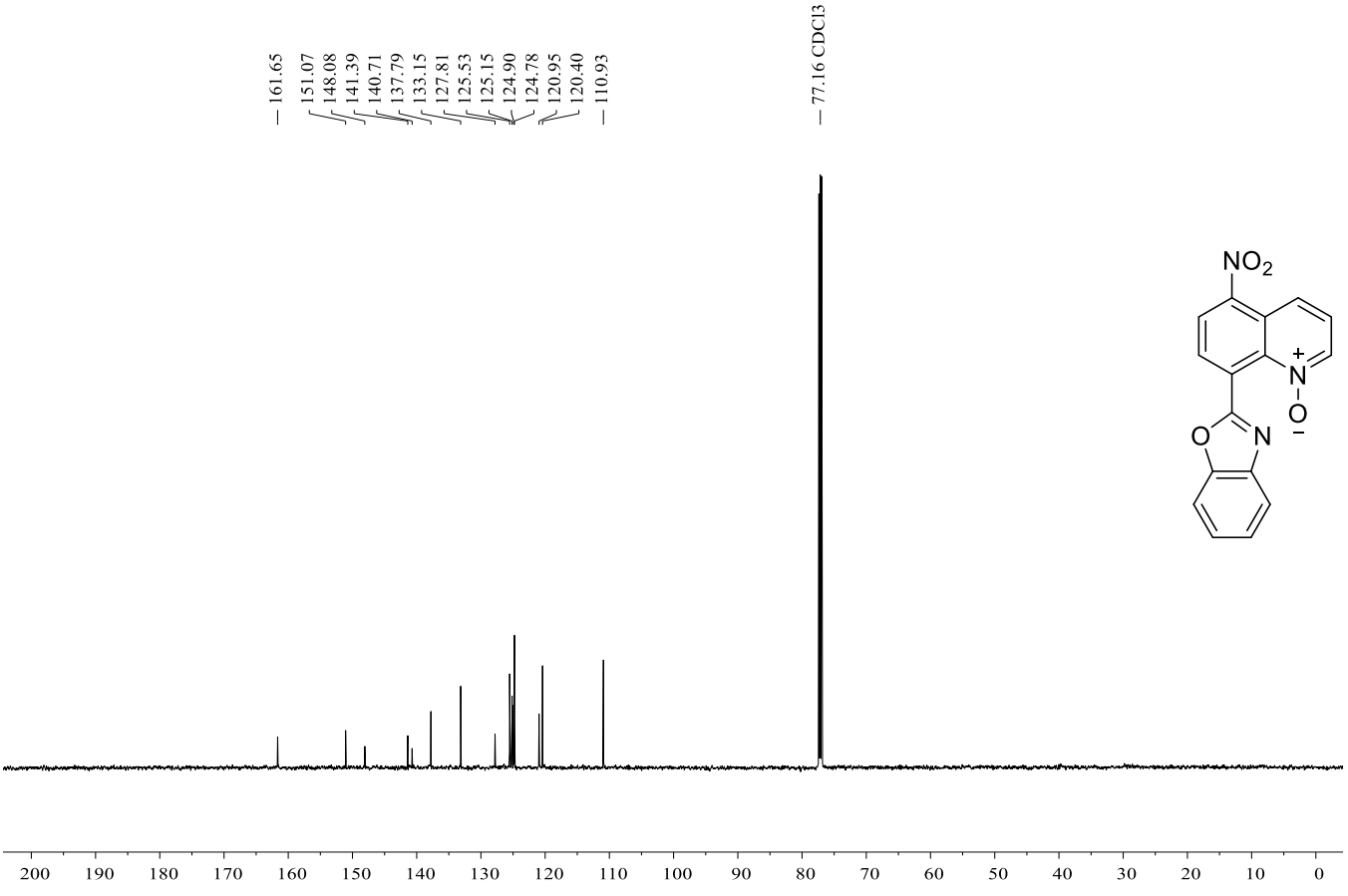


*8-(benzo[d]oxazol-2-yl)-5-nitroquinoline 1-oxide (Table 2, Entry **3j**)*

^{1}H NMR (600 MHz)

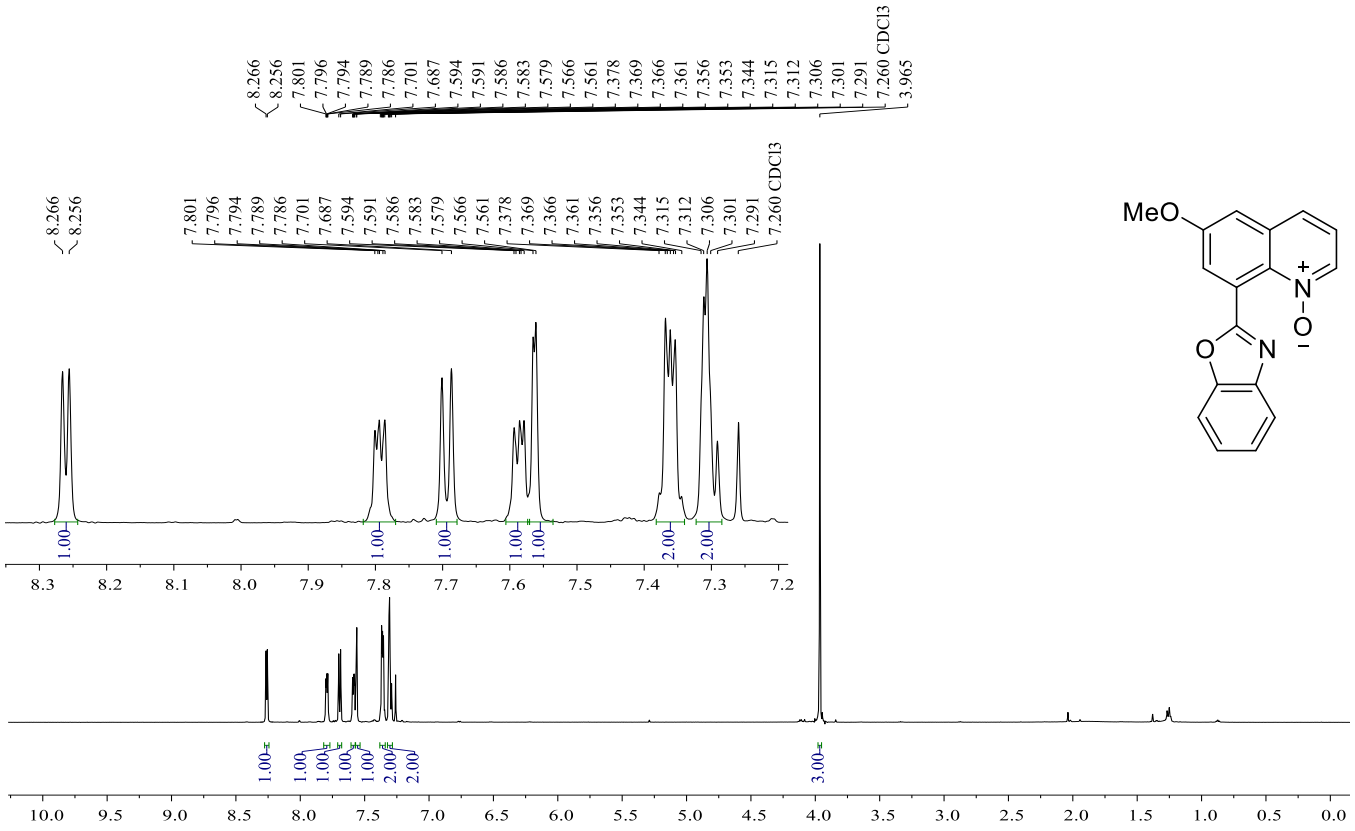


^{13}C{^{1}H} NMR (150 MHz)

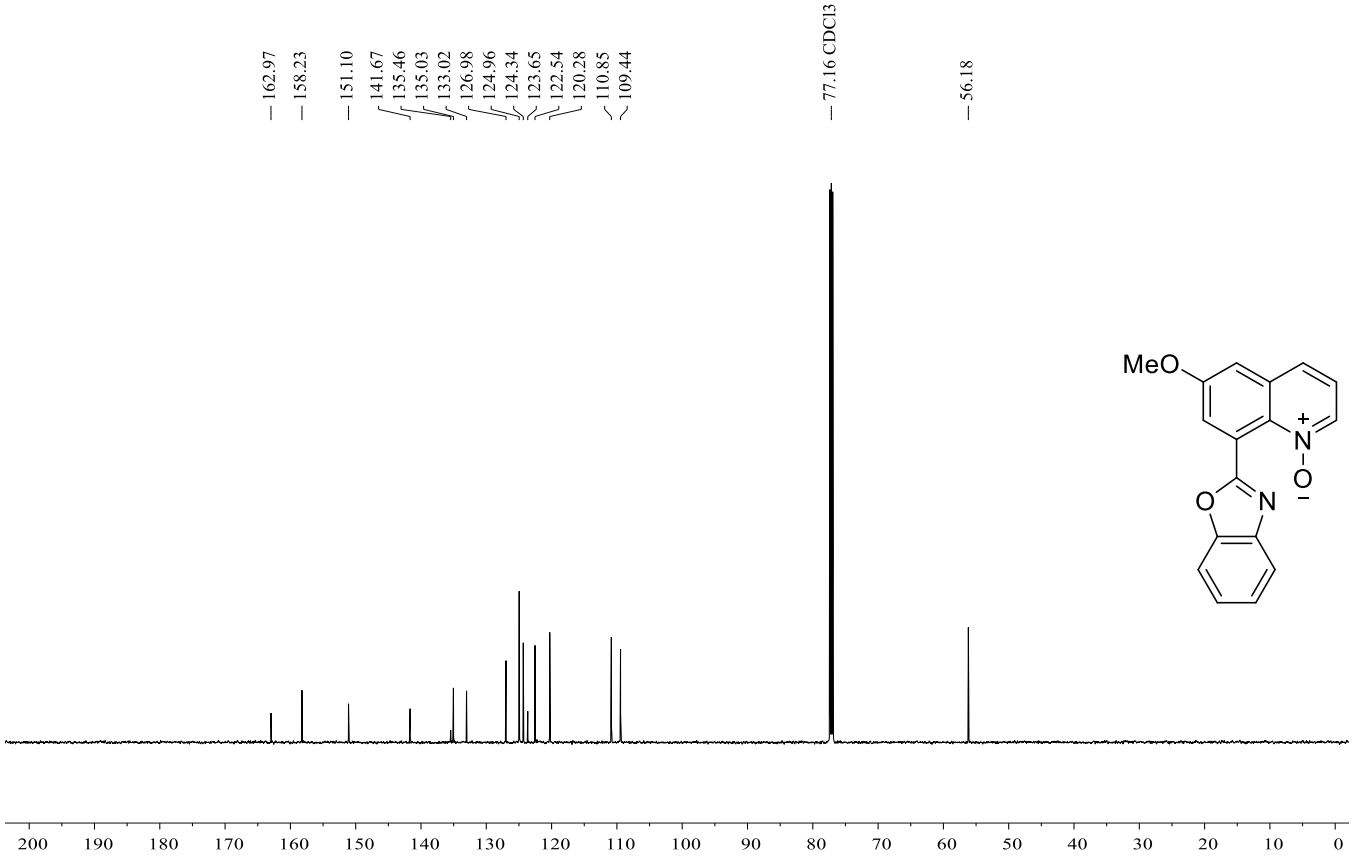


*8-(benzo[d]oxazol-2-yl)-6-methoxyquinoline 1-oxide (Table 2, Entry **3k**)*

^{1}H NMR (600 MHz)

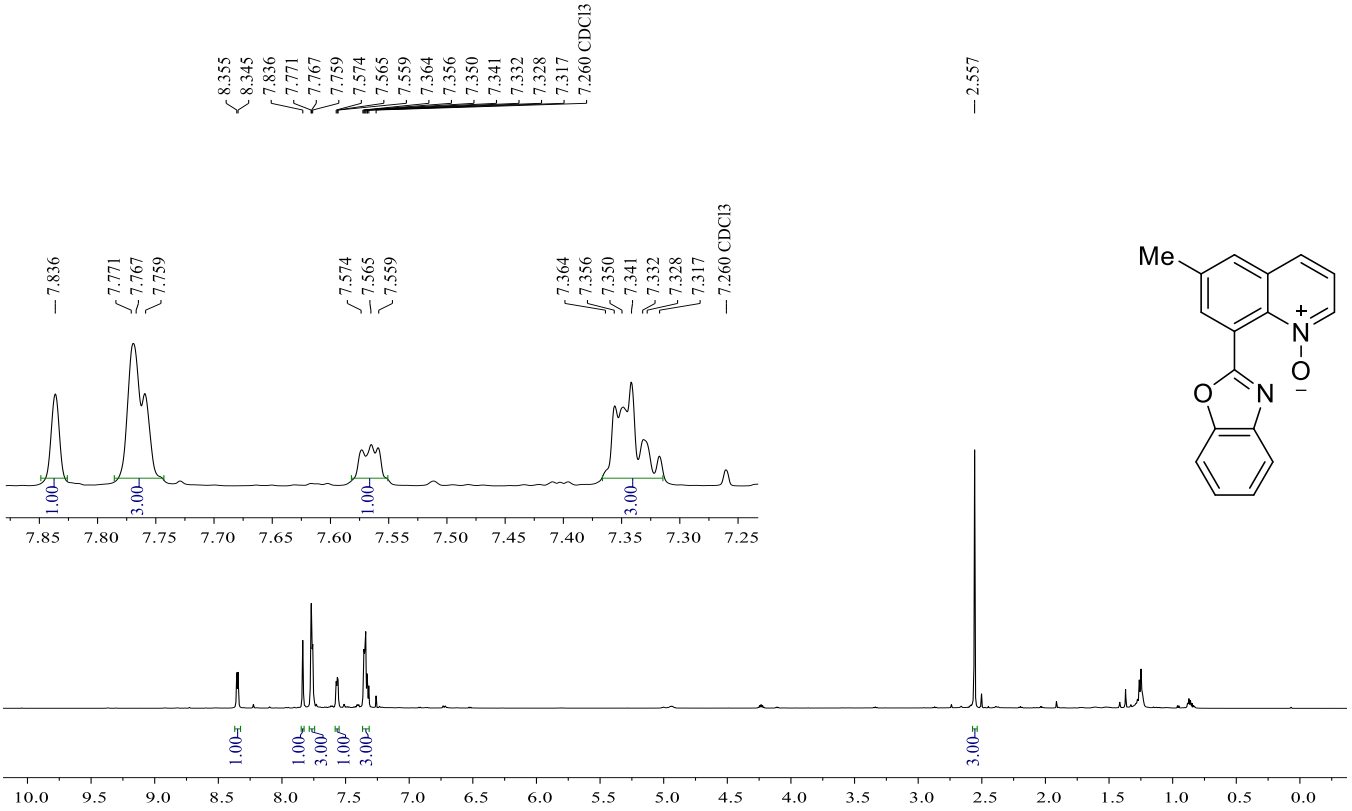


^{13}C{^{1}H} NMR (150 MHz)

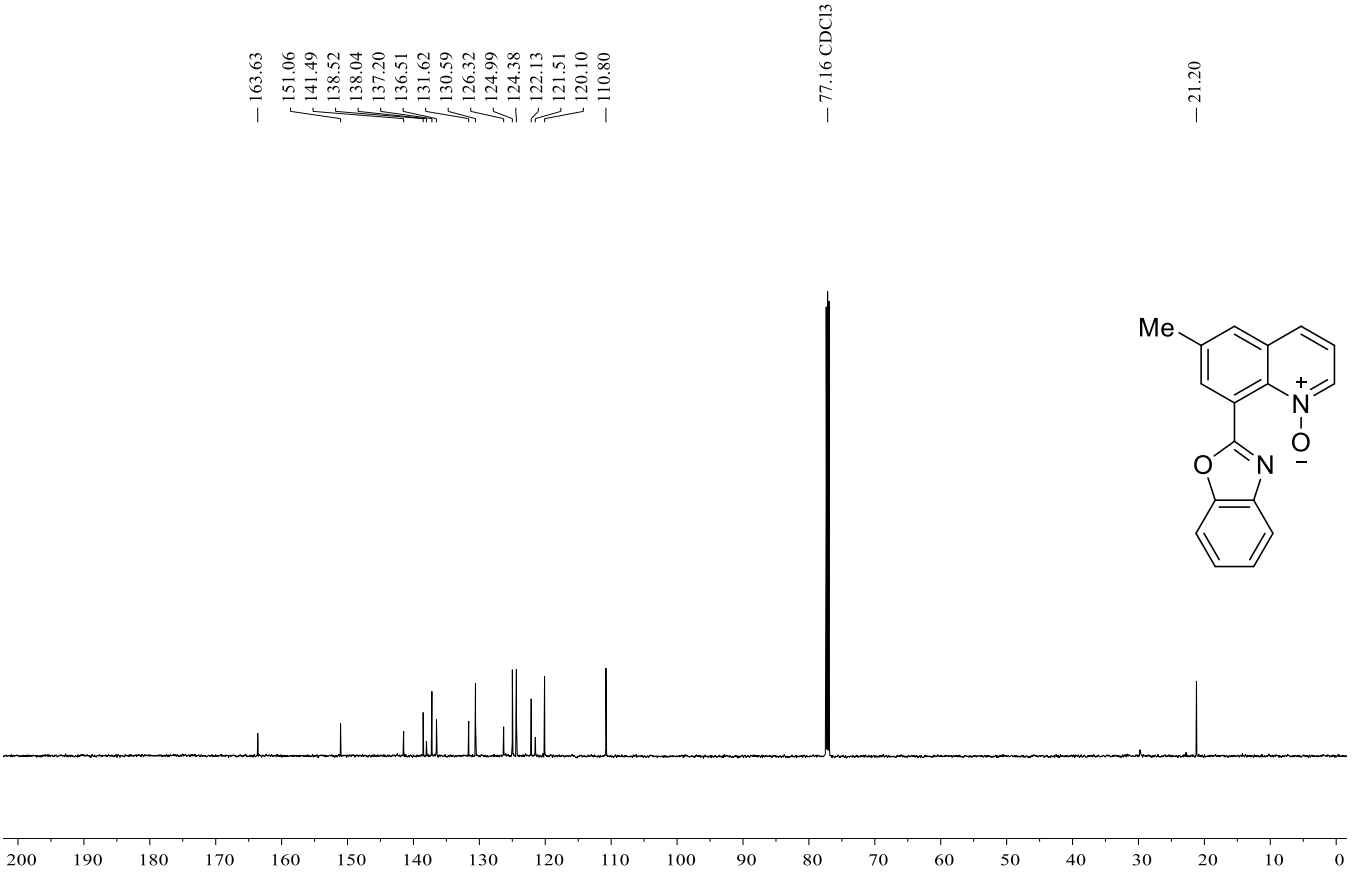


*8-(benzo[d]oxazol-2-yl)-6-methylquinoline 1-oxide (Table 2, Entry **3l**)*

^{1}H NMR (600 MHz)

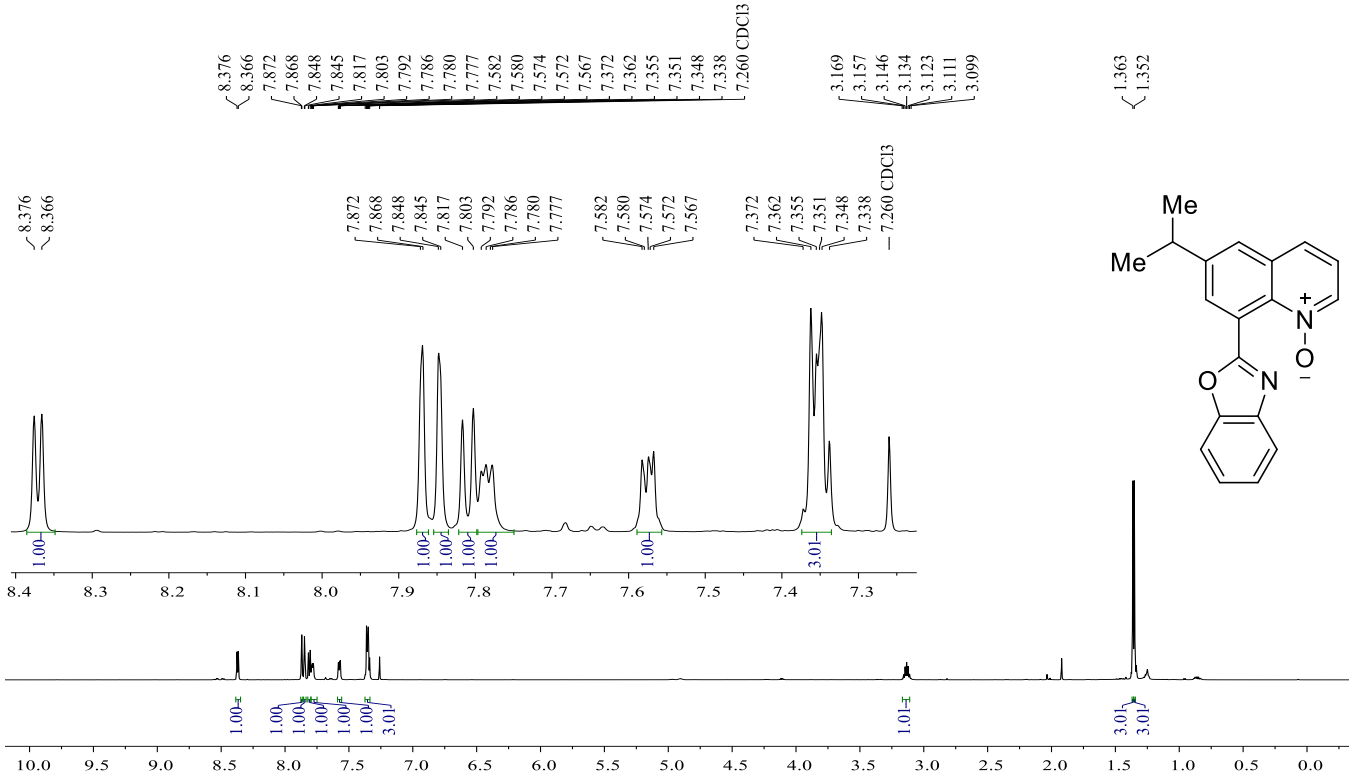


^{13}C{^{1}H} NMR (150 MHz)

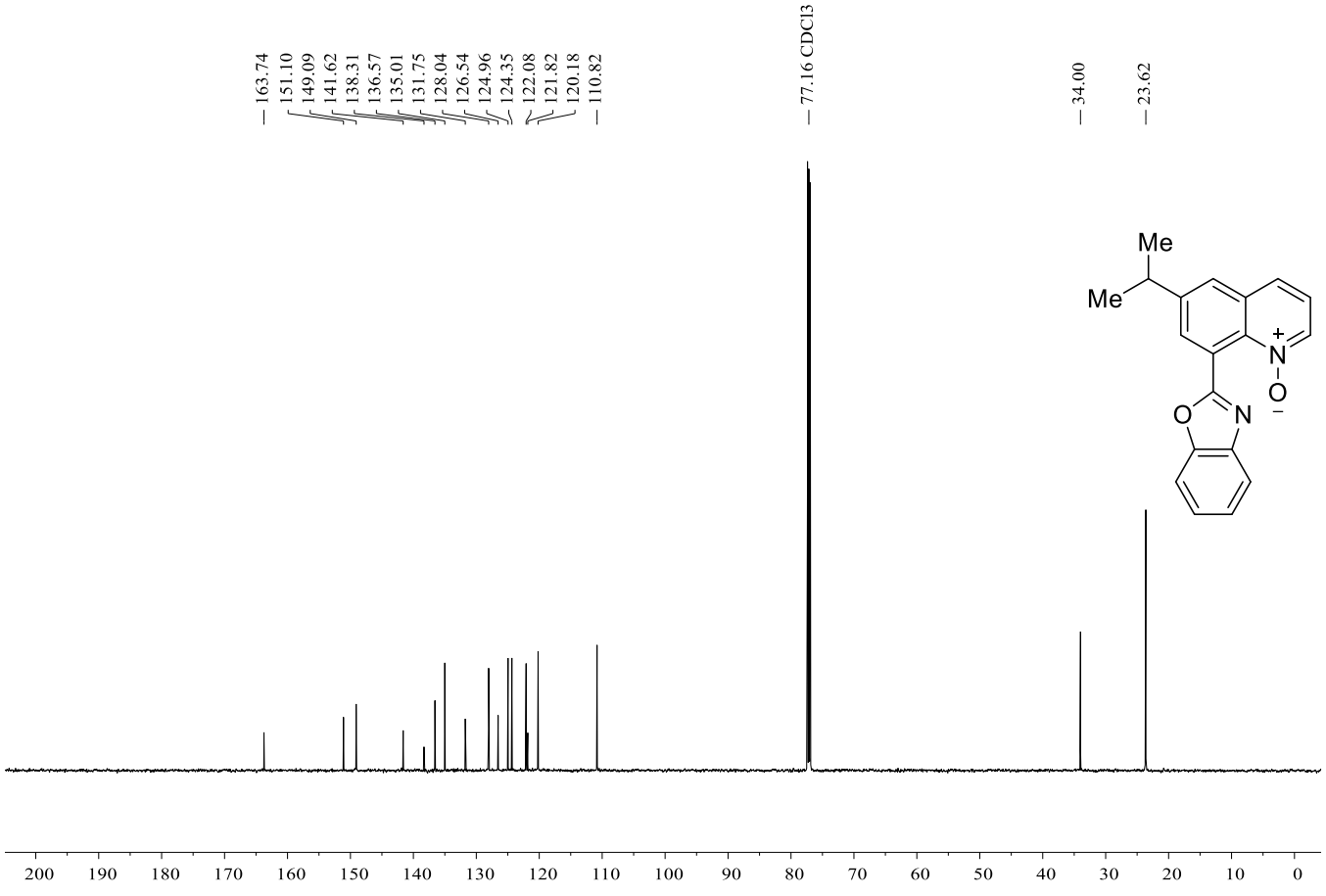


*8-(benzo[d]oxazol-2-yl)-6-isopropylquinoline 1-oxide (Table 2, Entry **3m**)*

^{1}H NMR (600 MHz)

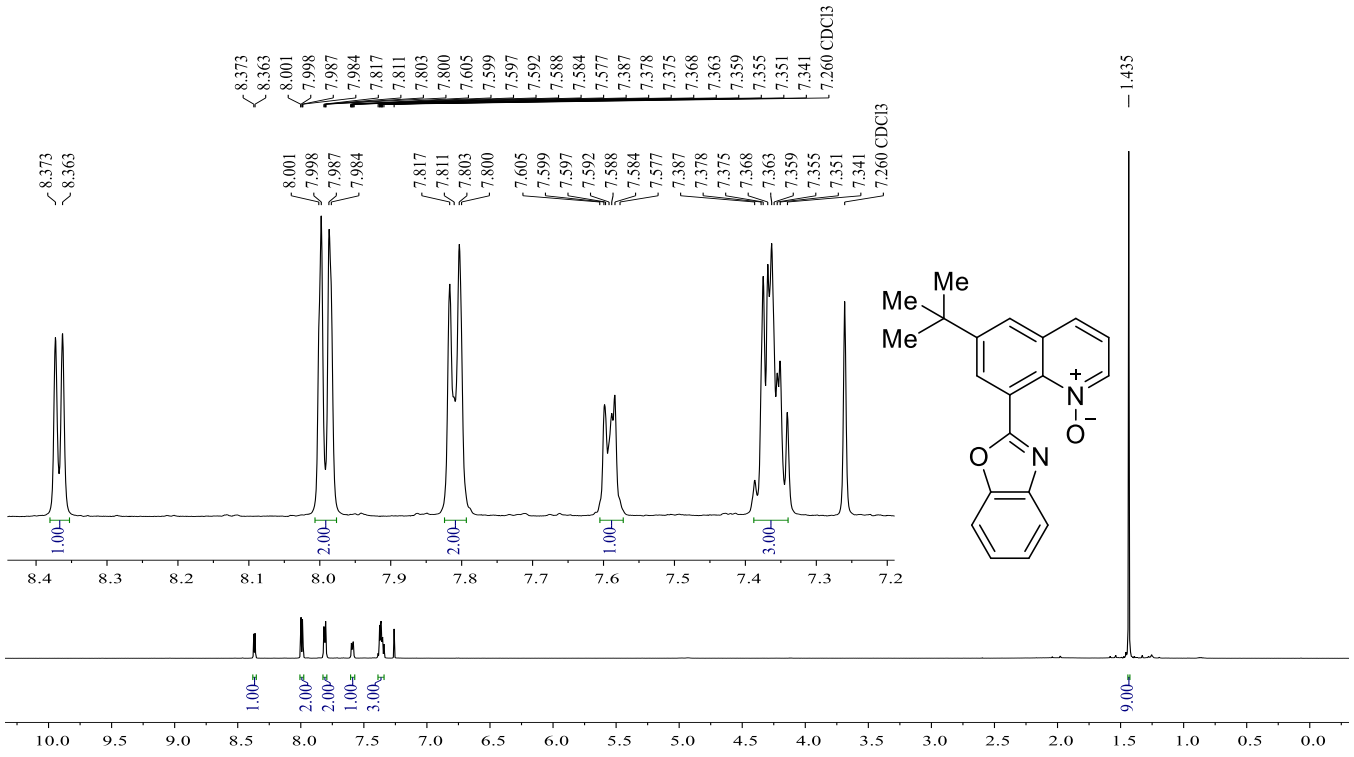


^{13}C{^{1}H} NMR (150 MHz)

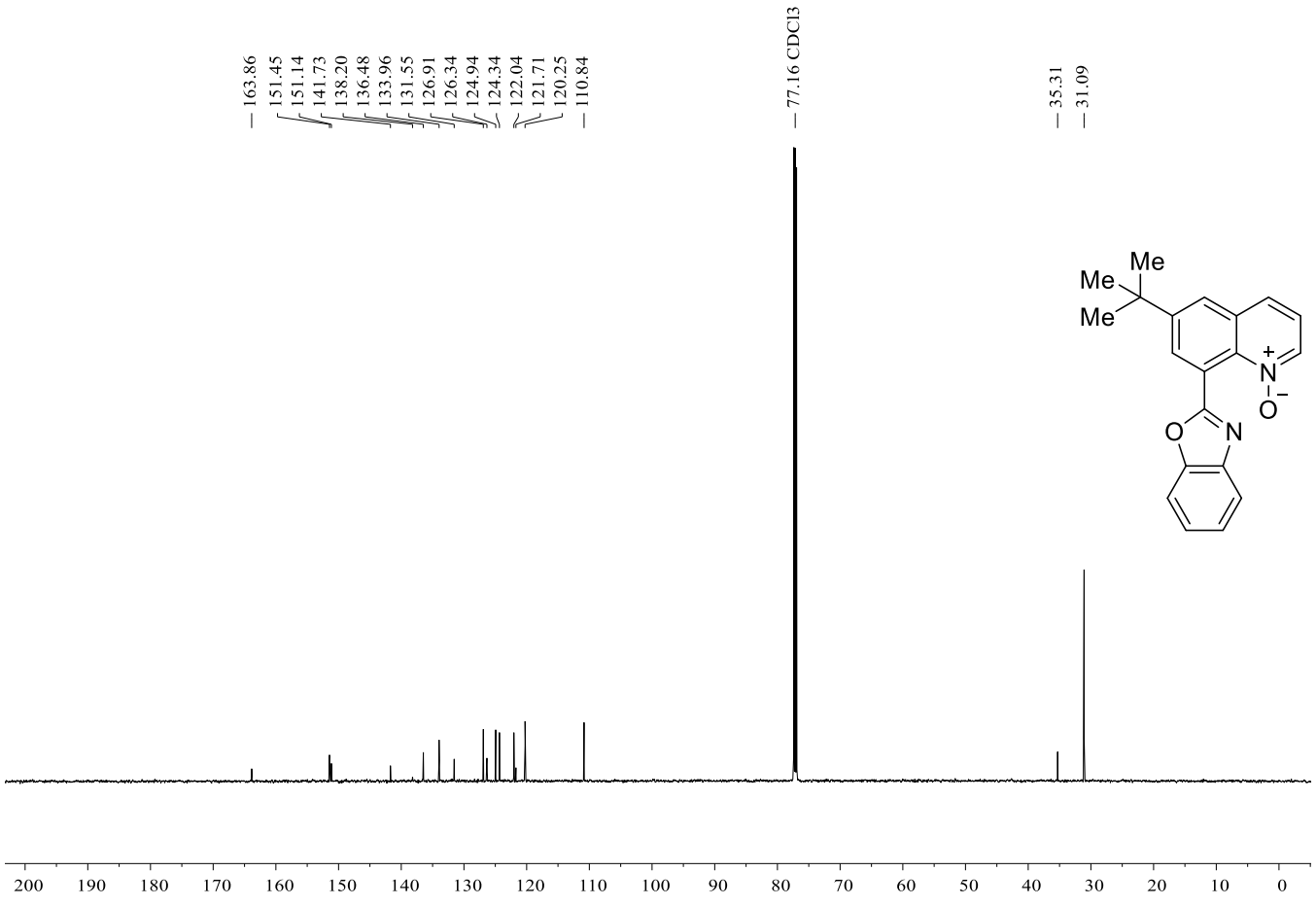


*8-(benzo[d]oxazol-2-yl)-6-(tert-butyl)quinoline 1-oxide (Table 2, Entry **3n**)*

^{1}H NMR (600 MHz)

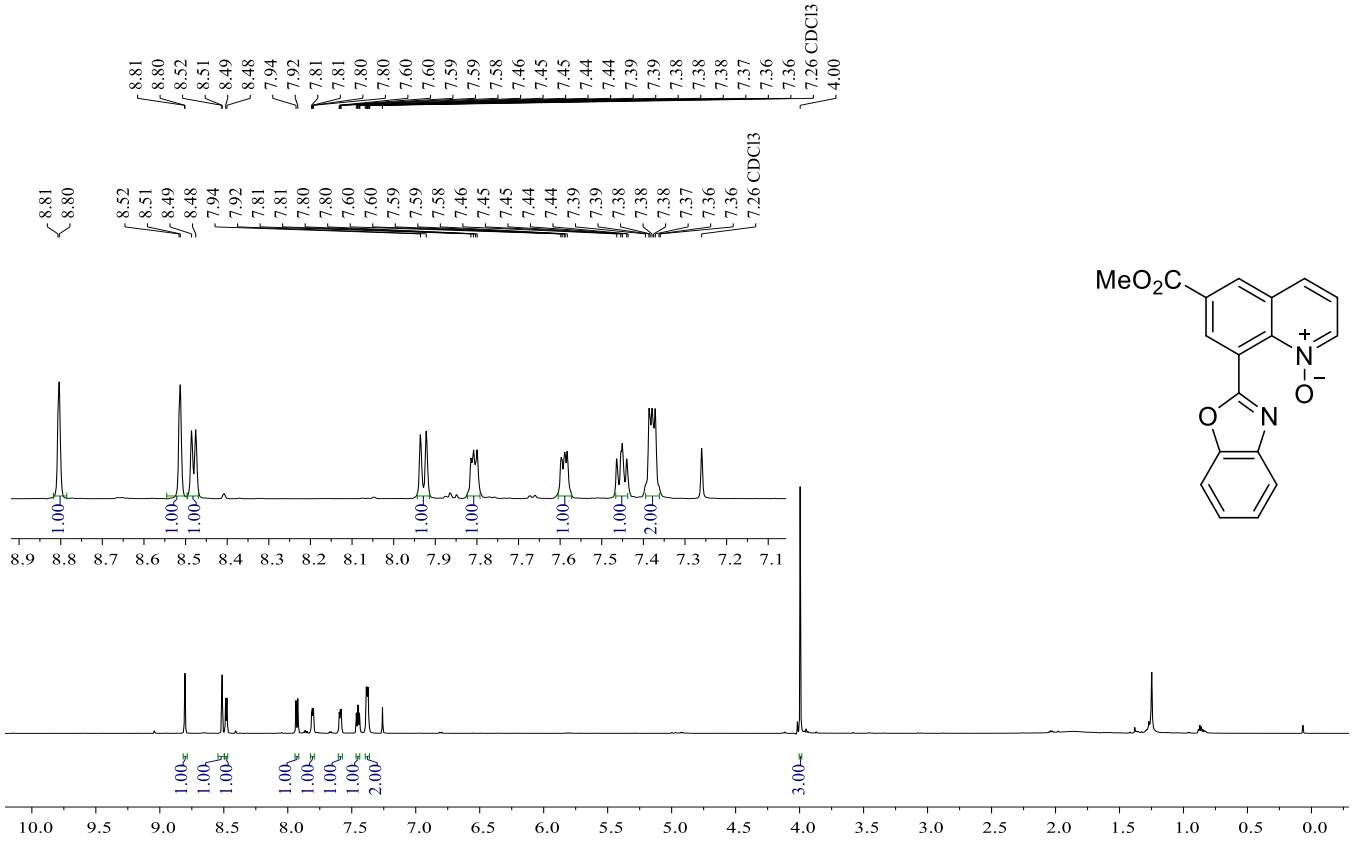


^{13}C{^{1}H} NMR (150 MHz)

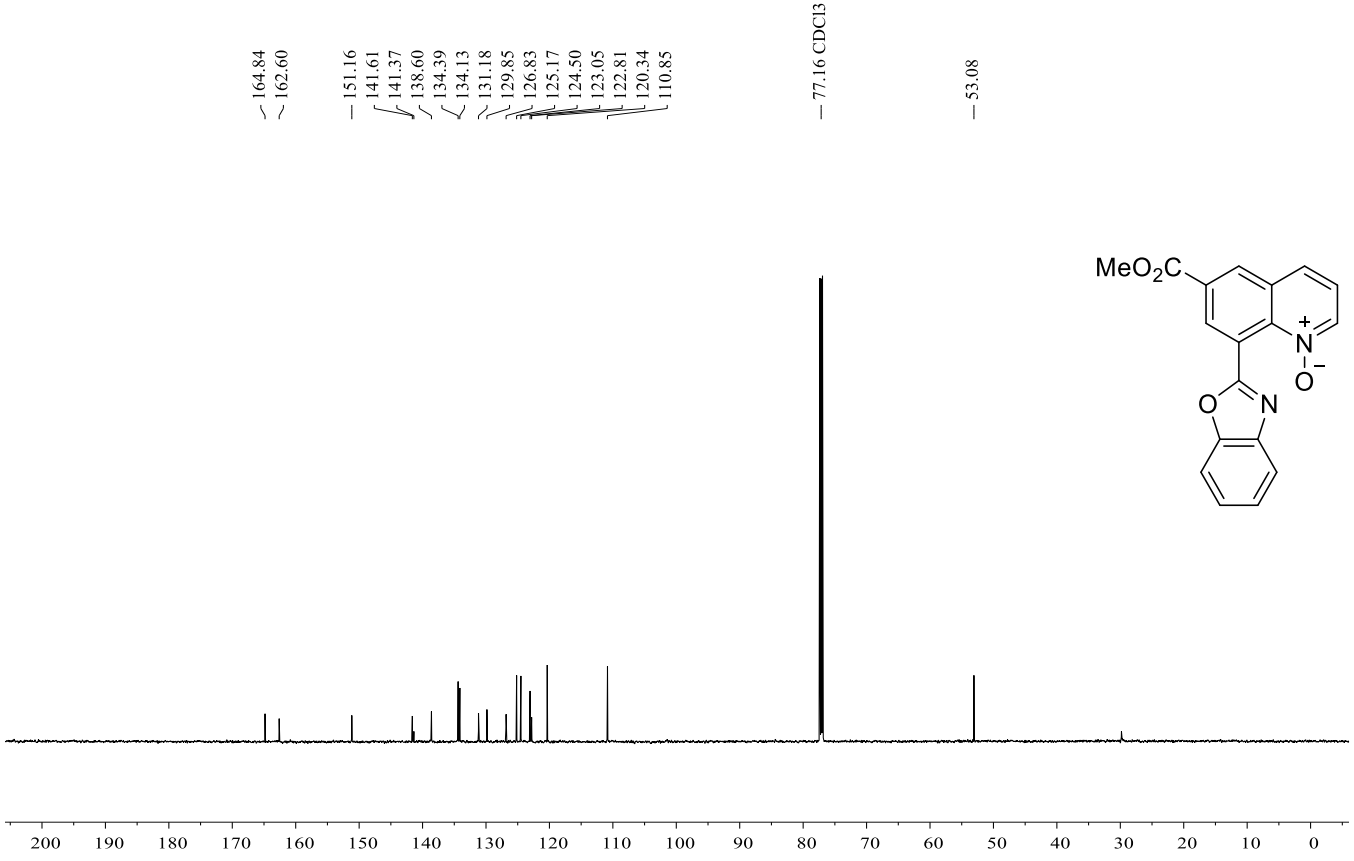


*8-(benzo[d]oxazol-2-yl)-6-(methoxycarbonyl)quinoline 1-oxide (Table 2, Entry **3o**)*

^{1}H NMR (600 MHz)

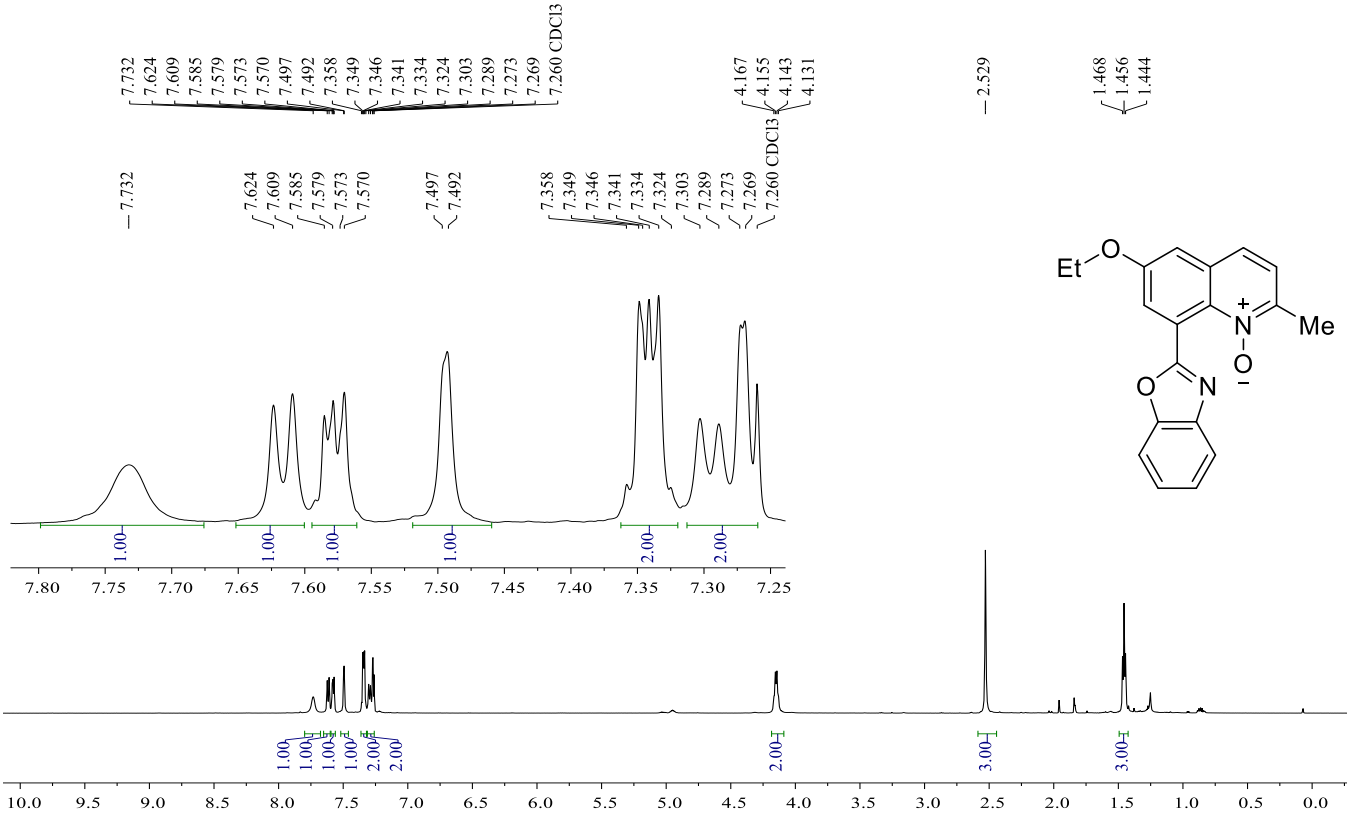


^{13}C{^{1}H} NMR (150 MHz)

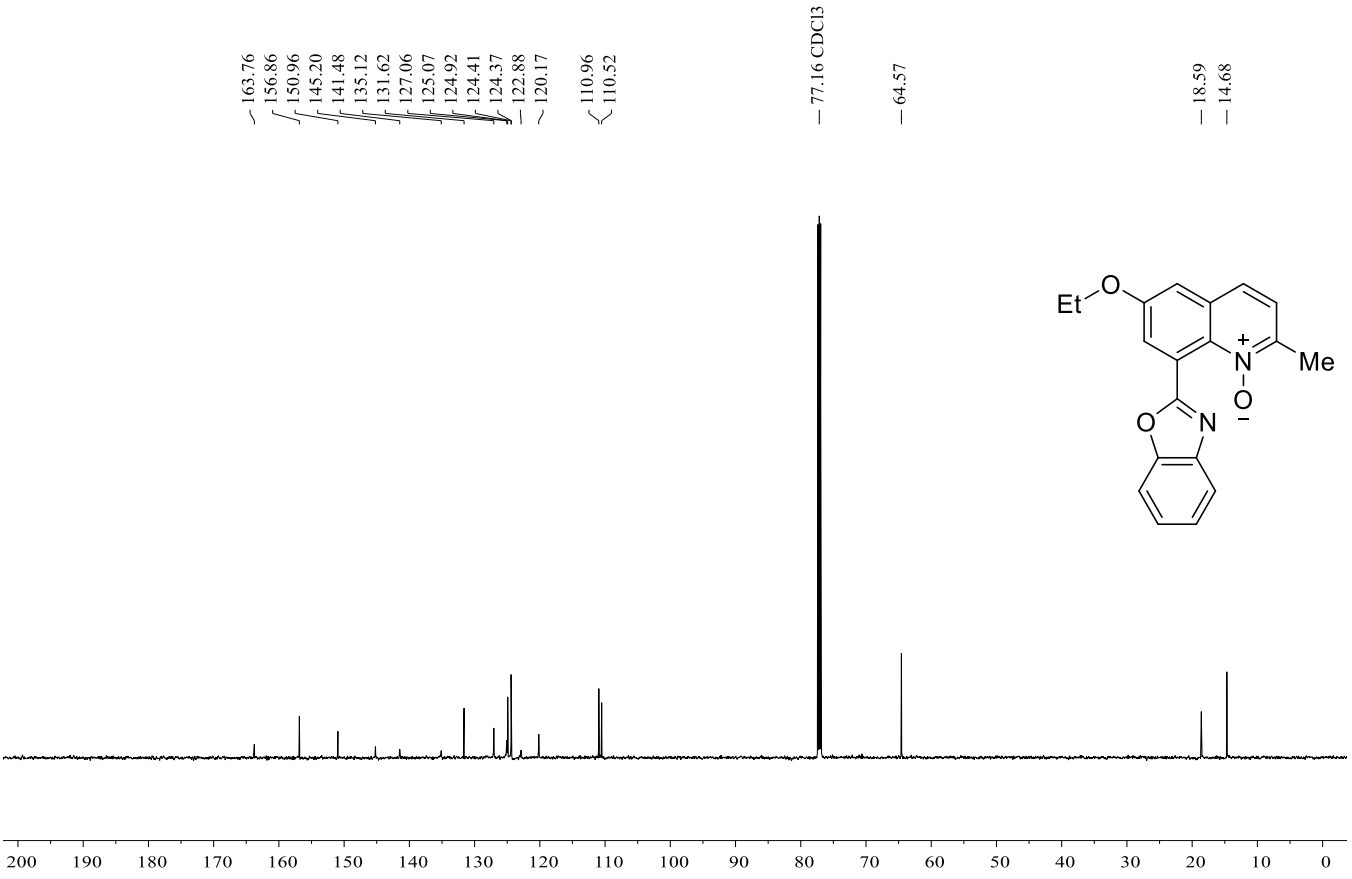


*8-(benzo[d]oxazol-2-yl)-6-ethoxy-2-methylquinoline 1-oxide (Table 2, Entry **3p**)*

^{1}H NMR (600 MHz)

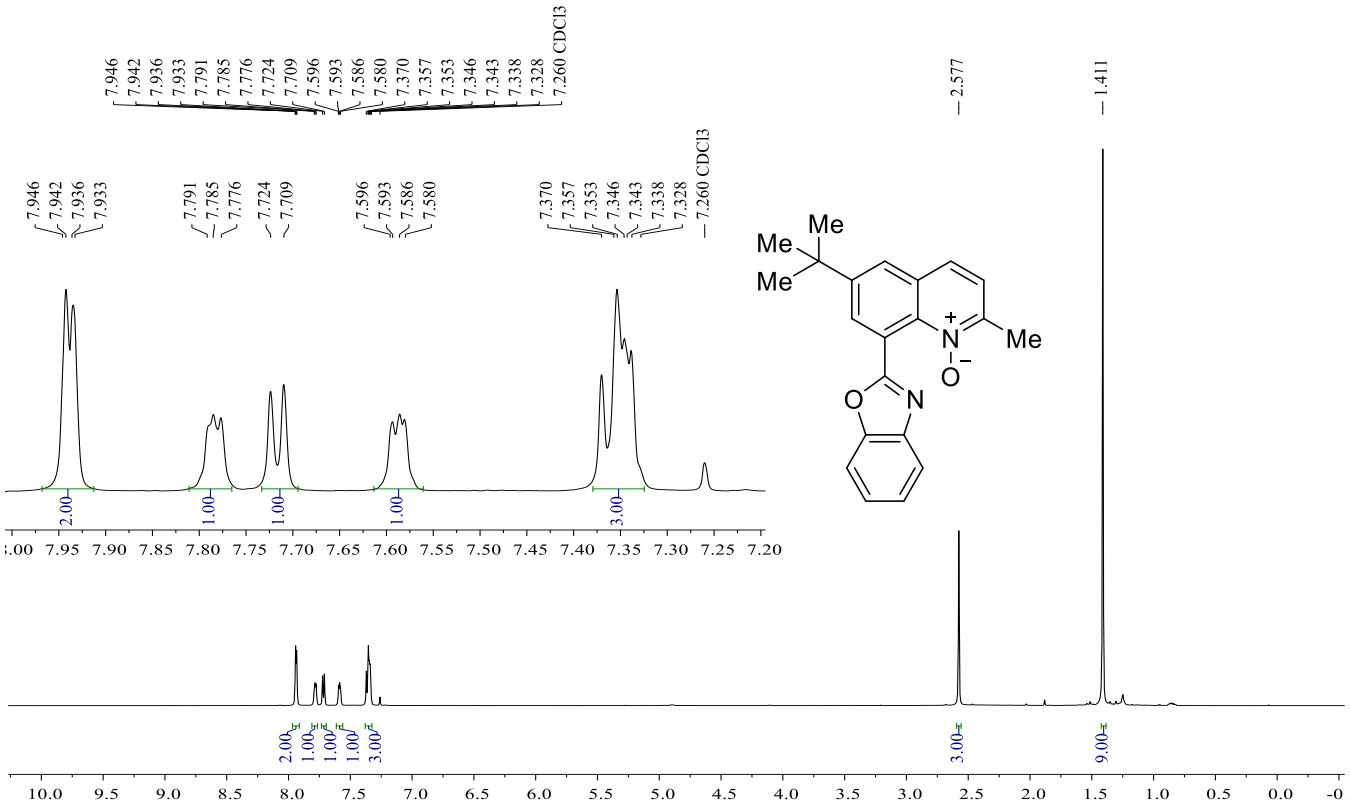


^{13}C{^{1}H} NMR (150 MHz)

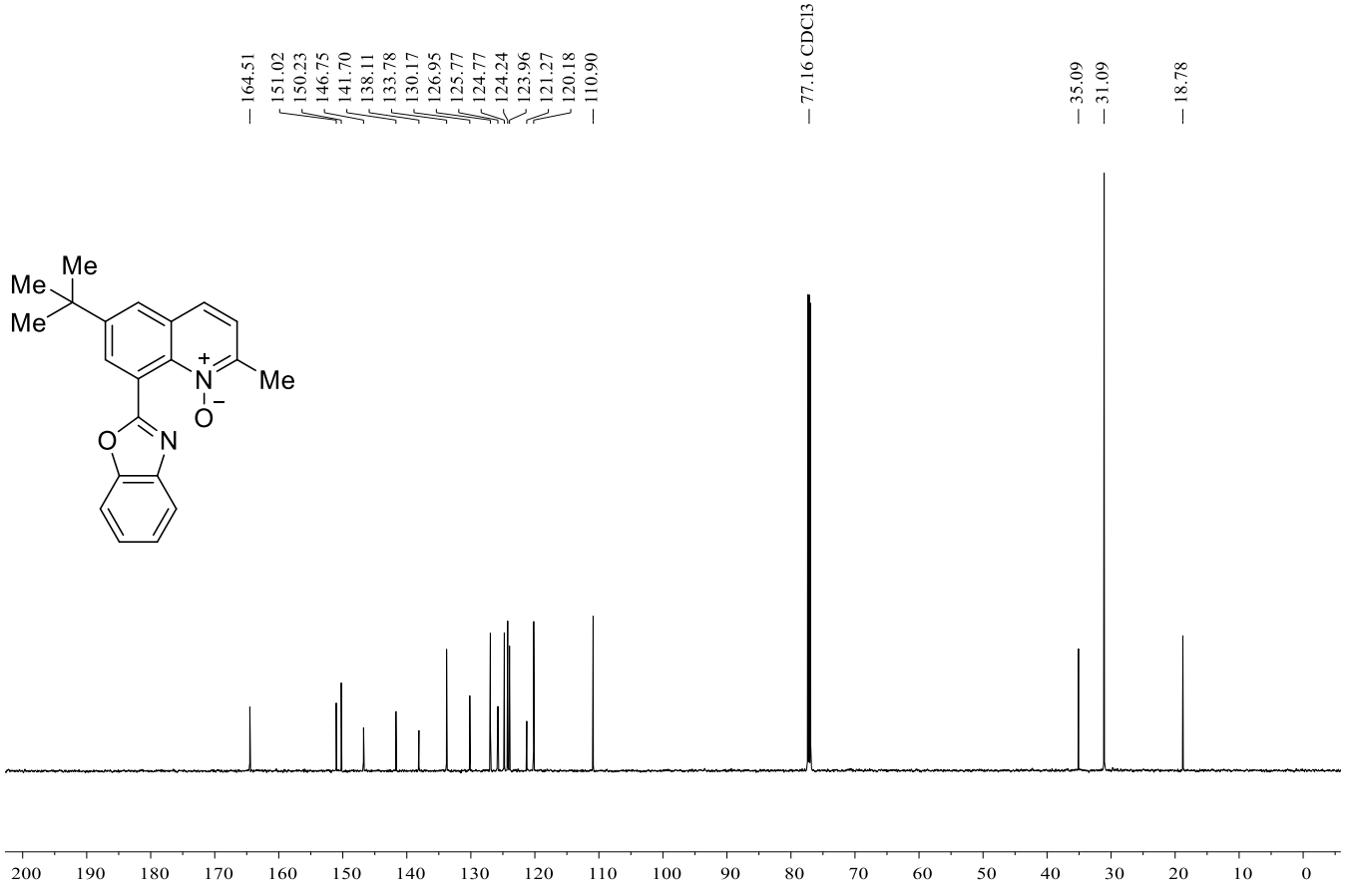


*8-(benzo[d]oxazol-2-yl)-6-(tert-butyl)-2-methylquinoline 1-oxide (Table 2, Entry **3q**)*

^{1}H NMR (600 MHz)

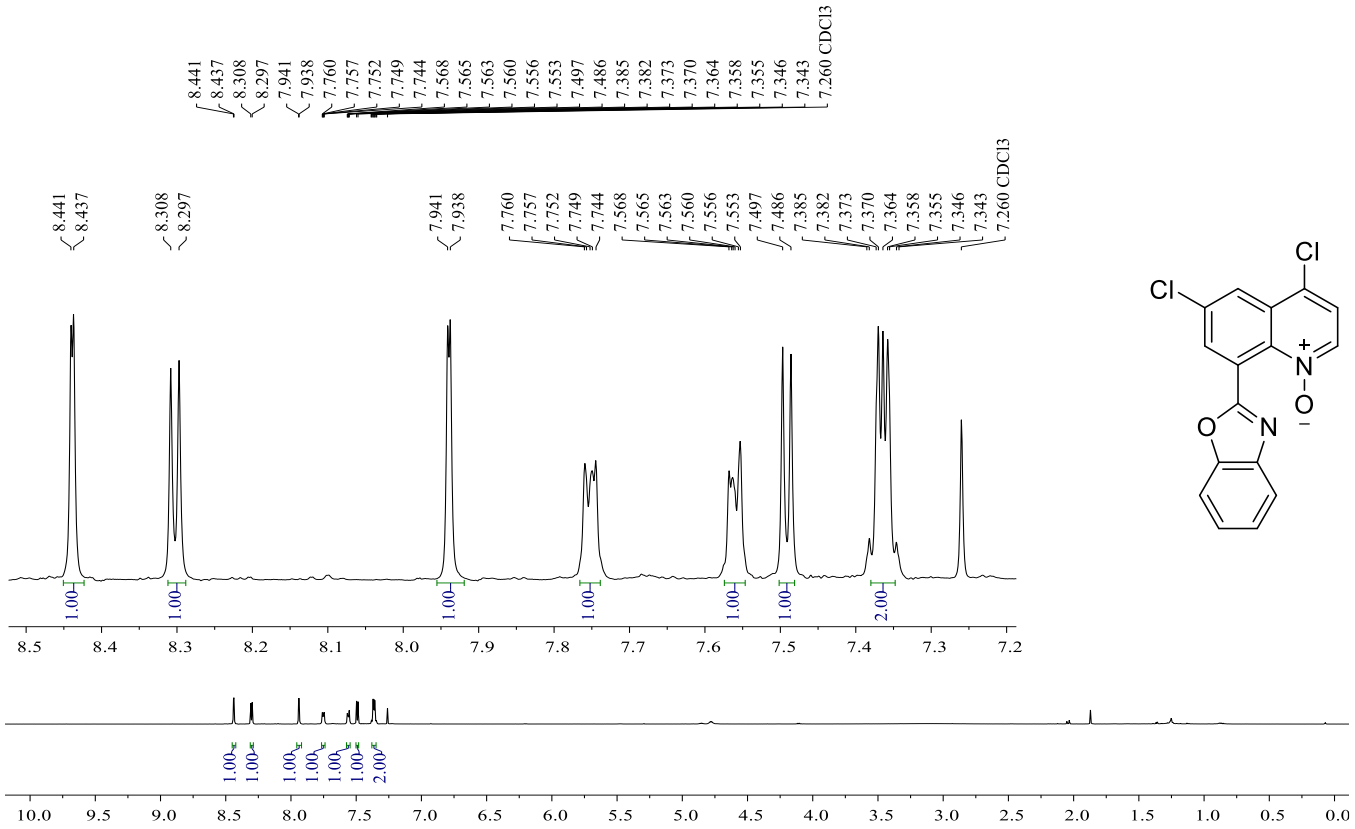


^{13}C{^{1}H} NMR (150 MHz)

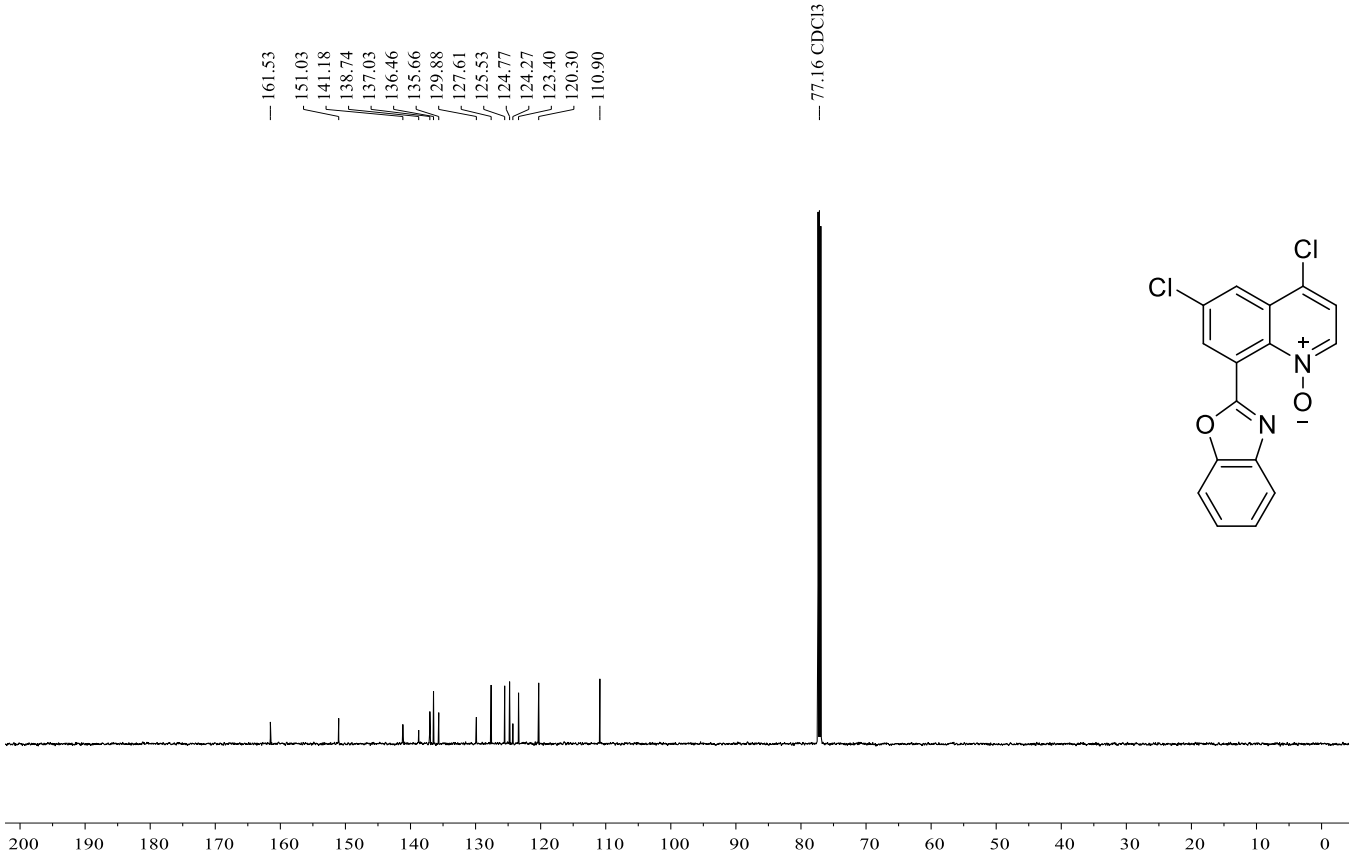


*8-(benzo[d]oxazol-2-yl)-4,6-dichloroquinoline 1-oxide (Table 2, Entry **3r**)*

^{1}H NMR (600 MHz)

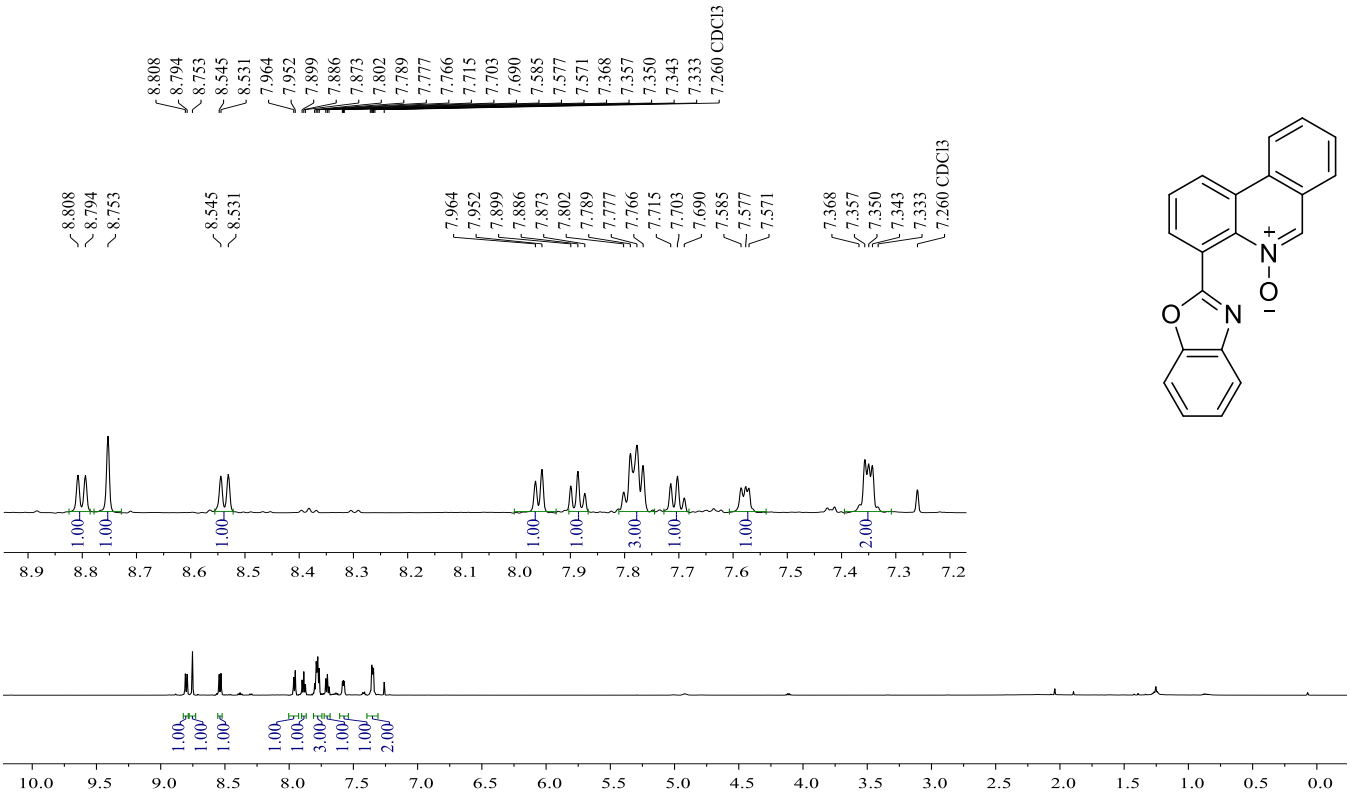


^{13}C{^{1}H} NMR (150 MHz)

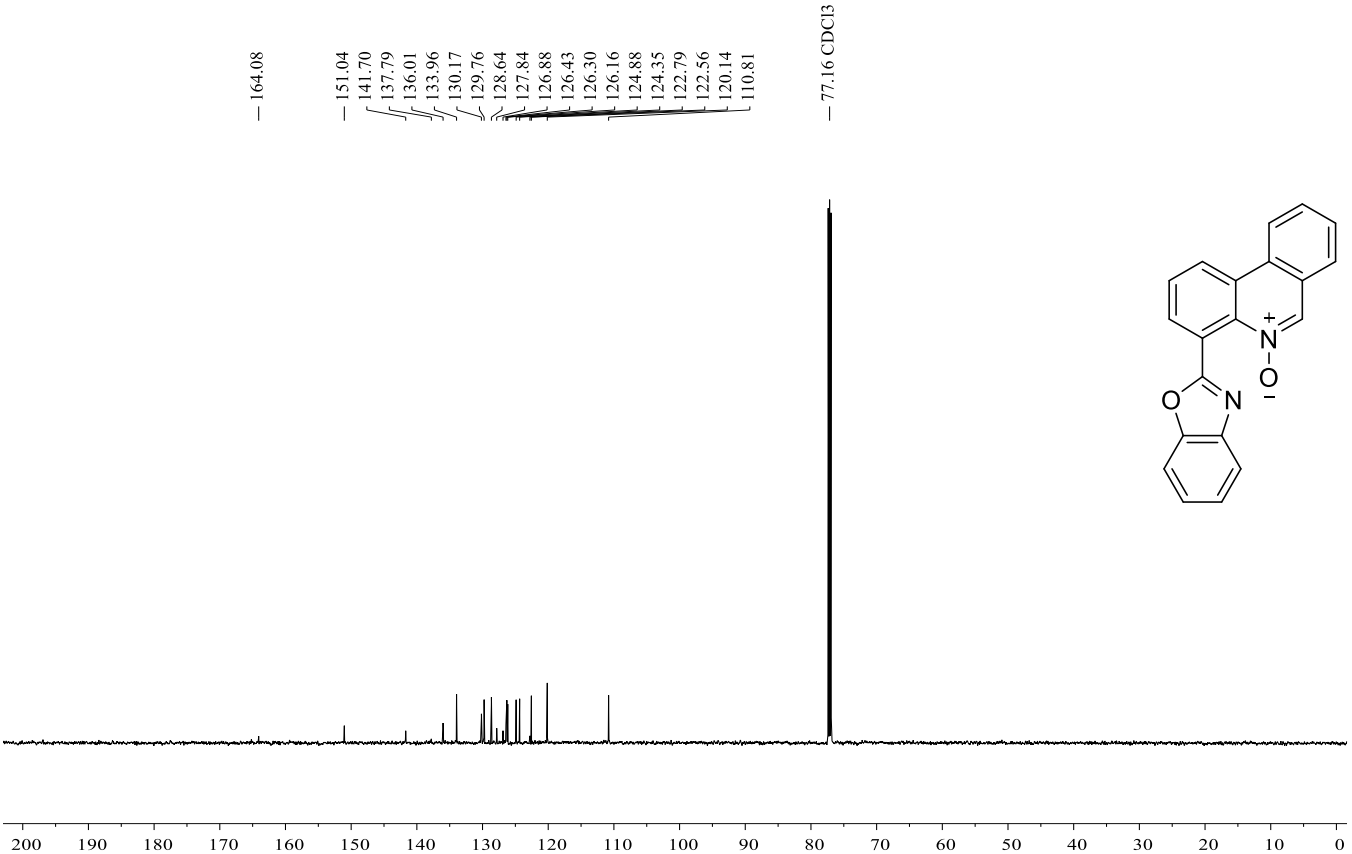


*4-(benzo[d]oxazol-2-yl)phenanthridine 5-oxide (Table 2, Entry **3s**)*

^{1}H NMR (600 MHz)

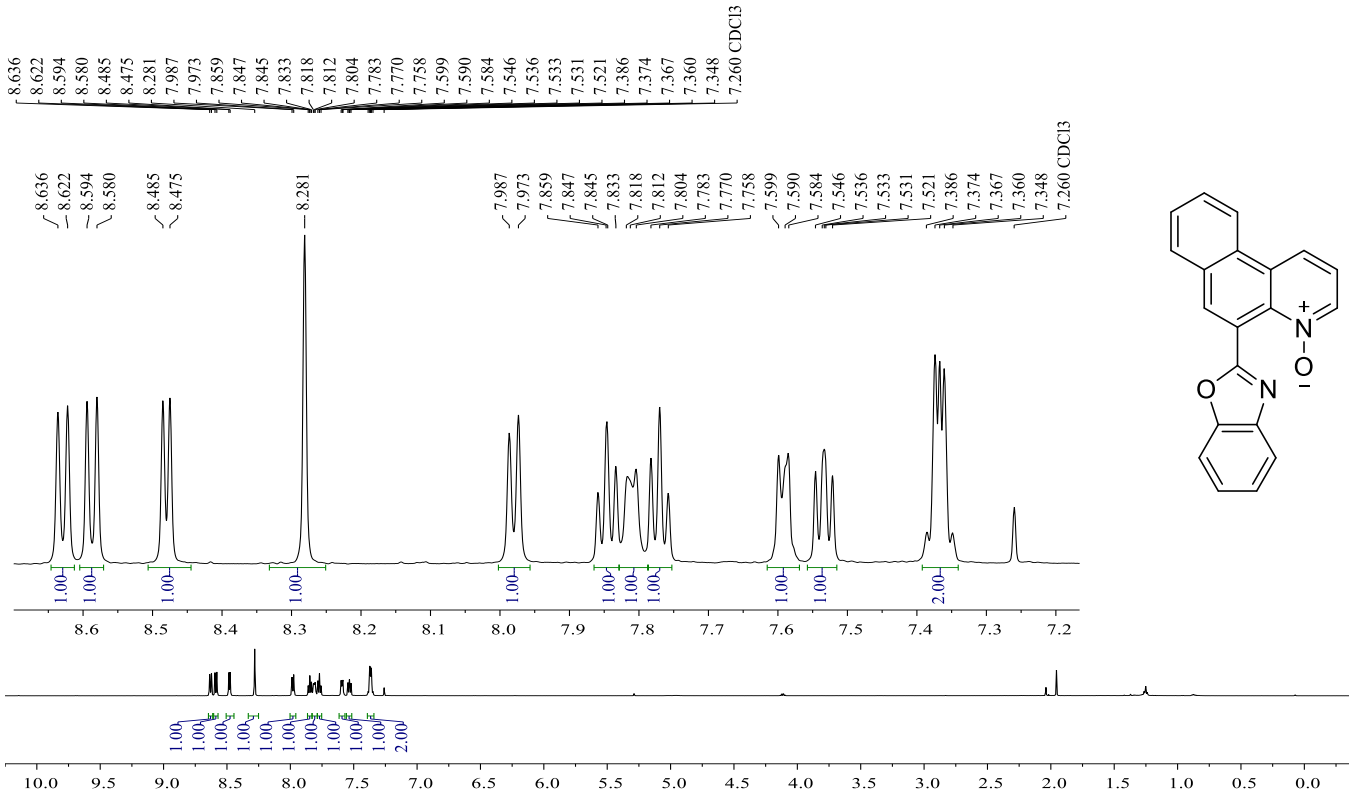


^{13}C{^{1}H} NMR (150 MHz)

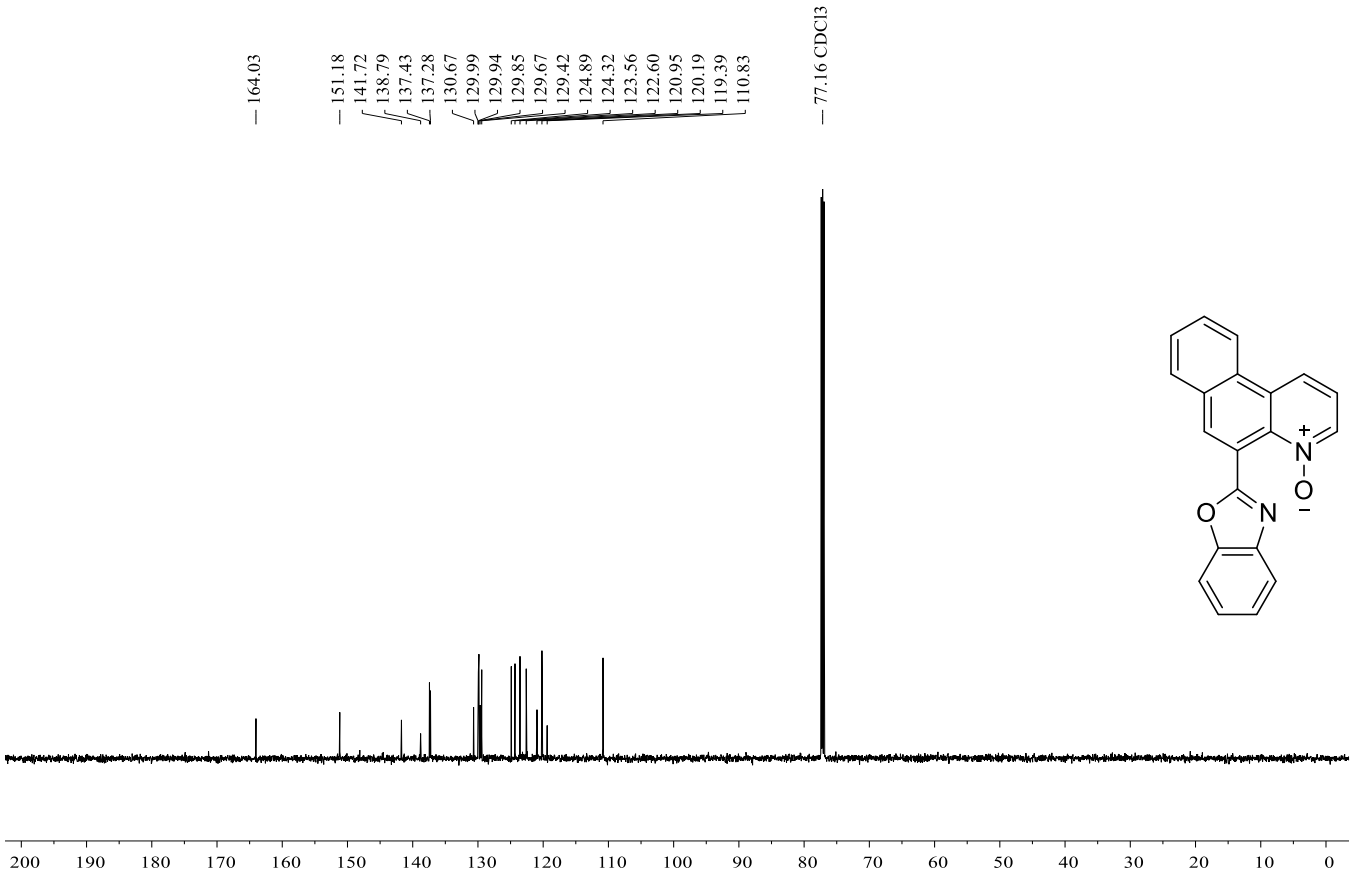


*5-(benzo[d]oxazol-2-yl)benzo[f]quinoline 4-oxide (Table 2, Entry **3t**)*

^{1}H NMR (600 MHz)

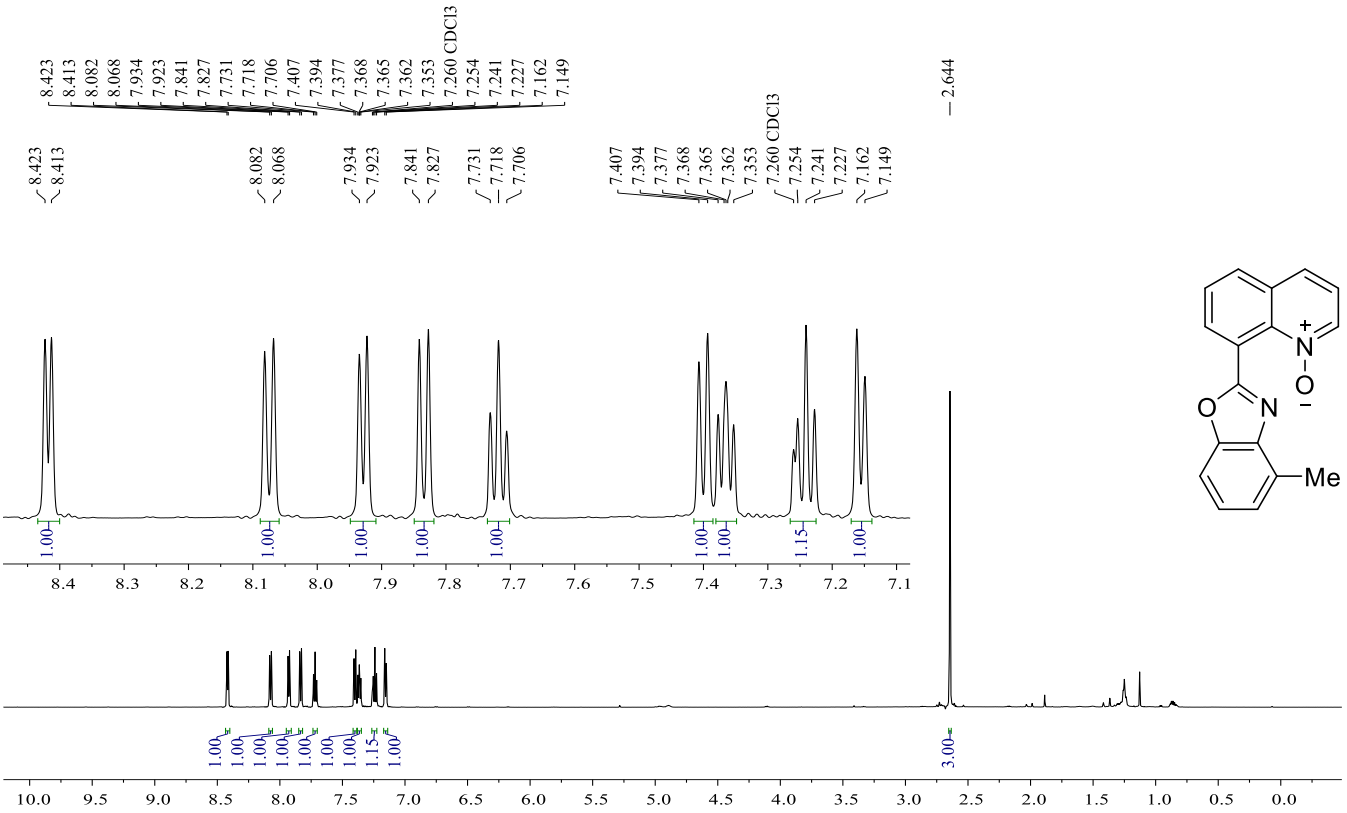


^{13}C{^{1}H} NMR (150 MHz)

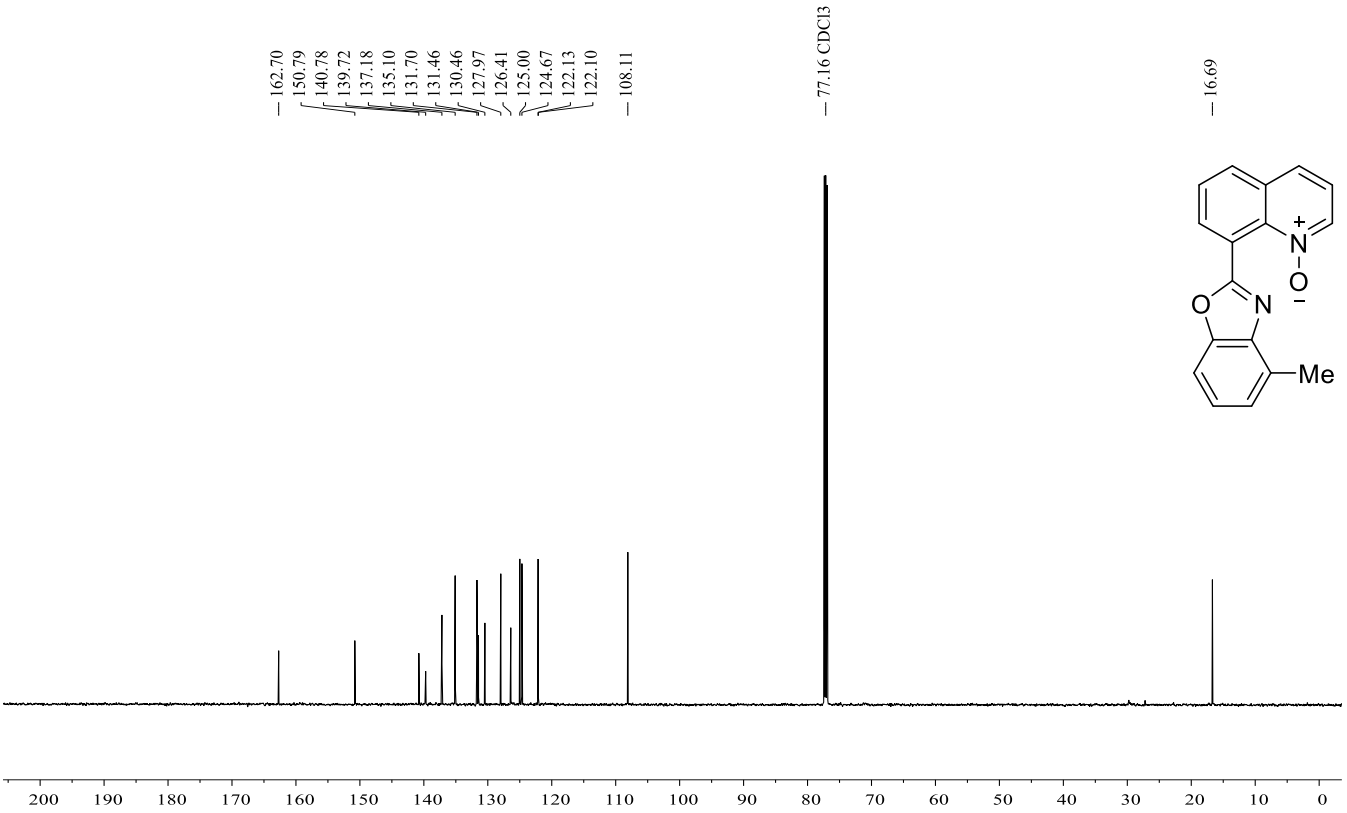


*8-(4-methylbenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3u**)*

^{1}H NMR (600 MHz)

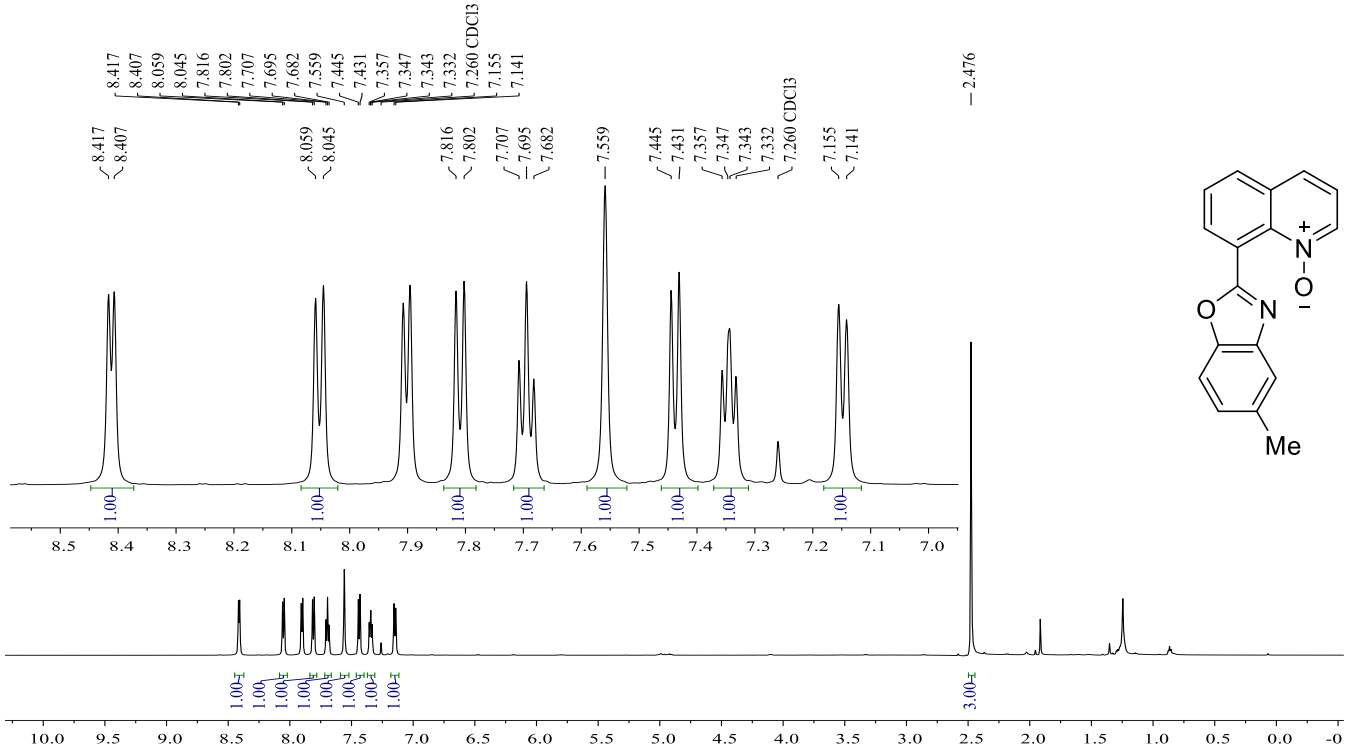


^{13}C{^{1}H} NMR (150 MHz)

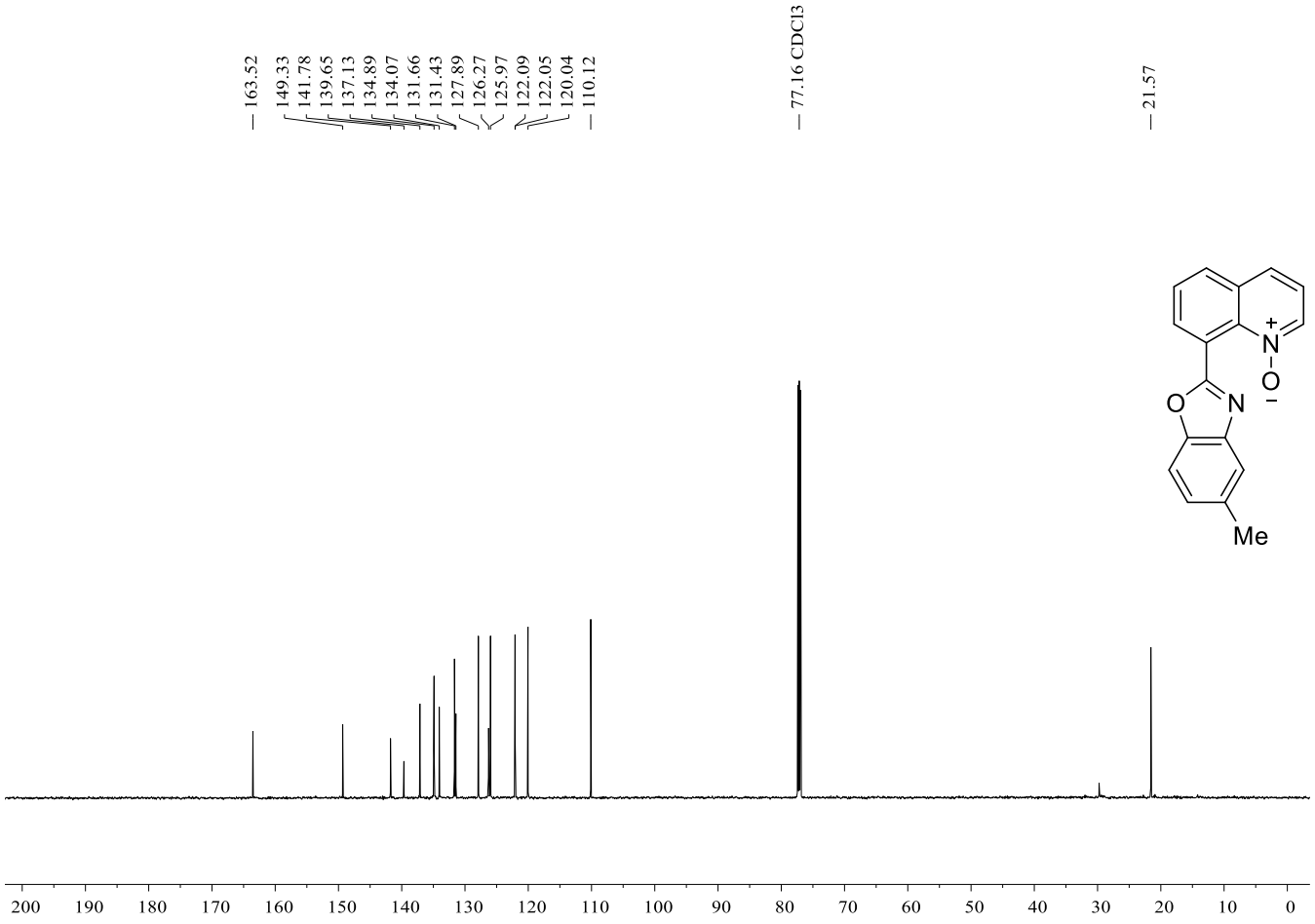


*8-(5-methylbenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3v**)*

^{1}H NMR (600 MHz)

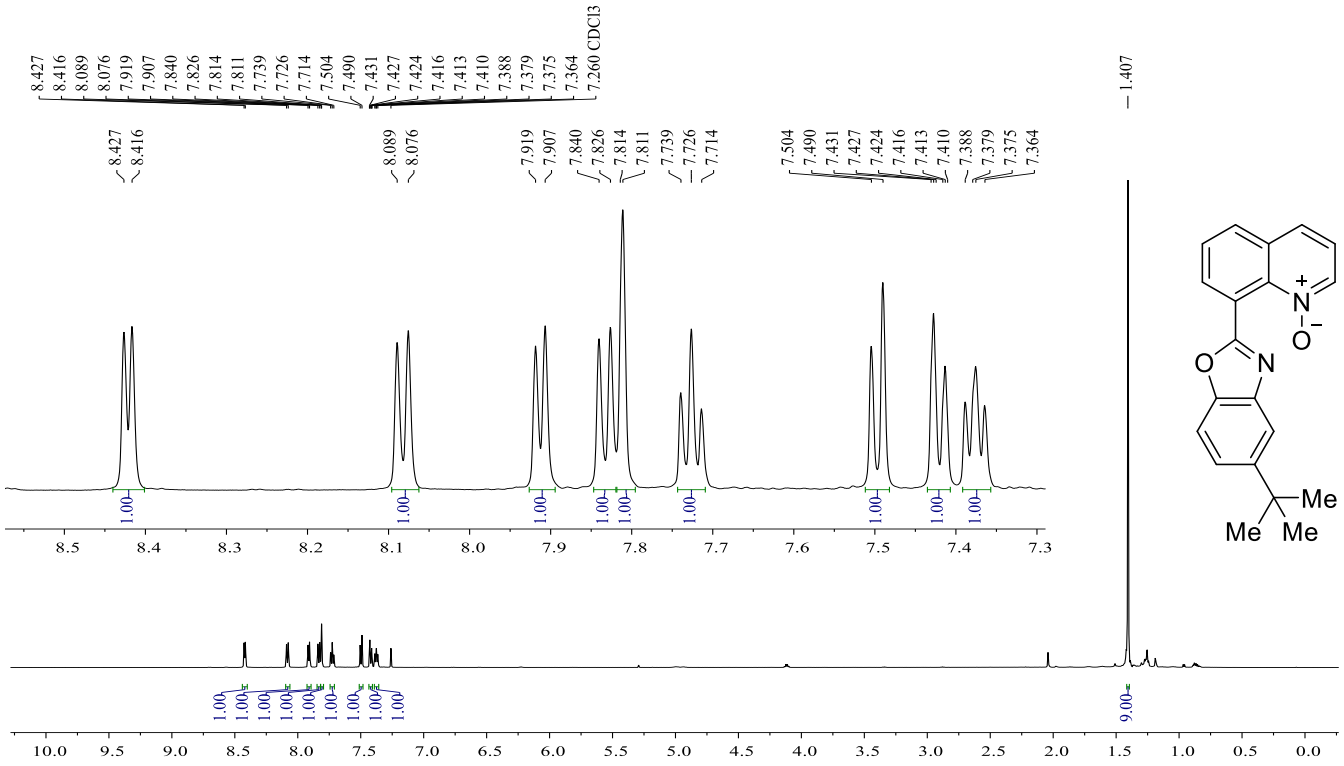


^{13}C{^{1}H} NMR (150 MHz)

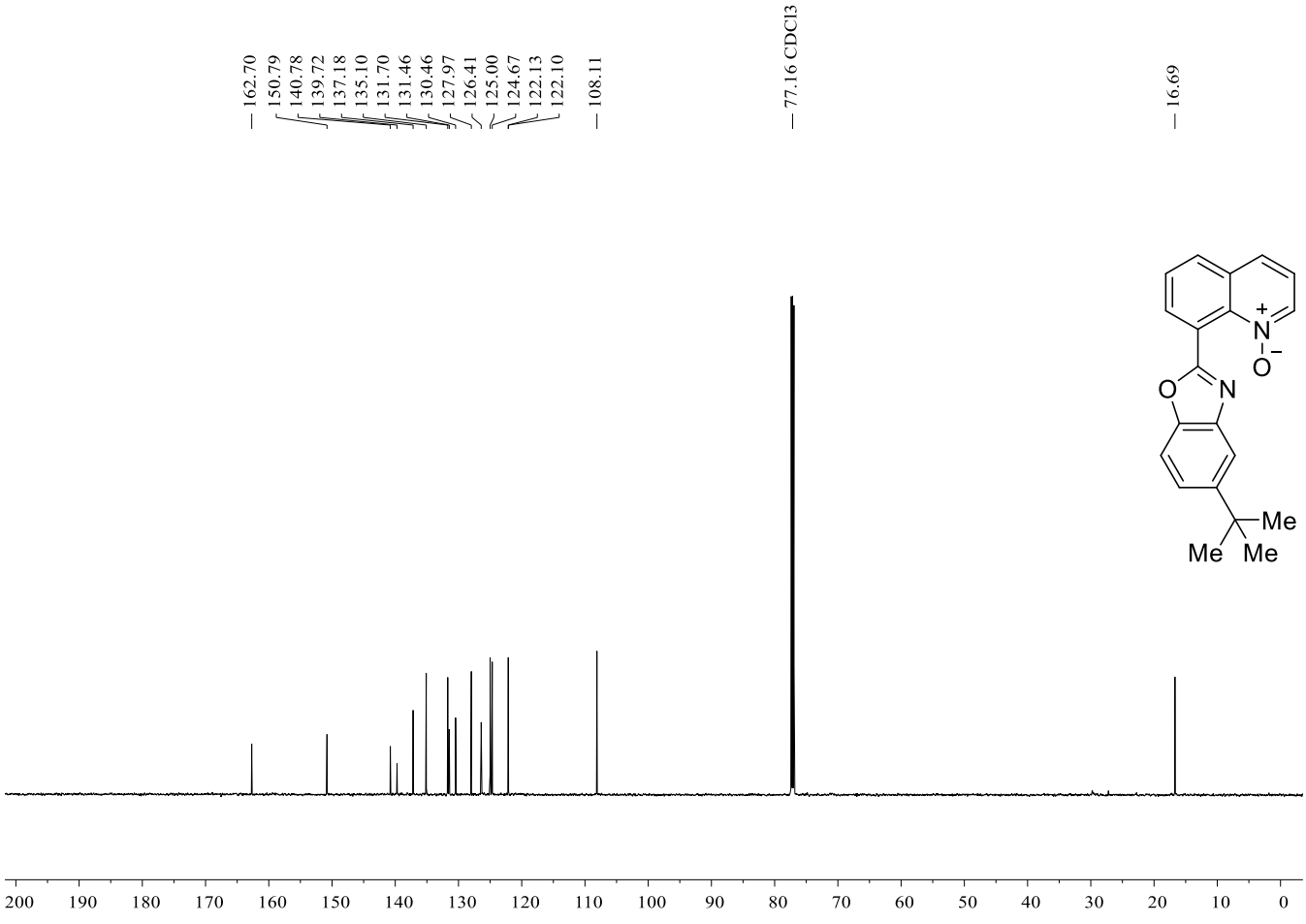


*8-(5-(tert-butyl)benzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3w**)*

^{1}H NMR (600 MHz)

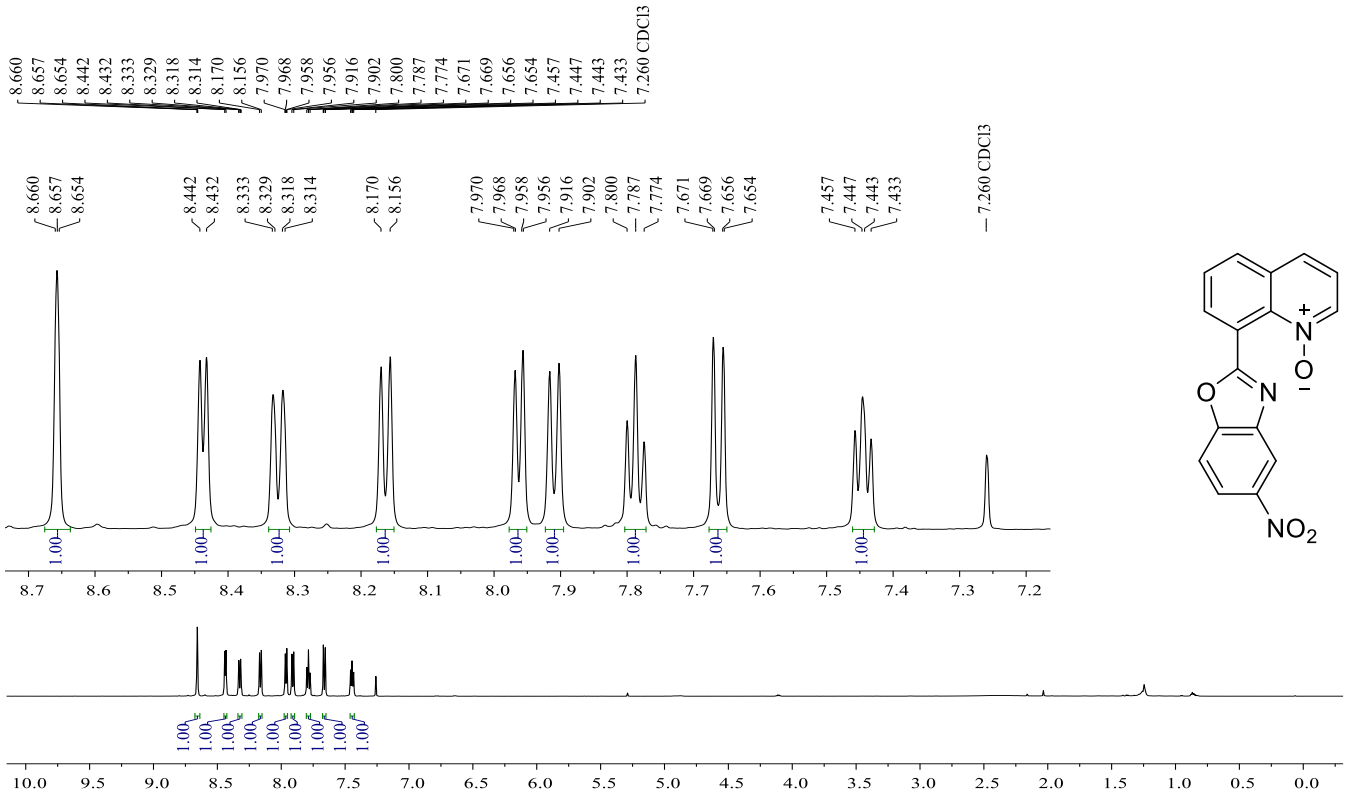


^{13}C{^{1}H} NMR (150 MHz)

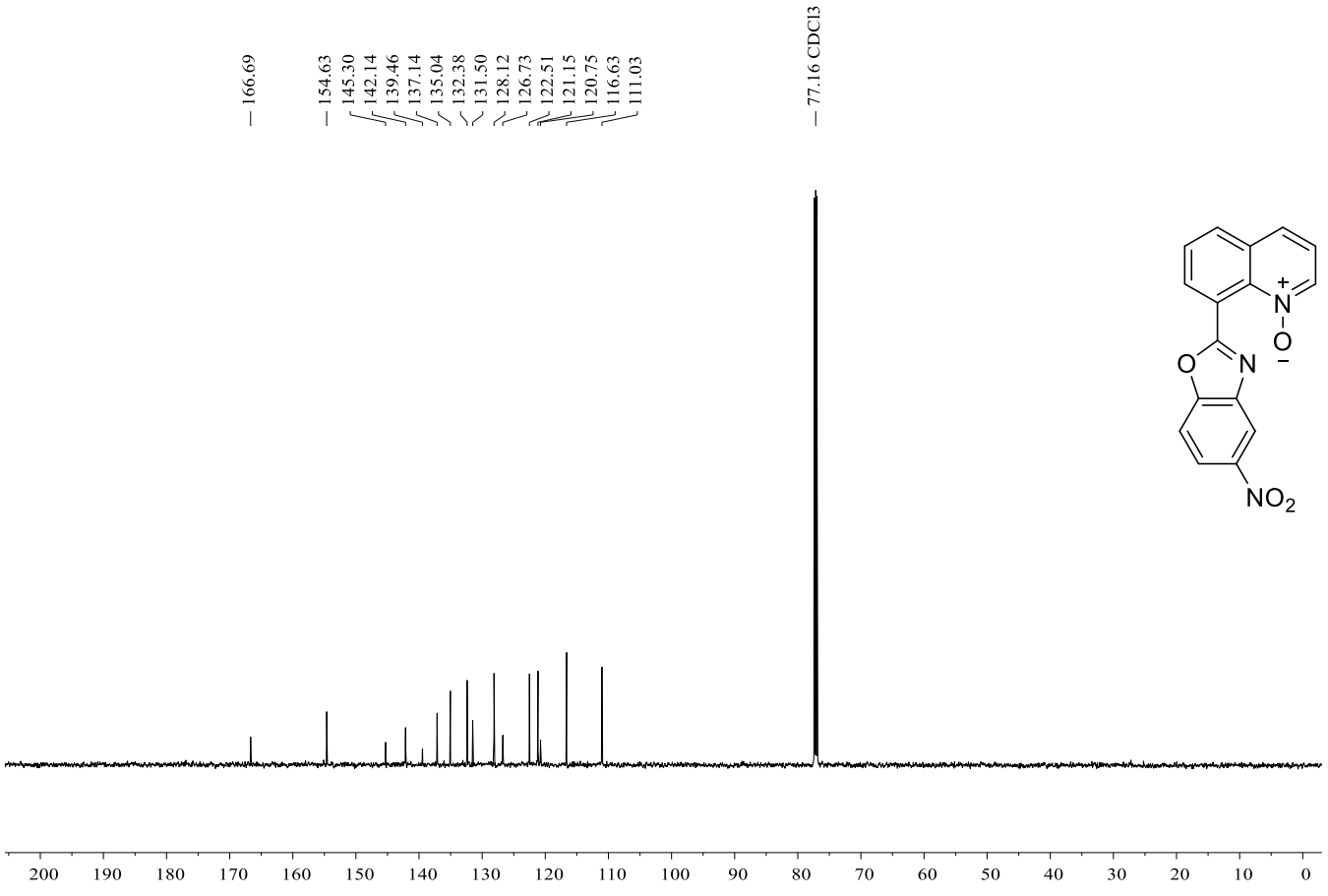


*8-(5-nitrobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3x**)*

^{1}H NMR (600 MHz)

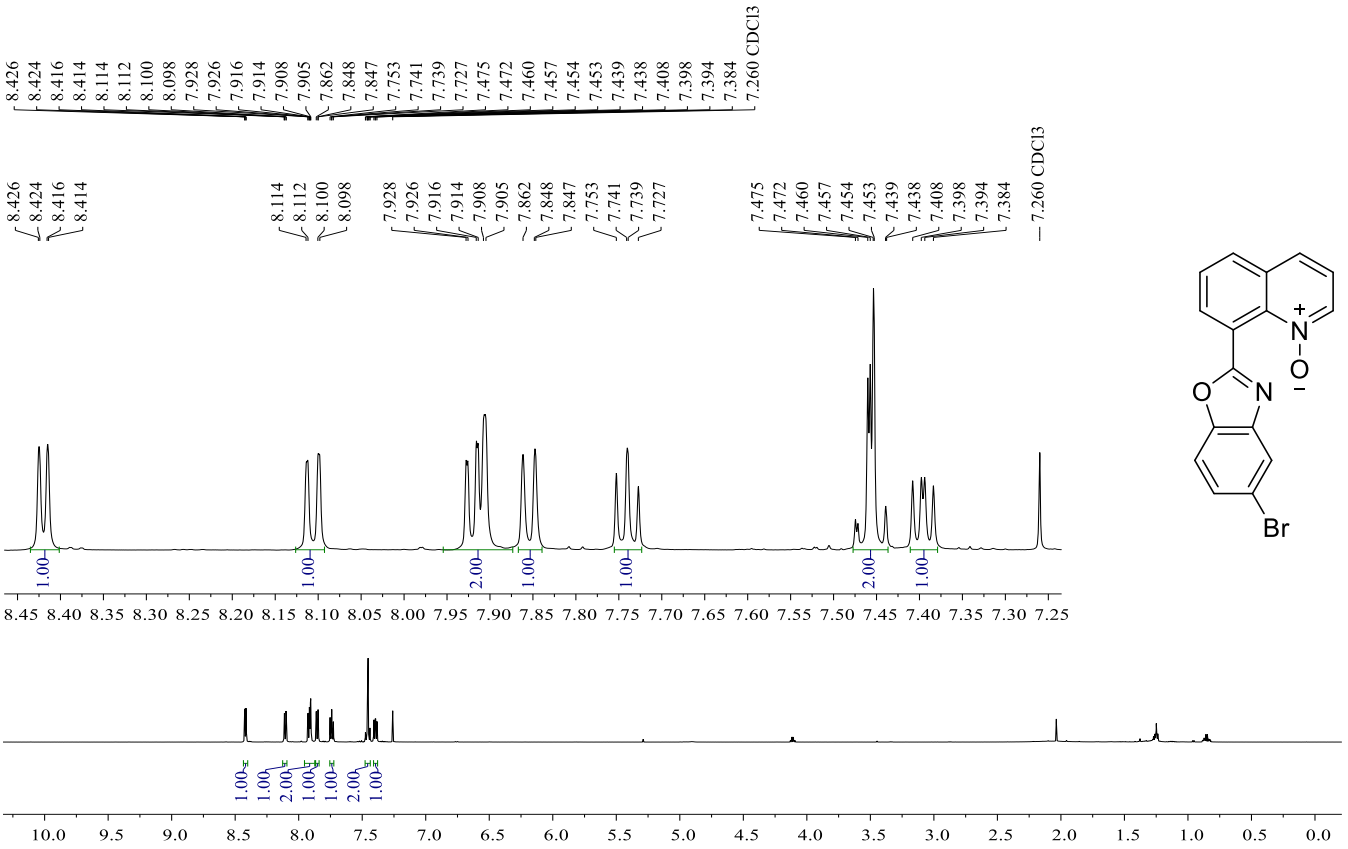


^{13}C{^{1}H} NMR (150 MHz)

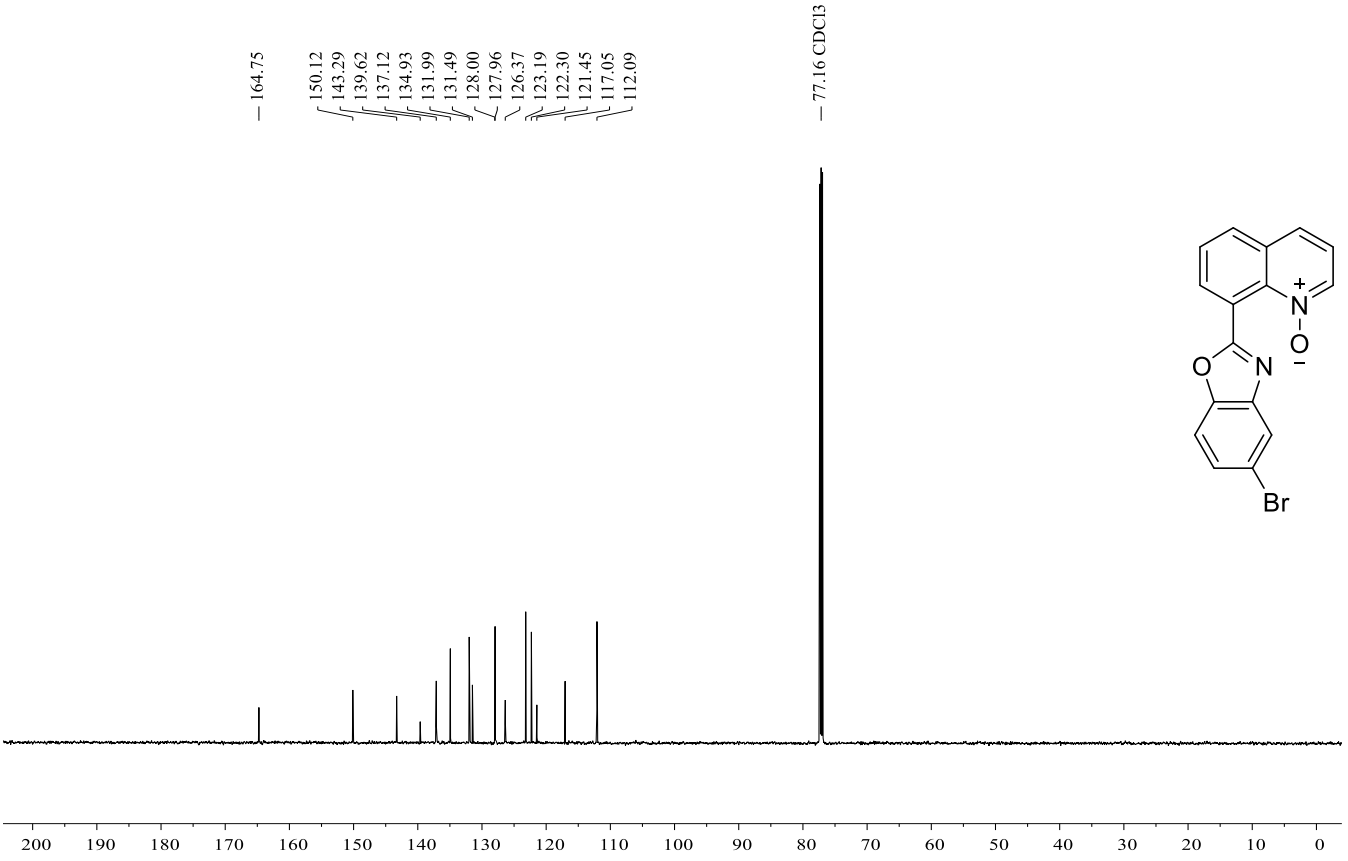


*8-(5-bromobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3y**)*

^{1}H NMR (600 MHz)

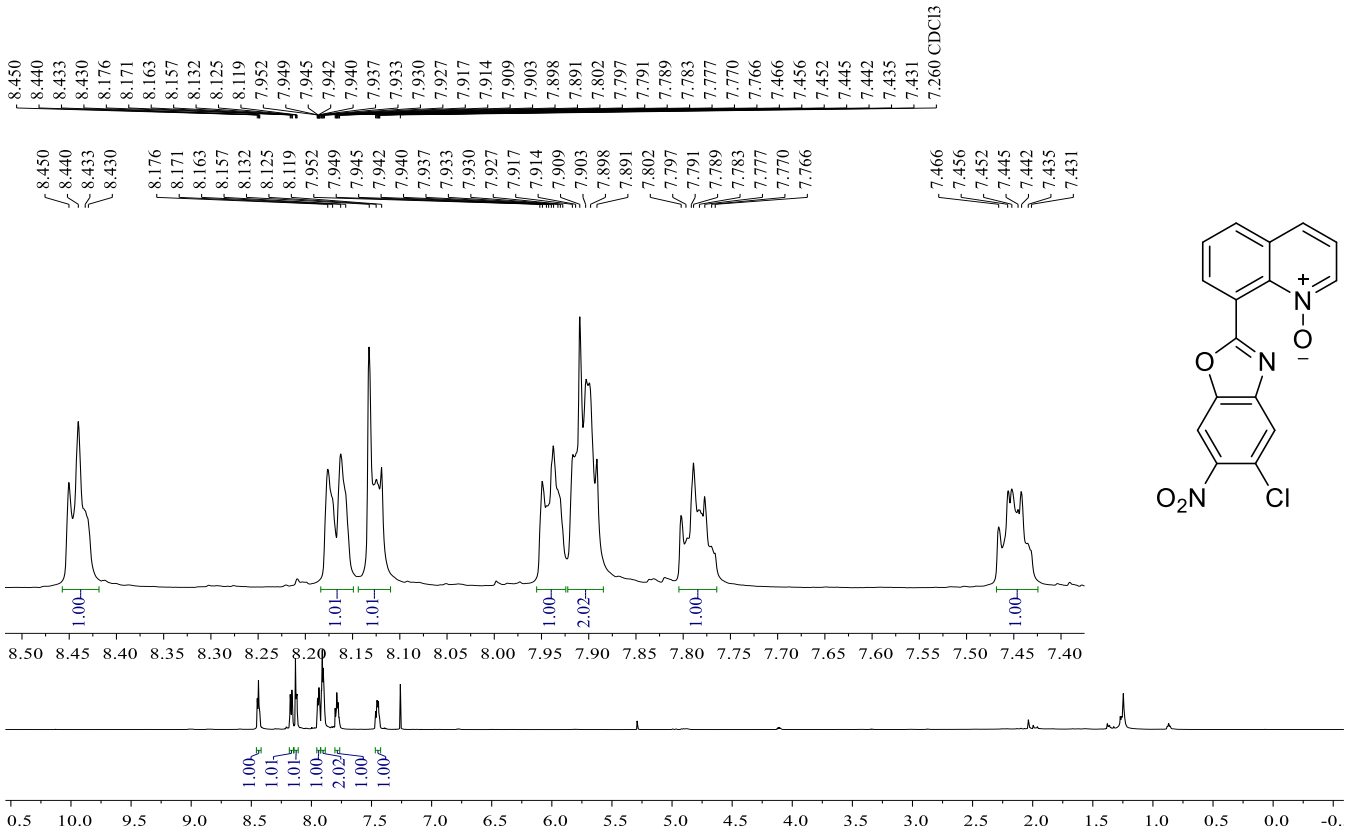


^{13}C{^{1}H} NMR (150 MHz)

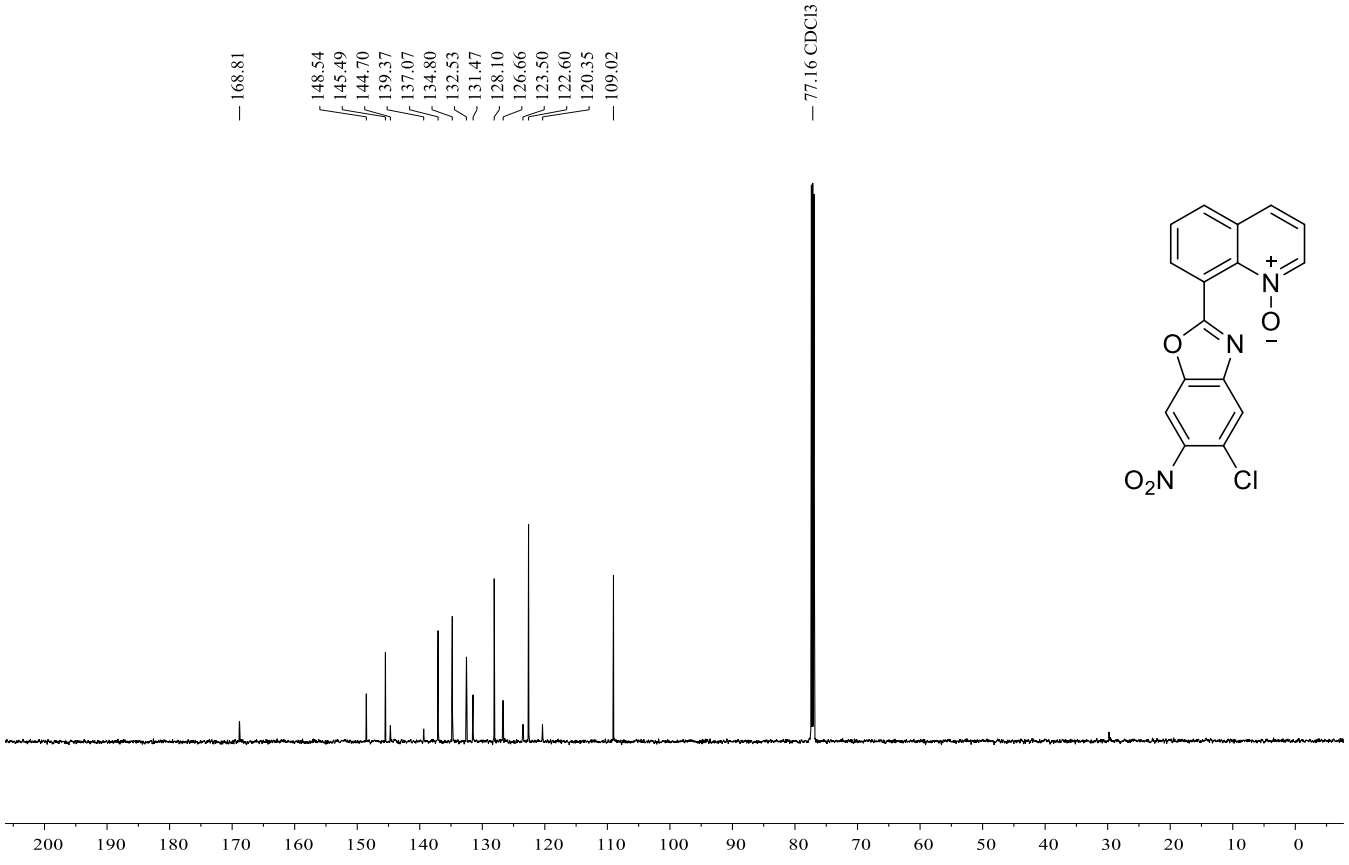


*8-(5-chloro-6-nitrobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3z**)*

^{1}H NMR (600 MHz)

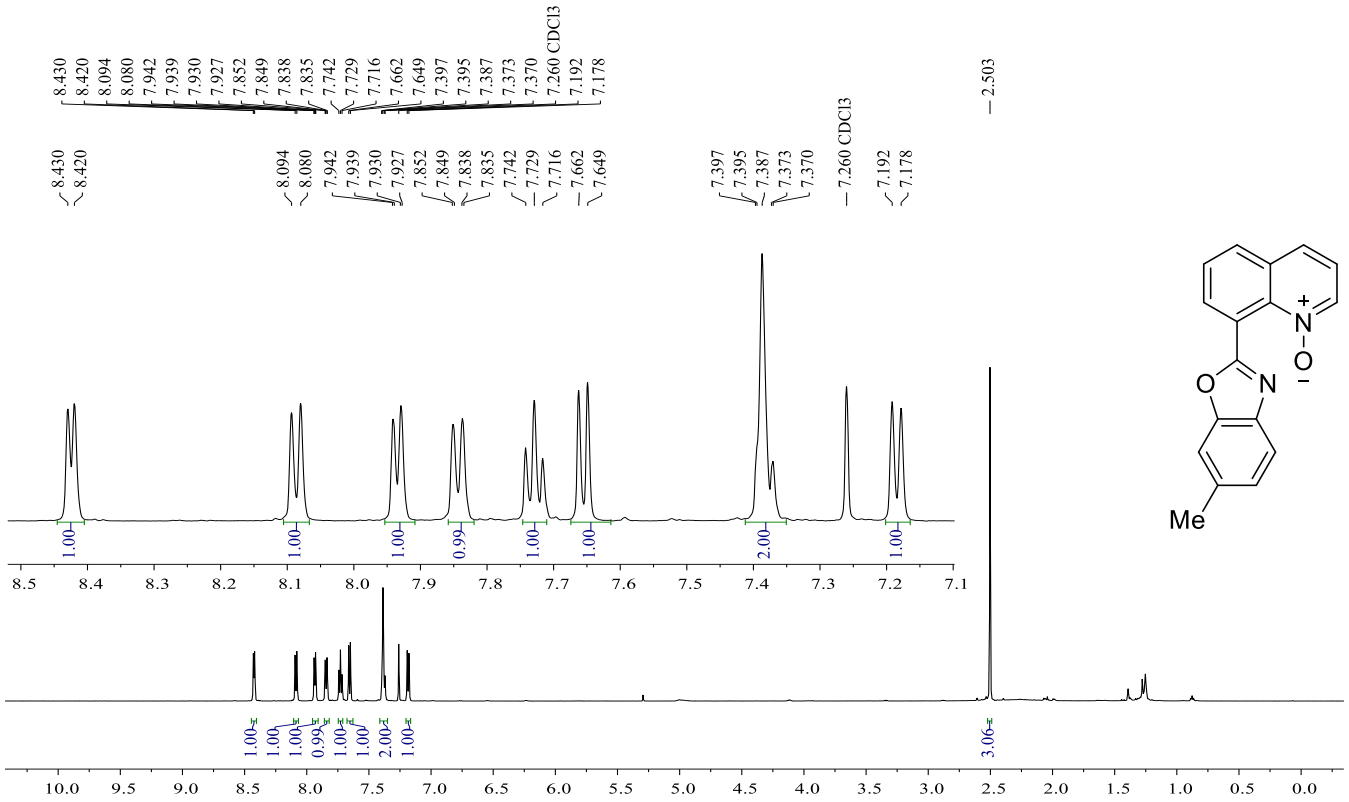


^{13}C{^{1}H} NMR (150 MHz)

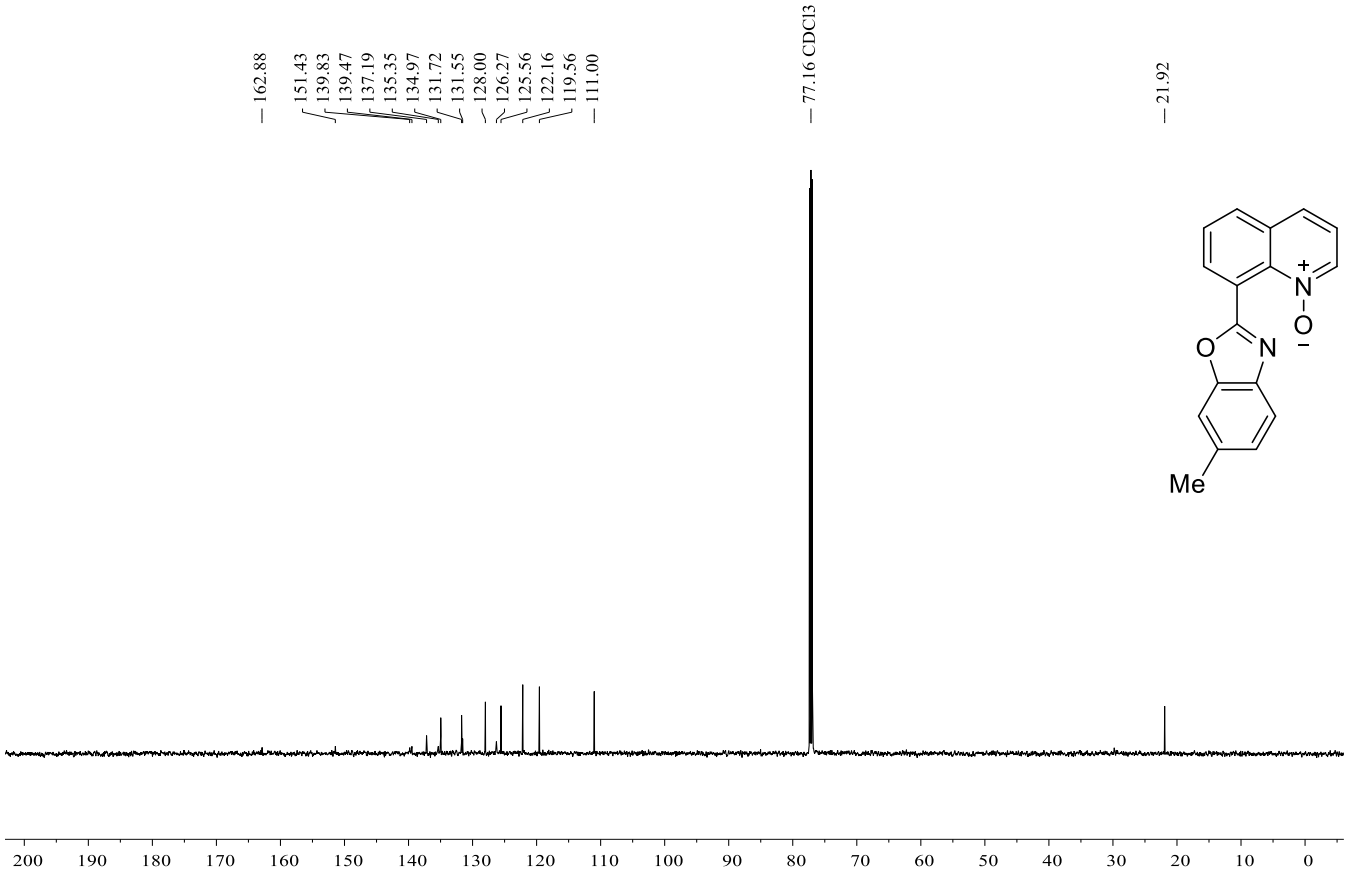


*8-(6-methylbenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3za**)*

^{1}H NMR (600 MHz)

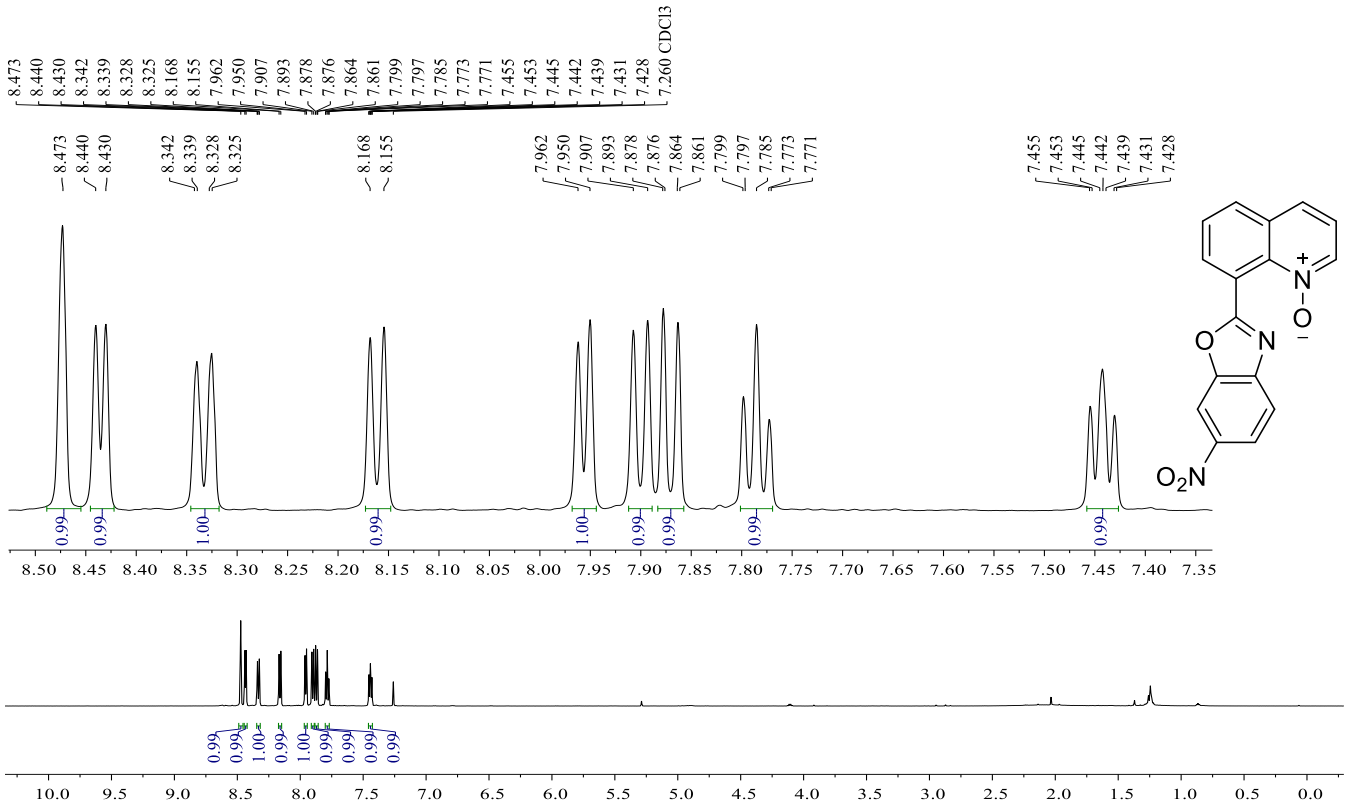


^{13}C{^{1}H} NMR (150 MHz)

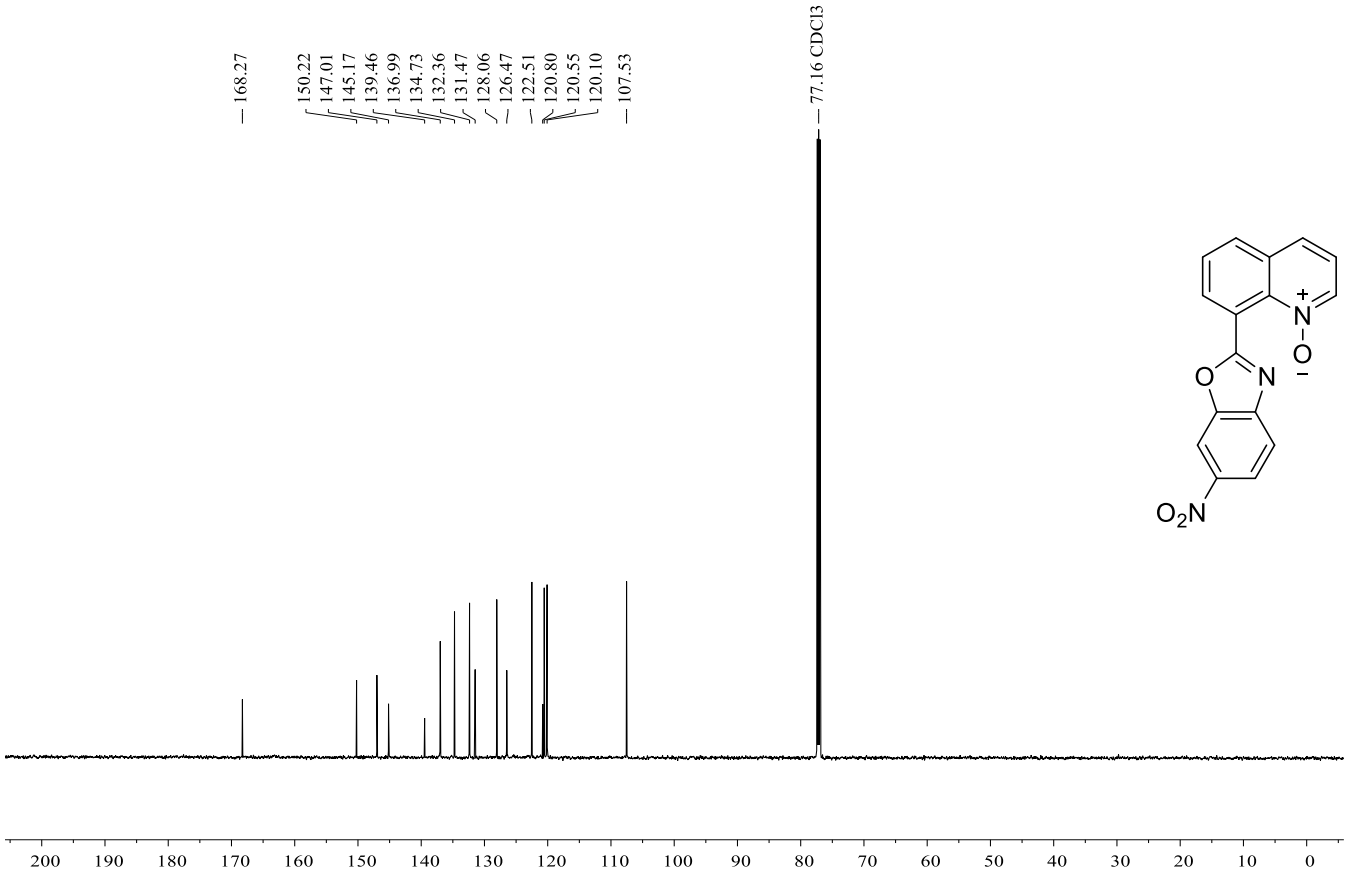


*8-(6-nitrobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3zb**)*

^{1}H NMR (600 MHz)

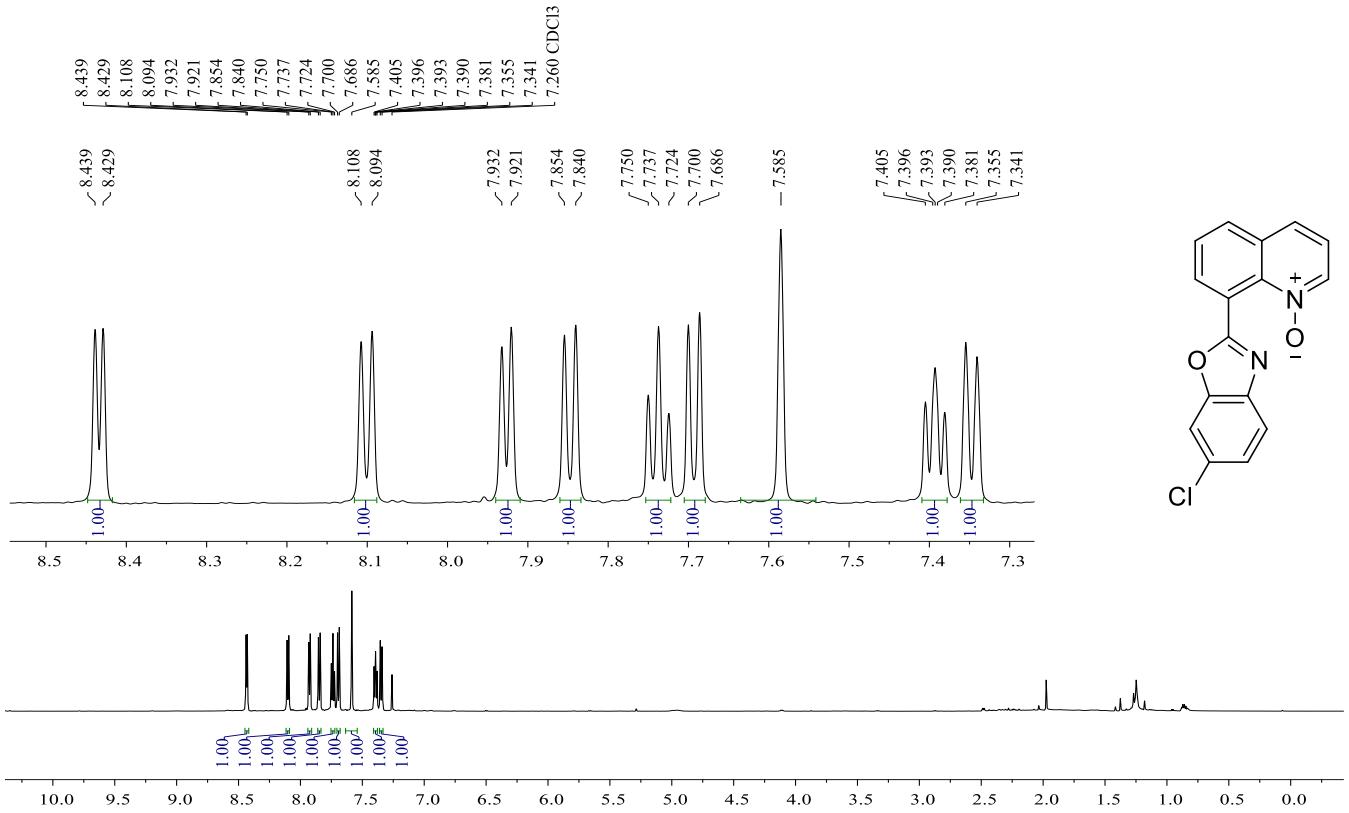


^{13}C{^{1}H} NMR (150 MHz)

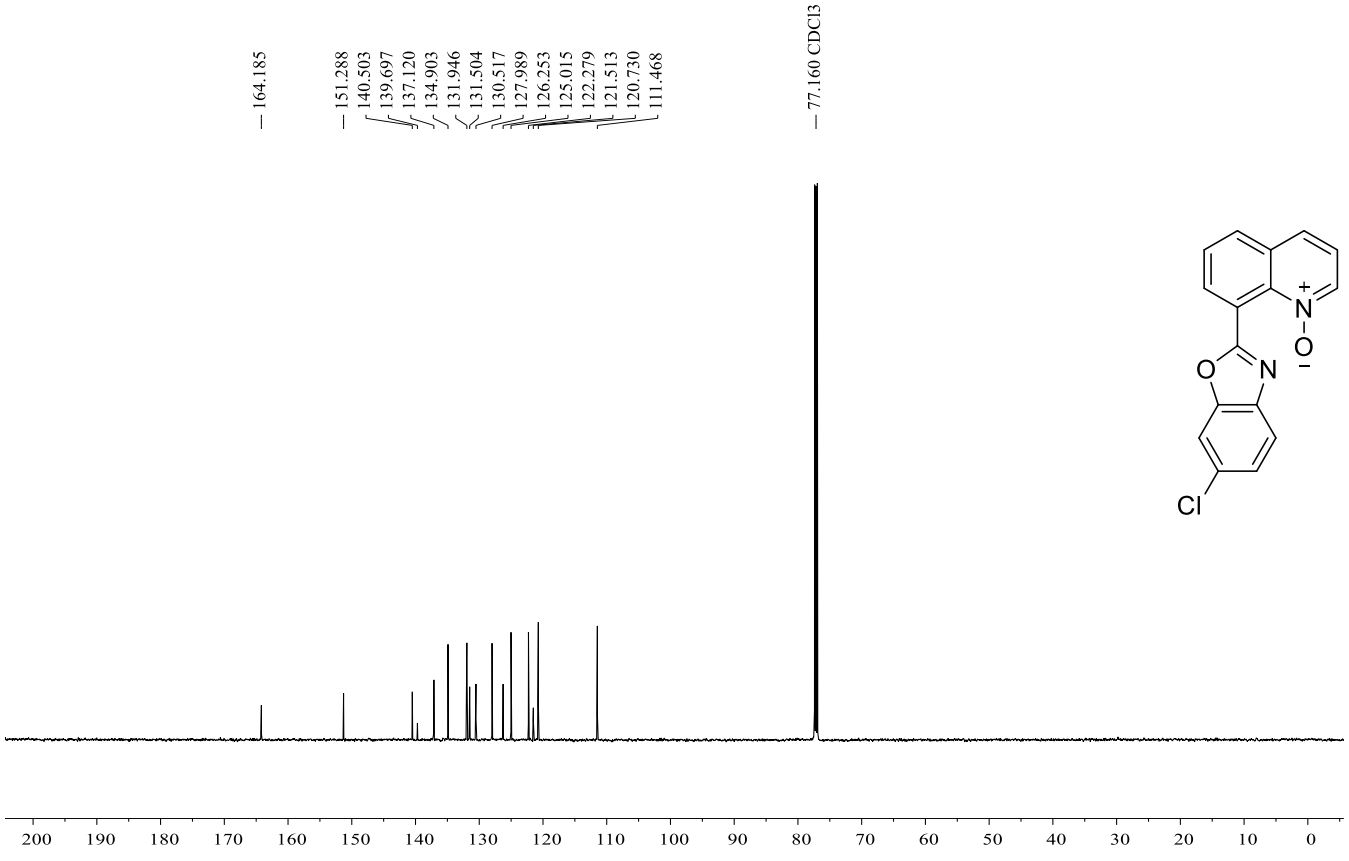


*8-(6-chlorobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3zc**)*

^{1}H NMR (600 MHz)

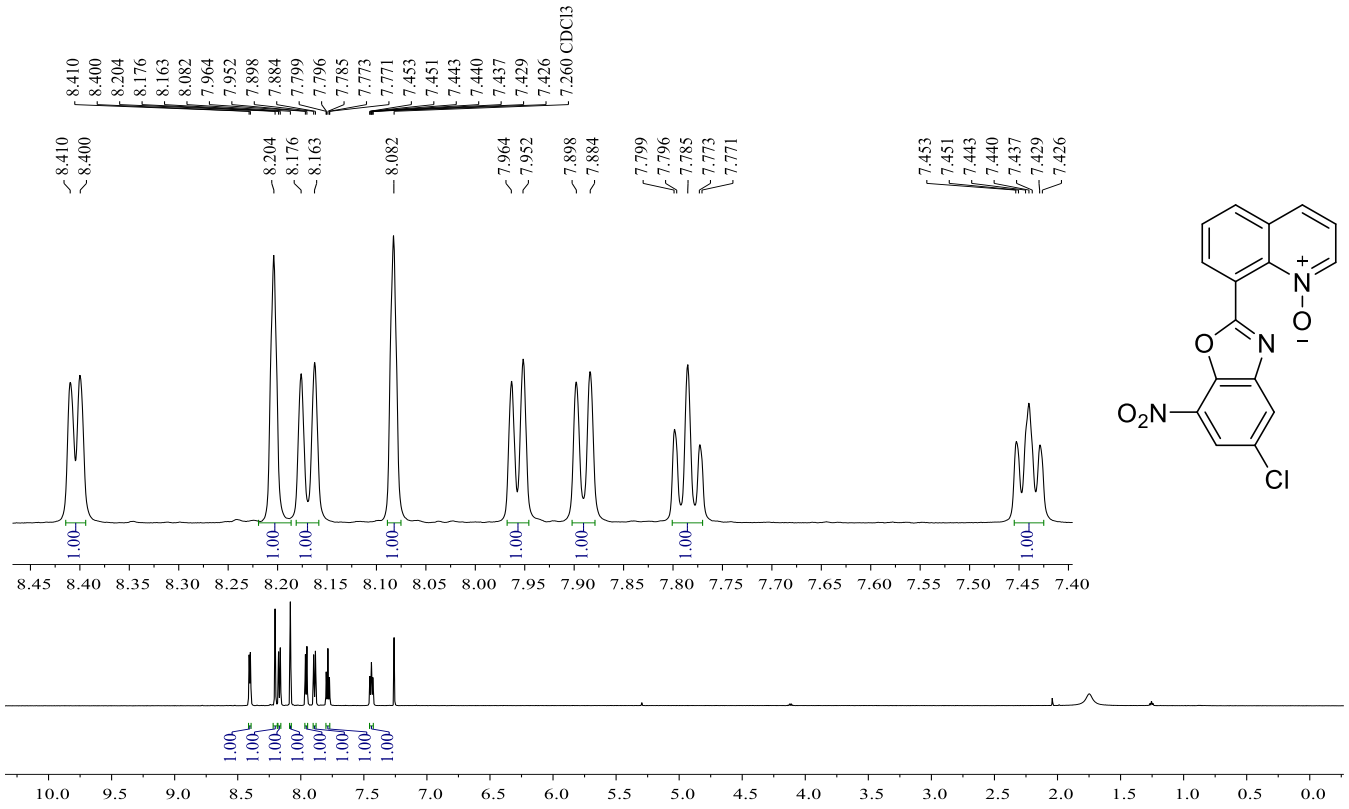


^{13}C{^{1}H} NMR (150 MHz)

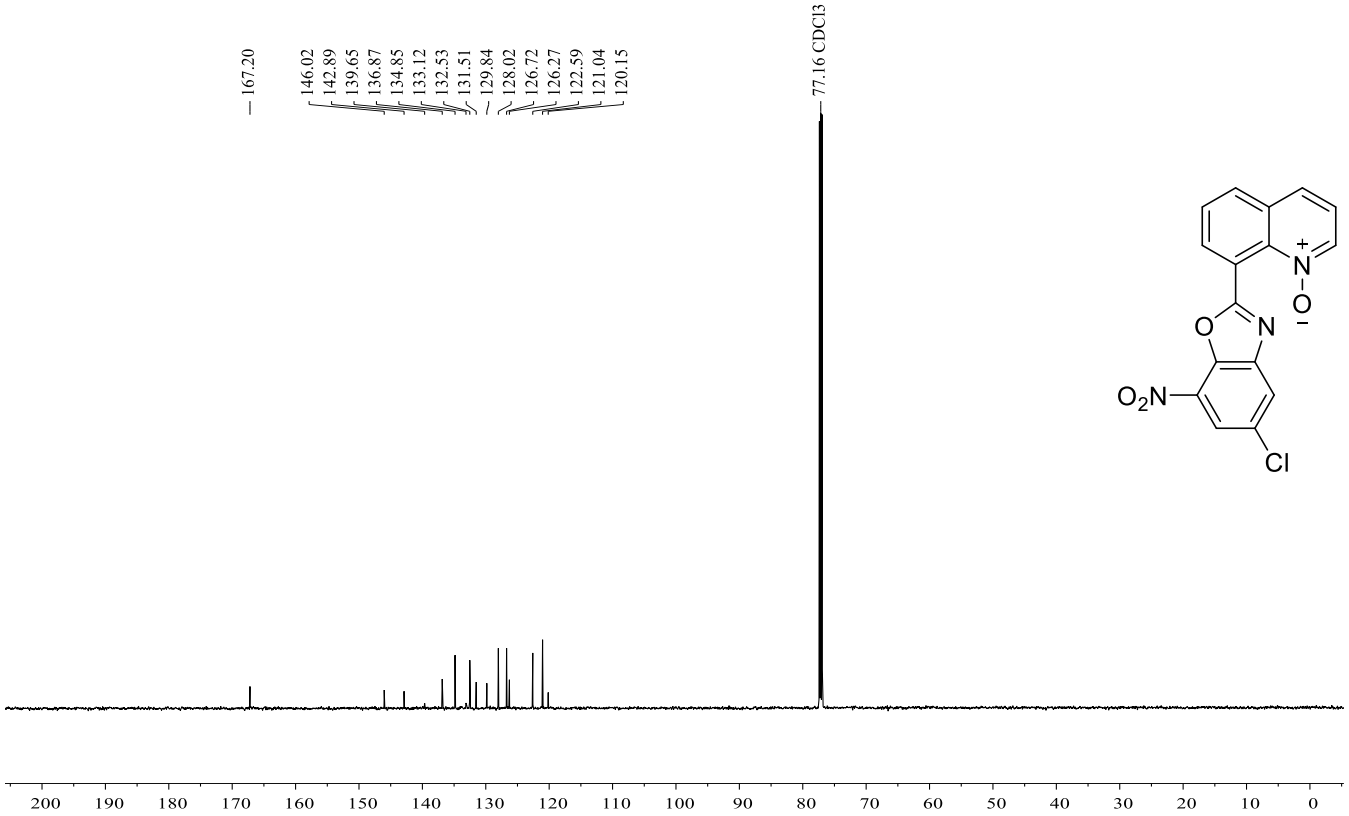


*8-(5-chloro-7-nitrobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3zd**)*

^{1}H NMR (600 MHz)

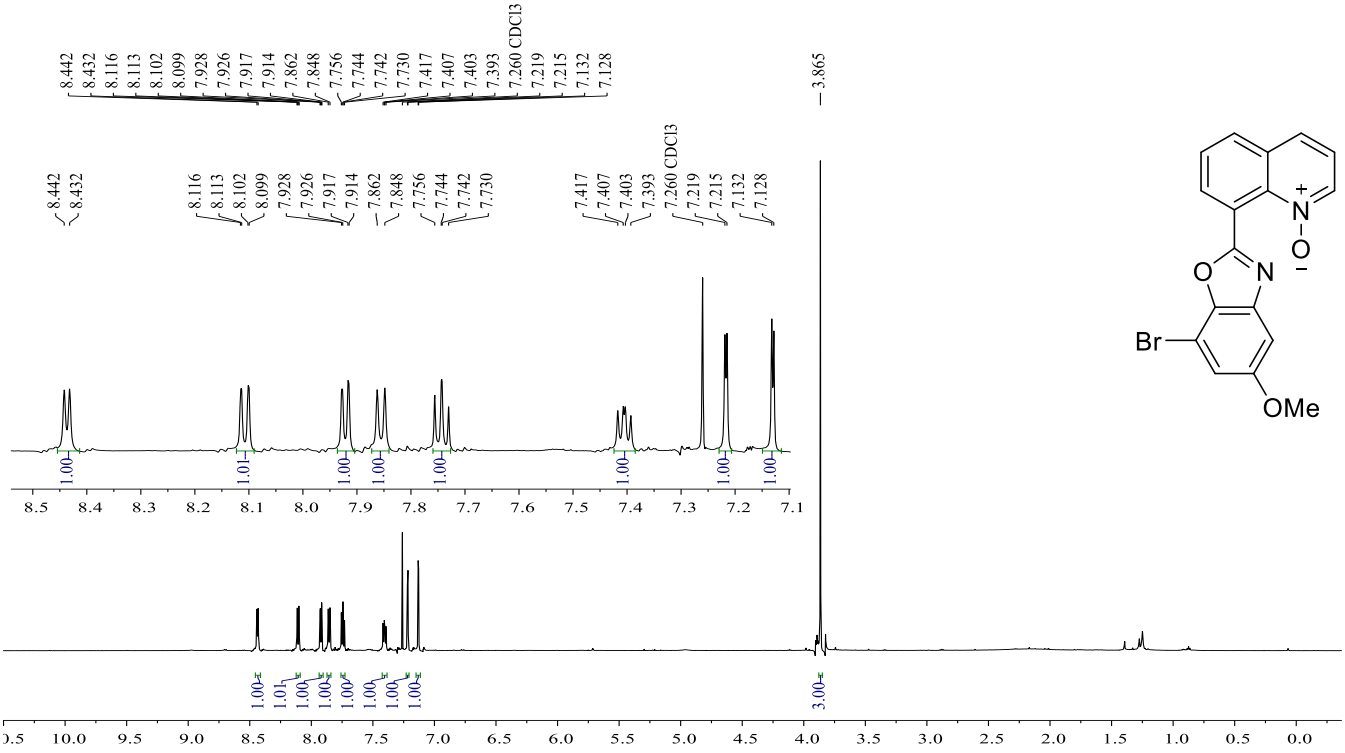


^{13}C{^{1}H} NMR (150 MHz)

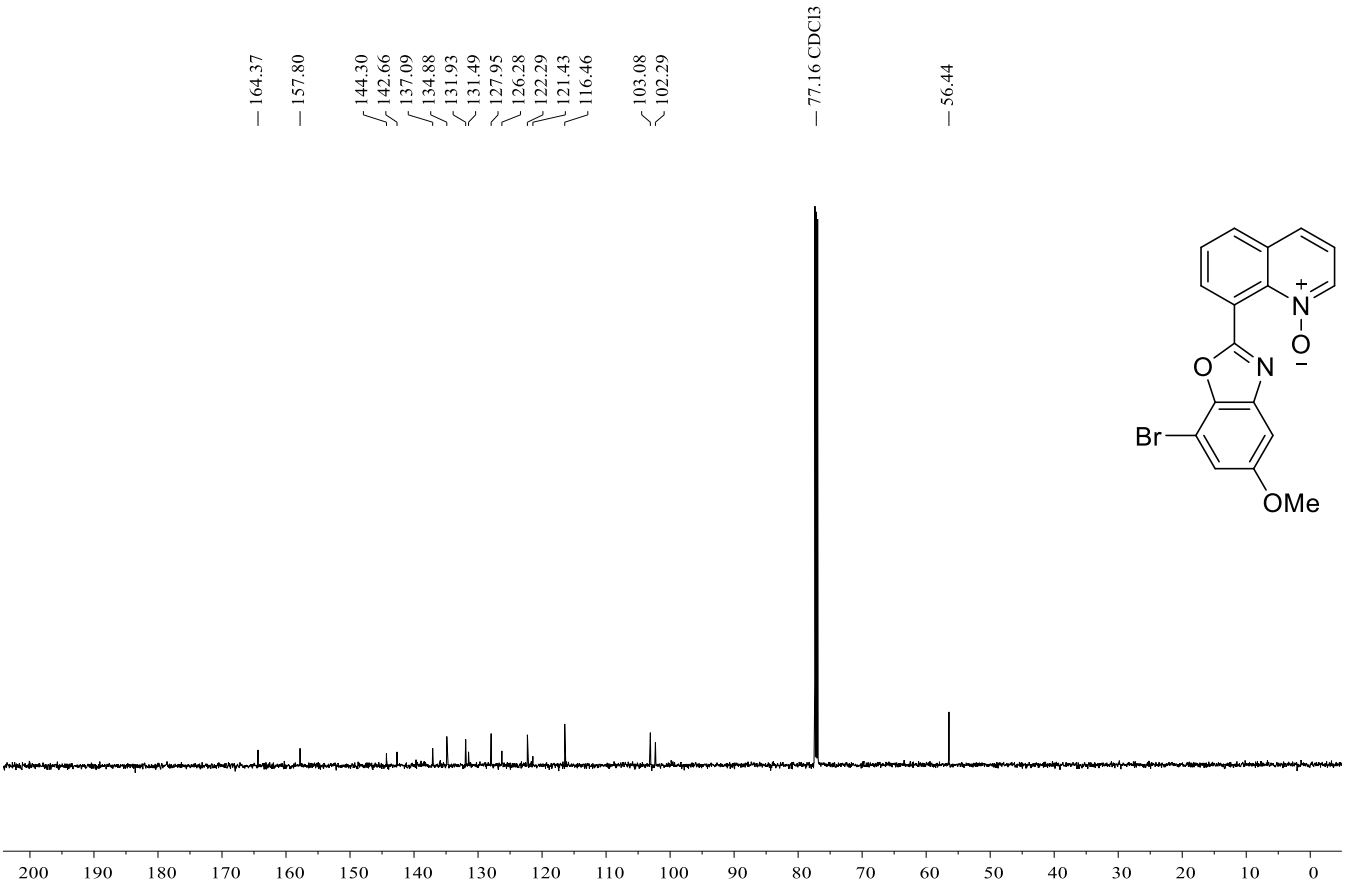


*8-(5-methoxy-7-bromobenzo[d]oxazol-2-yl)quinoline 1-oxide (Table 2, Entry **3ze**)*

^{1}H NMR (600 MHz)

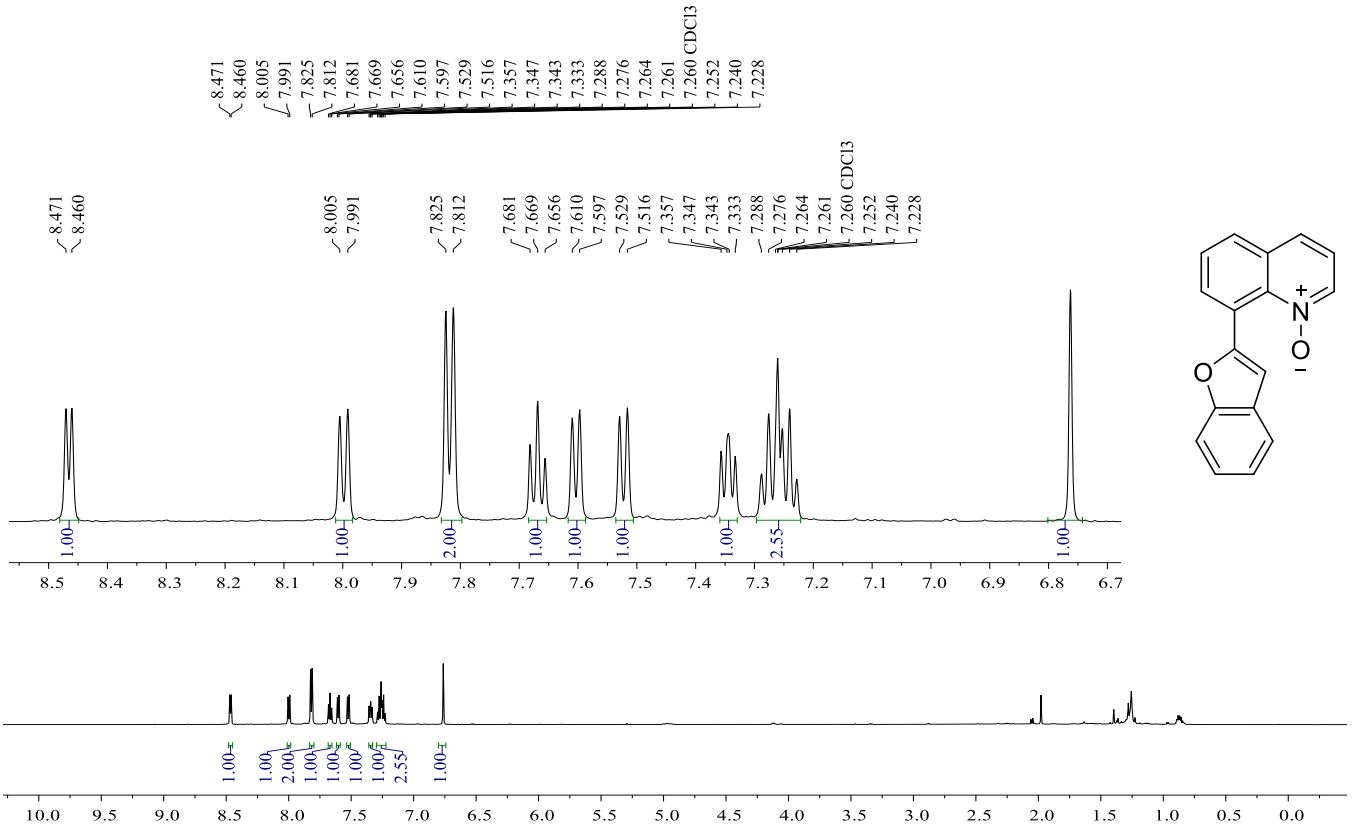


^{13}C{^{1}H} NMR (150 MHz)

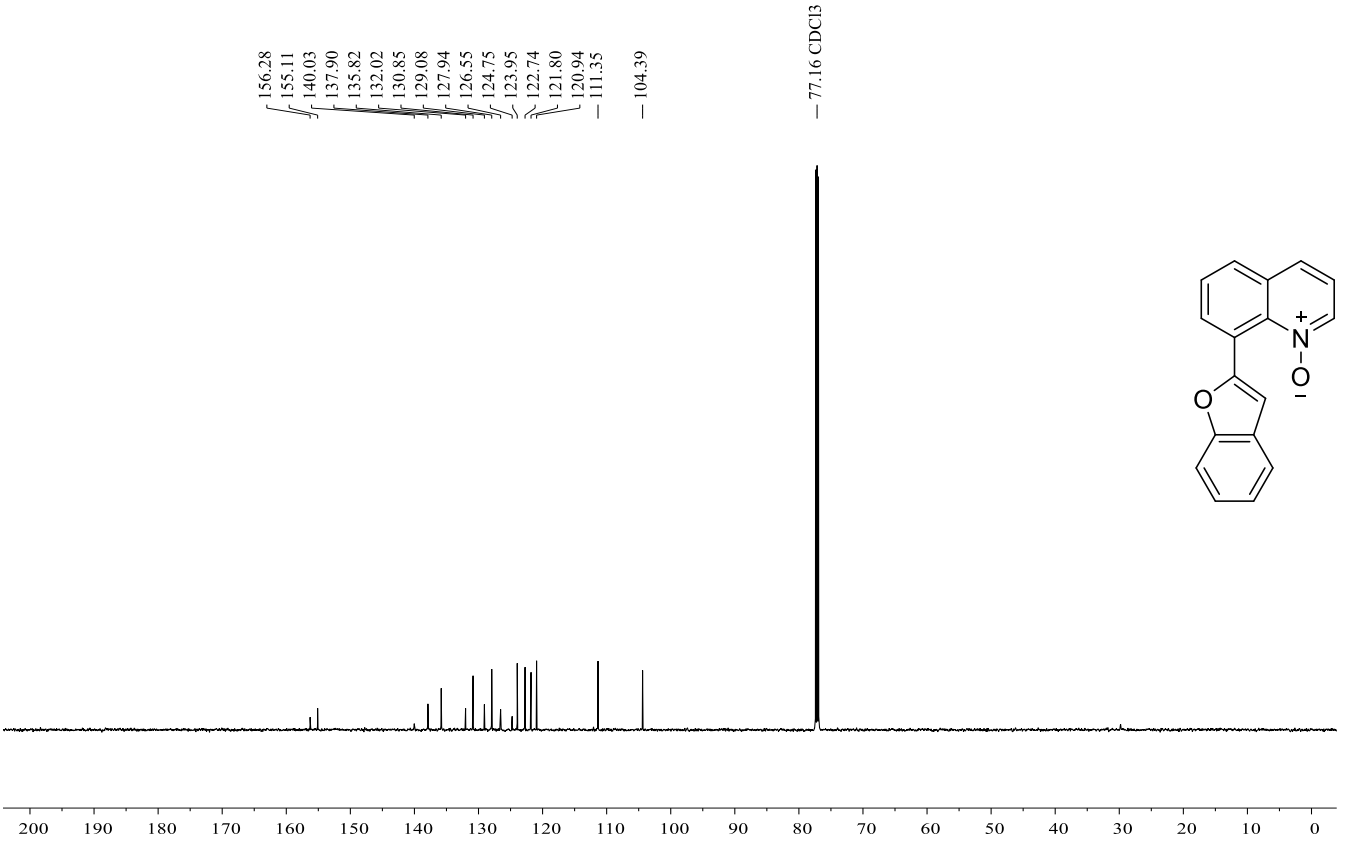


*8-(benzofuran-2-yl)quinoline 1-oxide (Table 3, Entry **6a**)*

^{1}H NMR (600 MHz)

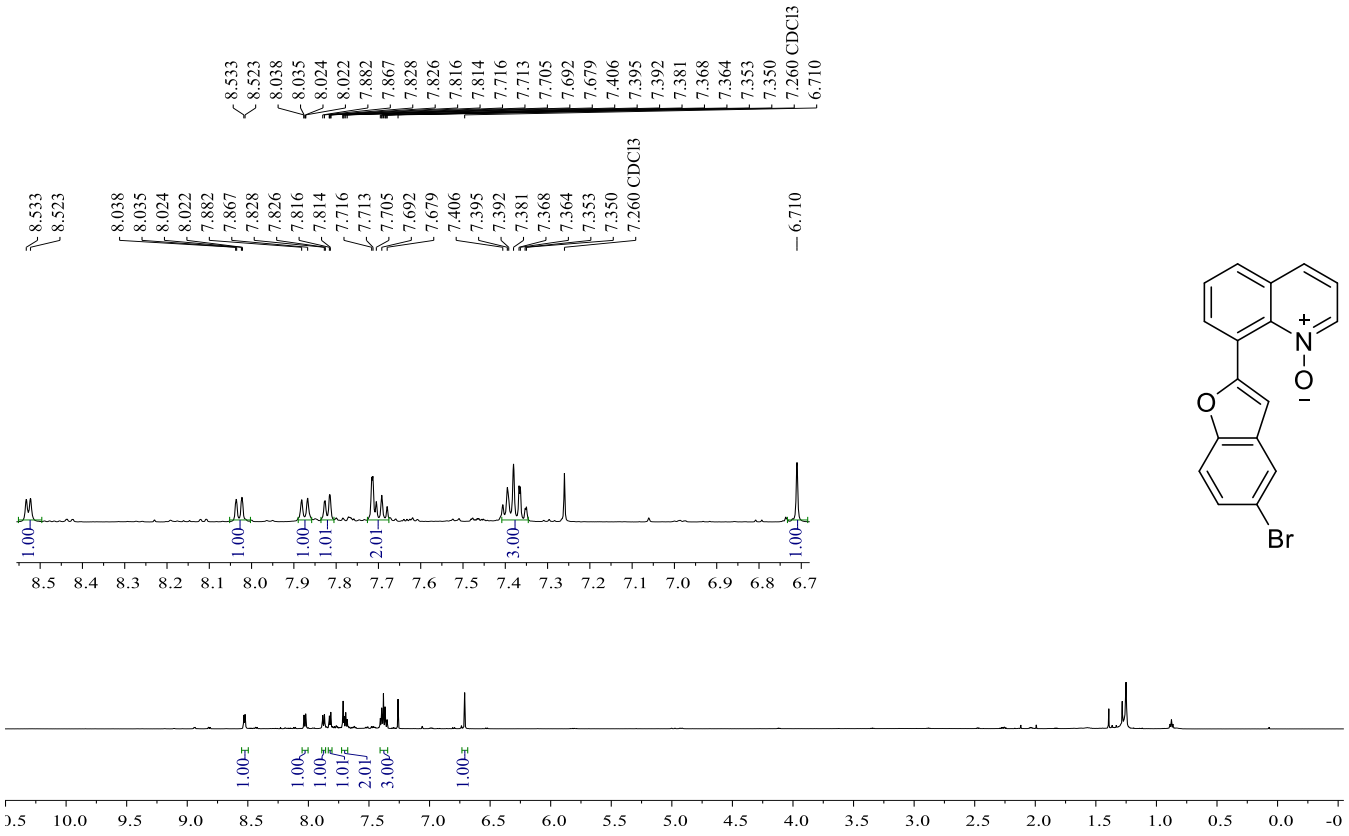


^{13}C{^{1}H} NMR (150 MHz)

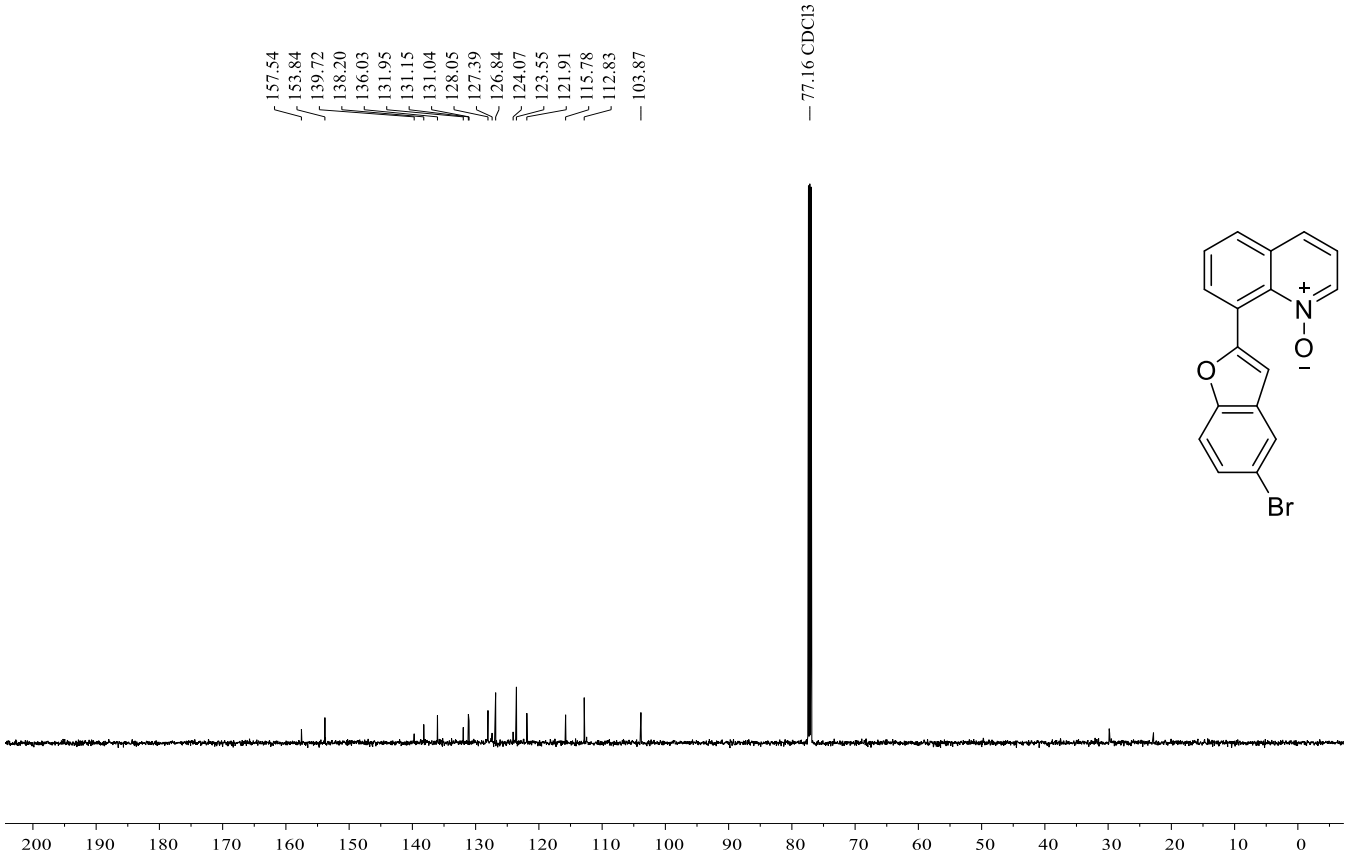


*8-(5-bromobenzofuran-2-yl)quinoline 1-oxide (Table 3, Entry **6b**)*

^{1}H NMR (600 MHz)

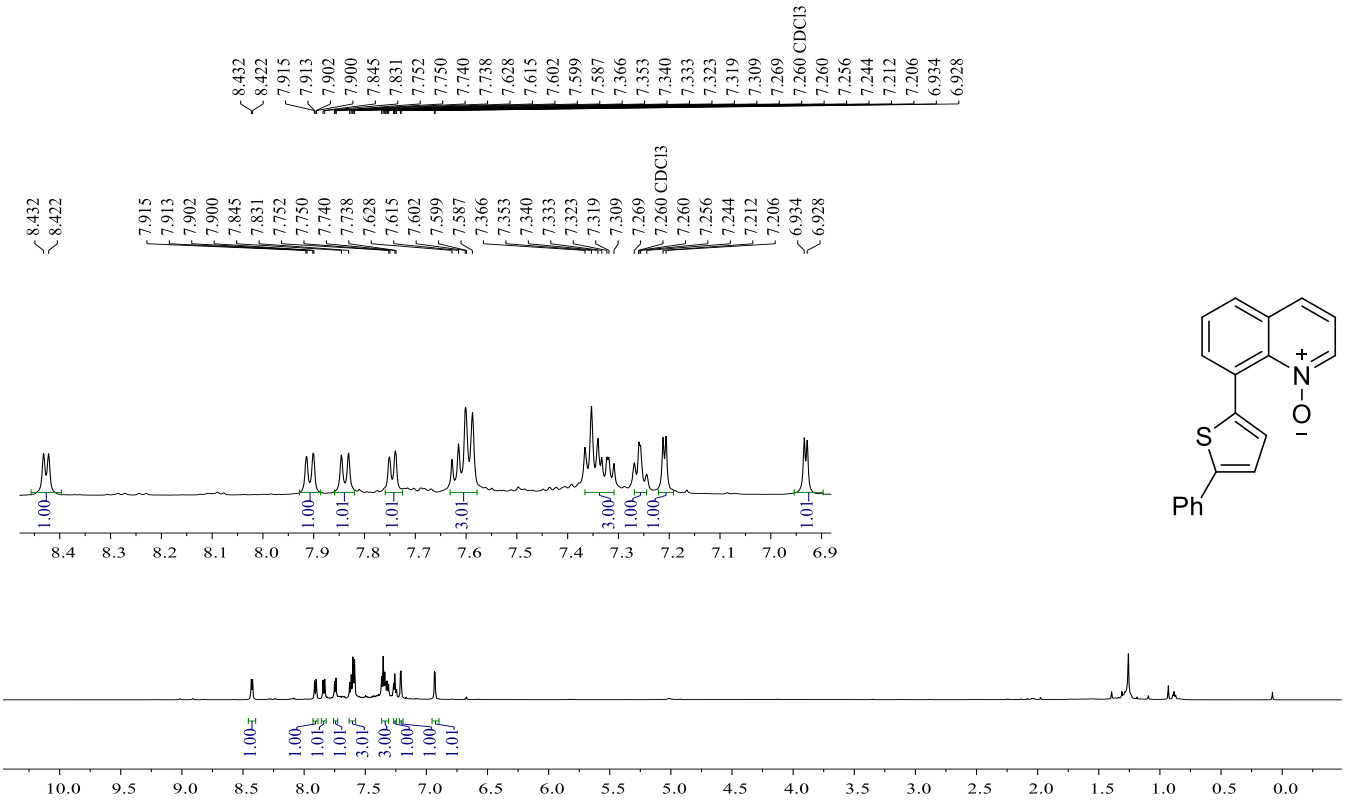


^{13}C{^{1}H} NMR (150 MHz)

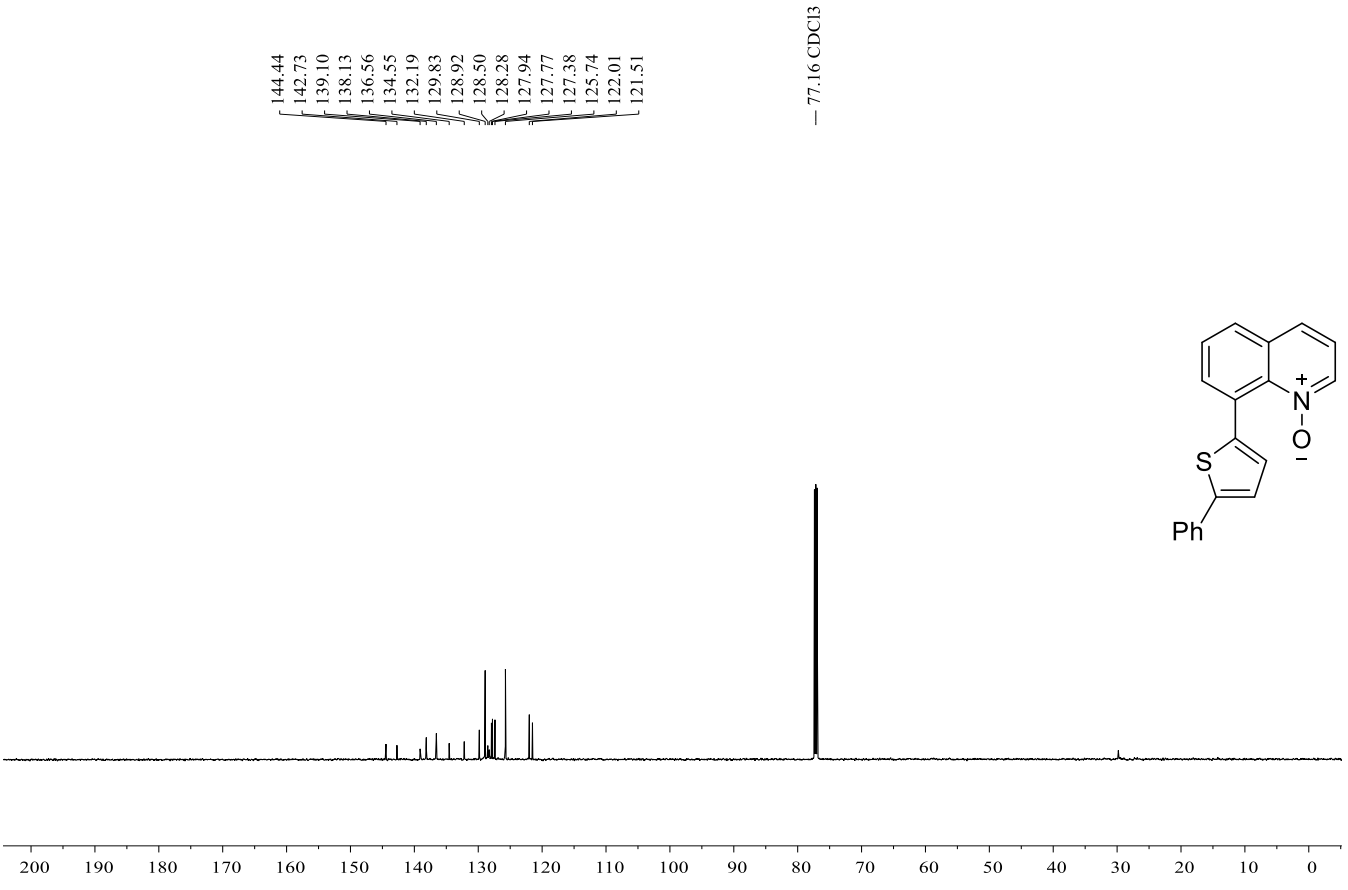


*8-(5-phenylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6c**)*

^{1}H NMR (600 MHz)

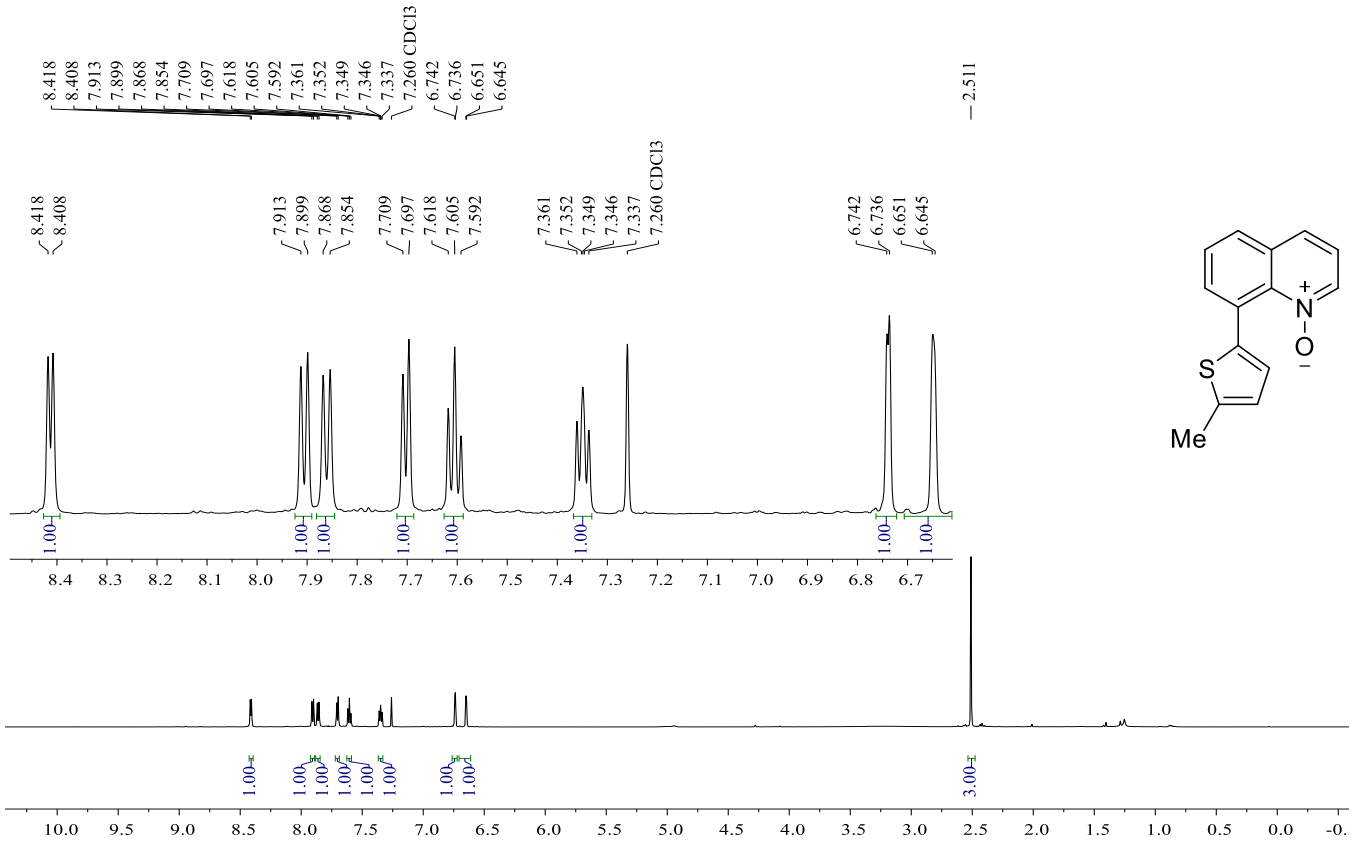


^{13}C{^{1}H} NMR (150 MHz)

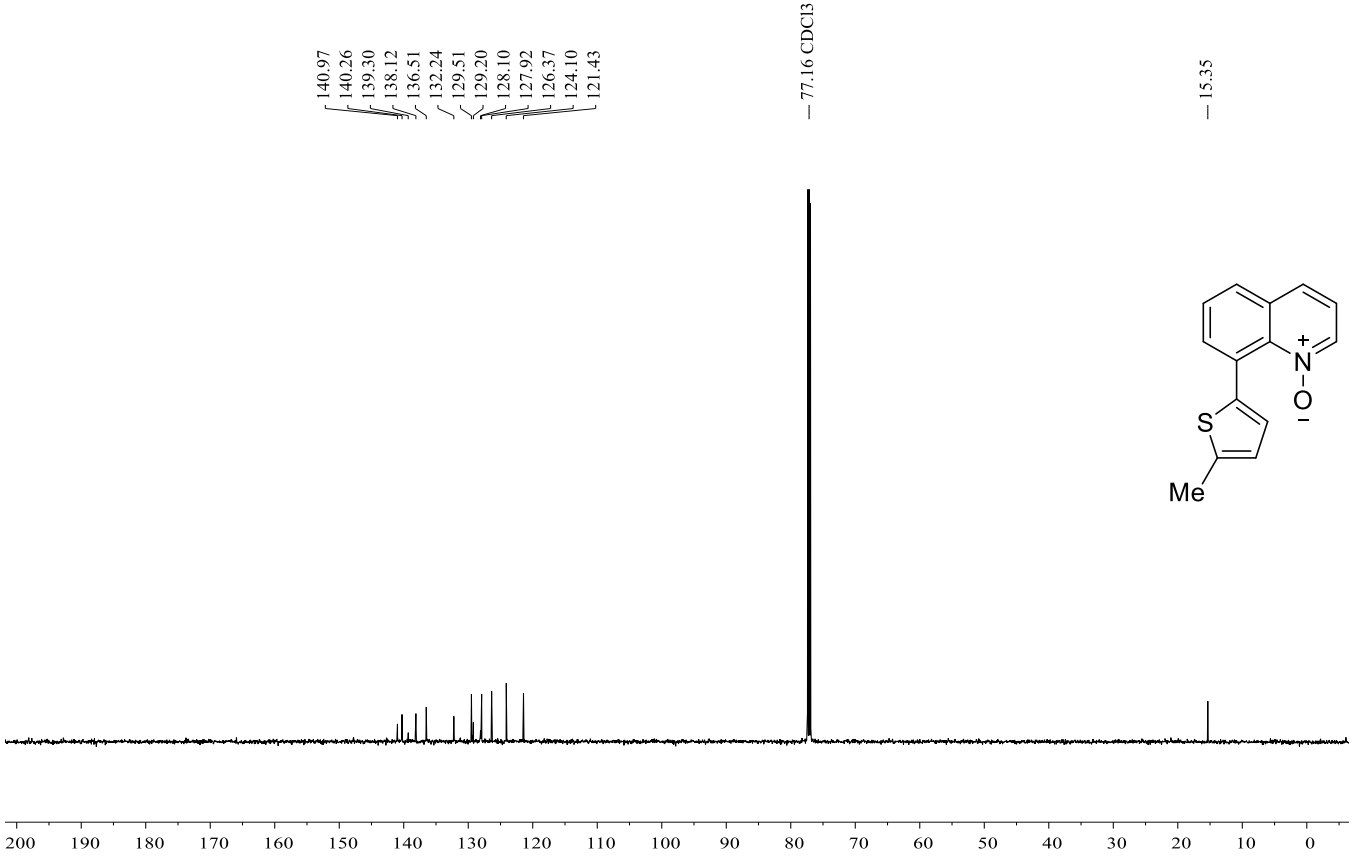


*8-(5-methylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6d**)*

^{1}H NMR (600 MHz)

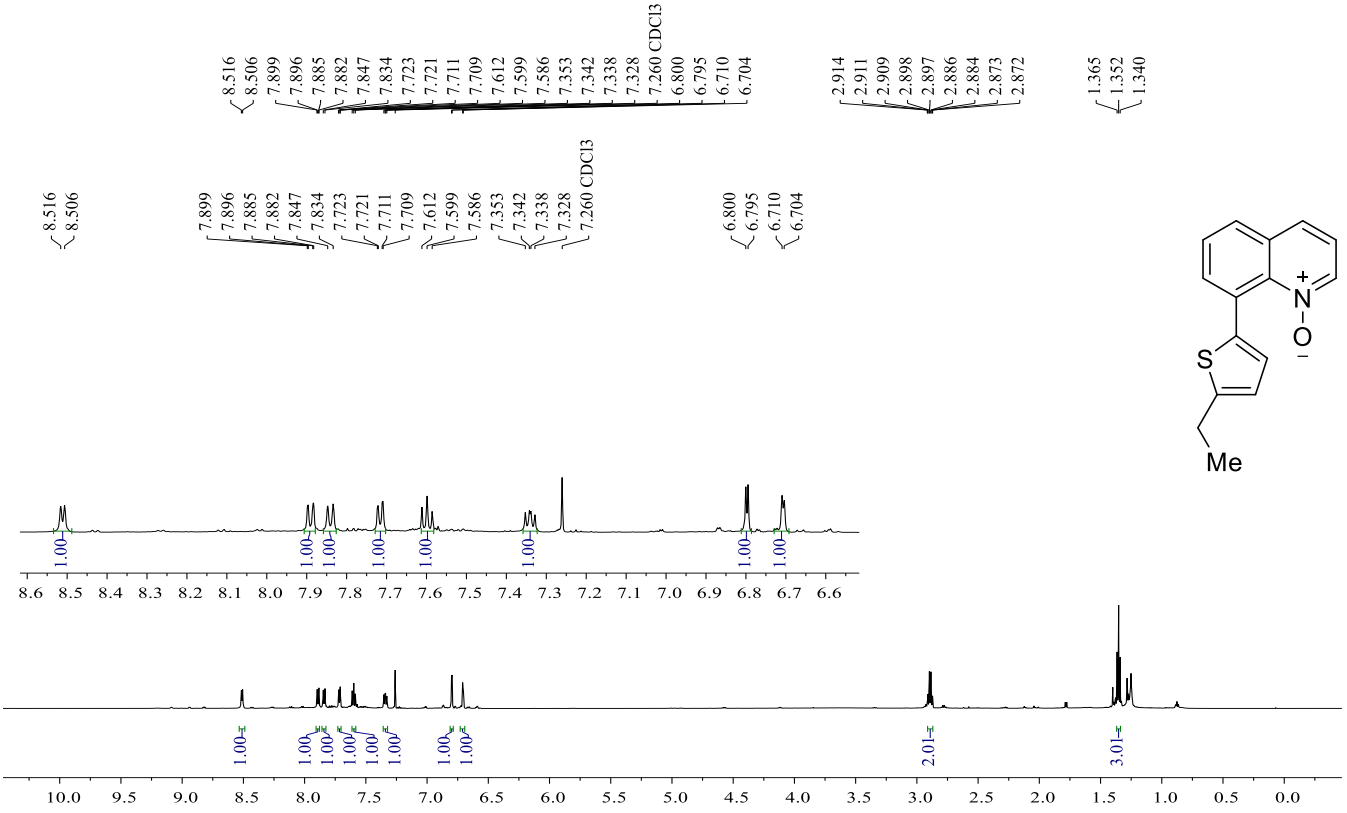


^{13}C{^{1}H} NMR (150 MHz)

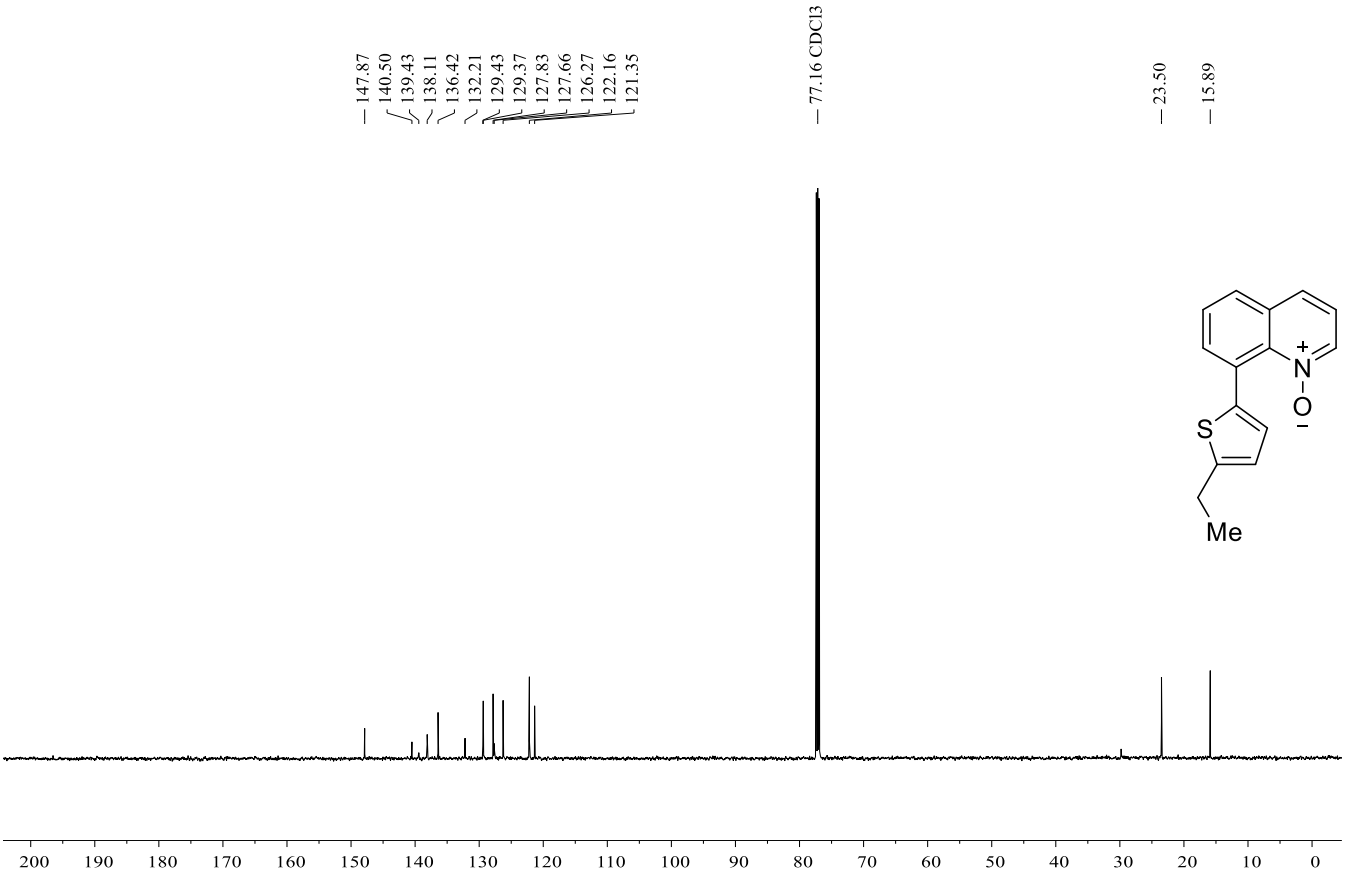


*8-(5-ethylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6e**)*

^{1}H NMR (600 MHz

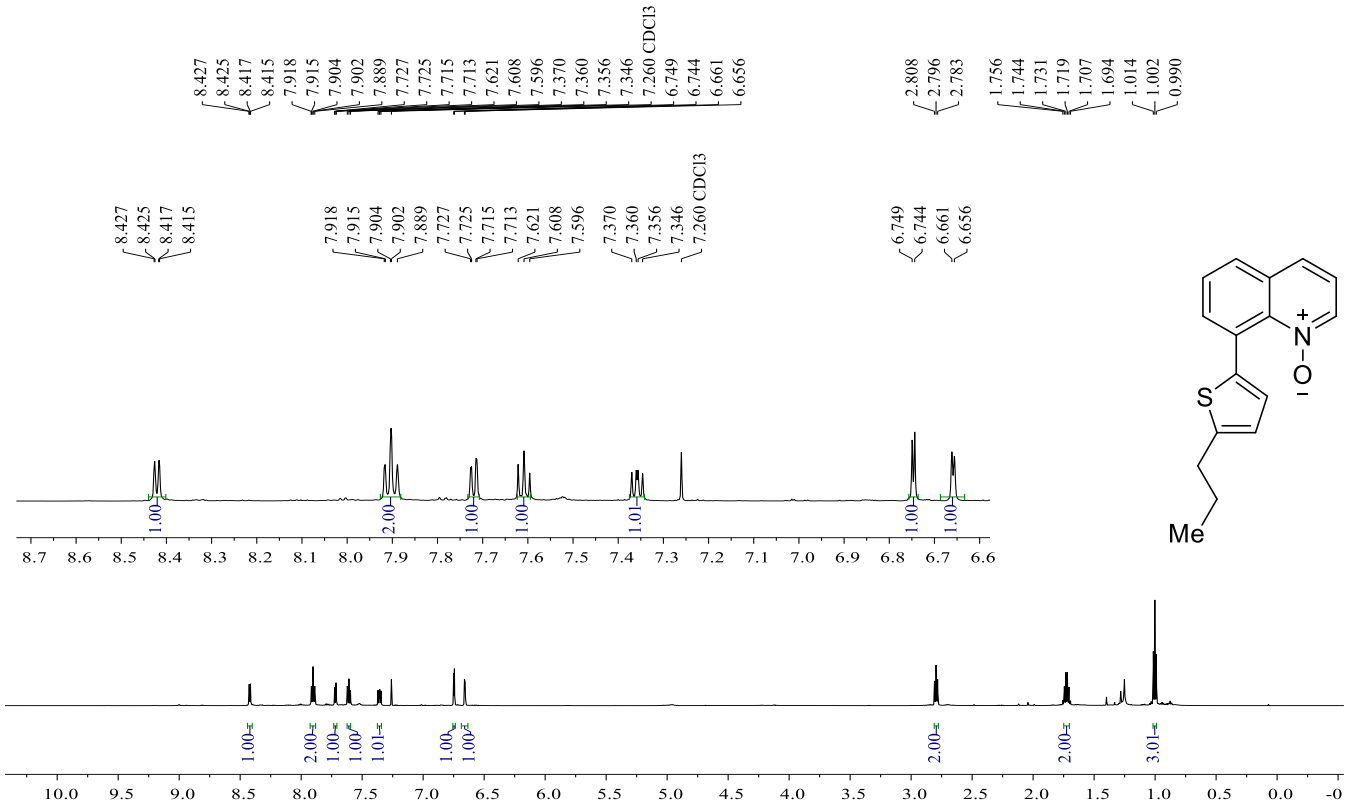


^{13}C{^{1}H} NMR (150 MHz)

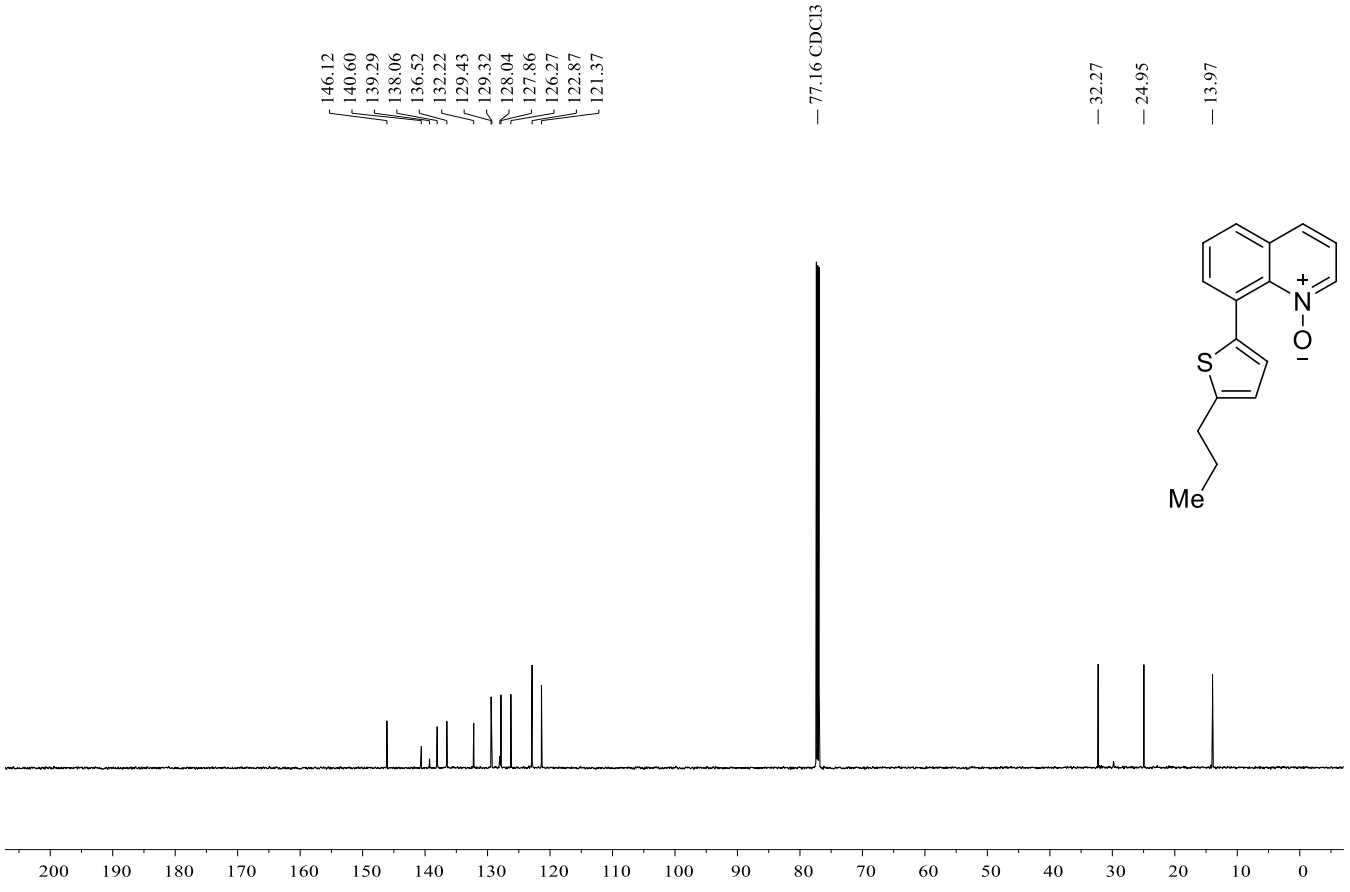


*8-(5-propylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6f**)*

^{1}H NMR (600 MHz)

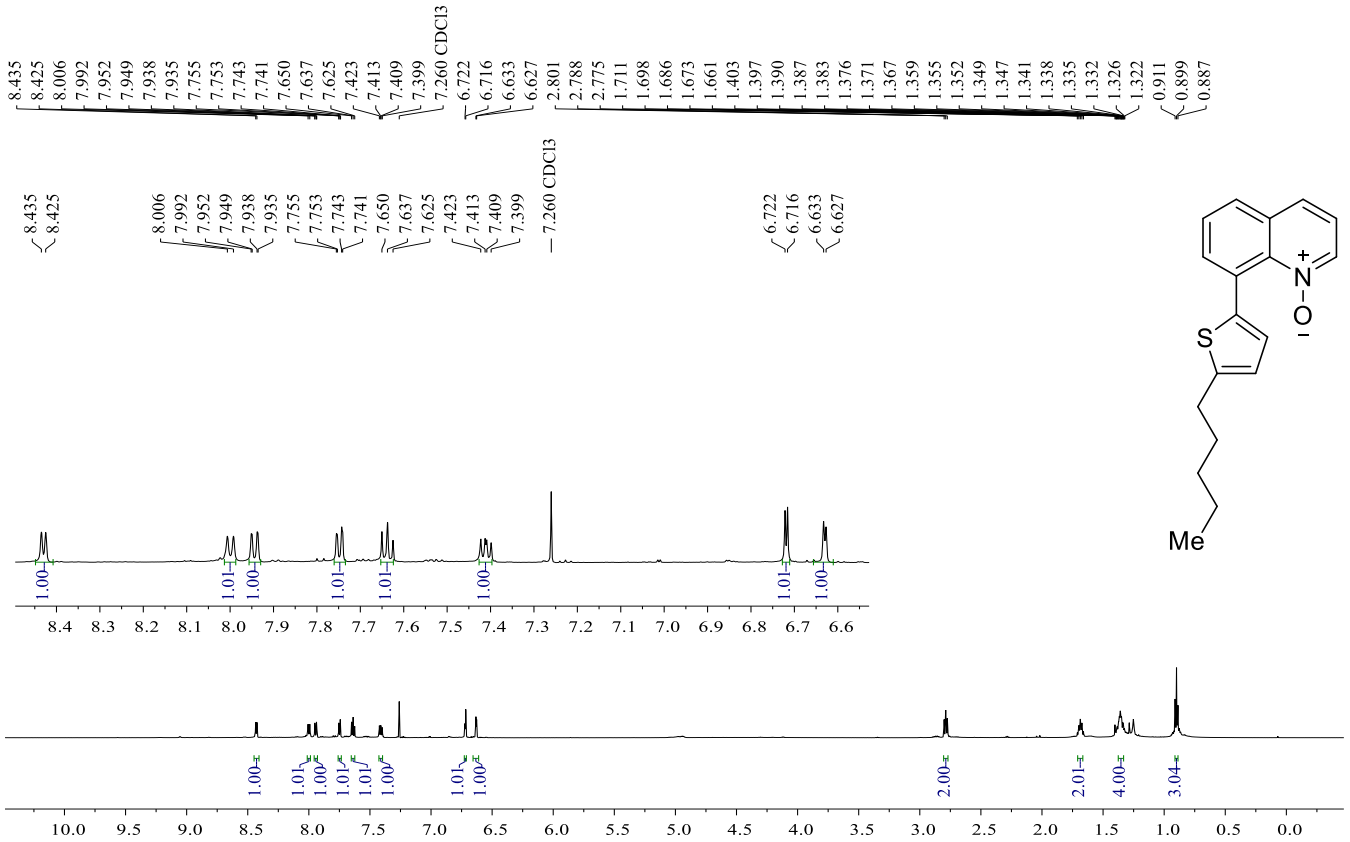


^{13}C{^{1}H} NMR (150 MHz)

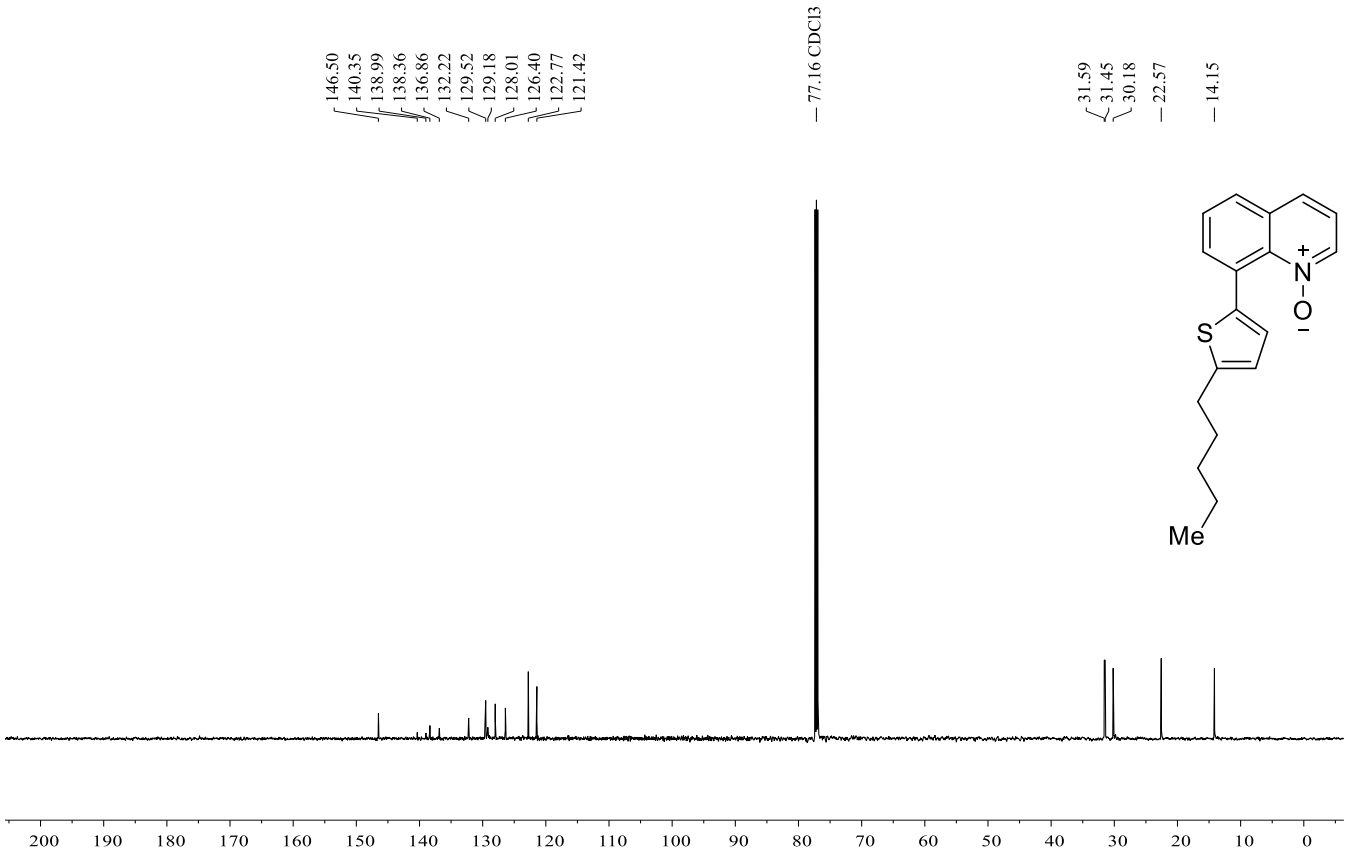


*8-(5-pentylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6g**)*

^{1}H NMR (600 MHz)

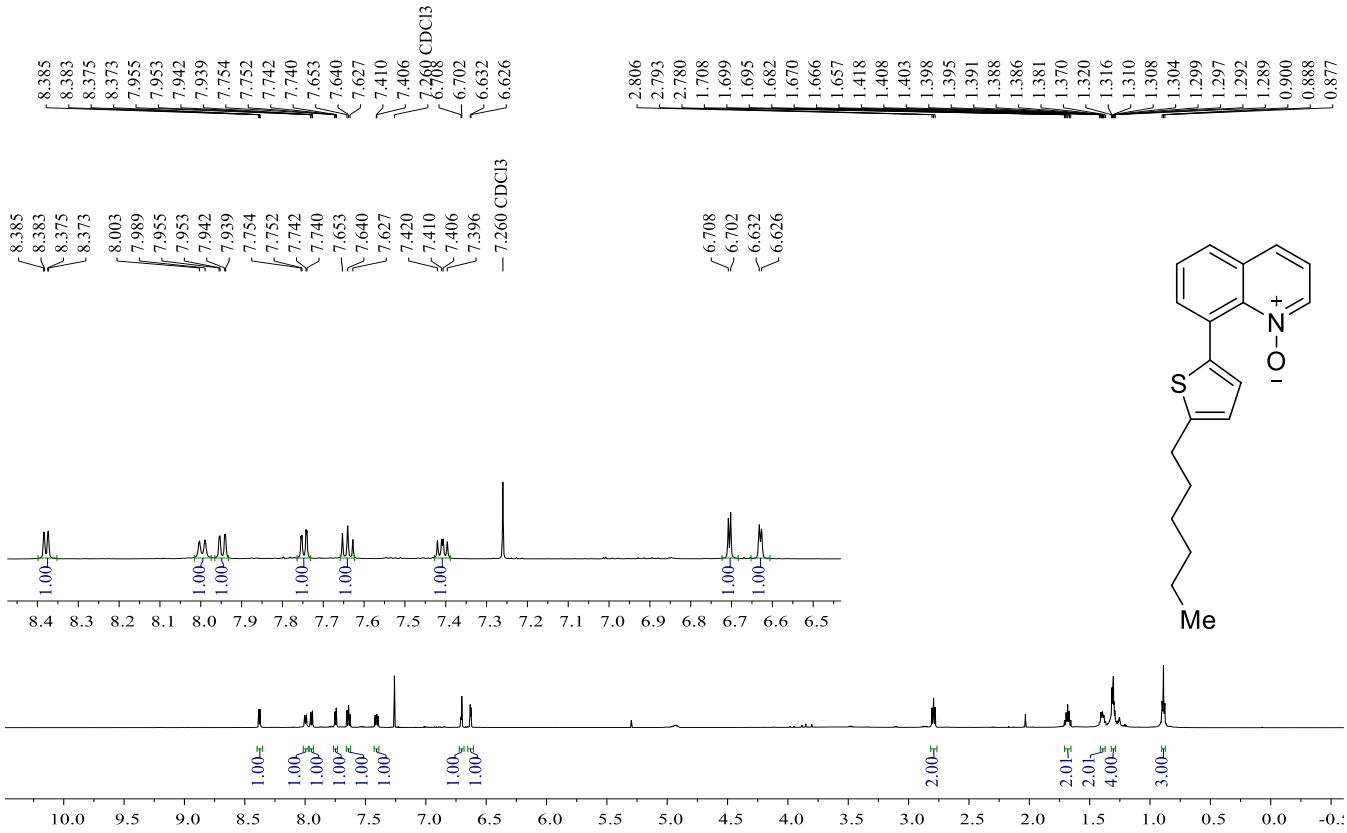


^{13}C{^{1}H} NMR (150 MHz)

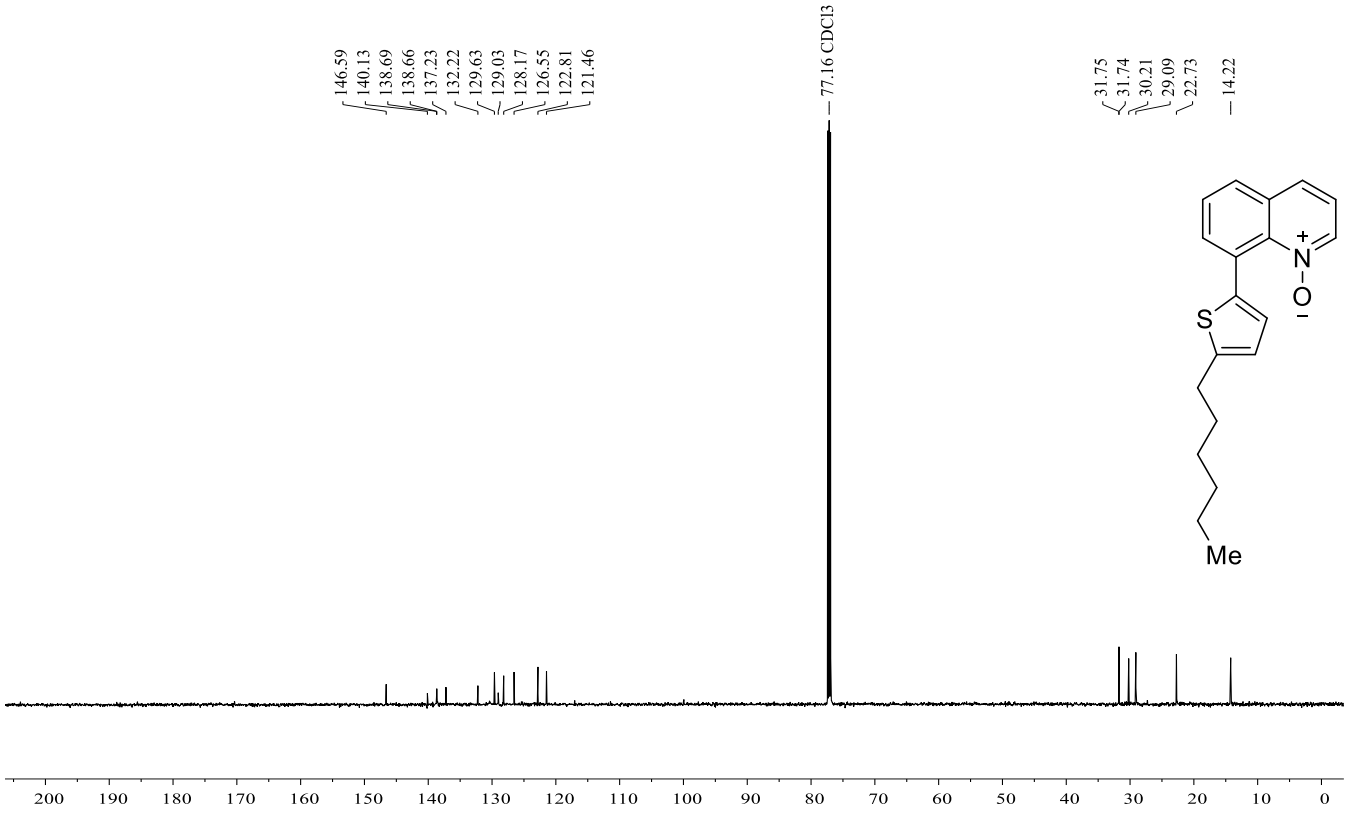


*8-(5-hexylthiophen-2-yl)quinoline 1-oxide (Table 3, Entry **6h**)*

^{1}H NMR (600 MHz)

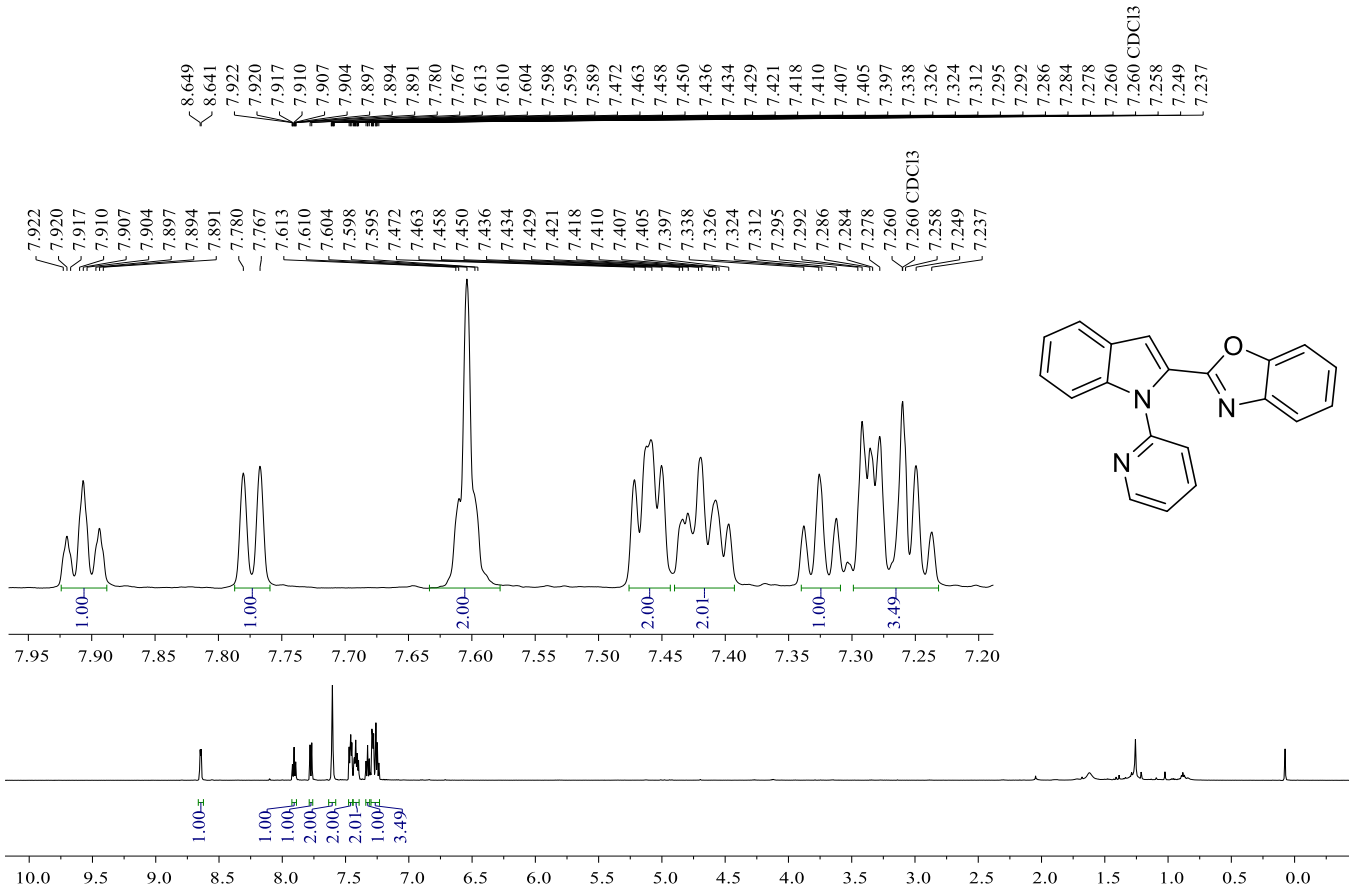


^{13}C{^{1}H} NMR (150 MHz)

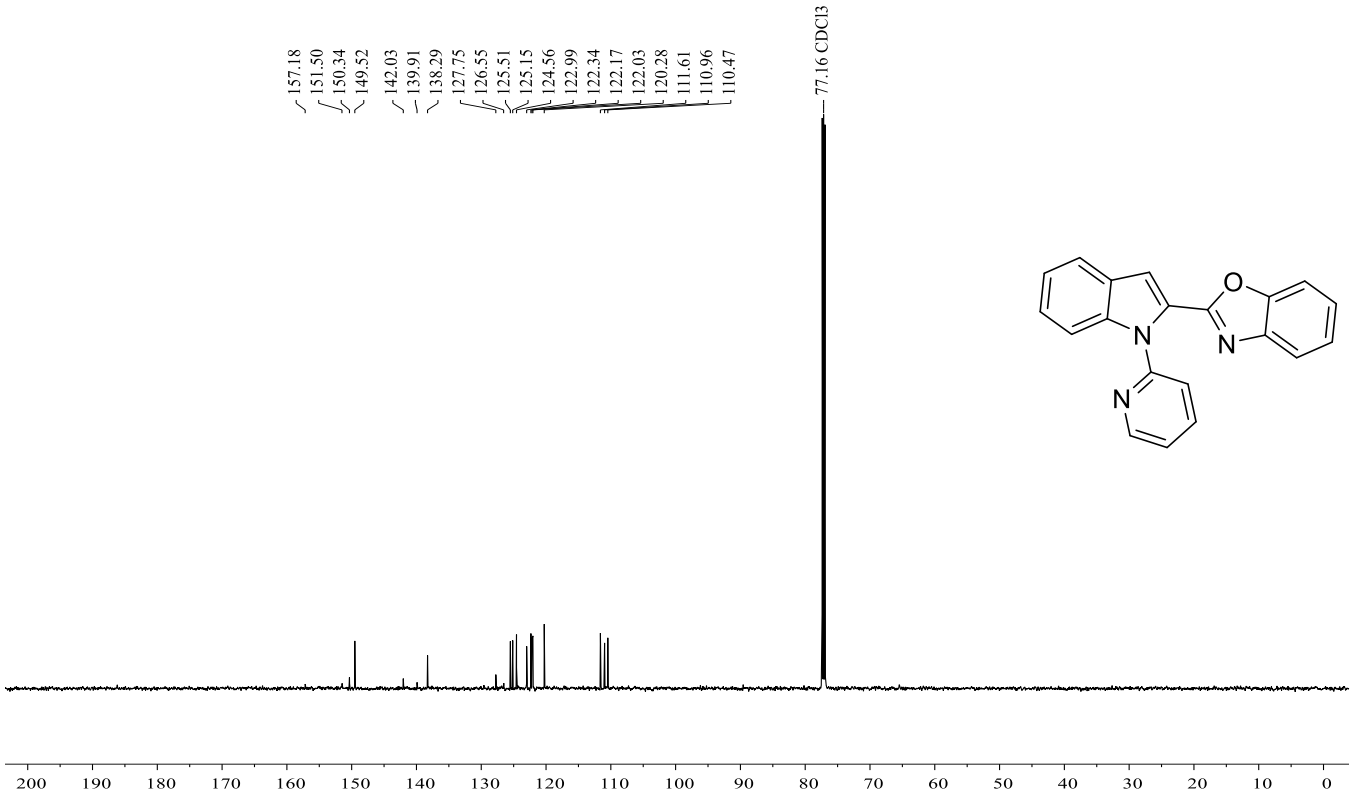


*2-(1-(pyridin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6i**)*

^{1}H NMR (600 MHz)

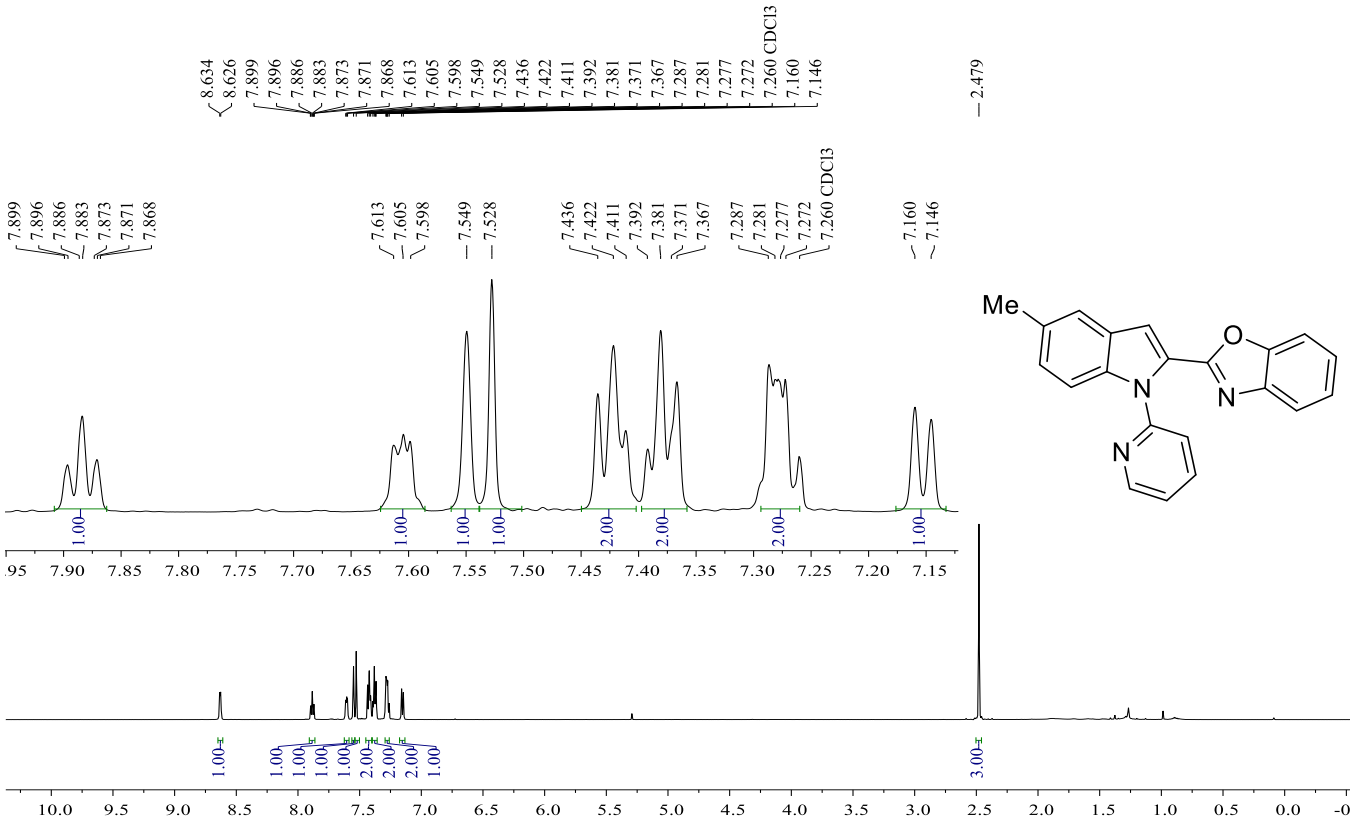


^{13}C{^{1}H} NMR (150 MHz)

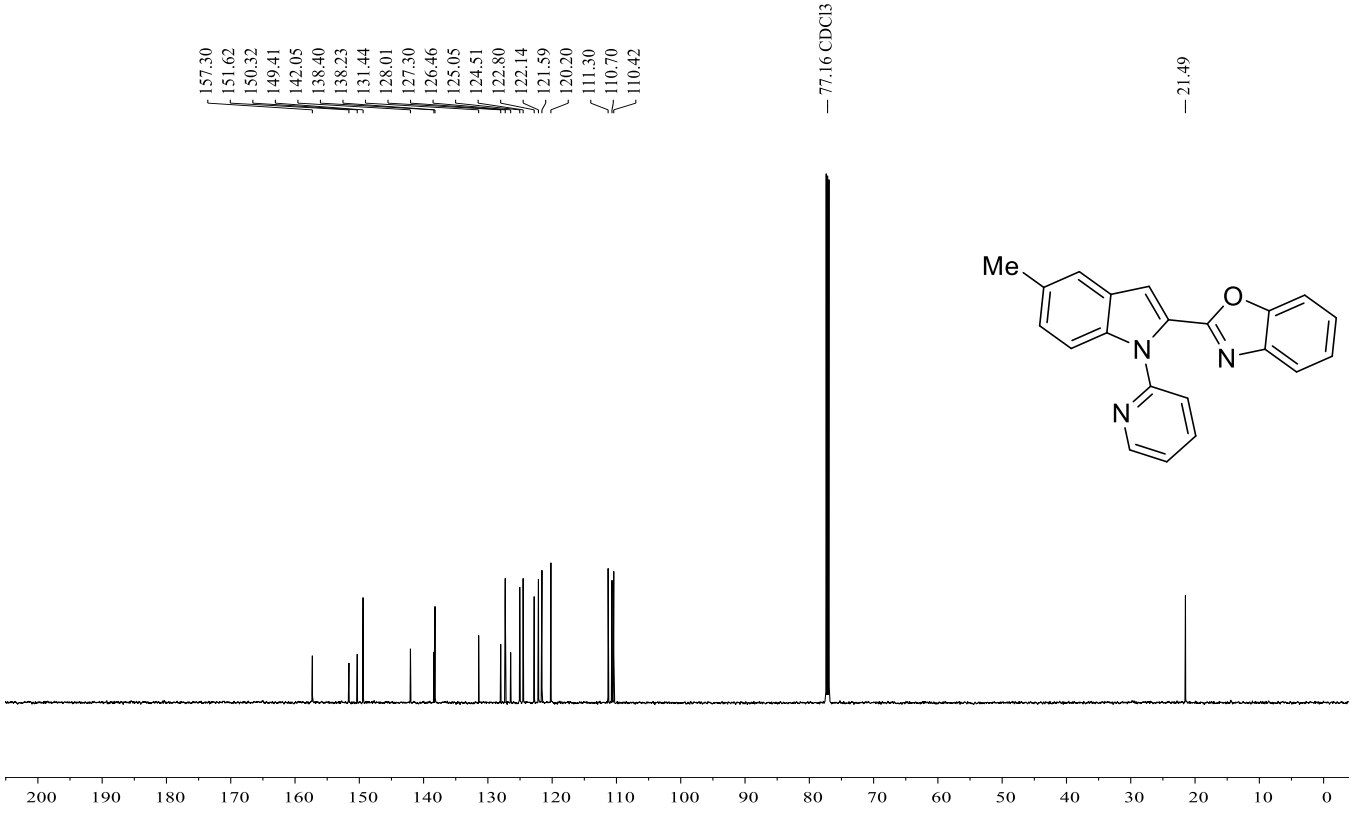


*2-(5-methyl-1-(pyridin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6j**)*

^{1}H NMR (600 MHz)

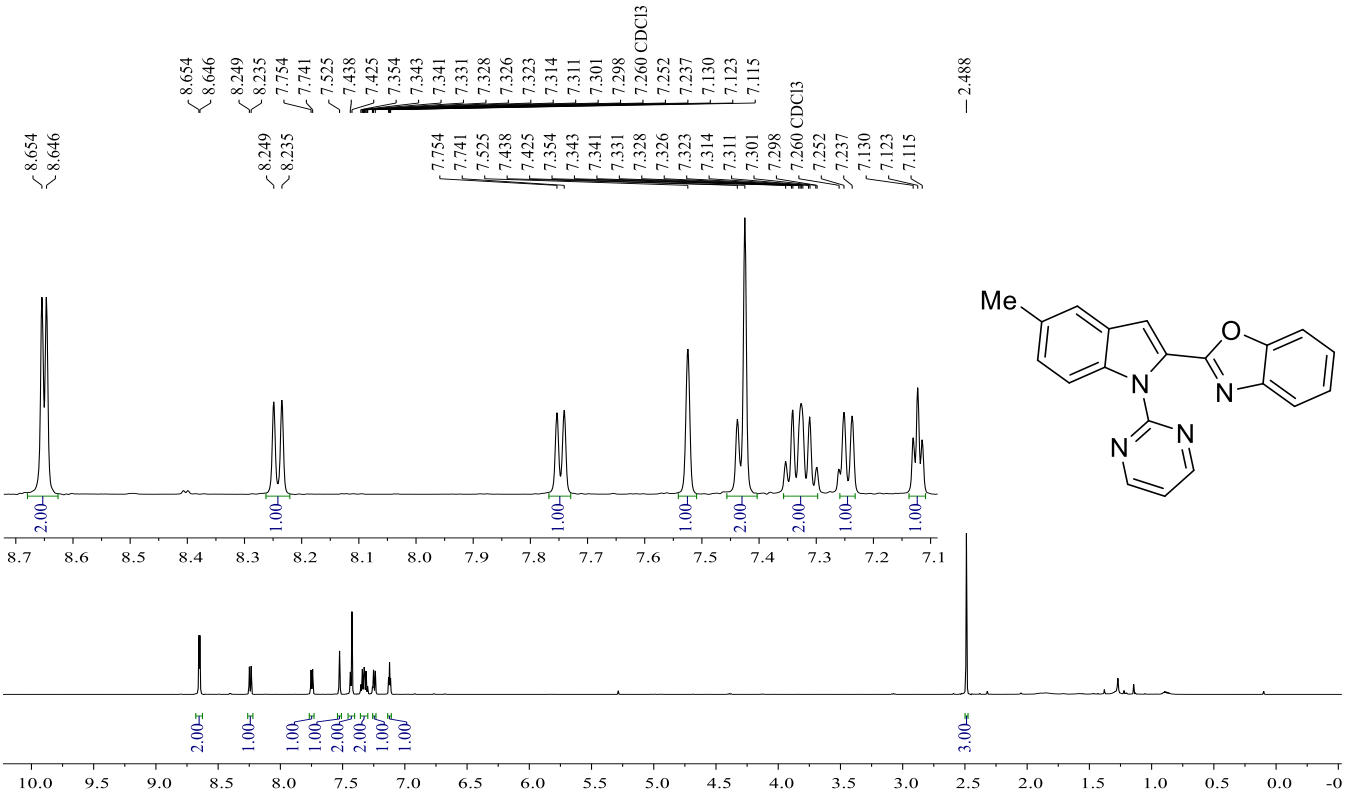


^{13}C{^{1}H} NMR (150 MHz)

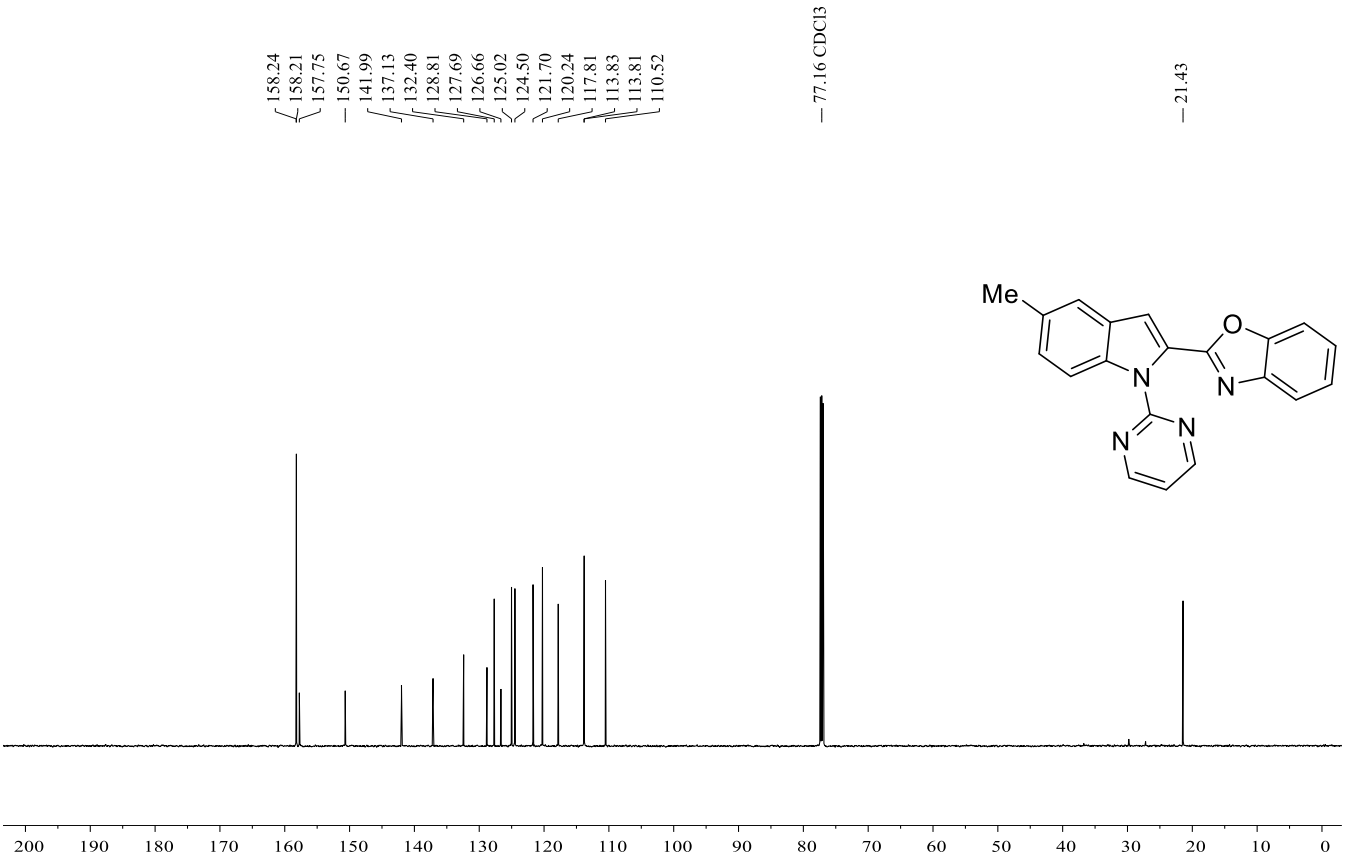


*2-(5-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6k**)*

^{1}H NMR (600 MHz)

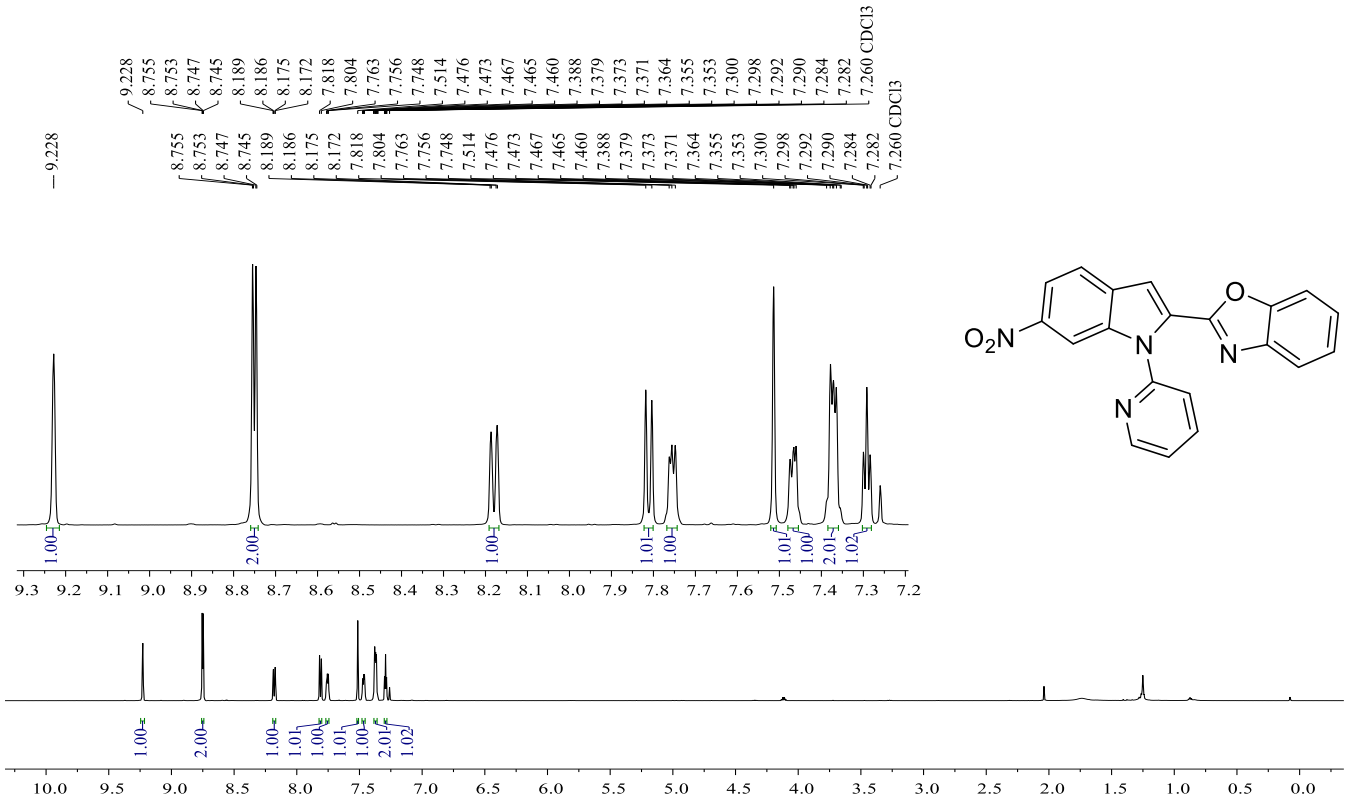


^{13}C{^{1}H} NMR (150 MHz)

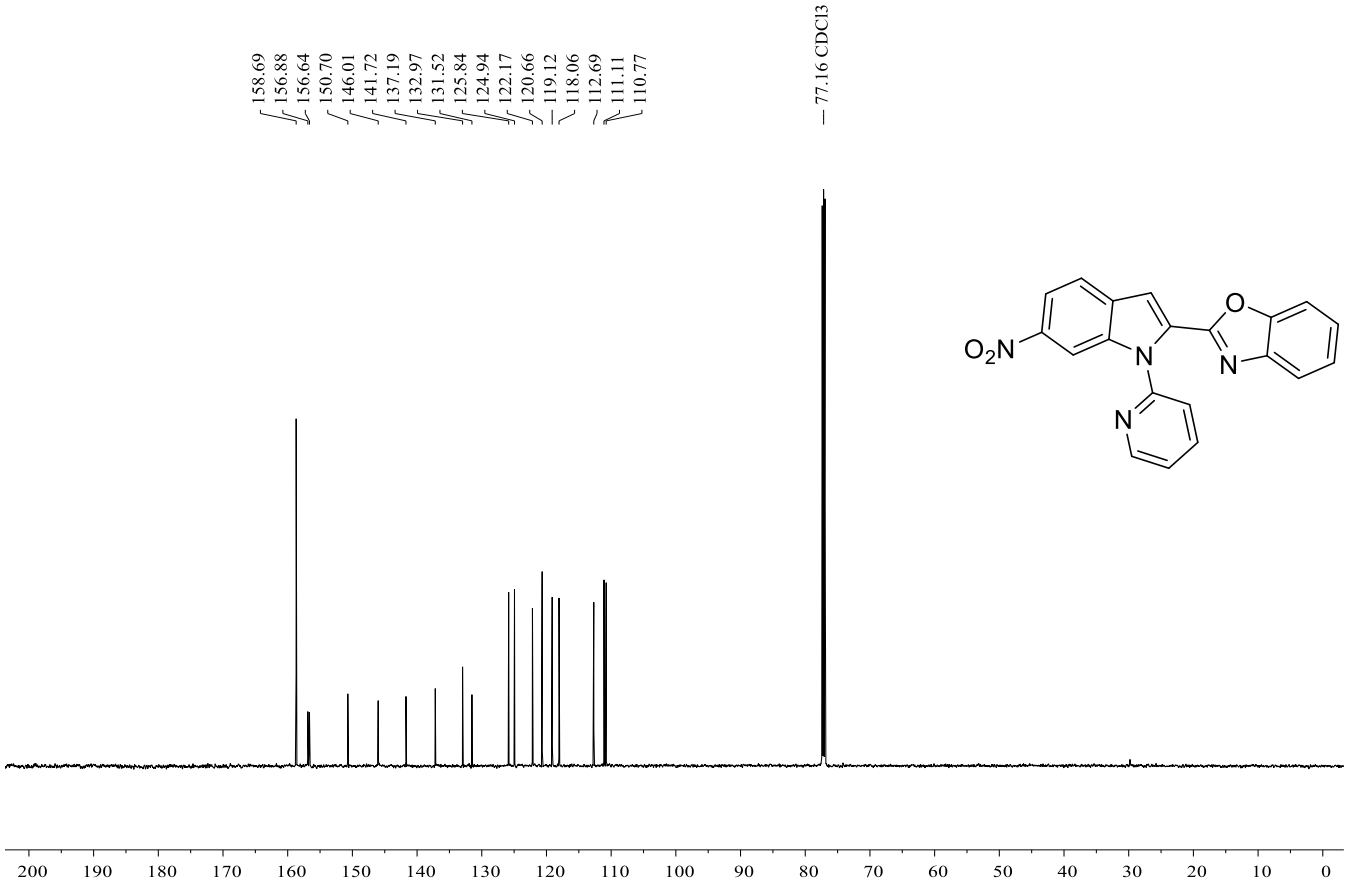


*2-(6-nitro-1-(pyridin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6l**)*

^{1}H NMR (600 MHz)

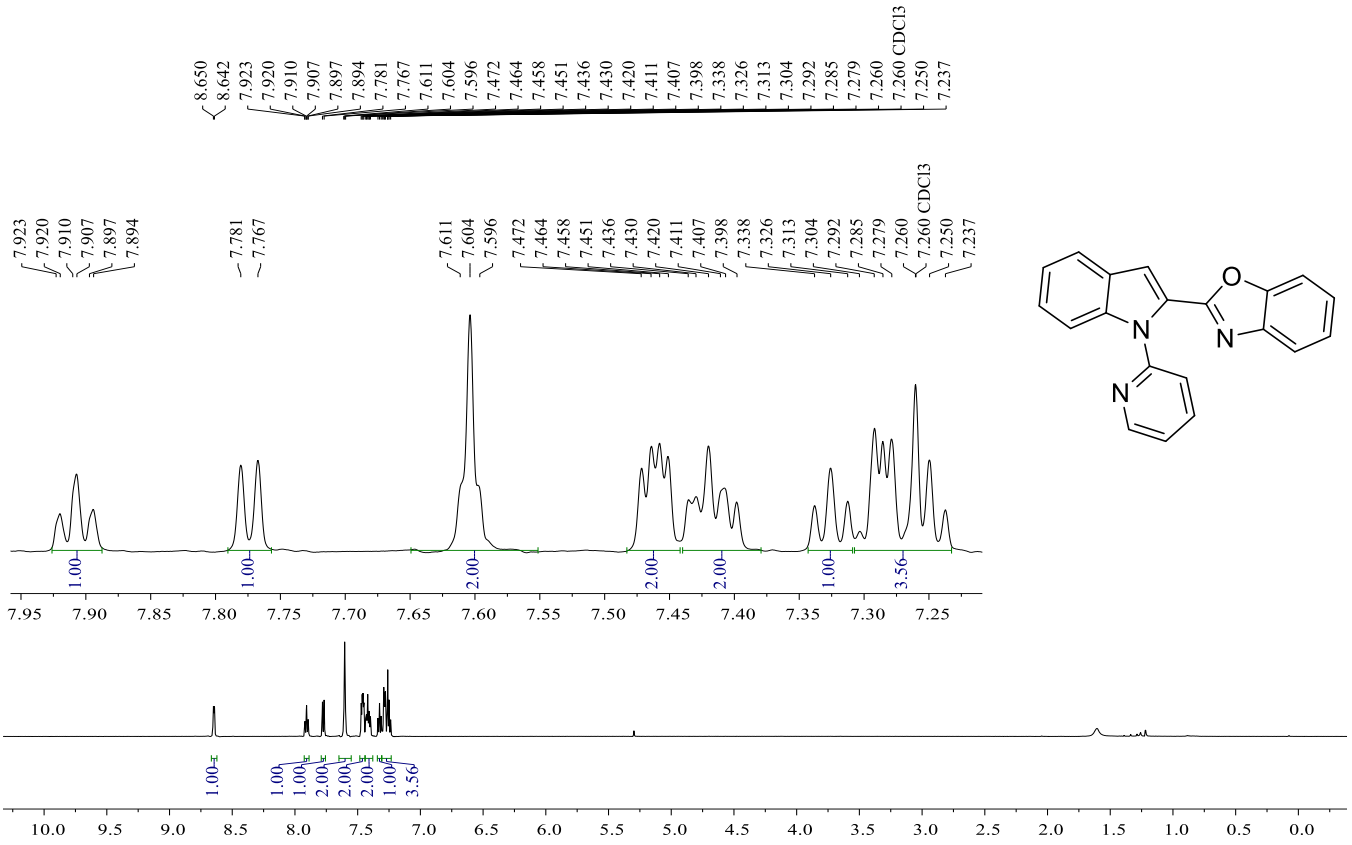


^{13}C{^{1}H} NMR (150 MHz)

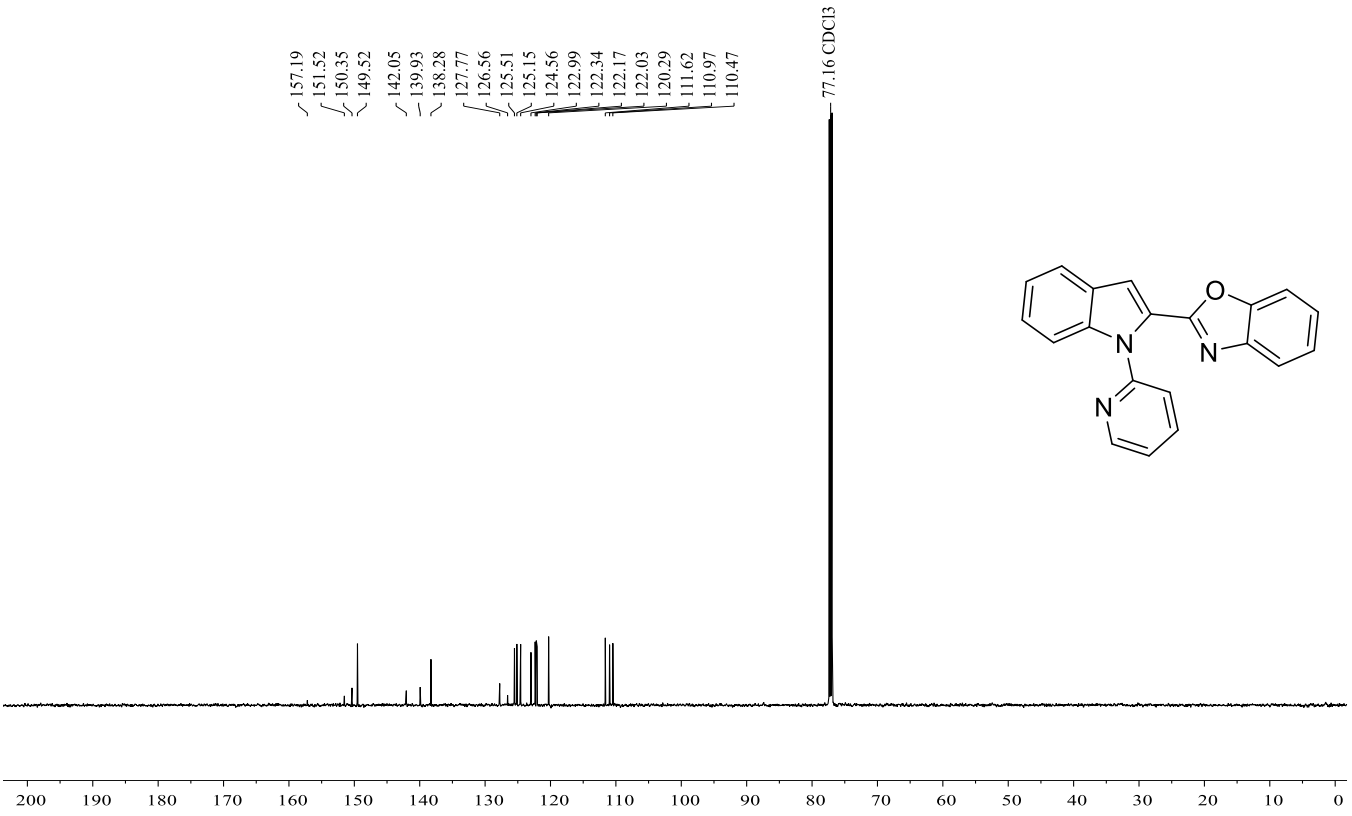


*2-(1-(pyridin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6i**)*

^{1}H NMR (600 MHz)

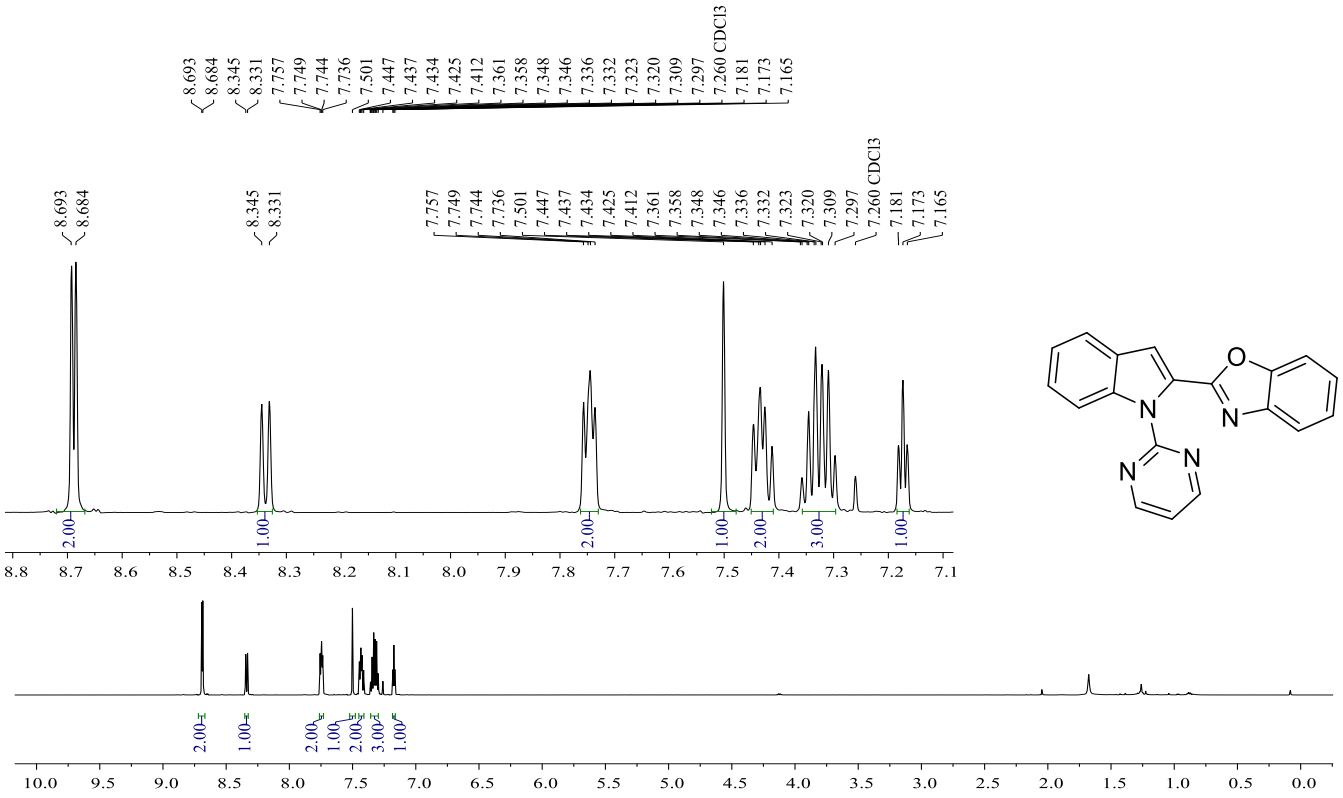


^{13}C{^{1}H} NMR (150 MHz)

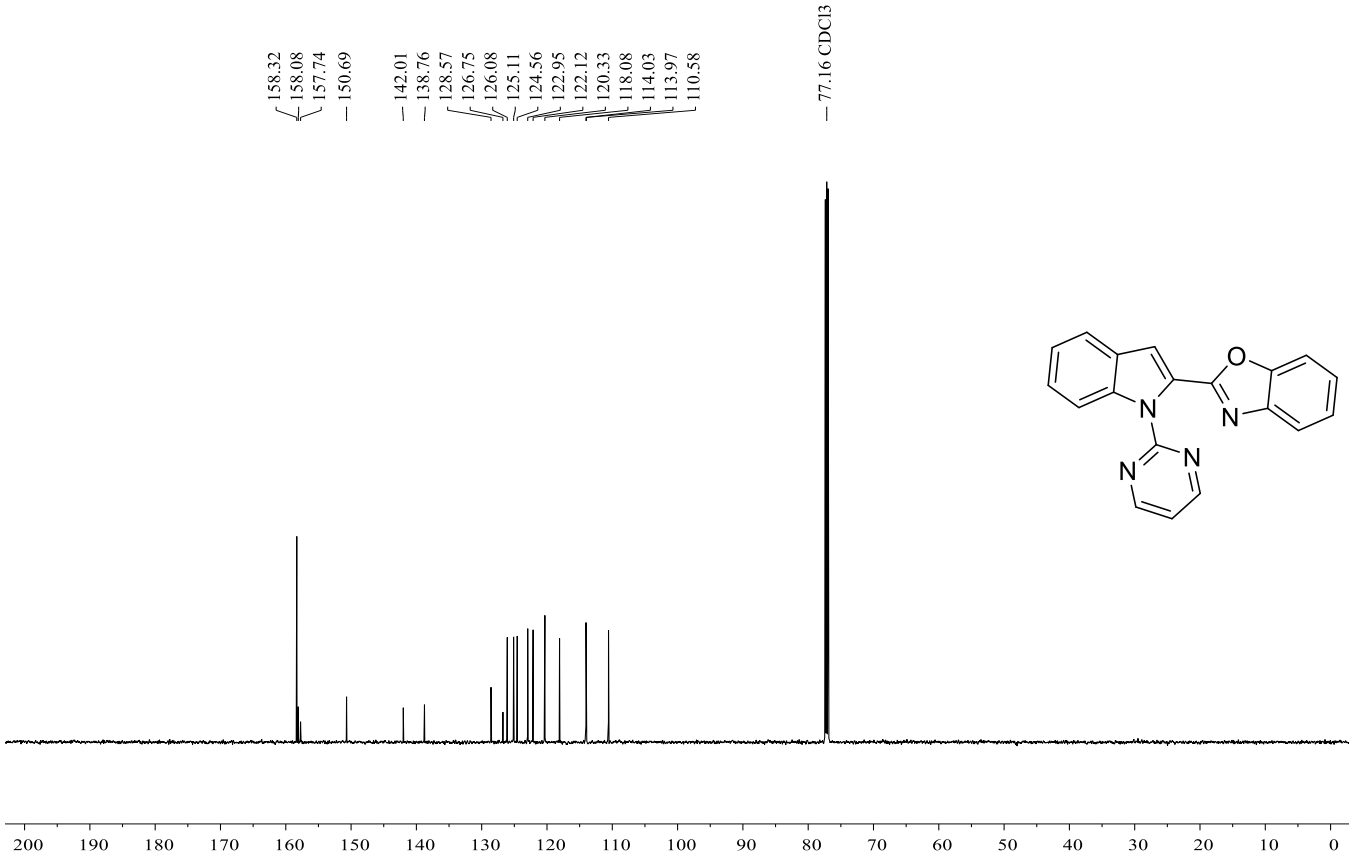


*2-(1-(pyrimidin-2-yl)-1H-indol-2-yl)benzo[d]oxazole (Table 3, Entry **6m**)*

^{1}H NMR (600 MHz)

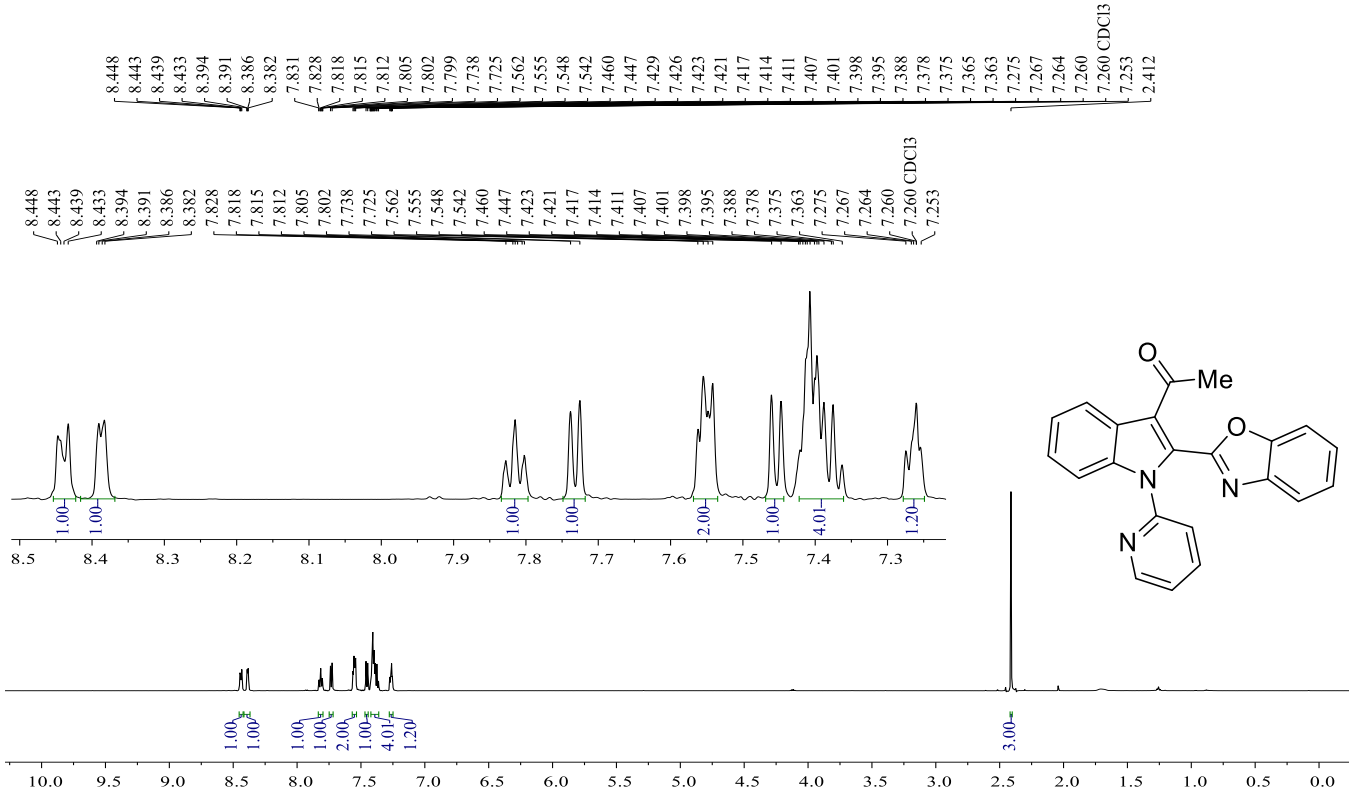


^{13}C{^{1}H} NMR (150 MHz)

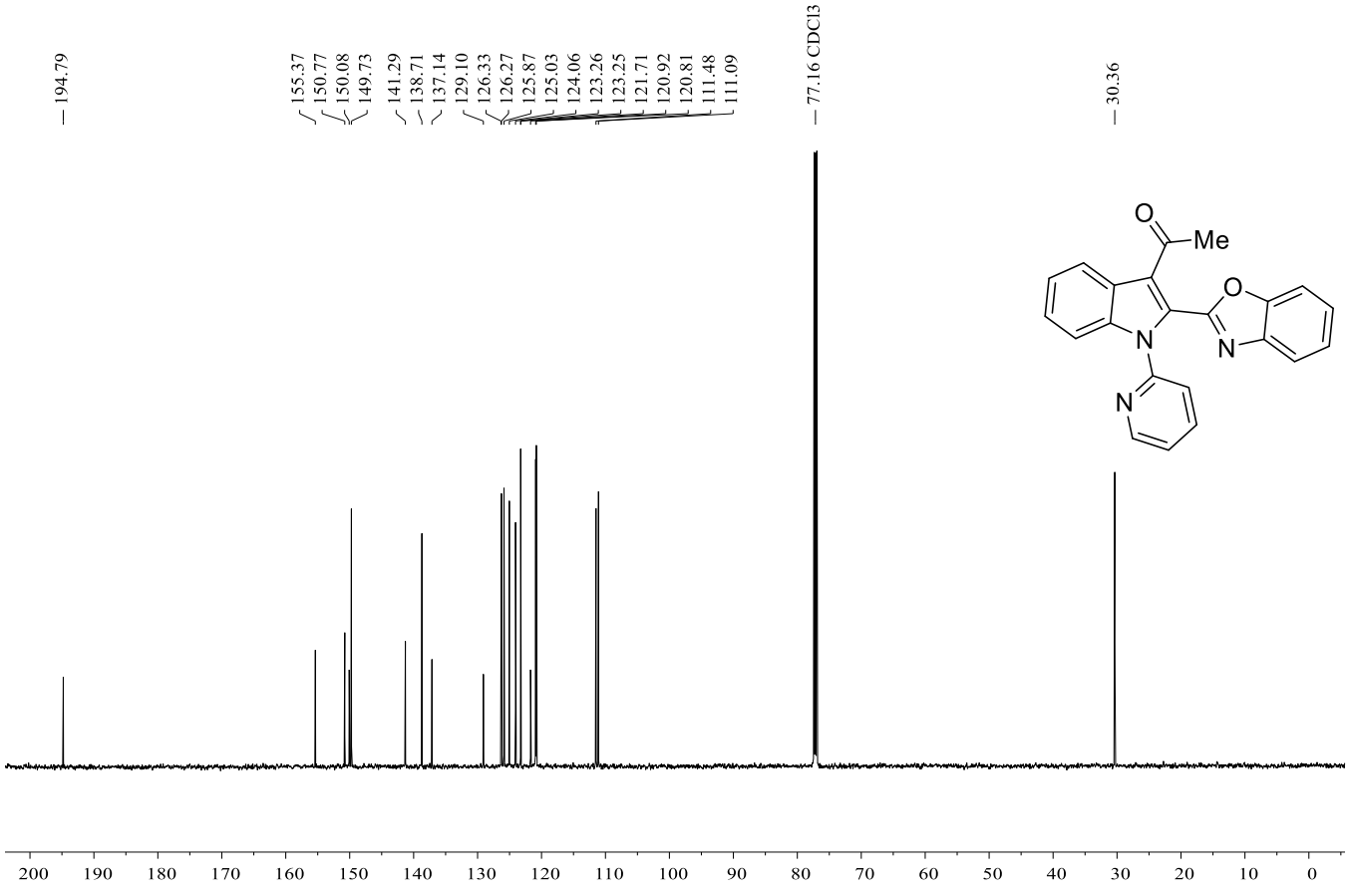


*1-(2-(benzo[d]oxazol-2-yl)-1-(pyridin-2-yl)-1H-indol-3-yl)ethan-1-one (Table 3, Entry **6n**)*

^{1}H NMR (600 MHz)

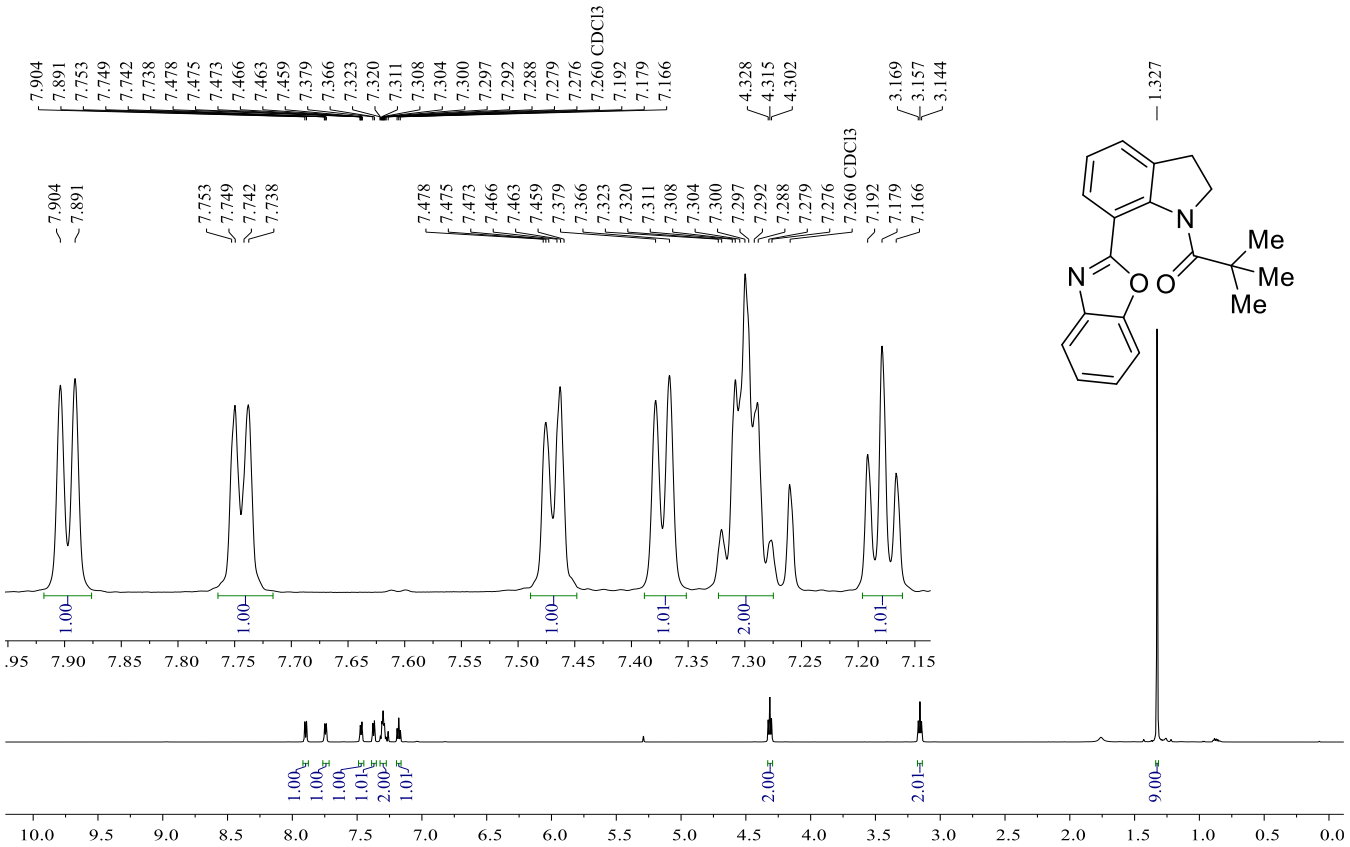


^{13}C{^{1}H} NMR (150 MHz)

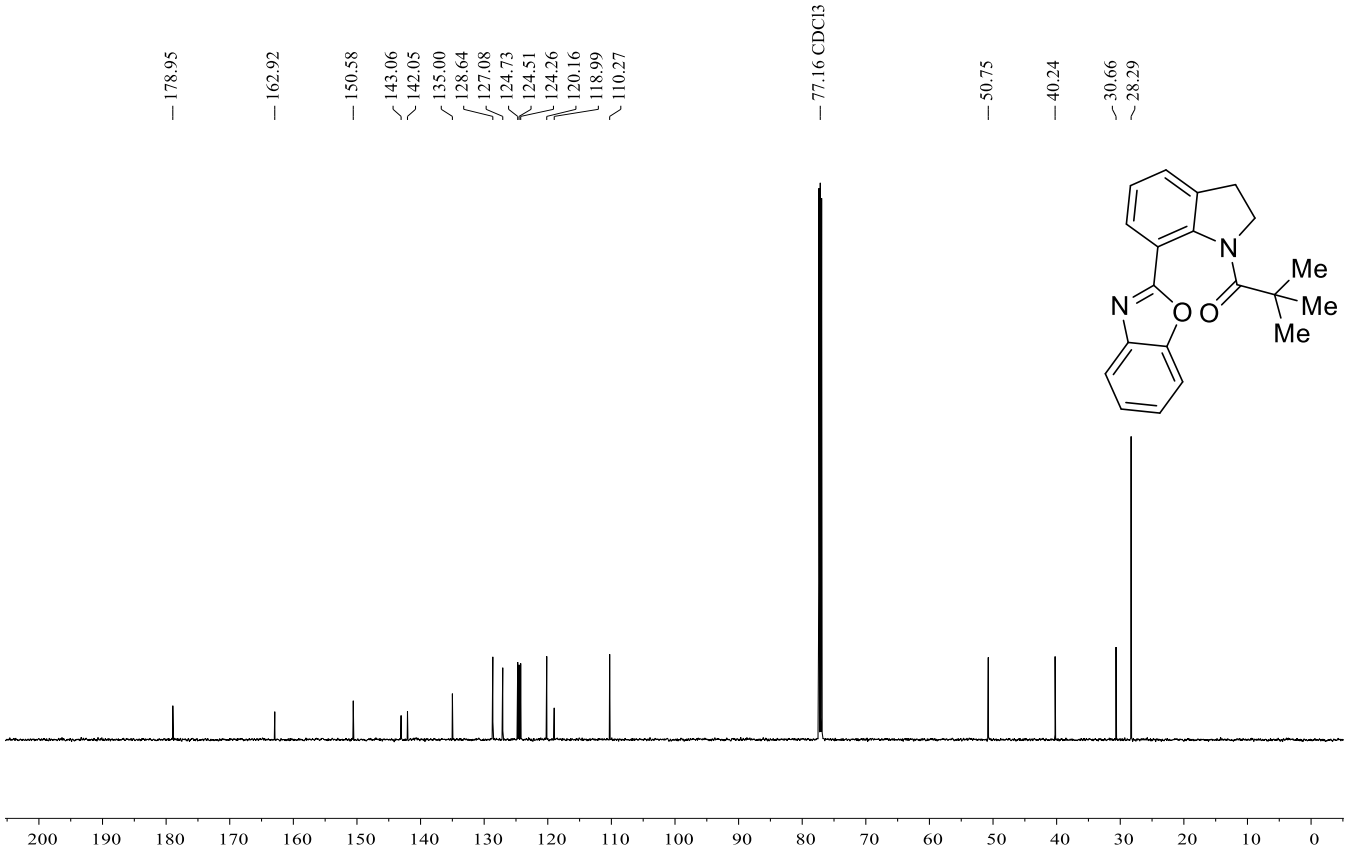


*1-(7-(benzo[d]oxazol-2-yl)indolin-1-yl)-2,2-dimethylpropan-1-one (Table 3, Entry **6o**)*

^{1}H NMR (600 MHz)

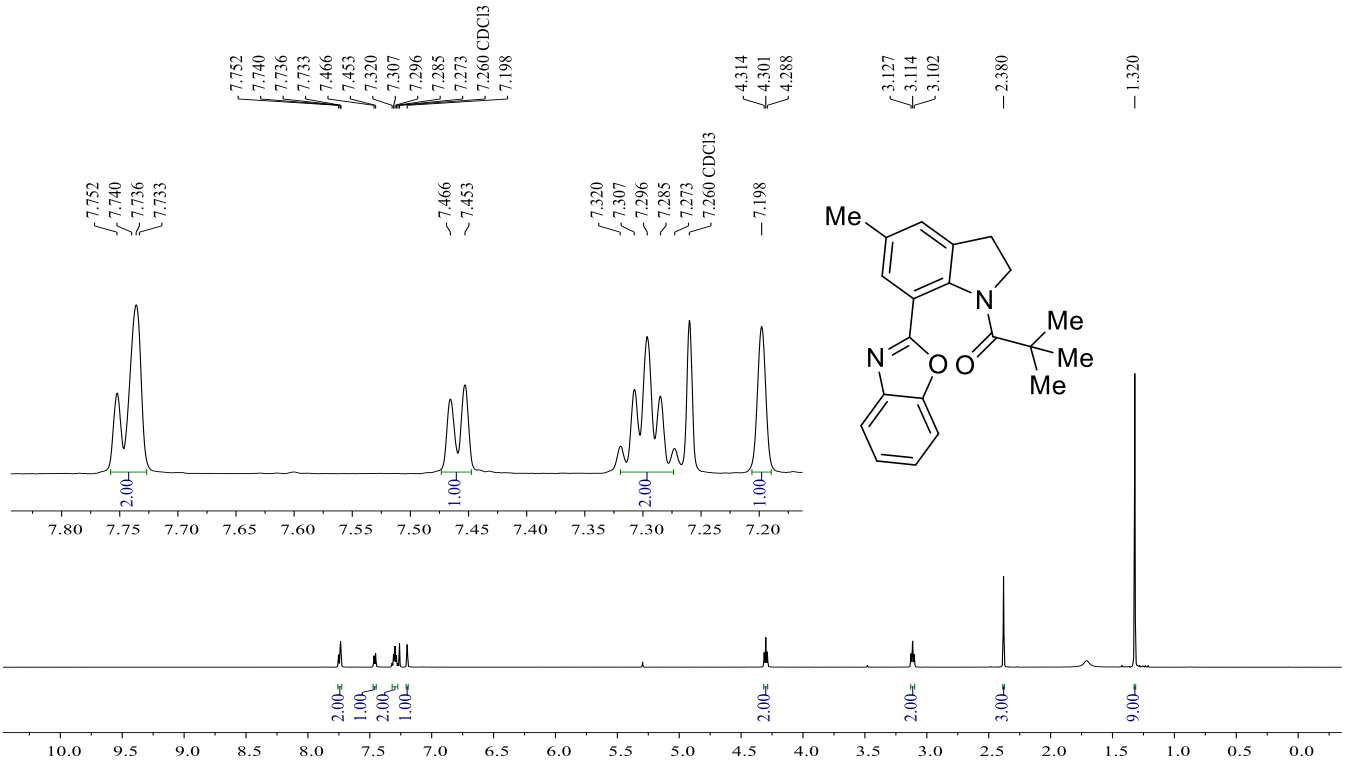


^{13}C{^{1}H} NMR (150 MHz)

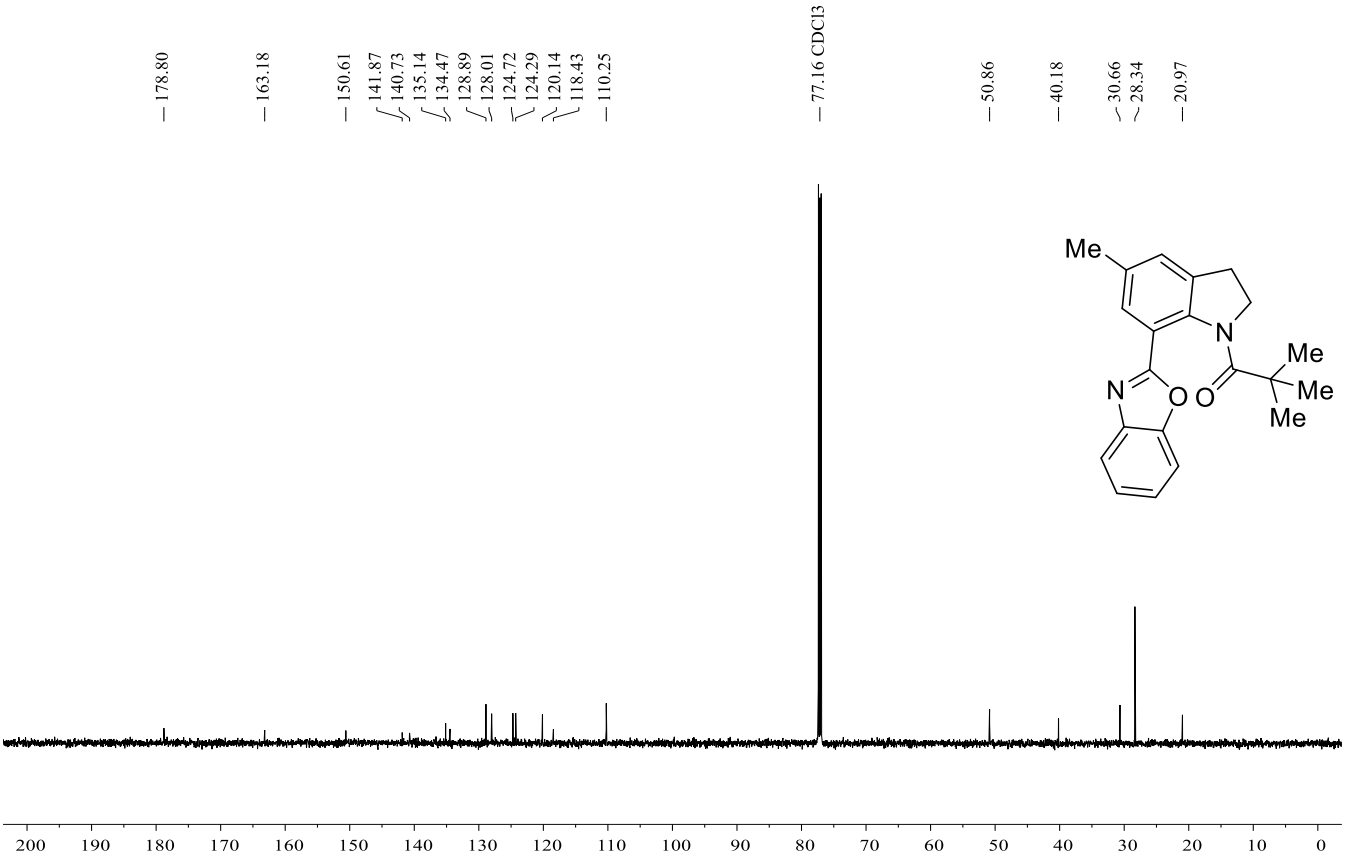


*1-(7-(benzo[d]oxazol-2-yl)indolin-1-yl)-2,2-dimethylpropan-1-one (Table 3, Entry **6p**)*

^{1}H NMR (600 MHz)

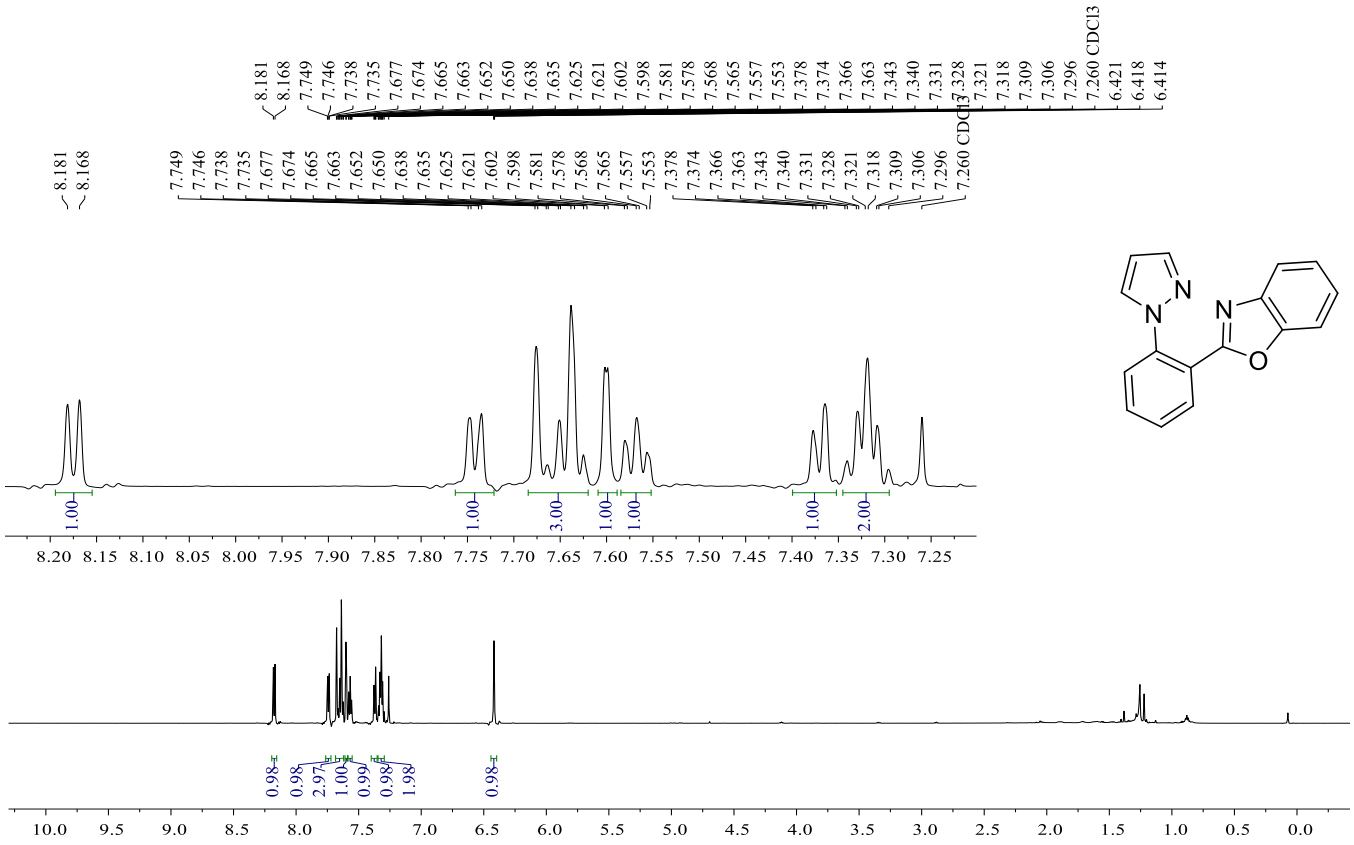


^{13}C{^{1}H} NMR (150 MHz)

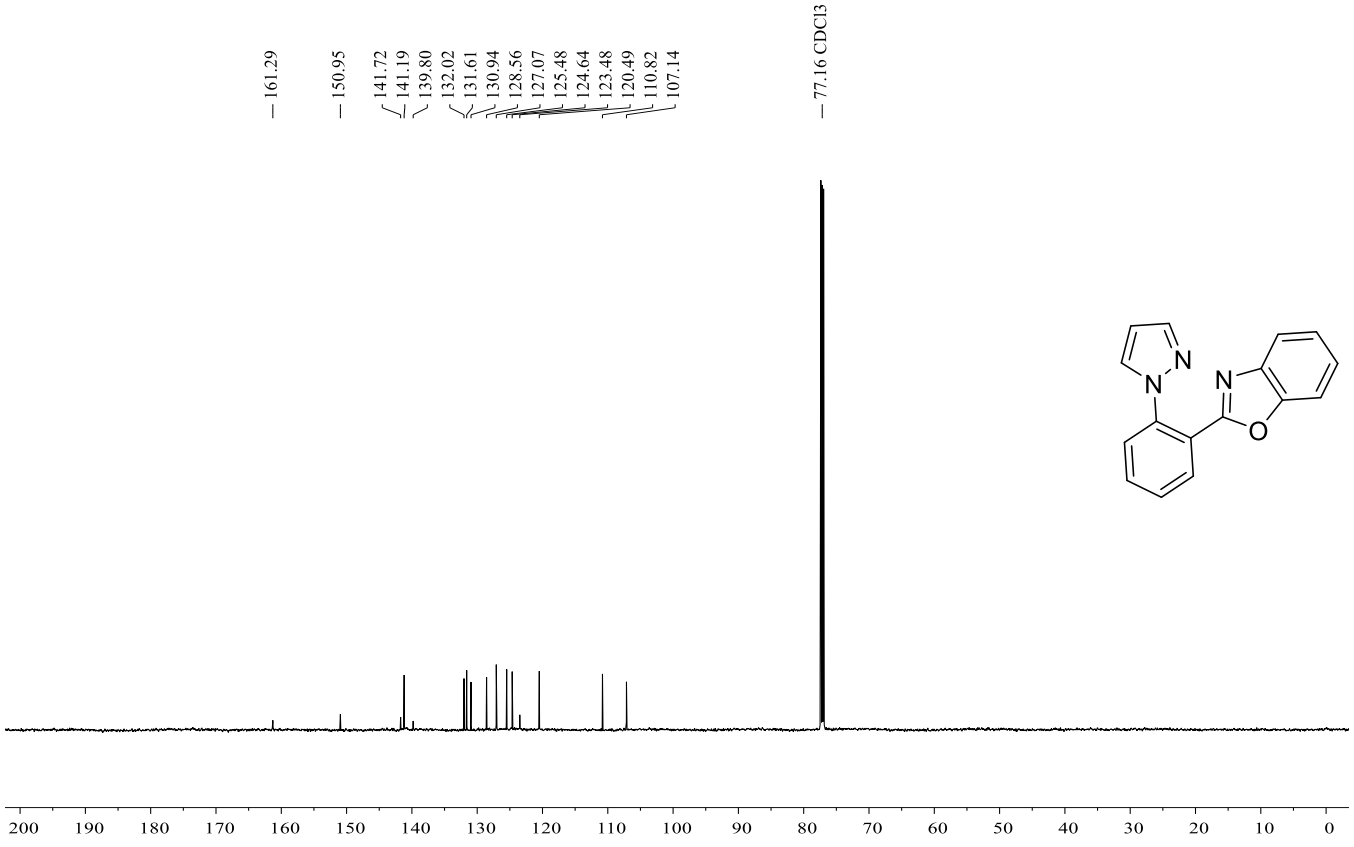


*2-(2-(1H-pyrazol-1-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6q**)*

^{1}H NMR (600 MHz)

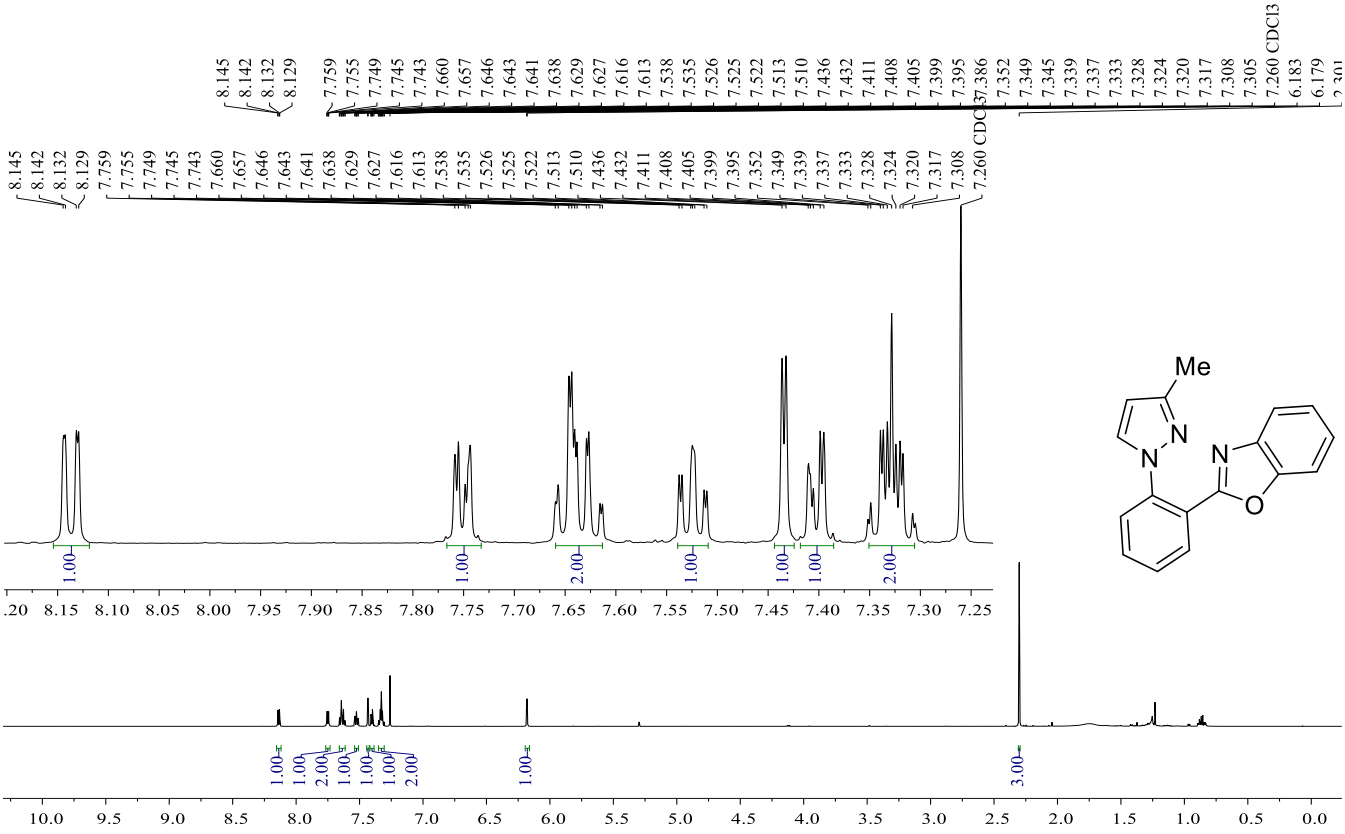


^{13}C{^{1}H} NMR (150 MHz)

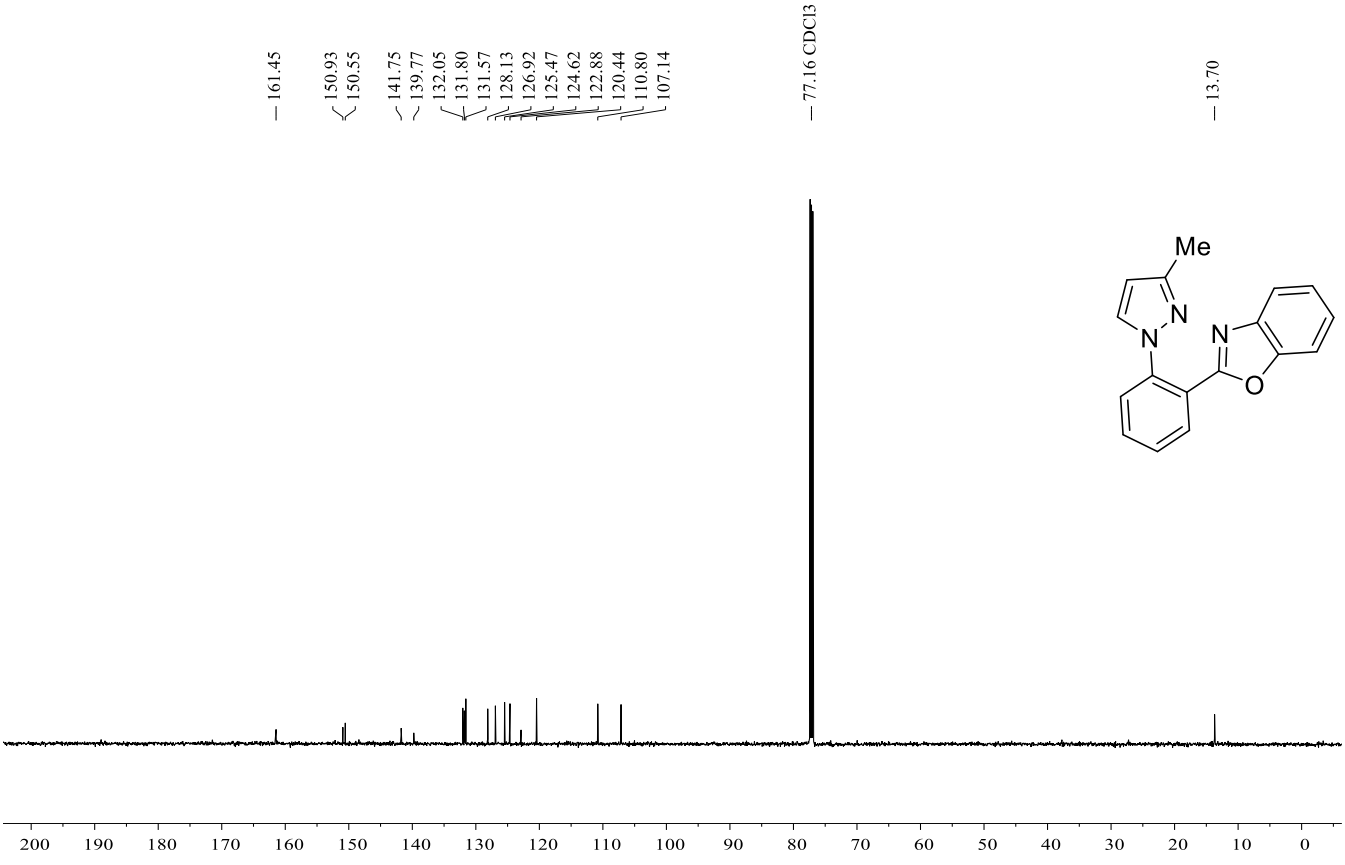


*2-(2-(3-methyl-1H-pyrazol-1-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6r**)*

^{1}H NMR (600 MHz)

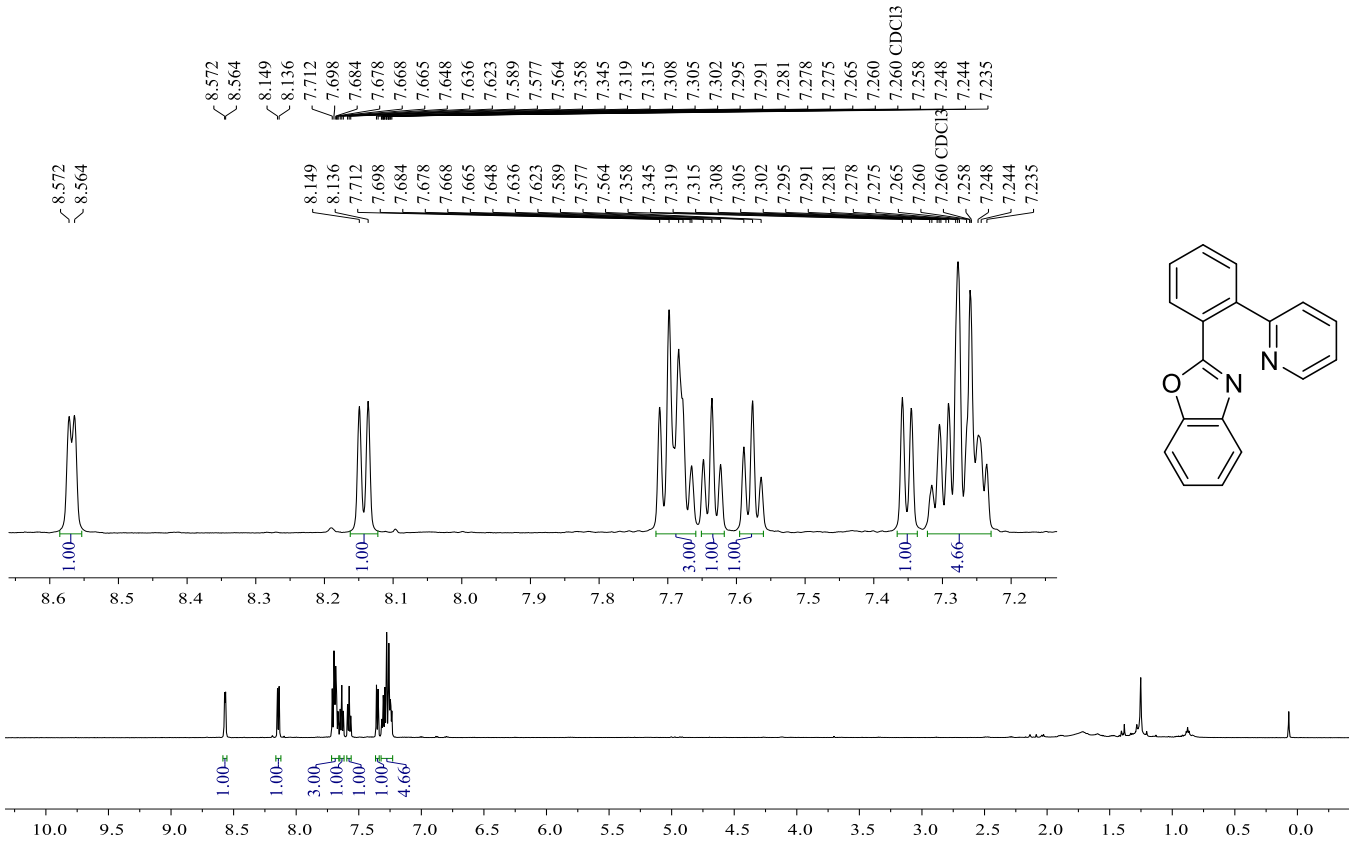


^{13}C{^{1}H} NMR (150 MHz)

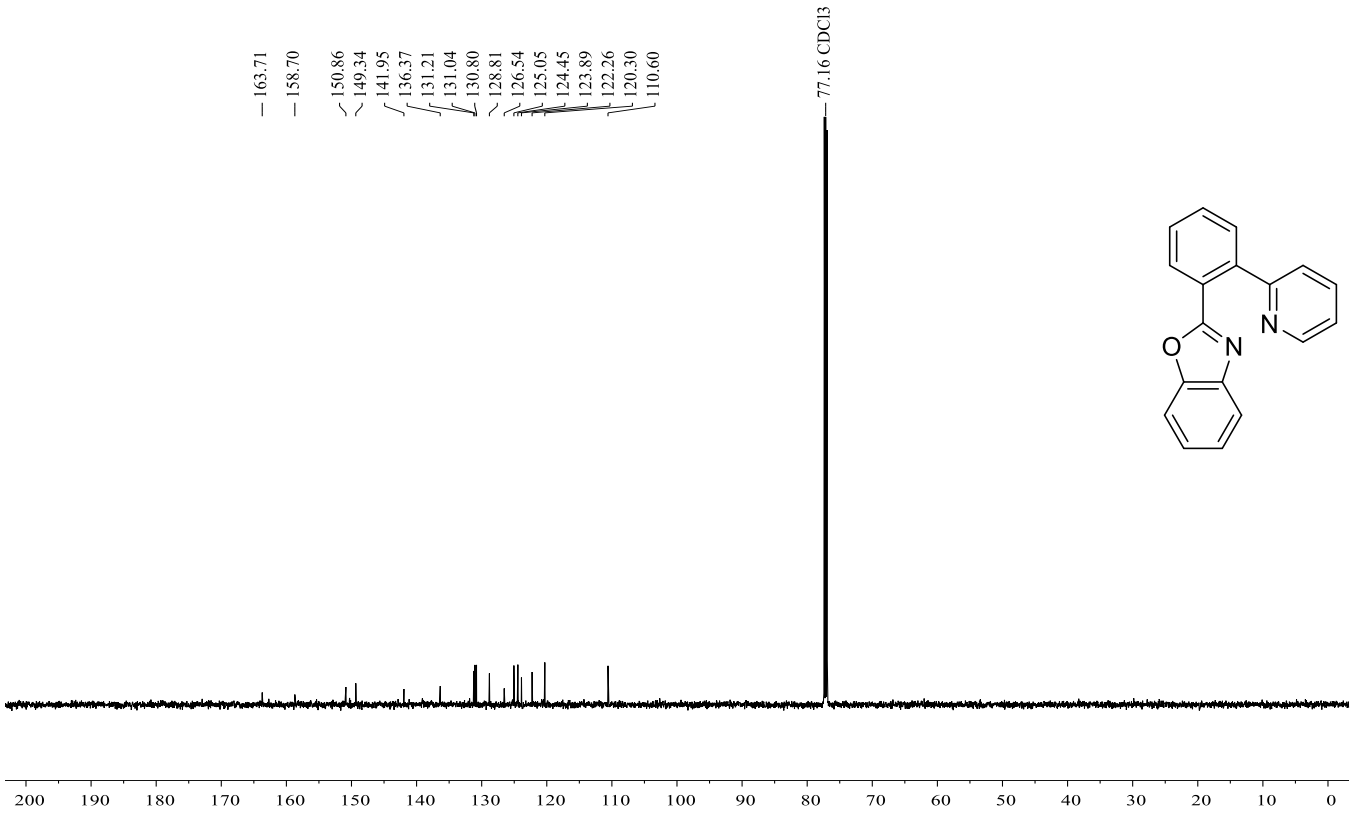


*2-(2-(pyridin-2-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6s**)*

^{1}H NMR (600 MHz)

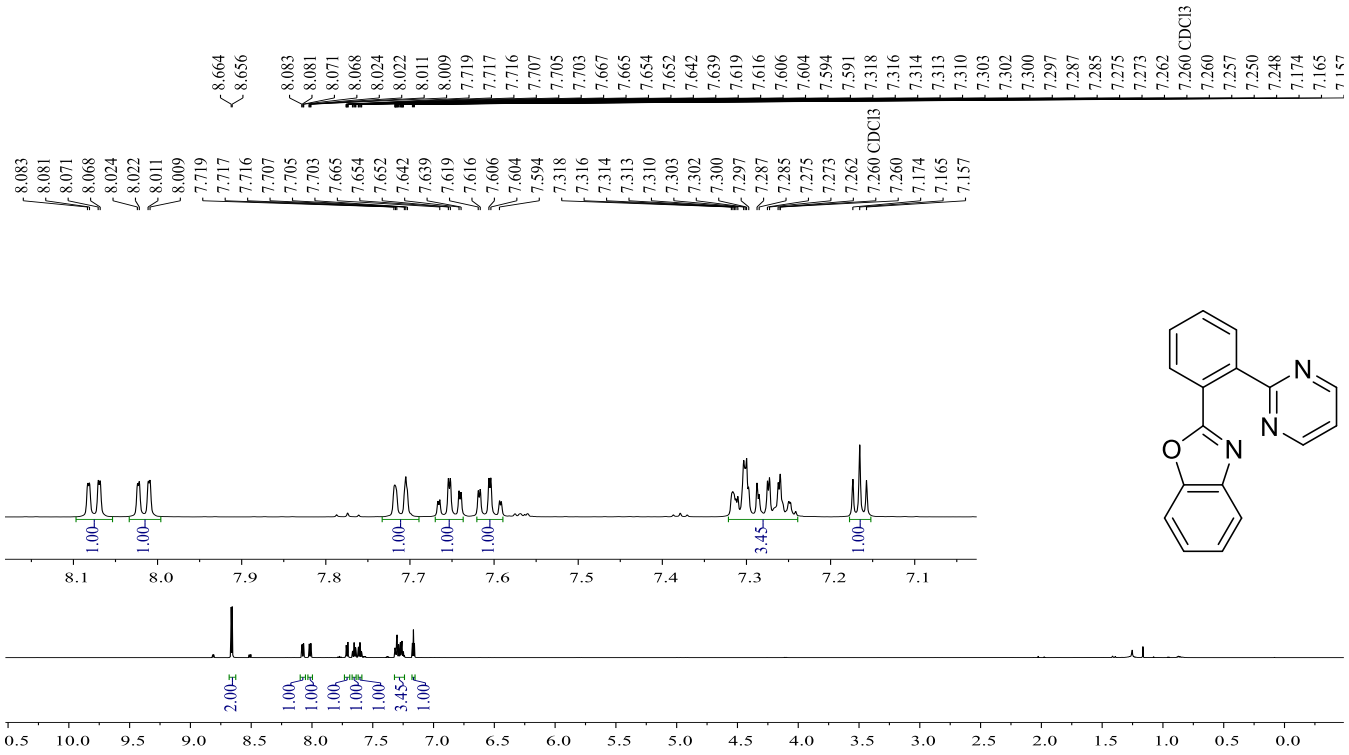


^{13}C{^{1}H} NMR (150 MHz)

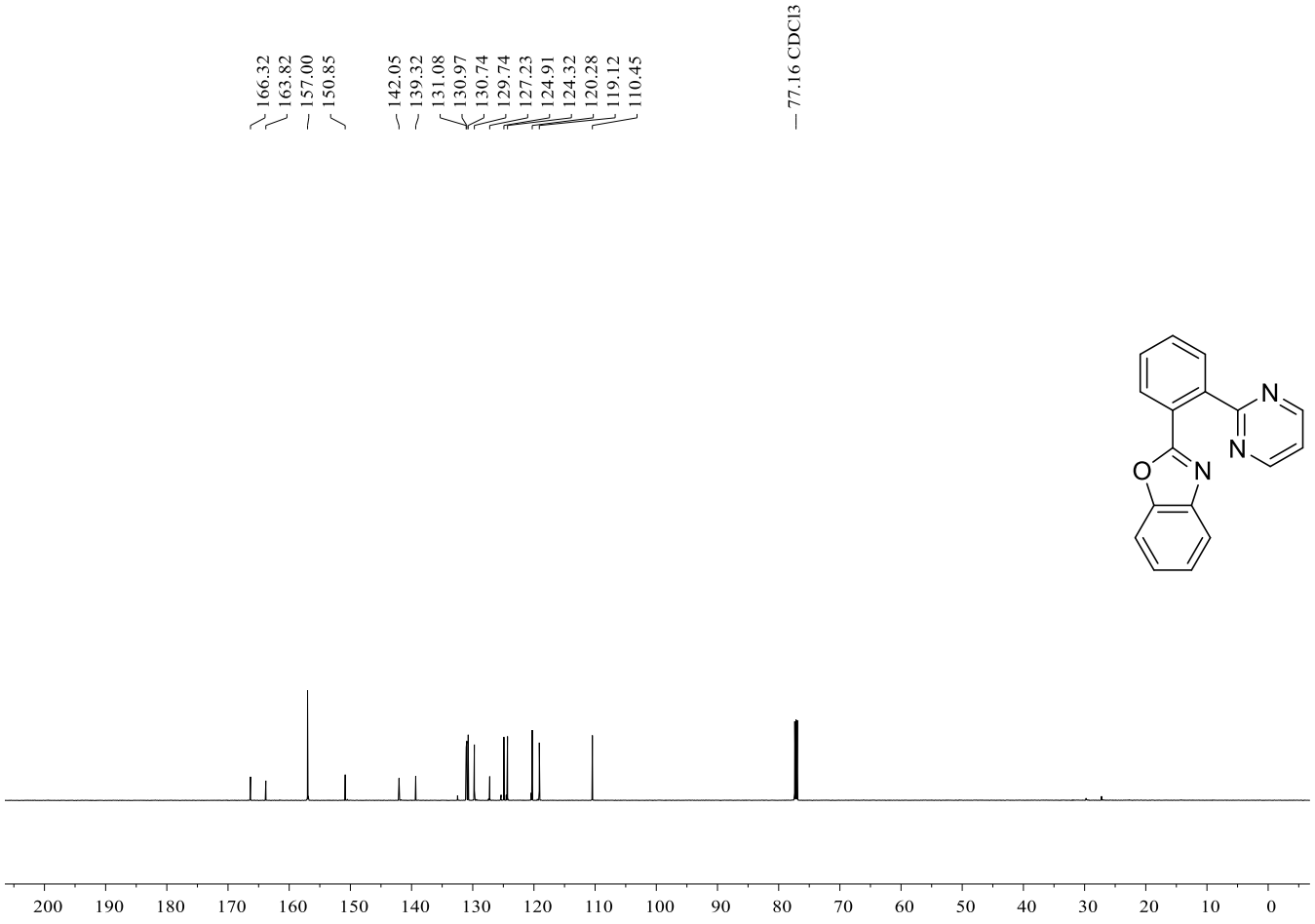


*2-(2-(pyrimidin-2-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6t**)*

^{1}H NMR (600 MHz)

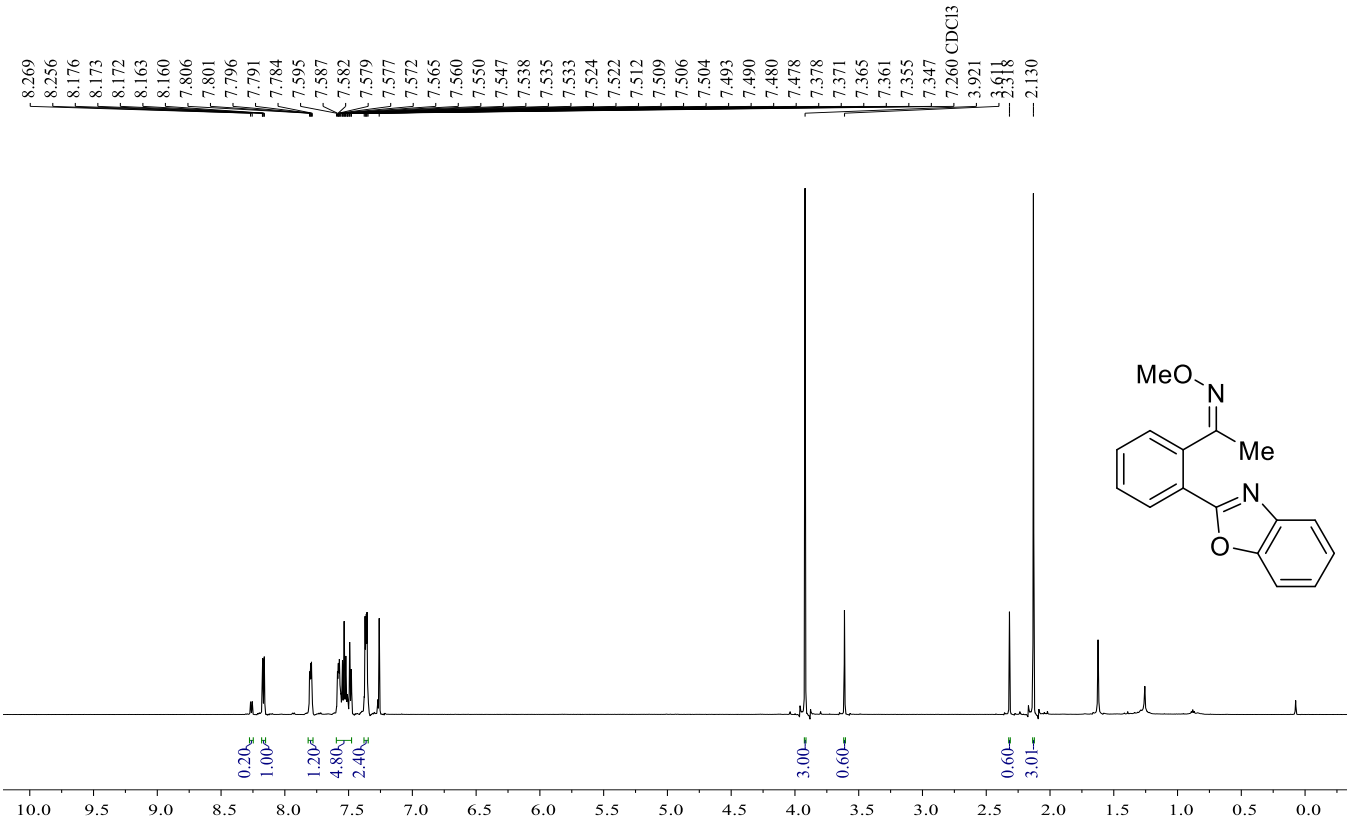


^{13}C{^{1}H} NMR (150 MHz)

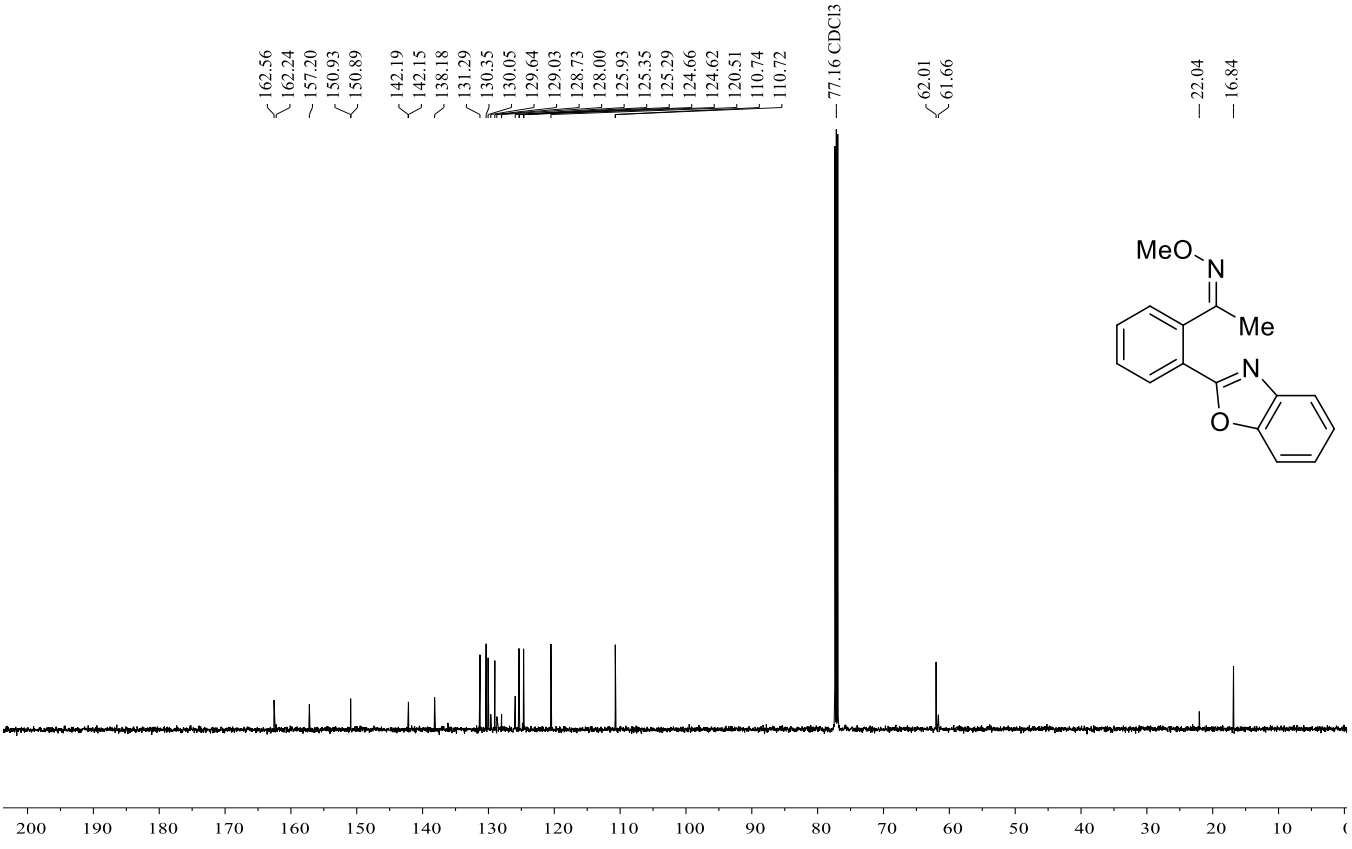


*1-(2-(benzo[d]oxazol-2-yl)phenyl)ethan-1-one O-methyl oxime (Table 3, Entry **6u**)*

^{1}H NMR (600 MHz)

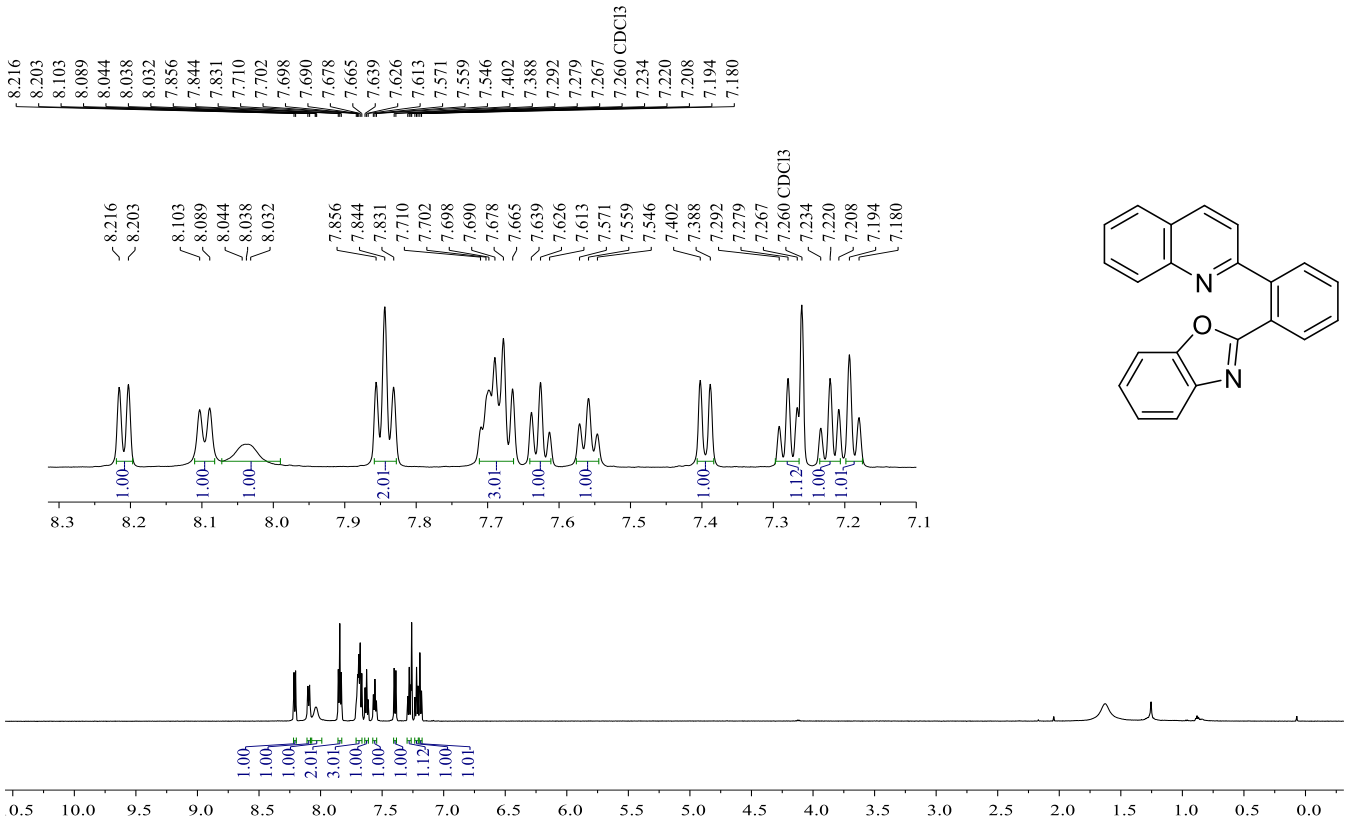


^{13}C{^{1}H} NMR (150 MHz)

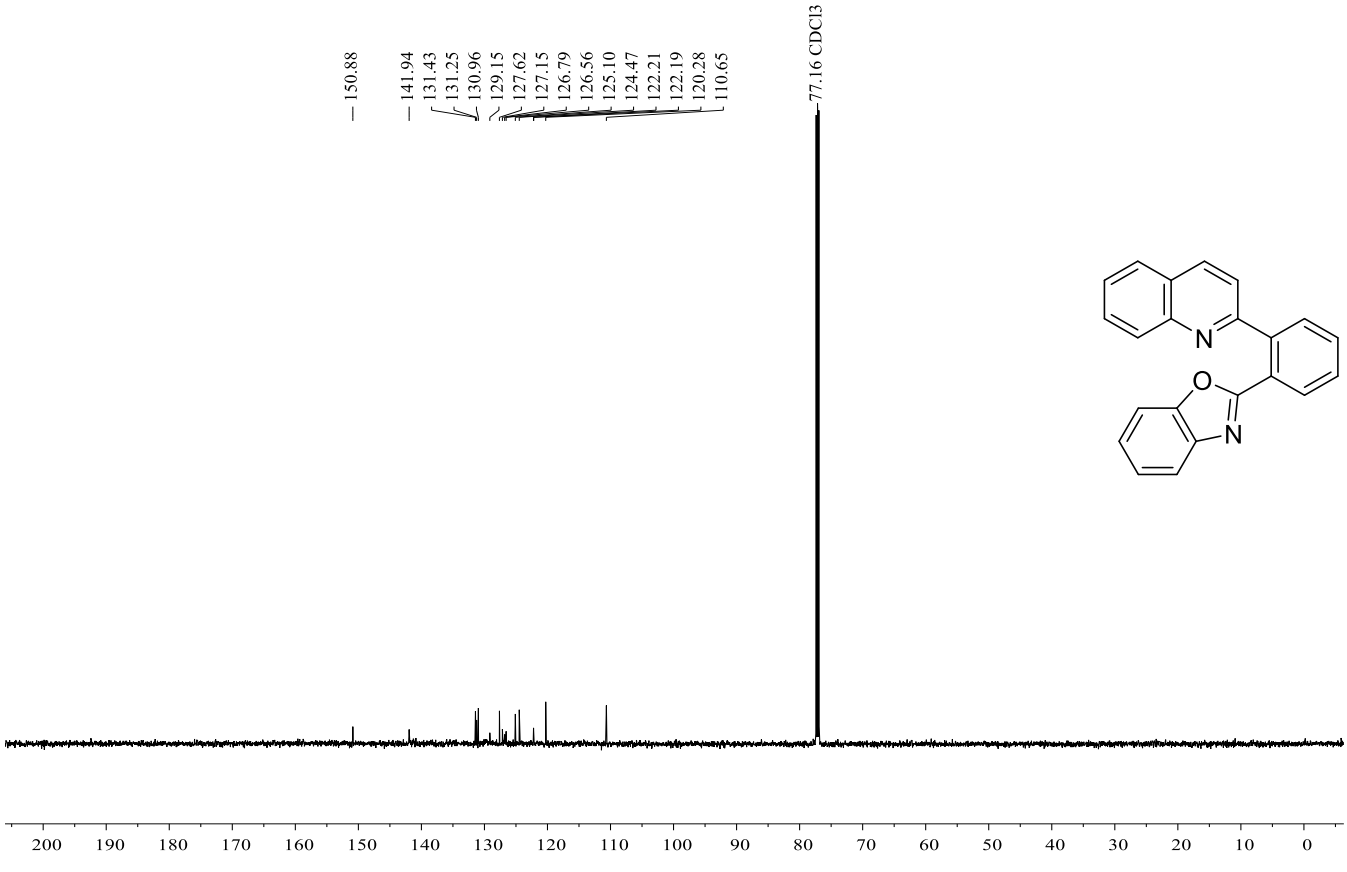


*2-(2-(quinolin-2-yl)phenyl)benzo[d]oxazole (Table 3, Entry **6v**)*

^{1}H NMR (600 MHz)

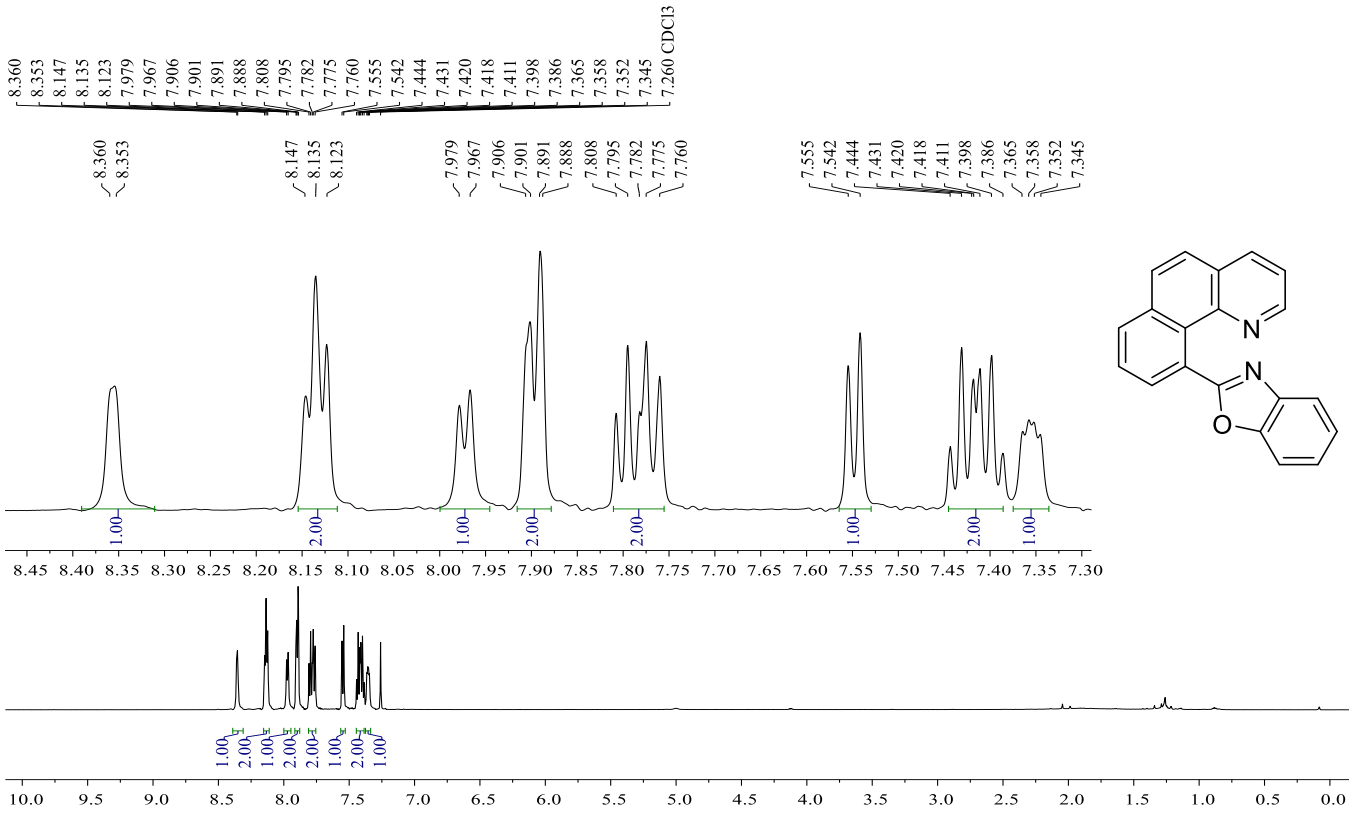


^{13}C{^{1}H} NMR (150 MHz)

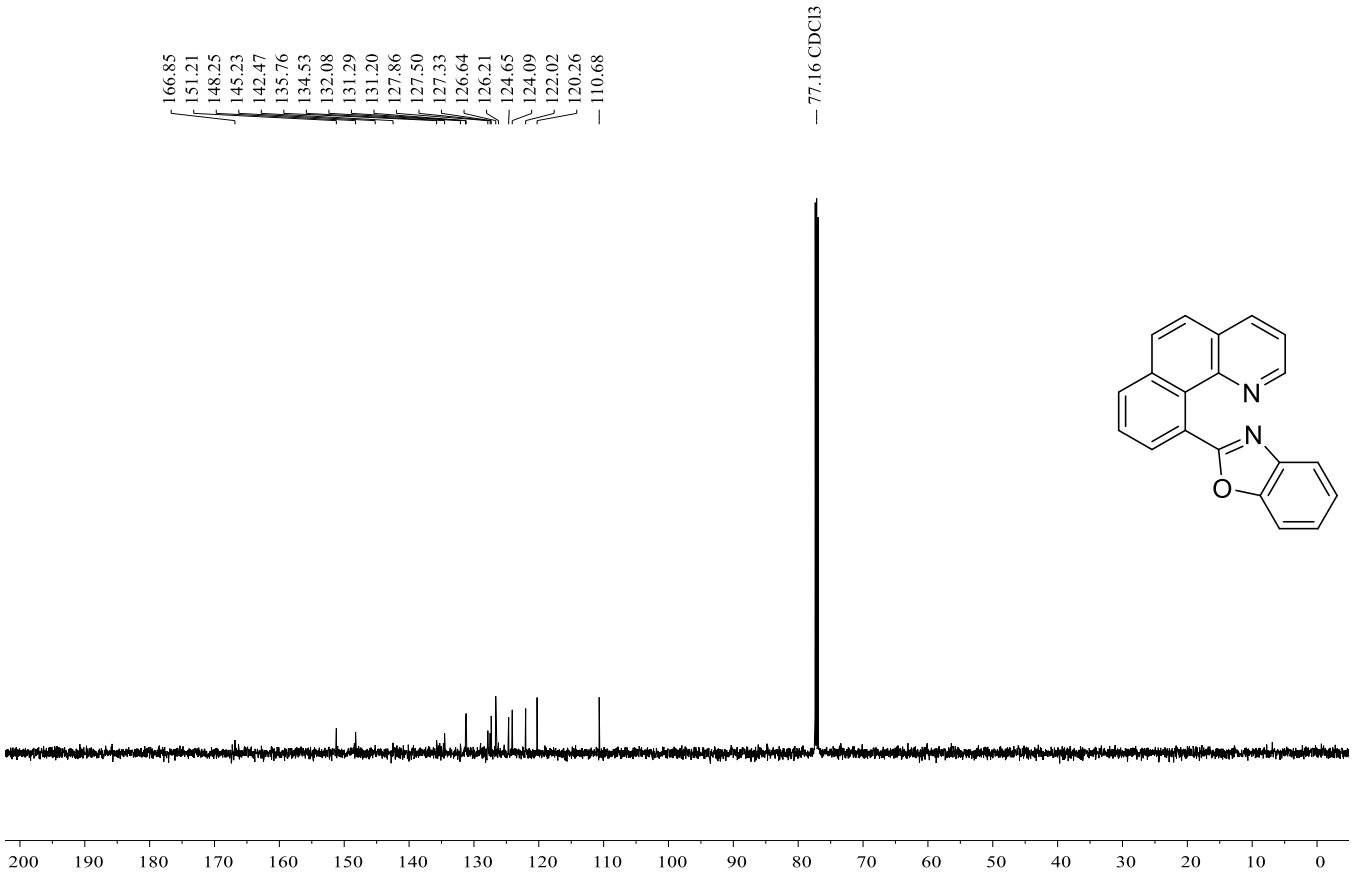


*2-(benzo[h]quinolin-10-yl)benzo[d]oxazole (Table 3, Entry **6w**)*

^{1}H NMR (600 MHz)

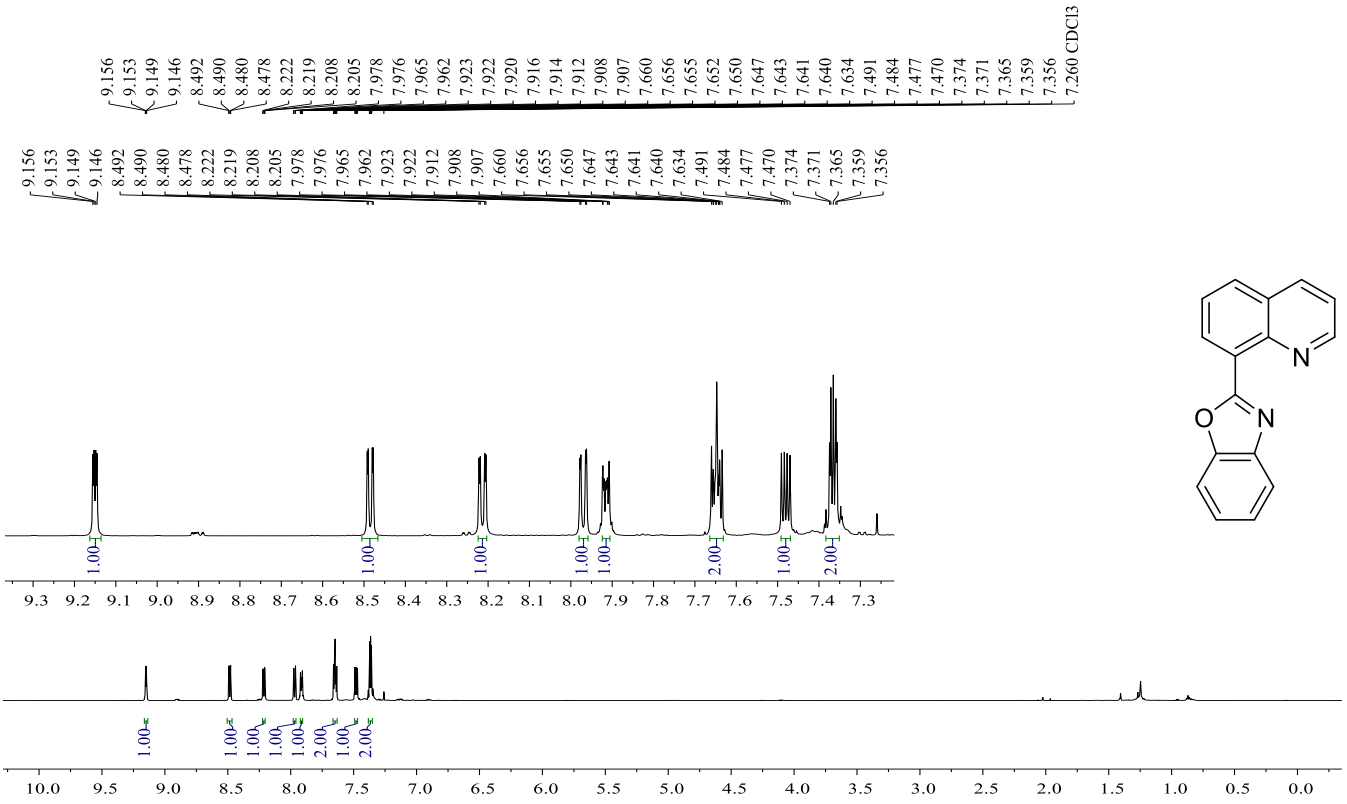


^{13}C{^{1}H} NMR (150 MHz)

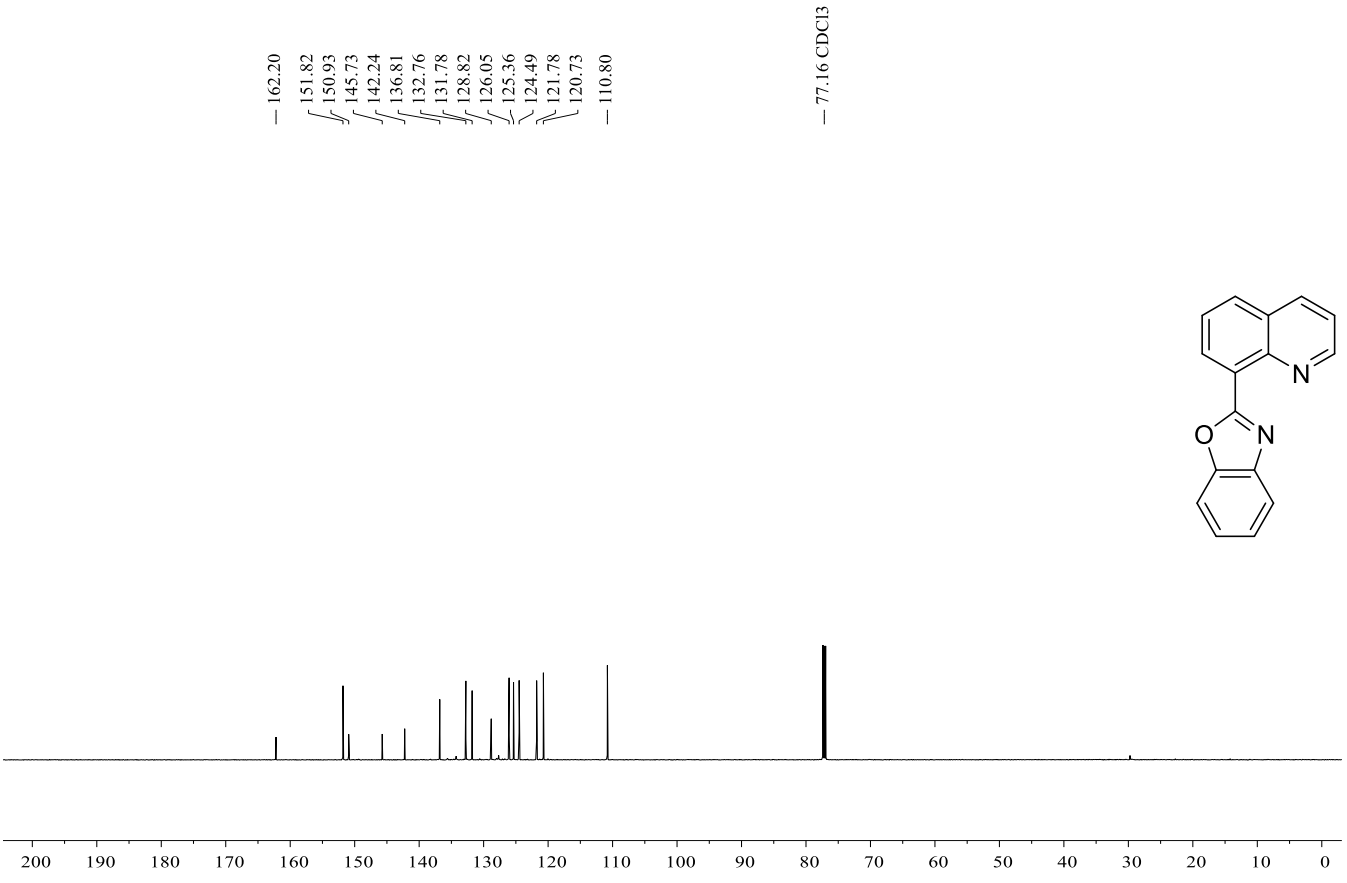


*2-(quinolin-8-yl)benzo[d]oxazole (Scheme 5, Entry **7a**)*

^{1}H NMR (600 MHz)

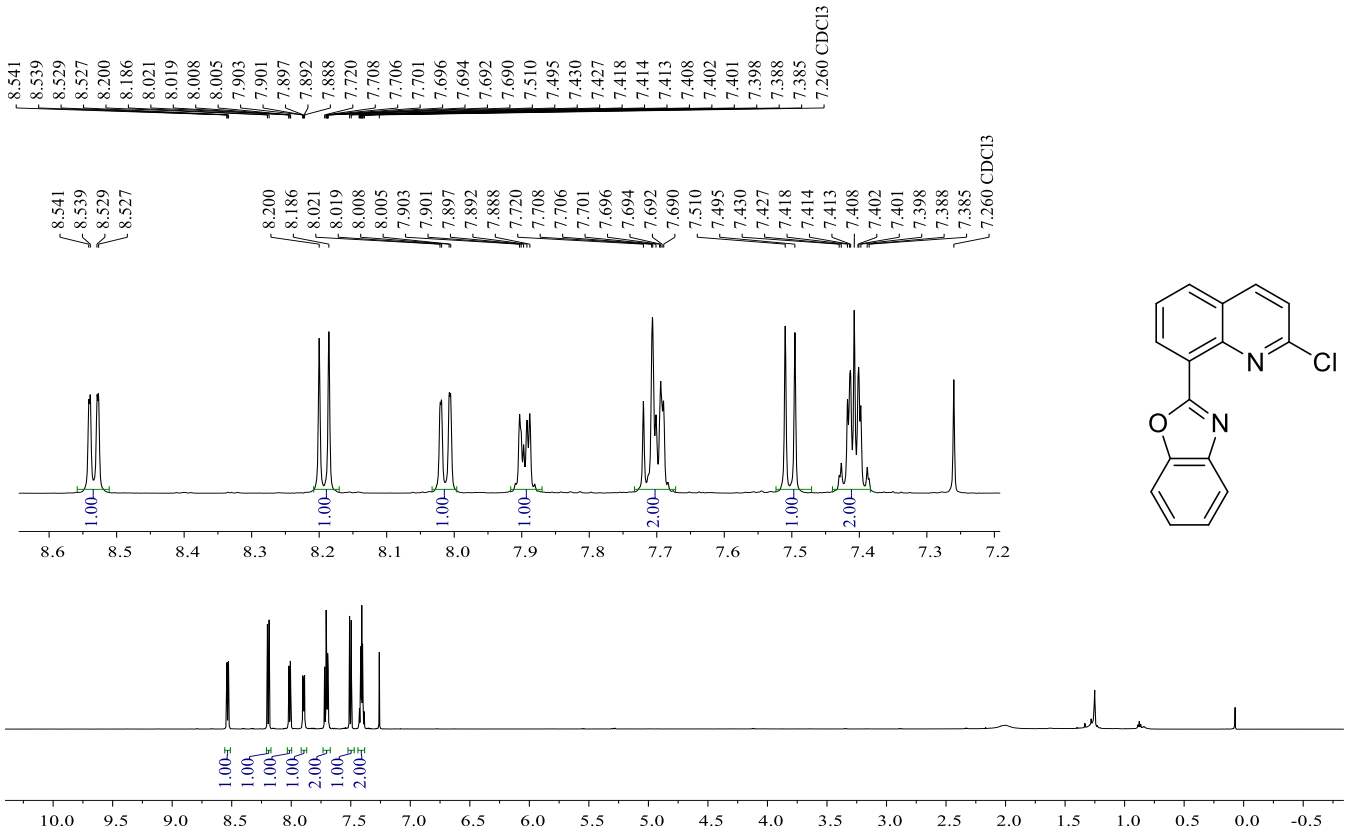


^{13}C{^{1}H} NMR (150 MHz)

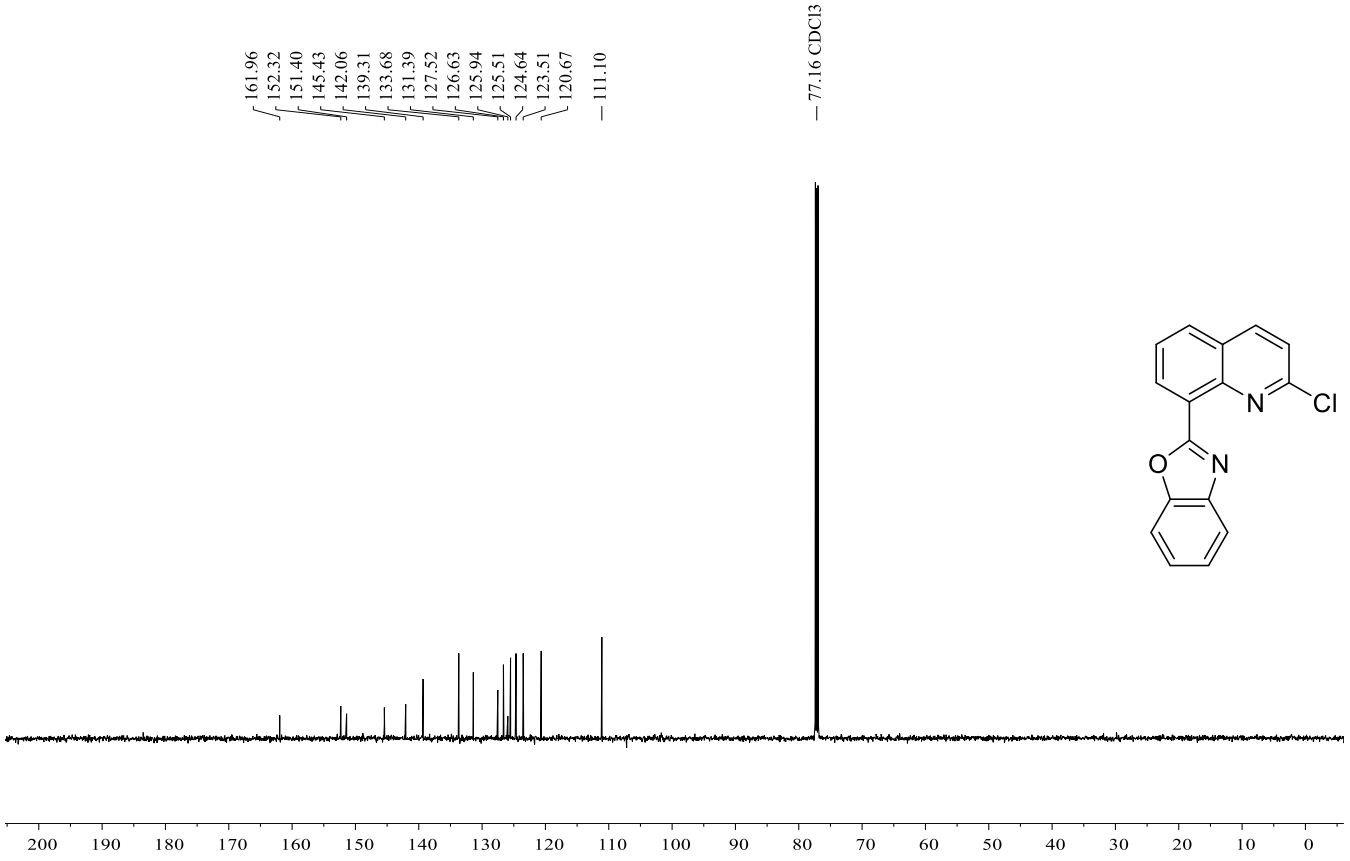


*2-(2-chloroquinolin-8-yl)benzo[d]oxazole (Scheme 5, Entry **7b**)*

^{1}H NMR (600 MHz)

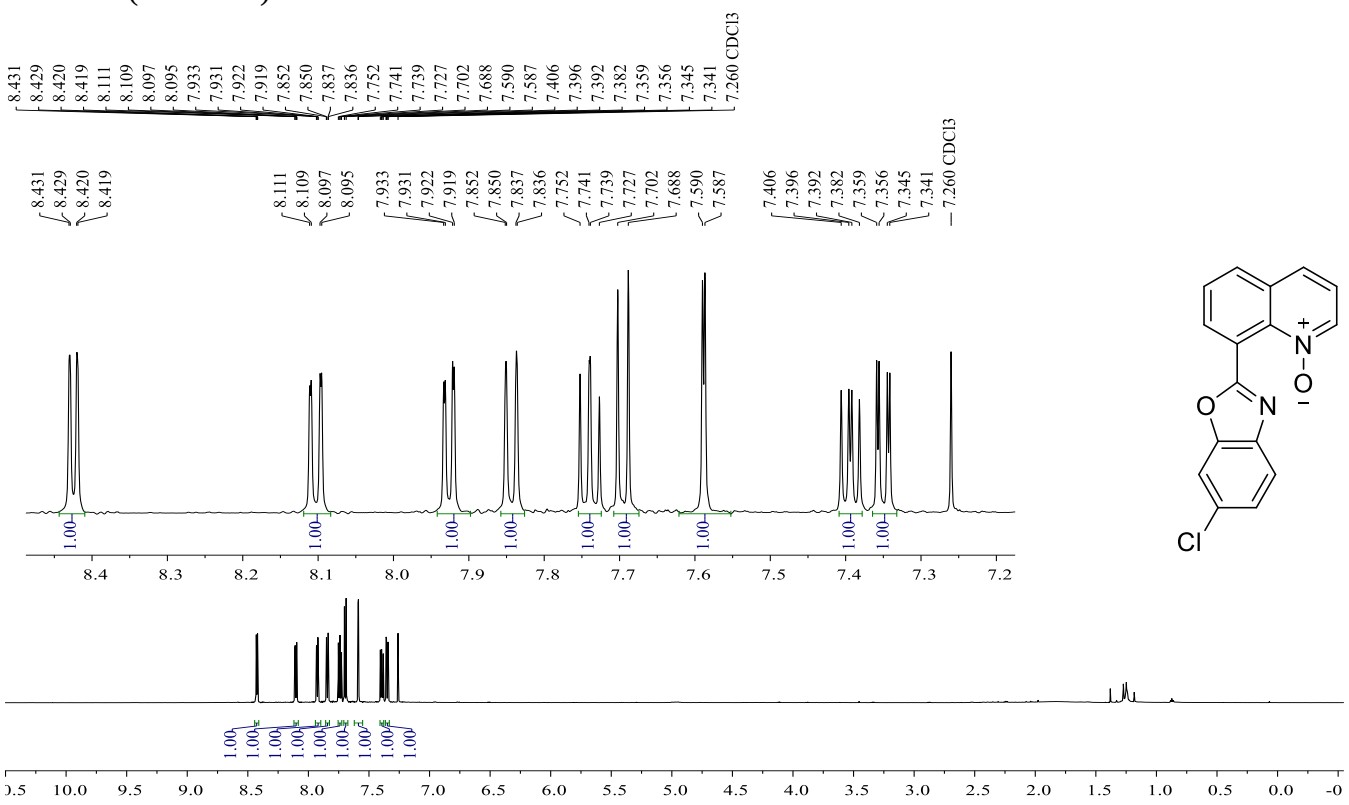


^{13}C{^{1}H} NMR (150 MHz)

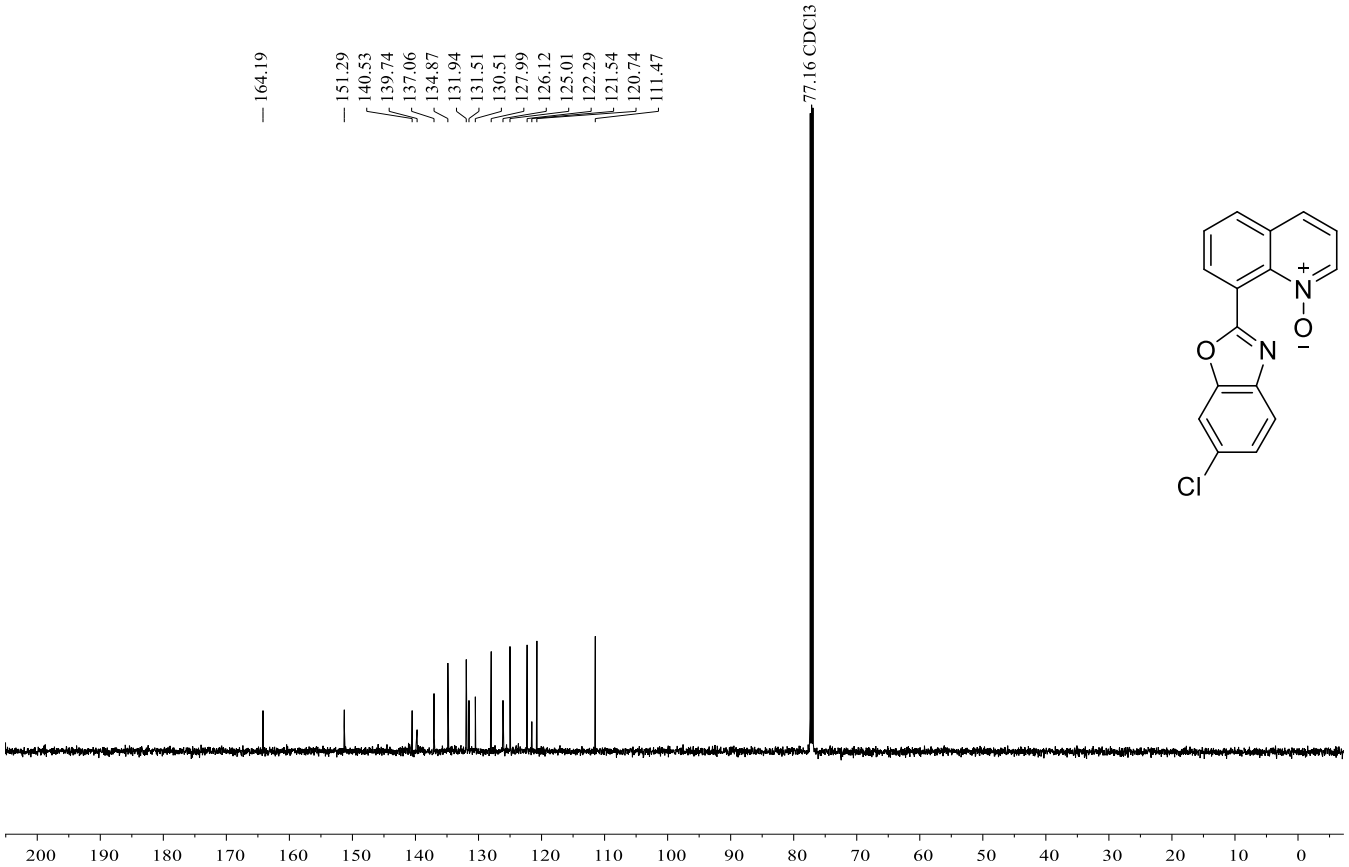


*8-(6-chlorobenzo[d]oxazol-2-yl)quinoline 1-oxide (Scheme 5, Entry **3zc**)*

^{1}H NMR (600 MHz)

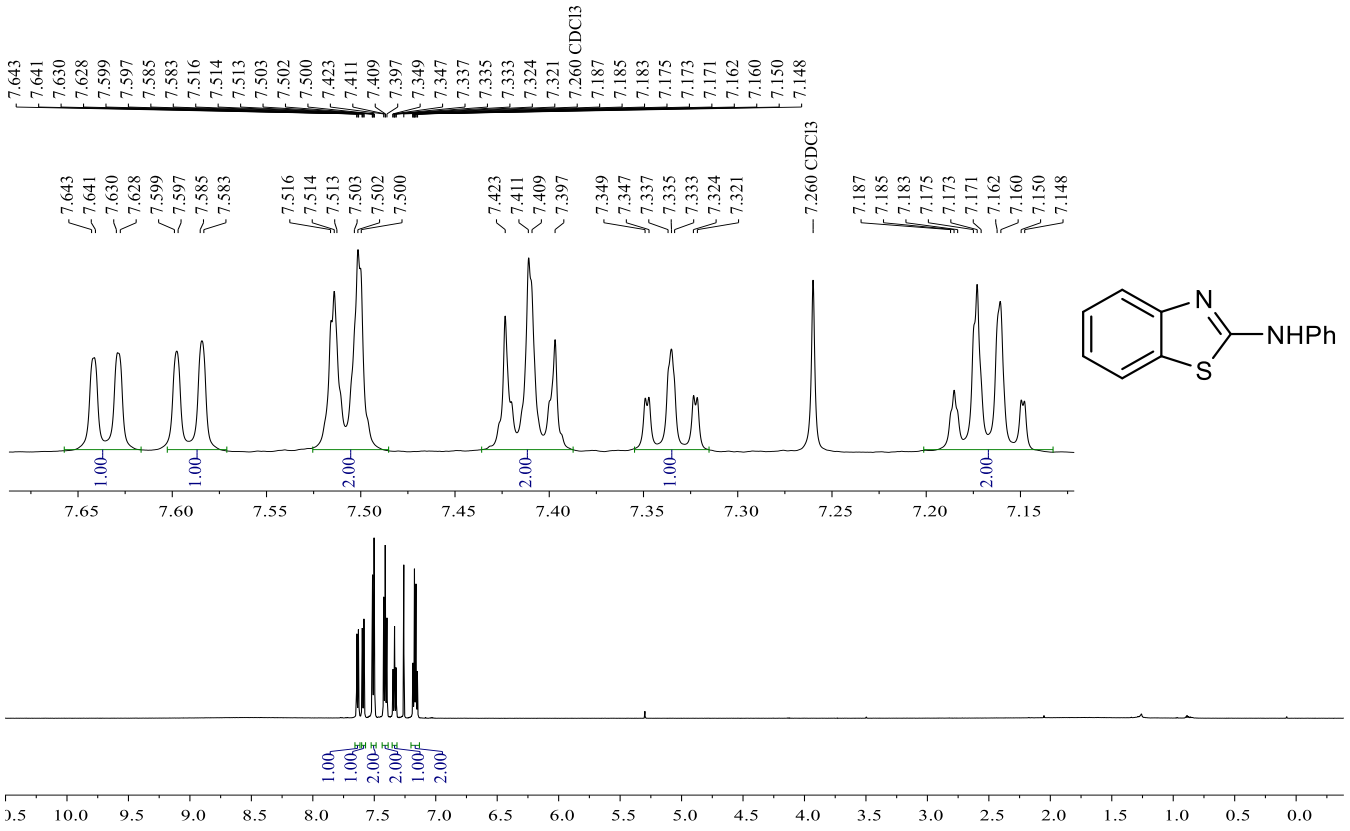


^{13}C{^{1}H} NMR (150 MHz)

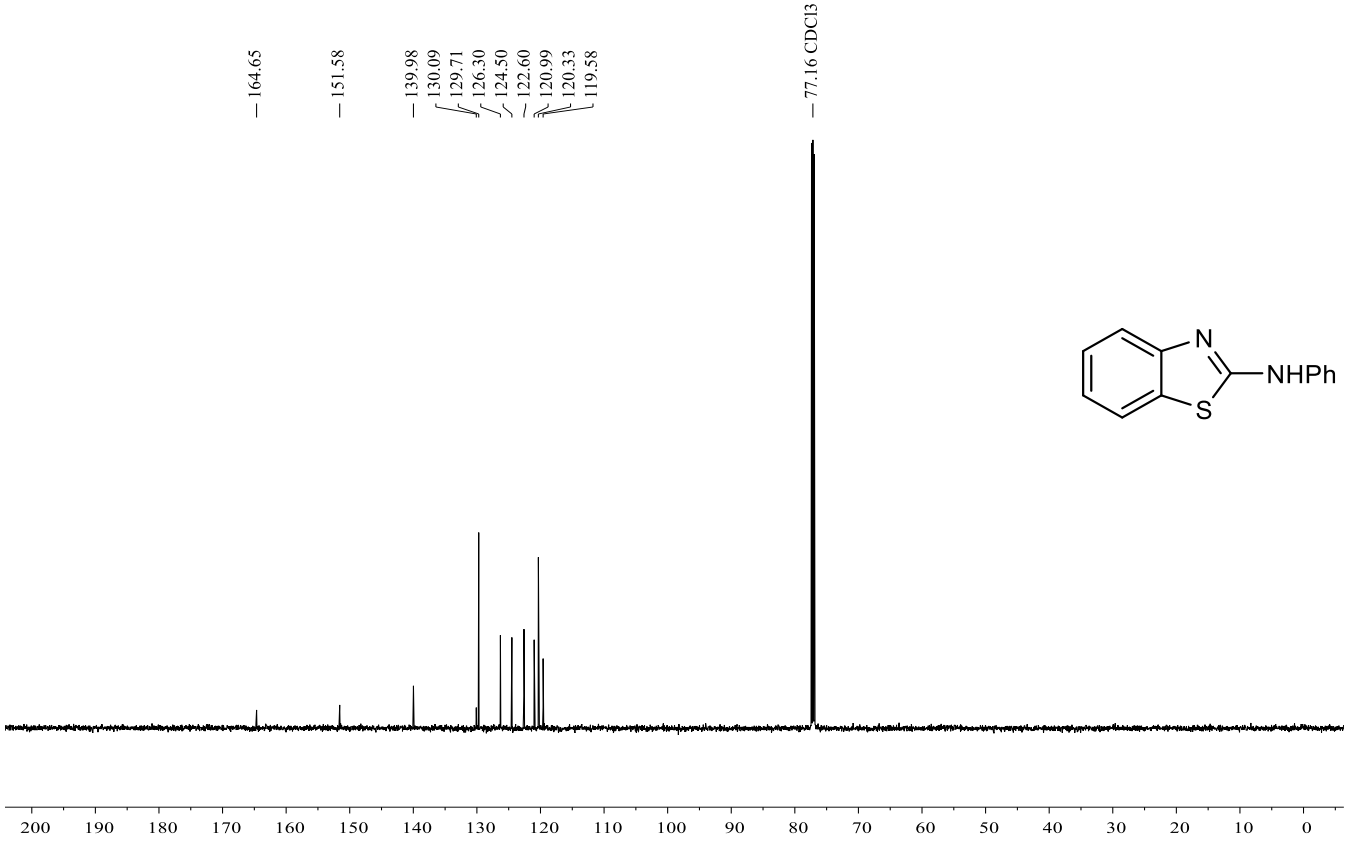


*N-phenylbenzo[d]thiazol-2-amine (Scheme 3c (i), Entry **8a**)*

^{1}H NMR (600 MHz)

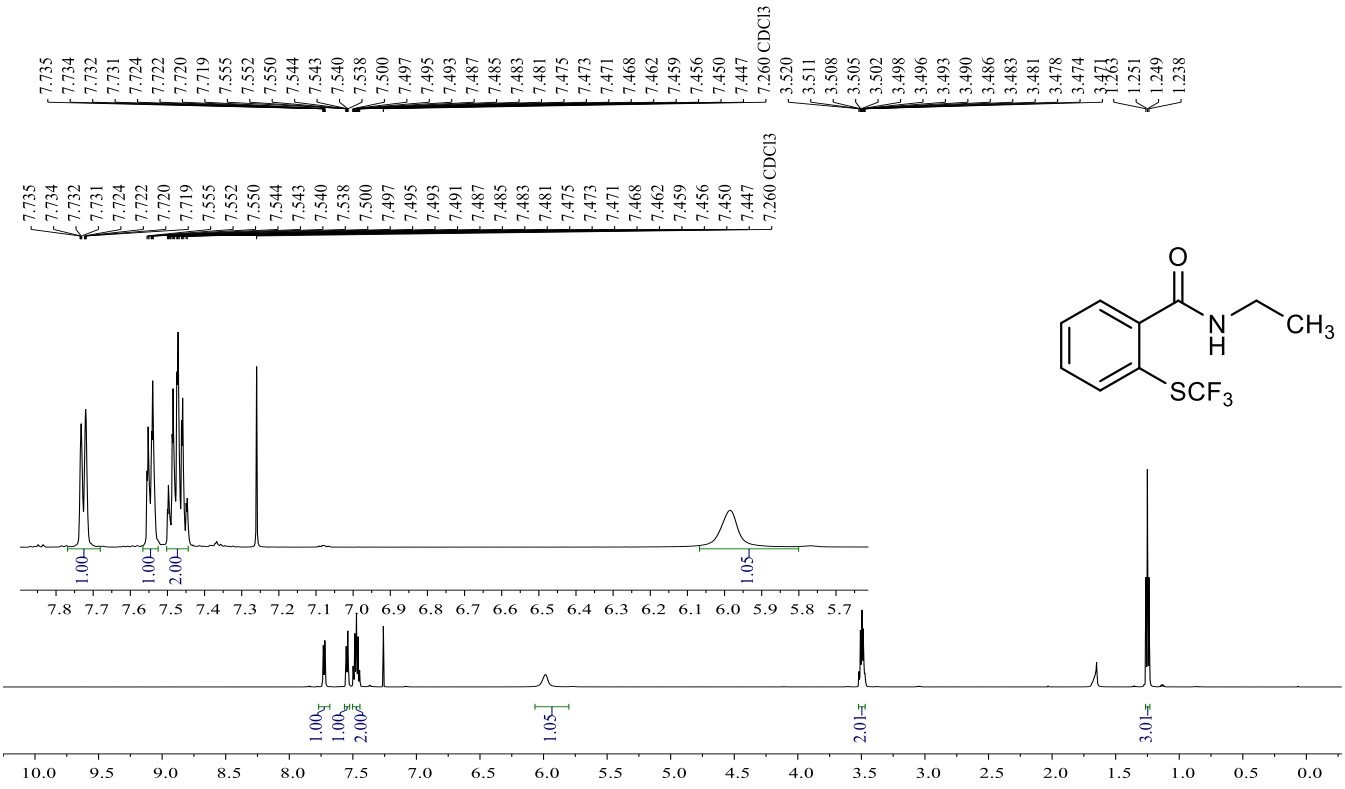


^{13}C{^{1}H} NMR (150 MHz)

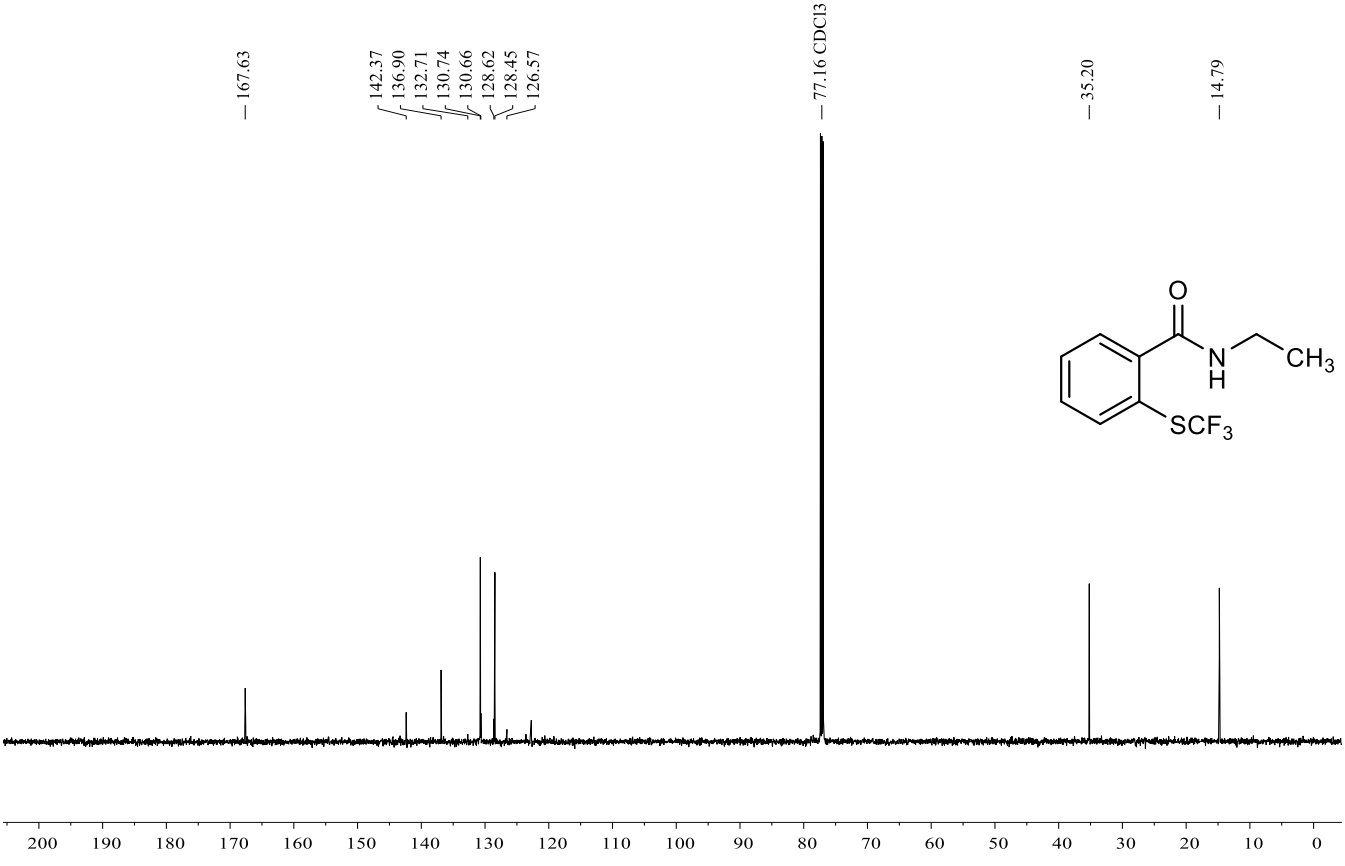


*N-ethyl-2-((trifluoromethyl)thio)benzamide (Scheme 3c (i), Entry **8b**)*

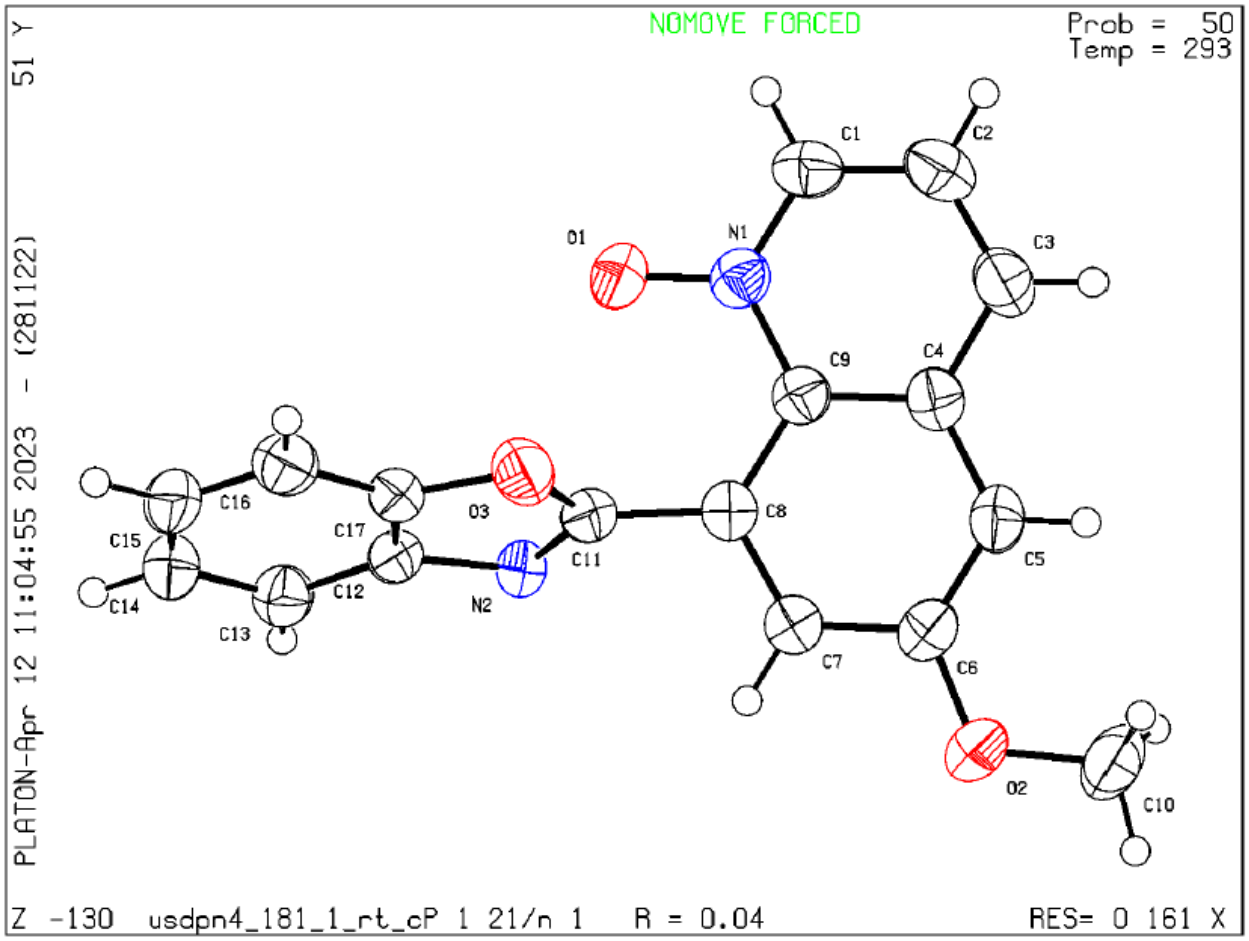
^{1}H NMR (600 MHz)



^{13}C{^{1}H} NMR (150 MHz)



13. X-ray data of 3k



ORTEP Diagram of **3k.** Ellipsoids displayed at 50% probability.

Crystal data and structure refinement

Identification code	USDPN4_181_1_Rt_Cu
Empirical formula	$C_{17}H_{12}N_2O_3$
Formula weight	292.29
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.7671(6)
b/Å	8.6079(6)
c/Å	18.2552(12)
α/°	90.00
β/°	93.710(6)
γ/°	90.00
Volume/Å^3	1374.75(16)
Z	4
ρ_{calc}g/cm^3	1.412
μ/mm^{-1}	0.813
F(000)	608.0

Crystal size/mm^3	0.49 × 0.363 × 0.244
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.72 to 132.6
Index ranges	$-10 \leq h \leq 9$, $-5 \leq k \leq 10$, $-21 \leq l \leq 21$
Reflections collected	4980
Independent reflections	2406 [R_{int} = 0.0216, R_{sigma} = 0.0269]
Data/restraints/parameters	2406/0/200
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0431, wR_2 = 0.1152
Final R indexes [all data]	R_1 = 0.0522, wR_2 = 0.1244
Largest diff. peak/hole / e Å^{-3}	0.18/-0.24

Bond Lengths

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O3	C17	1.390(2)	C17	C16	1.375(2)
O3	C11	1.350(2)	C8	C11	1.469(2)
O1	N1	1.2945(19)	C8	C7	1.367(2)
N2	C12	1.393(2)	C13	C14	1.383(3)
N2	C11	1.297(2)	C4	C5	1.412(3)
O2	C6	1.355(2)	C4	C3	1.416(3)
O2	C10	1.431(2)	C6	C7	1.409(2)
N1	C9	1.394(2)	C6	C5	1.366(3)
N1	C1	1.343(2)	C16	C15	1.379(3)
C12	C17	1.380(2)	C14	C15	1.391(3)
C12	C13	1.383(2)	C1	C2	1.389(3)
C9	C8	1.421(2)	C3	C2	1.354(3)
C9	C4	1.410(2)			

Bond Angles

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	O3	C17	103.58(14)	C14	C13	C12	116.02(17)
C11	N2	C12	104.54(14)	C9	C4	C5	118.98(17)
C6	O2	C10	117.33(17)	C9	C4	C3	118.88(17)
O1	N1	C9	119.39(15)	C5	C4	C3	122.13(17)
O1	N1	C1	120.58(15)	O3	C11	C8	120.98(16)
C1	N1	C9	120.02(16)	N2	C11	O3	115.73(15)
C17	C12	N2	108.32(15)	N2	C11	C8	123.13(16)
C17	C12	C13	121.80(16)	O2	C6	C7	114.19(17)
C13	C12	N2	129.88(16)	O2	C6	C5	125.87(17)
N1	C9	C8	120.58(15)	C5	C6	C7	119.93(17)
N1	C9	C4	119.33(16)	C8	C7	C6	121.61(18)
C4	C9	C8	120.07(16)	C6	C5	C4	120.51(17)
C12	C17	O3	107.74(14)	C17	C16	C15	116.34(18)

C16	C17	O3	129.94(17)	C13	C14	C15	121.87(18)
C16	C17	C12	122.30(17)	C16	C15	C14	121.60(17)
C9	C8	C11	123.85(15)	N1	C1	C2	121.31(18)
C7	C8	C9	118.72(16)	C2	C3	C4	119.44(18)
C7	C8	C11	117.42(16)	C3	C2	C1	120.72(18)

14. Computational Methods

The Gaussian16 software was used for the quantum mechanical calculations.[12] The DFT method, B3LYP[13] functional with Grimme's third generation empirical dispersion correction including Becke-Johanson damping was used for all calculations.[14] For geometry optimization, SDD[15] basis sets with the associated effective core potentials was used for Rh and Ag. The 6-31G** basis sets (BS1) were used for other atoms.[16] All calculations were performed with inclusion of solvent effect using SMD implicit solvation method with HFIP as solvent.[17] All stationary points were confirmed by hessian calculation at same level of theory with no imaginary frequency for minima and only one imaginary frequency for transition states (TSs) corresponding to expected atom displacement for the desired reaction.

The energies of stationary points were further calculated using SMD_{HFIP}/B3LYP-D3BJ/SDD(Rh,Ag),6-311++G**(other atoms) method. These computed electronic energies were then added to the thermal corrections obtained at SMD_{HFIP}/B3LYP-D3BJ/SDD(Rh,Ag),6-31G**(other atoms) level of theory to get free energy. Furthermore, the quasiharmonic corrections for entropy proposed by Grimme[18] using a frequency cut-off of 100 cm^{-1}, correction for standard state of 1 M for all species and for temperature (373.15 K) were also applied using GoodVibes v3.0.1 program.[19] The Gibbs free energies were reported in the paper. The molecular geometries in the Figures were generated using open source Pymol program.[20]

HFIP solvent is not implemented in Gaussian16 program, so we used "Solvent=Generic,Read" options in the SCRF keyword. Following parameters were used for the solvent[21]

Eps=16.7
EpsInf=1.62562
HbondAcidity=0.77
HbondBasicity=0.10
SurfaceTensionAtInterface=23.23
CarbonAromaticity=0.0
ElectronegativeHalogenicity=0.6

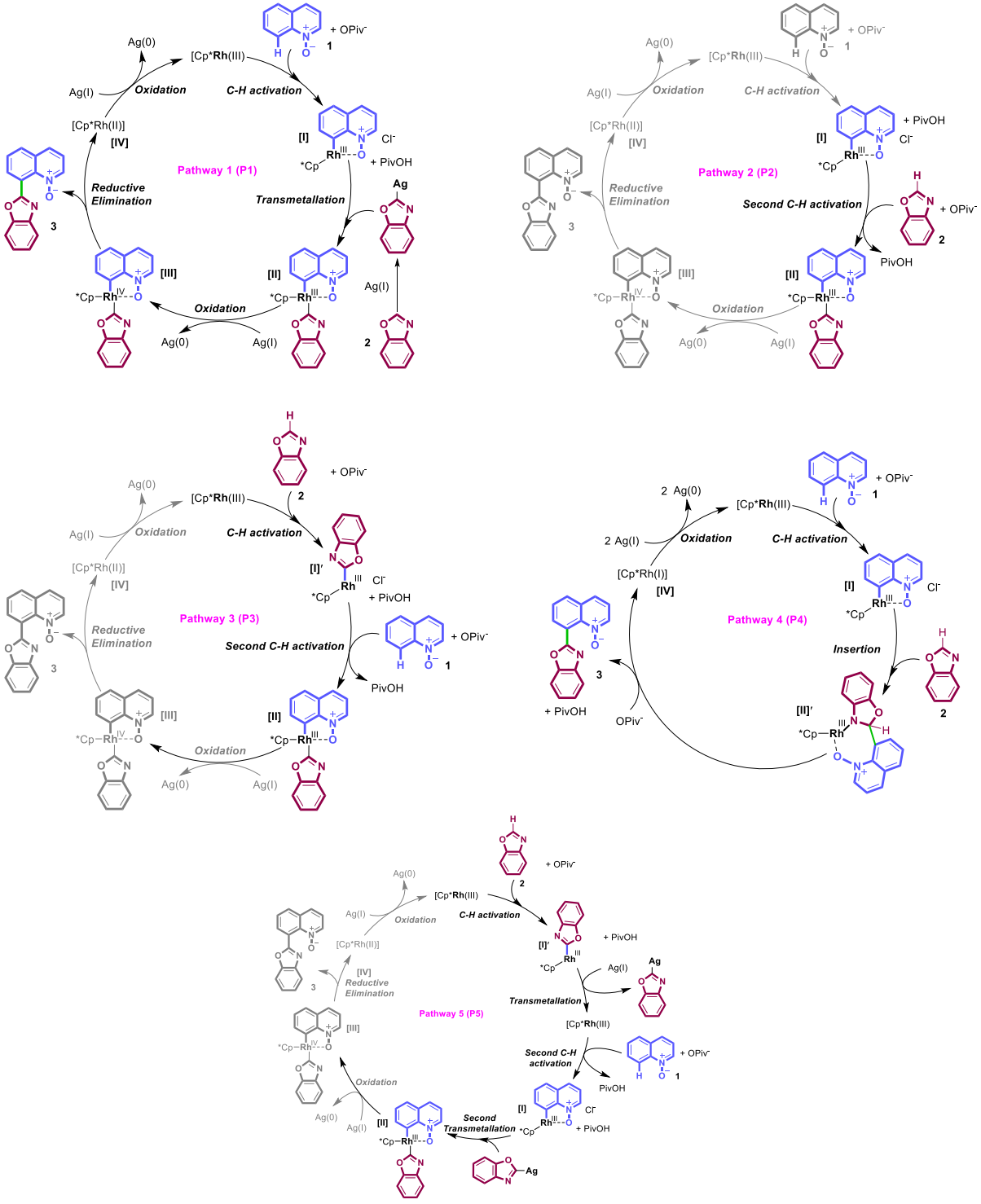


Figure S1. Different pathways examined in this study.

Initially, the activation of **2a** by Ag_2O takes place (Figure S2). The isolated Ag_2O molecule is used for DFT calculations. It is based on the assumption that Ag_2O is partially dissolved in the solvent,[22] although the possibility of Ag_2O catalysed C-H activation under heterogenous conditions cannot be excluded. The coordination of **2a** to 'Ag' of Ag_2O through *N*-atom is exergonic by 9.7 kcal/mol, and will generate the complex **A**. Further, **2a** will decoordinate from Ag_2O and form a complex **B**, which has weak C(2)-H---O interaction. It will be followed by the deprotonation of C(2)-H of **2a** by *O*-atom of Ag_2O (**TS1**) with 21.2 kcal/mol barrier.[22]

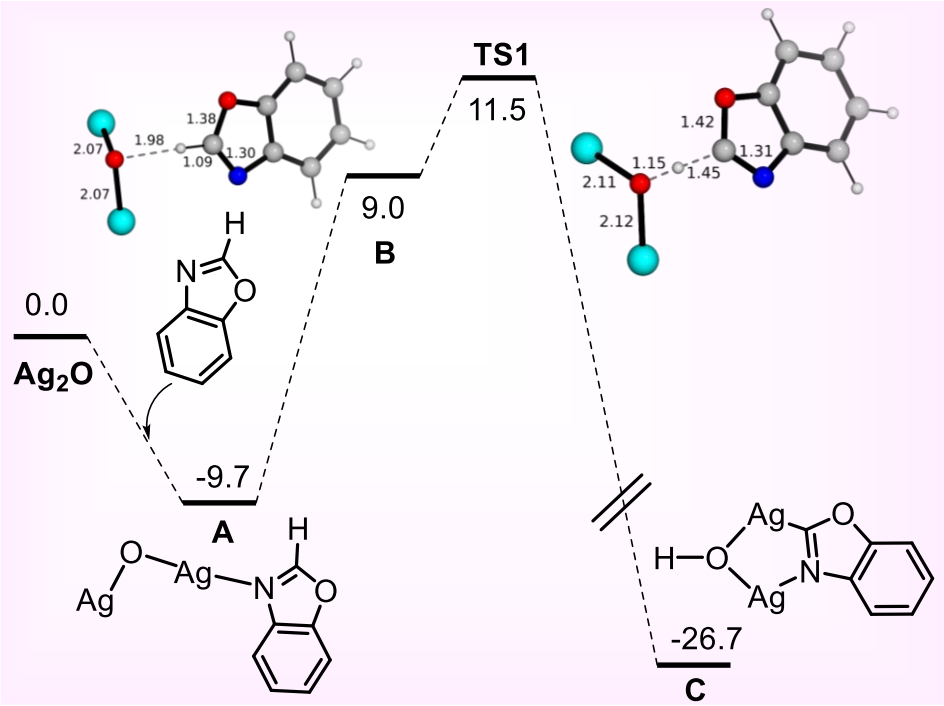


Figure S2. The free energy profile for abstraction of C2-proton of benzoxazole **2a** by Ag_2O.

The deprotonation of **2a** is a highly exergonic process and leads to the formation of species **C**, where Ag of Ag_2O is coordinated to C(2) and *N*-atom. The reaction between Ag_2O and **2a** might finish before the initiation of catalytic reaction, as these reagents are present in high concentration, and this process has a relatively lower barrier than the catalytic processes discussed later. Since HFIP coordination with Ag_2O is endergonic (Figure S2, SI), and PivOH is not crucial in the transmetallation step (Scheme 2a); the HFIP and PivOH involvement are not considered in this step. Furthermore, **2a** concentration is low in comparison to Ag_2O, hence the involvement of more than one molecule of **2a** is not explored.

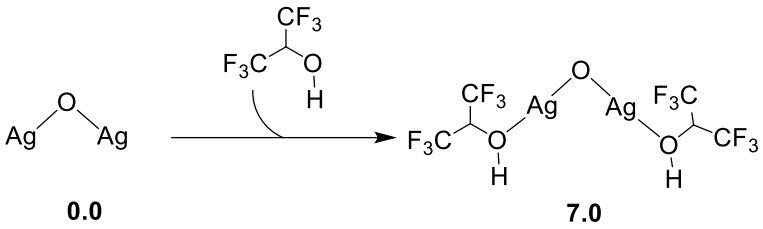


Figure S3. Thermodynamics for HFIP coordination to Ag_2O. Free energies are given in kcal/mol.

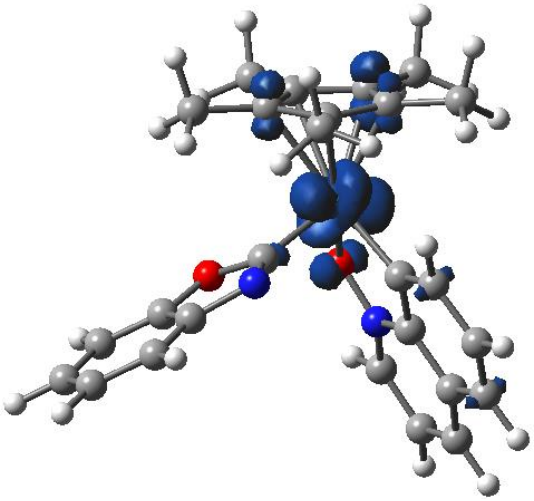


Figure S4. The spin density distribution on $^{2}\mathbf{H}^{\mathbf{IV}}$, Rh(IV) complex.

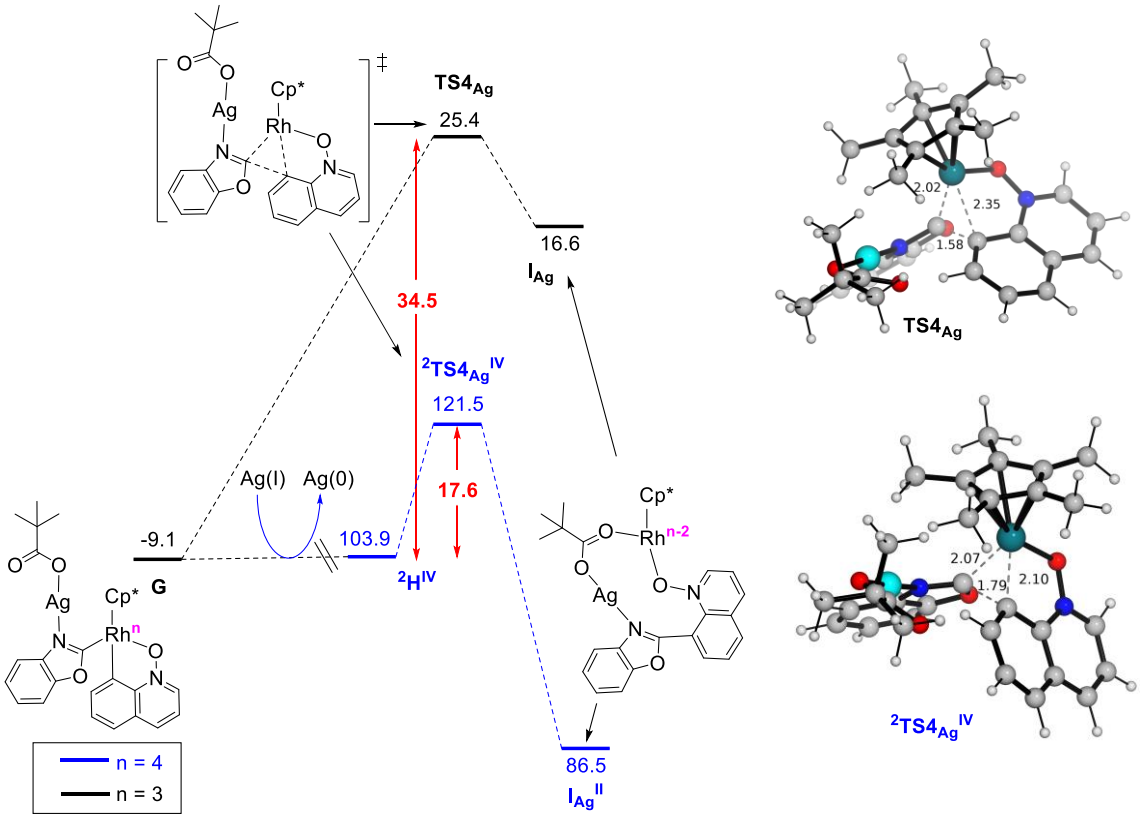


Figure S5. The Free energy profile for reductive elimination with Ag-PivO. Free energies are given in kcal/mol.

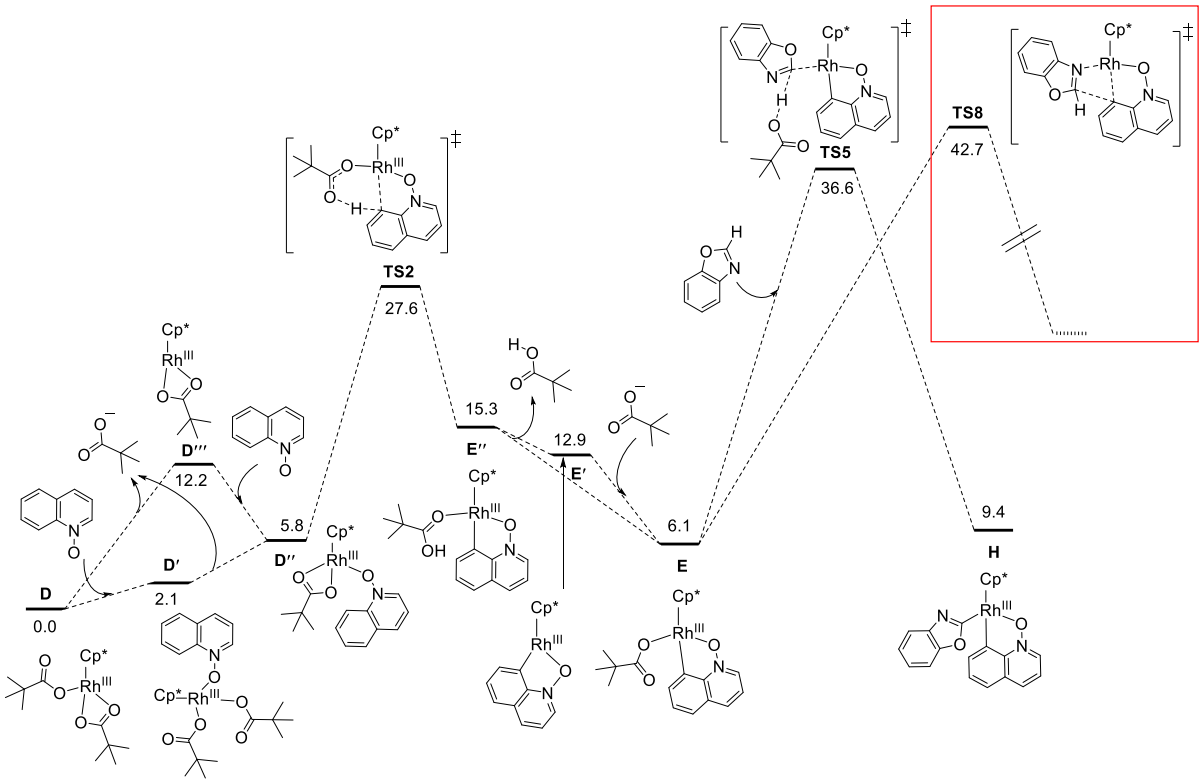


Figure S6. Free energy profile for C-H activation of both substrates (**1a** and **2a**) by Cp*Rh(III) catalyst (Pathway 2, Figure S1), where **1a** reacts first. Free energies are given in kcal/mol. Another possible path the involving carbometalation of **2a** by **E** (addition of **2a** to Rh-C bond of intermediate **E**) and followed by H-elimination (Pathway 4, Figure S1) was not explored fully as carbometalation step (**TS8**) have high barrier. Free energies are given in kcal/mol.

Description of C-H bond activation: The C-H activation of **1a** leading to formation of intermediate **E** involves more than one step (Figure S6). First, $PivO^-$ decoordinates from Rh (**D**) and **1a** coordinates to it to forms intermeidate **D″**. These two processes can take place in different sequences and both paths (through intermediate **D′** or **D″**) ares feasible under the reaction conditions. From intermediate **E″** the C(8)-H activation of **1a** occurs *via* CMD process through a transition state (**TS2**) with 27.6 kcal/mol barrier. It leads to the formation of intermediate **E″**. In next step PivOH decoordinates froming intermediate **E′**. Then $PivO^-$ coordinates to Rh forming intermediate **E**. Alternatively, the $PivO^-$ can also abstracts proton from PivOH of intermediate **E″** forming **E**.

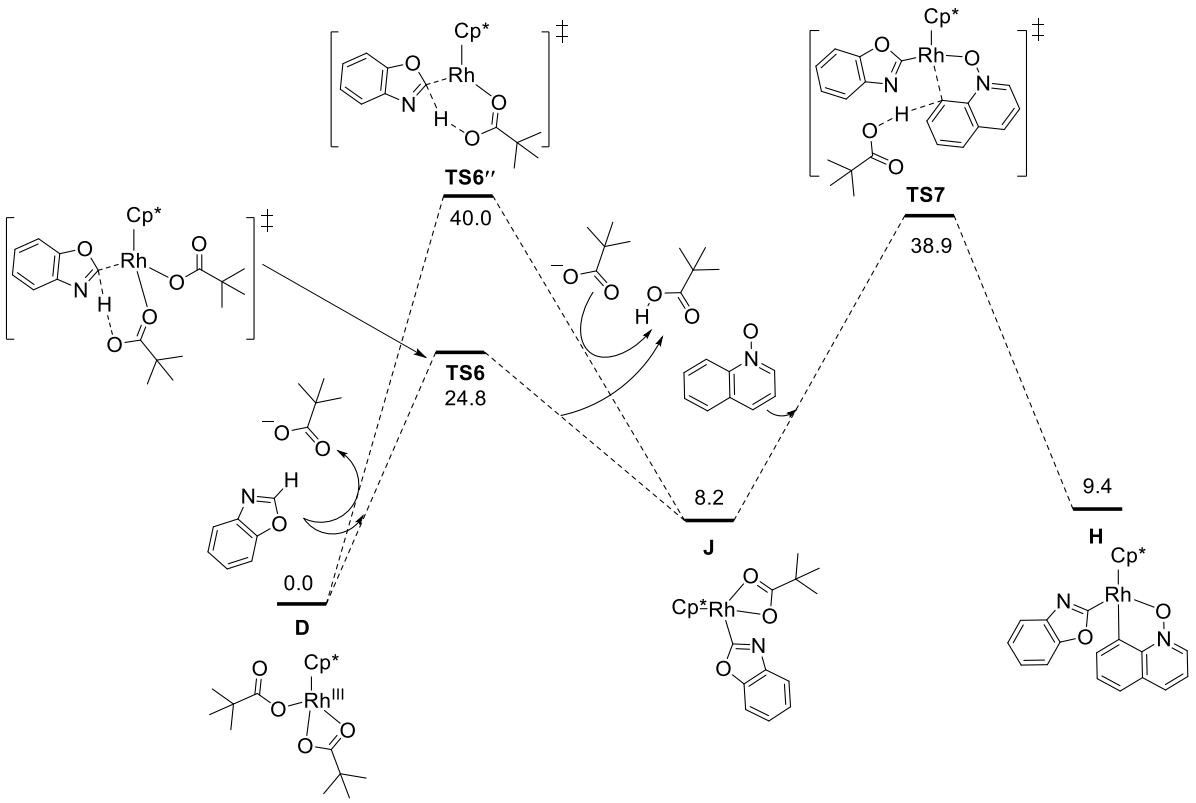


Figure S7. Free energy profile for C-H activation of both substrates (**1a** and **2a**) by Cp*Rh(III) catalyst, where **2a** reacts first (Pathway 3, Figure S1). Free energies are given in kcal/mol.

- Besides the most probable pathway described in Figure 1 (main text) and Figure S2 (SI) the other possible pathways were also explored (Figure S1, SI). In pathway-2, the C-H activation of **2a** by Rh(III)-complex **E** forming **H** has 36.6 kcal/mol barrier (Figure S6 , SI).

- In pathway-3, leading to intermediate **H**, although the first C-H activation of **2a** by Rh-catalyst (**D**) has a relatively lower barrier (24.8 kcal/mol), but then the barrier for C-H activation of **1a** is high (38.9 kcal/mol, Figure S7, SI).

- Furthermore, we also considered the carbometalation of **2a** by **E** (pathway 4), but the barrier for the process was 42.7 kcal/mol (Figure S6, SI).

"All these pathways have high activation barriers (>35 kcal/mol), and the reaction is less likely to proceed through these pathways."

- In another probable pathway (pathway-5, Figure S1), the first step involves C-H activation of **2a** by Rh-catalyst (**D**) leading to the formation of intermediate **J** (Figure S7). The intermediate **J** then further reacts with Ag_2O and PivOH undergoing transmetallation forming intermediate **C** and **D**. The transmetallation step was not explored by DFT, as the barrier is expected to be approximately similar to the transmetallation of **E**. Afterwards, the reaction proceeds by mechanism as described in Figure 1 (main text). The free energy profile for this reaction is not shown, as the processes involved in this reaction are already described in Figure S7 and Figure 1 (main text). This pathway is feasible under the reaction conditions, but as the barrier for C-H activation of **2a** by Rh(III)-species **D** (24.8 kcal/mol, Figure S7) is higher than

C-H activation of **2a** by Ag_2O (21.2 kcal/mol, Figure S2). Hence, the reaction is less likely to proceed through this pathway.

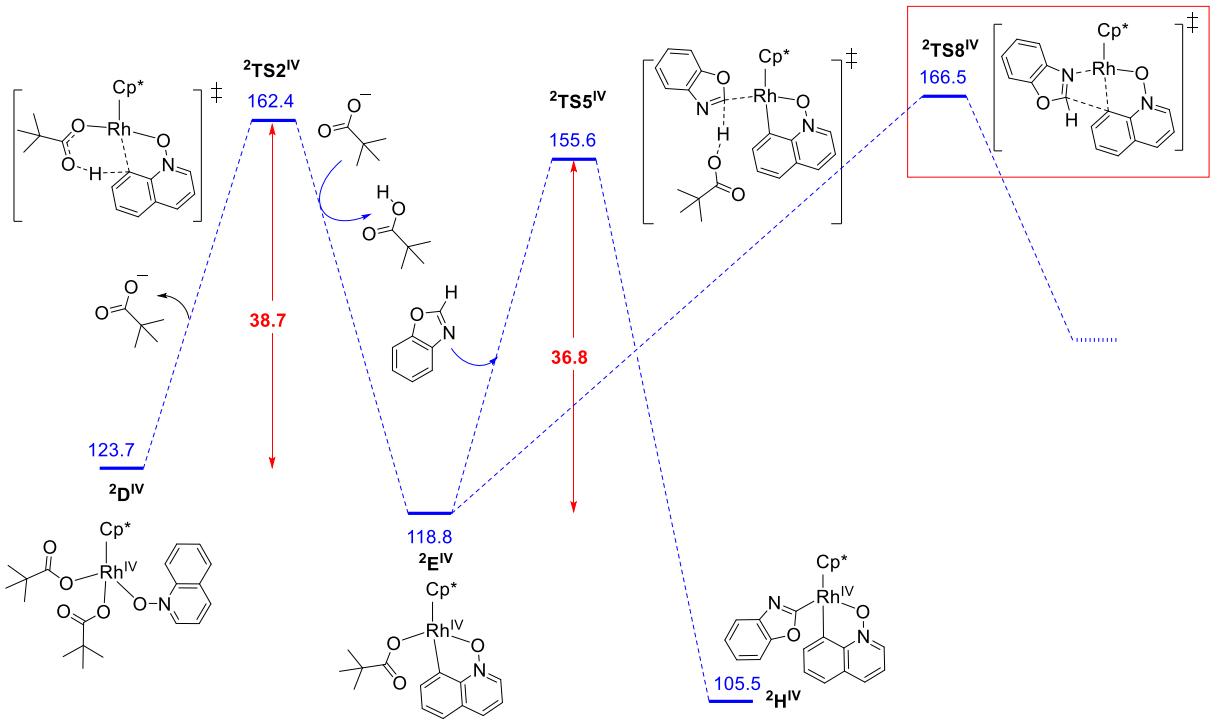


Figure S8. Free energy profile for C-H activation of both substrates (**1a** and **2a**) by Cp*Rh(IV) catalyst. Another possible path the involving carbometalation of **2a** by **E** (addition of **2a** to Rh-C bond of intermediate **E**) and followed by H-elimination was not explored fully as TS for carbometalation, **TS8** (in inset) have high barrier. Free energies are given in kcal/mol.

- Besides checking the effect of oxidation before reductive elimination, we also explored the effect of oxidation on the C-H activation of **1a** as well as **2a** by Cp*Rh. However, this seems unlikely due to high free energy barriers (>35 kcal/mol) (Figure S8). It shows that oxidation doesn't have any role in other steps.

Table S9. Computed total electronic energies (E_SPC), total electronic energy (E) at lower level of theory, zero-point energy correction (ZPE), enthalpy (H_SPC), temperature*entropy (T.S) term, T.S with quasiharmonic correction by Grimme (T.qh-S), free energy (with quasiharmonic corrections for entropy and correction for solution phase standard state of 1 mole/litre, qh-G(T)_SPC) and relative energy w.r.t. substrates and catalyst (ΔG_qh-G(T)_SPC). The energies are at 373.15 K temperature. The E_SPC is at SMD_{HFIP}/B3LYP-D3BJ/SDD(Rh,Ag),6-311++G**(other atoms) level of theory. The E and energy corrections are at SMD_{HFIP}/B3LYP-D3BJ/SDD(Rh,Ag),6-31G** level of theory. All energies are in hartee, except ΔG_qh-G(T)_SPC which is in kcal/mol

	E_SPC	E	ZPE	H_SPC	T.S	T.qh-S	G(T)_SPC	qh-G(T)_SPC	ΔG_ qh-G(T)_SPC
2a	-399.860215	-399.754317	0.106014	-399.744027	0.045787	0.04579	-399.789815	-399.789818	
1a	-477.273606	-477.145221	0.140396	-477.12027	0.051892	0.051818	-477.172163	-477.172088	
PivOH	-347.168476	-347.065827	0.146472	-347.008518	0.053068	0.051879	-347.061587	-347.060398	
PivO-	-346.699062	-346.576581	0.133769	-346.552454	0.051062	0.050516	-346.603515	-346.602969	
3a	-875.934533	-875.706732	0.226051	-875.685701	0.075752	0.072835	-875.761453	-875.758536	
HFIP	-790.083089	-789.806888	0.062256	-790.006156	0.057966	0.056636	-790.064122	-790.062792	
Ag0H	-222.86923	-222.834065	0.011313	-222.852523	0.033706	0.033707	-222.88623	-222.88623	
Ag_2(OH)(PivOH)	-716.514562	-716.39229	0.148535	-716.344563	0.081651	0.075397	-716.426214	-716.41996	
Ag_2O	-369.255807	-369.226864	0.002086	-369.247013	0.042782	0.042037	-369.289795	-369.28905	**0.0**
A	-769.155095	-769.027904	0.109959	-769.027216	0.071229	0.067117	-769.098445	-769.094333	**-9.7**
$Ag_2O(BOxZ)_2$	-1169.055952	-1168.83098	0.217727	-1168.809009	0.098572	0.090409	-1168.907581	-1168.899418	**-19.3**
B	-769.12415	-768.994231	0.108462	-768.998315	0.071275	0.066469	-769.06959	-769.064784	**8.8**
TS1	-769.113104	-768.981675	0.102702	-768.992458	0.074245	0.068045	-769.066703	-769.060503	**11.5**
C	-769.179431	-769.049991	0.107348	-769.053325	0.071183	0.068124	-769.124508	-769.121449	**-26.7**
$Ag_2O(HFIP)_2$	-1949.462921	-1948.91172	0.130977	-1949.294361	0.121811	0.109176	-1949.416172	-1949.403537	**7.0**
D	-1194.070402	-1193.800955	0.494656	-1193.527034	0.137918	0.126909	-1193.664952	-1193.653943	0.0
D′	-1671.372279	-1670.982634	0.637785	-1670.672519	0.161187	0.150122	-1670.833706	-1670.822641	**2.1**
D″	-1324.639237	-1324.351049	0.501643	-1324.089197	0.132893	0.124573	-1324.22209	-1324.213769	5.8
D‴	-847.326377	-847.154144	0.35901	-846.932496	0.105497	0.098977	-847.037993	-847.031473	12.2
TS2	-1324.601019	-1324.313556	0.496753	-1324.056636	0.129975	0.122516	-1324.186611	-1324.179152	27.6
E	-1324.171004	-1323.876884	0.489529	-1323.633931	0.128892	0.121996	-1323.762823	-1323.755927	6.1
E′	-977.434559	-977.239063	0.353863	-977.046748	0.098771	0.095364	-977.145519	-977.142112	12.9
E″	-1324.623954	-1324.335516	0.501682	-1324.073911	0.133785	0.124834	-1324.207696	-1324.198745	15.3
TS5	-1724.004361	-1723.606509	0.592152	-1723.353794	0.153611	0.143265	-1723.507406	-1723.497059	36.6
TS8	-1377.273749	-1376.978945	0.460419	-1376.769065	0.12159	0.115402	-1376.890655	-1376.884467	42.7
TS8′	-1377.268919	-1376.975197	0.460646	-1376.764272	0.120154	0.114543	-1376.884426	-1376.878814	46.2
TS6	-1593.915745	-1593.546743	0.597641	-1593.259347	0.155705	0.144864	-1593.415053	-1593.404211	24.8
TS6′	-1593.911787	-1593.542251	0.598205	-1593.25509	0.153853	0.14382	-1593.408942	-1593.39891	28.1
TS6″	-1247.167882	-1246.896043	0.463304	-1246.659864	0.124938	0.117149	-1246.784802	-1246.777013	40.0
J	-1246.751578	-1246.476914	0.454657	-1246.251725	0.126226	0.118588	-1246.37795	-1246.370313	8.2
TS7	-1723.999467	-1723.602011	0.59086	-1723.349887	0.153569	0.143593	-1723.503456	-1723.49348	38.9
H	-1376.855654	-1376.55606	0.448059	-1376.362677	0.124439	0.117327	-1376.487116	-1376.480005	-8.1
TS4	-1376.799437	-1376.499281	0.445543	-1376.309439	0.121643	0.115796	-1376.431082	-1376.425235	26.3
I	-1376.812991	-1376.513077	0.447878	-1376.320151	0.125185	0.117801	-1376.445336	-1376.437952	18.3
$^2H^{IV}$	-1376.677865	-1376.383577	0.44892	-1376.184056	0.125048	0.117922	-1376.309105	-1376.301979	103.6
$^2TS4^{IV}$	-1376.65761	-1376.363924	0.447443	-1376.165831	0.122331	0.116472	-1376.288162	-1376.282303	116.0
$^2I^{IV}$	-1376.704788	-1376.41163	0.450813	-1376.209508	0.124319	0.117347	-1376.333826	-1376.326854	88.0
F	-1870.488311	-1870.099084	0.584589	-1869.841935	0.164891	0.151569	-1870.006826	-1869.993504	4.6
F′	-1870.484606	-1870.093673	0.585032	-1869.837851	0.164524	0.151409	-1870.002375	-1869.98926	7.3
TS3	-1870.482728	-1870.092273	0.584491	-1869.837377	0.161559	0.149138	-1869.998935	-1869.986515	9.0
G′	-1870.493108	-1870.103139	0.583454	-1869.847261	0.169871	0.154167	-1870.017131	-1870.001427	-0.4
G	-1870.511457	-1870.120876	0.5854	-1869.864631	0.163976	0.150783	-1870.028607	-1870.015415	-9.1
H	-1376.855654	-1376.55606	0.448059	-1376.362677	0.124439	0.117327	-1376.487116	-1376.480005	-8.1
$TS4_{Ag}$	-1870.45445	-1870.062805	0.582985	-1869.810534	0.162103	0.149864	-1869.972637	-1869.960398	25.4
I_{Ag}	-1870.471214	-1870.081826	0.58441	-1869.825778	0.15912	0.148542	-1869.984898	-1869.97432	16.6
$^2G^{IV}$	-1870.330222	-1869.944416	0.585641	-1869.682967	0.166425	0.152289	-1869.849393	-1869.835257	103.9
$^2TS4_{Ag}{}^{IV}$	-1870.302898	-1869.916981	0.584677	-1869.657532	0.161497	0.149726	-1869.819029	-1869.807257	121.5
$^2I_{Ag}{}^{IV}$	-1870.361373	-1869.978688	0.587165	-1869.713109	0.160954	0.149926	-1869.874063	-1869.863035	86.5
$^2D^{IV}$	-1671.178977	-1670.796177	0.638196	-1670.479043	0.159464	0.149886	-1670.638508	-1670.628929	**123.7**
$^2TS2^{IV}$	-1324.388109	-1324.104816	0.497991	-1323.84317	0.127541	0.121098	-1323.970711	-1323.964268	162.4
$^2E^{IV}$	-1323.988635	-1323.700074	0.488999	-1323.451447	0.13346	0.12489	-1323.584907	-1323.576336	118.8
$^2TS5^{IV}$	-1723.816321	-1723.420922	0.594516	-1723.163357	0.155273	0.144083	-1723.31863	-1723.307439	155.6
$^2H^{IV}$	-1376.704788	-1376.41163	0.450813	-1376.209508	0.124319	0.117347	-1376.333826	-1376.326854	105.5
$^2TS8^{IV}$	-1377.077126	-1376.788761	0.460901	-1376.572207	0.120252	0.114995	-1376.692459	-1376.687202	166.5

Cartesian Coordinates in xyz format

14
2a Eopt -399.754317
C 0.514718 0.584585 -0.000000
C -0.000000 -0.717781 -0.000000
C -1.352946 -1.019216 0.000000
C -2.212633 0.082676 0.000000
C -1.723064 1.402667 0.000000
C -0.355120 1.677226 0.000000
H -1.717061 -2.040505 0.000000
H -3.285284 -0.085018 0.000000
H -2.430757 2.226130 0.000000
H 0.022776 2.694385 0.000000
C 2.169697 -0.754145 -0.000000
H 3.133583 -1.243946 -0.000000
N 1.917423 0.513540 -0.000000
O 1.076360 -1.585236 -0.000000
18
1a Eopt -477.145221
C -2.023131 1.438437 0.000024
C -0.725904 1.896370 -0.000044
C 0.332772 0.953882 -0.000049
C 0.031388 -0.437077 -0.000007
C -2.291365 0.063256 0.000019
H 1.943677 2.390733 -0.000254
H -2.866231 2.120380 0.000083
H -0.500325 2.957498 -0.000217
C 1.701323 1.332257 -0.000027
C 1.052005 -1.406728 -0.000134
H -3.290562 -0.352308 0.000148
C 2.368863 -0.997152 -0.000012
C 2.695812 0.379557 0.000123
H 3.162509 -1.737867 0.000148
H 3.738178 0.682995 0.000522
N -1.306617 -0.854305 0.000065
O -1.583203 -2.120683 0.000041
H 0.774121 -2.452636 -0.000562
17
PivOH Eopt -347.065827
O -1.517054 1.257472 -0.000144
C -0.939463 0.183131 -0.000157
O -1.612767 -0.986380 -0.000115
H -2.566315 -0.786026 -0.000003
C 0.964064 -0.807075 -1.262315
H 0.669964 -0.273392 -2.172446
H 0.494035 -1.794120 -1.274780
C 0.571448 -0.012044 -0.000028
C 1.253986 1.360379 -0.001132
H 0.977101 1.941678 0.883512
H 0.977173 1.940208 -0.886768
C 0.963765 -0.804872 1.263774
H 0.493630 -1.791850 1.277876
H 0.669532 -0.269547 2.172897
H 2.340751 1.231321 -0.000986
H 2.050107 -0.943138 -1.284355
H 2.049792 -0.940990 1.286257
16
PivO- Eopt -346.576581
O -1.622993 1.151453 -0.000079
C -1.038114 0.030269 -0.000083
O -1.612697 -1.099158 -0.000041
C 0.994072 -0.746606 -1.255769
H 0.678055 -0.228916 -2.169742
H 0.572921 -1.756258 -1.279753
C 0.522193 0.009014 -0.000018
C 1.103323 1.426655 0.000252
H 0.778530 1.987701 0.882577
H 0.778536 1.988062 -0.881850
C 0.993770 -0.746914 1.255669
H 0.572626 -1.756583 1.279341
H 0.677524 -0.229456 2.169693
H 2.200165 1.398279 0.000245
H 2.088007 -0.827693 -1.278593
H 2.087697 -0.828005 1.278732

30
3a Eopt -875.706732
C 3.912841 -1.943979 0.060204
C 4.244591 -0.626900 -0.155431
C 3.219645 0.350914 -0.144534
C 1.868302 -0.046347 0.067037
C 2.584177 -2.302038 0.309066
H 4.530788 2.030343 -0.481532
H 4.661762 -2.727948 0.061019
H 5.271135 -0.320668 -0.324760
C 3.499363 1.731315 -0.322682
C 0.825051 0.917144 0.056519
H 2.262941 -3.313729 0.519099
C 1.153692 2.253942 -0.100003
C 2.490858 2.664715 -0.281937
H 0.357005 2.990232 -0.104963
H 2.712473 3.719564 -0.406318
N 1.590205 -1.392216 0.331062
O 0.380333 -1.757554 0.614079
C -0.602843 0.571648 0.147145
C -2.493298 -0.180235 -0.630235
C -2.686283 0.455548 0.603739
N -1.451179 0.938439 1.057760
O -1.153240 -0.087090 -0.935784
C -3.964842 0.520321 1.160530
C -5.006570 -0.067203 0.439958
H -4.136193 1.008258 2.114631
H -6.014556 -0.037099 0.842570
C -4.784312 -0.699105 -0.797283
C -3.508580 -0.769124 -1.366314
H -5.622406 -1.145094 -1.324039
H -3.323614 -1.253965 -2.318506
12
HFIP Eopt -789.806888
C 0.001342 0.558097 -0.508177
H 0.000491 0.538405 -1.602996
C -1.272782 -0.150147 -0.037213
C 1.276461 -0.143417 -0.041945
F 1.393650 -0.127868 1.298902
F 2.353539 0.481337 -0.552537
F 1.310434 -1.427371 -0.446949
F -1.332720 -0.242806 1.304373
F -1.371918 -1.394538 -0.543336
F -2.350149 0.549342 -0.446094
O 0.037538 1.857799 0.026250
H -0.356447 2.469154 -0.612227
3
Ag0H Eopt -222.834065
Ag 0.016766 -0.338369 -0.000000
O 0.016766 1.740716 0.000000
H -0.922155 1.977632 0.000000
20
Ag_2(OH)(PivO) Eopt -716.392290
C -1.554528 0.032874 0.007658
O -0.995166 -1.111340 0.001437
O -0.966280 1.159325 0.013892
C -3.574890 -0.767214 1.237157
H -3.194572 -1.792234 1.220448
H -3.237589 -0.290531 2.164526
C -3.558787 -0.692630 -1.283532
H -3.210739 -0.161058 -2.176425
H -3.176736 -1.716500 -1.323174
C -3.098108 0.022095 0.002339
C -3.667465 1.444897 0.040496
H -3.350054 1.977829 0.942051
H -3.345633 2.027222 -0.828116
H -4.652920 -0.730598 -1.318166
H -4.669392 -0.805296 1.256098
H -4.762162 1.405209 0.036736
Ag 1.199835 -1.382684 -0.001169
O 2.971560 -0.033270 -0.092046
Ag 1.244398 1.377723 -0.002640
H 3.362642 -0.038727 0.794067
3
Ag_2O Eopt -369.226864

Ag 1.547548 -0.106596 0.000000
O 0.000000 1.252580 0.000000
Ag -1.547548 -0.106609 -0.000000
17
A Eopt -769.027904
Ag -2.988325 0.868144 -0.231488
O -2.627221 -1.035762 0.480670
Ag -0.618787 -0.982567 0.219359
C 3.615790 -0.212798 -0.212814
C 2.305540 0.189399 0.053639
C 2.014330 1.521176 0.346502
C 3.091209 2.407135 0.355048
C 4.405516 1.979854 0.082323
C 4.702306 0.646582 -0.210744
C 2.289989 -1.931956 -0.343072
H 0.999029 1.841088 0.556763
H 2.914805 3.454653 0.577794
H 5.211877 2.706142 0.100689
H 5.709314 0.305357 -0.421090
N 1.488881 -0.950107 -0.042151
O 3.588921 -1.577342 -0.464914
H 2.035347 -2.970165 -0.500348
31
$Ag_2O(BOxZ)_2$ Eopt -1168.830980
Ag 1.550828 -1.817007 -0.087421
O 0.139045 -3.282977 -0.171473
Ag -1.385893 -1.942449 -0.006141
C -3.706855 1.682724 0.206230
C -2.678705 0.893605 -0.312762
C -1.720980 1.441305 -1.165576
C -1.843623 2.801125 -1.450301
C -2.885447 3.580332 -0.910218
C -3.852984 3.033879 -0.062961
C -3.906713 -0.351259 0.951934
H -0.920623 0.835318 -1.575671
H -1.115911 3.273412 -2.102273
H -2.940350 4.635212 -1.159556
H -4.660480 3.622412 0.356914
N -2.846627 -0.405714 0.197742
O -4.491028 0.867540 1.010685
H -4.357025 -1.151904 1.520785
C 3.662322 1.935174 0.159864
C 2.525249 1.131689 0.258702
C 1.281359 1.688070 0.552789
C 1.241449 3.070763 0.727218
C 2.400821 3.863740 0.620943
C 3.651347 3.309657 0.334306
C 4.204151 -0.138806 -0.214404
H 0.395364 1.069464 0.635226
H 0.292441 3.549501 0.946459
H 2.322620 4.936453 0.766532
H 4.550134 3.909702 0.251668
N 2.922562 -0.193301 0.007873
O 4.733239 1.104427 -0.140509
H 4.871943 -0.955910 -0.446179
17
B Eopt -768.994231
C 2.828530 -0.809557 0.037480
C 3.002384 0.510860 0.472017
C 4.174994 1.232422 0.313460
C 5.216072 0.555214 -0.328433
C 5.068391 -0.770660 -0.777019
C 3.876308 -1.475241 -0.602219
H 4.277235 2.252768 0.666397
H 6.161725 1.065608 -0.483166
H 5.905396 -1.255675 -1.270092
H 3.764055 -2.498688 -0.945727
C 0.994670 -0.193471 0.953858
H -0.028946 -0.073935 1.320208
N 1.526341 -1.219548 0.366049
O 1.817080 0.907974 1.061692
O -1.985546 0.206004 1.182433
Ag -2.132364 -1.439140 -0.070299
Ag -1.705598 1.563343 -0.359868
17
TS1 Eopt -768.981675
C 2.949458 -0.799947 0.122647
C 2.996112 0.589235 0.295451
C 4.126834 1.356375 0.053614
C 5.258794 0.662170 -0.388917
C 5.237067 -0.731823 -0.571517
C 4.085907 -1.482665 -0.318477
H 4.133727 2.431485 0.201666
H 6.172391 1.212525 -0.594197
H 6.136699 -1.234037 -0.915737
H 4.071902 -2.559807 -0.457383
C 0.970909 -0.193129 0.818553
H -0.450773 -0.047526 1.062304
N 1.663788 -1.246387 0.457610
O 1.754347 0.987231 0.731268
O -1.591158 0.052954 1.110060
Ag -2.116138 -1.574348 -0.136444
Ag -1.857617 1.663695 -0.231613
17
C Eopt -769.049991
C 2.140197 -0.355778 0.001380
C 2.620606 0.956353 0.005978
C 3.969172 1.278633 0.008177
C 4.853714 0.195347 0.004119
C 4.390838 -1.133480 -0.001610
C 3.027218 -1.432878 -0.002812
H 4.314089 2.306918 0.012434
H 5.922629 0.385562 0.005125
H 5.113563 -1.943920 -0.005311
H 2.666965 -2.457208 -0.007239
C 0.393759 0.997014 0.004111
H -3.536350 -0.518699 0.819148
N 0.743073 -0.286087 0.001173
O 1.525734 1.803348 0.007678
O -3.156008 -0.436811 -0.067647
Ag -1.164332 -1.518919 -0.003589
Ag -1.708290 1.311821 -0.006383
27
$Ag_2O(HFIP)_2$ Eopt -1948.911720
Ag -1.778522 -1.894576 0.072613
O -0.144233 -3.097143 -0.154270
Ag 1.137919 -1.525102 0.102769
O 2.490210 0.182152 0.533171
C 3.822348 0.238920 0.062930
O -3.494699 -0.503599 0.328273
C -3.535377 0.748245 -0.328283
H -3.258299 0.576441 -1.369766
H 4.218277 -0.777555 0.092290
C -2.515013 1.726677 0.270637
C -4.974946 1.278091 -0.310692
C 4.671899 1.089217 1.015229
C 3.862780 0.716566 -1.391981
F -1.261621 1.258507 0.092495
F -2.702136 1.889109 1.593871
F -2.591551 2.929656 -0.317499
F -5.396630 1.519241 0.947161
F -5.795113 0.360955 -0.849923
F -5.088751 2.413175 -1.016228
F 4.544516 0.616896 2.266807
F 4.288841 2.381111 1.021195
F 5.969849 1.039890 0.674883
F 5.120387 0.775650 -1.853303
F 3.305106 1.936364 -1.524544
F 3.168486 -0.134477 -2.172946
H -3.742792 -0.425133 1.265764
H 2.038293 1.038816 0.446584
58
D Eopt -1193.800955
Rh 0.805108 -0.005418 -0.070681
C 2.904631 0.435123 0.167466
C 2.479041 -0.433165 1.233875
C 2.689896 -0.271293 -1.077935
C 1.987967 -1.661014 0.660647
C 2.123939 -1.559628 -0.777090
C 2.484433 -0.096296 2.685265

H	3.433397	-0.416824	3.133236
H	2.382304	0.979387	2.842973
H	1.673507	-0.604535	3.211047
C	3.481235	1.805230	0.311273
H	3.093794	2.304199	1.202512
H	4.573616	1.754766	0.399412
H	3.242212	2.424118	-0.556889
C	2.974930	0.275820	-2.434799
H	2.747402	1.343542	-2.483791
H	4.039686	0.148309	-2.666843
H	2.395121	-0.238459	-3.203587
C	1.740258	-2.618602	-1.755275
H	1.559740	-2.199307	-2.747001
H	2.544601	-3.359786	-1.839666
H	0.835806	-3.139290	-1.431766
C	1.491705	-2.853562	1.407417
H	0.711884	-3.374787	0.848326
H	2.318160	-3.557246	1.570060
H	1.086272	-2.573339	2.380844
C	-0.647440	2.146457	0.016483
O	-0.352610	1.522828	1.087830
O	-0.084710	1.775232	-1.069294
C	-1.268268	4.368994	-0.947218
H	-0.341733	4.838909	-0.599013
H	-1.102402	3.994755	-1.960926
C	-1.937995	3.784834	1.415954
H	-2.274952	2.997101	2.095264
H	-1.022390	4.221914	1.828287
C	-1.705598	3.239889	0.000449
C	-2.995728	2.571313	-0.528747
H	-2.849533	2.185683	-1.542121
H	-3.297434	1.739932	0.116974
H	-2.044472	5.140155	-0.988640
H	-2.705290	4.565565	1.389345
H	-3.809760	3.303551	-0.550507
C	-1.784620	-1.393576	0.307707
O	-1.488606	-1.392541	1.518762
O	-1.059114	-0.863886	-0.622414
C	-2.836727	-3.617768	0.058277
H	-2.007852	-3.977420	-0.562308
H	-2.599977	-3.833213	1.104523
C	-3.395696	-1.831045	-1.625769
H	-3.539096	-0.761114	-1.807204
H	-2.594397	-2.180036	-2.283679
C	-3.073559	-2.107825	-0.152761
C	-4.236847	-1.637572	0.737201
H	-4.018711	-1.815483	1.793337
H	-4.426665	-0.566402	0.604385
H	-3.733298	-4.184465	-0.216701
H	-4.318402	-2.349805	-1.909926
H	-5.154025	-2.177517	0.477093

76

D′ Eopt -1670.982634

Rh	-0.907468	-0.845487	-0.216569
C	-0.759549	-3.024495	-0.127116
C	-1.341275	-2.549244	1.097447
C	-1.647447	-2.634793	-1.210109
C	-2.552279	-1.841749	0.782449
C	-2.746375	-1.912196	-0.656249
C	-0.814997	-2.759726	2.477446
H	-1.352204	-3.594929	2.944752
H	0.249738	-2.987507	2.471260
H	-0.974026	-1.873236	3.096164
C	0.446957	-3.893147	-0.266579
H	1.187277	-3.668585	0.501571
H	0.159921	-4.948786	-0.174313
H	0.915285	-3.763326	-1.244982
C	-1.414438	-2.933812	-2.652797
H	-0.358826	-2.820581	-2.912461
H	-1.702267	-3.970251	-2.868007
H	-2.001120	-2.276407	-3.297321
C	-3.902239	-1.325369	-1.396244
H	-3.646380	-1.119005	-2.437696
H	-4.748392	-2.023657	-1.385238
H	-4.231679	-0.392758	-0.932632
C	-3.519156	-1.270768	1.765559
H	-4.053981	-0.414627	1.350688
H	-4.259884	-2.034861	2.035922
H	-3.014839	-0.948965	2.678355
C	1.483964	-0.263713	1.577692
O	0.471477	0.241585	0.959490
O	1.904505	-1.428141	1.443831
C	1.628517	0.234782	3.984934
H	0.541240	0.356741	4.043353
H	1.868023	-0.815651	4.178986
C	1.797988	2.146120	2.356361
H	2.125306	2.473304	1.364485
H	0.719406	2.310644	2.424286
C	2.158095	0.675406	2.603498
C	3.681330	0.486375	2.545120
H	3.952898	-0.562778	2.688187
H	4.081198	0.807548	1.578250
H	2.080954	0.842540	4.776752
H	2.290364	2.781610	3.101851
H	4.167565	1.080027	3.327420
C	-2.170411	1.877573	0.293250
O	-2.104791	1.653506	1.517817
O	-1.757185	1.081010	-0.633494
C	-4.127546	3.412507	0.522091
H	-4.838418	2.633339	0.222204
H	-4.015103	3.368246	1.608285
C	-2.970233	3.275890	-1.700768
H	-2.021353	3.201100	-2.239386
H	-3.618749	2.465597	-2.048672
C	-2.771699	3.221940	-0.181562
C	-1.792561	4.327656	0.260807
H	-1.653854	4.313169	1.345850
H	-0.810743	4.193324	-0.207531
H	-4.561037	4.383289	0.257178
H	-3.437883	4.226893	-1.980806
H	-2.174362	5.313748	-0.026752
C	1.853550	2.915912	-1.631133
C	3.174749	2.613515	-1.388549
C	3.582994	1.258921	-1.341139
C	2.614297	0.233411	-1.538779
C	0.926681	1.884561	-1.821479
H	5.668763	1.646519	-0.942291
H	1.500602	3.939201	-1.676955
H	3.909888	3.396430	-1.233516
C	4.925510	0.870003	-1.093646
C	2.973517	-1.126677	-1.496204
H	-0.127182	2.043665	-1.993403
C	4.287451	-1.461354	-1.247661
C	5.268861	-0.462164	-1.045710
H	4.572419	-2.507739	-1.203380
H	6.296527	-0.752213	-0.851451
N	1.299069	0.602949	-1.777069
O	0.385974	-0.354052	-1.954462
H	2.212114	-1.878225	-1.644930

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D″ Eopt -1324.351049

C	-2.389398	-2.317879	-2.137942
C	-3.606337	-1.936295	-1.615510
C	-3.674926	-1.423470	-0.299371
C	-2.477394	-1.308797	0.464890
C	-1.234814	-2.204634	-1.357165
H	-5.805162	-1.072306	-0.281663
H	-2.296435	-2.708690	-3.144046
H	-4.515773	-2.017170	-2.201793
C	-4.888850	-0.987788	0.293743
C	-2.489209	-0.774641	1.768387
H	-0.247195	-2.484796	-1.699742
C	-3.689595	-0.354602	2.301693
C	-4.894403	-0.462644	1.565742
H	-3.710434	0.064287	3.302699
H	-5.824752	-0.126211	2.011670
Rh	1.262485	-0.127794	0.115552
O	-0.166903	-1.659093	0.618293
N	-1.290861	-1.731347	-0.110174
C	3.079082	0.864011	-0.483994

C 3.110126 0.649132 0.934592
C 2.993479 -0.438397 -1.122554
C 3.013769 -0.773030 1.182434
C 2.973506 -1.441823 -0.098009
C 3.165265 1.706258 1.982165
H 4.207508 1.857763 2.289873
H 2.779528 2.657257 1.610193
H 2.592921 1.417223 2.866618
C 3.130946 2.176509 -1.191755
H 2.760544 2.983079 -0.555753
H 4.164445 2.412558 -1.473343
H 2.530396 2.153646 -2.103954
C 2.929889 -0.667778 -2.593512
H 2.342229 0.110997 -3.086242
H 3.942697 -0.640187 -3.014446
H 2.490525 -1.639087 -2.828698
C 2.902697 -2.917807 -0.293723
H 2.609167 -3.174210 -1.313081
H 3.888341 -3.359613 -0.103380
H 2.193617 -3.373856 0.402211
C 3.024606 -1.443883 2.514015
H 2.430685 -2.360867 2.495584
H 4.052073 -1.713061 2.789529
H 2.628383 -0.787687 3.291955
C -0.658116 1.631157 -0.235825
O -0.158429 1.422310 0.917767
O -0.229826 0.935316 -1.218459
C -1.124775 3.737137 -1.434238
H -0.218331 4.191199 -1.018700
H -0.870764 3.277174 -2.393530
C -2.108092 3.368528 0.862982
H -2.512758 2.639528 1.571590
H -1.247363 3.856792 1.329924
C -1.723100 2.698530 -0.461814
C -2.961128 2.039262 -1.099447
H -2.696068 1.486348 -2.004789
H -3.442865 1.351331 -0.400351
H -1.562628 -0.697396 2.319880
H -3.689560 2.811394 -1.368412
H -1.852438 4.534878 -1.615195
H -2.874463 4.129252 0.681277

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D‴ Eopt -847.154144

Rh -0.392776 0.007477 -0.305349
C -1.937159 1.157465 0.662543
C -2.425854 0.730447 -0.609558
C -1.588066 -0.027850 1.427467
C -2.411567 -0.725030 -0.635662
C -1.921356 -1.190606 0.623038
C -2.893080 1.601758 -1.723757
H -3.985158 1.697432 -1.673643
H -2.463285 2.603044 -1.659679
H -2.643582 1.172220 -2.696848
C -1.765236 2.559474 1.133367
H -1.706807 3.259664 0.298306
H -2.623951 2.840171 1.755841
H -0.863646 2.662299 1.741691
C -1.073921 -0.049130 2.823314
H -0.486366 0.844142 3.045086
H -1.922943 -0.077972 3.518685
H -0.458014 -0.932174 3.006472
C -1.728285 -2.605151 1.047492
H -0.822220 -2.713706 1.648198
H -2.579371 -2.918524 1.664641
H -1.662509 -3.278176 0.191119
C -2.842137 -1.559161 -1.792254
H -2.512796 -1.122471 -2.738827
H -2.455035 -2.576974 -1.722783
H -3.937941 -1.610600 -1.815124
C 2.154004 0.034676 -0.120013
O 1.490120 -1.062195 -0.072734
O 1.483141 1.124088 -0.126724
C 4.082636 -0.677435 -1.486439
H 3.711742 -0.124994 -2.356664
H 3.694712 -1.698941 -1.531874
C 4.178065 -0.800831 1.034334
H 3.875449 -0.338674 1.980201
H 3.791750 -1.823377 1.009379
C 4.228290 1.444705 -0.122669
H 3.928426 1.958880 0.795666
H 3.882014 2.037734 -0.974296
C 3.670404 0.017010 -0.170680
H 5.174519 -0.719357 -1.550583
H 5.271511 -0.843983 1.011097
H 5.321888 1.410697 -0.152820

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TS2 Eopt -1324.313556

C -3.712803 -2.215785 -1.974160
C -4.087397 -2.322979 -0.652281
C -3.203304 -1.878916 0.361227
C -1.942713 -1.341791 -0.007921
C -2.481621 -1.637689 -2.308653
H -4.472403 -2.325672 2.053211
H -4.358994 -2.545949 -2.778693
H -5.050850 -2.738942 -0.376466
C -3.510149 -1.926758 1.747970
C -0.973564 -0.897484 0.934678
H -2.141581 -1.482564 -3.324619
C -1.335913 -0.986421 2.273504
C -2.597457 -1.481323 2.679526
H -0.618484 -0.695737 3.034671
H -2.837249 -1.528289 3.737345
Rh 0.181579 0.692208 -0.121326
O -0.499324 -0.621038 -1.703232
N -1.650809 -1.213989 -1.352744
C -0.273999 2.309515 1.287833
C 1.012027 2.533154 0.702857
C -1.254710 2.274943 0.220682
C 0.840535 2.688178 -0.729634
C -0.558678 2.550458 -1.014455
C 2.309050 2.631179 1.432671
H 2.523868 3.681785 1.664709
H 2.280793 2.076619 2.373006
H 3.132760 2.248088 0.826159
C -0.561274 2.210493 2.747417
H 0.227142 1.674643 3.280252
H -0.614404 3.224744 3.163301
H -1.514113 1.717339 2.939696
C -2.729869 2.108130 0.388299
H -2.960650 1.452121 1.230276
H -3.201747 3.080229 0.576711
H -3.184388 1.684620 -0.510092
C -1.187308 2.616410 -2.364183
H -2.092335 2.007346 -2.412734
H -1.467378 3.654242 -2.583540
H -0.498831 2.281463 -3.142706
C 1.935324 2.973349 -1.702710
H 2.849117 2.438706 -1.431105
H 1.654788 2.683003 -2.717232
H 2.164076 4.046396 -1.707909
H 0.276795 -1.341581 0.770677
C 2.257963 -1.440911 0.094755
O 2.073067 -0.278337 -0.373527
O 1.344815 -2.091269 0.706586
C 3.411736 -3.397360 -0.891477
H 2.714295 -4.076036 -0.392983
H 3.016775 -3.165672 -1.886727
C 4.144208 -2.467181 1.339929
H 4.271389 -1.567244 1.951970
H 3.457675 -3.142190 1.857750
C 3.622672 -2.111613 -0.066474
C 4.609817 -1.179966 -0.778101
H 4.253725 -0.907103 -1.775884
H 4.769482 -0.258645 -0.209691
H 5.117715 -2.960807 1.256384
H 5.575259 -1.684574 -0.886304
H 4.368490 -3.914433 -1.016967

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E Eopt -1323.876884

C 3.382717 -2.696913 -1.655909

C	3.711852	-2.621981	-0.319468
C	2.800944	-2.037582	0.594727
C	1.560680	-1.539440	0.103670
C	2.151378	-2.202676	-2.107938
H	3.991734	-2.253193	2.388280
H	4.058023	-3.130153	-2.384424
H	4.665318	-2.994935	0.040862
C	3.054964	-1.885120	1.981719
C	0.588088	-0.895464	0.909453
H	1.828806	-2.229921	-3.140747
C	0.900150	-0.772359	2.253841
C	2.119458	-1.266147	2.784108
H	0.212648	-0.265314	2.923944
H	2.320797	-1.142017	3.844890
Rh	-0.949571	-0.141562	-0.160308
O	0.119267	-1.187334	-1.697969
N	1.288936	-1.655680	-1.247261
C	-2.603837	-0.788652	1.111741
C	-2.535764	0.649738	1.099891
C	-2.833905	-1.219932	-0.234486
C	-2.857010	1.098189	-0.254073
C	-3.041100	-0.036131	-1.069122
C	-2.423674	1.531482	2.302120
H	-3.412296	1.683707	2.755599
H	-1.774198	1.087071	3.060325
H	-2.015464	2.509278	2.042019
C	-2.505341	-1.663342	2.319031
H	-1.871728	-1.216593	3.087650
H	-3.502978	-1.807969	2.752801
H	-2.101186	-2.647708	2.071930
C	-2.975598	-2.630371	-0.708549
H	-2.455939	-3.326697	-0.046213
H	-4.033988	-2.919497	-0.740799
H	-2.569078	-2.748830	-1.716747
C	-3.349837	-0.079274	-2.531701
H	-2.701965	-0.793458	-3.049927
H	-4.386749	-0.396353	-2.699764
H	-3.217624	0.899448	-2.998201
C	-2.899727	2.533291	-0.668260
H	-2.072007	3.091611	-0.222146
H	-2.841608	2.642029	-1.753327
H	-3.833214	2.999293	-0.328565
C	1.023719	2.152479	0.128798
O	0.465854	1.347823	-0.716415
O	0.589419	2.404473	1.267002
C	2.829772	3.853575	0.599900
H	2.095910	4.661781	0.685011
H	2.995403	3.445992	1.601235
C	2.152672	3.365031	-1.773561
H	1.825403	2.602347	-2.484964
H	1.401418	4.163231	-1.760197
C	2.349559	2.768015	-0.369712
C	3.383010	1.622475	-0.427390
H	3.503899	1.152065	0.554717
H	3.079174	0.850901	-1.140200
H	3.092666	3.794270	-2.138655
H	4.359448	2.010991	-0.738770
H	3.772168	4.285664	0.245163

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E′		Eopt	-977.239063
Rh	-0.590631	-0.161176	-0.218741
C	-2.536487	-1.059491	0.523235
C	-1.980558	-0.005887	1.373565
C	-2.782738	-0.499185	-0.740085
C	-2.008856	1.240676	0.632780
C	-2.418659	0.925455	-0.693037
C	-1.641918	-0.157379	2.816593
H	-2.553662	-0.050703	3.419504
H	-1.218587	-1.143303	3.023083
H	-0.931728	0.606361	3.140570
C	-2.708119	-2.480675	0.948345
H	-1.835611	-2.829445	1.508681
H	-3.581142	-2.577931	1.604907
H	-2.852139	-3.141187	0.091075
C	-3.292156	-1.187093	-1.961610
H	-3.280930	-2.272708	-1.848389
H	-4.324267	-0.874186	-2.163157
H	-2.696243	-0.921635	-2.840192
C	-2.591758	1.877192	-1.828994
H	-2.324864	1.409022	-2.780208
H	-3.641954	2.189309	-1.897233
H	-1.980113	2.772268	-1.698642
C	-1.734595	2.592737	1.202134
H	-0.907900	2.570568	1.915480
H	-1.505316	3.320589	0.421823
H	-2.626297	2.945621	1.735109
C	4.327460	-1.909718	-0.101007
C	4.659424	-0.570857	-0.056497
C	3.635219	0.406556	-0.056841
C	2.280656	-0.021768	-0.103248
C	2.982396	-2.298234	-0.151278
H	4.889730	2.167854	0.016843
H	5.085167	-2.684153	-0.101938
H	5.697721	-0.256814	-0.023974
C	3.867329	1.805518	-0.020285
C	1.161891	0.851735	-0.104985
H	2.647937	-3.327048	-0.194717
C	1.462822	2.207219	-0.069105
C	2.799760	2.678579	-0.033354
H	0.662643	2.940120	-0.065621
H	2.981137	3.749259	-0.010206
O	0.729605	-1.762107	-0.221594
N	2.021612	-1.373480	-0.156379

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E″		Eopt	-1324.335516
C	-3.919318	-2.039558	-1.938438
C	-4.178589	-2.264071	-0.602893
C	-3.324954	-1.705593	0.379303
C	-2.218131	-0.919283	-0.042457
C	-2.816366	-1.265529	-2.321667
H	-4.333962	-2.483163	2.128790
H	-4.550981	-2.450520	-2.717002
H	-5.027372	-2.865340	-0.293587
C	-3.499179	-1.885714	1.776678
C	-1.298419	-0.297865	0.844456
H	-2.551263	-1.052405	-3.349297
C	-1.525463	-0.518572	2.196221
C	-2.611380	-1.309172	2.656644
H	-0.859342	-0.086501	2.935865
H	-2.739787	-1.453919	3.725607
Rh	0.103543	0.817216	-0.136199
O	-0.954381	-0.008677	-1.779594
N	-2.011527	-0.740660	-1.394359
C	0.093192	2.504694	1.252521
C	1.444379	2.132893	0.980226
C	-0.516812	2.851515	-0.011525
C	1.730504	2.432120	-0.428410
C	0.542637	2.878140	-1.026291
C	2.464972	1.670195	1.967807
H	3.076354	2.515529	2.308500
H	1.995214	1.218455	2.844285
H	3.138952	0.935272	1.519479
C	-0.553591	2.606895	2.592670
H	-0.063520	1.969888	3.331376
H	-0.469813	3.643706	2.942601
H	-1.613939	2.351735	2.556040
C	-1.912909	3.339032	-0.219154
H	-2.587015	2.943731	0.544032
H	-1.945867	4.434940	-0.167503
H	-2.288785	3.038765	-1.200910
C	0.312792	3.241396	-2.455560
H	-0.583864	2.747428	-2.841870
H	0.156821	4.322663	-2.549394
H	1.159674	2.962294	-3.085038
C	3.063096	2.225036	-1.068523
H	3.464933	1.235895	-0.828711
H	3.007787	2.318393	-2.154875
H	3.780111	2.967248	-0.696961
H	0.383443	-1.496089	1.279005
C	1.824433	-1.882917	0.117350

O 1.618127 -0.876735 -0.568980
O 1.098776 -2.167536 1.189679
C 2.223411 -4.261062 -0.433963
H 1.675883 -4.595368 0.451109
H 1.524164 -4.205010 -1.275077
C 3.850016 -2.990004 1.028904
H 4.323565 -2.024030 1.234084
H 3.312666 -3.311452 1.924855
C 2.909691 -2.899405 -0.190895
C 3.689154 -2.465042 -1.436660
H 3.032846 -2.380952 -2.307873
H 4.180604 -1.499696 -1.283670
H 4.639571 -3.718274 0.820077
H 4.459919 -3.209057 -1.658439
H 2.985084 -5.009443 -0.672930
73
TS5 Eopt -1723.606509
C -2.274309 2.644511 -0.489055
C -2.110125 2.568258 0.906113
C -0.754867 1.134419 0.026084
H -3.286108 3.531138 -2.189547
C -3.179024 3.496387 -1.110884
C -2.883499 3.380400 1.747821
H 0.430419 0.999775 -0.249957
C -3.793447 4.242556 1.143302
C -3.937602 4.300677 -0.259697
H -4.408879 4.889114 1.761382
H -4.658957 4.989996 -0.688010
Rh -0.725101 -1.138300 -0.178078
N -1.141125 1.622004 1.187082
C -3.008427 -1.263833 -0.654057
C -2.330301 -2.218941 -1.424276
C -2.696566 -1.506592 0.759127
C -1.582278 -3.086295 -0.510988
C -1.900808 -2.692505 0.836878
C -2.308585 -2.344302 -2.912466
H -2.896031 -3.213945 -3.232201
H -2.725831 -1.457272 -3.393790
H -1.287196 -2.487037 -3.278769
C -3.936881 -0.206299 -1.153021
H -3.648541 0.155475 -2.142168
H -4.952317 -0.616519 -1.227220
H -3.980255 0.645891 -0.474189
C -3.322004 -0.797476 1.916027
H -3.531403 0.247462 1.683154
H -4.271897 -1.280151 2.180777
H -2.674716 -0.825978 2.795656
C -1.526494 -3.428850 2.079945
H -1.487922 -2.765305 2.945363
H -2.283176 -4.197613 2.282617
H -0.560261 -3.927525 1.981804
C -0.783440 -4.278745 -0.923098
H -0.250289 -4.088913 -1.858317
H -0.052686 -4.549385 -0.157475
H -1.442111 -5.142204 -1.083278
H -2.769801 3.334033 2.826217
C 2.021684 2.586079 -0.431647
O 1.145912 3.471710 -0.392542
O 1.781700 1.319862 -0.529179
C 3.709931 4.468023 -0.365011
H 3.320242 4.897265 -1.293906
H 3.186332 4.947797 0.467280
C 4.273157 2.300023 -1.513747
H 4.161113 1.213042 -1.502097
H 3.895839 2.670221 -2.474123
C 3.522339 2.947357 -0.336194
C 4.052461 2.373958 0.993362
H 3.515599 2.801943 1.847847
H 3.933296 1.287606 1.028466
H 5.342395 2.535709 -1.459221
H 4.773826 4.720943 -0.292337
H 5.116894 2.607849 1.112304
O -1.427901 1.741628 -1.053633
C 4.375126 -1.784796 -1.221535
C 4.505237 -1.792946 0.151199
C 3.356859 -1.628354 0.963764
C 2.091725 -1.474295 0.332864
C 3.115135 -1.606789 -1.810046
H 4.334690 -1.680968 2.893864
H 5.232578 -1.898123 -1.874262
H 5.478192 -1.909487 0.617715
C 3.384375 -1.569299 2.381539
C 0.877179 -1.282425 1.036167
H 2.944355 -1.564186 -2.877954
C 0.970047 -1.218138 2.415321
C 2.215624 -1.357666 3.081047
H 0.078143 -1.051369 3.011309
H 2.241874 -1.296912 4.165673
O 0.840442 -1.259018 -1.620996
N 2.032206 -1.467280 -1.043841
57
TS8 Eopt -1376.978945
Rh 0.920178 -0.247303 -0.055471
C 2.903194 -1.262533 -0.015367
C 2.473197 -0.975117 1.312950
C 2.690225 1.065076 0.198047
C 2.970828 -0.012635 -0.736920
C 2.348653 0.480153 1.443875
C 3.202899 -2.607664 -0.587606
H 2.694823 -3.401913 -0.036997
H 2.904705 -2.669180 -1.637059
H 4.282055 -2.799254 -0.537851
C 3.417373 0.154823 -2.152480
H 3.005141 1.064842 -2.594057
H 4.511582 0.227470 -2.197628
H 3.113705 -0.696207 -2.766859
C 2.742629 2.524536 -0.112885
H 2.034144 3.088827 0.497616
H 3.748441 2.910326 0.094467
H 2.521907 2.719088 -1.164084
C 1.951975 1.191582 2.695115
H 1.163768 0.647748 3.222401
H 2.810785 1.271350 3.373012
H 1.593999 2.201552 2.482731
C 2.234571 -1.948193 2.418741
H 3.087524 -1.952826 3.109192
H 1.345363 -1.675835 2.994570
H 2.102221 -2.962837 2.037617
N -1.524024 0.809520 1.155771
O -0.813219 -0.319551 1.234729
C -0.505550 1.157793 -1.013575
C -0.166356 2.122393 -1.964346
H 0.445405 1.824414 -2.811982
C -0.648947 3.444954 -1.918358
H -0.345740 4.148490 -2.686883
C -1.548614 3.826110 -0.946127
H -1.976883 4.823183 -0.937077
C -1.918143 2.916265 0.080513
C -1.338186 1.621162 0.058211
C -2.790422 3.263800 1.140542
H -3.250538 4.246179 1.150367
C -3.024729 2.357539 2.152290
H -3.685020 2.584592 2.980591
C -2.350214 1.131800 2.156509
H -2.413503 0.406047 2.957399
C -2.531239 -1.644397 -1.093913
C -1.319926 -2.242322 -0.715232
C -1.331830 -3.385297 0.082190
C -2.577112 -3.888983 0.476312
C -3.774510 -3.269286 0.091133
C -3.771101 -2.115375 -0.708787
C -0.854516 -0.405754 -1.870493
H -0.405558 -3.857860 0.392941
H -2.616217 -4.779128 1.097052
H -4.723095 -3.687571 0.412832
H -4.687705 -1.622079 -1.014015
N -0.263835 -1.513359 -1.259280
O -2.259383 -0.538628 -1.880506
H -0.478381 -0.141073 -2.853346
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TS8′ Eopt -1376.975197

Rh	-0.100462	0.672921	-0.238412
C	-1.425331	2.390911	0.386087
C	-0.176416	2.863882	-0.102878
C	0.272228	1.536289	1.759598
C	-1.155298	1.486638	1.481336
C	0.881974	2.345545	0.767564
C	-2.773033	2.785632	-0.112653
H	-2.787272	2.908109	-1.198286
H	-3.534976	2.059972	0.171820
H	-3.049296	3.749378	0.334172
C	-2.182564	0.770260	2.295033
H	-1.765532	-0.127449	2.757224
H	-2.553144	1.419999	3.098211
H	-3.035878	0.475139	1.680149
C	0.963235	0.875212	2.904392
H	1.979578	0.571523	2.645578
H	1.027206	1.583908	3.739646
H	0.418341	-0.002483	3.253599
C	2.335949	2.655081	0.630963
H	2.622997	2.737321	-0.420334
H	2.566543	3.612320	1.115021
H	2.952765	1.884450	1.098860
C	0.042389	3.792395	-1.249217
H	0.195169	4.814294	-0.879021
H	0.932143	3.511292	-1.819364
H	-0.815557	3.801168	-1.924762
N	2.437652	-0.265821	-1.356880
O	1.399167	0.417157	-1.853824
C	0.850364	-1.255124	0.152367
C	0.662546	-1.998534	1.313820
H	-0.346506	-2.166904	1.675141
C	1.742785	-2.584262	2.007690
H	1.546153	-3.149636	2.913178
C	3.032910	-2.471140	1.533891
H	3.861432	-2.948591	2.046961
C	3.301397	-1.716074	0.359315
C	2.200232	-1.099621	-0.284264
C	4.599071	-1.528456	-0.176742
H	5.448894	-2.001635	0.303859
C	4.763485	-0.740027	-1.295835
H	5.739691	-0.573375	-1.735415
C	3.660499	-0.093677	-1.868259
H	3.723518	0.586902	-2.707765
C	-2.423478	-2.261323	-0.492957
C	-2.492262	-0.975154	-1.045752
C	-3.721565	-0.316932	-1.091588
C	-4.826505	-0.957732	-0.517899
C	-4.717128	-2.226063	0.069706
C	-3.494240	-2.914572	0.085630
C	-0.396493	-1.673082	-1.175134
H	-3.816632	0.652556	-1.564460
H	-5.792818	-0.462955	-0.536507
H	-5.594786	-2.694859	0.503371
H	-3.395349	-3.908746	0.507878
N	-1.233810	-0.612811	-1.543902
O	-1.139329	-2.741220	-0.662701
H	0.339966	-2.010640	-1.897824

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TS6 Eopt -1593.546743

C	-3.471053	-1.412996	-0.335595
C	-3.268135	-0.811829	-1.589590
C	-1.373625	-0.757568	-0.547551
H	-4.824580	-2.364821	1.066390
C	-4.697199	-1.907007	0.091465
C	-4.336556	-0.685111	-2.487322
H	-0.220903	-1.402724	-0.487678
C	-5.574627	-1.172433	-2.077706
C	-5.751514	-1.772848	-0.813076
H	-6.427737	-1.091464	-2.744331
H	-6.735207	-2.139167	-0.535450
Rh	-0.008826	0.670928	0.472384
N	-1.937725	-0.428513	-1.687528
C	-1.671969	1.737960	1.477332
C	-0.586187	1.571804	2.384805
C	-1.192192	2.488583	0.328921
C	0.571815	2.262399	1.837473
C	0.179486	2.846553	0.585326
C	-0.607840	0.846227	3.688290
H	-0.737330	1.560130	4.511155
H	-1.427210	0.125640	3.730758
H	0.332087	0.313469	3.853542
C	-3.077624	1.288142	1.688972
H	-3.127405	0.386103	2.300499
H	-3.625818	2.082792	2.211123
H	-3.590138	1.099991	0.744418
C	-2.017815	2.942271	-0.829313
H	-2.835689	2.248237	-1.030256
H	-2.451785	3.927745	-0.617890
H	-1.412463	3.026958	-1.734565
C	1.045996	3.650173	-0.323966
H	0.770202	3.495211	-1.368861
H	0.920040	4.716187	-0.096496
H	2.099264	3.395679	-0.199708
C	1.898152	2.371670	2.510978
H	2.199654	1.410441	2.935575
H	2.673845	2.699575	1.818446
H	1.838758	3.096585	3.332870
H	-4.197223	-0.223741	-3.459799
C	1.299106	-2.019623	0.745559
O	1.109337	-0.939287	1.375884
O	0.700598	-2.290561	-0.353764
C	2.689720	-2.702864	2.729099
H	3.136629	-1.708757	2.814985
H	1.810879	-2.739617	3.381102
C	3.565939	-2.892422	0.372520
H	3.331587	-3.160413	-0.661585
H	3.951284	-1.868179	0.386202
C	2.319383	-3.026175	1.276444
C	1.739307	-4.446382	1.172140
H	0.840391	-4.551458	1.789673
H	1.476677	-4.693350	0.140393
H	4.352621	-3.563641	0.732690
H	3.415612	-3.436931	3.093582
H	2.478885	-5.173391	1.523053
O	-2.279797	-1.391931	0.328177
C	2.444096	0.555802	-1.237857
O	1.152082	0.489676	-1.275686
O	3.115680	0.757966	-0.209696
C	2.655211	-0.971035	-3.216270
H	2.937776	-1.808551	-2.569962
H	1.570157	-0.995666	-3.347168
C	4.640229	0.386303	-2.470673
H	4.989299	1.326337	-2.032829
H	4.987161	-0.430976	-1.830869
C	3.114259	0.371280	-2.616310
C	2.661528	1.530796	-3.525619
H	1.575431	1.529062	-3.654695
H	2.956588	2.499613	-3.106466
H	5.110323	0.271592	-3.453642
H	3.124380	-1.125114	-4.194639
H	3.124644	1.437504	-4.514353

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TS6′ Eopt -1593.542251

C	-3.367264	-0.931641	-0.933387
C	-3.116372	0.168273	-1.771581
C	-1.237421	-0.350269	-0.831996
H	-4.788575	-2.353450	-0.119117
C	-4.622458	-1.506048	-0.775291
C	-4.161564	0.745706	-2.504892
H	-0.139838	-1.023785	-1.092829
C	-5.427442	0.185754	-2.358703
C	-5.653212	-0.919670	-1.510959
H	-6.264419	0.606075	-2.907794
H	-6.657491	-1.323928	-1.427658
Rh	0.148845	0.307030	0.796706
N	-1.769219	0.489620	-1.690587
C	-1.540181	0.993687	2.065112
C	-0.651864	0.185614	2.831474
C	-0.799403	2.129281	1.550652

C	0.650742	0.835579	2.836847
C	0.541960	2.045244	2.070589
C	-0.978390	-1.095642	3.522492
H	-1.197909	-0.908341	4.580884
H	-1.850045	-1.575863	3.072921
H	-0.137011	-1.791466	3.473717
C	-3.002933	0.776716	1.881097
H	-3.275436	-0.274765	1.975041
H	-3.538103	1.336344	2.658973
H	-3.348115	1.146884	0.914654
C	-1.391368	3.266725	0.787491
H	-2.141454	2.915922	0.075530
H	-1.883603	3.959483	1.482234
H	-0.628568	3.816163	0.236075
C	1.636134	3.030763	1.835748
H	1.521020	3.528453	0.872460
H	1.609711	3.793853	2.623904
H	2.616569	2.550950	1.866835
C	1.859779	0.334446	3.552248
H	1.898495	-0.757585	3.537867
H	2.776622	0.719264	3.101028
H	1.835878	0.655691	4.601241
H	-3.983340	1.595931	-3.155481
C	1.193042	-2.335450	-0.249753
O	1.049383	-1.666642	0.816414
O	0.689374	-1.973734	-1.369314
C	2.525983	-3.921509	1.186194
H	3.186602	-3.119558	1.529296
H	1.711391	-4.024427	1.909453
C	3.159861	-3.495307	-1.217434
H	2.794645	-3.304620	-2.230104
H	3.823515	-2.673461	-0.928935
C	1.990893	-3.639993	-0.222102
C	1.050657	-4.774544	-0.674938
H	0.199472	-4.876378	0.007493
H	0.664725	-4.588700	-1.680785
H	3.747144	-4.419371	-1.230579
H	3.097356	-4.855432	1.180763
H	1.595657	-5.724086	-0.683027
O	-2.189822	-1.273168	-0.338400
C	1.787493	1.634681	-1.361971
O	1.751994	0.644519	-0.532150
O	0.916943	2.518080	-1.459377
C	3.908327	0.442689	-2.136081
H	4.277418	0.312243	-1.114411
H	3.344763	-0.454808	-2.408260
C	3.839107	2.944455	-1.829324
H	3.227273	3.847995	-1.910035
H	4.178324	2.852618	-0.791079
C	3.039892	1.700038	-2.263424
C	2.568406	1.864002	-3.719300
H	1.992573	0.990383	-4.045530
H	1.934780	2.748098	-3.828618
H	4.723755	3.068548	-2.463772
H	4.774744	0.517724	-2.803188
H	3.430568	1.969798	-4.387065

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TS6″ Eopt -1246.896043

C	2.855849	1.862331	0.518395
C	2.564642	1.407220	-0.772236
C	0.657582	1.647901	0.301347
H	4.344724	2.432989	1.986406
C	4.145042	2.079897	0.980773
C	3.591022	1.133988	-1.677518
H	-0.833626	1.906634	0.581068
C	4.897108	1.335969	-1.231631
C	5.167893	1.799934	0.070496
H	5.726753	1.133034	-1.901499
H	6.199555	1.942037	0.377032
Rh	-0.092222	-0.479962	-0.197563
N	1.172066	1.295865	-0.873684
C	0.379739	-1.671017	1.527872
C	-0.881931	-2.119065	0.970695
C	1.407903	-1.873103	0.536335
C	-0.635506	-2.585353	-0.365135
C	0.775599	-2.420060	-0.638763
C	-2.198671	-2.093839	1.665644
H	-2.323946	-3.022704	2.236280
H	-2.262312	-1.259586	2.367198
H	-3.022838	-2.023212	0.954030
C	0.581074	-1.122278	2.895863
H	-0.306696	-0.592442	3.247156
H	0.774282	-1.952796	3.587239
H	1.435628	-0.444643	2.931582
C	2.866232	-1.630823	0.721579
H	3.051316	-0.825361	1.433533
H	3.331604	-2.543306	1.114881
H	3.357268	-1.381044	-0.219899
C	1.461283	-2.764988	-1.912860
H	2.365272	-2.169501	-2.052345
H	1.752503	-3.823091	-1.887173
H	0.803999	-2.619851	-2.772775
C	-1.652692	-3.123701	-1.310345
H	-2.636429	-2.687236	-1.126559
H	-1.372787	-2.932450	-2.348234
H	-1.734784	-4.209740	-1.177525
H	3.377463	0.778534	-2.680344
C	-2.564678	1.315641	-0.167707
O	-2.006886	0.374386	-0.791065
O	-1.926700	2.108106	0.632900
C	-4.645279	0.709379	-1.438515
H	-4.177532	0.951911	-2.397816
H	-4.508054	-0.359276	-1.251890
C	-4.301047	3.056348	-0.575741
H	-3.909810	3.675155	0.235525
H	-3.821968	3.368926	-1.509747
C	-4.062313	1.559069	-0.304145
C	-4.702987	1.160664	1.044728
H	-4.531819	0.102206	1.267029
H	-4.299117	1.758732	1.866508
H	-5.375670	3.243072	-0.665067
H	-5.718582	0.905139	-1.523201
H	-5.783483	1.327645	0.994501
O	1.659767	2.000357	1.196341

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J Eopt -1246.476914

Rh	-0.978641	-0.151164	-0.030200
C	-3.001101	-0.720965	0.867660
C	-3.162709	-0.629104	-0.523243
C	-1.928118	-1.683640	1.141478
C	-2.199073	-1.539794	-1.151187
C	-1.515372	-2.254854	-0.111380
C	-4.082020	0.264640	-1.289445
H	-4.873550	-0.323437	-1.769742
H	-4.553982	1.007370	-0.643378
H	-3.540682	0.792490	-2.080866
C	-3.700817	0.062481	1.928977
H	-4.293024	0.876761	1.507116
H	-4.371736	-0.589133	2.501952
H	-2.980545	0.489840	2.633798
C	-1.486437	-2.113730	2.501597
H	-1.504685	-1.275442	3.202896
H	-2.155266	-2.891593	2.892398
H	-0.472531	-2.519422	2.477737
C	-0.554819	-3.385375	-0.290873
H	0.194856	-3.401376	0.503400
H	-1.100870	-4.336286	-0.260286
H	-0.037868	-3.323369	-1.250189
C	-2.091992	-1.781157	-2.620244
H	-1.124172	-2.212913	-2.883750
H	-2.875954	-2.476505	-2.947350
H	-2.218521	-0.850524	-3.179720
C	-0.167962	2.298754	-0.008957
O	-0.539304	1.744551	-1.097223
O	-0.356359	1.658198	1.080969
C	0.320317	4.391758	1.281172
H	-0.741239	4.646541	1.371494
H	0.609020	3.813050	2.162498
C	0.209061	4.452259	-1.240557
H	0.415759	3.916303	-2.170648

H	-0.855291	4.710486	-1.223864
C	0.594667	3.613385	-0.014194
C	2.089063	3.215415	-0.088632
H	2.371530	2.591885	0.765800
H	2.300082	2.656693	-1.005881
H	0.894371	5.324086	1.280407
H	0.784436	5.383769	-1.246854
H	2.711692	4.116167	-0.081651
C	3.025077	-0.972317	-0.760441
C	2.999497	-0.931481	0.639619
C	4.113341	-1.131268	1.438889
C	5.311978	-1.387055	0.761654
C	5.364835	-1.434566	-0.642265
C	4.225476	-1.228110	-1.425371
C	0.978294	-0.545651	-0.185597
H	4.059679	-1.090748	2.521833
H	6.219475	-1.551524	1.334876
H	6.315018	-1.635581	-1.128547
H	4.268728	-1.263639	-2.509772
O	1.700506	-0.661713	1.016435
N	1.729754	-0.723944	-1.238302

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TS7 Eopt -1723.602011

C	3.087576	3.222983	-1.699215
C	3.621100	3.223950	-0.427944
C	3.044062	2.397573	0.567084
C	1.931832	1.592160	0.227493
C	2.018604	2.372508	-2.014008
H	4.364864	2.924558	2.197387
H	3.492526	3.848022	-2.486198
H	4.470692	3.851284	-0.178689
C	3.506049	2.325217	1.911278
C	1.222261	0.787212	1.164980
H	1.586503	2.284243	-3.002480
C	1.726284	0.768560	2.462388
C	2.868496	1.517734	2.829704
H	1.204998	0.192813	3.222178
H	3.231173	1.474607	3.852237
Rh	0.713392	-1.002085	-0.079159
O	0.511706	0.722508	-1.408055
N	1.491360	1.578395	-1.080566
C	1.660498	-2.740619	0.843269
C	0.797608	-3.193035	-0.213196
C	2.780903	-2.019299	0.228468
C	1.273025	-2.611031	-1.436192
C	2.540392	-1.934057	-1.151212
C	-0.362933	-4.122514	-0.071213
H	-0.014923	-5.155277	-0.198083
H	-0.825585	-4.038197	0.912926
H	-1.127095	-3.929099	-0.827237
C	1.572280	-3.132196	2.282052
H	0.536119	-3.307429	2.579067
H	2.137840	-4.055803	2.462101
H	1.986209	-2.355806	2.929517
C	3.959241	-1.478326	0.969999
H	3.698625	-1.219189	1.997048
H	4.753633	-2.234339	1.009268
H	4.368729	-0.588810	0.486110
C	3.361758	-1.217635	-2.173060
H	4.079638	-0.539333	-1.706994
H	3.921484	-1.934549	-2.786339
H	2.726106	-0.637380	-2.848560
C	0.677237	-2.778319	-2.795217
H	-0.391737	-2.994313	-2.734558
H	0.810584	-1.872677	-3.393174
H	1.162791	-3.605589	-3.328957
H	-0.033179	0.964158	1.083202
C	-1.277484	2.751347	0.523581
O	-0.284026	3.502580	0.485946
O	-1.280533	1.561579	1.034192
C	-3.815490	2.611118	0.605919
H	-3.786493	1.520325	0.613006
H	-3.851056	2.955720	1.645781
C	-2.565857	2.676779	-1.582962
H	-1.697854	3.077866	-2.117959
H	-2.505678	1.585997	-1.605741
C	-2.603822	3.201088	-0.130642
C	-2.687821	4.733415	-0.138304
H	-2.683702	5.135299	0.881227
H	-1.842522	5.173453	-0.674135
H	-3.470797	2.984564	-2.119917
H	-3.613099	5.060080	-0.626359
H	-4.744505	2.925164	0.116019
C	-3.295197	-1.413536	0.856323
C	-3.347934	-1.003378	-0.483256
C	-4.524386	-0.827492	-1.192960
C	-5.707003	-1.086865	-0.488723
C	-5.683000	-1.498664	0.854769
C	-4.480546	-1.669058	1.548156
H	-4.528594	-0.501267	-2.227573
H	-6.661326	-0.963036	-0.991852
H	-6.622591	-1.687062	1.366142
H	-4.465921	-1.983571	2.587365
C	-1.249850	-1.093988	0.219411
N	-1.952187	-1.470835	1.253280
O	-2.050900	-0.809708	-0.901238

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H Eopt -1376.556060

Rh	-0.902614	-0.340313	-0.163319
C	-1.804058	-2.433974	-0.199672
C	-2.492445	-1.674242	-1.169982
C	-2.896770	-0.666520	0.892405
C	-1.967558	-1.766473	1.084749
C	-3.172388	-0.572602	-0.491284
C	-1.044901	-3.704626	-0.406104
H	-0.845752	-3.885585	-1.465227
H	-0.088922	-3.677312	0.123046
H	-1.620794	-4.555585	-0.020516
C	-1.511696	-2.309033	2.402295
H	-1.465092	-1.522316	3.160109
H	-2.202425	-3.080957	2.767289
H	-0.518817	-2.756161	2.316458
C	-3.447816	0.192940	1.984162
H	-3.805065	1.152286	1.602261
H	-4.291835	-0.310620	2.472435
H	-2.697350	0.393869	2.752761
C	-4.028998	0.439060	-1.185715
H	-3.540205	0.809694	-2.092666
H	-4.988573	0.000537	-1.487992
H	-4.240094	1.296158	-0.541810
C	-2.581392	-1.931898	-2.641577
H	-3.557644	-2.358575	-2.905709
H	-2.468161	-1.003295	-3.210017
H	-1.808787	-2.628673	-2.974887
N	0.017951	2.201881	-1.242077
O	-0.454429	1.048653	-1.730253
C	-0.258817	1.225630	0.924141
C	-0.110477	1.374919	2.294026
H	-0.359011	0.549039	2.954375
C	0.371483	2.581601	2.862320
H	0.464977	2.654255	3.942731
C	0.731583	3.654469	2.074206
H	1.107498	4.574065	2.511504
C	0.624332	3.558641	0.662536
C	0.126065	2.335855	0.129756
C	0.993886	4.590464	-0.234963
H	1.379257	5.526675	0.156124
C	0.869557	4.389207	-1.593421
H	1.148569	5.154676	-2.308003
C	0.375446	3.174160	-2.086340
H	0.252948	2.950094	-3.138168
C	3.172485	-0.788986	-0.545885
C	2.939460	-1.822985	0.370714
C	4.007772	-2.596040	0.829497
C	5.282694	-2.291162	0.342131
C	5.489255	-1.247717	-0.576124
C	4.424233	-0.466907	-1.044284
C	1.005889	-0.921401	-0.056043
H	3.850574	-3.403546	1.538450
H	6.134735	-2.874212	0.679838

H 6.494402 -1.041091 -0.931572
H 4.570186 0.340548 -1.754444
N 1.569924 -1.864881 0.656595
O 1.956548 -0.209049 -0.823236
56
TS4 Eopt -1376.499281
Rh -0.753195 -0.555309 -0.192669
C -1.204298 -2.841095 -0.241287
C -1.985653 -2.187662 -1.209058
C -2.583174 -1.289187 0.878248
C -1.491319 -2.214936 1.045408
C -2.830891 -1.194305 -0.522094
C -0.221682 -3.949677 -0.451418
H 0.069094 -4.035313 -1.501671
H 0.686877 -3.795949 0.138518
H -0.647564 -4.914272 -0.143305
C -0.939370 -2.658778 2.364003
H -0.966420 -1.847789 3.096848
H -1.530106 -3.491677 2.769072
H 0.094361 -3.000181 2.272920
C -3.257173 -0.538743 1.980760
H -3.974536 0.186042 1.587487
H -3.798991 -1.220601 2.647983
H -2.530747 0.010609 2.594140
C -3.854509 -0.345388 -1.205663
H -3.482010 0.019667 -2.167081
H -4.769871 -0.918809 -1.405001
H -4.126259 0.521245 -0.597428
C -2.027308 -2.438913 -2.683880
H -2.939080 -2.982095 -2.965595
H -2.025348 -1.498590 -3.244757
H -1.169583 -3.030140 -3.014327
N -0.359496 2.115990 -1.279760
O -0.473487 0.866619 -1.756644
C 0.004318 1.075726 0.869129
C -0.154701 1.283752 2.289426
H -0.045898 0.426360 2.944249
C -0.325203 2.553919 2.822905
H -0.416345 2.655812 3.901903
C -0.351804 3.706039 2.031149
H -0.434087 4.691525 2.476815
C -0.305160 3.588036 0.621528
C -0.206697 2.279962 0.064252
C -0.375871 4.681828 -0.282218
H -0.408041 5.692919 0.110747
C -0.407823 4.453493 -1.645887
H -0.460685 5.275283 -2.351479
C -0.423980 3.152412 -2.145526
H -0.533792 2.885117 -3.187399
C 3.233115 0.038707 -0.444623
C 3.097948 -0.866879 0.621574
C 4.147606 -1.740788 0.930972
C 5.297704 -1.659563 0.147454
C 5.407396 -0.738780 -0.913251
C 4.367044 0.138696 -1.234877
C 1.251282 0.233442 0.482475
H 4.062360 -2.449492 1.748506
H 6.132524 -2.321335 0.357229
H 6.321427 -0.710664 -1.498366
H 4.438970 0.849863 -2.050514
N 1.849455 -0.700019 1.197102
O 2.068363 0.752345 -0.529333
56
I Eopt -1376.513077
Rh 0.343288 -0.835342 -0.146166
C 1.902446 -2.533058 -0.179139
C 0.646885 -3.016255 -0.648419
C 0.334755 -2.335216 1.560412
C 1.684689 -2.022062 1.161521
C -0.318880 -2.905110 0.430714
C 3.208218 -2.613032 -0.905011
H 3.909558 -1.844432 -0.571329
H 3.693670 -3.585083 -0.734957
H 3.077574 -2.499675 -1.985386
C 2.739391 -1.530658 2.108757
H 2.403678 -0.650447 2.665571
H 2.983799 -2.309212 2.843610
H 3.664893 -1.269796 1.592393
C -0.243289 -2.142934 2.927557
H -1.330997 -2.032408 2.891415
H -0.022552 -3.004420 3.575084
H 0.170572 -1.256658 3.417578
C -1.727193 -3.407736 0.404870
H -2.083273 -3.564384 -0.615484
H -1.803322 -4.370537 0.927691
H -2.414940 -2.713200 0.897807
C 0.377404 -3.625899 -1.989556
H 0.461745 -4.720699 -1.954804
H -0.630942 -3.388316 -2.341014
H 1.085379 -3.263243 -2.740187
N -2.137336 0.024920 -1.014574
O -0.955239 -0.072025 -1.649986
C -1.483200 2.206419 -0.036928
C -1.985036 3.413827 0.517445
H -1.298378 4.240278 0.648751
C -3.295504 3.537465 0.956006
H -3.621139 4.471060 1.404608
C -4.175100 2.465039 0.859106
H -5.192891 2.539729 1.228353
C -3.771037 1.267720 0.240384
C -2.425040 1.146115 -0.250621
C -4.686942 0.191196 0.048733
H -5.682312 0.271990 0.472282
C -4.320690 -0.893893 -0.712085
H -5.007385 -1.708666 -0.913241
C -3.047883 -0.940146 -1.277182
H -2.693887 -1.722348 -1.931474
C 1.916493 3.118511 -0.275020
C 2.088179 1.740022 -0.122974
C 3.371777 1.201725 -0.059572
C 4.446034 2.092298 -0.126043
C 4.248276 3.476135 -0.267075
C 2.963086 4.022367 -0.353953
C -0.064185 2.141500 -0.245675
H 3.523194 0.135396 0.025491
H 5.458728 1.704158 -0.074765
H 5.108460 4.136466 -0.317469
H 2.790028 5.085870 -0.476066
N 0.818000 1.139502 -0.113160
O 0.572262 3.376021 -0.357562
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$^{2}H^{IV}$ Eopt -1376.383577
Rh -0.832804 -0.459270 -0.175071
C -0.562219 -2.764603 0.022186
C -1.510479 -2.577318 -1.017310
C -2.394570 -1.638450 0.933457
C -1.084003 -2.138493 1.233677
C -2.643876 -1.882812 -0.467632
C 0.725540 -3.509027 -0.072199
H 1.446606 -3.156228 0.667176
H 0.541011 -4.572848 0.125265
H 1.169397 -3.425656 -1.066391
C -0.465958 -2.243661 2.588594
H -0.892265 -1.511802 3.277481
H -0.652108 -3.243060 3.001001
H 0.612863 -2.086206 2.544697
C -3.364924 -1.053492 1.903617
H -3.979197 -0.276941 1.442063
H -4.037368 -1.842748 2.263468
H -2.857433 -0.627165 2.770013
C -3.878399 -1.516091 -1.216454
H -3.649868 -1.252726 -2.252494
H -4.565568 -2.372527 -1.238386
H -4.401504 -0.681023 -0.745919
C -1.380340 -3.028023 -2.434909
H -1.926056 -3.967356 -2.587181
H -1.799884 -2.288997 -3.123079
H -0.336027 -3.197991 -2.704717
N -0.661574 2.119367 -1.410681
O -0.765530 0.832346 -1.794344

C	-0.829542	1.286995	0.815345
C	-0.891064	1.570501	2.169453
H	-0.936281	0.762718	2.891945
C	-0.872970	2.908015	2.635391
H	-0.936634	3.092430	3.703592
C	-0.759081	3.973929	1.764781
H	-0.730824	4.995348	2.129684
C	-0.672722	3.741179	0.368264
C	-0.718699	2.388579	-0.063748
C	-0.552231	4.755435	-0.611032
H	-0.521111	5.795052	-0.301962
C	-0.478216	4.415110	-1.948557
H	-0.381521	5.168613	-2.720839
C	-0.537207	3.072859	-2.338518
H	-0.500287	2.731765	-3.365299
C	3.200338	-0.464196	-0.633298
C	3.210288	-0.305636	0.758199
C	4.424667	-0.220679	1.441159
C	5.592846	-0.301285	0.679686
C	5.554246	-0.460432	-0.717444
C	4.342619	-0.545304	-1.412425
C	1.142183	-0.375200	0.154553
H	4.454995	-0.094393	2.518803
H	6.556376	-0.238168	1.176325
H	6.486012	-0.518769	-1.271677
H	4.300225	-0.667657	-2.489348
N	1.882441	-0.251531	1.212077
O	1.876680	-0.514691	-1.028754

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^{2}TS4^{IV} Eopt -1376.363924

Rh	1.052601	0.093562	-0.185816
C	1.821023	2.217649	-0.021143
C	2.532180	1.596021	-1.090723
C	3.019175	0.416270	0.870989
C	2.085391	1.466120	1.189229
C	3.251458	0.467482	-0.545655
C	0.994498	3.456320	-0.111203
H	0.206585	3.461923	0.642819
H	1.630903	4.334775	0.055449
H	0.532546	3.560104	-1.095918
C	1.634412	1.847722	2.561263
H	1.666889	0.993937	3.241435
H	2.296920	2.623416	2.965638
H	0.616879	2.240274	2.545584
C	3.640510	-0.532543	1.840434
H	3.892332	-1.484012	1.366105
H	4.567955	-0.104505	2.242822
H	2.975867	-0.731891	2.684472
C	4.118106	-0.457047	-1.334979
H	3.695905	-0.642714	-2.326173
H	5.111974	-0.013582	-1.476503
H	4.247431	-1.415890	-0.828355
C	2.550460	2.020688	-2.521071
H	3.455335	2.605336	-2.731402
H	2.557737	1.155557	-3.189966
H	1.685620	2.640930	-2.766354
N	-0.277793	-2.239326	-1.233515
O	0.499116	-1.248431	-1.696192
C	-0.297448	-1.077872	0.876187
C	-0.509421	-1.177087	2.256496
H	-0.296360	-0.317208	2.880771
C	-1.069853	-2.331123	2.829913
H	-1.213231	-2.367219	3.905129
C	-1.489162	-3.389899	2.044218
H	-1.975268	-4.254194	2.484358
C	-1.279369	-3.364869	0.640610
C	-0.635519	-2.224822	0.091946
C	-1.642082	-4.419955	-0.229183
H	-2.143279	-5.293793	0.173444
C	-1.343934	-4.329745	-1.574986
H	-1.612551	-5.116486	-2.269501
C	-0.636485	-3.228599	-2.063644
H	-0.306218	-3.120499	-3.088796
C	-2.832869	1.139728	-0.667648
C	-2.567927	1.861541	0.508671
C	-3.464932	2.846924	0.937870
C	-4.598098	3.062173	0.154921
C	-4.838470	2.322596	-1.019825
C	-3.950848	1.336263	-1.461706
C	-0.925446	0.502338	0.222331
H	-3.277493	3.417805	1.841568
H	-5.315804	3.819459	0.455150
H	-5.734896	2.523546	-1.598164
H	-4.124541	0.762948	-2.365705
N	-1.370357	1.419136	1.047638
O	-1.794533	0.260350	-0.851924

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^{2}I^{IV} Eopt -1376.411630

Rh	0.347579	-0.962783	-0.251526
C	1.405031	-2.931510	0.050331
C	0.047996	-3.147472	-0.355866
C	-0.019883	-2.045633	1.696644
C	1.364278	-2.163330	1.267505
C	-0.826964	-2.635728	0.687512
C	2.637456	-3.395549	-0.657798
H	3.465332	-2.693965	-0.521207
H	2.965979	-4.369347	-0.269503
H	2.465057	-3.512087	-1.731002
C	2.542455	-1.746090	2.092439
H	2.384326	-0.764681	2.548576
H	2.706739	-2.464064	2.906461
H	3.458185	-1.702670	1.499401
C	-0.490248	-1.435159	2.977643
H	-1.501953	-1.031034	2.881330
H	-0.507705	-2.181654	3.783417
H	0.170571	-0.625172	3.298379
C	-2.317797	-2.745132	0.703012
H	-2.725681	-2.824910	-0.306950
H	-2.628869	-3.644666	1.250377
H	-2.781395	-1.884669	1.193686
C	-0.409457	-3.880892	-1.577817
H	-0.591857	-4.940244	-1.354923
H	-1.342793	-3.461862	-1.964207
H	0.337183	-3.832223	-2.374761
N	-2.087882	0.345677	-1.209485
O	-0.884264	0.053836	-1.706400
C	-1.153978	2.230565	0.119140
C	-1.460056	3.316474	0.940691
H	-0.648727	3.950230	1.278239
C	-2.766357	3.600813	1.370525
H	-2.940431	4.452490	2.018766
C	-3.803428	2.792307	0.976133
H	-4.821765	2.983758	1.297718
C	-3.567016	1.689370	0.118386
C	-2.237093	1.405477	-0.323002
C	-4.649429	0.889667	-0.322978
H	-5.648084	1.120932	0.031650
C	-4.425445	-0.147063	-1.195777
H	-5.225761	-0.777369	-1.563752
C	-3.121943	-0.392460	-1.629267
H	-2.856113	-1.177995	-2.323814
C	2.319846	2.858387	-0.314374
C	2.365516	1.463312	-0.266402
C	3.581497	0.785310	-0.348431
C	4.727331	1.571891	-0.459114
C	4.660402	2.978636	-0.495865
C	3.442733	3.661344	-0.430220
C	0.278119	2.066809	-0.153440
H	3.621144	-0.297656	-0.334218
H	5.697555	1.089654	-0.523054
H	5.579366	3.549437	-0.582369
H	3.377495	4.742598	-0.466978
N	1.049849	1.005286	-0.156096
O	0.993764	3.233613	-0.244999

73

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C	-5.137990	-0.460936	0.433397
C	-5.097531	-0.986196	-0.863900
C	-3.120783	-1.307800	-0.000268
H	-6.256356	0.543960	1.993944

C	-6.257575	0.144472	0.984985
C	-6.231549	-0.917804	-1.677050
C	-7.372957	-0.313394	-1.144465
C	-7.387247	0.208553	0.161683
H	-8.271257	-0.243295	-1.751032
H	-8.293491	0.672170	0.540092
Rh	0.814038	1.201021	-0.010052
N	-3.818581	-1.509994	-1.091850
C	-1.135236	2.403261	-0.149338
C	-0.767955	2.337221	1.202638
C	-0.007316	2.962923	-0.901672
C	0.587225	2.892327	1.331666
C	0.999955	3.370870	0.048060
C	-1.549828	1.772557	2.344496
H	-1.891416	2.577454	3.007566
H	-2.422661	1.214910	2.001567
H	-0.929561	1.098732	2.943709
C	-2.408794	1.955266	-0.788148
H	-3.100749	1.537745	-0.058117
H	-2.896799	2.807280	-1.276598
H	-2.222751	1.200746	-1.558261
C	-0.025330	3.263035	-2.365210
H	-0.539290	2.472313	-2.918436
H	-0.552869	4.205868	-2.559994
H	0.989045	3.355295	-2.760766
C	2.210552	4.188205	-0.259199
H	2.621107	3.949301	-1.242529
H	1.935354	5.250566	-0.259949
H	2.994233	4.050587	0.488062
C	1.315184	3.049884	2.626439
H	1.196302	2.160757	3.251440
H	2.383047	3.213662	2.465255
H	0.920426	3.907451	3.186223
H	-6.221784	-1.319663	-2.685924
C	1.617947	-1.456210	1.562697
O	0.881185	-2.252147	0.897745
O	1.430717	-0.205522	1.650063
C	3.523949	-1.046772	3.182298
H	3.893727	-0.198693	2.598957
H	2.846602	-0.660801	3.950897
C	3.804677	-2.563148	1.196777
H	3.320126	-3.269817	0.516843
H	4.186811	-1.723696	0.609072
C	2.825823	-2.076246	2.286348
C	2.341960	-3.271127	3.127592
H	1.615852	-2.952289	3.884137
H	1.869392	-4.030741	2.499212
H	4.658723	-3.065457	1.664411
H	4.378034	-1.513134	3.685513
H	3.189575	-3.732009	3.646096
O	-3.899919	-0.661034	0.993351
C	2.438802	-2.546001	-3.307934
C	3.694951	-2.055591	-3.018789
C	3.831226	-0.936626	-2.160482
C	2.655478	-0.344918	-1.619614
C	1.299609	-1.937343	-2.762867
H	5.991160	-0.804817	-2.161212
H	2.299824	-3.405928	-3.952515
H	4.583098	-2.525050	-3.429559
C	5.074314	-0.378250	-1.766957
C	2.656006	0.747533	-0.715846
H	0.285010	-2.268078	-2.943972
C	3.902671	1.233932	-0.356888
C	5.098770	0.678775	-0.881568
H	3.982089	2.052358	0.351498
H	6.052683	1.095045	-0.569106
O	0.336401	-0.304655	-1.442600
N	1.429997	-0.877303	-1.962941
Ag	-1.122680	-1.643903	0.370161
73			
F′		Eopt -1870.093673	
C	-3.676757	-2.099914	-0.554125
C	-3.692633	-1.300251	-1.703711
C	-1.622844	-1.383330	-1.029124
H	-4.765875	-3.298919	0.886240
C	-4.809874	-2.683096	-0.005898
C	-4.899207	-1.053025	-2.363733
C	-6.055089	-1.627631	-1.830084
C	-6.012448	-2.428485	-0.673831
H	-7.010025	-1.455237	-2.317725
H	-6.932716	-2.858792	-0.290267
Rh	-0.466379	1.003831	0.848130
N	-2.384281	-0.878158	-1.968917
C	-2.001001	0.451793	2.480977
C	-0.712168	-0.187884	2.706409
C	-1.781413	1.843531	2.439628
C	0.284389	0.820788	2.891941
C	-0.354836	2.097388	2.652676
C	-0.494436	-1.658364	2.836172
H	-0.699261	-1.964668	3.871057
H	-1.164191	-2.219412	2.181836
H	0.533824	-1.929467	2.594826
C	-3.321650	-0.237858	2.350677
H	-3.196144	-1.306553	2.182693
H	-3.905746	-0.107832	3.270474
H	-3.911243	0.169516	1.525168
C	-2.807551	2.895426	2.184163
H	-3.673173	2.485802	1.658506
H	-3.155606	3.315802	3.136192
H	-2.395189	3.715992	1.591312
C	0.266800	3.445157	2.812623
H	-0.207536	4.178748	2.156128
H	0.147412	3.792841	3.847086
H	1.334525	3.419505	2.584964
C	1.682176	0.597849	3.368577
H	2.123728	-0.296064	2.923432
H	2.323092	1.452507	3.144945
H	1.677010	0.463681	4.457986
H	-4.932202	-0.437119	-3.257454
C	3.149062	-1.966959	0.095333
O	2.541635	-1.752044	-1.018544
O	2.574402	-2.024309	1.206479
C	5.348924	-1.322382	1.108055
H	5.199110	-0.256738	0.904104
H	4.943129	-1.538633	2.099772
C	5.248051	-1.861105	-1.347678
H	4.807437	-2.491748	-2.125372
H	5.060109	-0.816942	-1.615858
C	4.674434	-2.194782	0.034621
C	4.915570	-3.684313	0.355799
H	4.517207	-3.940470	1.342219
H	4.432025	-4.329316	-0.386842
H	6.332022	-2.023508	-1.352008
H	6.427815	-1.512293	1.126979
H	5.988809	-3.905289	0.348996
O	-2.377430	-2.159811	-0.116961
C	0.171773	3.228288	-3.842630
C	1.517104	3.043157	-3.599185
C	1.936634	2.476153	-2.371064
C	0.949514	2.099518	-1.418654
C	-0.774714	2.868923	-2.873959
H	4.072628	2.531855	-2.716998
H	-0.184317	3.655605	-4.772431
H	2.259710	3.324082	-4.339074
C	3.291901	2.251653	-2.017035
C	1.231927	1.484111	-0.170408
H	-1.843207	2.998826	-2.988579
C	2.577496	1.309355	0.117984
C	3.593761	1.689519	-0.794579
H	2.876200	0.834841	1.044248
H	4.631998	1.523435	-0.523285
O	-1.291313	2.013724	-0.789488
N	-0.375541	2.334224	-1.718127
Ag	0.427207	-1.417846	-0.847688
73			
TS3		Eopt -1870.092273	
C	-3.422214	-2.120568	-0.913943
C	-3.512490	-1.128996	-1.899969
C	-1.509780	-0.993359	-1.056349
H	-4.362883	-3.734875	0.185273

C	-4.463287	-2.976746	-0.584222
C	-4.701603	-0.964578	-2.616423
C	-5.764258	-1.814025	-2.302127
C	-5.648476	-2.801652	-1.305555
H	-6.703498	-1.713564	-2.837975
H	-6.498494	-3.442452	-1.090887
Rh	-0.585770	0.746337	0.928237
N	-2.289684	-0.451705	-1.960610
C	-2.004436	-0.175874	2.507416
C	-0.660890	-0.734377	2.598183
C	-1.896755	1.218967	2.680420
C	0.256251	0.316481	2.911304
C	-0.489756	1.555944	2.893608
C	-0.331057	-2.188499	2.526855
H	-0.486454	-2.643957	3.514199
H	-0.974609	-2.706441	1.813777
H	0.707126	-2.347471	2.234692
C	-3.276901	-0.944161	2.338857
H	-3.084493	-1.967457	2.019416
H	-3.817090	-0.984023	3.293290
H	-3.938487	-0.476888	1.604802
C	-3.010803	2.209891	2.627926
H	-3.872278	1.811709	2.087063
H	-3.334300	2.461942	3.645699
H	-2.693176	3.136935	2.143370
C	0.031209	2.913744	3.233519
H	-0.501162	3.689124	2.676535
H	-0.104833	3.116222	4.303774
H	1.096128	2.997467	3.006021
C	1.686392	0.148562	3.305146
H	2.162761	-0.665395	2.755410
H	2.257695	1.063876	3.141188
H	1.740883	-0.089833	4.375346
H	-4.791235	-0.204264	-3.386370
C	3.248113	-1.934224	-0.271284
O	2.659324	-1.535923	-1.343914
O	2.657622	-2.129752	0.816681
C	5.435991	-1.303178	0.743848
H	5.270476	-0.237655	0.550251
H	5.035582	-1.535862	1.734333
C	5.343733	-1.827061	-1.715650
H	4.890583	-2.438261	-2.502146
H	5.169411	-0.775709	-1.964642
C	4.770357	-2.175535	-0.337758
C	5.020299	-3.663612	-0.023458
H	4.617385	-3.928119	0.958469
H	4.546834	-4.309147	-0.772131
H	6.425153	-2.004980	-1.727626
H	6.517478	-1.478171	0.758560
H	6.095134	-3.876461	-0.024398
O	-2.164207	-2.048668	-0.376576
C	-0.143395	4.232415	-2.962711
C	1.210684	4.004217	-2.834098
C	1.681217	3.118457	-1.833731
C	0.733269	2.473596	-0.990685
C	-1.049922	3.599058	-2.102138
H	3.800100	3.292298	-2.239798
H	-0.537823	4.899501	-3.720111
H	1.922074	4.490866	-3.493647
C	3.050311	2.818461	-1.614145
C	1.068359	1.531431	0.018061
H	-2.122574	3.739133	-2.137249
C	2.426414	1.306007	0.196818
C	3.403335	1.938884	-0.612735
H	2.762492	0.594644	0.940319
H	4.452095	1.713113	-0.442284
O	-1.479631	2.174102	-0.334656
N	-0.604055	2.762961	-1.161288
Ag	0.568202	-1.079274	-1.000895
73			
G′	Eopt	-1870.103139	
C	-1.728309	-3.361419	0.024501
C	-1.777215	-2.913953	-1.302882
C	-1.111635	-1.229443	-0.094810
H	-2.009012	-4.965134	1.453714
C	-2.058697	-4.649713	0.416766
C	-2.180001	-3.787664	-2.317228
C	-2.522182	-5.090075	-1.946756
C	-2.463408	-5.514531	-0.606475
H	-2.842070	-5.793950	-2.709385
H	-2.738272	-6.535443	-0.359052
Rh	-1.112845	0.683326	0.747019
N	-1.379007	-1.577323	-1.339615
C	-1.702502	0.184626	2.916771
C	-0.274020	0.403726	2.795971
C	-2.349639	1.385860	2.531006
C	-0.061844	1.774040	2.396077
C	-1.343961	2.373248	2.181686
C	0.782217	-0.556186	3.246775
H	0.903011	-0.484499	4.336222
H	0.508573	-1.587291	3.011775
H	1.747273	-0.341644	2.784291
C	-2.360659	-1.048335	3.451354
H	-1.729271	-1.927024	3.316011
H	-2.556059	-0.936000	4.525565
H	-3.316626	-1.241263	2.957914
C	-3.822189	1.617525	2.461961
H	-4.377055	0.677043	2.451612
H	-4.150324	2.196910	3.334027
H	-4.089373	2.188858	1.568397
C	-1.618219	3.790560	1.789205
H	-2.525042	3.860774	1.181777
H	-1.762015	4.422663	2.674757
H	-0.790439	4.208111	1.210881
C	1.255891	2.472878	2.342315
H	2.065175	1.796820	2.063938
H	1.240758	3.307924	1.639277
H	1.485608	2.880239	3.335753
H	-2.224585	-3.461074	-3.351758
C	4.001794	-0.478239	0.108510
O	3.236253	-1.288249	-0.536610
O	3.587226	0.337938	0.964418
C	5.849732	0.869090	-0.845094
H	5.287795	1.031148	-1.772290
H	5.609563	1.682055	-0.153724
C	5.861243	-1.622117	-1.207376
H	5.608067	-2.605241	-0.797805
H	5.327015	-1.504626	-2.154876
C	5.507936	-0.500692	-0.223644
C	6.292066	-0.685240	1.088417
H	6.052163	0.106744	1.803123
H	6.056992	-1.648706	1.555344
H	6.936490	-1.609545	-1.418990
H	6.917903	0.921754	-1.083270
H	7.369787	-0.659476	0.892711
O	-1.305042	-2.312062	0.796972
C	-2.909396	2.166071	-3.958231
C	-1.607203	2.558128	-4.182629
C	-0.638881	2.396890	-3.161215
C	-1.037436	1.814168	-1.923726
C	-3.277294	1.626230	-2.718851
H	1.052519	3.227942	-4.224820
H	-3.674502	2.271400	-4.718376
H	-1.311499	2.989541	-5.133572
C	0.718904	2.785417	-3.291637
C	-0.155176	1.572301	-0.837030
H	-4.283370	1.319829	-2.463054
C	1.152951	2.007166	-1.019899
C	1.582584	2.603720	-2.233720
H	1.889103	1.875511	-0.234986
H	2.621364	2.909223	-2.324698
O	-2.747831	0.996771	-0.566075
N	-2.364550	1.476535	-1.756170
Ag	1.144377	-0.814407	-0.121109
73			
G	Eopt	-1870.120876	
C	1.867349	3.180168	-0.799626
C	0.632642	3.237279	-0.148824
C	1.117575	1.110084	-0.472737
H	3.554444	4.226723	-1.662734

C	2.597589	4.300894	-1.157333
C	0.060159	4.465047	0.177479
C	0.777944	5.611906	-0.173774
C	2.020508	5.533008	-0.826687
H	0.366264	6.588700	0.061695
H	2.546022	6.447954	-1.082293
Rh	1.041199	-0.872594	-0.643710
N	0.204358	1.917396	0.039037
C	-0.614941	-1.886004	-1.881509
C	-0.058394	-0.831649	-2.635290
C	0.436164	-2.860302	-1.597384
C	1.371692	-1.098010	-2.775652
C	1.633189	-2.404522	-2.203665
C	-0.773844	0.366011	-3.179426
H	-1.071271	0.194653	-4.221840
H	-1.676182	0.590346	-2.605022
H	-0.133919	1.252293	-3.162323
C	-2.031349	-2.039073	-1.423956
H	-2.628297	-1.151989	-1.636686
H	-2.500751	-2.894458	-1.926186
H	-2.078073	-2.230572	-0.347228
C	0.220155	-4.142462	-0.856571
H	-0.427475	-3.988261	0.012176
H	-0.263409	-4.891467	-1.497077
H	1.164806	-4.564189	-0.504096
C	2.938077	-3.129965	-2.264658
H	3.057881	-3.817224	-1.423668
H	2.995019	-3.717807	-3.189657
H	3.783803	-2.438795	-2.263834
C	2.325489	-0.302885	-3.611396
H	2.070026	0.759251	-3.601500
H	3.351935	-0.405842	-3.249514
H	2.303600	-0.643689	-4.654909
H	-0.900985	4.520727	0.679357
C	-4.328738	0.179639	0.243810
O	-3.495070	0.181480	1.231648
O	-4.104554	0.731573	-0.855292
C	-6.304568	-0.042371	1.770914
H	-5.649598	-0.168986	2.637216
H	-6.537445	1.024114	1.672094
C	-5.295448	-2.076634	0.678365
H	-4.825691	-2.488559	-0.221481
H	-4.609751	-2.218946	1.518746
C	-5.643847	-0.585983	0.490518
C	-6.593707	-0.420755	-0.701586
H	-6.847883	0.631407	-0.864255
H	-6.143862	-0.802969	-1.622693
H	-6.206112	-2.653135	0.876218
H	-7.241945	-0.574693	1.967488
H	-7.523064	-0.972043	-0.520166
O	2.170809	1.845348	-0.997211
C	1.663989	-1.035829	4.567444
C	3.008025	-0.987519	4.261539
C	3.418511	-0.941200	2.906383
C	2.421056	-0.951006	1.890144
C	0.706333	-1.046902	3.544639
H	5.556145	-0.861638	3.234350
H	1.316227	-1.066526	5.593325
H	3.756881	-0.975254	5.047174
C	4.771259	-0.868552	2.484634
C	2.702652	-0.886098	0.500832
H	-0.362508	-1.087120	3.710870
C	4.041961	-0.794010	0.156478
C	5.065036	-0.795812	1.139154
H	4.324576	-0.709423	-0.888803
H	6.101684	-0.730063	0.819489
O	0.165063	-1.029917	1.298801
N	1.092696	-1.010142	2.266173
Ag	-1.645948	1.101418	0.683173

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H Eopt -1376.556060

Rh	-0.902614	-0.340313	-0.163319
C	-1.804058	-2.433974	-0.199672
C	-2.492445	-1.674242	-1.169982
C	-2.896770	-0.666520	0.892405
C	-1.967558	-1.766473	1.084749
C	-3.172388	-0.572602	-0.491284
C	-1.044901	-3.704626	-0.406104
H	-0.845752	-3.885585	-1.465227
H	-0.088922	-3.677312	0.123046
H	-1.620794	-4.555585	-0.020516
C	-1.511696	-2.309033	2.402295
H	-1.465092	-1.522316	3.160109
H	-2.202425	-3.080957	2.767289
H	-0.518817	-2.756161	2.316458
C	-3.447816	0.192940	1.984162
H	-3.805065	1.152286	1.602261
H	-4.291835	-0.310620	2.472435
H	-2.697350	0.393869	2.752761
C	-4.028998	0.439060	-1.185715
H	-3.540205	0.809694	-2.092666
H	-4.988573	0.000537	-1.487992
H	-4.240094	1.296158	-0.541810
C	-2.581392	-1.931898	-2.641577
H	-3.557644	-2.358575	-2.905709
H	-2.468161	-1.003295	-3.210017
H	-1.808787	-2.628673	-2.974887
N	0.017951	2.201881	-1.242077
O	-0.454429	1.048653	-1.730253
C	-0.258817	1.225630	0.924141
C	-0.110477	1.374919	2.294026
H	-0.359011	0.549039	2.954375
C	0.371483	2.581601	2.862320
H	0.464977	2.654255	3.942731
C	0.731583	3.654469	2.074206
H	1.107498	4.574065	2.511504
C	0.624332	3.558641	0.662536
C	0.126065	2.335855	0.129756
C	0.993886	4.590464	-0.234963
H	1.379257	5.526675	0.156124
C	0.869557	4.389207	-1.593421
H	1.148569	5.154676	-2.308003
C	0.375446	3.174160	-2.086340
H	0.252948	2.950094	-3.138168
C	3.172485	-0.788986	-0.545885
C	2.939460	-1.822985	0.370714
C	4.007772	-2.596040	0.829497
C	5.282694	-2.291162	0.342131
C	5.489255	-1.247717	-0.576124
C	4.424233	-0.466907	-1.044284
C	1.005889	-0.921401	-0.056043
H	3.850574	-3.403546	1.538450
H	6.134735	-2.874212	0.679838
H	6.494402	-1.041091	-0.931572
H	4.570186	0.340548	-1.754444
N	1.569924	-1.864881	0.656595
O	1.956548	-0.209049	-0.823236

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$TS4_{Ag}$ Eopt -1870.062805

Rh	-1.335933	-0.909024	-0.676927
C	-0.111854	-1.151066	-2.529983
C	-1.467981	-1.566264	-2.727273
C	-0.531094	-3.070958	-1.222716
C	0.427921	-1.995081	-1.504834
C	-1.687881	-2.807009	-1.951812
C	0.599343	-0.057350	-3.259089
H	1.376347	0.398801	-2.638631
H	1.084742	-0.447147	-4.163575
H	-0.090309	0.734194	-3.564415
C	1.840065	-2.019307	-1.009924
H	1.893393	-2.096210	0.079082
H	2.359709	-2.893137	-1.425154
H	2.393961	-1.131552	-1.316604
C	-0.266218	-4.194678	-0.271660
H	-1.184123	-4.725941	-0.007705
H	0.427944	-4.923731	-0.710207
H	0.193556	-3.830753	0.652954
C	-2.977282	-3.563124	-1.952296
H	-3.823589	-2.894941	-1.758235
H	-3.153364	-4.033956	-2.927512

H	-2.983255	-4.347364	-1.191441
C	-2.443712	-1.008763	-3.713078
H	-2.411752	-1.573905	-4.654781
H	-3.466824	-1.067733	-3.330197
H	-2.224902	0.037497	-3.941390
N	-3.586421	-0.463102	1.131817
O	-3.391925	-0.589956	-0.180339
C	-1.238171	0.181320	1.407771
C	-0.151207	0.144346	2.277077
H	0.829150	0.418919	1.905341
C	-0.288000	-0.157114	3.645228
H	0.595158	-0.165014	4.275688
C	-1.535543	-0.367076	4.190045
H	-1.664886	-0.523408	5.256224
C	-2.682427	-0.401035	3.355371
C	-2.502175	-0.211182	1.956439
C	-3.982182	-0.639854	3.863981
H	-4.119610	-0.759385	4.933390
C	-5.046881	-0.724182	2.994258
H	-6.058880	-0.894257	3.341641
C	-4.818369	-0.662969	1.616505
H	-5.582515	-0.831292	0.868465
C	-1.838067	3.069355	-0.437032
C	-0.435818	3.025827	-0.519956
C	0.266705	4.178083	-0.885938
C	-0.472977	5.340119	-1.151617
C	-1.869166	5.359845	-1.056560
C	-2.584011	4.202711	-0.689625
C	-1.132735	0.970245	0.038553
H	1.350712	4.164461	-0.959551
H	0.053481	6.246653	-1.437340
H	-2.412722	6.275162	-1.269653
H	-3.666487	4.197345	-0.610544
N	-0.008525	1.759561	-0.196091
O	-2.291318	1.826012	-0.077522
C	4.310733	-0.153528	0.849222
O	4.076357	0.663682	-0.125611
O	3.469463	-0.445475	1.726162
C	6.782416	0.282018	0.674807
H	6.648484	0.827245	-0.263164
H	6.746985	1.004801	1.497967
C	5.751844	-1.777129	-0.351655
H	4.987514	-2.556222	-0.254347
H	5.584197	-1.248084	-1.294511
C	5.707068	-0.805320	0.846198
C	5.943681	-1.577150	2.149767
H	5.894962	-0.913139	3.018949
H	5.196323	-2.363999	2.286518
H	6.729944	-2.268502	-0.402110
H	7.779772	-0.171798	0.668512
H	6.934353	-2.044838	2.134309
Ag	2.016327	1.224161	-0.157636

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I_{Ag} Eopt -1870.081826

Rh	-0.271737	-0.873730	0.646000
C	-2.102306	-2.077792	0.076336
C	-1.937266	-1.983267	1.497365
C	-0.148138	-3.232505	0.695327
C	-0.937239	-2.722438	-0.434261
C	-0.759306	-2.791581	1.868095
C	-3.278646	-1.652467	-0.737759
H	-2.965114	-1.130307	-1.644807
H	-3.858235	-2.534199	-1.042832
H	-3.939245	-0.988752	-0.179831
C	-0.697260	-3.118850	-1.857625
H	0.367040	-3.110337	-2.103611
H	-1.071604	-4.137277	-2.032269
H	-1.215429	-2.453726	-2.555398
C	1.122631	-4.005591	0.541368
H	1.646582	-4.113688	1.494213
H	0.928953	-5.011459	0.147078
H	1.801151	-3.509661	-0.161063
C	-0.302017	-2.981646	3.277050
H	-0.226669	-2.019661	3.795579
H	-1.017731	-3.596112	3.837119
H	0.674032	-3.470444	3.323730
C	-2.924186	-1.441740	2.483924
H	-3.534523	-2.250042	2.908724
H	-2.415965	-0.941805	3.313915
H	-3.597237	-0.719604	2.017924
N	1.354347	1.002085	2.284631
O	0.343106	0.141788	2.400347
C	0.300863	2.035023	0.312659
C	0.415008	3.037788	-0.639732
H	-0.374036	3.111925	-1.377605
C	1.502583	3.934381	-0.695006
H	1.526677	4.694532	-1.469842
C	2.519182	3.840668	0.222172
H	3.371398	4.512293	0.199443
C	2.464759	2.850071	1.234934
C	1.348122	1.956159	1.276833
C	3.498427	2.740573	2.194733
H	4.333299	3.431890	2.148417
C	3.435125	1.766460	3.163867
H	4.207926	1.645766	3.913458
C	2.344899	0.895662	3.177442
H	2.220664	0.094755	3.894525
C	-3.074973	1.701152	0.593863
C	-2.885776	1.524373	-0.797144
C	-3.982987	1.686643	-1.652143
C	-5.229885	2.006649	-1.088023
C	-5.394097	2.166250	0.289549
C	-4.292280	2.009974	1.161915
C	-0.908091	1.091511	0.212494
H	-3.870953	1.546723	-2.724135
H	-6.087565	2.129643	-1.744841
H	-6.369163	2.412494	0.698843
H	-4.394724	2.128988	2.236526
N	-1.582743	1.208899	-1.040798
O	-1.882383	1.492787	1.245282
C	2.332697	-0.652983	-1.271750
O	1.722300	-0.736978	-2.389863
O	1.784197	-0.563430	-0.135510
C	4.258609	0.716418	-2.006124
H	3.852490	0.773976	-3.020357
H	3.879155	1.571417	-1.435470
C	4.369264	-1.799460	-2.178342
H	4.093560	-2.756467	-1.720639
H	3.946169	-1.768537	-3.185890
C	3.871634	-0.615995	-1.329751
C	4.486615	-0.681013	0.073557
H	4.184230	0.173140	0.684955
H	4.187938	-1.594358	0.598065
H	5.461058	-1.768768	-2.261544
H	5.348940	0.804323	-2.065577
H	5.579655	-0.674622	-0.001210
Ag	-0.320837	0.073852	-2.323817

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$^{2}G^{IV}$ Eopt -1869.944416

C	2.287753	2.626554	-1.323746
C	1.043327	2.947916	-0.777273
C	1.276751	0.775512	-0.687079
H	4.132877	3.286422	-2.246792
C	3.172832	3.564616	-1.826540
C	0.617049	4.272617	-0.708808
C	1.492534	5.239176	-1.208355
C	2.742339	4.893906	-1.754805
H	1.202391	6.284716	-1.176290
H	3.390608	5.678451	-2.132087
Rh	0.915542	-1.161823	-0.354202
N	0.439281	1.742244	-0.389220
C	-0.808135	-2.170974	-1.589568
C	-0.151504	-1.225381	-2.415043
C	0.154238	-3.174278	-1.197683
C	1.260843	-1.606183	-2.499319
C	1.431599	-2.829392	-1.774473
C	-0.776316	-0.066291	-3.113785
H	-1.088563	-0.376193	-4.119551
H	-1.660008	0.296073	-2.584683
H	-0.073814	0.761788	-3.228773

C	-2.241563	-2.173542	-1.167891
H	-2.761273	-1.268889	-1.481989
H	-2.756955	-3.037714	-1.603490
H	-2.325264	-2.258133	-0.079937
C	-0.144386	-4.369448	-0.362769
H	-0.905720	-4.146788	0.389419
H	-0.537982	-5.172954	-1.000489
H	0.750299	-4.748486	0.135725
C	2.675511	-3.650393	-1.710851
H	2.787988	-4.138843	-0.740324
H	2.632429	-4.433485	-2.478379
H	3.562518	-3.044609	-1.903092
C	2.276516	-0.977643	-3.395212
H	2.063599	0.076869	-3.571775
H	3.283155	-1.061694	-2.980406
H	2.267343	-1.493573	-4.363536
H	-0.349425	4.532224	-0.288682
C	-4.253918	0.514579	0.143471
O	-3.403208	0.644209	1.108703
O	-4.002292	0.816958	-1.043317
C	-6.202591	0.738005	1.705932
H	-5.540106	0.714336	2.575391
H	-6.351201	1.785017	1.418084
C	-5.383405	-1.535692	0.992615
H	-4.971761	-2.141340	0.177862
H	-4.689365	-1.577935	1.837286
C	-5.619024	-0.080077	0.539302
C	-6.582351	-0.056357	-0.652924
H	-6.757105	0.966278	-1.001907
H	-6.187972	-0.634911	-1.493417
H	-6.330907	-1.989721	1.303396
H	-7.174717	0.329465	2.003403
H	-7.547129	-0.487241	-0.363413
O	2.426432	1.248026	-1.256817
C	1.322488	0.203736	4.640258
C	2.682539	0.102352	4.411401
C	3.155060	-0.292883	3.137539
C	2.201446	-0.579306	2.124993
C	0.410975	-0.102281	3.623941
H	5.279595	-0.217692	3.538946
H	0.931687	0.509831	5.603022
H	3.394224	0.323605	5.199993
C	4.524081	-0.424237	2.788158
C	2.547289	-0.956806	0.806504
H	-0.665526	-0.063186	3.732426
C	3.898607	-1.047482	0.513328
C	4.877278	-0.803332	1.507652
H	4.219677	-1.294162	-0.493551
H	5.926826	-0.900154	1.246816
O	-0.014944	-0.824679	1.462731
N	0.864041	-0.487973	2.427177
Ag	-1.507407	1.294185	0.362978

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^{2}TS4$_{Ag}^{IV}$ Eopt -1869.916981

Rh	-1.484799	-1.143171	-0.453006
C	-0.167201	-1.632173	-2.226893
C	-1.481862	-2.128936	-2.506504
C	-0.664391	-3.251435	-0.621712
C	0.334763	-2.312183	-1.056004
C	-1.810443	-3.086383	-1.480654
C	0.573160	-0.679875	-3.106032
H	1.479844	-0.301785	-2.632346
H	0.867266	-1.198197	-4.027200
H	-0.049633	0.172335	-3.389258
C	1.714705	-2.225633	-0.491255
H	1.707874	-2.219580	0.600786
H	2.290826	-3.101296	-0.815720
H	2.241883	-1.336747	-0.837795
C	-0.521491	-4.216299	0.505095
H	-1.490590	-4.481027	0.934430
H	-0.051255	-5.142504	0.148186
H	0.113009	-3.809106	1.296859
C	-3.097553	-3.836162	-1.375159
H	-3.933443	-3.241012	-1.750656
H	-3.045677	-4.755333	-1.971631
H	-3.309520	-4.117708	-0.341237
C	-2.340850	-1.735525	-3.659792
H	-2.136252	-2.386452	-4.520326
H	-3.402330	-1.830736	-3.418990
H	-2.143948	-0.706008	-3.969254
N	-3.455201	-0.259491	1.482427
O	-3.429397	-0.864866	0.285023
C	-1.070439	-0.008647	1.270477
C	0.138470	0.112982	1.961354
H	1.079613	0.005657	1.434104
C	0.175374	0.440614	3.328294
H	1.141404	0.527260	3.815367
C	-0.986510	0.700445	4.030305
H	-0.955304	1.017480	5.067418
C	-2.250900	0.526125	3.406661
C	-2.263166	0.108269	2.050914
C	-3.487577	0.692645	4.073103
H	-3.495910	1.024231	5.105876
C	-4.665241	0.412992	3.407111
H	-5.629854	0.532629	3.885367
C	-4.630072	-0.092689	2.105172
H	-5.502678	-0.412871	1.550148
C	-1.942761	2.853941	-0.885978
C	-0.557523	2.843769	-1.082381
C	0.094447	3.965829	-1.600801
C	-0.701310	5.069316	-1.905446
C	-2.095105	5.057014	-1.699902
C	-2.753200	3.937643	-1.180951
C	-1.123595	0.887533	-0.278920
H	1.168866	3.966038	-1.755668
H	-0.237258	5.962833	-2.310947
H	-2.674456	5.940184	-1.949429
H	-3.824622	3.916823	-1.016587
N	-0.077787	1.605956	-0.678328
O	-2.297618	1.629696	-0.373333
C	4.294502	0.106269	0.756540
O	4.074456	0.669508	-0.388599
O	3.447276	0.055317	1.673478
C	6.774601	0.404803	0.450235
H	6.640181	0.687211	-0.597161
H	6.774615	1.319866	1.053374
C	5.666180	-1.817756	0.013776
H	4.882236	-2.518336	0.322578
H	5.495711	-1.550889	-1.033575
C	5.672095	-0.563299	0.913255
C	5.908589	-0.971558	2.372310
H	5.890591	-0.100782	3.035871
H	5.143853	-1.672998	2.717772
H	6.628840	-2.335996	0.084612
H	7.757724	-0.067211	0.555156
H	6.886537	-1.454992	2.472320
Ag	2.009932	1.199987	-0.542037

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^{2}I$_{Ag}^{IV}$ Eopt -1869.978688

Rh	0.100861	1.255194	0.540175
C	1.550389	2.594516	-0.577755
C	2.014958	2.304208	0.748415
C	-0.000614	3.441746	0.974316
C	0.252656	3.194750	-0.440030
C	1.082784	2.887856	1.705456
C	2.277483	2.351718	-1.862012
H	1.594175	2.054051	-2.663849
H	2.789202	3.266675	-2.192587
H	3.035053	1.574262	-1.752256
C	-0.622380	3.665060	-1.559152
H	-1.680436	3.578043	-1.298557
H	-0.423632	4.721081	-1.785143
H	-0.449300	3.088451	-2.470842
C	-1.209716	4.132765	1.518799
H	-1.364015	3.898149	2.575366
H	-1.112036	5.222703	1.428788
H	-2.110698	3.840412	0.970880
C	1.262704	2.863574	3.189631
H	1.672098	1.903979	3.520216
H	1.963035	3.645288	3.512004

H	0.316502	3.028216	3.711836
C	3.310794	1.653273	1.120607
H	4.055650	2.407930	1.405668
H	3.183271	0.980985	1.973931
H	3.721900	1.074632	0.292207
N	-0.720172	-1.214668	1.936860
O	0.423679	-0.567780	1.681890
C	-0.121240	-2.867071	0.236443
C	-0.534714	-3.925990	-0.557100
H	0.155497	-4.327353	-1.291776
C	-1.817089	-4.496346	-0.415999
H	-2.104183	-5.324168	-1.055123
C	-2.682319	-4.017755	0.539329
H	-3.664444	-4.458327	0.676690
C	-2.311988	-2.927664	1.368737
C	-1.028534	-2.335778	1.190390
C	-3.186213	-2.403510	2.350753
H	-4.158976	-2.862708	2.490212
C	-2.795198	-1.319112	3.102999
H	-3.435126	-0.887639	3.863011
C	-1.554614	-0.724319	2.857589
H	-1.204540	0.168787	3.359158
C	3.376352	-2.107824	0.422457
C	3.059472	-1.543536	-0.816599
C	4.045816	-0.938449	-1.594000
C	5.335394	-0.911345	-1.061056
C	5.628190	-1.471380	0.197023
C	4.646376	-2.093889	0.973834
C	1.245288	-2.359679	0.032874
H	3.814895	-0.509411	-2.562913
H	6.134381	-0.445454	-1.628882
H	6.644933	-1.424149	0.573426
H	4.861564	-2.536865	1.939457
N	1.687475	-1.734259	-1.029710
O	2.211222	-2.649582	0.944609
C	-2.473743	0.550771	-1.004512
O	-1.822664	0.433353	-2.093142
O	-1.948494	0.674999	0.143599
C	-4.398604	-0.870979	-1.659746
H	-3.960281	-1.037307	-2.647879
H	-4.058847	-1.672078	-0.993682
C	-4.451469	1.617090	-2.085958
H	-4.171117	2.609553	-1.715374
H	-3.997663	1.478045	-3.070768
C	-4.006682	0.514633	-1.106137
C	-4.663959	0.734869	0.261297
H	-4.380834	-0.046160	0.971836
H	-4.380316	1.701459	0.689231
H	-5.540334	1.595675	-2.200877
H	-5.487766	-0.942872	-1.748663
H	-5.753697	0.718120	0.152698
Ag	0.210612	-0.344774	-1.859710

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^{2}D^{IV} Eopt -1670.796177

Rh	-0.906128	-0.745476	-0.297522
C	-1.439558	-2.841223	0.403031
C	-2.145842	-1.904987	1.240906
C	-1.861398	-2.629848	-0.968174
C	-3.037546	-1.165739	0.406208
C	-2.835687	-1.584613	-0.971383
C	-2.016224	-1.760871	2.717784
H	-2.787846	-2.359630	3.217124
H	-1.038158	-2.097927	3.061360
H	-2.148164	-0.718196	3.014261
C	-0.507947	-3.911981	0.843226
H	-0.204647	-3.786122	1.880768
H	-1.022371	-4.876559	0.737529
H	0.384637	-3.948419	0.213429
C	-1.386429	-3.393432	-2.154197
H	-0.416945	-3.858882	-1.968910
H	-2.107906	-4.188173	-2.380195
H	-1.309433	-2.749949	-3.033581
C	-3.587561	-1.058497	-2.143584
H	-3.078594	-1.290398	-3.080649
H	-4.585581	-1.513153	-2.171776
H	-3.716158	0.024057	-2.068917
C	-4.077097	-0.201402	0.844415
H	-4.175320	0.627366	0.140965
H	-5.036755	-0.735954	0.857256
H	-3.882786	0.189329	1.841509
C	1.277705	-0.350992	1.680754
O	0.593905	0.238927	0.748841
O	1.260347	-1.572860	1.894539
C	1.219100	0.848968	3.820488
H	0.278715	1.334398	3.538689
H	0.984806	-0.088521	4.335017
C	2.408138	1.926426	1.883230
H	3.003311	1.776103	0.978367
H	1.492253	2.452385	1.605218
C	2.100556	0.593548	2.577538
C	3.405167	-0.104577	2.987684
H	3.204402	-1.055942	3.486962
H	4.035052	-0.305401	2.114476
H	1.746102	1.503774	4.523109
H	2.980814	2.570501	2.559806
H	3.971232	0.533429	3.674834
C	-1.742133	2.042465	0.346762
O	-1.738707	1.751267	1.545550
O	-1.579833	1.186379	-0.632453
C	-2.951272	4.186629	0.783534
H	-3.936280	3.719720	0.672807
H	-2.661999	4.127099	1.835445
C	-2.341137	3.604877	-1.586724
H	-1.597788	3.170646	-2.260661
H	-3.294355	3.093720	-1.757664
C	-1.909631	3.504853	-0.117611
C	-0.531465	4.172203	0.075292
H	-0.223737	4.135322	1.124444
H	0.236793	3.676577	-0.526726
H	-3.044856	5.242659	0.509219
H	-2.470558	4.657733	-1.859736
H	-0.581905	5.222393	-0.232264
C	2.171453	2.340637	-2.343180
C	3.429171	1.968854	-1.918547
C	3.665328	0.644660	-1.479869
C	2.591627	-0.291228	-1.491504
C	1.136432	1.400565	-2.340117
H	5.749484	0.914910	-0.987279
H	1.955443	3.346618	-2.680980
H	4.246112	2.683103	-1.908271
C	4.927439	0.206453	-1.001793
C	2.769696	-1.615733	-1.051395
H	0.123056	1.614736	-2.649802
C	4.011116	-1.997490	-0.587693
C	5.094584	-1.087105	-0.561954
H	4.157581	-3.012886	-0.233968
H	6.060067	-1.415858	-0.191838
N	1.359629	0.147935	-1.940101
O	0.341152	-0.734759	-1.962782
H	1.936157	-2.303889	-1.068501

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^{2}TS2^{IV} Eopt -1324.104816

C	-4.064464	-1.816059	-1.874842
C	-4.230527	-2.165292	-0.549766
C	-3.178430	-1.933850	0.368996
C	-1.976990	-1.366627	-0.108271
C	-2.884085	-1.190767	-2.295655
H	-4.173113	-2.625457	2.159737
H	-4.846875	-1.976436	-2.606380
H	-5.159133	-2.603881	-0.200648
C	-3.255305	-2.201680	1.764935
C	-0.841827	-1.132652	0.720240
H	-2.710321	-0.829141	-3.301313
C	-0.986032	-1.408796	2.080691
C	-2.190535	-1.927254	2.600324
H	-0.135274	-1.271316	2.739957
H	-2.267541	-2.138381	3.661578
Rh	0.212009	0.605433	-0.172909
O	-0.804697	-0.279900	-1.799629
N	-1.898739	-0.978289	-1.419446

C	-0.058711	1.990913	1.514054
C	1.033331	2.508913	0.724154
C	-1.255163	2.025140	0.691619
C	0.520068	2.883024	-0.564214
C	-0.886018	2.565437	-0.587650
C	2.438282	2.663596	1.182363
H	2.580354	3.691750	1.538733
H	2.667067	1.983596	2.003850
H	3.143193	2.490199	0.366869
C	0.016352	1.638852	2.956019
H	0.920697	1.069722	3.182322
H	0.059769	2.572337	3.532165
H	-0.857089	1.075633	3.282586
C	-2.641097	1.704075	1.128523
H	-2.652009	0.983290	1.946315
H	-3.116519	2.627566	1.482232
H	-3.239657	1.317185	0.301724
C	-1.796472	2.774191	-1.740554
H	-2.668895	2.121770	-1.687203
H	-2.146716	3.814490	-1.723741
H	-1.281916	2.611579	-2.689905
C	1.290138	3.478284	-1.684072
H	2.362478	3.315565	-1.567175
H	0.965076	3.076289	-2.646927
H	1.108739	4.561283	-1.702719
H	0.211966	-1.597013	0.291257
C	2.333273	-1.490505	-0.138875
O	2.134525	-0.215563	-0.069258
O	1.403259	-2.330366	-0.068813
C	3.871253	-3.467259	-0.336911
H	3.503388	-3.897471	0.599333
H	3.285950	-3.888944	-1.159123
C	4.607599	-1.366858	0.854877
H	4.581135	-0.274102	0.865246
H	4.230416	-1.733580	1.815713
C	3.786984	-1.936836	-0.318561
C	4.293704	-1.354858	-1.653453
H	3.693625	-1.717739	-2.494916
H	4.261250	-0.261789	-1.647981
H	5.649879	-1.686018	0.756145
H	5.329745	-1.668191	-1.815747
H	4.914419	-3.771369	-0.467172

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^{2}E^{IV} Eopt -1323.700074

C	3.223061	-3.215775	-1.451547
C	3.681552	-2.837851	-0.206638
C	2.894792	-1.986611	0.607807
C	1.637409	-1.553103	0.107161
C	1.979997	-2.761619	-1.914018
H	4.227338	-1.838231	2.305571
H	3.803651	-3.862562	-2.098125
H	4.643038	-3.183554	0.158738
C	3.274368	-1.523301	1.893255
C	0.773859	-0.692533	0.820600
H	1.557034	-3.013124	-2.878360
C	1.194733	-0.250428	2.054628
C	2.440115	-0.677218	2.589800
H	0.597571	0.446841	2.626610
H	2.735815	-0.312967	3.569091
Rh	-0.835844	-0.156609	-0.290728
O	0.041255	-1.530330	-1.581353
N	1.242919	-1.963213	-1.142553
C	-2.241128	-1.179022	1.073721
C	-2.253640	0.230061	1.401174
C	-2.778045	-1.317824	-0.252501
C	-2.785903	0.942562	0.267245
C	-3.172258	-0.015994	-0.725806
C	-1.980282	0.833209	2.735404
H	-2.938706	1.095494	3.201618
H	-1.467464	0.136693	3.398668
H	-1.390163	1.746749	2.644539
C	-1.873660	-2.296266	1.990935
H	-1.144782	-1.976758	2.737053
H	-2.770975	-2.645358	2.516653
H	-1.456867	-3.141863	1.439331
C	-2.960675	-2.596377	-0.995414
H	-2.276138	-3.366751	-0.636454
H	-3.986145	-2.958016	-0.849808
H	-2.804155	-2.458866	-2.067967
C	-3.817368	0.272098	-2.034123
H	-3.468346	-0.414012	-2.810366
H	-4.903996	0.139011	-1.944968
H	-3.632804	1.298625	-2.357035
C	-3.016681	2.413862	0.193735
H	-2.336458	2.955166	0.850714
H	-2.888140	2.785900	-0.825487
H	-4.046892	2.633585	0.501616
C	0.778340	2.364318	-0.100546
O	0.477981	1.344432	-0.858587
O	0.204763	2.636921	0.960798
C	2.121798	4.465886	0.210990
H	1.228158	5.092479	0.124845
H	2.276756	4.244786	1.270757
C	1.789462	3.521296	-2.099692
H	1.712409	2.616941	-2.709254
H	0.883214	4.117762	-2.254812
C	1.979213	3.180227	-0.611709
C	3.228831	2.292308	-0.428272
H	3.353930	1.999097	0.619984
H	3.158511	1.382264	-1.031299
H	2.642703	4.105509	-2.461032
H	4.125420	2.841088	-0.736313
H	2.979699	5.044338	-0.147845

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^{2}TS5^{IV} Eopt -1723.420922

C	-2.023626	2.796689	-0.522489
C	-1.803622	2.689823	0.866390
C	-0.416046	1.368985	-0.107954
H	-3.143900	3.676182	-2.158944
C	-2.994685	3.613390	-1.087068
C	-2.591173	3.428841	1.764960
H	0.618874	1.038286	-0.430087
C	-3.567261	4.250025	1.217859
C	-3.763191	4.341450	-0.180540
H	-4.198112	4.841911	1.873123
H	-4.538424	5.000489	-0.558668
Rh	-0.867447	-0.955438	-0.292509
N	-0.784274	1.790588	1.086580
C	-3.211677	-0.838037	-0.053758
C	-2.961553	-1.555771	-1.267169
C	-2.579624	-1.531181	1.042793
C	-2.135682	-2.681349	-0.941930
C	-1.918734	-2.690986	0.499065
C	-3.444094	-1.161815	-2.617760
H	-4.501053	-1.436091	-2.729791
H	-3.369608	-0.079356	-2.757269
H	-2.879546	-1.660721	-3.407209
C	-4.103558	0.339879	0.080248
H	-4.091023	0.966064	-0.812413
H	-5.130307	-0.029894	0.208456
H	-3.861137	0.943036	0.954866
C	-2.762473	-1.186432	2.479165
H	-2.616850	-0.117769	2.655456
H	-3.791385	-1.432489	2.771053
H	-2.087091	-1.751301	3.121058
C	-1.276015	-3.795126	1.263926
H	-0.949013	-3.461798	2.249111
H	-2.005933	-4.603716	1.396862
H	-0.417394	-4.204584	0.727733
C	-1.647525	-3.716575	-1.890057
H	-1.451544	-3.294120	-2.877544
H	-0.740109	-4.197849	-1.521987
H	-2.420442	-4.488424	-1.998819
H	-2.433639	3.355778	2.835819
C	2.599358	2.229635	-0.772451
O	1.838431	3.223337	-0.854877
O	2.216702	1.012032	-0.897830
C	4.495875	3.908033	-0.622175
H	4.351641	4.228946	-1.659637
H	3.894528	4.564008	0.013492

C	4.966378	1.541333	-1.332998
H	4.708947	0.487393	-1.203284
H	4.834216	1.793631	-2.391741
C	4.097953	2.439096	-0.436752
C	4.280311	2.028620	1.039036
H	3.657673	2.646456	1.696512
H	3.999246	0.982659	1.192106
H	6.027688	1.668140	-1.088637
H	5.551720	4.054028	-0.366025
H	5.325041	2.152852	1.347905
O	-1.152489	1.954152	-1.142956
C	4.094120	-2.411670	-0.925121
C	4.185373	-2.210246	0.437075
C	3.045250	-1.794631	1.167236
C	1.829443	-1.609825	0.458810
C	2.876171	-2.206467	-1.588726
H	3.940968	-1.652563	3.131415
H	4.951013	-2.719395	-1.511868
H	5.125583	-2.359289	0.957776
C	3.028779	-1.520728	2.558975
C	0.635457	-1.169642	1.068039
H	2.731115	-2.330585	-2.654321
C	0.669922	-0.897029	2.416417
C	1.869233	-1.079526	3.157419
H	-0.204955	-0.519990	2.929912
H	1.861488	-0.855529	4.219823
O	0.633438	-1.618420	-1.527486
N	1.807086	-1.832167	-0.890710

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^{2}H^{IV} Eopt -1376.411630

Rh	0.347579	-0.962783	-0.251526
C	1.405031	-2.931510	0.050331
C	0.047996	-3.147472	-0.355866
C	-0.019883	-2.045633	1.696644
C	1.364278	-2.163330	1.267505
C	-0.826964	-2.635728	0.687512
C	2.637456	-3.395549	-0.657798
H	3.465332	-2.693965	-0.521207
H	2.965979	-4.369347	-0.269503
H	2.465057	-3.512087	-1.731002
C	2.542455	-1.746090	2.092439
H	2.384326	-0.764681	2.548576
H	2.706739	-2.464064	2.906461
H	3.458185	-1.702670	1.499401
C	-0.490248	-1.435159	2.977643
H	-1.501953	-1.031034	2.881330
H	-0.507705	-2.181654	3.783417
H	0.170571	-0.625172	3.298379
C	-2.317797	-2.745132	0.703012
H	-2.725681	-2.824910	-0.306950
H	-2.628869	-3.644666	1.250377
H	-2.781395	-1.884669	1.193686
C	-0.409457	-3.880892	-1.577817
H	-0.591857	-4.940244	-1.354923
H	-1.342793	-3.461862	-1.964207
H	0.337183	-3.832223	-2.374761
N	-2.087882	0.345677	-1.209485
O	-0.884264	0.053836	-1.706400
C	-1.153978	2.230565	0.119140
C	-1.460056	3.316474	0.940691
H	-0.648727	3.950230	1.278239
C	-2.766357	3.600813	1.370525
H	-2.940431	4.452490	2.018766
C	-3.803428	2.792307	0.976133
H	-4.821765	2.983758	1.297718
C	-3.567016	1.689370	0.118386
C	-2.237093	1.405477	-0.323002
C	-4.649429	0.889667	-0.322978
H	-5.648084	1.120932	0.031650
C	-4.425445	-0.147063	-1.195777
H	-5.225761	-0.777369	-1.563752
C	-3.121943	-0.392460	-1.629267
H	-2.856113	-1.177995	-2.323814
C	2.319846	2.858387	-0.314374
C	2.365516	1.463312	-0.266402
C	3.581497	0.785310	-0.348431
C	4.727331	1.571891	-0.459114
C	4.660402	2.978636	-0.495865
C	3.442733	3.661344	-0.430220
C	0.278119	2.066809	-0.153440
H	3.621144	-0.297656	-0.334218
H	5.697555	1.089654	-0.523054
H	5.579366	3.549437	-0.582369
H	3.377495	4.742598	-0.466978
N	1.049849	1.005286	-0.156096
O	0.993764	3.233613	-0.244999

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^{2}TS8^{IV} Eopt -1376.788761

Rh	1.122928	-0.184418	0.081950
C	3.069298	-0.943695	-0.687244
C	3.038196	-1.151797	0.736323
C	2.831981	1.143944	0.325002
C	2.932280	0.464217	-0.949834
C	2.877796	0.140052	1.358113
C	3.233194	-2.003027	-1.720371
H	2.763342	-2.940098	-1.414121
H	2.816590	-1.691522	-2.679870
H	4.303846	-2.195842	-1.865200
C	2.991879	1.093297	-2.301495
H	2.646341	2.127194	-2.281134
H	4.028290	1.093179	-2.660398
H	2.392732	0.536115	-3.027107
C	2.778824	2.616575	0.550555
H	2.137955	2.866405	1.398990
H	3.789235	2.981410	0.773748
H	2.413975	3.147411	-0.329327
C	2.799030	0.386181	2.825316
H	2.261063	-0.418135	3.332747
H	3.813755	0.423985	3.240734
H	2.307127	1.334850	3.047323
C	3.169585	-2.452510	1.449782
H	4.210836	-2.600916	1.763989
H	2.547283	-2.475173	2.348010
H	2.890023	-3.289456	0.806738
N	-1.413003	0.189100	1.416781
O	-0.306058	-0.544807	1.575382
C	-0.379672	1.229532	-0.517141
C	-0.297371	2.416499	-1.264468
H	0.458424	2.497193	-2.038306
C	-1.250990	3.441590	-1.143010
H	-1.149028	4.337431	-1.745887
C	-2.365671	3.265807	-0.345960
H	-3.159798	4.005424	-0.330405
C	-2.490838	2.117788	0.485140
C	-1.435738	1.172797	0.455971
C	-3.580361	1.901324	1.357112
H	-4.402833	2.608400	1.373645
C	-3.571874	0.798629	2.192544
H	-4.395030	0.589184	2.864619
C	-2.454884	-0.035025	2.234607
H	-2.332609	-0.856336	2.928652
C	-2.565540	-1.016825	-1.425668
C	-1.529068	-1.789660	-0.834387
C	-1.843046	-2.876731	0.003667
C	-3.186288	-3.132938	0.214544
C	-4.200979	-2.344485	-0.387447
C	-3.910553	-1.264605	-1.224765
C	-0.631868	-0.082011	-1.860428
H	-1.058619	-3.461509	0.470099
H	-3.480449	-3.954729	0.858504
H	-5.239210	-2.587486	-0.186703
H	-4.682146	-0.656546	-1.681538
N	-0.329087	-1.259227	-1.200824
O	-1.992843	-0.014537	-2.158909
H	0.009046	0.274454	-2.657800

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