

Electronic Supplementary Information

Rhodium-Catalyzed Annulative Approach to N-N Axially Chiral Biaryls via C-H Activation and Dynamic Kinetic Transformation

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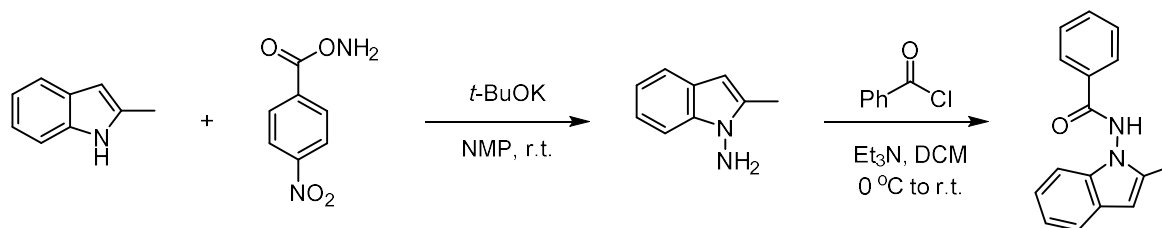
1. General Information:

Commercially available chemicals were obtained from Adamas, Acros Organics, Aldrich Chemical Co., Alfa Aesar, and TCI and used as received unless otherwise noted. All air- and moisture-sensitive manipulations were carried out with standard Schlenk techniques under nitrogen or in a glove box under argon. The ^1H NMR spectra were recorded on 400 MHz or 600 MHz NMR spectrometer. The ^{13}C NMR spectra were recorded at 100 MHz or 150 MHz. The ^{19}F NMR spectra were recorded at 376 MHz. The ^{31}P NMR spectra were recorded at 243 MHz. Chemical shifts were expressed in parts per million (δ) downfield from the internal standard tetramethylsilane (TMS), and were reported as s (singlet), d (doublet), t (triplet), dd (doublets of doublet), and m (multiplet). The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale (CDCl_3 : $\delta \text{H} = 7.26 \text{ ppm}$, $\delta \text{C} = 77.16 \text{ ppm}$). The coupling constants J were given in Hz. High resolution mass spectra (HRMS) were obtained via ESI mode by using a MicroTOF mass spectrometer. Column chromatography was performed on silica gel 200-300 mesh. The enantiomeric excess (ee) of the products were determined by high-performance liquid chromatography (HPLC) with a chiral stationary phase in comparison with the authentic racemate sample with n -hexane and i -PrOH as solvents. All the chiral stationary phases including Chiralcel IE, IC, OZ-H, OD-3, IJ-3 used in this study were purchased from Daicel Chiral Technologies. Optical rotations were reported as follows: $[\alpha]_{\text{D}}^{\text{T}} = (c$: g/100mL, in CHCl_3).

Chiral rhodium catalysts,^[1] and alkynes,^[2] were prepared according to published procedures.

2. General Procedure for the Preparation of Unpublished Substrates

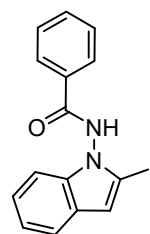
2.1 The 2-methyl substituted *N*-indol benzamides was obtained from the following step.



To a solution of 2-methyl indole (25.0 mmol) in 60 mL *N*-methylpyrrolidone (NMP) were added 30 mL *t*-BuOK (1M in THF) and the reaction mixture was stirred at r.t. for 0.5 h. Then, a solution of *O*-(4-Nitrobenzoyl)hydroxylamine (5.46 g, 30.0 mmol) was added to the mixture, which was stirred at r.t. for 12 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with saturated brine and the aqueous layer was extracted with EtOAc (3×30 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and then concentrated under reduced pressure. The residue was purified by flash column chromatography (silica gel, petroleum ether/dichloromethane 5/1 to 2/1) to afford the aminoindole.^[3]

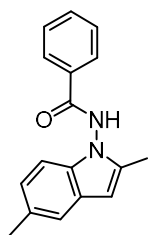
To a stirring solution of aminoindole (4.0 mmol), Et₃N (1.12 mL, 8.0 mmol) in CH₂Cl₂ (20 mL) were added benzoyl chloride (0.84 g, 6.0 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 10 minutes. Then, the reaction mixture was stirred at room temperature for 12 h. After the completion of the reaction, the reaction mixture was washed with saturated NaHCO₃ solution, saturated brine, and dried over Na₂SO₄. The solvent was concentrated and the residue was purified by silica gel flash chromatography to afford the desired 2-methyl substituted *N*-indol benzamides.

2.2 Characterization of unreported 2-methyl substituted *N*-indol benzamides is listed below.



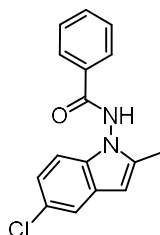
N-(2-methyl-1H-indol-1-yl)benzamide (3a)

The title compound was isolated as a white solid. ¹H NMR (600 MHz, CDCl₃) δ 8.33 (s, 1H), 7.78 (d, *J* = 7.4 Hz, 2H), 7.62 – 7.57 (m, 1H), 7.55 – 7.51 (m, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.16 – 7.07 (m, 3H), 6.28 (s, 1H), 2.23 (s, 3H). ¹³C NMR (150 MHz, CDCl₃) δ 166.8, 137.4, 136.5, 132.9, 131.6, 129.0, 127.6, 126.5, 121.8, 120.8, 120.2, 108.3, 99.6, 11.6. HRMS (ESI): calcd. for C₁₆H₁₄N₂NaO⁺ [M+Na]⁺ : 273.0998, found : 273.0992.



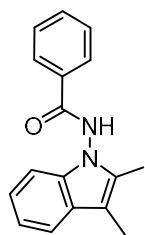
***N*-(2,5-dimethyl-1H-indol-1-yl)benzamide (4a)**

The title compound was isolated as a white solid. ¹H NMR (600 MHz, CDCl₃) δ 8.19 (s, 1H), 7.75 (d, *J* = 7.4 Hz, 2H), 7.62 – 7.56 (m, 1H), 7.45 (d, *J* = 7.5 Hz, 2H), 7.31 (s, 1H), 6.95 (s, 2H), 6.19 (s, 1H), 2.42 (s, 3H), 2.18 (s, 3H). ¹³C NMR (150 MHz, CDCl₃) δ 166.8, 137.5, 134.8, 132.7, 131.7, 130.0, 129.0, 127.6, 126.7, 123.2, 120.1, 108.0, 99.1, 21.6, 11.5. **HRMS (ESI):** calcd. for C₁₇H₁₆N₂NaO⁺ [M+Na]⁺ : 287.1155, found : 287.1145.



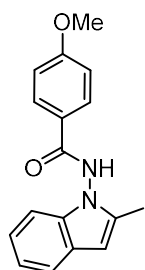
***N*-(5-chloro-2-methyl-1H-indol-1-yl)benzamide (5a)**

The title compound was isolated as a white solid. ¹H NMR (600 MHz, CDCl₃) δ 8.68 (s, 1H), 7.75 (d, *J* = 7.5 Hz, 2H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 2.0 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.05 (dd, *J* = 8.6, 1.9 Hz, 1H), 6.97 (d, *J* = 8.5 Hz, 1H), 6.18 (s, 1H), 2.18 (s, 3H). ¹³C NMR (150 MHz, CDCl₃) δ 166.9, 138.8, 134.9, 133.1, 131.2, 130.3, 129.1, 128.6, 127.51, 127.48, 126.3, 121.9, 119.7, 109.3, 99.3, 11.6. **HRMS (ESI):** calcd. for C₁₆H₁₃ClN₂NaO⁺ [M+Na]⁺ : 307.0609, found : 307.0598.



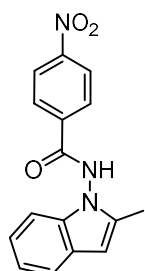
***N*-(2,3-dimethyl-1H-indol-1-yl)benzamide (6a)**

The title compound was isolated as a white solid. ¹H NMR (600 MHz, CDCl₃) δ 8.26 (s, 1H), 7.87 – 7.81 (m, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.53 – 7.46 (m, 3H), 7.18 – 7.09 (m, 3H), 2.24 (s, 3H), 2.19 (s, 3H). ¹³C NMR (150 MHz, CDCl₃) δ 167.0, 136.0, 133.0, 132.8, 131.8, 129.0, 127.6, 127.3, 121.8, 120.3, 118.4, 108.0, 106.7, 9.3, 9.0. **HRMS (ESI):** calcd. for C₁₇H₁₆N₂NaO⁺ [M+Na]⁺ : 287.1155, found : 287.1144.



4-methoxy-*N*-(2-methyl-1H-indol-1-yl)benzamide (7a)

The title compound was isolated as a white solid. ¹H NMR (600 MHz, CDCl₃) δ 8.38 (s, 1H), 7.76 (d, *J* = 8.3 Hz, 2H), 7.55 – 7.50 (m, 1H), 7.16 – 7.08 (m, 3H), 6.89 (d, *J* = 8.3 Hz, 2H), 6.28 (s, 1H), 3.88 (s, 3H), 2.25 (s, 3H). ¹³C NMR (150 MHz, CDCl₃) δ 166.3, 163.3, 137.5, 136.6, 129.5, 126.5, 123.7, 121.7, 120.7, 120.2, 114.2, 108.3, 99.5, 55.7, 11.6. **HRMS (ESI):** calcd. for C₁₇H₁₆N₂NaO₂⁺ [M+Na]⁺ : 303.1104, found : 303.1093.

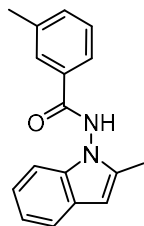


***N*-(2-methyl-1H-indol-1-yl)-4-nitrobenzamide (8a)**

The title compound was isolated as a white solid. ¹H NMR (600 MHz, CDCl₃) δ 8.79 (s, 1H), 8.13 (d, *J* = 7.9 Hz, 2H), 7.78 (d, *J* = 7.8 Hz, 2H), 7.57 – 7.49 (m, 1H), 7.17 – 7.10 (m, 2H), 7.07 (d, *J* = 7.3 Hz, 1H), 6.30 (s, 1H), 2.23 (s, 3H). ¹³C NMR (150 MHz, CDCl₃)

δ 165.3, 150.4, 136.9, 136.7, 136.3, 128.7, 126.6, 124.2, 122.1, 121.2, 120.5, 108.1, 100.2, 11.6.

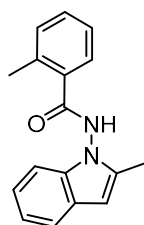
HRMS (ESI): calcd. for $C_{16}H_{13}N_3NaO_3^+$ $[M+Na]^+$: 318.0849, found : 318.0838.



3-methyl-N-(2-methyl-1H-indol-1-yl)benzamide (9a)

The title compound was isolated as a white solid. 1H NMR (600 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.70 (s, 1H), 7.64 (d, J = 7.6 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.43 (d, J = 7.7 Hz, 1H), 7.38 (t, J = 7.6 Hz, 1H), 7.17 – 7.10 (m, 3H), 6.29 (s, 1H), 2.45 (s, 3H), 2.28 (s, 3H). ^{13}C

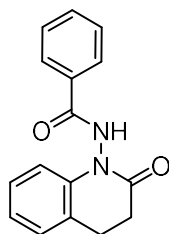
NMR (150 MHz, $CDCl_3$) δ 167.2, 138.8, 137.4, 136.3, 133.5, 131.4, 128.7, 128.3, 126.3, 124.5, 121.5, 120.6, 120.0, 108.4, 99.3, 21.4, 11.4. **HRMS (ESI):** calcd. for $C_{17}H_{16}N_2NaO^+$ $[M+Na]^+$: 287.1155, found : 287.1145.



2-methyl-N-(2-methyl-1H-indol-1-yl)benzamide (10a)

The title compound was isolated as a white solid. 1H NMR (600 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.44 – 7.36 (m, 2H), 7.34 (d, J = 7.5 Hz, 1H), 7.28 – 7.18 (m, 2H), 7.08 (t, J = 7.5 Hz, 1H), 7.01 (t, J = 7.4 Hz, 1H), 6.97 (d, J = 8.0 Hz, 1H), 6.17 (s, 1H), 2.38 (s, 3H), 2.15

(s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.0, 137.22, 137.19, 136.2, 132.8, 131.4, 131.1, 127.2, 126.3, 125.9, 121.6, 120.7, 120.1, 108.2, 99.4, 19.9, 11.5. **HRMS (ESI):** calcd. for $C_{17}H_{16}N_2NaO^+$ $[M+Na]^+$: 287.1155, found : 287.1143.



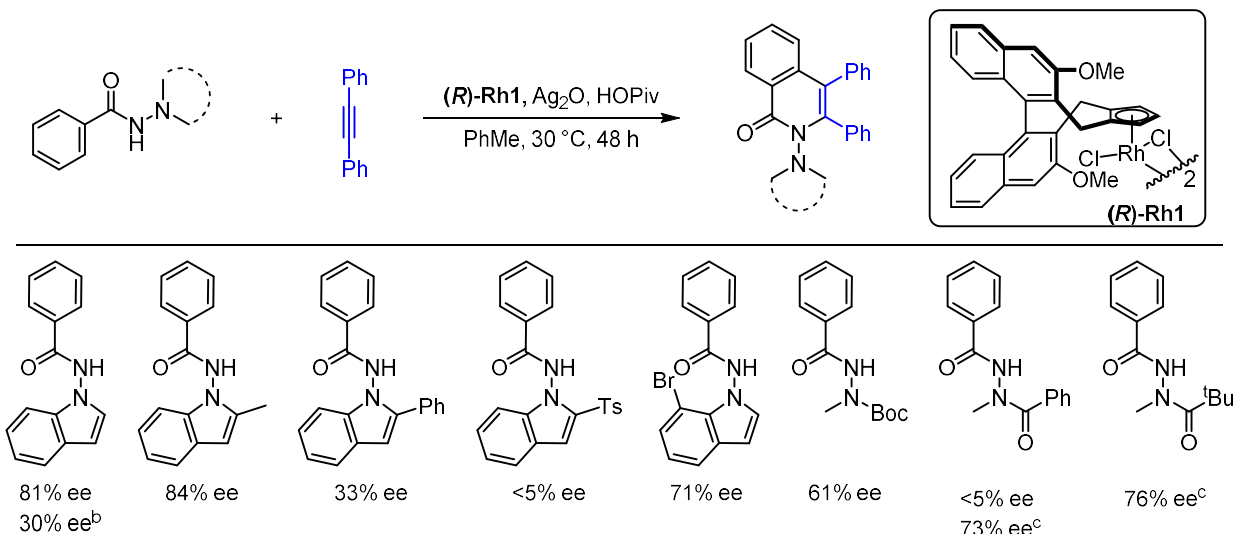
N-(2-oxo-3,4-dihydroquinolin-1(2H)-yl)benzamide (21a)

The title compound was isolated as a white solid. 1H NMR (600 MHz, $CDCl_3$) δ 9.29 (s, 1H), 7.88 (d, J = 7.3 Hz, 2H), 7.48 (t, J = 7.4 Hz, 1H), 7.35 (t, J = 7.4 Hz, 2H), 7.18 (q, J = 8.0 Hz, 2H), 7.12 – 7.08 (m, 1H), 7.05 – 7.00 (m, 1H), 3.06 (d, J = 11.0 Hz, 1H),

2.95 – 2.76 (m, 2H), 2.67 (d, J = 11.3 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.4, 166.6, 139.7, 132.5, 131.4, 128.8, 128.7, 127.9, 127.79, 127.77, 125.0, 123.9, 114.20, 114.17, 31.5, 25.0. **HRMS (ESI):** calcd. for $C_{16}H_{14}N_2NaO_2^+$ $[M+Na]^+$: 289.0947, found : 289.0937.

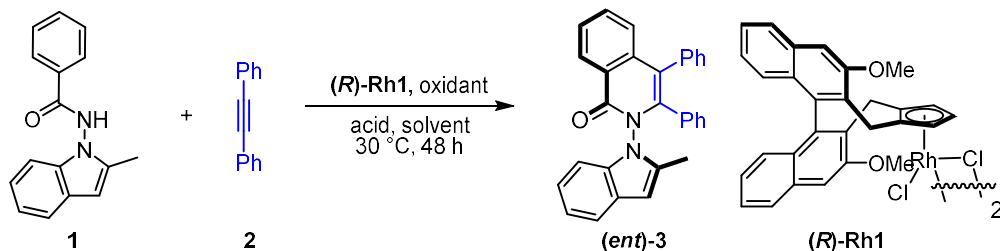
3. Experimental Section

3.1 Tables of the Optimization Studies on NH Amide Directing Groups.



[a] Reaction conditions: arene (0.1 mmol), alkyne (0.15 mmol), **(R)-Rh1** (3 mol%), Ag_2O (2.0 equiv) and HOPiv (2.0 equiv) in toluene (2 mL), 30 °C, 24 h. The ee was determined by HPLC analysis using a chiral stationary phase. [b] Ag_2O (1.0 equiv), Ag_2CO_3 (0.5 equiv) and MesCOOH (2.0 equiv), 60 °C, 48 h. [c] TFE.

3.2 Tables of the Optimization of Reaction Conditions of synthesis of (*ent*)-3.

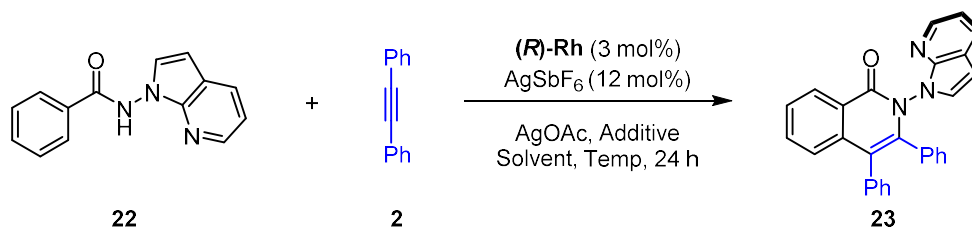


Entry	Oxidant	Additive	Acid	Solvent	yield [%]	ee [%]
1	Ag_2CO_3	-	HOPiv	MeOH	20	88
2	Ag_2O	-	HOPiv	MeOH	32	88
3	Ag_2O	-	HOPiv	DCE	34	72
4	Ag_2O	-	HOPiv	PhMe	49	84
5	Ag_2O	-	MesCOOH	PhMe	55	88
6	Ag_2CO_3	-	MesCOOH	PhMe	39	98
7	Ag_2O (2.0 eq)	Ag_2CO_3 (0.5 eq)	MesCOOH	PhMe	52	89
8	Ag_2O (1.0 eq)	Ag_2CO_3 (0.5 eq)	MesCOOH	PhMe	56	95
9	Ag_2O (1.0 eq)	Ag_2CO_3 (1.0 eq)	MesCOOH	PhMe	51	95

10	Ag ₂ O (1.0 eq)	Ag ₂ CO ₃ (0.5 eq)	MesCOOH	PhMe	60	94 (40 °C)
11	Ag ₂ O (1.2 eq)	Ag ₂ CO ₃ (0.6 eq)	MesCOOH	PhMe	58	92 (40 °C)
12	Ag ₂ O (1.4 eq)	Ag ₂ CO ₃ (0.7 eq)	MesCOOH	PhMe	62	92 (60 °C)
13	Ag ₂ O (1.0 eq)	Ag ₂ CO ₃ (0.5 eq)	MesCOOH	PhMe	70	94 (60 °C)

[a] Reaction conditions: **1** (0.1 mmol), **2** (0.15 mmol), (*R*)-**Rh1** (3 mol%), Oxidant (1.0 equiv), Additive (0.5 equiv) and Acid (2.0 equiv) in solvent (2 mL), 30 °C, 48 h. The ee was determined by HPLC analysis using a chiral stationary phase.

3.3 Tables of the Optimization of Reaction Conditions of synthesis of **23**.

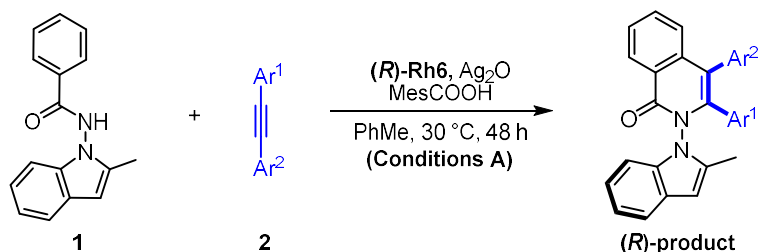


Entry	Rh cat.	Additive	Solvent	Temp (°C)	yield [%]	ee [%]
1	(<i>R</i>)-Rh1	PivOH	EtOH	40	60	80
2	(<i>R</i>)-Rh2	PivOH	EtOH	40	35	53
3	(<i>R</i>)-Rh5	PivOH	EtOH	40	12	8
4	(<i>R</i>)-Rh6	PivOH	EtOH	40	42	-62
5	(<i>R</i>)-Rh1	AcOH	EtOH	40	60	88
6	(<i>R</i>)-Rh1	1-AdCOOH	EtOH	40	trace	-
7	(<i>R</i>)-Rh1	PhCOOH	EtOH	40	55	80
8	(<i>R</i>)-Rh1	MesCOOH	EtOH	40	39	85
9	(<i>R</i>)-Rh1	4-CF ₃ -PhCOOH	EtOH	40	62	84
10	(<i>R</i>)-Rh1	NaOAc	EtOH	40	68	68
11	(<i>R</i>)-Rh1	NaOPiv	EtOH	40	65	77
12	(<i>R</i>)-Rh1	Zn(OAc) ₂	EtOH	40	23	68
13	(<i>R</i>)-Rh1	AcOH	THF	40	trace	-
14	(<i>R</i>)-Rh1	AcOH	EA	40	44	91
15	(<i>R</i>)-Rh1	AcOH	PhCl	40	57	90
16	(<i>R</i>)-Rh1	AcOH	DCM	40	89	90
17	(<i>R</i>)-Rh1	AcOH	DCE	40	87	92
18	(<i>R</i>)-Rh1	AcOH	DCE	25	87	94
19	(<i>R</i>)-Rh1	AcOH	DCE	10	56	94

[a]Reaction conditions: **22** (0.05 mmol), **2** (0.05 mmol), (*R*)-**Rh** (3 mol%), AgSbF₆ (12 mol%), oxidant (2 equiv) and additive (1 equiv) in solvent (1 mL), 24 h. Isolated yield. The ee was determined by HPLC analysis using a chiral stationary phase.

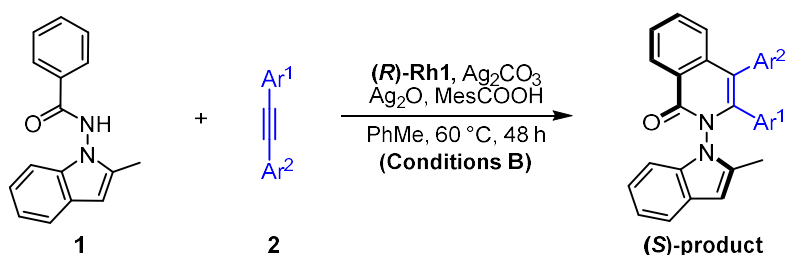
3.4 Typical General Procedure for the Asymmetric Catalysis

General procedure for the synthesis of 3-14 and 21.



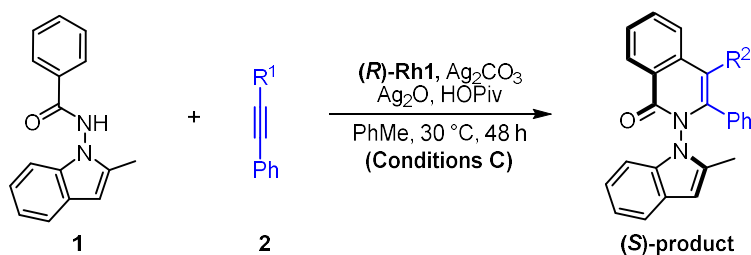
Conditions A: A scew-cap vial (8 mL) was charged with *N*-indol benzamides **1** (0.1 mmol), alkynes **2** (0.15 mmol), (*R*)-**Rh6** (3 mol%), Ag₂O (1.5 equiv), and MesCOOH (1.2 equiv) in toluene (2 mL) and the mixture was stirred at 30 °C for 48 h. The reaction mixture was evaporated under vacuum and the residue was purified by preparative TLC to give the corresponding product.

General procedure for the synthesis of (ent)-3 and (ent)-15.



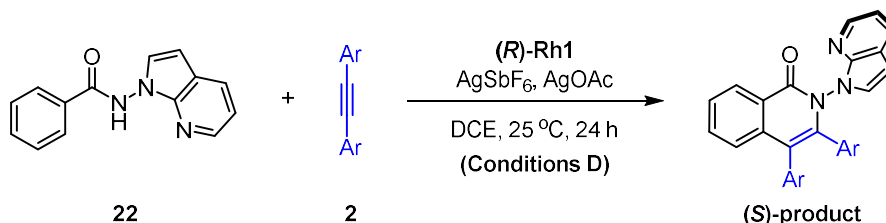
Conditions B: A scew-cap vial (8 mL) was charged with *N*-indol benzamides **1** (0.1 mmol), alkynes **2** (0.15 mmol), (*R*)-**Rh1** (3 mol%), Ag₂O (1.0 equiv), Ag₂CO₃ (0.5 equiv) and MesCOOH (2.0 equiv) in toluene (2 mL) and the mixture was stirred at 60 °C for 48 h. The reaction mixture was evaporated under vacuum and the residue was purified by preparative TLC to give the corresponding product.

General procedure for the synthesis of (ent)-16-19.



Conditions C: A scew-cap vial (8 mL) was charged with *N*-indol benzamides **1** (0.1 mmol), alkynes **2** (0.15 mmol), (*R*)-**Rh1** (3 mol%), Ag₂CO₃(1.0 equiv), Ag₂O (0.5 equiv) and HOPiv (2.0 equiv) in toluene (2 mL) and the mixture was stirred at 30 °C for 48 h. The reaction mixture was evaporated under vacuum and the residue was purified by preparative TLC to give the corresponding product.

General procedure for the synthesis of 23-39.



Conditions D: A scew-cap vial (8 mL) was charged with *N*-(7-azaindol-1-yl)benzamide **22** (0.1 mmol), **2** (0.1 mmol), (*R*)-**Rh1** (3 mol%), AgSbF₆ (12 mol%), AgOAc (2.0 equiv) and HOAc (1.0 equiv). in DCE (1 mL) and the mixture was stirred at 25 °C for 24 h. The reaction mixture was evaporated under vacuum and the residue was purified by preparative TLC to give the corresponding product.

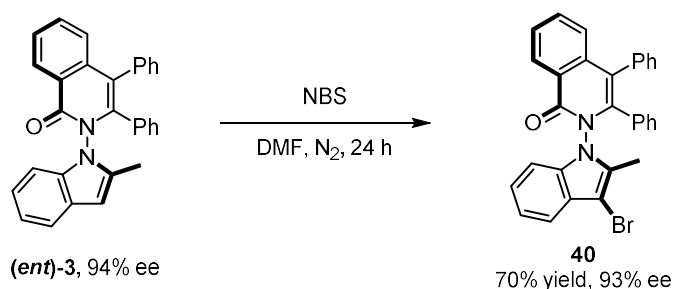
General procedure for the synthesis of racemic product 3-21.

A similar synthetic procedure was followed for synthesis of racemic products except that [Cp*RhCl₂]₂ (4 mol %) was used at 80 °C for 24 h.

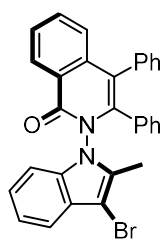
General procedure for the synthesis of racemic product 23-39.

A similar synthetic procedure was followed for synthesis of racemic products except that racemic Rh-**1** (3 mol %) was used.

3.5 Transformations and application



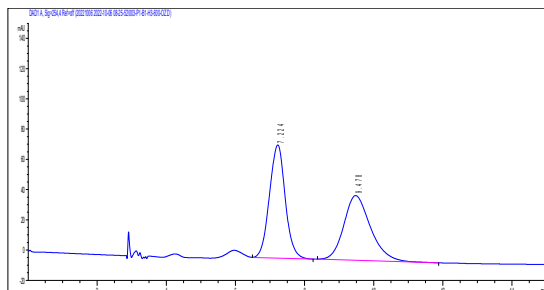
To a stirring solution of **(ent)-3** (0.1 mmol, 94% ee) in DMF (2 mL) was added NBS (2.2 equiv) under N₂ atmosphere. The resulting mixture was allowed to stir at 25 °C for 24 h. The reaction was quenched by the addition of water and the mixture was extracted with EtOAc. The organic phase was separated, washed with water and brine, dried over anhydrous Na₂SO₄, filtered and concentrated. The residue was purified by a silica gel chromatography to give compound **40** (35.3 mg, 70%, 93% ee) as a solid.^[4]



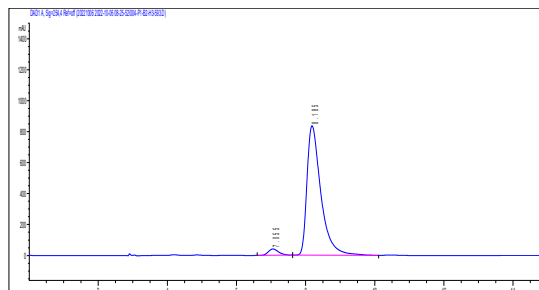
(R)-2-(3-bromo-2-methyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (40)

¹H NMR (600 MHz, CDCl₃) δ 8.52 (dd, J = 8.0, 1.4 Hz, 1H), 7.71 – 7.65 (m, 1H), 7.61 – 7.56 (m, 1H), 7.40 – 7.33 (m, 2H), 7.31 – 7.27 (m, 1H), 7.25 (d, J = 7.6 Hz, 1H), 7.23 – 7.17 (m, 3H), 7.16 – 7.10 (m, 3H), 7.05 – 6.89 (m, 4H), 6.77 (t, J = 7.6 Hz, 1H), 2.24 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 160.9, 142.5, 137.6, 136.3, 135.6, 134.5, 133.6, 131.9, 131.6, 131.5, 129.8, 129.7, 128.9, 128.6, 128.5, 128.2, 127.7, 127.5, 127.42, 127.38, 126.3, 126.0, 125.5, 123.3, 121.5, 120.1, 119.0, 109.0, 91.1, 11.0. **HRMS (ESI)**: calcd. for C₃₀H₂₁BrN₂NaO⁺ [M+Na]⁺ : 527.0729, found : 527.0722. **[α]_D²⁰** = -36 (c = 0.1, CHCl₃).

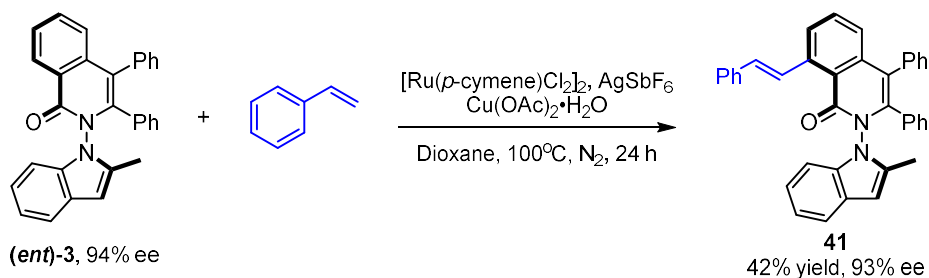
HPLC analysis: Daicel Chiralpak OZ-H column (hexane: 2-propanol = 95:5, v = 1.0 mL/min, 40 °C, 254 nm). tr (minor) = 7.055 min, tr (major) = 8.185 min, 93% ee.



No.	Time	Area	Area (%)
1	7.224	2377.9	50.90
2	9.478	2293.7	49.10

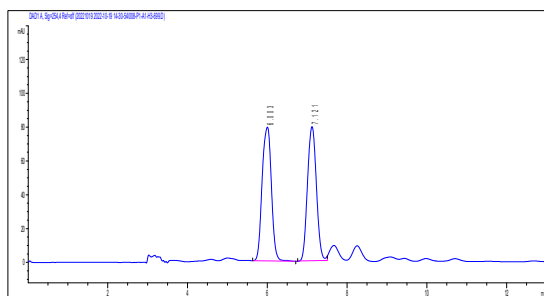


No.	Time	Area	Area (%)
1	7.055	841.8	3.48
2	8.185	23377.3	96.52

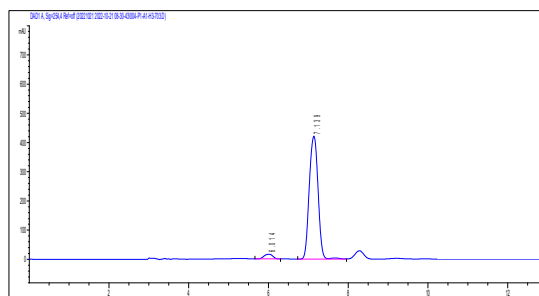


Under N₂ atmosphere, **(ent)-3** (0.1 mmol, 94% ee), styrene (0.15 mmol), [Ru(*p*-cymene)Cl₂]₂ (5 mol%), AgSbF₆ (20 mol%), Cu(OAc)₂·H₂O (2.2 equiv) in 1,4-dioxane (2 mL) were charged into a Schlenk. The mixture was stirred at 100 °C for 24 h, The reaction mixture was washed with saturated NaHCO₃ solution and was extracted with CH₂Cl₂ (three times) and the combined organic layers were dried over anhydrous Na₂SO₄. The residue was purified by a silica gel chromatography to give compound **41** (22.2 mg, 42%, 93% ee) as a solid.^[5]

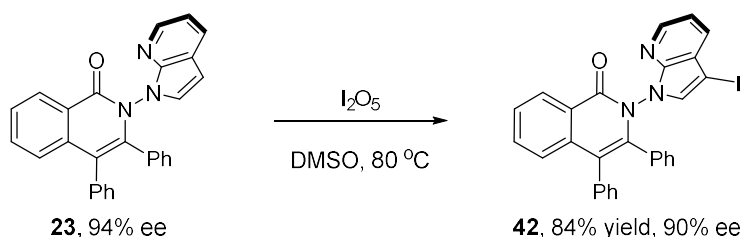
(S, E)-2-(2-methyl-1H-indol-1-yl)-3,4-diphenyl-8-styrylisoquinolin-1(2H)-one (41) ¹H NMR (600 MHz, CDCl₃) δ 8.62 (d, *J* = 16.1 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.28 (t, *J* = 7.7 Hz, 3H), 7.26 – 7.23 (m, 2H), 7.22 – 7.17 (m, 3H), 7.16 – 7.11 (m, 3H), 7.06 – 6.99 (m, 3H), 6.99 – 6.94 (m, 2H), 6.93 – 6.89 (m, 1H), 6.75 (t, *J* = 7.6 Hz, 1H), 6.16 – 6.09 (m, 1H), 2.26 (s, 3H). ¹³C NMR (150 MHz, CDCl₃) δ 161.3, 142.9, 142.3, 139.2, 137.7, 136.7, 136.5, 136.4, 132.7, 132.2, 131.9, 131.8, 131.7, 130.2, 129.7, 129.6, 128.6, 128.5, 128.4, 128.2, 127.8, 127.4, 127.3, 127.2, 127.0, 126.4, 126.0, 122.5, 121.9, 120.7, 120.3, 119.6, 108.9, 100.2, 12.2. **HRMS (ESI)**: calcd. for C₃₈H₂₈N₂NaO⁺ [M+Na]⁺ : 551.2094, found : 551.2091. [*α*]_D²⁰ = -53 (c = 0.1, CHCl₃). **HPLC analysis**: Daicel Chiralpak IE column (hexane: 2-propanol = 85:15, v = 1.0 mL/min, 40 °C, 254 nm). tr (minor) = 6.014 min, tr (major) = 7.139 min, 93% ee.



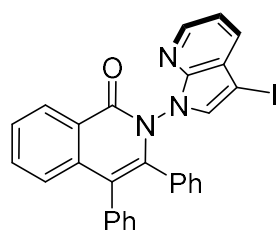
No.	Time	Area	Area (%)
1	6.003	1278.4	50.89
2	7.121	1233.5	49.11



No.	Time	Area	Area (%)
1	6.014	246.1	3.67
2	7.139	6466.5	96.33



A screw-cap vial (8 mL) was charged with **26** (41.3 mg, 0.1 mmol, 1.0 equiv), in DMSO (1.0 mL), then I_2O_5 (40.1 mg, 0.12 mmol, 1.2 equiv) was added slowly. The reaction was allowed to warm to 80 °C and stirred for 12 h. After the reaction was complete (monitored by TLC). Then the residue was purified by silica gel column chromatography (PE/EA = 2:1) to afford the desired product **42** (45.3 mg, 84%, 90% ee) as a white solid.

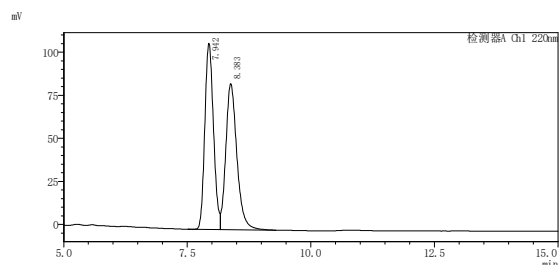


(S)-2-(3-iodo-1H-pyrrolo[2,3-b]pyridin-1-yl)-3,4-diphenylisoquinolin-

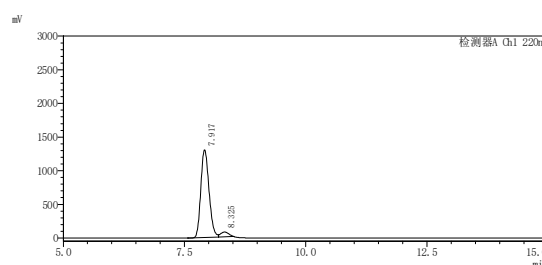
1(2H)-one (42) 1H NMR (600 MHz, $CDCl_3$) δ 8.51 (dd, J = 8.0, 1.5 Hz, 1H), 8.32 (dd, J = 4.8, 1.5 Hz, 1H), 7.62 (ddd, J = 8.5, 7.1, 1.5 Hz, 1H), 7.58 (dd, J = 7.9, 1.5 Hz, 1H), 7.55 – 7.50 (m, 1H), 7.31 – 7.22 (m, 3H), 7.22 – 7.15 (m,

4H), 7.12 (dd, J = 7.9, 4.8 Hz, 1H), 7.10 – 7.05 (m, 2H), 7.01 – 6.95 (m, 1H), 6.93 – 6.88 (m, 1H), 6.71 (td, J = 7.6, 1.7 Hz, 1H). **^{13}C NMR (150 MHz, $CDCl_3$)** δ 160.9, 146.6, 145.2, 141.9, 137.8, 135.4, 133.4, 132.8, 131.9, 131.5, 131.3, 129.9, 129.7, 128.6, 128.3, 128.2, 128.0, 127.4, 127.2, 127.1, 127.0, 126.1, 125.2, 121.5, 119.5, 117.9. **HRMS (ESI-TOF) (m/z):** Calcd for $C_{28}H_{19}IN_3O^+$, ($[M + H]^+$), 540.0567, found 540.0560. **$[\alpha]_D^{20}$** = -16 (c = 0.1, $CHCl_3$).

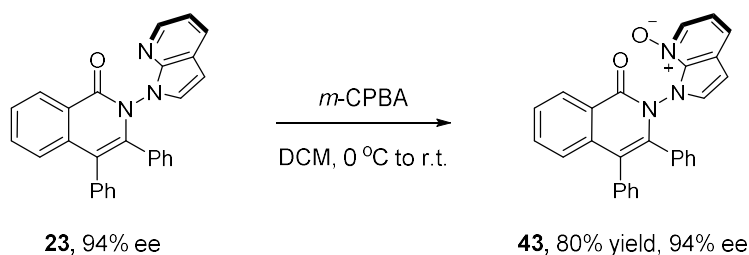
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 7.917 min, tr (minor) = 8.325 min, 90% ee.



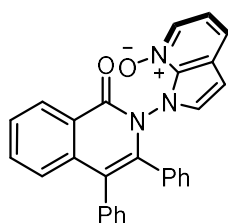
No.	Time	Area	Area (%)
1	7.942	1315814	49.73
2	8.383	1330267	50.27



No.	Time	Area	Area (%)
1	7.917	15265906	94.92
2	8.325	816691	5.08



A screw-cap vial (8 mL) was charged with **23** (41.3 mg, 0.1 mmol, 1.0 equiv), in DCM (1.0 mL). The resulted mixture was stirred at 0 °C, then *m*-CPBA (20.6 mg, 0.12 mmol, 1.2 equiv) was added slowly. The reaction was allowed to warm to room temperature and stirred for 12 h. After the reaction was complete (monitored by TLC), the solvent was removed under reduced pressure. Then the residue was purified by silica gel column chromatography (PE/EA = 1:1) to afford the desired product **43** (34.3 mg, 80%, 94% ee) as a white solid.

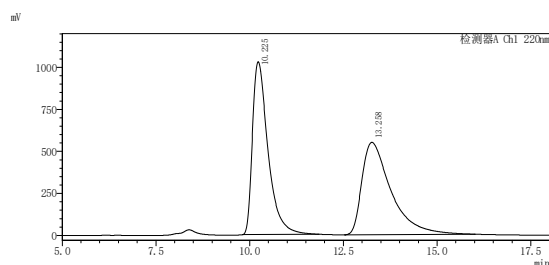


(S)-1-(1-oxo-3,4-diphenylisoquinolin-2(1H)-yl)-1H-pyrrolo[2,3-b]pyridine 7-

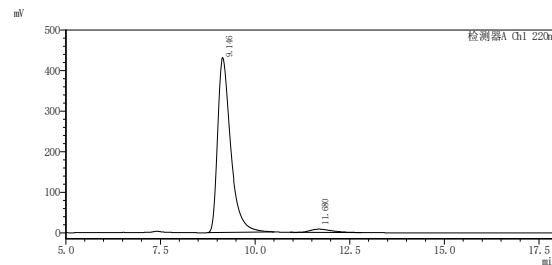
oxide (43) ¹H NMR (600 MHz, CDCl₃) δ 8.50 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.03 (d, *J* = 6.2 Hz, 1H), 7.60 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.55 – 7.45 (m, 2H), 7.40 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.28 – 7.21 (m, 4H), 7.20 – 7.14 (m, 2H), 7.12 (dd, *J* = 7.7,

1.6 Hz, 1H), 7.05 – 6.92 (m, 4H), 6.89 (td, *J* = 7.6, 1.6 Hz, 1H), 6.39 (dd, *J* = 3.8, 1.3 Hz, 1H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.3, 141.5, 137.7, 135.6, 134.7, 133.2, 132.8, 131.9, 131.2, 130.8, 130.0, 128.8, 128.3, 128.0, 127.8, 127.2, 127.1, 126.0, 124.40, 124.37, 120.6, 118.9, 117.9, 102.2. **HRMS (ESI-TOF) (m/z):** Calcd for C₂₈H₂₀N₃O₂⁺, ([M + Na]⁺), 430.1550, found 430.1552. [α]_D²⁰ = -12 (c = 0.1, CHCl₃).

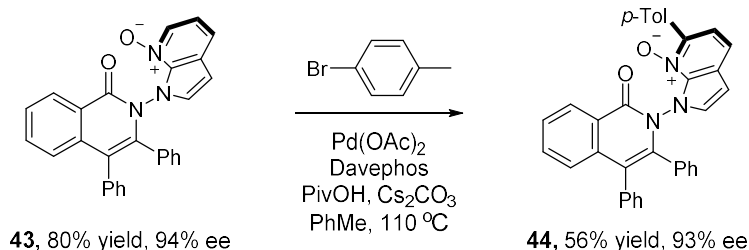
HPLC conditions: Daicel Chiralpak IJ-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 9.146 min, tr (minor) = 11.680 min, 94% ee.



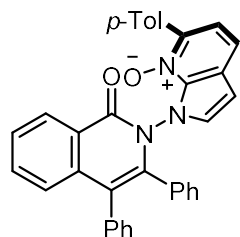
No.	Time	Area	Area (%)
1	10.225	29794005	50.03
2	13.258	29754627	49.97



No.	Time	Area	Area (%)
1	9.146	10351486	96.99
2	11.680	321575	3.01



In a N₂-filled glove box, a screw-cap vial (8 mL) was charged with **43** (42.9 mg, 0.1 mmol, 1.0 equiv), 1-bromo-4-methylbenzene (17 mg, 0.1 mmol, 1.0 equiv), Pd(OAc)₂ (2.2 mg, 0.01 mmol, 10 mol %), Davephos (7.9 mg, 0.02 mmol, 20 mol %), PivOH (3 mg, 0.03 mmol, 30 mol%) and Cs₂CO₃ (65.2 mg, 0.2 mmol, 2.0 equiv) in toluene (1.0 mL). The reaction mixture was then stirred at 110 °C in a preset oil bath for 12 h. After the reaction was complete (monitored by TLC), the reaction mixture was allowed to cool to room temperature. The resulting mixture was then concentrated and purified by silica gel chromatography using PE: EA (3:1) as the eluent to yield compound **44** (29.1 mg, 56%, 93% ee) as a white solid.

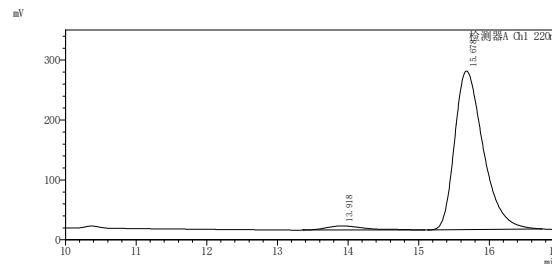
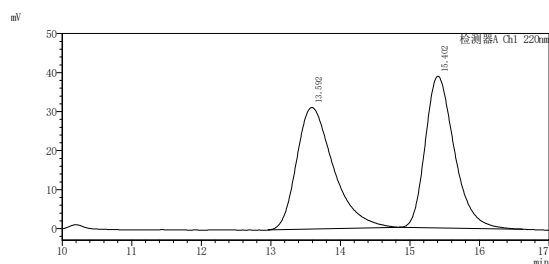


(S)-1-(1-oxo-3,4-diphenylisoquinolin-2(1H)-yl)-6-(p-tolyl)-1H-pyrrolo[2,3-b]pyridine 7-oxide (44**)** ¹H NMR (600 MHz, CDCl₃) δ 8.48 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.76 – 7.69 (m, 2H), 7.64 – 7.54 (m, 2H), 7.48 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H),

7.36 (d, *J* = 8.2 Hz, 1H), 7.27 – 7.21 (m, 7H), 7.20 – 7.15 (m, 2H), 7.12 (d, *J* =

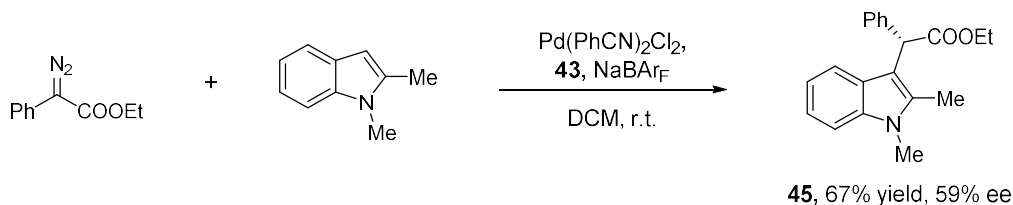
8.2 Hz, 1H), 7.09 (dt, *J* = 7.7, 1.7 Hz, 1H), 6.99 (td, *J* = 7.5, 1.6 Hz, 1H), 6.97 – 6.89 (m, 3H), 6.38 (d, *J* = 3.7 Hz, 1H), 2.37 (s, 3H). ¹³C NMR (150 MHz, CDCl₃) δ 161.1, 144.8, 141.6, 139.0, 137.8, 135.8, 133.0, 131.9, 131.5, 131.4, 130.5, 130.0, 129.5, 128.9, 128.7, 128.2, 127.9, 127.8, 127.6, 127.04, 126.98, 125.9, 124.7, 122.7, 119.9, 119.5, 118.6, 101.9, 21.4. HRMS (ESI-TOF) (*m/z*): Calcd for C₃₅H₂₅N₃O₂⁺, ([M + H]⁺), 520.2020, found 520.2018. [α]_D²⁰ = -18 (*c* = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 15.678 min, tr (minor) = 13.918 min, 94% ee.

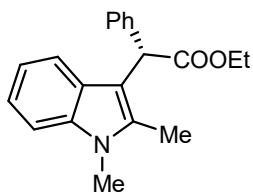


No.	Time	Area	Area (%)
1	13.592	1149807	50.44
2	15.402	1129786	49.56

No.	Time	Area	Area (%)
1	13.918	263059	3.41
2	15.678	7441425	96.59



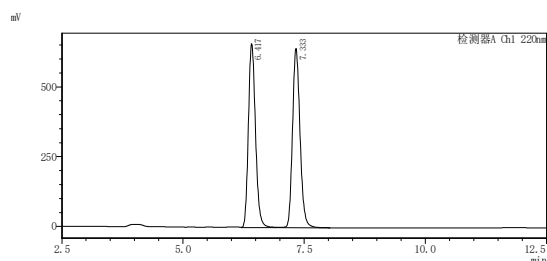
A screw-cap vial (8 mL) was charged with ethyl 2-diazo-2-phenylacetate (19.0 mg, 0.1 mmol, 1.0 equiv), 1,2-dimethyl-1H-indole (14.5 mg, 0.1 mmol, 1.0 equiv), Pd(PhCN)₂Cl₂ (2.6 mg, 10 mol%), **43** (4.3 mg, 10 mol%) and NaBARF (21.3 mg, 24 mol%) in DCM (1 mL) was stirred in a vial at 25 °C for 12 h. The reaction mixture was evaporated under vacuum and the residue was purified by preparative TLC to give the corresponding product **45** (20.6 mg, 67%, 59% ee) as a white solid.



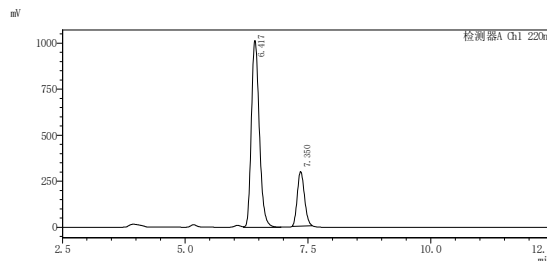
ethyl (S)-2-(1,2-dimethyl-1H-indol-3-yl)-2-phenylacetate (45) ¹H NMR (600 MHz, CDCl₃) δ 7.49 (dt, J = 8.0, 1.0 Hz, 1H), 7.30 – 7.23 (m, 5H), 7.22 – 7.18 (m, 1H), 7.14 (ddd, J = 8.1, 7.0, 1.2 Hz, 1H), 7.02 (ddd, J = 8.0, 6.9, 1.0 Hz, 1H), 5.29 (s, 1H), 4.26 – 4.13 (m, 2H), 3.66 (s, 3H), 2.35 (s, 3H), 1.25 – 1.20 (m, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 173.2, 139.1, 136.7, 134.7, 128.2, 126.9, 126.6, 120.7, 119.5, 119.2, 108.6, 107.9, 61.0, 48.4, 29.6, 14.2, 10.8. **HRMS** (ESI-TOF) (m/z): Calcd for C₂₀H₂₂NO₂⁺, ([M + H]⁺), 308.1645, found 308.1640. $[\alpha]_D^{20}$ = 42 (c = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak IC column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 6.417 min, tr (minor) = 7.350 min, 59% ee.



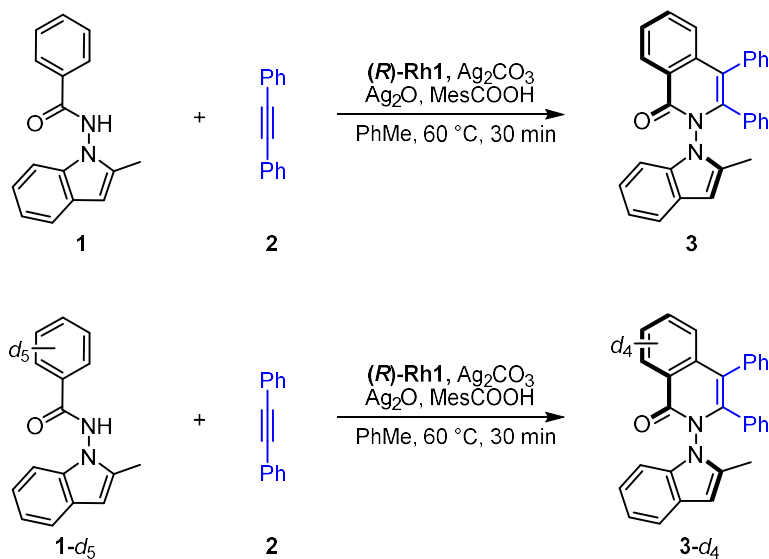
No.	Time	Area	Area (%)
1	6.417	6721273	49.23
2	7.333	6932609	50.77



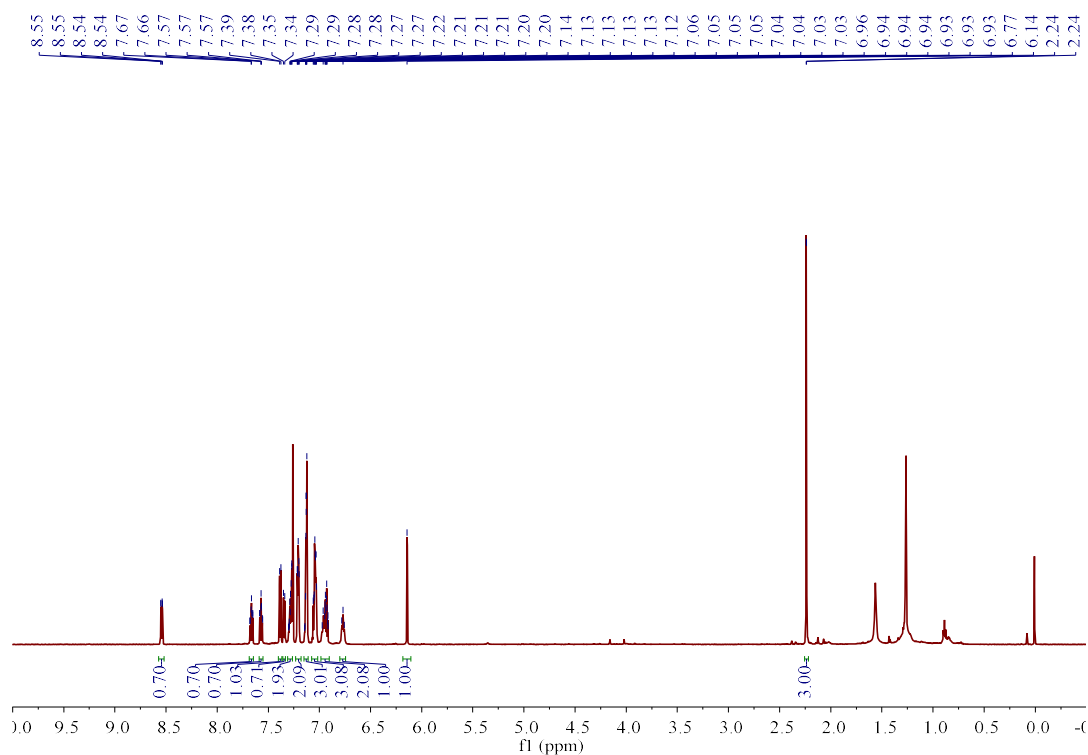
No.	Time	Area	Area (%)
1	6.417	11474131	79.27
2	7.350	3000574	20.73

3.6 Mechanistic Studies

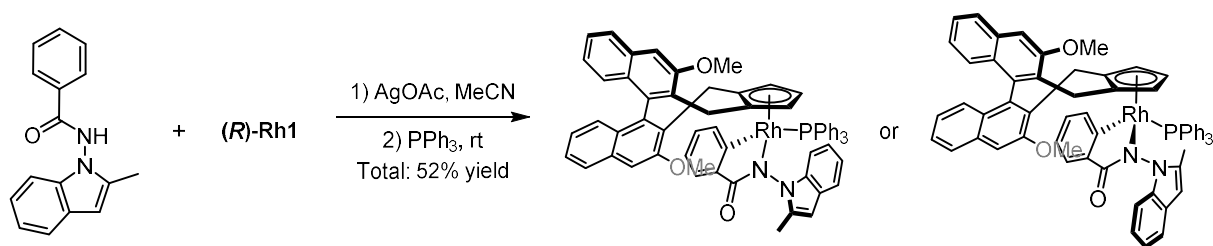
(a) Parallel Kinetic Isotope Effect Experiment



To two tubes equipped with a magnetic stir bar was charged with **1** (1.0 equiv) or **1-d₅** (1.0 equiv), diphenylacetylene **2** (1.5 equiv), $(R)\text{-Rh1}$ (3 mol%), Ag_2O (1.0 equiv), Ag_2CO_3 (0.5 equiv) and MesCOOH (2.0 equiv) and toluene (2 mL). After stirring at $60\text{ }^\circ\text{C}$ for 30 min, The two mixtures were combined and were rapidly evaporated under vacuum and the residue was purified by flash chromatography on silica gel (PE : EA = 5 : 1 as the eluent) to afford the mixed isotopic products. The KIE was determined by ^1H NMR (600 MHz, CDCl_3) analysis to be ($k_{\text{H}}/k_{\text{D}} = 0.70/0.30 = 2.3$).



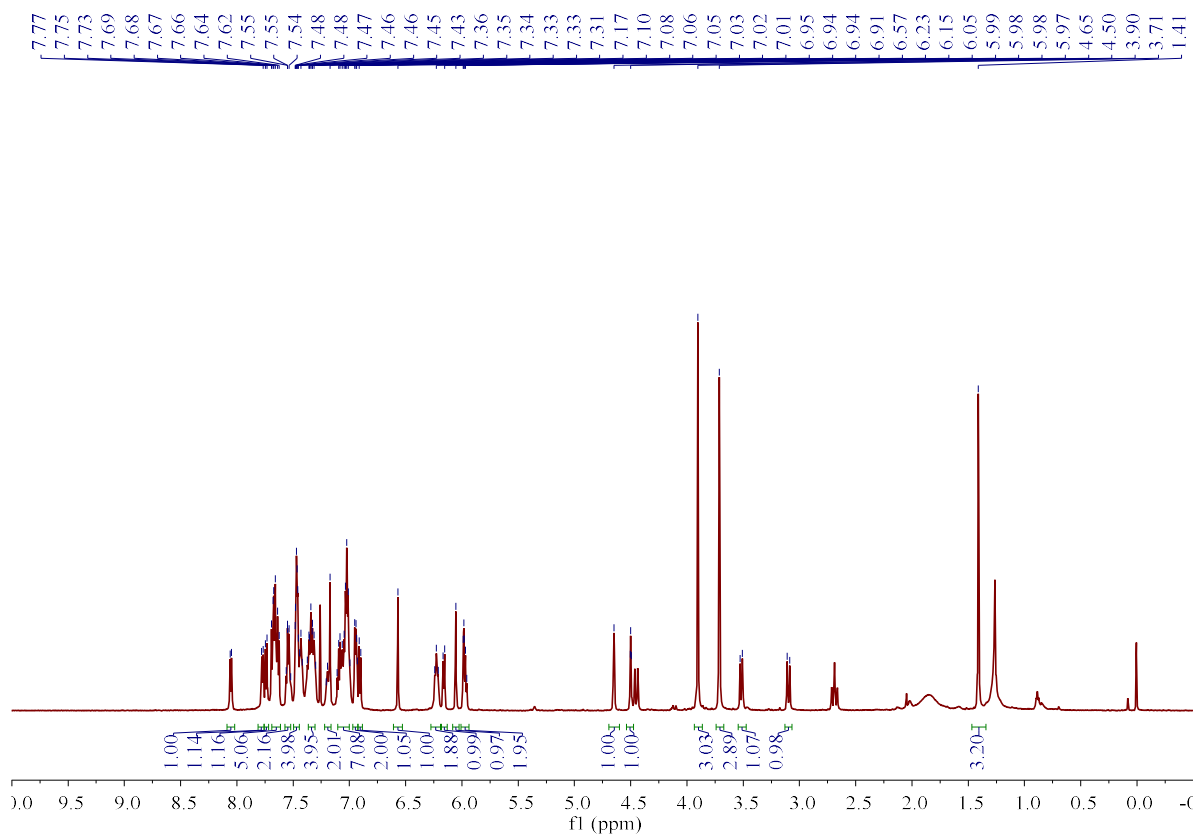
(b) Synthesis of rhodium complexes 46.



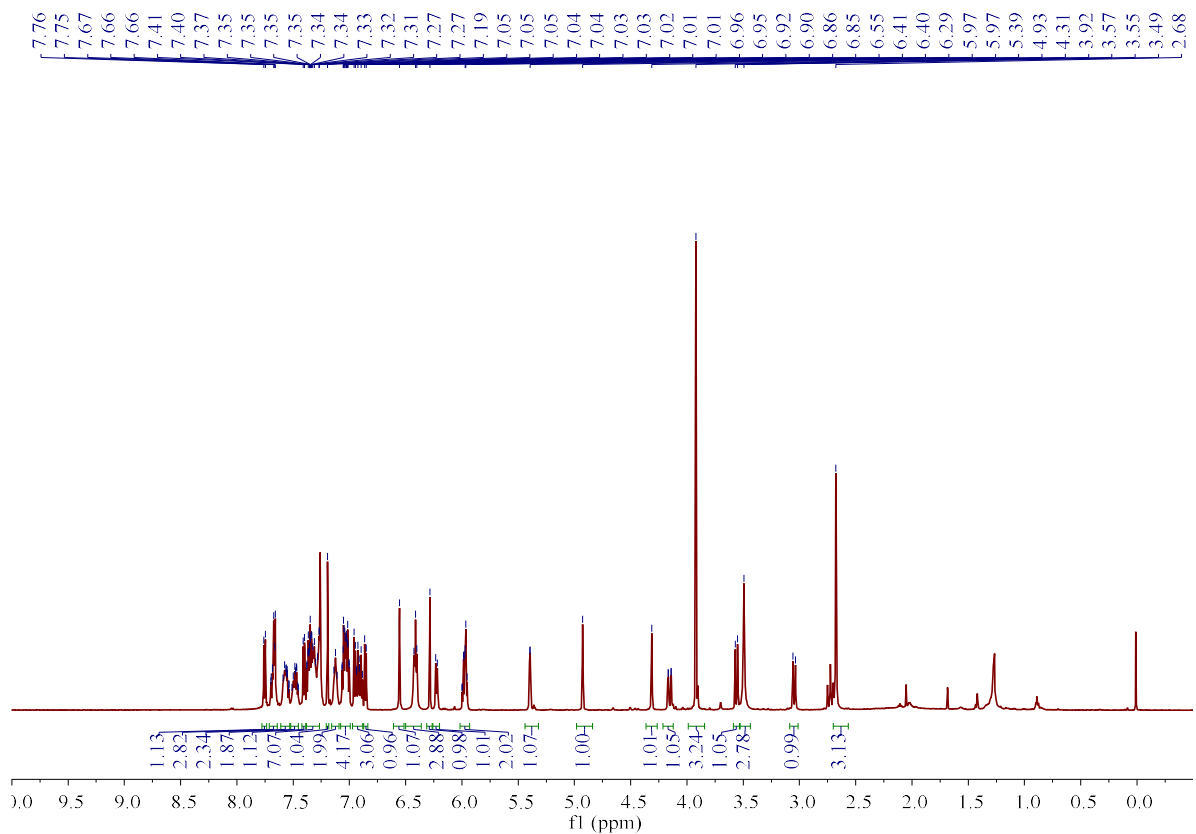
A mixture of N-indol benzamides (25.0 mg, 0.1 mmol, 2.0 equiv), **(R)-Rh1** (57.8 mg, 0.05 mmol) and silver acetate (33.4 mg, 0.2 mmol, 4.0 equiv) in acetonitrile (5 mL) was stirred for 20 min at room temperature under N₂ atmosphere. Another portion of triphenylphosphine (26.2 mg, 0.1 mmol, 2.0 equiv) was added and the mixture was allowed to stir for additional 40 min at room temperature. The resulting crude mixture was filtered through PTFE syringe filter washing with acetonitrile (10 mL) and concentrated under reduced pressure. **46** was purified by deactivated silica gel chromatography (PE/EA/DCM = 2:1:1). Product **46** was totally isolated in 52% yield as a yellow solid.

¹H NMR (600 MHz, CDCl₃) δ 8.05 (d, J = 8.2 Hz, 1H), 7.77 (d, J = 7.3 Hz, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.69 – 7.61 (m, 5H), 7.57 – 7.52 (m, 2H), 7.50 – 7.45 (m, 4H), 7.37 – 7.30 (m, 4H), 7.22 – 7.16 (m, 2H), 7.10 – 7.00 (m, 7H), 6.94 (dd, J = 8.0, 4.9 Hz, 2H), 6.91 (d, J = 8.5 Hz, 1H), 6.57 (s, 1H), 6.23 (t, J = 9.3 Hz, 2H), 6.16 (d, J = 7.7 Hz, 1H), 6.05 (s, 1H), 6.01 – 5.94 (m, 2H), 4.65 (s, 1H), 4.50 (t, J = 2.7 Hz, 1H), 3.90 (s, 3H), 3.71 (s, 3H), 3.52 (d, J = 12.9 Hz, 1H), 3.10 (d, J = 13.0 Hz, 1H), 1.41 (s, 3H) or the isomer **¹H NMR (600 MHz, CDCl₃)** δ 7.75 (d, J = 8.1 Hz, 1H), 7.71 – 7.64 (m, 3H), 7.61 – 7.53 (m, 2H), 7.52 – 7.45 (m, 2H), 7.40 (d, J = 7.8 Hz, 1H), 7.38 – 7.27 (m, 7H), 7.19 (s, 1H), 7.13 (d, J = 7.8 Hz, 2H), 7.08 – 6.99 (m, 4H), 6.97 – 6.88 (m, 3H), 6.86 (d, J = 8.5 Hz, 1H), 6.55 (s, 1H), 6.41 (t, J = 7.8 Hz, 3H), 6.29 (s, 1H), 6.23 (d, J = 8.1 Hz, 1H), 6.02 – 5.93 (m, 2H), 5.40 (d, J = 2.4 Hz, 1H), 4.93 (s, 1H), 4.31 (s, 1H), 4.15 (dd, J = 15.5, 2.3 Hz, 1H), 3.92 (s, 3H), 3.56 (d, J = 13.0 Hz, 1H), 3.49 (s, 3H), 3.05 (d, J = 13.0 Hz, 1H), 2.68 (s, 3H).

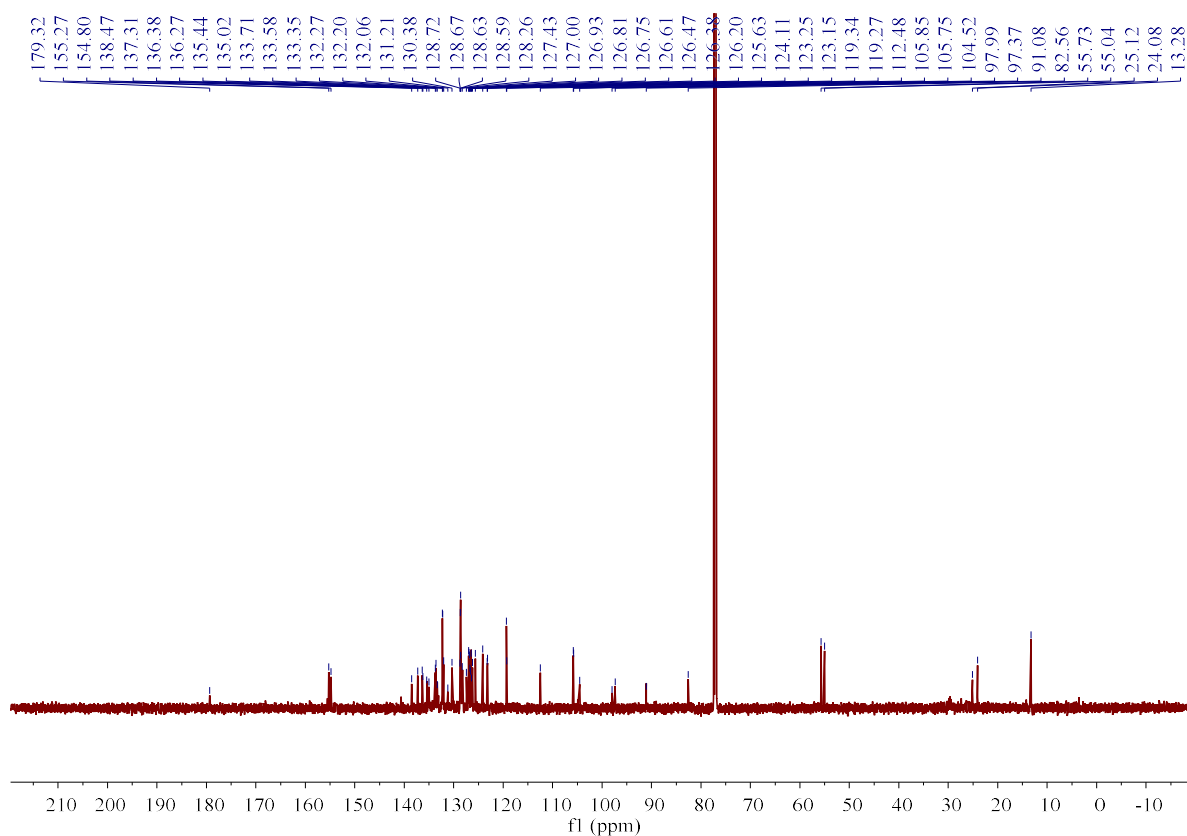
¹³C NMR (150 MHz, CDCl₃) δ 179.3, 155.3, 154.8, 138.5, 137.3, 136.4, 136.3, 135.4, 135.0, 133.7, 133.6, 132.3, 132.2, 132.1, 131.2, 130.4, 128.72, 128.67, 128.63, 128.59, 127.4, 127.0, 126.9, 126.8, 126.7, 126.6, 126.5, 126.4, 126.2, 125.6, 124.1, 123.3, 123.2, 119.34, 119.27, 112.5, 105.9, 105.8, 104.5, 98.0, 97.4, 91.1, 82.6, 55.7, 55.0, 25.1, 24.1, 13.3. **³¹P NMR (243 MHz, CDCl₃)** δ 38.6 (d, J = 159.6 Hz), 29.3. **HRMS (ESI):** calcd. for C₆₃H₅₁N₂O₃PRh⁺ [M+H]⁺: 1017.2687, found : 1018.2687.



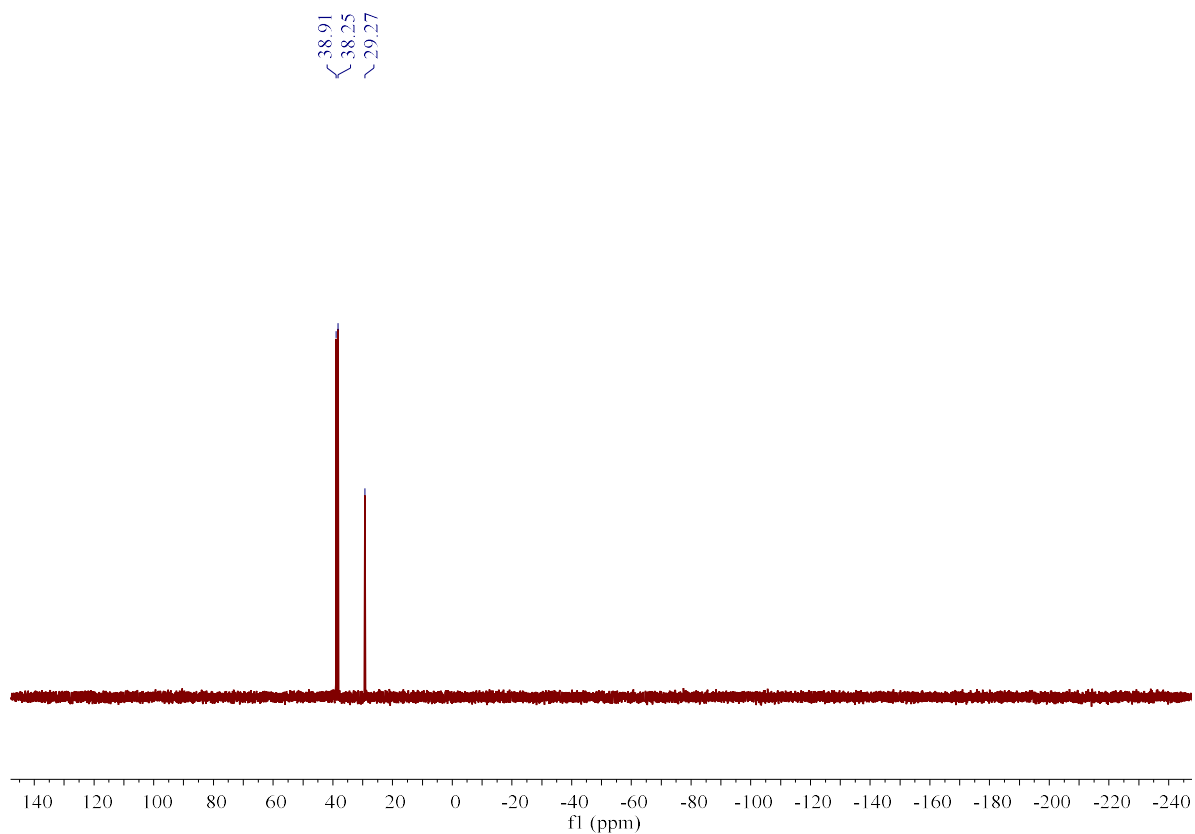
¹H NMR (600 MHz, CDCl₃) spectrum of 46.



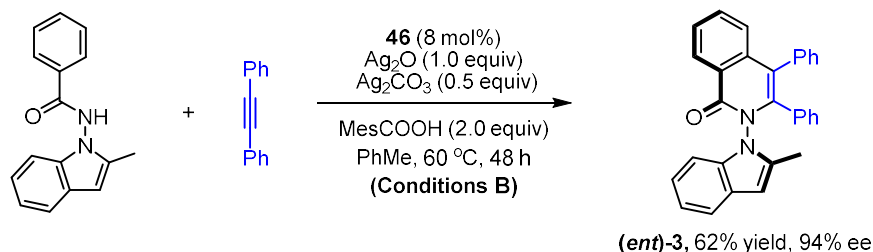
¹H NMR (600 MHz, CDCl₃) spectrum of 46 (the isomer).



^{13}C NMR (150 MHz, CDCl_3) spectrum of 46.

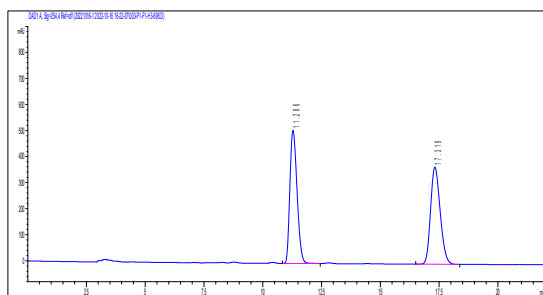


^{31}P NMR (243 MHz, CDCl_3) spectrum of 46.

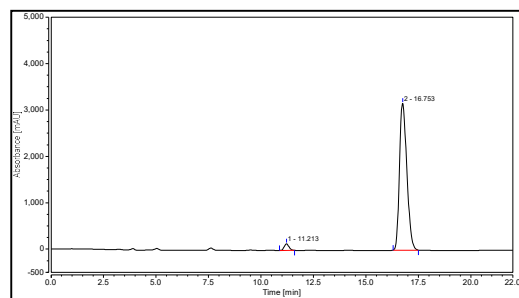


A scew-cap vial (8 mL) was charged with *N*-indol benzamides **1** (0.1 mmol), alkynes **2** (0.15 mmol), **46** (8 mol%), Ag₂O (1.0 equiv), Ag₂CO₃ (0.5 equiv) and MesCOOH (2.0 equiv) in toluene (2 mL) and the mixture was stirred at 60 °C for 48 h. The reaction mixture was evaporated under vacuum and the residue was purified by preparative TLC to give the corresponding product (*ent*)-3 (26.4 mg, 62% yield, 94% ee).

HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 85:15, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (minor) = 11.213 min, tr (major) = 16.753 min, 94% ee.



No.	Time	Area	Area (%)
1	11.286	10817.0	50.50
2	17.319	10604.8	49.50



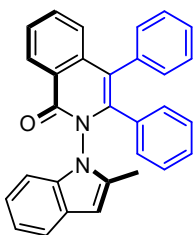
No.	Time	Area	Area (%)
1	11.213	37.3	2.81
2	16.753	1289.1	97.19

3.7 Determination of Rotational Barrier for (*ent*)-3 and 23.

The enantiomerisation barrier, corresponding to the barrier to rotation for the following atropisomers, was obtained by kinetic of racemisation of an enantiomer. The slope of the first order kinetic line gives the racemisation constant ($k_{\text{racemisation}} = 2 \times k_{\text{enantiomerisation}}$). Eyring equation gives the enantiomerisation barrier ($\Delta G^{\ddagger}_{\text{enantiomerization}}$) from enantiomerisation constant ($k_{\text{enantiomerisation}}$), $R = 8.31451 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$, $h = 6.62608 \times 10^{-34} \text{ Js}$ and $k_B = 1.38066 \times 10^{-23} \text{ J/K}$. Reactions were conducted at 1 mg/mL concentration. The diastereomeric ratio (dr) and diastereomeirc excess (de) value were determined by HPLC.

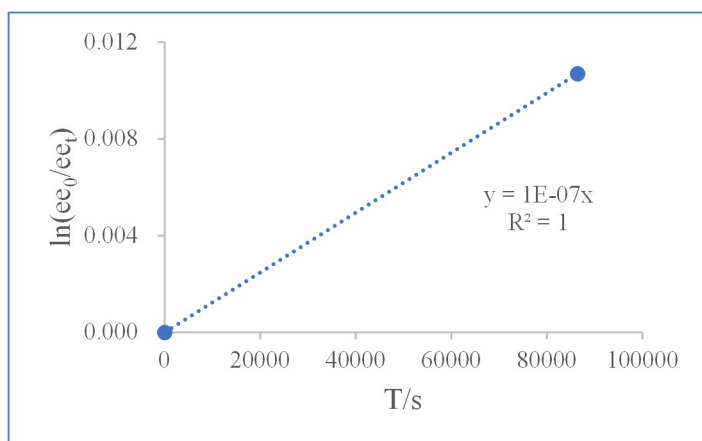
$$\Delta G^{\ddagger}_{\text{enantiomerization}} = RT \times \ln \frac{k_B \times T}{h \times k_{\text{enantiomerisation}}}$$

Racemization of (*ent*)-**3** in DMF at 150 °C.



(*ent*)-**3**. $\Delta G^{\ddagger} = 39.2 \text{ kcal/mol}$ (150 °C, DMF)

T/s	ee	ln (ee ₀ /ee _t)
0	94	0
86400	93	0.0106953



$$k_{\text{racemization}} (150 \text{ °C}) = 1.0 \times 10^{-7} \text{ s}^{-1}$$

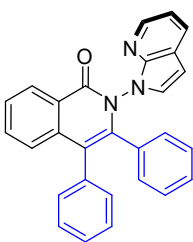
$$k_{\text{enantiomerization}} (150 \text{ °C}) = 5.0 \times 10^{-8} \text{ s}^{-1}$$

Employing the Eyring equation: $\Delta G^{\ddagger}_{\text{enantiomerization}} = RT \times \ln \frac{k_B \times T}{h k_{\text{enantiomerisation}}}$

$$\Delta G^{\ddagger} = 8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} \times 423.15 \text{ K} \times \ln \frac{1.381 \times 10^{-23} \text{ J} \cdot \text{K}^{-1} \times 423.15 \text{ K}}{5.0 \times 10^{-8} \text{ s}^{-1} \times 6.626 \times 10^{-34} \text{ J} \cdot \text{s}}$$

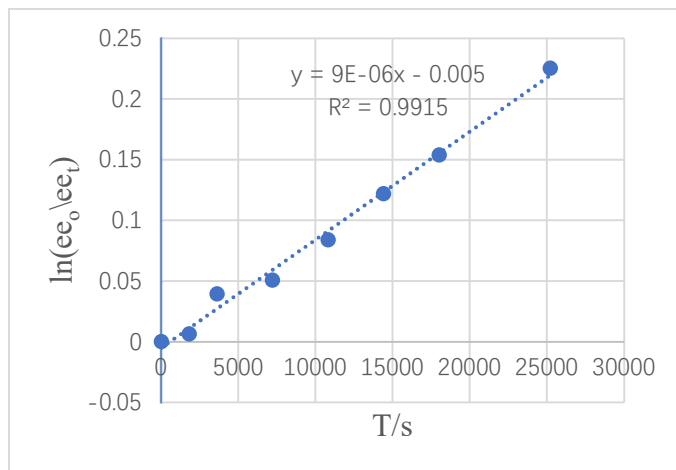
$$\Delta G^{\ddagger} = 164.0 \text{ kJ} \cdot \text{mol}^{-1} = 39.2 \text{ kcal} \cdot \text{mol}^{-1}$$

Racemization of **23** in mesitylene at 120 °C.



23. $\Delta G^\ddagger = 32.8$ kcal/mol (120 °C, mesitylene)

T/s	ee	ln (ee ₀ /ee _t)
0	93.2	0.000000
1800	92.6	0.006458
3600	89.6	0.039393
7200	88.6	0.050616
10800	85.8	0.083894
14400	82.6	0.121949
18000	80.0	0.153972
25200	74.4	0.225292



$$k_{\text{racemization}} (120\text{ }^\circ\text{C}) = 9.0 \times 10^{-6} \text{ s}^{-1}$$

$$k_{\text{enantiomerization}} (120\text{ }^\circ\text{C}) = 4.5 \times 10^{-6} \text{ s}^{-1}$$

Employing the Eyring equation: $\Delta G^\ddagger_{\text{enantiomerization}} = RT \times \ln \frac{k_B \times T}{h k_{\text{enantiomerisation}}}$

$$\Delta G^\ddagger = 8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} \times 393.15 \text{ K} \times \ln \frac{1.381 \times 10^{-23} \text{ J} \cdot \text{K}^{-1} \times 393.15 \text{ K}}{4.5 \times 10^{-6} \text{ s}^{-1} \times 6.626 \times 10^{-34} \text{ J} \cdot \text{s}}$$

$$\Delta G^\ddagger = 137.4 \text{ kJ} \cdot \text{mol}^{-1} = 32.8 \text{ kcal} \cdot \text{mol}^{-1}$$

4. X-Ray Crystallographic Data

X-ray crystal structure of (*S*)-(*ent*)-3 (CCDC 2213499)

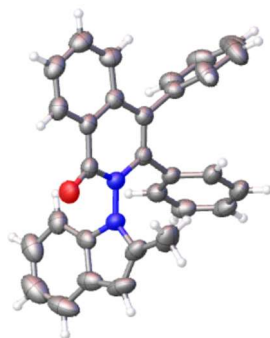


Table S4 Crystal data and structure refinement for (*ent*)-3.

Identification code	(<i>ent</i>)-3
Empirical formula	C ₃₀ H ₂₂ N ₂ O
Formula weight	426.49
Temperature/K	180.00
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	9.5313(3)
b/Å	14.4824(5)
c/Å	16.6299(5)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	2295.53(13)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.234
μ/mm^{-1}	0.586
F(000)	896.0
Crystal size/mm ³	0.45 × 0.3 × 0.1
Radiation	CuK α (λ = 1.54178)
2 θ range for data collection/°	8.096 to 136.56
Index ranges	-11 ≤ h ≤ 11, -16 ≤ k ≤ 17, -19 ≤ l ≤ 20
Reflections collected	34480

Independent reflections	4169 [$R_{\text{int}} = 0.0316$, $R_{\text{sigma}} = 0.0149$]
Data/restraints/parameters	4169/93/299
Goodness-of-fit on F^2	1.067
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0288$, $wR_2 = 0.0732$
Final R indexes [all data]	$R_1 = 0.0301$, $wR_2 = 0.0747$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.15/-0.14
Flack parameter	-0.03(7)

5. ECD Spectrum and DFT Calculations of N-N Single-axis Product 23.

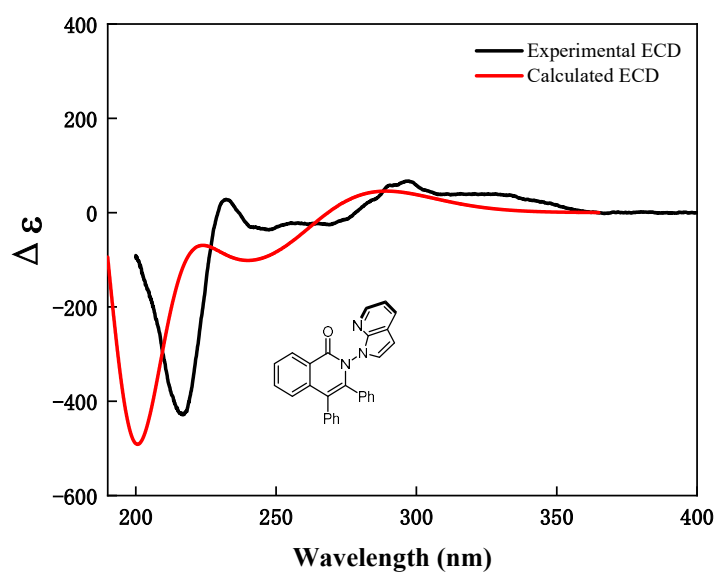


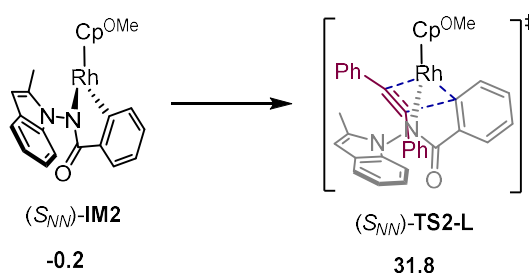
Figure 1. Comparison of calculated (red line) and experimental (black line) ECD spectra of N-N single-axis product (*S*)-23.

6. Theoretical Calculation

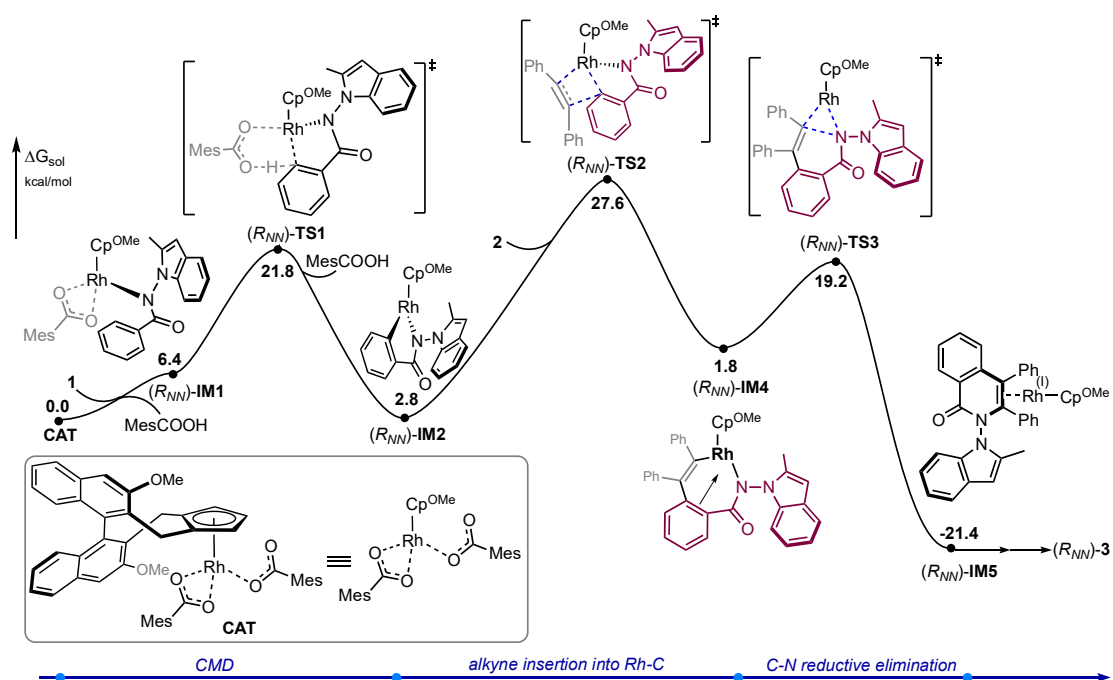
6.1 Computational details

All the calculations were performed using the Gaussian 09^[6]. The geometry optimizations were carried out at the B3LYP-D3(BJ)^[7] level of theory with a basis set of def2-SVP^[8] for all atoms. Frequencies were computed analytically at the same level of theory to confirm whether the structures are minima (no imaginary frequencies) or transition states (only one imaginary frequency). Key transition-state structures were confirmed to connect the correct reactants and products by intrinsic reaction coordinate (IRC) calculations^[9]. Because the harmonic oscillator approximation may lead to spurious results for the computed entropies in molecules with low-frequency vibrational modes, the quasi-harmonic approximation from Grimme^[10] was applied to compute the thermal corrections with a cutoff frequency of 100 cm⁻¹ using GoodVibes^[11]. To obtain better accuracy, single-point energies for the optimized geometries were calculated at the M06^[12] level of theory with a larger basis set of def2-TZVPP^[13] for all atoms. Solvation effects (toluene, $\epsilon = 2.3741$) were taken into account by performing single-point calculations using the SMD model^[14]. To correct the Gibbs free energies under a pressure of 1 atm to the standard state in solution (1 mol/L), a correction of 1.89 kcal/mol is added to the energies of all species. The final free energies reported in the article (ΔG_{sol}) are the large basis set solution-phase single-point energies corrected by gas-phase Gibbs free energy correction (at 298.15 K). All 3D structures of the optimized geometries were generated using CYLview^[15].

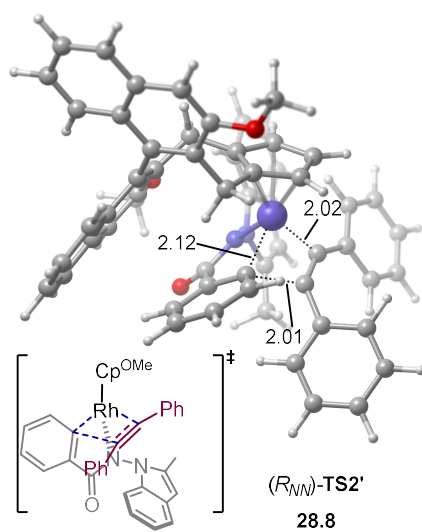
2. The alkyne insertion transition state from intermediate (S_{NN})-IM2



6.2 The whole calculated energy profile for the pathway leading to product (R_{NN})-3



6.3 Optimized geometries of alkyne insertion transition states (R_{NN})-TS2'



6.4 Table of calculated energies and energy corrections

Stationary point	Single-point energy M06-SMD def2-TZVPP (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
1	-802.5867964	0.223365
2	-539.2382104	0.154957
MesCOOH	-538.6158937	0.161251
CAT	-2455.604162	0.7428
(S_{NN})- IM1	-2719.57107	0.810315
(R_{NN})- IM1	-2719.569059	0.809129
(S_{NN})- TS1	-2719.539937	0.805086
(R_{NN})- TS1	-2719.540166	0.804817
(S_{NN})- IM2	-2180.94017	0.621264
(S_{NN})- IM3	-2180.936126	0.620597
(S_{NN})- IM4	-2720.200233	0.80824
(S_{NN})- IM5	-2720.240303	0.807829
(R_{NN})- IM2	-2180.935254	0.621211
(R_{NN})- IM4	-2720.202346	0.8065
(R_{NN})- IM5	-2720.241481	0.80861
(S_{NN})- TS2	-2720.16477	0.806715
(S_{NN})- TS3	-2720.182236	0.807474
(S_{NN})- TS2-L	-2720.152005	0.80394
(R_{NN})- TS2	-2720.159337	0.804557
(R_{NN})- TS2'	-2720.158895	0.806079
(R_{NN})- TS3	-2720.174776	0.806642

6.5 Cartesian coordinates

1

N	-5.61253700	-4.72905900	-2.37424900
C	-6.48860500	-5.41642000	-3.20218500
C	-5.91743700	-5.81571400	-4.53020900
C	-4.81698200	-5.17802600	-5.12431700
C	-6.55040800	-6.86891600	-5.20704000
C	-4.34451100	-5.60381800	-6.36753300
H	-4.34093700	-4.32256000	-4.63974100
C	-6.07295500	-7.29752100	-6.44458600
H	-7.41886700	-7.33591500	-4.73952600
C	-4.96733600	-6.66761500	-7.02589300
H	-3.49313800	-5.09686300	-6.82734000
H	-6.56603000	-8.12400400	-6.96149700
H	-4.59539500	-7.00091200	-7.99764900
O	-7.62906900	-5.66047400	-2.86883200
N	-5.98306800	-4.37969600	-1.10826100
C	-6.73601000	-3.24965900	-0.78009000
C	-5.73451100	-5.13509800	0.02778200
C	-6.94700500	-3.25805500	0.57716900
C	-6.32028400	-4.43724000	1.12002300
H	-7.50459400	-2.50461200	1.12938600
C	-7.19614600	-2.31308100	-1.84117700
H	-6.35622300	-1.94769600	-2.45490700
H	-7.90729200	-2.81367600	-2.51949300
H	-7.69815900	-1.44765800	-1.38877100
C	-6.19366800	-4.98428900	2.40896700
C	-5.50634800	-6.18530400	2.57136400
C	-4.93957600	-6.85753500	1.46908100
C	-5.04524200	-6.33976700	0.17837900
H	-6.63216400	-4.47400500	3.27008500
H	-5.40586600	-6.61868300	3.56925500
H	-4.41293800	-7.80156400	1.62724700
H	-4.61743100	-6.85863500	-0.68197700
H	-4.62095400	-4.68822800	-2.58546000

2

C	-1.09649000	1.32357700	0.01335400
C	0.12255800	1.32357600	0.01487000
C	-2.52281200	1.32360700	0.01158100
C	-3.24268700	2.15412500	0.89683300
C	-3.24054700	0.49313900	-0.87544700
C	-4.63625300	2.15090000	0.89159500
H	-2.69276200	2.79843500	1.58523700

C	-4.63412300	0.49648300	-0.87367800
H	-2.68896500	-0.15121800	-1.56248000
C	-5.33739800	1.32372400	0.00808100
H	-5.18071200	2.79896100	1.58257600
H	-5.17691400	-0.15153500	-1.56600900
H	-6.42986800	1.32377000	0.00671800
C	1.54887900	1.32356200	0.01665500
C	2.26878500	0.49304300	-0.86856600
C	2.26658500	2.15405700	0.90368600
C	3.66235200	0.49629600	-0.86330500
H	1.71889000	-0.15129200	-1.55697000
C	3.66015900	2.15074200	0.90194100
H	1.71497700	2.79841200	1.59070100
C	4.36346700	1.32350100	0.02020400
H	4.20683300	-0.15176600	-1.55426600
H	4.20292500	2.79878200	1.59427200
H	5.45593700	1.32347800	0.02158400

MesCOOH

O	7.92500400	-8.76404200	4.81767900
O	7.45144500	-6.75645000	5.65950900
C	7.80822200	-7.89773100	5.85028700
H	7.70331900	-8.25258800	4.02067500
C	8.12610000	-8.49424500	7.18012500
C	7.43363800	-7.99722200	8.31604900
C	9.11100200	-9.50249500	7.33163300
C	7.72214000	-8.54332300	9.56992200
C	9.37386800	-9.99430600	8.61624500
C	8.68714600	-9.54088200	9.74532000
H	7.17722400	-8.16926500	10.44111200
H	10.14546900	-10.75977700	8.73500400
C	6.39102700	-6.90961400	8.23319800
H	6.84609800	-5.94572900	7.96397500
H	5.64077500	-7.11306500	7.45502300
H	5.87536500	-6.80392200	9.19838000
C	9.91908900	-10.06624600	6.18615300
H	9.30446300	-10.71599300	5.54589300
H	10.31950100	-9.27862300	5.53234200
H	10.76139100	-10.65675400	6.57365500
C	8.95943400	-10.11679600	11.11037400
H	8.16732700	-10.82908500	11.39927800
H	9.91720500	-10.65656600	11.13930500
H	8.98206500	-9.33038800	11.88083000

CAT

C	0.67124500	1.63605500	-3.54787300
C	0.24255900	0.51477400	-4.32332800
C	1.00606600	-0.62856300	-3.88337500
C	1.85403100	-0.23499800	-2.81472300
C	1.64553100	1.19648700	-2.59866900
C	2.72532100	-1.14985000	-1.99450200
C	2.37392800	2.08878700	-1.62798400
H	0.23092300	2.63050200	-3.55838500
H	0.89778600	-1.64893500	-4.24893200
O	0.61124500	2.98230700	0.23727400
O	4.69157300	-1.73522300	-3.80618200
C	2.42124400	1.56034200	-0.21098900
C	1.45041600	2.04480400	0.72612500
C	1.42431600	1.57204200	2.02172800
C	2.33618600	0.56714300	2.43786300
C	2.28521200	0.01060400	3.74526000
C	3.16038800	-0.98394000	4.12861400
C	4.13292000	-1.46591700	3.21992400
C	4.21416500	-0.93845600	1.94706900
C	3.32570400	0.08500100	1.52137300
C	3.36478500	0.63213900	0.19638500
C	-0.20642900	3.73233900	1.11216800
C	4.12543700	-0.61668200	-1.81951500
C	4.43665100	0.21470500	-0.75803300
C	5.76885600	0.72587000	-0.59968900
C	6.13054600	1.59602400	0.46459000
C	7.42173400	2.06640100	0.58863200
C	8.41099400	1.69034100	-0.35107400
C	8.08851700	0.85648400	-1.40124400
C	6.76714800	0.35625500	-1.55794600
C	6.41836200	-0.48553600	-2.64991200
C	5.12602000	-0.94968300	-2.78560600
C	5.60886400	-2.12552300	-4.80257000
H	0.68594700	1.93764900	2.73442500
H	1.52703300	0.37896400	4.44098600
H	3.10176300	-1.40584900	5.13486700
H	4.81963900	-2.25773300	3.52770500
H	4.96206700	-1.31158000	1.24575900
H	-0.90934000	3.09343400	1.66610900
H	-0.78123700	4.41377000	0.47440800
H	0.40873100	4.30263900	1.83073500
H	5.36966600	1.88720200	1.18922000
H	7.68227700	2.73229100	1.41439100

H	9.43147000	2.06620300	-0.24481200
H	8.84804400	0.56951300	-2.13324900
H	7.19181800	-0.74212400	-3.37306200
H	5.05221500	-2.74559000	-5.51731800
H	6.43979300	-2.71790100	-4.38019400
H	6.02929900	-1.25203200	-5.33172100
H	2.75218500	-2.13320600	-2.47948400
H	2.26040000	-1.26911800	-1.00670000
H	3.39985400	2.21842000	-2.00859000
H	1.88100200	3.06729200	-1.63469800
H	-0.50415000	0.52539500	-5.11464600
Rh	-0.19788500	0.11919700	-2.25864200
O	-1.38886700	-1.62739600	-1.79270100
O	-0.12283100	-0.72256500	-0.28296400
C	-1.02136600	-1.57760400	-0.57759700
C	-1.62811300	-2.43771400	0.46703700
C	-0.82000200	-2.95304500	1.50797900
C	-3.02127000	-2.69688700	0.43286600
C	-1.42866300	-3.73239500	2.49865100
C	-3.57870100	-3.46117800	1.46227400
C	-2.80309800	-3.99020300	2.50106500
H	-0.80633500	-4.14622700	3.29690100
H	-4.65600500	-3.64991500	1.45073900
C	0.66681200	-2.70617000	1.58294400
H	1.16570500	-2.92025600	0.62577900
H	0.88701100	-1.65571500	1.81480200
H	1.12586800	-3.33512600	2.35823500
C	-3.92113700	-2.15968000	-0.65352000
H	-3.73098500	-1.09639600	-0.85884800
H	-3.74584300	-2.68486100	-1.60421600
H	-4.97638800	-2.28553800	-0.37153000
C	-3.44415500	-4.79860700	3.59958500
H	-4.04857000	-4.15409900	4.26077200
H	-4.12237600	-5.56448600	3.19066900
H	-2.69199800	-5.30370100	4.22297700
O	-1.36811600	3.16306300	-2.06591300
O	-1.85298400	1.03921900	-1.49720500
C	-2.03748300	2.32487100	-1.46749300
C	-3.19971000	2.74450500	-0.59482900
C	-3.40482800	2.16828500	0.67870300
C	-4.06206000	3.77132400	-1.05531400
C	-4.45933000	2.64640100	1.47289700
C	-5.11535200	4.18929100	-0.23798600
C	-5.32930900	3.64562800	1.03527100

H	-4.60376200	2.21205000	2.46671500
H	-5.78749500	4.97109700	-0.60471000
C	-2.55134300	1.05835900	1.24568000
H	-2.95519900	0.07582600	0.96046000
H	-1.51826000	1.06901600	0.88532000
H	-2.55312000	1.09958300	2.34594700
C	-3.88555400	4.42490700	-2.40460100
H	-2.96809800	5.02947500	-2.43028100
H	-3.77680900	3.68017200	-3.20774400
H	-4.74862000	5.06572600	-2.63815500
C	-6.46984400	4.13007000	1.89399200
H	-6.42035100	5.22084800	2.04771500
H	-7.44283000	3.91801900	1.41942000
H	-6.46595400	3.64753100	2.88241300

(S_{NN}) -IM1

C	0.10436600	-2.22911500	-2.25054300
C	-0.52647000	-3.21381700	-1.43023800
C	0.03080600	-3.08345900	-0.11670700
C	0.98174300	-2.01045700	-0.12968400
C	1.05710600	-1.49339800	-1.48156800
C	1.72199900	-1.46699200	1.06090900
C	2.02890600	-0.48263600	-2.03314700
H	-0.13710700	-2.03407300	-3.29485400
H	-0.23223400	-3.67913500	0.75370700
O	0.70794000	1.80144000	-2.76611100
O	3.24806200	-3.65410000	1.59689200
C	2.18519100	0.79072100	-1.23242500
C	1.47711500	1.95991800	-1.65808900
C	1.60672800	3.15309100	-0.97930100
C	2.41267100	3.23165700	0.18559600
C	2.50577500	4.43235300	0.94032300
C	3.26455500	4.48764800	2.08997800
C	3.96673200	3.34149800	2.53533800
C	3.89943200	2.16336100	1.82053200
C	3.12655000	2.07385100	0.63113600
C	3.01858300	0.86090400	-0.12701700
C	0.20956500	2.95319400	-3.41542800
C	3.20970200	-1.44224500	0.80830100
C	3.82923900	-0.33508000	0.25506800
C	5.24242400	-0.34574100	-0.00412900
C	5.91821900	0.75466600	-0.59834800
C	7.27775200	0.71213800	-0.83092500
C	8.02517400	-0.43782400	-0.48222300

C	7.39643600	-1.52695900	0.08388700
C	5.99682800	-1.51570200	0.33253500
C	5.33528900	-2.64503200	0.88871700
C	3.97324300	-2.61574700	1.10495900
C	3.91288200	-4.84950200	1.93817800
H	1.06272600	4.04181500	-1.29435400
H	1.94745200	5.30754900	0.59900000
H	3.32124700	5.41516900	2.66477500
H	4.55951400	3.39012600	3.45149400
H	4.43610200	1.28011300	2.16927700
H	-0.49764300	3.50860800	-2.78060900
H	-0.31537100	2.60140500	-4.31252700
H	1.03346500	3.62658500	-3.71088300
H	5.34529700	1.64184600	-0.86878900
H	7.77967600	1.56874500	-1.28646600
H	9.10177100	-0.46265800	-0.66718100
H	7.96815800	-2.42074800	0.34706700
H	5.92781300	-3.52870100	1.12295300
H	3.14569500	-5.53996400	2.31188700
H	4.66611600	-4.68338100	2.72844200
H	4.41095400	-5.30085400	1.06181800
H	1.49226700	-2.08135000	1.93670500
H	1.35670800	-0.45156500	1.26598300
H	3.00919000	-0.98140000	-2.10809400
H	1.71075500	-0.22779600	-3.05053200
H	-1.27880000	-3.92982400	-1.74737700
N	-2.74205900	-1.53746100	0.45562700
Rh	-0.96894400	-1.24441200	-0.60237500
O	-1.98244600	0.49698300	-1.43661100
O	-0.80717600	0.62880200	0.36803600
C	-1.55391800	1.22314400	-0.47930800
C	-3.75483300	-2.42482800	0.18859300
C	-3.72117200	-3.05911100	-1.17554600
C	-3.53509600	-2.30364300	-2.34297300
C	-3.95052500	-4.43767100	-1.27658600
C	-3.53300000	-2.93147300	-3.59114600
H	-3.38372600	-1.22628800	-2.27041300
C	-3.92610300	-5.06750800	-2.52292000
H	-4.14078300	-5.00566300	-0.36359900
C	-3.71081000	-4.31582600	-3.68362900
H	-3.39240300	-2.33590000	-4.49687500
H	-4.08431000	-6.14668000	-2.59194800
H	-3.69805000	-4.80708200	-4.65977300
O	-4.66344300	-2.68818900	0.96576700

N	-2.92978200	-0.78631500	1.59427900
C	-3.78951400	0.30700700	1.68371200
C	-2.16265300	-0.86999400	2.73757200
C	-3.57680300	0.93442700	2.89158300
C	-2.54010200	0.21576100	3.58243100
H	-4.11698500	1.80847600	3.24907600
C	-4.77628300	0.58830600	0.60627800
H	-5.22712800	1.57913200	0.75149300
H	-4.29968300	0.55464100	-0.38348000
H	-5.57225700	-0.17413400	0.61066900
C	-1.87725300	0.37743800	4.81138300
C	-0.87611000	-0.52363900	5.16944200
C	-0.53408600	-1.60133600	4.32664500
C	-1.17686500	-1.78897200	3.10344600
H	-2.14402500	1.20307300	5.47626400
H	-0.35422200	-0.40230700	6.12181000
H	0.23931700	-2.30677700	4.64129100
H	-0.94101800	-2.63405500	2.46019800
C	-1.86785700	2.66355400	-0.35726800
C	-1.33682100	3.41437000	0.73045800
C	-2.64942200	3.31212000	-1.35527500
C	-1.55519600	4.79738600	0.75354500
C	-2.83552200	4.69568700	-1.26900300
C	-2.29025800	5.46020000	-0.23218000
H	-1.13568200	5.37318400	1.58253300
H	-3.42960300	5.19250400	-2.04080500
C	-0.57137100	2.81411800	1.87952000
H	-1.16487400	2.04028500	2.38348000
H	0.35095600	2.32571500	1.54641500
H	-0.30997800	3.59652300	2.60540700
C	-3.30053000	2.59694100	-2.51458300
H	-4.01702800	1.83967800	-2.16646200
H	-3.83713700	3.31918500	-3.14669900
H	-2.57106400	2.05289400	-3.12822600
C	-2.52992600	6.94529900	-0.15902100
H	-3.50330200	7.15944600	0.31566400
H	-1.75626400	7.45132500	0.43721200
H	-2.55164300	7.40126300	-1.16076300

(R_{NN}) -IM1

C	-0.22197000	-2.53934300	-1.77390500
C	-0.71902500	-3.34025900	-0.71433400
C	0.03564600	-3.02291100	0.45719300
C	1.07504700	-2.07989300	0.08852700

C	0.93074100	-1.79234900	-1.29821700
C	2.04857200	-1.45324200	1.05218100
C	1.83444000	-0.94994800	-2.15989400
H	-0.61691700	-2.51232200	-2.78814000
H	-0.10224900	-3.45111100	1.44815500
O	0.37583100	1.15670900	-3.05647500
O	3.70959500	-3.55477400	1.57935000
C	2.07334600	0.43524000	-1.60660900
C	1.23481000	1.49915200	-2.06910800
C	1.33907600	2.76138000	-1.52196100
C	2.29507500	3.02684100	-0.50585200
C	2.38474200	4.30461100	0.10931600
C	3.30618900	4.54801800	1.10568700
C	4.18350500	3.52221000	1.53257400
C	4.11935800	2.27010200	0.95619800
C	3.17792500	1.98698300	-0.06990600
C	3.04671800	0.68377500	-0.65346000
C	-0.50312400	2.13539500	-3.56488000
C	3.46930300	-1.46081200	0.54007100
C	3.95637900	-0.42868100	-0.24369100
C	5.30840400	-0.45349800	-0.72650100
C	5.84264200	0.57289700	-1.55235000
C	7.14739600	0.51833800	-1.99778500
C	7.97796000	-0.57041600	-1.64016300
C	7.48528600	-1.58769400	-0.84996200
C	6.14475800	-1.56234300	-0.37751400
C	5.61743200	-2.61976100	0.41354900
C	4.30852700	-2.57854300	0.84828900
C	4.45637400	-4.69675900	1.93393500
H	0.68105300	3.56923800	-1.83720400
H	1.69516300	5.08857300	-0.21103000
H	3.35591300	5.53403600	1.57381900
H	4.90843700	3.72193000	2.32490400
H	4.78810700	1.47614300	1.29139900
H	-1.15338000	2.52734200	-2.77001300
H	-1.12177400	1.63663800	-4.32176300
H	0.05185000	2.96716500	-4.03373100
H	5.20493500	1.41264800	-1.82961800
H	7.54146300	1.31765000	-2.62943000
H	9.01050800	-0.60522000	-1.99581900
H	8.12123300	-2.43415700	-0.57795200
H	6.26783700	-3.46031700	0.65307300
H	3.78351900	-5.34620600	2.50883000
H	5.32796000	-4.43443000	2.55936600

H	4.81112200	-5.24227300	1.04165200
H	1.99203500	-1.99669000	2.00251300
H	1.72710600	-0.42108000	1.24484200
H	2.79312100	-1.48291700	-2.25768800
H	1.39046400	-0.87395900	-3.15826600
H	-1.58107700	-4.00180300	-0.75809300
N	-2.97815500	-1.36620300	0.19480200
Rh	-0.92973800	-1.23158100	-0.17566600
O	-1.40414600	0.84696700	-0.77236800
O	-0.60228800	0.38119300	1.17591200
C	-1.06714300	1.26344600	0.37860100
C	-3.80377600	-0.46443100	0.84144600
C	-3.30890700	0.04350800	2.16381100
C	-2.50995200	-0.73973800	3.00770300
C	-3.71184800	1.31627300	2.58782900
C	-2.09430700	-0.24545700	4.24322500
H	-2.20764000	-1.73365400	2.67698300
C	-3.27526700	1.82361700	3.81151900
H	-4.36188000	1.90264200	1.93765800
C	-2.46385800	1.04368400	4.64124700
H	-1.47262900	-0.86253500	4.89670000
H	-3.56791200	2.83014000	4.11902600
H	-2.12420900	1.43840500	5.60220500
O	-4.89737300	-0.11859400	0.41104900
N	-3.62311900	-2.12995700	-0.76070000
C	-3.86012800	-1.81544100	-2.09692100
C	-3.94299100	-3.45400700	-0.53033000
C	-4.32606800	-2.94746500	-2.73364200
C	-4.38797500	-4.00960300	-1.76464600
H	-4.62535100	-2.99871100	-3.77861200
C	-3.65481900	-0.44017400	-2.62622900
H	-3.92478100	-0.40762500	-3.69068800
H	-4.28765900	0.26820700	-2.07019500
H	-2.61608800	-0.10160200	-2.50570600
C	-4.75297800	-5.36737500	-1.79584000
C	-4.65547300	-6.12442800	-0.62919800
C	-4.20352300	-5.55116400	0.57846800
C	-3.84200400	-4.20552700	0.64444500
H	-5.10641500	-5.82316900	-2.72440100
H	-4.93696200	-7.18019300	-0.64634000
H	-4.14446100	-6.16909500	1.47779200
H	-3.49903400	-3.74212700	1.57043500
C	-1.22612900	2.67661900	0.79227600
C	-0.38576300	3.21577800	1.79848100

C	-2.24238300	3.47697100	0.20318200
C	-0.53310100	4.56492700	2.14109800
C	-2.35355800	4.81206200	0.60152900
C	-1.50035500	5.38280400	1.55357500
H	0.13096000	4.98449500	2.90098000
H	-3.14381800	5.42502300	0.15908200
C	0.64771500	2.40796900	2.53859700
H	0.16002100	1.65904000	3.17883400
H	1.30686400	1.85972000	1.85516600
H	1.26979500	3.06687600	3.15908200
C	-3.25923700	2.94696700	-0.77892200
H	-3.75225300	2.03624500	-0.41194400
H	-4.03363000	3.70532800	-0.96185400
H	-2.80744100	2.67519400	-1.74154400
C	-1.62873500	6.83691900	1.92600300
H	-2.68125600	7.11712400	2.09023300
H	-1.06307000	7.07316600	2.83903000
H	-1.24628200	7.48528800	1.11879600

(S_{NN}) -TS1

C	0.26080600	-3.31981300	-1.16309700
C	-0.36768400	-3.80314200	0.02906700
C	0.16026400	-3.03576600	1.12348000
C	1.04334700	-2.05704800	0.59814400
C	1.12437100	-2.23179200	-0.84181200
C	1.71782500	-0.98551800	1.40297700
C	2.04731500	-1.52397700	-1.80345600
H	0.07928600	-3.69544300	-2.16818500
H	-0.09433200	-3.14441500	2.17411600
O	0.51499100	0.00182900	-3.50300600
O	3.46539000	-2.48286000	2.87623900
C	2.01893100	-0.01644400	-1.68542500
C	1.16753600	0.73189500	-2.56099600
C	1.05475000	2.10023500	-2.43493400
C	1.76776500	2.79270000	-1.42116900
C	1.61114800	4.19097900	-1.22951700
C	2.29323700	4.84717300	-0.22781400
C	3.16691300	4.13292400	0.62627200
C	3.34277500	2.77401000	0.46134300
C	2.65139900	2.06850300	-0.56030300
C	2.77441700	0.64986800	-0.73400100
C	-0.26618300	0.67970300	-4.46789600
C	3.20259000	-0.91894900	1.14635500
C	3.71180000	-0.12677900	0.13299800

C	5.12466500	-0.07524200	-0.11334700
C	5.68918000	0.70954600	-1.15515100
C	7.05334700	0.74002400	-1.36092400
C	7.91572900	-0.01786200	-0.53322300
C	7.39713700	-0.79737100	0.47964900
C	5.99637400	-0.85288400	0.71561700
C	5.44873400	-1.67069400	1.74237100
C	4.08401800	-1.71552500	1.94332800
C	4.24702800	-3.29124400	3.72595000
H	0.39783700	2.67432200	-3.08530900
H	0.91461500	4.73293800	-1.87236100
H	2.15017200	5.92055900	-0.08285200
H	3.69962600	4.65878600	1.42187700
H	4.01073100	2.22303000	1.12465500
H	-1.12843700	1.17375700	-3.99638300
H	-0.63145800	-0.08308400	-5.16676600
H	0.33813300	1.41976200	-5.02015000
H	5.02531300	1.29422800	-1.79293600
H	7.47029500	1.35091300	-2.16478600
H	8.99499500	0.01336100	-0.70100700
H	8.05990400	-1.38907100	1.11658900
H	6.13073400	-2.26244800	2.35212900
H	3.54769600	-3.81596800	4.38963200
H	4.94097500	-2.68638200	4.33619300
H	4.83179400	-4.03389800	3.15460700
H	1.51751800	-1.16393900	2.46575200
H	1.25731400	-0.02995500	1.12971900
H	3.07217400	-1.88415400	-1.62106800
H	1.77187500	-1.81646100	-2.82341300
H	-1.06770600	-4.63330100	0.09365600
N	-2.86709300	-1.69038600	0.62179800
Rh	-0.99409300	-1.74210200	-0.28255400
O	-2.07172800	0.78761400	-1.69121100
O	-0.89537800	0.32229500	0.11904400
C	-1.46888400	1.16283100	-0.64301900
C	-3.99205500	-1.93835900	-0.12088700
C	-3.61611700	-2.23559800	-1.54120800
C	-2.33884900	-1.82977100	-1.98605200
C	-4.49534500	-2.91058600	-2.38711900
C	-1.94860300	-2.16581500	-3.29734600
H	-2.03847200	-0.58417700	-1.72020700
C	-4.09202800	-3.23131200	-3.68613800
H	-5.48066100	-3.18476200	-2.00354800
C	-2.81650400	-2.86530500	-4.13764700

H	-0.96819800	-1.84964700	-3.65497900
H	-4.77075100	-3.77086200	-4.35146600
H	-2.50493700	-3.11886100	-5.15442300
O	-5.14308500	-1.92105800	0.28920900
N	-3.04249600	-1.27698700	1.91335500
C	-3.39229500	0.01577600	2.31206400
C	-2.67976000	-2.02103200	3.02046200
C	-3.19953300	0.11906000	3.67193400
C	-2.74021300	-1.15765100	4.15257900
H	-3.42046900	0.99991900	4.27127500
C	-4.02243500	0.97112900	1.36049800
H	-3.86199700	2.00868300	1.68238300
H	-3.63698700	0.85293200	0.34231400
H	-5.10568100	0.77409400	1.30305000
C	-2.40677800	-1.67886100	5.41469400
C	-2.04298200	-3.02052900	5.52286100
C	-2.02411400	-3.86362800	4.39222200
C	-2.34808700	-3.37372600	3.12627200
H	-2.44383400	-1.04118600	6.30168500
H	-1.78738800	-3.43352600	6.50177800
H	-1.76977000	-4.91970400	4.51213400
H	-2.37502600	-4.02004700	2.24855200
C	-1.45358800	2.61430800	-0.27392800
C	-0.86739400	3.05297100	0.94872100
C	-2.05070800	3.57444700	-1.14086000
C	-0.86585800	4.41954800	1.24553500
C	-2.00131300	4.92955400	-0.79010200
C	-1.40823700	5.37848700	0.39024100
H	-0.40527800	4.74404000	2.18192400
H	-2.45577000	5.65863500	-1.46593400
C	-0.21956300	2.15356900	1.96999900
H	-0.85450100	1.30501900	2.25110000
H	0.71994200	1.74552300	1.57532900
H	0.02238800	2.73390500	2.87129700
C	-2.76333400	3.24934700	-2.43197700
H	-3.16991900	4.17081300	-2.87279600
H	-2.09351600	2.78242300	-3.16669000
H	-3.58211200	2.53421900	-2.27979600
C	-1.32581100	6.84419200	0.72300100
H	-1.55575200	7.02958900	1.78377300
H	-0.30484900	7.22455600	0.54389800
H	-2.01576700	7.44144700	0.10919000

(R_{NN}) -TS1

C	-0.36061400	-0.67875300	-2.59220000
C	-1.05637800	-1.49298700	-3.54747400
C	-0.31897600	-2.72472900	-3.66130600
C	0.75122400	-2.71095600	-2.73812700
C	0.73009100	-1.41713000	-2.06516000
C	1.80604000	-3.76853000	-2.57919000
C	1.76326200	-0.83528600	-1.13744800
H	-0.64768300	0.32328000	-2.28081900
H	-0.56834800	-3.55860600	-4.31380100
O	0.97578700	-0.87756000	1.48189800
O	2.71843800	-3.72210800	-5.15008100
C	2.42193300	-1.76796100	-0.14530000
C	1.98173900	-1.74002300	1.21834800
C	2.59556000	-2.52689200	2.17268700
C	3.65631500	-3.39782500	1.81597400
C	4.26520700	-4.25331900	2.77409100
C	5.26033900	-5.13443900	2.40662500
C	5.69379300	-5.19636300	1.05998600
C	5.12981400	-4.36908700	0.11007300
C	4.10476300	-3.44838400	0.45802300
C	3.47479800	-2.59447100	-0.50791100
C	0.58438600	-0.68053600	2.82410200
C	3.16197900	-3.18556900	-2.90579800
C	3.94952300	-2.60665700	-1.92454200
C	5.20404100	-1.99540000	-2.26312000
C	6.02926000	-1.36195700	-1.29443900
C	7.23094700	-0.78627900	-1.65284800
C	7.66169000	-0.81622200	-3.00063000
C	6.87763100	-1.41269200	-3.96585300
C	5.63251600	-2.01047300	-3.62946100
C	4.80361600	-2.60469300	-4.62054100
C	3.59126400	-3.16259700	-4.27068400
C	3.05578200	-3.75240100	-6.51837900
H	2.25979800	-2.51962800	3.20789300
H	3.91760800	-4.20816100	3.80886900
H	5.71483200	-5.78990700	3.15351800
H	6.47767300	-5.90111400	0.77352100
H	5.46432200	-4.42072800	-0.92666600
H	0.18054900	-1.60635600	3.26556900
H	-0.19976500	0.08412100	2.80116400
H	1.43322800	-0.32886300	3.43662700
H	5.69907800	-1.33782000	-0.25558200

H	7.85238500	-0.30485900	-0.89444500
H	8.61581400	-0.36047800	-3.27591500
H	7.20276500	-1.43003800	-5.00939000
H	5.14534400	-2.59367100	-5.65497900
H	3.19208600	-2.73501300	-6.92571300
H	2.21973700	-4.23876300	-7.03769200
H	3.97857800	-4.33240400	-6.69631200
H	1.57672400	-4.60557900	-3.24950200
H	1.80398100	-4.14257500	-1.55213700
H	2.54746700	-0.40589500	-1.78455800
H	1.29844000	-0.00346500	-0.59477300
H	-1.91936200	-1.20176000	-4.14189800
N	-2.85293700	-1.57782900	-0.74770500
Rh	-1.21877100	-2.49020400	-1.65135100
O	-2.27263500	-4.89526200	0.15989900
O	-0.66047800	-3.35881200	0.20611800
C	-1.26516600	-4.36353400	0.69220200
C	-4.10279400	-1.88093900	-1.24548200
C	-4.03978300	-3.06369700	-2.16479600
C	-2.86050400	-3.84000100	-2.17562700
C	-5.09834100	-3.34480400	-3.02731700
C	-2.76615900	-4.90373300	-3.09578600
H	-2.45577300	-4.22556000	-1.02791400
C	-4.98069800	-4.39874200	-3.93828200
H	-5.99173000	-2.71838900	-2.97819500
C	-3.81529400	-5.17772500	-3.97383700
H	-1.87905300	-5.54291600	-3.08716600
H	-5.80185700	-4.61980300	-4.62481000
H	-3.73699700	-6.00953100	-4.67847600
O	-5.12803800	-1.26166400	-1.01398900
N	-2.75482200	-0.37688800	-0.09754900
C	-2.59667600	-0.21937400	1.27533700
C	-2.79212400	0.86636200	-0.70716300
C	-2.47842200	1.12420700	1.55421800
C	-2.58854400	1.84218200	0.31031700
H	-2.36884900	1.55412300	2.54792300
C	-2.63772700	-1.40219400	2.17058100
H	-3.56758300	-1.96722800	2.00900300
H	-1.79999000	-2.08209500	1.96720900
H	-2.59752400	-1.08825300	3.22201400
C	-2.55794400	3.19926600	-0.05354100
C	-2.73847600	3.54890100	-1.39082400
C	-2.96847000	2.56594000	-2.37538500
C	-3.00552000	1.21150700	-2.04409700

H	-2.40174000	3.97037300	0.70523700
H	-2.71859000	4.60204700	-1.68146100
H	-3.13606800	2.87075400	-3.41122100
H	-3.22033000	0.44781300	-2.79190500
C	-0.71559800	-4.93059800	1.97378800
C	-1.49442300	-4.97258700	3.14414000
C	0.61005900	-5.42513300	1.97577700
C	-0.89161900	-5.42502700	4.33078100
C	1.15681900	-5.88891200	3.17101500
C	0.42824000	-5.87386900	4.37028300
H	-1.48855900	-5.43746900	5.24768000
H	2.18033500	-6.27188400	3.16472000
C	-2.95008100	-4.57516300	3.19133300
H	-3.10581100	-3.72682500	3.87602600
H	-3.34839300	-4.31085800	2.20727700
H	-3.55120900	-5.41426400	3.57692700
C	1.40904300	-5.49511500	0.70333200
H	0.86075400	-6.04597100	-0.07856600
H	1.59762000	-4.48758700	0.32009000
H	2.37597700	-5.98871200	0.86428400
C	1.05861200	-6.36200800	5.64963700
H	0.38356300	-6.23744400	6.50874400
H	1.32315100	-7.43043800	5.57980900
H	1.99164800	-5.81624000	5.86794800

(S_{NN}) -IM2

C	0.26035500	-4.27479800	-1.42116000
C	-0.35887400	-4.87669900	-0.30182200
C	0.05441800	-4.15860700	0.89301000
C	0.84773400	-3.07345200	0.50832700
C	0.94708900	-3.09984400	-0.95985600
C	1.41631100	-2.01562000	1.41146600
C	1.81794400	-2.23275200	-1.82757500
H	0.18185900	-4.59002100	-2.45900300
H	-0.26912400	-4.37096700	1.90989000
O	0.22528300	-0.60065400	-3.32772700
O	3.15271000	-3.55420400	2.83837500
C	1.75934300	-0.74786500	-1.55023800
C	0.91109500	0.06598200	-2.37137200
C	0.84564100	1.43176800	-2.17916200
C	1.58693400	2.04956200	-1.13738300
C	1.49032100	3.44476400	-0.88512500
C	2.17354600	4.02412300	0.16350700
C	2.98704000	3.23095000	1.00799100

C	3.10931200	1.87531200	0.78062900
C	2.42177600	1.25004500	-0.29416300
C	2.51311300	-0.15965800	-0.54736300
C	-0.70700200	0.10523100	-4.12092800
C	2.90662200	-1.87592900	1.21557900
C	3.43107300	-1.00197000	0.27869100
C	4.85004100	-0.91892600	0.07135300
C	5.43097500	-0.05942500	-0.90053300
C	6.79900200	-0.00363400	-1.07252800
C	7.65035500	-0.80898900	-0.27915300
C	7.11658800	-1.66083000	0.66508700
C	5.71139600	-1.74470600	0.86343700
C	5.14992200	-2.63753600	1.81709300
C	3.78159200	-2.71380600	1.97816700
C	3.92641800	-4.40339900	3.65416300
H	0.20797900	2.05677600	-2.80253600
H	0.85046400	4.05106100	-1.53126800
H	2.08296700	5.09705700	0.34897500
H	3.51787800	3.69426400	1.84265800
H	3.73365900	1.26453100	1.43365200
H	-1.48409400	0.57537800	-3.49666400
H	-1.18366200	-0.63595600	-4.77150200
H	-0.20845400	0.87665400	-4.73364700
H	4.77730900	0.56257000	-1.51262200
H	7.22726900	0.66412700	-1.82345700
H	8.73274100	-0.75713800	-0.41944200
H	7.77037000	-2.28980300	1.27501400
H	5.82491300	-3.26186000	2.40159300
H	3.21998900	-4.98025500	4.26497400
H	4.59469700	-3.82854900	4.31955300
H	4.53781200	-5.09882500	3.05189400
H	1.18249100	-2.27538300	2.44993500
H	0.92815300	-1.05636800	1.20279400
H	2.85421900	-2.58385000	-1.68723600
H	1.54306700	-2.41422800	-2.87314600
H	-1.00233000	-5.75515700	-0.31955100
N	-2.14026600	-1.36102600	0.30048300
Rh	-1.13333500	-2.83715000	-0.53186700
C	-3.11101200	-0.67455700	-0.43763100
C	-3.19855800	-1.25400900	-1.81322100
C	-2.32365400	-2.31937700	-2.10102700
C	-4.11084300	-0.76983100	-2.75085500
C	-2.39374700	-2.90082100	-3.37232200
C	-4.16871900	-1.36262800	-4.01674100

H	-4.76649500	0.05890100	-2.47171200
C	-3.31395800	-2.42779800	-4.32033800
H	-1.73505400	-3.72972600	-3.64210700
H	-4.88115300	-1.00123700	-4.76219100
H	-3.36178100	-2.89716400	-5.30719900
O	-3.76978800	0.25680100	-0.01883200
N	-1.88430800	-0.92660300	1.58038500
C	-1.22626500	0.25711600	1.92579600
C	-1.98060000	-1.74846100	2.69115400
C	-0.91351000	0.20376800	3.26614400
C	-1.36875100	-1.06042700	3.77869800
H	-0.41053200	0.99262400	3.82132500
C	-0.97498000	1.31427900	0.91355200
H	-0.23929300	2.03781700	1.28684400
H	-0.58775900	0.87744300	-0.01766700
H	-1.90896300	1.83806300	0.65656800
C	-1.31525500	-1.69680700	5.03231400
C	-1.85509500	-2.97359100	5.17030600
C	-2.46432900	-3.62950000	4.07896900
C	-2.53838700	-3.02313200	2.82514400
H	-0.85402600	-1.19353200	5.88588600
H	-1.81632400	-3.47472600	6.14060100
H	-2.89542400	-4.62354600	4.22126100
H	-3.01602900	-3.51587800	1.97663700

(S_{NN}) -IM3

C	-0.06338100	0.43602700	-2.16635100
C	-0.73151300	0.21937600	-3.37142500
C	-0.25850800	-1.04327400	-3.92132600
C	0.74649200	-1.57144100	-3.08359700
C	0.79841700	-0.71815500	-1.91009300
C	1.62875500	-2.75310200	-3.38381800
C	1.73030100	-0.83463100	-0.73140500
H	-0.22539600	1.25491800	-1.46779000
H	-0.57967100	-1.48452200	-4.86388800
O	0.29411500	-1.81143900	1.42416400
O	3.13782400	-1.67885500	-5.41662800
C	1.92928400	-2.24696400	-0.22433400
C	1.13817700	-2.71874800	0.87442700
C	1.25770800	-4.01835300	1.32057400
C	2.14980100	-4.92025300	0.68739600
C	2.24061000	-6.28105500	1.08872400
C	3.10080900	-7.15129700	0.45317300
C	3.91340300	-6.69790600	-0.61459400

C	3.84851900	-5.38253900	-1.02597800
C	2.97013000	-4.46210700	-0.39185500
C	2.84816100	-3.09923300	-0.81692400
C	-0.39607000	-2.14324600	2.61727400
C	3.08676500	-2.41296000	-3.18628400
C	3.68122600	-2.59354700	-1.94975900
C	5.05908200	-2.25524800	-1.74438200
C	5.70387900	-2.41563600	-0.48798000
C	7.03276300	-2.08136600	-0.32621300
C	7.77557900	-1.56641400	-1.41567900
C	7.17490400	-1.39084000	-2.64489100
C	5.80752800	-1.72439600	-2.84435300
C	5.17026000	-1.52905800	-4.10105200
C	3.83853000	-1.85356500	-4.26570700
C	3.79602800	-1.13196400	-6.53664700
H	0.64122900	-4.38757400	2.13771600
H	1.60609800	-6.62771800	1.90810300
H	3.15613900	-8.19540400	0.77068900
H	4.59112800	-7.39358300	-1.11466800
H	4.47060400	-5.03437900	-1.85173300
H	-1.06560900	-3.00239400	2.46814500
H	-1.00438000	-1.26834600	2.87509400
H	0.31601300	-2.36381200	3.43107300
H	5.13074600	-2.81226200	0.35103100
H	7.51427600	-2.21310400	0.64537000
H	8.82755400	-1.30448500	-1.27915500
H	7.74482000	-0.98782500	-3.48615600
H	5.75691700	-1.11118100	-4.91855200
H	4.18011000	-0.11809200	-6.32622200
H	3.05231200	-1.07514300	-7.34213300
H	4.63673300	-1.76858500	-6.86480300
H	1.44779700	-3.07058400	-4.41803500
H	1.38221000	-3.58954000	-2.72324800
H	2.70165700	-0.41475600	-1.04178800
H	1.34484900	-0.19885700	0.07358300
H	-1.50499900	0.85304200	-3.80192900
N	-2.53659200	-1.17954300	-0.54981600
Rh	-1.17212700	-1.49353400	-1.94117400
C	-2.85649600	-2.19255800	0.35511600
C	-2.18544800	-3.46072800	-0.05532900
C	-1.35954800	-3.39236000	-1.19404900
C	-2.38395900	-4.64921800	0.64679800
C	-0.77111600	-4.58033300	-1.64015900
C	-1.74914800	-5.81699400	0.21146400

H	-3.03808000	-4.64068800	1.52274600
C	-0.95502400	-5.77992600	-0.93763200
H	-0.16073300	-4.59940500	-2.54352500
H	-1.88268500	-6.75427900	0.75685700
H	-0.46462000	-6.69060500	-1.29107400
O	-3.58276700	-2.05239300	1.32066800
N	-3.05585800	0.06846500	-0.29891300
C	-4.24922200	0.53632700	-0.84323000
C	-2.41256600	1.09038600	0.37289600
C	-4.38517600	1.86788000	-0.51863300
C	-3.22972200	2.25184300	0.24903900
H	-5.23042400	2.49807600	-0.78729200
C	-5.14003500	-0.38213400	-1.60352500
H	-4.62411700	-0.81618000	-2.47619400
H	-5.46688300	-1.22356000	-0.97057100
H	-6.02934500	0.15802500	-1.95490500
C	-2.78532000	3.45048600	0.83562100
C	-1.56277600	3.46893100	1.50435700
C	-0.77007900	2.30601400	1.60461400
C	-1.18470900	1.09882500	1.04095900
H	-3.39157900	4.35712500	0.76285400
H	-1.21107700	4.39726000	1.96103500
H	0.18261300	2.34843000	2.13855200
H	-0.58435400	0.19348200	1.10974000

(S_{NN}) -IM4

C	1.12659600	-1.76593400	0.64383300
C	1.41656600	-0.38047200	0.38660200
C	1.62941400	-0.24796700	-1.00506800
C	1.54468200	-1.56452700	-1.59940100
C	1.27073600	-2.51419600	-0.58157700
C	1.75572900	-1.83947700	-3.05953500
C	1.22083800	-4.01953600	-0.71038100
H	0.92604700	-2.19650900	1.62223000
H	1.86927400	0.66440600	-1.54683200
O	-1.38917400	-4.88962700	-0.45918600
O	4.41026400	-1.19308000	-3.24506000
C	0.43956600	-4.54216100	-1.90024700
C	-0.92052200	-4.96380000	-1.72153700
C	-1.66309100	-5.42431100	-2.79188500
C	-1.10829800	-5.45193300	-4.09838900
C	-1.87889600	-5.84386900	-5.22727500
C	-1.33712200	-5.82822600	-6.49583600
C	0.00525000	-5.42292700	-6.69178700

C	0.78012500	-5.04395300	-5.61411300
C	0.24968500	-5.04611600	-4.29574200
C	1.01501200	-4.62275300	-3.15900200
C	-2.73921800	-5.23963000	-0.18946400
C	2.80227800	-2.90531500	-3.27297900
C	2.44828900	-4.24080200	-3.33155600
C	3.44698400	-5.25535000	-3.51350400
C	3.12889900	-6.63950100	-3.56392600
C	4.11519600	-7.58812400	-3.74214100
C	5.46793000	-7.19365800	-3.87357400
C	5.80930900	-5.85831900	-3.81803600
C	4.81726400	-4.85713700	-3.63405400
C	5.15959400	-3.47872500	-3.55257400
C	4.17879900	-2.52696600	-3.36240600
C	5.73793400	-0.72471300	-3.30546600
H	-2.69822600	-5.73456100	-2.65816200
H	-2.91667500	-6.14960600	-5.07204600
H	-1.94469700	-6.12677800	-7.35351300
H	0.42757400	-5.41035600	-7.69918700
H	1.81346400	-4.72940600	-5.76626300
H	-3.43551800	-4.57379300	-0.72316800
H	-2.87413100	-5.10737000	0.89043400
H	-2.93196100	-6.29235300	-0.45831400
H	2.08725100	-6.94551100	-3.46084200
H	3.85206000	-8.64761400	-3.78040900
H	6.24291900	-7.95081300	-4.01511000
H	6.85399000	-5.55033200	-3.91201900
H	6.21006000	-3.20131000	-3.63398300
H	5.69338000	0.36454900	-3.17608000
H	6.20679700	-0.95441200	-4.27883100
H	6.35827300	-1.15950200	-2.50183700
H	2.05352300	-0.90987500	-3.55724300
H	0.81253000	-2.16838400	-3.51131100
H	2.25742100	-4.38770300	-0.78054000
H	0.79764200	-4.43595900	0.21067600
H	1.44184400	0.41789500	1.12423700
N	-2.28612800	-1.78491800	-0.09928400
Rh	-0.46870600	-0.90436300	-0.61648800
C	-2.98305000	-1.89753200	-1.24816500
C	-2.15799400	-1.28872300	-2.37047900
C	-1.73264500	0.08465700	-2.38227700
C	-1.94420400	-2.08889000	-3.51749500
C	-1.06482900	0.55613500	-3.55161800
C	-1.29015800	-1.59739000	-4.62981700

H	-2.32309200	-3.10828400	-3.50238000
C	-0.84337400	-0.25786100	-4.64355600
H	-0.76308000	1.60534600	-3.57483600
H	-1.12793200	-2.24488900	-5.49449200
H	-0.33401500	0.13826300	-5.52525200
O	-4.07856100	-2.41119900	-1.44979600
N	-2.92434800	-1.88301200	1.11234800
C	-4.01430600	-1.09733500	1.52999000
C	-2.37103800	-2.51399700	2.21502700
C	-4.16588500	-1.25298800	2.88785000
C	-3.13115900	-2.12864700	3.35727500
H	-4.94404500	-0.78147700	3.48364300
C	-4.84966600	-0.30783300	0.58585600
H	-5.52828700	0.34035700	1.15568200
H	-4.23627500	0.32635200	-0.06753000
H	-5.43183400	-0.97178900	-0.07054600
C	-2.75428000	-2.61822900	4.61960600
C	-1.65176800	-3.46475500	4.72106800
C	-0.92819400	-3.85097700	3.57386400
C	-1.28223900	-3.38446100	2.30702800
H	-3.32086900	-2.33421400	5.51013400
H	-1.35101800	-3.84785600	5.69929700
H	-0.08596900	-4.54036100	3.67476500
H	-0.76976000	-3.71380100	1.40865300
C	-2.08536300	1.08821700	-1.31141000
C	-1.55468300	0.73925900	-0.11606700
C	-2.89000000	2.25789000	-1.73483700
C	-2.50021700	3.57505800	-1.43362700
C	-4.05110400	2.05931200	-2.50466200
C	-3.26339400	4.66037400	-1.86599700
H	-1.58881800	3.73816000	-0.85449300
C	-4.81613900	3.14505800	-2.93307500
H	-4.35740900	1.04028800	-2.75353400
C	-4.42655300	4.44938900	-2.61370400
H	-2.94571100	5.67755500	-1.62357200
H	-5.72242500	2.97196400	-3.51852800
H	-5.02395000	5.29948700	-2.95163800
C	-1.80231900	1.20836600	1.25228900
C	-2.75082900	2.21510700	1.54775200
C	-1.18369900	0.56807400	2.34487500
C	-3.04424500	2.56442700	2.86301200
H	-3.28259900	2.71265300	0.74050600
C	-1.48086100	0.91362500	3.66159400
H	-0.50551700	-0.25930600	2.15810200

C	-2.40932300	1.91950500	3.93009200
H	-3.78683400	3.34254300	3.05732300
H	-1.00451200	0.36794800	4.47872800
H	-2.65109300	2.18893500	4.96097600

(S_{NN}) -IM5

C	1.58130400	0.34453300	-1.07174500
C	0.89280000	1.53538400	-0.63025900
C	-0.17143700	1.76695200	-1.52690500
C	-0.17693300	0.69963000	-2.50342200
C	0.97939900	-0.12866400	-2.26198300
C	-1.06459600	0.64926900	-3.72045300
C	1.57700800	-1.19420600	-3.14461600
H	2.44702800	-0.10167400	-0.58420000
H	-0.86833700	2.60143900	-1.50984900
O	1.04270100	-3.75984600	-2.29036600
O	-0.48867300	3.12376500	-4.72243400
C	0.62800400	-2.09169700	-3.90668800
C	0.40719400	-3.42977100	-3.44453400
C	-0.37791800	-4.30769500	-4.16181200
C	-1.03483600	-3.88491600	-5.34511100
C	-1.89893000	-4.75376100	-6.06561400
C	-2.57155200	-4.31470300	-7.18662200
C	-2.40613000	-2.98303200	-7.63890900
C	-1.56500600	-2.12044400	-6.96599800
C	-0.85630100	-2.54376900	-5.80869200
C	0.02286700	-1.67260000	-5.08248600
C	0.95265800	-5.08775200	-1.82777400
C	-0.23302200	0.80198300	-4.97045700
C	0.30202800	-0.30233800	-5.61070300
C	1.14354000	-0.14141200	-6.76400500
C	1.73839000	-1.24334600	-7.43643200
C	2.53952600	-1.05224000	-8.54390900
C	2.78537600	0.25411700	-9.02881800
C	2.23199000	1.34476100	-8.39095200
C	1.40568500	1.18136400	-7.24601000
C	0.84936800	2.30129600	-6.56818900
C	0.06265000	2.11745800	-5.45004200
C	-0.24400500	4.45682200	-5.10719200
H	-0.55051500	-5.32418200	-3.81342800
H	-2.03194700	-5.77678600	-5.70438200
H	-3.23742400	-4.99235500	-7.72646500
H	-2.94708700	-2.63859600	-8.52318200
H	-1.43882200	-1.09475100	-7.31451300

H	-0.08836800	-5.36052100	-1.58158300
H	1.56769800	-5.14508900	-0.92072300
H	1.34252600	-5.80244200	-2.57387200
H	1.55246400	-2.25145600	-7.06471900
H	2.98644000	-1.91208600	-9.04819100
H	3.41863300	0.39726100	-9.90771100
H	2.42529300	2.35645200	-8.75731800
H	1.07014300	3.29813500	-6.94847600
H	-0.77016500	5.09424500	-4.38469800
H	-0.62976100	4.66483700	-6.12105200
H	0.83419600	4.69451000	-5.08176100
H	-1.81003300	1.44853200	-3.65849200
H	-1.60171900	-0.30346100	-3.76599700
H	2.21566500	-0.67747100	-3.88212300
H	2.23749900	-1.81493100	-2.52718700
H	1.15146700	2.13754000	0.23880700
N	-2.75208500	0.08039300	1.45237900
Rh	-0.54984500	-0.16887700	-0.46019500
C	-1.64426500	0.07763400	2.28378100
C	-0.53689600	-0.75914100	1.72636700
C	-0.81801400	-1.88701300	0.85007800
C	0.70030500	-0.75062100	2.45368300
C	0.10972700	-2.98481800	0.82954200
C	1.58984400	-1.78665900	2.35006900
H	0.87209900	0.08604900	3.13272000
C	1.27274700	-2.92588400	1.54871900
H	-0.12152400	-3.84834400	0.21313400
H	2.52552800	-1.76731800	2.91316900
H	1.97485400	-3.76272700	1.50871700
O	-1.59281100	0.66980700	3.34117400
N	-3.80783800	0.88409600	1.76785200
C	-5.00819000	0.44387300	2.32714700
C	-3.88014200	2.23763700	1.48604600
C	-5.87046500	1.51234700	2.38157300
C	-5.18592600	2.66486400	1.84978600
H	-6.88239400	1.48290500	2.77999500
C	-5.14927500	-0.95934100	2.80185200
H	-6.16655400	-1.13003000	3.17846800
H	-4.94887300	-1.68737400	2.00052900
H	-4.43549500	-1.16852500	3.61644800
C	-5.53032000	4.01233800	1.64093000
C	-4.58498600	4.87671500	1.09281700
C	-3.29151500	4.42581700	0.75448400
C	-2.92037200	3.09630100	0.94869000

H	-6.52637900	4.37510800	1.90681400
H	-4.84443900	5.92540600	0.92855100
H	-2.56695300	5.13171600	0.34094300
H	-1.92414100	2.73029900	0.69823400
C	-1.93227900	-1.72343000	-0.05954200
C	-2.58649800	-0.42309900	0.08007500
C	-2.42383600	-2.80584900	-0.94735800
C	-2.73782600	-2.57778800	-2.29547700
C	-2.69830100	-4.07305600	-0.40288800
C	-3.33269200	-3.57032600	-3.07049100
H	-2.52304900	-1.60635400	-2.73362000
C	-3.27186500	-5.07882900	-1.18639300
H	-2.48458200	-4.26238500	0.65123000
C	-3.59948000	-4.82719300	-2.52142900
H	-3.57726800	-3.36516100	-4.11326100
H	-3.48097600	-6.05601800	-0.74366300
H	-4.05925100	-5.60681500	-3.13344700
C	-3.75264500	-0.06239300	-0.79185700
C	-4.89301700	-0.88124100	-0.81501400
C	-3.75895000	1.10893300	-1.55683400
C	-6.00208600	-0.54223100	-1.58930100
H	-4.90510100	-1.80303900	-0.23259000
C	-4.86715900	1.45479500	-2.33194500
H	-2.88824800	1.75761700	-1.52972200
C	-5.99213600	0.62812300	-2.35302400
H	-6.87720900	-1.19609500	-1.59641600
H	-4.84996900	2.37757000	-2.91621500
H	-6.86034900	0.89578800	-2.96000000

(R_{NN})-IM2

C	-0.68761700	0.60511200	-2.17373100
C	-1.45881300	0.28896400	-3.29378500
C	-0.87079500	-0.88808000	-3.91160800
C	0.29096800	-1.26481000	-3.20502200
C	0.36634500	-0.40159100	-2.03728400
C	1.29025400	-2.30396300	-3.63706800
C	1.45089500	-0.34723000	-0.99116000
H	-0.89513000	1.39430600	-1.45201400
H	-1.23896000	-1.38106500	-4.81039200
O	0.60316700	-1.49580500	1.39014100
O	2.30207400	-1.06025900	-5.87253600
C	1.96496200	-1.69559500	-0.53480200
C	1.46132000	-2.26934900	0.67869900
C	1.86059900	-3.52758700	1.07903700

C	2.77297400	-4.28074500	0.29828400
C	3.15065900	-5.60168700	0.66345600
C	4.03571400	-6.32420300	-0.10862300
C	4.58602600	-5.75525500	-1.28306000
C	4.23746100	-4.47568500	-1.66376700
C	3.32459500	-3.70765300	-0.89055900
C	2.90844500	-2.39151700	-1.27494200
C	0.20967100	-1.93433600	2.67809000
C	2.68637500	-1.72936300	-3.65418400
C	3.46803200	-1.77173500	-2.51398300
C	4.78211800	-1.19800100	-2.50546400
C	5.61118700	-1.21015200	-1.35131300
C	6.87200000	-0.65003000	-1.37907500
C	7.35833400	-0.04906300	-2.56484700
C	6.57320500	-0.01390800	-3.69846700
C	5.26922100	-0.58000400	-3.70226700
C	4.44071900	-0.53211500	-4.85764600
C	3.17454600	-1.08174500	-4.83156200
C	2.69073600	-0.43191100	-7.07291000
H	1.45601500	-3.98291100	1.98049400
H	2.71923000	-6.03766800	1.56793700
H	4.31394800	-7.33974500	0.18342100
H	5.28615300	-6.33386900	-1.88998600
H	4.65698500	-4.04016600	-2.57169900
H	-0.37961300	-2.86152800	2.62178400
H	-0.41998300	-1.14377600	3.09905000
H	1.08988300	-2.09274000	3.32456300
H	5.23513700	-1.67403400	-0.43850600
H	7.49784000	-0.66960300	-0.48400000
H	8.35838100	0.39094300	-2.57893700
H	6.94427700	0.45505700	-4.61354300
H	4.82838700	-0.04490000	-5.75173300
H	2.91861600	0.63710300	-6.91491200
H	1.84234100	-0.52111200	-7.76382000
H	3.57441800	-0.92053300	-7.52031800
H	1.01165200	-2.66222100	-4.63541100
H	1.27761400	-3.15866400	-2.95379300
H	2.28365800	0.23758800	-1.41742200
H	1.06816000	0.21250000	-0.12895900
H	-2.37489600	0.78710700	-3.60601400
N	-2.68730100	-1.24721000	-0.29721400
Rh	-1.45499900	-1.44805900	-1.82391000
C	-2.69888100	-2.19579800	0.72046300
C	-1.89989400	-3.38476100	0.29308000

C	-1.23439300	-3.28374500	-0.94518000
C	-1.83184600	-4.53591300	1.07705000
C	-0.52004700	-4.39870200	-1.39347900
C	-1.08883600	-5.63179500	0.62389100
H	-2.36868300	-4.55789100	2.02918600
C	-0.44383100	-5.56190200	-0.61352100
H	-0.00836400	-4.38585400	-2.35699300
H	-1.02060300	-6.53953400	1.22828200
H	0.13529400	-6.41527700	-0.97554600
O	-3.26124300	-2.06676200	1.79309100
N	-3.35111900	-0.05710200	-0.11321700
C	-2.93279500	1.00848500	0.68661100
C	-4.28778800	0.39463300	-1.03172300
C	-3.63108800	2.13523900	0.31216800
C	-4.49737200	1.77953600	-0.78202800
H	-3.54636400	3.11068500	0.78711800
C	-1.90670300	0.81804600	1.74473000
H	-2.29256300	0.14907100	2.52995800
H	-0.99782700	0.34704400	1.33864500
H	-1.63926500	1.78534800	2.19094200
C	-5.40879800	2.48055600	-1.59167100
C	-6.05874700	1.80415800	-2.62216700
C	-5.82158100	0.43330900	-2.85830500
C	-4.93287900	-0.29135300	-2.06416200
H	-5.59822100	3.54283800	-1.41784800
H	-6.76596800	2.34117700	-3.25895300
H	-6.34952100	-0.07152200	-3.67096600
H	-4.74643100	-1.35347100	-2.23077600

(R_{NN}) -IM4

C	-0.85882400	-0.21617200	-3.19021500
C	-1.96081000	0.61210400	-2.79004100
C	-3.09247200	0.26562500	-3.60266700
C	-2.71776400	-0.83153500	-4.40843600
C	-1.31237400	-1.13623200	-4.18028000
C	-3.60350600	-1.54454000	-5.38570800
C	-0.38094300	-2.00522600	-4.99726600
H	0.15236300	-0.16421800	-2.79203000
H	-4.08179200	0.71438600	-3.57294000
O	0.37858600	-4.41638000	-3.82996000
O	-4.33230600	0.66760400	-6.80495200
C	-0.88843900	-3.33602400	-5.51477500
C	-0.43502000	-4.55466000	-4.90828400
C	-0.82827800	-5.78317000	-5.40120500

C	-1.74812300	-5.87132900	-6.47732800
C	-2.22964200	-7.12426000	-6.94688700
C	-3.14795500	-7.18886700	-7.97366900
C	-3.62278900	-6.00035600	-8.57924800
C	-3.16572500	-4.77113800	-8.15044000
C	-2.21994800	-4.67065600	-7.09382500
C	-1.73047900	-3.40942100	-6.61559000
C	0.85191100	-5.57738500	-3.17212700
C	-3.06217000	-1.30801000	-6.77590100
C	-2.13545800	-2.16632600	-7.33861800
C	-1.55293600	-1.87579100	-8.61918400
C	-0.57524700	-2.71351800	-9.22135000
C	-0.03474300	-2.40281800	-10.45247200
C	-0.44849700	-1.23652200	-11.13875000
C	-1.38929500	-0.39895800	-10.57665200
C	-1.96143000	-0.68888800	-9.30816700
C	-2.91614000	0.17901100	-8.70964300
C	-3.44184700	-0.11360700	-7.46829400
C	-4.74956000	1.87905300	-7.39290200
H	-0.47599800	-6.70850800	-4.94816800
H	-1.86376700	-8.03836600	-6.47219800
H	-3.51362600	-8.15827400	-8.32054200
H	-4.35413700	-6.05820600	-9.38849600
H	-3.53443400	-3.85728200	-8.61723800
H	0.02275800	-6.18786400	-2.77875600
H	1.45288400	-5.23244000	-2.32282100
H	1.47435200	-6.19205800	-3.84451100
H	-0.25332700	-3.61277000	-8.69528700
H	0.71580600	-3.05864000	-10.89945700
H	-0.01738500	-0.99867400	-12.11414000
H	-1.70657900	0.50687600	-11.09982800
H	-3.20696400	1.07973800	-9.24903000
H	-3.89715800	2.55886800	-7.56784200
H	-5.44489200	2.34828600	-6.68491500
H	-5.27045900	1.70749900	-8.35151400
H	-4.62733400	-1.16477700	-5.29536600
H	-3.61566800	-2.61894200	-5.16254900
H	-0.07749100	-1.40260700	-5.87119700
H	0.52356200	-2.17367300	-4.40091100
H	-1.92344000	1.40509400	-2.04595300
N	-3.40205400	-1.24043200	-0.40141300
Rh	-2.35579300	-1.44705500	-2.20520300
C	-4.23721300	-2.29341300	-0.27209900
C	-4.10078700	-3.14235100	-1.52259500

C	-2.90795400	-3.86743000	-1.81800500
C	-5.23888000	-3.29229700	-2.35031300
C	-2.92872200	-4.72381600	-2.94886400
C	-5.21094800	-4.11658800	-3.46127700
H	-6.14624800	-2.74986200	-2.07713500
C	-4.04279800	-4.84582400	-3.75903600
H	-2.04462200	-5.31597700	-3.16052000
H	-6.09389700	-4.21355700	-4.09705500
H	-4.01061000	-5.50971800	-4.62541100
O	-5.00287600	-2.57233600	0.63666900
N	-3.21868000	-0.39034000	0.65568900
C	-2.64512000	-0.71149300	1.89070300
C	-3.42868000	0.97350700	0.58082900
C	-2.46750400	0.45720300	2.60020600
C	-2.94660200	1.54683000	1.79325500
H	-2.06470000	0.51917700	3.60904400
C	-2.37040800	-2.11975600	2.28809400
H	-3.31503700	-2.67048200	2.41709100
H	-1.79219500	-2.65700900	1.52301200
H	-1.80593200	-2.13737600	3.22998500
C	-3.04097700	2.93927800	1.96369300
C	-3.60562000	3.71211400	0.95062700
C	-4.09797900	3.11773300	-0.23028500
C	-4.02116900	1.73904200	-0.42747300
H	-2.68092800	3.40764900	2.88331900
H	-3.68258400	4.79486500	1.07634000
H	-4.55975300	3.74588000	-0.99619700
H	-4.42682200	1.26085900	-1.31797400
C	-1.63904200	-3.78579700	-0.99226100
C	-1.07874500	-2.56493800	-1.11965300
C	-1.15969700	-4.97345200	-0.25830800
C	-1.91606800	-6.16329200	-0.25362600
C	0.04517600	-4.96275900	0.47740700
C	-1.47517100	-7.29985500	0.42677100
H	-2.86988000	-6.19816700	-0.78138400
C	0.48218400	-6.09854200	1.15615800
H	0.64326700	-4.05453500	0.52184300
C	-0.26891800	-7.27888000	1.12982100
H	-2.08588900	-8.20604900	0.41155600
H	1.41963500	-6.05951500	1.71676900
H	0.07766900	-8.16762100	1.66224300
C	0.21257100	-1.99220600	-0.72104000
C	0.30746600	-0.98499100	0.25787200
C	1.38454800	-2.36392500	-1.41127000

C	1.53908900	-0.40384800	0.56372200
H	-0.58598200	-0.64623300	0.77903900
C	2.61216400	-1.77373300	-1.10783300
H	1.30759200	-3.10033800	-2.20889500
C	2.69853800	-0.79537800	-0.11220500
H	1.58582400	0.36905300	1.33475400
H	3.50709600	-2.07701200	-1.65744400
H	3.65977800	-0.33439000	0.12679200

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C	-0.80953800	-0.50635800	-2.58178300
C	-1.14770300	0.10773100	-1.31626100
C	-2.45270400	0.62680600	-1.43124800
C	-2.93096500	0.33679400	-2.76439000
C	-1.87593700	-0.28064800	-3.50437500
C	-4.27229000	0.75792800	-3.29973400
C	-1.80326000	-0.53644900	-4.98995800
H	0.15111700	-0.95660100	-2.82778700
H	-3.02133800	1.15122400	-0.66586900
O	-2.05984600	-3.20669800	-5.61178200
O	-4.02217700	3.44997200	-2.88680000
C	-3.05408700	-1.06986500	-5.65636600
C	-3.13556000	-2.46482200	-5.97383100
C	-4.24065400	-2.98429700	-6.61797200
C	-5.34771800	-2.15407500	-6.93373900
C	-6.52571400	-2.67772100	-7.53370400
C	-7.60523700	-1.86286700	-7.80512700
C	-7.55211900	-0.48382400	-7.49042400
C	-6.41886800	0.05392300	-6.91488900
C	-5.29039600	-0.75906400	-6.62230100
C	-4.10254800	-0.23460000	-6.01113900
C	-1.99682600	-4.55594600	-6.02061100
C	-4.09558400	1.70675000	-4.45914700
C	-3.99687200	1.23364500	-5.75497100
C	-3.76847000	2.13575800	-6.84894600
C	-3.63693100	1.69080000	-8.19211800
C	-3.42191000	2.58670800	-9.21980300
C	-3.32503900	3.97213300	-8.94846600
C	-3.43671700	4.43374600	-7.65335600
C	-3.65519800	3.53643500	-6.57291300
C	-3.74908300	3.99943800	-5.23119500
C	-3.94870800	3.10642600	-4.19860900
C	-3.87548900	4.80414900	-2.52720100
H	-4.30099600	-4.04273200	-6.86737900

H	-6.56374100	-3.74414400	-7.77153500
H	-8.50522400	-2.28123200	-8.26225000
H	-8.41202200	0.15539400	-7.70298800
H	-6.38017600	1.11602300	-6.67023000
H	-2.79134300	-5.16053100	-5.55174700
H	-1.02854400	-4.93914200	-5.68396600
H	-2.07630200	-4.64434000	-7.11810100
H	-3.70997900	0.62339400	-8.40297500
H	-3.32550400	2.22594900	-10.24641900
H	-3.15715000	4.67560500	-9.76757100
H	-3.35509500	5.50253100	-7.43845800
H	-3.64860300	5.06821900	-5.04500100
H	-2.89142800	5.20081800	-2.83403000
H	-3.95683800	4.84963100	-1.43337600
H	-4.66628900	5.43206300	-2.97495900
H	-4.84247000	1.23784400	-2.49584400
H	-4.83960200	-0.12167100	-3.62669300
H	-1.54294600	0.42113400	-5.47285800
H	-0.97535500	-1.22991900	-5.17980600
H	-0.50420100	0.18119000	-0.44319900
N	-3.08163400	-3.13260400	0.78621600
Rh	-2.53433100	-1.61367000	-1.66030000
C	-4.31024900	-2.54509600	0.52243900
C	-4.56087700	-2.40243100	-0.94558500
C	-3.92414500	-3.28556700	-1.91088300
C	-5.77910200	-1.74828400	-1.32269800
C	-4.58007600	-3.52295600	-3.16606300
C	-6.34018600	-1.95568900	-2.55492300
H	-6.26170500	-1.12148300	-0.57140300
C	-5.74279500	-2.86935600	-3.47554400
H	-4.11422100	-4.20231800	-3.87658900
H	-7.26663600	-1.44800200	-2.83146100
H	-6.21416100	-3.03413600	-4.44546200
O	-5.09162700	-2.21065700	1.38773100
N	-2.65941100	-3.21228100	2.08101500
C	-2.76286200	-4.34640700	2.88712400
C	-2.00545700	-2.19993100	2.76184700
C	-2.14567400	-4.07584600	4.08478700
C	-1.64913700	-2.72299500	4.03448400
H	-2.07465400	-4.76454400	4.92400600
C	-3.51618100	-5.54093800	2.41813300
H	-4.58022700	-5.29377600	2.26469900
H	-3.13062300	-5.92185600	1.45932300
H	-3.45002000	-6.34542000	3.16272000

C	-0.94484600	-1.89230900	4.92434200
C	-0.62698400	-0.59362600	4.53225300
C	-1.00517800	-0.09908700	3.26613800
C	-1.70204300	-0.89817500	2.36110000
H	-0.65305800	-2.26185500	5.91061900
H	-0.08101500	0.05837800	5.21840700
H	-0.75313100	0.92869900	2.99322600
H	-2.00677200	-0.53487900	1.37937200
C	-2.58631600	-3.71939300	-1.58331700
C	-2.10664100	-3.20256200	-0.30653700
C	-1.81219000	-4.69751300	-2.38637100
C	-0.50361600	-4.43307500	-2.81810600
C	-2.34977300	-5.97570100	-2.60882100
C	0.26114800	-5.43131600	-3.42005700
H	-0.09086800	-3.43743500	-2.66097300
C	-1.58960500	-6.97254000	-3.22698800
H	-3.36490800	-6.19491200	-2.26930100
C	-0.27639100	-6.70716100	-3.62313300
H	1.28421400	-5.21196900	-3.73458400
H	-2.02109300	-7.96397100	-3.38547400
H	0.32504100	-7.48920300	-4.09262500
C	-0.74078000	-3.60726400	0.16834700
C	-0.48999300	-4.96057200	0.44716100
C	0.29558900	-2.68720600	0.35149500
C	0.76010000	-5.37996300	0.89903200
H	-1.28035700	-5.69514100	0.28873500
C	1.55088400	-3.10111200	0.80309200
H	0.10838100	-1.63848000	0.14311000
C	1.78718500	-4.44894100	1.07870600
H	0.93418800	-6.43809700	1.10765100
H	2.34396400	-2.36339700	0.94502200
H	2.76821700	-4.77434600	1.43310800

(S_{NV})-TS2

C	1.18813200	-1.67494600	0.81345800
C	1.46209300	-0.29704300	0.60366500
C	1.64781100	-0.10906500	-0.79614100
C	1.59112100	-1.39701600	-1.44519800
C	1.30385100	-2.37264400	-0.45912200
C	1.79433800	-1.62111100	-2.91900000
C	1.28087300	-3.87455900	-0.63294800
H	1.00622200	-2.15074000	1.77326200
H	1.87812500	0.82966700	-1.29713000
O	-1.22612400	-4.94636600	-0.25790900

O	4.47351700	-1.06153300	-3.15709500
C	0.45132400	-4.36656800	-1.80031700
C	-0.87851400	-4.84715600	-1.55726700
C	-1.70047400	-5.20594900	-2.60686500
C	-1.24078200	-5.11281500	-3.94523900
C	-2.09137600	-5.40444700	-5.04663600
C	-1.63739500	-5.29058600	-6.34417800
C	-0.30413200	-4.88768900	-6.59943800
C	0.54804000	-4.60743500	-5.55052100
C	0.10647200	-4.70532200	-4.20376300
C	0.94929900	-4.36725200	-3.09425700
C	-2.48779200	-5.49679600	0.09730700
C	2.79757200	-2.70741500	-3.20692500
C	2.38526100	-4.02172000	-3.32169200
C	3.33358100	-5.06275300	-3.60136400
C	2.95752900	-6.42854200	-3.71469100
C	3.89576700	-7.40260300	-3.98960000
C	5.25687500	-7.05391000	-4.15850500
C	5.65472100	-5.73822500	-4.04277800
C	4.71327100	-4.71174100	-3.75917500
C	5.11598600	-3.35477800	-3.61584200
C	4.18317700	-2.37797800	-3.33372400
C	5.81403600	-0.64163700	-3.26251500
H	-2.72457400	-5.52609500	-2.42363100
H	-3.12011500	-5.71371300	-4.84430500
H	-2.30634400	-5.51319900	-7.17919600
H	0.04951800	-4.79949800	-7.62931900
H	1.57490700	-4.29487200	-5.74653600
H	-3.30791900	-4.85708600	-0.26156200
H	-2.50226700	-5.52690900	1.19358200
H	-2.58973600	-6.52058700	-0.30291800
H	1.90947200	-6.69934600	-3.58324900
H	3.58767700	-8.44707500	-4.07592400
H	5.99341700	-7.83093100	-4.37701200
H	6.70630400	-5.46574800	-4.16550900
H	6.17307200	-3.11501500	-3.72632000
H	5.82027200	0.44113900	-3.08086300
H	6.22566400	-0.84195800	-4.26781400
H	6.45526000	-1.13765300	-2.51236300
H	2.12007000	-0.67952900	-3.37603400
H	0.83956300	-1.89679400	-3.37976800
H	2.32423800	-4.20466400	-0.76362800
H	0.91531900	-4.33323400	0.29170600
H	1.47225900	0.48077000	1.36435300

N	-2.18996300	-1.93540600	-0.11230100
Rh	-0.43709200	-0.82020100	-0.46415400
C	-2.92516300	-2.29665200	-1.20440900
C	-2.36607000	-1.69171900	-2.44784200
C	-1.46331400	-0.61734000	-2.32149900
C	-2.71943900	-2.17545200	-3.71034800
C	-0.90379800	-0.05589500	-3.48289700
C	-2.14279600	-1.62684800	-4.85572200
H	-3.42794500	-3.00232400	-3.76321800
C	-1.23002700	-0.56890600	-4.73721000
H	-0.22652000	0.79637500	-3.40202600
H	-2.39016800	-2.03194300	-5.83883600
H	-0.77570300	-0.13635800	-5.63194400
O	-3.94561300	-2.98666500	-1.20638400
N	-2.83268800	-2.01088400	1.10440200
C	-3.99099700	-1.29211200	1.44355400
C	-2.29600000	-2.57190400	2.25020300
C	-4.19587800	-1.40620000	2.79920600
C	-3.13025200	-2.19496400	3.34459300
H	-5.02436700	-0.95934100	3.34408700
C	-4.82763900	-0.58684800	0.43492400
H	-5.55228200	0.05810600	0.94959100
H	-4.21922800	0.03844000	-0.23361000
H	-5.36226900	-1.30937600	-0.20004700
C	-2.78011800	-2.60871500	4.64171200
C	-1.63366200	-3.37848700	4.82569200
C	-0.83978300	-3.76602600	3.72569000
C	-1.16506000	-3.37349900	2.42707700
H	-3.40323900	-2.32604700	5.49418400
H	-1.35323600	-3.70279600	5.83089200
H	0.03542900	-4.39998400	3.88983000
H	-0.59902300	-3.71137200	1.56563000
C	-1.90778200	0.87216300	-1.06320000
C	-1.62728900	0.67068800	0.18983800
C	-2.42336600	1.94737800	-1.90712200
C	-2.01015600	3.26895700	-1.65256900
C	-3.38409300	1.71310500	-2.90900000
C	-2.55072100	4.33147200	-2.37872600
H	-1.26175500	3.44979800	-0.87847300
C	-3.92346900	2.77752500	-3.62754300
H	-3.70508100	0.69074100	-3.11203400
C	-3.50792200	4.08881300	-3.36763900
H	-2.21945100	5.35231000	-2.17385000
H	-4.67491800	2.58402900	-4.39648800

H	-3.92985300	4.92005100	-3.93748500
C	-1.96369800	1.13741300	1.51785300
C	-2.95019000	2.13369600	1.68575300
C	-1.36879800	0.57339600	2.66024300
C	-3.32535500	2.54409900	2.96125100
H	-3.42736200	2.56852200	0.80596900
C	-1.74847400	0.98794600	3.93540400
H	-0.64443400	-0.23016400	2.54042800
C	-2.72647700	1.97237500	4.09115900
H	-4.09534000	3.31052400	3.07887600
H	-1.29696600	0.51559800	4.81009900
H	-3.03125500	2.28959400	5.09129400

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C	-1.28017600	-1.71420900	-4.67880800
C	-0.01558200	-1.99054900	-4.06101900
C	0.39920000	-0.79844500	-3.39550900
C	-0.62999400	0.17630100	-3.54716800
C	-1.66603800	-0.38396200	-4.39795700
C	-0.52629800	1.61635700	-3.12659000
C	-2.78477500	0.32429700	-5.11732200
H	-1.86674500	-2.41889600	-5.26649900
H	1.32672600	-0.64874400	-2.84885300
O	-5.18258100	-0.07070700	-3.84657500
O	1.87297600	2.12622800	-4.31701000
C	-3.47806300	1.45661300	-4.39834500
C	-4.74832800	1.21132500	-3.78321000
C	-5.44800100	2.23561900	-3.17775800
C	-4.89727000	3.54174200	-3.10923400
C	-5.57535000	4.59687600	-2.44013700
C	-5.00801900	5.84891900	-2.33292400
C	-3.73183900	6.10127700	-2.89157300
C	-3.05205300	5.09878400	-3.55249300
C	-3.61287400	3.79937900	-3.68575000
C	-2.92831400	2.72855700	-4.35088200
C	-6.39485100	-0.40771500	-3.20227700
C	-0.44998800	2.47714000	-4.36901100
C	-1.59174900	2.98122400	-4.97139100
C	-1.50167300	3.73052400	-6.19342600
C	-2.64821000	4.24327900	-6.85909400
C	-2.52752900	4.96188400	-8.03098300
C	-1.25067300	5.19866800	-8.59344700
C	-0.11986300	4.70501600	-7.97701900
C	-0.21130800	3.95870800	-6.77072400

C	0.94597300	3.42796300	-6.13757800
C	0.82863900	2.69414800	-4.97534500
C	3.17377700	2.28488300	-4.83429800
H	-6.41196500	2.05629600	-2.70450600
H	-6.55446300	4.39308300	-1.99920900
H	-5.53943300	6.64761700	-1.80994300
H	-3.28324400	7.09268200	-2.79583500
H	-2.06736000	5.29617400	-3.97744400
H	-6.31529400	-0.26170100	-2.11167200
H	-6.56791000	-1.46898400	-3.41068700
H	-7.23854600	0.18482200	-3.59708300
H	-3.63297500	4.06186300	-6.42746200
H	-3.42018400	5.34959500	-8.52706600
H	-1.16298500	5.77087800	-9.52018700
H	0.86796300	4.87974100	-8.41151300
H	1.91647200	3.60702500	-6.59916800
H	3.26262600	1.85627100	-5.84834000
H	3.84934700	1.74763900	-4.15592700
H	3.46960400	3.34833600	-4.87158100
H	0.36920500	1.75019900	-2.50922900
H	-1.39396100	1.90532000	-2.53203000
H	-2.35251200	0.73089900	-6.04808600
H	-3.53139700	-0.42485400	-5.40860500
H	0.54185900	-2.92334700	-4.12268200
N	-2.62512000	-0.92171400	-0.80771800
Rh	-1.43733100	-1.64176100	-2.40421800
C	-3.85854600	-1.48481800	-0.61562900
C	-4.06439000	-2.63831100	-1.54480400
C	-2.95746500	-3.13365200	-2.26174900
C	-5.33030200	-3.20268700	-1.71867400
C	-3.16662900	-4.13495900	-3.23088400
C	-5.52146600	-4.21227900	-2.66315200
H	-6.14900100	-2.81424300	-1.10905300
C	-4.44052700	-4.65632900	-3.44056700
H	-2.31495500	-4.54508500	-3.77785000
H	-6.51127500	-4.65340700	-2.80369800
H	-4.59035200	-5.43680000	-4.19058900
O	-4.70527500	-1.12177000	0.19290200
N	-2.20331500	-0.07951900	0.19737500
C	-2.24509900	1.31180900	0.16615800
C	-1.58651800	-0.49370800	1.37040100
C	-1.56209000	1.80091600	1.25822500
C	-1.12827800	0.67634500	2.04220800
H	-1.45205700	2.85415800	1.50912600

C	-3.11351200	2.01253900	-0.81119300
H	-3.12217000	1.49902700	-1.77730500
H	-4.15644600	2.00623900	-0.45424400
H	-2.80567800	3.05619300	-0.95180400
C	-0.42270600	0.53228300	3.25043100
C	-0.21475000	-0.74429300	3.76584600
C	-0.72025700	-1.88429200	3.10638500
C	-1.41682200	-1.77249600	1.90607100
H	-0.05348300	1.41406000	3.78084800
H	0.33196600	-0.86737400	4.70411000
H	-0.56425400	-2.87302000	3.54399900
H	-1.81198500	-2.64835300	1.39445900
C	-1.39400700	-3.66662400	-1.18684100
C	-0.51132800	-2.73660400	-0.98562000
C	-1.60061700	-5.09299900	-0.94509400
C	-0.58680300	-6.00623600	-1.28978800
C	-2.77309000	-5.57242400	-0.33224000
C	-0.73790300	-7.36706100	-1.01643900
H	0.31614800	-5.63712600	-1.78014000
C	-2.91741500	-6.93058300	-0.05885300
H	-3.56654900	-4.86929400	-0.07603200
C	-1.90257500	-7.83224900	-0.40035900
H	0.05561900	-8.06664200	-1.28986400
H	-3.82844100	-7.29021400	0.42492900
H	-2.02189800	-8.89727600	-0.18791500
C	0.67996300	-2.47072100	-0.19796200
C	1.12432300	-1.15010400	-0.00524500
C	1.35749400	-3.51803900	0.45602500
C	2.20316200	-0.88124600	0.83312400
H	0.57723500	-0.33448400	-0.47727200
C	2.44597900	-3.24577400	1.28278600
H	1.01348700	-4.54481200	0.32797900
C	2.86904000	-1.92745900	1.47809700
H	2.51083900	0.15278600	1.00103200
H	2.95981100	-4.06684400	1.78854900
H	3.71087800	-1.71475700	2.14117500

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C	-0.58797000	1.58730900	-2.06777000
C	-1.10705300	0.56372100	-2.90107100
C	-0.31197400	-0.59503000	-2.65748200
C	0.80043800	-0.23892700	-1.79197200
C	0.62611600	1.10566500	-1.41731800
C	1.86710600	-1.19289300	-1.32646100

C	1.56042100	1.96200300	-0.59616200
H	-0.97439100	2.60005300	-1.99496400
H	-0.43353700	-1.57279900	-3.12260300
O	0.41793700	2.62170700	1.81238000
O	3.22222200	-1.57657000	-3.67368600
C	2.04726100	1.34150900	0.69656600
C	1.41164500	1.71407000	1.92792200
C	1.84029000	1.18909100	3.13003100
C	2.88827100	0.23369300	3.16566800
C	3.30146800	-0.37076700	4.38423800
C	4.29246500	-1.33033400	4.40050900
C	4.91825600	-1.72733800	3.19411400
C	4.54622300	-1.14895300	1.99744200
C	3.53066500	-0.15713500	1.94879700
C	3.10978700	0.45136300	0.71951900
C	-0.21636200	3.12192100	2.98194000
C	3.24840100	-0.62056000	-1.52586500
C	3.84441900	0.15486500	-0.54731900
C	5.14669600	0.72461500	-0.75852000
C	5.78591600	1.54914500	0.20674200
C	7.03890800	2.07800900	-0.02803800
C	7.70968400	1.80889200	-1.24452100
C	7.10994300	1.02323600	-2.20670500
C	5.81903900	0.46680400	-1.99616700
C	5.18022900	-0.32172800	-2.99277700
C	3.92092400	-0.83887800	-2.77024500
C	3.80148100	-1.83869400	-4.93040200
H	1.35474900	1.46860600	4.06348300
H	2.80811600	-0.06839700	5.31161600
H	4.59412600	-1.78919100	5.34530600
H	5.69735200	-2.49290400	3.21194900
H	5.02679800	-1.45552400	1.06734000
H	-0.75879200	2.32034500	3.50604800
H	-0.93362000	3.87523100	2.63446700
H	0.52202800	3.59562200	3.65175400
H	5.27093500	1.75982900	1.14426000
H	7.51468600	2.70772100	0.72720500
H	8.70246000	2.22941700	-1.42235000
H	7.62066300	0.81974700	-3.15170900
H	5.70599800	-0.49273600	-3.93151400
H	3.07254400	-2.43483000	-5.49500900
H	4.74069100	-2.41232400	-4.83481700
H	4.01168900	-0.90588300	-5.48339700
H	1.76699400	-2.13253400	-1.88265200

H	1.71960100	-1.42552500	-0.26290800
H	2.43271500	2.19566100	-1.22837000
H	1.06358800	2.91314900	-0.37323800
H	-1.97938300	0.63192000	-3.54751300
N	-2.05959500	0.44401000	1.20843100
Rh	-1.25379200	-0.13840600	-0.75948300
C	-1.54659100	-0.12886600	2.35181400
C	-0.76393700	-1.36027200	2.08286000
C	-0.99220900	-2.18770300	0.94332300
C	0.24061000	-1.68915100	3.00095500
C	-0.07398100	-3.24834500	0.72995000
C	1.11381900	-2.74958500	2.78249100
H	0.33135500	-1.05484700	3.88110000
C	0.96118300	-3.51348400	1.61999200
H	-0.18272700	-3.86870500	-0.15961000
H	1.92228000	-2.95253000	3.48598700
H	1.65446000	-4.33031200	1.40452300
O	-1.70994300	0.31847300	3.48625900
N	-3.07090100	1.35818700	1.41202200
C	-4.31303700	1.04286200	1.98576500
C	-3.14009600	2.61807100	0.84040900
C	-5.17113000	2.09810000	1.77888000
C	-4.46520300	3.10684100	1.04298600
H	-6.20039500	2.14301600	2.12796700
C	-4.55064900	-0.22141200	2.73498800
H	-5.63062600	-0.39626700	2.83091100
H	-4.10400100	-1.08899000	2.23006800
H	-4.09207900	-0.16908000	3.73428900
C	-4.80615300	4.37484400	0.53892600
C	-3.84123100	5.12401000	-0.13034400
C	-2.52545300	4.63796800	-0.28117200
C	-2.15803100	3.38481200	0.20888200
H	-5.81614800	4.76812600	0.68083700
H	-4.09741500	6.11079100	-0.52370800
H	-1.77362800	5.26251400	-0.77077000
H	-1.13548300	3.02669600	0.16161000
C	-2.16610800	-2.09697800	0.02730600
C	-2.91672200	-0.96214800	-0.29600700
C	-2.60743100	-3.35348100	-0.65604300
C	-2.88175800	-3.37352900	-2.03213600
C	-2.83965800	-4.51832900	0.09680200
C	-3.37854800	-4.52658300	-2.64349800
H	-2.70972700	-2.46998000	-2.61914400
C	-3.33946200	-5.66882000	-0.51322000

H	-2.63027100	-4.51195800	1.16829000
C	-3.61008500	-5.67751000	-1.88619400
H	-3.58644500	-4.52511000	-3.71615200
H	-3.52259500	-6.56364700	0.08659000
H	-3.99976500	-6.58004100	-2.36286800
C	-4.29219800	-0.70879200	-0.63134900
C	-5.33140300	-1.57684000	-0.22522700
C	-4.62419400	0.49092200	-1.29589400
C	-6.65741900	-1.24590700	-0.47594800
H	-5.08171200	-2.50574900	0.28883700
C	-5.95388200	0.82128700	-1.53622000
H	-3.82013500	1.17006300	-1.58014200
C	-6.97259000	-0.04356000	-1.12500000
H	-7.45568800	-1.92094300	-0.15893600
H	-6.19764400	1.76599400	-2.02618000
H	-8.01788600	0.21914700	-1.30494800

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C	-0.73682200	0.02941500	-3.22066300
C	-1.85841400	0.70618900	-2.68123400
C	-3.02183000	0.26595000	-3.41905500
C	-2.61504900	-0.68888700	-4.37408800
C	-1.18391000	-0.86527800	-4.24729400
C	-3.52448300	-1.37642500	-5.35483400
C	-0.25175800	-1.59068100	-5.18595100
H	0.29842500	0.14163300	-2.90448700
H	-4.04008100	0.61737500	-3.28063300
O	0.89603100	-3.74577000	-3.95227800
O	-4.32712200	0.74877500	-6.87374400
C	-0.66531400	-2.99647100	-5.54564000
C	-0.05129000	-4.09273800	-4.85554400
C	-0.41663500	-5.39498800	-5.13396700
C	-1.45487000	-5.66753700	-6.06502200
C	-1.92027700	-6.99111700	-6.29390600
C	-2.94969700	-7.23689200	-7.17869500
C	-3.55573900	-6.16759700	-7.88128000
C	-3.11883100	-4.87292100	-7.68723200
C	-2.06567300	-4.58624600	-6.77765100
C	-1.61397000	-3.24822900	-6.52456500
C	1.63666200	-4.75940100	-3.30589400
C	-3.04352100	-1.21577400	-6.77661400
C	-2.15010000	-2.11195500	-7.33602400
C	-1.68135000	-1.93638000	-8.68264700
C	-0.74894800	-2.82073600	-9.29026300

C	-0.32302000	-2.62288300	-10.58793600
C	-0.80845500	-1.52554200	-11.33793100
C	-1.70496600	-0.64299100	-10.77247800
C	-2.16096800	-0.81800600	-9.43749700
C	-3.06672000	0.09915300	-8.83744900
C	-3.48665700	-0.08580700	-7.53606100
C	-4.80893100	1.89815300	-7.53176000
H	0.05556000	-6.23284400	-4.62361900
H	-1.45150000	-7.81374100	-5.74749800
H	-3.30118100	-8.25902600	-7.33831100
H	-4.37242900	-6.36943100	-8.57792700
H	-3.58710600	-4.04776800	-8.22554700
H	0.99130700	-5.39144700	-2.67383400
H	2.36984100	-4.24733800	-2.67147700
H	2.16397800	-5.39660600	-4.03735800
H	-0.37060700	-3.66668600	-8.71580200
H	0.39228400	-3.31487800	-11.03825800
H	-0.46776900	-1.37648700	-12.36534800
H	-2.07695500	0.21050000	-11.34537500
H	-3.40867600	0.94912800	-9.42696000
H	-3.98423000	2.56589200	-7.83785800
H	-5.45059400	2.42485100	-6.81359300
H	-5.40397200	1.63645300	-8.42478200
H	-4.53177400	-0.95736700	-5.24846500
H	-3.58920500	-2.44394300	-5.11590000
H	-0.17991600	-0.99252900	-6.10940400
H	0.74515900	-1.61162200	-4.73102500
H	-1.85637100	1.45345700	-1.89143300
N	-3.16415200	-1.33554800	-0.41819500
Rh	-2.10340500	-1.44280700	-2.21539700
C	-4.06163700	-2.31897400	-0.09404500
C	-4.20732500	-3.27555800	-1.23438500
C	-3.22165500	-3.25774500	-2.24132000
C	-5.30918800	-4.12295500	-1.33945400
C	-3.37504300	-4.07487900	-3.36940200
C	-5.45738600	-4.93256800	-2.47191900
H	-6.04528000	-4.11668800	-0.53227300
C	-4.50004800	-4.89390400	-3.49354500
H	-2.60508400	-4.09263100	-4.13599100
H	-6.32311000	-5.59322300	-2.56097100
H	-4.61074400	-5.51960900	-4.38296500
O	-4.67727600	-2.41536200	0.96025200
N	-2.92484800	-0.37570700	0.53449700
C	-2.12912100	-0.50947300	1.67378500

C	-3.33448500	0.93904700	0.41201000
C	-1.97667300	0.73330000	2.24944300
C	-2.72324600	1.67976700	1.46499300
H	-1.42897500	0.93315300	3.16814500
C	-1.67798600	-1.83973000	2.16338400
H	-2.55210000	-2.48867000	2.33181600
H	-1.01463000	-2.33965900	1.44640400
H	-1.12830800	-1.71951700	3.10639400
C	-2.97201700	3.06136000	1.54958300
C	-3.81719300	3.65865300	0.61594200
C	-4.44165100	2.89584300	-0.39354500
C	-4.21280600	1.52478200	-0.50303800
H	-2.51652600	3.65595300	2.34579800
H	-4.01755200	4.73119600	0.67685100
H	-5.12828000	3.38438500	-1.08939800
H	-4.71742900	0.91239900	-1.24895700
C	-1.39543800	-3.57852300	-1.39087800
C	-0.72138500	-2.50009700	-1.17339000
C	-1.47268300	-4.97978800	-0.98778700
C	-1.58388700	-6.05515400	-1.88539400
C	-1.38564000	-5.25578500	0.39153900
C	-1.58971900	-7.36869100	-1.41832600
H	-1.66646000	-5.85758400	-2.95038400
C	-1.38884300	-6.57211600	0.85319600
H	-1.32951100	-4.42633700	1.09518700
C	-1.49053700	-7.63440100	-0.04899500
H	-1.67741200	-8.19185600	-2.13164000
H	-1.32635600	-6.76546400	1.92658300
H	-1.50262400	-8.66487800	0.31360000
C	0.50446800	-2.07743000	-0.51663800
C	0.71111500	-0.73055000	-0.17008600
C	1.48365300	-3.02767100	-0.16124400
C	1.86732400	-0.34214800	0.50658400
H	-0.06161000	0.00042800	-0.40481400
C	2.64244200	-2.63398200	0.50516300
H	1.31785500	-4.07836400	-0.40172200
C	2.83984700	-1.28902100	0.83963700
H	2.00323600	0.70584500	0.78275900
H	3.39412100	-3.38062700	0.77285500
H	3.74660800	-0.98291000	1.36659500

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C	1.20044900	-1.76310900	0.78249000
C	1.46376500	-0.37874400	0.59804700
C	1.63476600	-0.16475300	-0.79923700
C	1.57804200	-1.44040800	-1.47083600
C	1.30651700	-2.43718400	-0.50175800
C	1.77759500	-1.63876300	-2.94821700
C	1.28360400	-3.93846100	-0.68595000
H	1.04582600	-2.26542800	1.73206300
H	1.85324600	0.78422500	-1.28562400
O	-1.19928000	-5.11456200	-0.36951100
O	4.44383600	-1.01020800	-3.16388200
C	0.48362000	-4.43463800	-1.87289800
C	-0.83248100	-4.96630100	-1.66145400
C	-1.62651000	-5.32910500	-2.73074000
C	-1.15087300	-5.19495200	-4.05976100
C	-1.97603700	-5.48812400	-5.17979700
C	-1.50375900	-5.33949500	-6.46721800
C	-0.17695100	-4.89895400	-6.69273000
C	0.65009200	-4.61458100	-5.62512500
C	0.18831300	-4.74619300	-4.28796700
C	1.00189000	-4.40264500	-3.15883800
C	-2.44623100	-5.72141100	-0.05920100
C	2.80995200	-2.69645200	-3.23915300
C	2.43198500	-4.01996900	-3.36091400
C	3.40881600	-5.03708200	-3.63058000
C	3.06766500	-6.41133000	-3.75145500
C	4.03303300	-7.36178700	-4.01507200
C	5.38729500	-6.97971500	-4.16513600
C	5.75121500	-5.65478500	-4.04259100
C	4.78129400	-4.65210600	-3.77015700
C	5.14846300	-3.28569700	-3.62005900
C	4.18848200	-2.33264500	-3.34806700
C	5.77562900	-0.55792400	-3.24295300
H	-2.64203000	-5.68654700	-2.57089500
H	-2.99950500	-5.82750300	-5.00039700
H	-2.15288800	-5.56371100	-7.31727100
H	0.19127000	-4.78403700	-7.71482500
H	1.67135500	-4.27183200	-5.79833900
H	-3.28202300	-5.09465100	-0.40453500
H	-2.47979400	-5.79976000	1.03443800
H	-2.50636700	-6.73242300	-0.49819300
H	2.02481700	-6.70811900	-3.63487400
H	3.75171200	-8.41328600	-4.10732400

H	6.14551800	-7.73808400	-4.37482200
H	6.79733100	-5.35644100	-4.15115200
H	6.20059300	-3.01955300	-3.71667000
H	5.75269200	0.52357900	-3.05525100
H	6.21000100	-0.74225000	-4.24172300
H	6.41489100	-1.04318100	-2.48410900
H	2.07793700	-0.68440400	-3.39569200
H	0.82974700	-1.93599700	-3.40962600
H	2.32974500	-4.27080800	-0.79117100
H	0.89373500	-4.39621600	0.22956400
H	1.48187300	0.38492000	1.37271600
N	-2.14986700	-2.08043800	-0.09628000
Rh	-0.44902500	-0.90547800	-0.44888900
C	-2.86867400	-2.45714300	-1.20353000
C	-2.33141900	-1.81726700	-2.44002900
C	-1.48173300	-0.70325800	-2.29417100
C	-2.66811200	-2.28971200	-3.71143800
C	-0.95388200	-0.08980600	-3.44375700
C	-2.12441000	-1.68766600	-4.84640400
H	-3.34075100	-3.14459800	-3.78163700
C	-1.26235000	-0.59016100	-4.70787000
H	-0.31821500	0.79236700	-3.34578400
H	-2.35914600	-2.08032700	-5.83770800
H	-0.83483200	-0.11628900	-5.59486800
O	-3.86500500	-3.17513000	-1.21300200
N	-2.85957000	-2.09093500	1.08576400
C	-2.48109800	-2.69474400	2.28355700
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C	-1.25363100	-3.52818100	2.41492400
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H	-6.52235200	0.66183900	0.23415500
H	-4.51577300	-0.50371600	-0.64728700
C	-2.00272400	0.74201300	-1.00330800

C	-1.67701200	0.54543900	0.23846300
C	-2.62064500	1.77982300	-1.82310700
C	-2.33090300	3.12750200	-1.53516900
C	-3.56473100	1.48476900	-2.82481500
C	-2.97771300	4.15402400	-2.22486100
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C	-4.20909300	2.51329700	-3.50820400
H	-3.79159000	0.44406100	-3.05829200
C	-3.91787300	3.85027500	-3.21312900
H	-2.74271600	5.19533800	-1.99180900
H	-4.94642000	2.27067500	-4.27685800
H	-4.42302200	4.65347400	-3.75478800
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C	-3.47263600	2.25595500	3.05091100
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H	-0.58873500	-0.29296900	2.56186600
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H	-1.26564000	0.38377400	4.85660700
H	-3.13552800	2.00254600	5.17407000

(R_{NN})-TS3

C	-0.54107500	0.43541300	-1.08272300
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C	0.11979200	-0.33781000	-2.06384500
C	-0.62612000	-1.41011500	-4.35342800
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C	3.64931800	-5.90519600	-5.38030800
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H	0.82970800	1.72088300	-7.52581400
H	-1.21904900	2.54914800	-6.74264900
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C	-6.22618200	-2.49513400	-3.11562300
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C	-5.22999400	-2.97363500	-3.97740400
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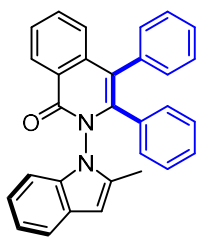
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H	1.25893600	-2.90253200	3.02776000
H	1.25139700	-5.36725800	3.42170500

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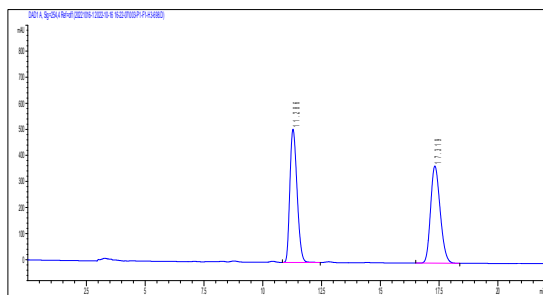
8. Characterization Data and HPLC Chromatograms



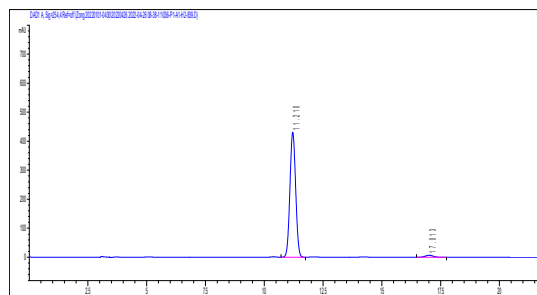
(*R*)-2-(2-methyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (3)

The title compound was isolated as a white solid (29.0 mg, 68%). **¹H NMR (400 MHz, CDCl₃)** δ 8.54 (dd, J = 8.0, 1.5 Hz, 1H), 7.70 – 7.63 (m, 1H), 7.61 – 7.53 (m, 1H), 7.36 (dd, J = 15.6, 7.9 Hz, 2H), 7.31 – 7.26 (m, 2H), 7.23 – 7.18 (m, 2H), 7.13 (d, J = 4.1 Hz, 3H), 7.08 – 7.00 (m, 3H), 6.99 – 6.89 (m, 2H), 6.78 (t, J = 7.1 Hz, 1H), 6.14 (s, 1H), 2.24 (s, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 161.0, 142.8, 137.6, 136.9, 136.6, 135.8, 133.4, 132.2, 131.7, 131.6, 129.9, 129.7, 128.9, 128.44, 128.42, 128.2, 127.5, 127.4, 127.2, 126.6, 126.2, 125.6, 121.9, 120.8, 120.2, 119.8, 108.7, 100.4, 12.1. **HRMS (ESI)**: calcd. for C₃₀H₂₂N₂NaO⁺ [M+Na]⁺: 449.1624, found : 449.1624. $[\alpha]_D^{20}$ = +84 (c = 0.1, CHCl₃).

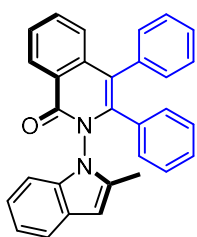
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 85:15, v = 1.0 mL/min, 40 °C, 254 nm). t_r (major) = 11.210 min, t_r (minor) = 17.013 min, -96% ee.



No.	Time	Area	Area (%)
1	11.286	10817.0	50.50
2	17.319	10604.8	49.50



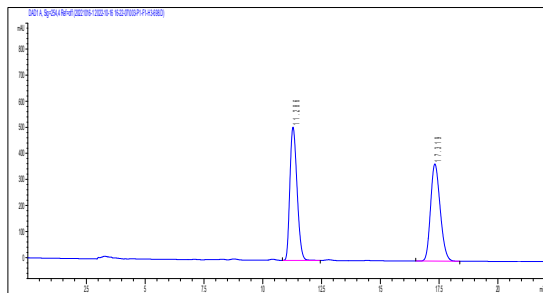
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2	17.013	158.4	2.13



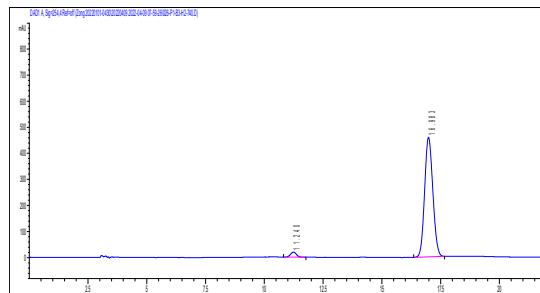
(*S*)-2-(2-methyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one ((*ent*)-3)

The title compound was isolated as a white solid (29.9 mg, 70%). **¹H NMR (400 MHz, CDCl₃)** δ 8.54 (dd, J = 8.0, 1.5 Hz, 1H), 7.70 – 7.63 (m, 1H), 7.61 – 7.53 (m, 1H), 7.36 (dd, J = 15.6, 7.9 Hz, 2H), 7.31 – 7.26 (m, 2H), 7.23 – 7.18 (m, 2H), 7.13 (d, J = 4.1 Hz, 3H), 7.08 – 7.00 (m, 3H), 6.99 – 6.89 (m, 2H), 6.78 (t, J = 7.1 Hz, 1H), 6.14 (s, 1H), 2.24 (s, 3H). **¹³C NMR (100 MHz, CDCl₃)** δ 161.0, 142.8, 137.6, 136.9, 136.6, 135.8, 133.4, 132.2, 131.7, 131.6, 129.9, 129.7, 128.9, 128.44, 128.42, 128.2, 127.5, 127.4, 127.2, 126.6, 126.2, 125.6, 121.9, 120.8, 120.2, 119.8, 108.7, 100.4, 12.1. **HRMS (ESI)**: calcd. for C₃₀H₂₂N₂NaO⁺ [M+Na]⁺ : 449.1624, found : 449.1624. $[\alpha]_D^{20}$ = -88 (c = 0.1, CHCl₃).

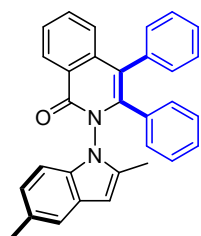
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 85:15, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (minor) = 11.240 min, tr (major) = 16.983 min, 94% ee.



No.	Time	Area	Area (%)
1	11.286	10817.0	50.50
2	17.319	10604.8	49.50



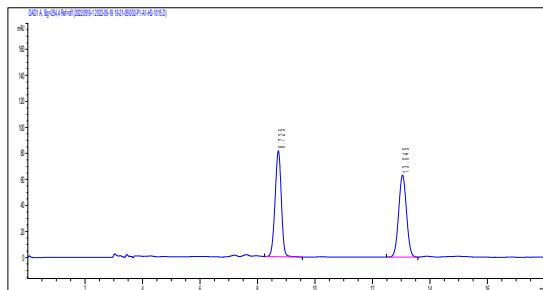
No.	Time	Area	Area (%)
1	11.240	333.2	2.91
2	16.983	11129.5	97.09



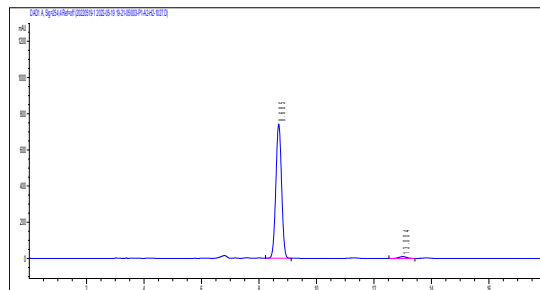
(*R*)-2-(2,5-dimethyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (4)

The title compound was isolated as a white solid (20.3 mg, 46%). **¹H NMR (400 MHz, CDCl₃)** δ 8.52 (d, $J = 8.0$ Hz, 1H), 7.65 (t, $J = 7.6$ Hz, 1H), 7.55 (t, $J = 7.6$ Hz, 1H), 7.34 (d, $J = 8.2$ Hz, 1H), 7.31 – 7.27 (m, 2H), 7.23 – 7.19 (m, 2H), 7.18 (s, 1H), 7.15 – 7.09 (m, 1H), 7.09 – 7.01 (m, 3H), 7.00 (s, 1H), 6.99 – 6.90 (m, 3H), 6.84 – 6.77 (m, 1H), 6.06 (s, 1H), 2.38 (s, 3H), 2.20 (s, 3H). **¹³C NMR (100 MHz, CDCl₃)** 161.0, 142.9, 137.6, 136.8, 135.9, 135.5, 133.3, 132.3, 131.7, 131.6, 130.0, 129.7, 128.8, 128.44, 128.39, 128.1, 127.4, 127.35, 127.31, 127.2, 126.9, 126.2, 125.6, 123.4, 120.2, 119.7, 108.4, 100.1, 21.6, 12.1. **HRMS (ESI):** calcd. for C₃₁H₂₄N₂NaO⁺ [M+Na]⁺ : 463.1781, found : 463.1771. **[α]_D²⁰ = +64** (c = 0.1, CHCl₃).

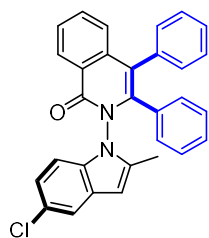
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (major) = 8.685 min, tr (minor) = 13.004 min, -96% ee.



No.	Time	Area	Area (%)
1	8.725	1227.0	50.74
2	13.045	1191.1	49.26



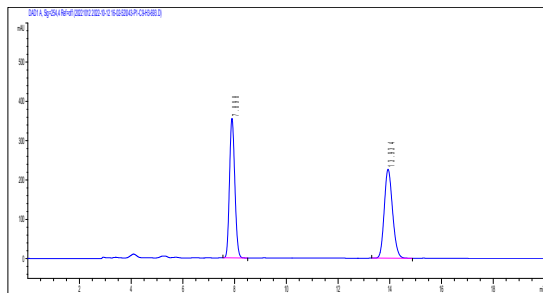
No.	Time	Area	Area (%)
1	8.685	10276.6	98.22
2	13.004	186.1	1.78



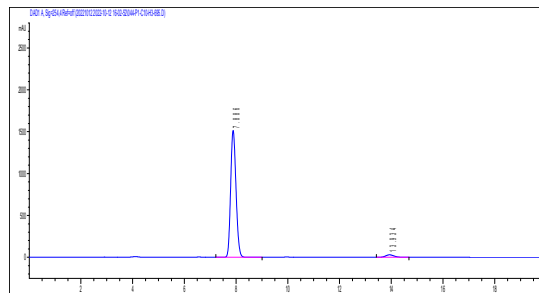
(R)-2-(5-chloro-2-methyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (5)

The title compound was isolated as a white solid (30.8 mg, 67%). **¹H NMR (600 MHz, CDCl₃)** δ 8.53 (dd, J = 8.0, 1.4 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.61 – 7.54 (m, 1H), 7.37 – 7.32 (m, 2H), 7.31 – 7.27 (m, 1H), 7.26 – 7.24 (m, 1H), 7.23 – 7.19 (m, 2H), 7.15 – 7.11 (m, 1H), 7.09 (dd, J = 8.6, 1.9 Hz, 1H), 7.07 – 7.01 (m, 2H), 7.01 – 6.93 (m, 3H), 6.80 (t, J = 6.9 Hz, 1H), 6.09 (s, 1H), 2.23 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 160.9, 142.4, 138.3, 137.5, 135.6, 135.3, 133.6, 131.9, 131.6, 131.5, 129.8, 129.6, 128.8, 128.6, 128.5, 128.2, 127.7, 127.6, 127.5, 127.40, 127.36, 126.4, 126.3, 125.5, 122.1, 120.0, 119.8, 109.7, 100.1, 12.1. **HRMS (ESI):** calcd. for C₃₀H₂₂ClN₂NO⁺ [M+H]⁺: 461.1415, found : 461.1422. [α]_D²⁰ = +80 (c = 0.1, CHCl₃).

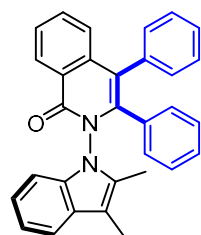
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, v = 1.0 mL/min, 40 °C, 254 nm). tr (major) = 7.886 min, tr (minor) = 13.934 min, -94% ee.



No.	Time	Area	Area (%)
1	7.898	5076.3	50.17
2	13.934	5041.3	49.83



No.	Time	Area	Area (%)
1	7.886	21728.6	97.09
2	13.934	651.6	2.91

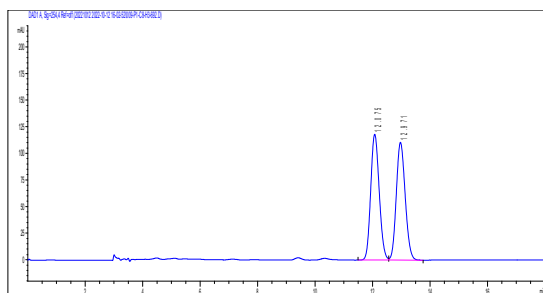


(R)-2-(2,3-dimethyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (6)

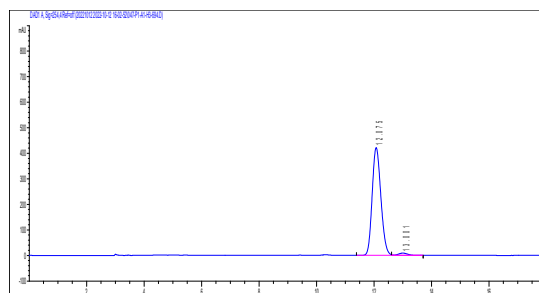
The title compound was isolated as a white solid (20.3 mg, 46%). **¹H NMR (600 MHz, CDCl₃)** δ 8.52 (dd, J = 8.0, 1.4 Hz, 1H), 7.67 – 7.63 (m, 1H), 7.57 – 7.53 (m, 1H), 7.35 (dd, J = 16.4, 8.0 Hz, 2H), 7.30 – 7.26 (m, 2H), 7.23 – 7.18 (m, 2H), 7.15 – 7.10 (m, 3H), 7.08 – 7.01 (m, 3H), 6.97 – 6.91 (m, 2H), 6.78 (t, J = 7.5 Hz, 1H), 2.14 (s, 3H), 2.11 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** 161.1, 143.1, 137.6, 136.6, 135.9, 133.3, 132.5, 132.4, 131.69, 131.65, 129.9, 129.8, 128.8, 128.4, 128.3, 128.1, 127.6, 127.4, 127.3, 127.2, 127.1, 126.2, 125.6, 122.0, 120.3, 119.6, 118.3, 108.5, 107.5, 9.8, 9.0. **HRMS (ESI):** calcd. for C₃₁H₂₅N₂O⁺ [M+H]⁺: 441.1961, found : 441.1968. [α]_D²⁰ = +66 (c = 0.1, CHCl₃).

HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 85:15, v = 1.0 mL/min, 40 °C,

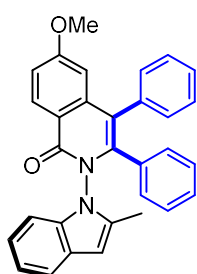
254 nm). tr (major) = 12.075 min, tr (minor) = 13.001 min, -96% ee.



No.	Time	Area	Area (%)
1	12.075	2436.2	50.52
2	12.971	2386.1	49.48



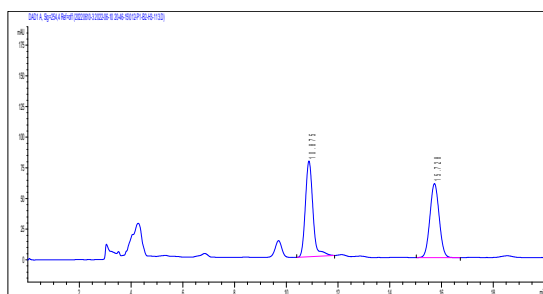
No.	Time	Area	Area (%)
1	12.075	8888.8	97.84
2	13.001	196.3	2.16



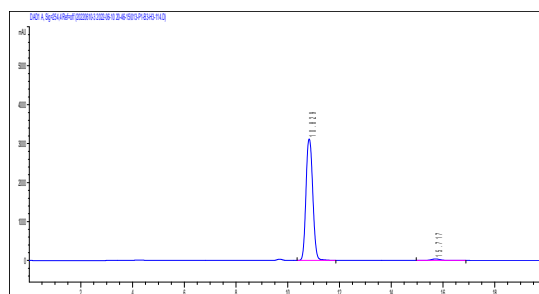
(R)-6-methoxy-2-(2-methyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (7)

The title compound was isolated as a white solid (33.3 mg, 73%). **¹H NMR (600 MHz, CDCl₃)** δ 8.48 (d, J = 8.9 Hz, 1H), 7.38 (d, J = 7.8 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.24 – 7.18 (m, 2H), 7.16 – 7.12 (m, 4H), 7.06 – 7.02 (m, 3H), 6.98 – 6.90 (m, 2H), 6.77 (t, J = 7.3 Hz, 1H), 6.71 (d, J = 2.5 Hz, 1H), 6.14 (s, 1H), 3.76 (s, 3H), 2.24 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** 163.7, 160.7, 143.4, 139.7, 137.0, 136.7, 135.8, 132.3, 131.6, 131.5, 131.1, 129.8, 129.6, 128.5, 128.4, 128.2, 127.4, 127.2, 126.5, 121.9, 120.7, 120.2, 119.4, 119.3, 115.9, 108.7, 108.5, 100.3, 55.5, 12.0. **HRMS (ESI):** calcd. for C₃₁H₂₅N₂O₂⁺ [M+H]⁺: 457.1911, found : 457.1918. **[α]_D²⁰** = +114 (c = 0.1, CHCl₃).

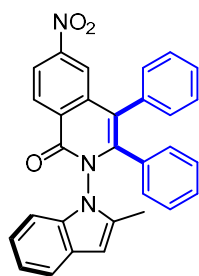
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, v = 1.0 mL/min, 40 °C, 254 nm). tr (major) = 10.829 min, tr (minor) = 15.717 min, -97% ee.



No.	Time	Area	Area (%)
1	10.875	1579.9	51.18
2	15.728	1507.1	48.82



No.	Time	Area	Area (%)
1	10.829	56799.0	98.37
2	15.717	938.8	1.63

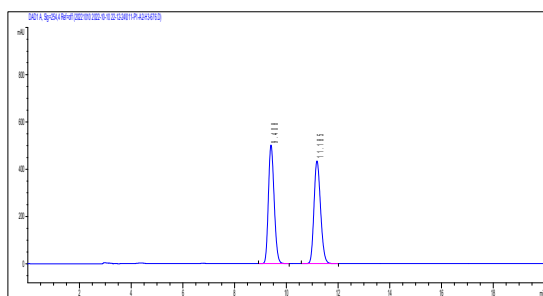


(R)-2-(2-methyl-1H-indol-1-yl)-6-nitro-3,4-diphenylisoquinolin-1(2H)-one (8)

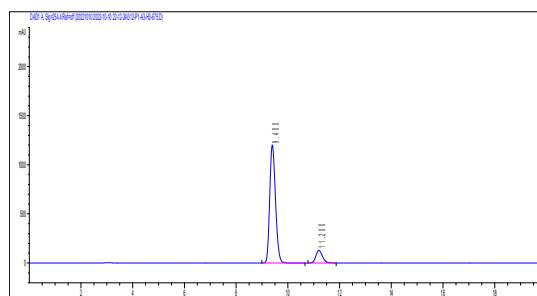
The title compound was isolated as a white solid (26.8 mg, 57%). **¹H NMR (600 MHz, CDCl₃)** δ 8.68 (d, J = 8.8 Hz, 1H), 8.29 (dd, J = 8.8, 2.2 Hz, 1H), 8.20 (d, J = 2.2 Hz, 1H), 7.40 (d, J = 7.8 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.27 – 7.22 (m, 3H), 7.17 – 7.13 (m, 1H), 7.13 – 7.09 (m, 2H), 7.09 – 7.05 (m, 1H), 7.04 (d, J = 7.8 Hz, 2H),

7.01 – 6.95 (m, 2H), 6.80 (t, J = 7.3 Hz, 1H), 6.17 (s, 1H), 2.23 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 159.8, 151.1, 145.4, 138.5, 136.7, 136.3, 134.3, 131.5, 131.4, 131.3, 131.0, 129.6, 129.4, 129.1, 128.93, 128.91, 128.7, 128.2, 127.5, 126.7, 122.2, 121.7, 121.1, 120.4, 119.5, 108.5, 101.0, 12.0. **HRMS (ESI)**: calcd. for C₃₀H₂₂N₃O₃⁺ [M+H]⁺: 472.1656, found : 472.1655. [α]_D²⁰ = +20 (c = 0.1, CHCl₃).

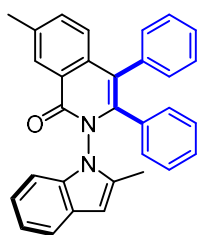
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 80:20, v = 1.0 mL/min, 40 °C, 254 nm). tr (major) = 9.400 min, tr (minor) = 11.200 min, -78% ee.



No.	Time	Area	Area (%)
1	9.408	7755.0	50.28
2	11.185	7669.4	49.72



No.	Time	Area	Area (%)
1	9.400	18627.8	89.24
2	11.200	2246.9	10.76

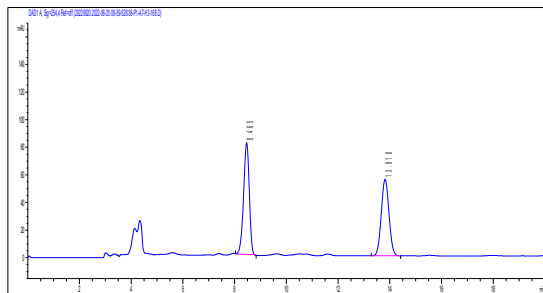


(R)-7-methyl-2-(2-methyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (9)

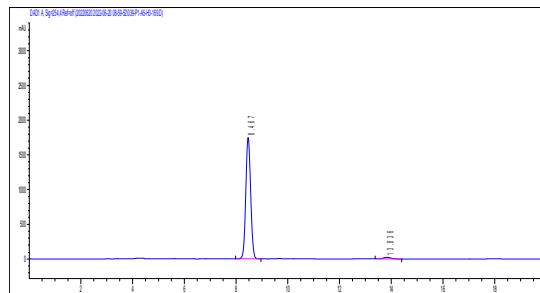
The title compound was isolated as a white solid (30.4 mg, 69%). **¹H NMR (600 MHz, CDCl₃)** δ 8.36 (s, 1H), 7.49 (d, J = 8.4 Hz, 1H), 7.39 (d, J = 7.8 Hz, 1H), 7.27 (d, J = 7.4 Hz, 3H), 7.23 – 7.17 (m, 2H), 7.16 – 7.11 (m, 3H), 7.07 – 7.01 (m, 3H),

6.98 – 6.90 (m, 2H), 6.76 (t, J = 6.2 Hz, 1H), 6.14 (s, 1H), 2.52 (s, 3H), 2.24 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.0, 141.8, 137.8, 136.9, 136.6, 136.0, 135.2, 134.8, 132.2, 131.7, 131.6, 130.0, 129.8, 128.5, 128.4, 128.3, 128.1, 127.3, 127.2, 126.5, 126.2, 125.5, 121.9, 120.7, 120.2, 119.8, 108.8, 100.3, 21.5, 12.0. **HRMS (ESI)**: calcd. for C₃₁H₂₅N₂O⁺ [M+H]⁺: 441.1961, found : 441.1966. [α]_D²⁰ = +36 (c = 0.1, CHCl₃).

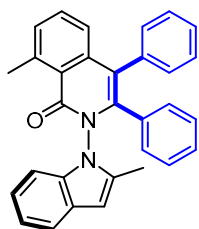
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (major) = 8.467 min, tr (minor) = 13.836 min, -96% ee.



No.	Time	Area	Area (%)
1	8.465	1239.6	51.95
2	13.818	1146.4	48.05



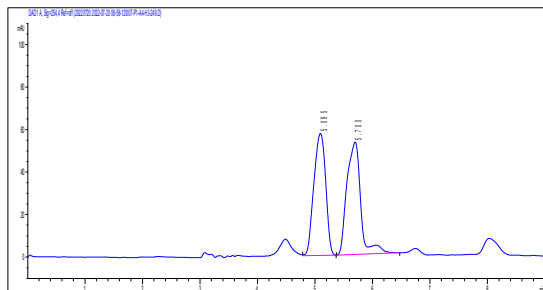
No.	Time	Area	Area (%)
1	8.467	22900.7	98.07
2	13.836	451.2	1.93



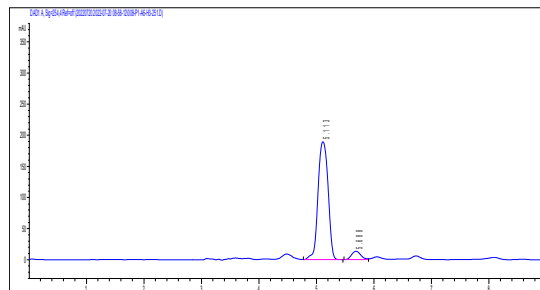
(*R*)-8-methyl-2-(2-methyl-1H-indol-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (10)

The title compound was isolated as a white solid (14.6 mg, 33%). **¹H NMR (600 MHz, CDCl₃)** δ 7.48 (t, $J = 7.8$ Hz, 1H), 7.38 (d, $J = 7.8$ Hz, 1H), 7.33 (d, $J = 7.4$ Hz, 1H), 7.28 (d, $J = 7.9$ Hz, 1H), 7.23 (d, $J = 7.6$ Hz, 1H), 7.22 – 7.18 (m, 2H), 7.17 – 7.09 (m, 4H), 7.08 – 7.00 (m, 3H), 6.98 – 6.89 (m, 2H), 6.77 (t, $J = 7.7$ Hz, 1H), 6.15 (s, 1H), 2.91 (s, 3H), 2.25 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** 161.4, 143.2, 142.7, 139.3, 136.9, 136.8, 136.5, 132.5, 132.4, 131.8, 131.7, 130.7, 129.7, 129.6, 128.4, 128.3, 128.2, 127.3, 127.23, 127.18, 126.6, 124.6, 124.1, 121.8, 120.7, 120.2, 119.5, 108.8, 100.3, 24.2, 12.2. **HRMS (ESI):** calcd. for C₃₁H₂₅N₂O⁺ [M+H]⁺: 441.1961, found : 441.1958. **[α]_D²⁰ = +20** ($c = 0.1$, CHCl₃).

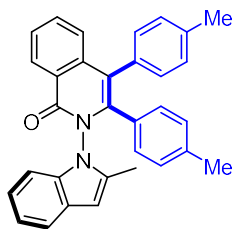
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 80:20, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (major) = 5.113 min, tr (minor) = 5.688 min, -88% ee.



No.	Time	Area	Area (%)
1	5.095	819.2	48.16
2	5.700	881.8	51.84



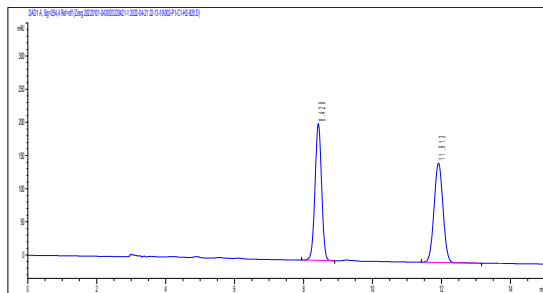
No.	Time	Area	Area (%)
1	5.113	2307.6	93.91
2	5.688	149.7	6.09



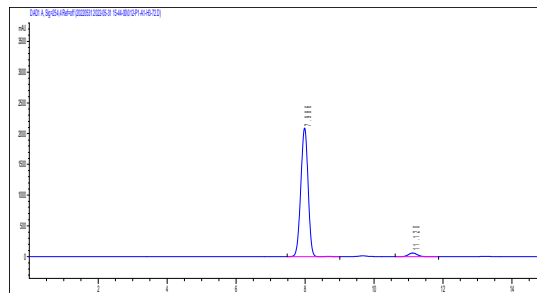
(R)-2-(2-methyl-1H-indol-1-yl)-3,4-di-p-tolylisoquinolin-1(2H)-one (11)

The title compound was isolated as a white solid (39.5 mg, 87%). **¹H NMR (600 MHz, CDCl₃)** δ 8.53 (d, J = 8.4 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.57 – 7.52 (m, 1H), 7.41 (d, J = 7.8 Hz, 1H), 7.35 (d, J = 8.2 Hz, 1H), 7.18 – 7.10 (m, 5H), 7.08 – 7.04 (m, 1H), 7.04 – 7.00 (m, 2H), 6.94 (d, J = 7.8 Hz, 2H), 6.77 (d, J = 7.7 Hz, 1H), 6.58 (d, J = 7.6 Hz, 1H), 2.31 (s, 3H), 2.23 (s, 3H), 2.05 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.1, 142.8, 138.0, 137.9, 137.1, 136.8, 136.7, 133.3, 132.9, 131.5, 131.4, 129.8, 129.5, 129.4, 129.2, 128.8, 128.7, 128.0, 127.3, 126.6, 126.2, 125.5, 121.9, 120.7, 120.2, 119.7, 108.8, 100.3, 21.32, 21.25, 12.0. **HRMS (ESI)**: calcd. for C₃₂H₂₇N₂O⁺ [M+H]⁺: 455.2118, found : 455.2103. **[α]_D²⁰** = +102 (c = 0.1, CHCl₃).

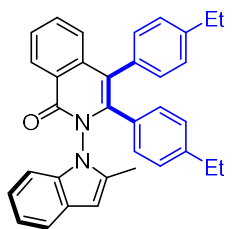
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, v = 1.0 mL/min, 40 °C, 254 nm). tr (major) = 7.986 min, tr (minor) = 11.120 min, -93% ee.



No.	Time	Area	Area (%)
1	8.428	2736.4	50.31
2	11.913	2702.3	49.69



No.	Time	Area	Area (%)
1	7.986	30651.6	96.56
2	11.120	1093.1	3.44

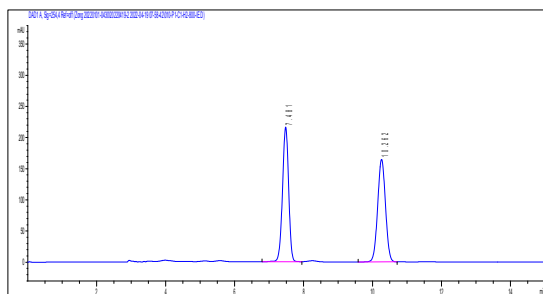


(R)-3,4-bis(4-ethylphenyl)-2-(2-methyl-1H-indol-1-yl)isoquinolin-1(2H)-one (12)

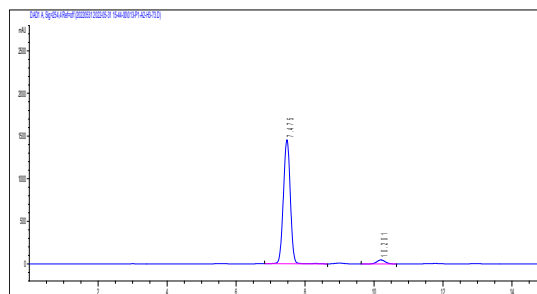
The title compound was isolated as a white solid (40.0 mg, 83%). **¹H NMR (600 MHz, CDCl₃)** δ 8.54 (d, J = 8.0 Hz, 1H), 7.68 – 7.63 (m, 1H), 7.57 – 7.52 (m, 1H), 7.39 (t, J = 8.3 Hz, 2H), 7.18 (d, J = 7.5 Hz, 1H), 7.15 – 7.11 (m, 3H), 7.08 – 7.00 (m, 3H), 6.94 (d, J = 7.8 Hz, 2H), 6.78 (s, 1H), 6.60 (s, 1H), 6.16 (s, 1H), 2.61 (q, J = 7.6 Hz, 2H), 2.36 (q, J = 7.6 Hz, 2H), 2.23 (s, 3H), 1.21 (t, J = 7.6 Hz, 3H), 0.99 (t, J = 7.6 Hz, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.1, 144.2, 143.1, 142.9, 137.9, 137.1, 136.8, 133.2, 133.1, 131.6, 131.5, 129.9, 129.6, 128.7, 127.8, 127.5, 127.3, 126.7, 126.6, 126.3, 125.6, 121.9, 120.7, 120.1, 119.8, 108.8, 100.3, 28.6, 28.4, 15.5, 14.9, 12.1. **HRMS (ESI)**: calcd. for C₃₄H₃₁N₂O⁺ [M+H]⁺: 483.2431, found : 483.2439. **[α]_D²⁰** = +110

(c = 0.1, CHCl₃).

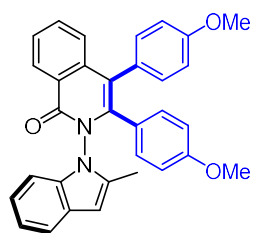
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, v = 1.0 mL/min, 40 °C, 254 nm). tr (major) = 7.475 min, tr (minor) = 10.201 min, -93% ee.



No.	Time	Area	Area (%)
1	7.481	2676.9	50.82
2	10.262	2590.2	49.18



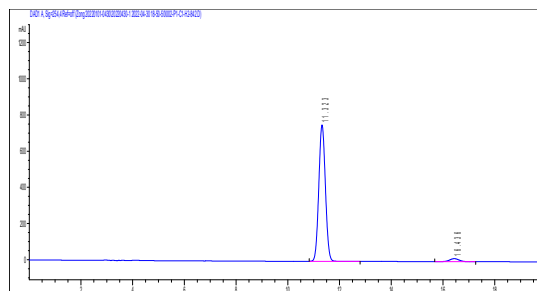
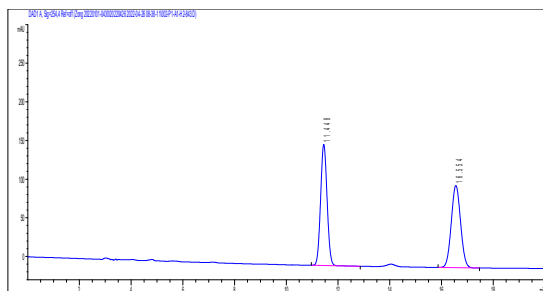
No.	Time	Area	Area (%)
1	7.475	20288.2	96.36
2	10.201	766.1	3.64



(*R*)-3,4-bis(4-methoxyphenyl)-2-(2-methyl-1H-indol-1-yl)isoquinolin-1(2H)-one (13)

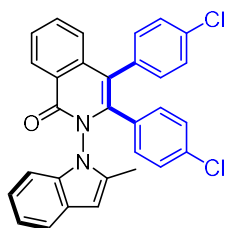
The title compound was isolated as a white solid (40.3 mg, 83%). **¹H NMR (600 MHz, CDCl₃)** δ 8.52 (d, *J* = 7.9 Hz, 1H), 7.67 – 7.63 (m, 1H), 7.57 – 7.52 (m, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 8.2 Hz, 1H), 7.18 (dd, *J* = 8.5, 2.3 Hz, 1H), 7.16 – 7.10 (m, 2H), 7.08 – 7.04 (m, 1H), 7.02 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 2H), 6.85 (dd, *J* = 8.5, 2.8 Hz, 1H), 6.76 (dd, *J* = 8.5, 2.8 Hz, 1H), 6.49 (s, 1H), 6.30 (s, 1H), 6.16 (s, 1H), 3.78 (s, 3H), 3.56 (s, 3H), 2.21 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.1, 159.1, 158.6, 142.8, 138.0, 137.0, 136.7, 133.3, 132.7, 132.6, 131.3, 130.9, 128.8, 128.2, 127.3, 126.6, 126.2, 125.5, 124.7, 121.9, 120.7, 120.2, 119.6, 113.9, 113.7, 112.9, 112.6, 108.7, 100.4, 55.3, 55.0, 12.0. **HRMS (ESI):** calcd. for C₃₂H₂₇N₂O₃⁺ [M+H]⁺: 487.2016, found : 487.2015. [α]_D²⁰ = +118 (c = 0.1, CHCl₃).

HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, v = 1.0 mL/min, 40 °C, 254 nm). tr (major) = 11.323 min, tr (minor) = 16.436 min, -94% ee.



No.	Time	Area	Area (%)
1	11.448	2727.6	50.71
2	16.554	2651.6	49.29

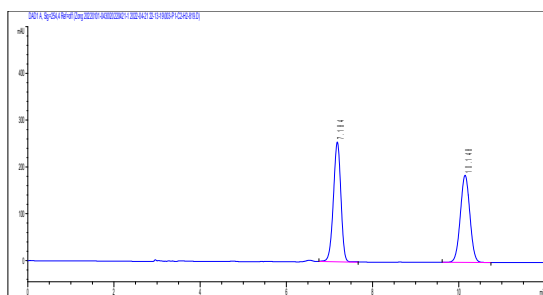
No.	Time	Area	Area (%)
1	11.323	13331.6	96.90
2	16.436	427.1	3.10



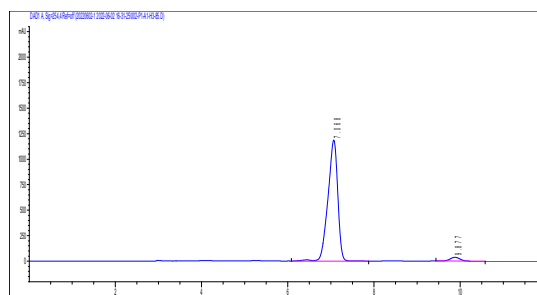
(*R*)-3,4-bis(4-chlorophenyl)-2-(2-methyl-1H-indol-1-yl)isoquinolin-1(2H)-one (14)

The title compound was isolated as a white solid (19.8 mg, 40%). **¹H NMR (600 MHz, CDCl₃)** δ 8.53 (dd, J = 8.0, 1.4 Hz, 1H), 7.71 – 7.66 (m, 1H), 7.61 – 7.57 (m, 1H), 7.41 (d, J = 8.2 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.23 (dd, J = 8.2, 2.3 Hz, 1H), 7.19 (dd, J = 8.3, 2.2 Hz, 1H), 7.13 (t, J = 7.5 Hz, 1H), 7.09 – 7.03 (m, 3H), 7.01 – 6.93 (m, 3H), 6.78 (d, J = 7.8 Hz, 1H), 6.18 (s, 1H), 2.21 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 160.8, 141.8, 137.1, 136.9, 136.4, 134.8, 134.0, 133.8, 133.7, 132.9, 132.8, 131.1, 130.9, 130.4, 129.0, 128.7, 127.93, 127.90, 126.6, 126.0, 125.7, 122.2, 121.1, 120.5, 118.9, 108.5, 100.9, 12.1. **HRMS (ESI):** calcd. for C₃₀H₂₁Cl₂N₂O⁺ [M+H]⁺: 495.1025, found : 495.1021. [α]_D²⁰ = +124 (c = 0.1, CHCl₃).

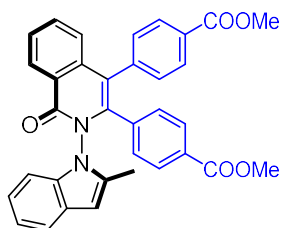
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, v = 1.0 mL/min, 40 °C, 254 nm). tr (major) = 7.068 min, tr (minor) = 9.877 min, -94% ee.



No.	Time	Area	Area (%)
1	7.184	3089.0	51.94
2	10.148	2857.6	48.06



No.	Time	Area	Area (%)
1	7.068	18696.9	96.98
2	9.877	582.2	3.02

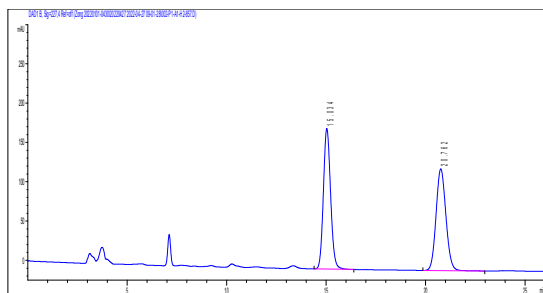


(*S*)-dimethyl 4,4'-(2-(2-methyl-1H-indol-1-yl)-1-oxo-1,2-dihydroisoquinoline-3,4-diyl)dibenzoate ((*ent*)-15)

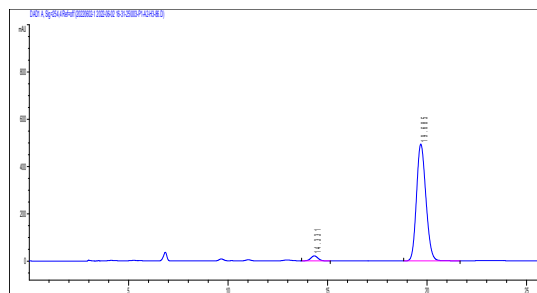
The title compound was isolated as a white solid (29.8 mg, 55%). **¹H NMR (600 MHz, CDCl₃)** δ 8.54 (dd, J = 8.1, 1.4 Hz, 1H), 7.96 (dd, J = 8.1, 1.8 Hz, 1H), 7.88 (dd, J = 8.0, 1.8 Hz, 1H), 7.71 – 7.67 (m, 1H), 7.66 – 7.63 (m, 1H), 7.60 (t, J = 7.4 Hz, 1H),

7.47 – 7.43 (m, 1H), 7.38 (d, $J = 7.8$ Hz, 1H), 7.35 (dd, $J = 8.1, 1.8$ Hz, 1H), 7.27 (d, $J = 8.3$ Hz, 1H), 7.20 (dd, $J = 8.1, 1.8$ Hz, 1H), 7.16 – 7.09 (m, 4H), 7.07 – 7.04 (m, 1H), 6.14 (s, 1H), 3.89 (s, 3H), 3.76 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 166.7, 166.2, 160.8, 141.9, 140.3, 136.8, 136.7, 136.4, 136.3, 133.8, 131.73, 131.66, 130.2, 129.9, 129.7, 129.6, 129.5, 129.1, 128.73, 128.70, 128.1, 126.6, 126.0, 125.7, 122.2, 121.1, 120.5, 119.1, 108.5, 100.9, 52.4, 52.2, 12.0. HRMS (ESI): calcd. for $\text{C}_{34}\text{H}_{27}\text{N}_2\text{O}_5^+$ $[\text{M}+\text{H}]^+$: 543.1914, found : 543.1908. $[\alpha]_{\text{D}}^{20} = -112$ ($c = 0.1$, CHCl_3).

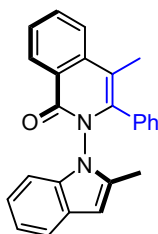
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (minor) = 14.331 min, tr (major) = 19.685 min, 94% ee.



No.	Time	Area	Area (%)
1	15.034	4505.6	50.29
2	20.762	4453.9	49.71



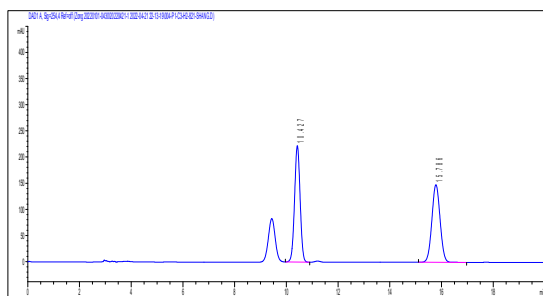
No.	Time	Area	Area (%)
1	14.331	522.1	3.11
2	19.685	16271.3	96.89



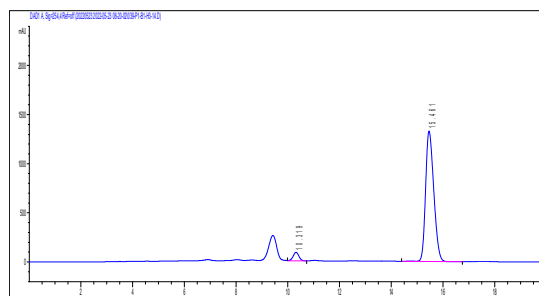
(S)-4-methyl-2-(2-methyl-1H-indol-1-yl)-3-phenylisoquinolin-1(2H)-one ((ent)-16)

The title compound was isolated as a white solid (21.8 mg, 60%). ^1H NMR (600 MHz, CDCl_3) δ 8.53 (d, $J = 7.9$ Hz, 1H), 7.87 – 7.82 (m, 2H), 7.62 – 7.57 (m, 1H), 7.37 (d, $J = 8.4$ Hz, 1H), 7.29 – 7.26 (m, 2H), 7.20 – 7.16 (m, 1H), 7.16 – 7.13 (m, 1H), 7.11 – 7.08 (m, 1H), 7.05 – 6.98 (m, 3H), 6.12 (s, 1H), 2.20 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 160.9, 141.6, 137.4, 136.7, 136.5, 133.4, 132.5, 129.1, 129.0, 128.8, 127.8, 127.7, 127.2, 126.4, 125.7, 123.9, 121.7, 120.5, 120.0, 111.6, 108.6, 100.1, 15.1, 11.9. HRMS (ESI): calcd. for $\text{C}_{25}\text{H}_{20}\text{N}_2\text{NaO}^+$ $[\text{M}+\text{Na}]^+$: 387.1468, found : 387.1468. $[\alpha]_{\text{D}}^{20} = +34$ ($c = 0.1$, CHCl_3).

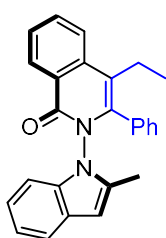
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (minor) = 10.319 min, tr (major) = 15.461 min, 91% ee.



No.	Time	Area	Area (%)
1	10.427	3314.1	50.34
2	15.786	3269.3	49.66



No.	Time	Area	Area (%)
1	10.319	1337.9	4.40
2	15.461	29085.5	95.60

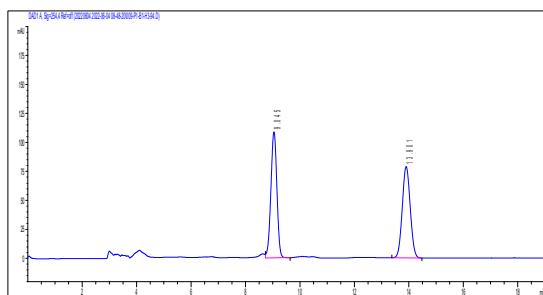


(S)-4-ethyl-2-(2-methyl-1H-indol-1-yl)-3-phenylisoquinolin-1(2H)-one ((ent)-17)

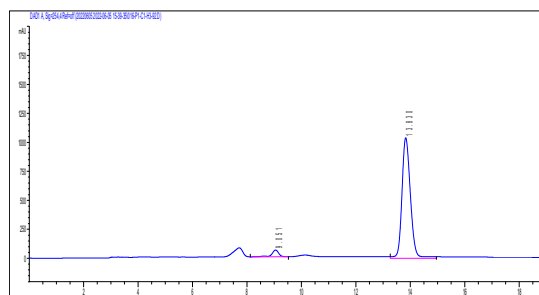
The title compound was isolated as a white solid (17.4 mg, 46%). ¹H NMR (600 MHz, CDCl₃) δ 8.52 (d, *J* = 8.1 Hz, 1H), 7.87 – 7.78 (m, 2H), 7.60 – 7.53 (m, 1H), 7.33 (d, *J* = 7.9 Hz, 1H), 7.30 – 7.22 (m, 2H), 7.19 – 7.13 (m, 2H), 7.09 – 7.05 (m, 1H), 7.04 – 6.94 (m, 3H), 6.09 (s, 1H), 2.60 – 2.45 (m, 2H), 2.20 (s, 3H), 1.16 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 160.9, 141.7, 136.8, 136.6, 136.5, 133.5, 132.4, 129.3, 129.03, 128.98, 128.8, 127.84, 127.81, 127.2, 126.5, 126.3, 124.0, 121.7, 120.7, 120.1, 117.8, 108.7, 100.2, 21.9, 14.9, 12.0. HRMS (ESI): calcd. for C₂₆H₂₃N₂O⁺ [M+H]⁺: 379.1805, found : 379.1801. [α]_D²⁰ = +24 (c = 0.1, CHCl₃).

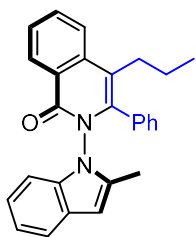
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, v = 1.0 mL/min, 40 °C, 254 nm). tr (minor) = 9.051 min, tr (major) = 13.830 min, 91% ee.



No.	Time	Area	Area (%)
1	9.045	1656.6	50.88
2	13.901	1599.2	49.12



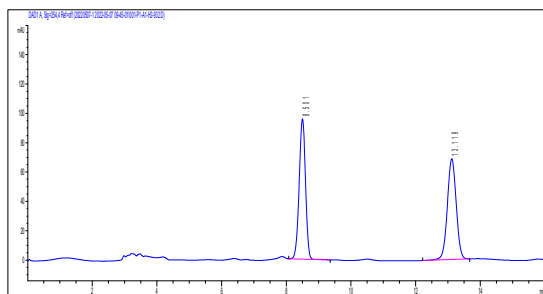
No.	Time	Area	Area (%)
1	9.051	1008.7	4.29
2	13.830	22483.1	95.71



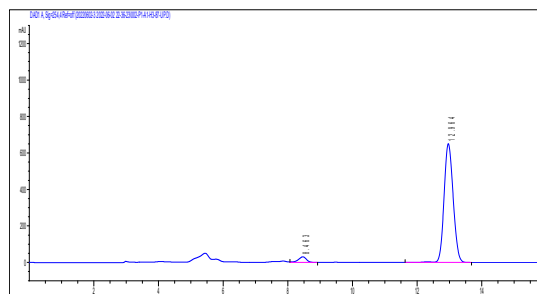
(S)-2-(2-methyl-1H-indol-1-yl)-3-phenyl-4-propylisoquinolin-1(2H)-one ((ent)-18)

The title compound was isolated as a white solid (15.7 mg, 40%). **¹H NMR (600 MHz, CDCl₃)** δ 8.52 (d, J = 7.9 Hz, 1H), 7.84 – 7.78 (m, 2H), 7.59 – 7.54 (m, 1H), 7.34 (d, J = 7.7 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.18 – 7.12 (m, 2H), 7.09 – 7.05 (m, 1H), 7.03 – 6.95 (m, 3H), 6.09 (s, 1H), 2.46 (td, J = 7.3, 2.9 Hz, 2H), 2.20 (s, 3H), 1.61 (dd, J = 7.3, 2.7 Hz, 2H), 0.86 (t, J = 7.3 Hz, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.0, 142.0, 136.81, 136.76, 136.6, 133.4, 132.5, 129.3, 129.2, 128.97, 128.95, 127.78, 127.76, 127.2, 126.5, 126.3, 124.1, 121.8, 120.7, 120.1, 116.6, 108.7, 100.2, 30.8, 23.7, 14.4, 12.0. **HRMS (ESI)**: calcd. for C₂₇H₂₅N₂O⁺ [M+H]⁺: 393.1961, found : 393.1963. **[α]_D²⁰** = +44 (c = 0.1, CHCl₃).

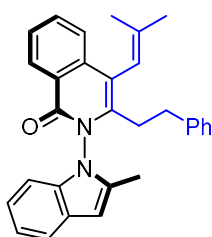
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 75:25, v = 1.0 mL/min, 40 °C, 254 nm). tr (minor) = 8.463 min, tr (major) = 12.964 min, 92% ee.



No.	Time	Area	Area (%)
1	8.501	1303.4	50.00
2	13.119	1303.3	50.00



No.	Time	Area	Area (%)
1	8.463	521.2	3.94
2	12.964	12716.2	96.06

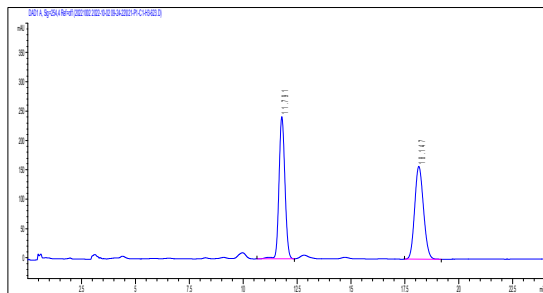


(S)-2-(2-methyl-1H-indol-1-yl)-4-(2-methylprop-1-en-1-yl)-3-phenethylisoquinolin-1(2H)-one ((ent)-19)

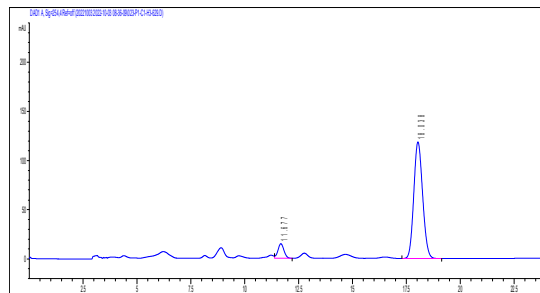
The title compound was isolated as a white solid (16.8 mg, 39%). **¹H NMR (600 MHz, CDCl₃)** δ 8.51 (d, J = 7.9 Hz, 1H), 7.91 (d, J = 8.2 Hz, 1H), 7.86 – 7.80 (m, 1H), 7.56 (t, J = 7.5 Hz, 1H), 7.49 (d, J = 7.5 Hz, 1H), 7.26 – 7.22 (m, 2H), 7.22 – 7.18 (m, 1H), 7.13 – 6.99 (m, 4H), 6.72 (s, 1H), 6.31 (s, 1H), 5.00 – 4.75 (m, 1H), 3.27 – 2.76 (m, 4H), 2.08 (s, 3H), 1.72 – 1.36 (m, 6H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.0, 141.1, 139.5, 136.6, 136.2, 133.3, 129.4, 128.8, 128.5, 126.8, 126.6, 126.3, 126.0, 123.9, 121.8, 120.7, 120.1, 114.1, 108.4, 100.1, 35.6, 29.9, 24.8, 20.4, 11.5. **HRMS (ESI)**: calcd. for C₃₀H₂₉N₂O⁺ [M+H]⁺: 433.2274, found : 433.2280.

[α]_D²⁰ = +12 (c = 0.1, CHCl₃).

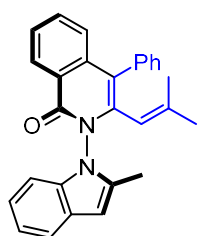
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 80:20, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (minor) = 11.677 min, tr (major) = 18.038 min, 84% ee.



No.	Time	Area	Area (%)
1	11.791	4625.0	50.71
2	18.147	4495.5	49.29



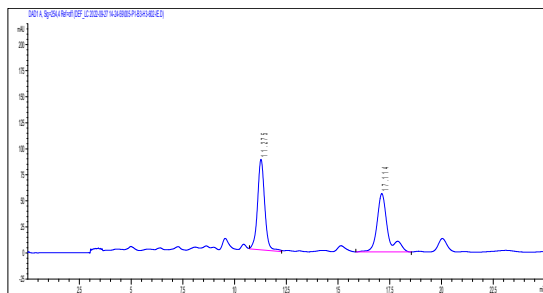
No.	Time	Area	Area (%)
1	11.677	286.7	7.80
2	18.038	3388.8	92.20



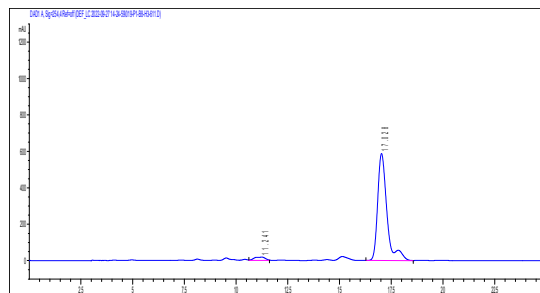
(S)-2-(2-methyl-1H-indol-1-yl)-3-(2-methylprop-1-en-1-yl)-4-phenylisoquinolin-1(2H)-one ((ent)-20)

The title compound was isolated as a white solid (17.0 mg, 42%). **¹H NMR (600 MHz, CDCl₃)** δ 8.50 (d, $J = 8.0$ Hz, 1H), 7.82 – 7.69 (m, 2H), 7.59 – 7.54 (m, 1H), 7.44 – 7.34 (m, 1H), 7.24 – 6.87 (m, 8H), 6.24 – 3.07 (m, 1H), 5.96 – 5.73 (m, 1H), 2.32 – 2.08 (m, 3H), 1.80 – 1.67 (m, 3H), 1.54 – 1.37 (m, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.1, 139.6, 136.6, 133.4, 128.9, 128.6, 127.5, 127.4, 125.7, 125.6, 121.9, 120.7, 118.7, 115.4, 108.6, 100.3, 25.0, 11.9. **HRMS (ESI):** calcd. for C₂₈H₂₄N₂NaO⁺ [M+Na]⁺: 427.1781, found : 427.1776. **[α]_D²⁰ = -24** (c = 0.1, CHCl₃).

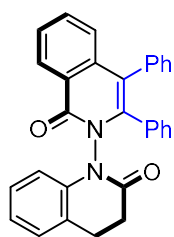
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 85:15, $v = 1.0$ mL/min, 40 °C, 254 nm). tr (minor) = 11.241 min, tr (major) = 17.028 min, 93% ee.



No.	Time	Area	Area (%)
1	11.275	2097.3	50.98
2	17.114	2016.8	49.02



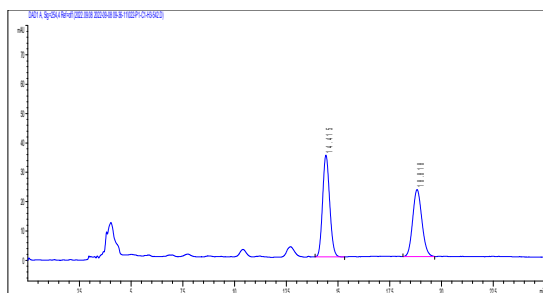
No.	Time	Area	Area (%)
1	11.241	668.4	3.52
2	17.028	18302	96.48



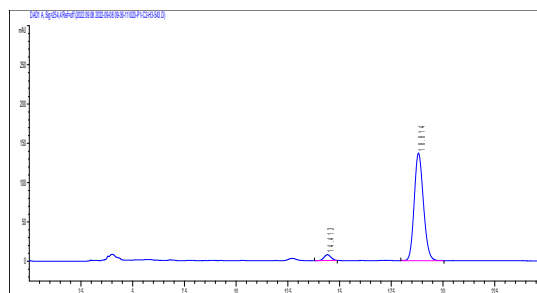
(*R*)-1-(1-oxo-3,4-diphenylisoquinolin-2(1H)-yl)-3,4-dihydroquinolin-2(1H)-one (21)

The title compound was isolated as a white solid (13.7 mg, 31%). **¹H NMR (600 MHz, CDCl₃)** δ 8.59 (dd, J = 8.1, 1.4 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.58 – 7.53 (m, 1H), 7.30 (dt, J = 7.7, 1.6 Hz, 1H), 7.26 (d, J = 8.1 Hz, 1H), 7.23 – 7.14 (m, 6H), 7.12 – 7.09 (m, 1H), 7.09 – 7.04 (m, 1H), 7.01 (d, J = 7.3 Hz, 1H), 6.97 (td, J = 7.4, 1.1 Hz, 1H), 6.79 (td, J = 7.6, 1.5 Hz, 1H), 6.72 (d, J = 8.0 Hz, 1H), 6.63 (d, J = 7.7 Hz, 1H), 2.75 (dt, J = 15.9, 5.7 Hz, 1H), 2.64 (dt, J = 15.5, 5.1 Hz, 1H), 2.49 (dt, J = 15.8, 4.7 Hz, 1H), 2.06 (td, J = 14.5, 5.0 Hz, 1H). **¹³C NMR (150 MHz, CDCl₃)** δ 167.9, 159.9, 142.0, 139.4, 137.9, 135.7, 133.3, 132.5, 131.6, 131.4, 130.1, 129.5, 128.9, 128.5, 128.3, 128.1, 127.7, 127.5, 127.30, 127.26, 126.9, 126.2, 125.7, 125.3, 123.8, 120.1, 114.1, 31.4, 24.5. **HRMS (ESI)**: calcd. for C₃₀H₂₂N₂NaO₂⁺ [M+Na]⁺: 465.1573, found : 465.1574. **[α]_D²⁰** = +56 (c = 0.1, CHCl₃).

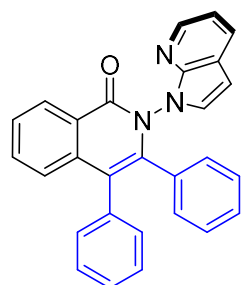
HPLC analysis: Daicel Chiralpak IE column (hexane: 2-propanol = 70:30, v = 1.0 mL/min, 40 °C, 254 nm). tr (minor) = 14.413 min, tr (major) = 18.814 min, -92% ee.



No.	Time	Area	Area (%)
1	14.415	822.3	53.84
2	18.818	704.9	46.16



No.	Time	Area	Area (%)
1	14.413	172.2	3.91
2	18.814	4228.2	96.09

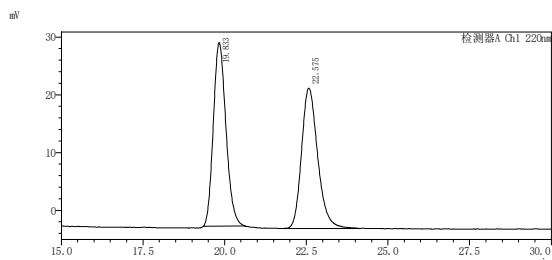


(*S*)-3,4-diphenyl-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (23)

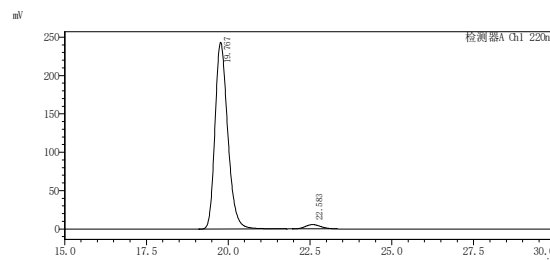
The title compound was isolated as a white solid (35.9 mg, 87%). **¹H NMR (600 MHz, CDCl₃)** δ 8.52 (dd, J = 8.0, 1.8 Hz, 1H), 8.32 (dd, J = 4.7, 1.9 Hz, 1H), 7.76 (dd, J = 7.8, 1.8 Hz, 1H), 7.63 – 7.56 (m, 1H), 7.51 (t, J = 7.7 Hz, 1H), 7.31 – 7.14 (m, 6H), 7.08 – 7.11 (m, 3H), 7.04 (ddd, J = 7.5, 4.7, 1.8 Hz, 1H), 6.95 (t, J = 7.6 Hz, 1H), 6.91 – 6.80 (m, 1H), 6.70 (t, J = 7.6 Hz, 1H), 6.34 (dd, J = 3.9, 1.8 Hz, 1H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.1, 147.3, 143.8, 142.0, 137.6, 135.6, 133.2, 132.2, 131.6, 131.3, 129.8, 129.7, 129.4, 128.8, 128.6, 128.2, 128.1, 127.9, 127.23, 127.16, 126.94, 126.92, 126.0, 125.3, 119.3, 118.6,

117.1, 100.5. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{28}H_{20}N_3O^+ [M + H]^+$, 414.1601, found 414.1603. $[\alpha]_D^{20} = -12$ ($c = 0.1$, $CHCl_3$).

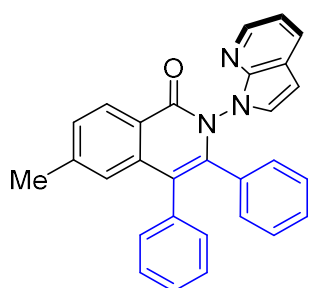
HPLC conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 19.767 min, tr (minor) = 22.583 min, 94% ee.



No.	Time	Area	Area (%)
1	19.833	855696	50.63
2	22.575	834444	49.37



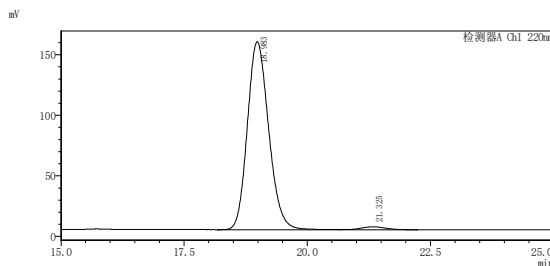
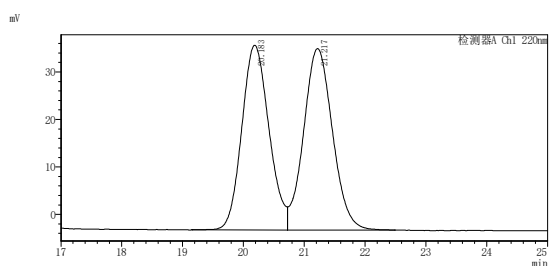
No.	Time	Area	Area (%)
1	19.767	6594297	97.29
2	22.583	183611	2.71



(S)-6-methyl-3,4-diphenyl-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (24)

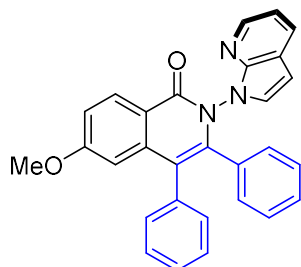
The title compound was isolated as a white solid (34.2 mg, 80%). **1H NMR** (600 MHz, $CDCl_3$) δ 8.41 (d, $J = 8.1$ Hz, 1H), 8.32 (dd, $J = 4.7, 1.5$ Hz, 1H), 7.76 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.34 (dd, $J = 8.2, 1.6$ Hz, 1H), 7.27 – 7.16 (m, 5H), 7.12 – 7.02 (m, 5H), 6.94 (td, $J = 7.6, 1.4$ Hz, 1H), 6.88 (tt, $J = 7.5, 1.3$ Hz, 1H), 6.70 (td, $J = 7.7, 1.4$ Hz, 1H), 6.34 (dd, $J = 3.8, 0.9$ Hz, 1H), 2.38 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.0, 146.9, 144.0, 142.0, 137.7, 135.8, 132.4, 131.6, 131.4, 129.9, 129.8, 129.4, 128.84, 128.79, 128.7, 128.2, 128.0, 127.9, 127.1, 126.9, 126.9, 125.8, 123.1, 119.2, 118.6, 117.1, 100.5, 22.1. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{29}H_{22}N_3O^+ [M + H]^+$, 428.1757, found 428.1752. $[\alpha]_D^{20} = -14$ ($c = 0.1$, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm). tr (major) = 18.983 min, tr (minor) = 21.325 min, 96% ee.



No.	Time	Area	Area (%)
1	20.183	1208956	48.91
2	21.217	1262736	51.09

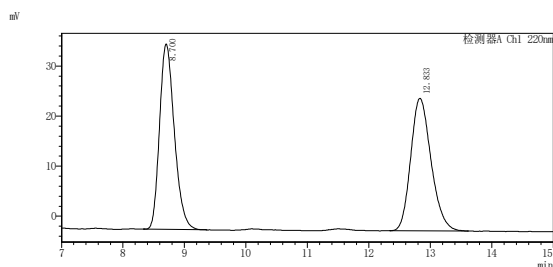
No.	Time	Area	Area (%)
1	18.983	4678935	98.24
2	21.325	83815	1.76



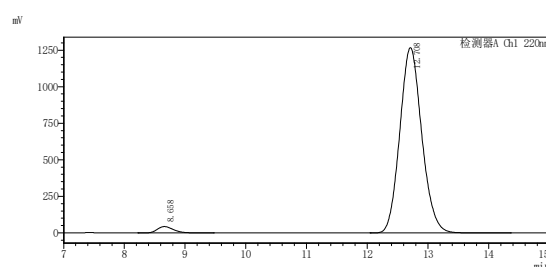
(S)-6-methoxy-3,4-diphenyl-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)-isoquinolin-1(2H)-one (25)

The title compound was isolated as a white solid (35.9 mg, 81%). **¹H NMR (600 MHz, CDCl₃)** δ 8.45 (dd, J = 8.9, 1.2 Hz, 1H), 8.32 (dd, J = 4.8, 1.5 Hz, 1H), 7.76 (dt, J = 7.8, 1.4 Hz, 1H), 7.26 – 7.20 (m, 2H), 7.20 – 7.14 (m, 3H), 7.13 – 7.06 (m, 4H), 7.04 (ddd, J = 7.8, 4.8, 1.2 Hz, 1H), 6.94 (td, J = 7.6, 1.4 Hz, 1H), 6.90 – 6.85 (m, 1H), 6.70 (td, J = 7.6, 1.4 Hz, 1H), 6.64 (d, J = 2.4 Hz, 1H), 6.33 (dd, J = 3.8, 1.2 Hz, 1H), 3.72 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 163.5, 160.7, 146.9, 144.0, 142.6, 139.8, 135.7, 132.4, 131.5, 131.3, 130.9, 129.8, 129.7, 129.3, 128.9, 128.3, 128.1, 127.9, 127.2, 126.92, 126.90, 119.1, 119.0, 118.6, 117.0, 115.6, 108.3, 100.4, 55.4. **HRMS (ESI-TOF) (m/z):** Calcd for C₂₉H₂₂N₃O₂⁺ [M + H]⁺, 444.1707, found 444.1710. **[α]_D²⁰** = -25 (c = 0.1, CHCl₃).

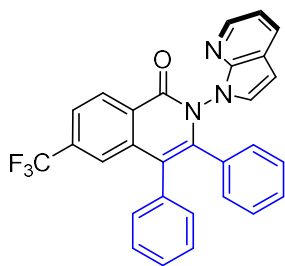
HPLC conditions: Daicel Chiralpak IC column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 12.708 min, tr (minor) = 8.658 min, 95% ee.



No.	Time	Area	Area (%)
1	8.700	620063	50.38
2	12.833	610643	49.62



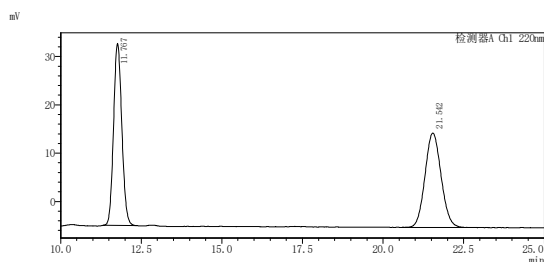
No.	Time	Area	Area (%)
1	8.658	814777	2.49
2	12.708	31867452	97.51



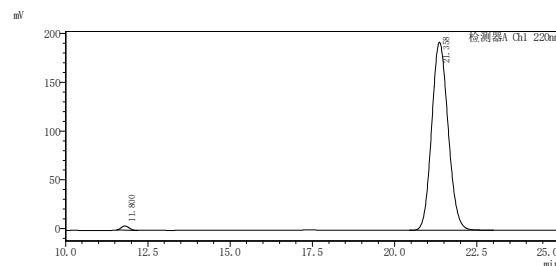
(S)-3,4-diphenyl-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)-6-(trifluoromethyl)-isoquinolin-1(2H)-one (26)

The title compound was isolated as a white solid (36.6 mg, 76%). ¹H NMR (600 MHz, CDCl₃) δ 8.64 (d, *J* = 8.3 Hz, 1H), 8.32 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.79 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.74 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.55 (s, 1H), 7.28 (td, *J* = 7.3, 2.7 Hz, 1H), 7.23 – 7.16 (m, 4H), 7.06–7.09 (m, 4H), 6.98 (t, *J* = 7.6 Hz, 1H), 6.94 – 6.90 (m, 1H), 6.73 (t, *J* = 7.6 Hz, 1H), 6.39 – 6.36 (m, 1H). ¹³C NMR (150 MHz, CDCl₃) δ 160.3, 146.7, 144.2, 143.7, 137.9, 134.6, 131.7, 131.4, 131.1, 129.7, 129.62, 129.56, 129.55, 128.6, 128.4, 128.3, 127.7, 127.6, 127.09, 127.07, 124.4 (q, *J* = 273.8 Hz), 123.3, 123.2, 119.1, 118.6, 117.3, 100.9. HRMS (ESI-TOF) (*m/z*): Calcd for C₂₉H₁₉F₃N₃⁺ [*M* + *H*]⁺, 482.1475, found 482.1478. [α]_D²⁰ = -11 (*c* = 0.1, CHCl₃).

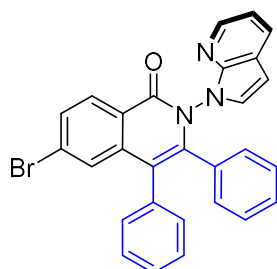
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm). *tr* (major) = 21.358 min, *tr* (minor) = 11.800 min, 98% ee.



No.	Time	Area	Area (%)
1	11.767	671472	49.69
2	21.542	679741	50.31



No.	Time	Area	Area (%)
1	11.800	70676	1.04
2	21.358	6695564	98.95

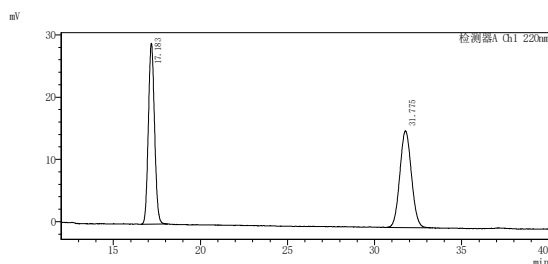


(S)-6-bromo-3,4-diphenyl-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (27)

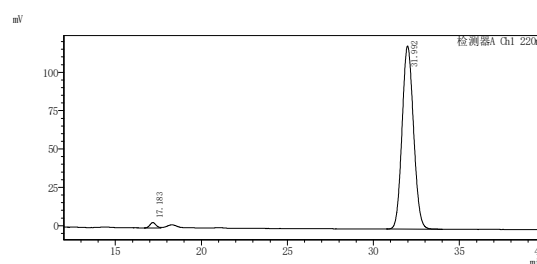
The title compound was isolated as a white solid (38.3 mg, 78%). ¹H NMR (600 MHz, CDCl₃) δ 8.36 (d, *J* = 8.5 Hz, 1H), 8.32 (dd, *J* = 4.8, 1.5 Hz, 1H), 7.77 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.62 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.42 (d, *J* = 1.9 Hz, 1H), 7.29 – 7.25 (m, 1H), 7.22 – 7.18 (m, 3H), 7.17 – 7.14 (m, 1H), 7.11 – 7.03 (m, 4H), 6.96 (t, *J* = 7.6 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 6.71 (t, *J* = 7.6 Hz, 1H), 6.35 (d, *J* = 3.8 Hz, 1H). ¹³C NMR (150 MHz, CDCl₃) δ 160.6, 146.7, 144.1, 143.5, 139.1, 134.8, 131.9, 131.5, 131.2, 130.6, 130.4, 129.7,

129.6, 129.5, 128.8, 128.6, 128.54, 128.49, 128.3, 128.2, 127.5, 127.0, 124.1, 118.6, 118.4, 117.3, 100.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{28}H_{19}BrN_3^+ [M + H]^+$, 492.0706, found 492.0703. $[\alpha]_D^{20} = -15$ ($c = 0.1$, $CHCl_3$).

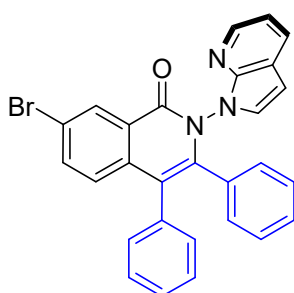
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 31.992 min, tr (minor) = 17.183 min, 97% ee.



No.	Time	Area	Area (%)
1	17.183	716093	49.83
2	31.775	720975	50.17



No.	Time	Area	Area (%)
1	17.183	86638	1.54
2	31.992	5538071	98.46

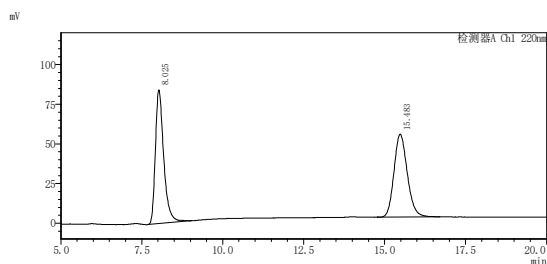


(S)-7-bromo-3,4-diphenyl-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (28)

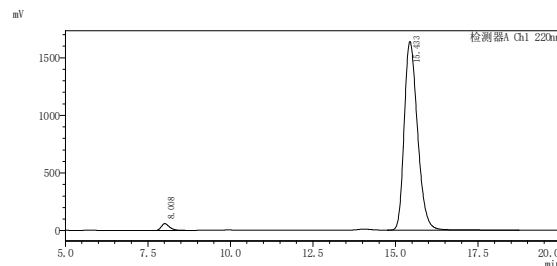
The title compound was isolated as a white solid (32.9 mg, 67%). **1H NMR** (600 MHz, $CDCl_3$) δ 8.64 (d, $J = 2.2$ Hz, 1H), 8.32 (d, $J = 4.8$ Hz, 1H), 7.77 (d, $J = 7.8$ Hz, 1H), 7.68 (dd, $J = 8.8, 2.2$ Hz, 1H), 7.27 – 7.23 (m, 1H), 7.18 – 7.20 (m, 3H), 7.15 (d, $J = 8.4$ Hz, 2H), 7.05 – 7.07 (m, 4H), 6.96 (t, $J = 7.6$

Hz, 1H), 6.90 (t, $J = 7.5$ Hz, 1H), 6.71 (t, $J = 7.6$ Hz, 1H), 6.35 (d, $J = 3.8$ Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.9, 145.8, 144.7, 142.6, 137.1, 136.1, 135.1, 131.9, 131.4, 131.2, 131.1, 129.7, 129.6, 129.5, 128.5, 128.4, 128.3, 128.1, 127.9, 127.4, 127.0, 126.7, 121.3, 118.9, 118.6, 117.2, 100.7. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{28}H_{19}BrN_3^+ [M + H]^+$, 492.0706, found 492.0703. $[\alpha]_D^{20} = -14$ ($c = 0.1$, $CHCl_3$).

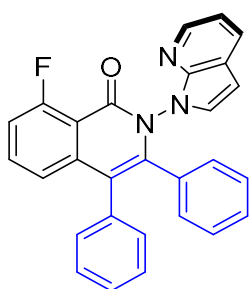
HPLC conditions: Daicel Chiralpak OD-3 column (70: 30 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm). tr (major) = 15.433 min, tr (minor) = 8.008 min, 95% ee.



No.	Time	Area	Area (%)
1	8.025	1514137	50.31
2	15.483	1495476	49.69



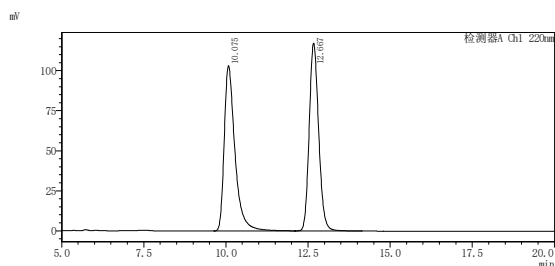
No.	Time	Area	Area (%)
1	8.008	1065588	2.27
2	15.433	45836809	97.73



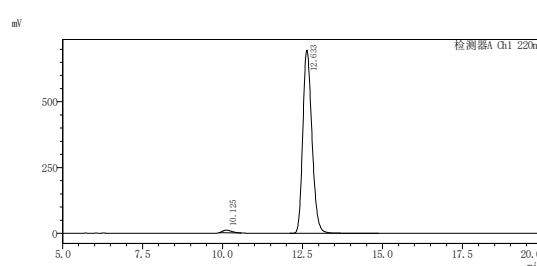
(S)-8-fluoro-3,4-diphenyl-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (29)

The title compound was isolated as a white solid (33.2 mg, 77%). **¹H NMR (600 MHz, CDCl₃)** δ 8.32 (dd, J = 4.8, 1.5 Hz, 1H), 7.76 (dd, J = 7.8, 1.5 Hz, 1H), 7.51 (td, J = 8.2, 5.0 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.22 – 7.10 (m, 6H), 7.10 – 7.06 (m, 2H), 7.06 – 7.00 (m, 2H), 6.96 (td, J = 7.6, 1.4 Hz, 1H), 6.89 (tt, J = 7.5, 1.3 Hz, 1H), 6.72 (td, J = 7.6, 1.4 Hz, 1H), 6.35 (d, J = 3.8 Hz, 1H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.0, 156.9, 145.8, 143.0, 142.4, 139.3, 134.6, 133.0, 131.0, 130.5, 130.3, 128.5, 128.3, 127.9, 127.3, 127.2, 127.0, 126.3, 126.0, 120.9, 117.7, 117.4, 116.1, 113.5, 113.3, 113.1, 99.7. **HRMS (ESI-TOF)** (m/z): Calcd for C₂₈H₁₉FN₃⁺ [$M + H$]⁺, 432.1507, found 432.1515. **[α]_D²⁰** = -7 (c = 0.1, CHCl₃).

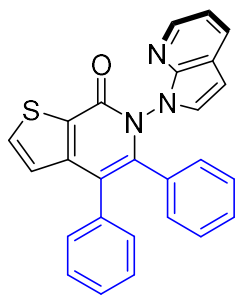
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 12.633 min, tr (minor) = 10.125 min, 98% ee.



No.	Time	Area	Area (%)
1	10.075	2356666	50.05
2	12.667	2351884	49.95



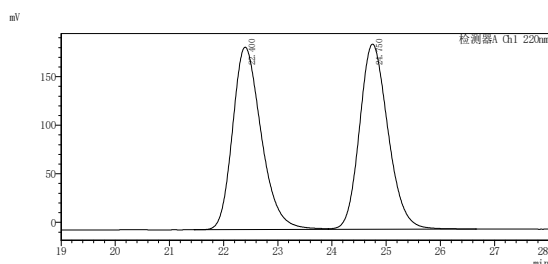
No.	Time	Area	Area (%)
1	10.125	185635	1.22
2	12.633	13900388	98.78



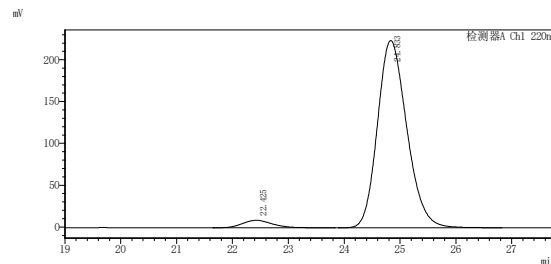
(S)-4,5-diphenyl-6-(1H-pyrrolo[2,3-b]pyridin-1-yl)thieno[2,3-c]pyridin-7(6H)-one (30)

The title compound was isolated as a white solid (21.8 mg, 52%). **¹H NMR (600 MHz, CDCl₃)** δ 8.33 (dd, J = 4.8, 1.4 Hz, 1H), 7.77 (dd, J = 7.8, 1.4 Hz, 1H), 7.71 (dd, J = 5.3, 1.2 Hz, 1H), 7.25 – 7.14 (m, 5H), 7.13 – 7.04 (m, 4H), 7.01 (dd, J = 5.3, 1.3 Hz, 1H), 6.97 (t, J = 7.6 Hz, 1H), 6.95 – 6.90 (m, 1H), 6.74 (t, J = 7.6 Hz, 1H), 6.35 (d, J = 3.7 Hz, 1H). **¹³C NMR (150 MHz, CDCl₃)** δ 156.2, 147.5, 146.6, 144.8, 143.5, 136.9, 134.3, 131.8, 130.8, 130.5, 130.0, 129.9, 129.5, 128.8, 128.7, 128.3, 128.2, 128.0, 127.2, 127.06, 127.05, 125.3, 118.6, 117.7, 117.2, 101.9. **HRMS (ESI-TOF)** (m/z): Calcd for C₂₆H₁₈N₃OS⁺ [M + H]⁺, 420.1165, found 420.1169. **[α]_D²⁰** = -20 (c = 0.1, CHCl₃).

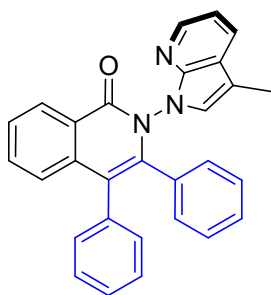
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 24.833 min, tr (minor) = 22.425 min, 92% ee.



No.	Time	Area	Area (%)
1	22.400	6927354	49.85
2	24.750	6969582	50.15



No.	Time	Area	Area (%)
1	22.425	335575	3.94
2	24.833	8170492	96.06



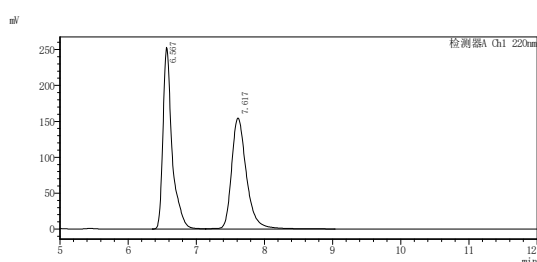
(S)-2-(3-methyl-1H-pyrrolo[2,3-b]pyridin-1-yl)-3,4-diphenylisoquinolin-1(2H)-one (31)

The title compound was isolated as a white solid (38.4 mg, 90%). **¹H NMR (600 MHz, CDCl₃)** δ 8.50 (dd, J = 8.0, 1.6 Hz, 1H), 8.29 (dd, J = 4.8, 1.6 Hz, 1H), 7.72 (dd, J = 7.8, 1.6 Hz, 1H), 7.59 (ddd, J = 8.4, 7.0, 1.6 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.30 – 7.20 (m, 4H), 7.20 – 7.14 (m, 4H), 7.08 (d, J = 7.9 Hz, 1H), 7.03 (dd, J = 7.8, 4.8 Hz, 1H), 6.96 (td, J = 7.6, 1.5 Hz, 1H), 6.89 (ddd, J = 9.0, 6.9, 1.5 Hz, 1H), 6.86 – 6.83 (m, 1H), 6.73 (td, J = 7.7, 1.6 Hz, 1H), 2.15 (s, 3H).

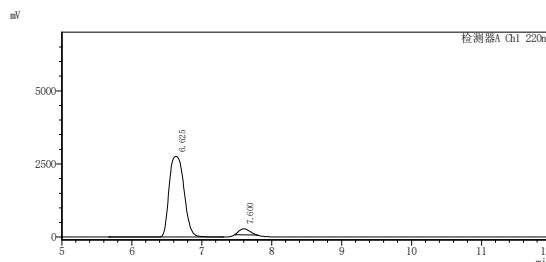
¹³C NMR (150 MHz, CDCl₃) δ 161.2, 147.4, 143.9, 142.2, 137.6, 135.7, 133.1, 132.4, 131.6, 131.4, 129.9, 129.8, 128.6, 128.2, 128.0, 127.9,

127.4, 127.13, 127.11, 126.91, 126.89, 126.0, 125.9, 125.4, 119.6, 119.2, 116.5, 110.1, 9.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{29}H_{22}N_3O^+$ $[M + H]^+$, 428.1757, found 428.1759. $[\alpha]_D^{20} = -25$ ($c = 0.1$, $CHCl_3$).

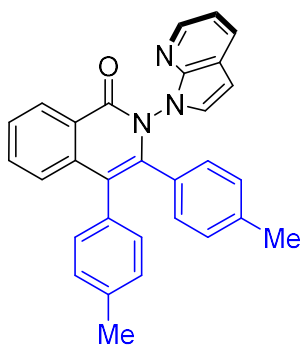
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 6.625 min, tr (minor) = 7.600 min, 91% ee.



No.	Time	Area	Area (%)
1	6.567	2343848	50.08
2	7.617	2336151	49.92



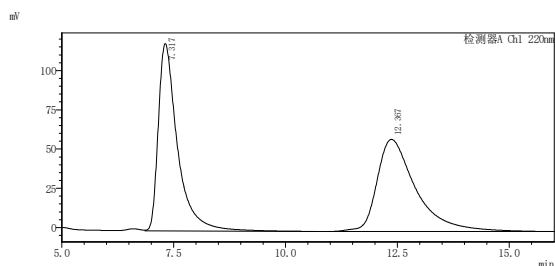
No.	Time	Area	Area (%)
1	6.625	40691890	95.26
2	7.600	2039277	4.74



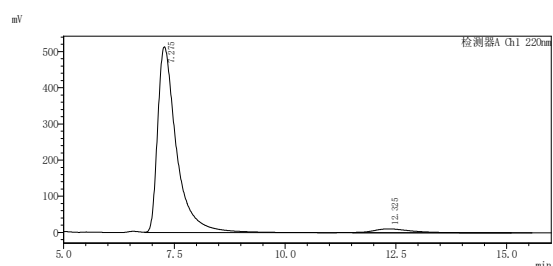
(S)-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)-3,4-di-p-tolylisoquinolin-1(2H)-one (32)

The title compound was isolated as a white solid (40.6 mg, 92%). **1H NMR** (600 MHz, $CDCl_3$) δ 8.50 (dd, $J = 8.0, 1.4$ Hz, 1H), 8.32 (dd, $J = 4.8, 1.5$ Hz, 1H), 7.77 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.58 (ddd, $J = 8.4, 7.2, 1.5$ Hz, 1H), 7.49 (ddd, $J = 8.2, 7.1, 1.2$ Hz, 1H), 7.30 – 7.25 (m, 1H), 7.11 (dd, $J = 7.8, 1.9$ Hz, 1H), 7.08 – 7.02 (m, 4H), 7.01 – 6.94 (m, 3H), 6.75 (dd, $J = 7.8, 1.8$ Hz, 1H), 6.51 (dd, $J = 7.9, 1.8$ Hz, 1H), 6.35 (d, $J = 3.8$ Hz, 1H), 2.27 (s, 3H), 2.02 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.1, 146.9, 144.0, 142.1, 137.9, 137.7, 136.6, 133.1, 132.7, 131.4, 131.2, 129.7, 129.50, 129.45, 129.3, 129.0, 128.8, 128.6, 128.5, 127.7, 127.0, 126.1, 125.3, 119.3, 118.6, 117.0, 100.5, 21.2, 21.1. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{30}H_{24}N_3O^+$ $[M + H]^+$, 442.1914, found 442.1916. $[\alpha]_D^{20} = -13$ ($c = 0.1$, $CHCl_3$).

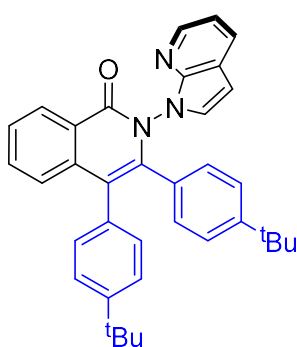
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm). tr (major) = 7.275 min, tr (minor) = 12.325 min, 92% ee.



No.	Time	Area	Area (%)
1	7.317	3573383	50.08
2	12.367	3562054	49.92

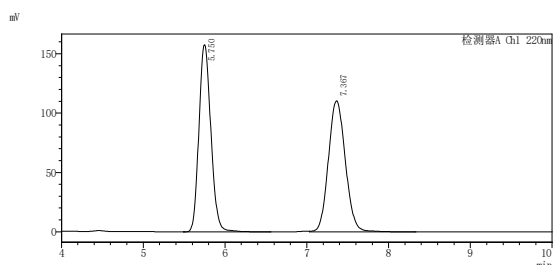


No.	Time	Area	Area (%)
1	7.275	15363877	95.96
2	12.325	647173	4.04

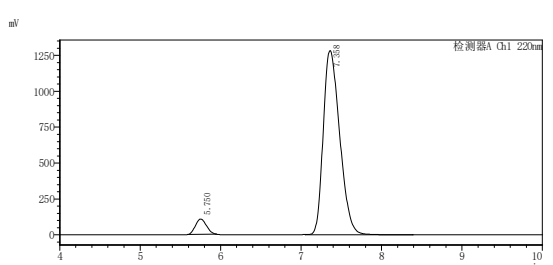


(*S*)-3,4-bis(4-(tert-butyl)phenyl)-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (33)

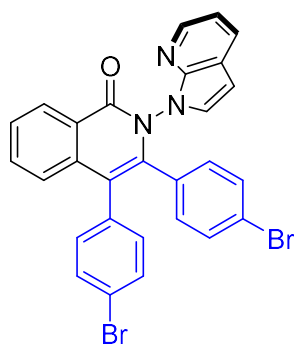
The title compound was isolated as a white solid (46.2 mg, 88%). **¹H NMR (600 MHz, CDCl₃)** δ 8.43 (dd, J = 8.1, 1.4 Hz, 1H), 8.25 (dd, J = 4.8, 1.5 Hz, 1H), 7.69 (dd, J = 7.8, 1.5 Hz, 1H), 7.52 (ddd, J = 8.4, 7.1, 1.5 Hz, 1H), 7.41 (ddd, J = 8.2, 7.2, 1.2 Hz, 1H), 7.30 (dt, J = 8.1, 1.0 Hz, 1H), 7.16 (dd, J = 8.1, 2.2 Hz, 1H), 7.08 (dd, J = 8.1, 2.2 Hz, 1H), 7.04 (dd, J = 8.1, 2.0 Hz, 1H), 7.00 (d, J = 3.8 Hz, 1H), 6.98 – 6.93 (m, 2H), 6.89 (d, J = 8.4 Hz, 1H), 6.85 (t, J = 6.0 Hz, 2H), 6.62 (d, J = 8.4 Hz, 1H), 6.26 (d, J = 3.8 Hz, 1H), 1.16 (s, 9H), 0.95 (s, 9H). **¹³C NMR (150 MHz, CDCl₃)** δ 172.4, 168.8, 160.1, 149.8, 148.7, 146.0, 143.0, 141.2, 136.8, 132.0, 131.7, 130.2, 129.9, 128.7, 128.4, 127.9, 127.5, 126.0, 125.1, 124.2, 123.9, 123.5, 122.6, 118.5, 117.7, 116.0, 99.5, 33.4, 33.3, 30.2, 29.9. **HRMS (ESI-TOF) (m/z):** Calcd for C₃₆H₃₆N₃⁺ [M + H]⁺, 526.2853, found 526.2853. **[α]_D²⁰** = -16 (c = 0.1, CHCl₃). **HPLC conditions:** Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm). tr (major) = 7.358 min, tr (minor) = 5.750 min, 90% ee.



No.	Time	Area	Area (%)
1	5.750	1603324	50.08
2	7.367	1597945	49.92



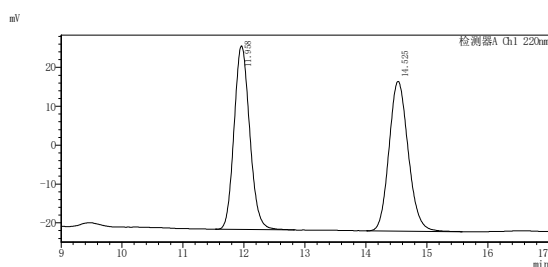
No.	Time	Area	Area (%)
1	5.750	1006383	5.21
2	7.358	18299696	94.79



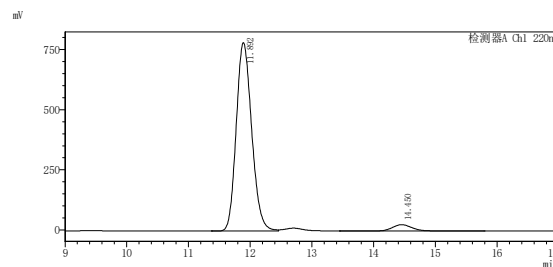
(S)-3,4-bis(4-bromophenyl)-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)-isoquinolin-1(2H)-one (34)

The title compound was isolated as a white solid (52.9 mg, 93%). ¹H NMR (600 MHz, CDCl₃) δ 8.54 – 8.47 (m, 1H), 8.30 (dd, *J* = 4.8, 1.4 Hz, 1H), 7.81 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.66 – 7.60 (m, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.42 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.38 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.22 (d, *J* = 8.2 Hz, 1H), 7.13 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.06 – 7.09 (m, 3H), 7.05 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.02 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.95 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.90 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.41 (d, *J* = 3.8 Hz, 1H). ¹³C NMR (150 MHz, CDCl₃) δ 160.9, 146.8, 144.2, 141.0, 137.1, 134.3, 133.4, 133.1, 132.9, 131.8, 131.5, 131.3, 131.2, 130.5, 129.6, 128.8, 128.5, 127.7, 125.8, 125.4, 122.8, 121.7, 118.7, 118.3, 117.4, 101.1. HRMS (ESI-TOF) (*m/z*): Calcd for C₂₈H₁₈Br₂N₃⁺ [*M* + *H*]⁺, 569.9811, found 569.9816. [α]_D²⁰ = -10 (*c* = 0.1, CHCl₃).

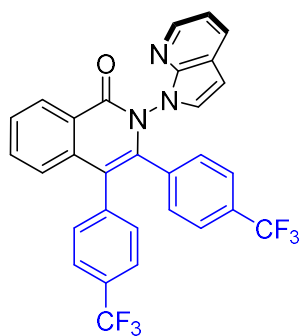
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm). *tr* (major) = 11.892 min, *tr* (minor) = 14.450 min, 92% ee.



No.	Time	Area	Area (%)
1	11.958	843032	49.95
2	14.525	844666	50.05



No.	Time	Area	Area (%)
1	11.892	13653436	95.89
2	14.450	585879	4.11

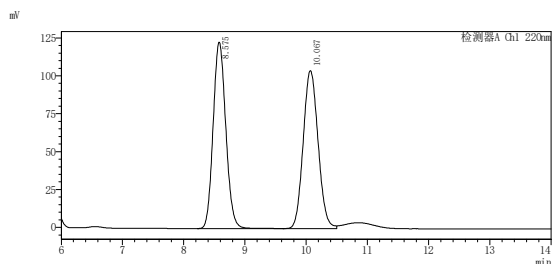


(S)-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)-3,4-bis(4-(trifluoromethyl)phenyl)isoquinolin-1(2H)-one (35)

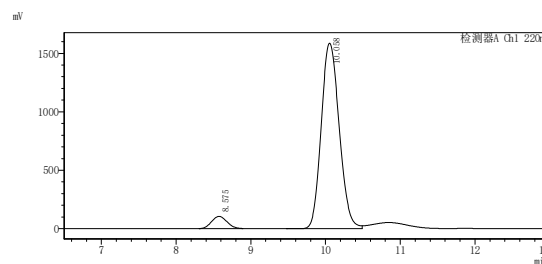
The title compound was isolated as a white solid (47.8 mg, 87%). ¹H NMR (600 MHz, CDCl₃) δ 8.53 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.31 (dd, *J* = 4.8, 1.5 Hz, 1H), 7.80 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.66 (ddd, *J* = 8.4, 7.1, 1.5 Hz, 1H), 7.60 – 7.53 (m, 2H), 7.51 (dd, *J* = 8.0, 2.2 Hz, 1H), 7.40 – 7.28 (m, 3H), 7.27 – 7.24 (m, 1H), 7.22 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.18 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.12 – 7.06 (m, 2H), 7.02

(dd, $J = 8.3, 1.9$ Hz, 1H), 6.40 (dd, $J = 3.8, 1.3$ Hz, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 160.8, 146.8, 144.9, 140.9, 139.1, 136.8, 133.7, 131.9, 131.7, 130.4, 130.3, 130.1 (q, $J = 67.2$ Hz), 129.7, 128.9, 128.5, 128.0, 125.7, 125.5, 125.3, 124.2, 118.7, 118.3, 117.6, 101.7. HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{30}\text{H}_{18}\text{F}_6\text{N}_3^+$ [$\text{M} + \text{H}$] $^+$, 550.1349, found 550.1349. $[\alpha]_{\text{D}}^{20} = -20$ ($c = 0.1$, CHCl_3).

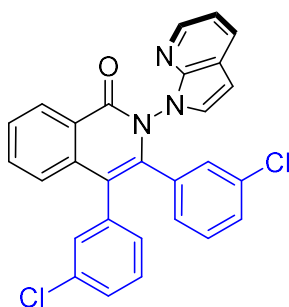
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm). tr (major) = 10.058 min, tr (minor) = 8.575 min, 90% ee.



No.	Time	Area	Area (%)
1	8.575	1768837	50.07
2	10.067	1763708	49.93



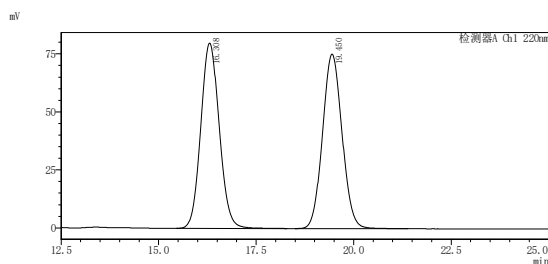
No.	Time	Area	Area (%)
1	8.575	1486849	5.30
2	10.058	26569745	94.70



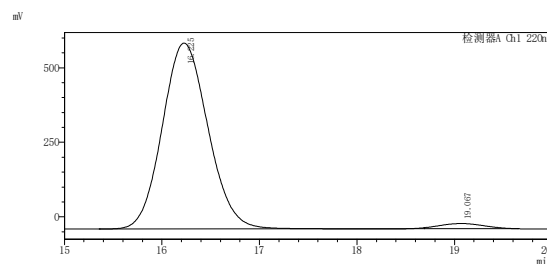
(*S*)-3,4-bis(3-chlorophenyl)-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (36)

The title compound was isolated as a white solid (41.8 mg, 87%). ^1H NMR (600 MHz, CDCl_3) δ 8.56 – 8.48 (m, 1H), 8.33 (dd, $J = 4.7, 1.4$ Hz, 1H), 7.81 (ddd, $J = 7.9, 4.1, 1.5$ Hz, 1H), 7.66 (t, $J = 7.7$ Hz, 1H), 7.57 (t, $J = 7.6$ Hz, 1H), 7.27 – 7.20 (m, 4H), 7.20 – 7.02 (m, 5H), 6.98 – 6.89 (m, 2H), 6.46 – 6.35 (m, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 160.8, 146.8, 144.8, 144.2, 140.8, 137.1, 133.5, 133.4, 132.9, 131.4, 131.2, 129.9, 129.7, 129.5, 128.8, 128.7, 128.4, 128.2, 127.83, 127.75, 125.8, 118.7, 118.2, 117.5, 116.9, 100.5. HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{28}\text{H}_{18}\text{Cl}_2\text{N}_3^+$ [$\text{M} + \text{H}$] $^+$, 482.0821, found 482.0823. $[\alpha]_{\text{D}}^{20} = -22$ ($c = 0.1$, CHCl_3).

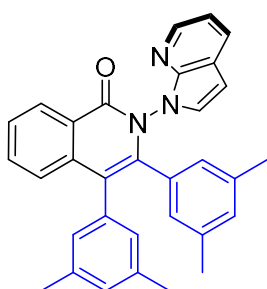
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 16.225 min, tr (minor) = 19.067 min, 95% ee.



No.	Time	Area	Area (%)
1	16.308	2631580	50.05
2	19.450	2626255	49.95



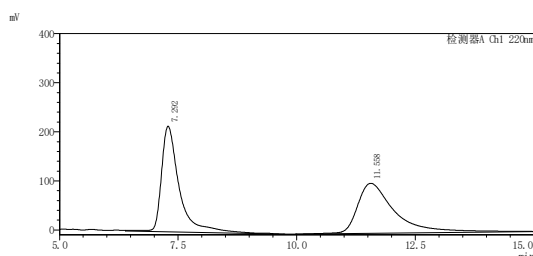
No.	Time	Area	Area (%)
1	16.225	20271034	97.34
2	19.067	554972	2.66



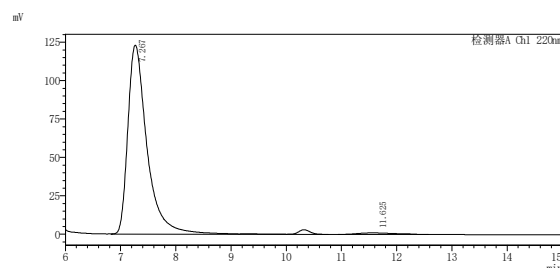
(S)-3,4-bis(3,5-dimethylphenyl)-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (37)

The title compound was isolated as a white solid (39.4 mg, 84%). **¹H NMR (600 MHz, CDCl₃)** δ 8.44 (dd, J = 8.0, 1.4 Hz, 1H), 8.26 (dd, J = 4.8, 1.5 Hz, 1H), 7.71 (dd, J = 7.8, 1.5 Hz, 1H), 7.52 (ddd, J = 8.5, 7.1, 1.5 Hz, 1H), 7.42 (dd, J = 8.2, 7.0 Hz, 1H), 7.21 (d, J = 8.2 Hz, 1H), 7.02 – 6.95 (m, 2H), 6.79 (s, 1H), 6.72 (s, 2H), 6.64 (s, 1H), 6.60 (s, 1H), 6.41 (s, 1H), 6.25 (d, J = 3.7 Hz, 1H), 2.17 (s, 3H), 2.09 (s, 3H), 1.98 (s, 3H), 1.65 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 160.2, 140.6, 136.9, 136.4, 136.0, 135.2, 134.9, 134.4, 132.0, 130.9, 128.5, 128.3, 128.1, 127.9, 127.6, 127.5, 126.7, 126.6, 125.9, 125.2, 124.2, 118.8, 117.7, 115.9, 99.3, 20.2, 20.1, 19.9, 19.6. **HRMS (ESI-TOF)** (m/z): Calcd for C₃₂H₂₈N₃O⁺ [M + H]⁺, 470.2227, found 470.2225. **[α]_D²⁰** = -22 (c = 0.1, CHCl₃).

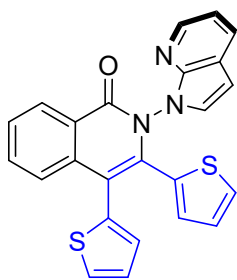
HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm). tr (major) = 7.267 min, tr (minor) = 11.625 min, 97% ee.



No.	Time	Area	Area (%)
1	7.292	5649932	50.37
2	11.558	5567142	49.63

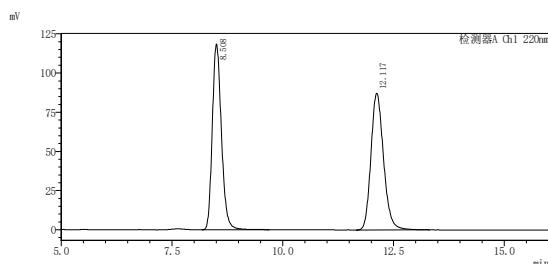


No.	Time	Area	Area (%)
1	7.267	3016000	98.48
2	11.625	46607	1.52

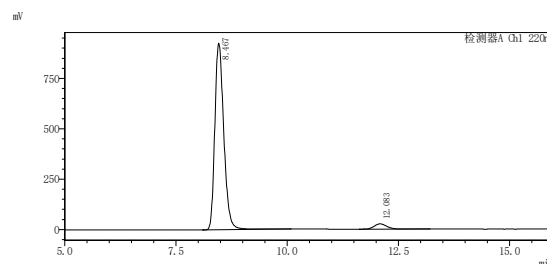


(S)-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)-3,4-di(thiophen-2-yl)isoquinolin-1(2H)-one (38)

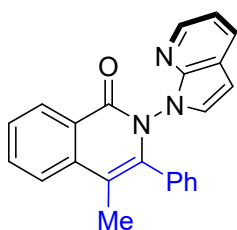
The title compound was isolated as a white solid (22.5 mg, 53%). **¹H NMR (600 MHz, CDCl₃)** δ 8.42 (ddd, J = 8.0, 1.4, 0.6 Hz, 1H), 8.26 (dd, J = 4.7, 1.5 Hz, 1H), 7.77 (dd, J = 7.8, 1.5 Hz, 1H), 7.60 (ddd, J = 8.4, 7.2, 1.4 Hz, 1H), 7.48 (ddd, J = 8.2, 7.2, 1.2 Hz, 1H), 7.43 (ddd, J = 8.2, 1.2, 0.6 Hz, 1H), 7.22 (dd, J = 5.0, 1.3 Hz, 1H), 7.07 (d, J = 3.8 Hz, 1H), 7.02 (dd, J = 7.8, 4.8 Hz, 1H), 6.94 (dd, J = 5.1, 1.2 Hz, 1H), 6.93 – 6.86 (m, 2H), 6.70 (dd, J = 3.6, 1.2 Hz, 1H), 6.46 (dd, J = 5.1, 3.6 Hz, 1H), 6.37 (d, J = 3.8 Hz, 1H). **¹³C NMR (150 MHz, CDCl₃)** δ 159.9, 145.9, 143.2, 136.5, 136.2, 135.1, 132.5, 130.6, 129.6, 129.1, 128.5, 127.8, 127.6, 127.0, 126.8, 125.9, 125.6, 125.2, 124.7, 124.3, 117.7, 116.3, 113.9, 99.7. **HRMS (ESI-TOF)** (m/z): Calcd for C₂₄H₁₆N₃OS₂⁺ [$M + H$]⁺, 426.0729, found 426.0729. **[α]_D²⁰** = -23 (c = 0.1, CHCl₃). **HPLC** conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm). t_r (major) = 8.467 min, t_r (minor) = 12.083 min, 92% ee.



No.	Time	Area	Area (%)
1	8.508	1698928	49.62
2	12.117	1725246	50.38



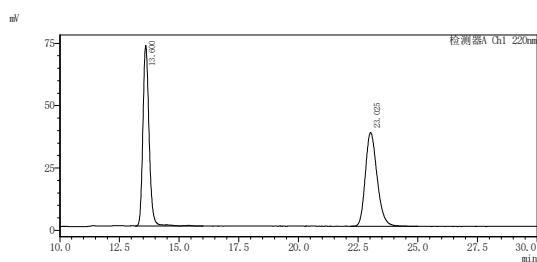
No.	Time	Area	Area (%)
1	8.467	13013169	96.16
2	12.083	520179	3.84



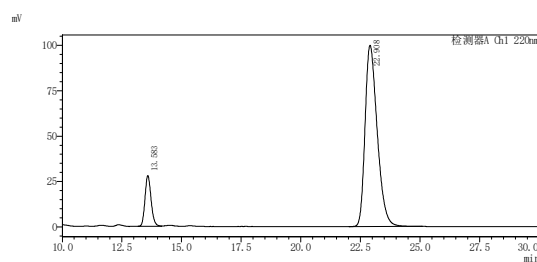
(S)-3-methyl-4-phenyl-2-(1H-pyrrolo[2,3-b]pyridin-1-yl)isoquinolin-1(2H)-one (39)

The title compound was isolated as a white solid (18.3 mg, 52%). **¹H NMR (600 MHz, CDCl₃)** δ 8.50 (dd, J = 7.6, 1.3 Hz, 1H), 8.29 (dd, J = 4.7, 1.5 Hz, 1H), 7.81 – 7.74 (m, 3H), 7.55 (ddd, J = 8.1, 6.4, 1.8 Hz, 1H), 7.29 – 7.19 (m, 3H), 7.16 – 7.12 (m, 1H), 7.08 – 7.01 (m, 2H), 6.95 (td, J = 7.6, 1.4 Hz, 1H), 6.33 (dd, J = 3.8, 1.0 Hz, 1H), 2.12 (s, 3H). **¹³C NMR (150 MHz, CDCl₃)** δ 161.1, 146.8, 144.1, 14.0, 137.6, 133.3, 132.8, 129.4, 129.34, 129.26, 128.9, 128.8, 128.6, 127.62, 127.60, 127.1, 125.6, 123.8, 118.6, 117.0, 111.3, 100.3, 14.9. **HRMS (ESI-TOF)** (m/z): Calcd for C₂₃H₁₈N₃O⁺ [$M + H$]⁺, 352.1444, found 352.1445. **[α]_D²⁰** = -11 (c = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak OD-3 column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 oC, 254 nm); tr (major) = 22.908 min, tr (minor) = 13.583 min, 75% ee.

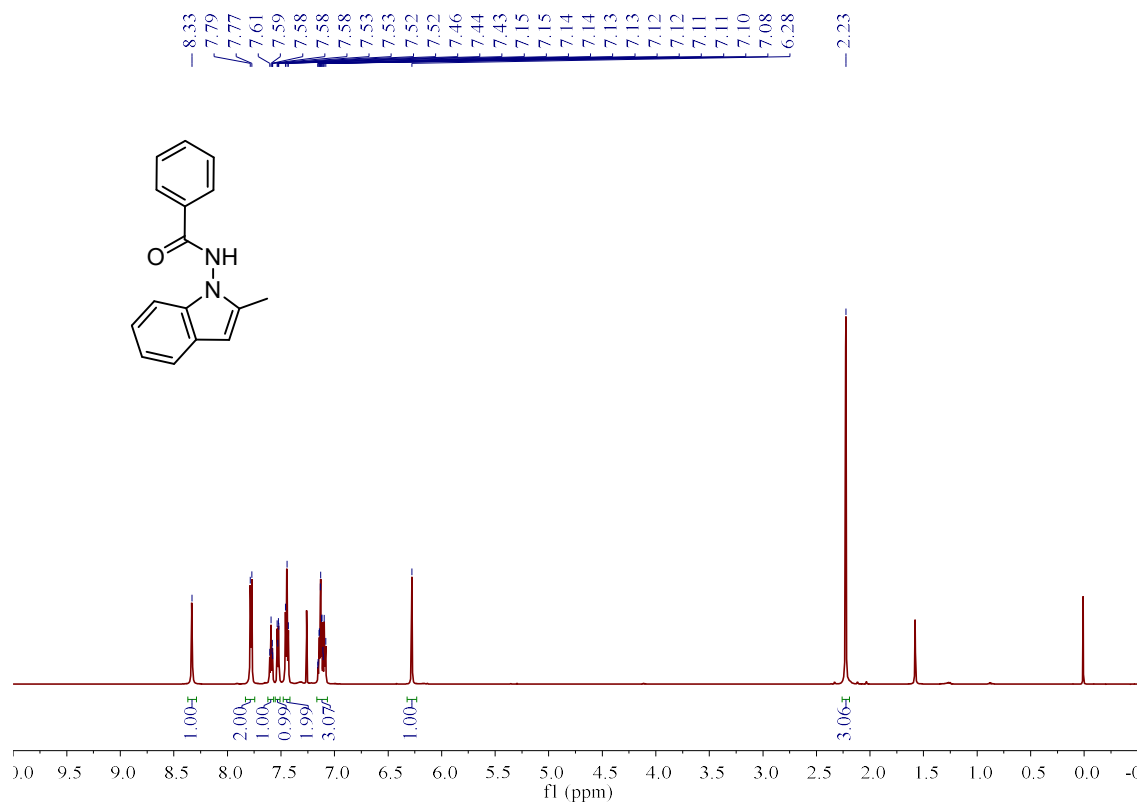


No.	Time	Area	Area (%)
1	13.600	1304010	50.27
2	23.025	1290256	49.73

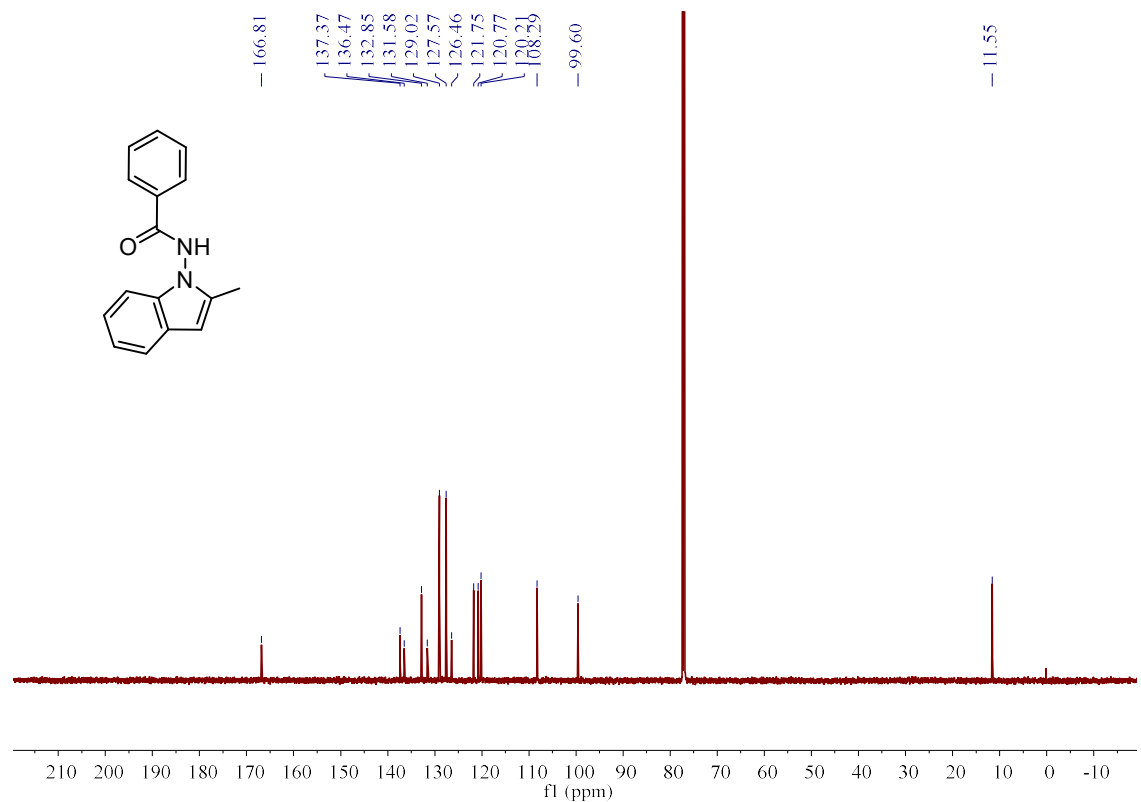


No.	Time	Area	Area (%)
1	13.583	497273	12.32
2	22.908	3539360	87.68

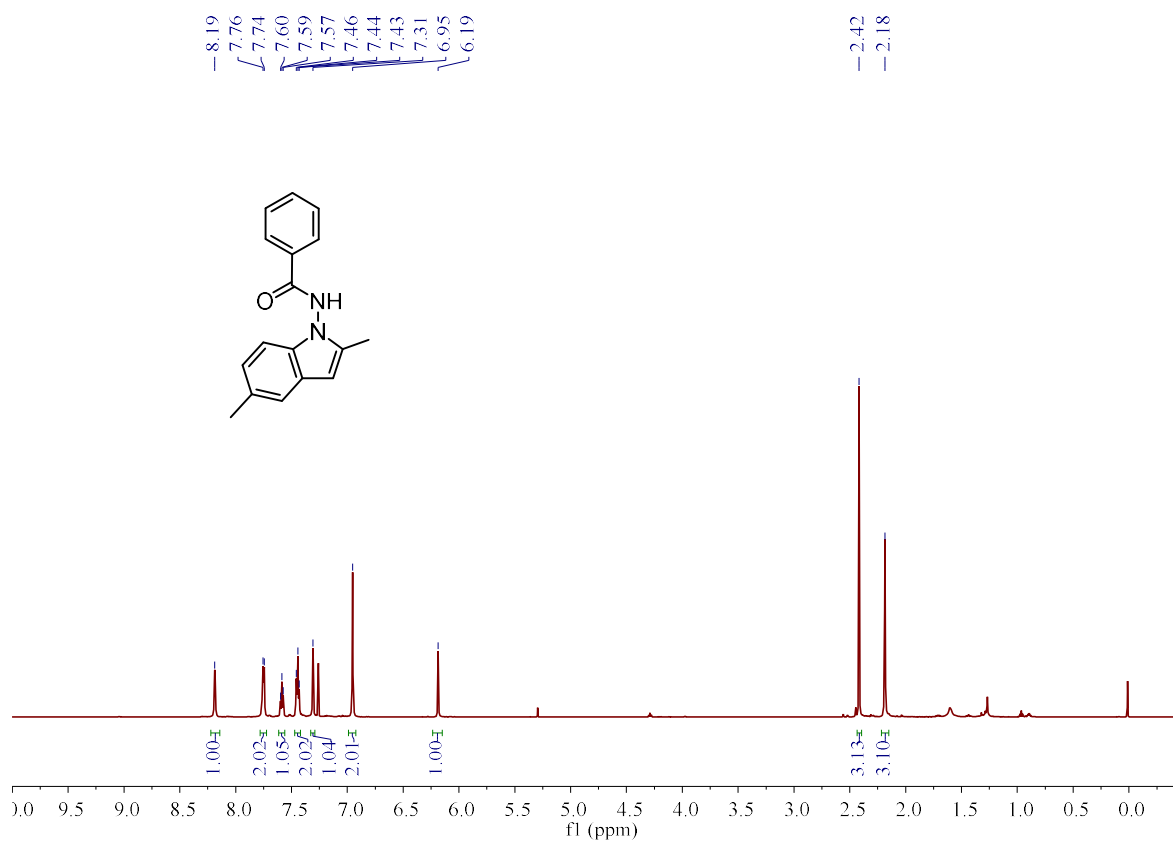
9. NMR Spectra



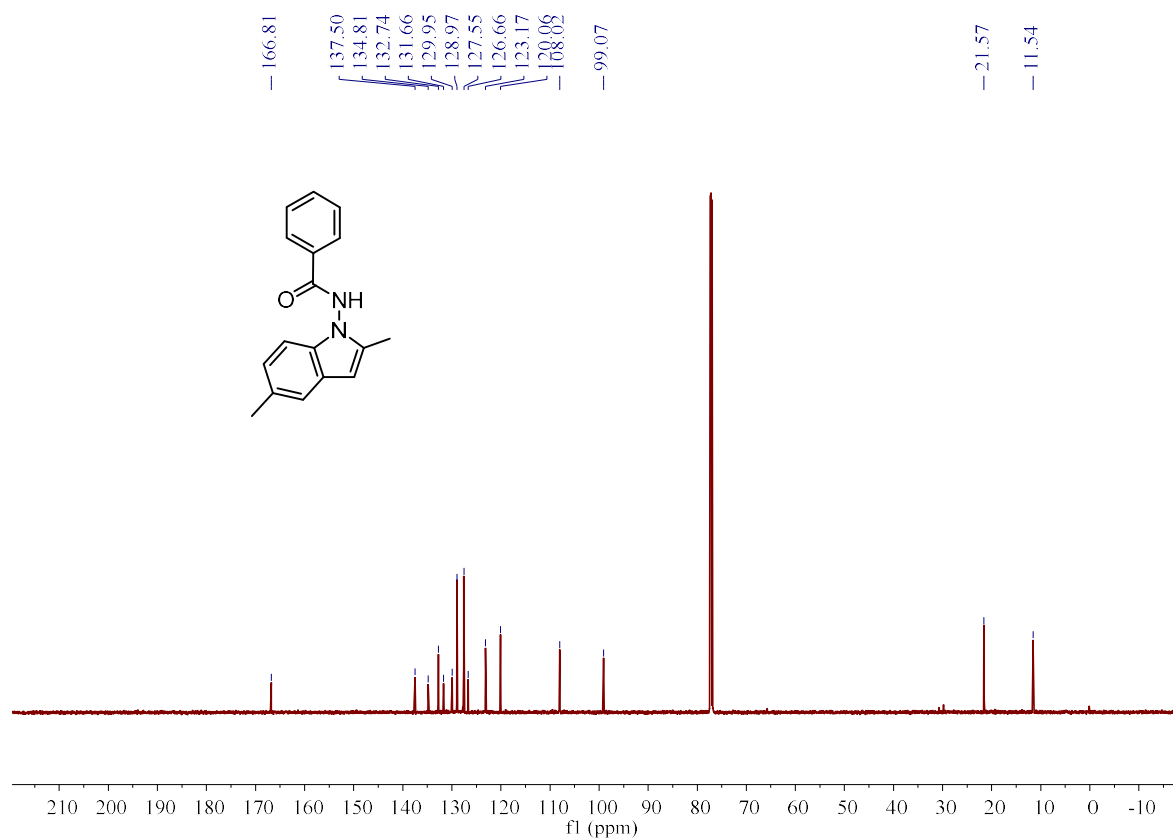
¹H NMR (600 MHz, CDCl₃) spectrum of 3a.



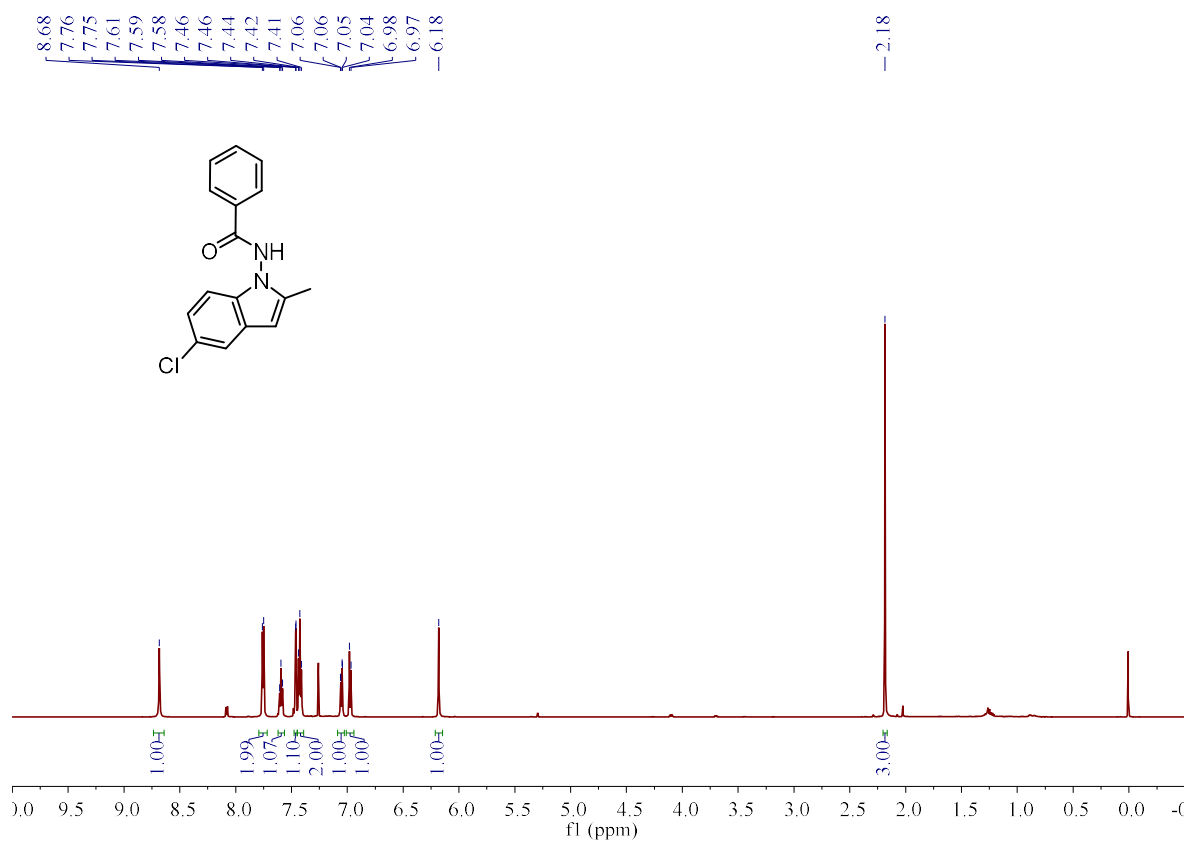
¹³C NMR (150 MHz, CDCl₃) spectrum of 3a.



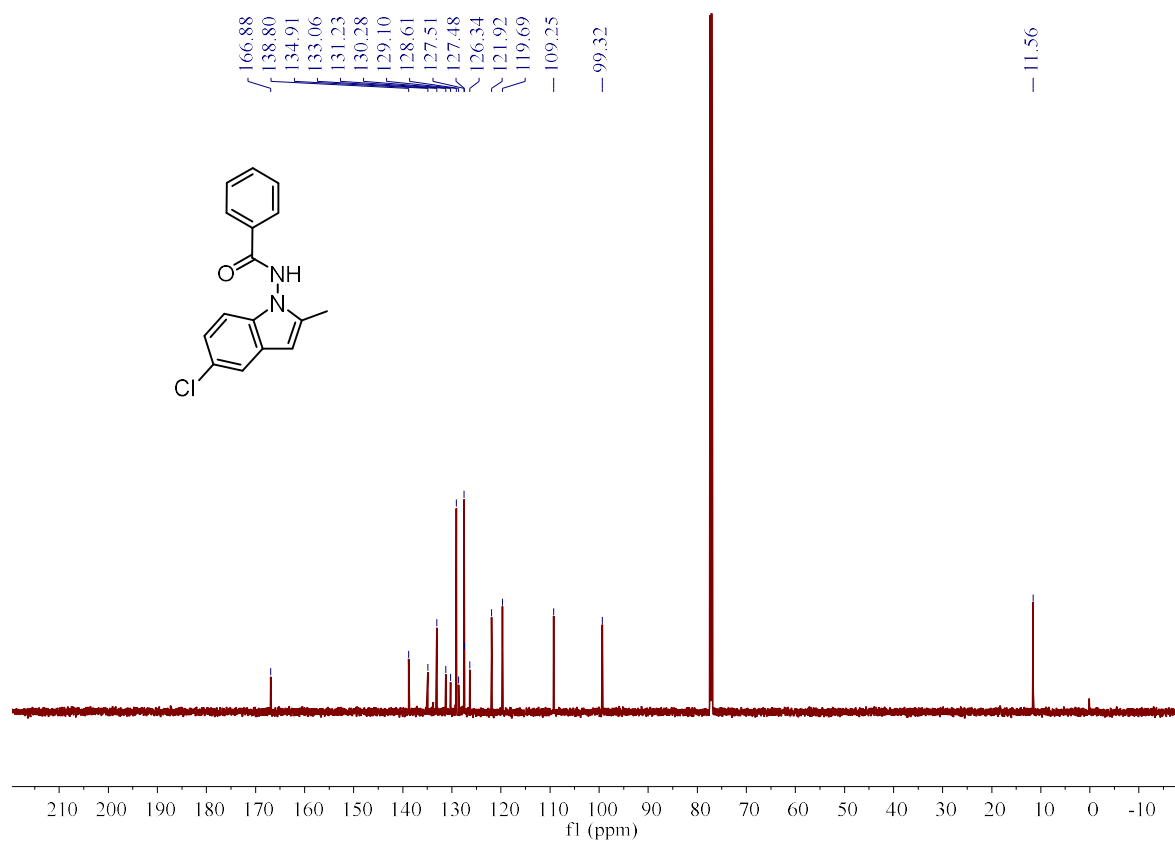
¹H NMR (600 MHz, CDCl₃) spectrum of 4a.



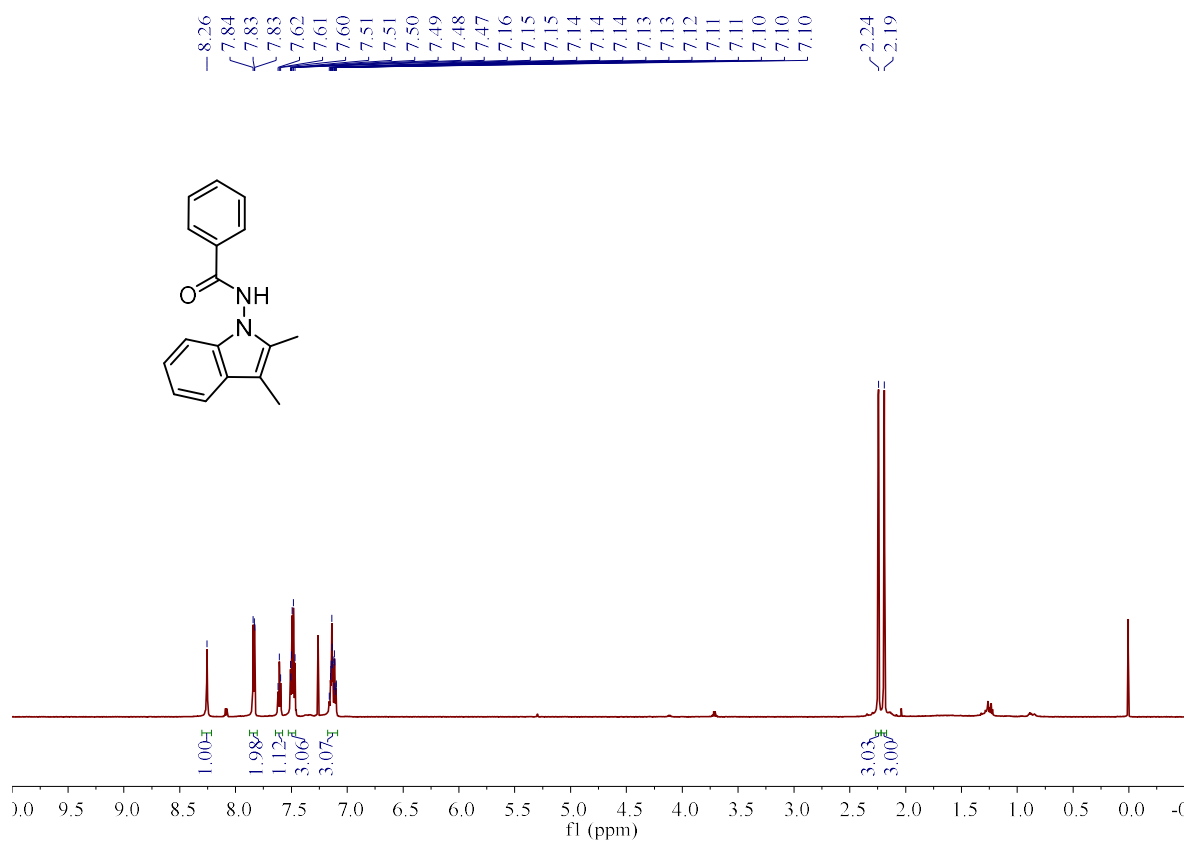
¹³C NMR (150 MHz, CDCl₃) spectrum of 4a.



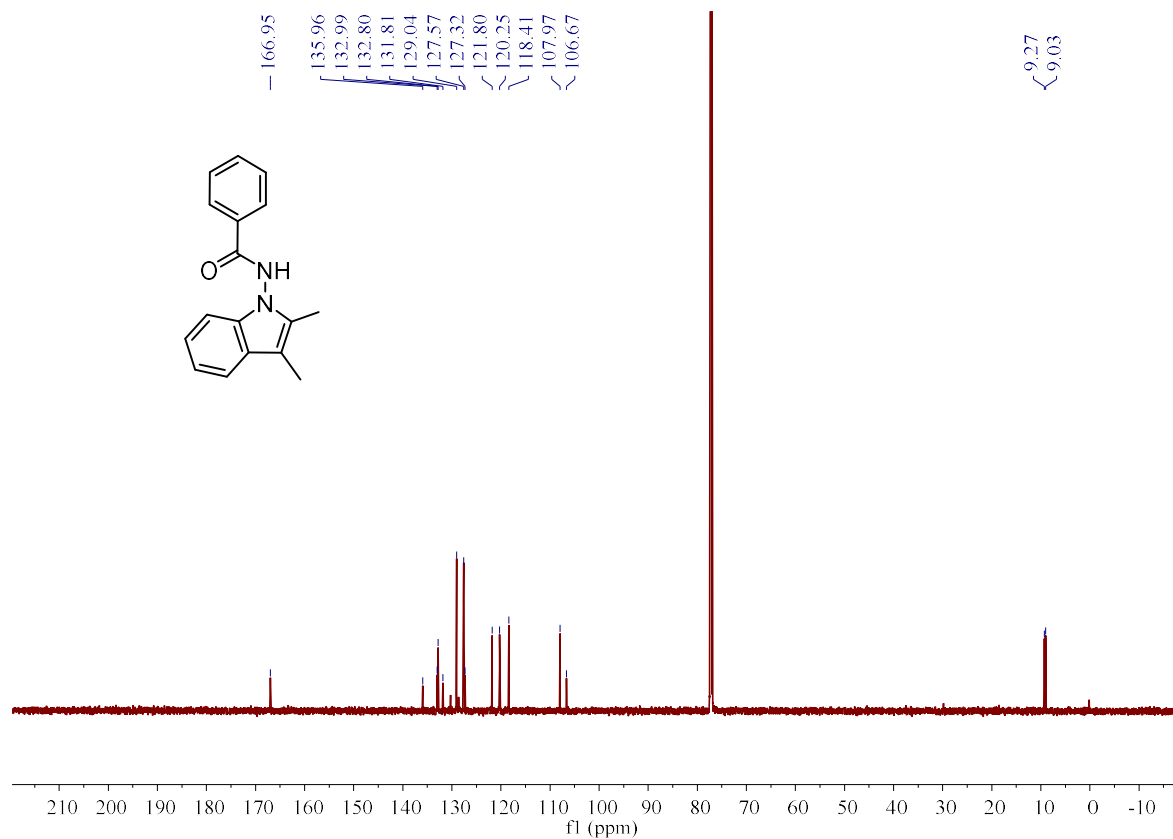
¹H NMR (600 MHz, CDCl₃) spectrum of 5a.



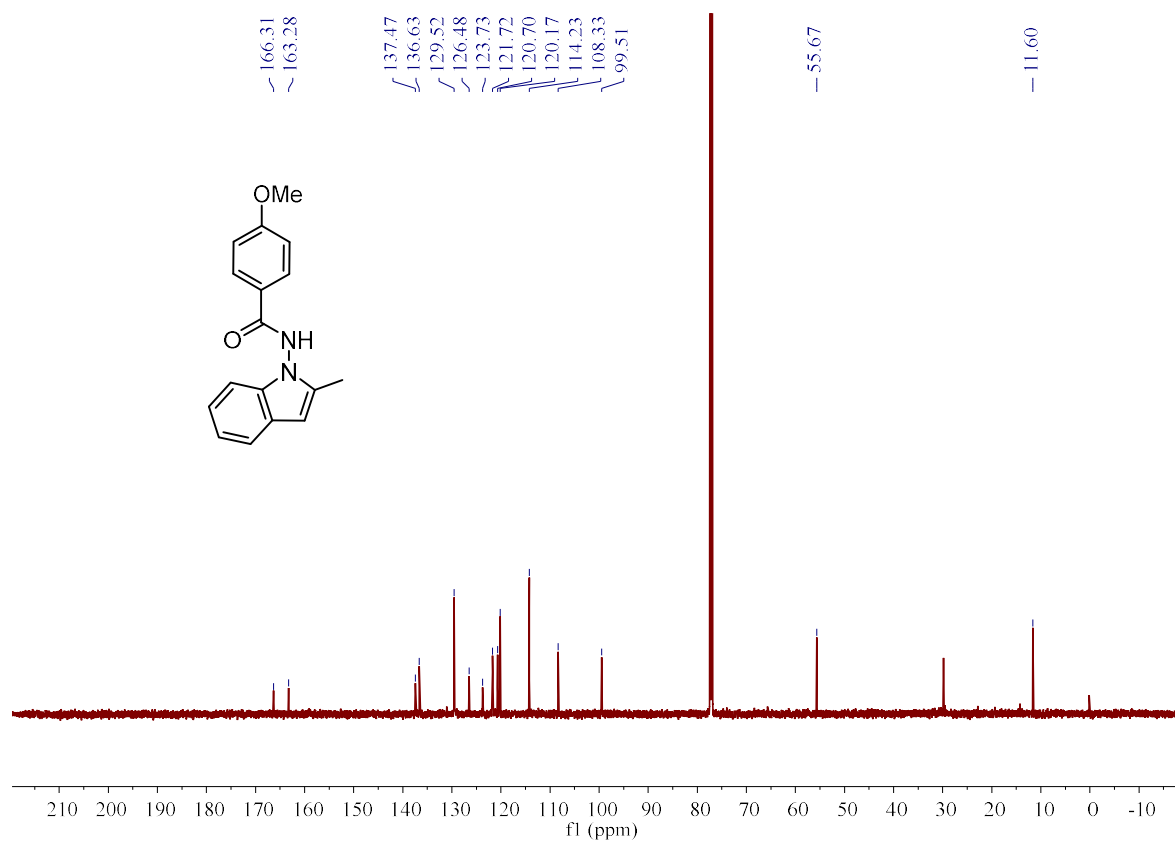
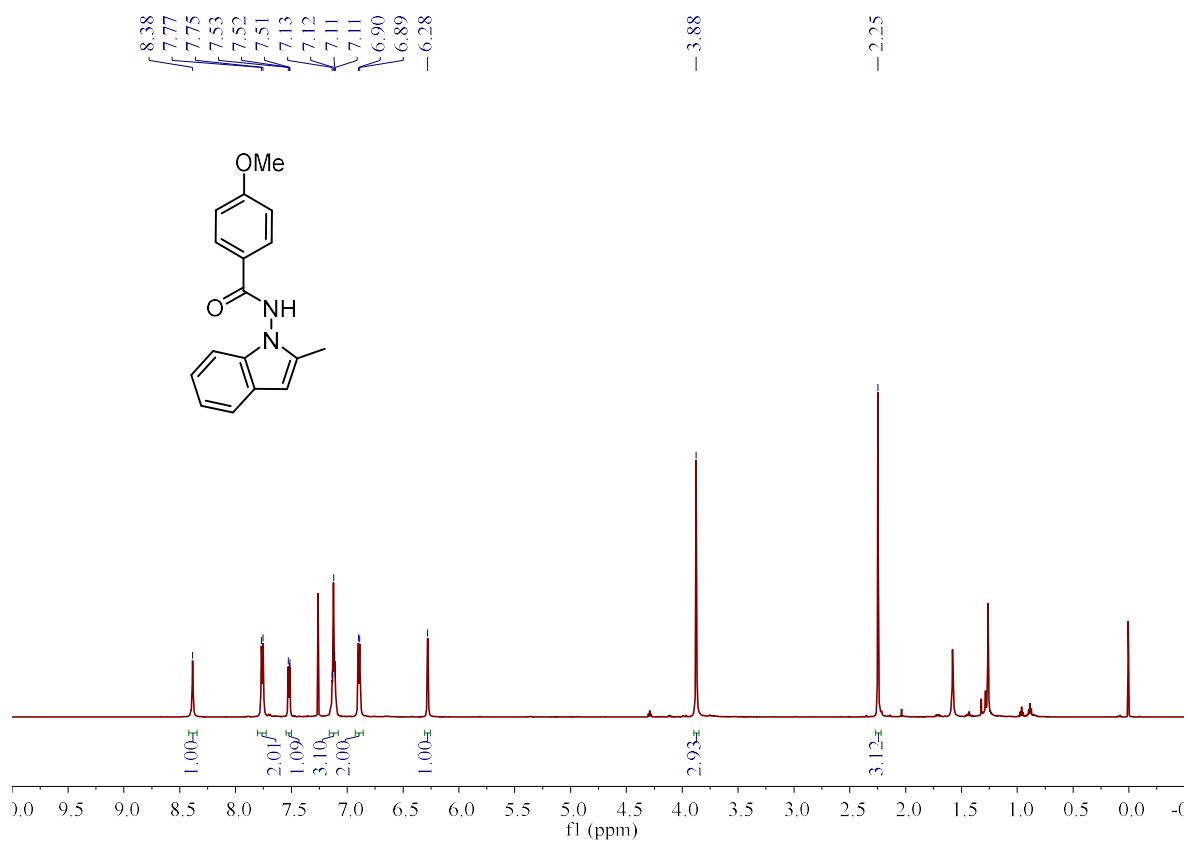
¹³C NMR (150 MHz, CDCl₃) spectrum of 5a.

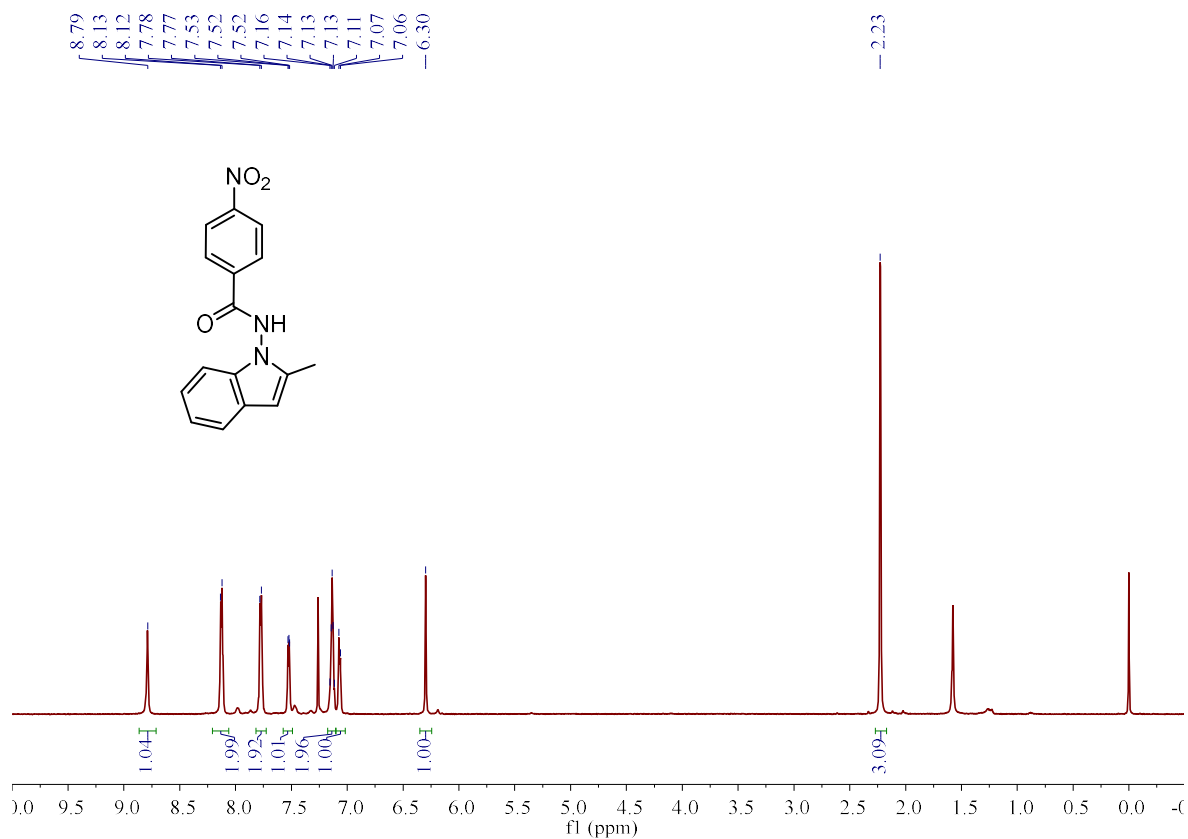


^1H NMR (600 MHz, CDCl_3) spectrum of 6a.

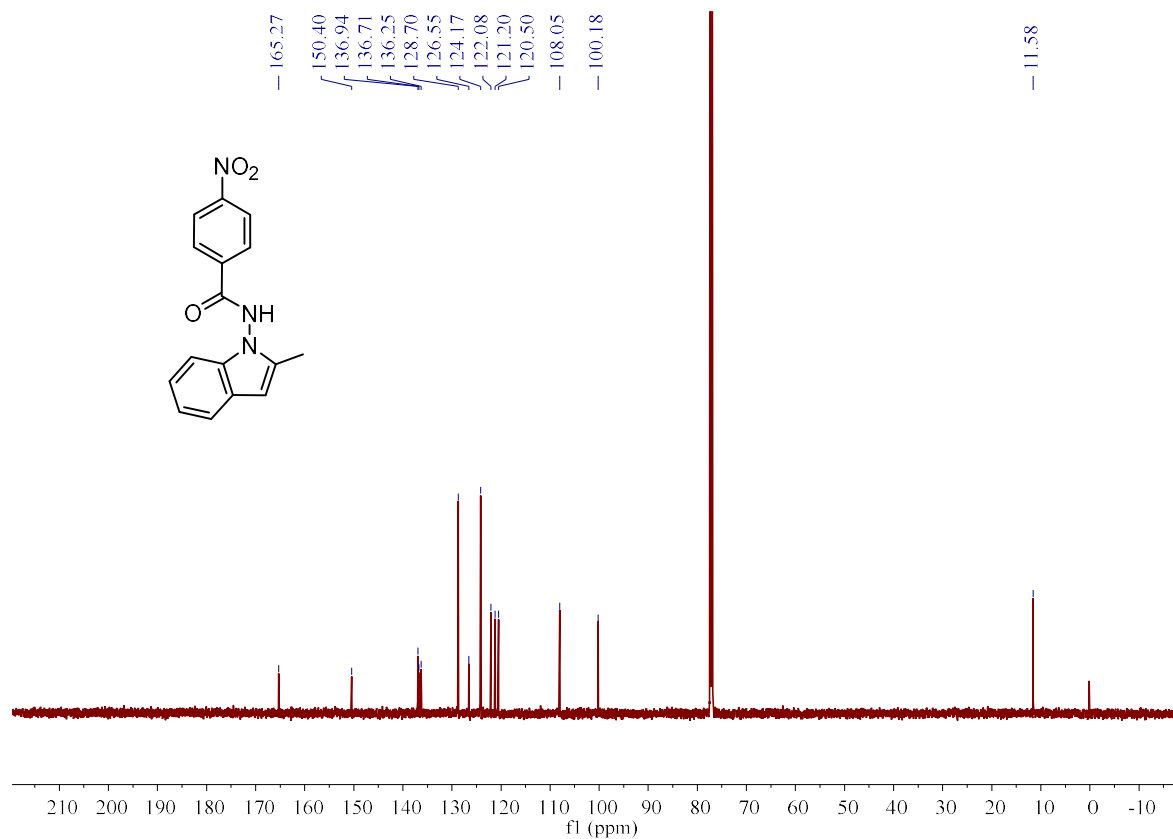


^{13}C NMR (150 MHz, CDCl_3) spectrum of 6a.

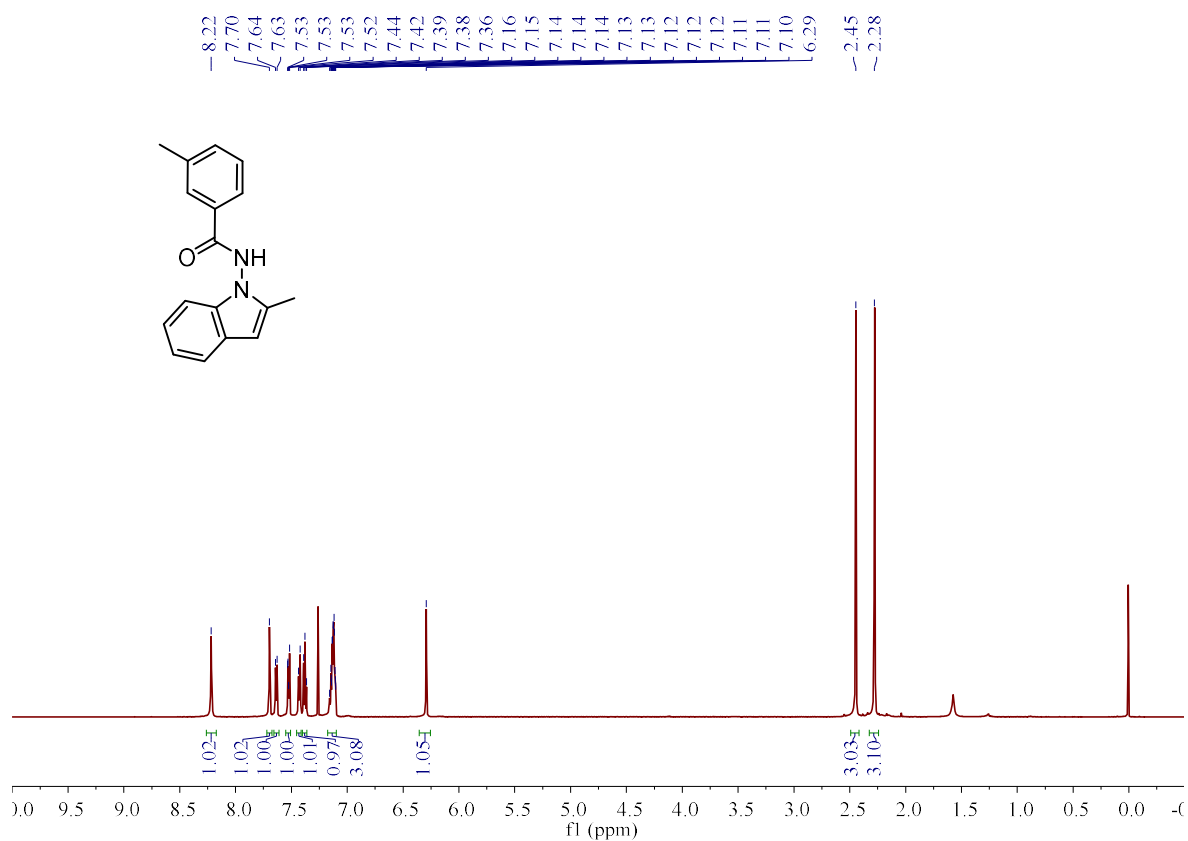




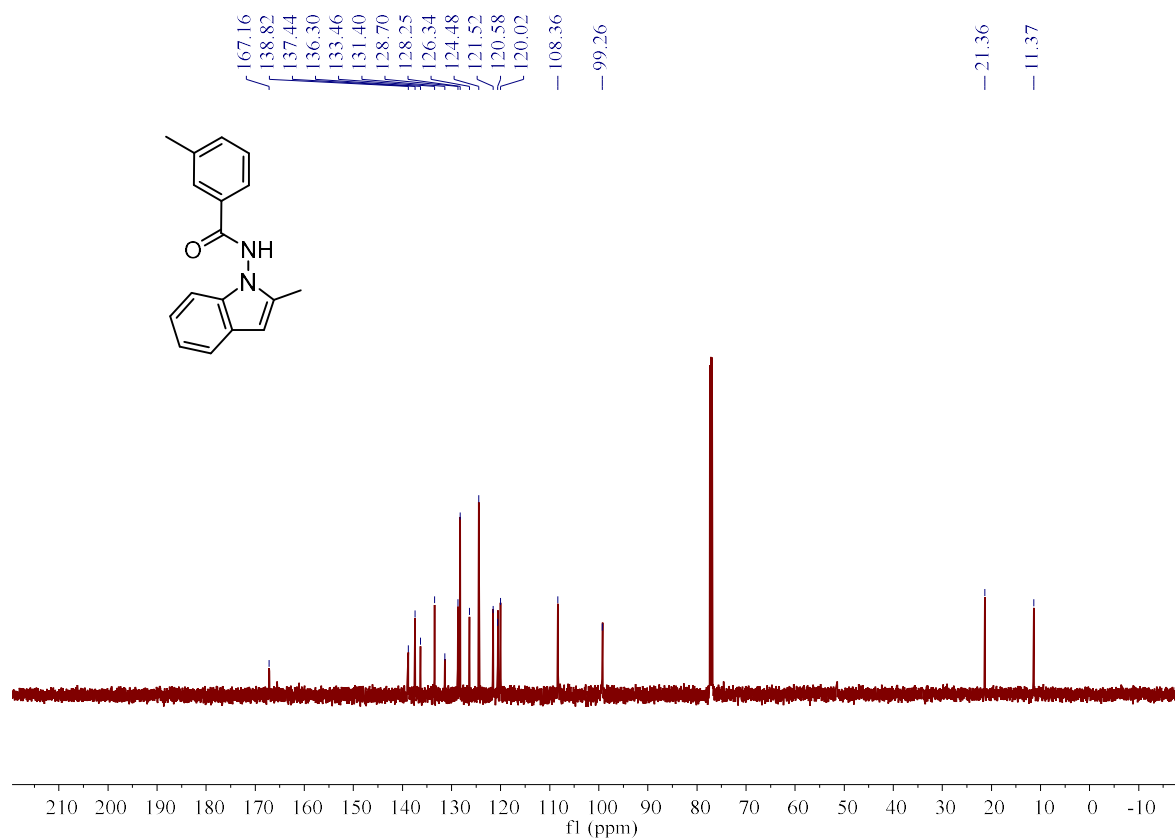
^1H NMR (600 MHz, CDCl_3) spectrum of 8a.



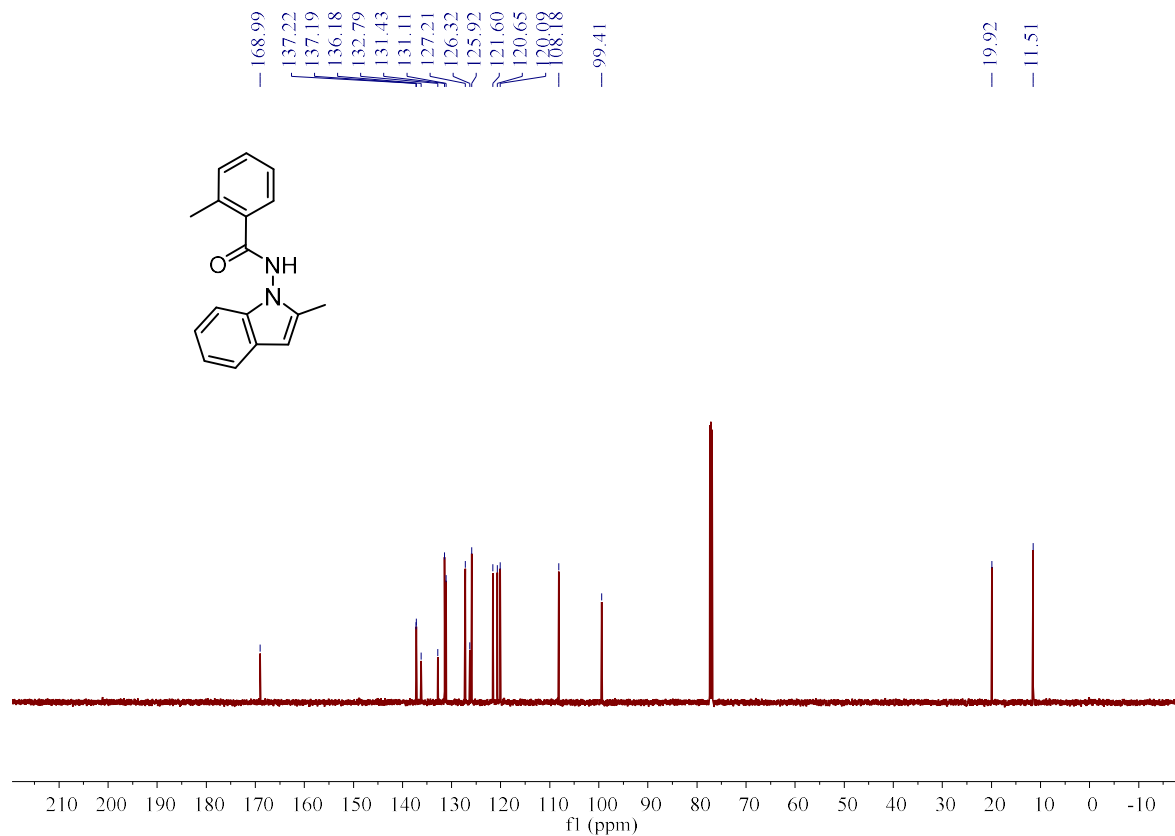
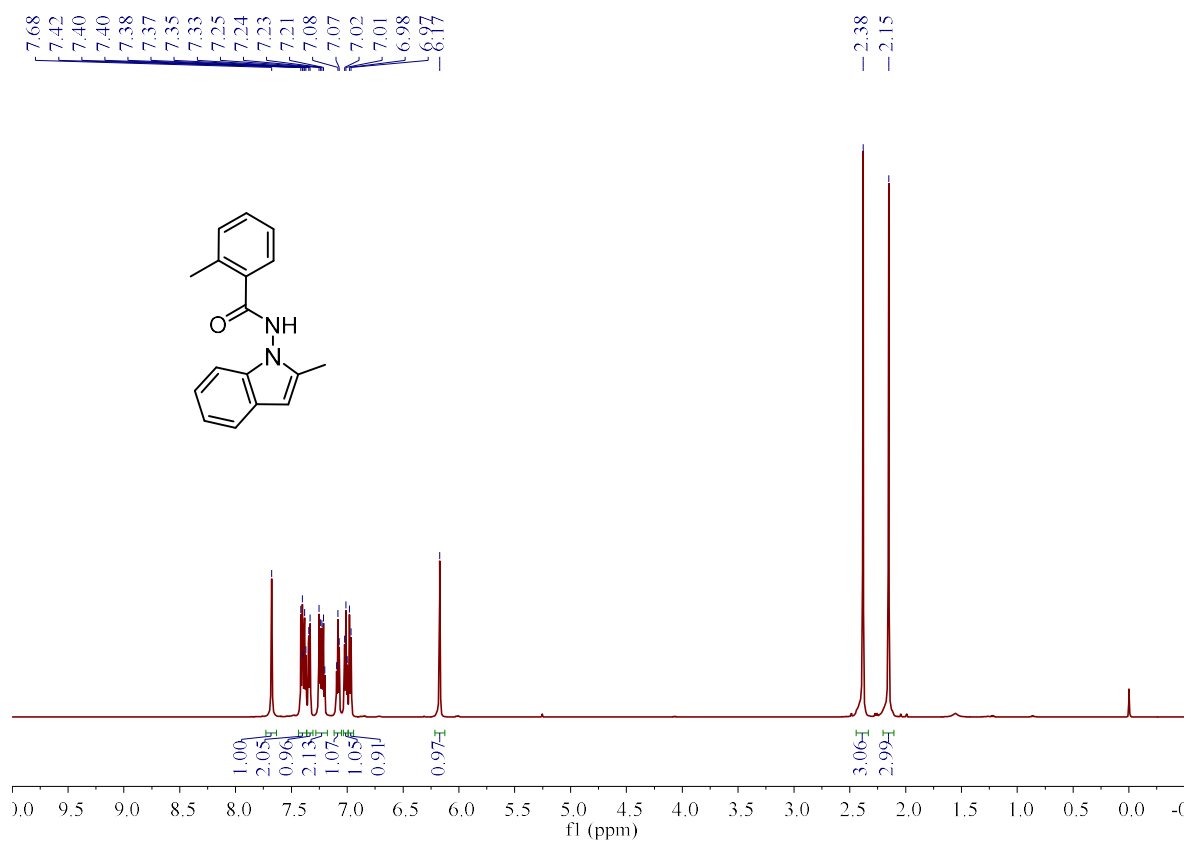
^{13}C NMR (150 MHz, CDCl_3) spectrum of 8a.

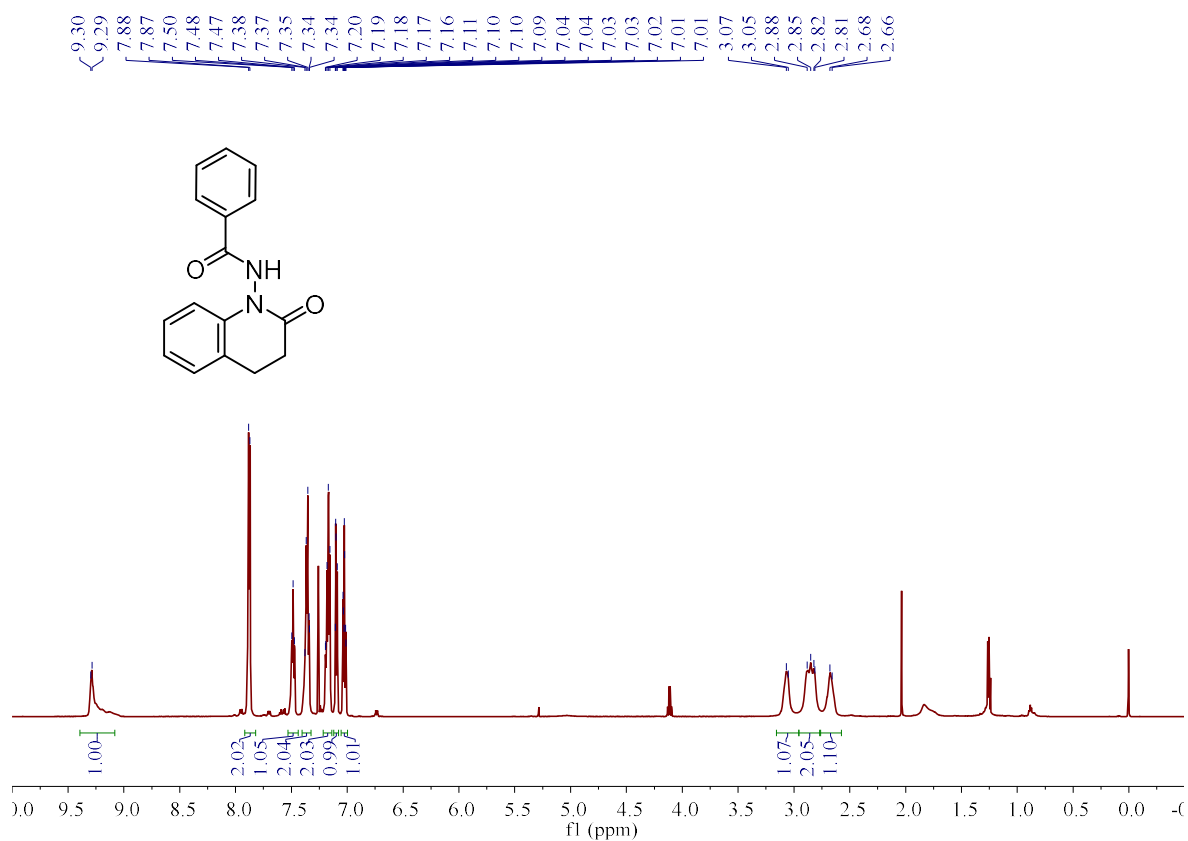


¹H NMR (600 MHz, CDCl₃) spectrum of 9a.

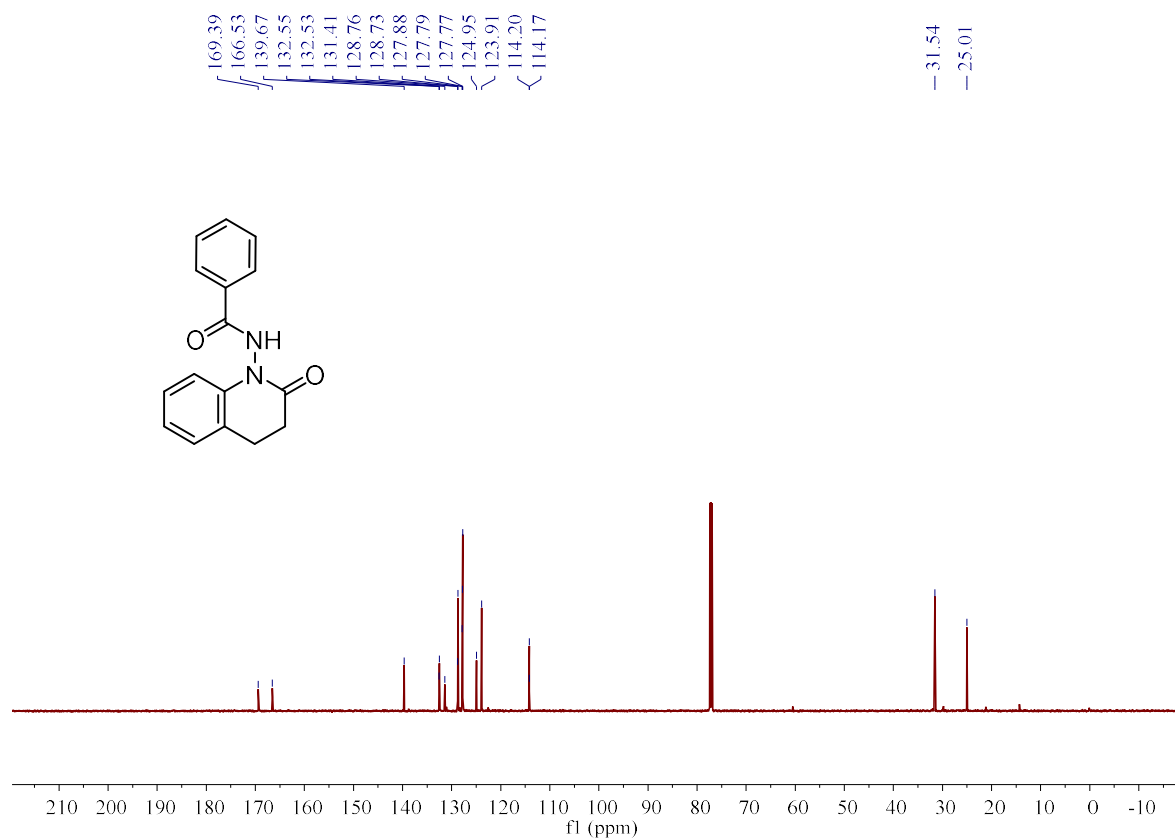


¹³C NMR (150 MHz, CDCl₃) spectrum of 9a.

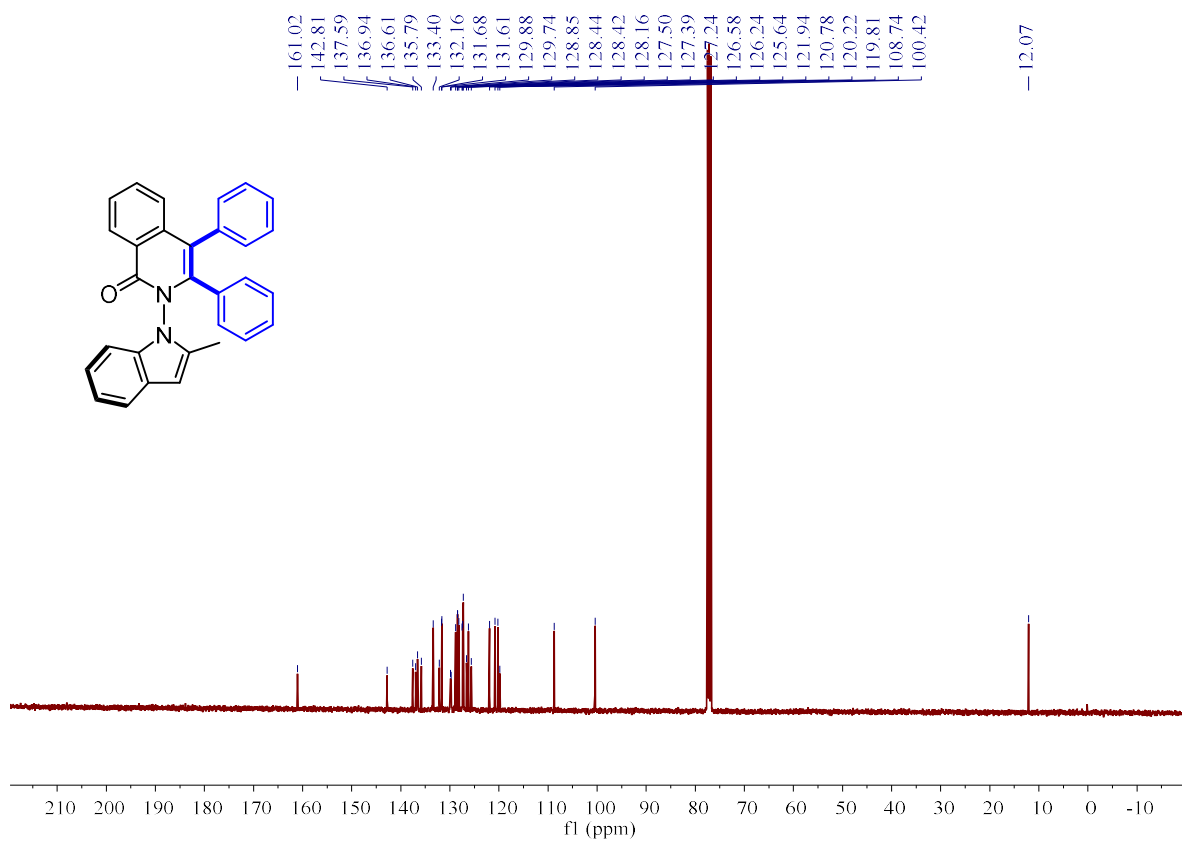
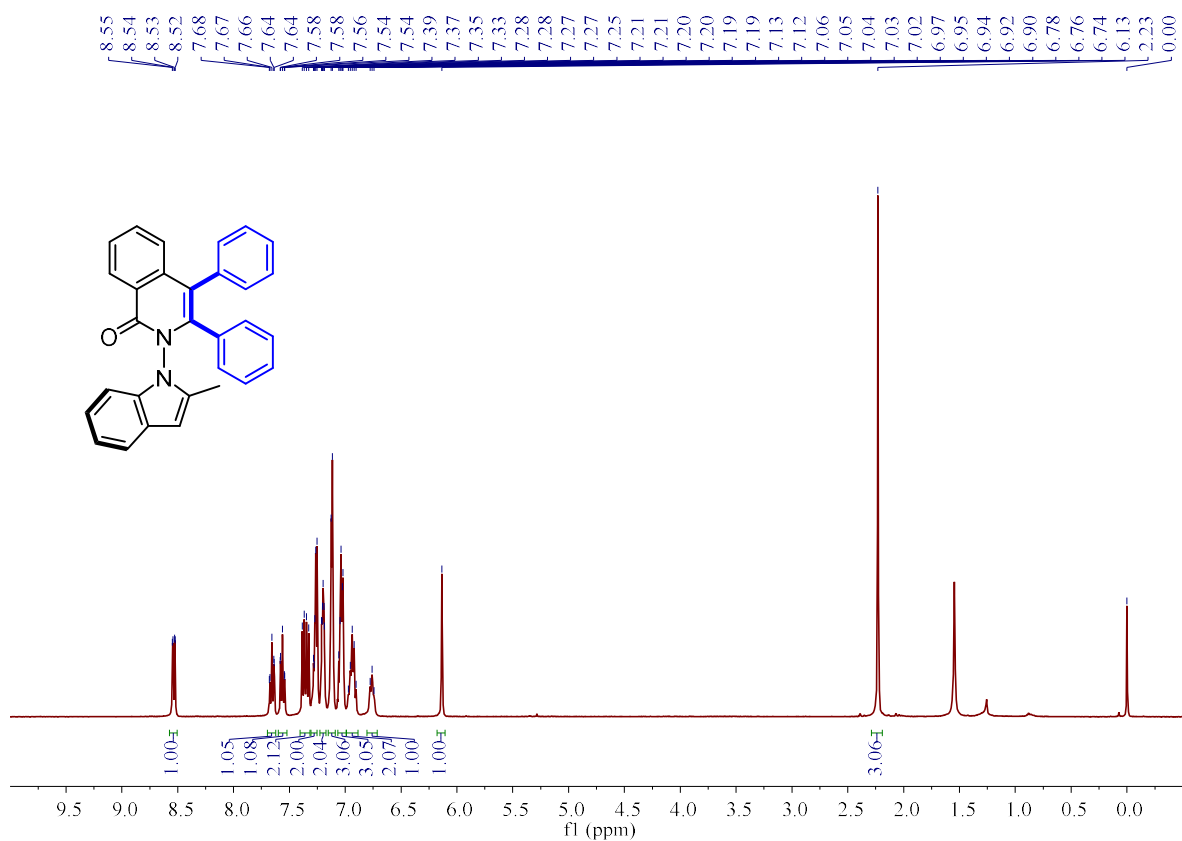


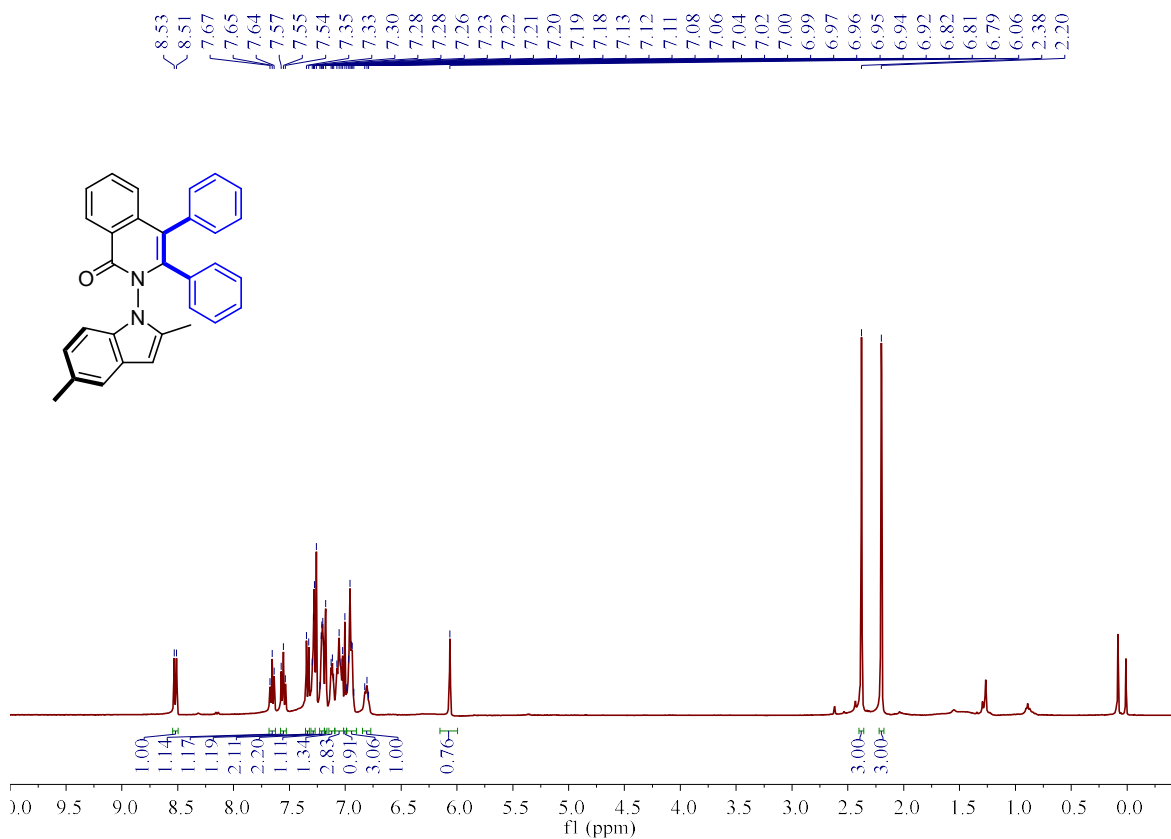


¹H NMR (600 MHz, CDCl₃) spectrum of 21a.

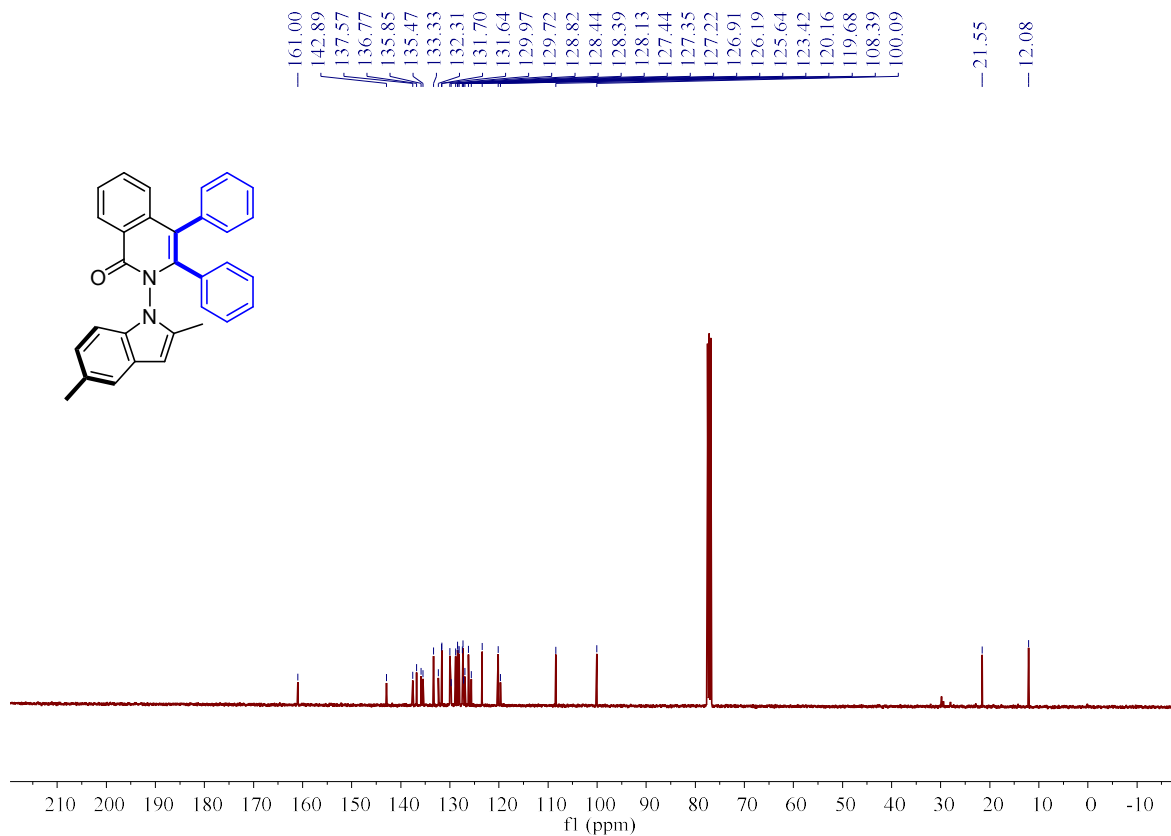


¹³C NMR (150 MHz, CDCl₃) spectrum of 21a.

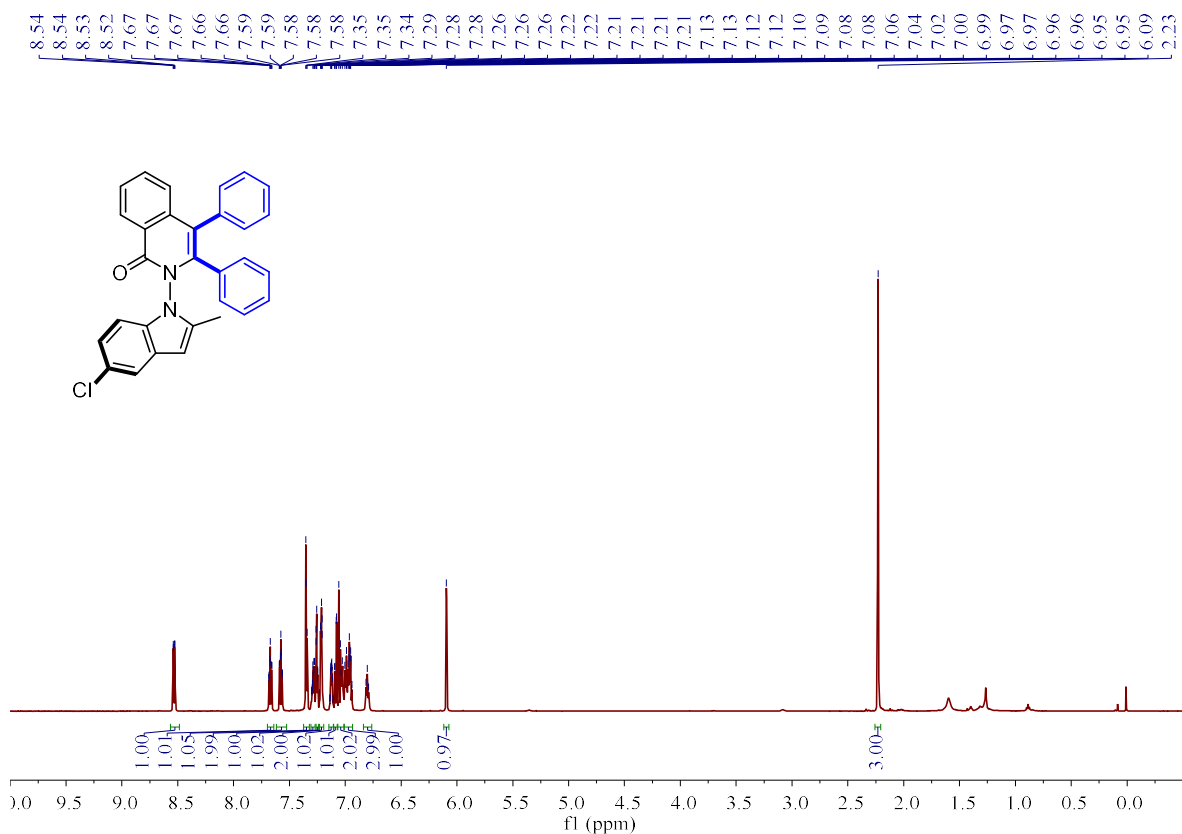




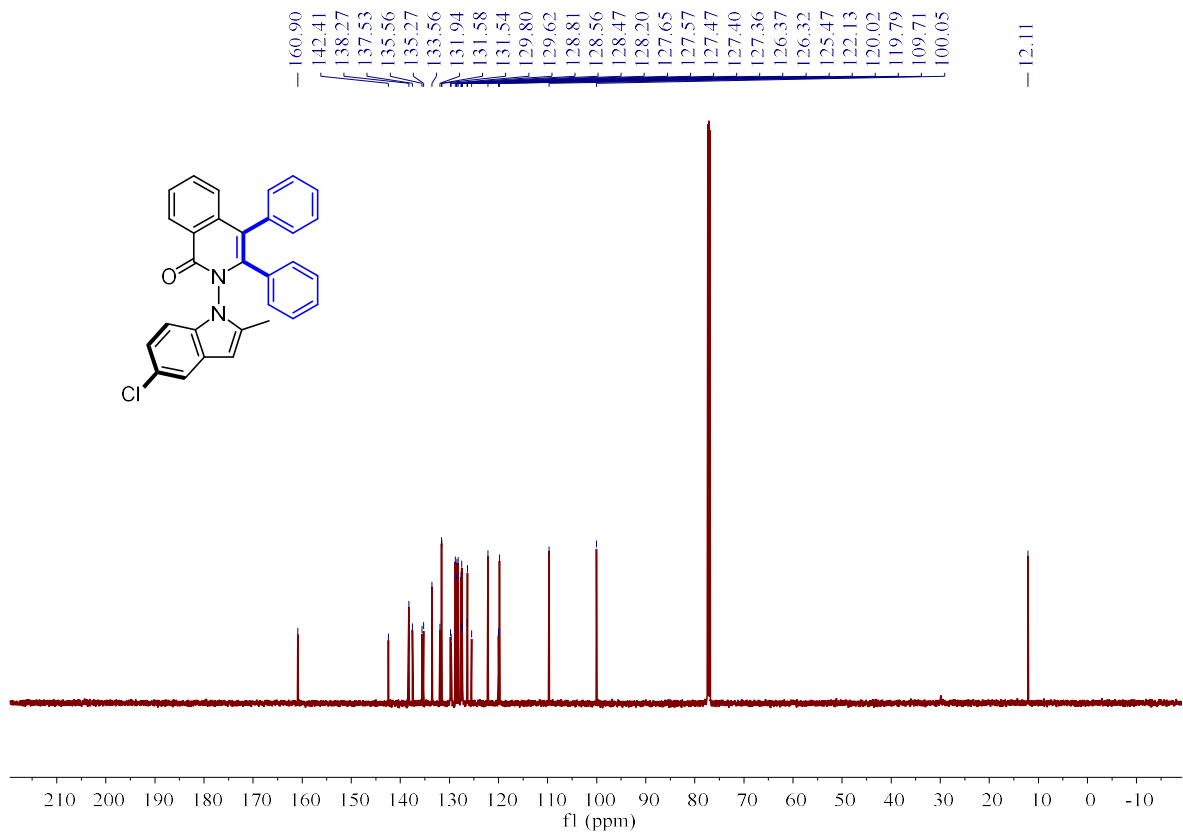
¹H NMR (400 MHz, CDCl₃) spectrum of 4.



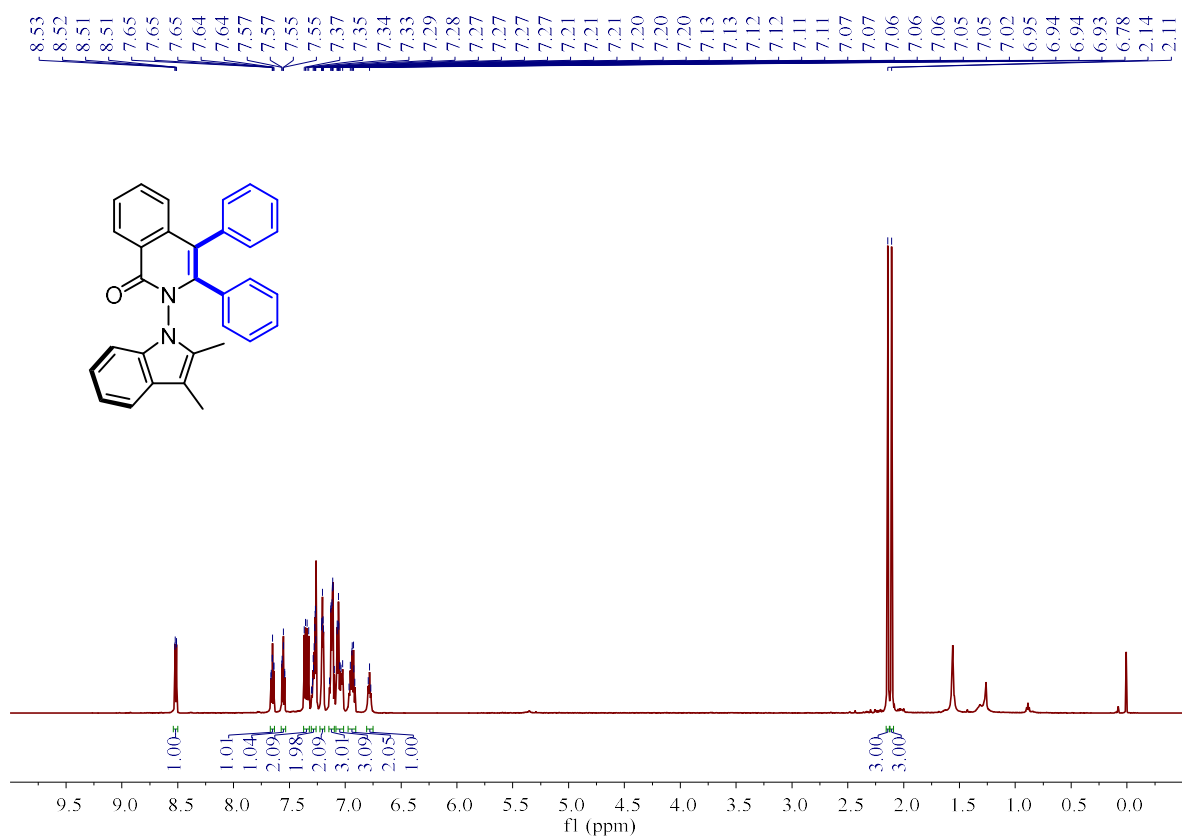
¹³C NMR (100 MHz, CDCl₃) spectrum of 4.



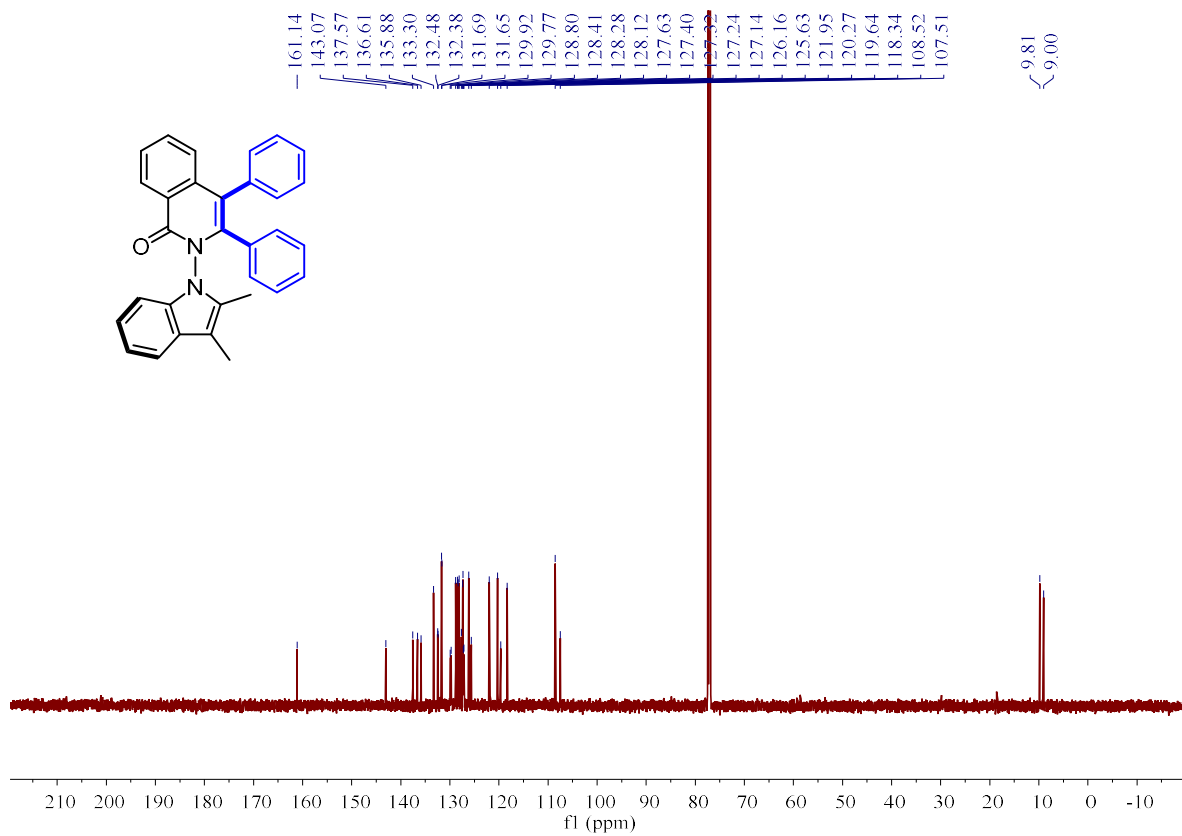
¹H NMR (600 MHz, CDCl₃) spectrum of 5.



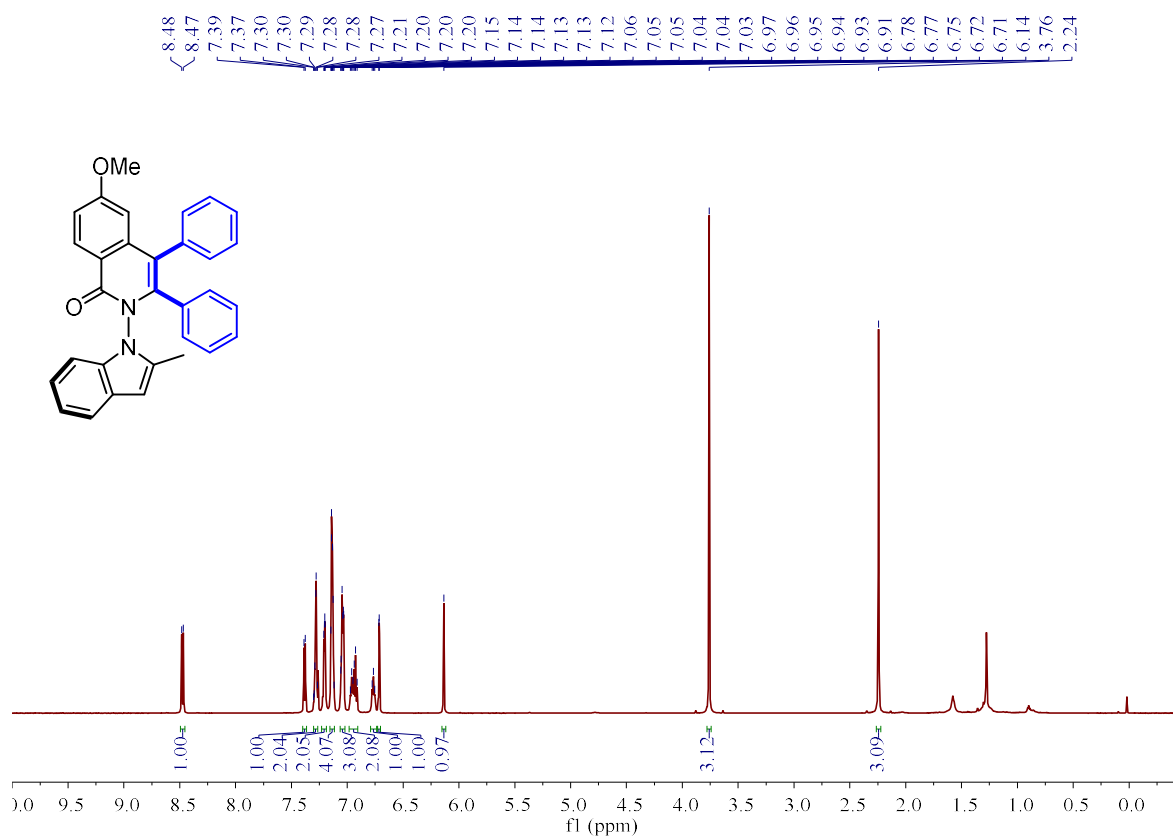
¹³C NMR (150 MHz, CDCl₃) spectrum of 5.



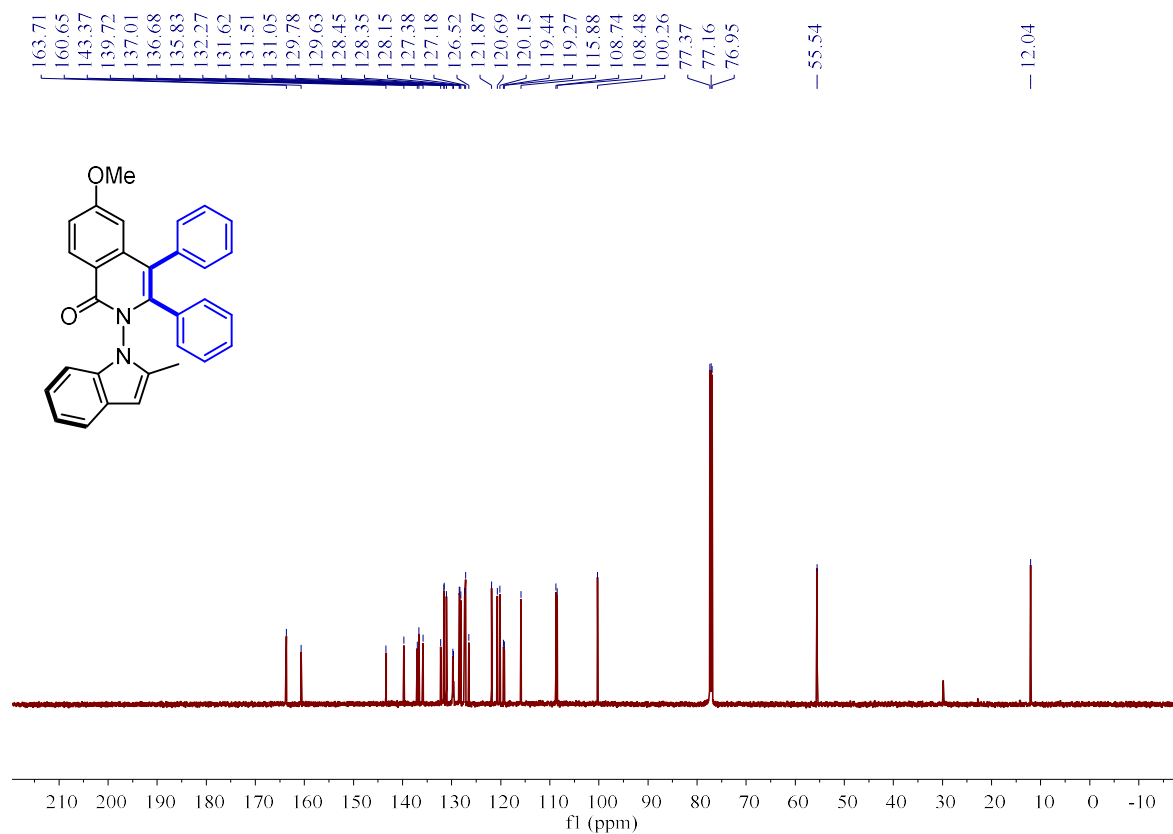
¹H NMR (600 MHz, CDCl₃) spectrum of 6.



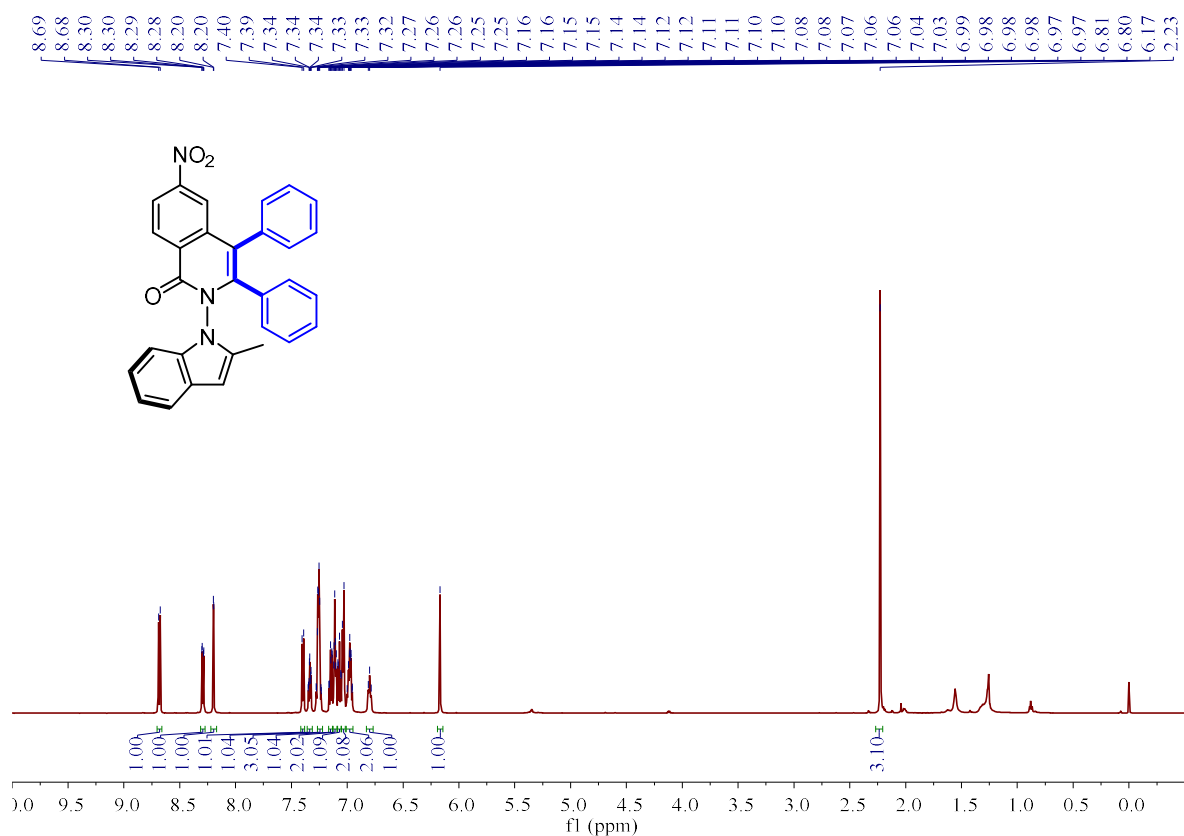
¹³C NMR (150 MHz, CDCl₃) spectrum of 6.



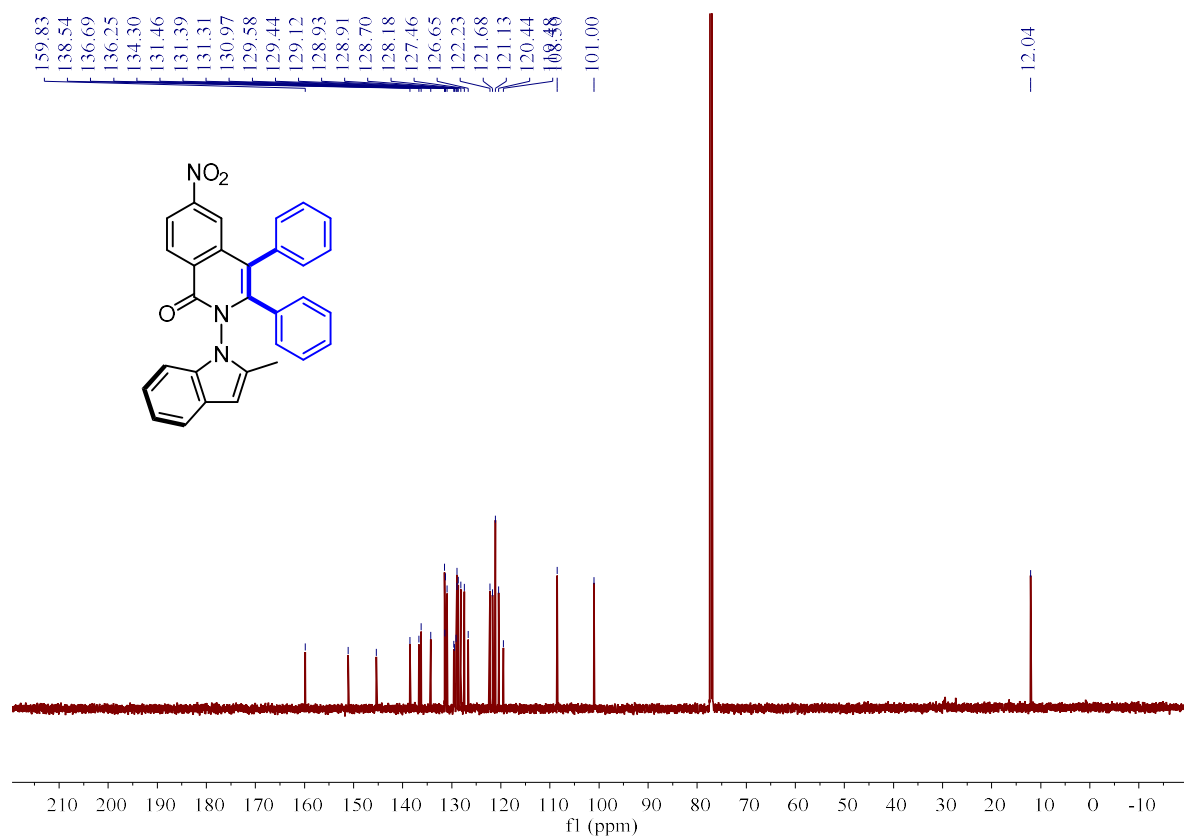
¹H NMR (600 MHz, CDCl₃) spectrum of 7.



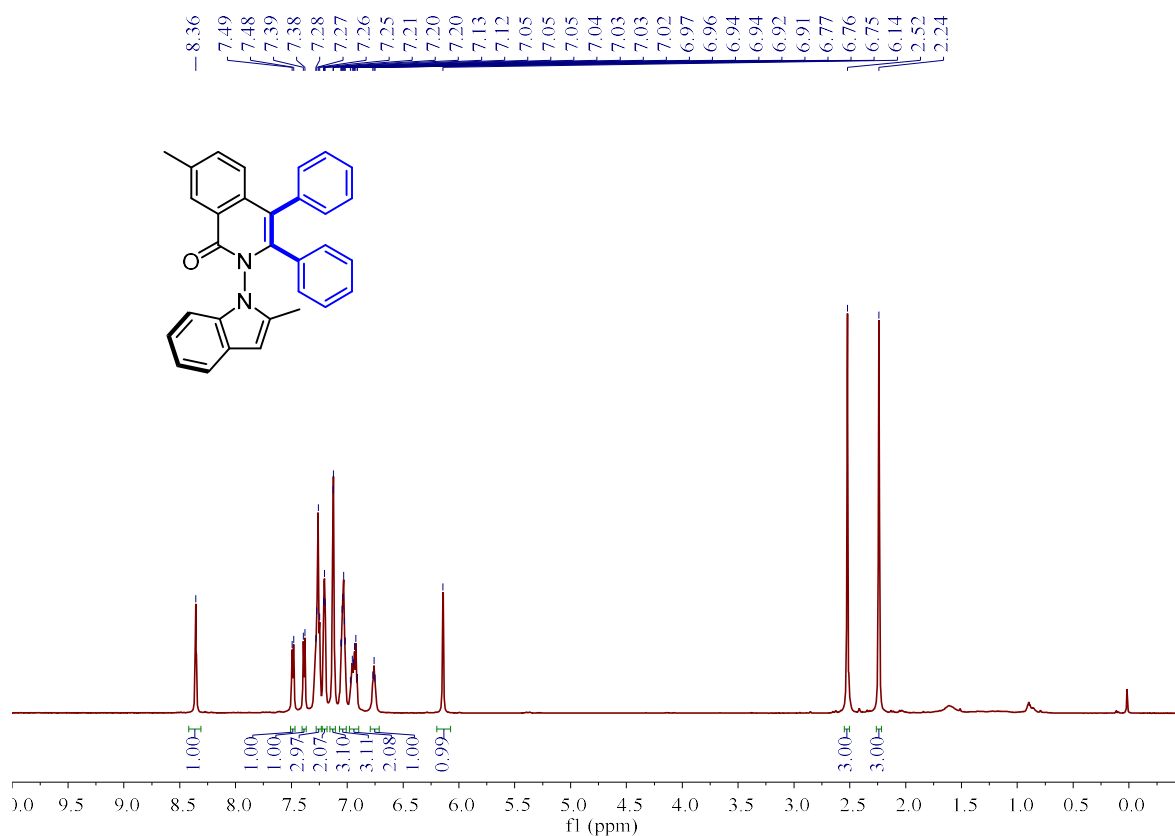
¹³C NMR (150 MHz, CDCl₃) spectrum of 7.



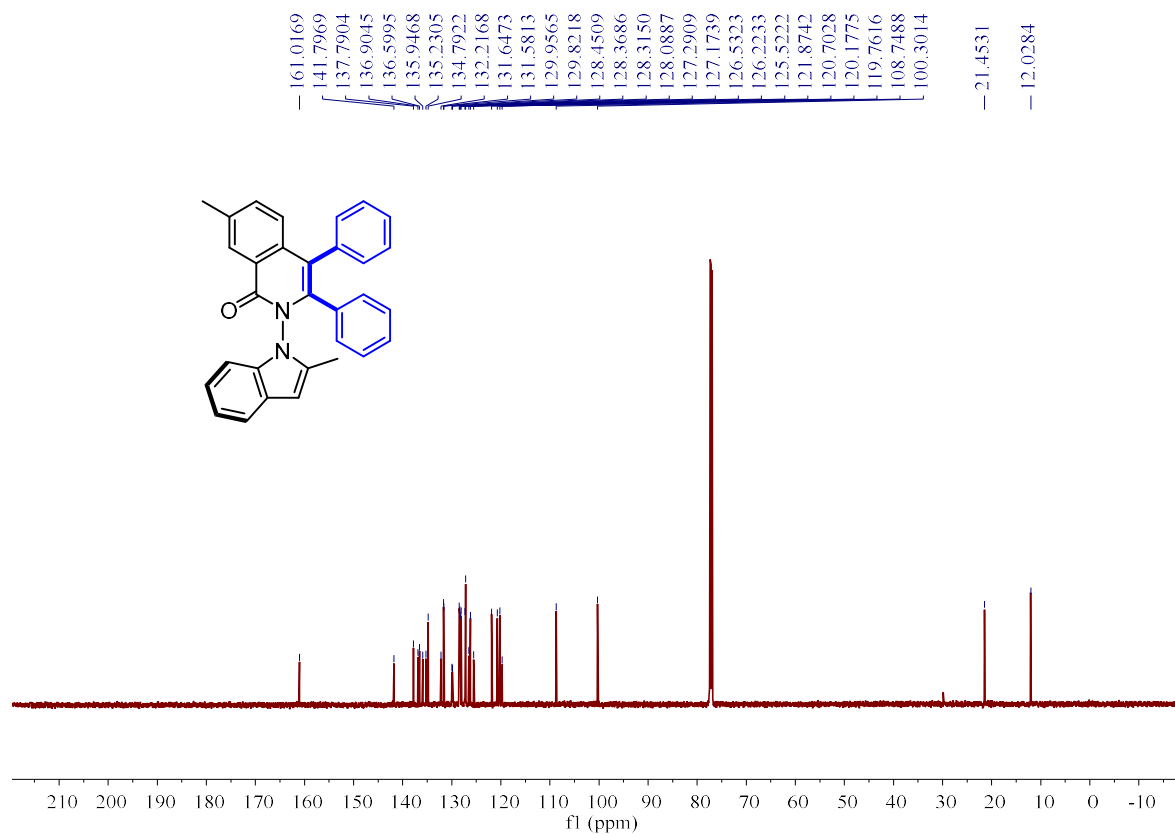
¹H NMR (600 MHz, CDCl₃) spectrum of 8.



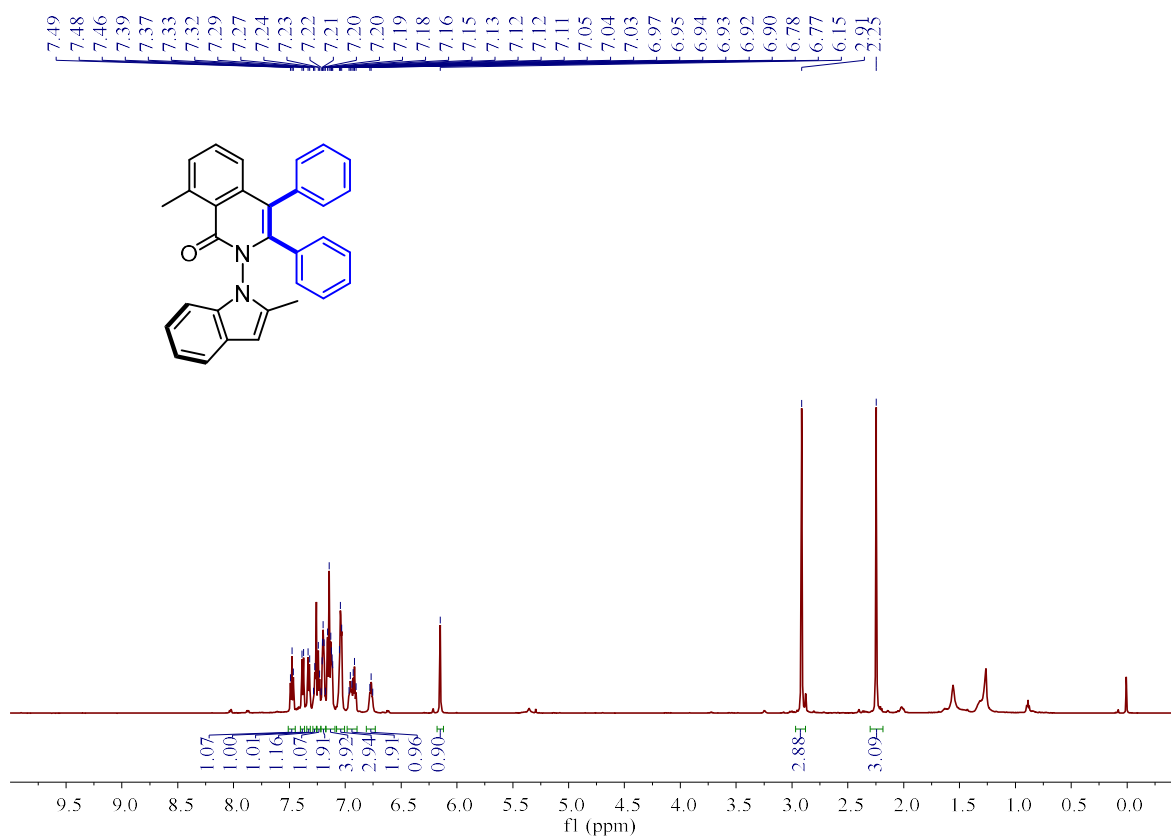
¹³C NMR (150 MHz, CDCl₃) spectrum of 8.



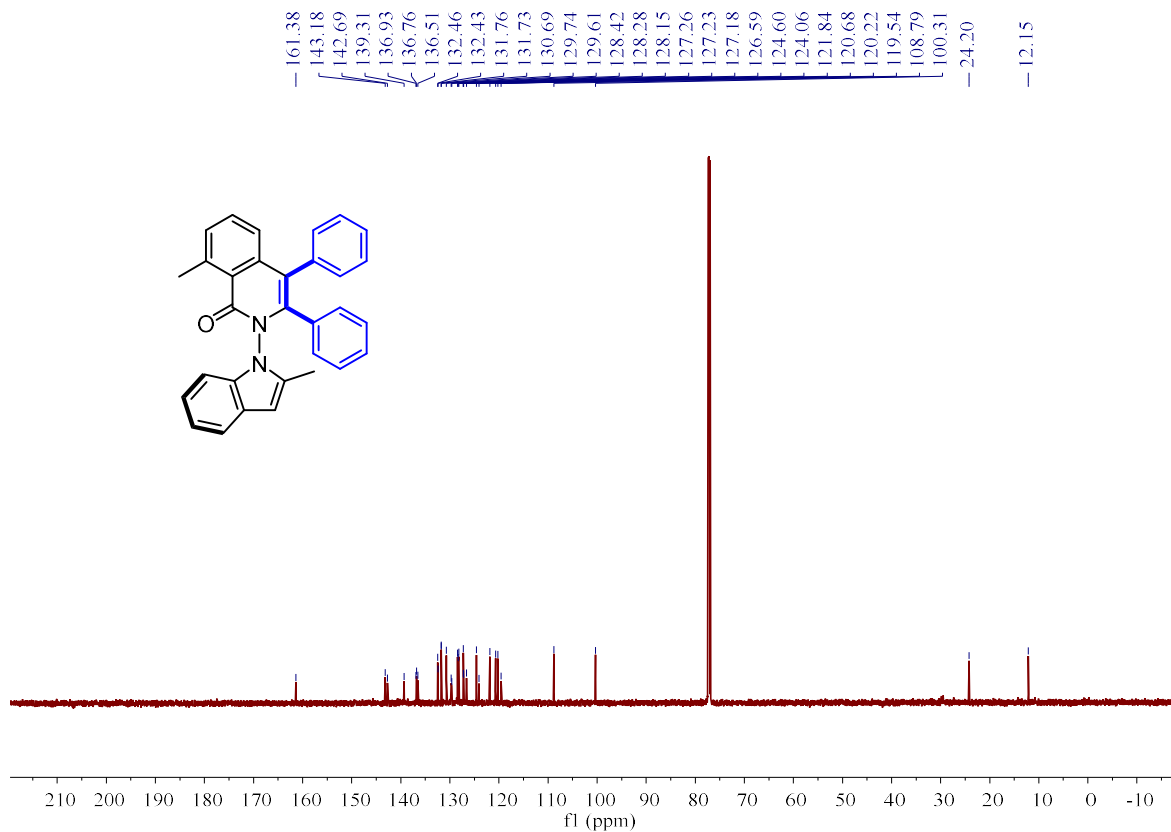
¹H NMR (600 MHz, CDCl₃) spectrum of 9.



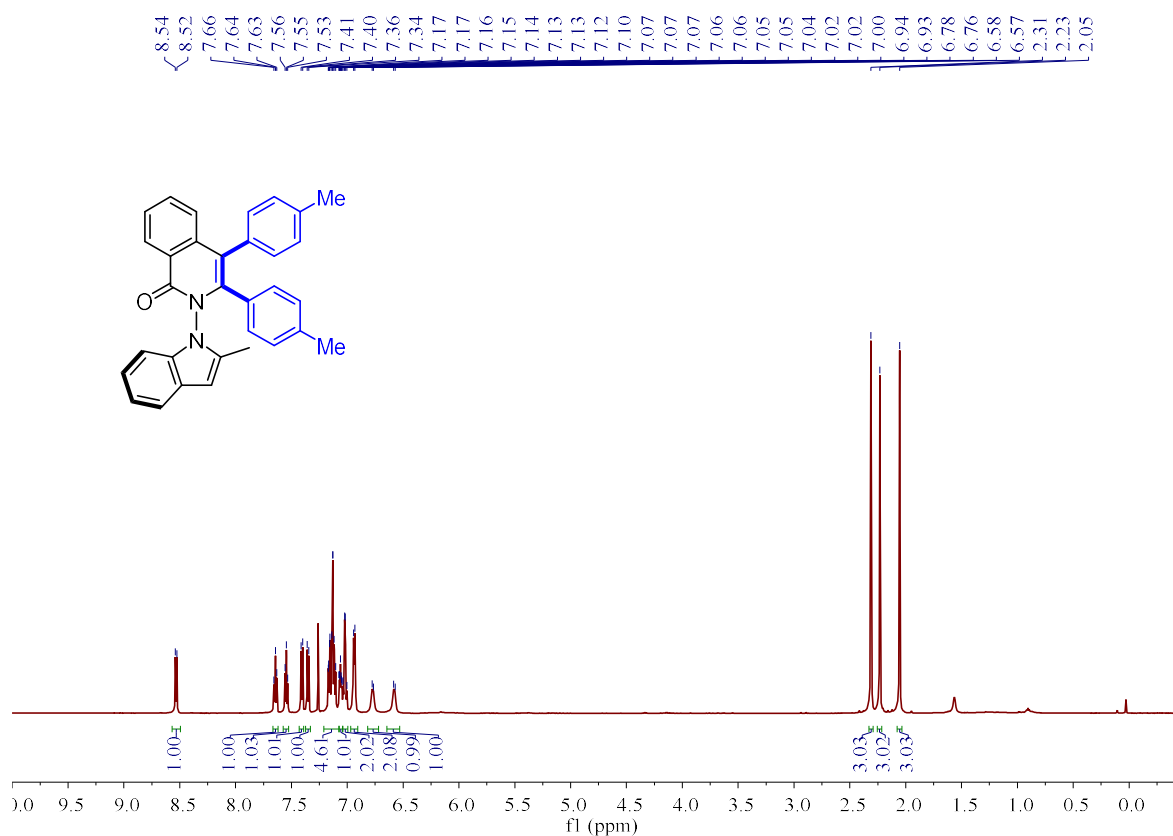
¹³C NMR (150 MHz, CDCl₃) spectrum of 9.



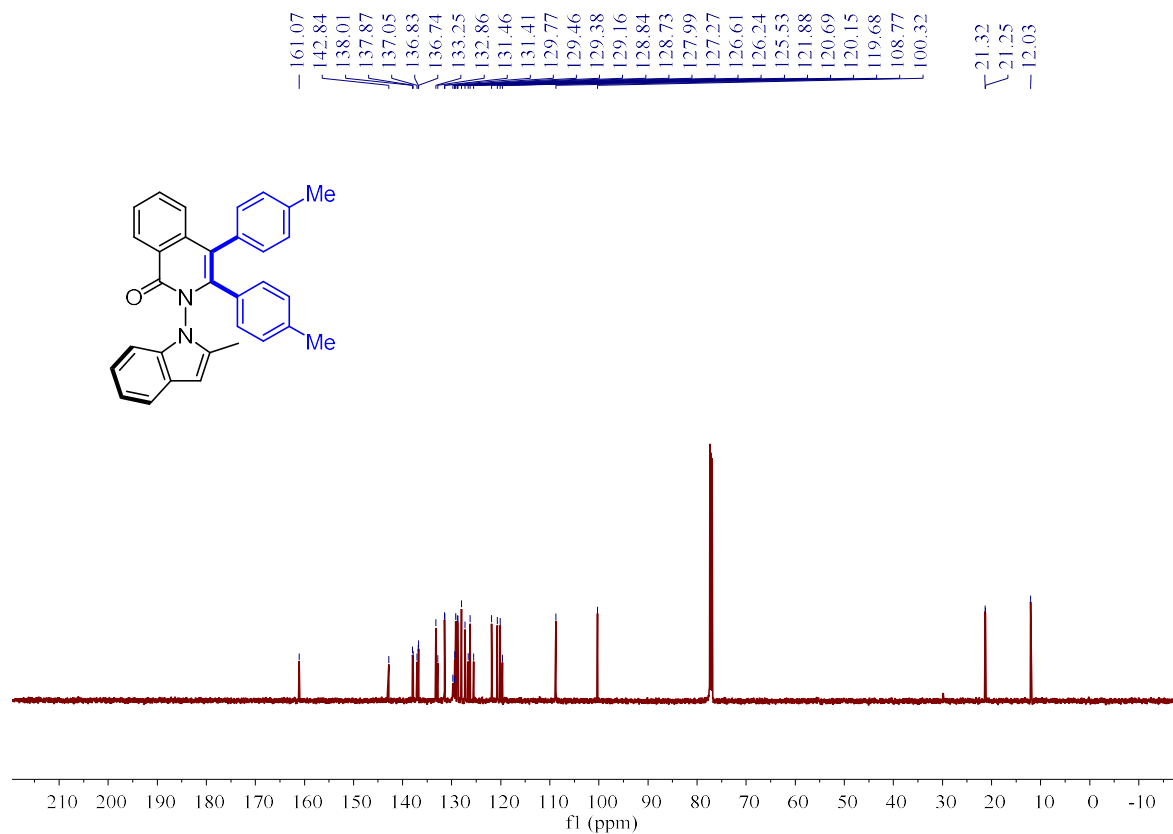
¹H NMR (600 MHz, CDCl₃) spectrum of 10.



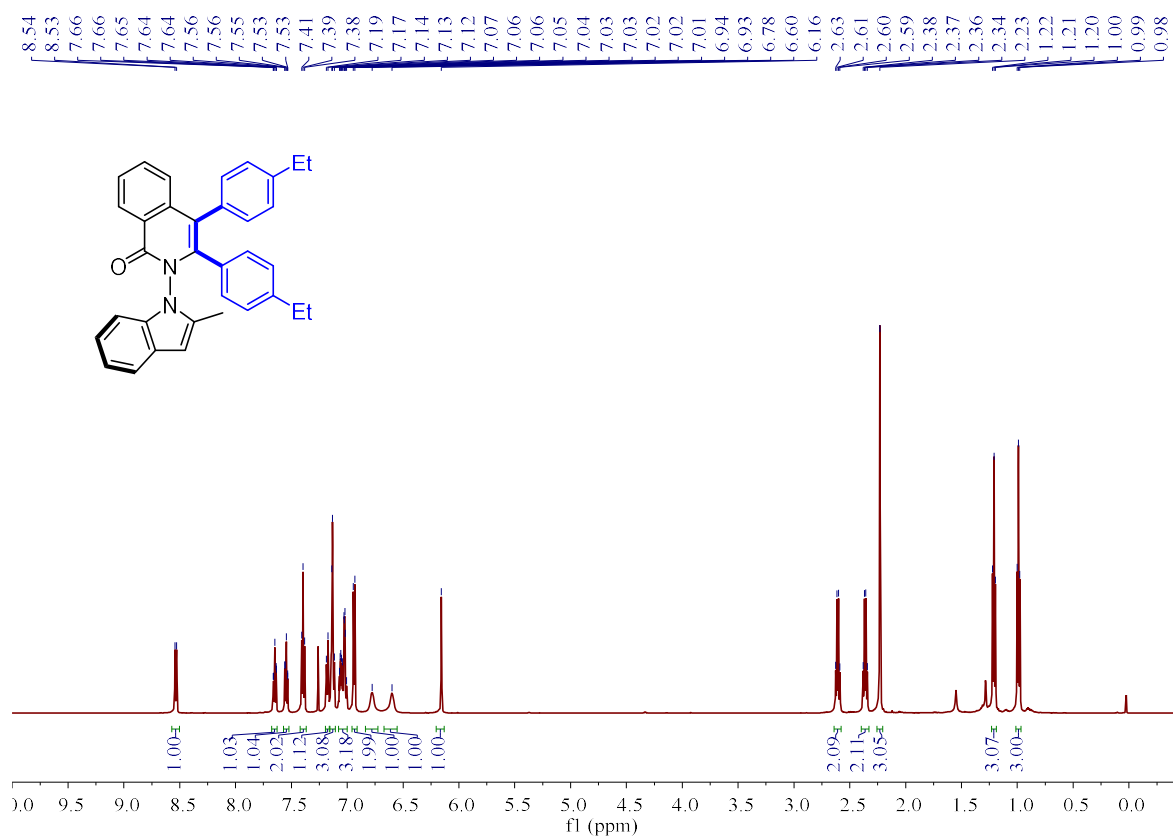
¹³C NMR (150 MHz, CDCl₃) spectrum of 10.



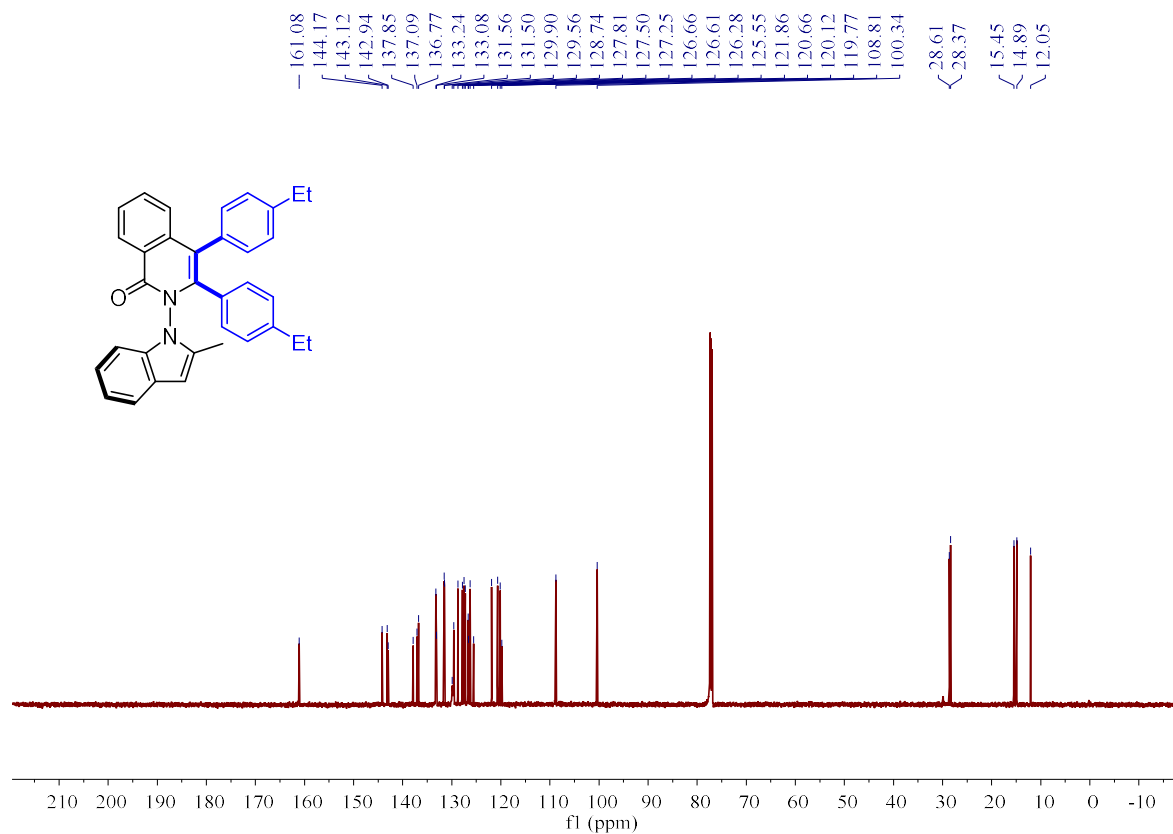
¹H NMR (600 MHz, CDCl₃) spectrum of 11.



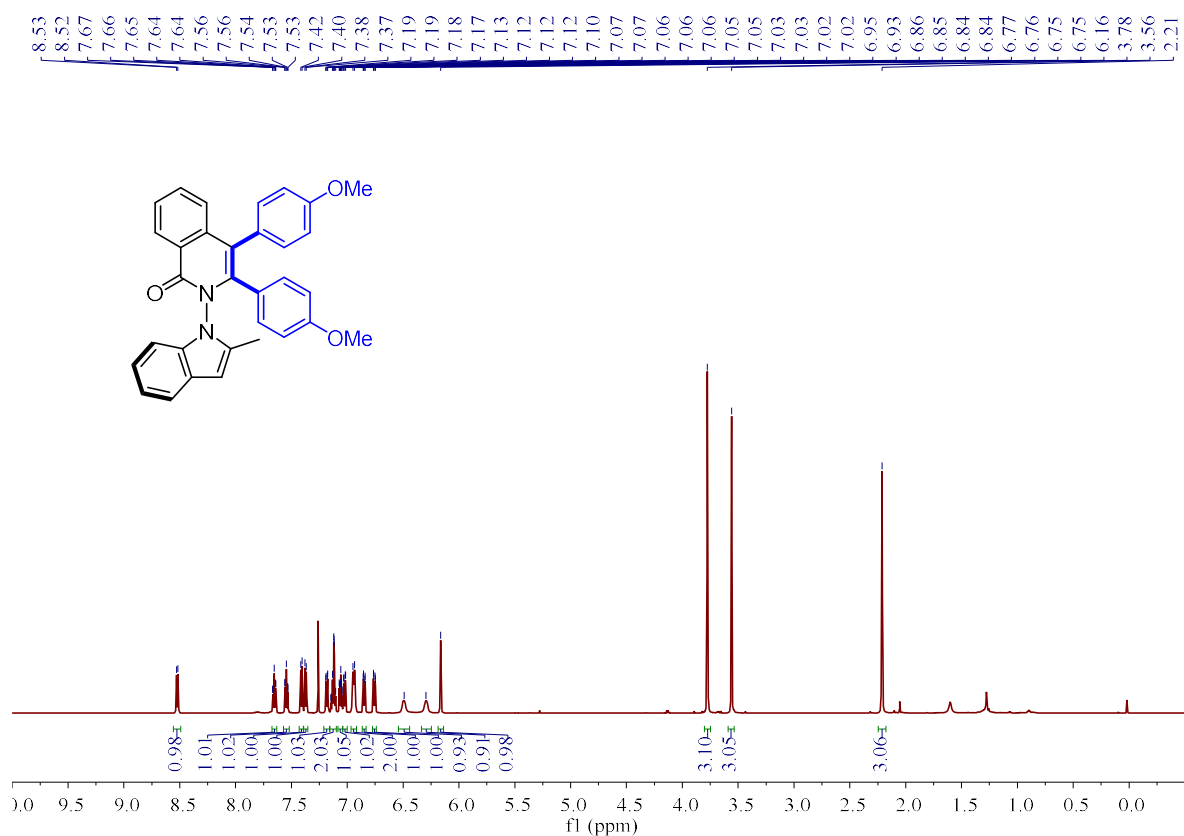
¹³C NMR (150 MHz, CDCl₃) spectrum of 11.



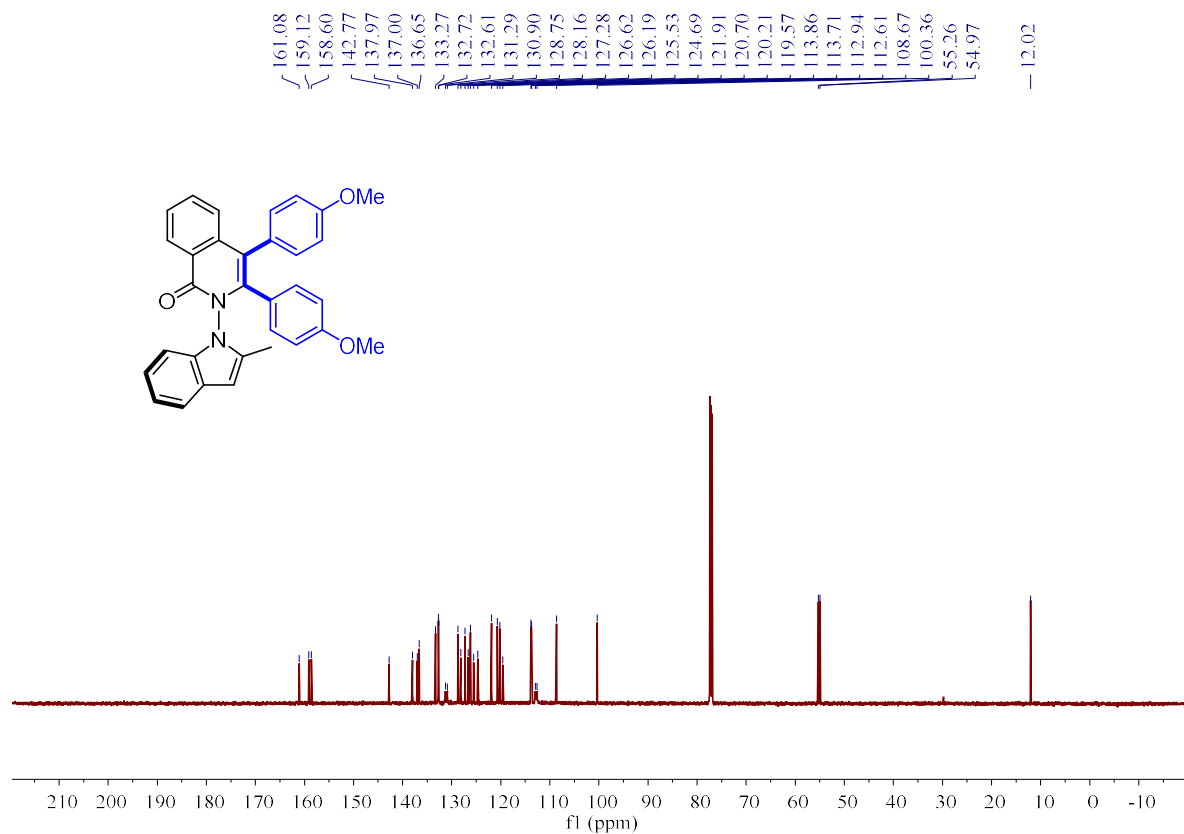
¹H NMR (600 MHz, CDCl₃) spectrum of 12.



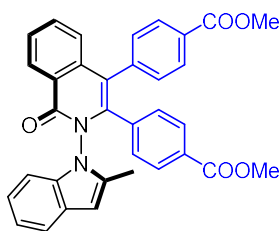
¹³C NMR (150 MHz, CDCl₃) spectrum of 12.



¹H NMR (600 MHz, CDCl₃) spectrum of 13.

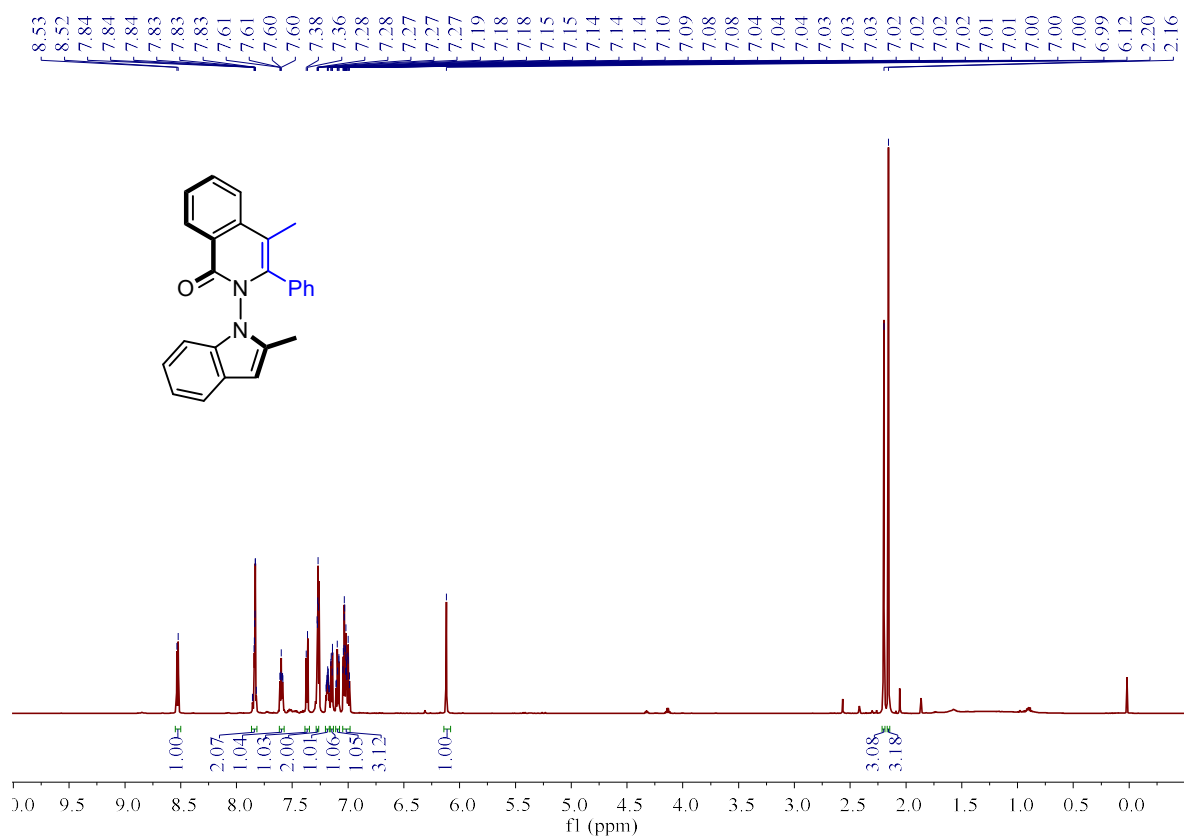


¹³C NMR (150 MHz, CDCl₃) spectrum of 13.

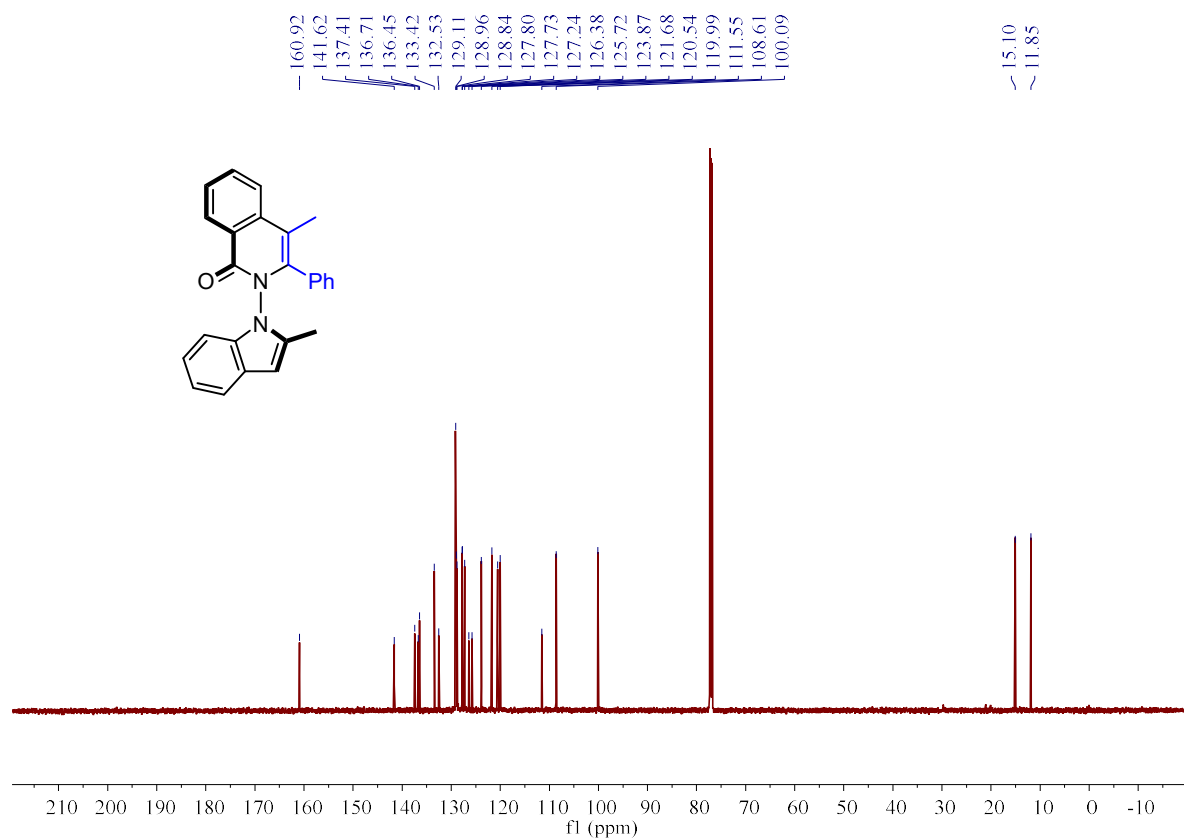


Chemical structure of compound 10 is shown in the top left. The ^{13}C NMR spectrum (CDCl₃) shows peaks at the following chemical shifts (ppm): 166.70, 166.24, 160.76, 141.88, 140.28, 136.83, 136.73, 136.36, 136.31, 133.75, 131.73, 131.66, 130.21, 129.89, 129.74, 129.62, 129.52, 129.08, 128.73, 128.70, 128.08, 126.59, 125.96, 125.72, 122.23, 121.11, 120.47, 119.07, 108.48, 100.91, 77.37, 77.16, 76.95, 52.35, 52.24, and 12.04.

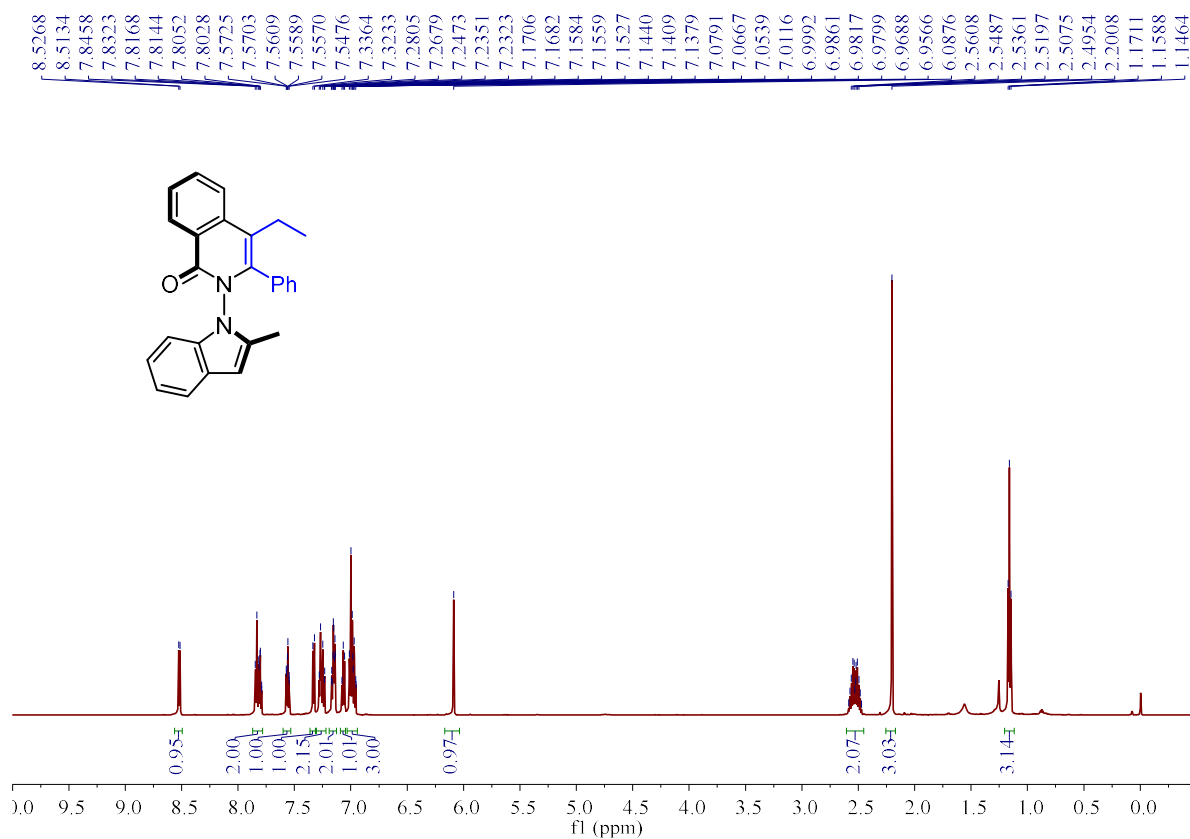
^{13}C NMR (150 MHz, CDCl_3) spectrum of (*ent*)-15.



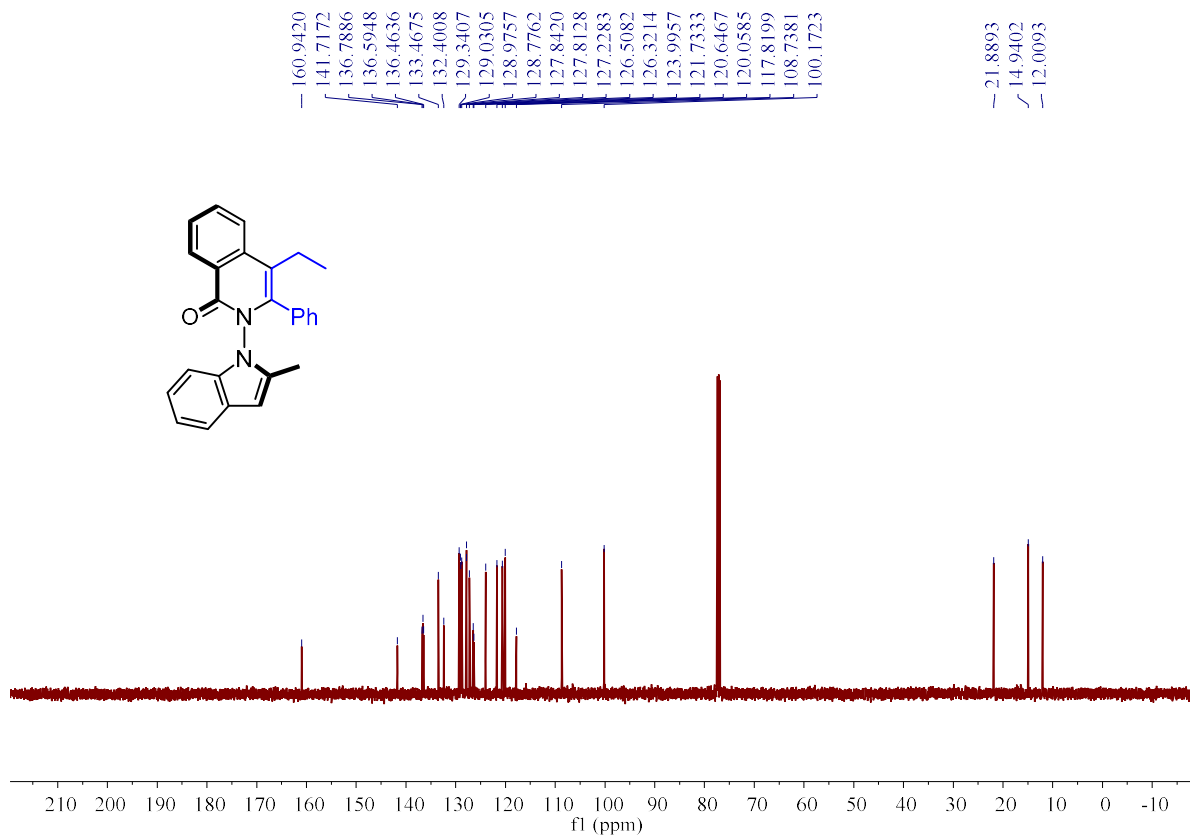
¹H NMR (600 MHz, CDCl₃) spectrum of (*ent*)-16.



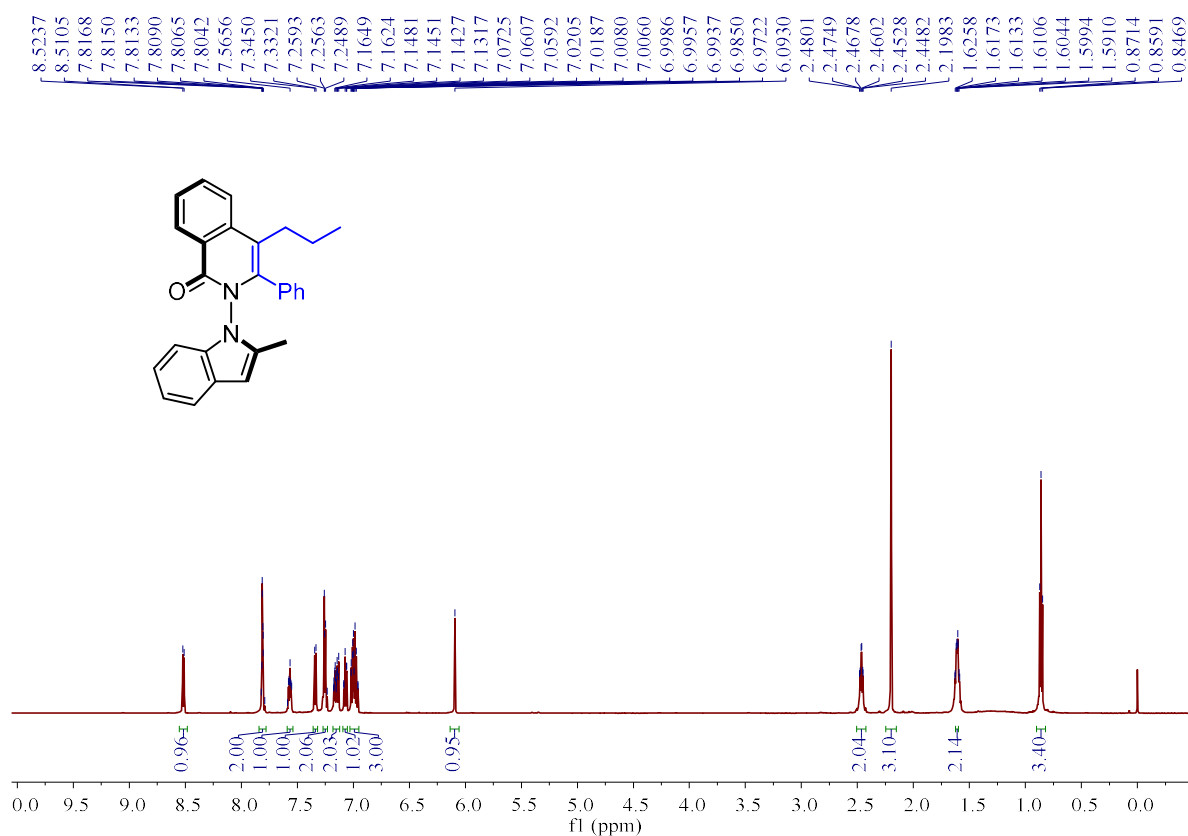
¹³C NMR (150 MHz, CDCl₃) spectrum of (*ent*)-16.



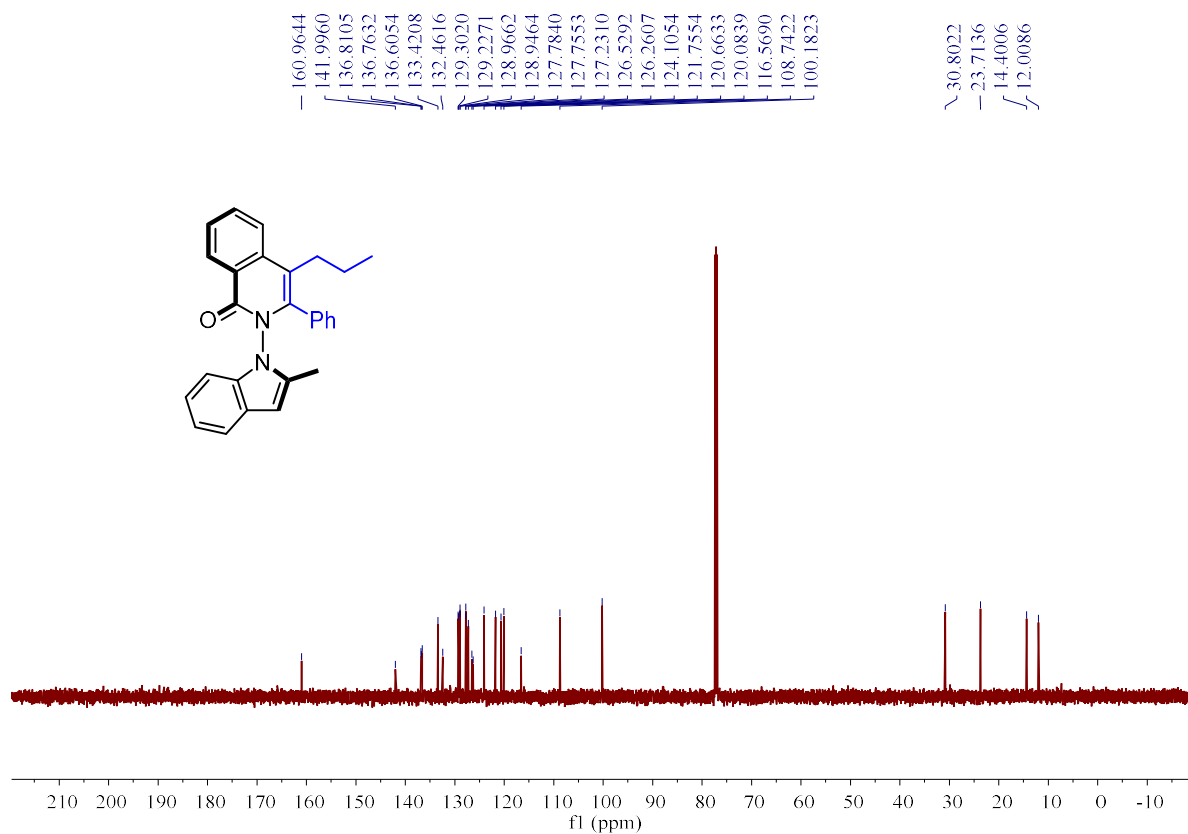
¹H NMR (600 MHz, CDCl₃) spectrum of (ent)-17.



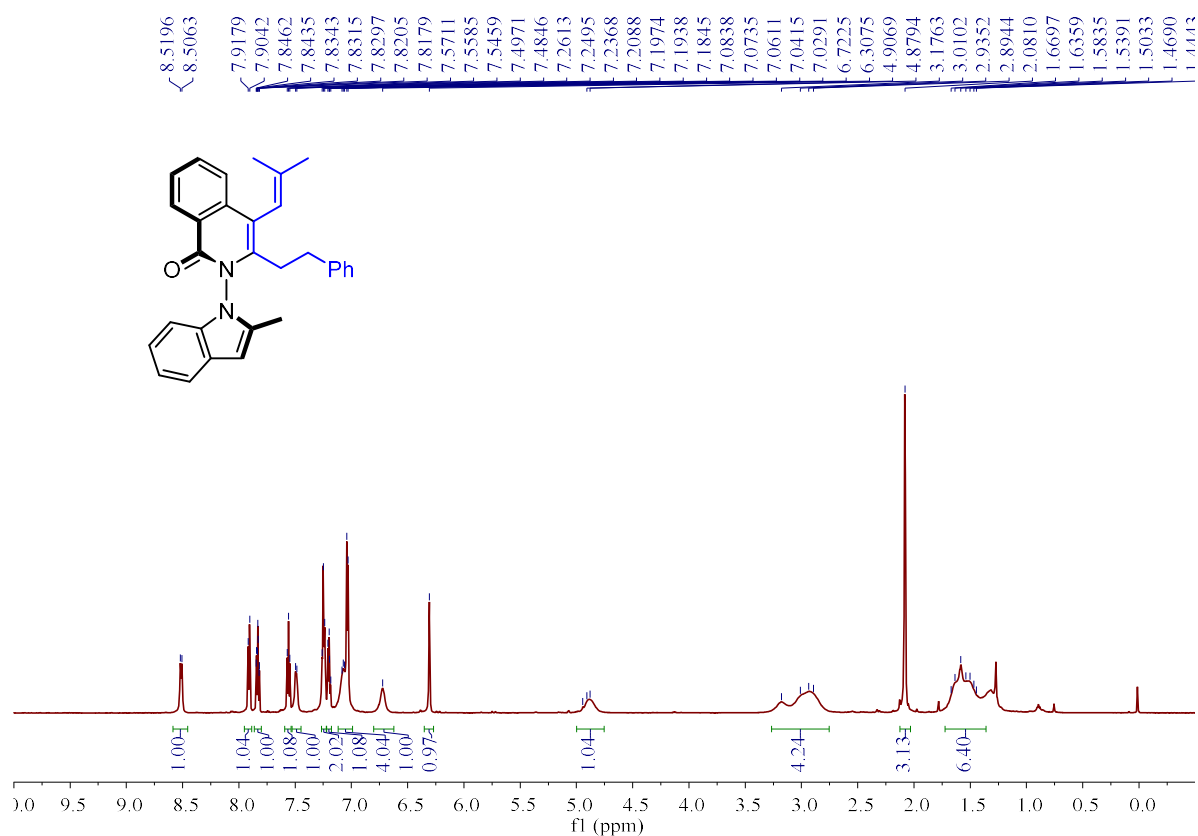
¹³C NMR (150 MHz, CDCl₃) spectrum of (ent)-17.



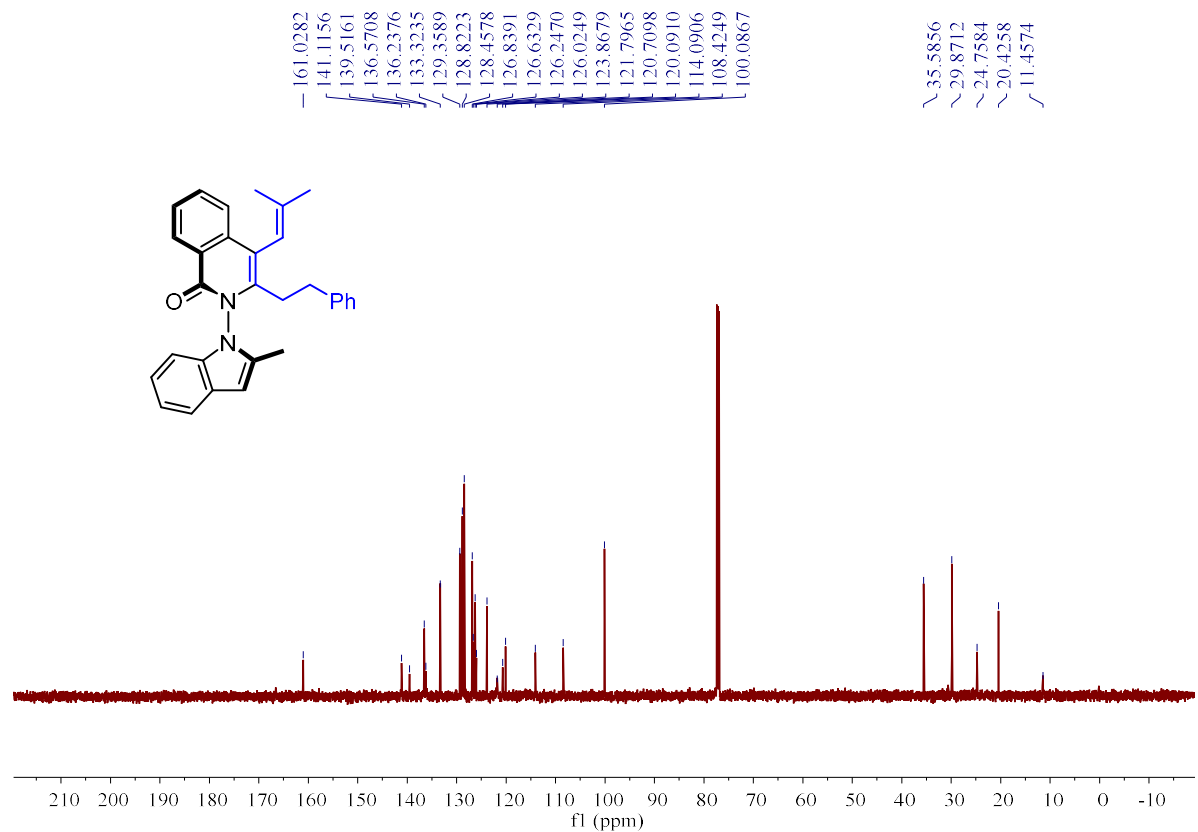
¹H NMR (600 MHz, CDCl₃) spectrum of (ent)-18.



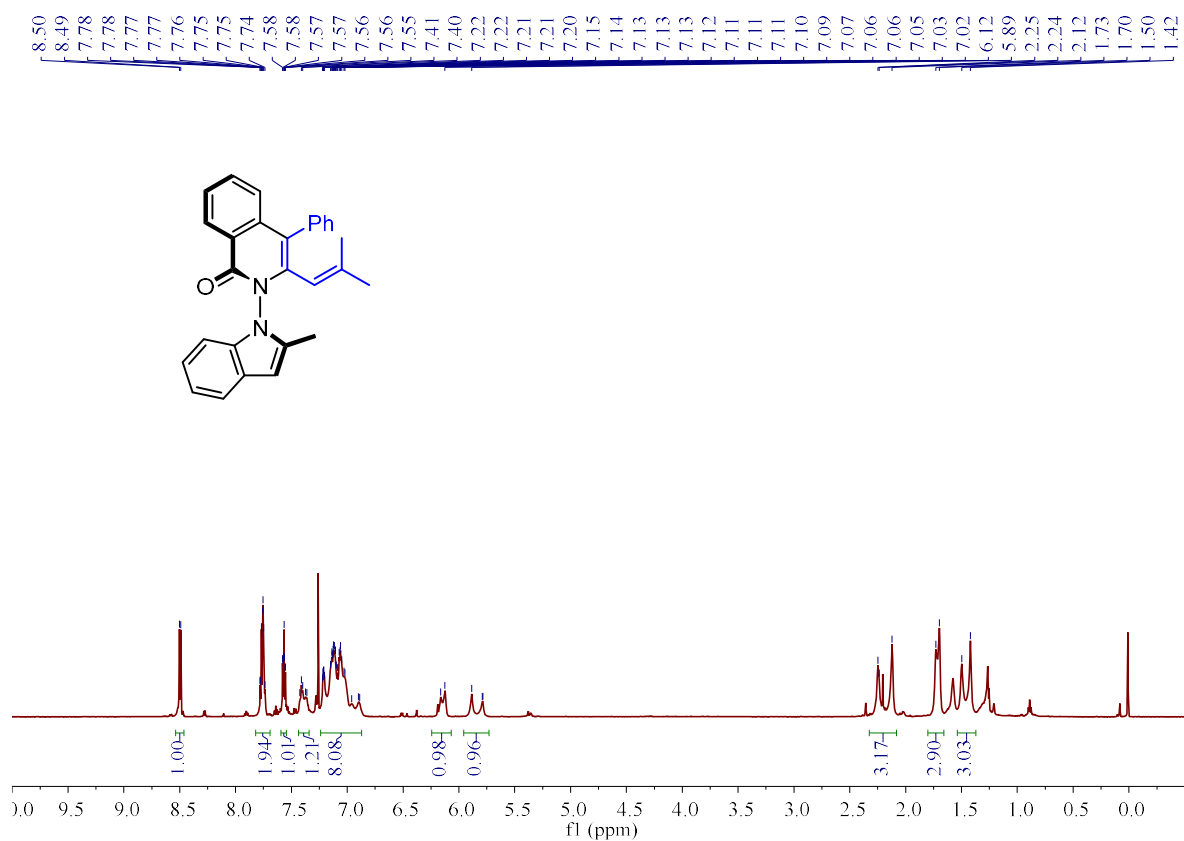
¹³C NMR (150 MHz, CDCl₃) spectrum of (ent)-18.



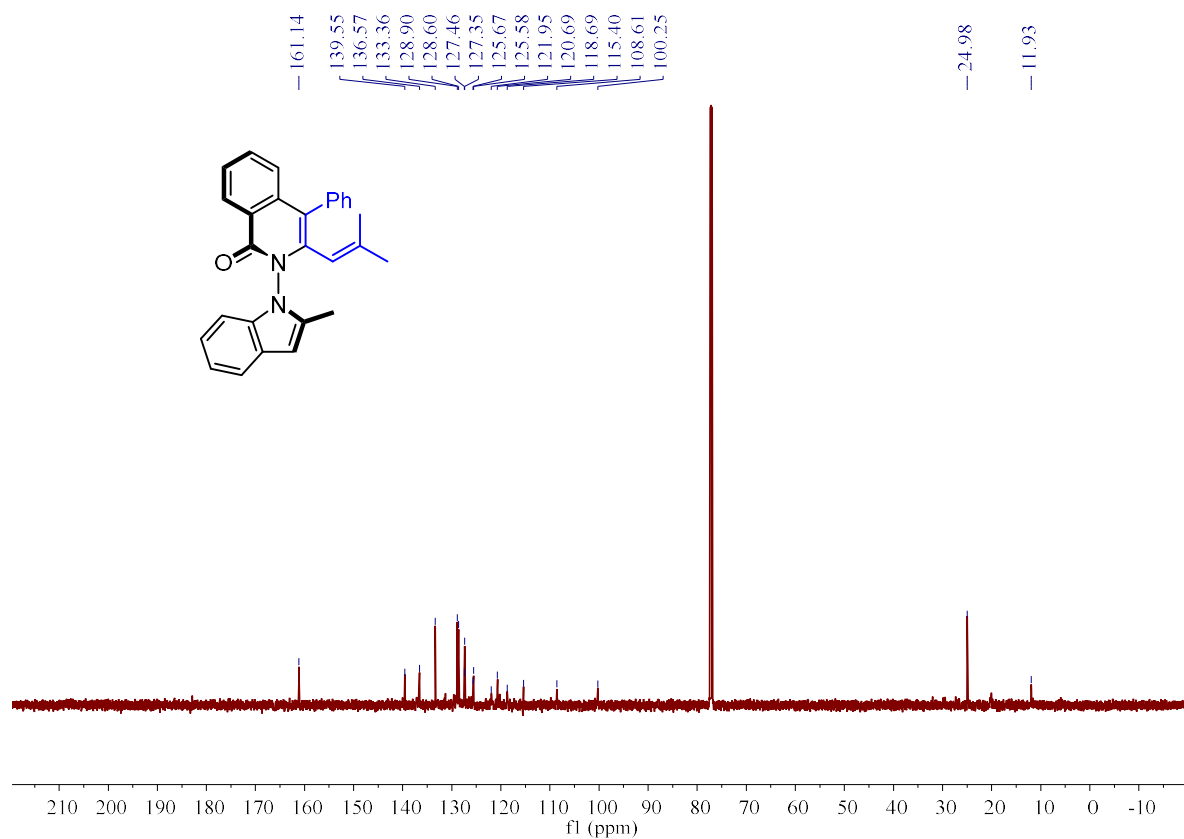
¹H NMR (600 MHz, CDCl₃) spectrum of (ent)-19.



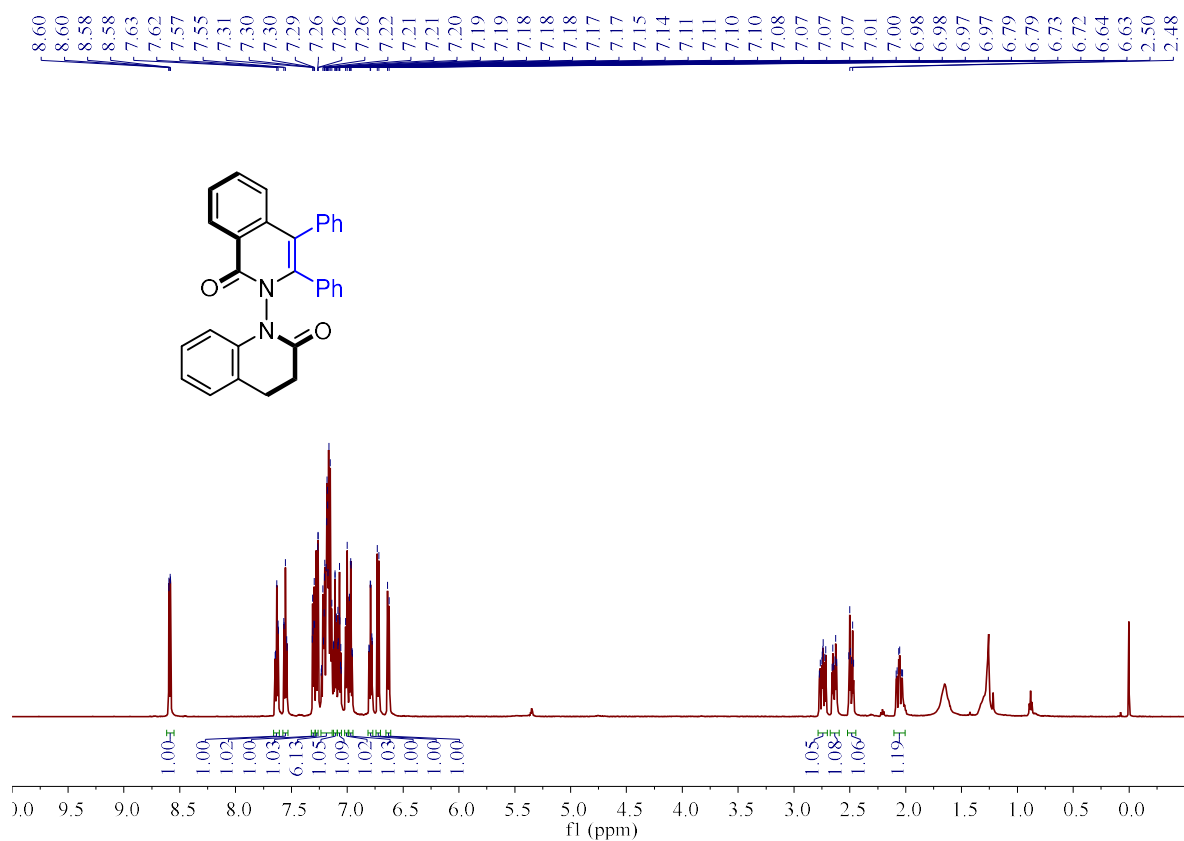
¹³C NMR (150 MHz, CDCl₃) spectrum of (ent)-19.



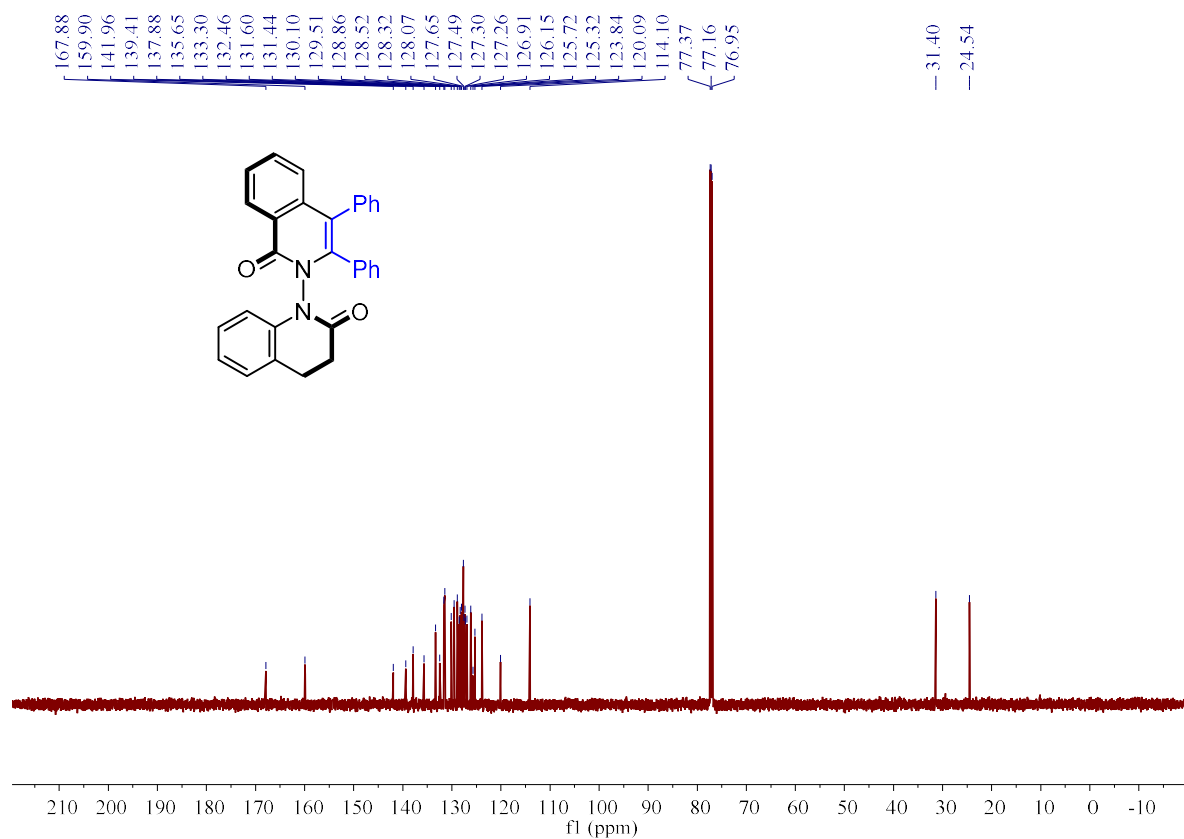
¹H NMR (600 MHz, CDCl₃) spectrum of (ent)-20.



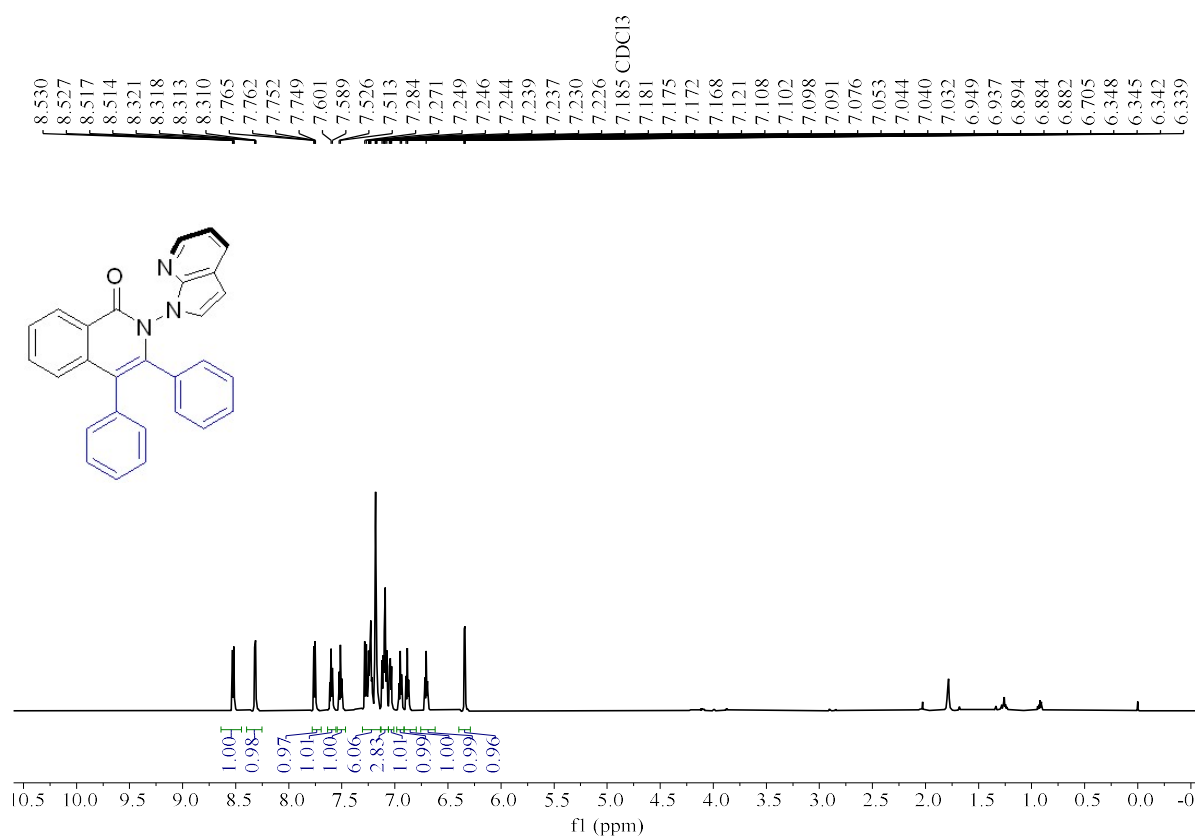
¹³C NMR (150 MHz, CDCl₃) spectrum of (ent)-20.



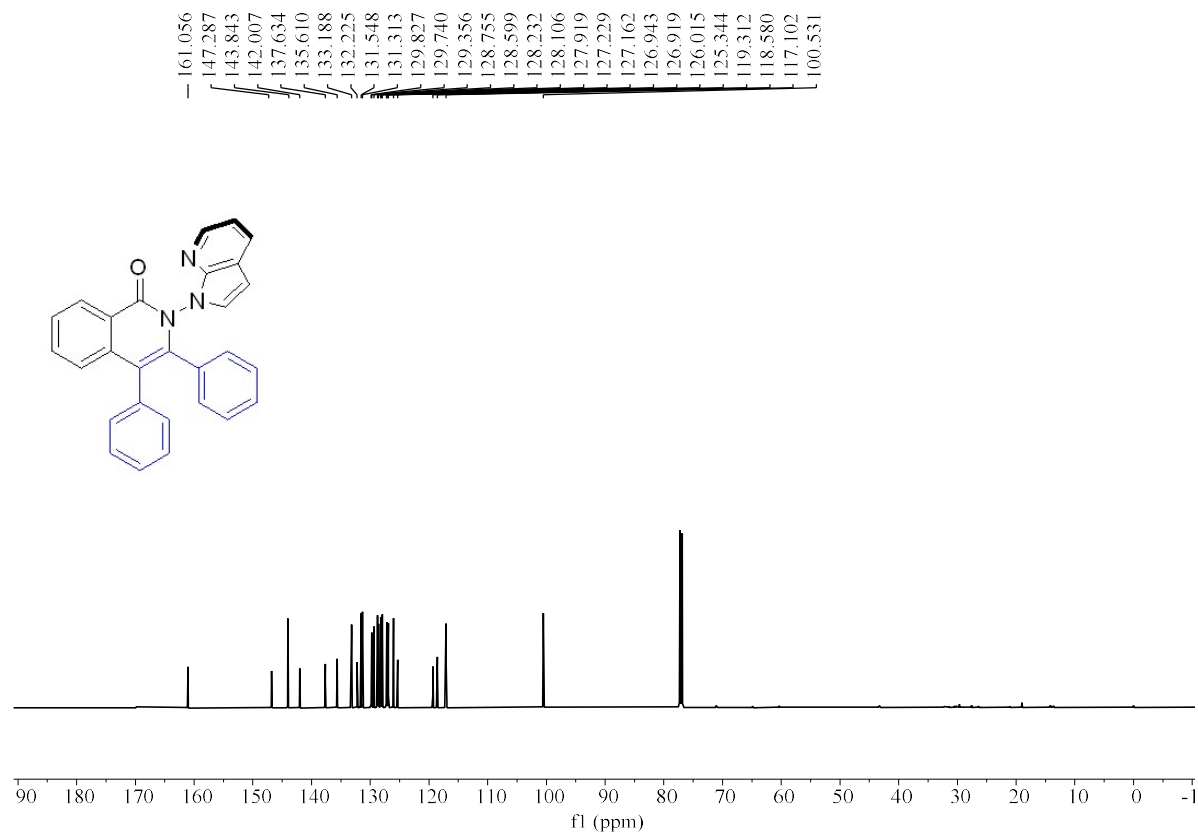
¹H NMR (600 MHz, CDCl₃) spectrum of 21.



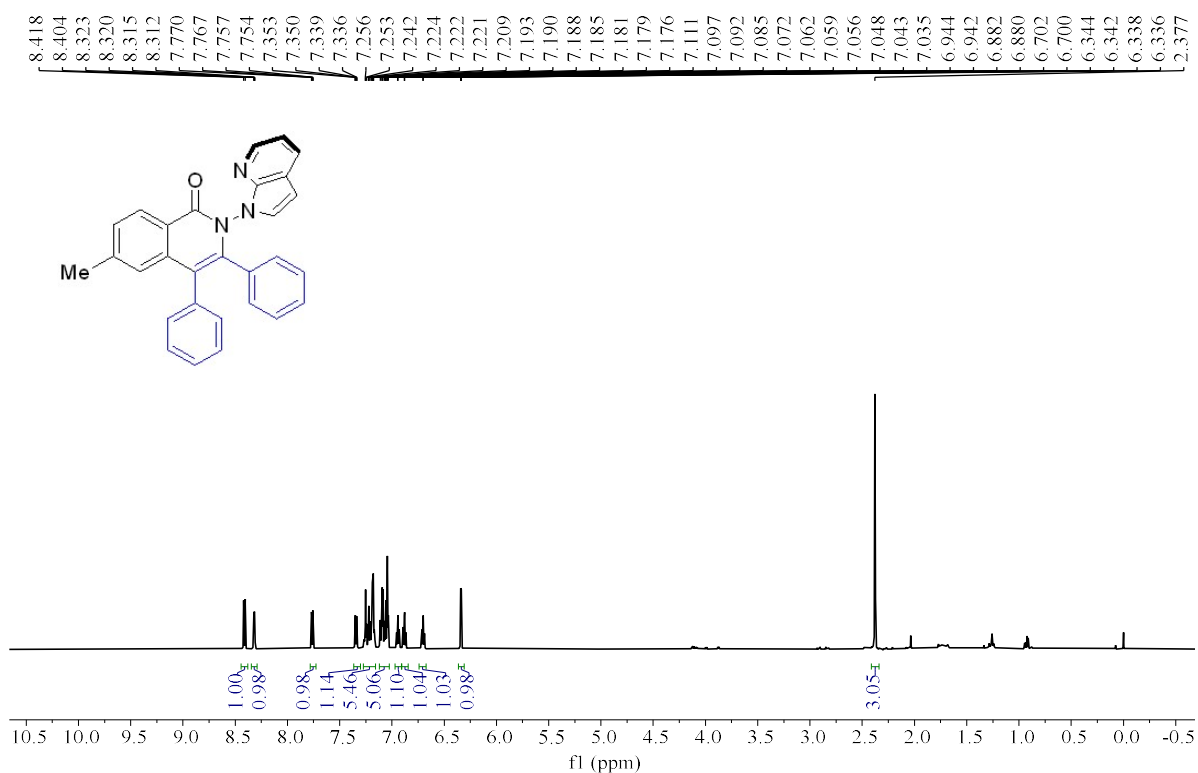
¹³C NMR (150 MHz, CDCl₃) spectrum of 21.

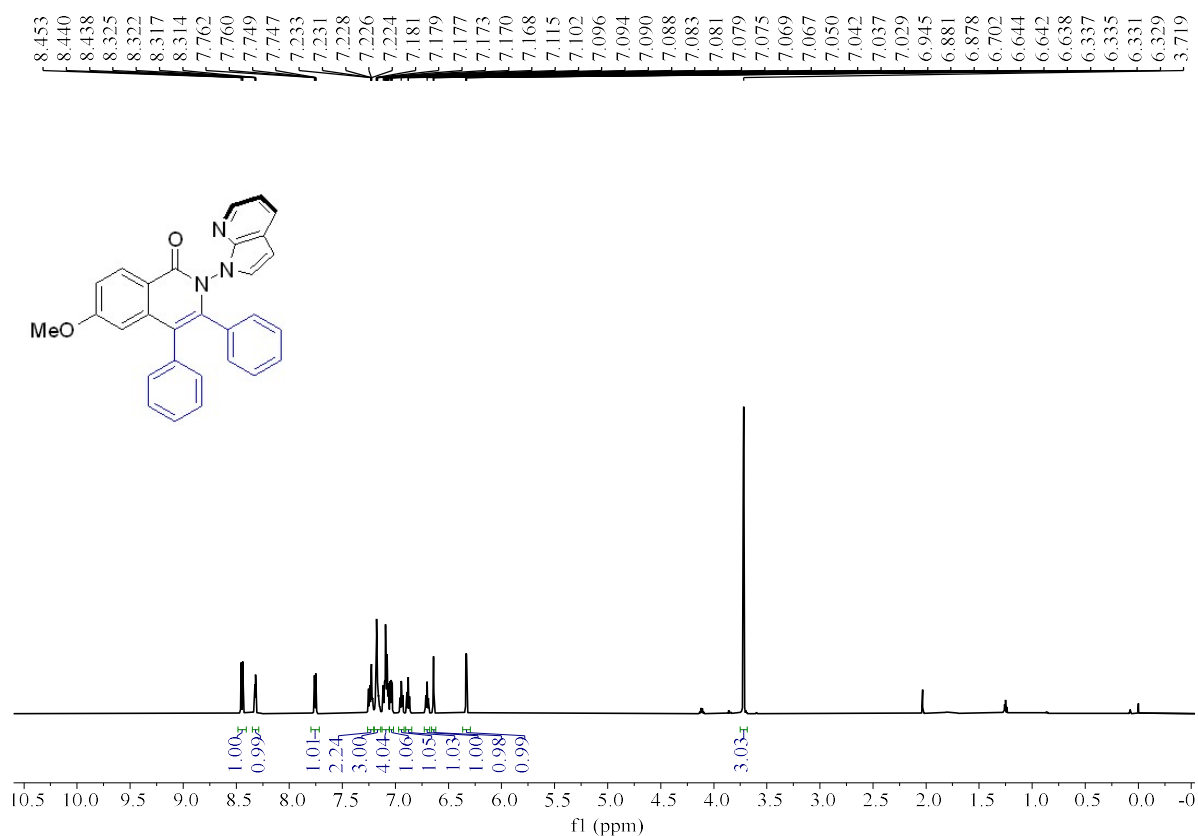


¹H NMR (600 MHz, CDCl₃) spectrum of 23.

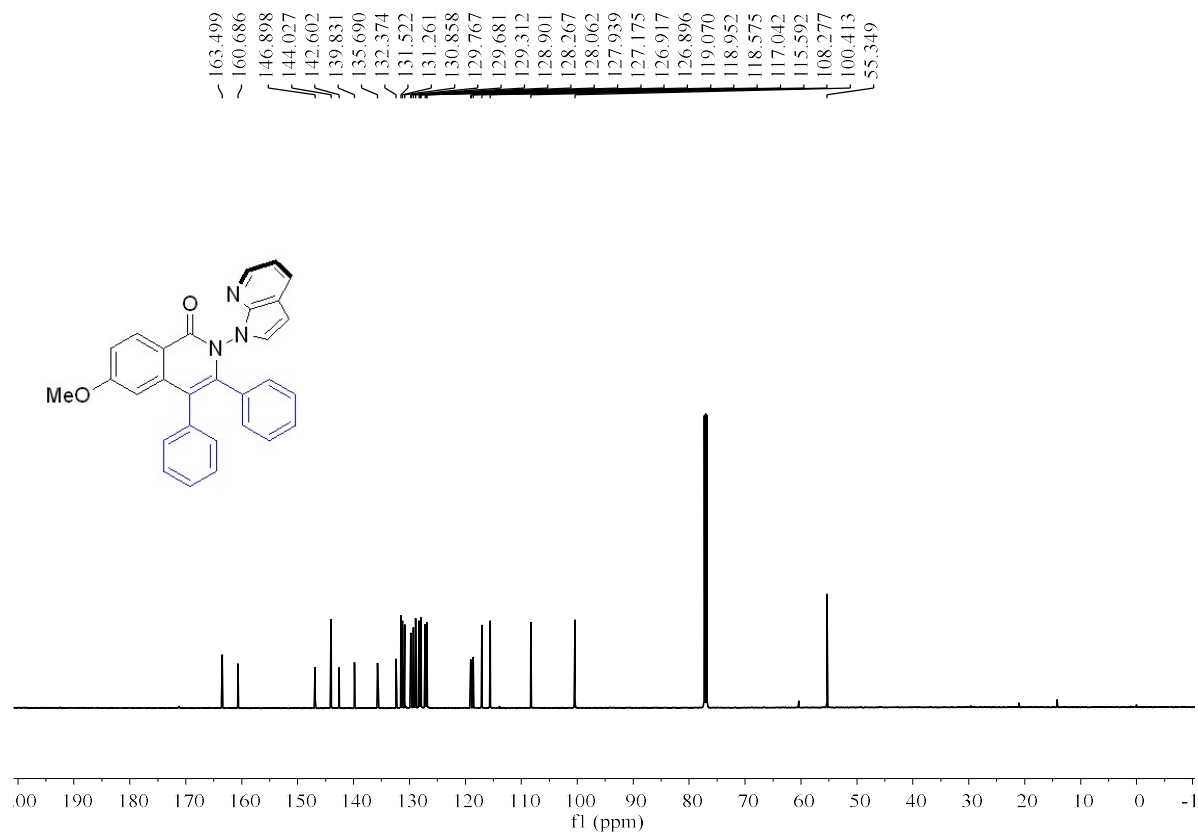


¹³C NMR (150 MHz, CDCl₃) spectrum of 23.

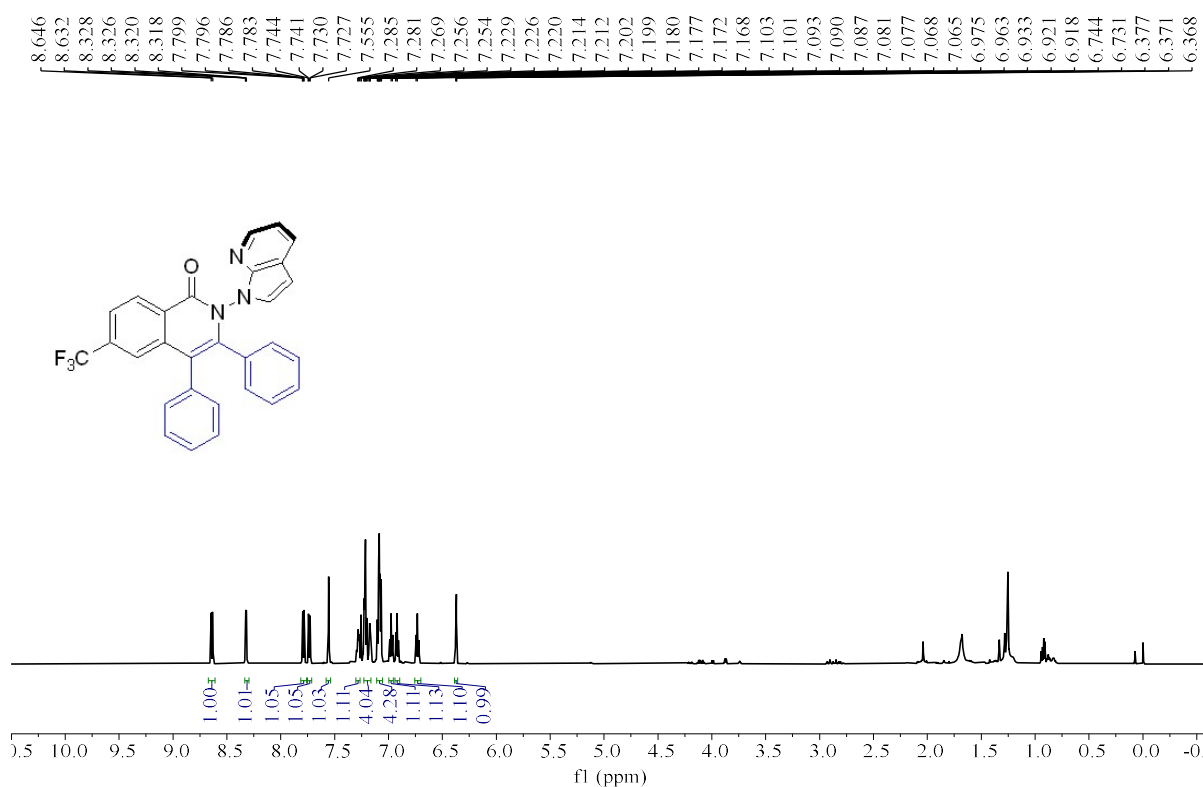




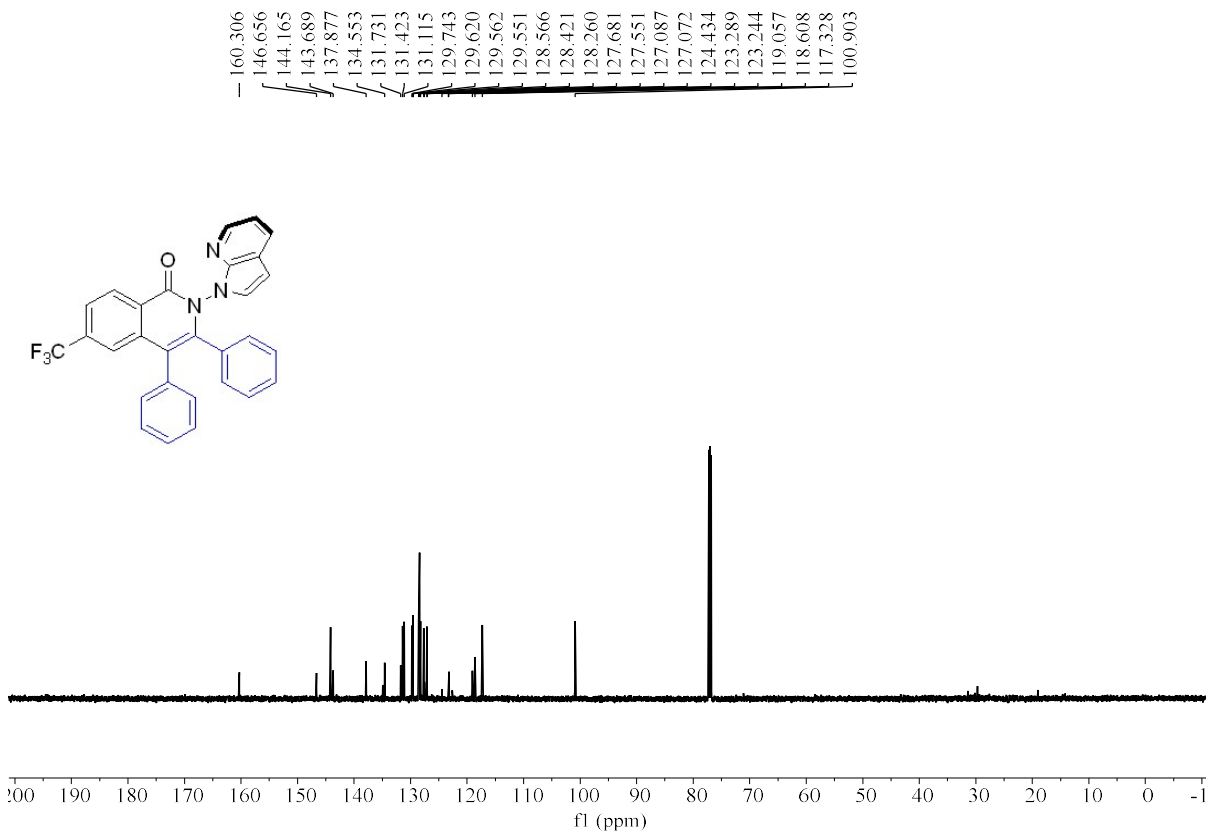
¹H NMR (600 MHz, CDCl₃) spectrum of 25.



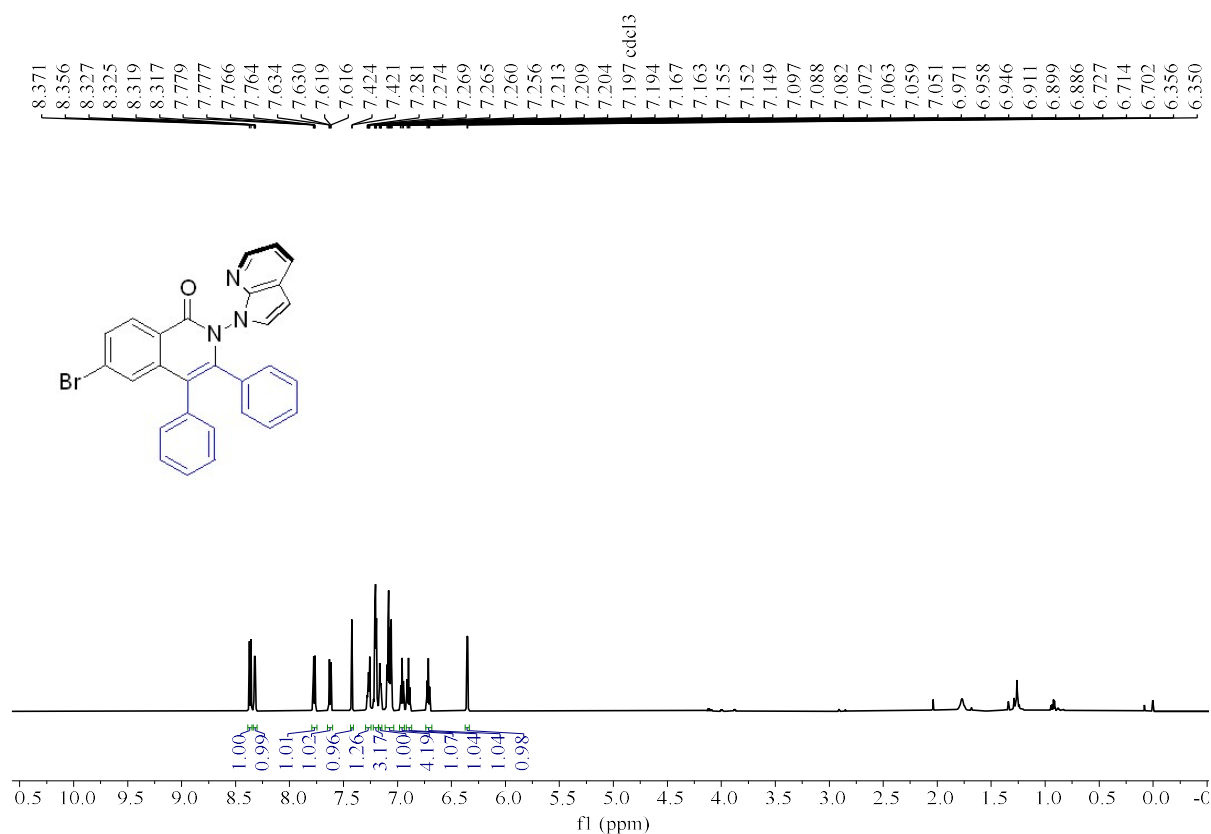
¹³C NMR (150 MHz, CDCl₃) spectrum of 25.



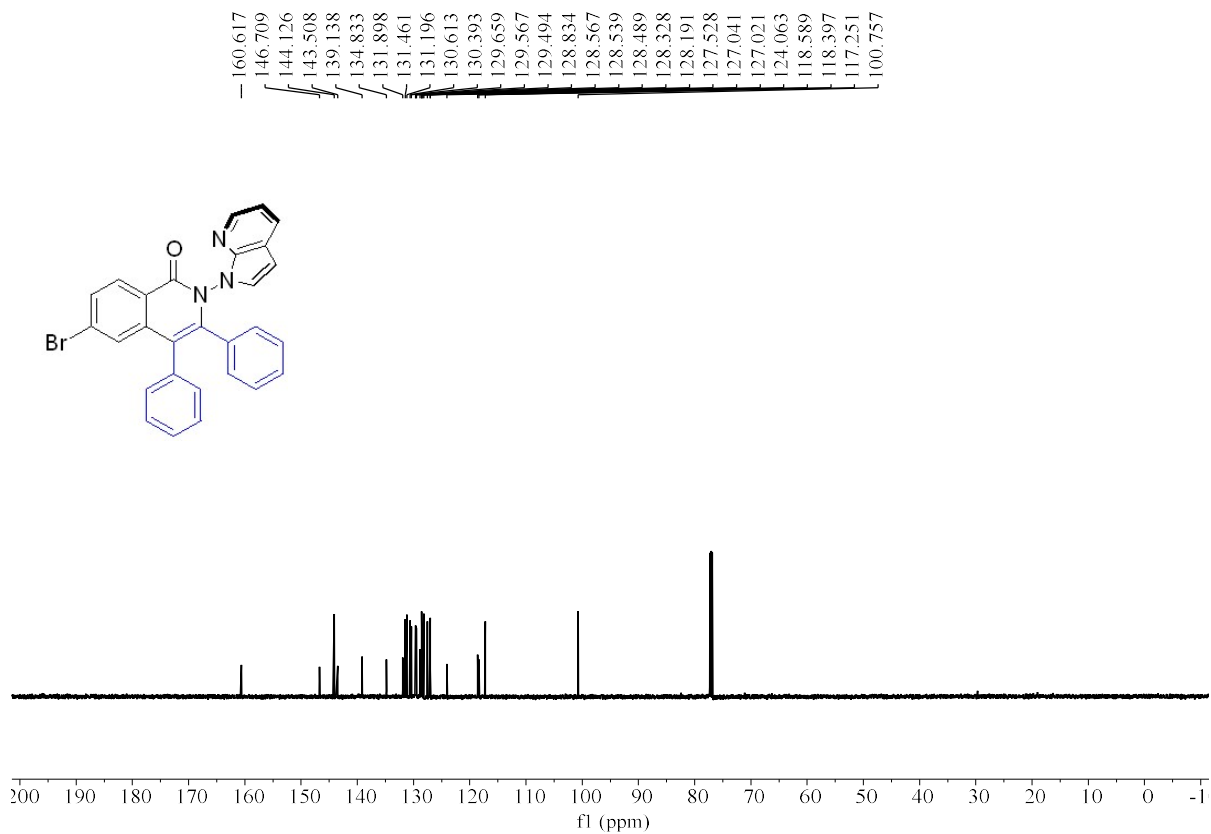
¹H NMR (600 MHz, CDCl₃) spectrum of 26.



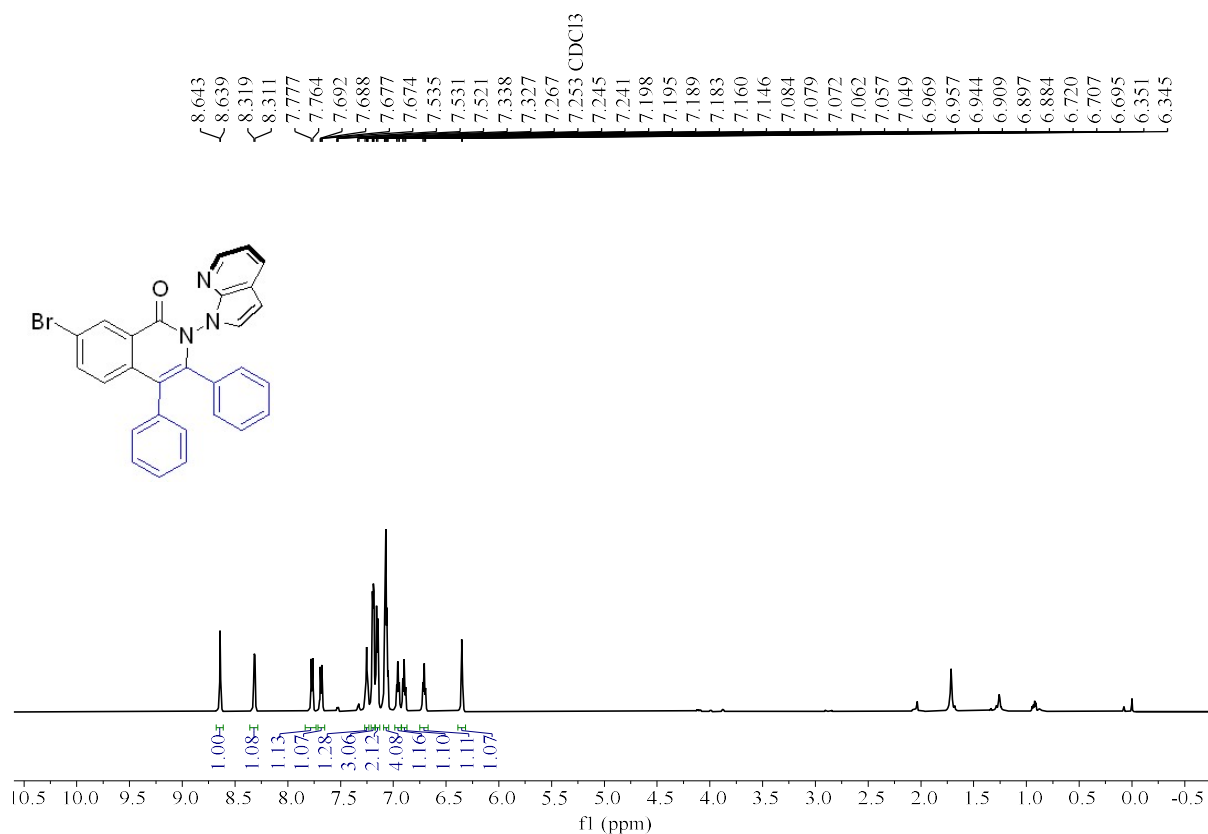
¹³C NMR (150 MHz, CDCl₃) spectrum of 26.



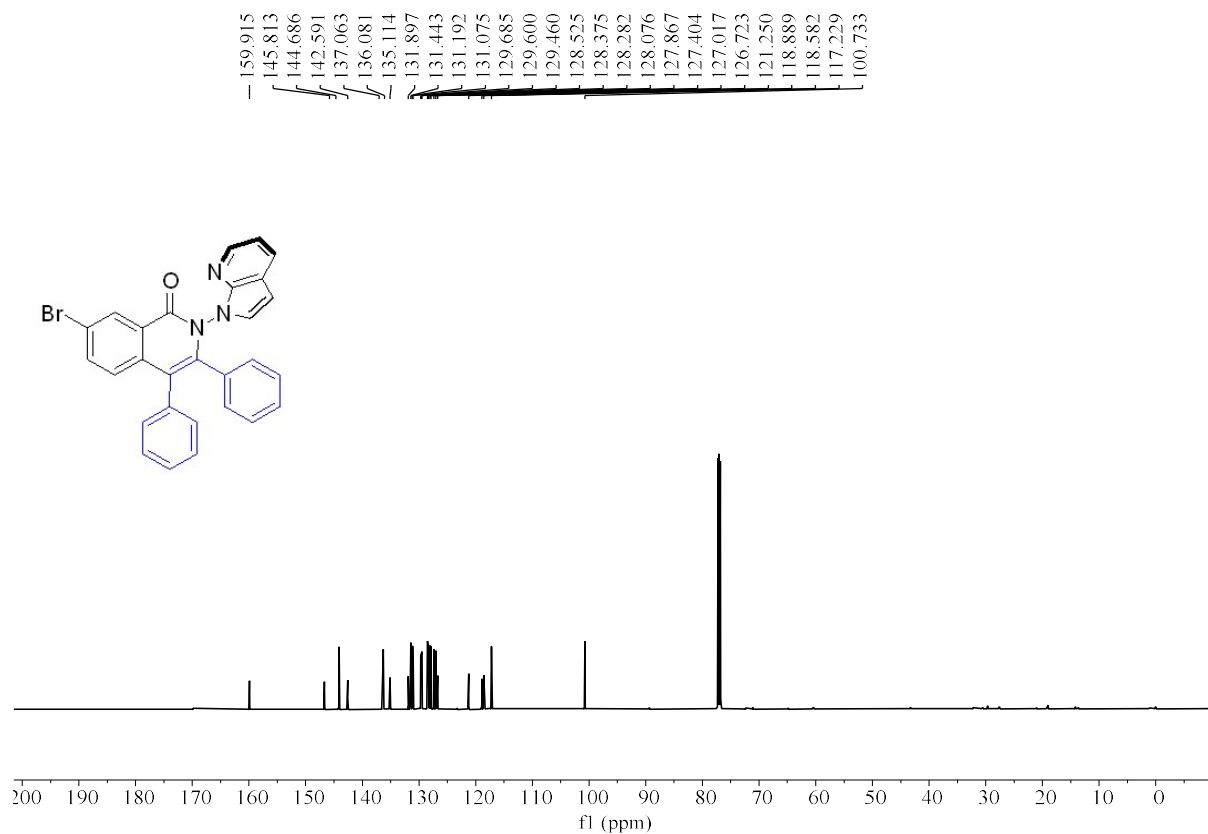
¹H NMR (600 MHz, CDCl₃) spectrum of 27.



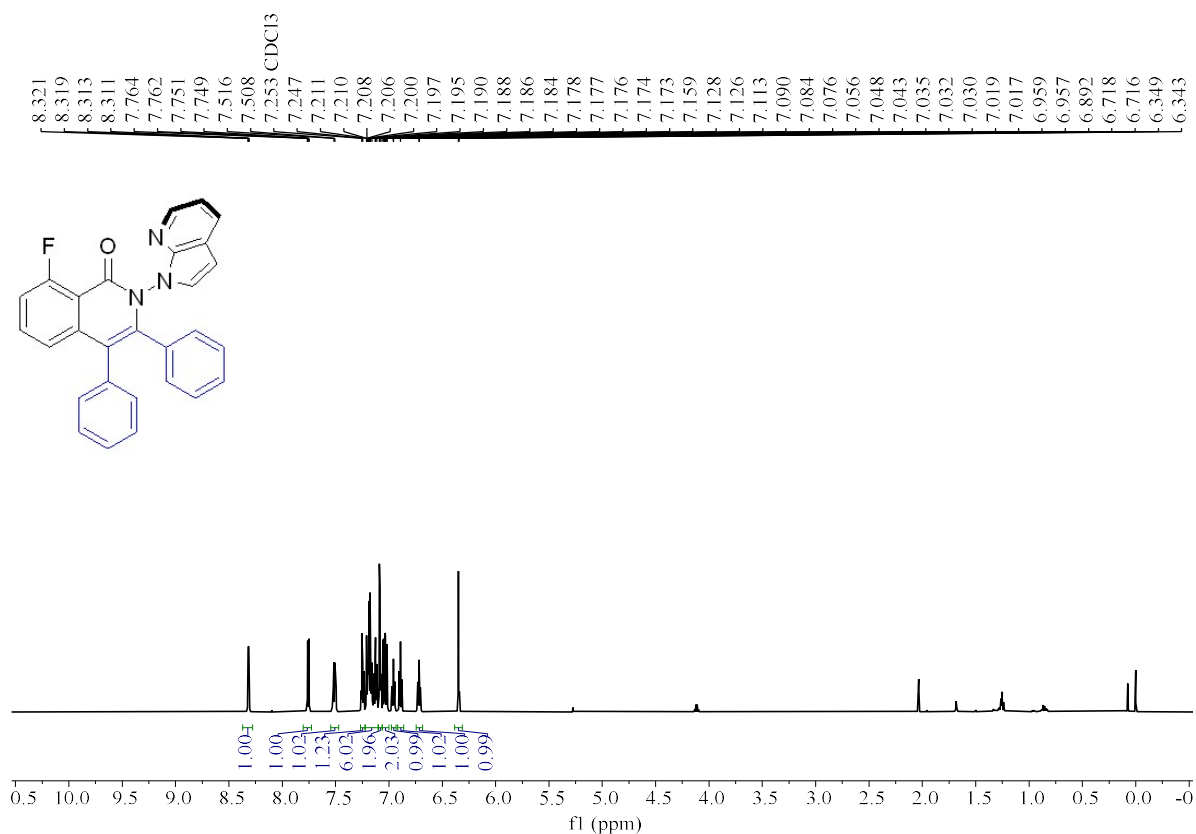
¹³C NMR (150 MHz, CDCl₃) spectrum of 27.



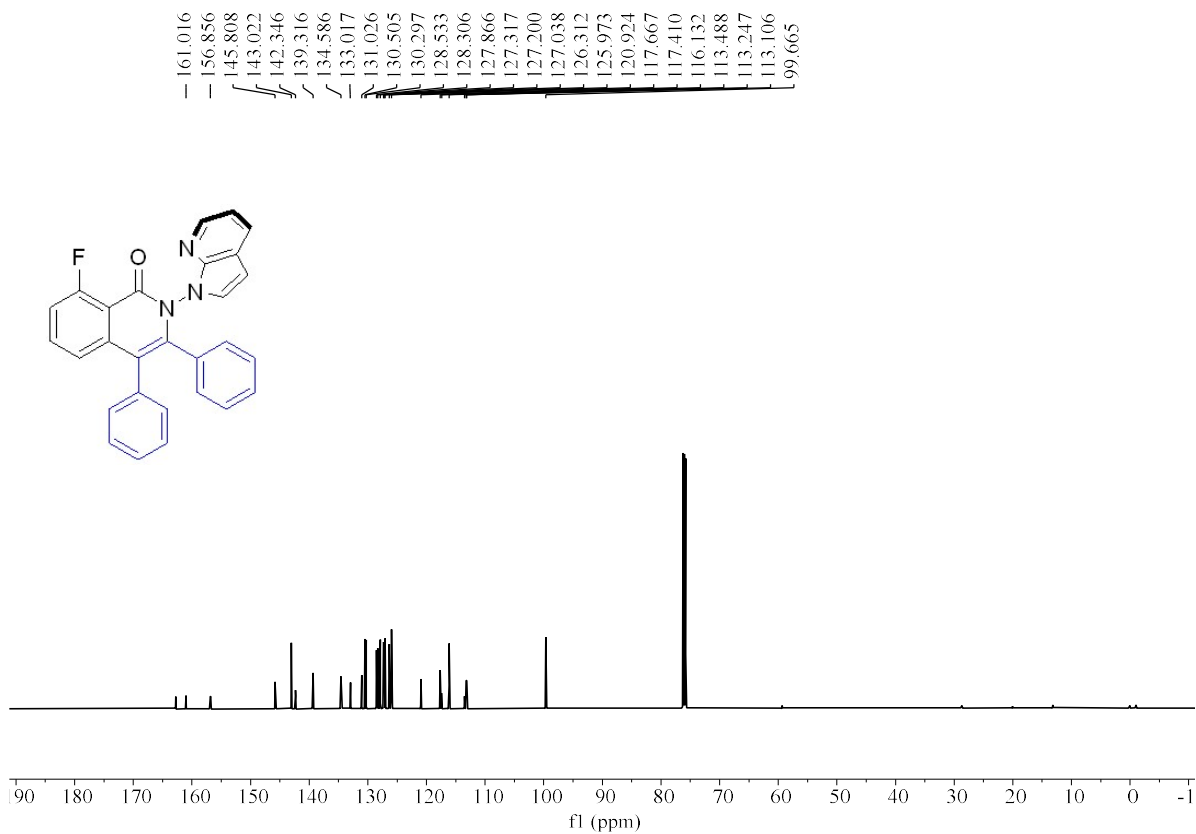
¹H NMR (600 MHz, CDCl₃) spectrum of 28.



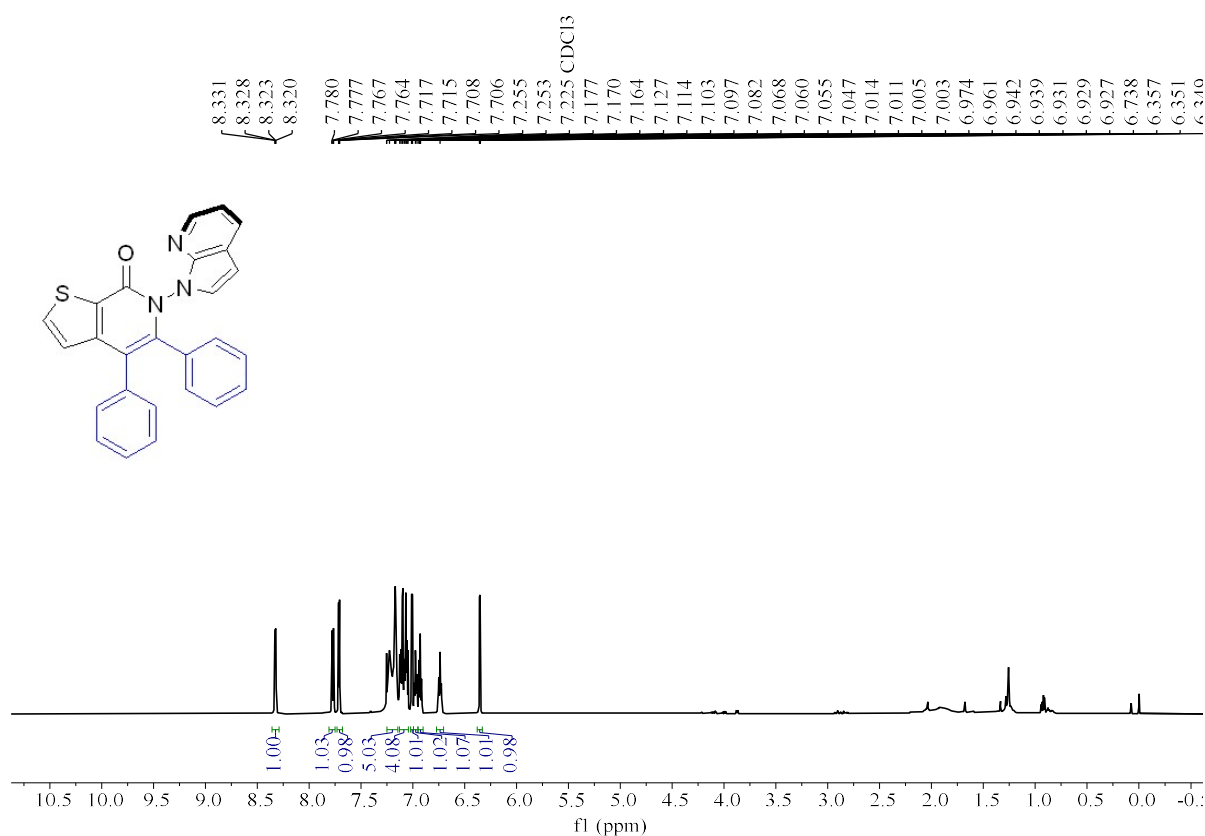
¹³C NMR (150 MHz, CDCl₃) spectrum of 28.



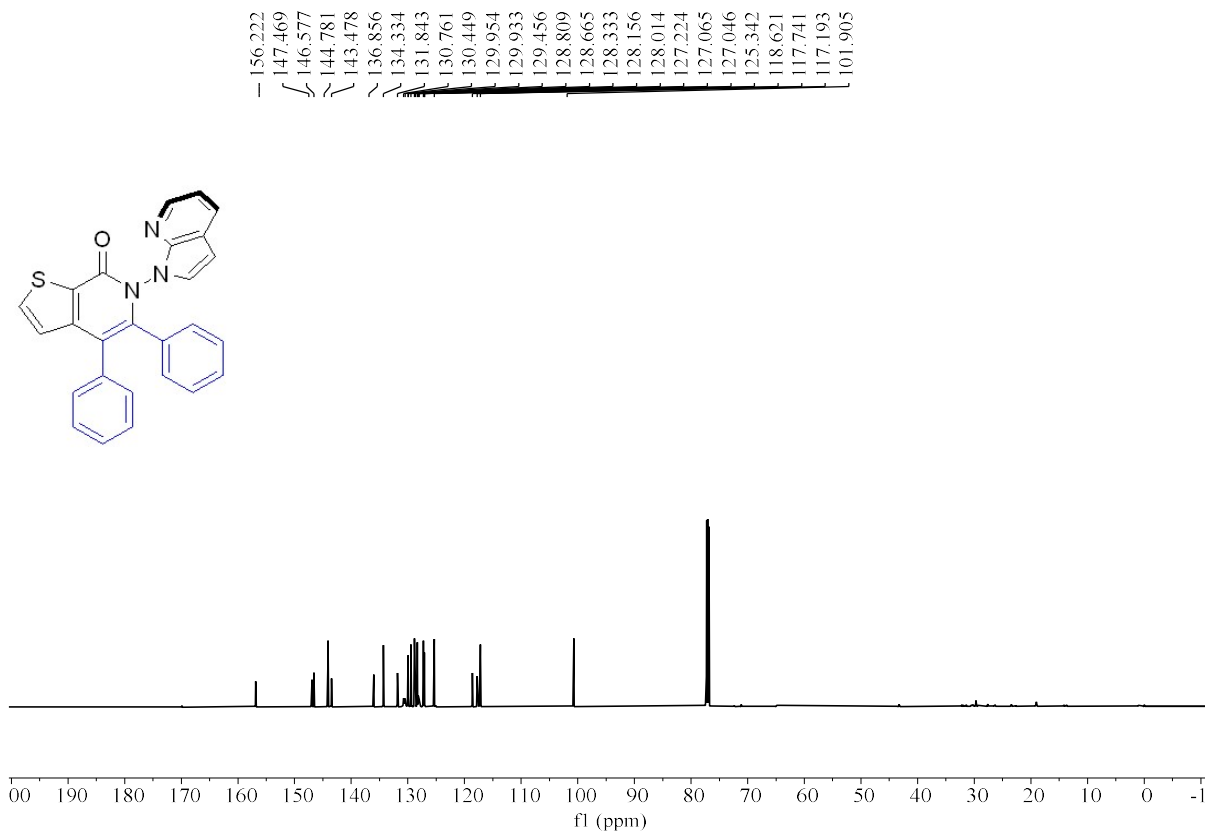
¹H NMR (600 MHz, CDCl₃) spectrum of 29.



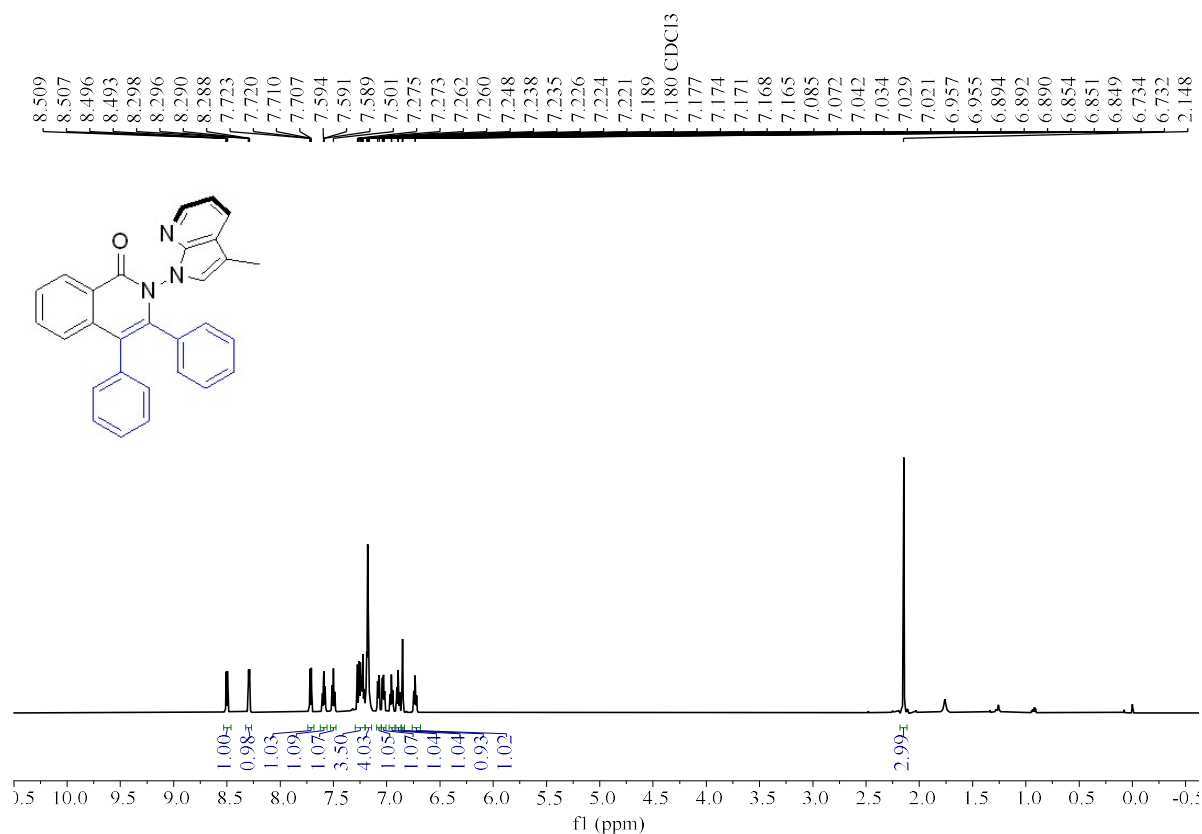
¹³C NMR (150 MHz, CDCl₃) spectrum of 29.



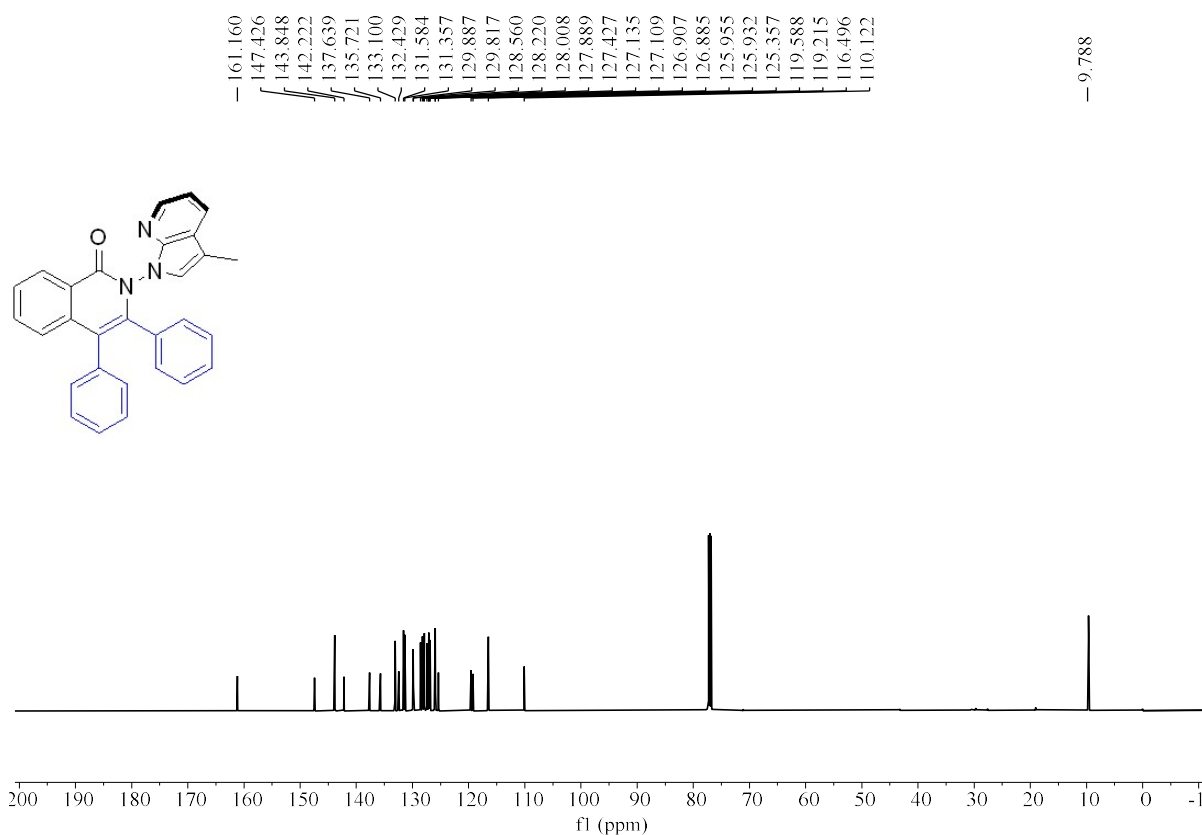
¹H NMR (600 MHz, CDCl₃) spectrum of 30.



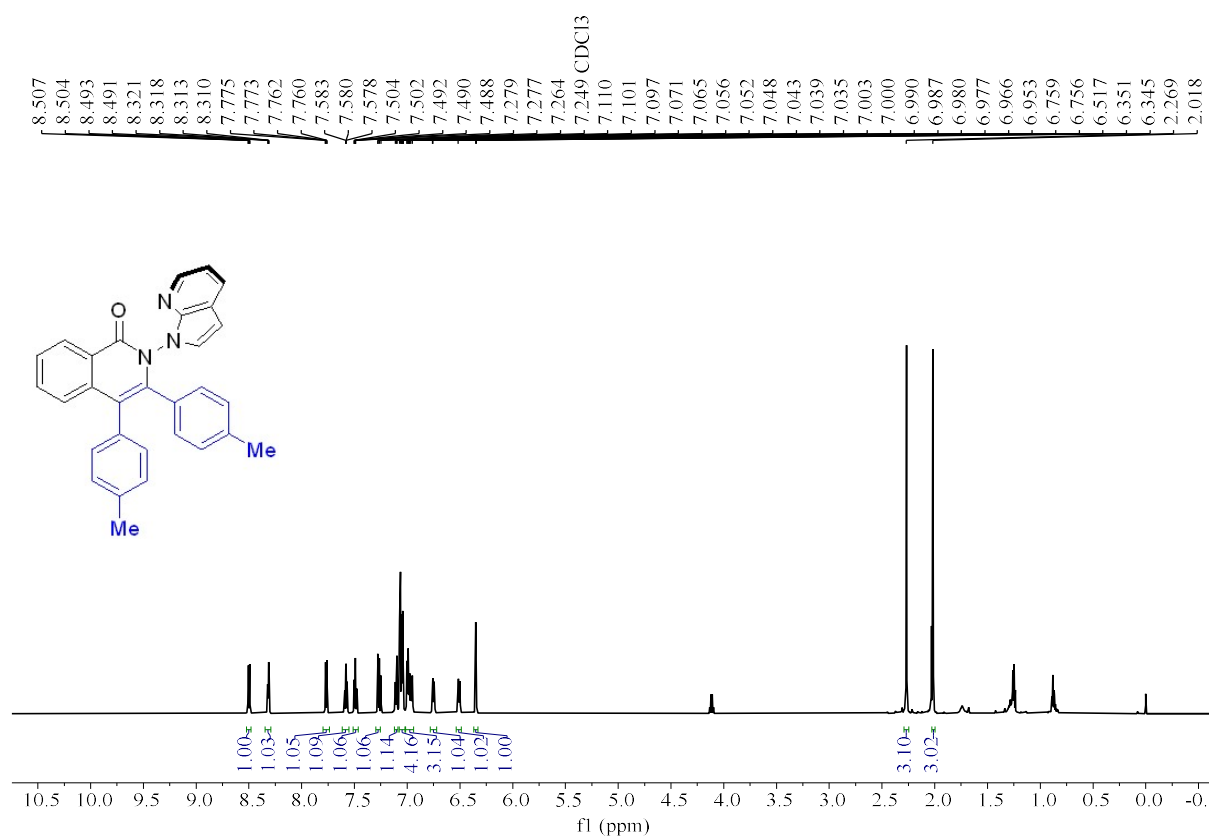
¹³C NMR (150 MHz, CDCl₃) spectrum of 30.



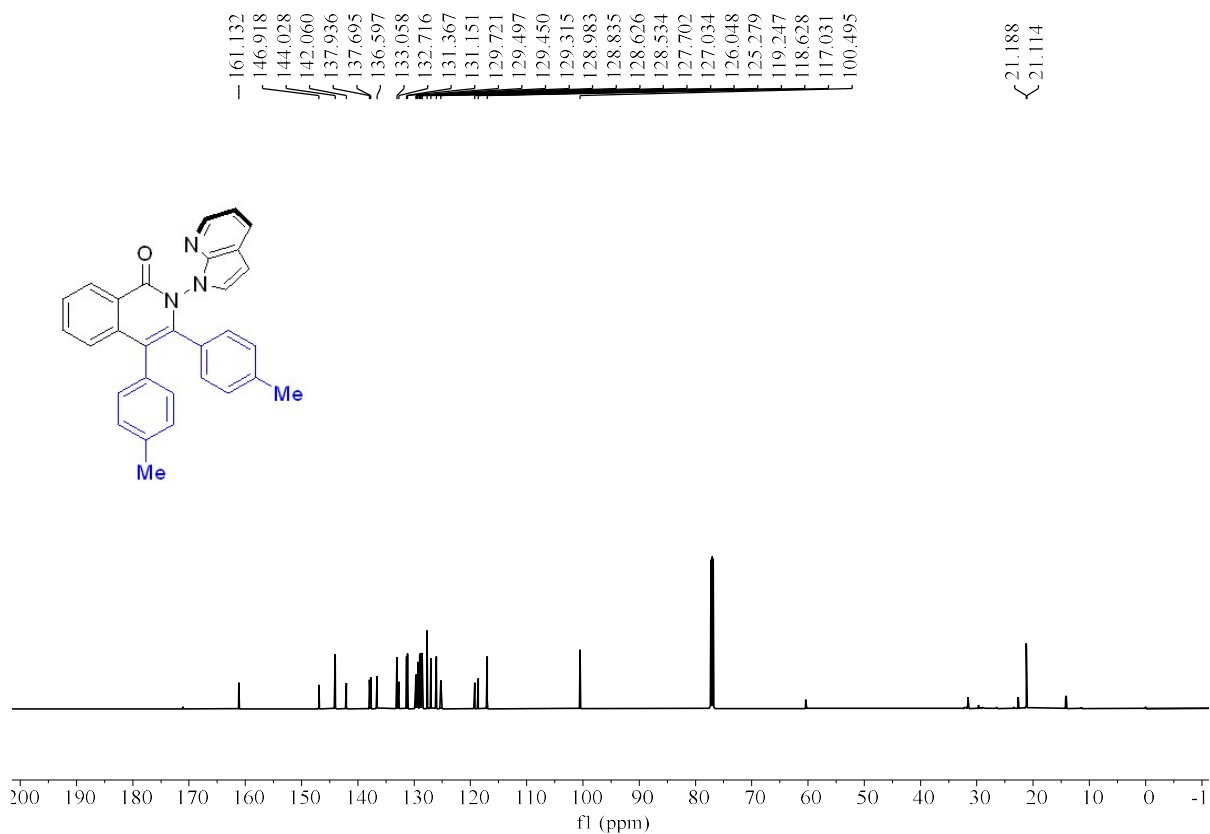
¹H NMR (600 MHz, CDCl₃) spectrum of 31.



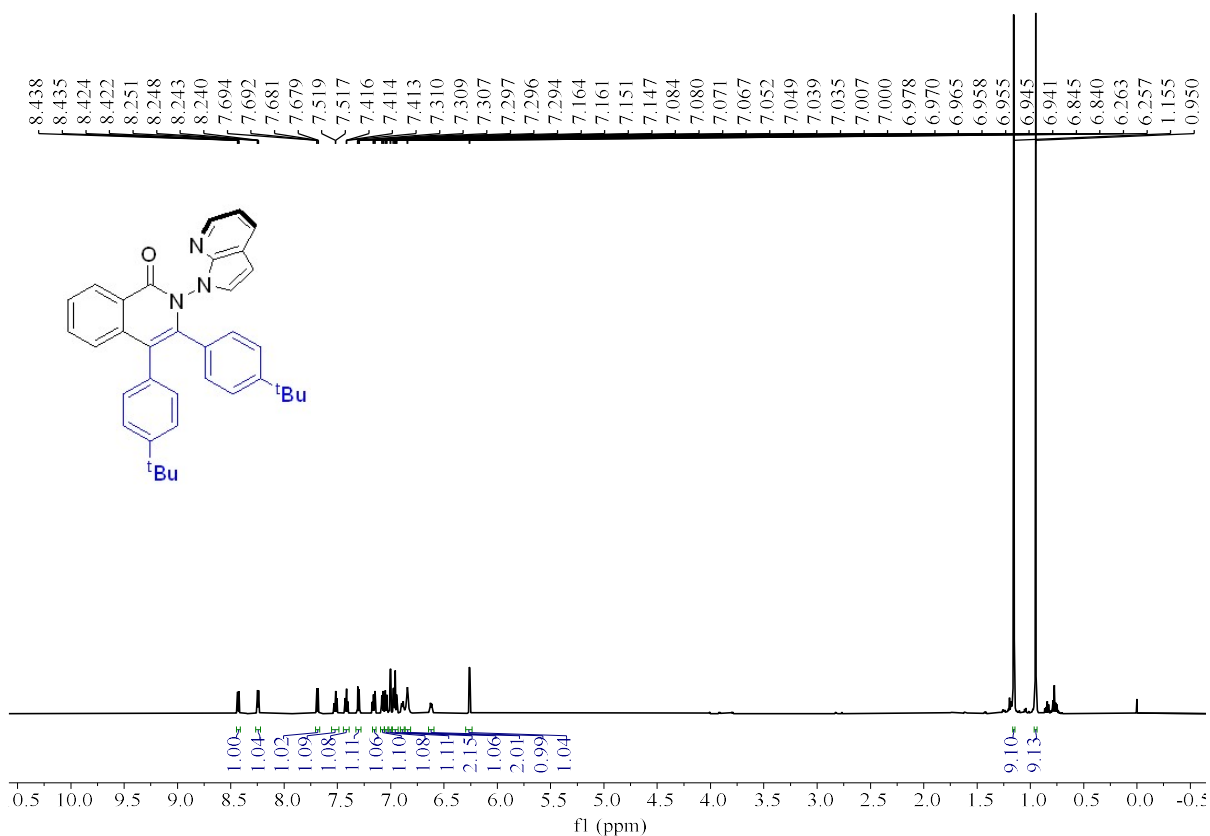
¹³C NMR (150 MHz, CDCl₃) spectrum of 31.



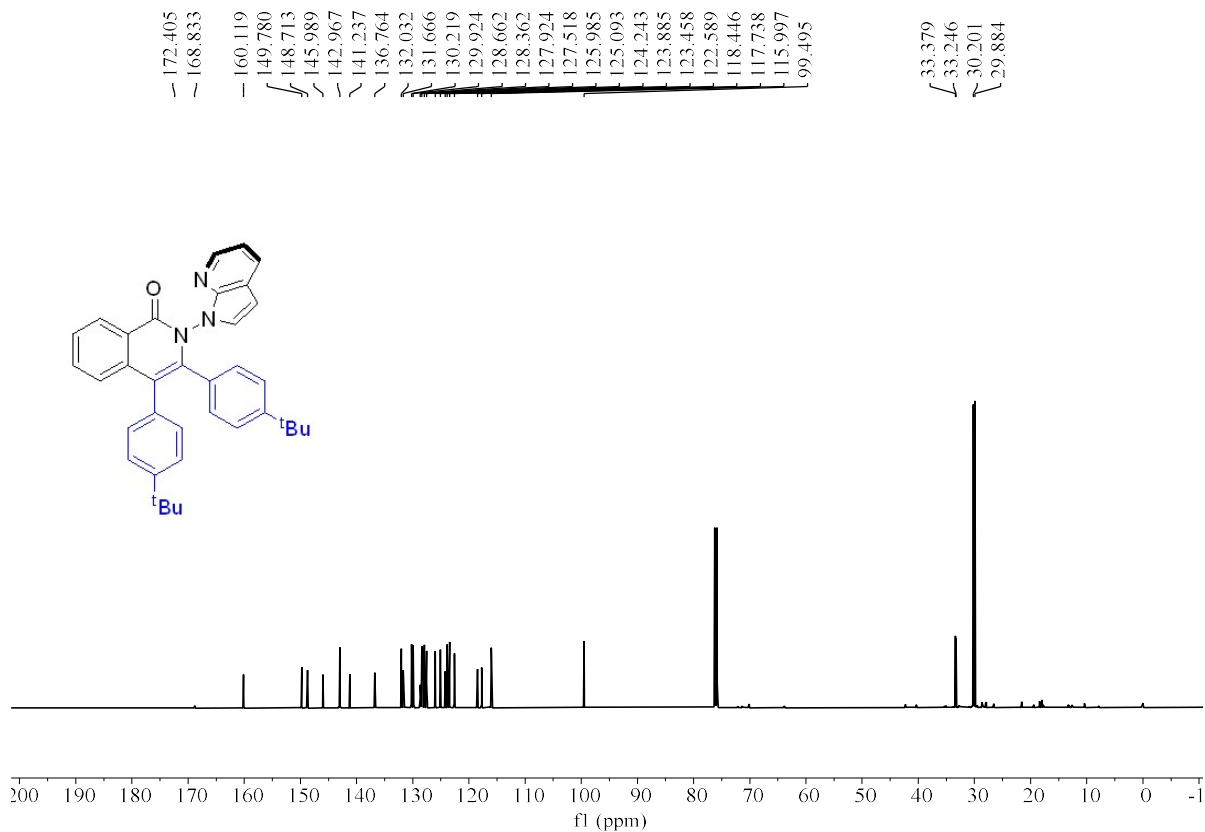
¹H NMR (600 MHz, CDCl₃) spectrum of 32.



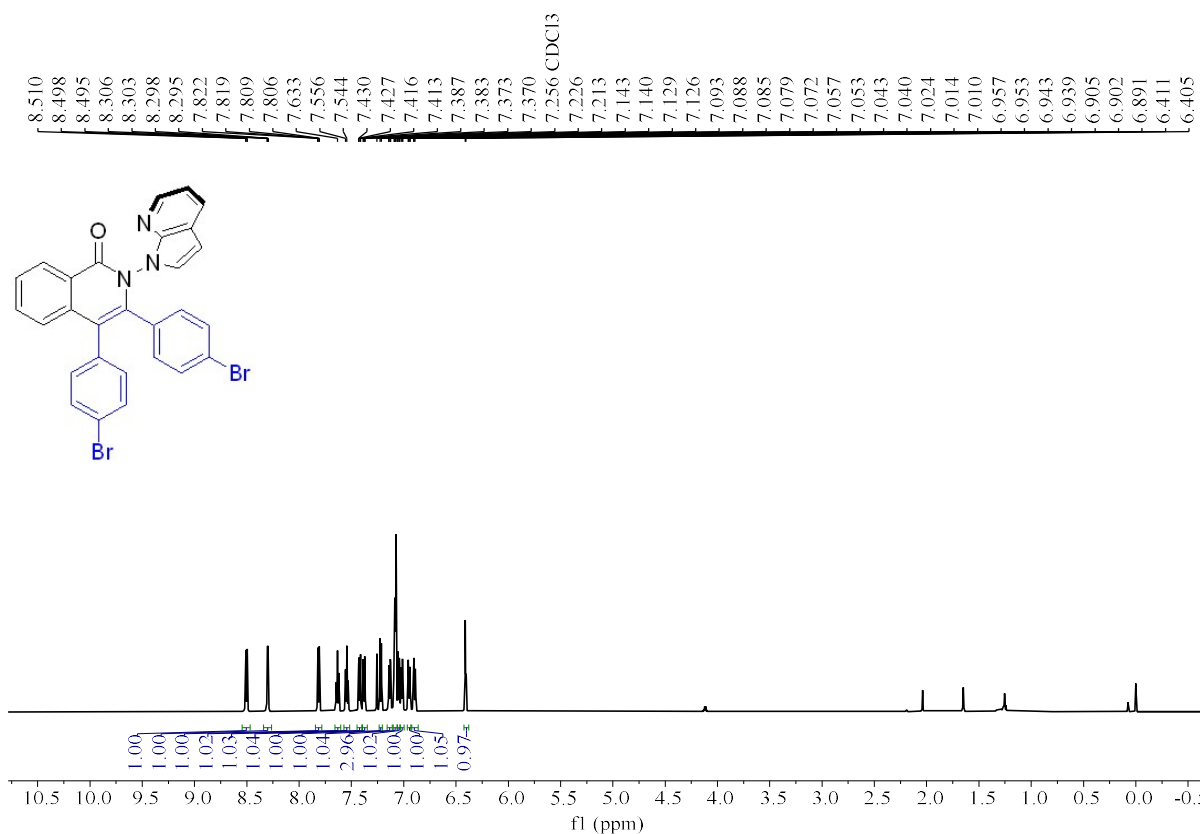
¹³C NMR (150 MHz, CDCl₃) spectrum of 32.



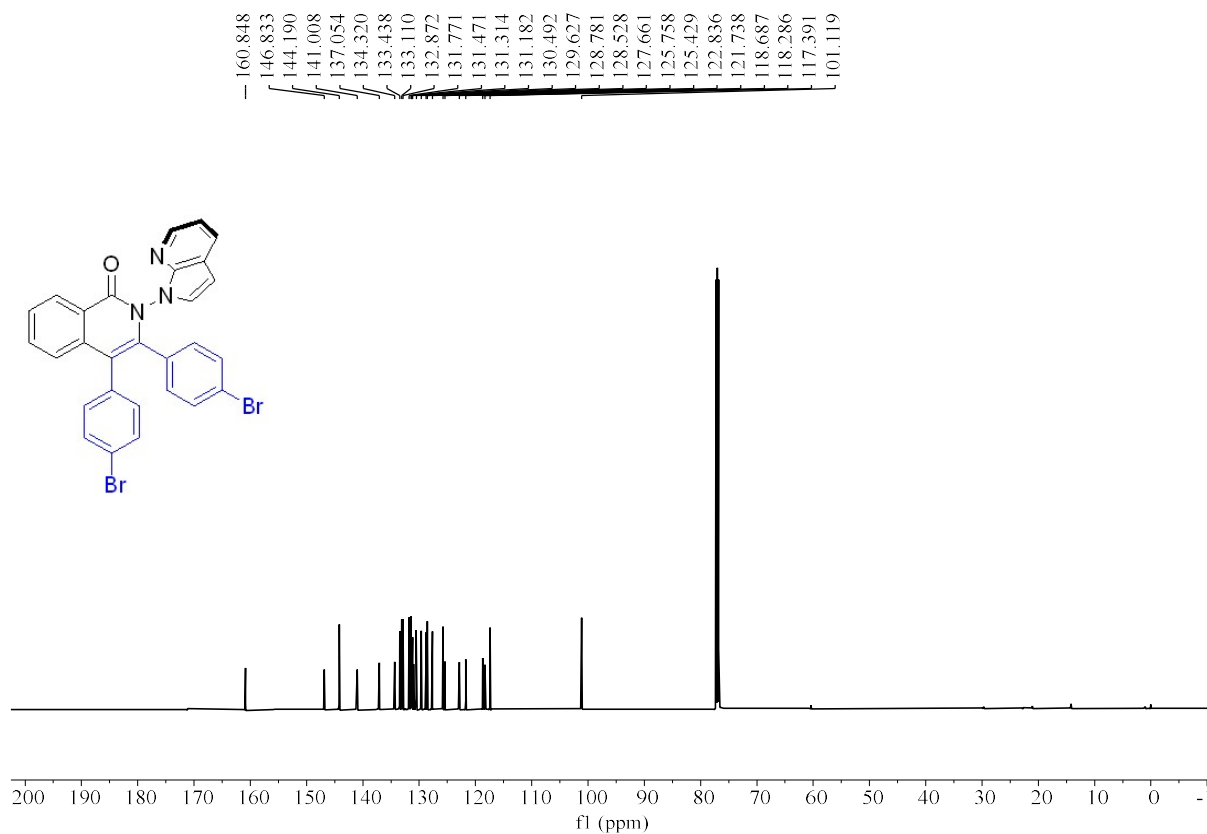
¹H NMR (600 MHz, CDCl₃) spectrum of 33.



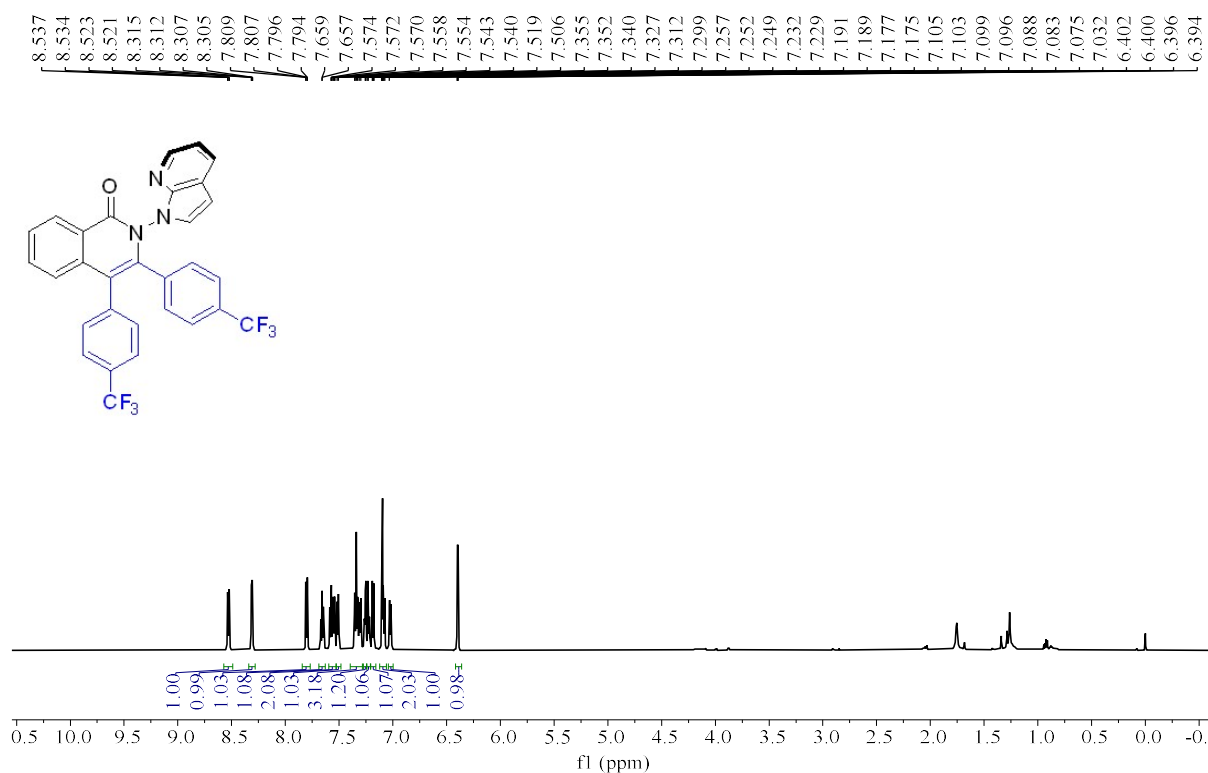
¹³C NMR (150 MHz, CDCl₃) spectrum of 33.



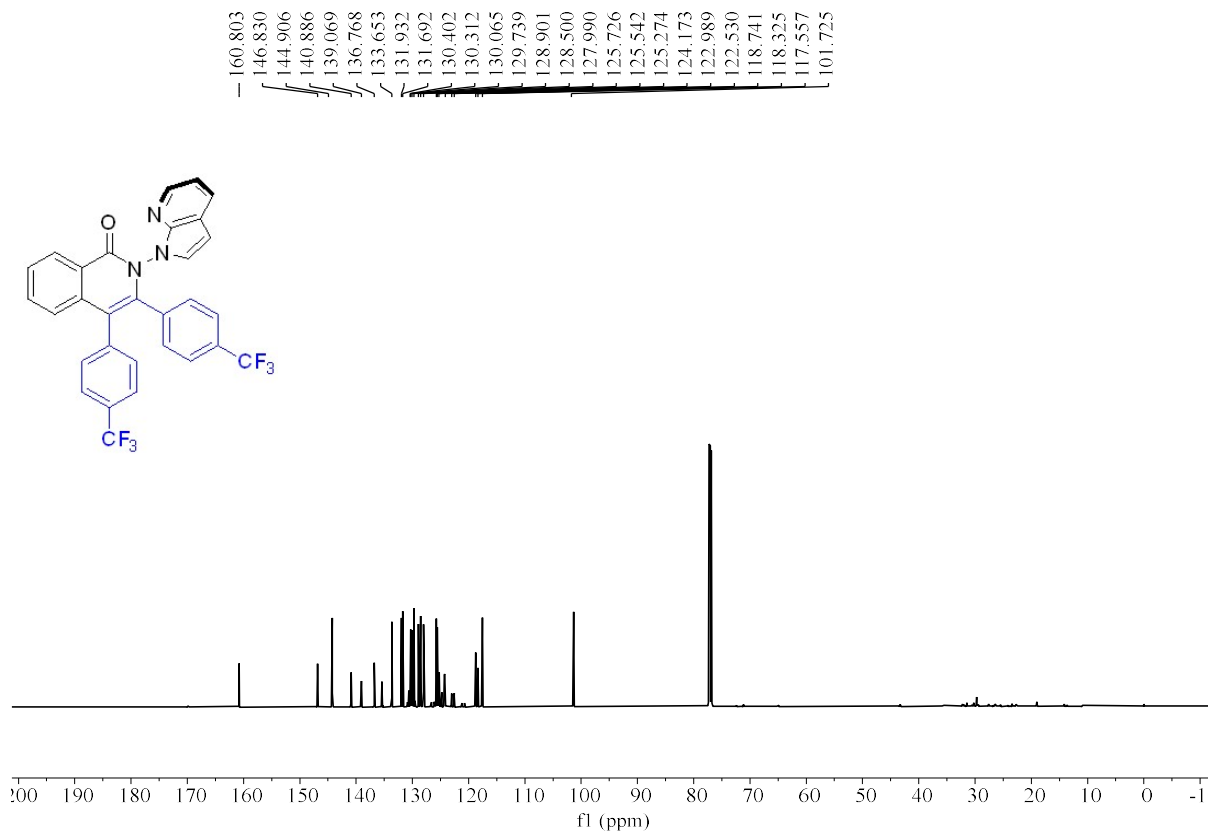
¹H NMR (600 MHz, CDCl₃) spectrum of 34.



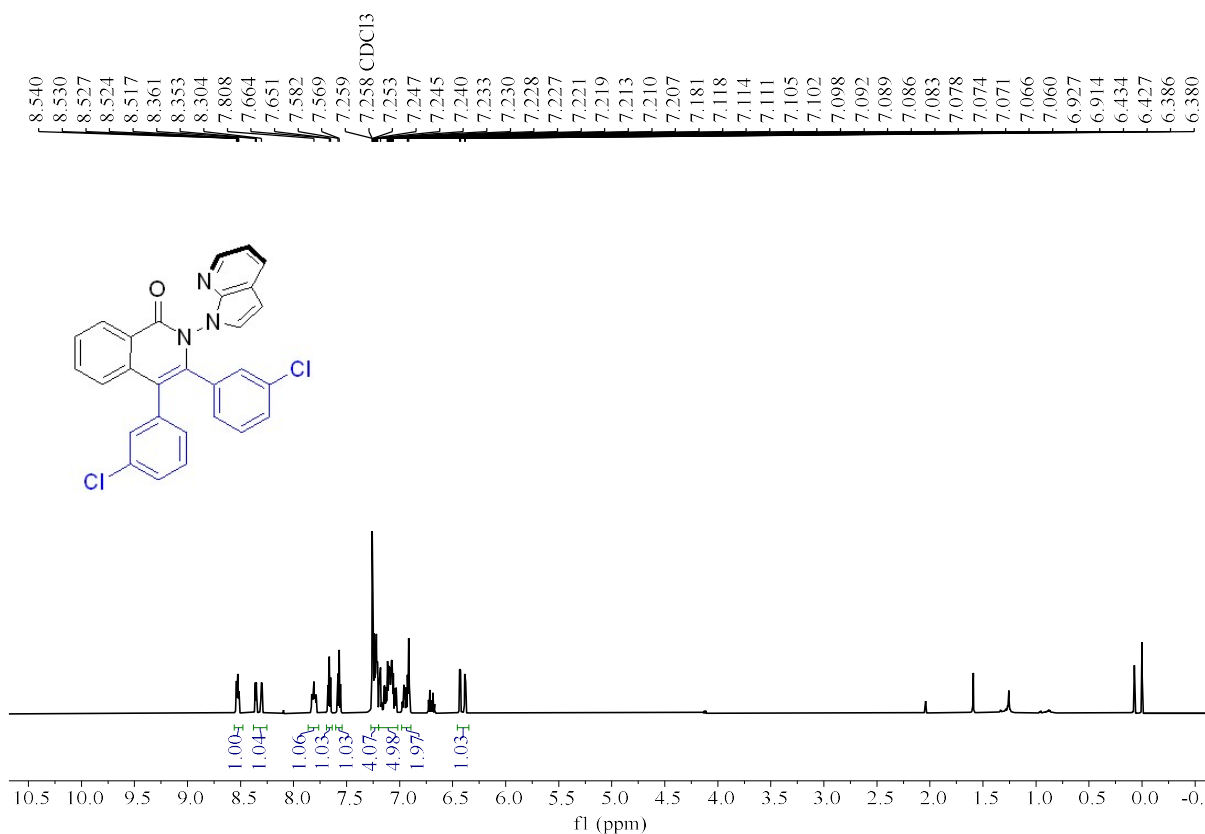
¹³C NMR (150 MHz, CDCl₃) spectrum of 34.



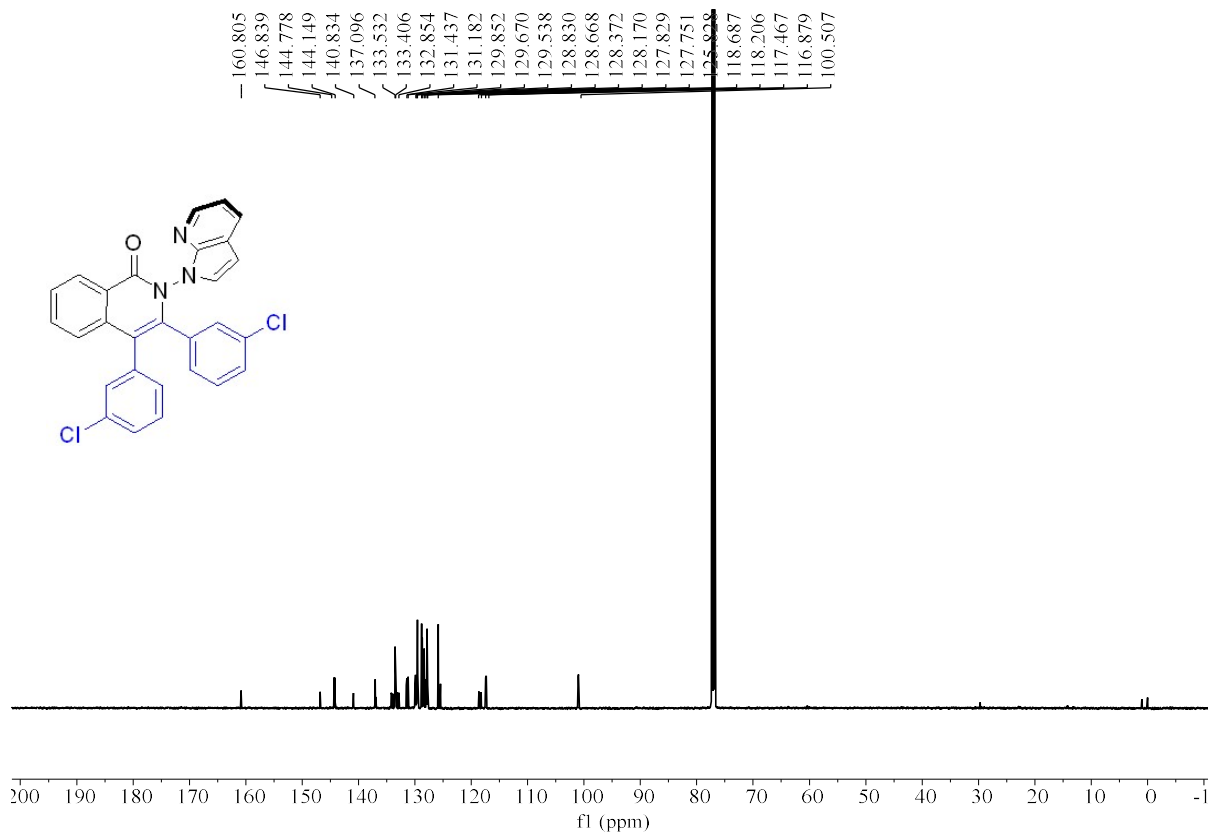
¹H NMR (600 MHz, CDCl₃) spectrum of 35.



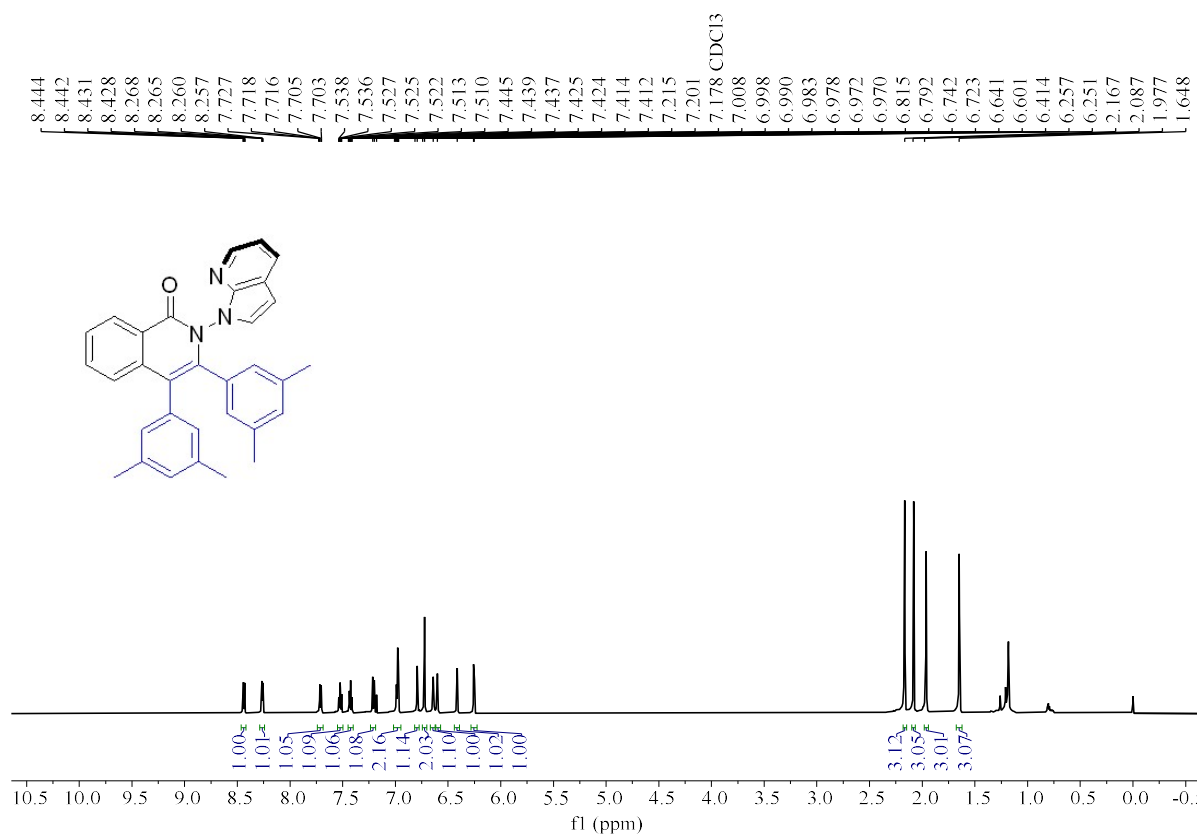
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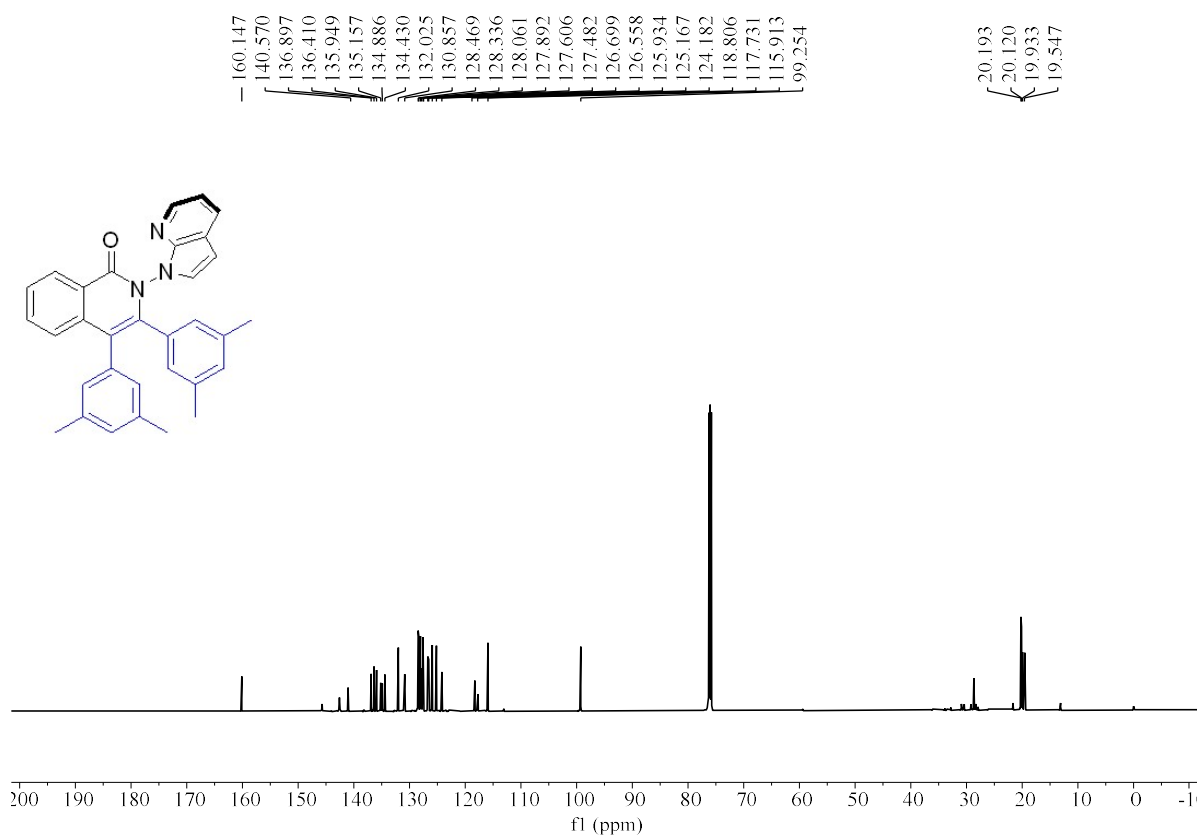
¹H NMR (600 MHz, CDCl₃) spectrum of 36.



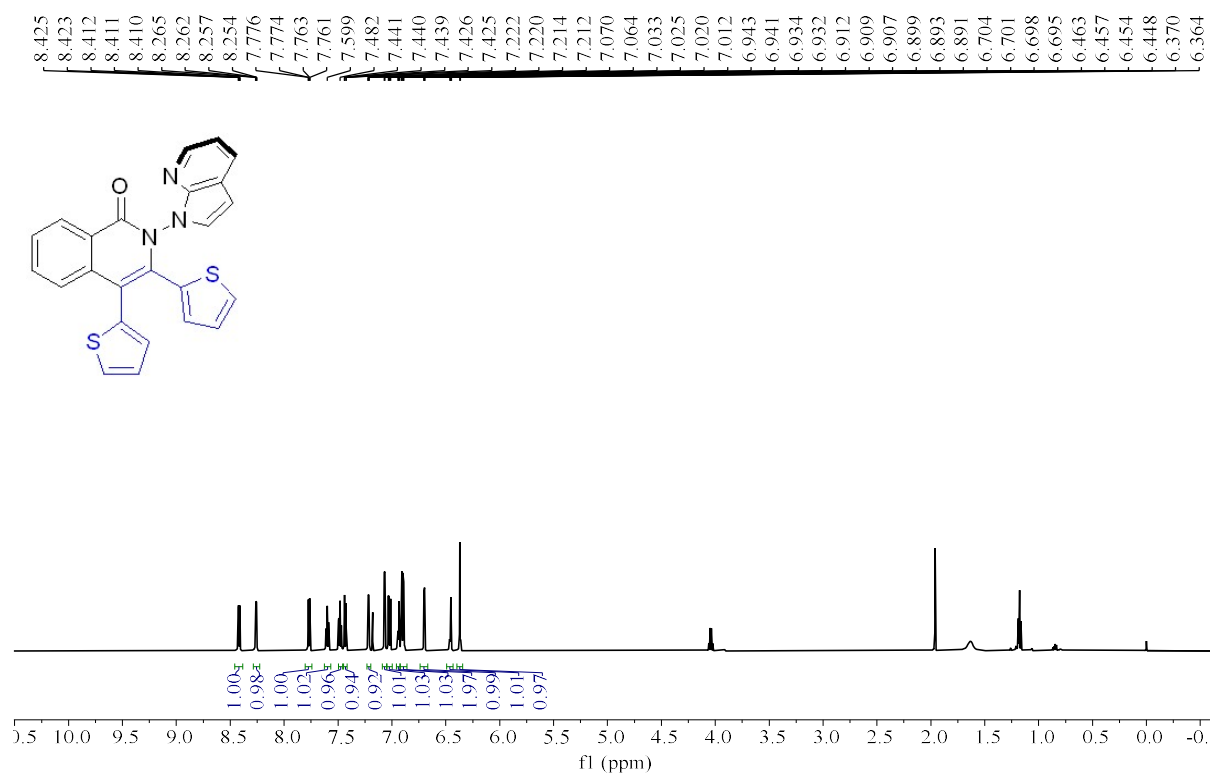
¹³C NMR (150 MHz, CDCl₃) spectrum of 36.



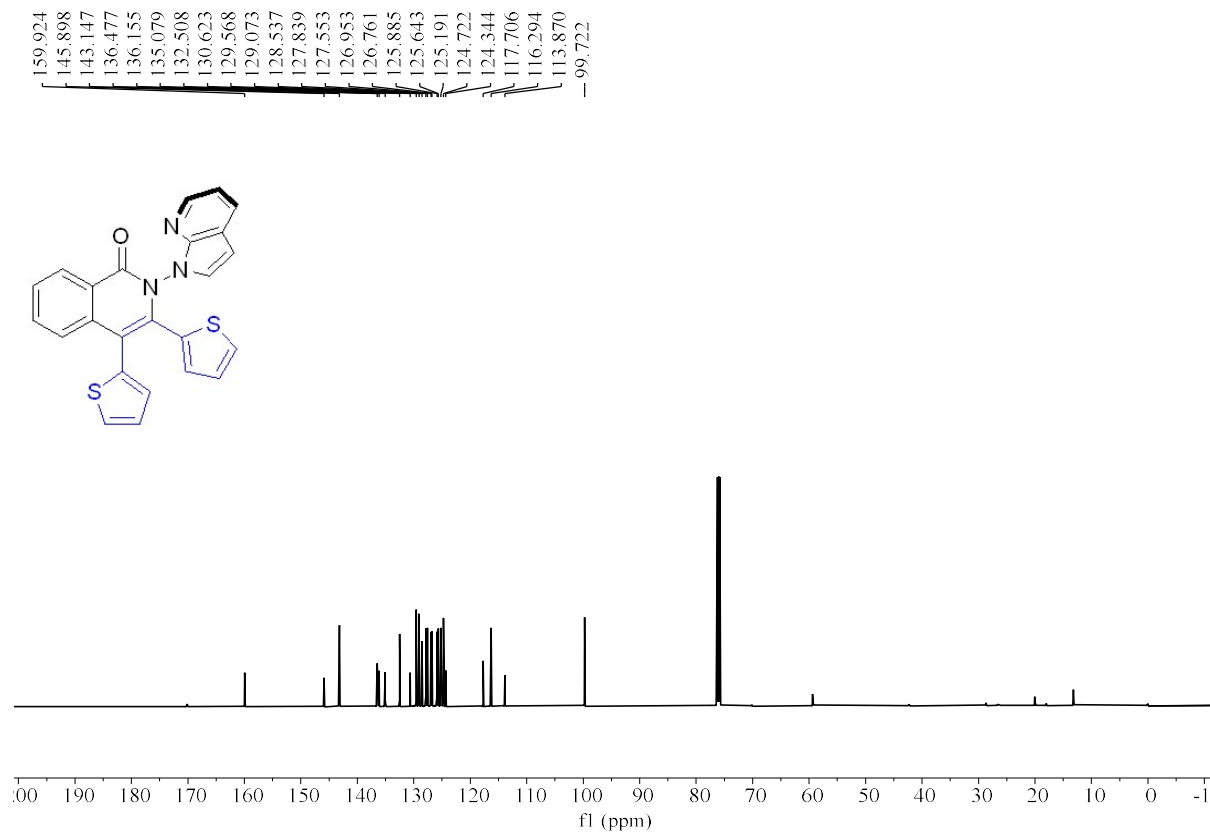
¹H NMR (600 MHz, CDCl₃) spectrum of 37.



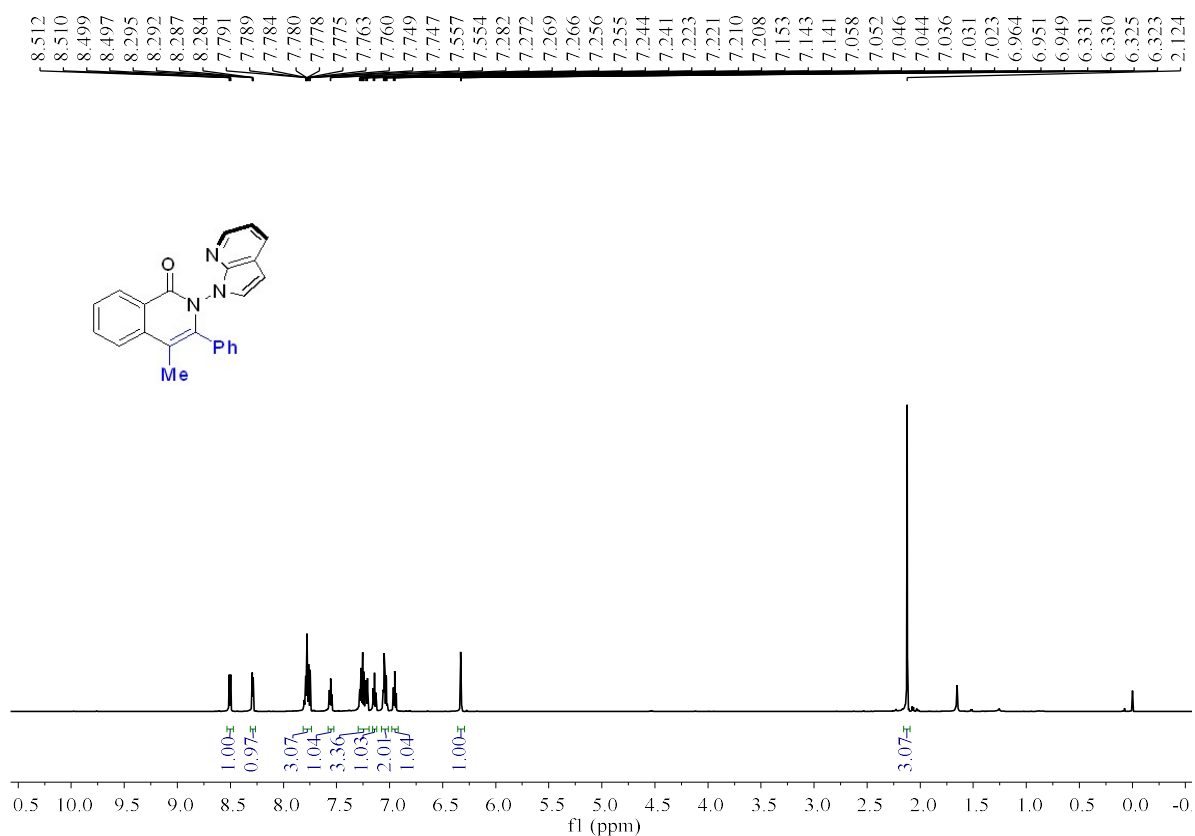
¹³C NMR (150 MHz, CDCl₃) spectrum of 37.



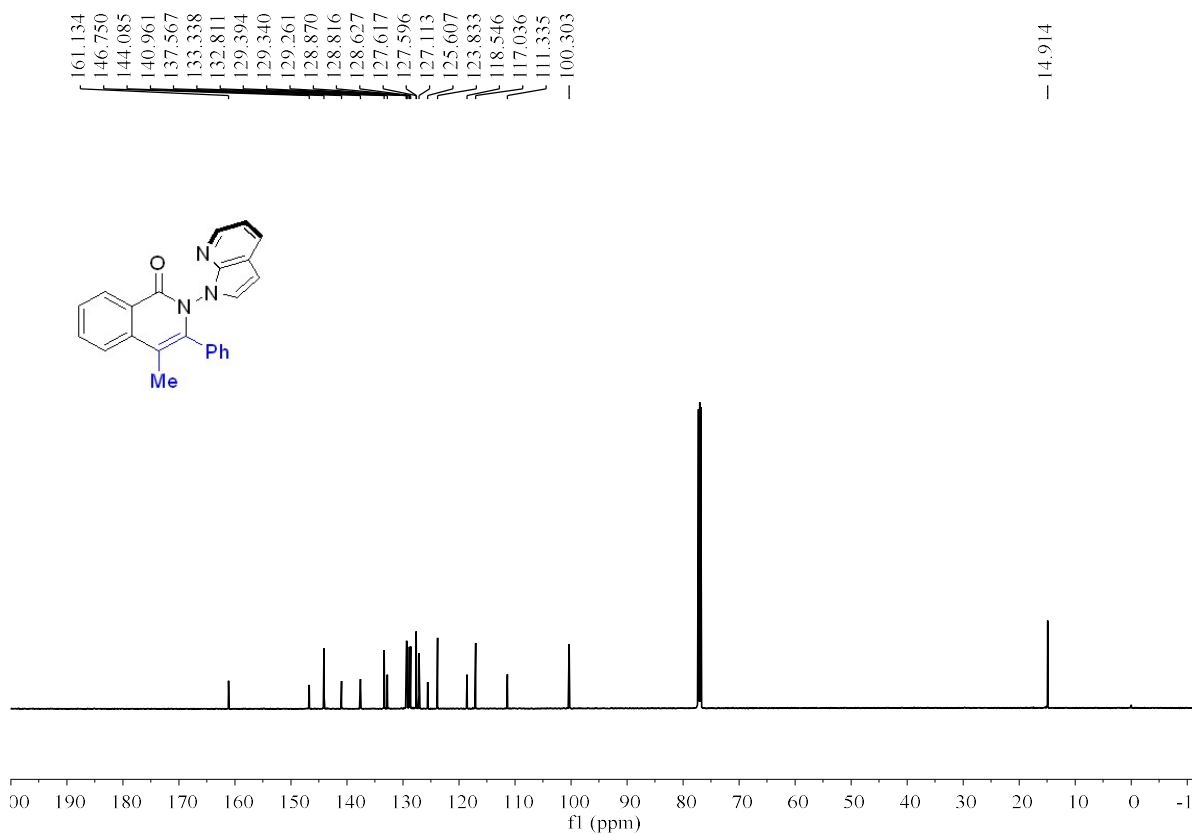
¹H NMR (600 MHz, CDCl₃) spectrum of 38.



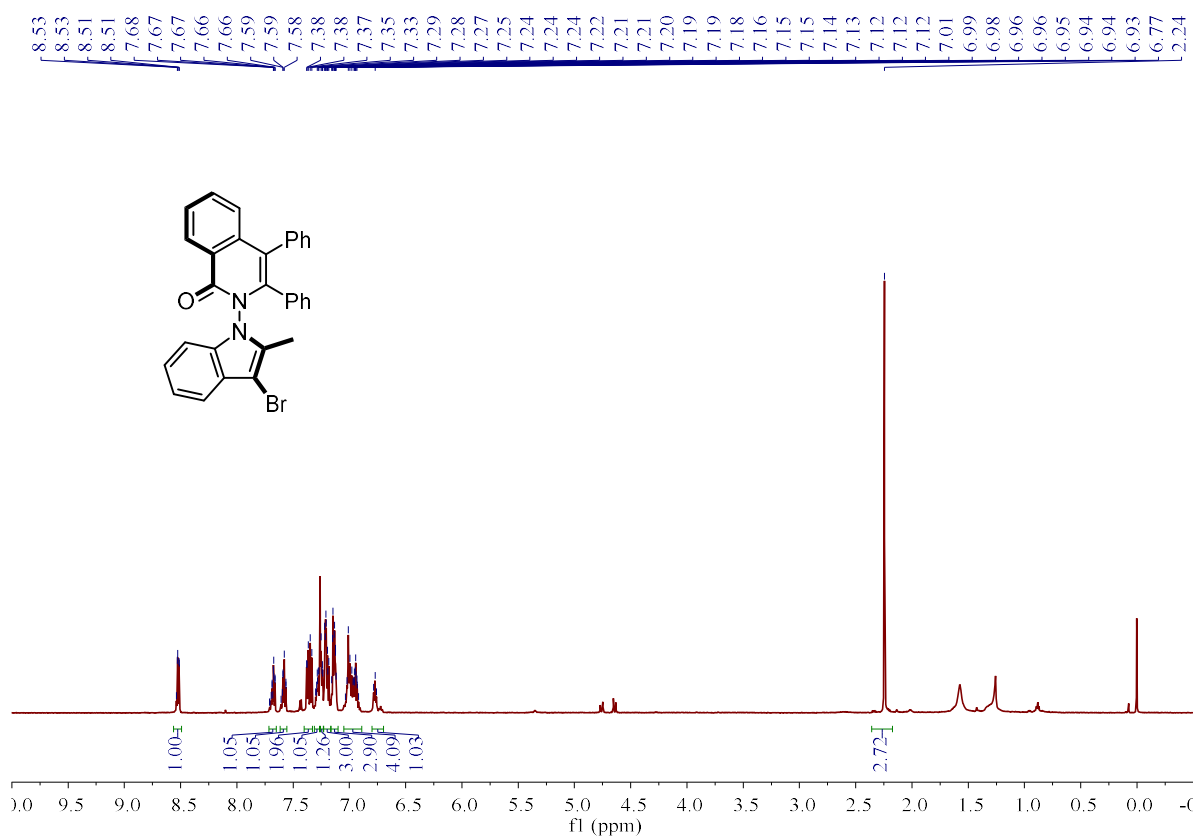
¹³C NMR (150 MHz, CDCl₃) spectrum of 38.



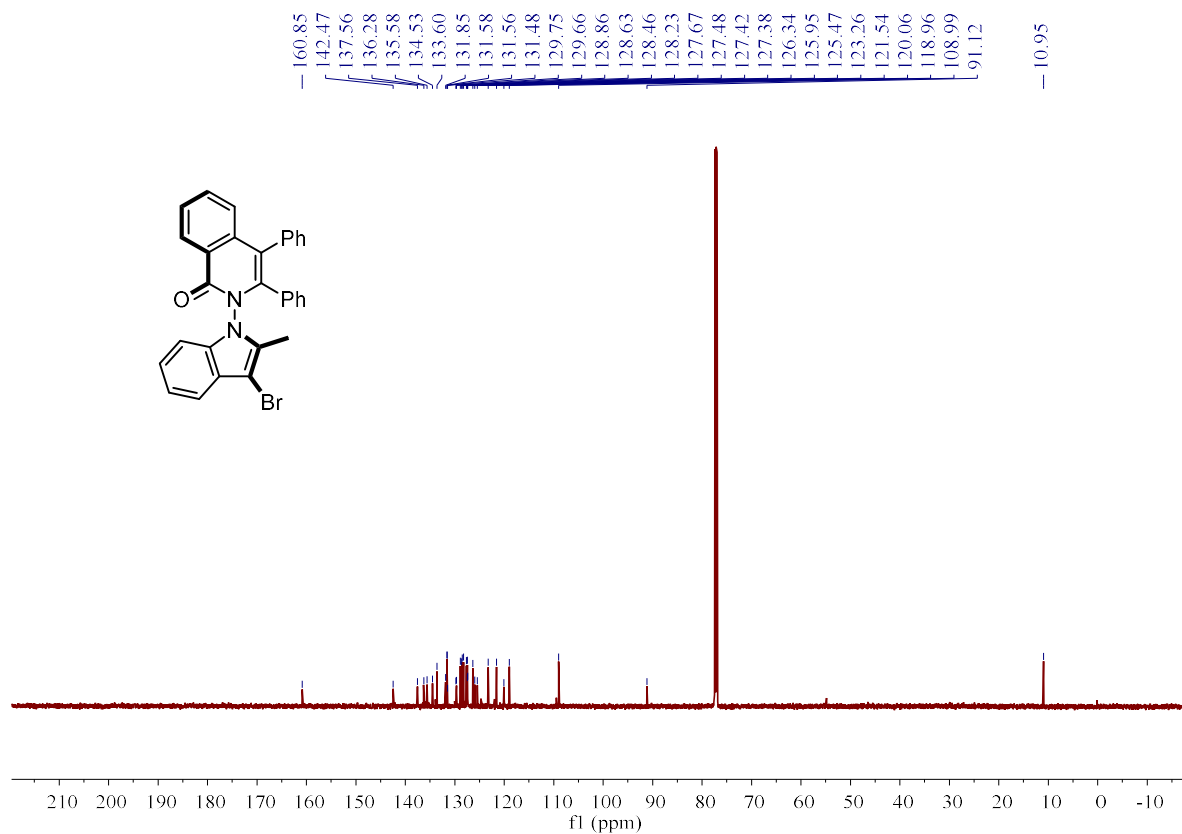
¹H NMR (600 MHz, CDCl₃) spectrum of 39.



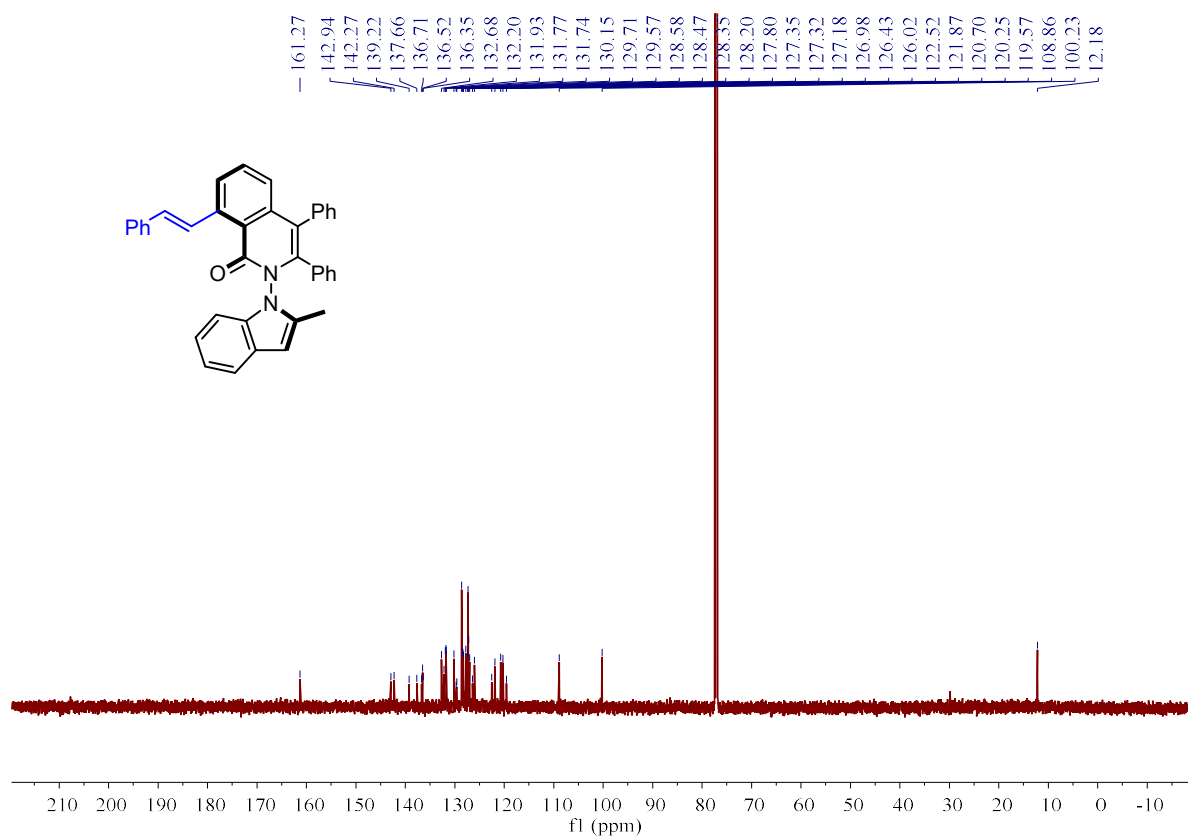
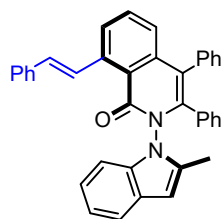
¹³C NMR (150 MHz, CDCl₃) spectrum of 39.

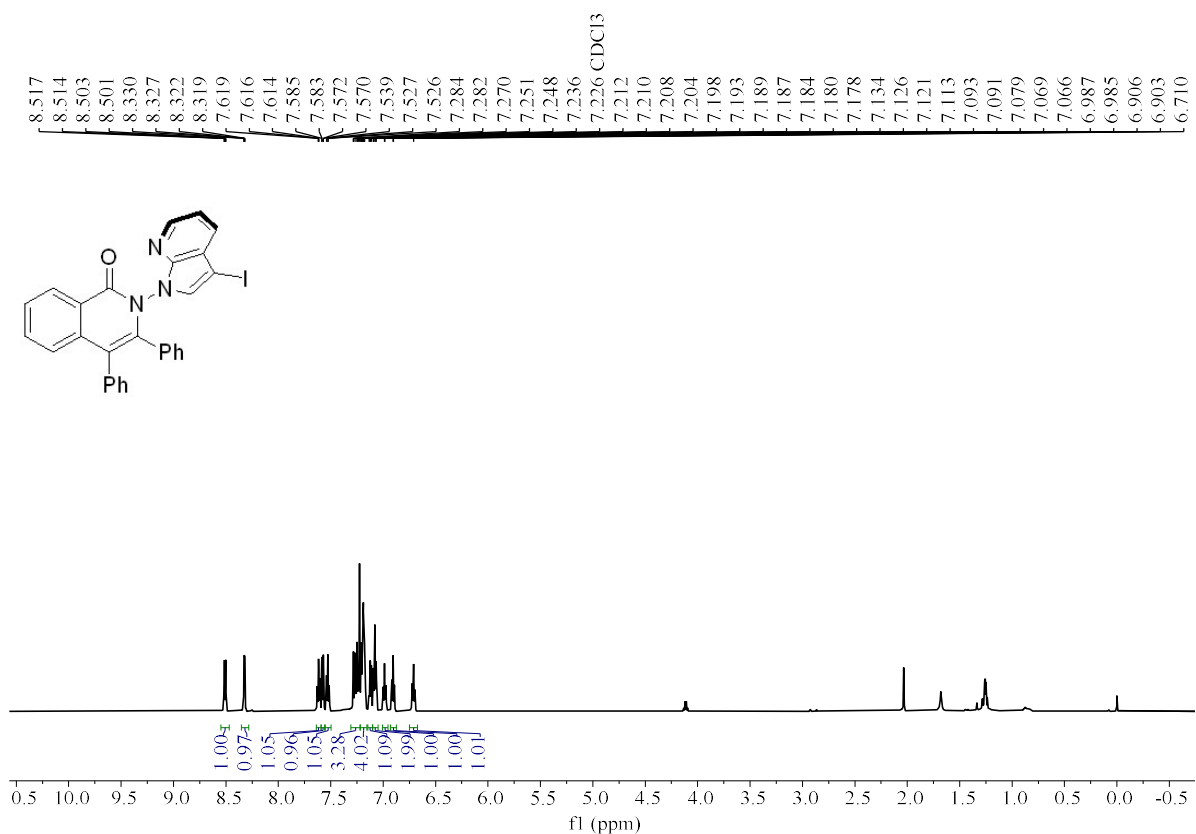


¹H NMR (600 MHz, CDCl₃) spectrum of 40.

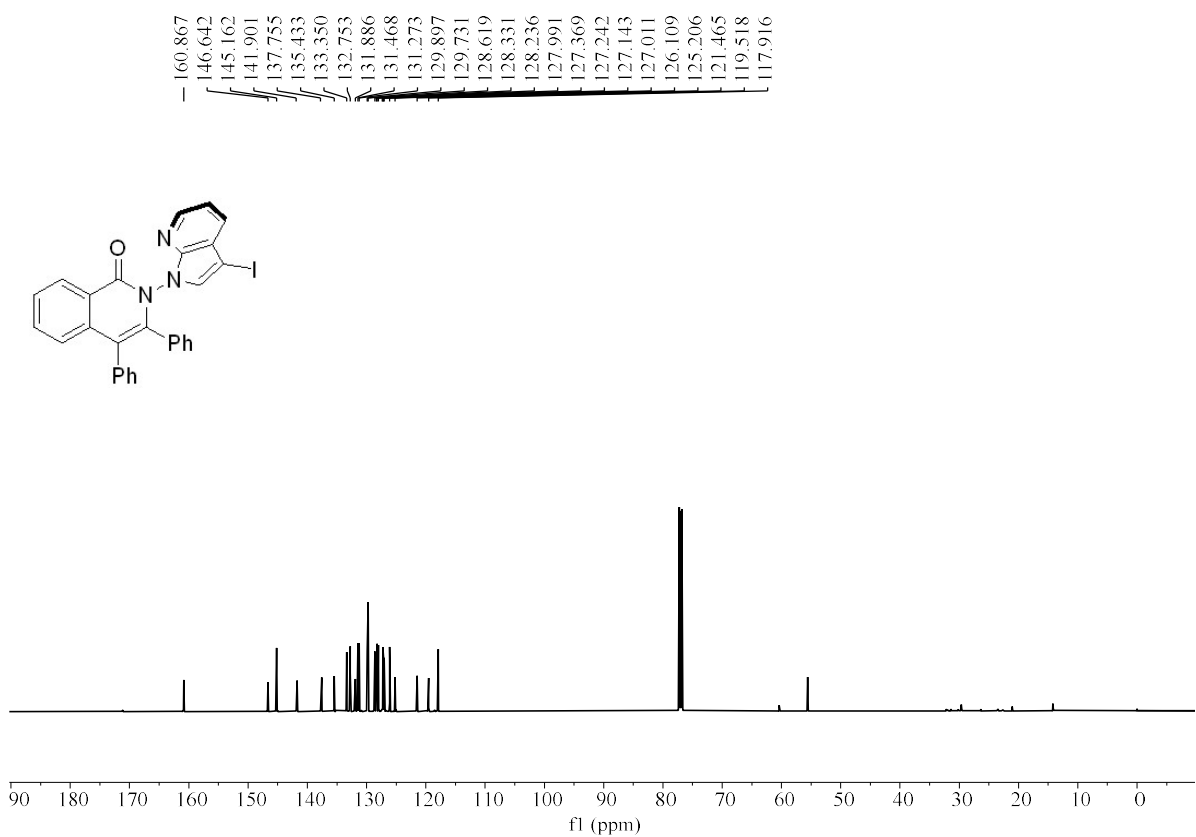


¹³C NMR (150 MHz, CDCl₃) spectrum of 40.

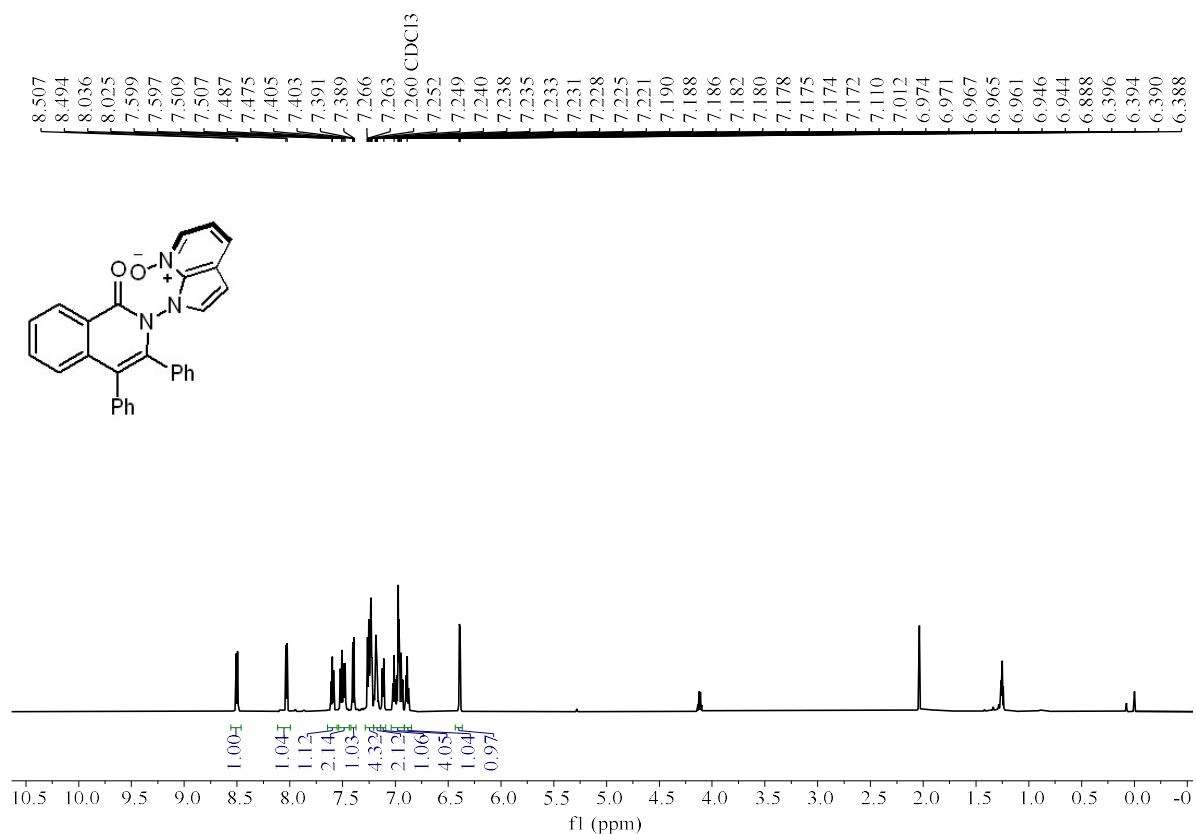




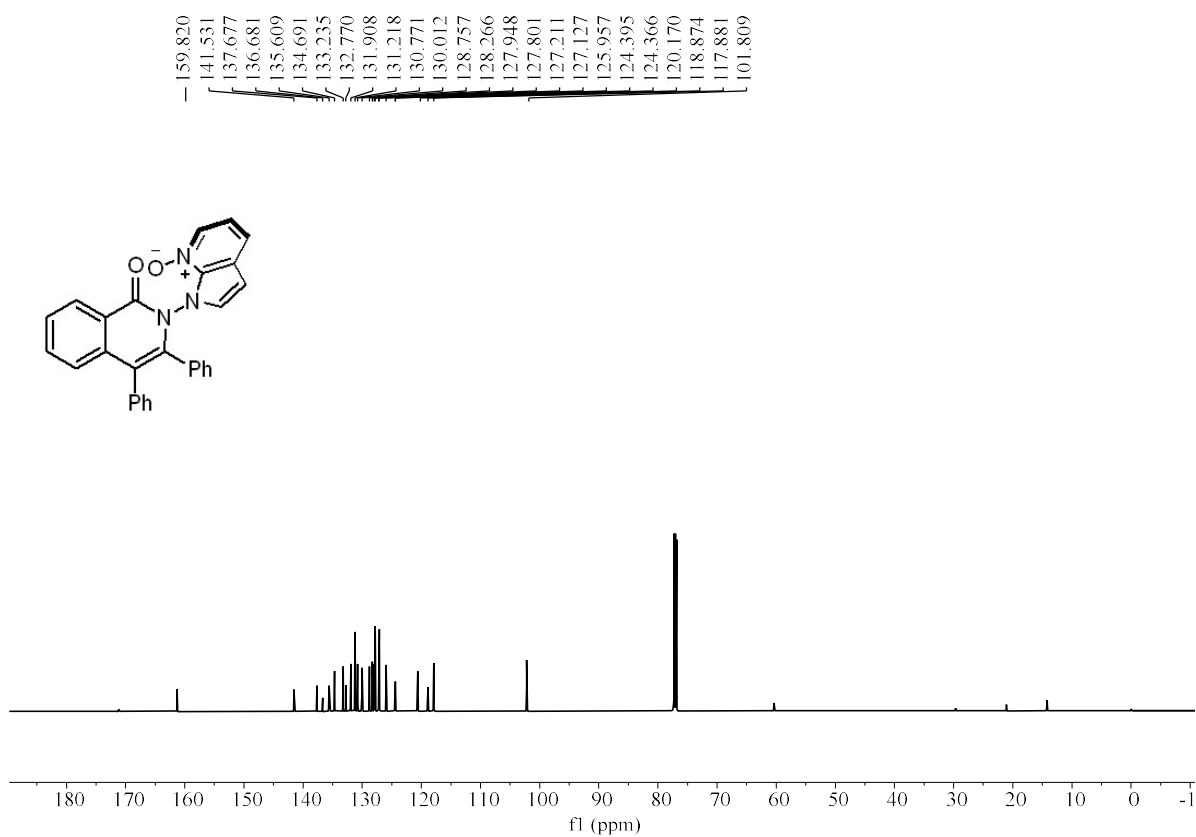
¹H NMR (600 MHz, CDCl₃) spectrum of 42.



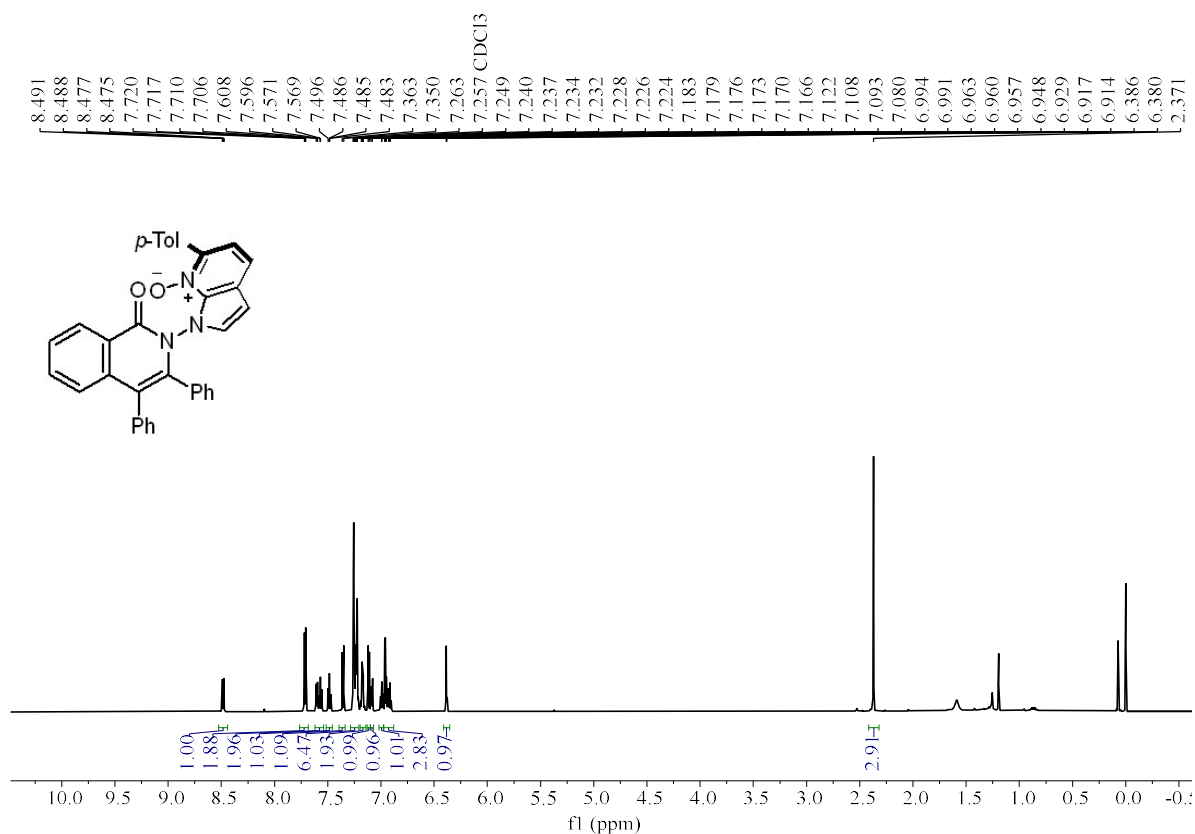
¹³C NMR (150 MHz, CDCl₃) spectrum of 42.

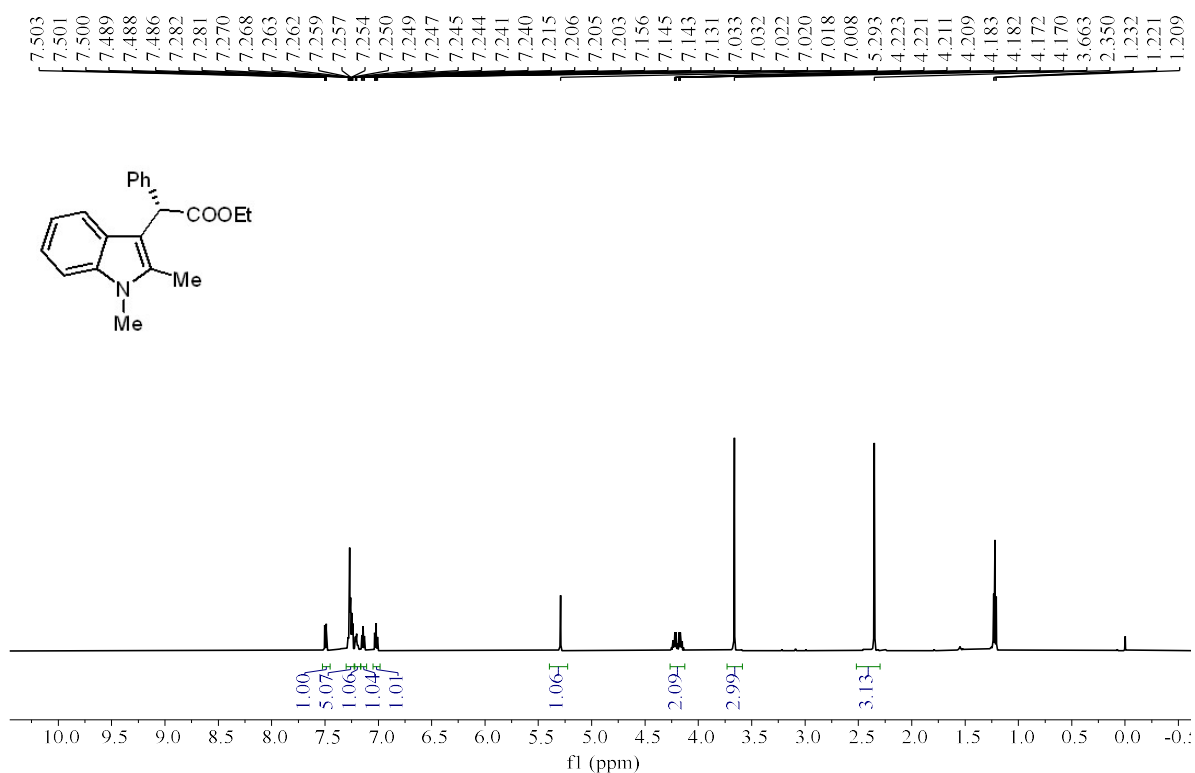


¹H NMR (600 MHz, CDCl₃) spectrum of 43.

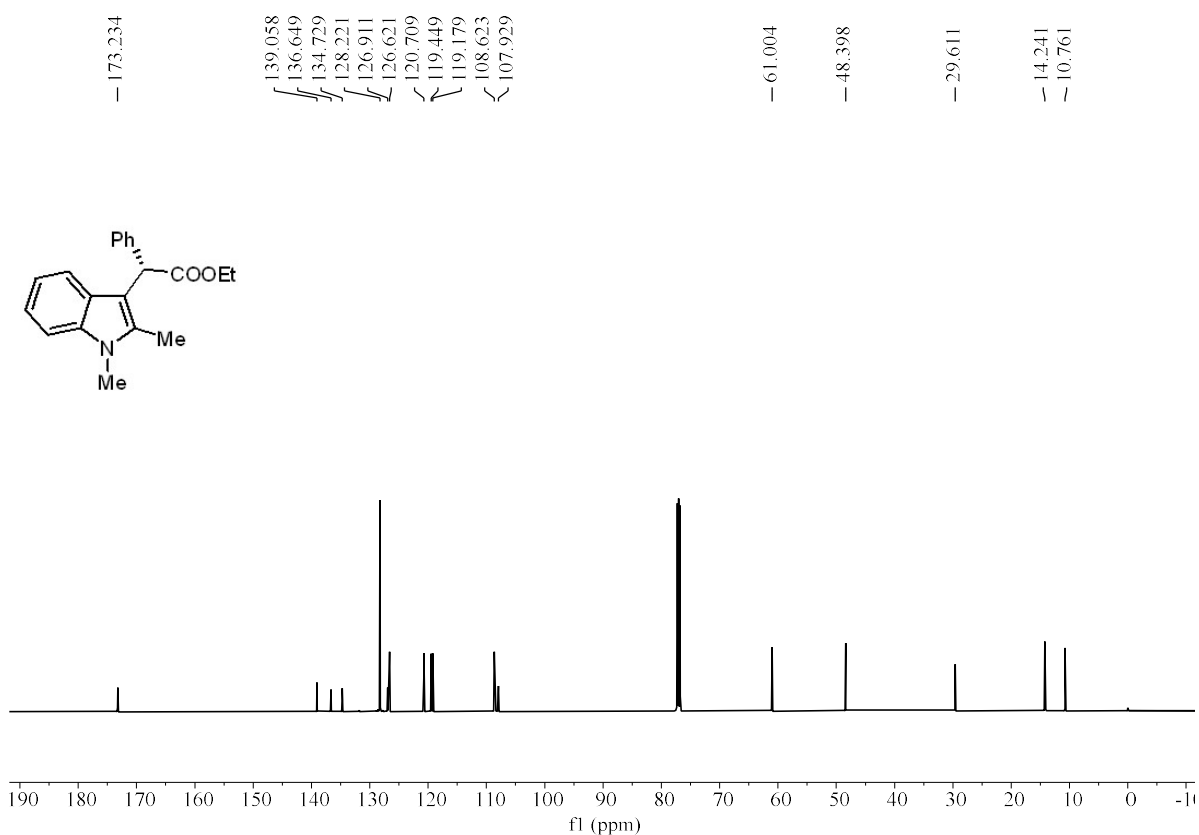


¹³C NMR (150 MHz, CDCl₃) spectrum of 43.





¹H NMR (600 MHz, CDCl₃) spectrum of 45.



¹³C NMR (150 MHz, CDCl₃) spectrum of 45.