

Experimental and Computational Studies on the Palladium-catalyzed Intramolecular Dearomatization, Electrophilic Addition, Intermolecular Coupling Sequence

Qing-Hui Liu,[†] Yue Ma,[†] Hong-Yu Zhang,[†] Yuecheng Zhang,^{*,†} Jiquan Zhao,[†]
Xiaohui Cao,^{*,‡} Ya-Ping Han,^{*,†} and Yong-Min Liang[§]

[†]School of Chemical Engineering and Technology, Hebei University of Technology, Tianjin 300130, China.

[‡]School of Pharmacy, Guangdong Pharmaceutical University, Guangzhou 510006, China

[§]State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, China

Supporting Information

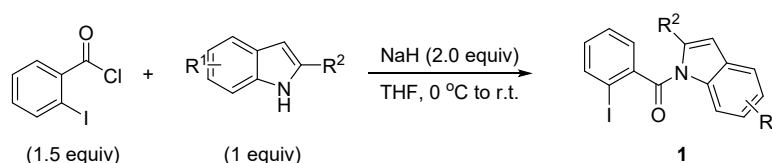
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1. General methods and materials

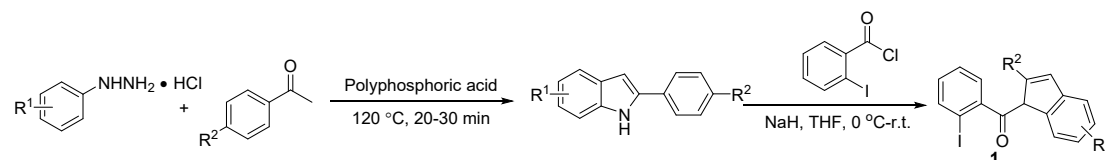
All reactions involving air- and moisture-sensitive reagents were carried out under an argon atmosphere. ^1H and ^{13}C NMR spectra were recorded on a Bruker AC-P 400 spectrometer (400 MHz for ^1H , 100 MHz for ^{13}C) in CDCl_3 (with TMS as internal standard). Chemical shifts (δ) were measured in ppm. Coupling constants, J , are reported in hertz. Mass data were measured with Thermo Scientific DSQ II mass spectrometer and Bruker O-TOF Compact Mass Spectrometry. Melting points (uncorrected) were obtained on Shanghai Inesa WRS-3 melting point apparatus. The starting materials were purchased from Innochem or Energy Chemicals and used without further purification. Solvents were dried and purified according to the procedure from "Purification of Laboratory Chemicals book". The crude products were purified by flash column chromatography on silica gel and the reported yields are the actual isolated yields of pure products. Thin-layer chromatography (TLC) was performed using 60 mesh silica gel plates visualized with short-wavelength UV light (254 nm).

2. General Procedures

2.1 Synthesis of substrates 1

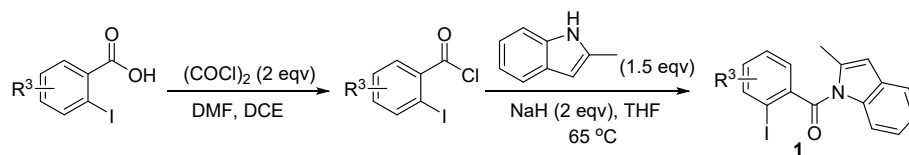


Synthesis of substrates 1a-1i, 1o: To a solution of indole derivative (1.0 equiv, 0.5 M) in THF was added 60% dispersion of NaH (1.2 equiv) in portions at 0 °C. After stirring at 0 °C for 30 min, a solution of acid chloride in THF was added dropwise to the reaction system. The mixture was then allowed to stir at room temperature. When the reaction was completed, the reaction mixture was quenched by aqueous NH_4Cl and extracted with EtOAc. The combined organic phase was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography using the indicated fluent to give the substrates.



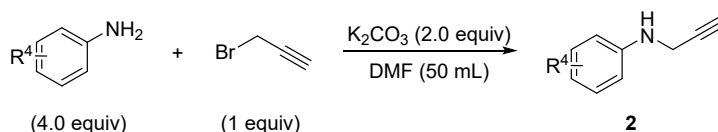
Synthesis of substrates 1j-1n: The appropriate substituted phenylhydrazine (1.0 mmol) and substituted acetophenone (1.0 mmol) were mixed in ethanol (20 mL) and a few drops of glacial AcOH were added. The solution was heated under reflux at 80 °C for 1-2 h. The solvents were evaporated in vacuo to give a solid that was added to polyphosphoric acid (PPA) (30 mL), and the mixture slowly heated to 120 °C and kept at this temperature for a few hours until the reaction was complete (TLC monitoring). The mixture was allowed to cool and then poured into cold water (50 mL). The acidic solution was neutralized by the slow addition of 1 M NaOH (aq) and the solid precipitate of crude

product was collected. Purification by column chromatography (hexane/ethyl acetate) gave the required indole products.



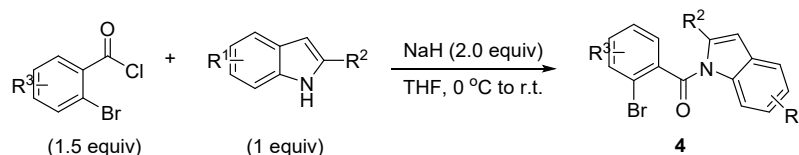
Synthesis of substrates 1p, 1q, 1r: In a flame dried flask under argon, oxalyl chloride (2.0 equiv) was added slowly to a solution of 2-iodo benzoic acid in DCM (0.5 M) with a few drops of DMF at 0 °C. The suspension was allowed to warm to room temperature and was stirred for 3 hours. The solvent was removed in-Vacuo, and the resulting yellow solid was put under argon. In a separate flame dried flask, to a solution of 2-methyl indole in THF (0.5 M) was added NaH (2.0 equiv) at 0 °C. The reaction was let stir until the gas evolution ceased. The yellow acyl chloride was suspended in THF and added *via* 3 aliquots dropwise at 0 °C. The reaction was allowed to warm to room temperature and was then heated to 65 °C overnight. Upon completion the reaction was quenched with H₂O and extracted 3 x EtOAc. The product was purified *via* silica gel chromatography with a solvent gradient of 100:1 pentane: triethylamine to 50:1:1 pentane: triethylamine: EtOAc.

2.2 Synthesis of substrates 2



To a mixture of K₂CO₃ (2.0 equiv) and *p*-toluidine (4.0 equiv) in DMF solvent was added 3-bromopropyne (1.0 equiv) dropwise at rt and stirred overnight. The reaction mixture was quenched with ice cold water and extracted with EtOAc (3x). The combined extracts were dried over anhydrous Na₂SO₄. The dried extracts were concentrated, and the crude product was purified by flash column chromatography on silica gel using 5% ethyl acetate in petroleum ether as eluent to afford the pure products.

2.3 Synthesis of substrates 4

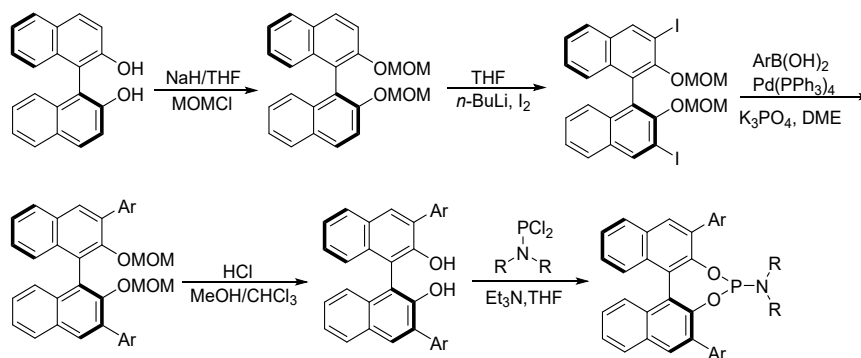


A 60% dispersion of NaH in mineral oil (2.0 equiv) was added to a stirred solution of the appropriate indole derivative (1 equiv, ~0.5 M) in THF at 0 °C and the corresponding solution was stirred for 5 minutes before warming to room temperature where it was stirred for 30 minutes. The solution of the sodium indolate was re-cooled to 0 °C at which time a solution of appropriate 2-bromobenzoyl chloride derivative (1.5 equiv, ~1 M) in THF was added dropwise. Once the addition was complete, the reaction was allowed to warm to room temperature and then was stirred at 65 °C for 30 minutes. At this time the extent of completion of the reaction was determined by conversion of the

indole derivate by TLC analysis. The reaction was cooled to room temperature and quenched with a saturated solution of NH_4Cl . The reaction mixture was then diluted with water and EtOAc, and after separating the layers, the aqueous layer was extracted with EtOAc (3x). The combined organic layers were washed sequentially with water and brine, dried over sodium sulfate, filtered and concentrated under reduced pressure. The crude *N*-(2-bromobenzoyl) indole derivative was purified by flash column gel chromatography using the indicated solvent system.

2.4 Synthesis of chiral phosphoramidite ligands $\text{L}_1\text{-L}_6$

The preparation of chiral phosphoramidite ligands $\text{L}_1\text{-L}_6$ were prepared according to the known method. [1, 2]

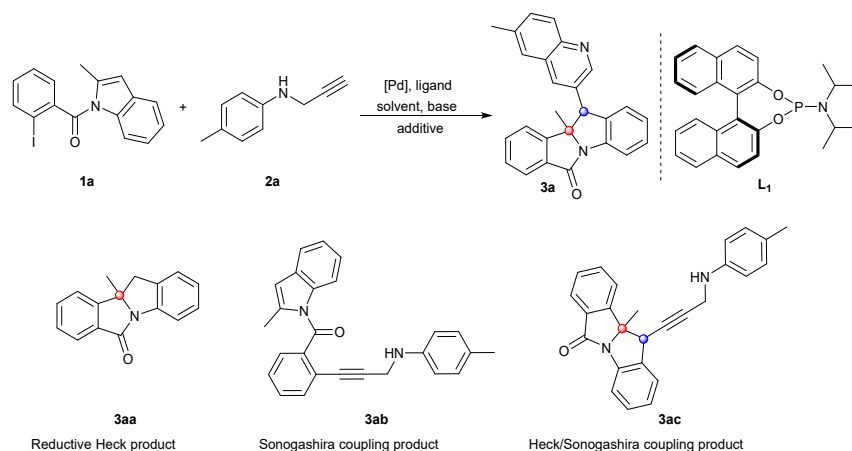


General Procedure a: To a solution of *N,N*-diisopropylamine (20.0 mmol) in dry THF (15 mL) at 0 °C was added *n*-BuLi (2.5 M in hexanes, 20 mmol) dropwise over 3 min under argon atmosphere. After stirring at 0 °C for 30 min, PCl_3 (60.0 mmol) was added to the reaction mixture in one portion. The resulting mixture was warmed to room temperature, stirred for 1 h, and then concentrated at room temperature. The remaining PCl_3 was removed under vacuum. dry THF (30 mL) was then added to the resulting residue. After stirring for 10 min, the mixture was cooled to 0 °C, followed by addition of a solution of 3,3'-disubstituted binaphthyl compound (10.0 mmol) and Et_3N (33.0 mmol) in dry THF (15 mL) over 2 min. The mixture was warmed to room temperature and stirred overnight. Then it was filtered and the solid was washed with THF. The residue was purified by chromatography on silica gel, eluting with PE:DCM = 10:1 (v/v) to afford the ligand $\text{L}_1\text{-L}_6$.

[1] *Org. Lett.* **2004**, 6, 2701-2704;

[2] *Angew. Chem. Int. Ed.* **2017**, 56, 7475-7478.

3. Optimization of the reaction conditions



entry	catalyst	ligand	base	solvent	3a	3aa	3ab	3ac	Recovery of 1a(%) ^b
					(%) ^b	(%) ^b	(%) ^b	(%) ^b	
1	Pd ₂ (dba) ₃	PPh ₃	Cs ₂ CO ₃	THF	24	trace	11	23	39
2	Pd ₂ (dba) ₃	PPh ₃	Cs ₂ CO ₃	MeCN	NR	65	13	trace	17
3	Pd ₂ (dba) ₃	PPh ₃	Cs ₂ CO ₃	DCE	50	trace	9	17	19
4	Pd ₂ (dba) ₃	PPh ₃	Cs ₂ CO ₃	dioxane	36	11	14	18	18
5	Pd ₂ (dba) ₃	PPh ₃	Cs ₂ CO ₃	PhMe	46	9	19	17	5
6	Pd ₂ (dba) ₃	PPh ₃	^t BuOLi	DCE	15	35	14	18	14
7	Pd ₂ (dba) ₃	PPh ₃	NaHCO ₃	DCE	48	30	7	6	5
8	Pd ₂ (dba) ₃	PPh ₃	KHCO ₃	DCE	47	4	41	4	trace
9	Pd ₂ (dba) ₃	PPh ₃	K ₂ CO ₃	DCE	55	25	6	5	4
10	Pd ₂ (dba) ₃	PPh ₃	Na ₂ CO ₃	DCE	43	28	7	5	12
11	Pd(PPh ₃) ₂ Cl ₂	PPh ₃	K ₂ CO ₃	DCE	48	6	15	27	trace
12	Pd(PPh ₂ Me) ₂ Cl ₂	PPh ₃	K ₂ CO ₃	DCE	46	32	5	7	6
13	Pd(OAc) ₂	PPh ₃	K ₂ CO ₃	DCE	20	17	26	35	trace
14	Pd(PPh ₃) ₄	PPh ₃	K ₂ CO ₃	DCE	59	15	8	10	4
15	Pd(PPh ₃) ₄	Xphos	K ₂ CO ₃	DCE	45	20	20	13	trace
16	Pd(PPh ₃) ₄	DPPP	K ₂ CO ₃	DCE	52	12	8	5	20
17	Pd(PPh ₃) ₄	DPPB	K ₂ CO ₃	DCE	43	15	25	8	5
18	Pd(PPh ₃) ₄	DPPF	K ₂ CO ₃	DCE	NR	17	70	10	trace
19	Pd(PPh ₃) ₄	L ₁	K ₂ CO ₃	DCE	78	10	trace	8	trace
20 ^c	Pd(PPh ₃) ₄	L ₁	K ₂ CO ₃	DCE	41	3	3	7	42
21 ^d	Pd(PPh ₃) ₄	L ₁	K ₂ CO ₃	DCE	63	3	5	5	20
22^e	Pd(PPh₃)₄	L₁	K₂CO₃	DCE	89	3	trace	5	trace
23 ^f	Pd(PPh ₃) ₄	L ₁	K ₂ CO ₃	DCE	55	3	4	trace	33

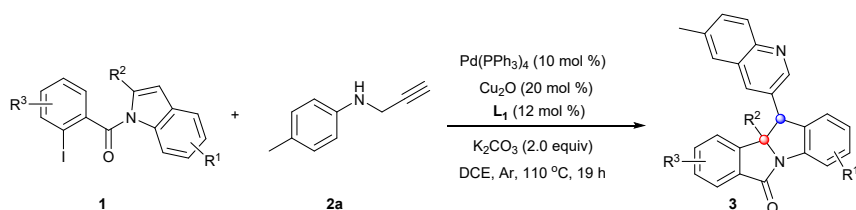
^aUnless otherwise noted, all reactions were performed with **1a** (0.1 mmol), **2a** (2.0 equiv), [Pd] (10 mol %), Cu₂O (20 mol %), ligand (12 mol %), and base (2.0 equiv) in solvent (1.0 mL) at 100 °C for 19 h.

^bYields are given for isolated products, diastereoselectivity of the product is > 20:1. ^cThe reaction was conducted at 80 °C. ^dThe reaction was conducted at 90 °C. ^eThe reaction was conducted at 110 °C. ^fThe reaction was conducted in the absence of Cu₂O.

The initial investigation began by employing aryl iodide **1a** as the starting point and 4-methyl-*N*-(prop-2-yn-1-yl)aniline **2a** as the coupling reagent. It has turned out that dearomative Heck annulation/phenyl electrophilic addition product **3a** was challenging to be obtained due to the reason that a series of by-products including reductive Heck by-product **3aa**, Sonogashira coupling by-product **3ab**, and Heck/Sonogashira coupling by-product **3ac** were observed in this transformation. To our gratification, the reaction worked well in the presence of Pd₂(dba)₃ (10 mol %), Cu₂O (20 mol %), PPh₃ (12 mol %), and Cs₂CO₃ (2.0 equiv) in tetrahydrofuran at 100 °C for 19 h and led to the desired product **3a**, Sonogashira coupling by-product **3ab**, and Heck/Sonogashira coupling by-product **3ac** in 24%, 11%, 23% yields, respectively. And 39% of the raw material **1a** was recycled (Table 1, entry 1). A subsequent exploration on the effect of solvent was investigated, the reactions in 1,2-dichloroethane, 1,4-dioxane, and toluene furnished the corresponding product **3a** in 50%, 36%, and 46% yields, respectively, while no product was observed in acetonitrile. Nevertheless, the reductive Heck by-product **3aa** was obtained in 65% yield in acetonitrile, which suggested that strong polar solvent was beneficial to the assembly of reductive Heck by-product (entries 2-5). Some representative inorganic bases were then examined, which revealed that K₂CO₃ was found to be superior to Cs₂CO₃, while ^tBuOLi, KHCO₃, NaHCO₃, and Na₂CO₃ were inefficient in promoting the efficiency of the transformation. Of note, the effect of base had a weak influence on the yield of this transformation (entries 6-10). Upon further screening of various palladium catalysts such as Pd(PPh₃)₂Cl₂, Pd(PPh₂Me)₂Cl₂, Pd(OAc)₂, and Pd(PPh₃)₄ indicated that Pd(PPh₃)₄ was optimal for the catalytic system, which afforded **3a** in 59% yield. And Pd(PPh₃)₂Cl₂, Pd(PPh₂Me)₂Cl₂, and Pd(OAc)₂ catalysts were favorable to form Heck/Sonogashira coupling by-product **3ac**, reductive Heck by-product **3aa**, and Heck/Sonogashira coupling by-product **3ac**, respectively (entries 11-14). Next, various monodentate and bis-monodentate phosphorus ligands were surveyed, regrettably, no better result was obtained. Among which, bis-monodentate phosphorus ligand DPPF could not furnish the desired product (entries 15-18). Gratifyingly, simply by switching from PPh₃ to phosphoramidite ligand **L**₁ under otherwise identical conditions did enhance remarkably the efficiency of the reaction, and the yield of **3a** was obviously increased to 78% (entry 19). Distinctly lower yields were observed by decreasing the temperature to 80 °C and 90 °C, leading to the desired product in 41% and 63% yields, respectively, accompanying the recovery of 42% and 20% raw material (entries 20-21). In sharp contrast, the result was sharply enhanced to 89% yield when carrying out the reaction at 110 °C (entry 22). Of note, a lower yield of 55% was obtained in the absence of Cu₂O with the recovery of 33% raw material, suggesting that Cu₂O may act as a critical additive in this transformation (entry 23). The molecular configuration of **3a** was definitely established by X-ray crystallographic analysis. Of note, the desired product was afforded with excellent diastereoselectivity (> 20:1), which was determined by ¹H NMR analysis. Ultimately, the optimized conditions were identified to be; aryl iodide **1a** (0.1 mmol) and 4-methyl-*N*-(prop-2-yn-1-yl)aniline **2a** (2.0 equiv) in the presence of Pd(PPh₃)₄ (10 mol %), Cu₂O (20 mol %), phosphoramidite ligand **L**₁ (12 mol %), and K₂CO₃ (2.0 equiv) in 1,2-dichloroethane at 110 °C for 19 h under an argon atmosphere.

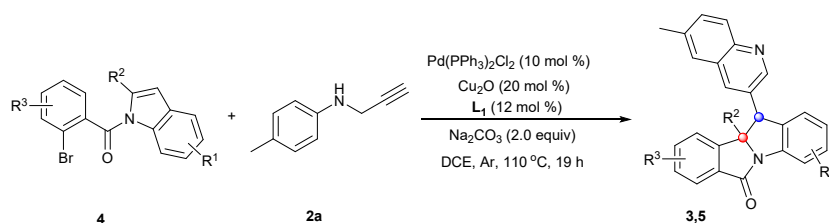
4. Procedure for the tandem cyclization of indoles with *N*-propargylated aniline.

4.1 Synthesis of products 3



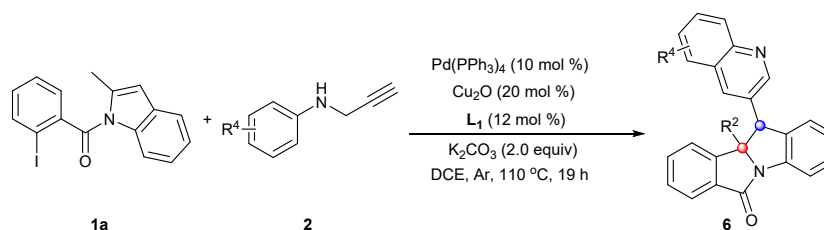
An oven-dried Schlenk tube charged with *N*-(2-Iodobenzoyl)indole derivative **1** (0.1 mmol), *N*-propargylated aniline **2a** (2.0 equiv), Pd(PPh₃)₄ (10 mol%), L₁ (12 mol%), K₂CO₃ (2.0 equiv), Cu₂O (20 mol%) in DCE (1.0 mL), the reactions were conducted under Ar atmosphere and stirred at 110 °C for 19.0 h. The reaction was monitored by TLC. Then, the reaction mixture was cooled down to room temperature and evaporated under reduced pressure. The residue was further purified by chromatography on silica gel to afford the corresponding products. Cs₂CO₃ (2.0 equiv) instead of K₂CO₃ (2.0 equiv) was used for the formation of **3g-3o**.

4.2 Synthesis of products 5



An oven-dried Schlenk tube charged with *N*-(2-bromobenzoyl)indole derivative **4** (0.1 mmol), *N*-propargylated aniline **2a** (2.0 equiv), Pd(PPh₃)₂Cl₂ (10 mol%), L₁ (12 mol%), Na₂CO₃ (2.0 equiv), Cu₂O (20 mol%) in DCE (1.0 mL), the reactions were conducted under Ar atmosphere and stirred at 110 °C for 19.0 h. The reaction was monitored by TLC. Then, the reaction mixture was cooled down to room temperature and evaporated under reduced pressure. The residue was further purified by chromatography on silica gel to afford the corresponding products.

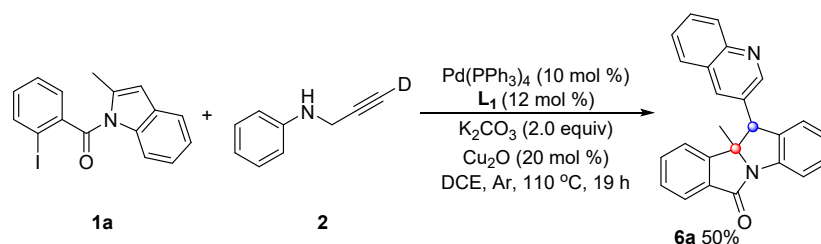
4.3 Synthesis of products 6



An oven-dried Schlenk tube charged with *N*-(2-Iodobenzoyl)indole derivative **1a** (0.1 mmol), *N*-propargylated aniline derivative **2** (4.0 equiv), Pd(PPh₃)₄ (10 mol%), L₁ (12 mol%), K₂CO₃ (2.0 equiv), Cu₂O (20 mol%) in DCE (1.0 mL) the reactions were conducted under Ar atmosphere and stirred at 110 °C for 19.0 h. The reaction was monitored by TLC. Then, the reaction mixture was cooled down to room temperature and evaporated under reduced pressure. The residue was further purified by chromatography on silica gel to afford the corresponding products.

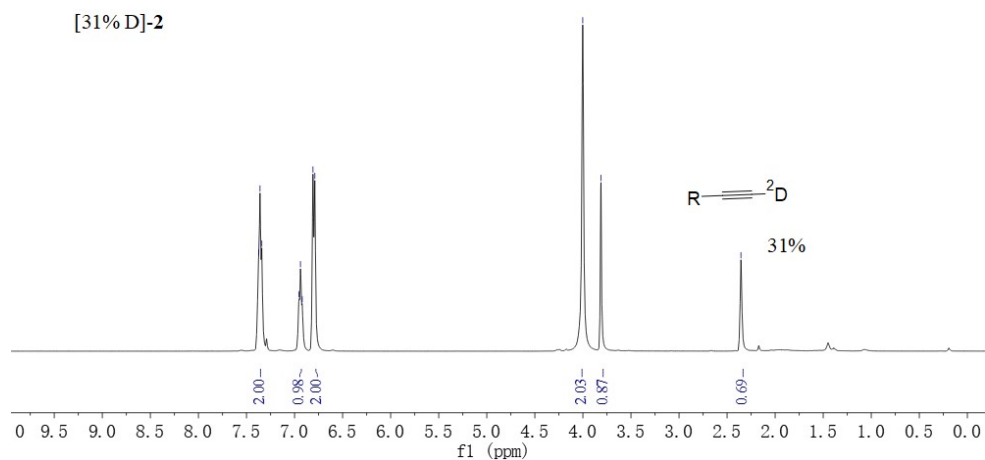
5. Mechanistic studies

5.1 H/D-exchange study

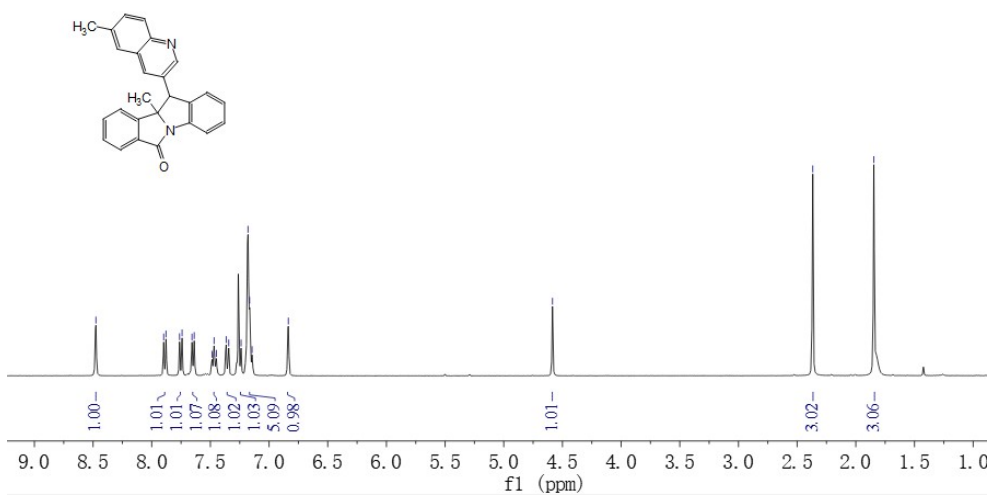


An oven-dried Schlenk tube charged with **1a** (0.1 mmol), [31% D]-**2** (2.0 equiv), Pd(PPh₃)₄ (10 mol%), L₁ (12 mol %), K₂CO₃ (2.0 equiv), Cu₂O (20 mol %) in DCE (1.0 mL) the reaction was conducted under Ar atmosphere and stirred at 110 °C for 19.0 h. The reaction was monitored by TLC. Then, the reaction mixture was cooled down to room temperature and evaporated under reduced pressure. The residue was further purified by chromatography on silica gel to afford the corresponding product **6a** in 50% yield with 0% D.

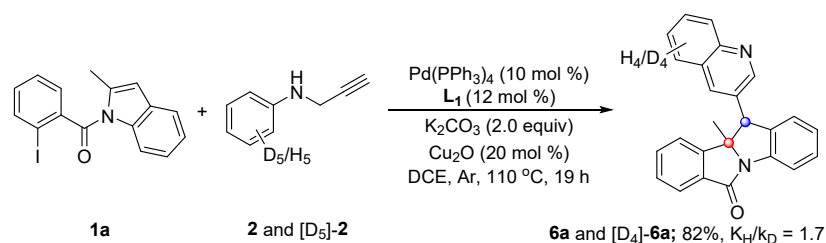
^1H NMR spectrum of [31% D]-2 (CDCl_3 , 400 MHz)



^1H NMR spectrum of **6a** (CDCl_3 , 400 MHz)



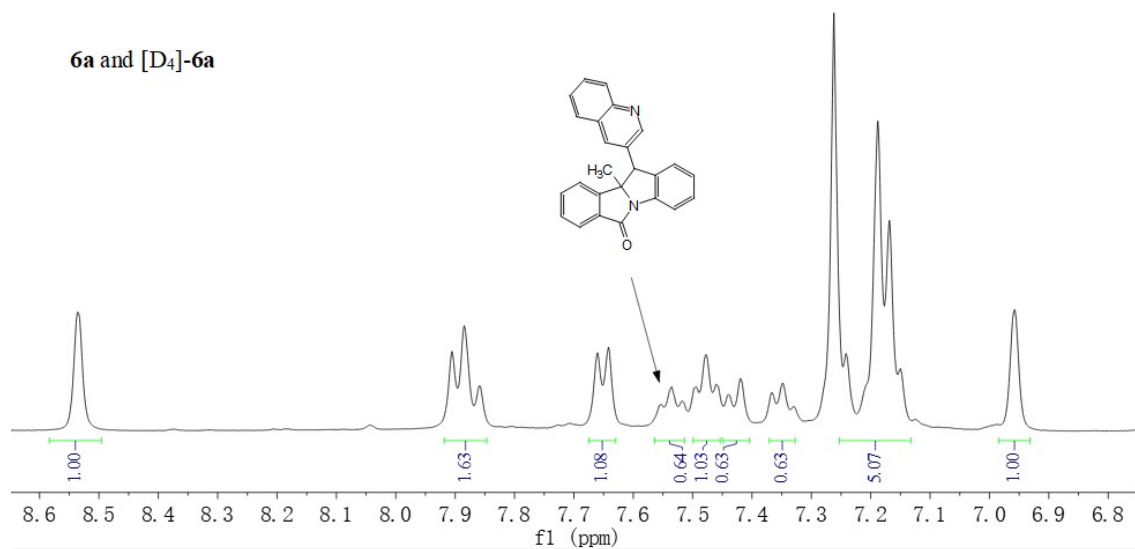
5.2 Intermolecular KIE competition



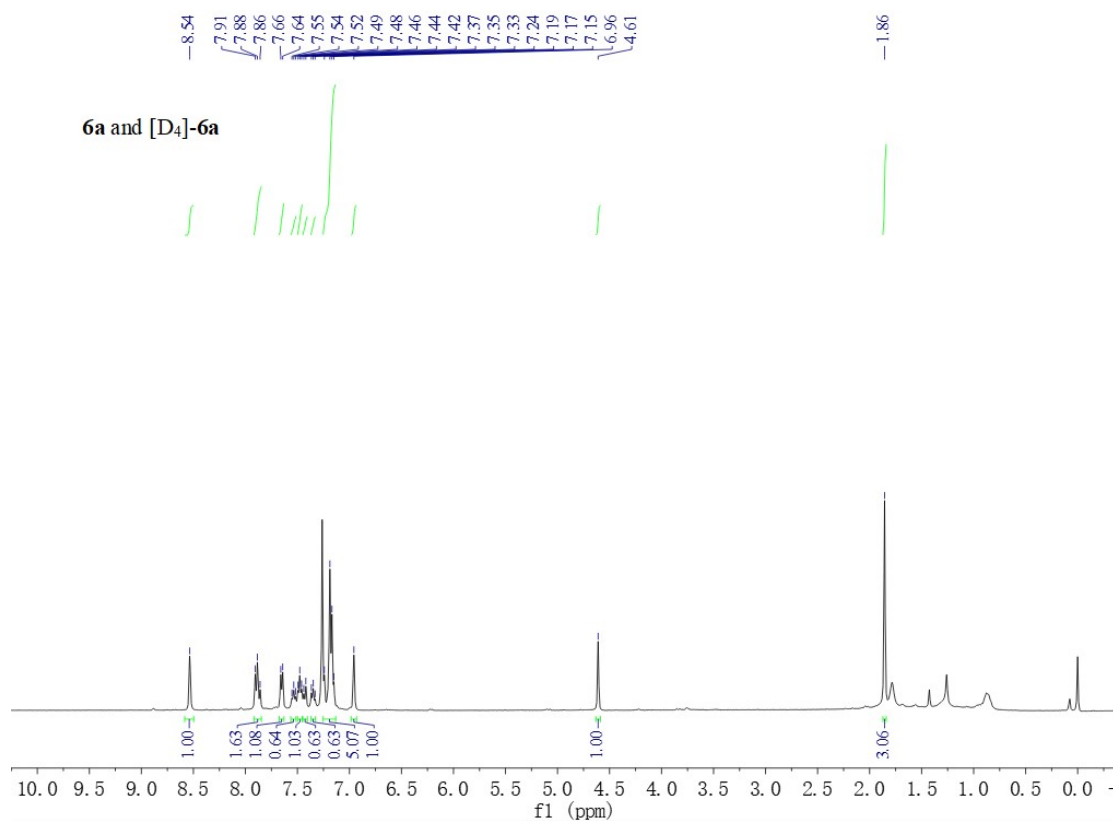
An oven-dried Schlenk tube charged with **1a** (0.1 mmol), **2** (1.0 equiv), $[\text{D}_5]\text{-2}$ (1.0 equiv), $\text{Pd(PPh}_3)_4$ (10 mol%), L_1 (12 mol%), K_2CO_3 (2.0 equiv), Cu_2O (20 mol%) in DCE (1.0 mL) the reaction was conducted under Ar atmosphere and stirred at 110 °C for 19.0 h. The reaction was monitored by TLC. Then, the reaction mixture was cooled down to room temperature and evaporated

under reduced pressure. The residue was further purified by chromatography on silica gel to afford the corresponding product mixture of **6a** and [D₄]-**6a** with a yield of 82%. The k_H/k_D was determined by ¹H-NMR spectroscopy.

¹H NMR spectrum of **6a** and [D₄]-**6a** (CDCl₃, 400 MHz)

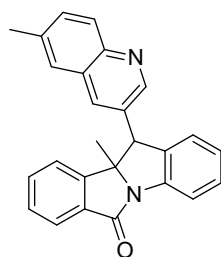


¹H NMR spectrum of **6a** and [D₄]-**6a** (CDCl₃, 400 MHz)

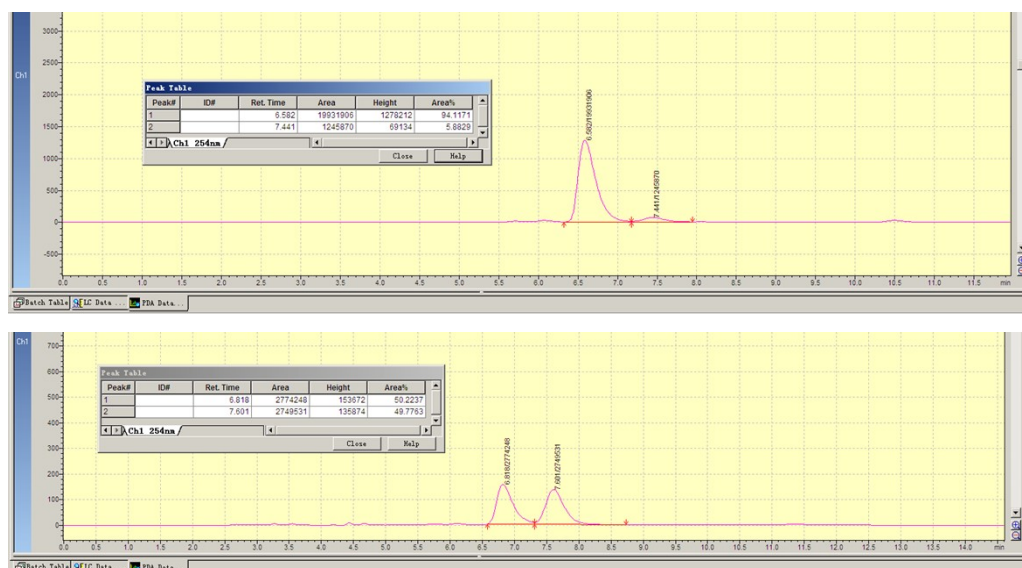


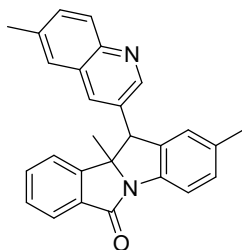
6. Characterization data of 3a-8

General procedure: ^1H and ^{13}C NMR spectra were recorded on a Bruker AC-P 400 spectrometer (400 MHz for ^1H , 100 MHz for ^{13}C) in CDCl_3 (with TMS as internal standard). Chemical shifts (δ) were measured in ppm. Coupling constants, J , are reported in hertz. Mass data were measured with Thermo Scientific DSQ II mass spectrometer and Bruker O-TOF Compact Mass Spectrometry. Melting points (uncorrected) were obtained on Shanghai Inesa WRS-3 melting point apparatus. Thin-layer chromatography (TLC) was performed using 60 mesh silica gel plates visualized with short-wavelength UV light (254 nm).

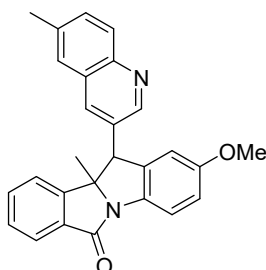


(3a) **10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.** Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid; m.p. = 209-211 °C 33.5 mg, 89% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.47 (s, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.46 (t, J = 8.0 Hz, 1H), 7.34 (d, J = 8.0 Hz, 1H), 7.23 (d, J = 8.0 Hz, 1H), 7.19-7.13 (m, 5H), 6.85 (s, 1H), 4.59 (s, 1H), 2.35 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.1, 149.6, 147.8, 145.5, 139.2, 137.9, 136.5, 133.5, 133.4, 132.7, 132.5, 131.5, 129.1, 128.4, 128.4, 127.4, 126.5, 125.2, 124.4, 122.8, 117.3, 76.0, 54.2, 28.2, 21.3; **HRMS** (ESI): m/z calcd for $\text{C}_{26}\text{H}_{21}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 377.1648. Found 377.1647. [Daicel Chiralpak AS-H column (25 cm \times 0.46 cm ID), n -hexane/ i -PrOH = 99/1, 1 mL/min, 254nm; t major = 22.65 min, t minor = 18.51 min].

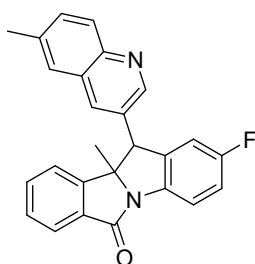




(3b) 10b-dimethyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid; m.p. = 237-239 °C 33.6 mg, 86% yield. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ : 8.47 (s, 1H), 7.77-7.74 (m, 2H), 7.64 (d, $J = 8.0$ Hz, 1H), 7.35 (d, $J = 8.0$ Hz, 1H), 7.23 (d, $J = 8.0$ Hz, 2H), 7.19-7.13 (m, 3H), 6.99 (s, 1H), 6.86 (s, 1H), 4.53 (s, 1H), 2.37 (s, 3H), 2.31 (s, 3H), 1.83 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ : 168.0, 149.7, 147.8, 145.5, 138.1, 136.9, 136.5, 135.1, 133.6, 133.5, 132.9, 132.4, 131.5, 129.7, 128.4, 127.5, 127.1, 126.6, 124.4, 122.7, 117.0, 76.2, 54.3, 28.2, 21.4, 21.2; **HRMS** (ESI): m/z calcd for $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}^+ [\text{M}+\text{H}]^+$ 391.1805. Found 391.1806.

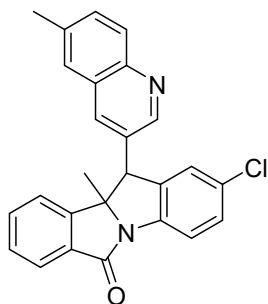


(3c) 2-methoxy-10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown liquid; 28.8 mg, 71% yield. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ : 8.48 (s, 1H), 7.79 (d, $J = 8.0$ Hz, 1H), 7.75 (d, $J = 8.0$ Hz, 1H), 7.63 (d, $J = 8.0$ Hz, 1H), 7.36 (d, $J = 8.0$ Hz, 1H), 7.23-7.14 (m, 4H), 7.00 (d, $J = 8.0$ Hz, 1H), 6.86 (s, 1H), 6.75 (s, 1H), 4.53 (s, 1H), 3.76 (s, 3H), 2.38 (s, 3H), 1.84 (s, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ : 168.1, 157.7, 149.6, 147.7, 145.5, 139.4, 136.6, 133.6, 133.3, 132.9, 132.9, 132.3, 131.6, 128.5, 128.4, 127.5, 126.6, 124.4, 122.7, 118.0, 114.3, 112.4, 76.4, 55.7, 54.6, 28.1, 21.4. **HRMS** (ESI): m/z calcd for $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}_2^+ [\text{M}+\text{H}]^+$ 407.1754. Found 407.1752.

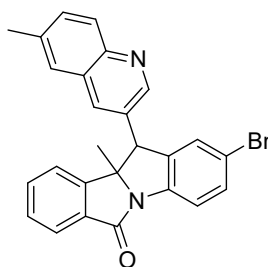


(3d) 2-fluoro-10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 205-207 °C; 35.1 mg, 89% yield. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ : 8.45 (s, 1H), 7.84-7.81 (m, 1H), 7.76 (d, $J = 8.0$ Hz, 1H), 7.64 (d, $J = 8.0$ Hz, 1H), 7.37 (d, $J = 8.0$ Hz, 1H), 7.24 (s, 1H), 7.20 (s, 1H), 7.19-7.15 (m, 3H), 6.91 (d, $J = 8.0$ Hz, 1H), 6.85 (s, 1H), 4.56 (s, 1H), 2.38 (s, 3H), 1.85 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ : 168.2, 161.7, 159.2, 149.4, 147.7, 145.6, 139.7, 139.6, 136.7, 133.4, 132.8, 132.6, 132.5, 131.7, 128.6, 128.5, 127.4, 126.5, 124.6, 122.8, 118.3, 118.2, 116.0,

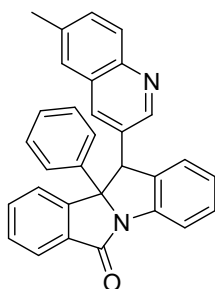
115.8, 114.0, 113.8, 76.5, 54.5, 28.1, 21.4; **HRMS** (ESI): m/z calcd for $C_{26}H_{20}FN_2O^+$ $[M+H]^+$ 395.1554. Found 395.1553.



(3e)2-chloro-10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 157-159 °C; 31.6 mg, 77% yield. **¹H NMR** (400 MHz, $CDCl_3$) δ : 8.45 (s, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.25 (s, 1H), 7.20 (d, J = 8.0 Hz, 1H), 7.17-7.15 (m, 3H), 6.86 (s, 1H), 4.56 (s, 1H), 2.39 (s, 3H), 1.84 (s, 3H); **¹³C NMR** (100 MHz, $CDCl_3$) δ : 168.1, 149.4, 147.6, 145.6, 139.6, 137.9, 136.8, 133.4, 132.8, 132.8, 132.4, 131.7, 130.4, 129.3, 128.7, 128.5, 127.4, 126.8, 126.6, 124.6, 122.8, 118.2, 76.3, 54.3, 28.3, 21.4; **HRMS** (ESI): m/z calcd for $C_{26}H_{20}ClN_2O^+$ $[M+H]^+$ 411.1259. Found 411.1259.

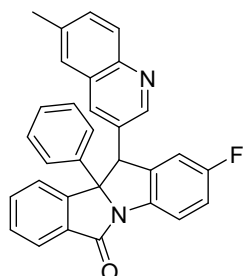


(3f)2-bromo-10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 90-92 °C; 29.5 mg, 65% yield. **¹H NMR** (400 MHz, $CDCl_3$) δ : 8.43 (s, 1H), 7.77 (d, J = 12.0 Hz, 2H), 7.69 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.32 (s, 1H), 7.25 (d, J = 8.0 Hz, 1H), 7.20 (d, J = 8.0 Hz, 1H), 7.16 (d, J = 8.0 Hz, 1H), 6.87 (s, 1H), 4.56 (s, 1H), 2.38 (s, 3H), 1.84 (s, 3H); **¹³C NMR** (100 MHz, $CDCl_3$) δ : 168.0, 149.3, 147.6, 145.6, 140.0, 138.3, 136.7, 133.4, 132.8, 132.7, 132.3, 132.2, 131.7, 129.6, 128.5, 128.5, 127.4, 126.5, 124.6, 122.8, 118.6, 117.9, 76.2, 54.2, 28.2, 21.4; **HRMS** (ESI): m/z calcd for $C_{26}H_{20}BrN_2O^+$ $[M+H]^+$ 455.0754. Found 455.0755.

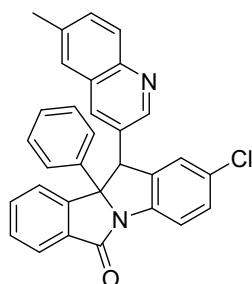


(3g) 11-(6-methylquinolin-3-yl)-10b-phenyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown

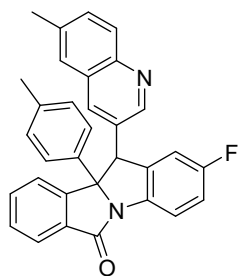
solid, m.p. = 249-251 °C; 30.6 mg, 70% yield. **¹H NMR** (400 MHz, CDCl₃) δ: 8.69 (s, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 3H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.39-7.36 (m, 3H), 7.31-7.29 (m, 2H), 7.22 (s, 1H), 7.18-7.06 (m, 4H), 6.99 (s, 1H), 5.23 (s, 1H), 2.38 (s, 3H); **¹³C NMR** (100 MHz, CDCl₃) δ: 168.7, 149.8, 147.1, 145.6, 143.1, 139.8, 137.6, 136.7, 134.0, 133.2, 132.7, 132.1, 131.7, 129.2, 129.0, 128.5, 128.5, 128.1, 127.6, 126.6, 126.2, 125.6, 125.0, 124.5, 123.8, 117.2, 81.2, 56.1, 21.4; **HRMS** (ESI): *m/z* calcd for C₃₁H₂₃N₂O⁺ [M+H]⁺ 439.1805. Found 439.1804.



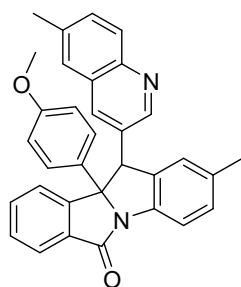
(3h)2-fluoro-11-(6-methylquinolin-3-yl)-10b-phenyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 108-110 °C; 32.4 mg, 71% yield. **¹H NMR** (400 MHz, CDCl₃) δ: 8.66 (s, 1H), 7.96-7.93 (m, 1H), 7.81-7.76 (m, 3H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 3H), 7.32-7.26 (m, 3H), 7.16 (t, *J* = 8.0 Hz, 2H), 7.10-7.07 (m, 1H), 7.01 (s, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 5.21 (s, 1H), 2.39 (s, 3H); **¹³C NMR** (100 MHz, CDCl₃) δ: 168.8, 161.8, 159.4, 149.6, 147.0, 145.7, 142.8, 139.5, 139.4, 136.9, 136.0, 133.9, 132.8, 132.4, 131.9, 131.8, 129.1, 128.6, 128.5, 128.3, 127.5, 126.6, 125.0, 124.5, 123.8, 118.2, 118.1, 116.1, 115.8, 113.8, 113.6, 81.7, 56.3, 21.4; **HRMS** (ESI): *m/z* calcd for C₃₁H₂₂FN₂O⁺ [M+H]⁺ 457.1711. Found 457.1714.



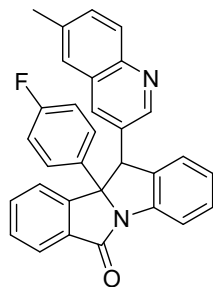
(3i)2-chloro-11-(6-methylquinolin-3-yl)-10b-phenyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 94-96 °C; 29.3 mg, 62% yield. **¹H NMR** (400 MHz, CDCl₃) δ: 8.66 (s, 1H), 7.96-7.93 (m, 1H), 7.81-7.76 (m, 3H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 3H), 7.30 (t, *J* = 8.0 Hz, 2H), 7.25 (s, 1H), 7.16 (t, *J* = 8.0 Hz, 2H), 7.10-7.07 (m, 1H), 7.01 (s, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 5.21 (s, 1H), 2.39 (s, 3H); **¹³C NMR** (100 MHz, CDCl₃) δ: 168.8, 161.8, 159.4, 149.6, 147.0, 145.7, 142.7, 139.5, 139.4, 136.9, 136.0, 133.9, 132.8, 132.4, 131.9, 131.8, 129.1, 128.6, 128.5, 128.3, 127.5, 126.6, 125.0, 124.5, 123.8, 118.2, 118.1, 116.1, 115.8, 113.8, 113.6, 81.7, 56.2, 21.4; **HRMS** (ESI): *m/z* calcd for C₃₁H₂₂ClN₂O⁺ [M+H]⁺ 473.1415. Found 473.1412.



(3j)2-fluoro-11-(6-methylquinolin-3-yl)-10b-(p-tolyl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 203-205 °C; 32.4 mg, 69% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.65 (s, 1H), 7.94-7.91 (m, 1H), 7.80 (d, *J* = 12.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.28-7.26 (m, 3H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 1H), 7.10-7.07 (m, 1H), 6.99 (s, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 5.19 (s, 1H), 2.40 (s, 3H), 2.31 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 168.8, 161.8, 159.4, 149.6, 147.2, 145.7, 139.7, 139.6, 139.5, 138.2, 136.9, 136.0, 133.9, 132.8, 132.5, 131.9, 131.8, 129.8, 128.5, 127.5, 126.6, 124.9, 124.5, 123.7, 118.2, 118.1, 116.1, 115.8, 113.8, 113.6, 81.6, 56.2, 21.4, 21.0; **HRMS** (ESI): *m/z* calcd for C₃₂H₂₄FN₂O⁺ [M+H]⁺ 471.1867. Found 471.1865.

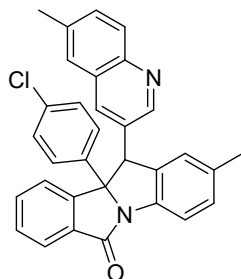


(3k)10b-(4-methoxyphenyl)-2-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 138-140 °C; 31.3 mg, 65% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.66 (s, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 12.0 Hz, 3H), 7.15-7.12 (m, 1H), 7.07-7.04 (m, 1H), 7.00 (s, 1H), 6.89 (s, 2H), 6.87 (s, 1H), 5.14 (s, 1H), 3.73 (s, 3H), 2.37 (s, 3H), 2.24 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 168.6, 159.3, 149.9, 147.4, 145.6, 137.9, 137.4, 136.6, 135.4, 135.0, 134.0, 133.3, 132.5, 132.1, 131.6, 129.7, 128.5, 128.3, 127.6, 126.8, 126.6, 126.2, 124.3, 123.7, 116.9, 114.3, 81.1, 56.0, 55.2, 21.4, 21.1; **HRMS** (ESI): *m/z* calcd for C₃₃H₂₇N₂O₂⁺ [M+H]⁺ 483.2067. Found 483.2066.

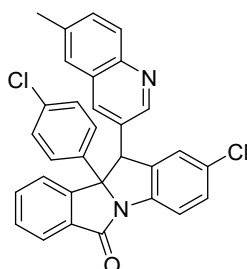


(3l)10b-(4-fluorophenyl)-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 258-260 °C; 29.2 mg, 64% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.66 (s, 1H), 7.99

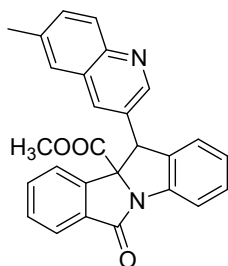
(d, $J = 8.0$ Hz, 1H), 7.80-7.73 (m, 3H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.47 (t, $J = 8.0$ Hz, 1H), 7.39 (d, $J = 12.0$ Hz, 1H), 7.25-7.20 (m, 2H), 7.16 (t, $J = 8.0$ Hz, 1H), 7.12-7.04 (m, 5H), 6.97 (s, 1H), 5.17 (s, 1H), 2.38 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ : 168.6, 163.6, 161.2, 149.7, 147.0, 145.7, 139.7, 138.9, 138.9, 137.5, 136.8, 134.0, 133.0, 132.8, 132.0, 131.7, 129.3, 128.6, 128.5, 127.5, 126.9, 126.8, 126.6, 126.2, 125.8, 124.6, 123.7, 117.3, 116.0, 115.8, 80.8, 56.2, 21.4; **HRMS** (ESI): m/z calcd for $\text{C}_{31}\text{H}_{22}\text{FN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 457.1711. Found 457.1710.



(3m)10b-(4-chlorophenyl)-2-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 224-226 °C; 27.7 mg, 57% yield. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ : 8.65 (s, 1H), 7.87 (d, $J = 8.0$ Hz, 1H), 7.79 (d, $J = 8.0$ Hz, 1H), 7.71 (d, $J = 8.0$ Hz, 2H), 7.60 (d, $J = 8.0$ Hz, 1H), 7.39 (d, $J = 8.0$ Hz, 1H), 7.34 (d, $J = 8.0$ Hz, 2H), 7.28 (s, 1H), 7.24 (s, 2H), 7.18-7.15 (m, 1H), 7.11-7.08 (m, 1H), 7.00 (s, 1H), 6.90 (s, 1H), 5.10 (s, 1H), 2.39 (s, 3H), 2.26 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ : 168.5, 149.7, 146.6, 145.7, 141.7, 137.5, 137.3, 136.7, 135.7, 134.0, 132.9, 132.7, 132.2, 131.7, 129.9, 129.1, 128.6, 128.5, 127.5, 126.8, 126.6, 126.5, 124.5, 123.6, 116.9, 81.0, 56.1, 21.4, 21.2; **HRMS** (ESI): m/z calcd for $\text{C}_{32}\text{H}_{24}\text{ClN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 487.1572. Found 487.1572.

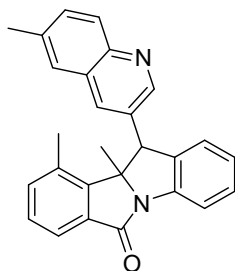


(3n)2-chloro-10b-(4-chlorophenyl)-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 248-250 °C; 24.3 mg, 48% yield. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ : 8.61 (s, 1H), 7.92 (d, $J = 12.0$ Hz, 1H), 7.80 (d, $J = 8.0$ Hz, 1H), 7.69 (d, $J = 8.0$ Hz, 2H), 7.62 (d, $J = 8.0$ Hz, 1H), 7.46-7.40 (m, 2H), 7.36 (d, $J = 8.0$ Hz, 2H), 7.23 (s, 2H), 7.19 (t, $J = 8.0$ Hz, 1H), 7.13 (d, $J = 8.0$ Hz, 1H), 7.10-7.09 (m, 1H), 7.00 (s, 1H), 5.13 (s, 1H), 2.41 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ : 168.5, 149.4, 146.5, 145.8, 141.2, 139.1, 138.3, 137.0, 134.3, 133.9, 133.0, 132.1, 132.0, 131.7, 131.0, 129.5, 129.3, 128.9, 128.6, 127.4, 126.6, 126.5, 126.4, 124.8, 123.7, 118.2, 81.0, 56.0, 21.4; **HRMS** (ESI): m/z calcd for $\text{C}_{31}\text{H}_{21}\text{Cl}_2\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 507.1025. Found 507.1022.



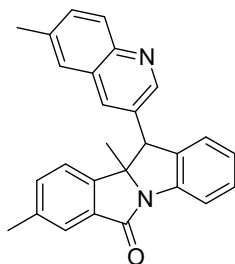
(3o) methyl 11-(6-methylquinolin-3-yl)-6-oxo-6H-isoindolo[2,1-a]indole-10b(11H)-carboxylate.

Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 194-196 °C; 32.4 mg, 77% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.56 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.50-7.45 (m, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.25-7.22 (m, 3H), 7.19-7.16 (m, 2H), 6.97 (s, 1H), 5.45 (s, 1H), 3.75 (s, 3H), 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 171.8, 168.1, 149.8, 145.7, 141.0, 139.8, 136.7, 136.3, 134.1, 133.2, 132.8, 132.0, 131.8, 129.7, 129.4, 128.5, 127.4, 126.6, 126.1, 125.6, 124.6, 124.0, 116.9, 80.8, 53.8, 51.2, 21.4; HRMS (ESI): *m/z* calcd for C₂₇H₂₁N₂O₃⁺ [M+H]⁺ 421.1547. Found 421.1548.



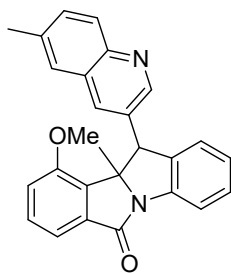
(3p) 10,10b-dimethyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 87-89 °C; 18.3 mg, 47% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.44 (s, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 4.0 Hz, 1H), 7.43-7.36 (m, 2H), 7.19 (s, 1H), 7.15 (t, *J* = 8.0 Hz, 2H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 4.58 (s, 1H), 2.38 (s, 3H), 2.28 (s, 3H), 1.87 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ: 167.4, 148.9, 145.7, 145.6, 139.2, 138.0, 136.6, 134.5, 133.8, 133.6, 133.4, 132.2, 131.6, 129.1, 129.0, 128.5, 127.5, 126.5, 126.3, 125.2, 122.4, 117.3, 76.2, 54.0, 26.5, 21.4, 19.0. HRMS (ESI): *m/z* calcd for C₂₇H₂₃N₂O⁺ [M+H]⁺ 391.1805. Found 391.1806.

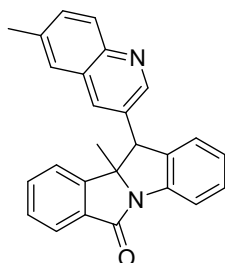


(3q) 8,10b-dimethyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

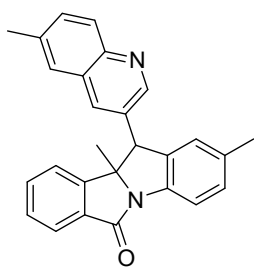
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 113-115 °C; 20.7 mg, 53% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.45 (s, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 12.0 Hz, 1H), 7.47-7.44 (m, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.19-7.13 (m, 3H), 7.06 (s, 2H), 6.87 (s, 1H), 4.56 (s, 1H), 2.37 (s, 3H), 2.19 (s, 3H), 1.81 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 168.2, 149.7, 145.1, 139.2, 138.5, 137.9, 136.4, 133.6, 133.5, 132.8, 132.1, 132.0, 131.4, 129.1, 128.5, 128.4, 126.6, 126.5, 125.1, 124.7, 122.5, 117.2, 75.8, 54.2, 28.4, 21.3, 21.1; HRMS (ESI): *m/z* calcd for C₂₇H₂₃N₂O⁺ [M+H]⁺ 391.1805. Found 391.1803.



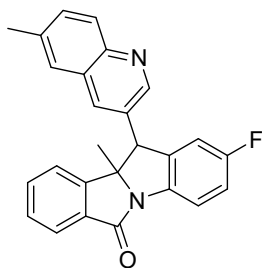
(3r)10-methoxy-10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown liquid; 30.5 mg, 75% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.43 (s, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.20-7.11 (m, 4H), 7.07 (d, *J* = 8.0 Hz, 1H), 6.87 (s, 1H), 6.70 (d, *J* = 8.0 Hz, 1H), 4.55 (s, 1H), 3.68 (s, 3H), 2.38 (s, 3H), 1.81 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 168.0, 159.9, 149.7, 145.5, 140.2, 139.2, 138.0, 136.5, 134.1, 133.7, 133.5, 131.5, 129.1, 128.5, 127.6, 126.6, 125.3, 123.6, 120.7, 117.3, 107.2, 75.7, 55.4, 54.3, 28.5, 21.4; HRMS (ESI): *m/z* calcd for C₂₇H₂₃N₂O₂⁺ [M+H]⁺ 407.1754. Found 407.1756.



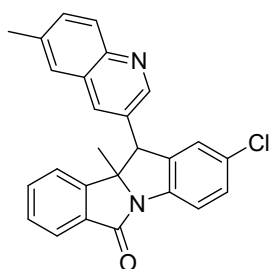
(5a)10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid; m.p. = 209-211 °C; 26.0 mg, 69% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.48 (s, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 12.0 Hz, 1H), 7.24 (s, 1H), 7.18-7.15 (m, 5H), 6.84 (s, 1H), 4.59 (s, 1H), 2.37 (s, 3H), 1.85 (s, 3H); HRMS (ESI): *m/z* calcd for C₂₆H₂₁N₂O⁺ [M+H]⁺ 377.1648. Found 377.1648.



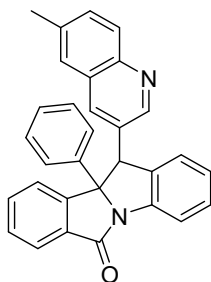
(5b)2,10b-dimethyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid; m.p. = 237-239 °C; 23.8 mg, 61% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.49 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 4.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.19-7.14 (m, 3H), 6.99 (s, 1H), 6.85 (s, 1H), 4.53 (s, 1H), 2.37 (s, 3H), 2.31 (s, 3H), 1.83 (s, 3H); HRMS (ESI): *m/z* calcd for C₂₇H₂₃N₂O⁺ [M+H]⁺ 391.1805. Found 391.1801.



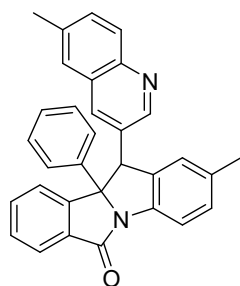
(5c)2-fluoro-10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 205-207 °C; 22.1 mg, 56% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.45 (s, 1H), 7.85-7.81 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.24-7.16 (m, 5H), 6.92 (d, *J* = 8.0 Hz, 1H), 6.85 (s, 1H), 4.56 (s, 1H), 2.38 (s, 3H), 1.85 (s, 3H); **HRMS** (ESI): *m/z* calcd for C₂₆H₂₀FN₂O⁺ [M+H]⁺ 395.1554. Found 395.1553.



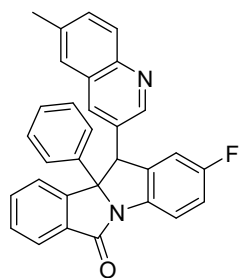
(5d)2-chloro-10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 157-159 °C; 29.6 mg, 72% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.44 (s, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.24-7.15 (m, 5H), 6.86 (s, 1H), 4.56 (s, 1H), 2.38 (s, 3H), 1.84 (s, 3H); **HRMS** (ESI): *m/z* calcd for C₂₆H₂₀ClN₂O⁺ [M+H]⁺ 411.1259. Found 411.1255.



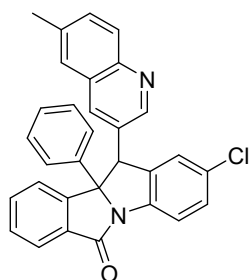
(5e)11-(6-methylquinolin-3-yl)-10b-phenyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 249-251 °C; 24.1 mg, 55% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.69(s, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 3H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.39-7.36 (m, 3H), 7.31-7.28 (m, 2H), 7.22 (s, 1H), 7.18-7.08(m, 4H), 6.99 (s, 1H), 5.23 (s, 1H), 2.38 (s, 3H); **HRMS** (ESI): *m/z* calcd for C₃₁H₂₃N₂O⁺ [M+H]⁺ 439.1805. Found 439.1804.



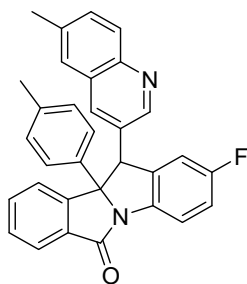
(5f)2-methyl-11-(6-methylquinolin-3-yl)-10b-phenyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 121-123 °C; 20.8 mg, 46% yield. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ : 8.67 (s, 1H), 7.87 (d, $J = 8.0$ Hz, 1H), 7.78 (d, $J = 8.0$ Hz, 2H), 7.65 (d, $J = 8.0$ Hz, 2H), 7.59 (d, $J = 8.0$ Hz, 1H), 7.37 (t, $J = 8.0$ Hz, 3H), 7.29 (d, $J = 4.0$ Hz, 2H), 7.24 (s, 2H), 7.15 (t, $J = 8.0$ Hz, 1H), 7.09-7.06 (m, 1H), 7.00 (s, 1H), 6.89 (s, 1H), 5.17 (s, 1H), 2.39 (s, 3H), 2.25 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ : 168.7, 149.8, 147.1, 145.5, 143.2, 137.8, 137.5, 136.7, 135.5, 134.1, 133.3, 132.6, 132.2, 131.7, 129.8, 129.0, 128.4, 128.4, 128.1, 127.6, 126.8, 126.6, 125.0, 124.4, 123.8, 116.9, 81.4, 56.1, 21.4, 21.2; **HRMS** (ESI): m/z calcd for $\text{C}_{32}\text{H}_{25}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 453.1961. Found 453.1963.



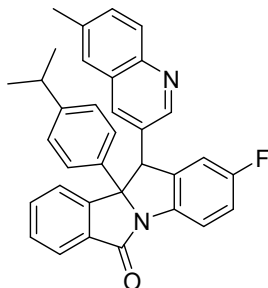
(5g)2-fluoro-11-(6-methylquinolin-3-yl)-10b-phenyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 108-110 °C; 23.3 mg, 51% yield. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ : 8.67 (s, 1H), 7.96-7.93 (m, 1H), 7.81-7.76 (m, 3H), 7.60 (d, $J = 8.0$ Hz, 1H), 7.41-7.38 (m, 3H), 7.30 (t, $J = 8.0$ Hz, 3H), 7.19-7.13 (m, 2H), 7.11-7.08 (m, 1H), 7.00 (s, 1H), 6.82 (d, $J = 8.0$ Hz, 1H), 5.21 (s, 1H), 2.40 (s, 3H); **HRMS** (ESI): m/z calcd for $\text{C}_{31}\text{H}_{22}\text{FN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 457.1711. Found 457.1707.



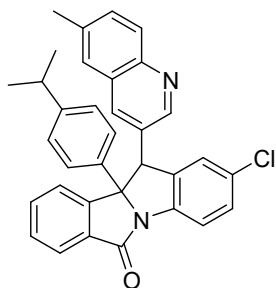
(5h)2-chloro-11-(6-methylquinolin-3-yl)-10b-phenyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 94-96 °C; 24.1 mg, 51% yield. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ : 8.67(s, 1H), 7.96-7.93 (m, 1H), 7.81-7.76 (m, 3H), 7.60 (d, $J = 8.0$ Hz, 1H), 7.41-7.38 (m, 3H), 7.30 (t, $J = 8.0$ Hz, 3H), 7.18-7.13 (m, 2H), 7.11-7.08(m, 1H), 7.00 (s, 1H), 6.82 (d, $J = 8.0$ Hz, 1H), 5.21 (s, 1H), 2.40 (s, 3H); **HRMS** (ESI): m/z calcd for $\text{C}_{31}\text{H}_{22}\text{ClN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 473.1415. Found 473.1413.



(5i)2-fluoro-11-(6-methylquinolin-3-yl)-10b-(p-tolyl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 203-205 °C; 25.9 mg, 55% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.65(s, 1H), 7.94-7.91 (m, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 4.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.28-7.26 (m, 3H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 1H), 7.10-7.07(m, 1H), 6.99(s, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 5.18 (s, 1H), 2.40 (s, 3H), 2.31 (s, 3H); **HRMS** (ESI): *m/z* calcd for C₃₂H₂₄FN₂O⁺ [M+H]⁺ 471.1867. Found 471.1866.

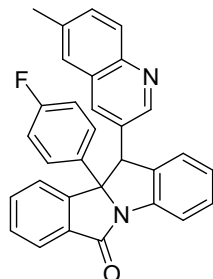


(5j)2-fluoro-10b-(4-isopropylphenyl)-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 125-127 °C; 25.4 mg, 51% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.66 (s, 1H), 7.95-7.92 (m, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.23 (s, 2H), 7.18-7.13 (m, 3H), 7.08 (t, *J* = 8.0 Hz, 1H), 6.98 (s, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 5.19 (s, 1H), 2.91-2.84 (m, 1H), 2.39 (s, 3H), 1.21 (s, 3H), 1.20 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 168.8, 161.8, 159.4, 149.5, 149.0, 147.2, 145.5, 140.0, 139.6, 139.5, 136.9, 136.1, 134.0, 132.7, 132.6, 131.9, 131.8, 128.5, 128.4, 127.5, 127.1, 126.6, 124.9, 124.5, 123.9, 118.2, 118.1, 116.0, 115.8, 113.8, 113.6, 81.6, 56.2, 33.6, 23.8, 21.4; **HRMS** (ESI): *m/z* calcd for C₃₄H₂₈FN₂O⁺ [M+H]⁺ 499.2180. Found 499.2183.

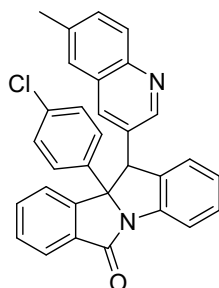


(5k)2-chloro-10b-(4-isopropylphenyl)-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 239-241 °C; 26.7 mg, 52% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.68 (s, 1H), 8.00 (s, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.29-7.25 (m, 2H), 7.23 (s, 2H), 7.16 (t, *J* = 8.0 Hz, 1H), 7.10-

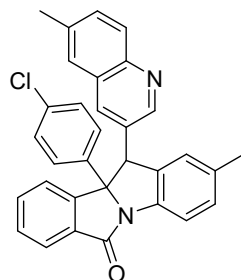
7.06 (m, 2H), 7.00 (d, $J = 8.0$ Hz, 1H), 6.96 (s, 1H), 5.18 (s, 1H), 2.90-2.83 (m, 1H), 2.39 (s, 3H), 1.21 (s, 3H), 1.19 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.6, 149.6, 149.0, 147.3, 145.6, 140.9, 140.0, 136.8, 136.2, 134.8, 133.9, 132.9, 132.9, 131.8, 131.6, 128.5, 128.5, 127.5, 127.1, 127.0, 126.6, 125.7, 124.9, 124.6, 123.9, 117.6, 81.6, 55.7, 33.6, 23.8, 21.4; HRMS (ESI): m/z calcd for $\text{C}_{34}\text{H}_{28}\text{ClN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 515.1885. Found 515.1886.



(5l)10b-(4-fluorophenyl)-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 258-260 °C; 25.1 mg, 55% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.64 (s, 1H), 7.99 (d, $J = 8.0$ Hz, 1H), 7.79-7.73 (m, 3H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.47 (t, $J = 8.0$ Hz, 1H), 7.39 (d, $J = 12.0$ Hz, 1H), 7.25-7.20 (m, 2H), 7.16 (t, $J = 8.0$ Hz, 1H), 7.12-7.04 (m, 5H), 6.97 (s, 1H), 5.17 (s, 1H), 2.38 (s, 3H); HRMS (ESI): m/z calcd for $\text{C}_{31}\text{H}_{22}\text{FN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 457.1711. Found 457.1714.

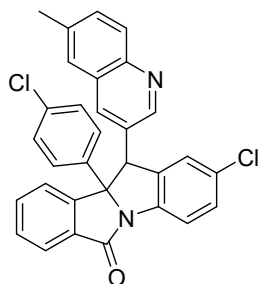


(5m)10b-(4-chlorophenyl)-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 241-243 °C; 25.5 mg, 54% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.63 (s, 1H), 7.99 (d, $J = 8.0$ Hz, 1H), 7.78 (d, $J = 12.0$ Hz, 1H), 7.72 (d, $J = 8.0$ Hz, 1H), 7.47 (t, $J = 8.0$ Hz, 2H), 7.39 (d, $J = 12.0$ Hz, 1H), 7.35 (d, $J = 8.0$ Hz, 2H), 7.22 (s, 1H), 7.18 (t, $J = 8.0$ Hz, 2H), 7.14-7.09 (m, 3H), 6.97 (s, 1H), 5.15 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.6, 149.6, 146.7, 145.6, 141.7, 139.7, 137.3, 136.8, 134.1, 134.1, 132.8, 132.0, 131.8, 129.4, 129.2, 128.7, 128.5, 127.5, 126.6, 126.5, 126.2, 125.8, 124.6, 123.7, 117.3, 80.8, 56.1, 21.4; HRMS (ESI): m/z calcd for $\text{C}_{31}\text{H}_{22}\text{ClN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 473.1415. Found 473.1413.

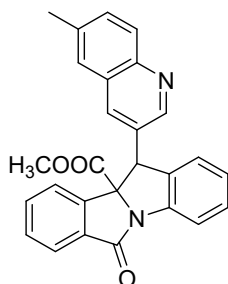


(5n)10b-(4-chlorophenyl)-2-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 224-226 °C; 23.3 mg, 48% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.64 (s,

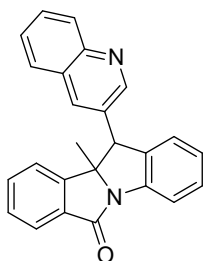
1H), 7.86 (d, $J = 8.0$ Hz, 1H), 7.79 (d, $J = 8.0$ Hz, 1H), 7.71 (d, $J = 8.0$ Hz, 2H), 7.60 (d, $J = 8.0$ Hz, 1H), 7.39 (d, $J = 8.0$ Hz, 1H), 7.34 (d, $J = 8.0$ Hz, 2H), 7.28 (s, 1H), 7.24 (s, 2H), 7.18-7.15 (m, 1H), 7.10 (t, $J = 8.0$ Hz, 1H), 7.00 (s, 1H), 6.90 (s, 1H), 5.10 (s, 1H), 2.39 (s, 3H), 2.26 (s, 3H); **HRMS** (ESI): m/z calcd for $C_{32}H_{24}ClN_2O^+$ $[M+H]^+$ 487.1572. Found 487.1573.



(5o)2-chloro-10b-(4-chlorophenyl)-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 224-226 °C; 24.3 mg, 48% yield. **1H NMR** (400 MHz, $CDCl_3$) δ : 8.63 (s, 1H), 7.95-7.91 (m, 1H), 7.80 (d, $J = 12.0$ Hz, 1H), 7.70 (d, $J = 8.0$ Hz, 2H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.41 (d, $J = 8.0$ Hz, 1H), 7.37 (d, $J = 12.0$ Hz, 2H), 7.24-7.15 (m, 4H), 7.12 (t, $J = 8.0$ Hz, 1H), 6.99 (s, 1H), 6.83 (d, $J = 8.0$ Hz, 1H), 5.13 (s, 1H), 2.41 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ : 168.7, 149.4, 146.5, 145.7, 141.3, 139.2, 137.0, 135.9, 134.3, 134.0, 133.0, 132.1, 132.0, 131.8, 129.3, 128.9, 128.5, 127.5, 126.6, 126.5, 124.7, 123.7, 118.3, 118.2, 116.3, 116.1, 113.8, 113.6, 81.3, 56.2, 21.4; **HRMS** (ESI): m/z calcd for $C_{31}H_{21}Cl_2N_2O^+$ $[M+H]^+$ 507.1025. Found 507.1023.

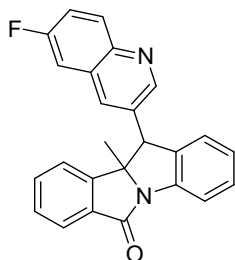


(5p)methyl 11-(6-methylquinolin-3-yl)-6-oxo-6H-isoindolo[2,1-a]indole-10b(11H)-carboxylate. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 194-196 °C; 24.4 mg, 58% yield. **1H NMR** (400 MHz, $CDCl_3$) δ : 8.57 (s, 1H), 7.93 (d, $J = 8.0$ Hz, 1H), 7.78 (d, $J = 8.0$ Hz, 1H), 7.66 (d, $J = 8.0$ Hz, 1H), 7.49-7.45 (m, 1H), 7.40-7.34 (m, 2H), 7.24-7.21 (m, 3H), 7.17 (d, $J = 4.0$ Hz, 2H), 6.97 (s, 1H), 5.45 (s, 1H), 3.75 (s, 3H), 2.39 (s, 3H); **HRMS** (ESI): m/z calcd for $C_{27}H_{21}N_2O_3^+$ $[M+H]^+$ 421.1547. Found 421.1546.



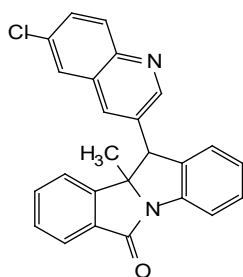
(6a)10b-methyl-11-(quinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 219-221 °C; 29.0 mg, 80% yield. **1H NMR** (400 MHz, $CDCl_3$) δ : 8.53 (s, 1H), 7.88 (t, $J = 8.0$ Hz, 2H), 7.65 (d, $J = 8.0$ Hz, 1H), 7.53 (t, $J = 8.0$ Hz, 1H), 7.49-7.46 (m, 1H), 7.43 (d, $J = 8.0$ Hz, 1H), 7.36-

7.33 (m, 1H), 7.24-7.15 (m, 5H), 6.96 (s, 1H), 4.61 (s, 1H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.1, 150.5, 147.8, 146.9, 139.2, 137.8, 134.1, 133.6, 132.7, 132.5, 129.2, 129.2, 128.8, 128.5, 127.7, 127.4, 126.6, 126.6, 125.3, 124.5, 122.8, 117.4, 76.0, 54.3, 28.3; HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{19}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 363.1492. Found 363.1491.



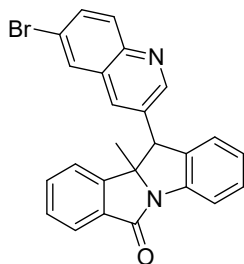
(6b) 11-(6-fluoroquinolin-3-yl)-10b-methyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 255-257 °C; 23.6 mg, 62% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.47 (s, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.85 (t, J = 4.0 Hz, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.48 (t, J = 8.0 Hz, 1H), 7.33-7.27 (m, 2H), 7.21-7.16 (m, 4H), 7.05 (d, J = 8.0 Hz, 1H), 6.91 (s, 1H), 4.60 (s, 1H), 1.86 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.0, 159.1, 149.9, 147.7, 144.0, 139.3, 137.5, 134.4, 133.5, 133.4, 132.7, 132.6, 131.4, 131.3, 129.4, 128.6, 126.5, 125.4, 124.6, 122.8, 119.6, 119.4, 117.5, 110.7, 110.5, 76.0, 54.2, 28.3; HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{18}\text{FN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 381.1398. Found 381.1399.



(6c) 11-(6-chloroquinolin-3-yl)-10b-methyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

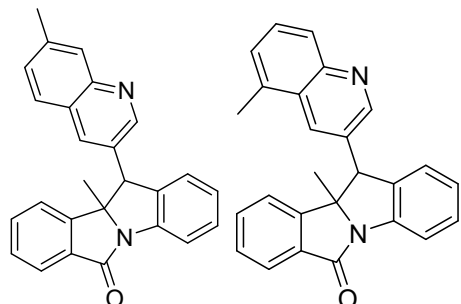
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 159-161 °C; 27.7 mg, 70% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.49 (s, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.50-7.45 (m, 2H), 7.43 (s, 1H), 7.29-7.27 (m, 1H), 7.21-7.16 (m, 4H), 6.88 (s, 1H), 4.60 (s, 1H), 1.86 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.0, 150.7, 147.6, 145.2, 139.3, 137.5, 134.6, 133.2, 132.7, 132.6, 132.5, 130.5, 130.2, 129.4, 128.6, 128.1, 126.5, 126.3, 125.4, 124.6, 122.7, 117.5, 76.0, 54.2, 28.2; HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{18}\text{ClN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 397.1102. Found 397.1101.



(6d) 11-(6-bromoquinolin-3-yl)-10b-methyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

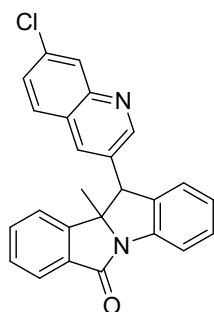
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); white solid, m.p. = 301-303 °C; 18.0 mg, 41% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.51 (s, 1H), 7.89 (d, J =

8.0 Hz, 1H), 7.73 (d, $J = 12.0$ Hz, 1H), 7.67 (d, $J = 4.0$ Hz, 1H), 7.59 (d, $J = 8.0$ Hz, 2H), 7.50-7.47 (m, 1H), 7.30-7.27 (m, 1H), 7.21-7.19 (m, 4H), 6.87 (s, 1H), 4.60 (s, 1H), 1.86 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.0, 150.9, 147.6, 145.5, 139.3, 137.5, 134.5, 133.1, 132.7, 132.6, 130.6, 129.7, 129.4, 128.7, 128.6, 126.5, 125.4, 124.7, 122.7, 120.7, 117.5, 76.0, 54.2, 28.2; HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{18}\text{BrN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 441.0597. Found 441.0595.



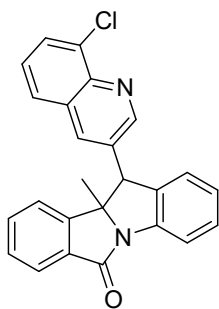
(6e,6e')10b-methyl-11-(7-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one/10b-methyl-11-(5-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 77-79 °C; 31.6 mg, 84% yield (1.38:1). ^1H NMR (400 MHz, CDCl_3) δ : 8.49 (d, $J = 8.0$ Hz, 1H), 7.89 (d, $J = 8.0$ Hz, 1H), 7.70 (t, $J = 8.0$ Hz, 1H), 7.67-7.64 (m, 1H), 7.48-7.45 (m, 1H), 7.41 (t, $J = 8.0$ Hz, 1H), 7.31 (d, $J = 8.0$ Hz, 0.54H), 7.23-7.13 (m, 6H), 6.89 (s, 0.5H), 4.60 (d, $J = 4.0$ Hz, 1H), 2.44 (s, 1.32H), 2.29 (s, 1.79H), 1.85 (d, $J = 8.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.2, 168.1, 150.5, 149.7, 147.9, 147.9, 147.1, 139.6, 139.2, 139.1, 138.2, 137.9, 134.5, 133.8, 133.2, 132.9, 132.8, 132.7, 132.6, 132.5, 130.7, 129.2, 128.9, 128.6, 128.5, 127.8, 127.3, 127.1, 127.1, 126.6, 126.5, 125.3, 124.5, 124.4, 122.8, 122.8, 117.5, 117.4, 76.0, 76.0, 54.5, 54.3, 28.1, 26.9, 21.7, 18.2; HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{21}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 377.1648. Found 377.1648.



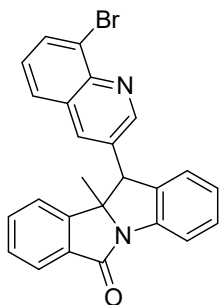
(6f)11-(7-chloroquinolin-3-yl)-10b-methyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 77-79 °C; 22.6 mg, 57% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.20 (s, 1H), 7.90 (d, $J = 8.0$ Hz, 1H), 7.78 (d, $J = 4.0$ Hz, 1H), 7.72 (d, $J = 8.0$ Hz, 2H), 7.47 (t, $J = 8.0$ Hz, 3H), 7.23-7.10 (m, 5H), 4.63 (s, 1H), 1.87 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ : 167.9, 150.8, 147.8, 147.4, 139.2, 137.5, 134.7, 132.9, 132.6, 131.1, 130.9, 129.4, 128.9, 128.6, 128.2, 126.8, 126.5, 125.5, 125.3, 124.8, 122.8, 117.5, 75.8, 54.7, 28.5. HRMS (ESI): m/z calcd for $\text{C}_{25}\text{H}_{18}\text{ClN}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 397.1102. Found 397.1104.



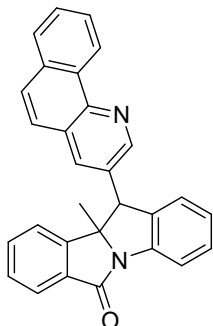
(6g)11-(8-chloroquinolin-3-yl)-10b-methyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 255-257 °C; 21.4 mg, 54% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.70 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.50-7.46 (m, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.30-7.27 (m, 1H), 7.20-7.17 (m, 4H), 6.94 (s, 1H), 4.64 (s, 1H), 1.87 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 168.0, 151.2, 147.6, 143.2, 139.2, 137.6, 134.7, 134.6, 133.0, 132.7, 132.7, 129.4, 128.9, 128.6, 126.9, 126.6, 126.5, 125.4, 124.6, 122.8, 117.5, 76.0, 54.0, 28.3; HRMS (ESI): *m/z* calcd for C₂₅H₁₈ClN₂O⁺ [M+H]⁺ 397.1102. Found 397.1104.



(6h)11-(8-bromoquinolin-3-yl)-10b-methyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

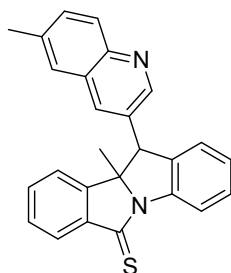
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); white solid, m.p. = 260-262 °C; 19.8 mg, 45% yield. ¹H NMR (400 MHz, CDCl₃) δ: 8.69 (s, 1H), 7.88 (t, *J* = 8.0 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.50-7.46 (m, 1H), 7.40 (d, *J* = 12.0 Hz, 1H), 7.30-7.28 (m, 1H), 7.23-7.17 (m, 5H), 6.93 (s, 1H), 4.64 (s, 1H), 1.86 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 168.0, 151.4, 147.6, 144.0, 139.2, 137.6, 134.8, 134.7, 133.0, 132.8, 129.4, 128.9, 128.7, 127.7, 127.1, 126.5, 125.4, 124.6, 124.2, 122.8, 117.5, 76.0, 54.0, 28.4; HRMS (ESI): *m/z* calcd for C₂₅H₁₈BrN₂O⁺ [M+H]⁺ 441.0597. Found 441.0599.



(6i)11-(benzo[h]quinolin-3-yl)-10b-methyl-10b,11-dihydro-6H-isoindolo[2,1-a]indol-6-one.

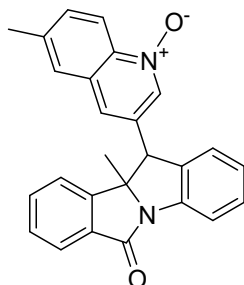
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:1 (v/v); brown solid, m.p. = 230-232 °C; 26.0 mg, 63% yield. ¹H NMR (400 MHz, CDCl₃) δ: 9.08 (d, *J* = 8.0 Hz, 1H), 8.60 (s, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.67-7.60 (m, 4H), 7.48 (t, *J* = 8.0 Hz,

1H), 7.28 (d, $J = 8.0$ Hz, 1H), 7.21-7.11 (m, 5H), 6.99 (s, 1H), 4.65 (s, 1H), 1.86 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 168.2, 148.4, 148.0, 145.1, 139.3, 138.0, 134.5, 134.2, 133.4, 132.8, 132.6, 130.9, 129.2, 128.5, 128.2, 127.9, 127.7, 127.0, 126.6, 125.9, 125.3, 125.2, 124.5, 124.2, 122.8, 117.4, 76.0, 54.3, 28.4; HRMS (ESI): m/z calcd for $\text{C}_{29}\text{H}_{21}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 413.1648. Found 413.1647.



(7)10b-methyl-11-(6-methylquinolin-3-yl)-10b,11-dihydro-6H-isoindolo[2,1-a]indole-6-thione.

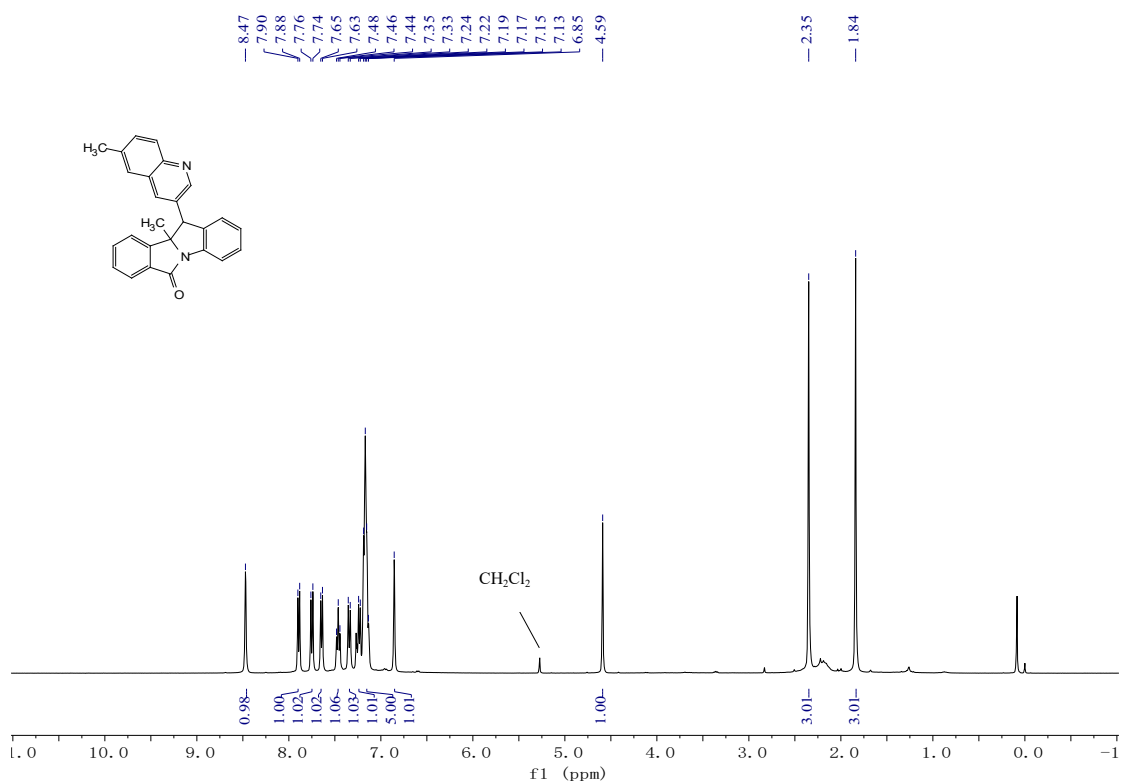
Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 1:2 (v/v); white solid, m.p. = 90-92 °C; 28.6 mg, 73% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.53 (d, $J = 8.0$ Hz, 2H), 7.88 (d, $J = 8.0$ Hz, 1H), 7.76 (d, $J = 8.0$ Hz, 1H), 7.53 (t, $J = 8.0$ Hz, 1H), 7.36 (d, $J = 8.0$ Hz, 1H), 7.29 (d, $J = 8.0$ Hz, 3H), 7.21-7.17 (m, 3H), 6.85 (s, 1H), 4.62 (s, 1H), 2.36 (s, 3H), 1.83 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ : 191.8, 149.3, 145.5, 145.0, 141.2, 139.7, 139.2, 136.7, 133.6, 132.9, 132.1, 131.8, 128.8, 128.8, 128.3, 127.6, 126.7, 126.6, 125.8, 121.9, 119.0, 83.7, 53.4, 28.0, 21.4. HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{21}\text{N}_2\text{S}^+$ $[\text{M}+\text{H}]^+$ 393.1420. Found 393.1421.



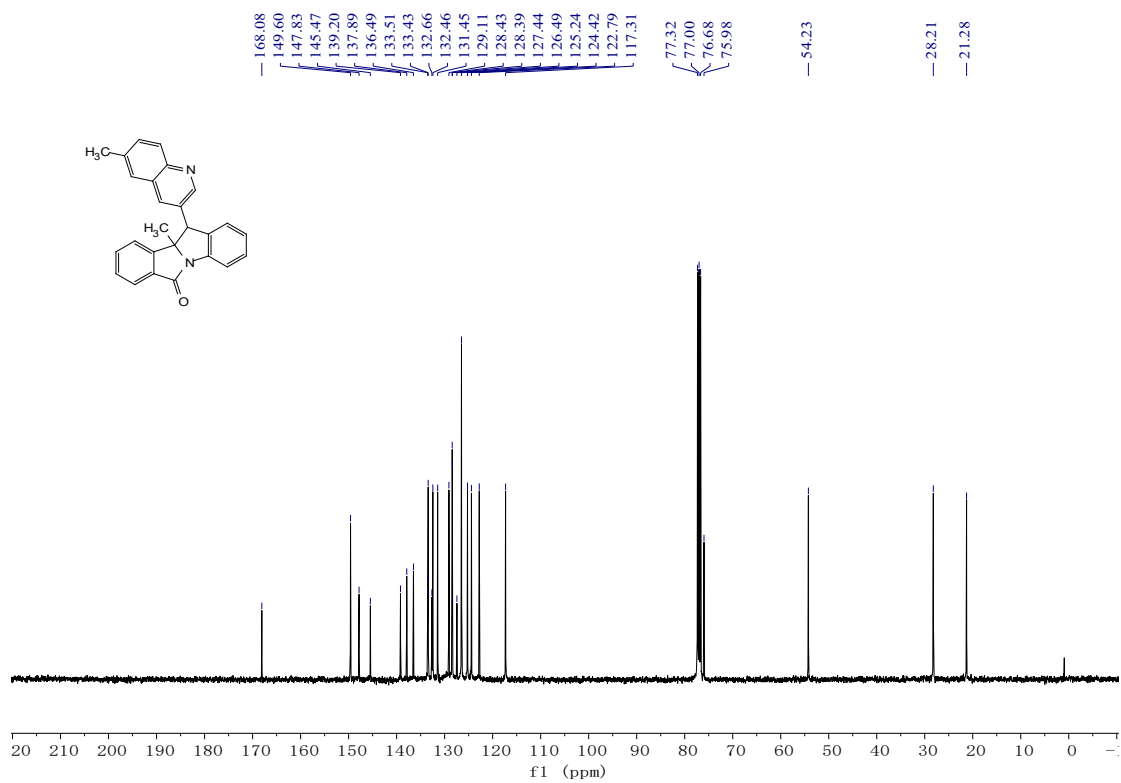
(8)6-methyl-3-(10b-methyl-6-oxo-10b,11-dihydro-6H-isoindolo[2,1-a]indol-11-yl)-114-quinolin-1-olate. Purified by chromatography on silica gel, eluting with ethyl acetate/petroleum ether 2:1 (v/v); white solid, m.p. = 267-269 °C; 33.3 mg, 85% yield. ^1H NMR (400 MHz, CDCl_3) δ : 8.37 (d, $J = 8.0$ Hz, 1H), 8.22 (s, 1H), 7.89 (d, $J = 8.0$ Hz, 1H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.49 (t, $J = 8.0$ Hz, 1H), 7.39 (d, $J = 8.0$ Hz, 1H), 7.33 (t, $J = 8.0$ Hz, 1H), 7.29 (d, $J = 8.0$ Hz, 1H), 7.24-7.17 (m, 4H), 6.48 (s, 1H), 4.45 (s, 1H), 2.36 (s, 3H), 1.84 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ : 167.9, 147.3, 139.1, 139.0, 138.3, 136.7, 134.8, 134.4, 132.7, 132.6, 132.2, 129.6, 129.5, 128.7, 126.8, 126.5, 125.4, 124.6, 123.8, 122.7, 118.9, 117.4, 75.7, 53.9, 28.2, 21.1. HRMS (ESI): m/z calcd for $\text{C}_{26}\text{H}_{21}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 393.1603. Found 393.1602.

7. NMR Charts

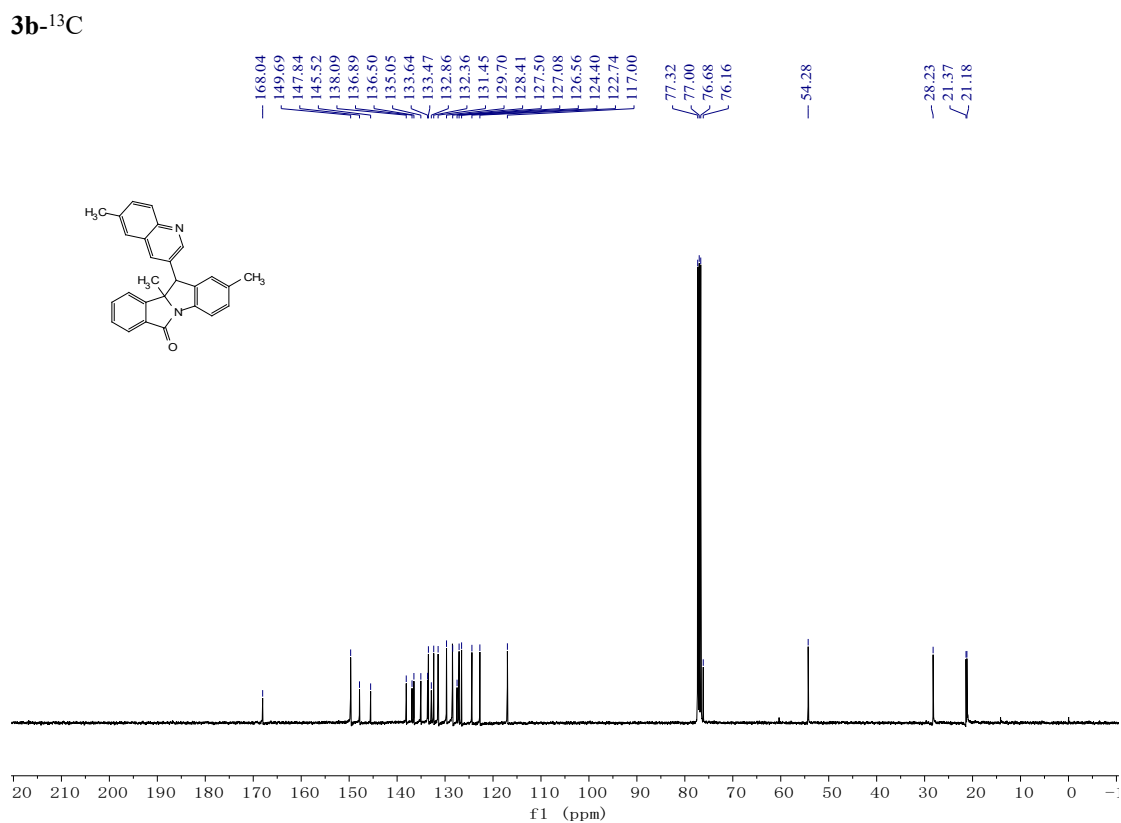
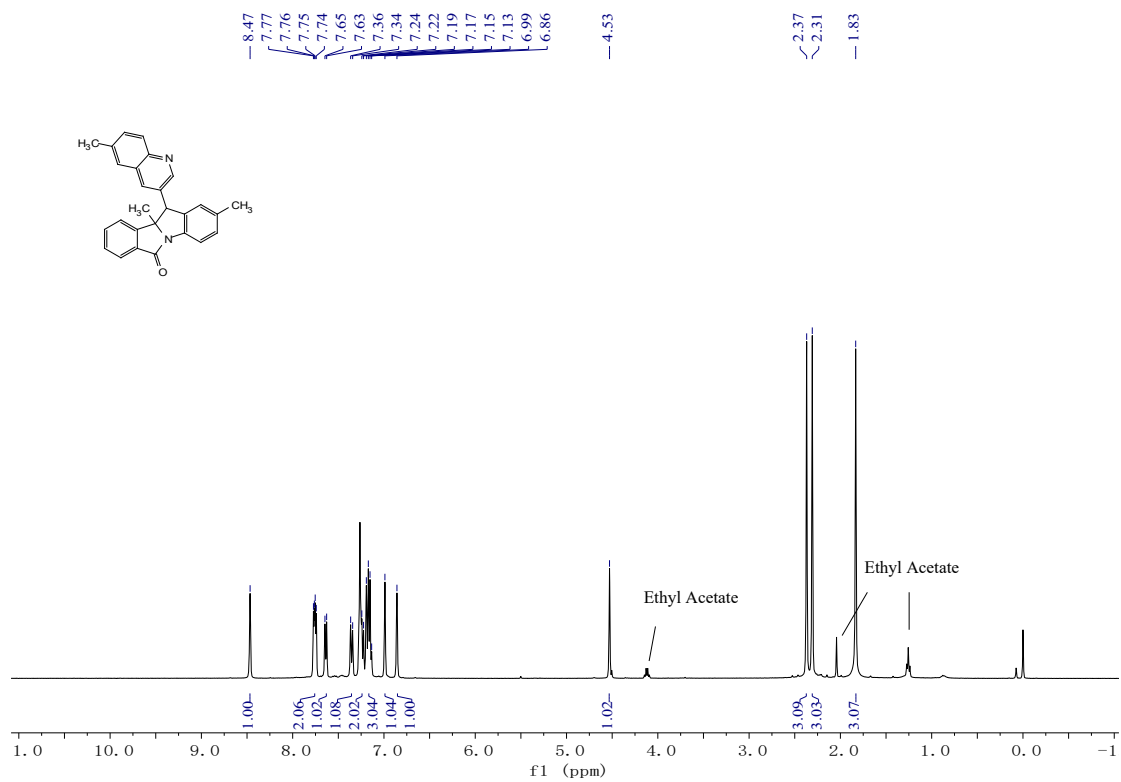
3a-¹H



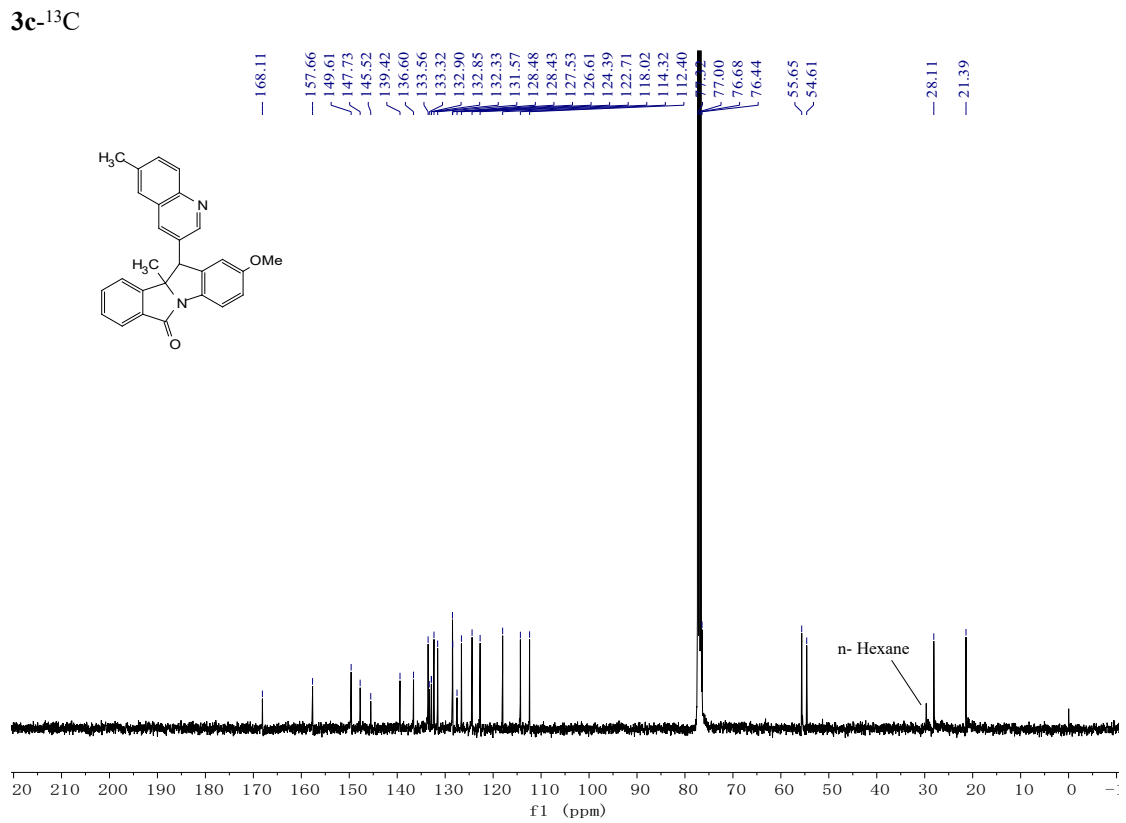
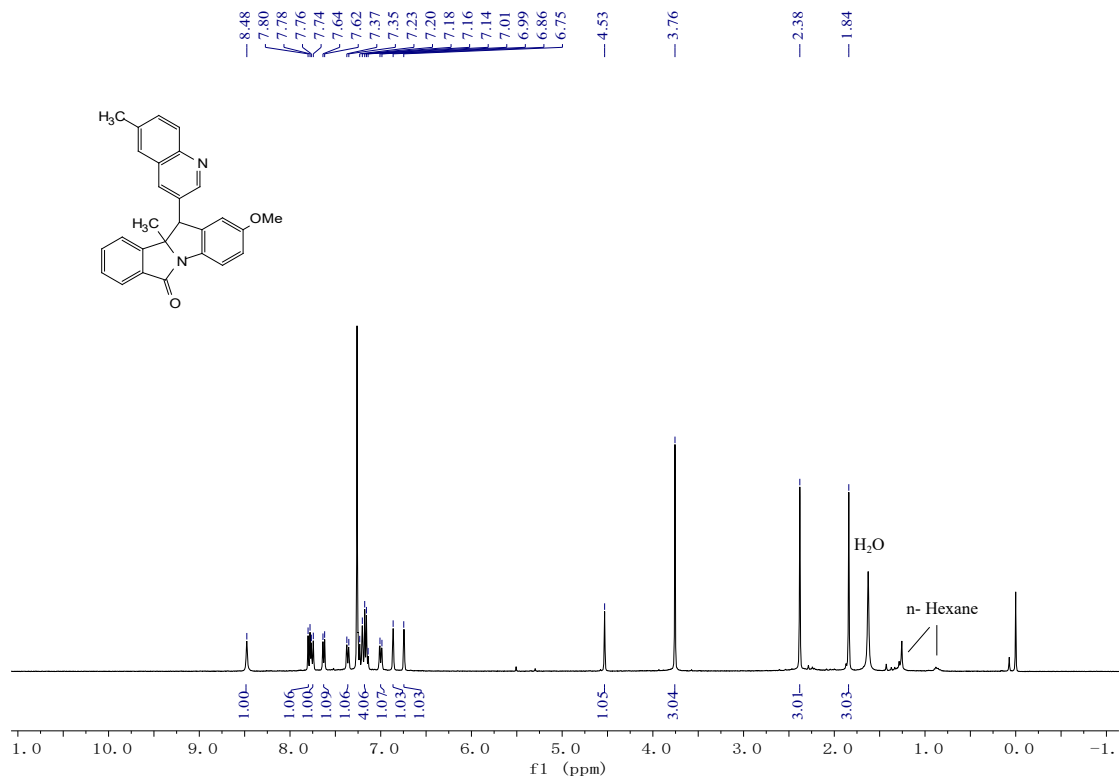
3a-¹³C



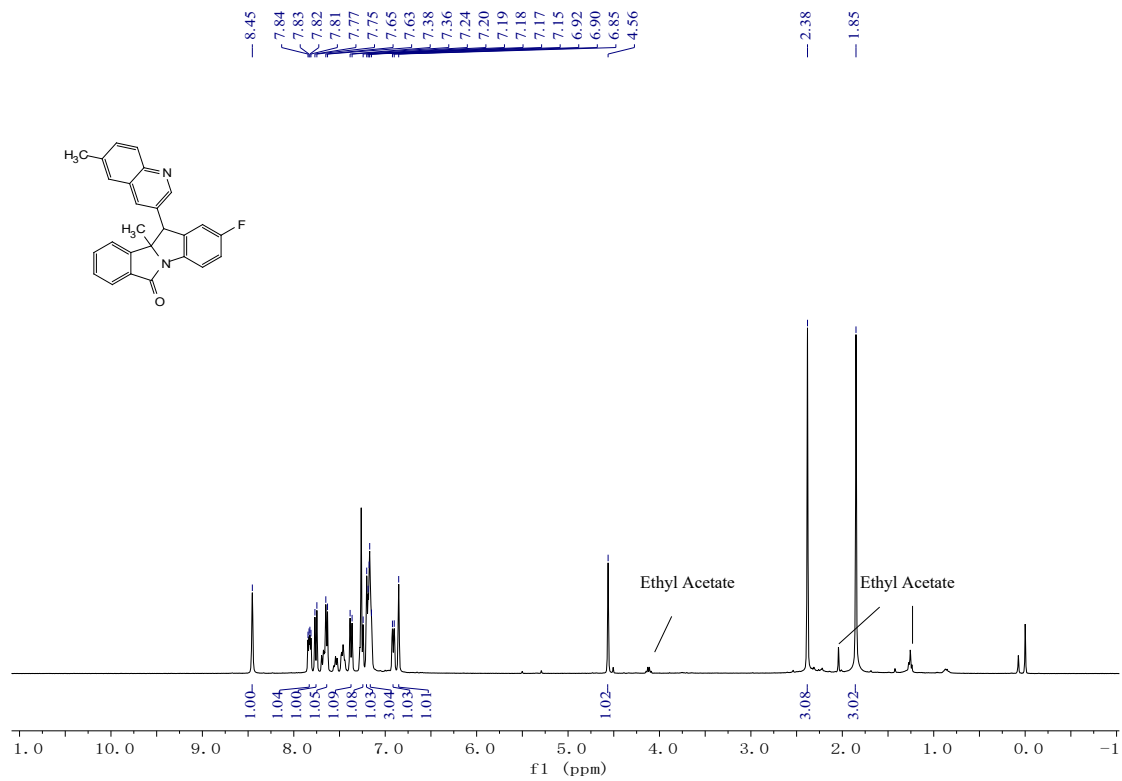
3b-¹H



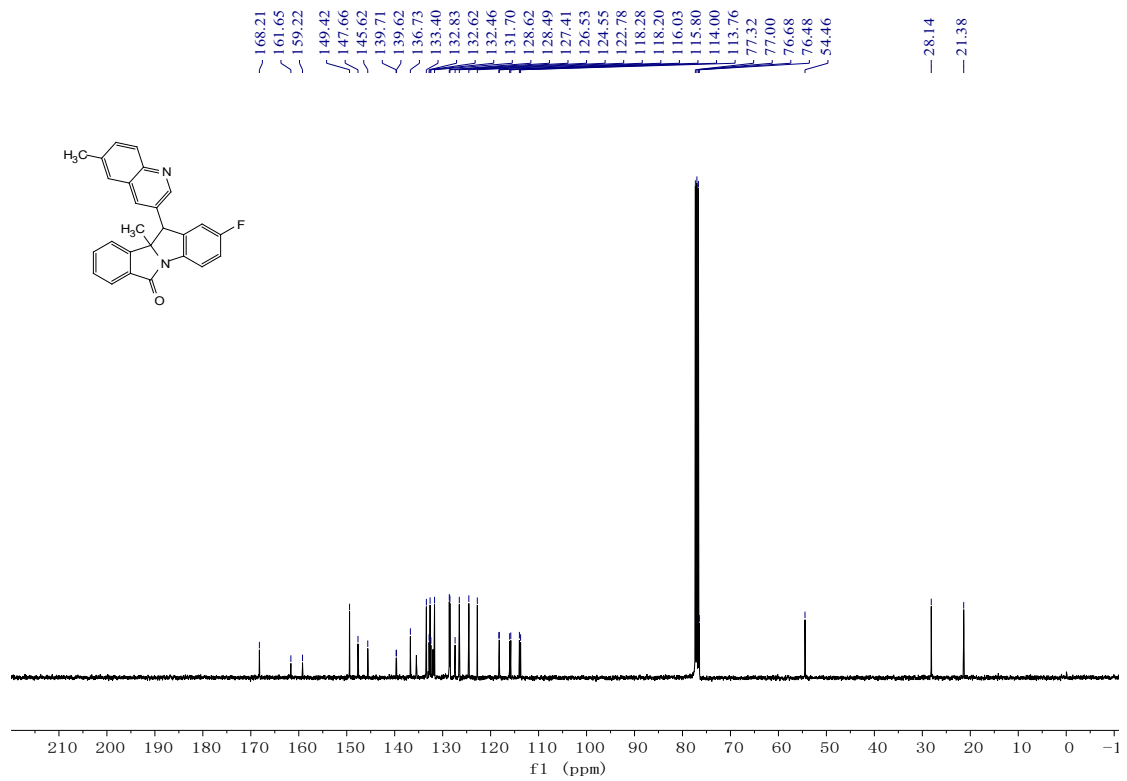
3c-¹H



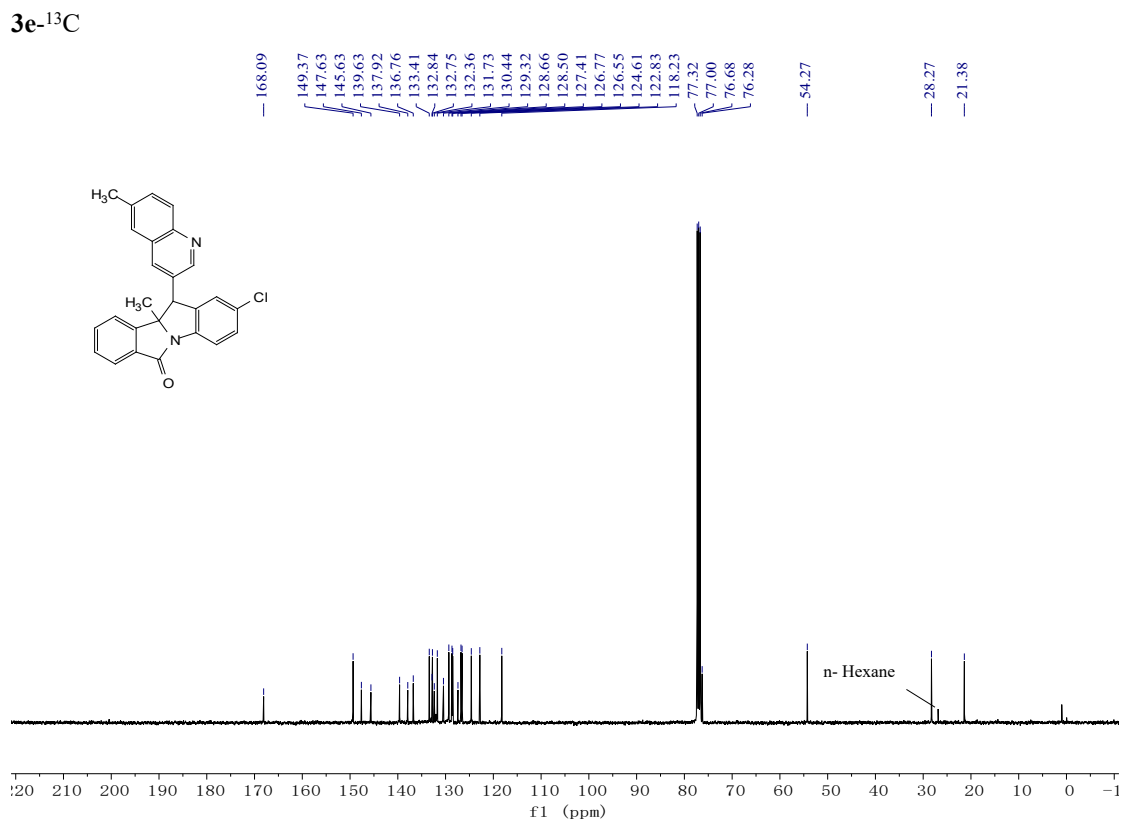
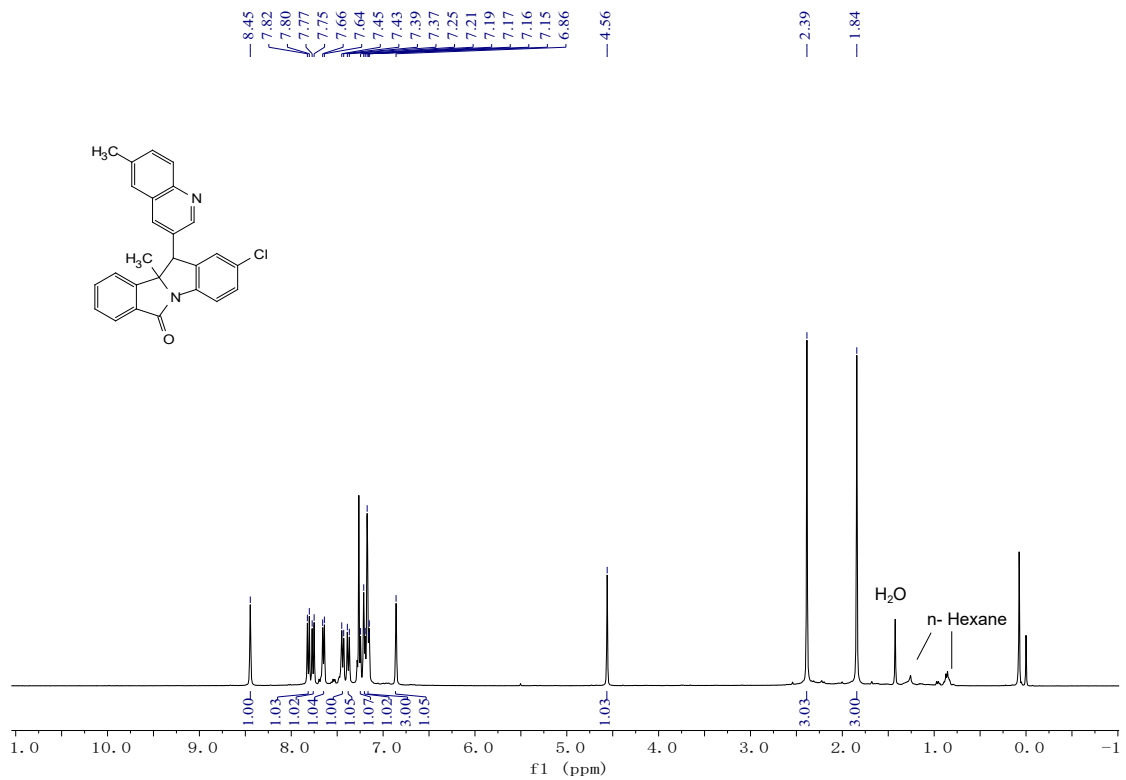
3d-¹H



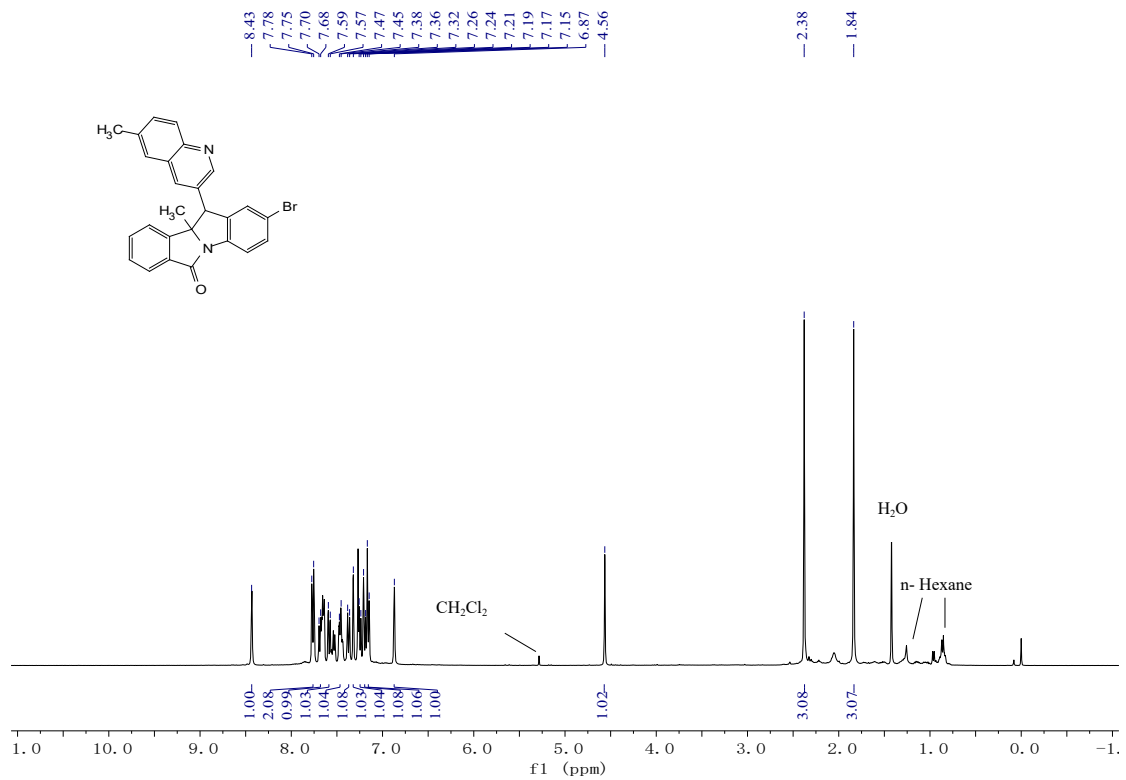
3d-¹³C



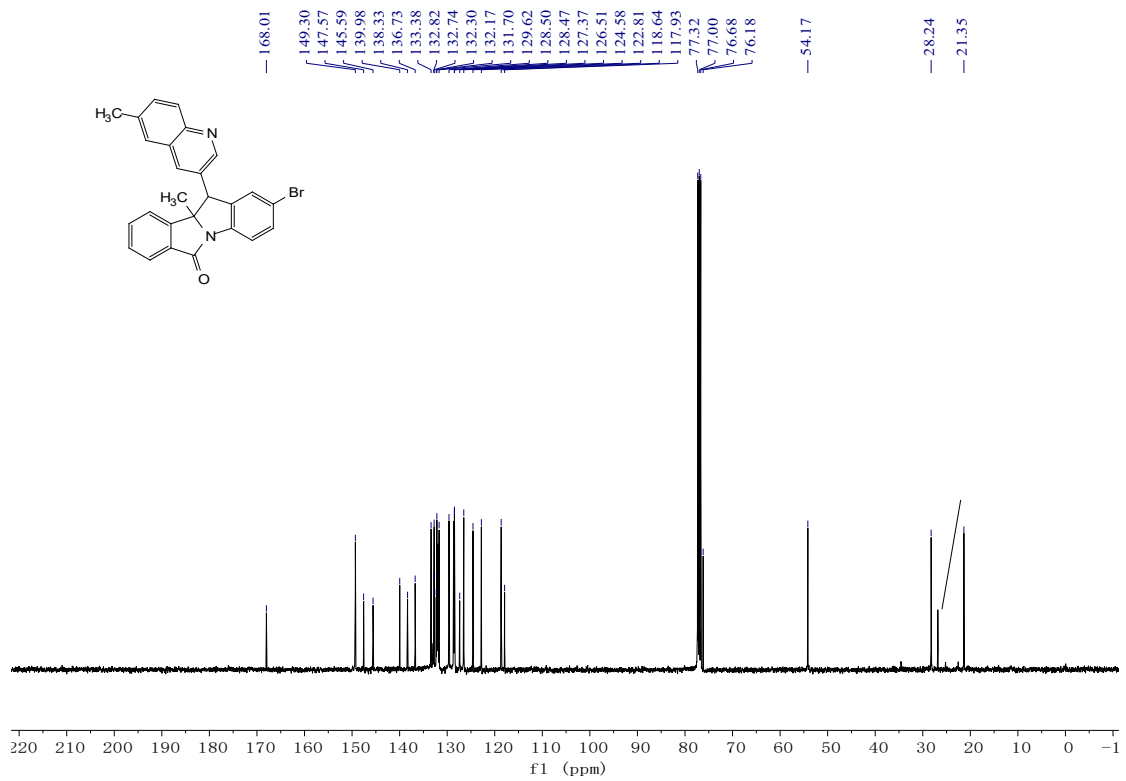
3e-¹H



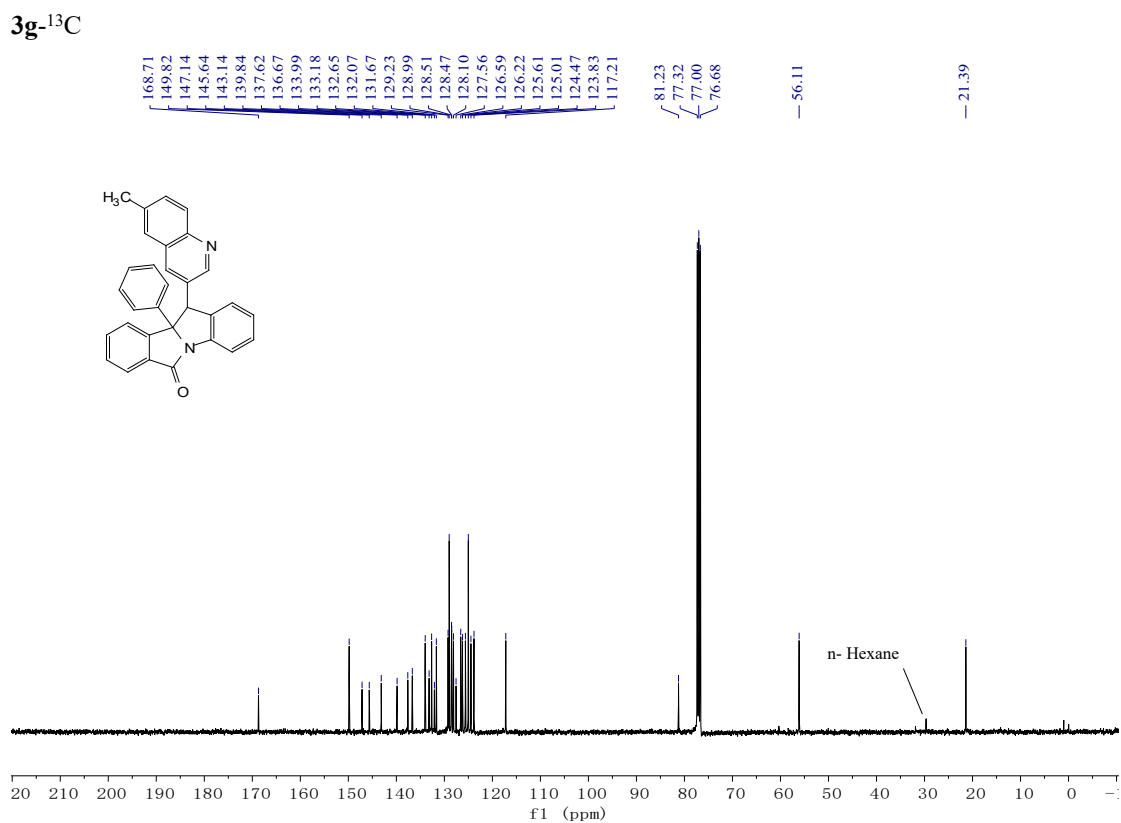
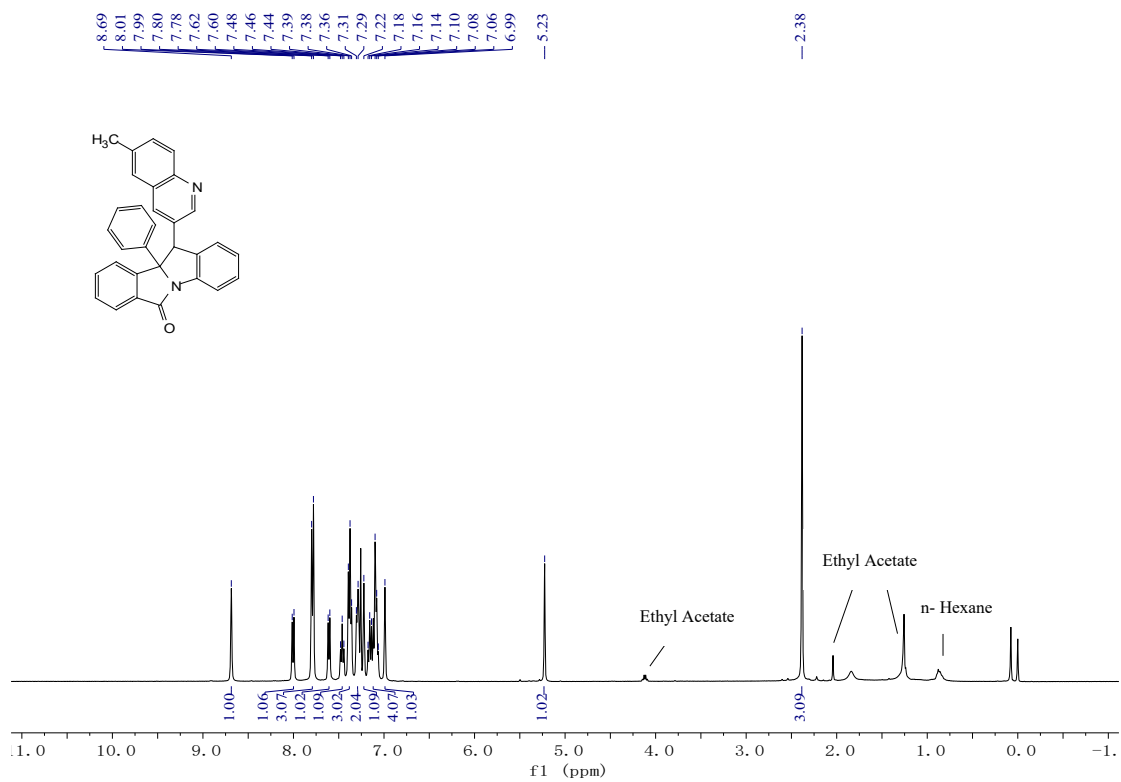
3f-¹H



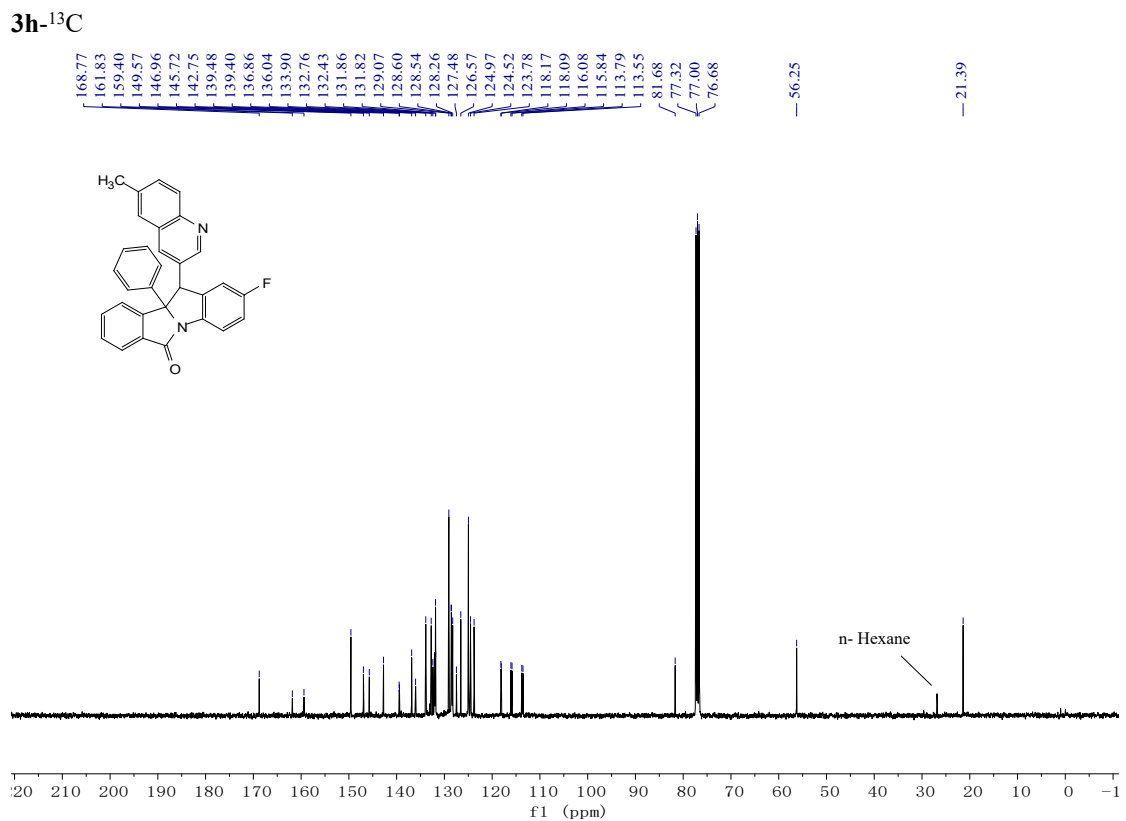
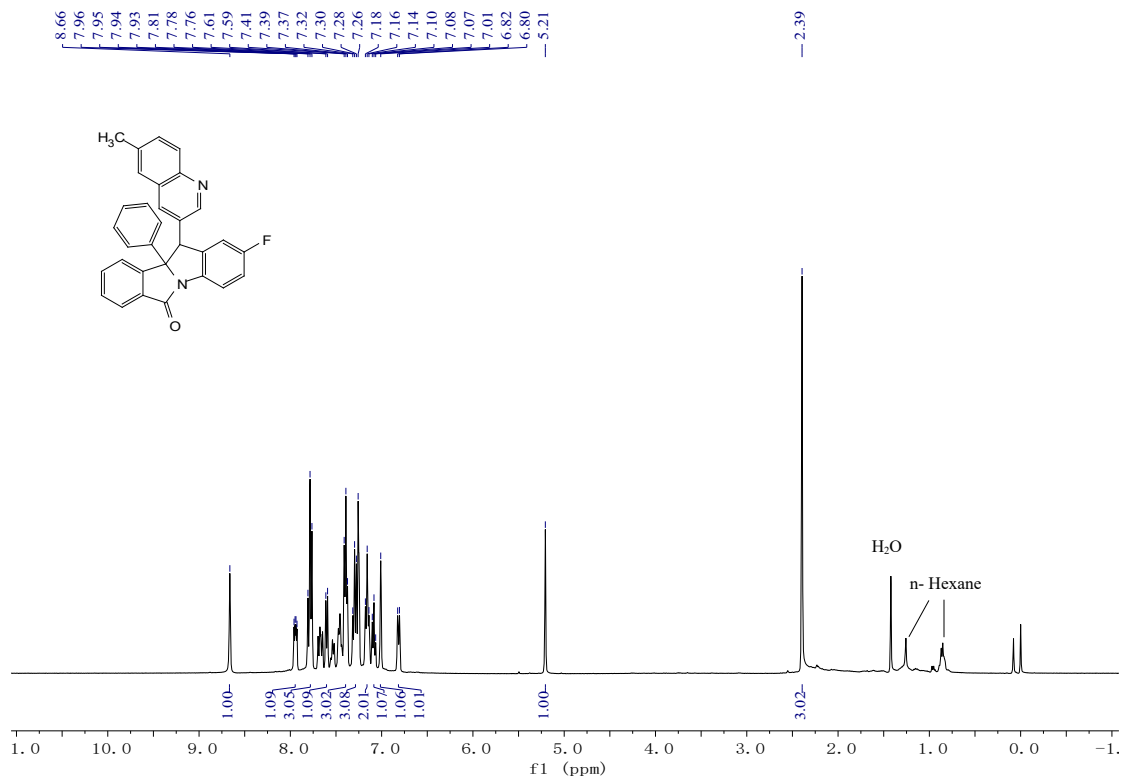
3f-¹³C



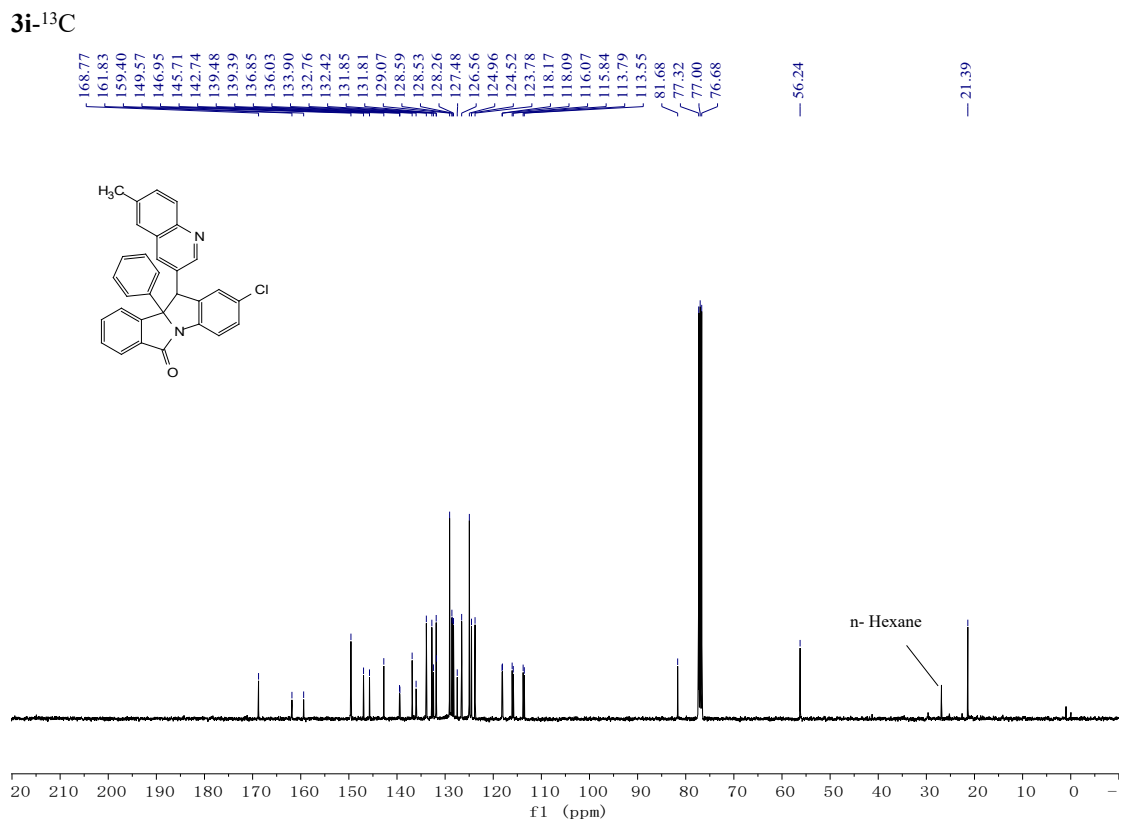
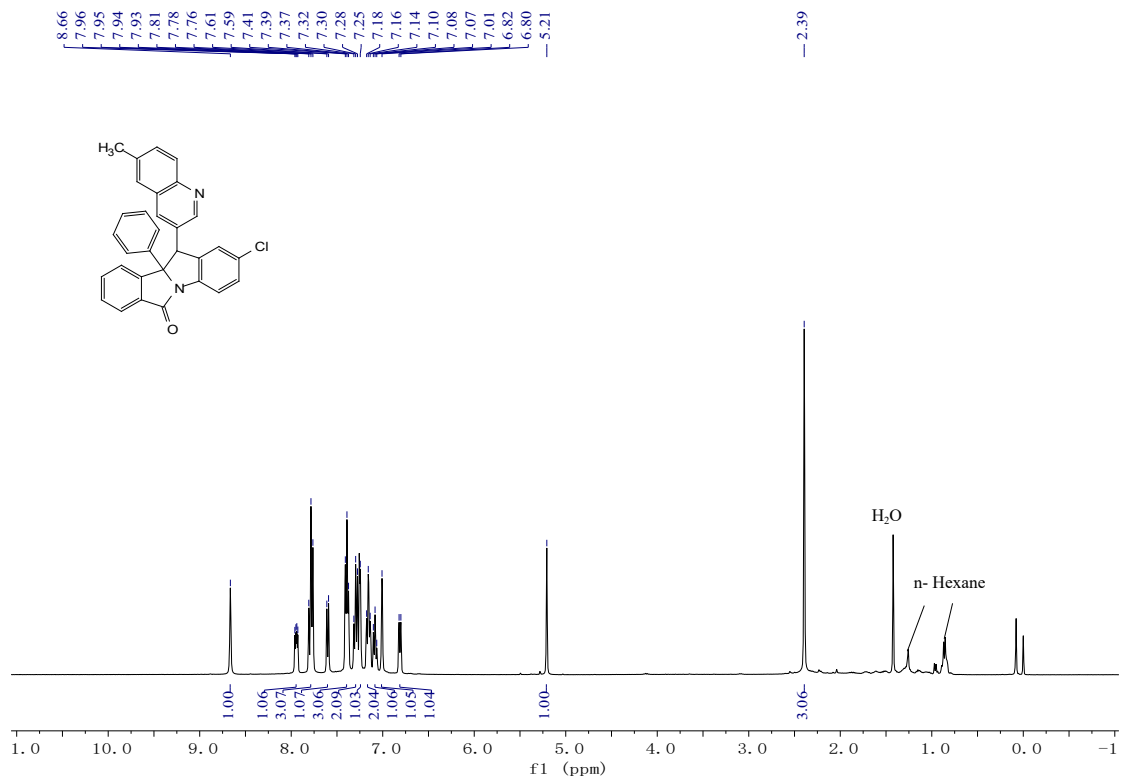
3g-¹H



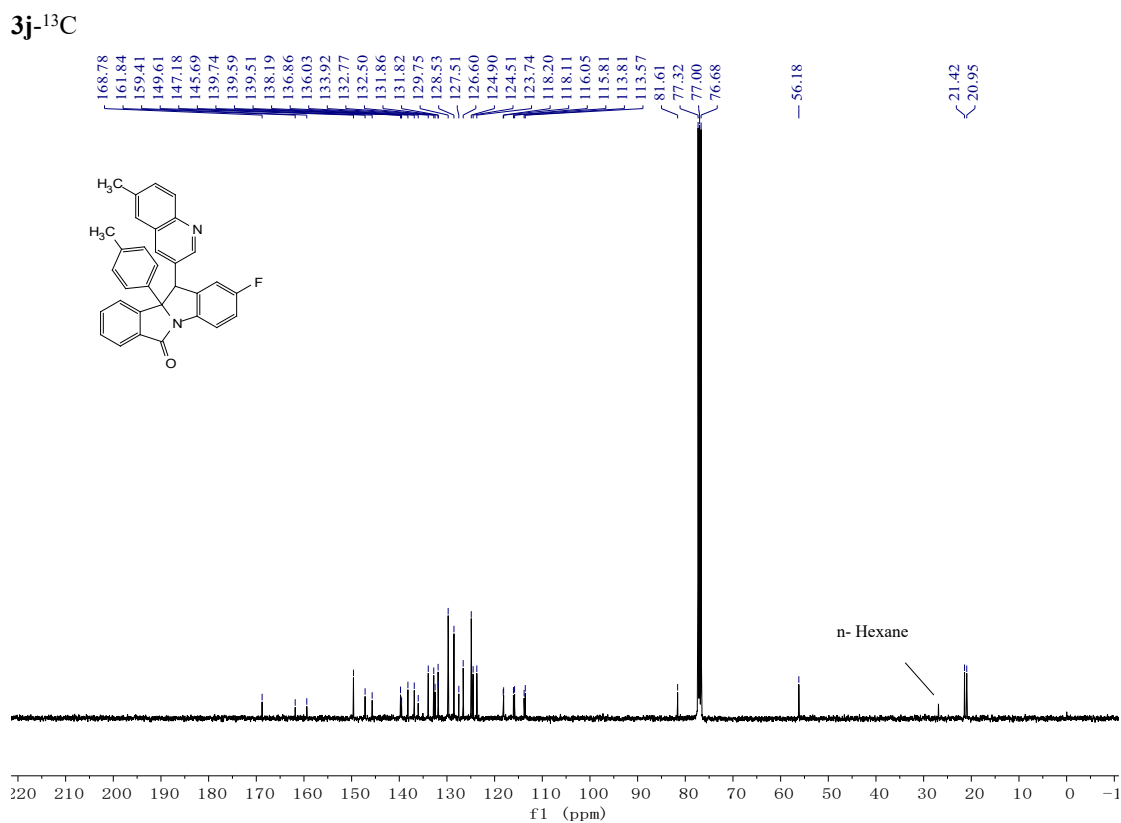
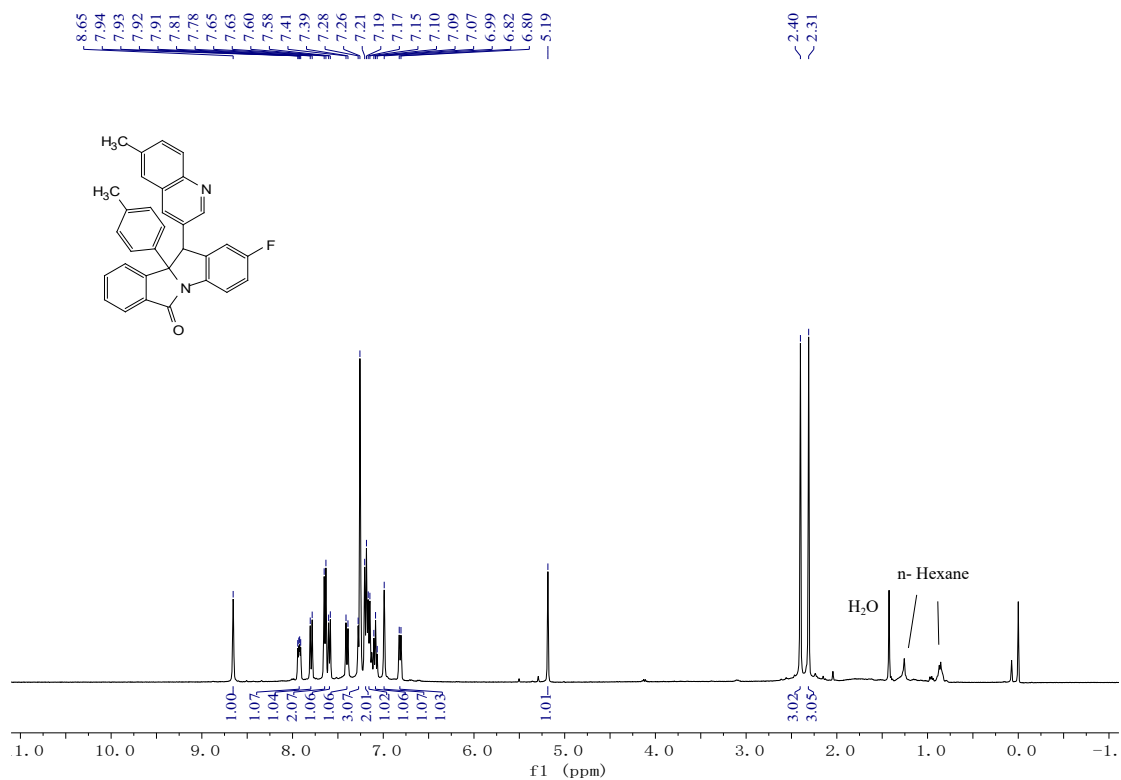
3h-¹H



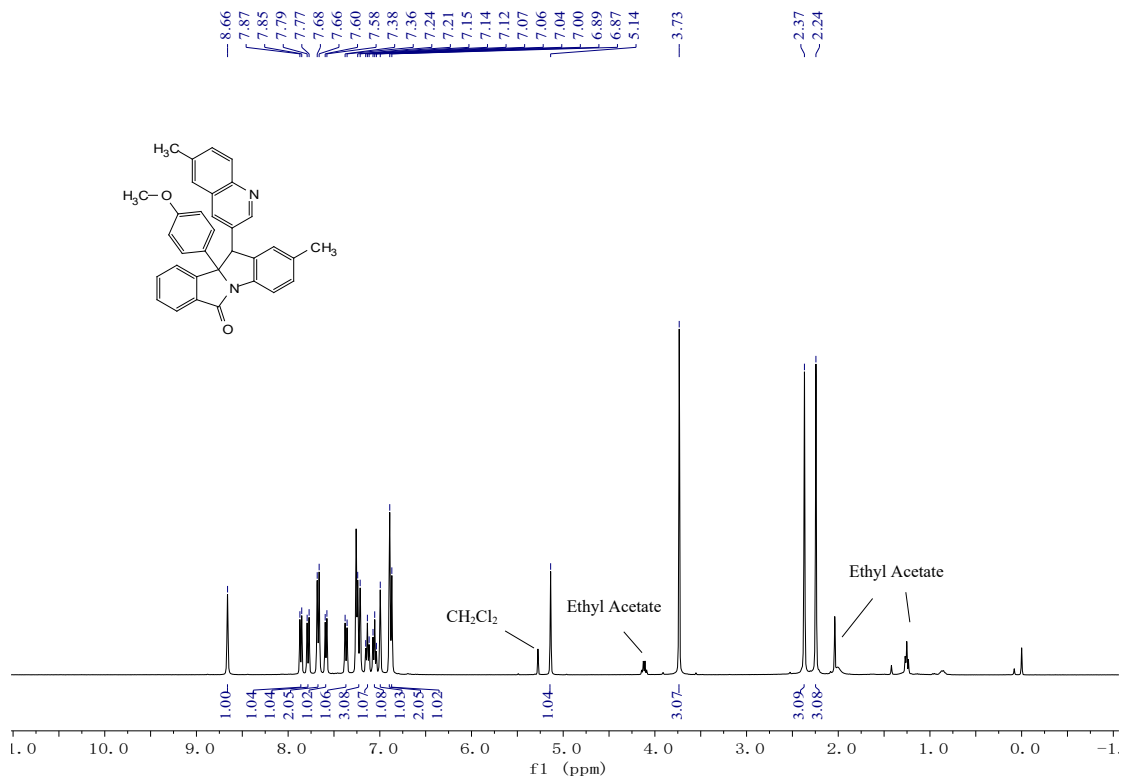
3i-¹H



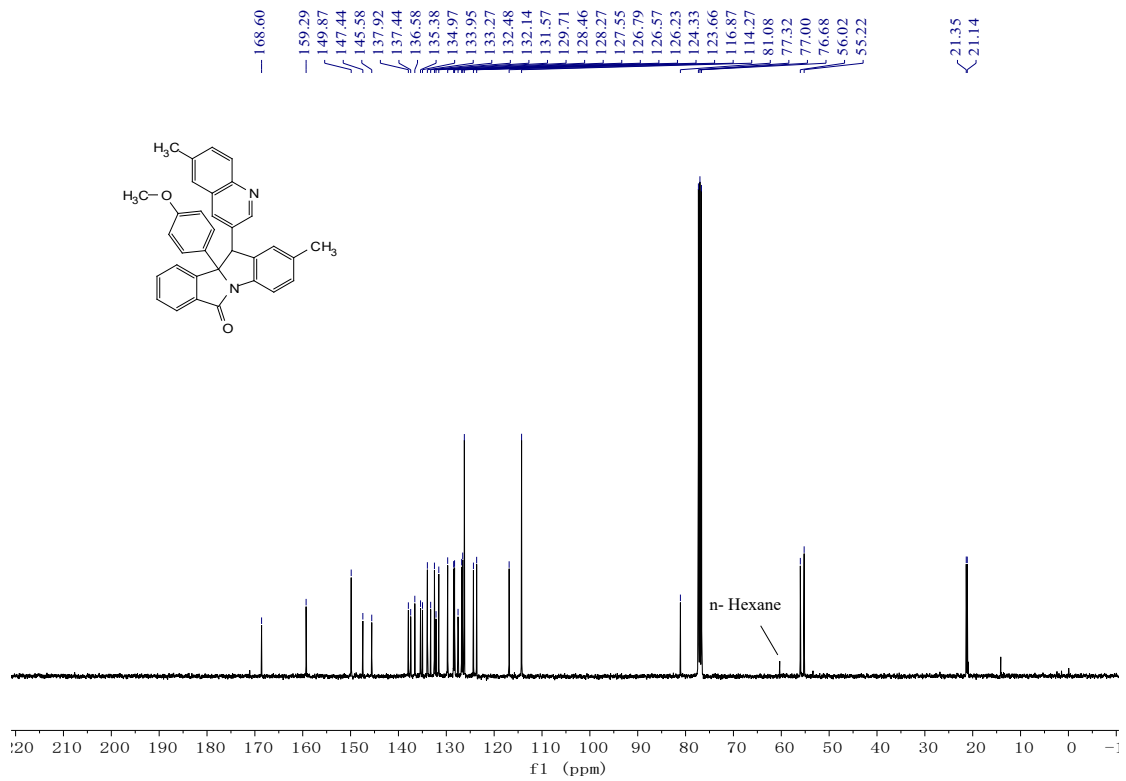
3j-¹H



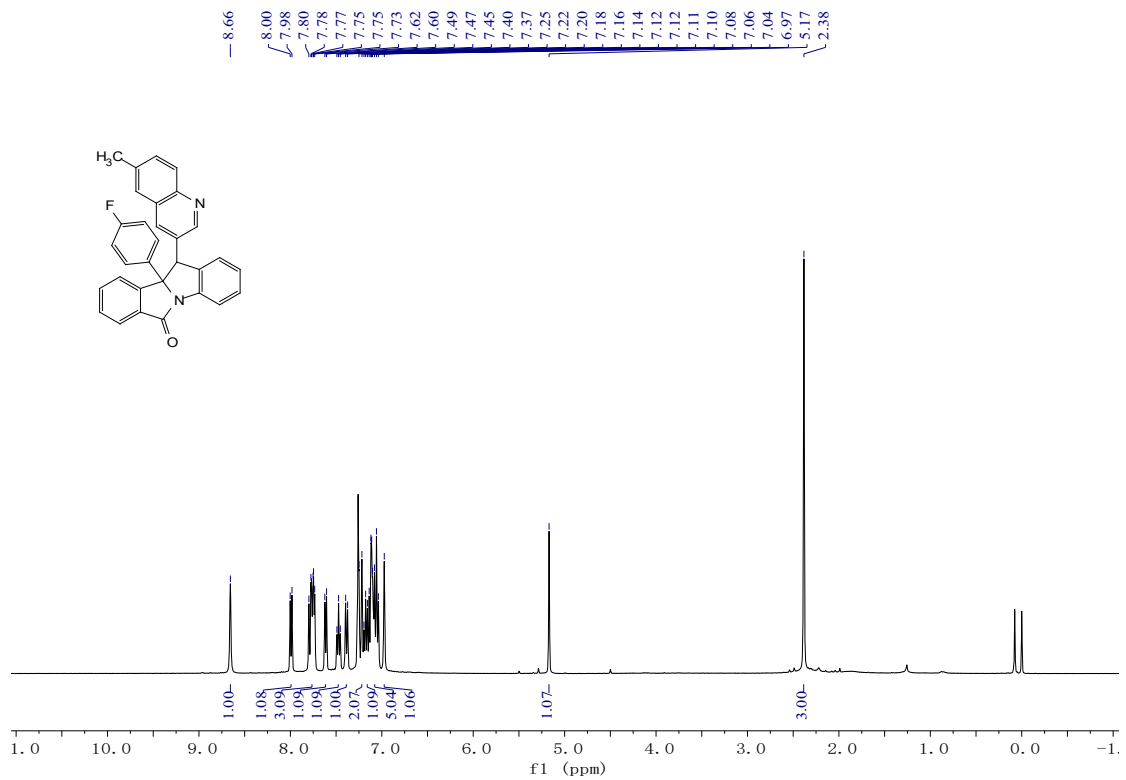
3k-¹H



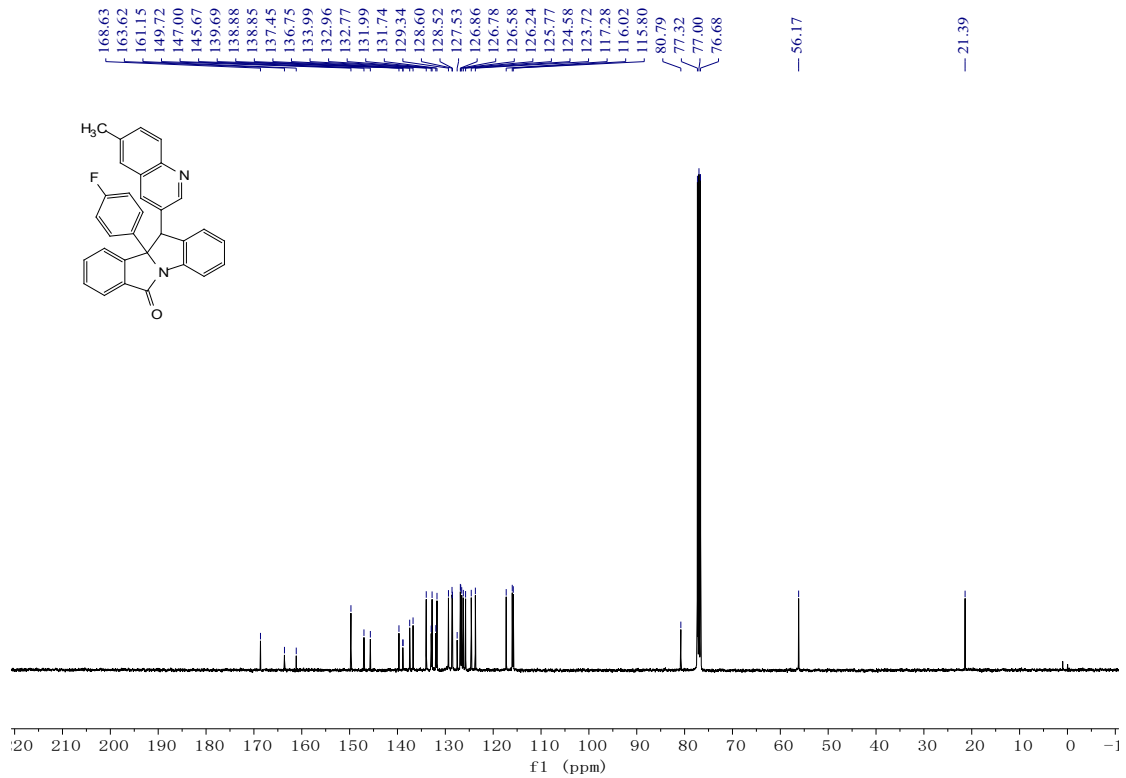
3k-¹³C



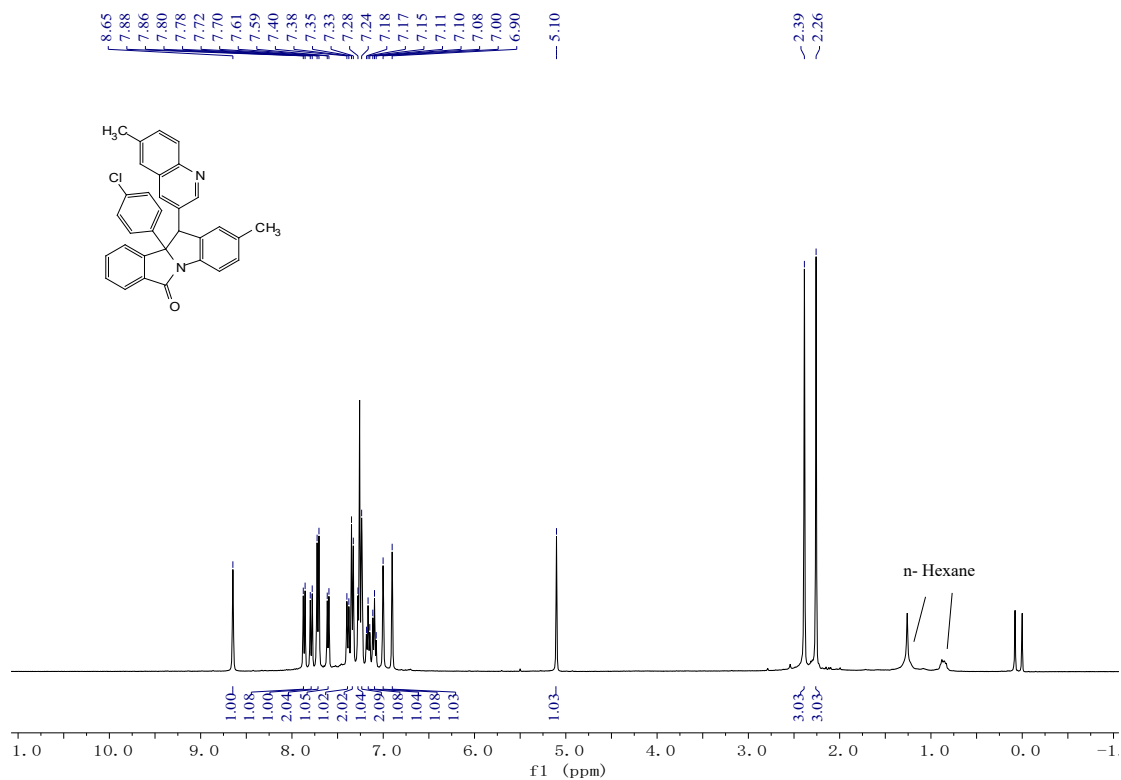
3l-¹H



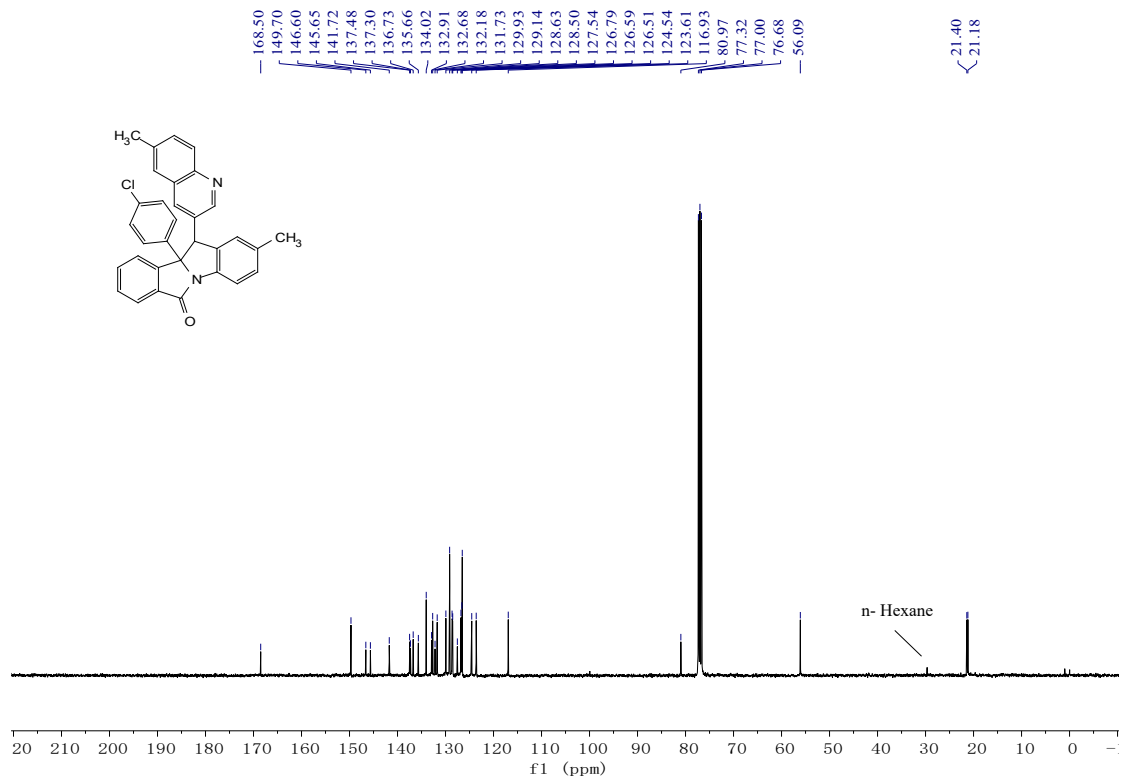
3l-¹³C



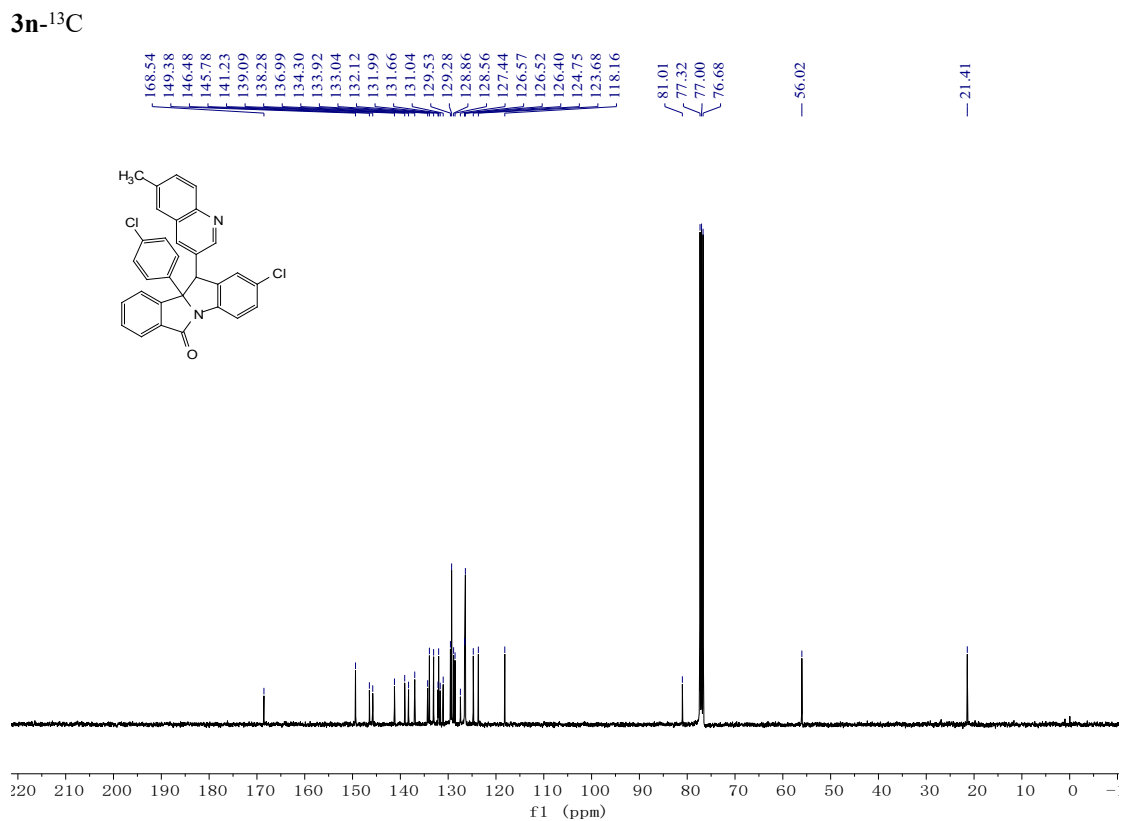
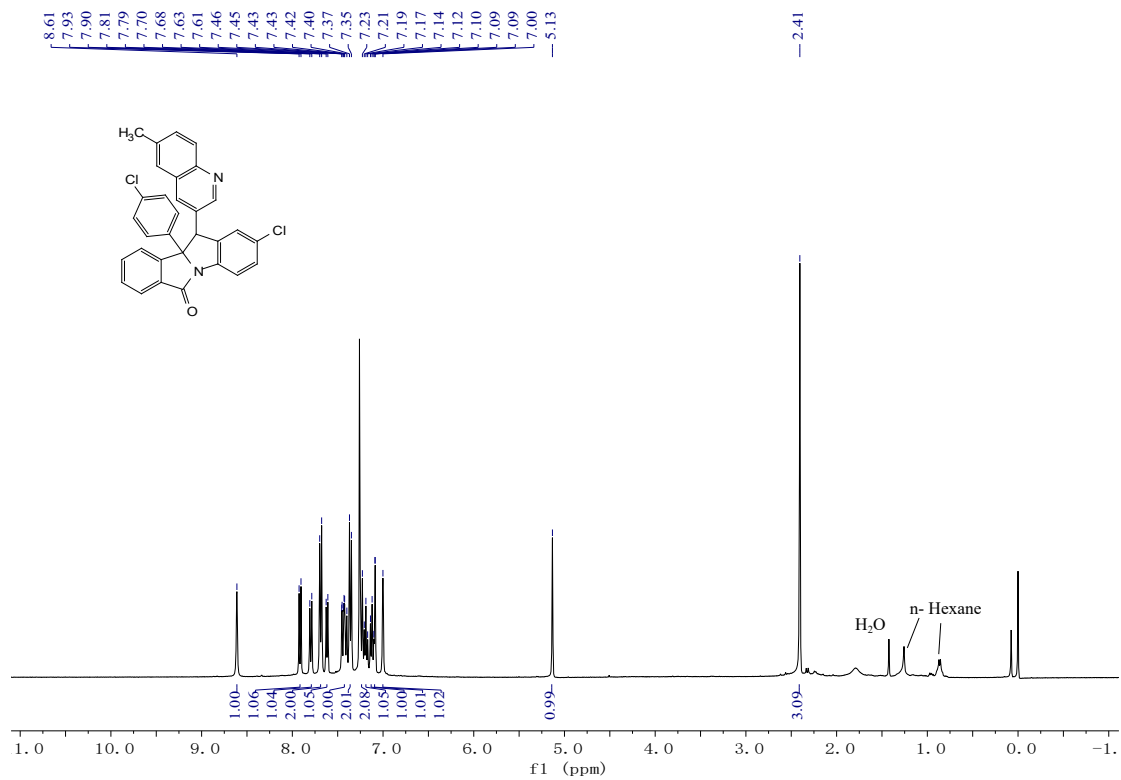
3m-¹H



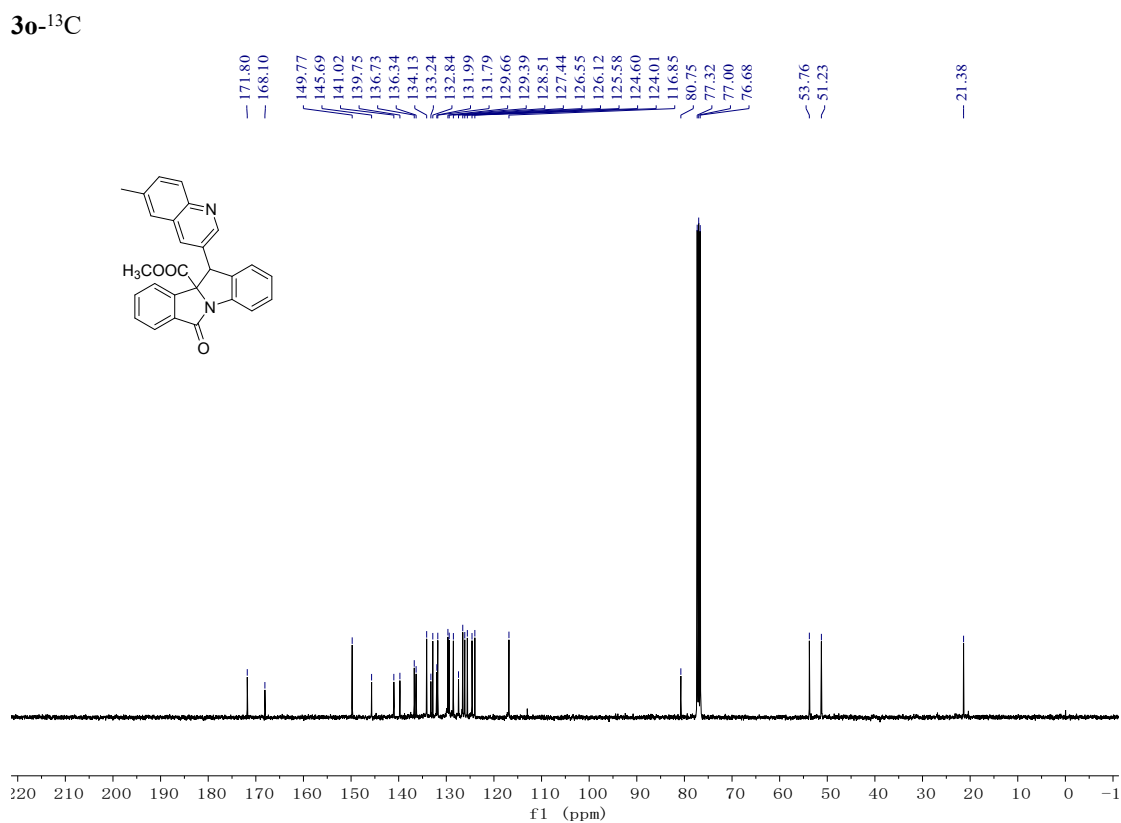
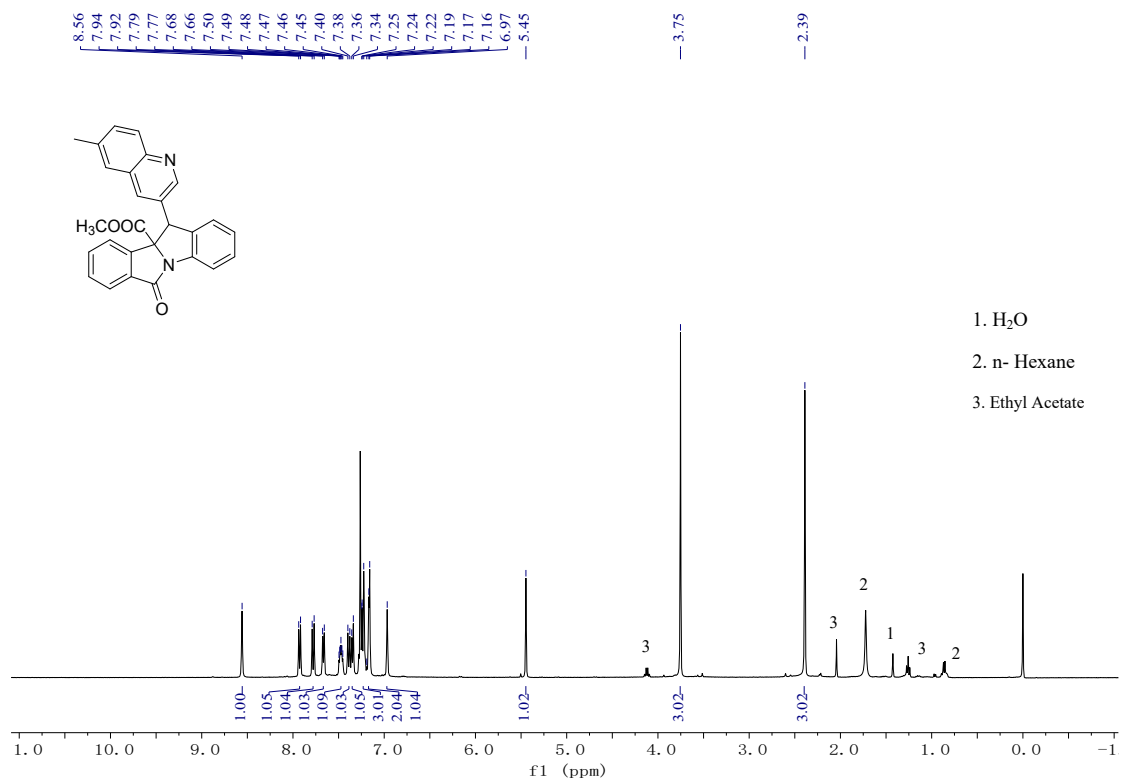
3m-¹³C



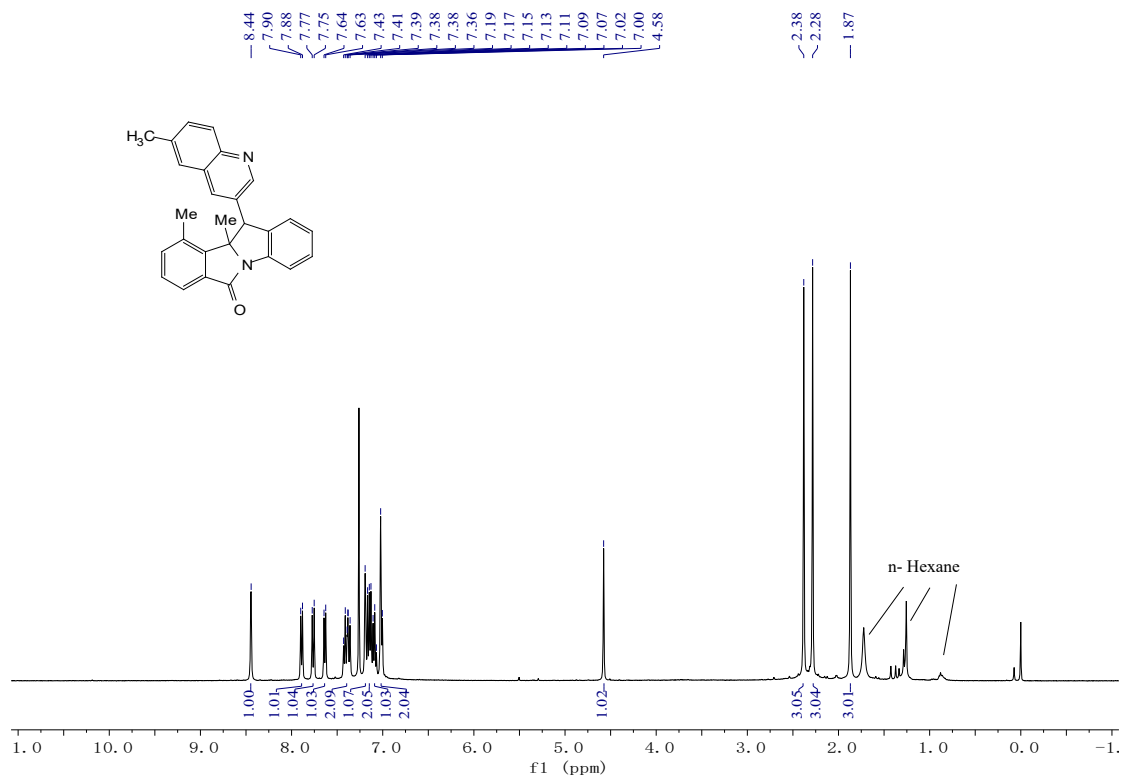
3n-¹H



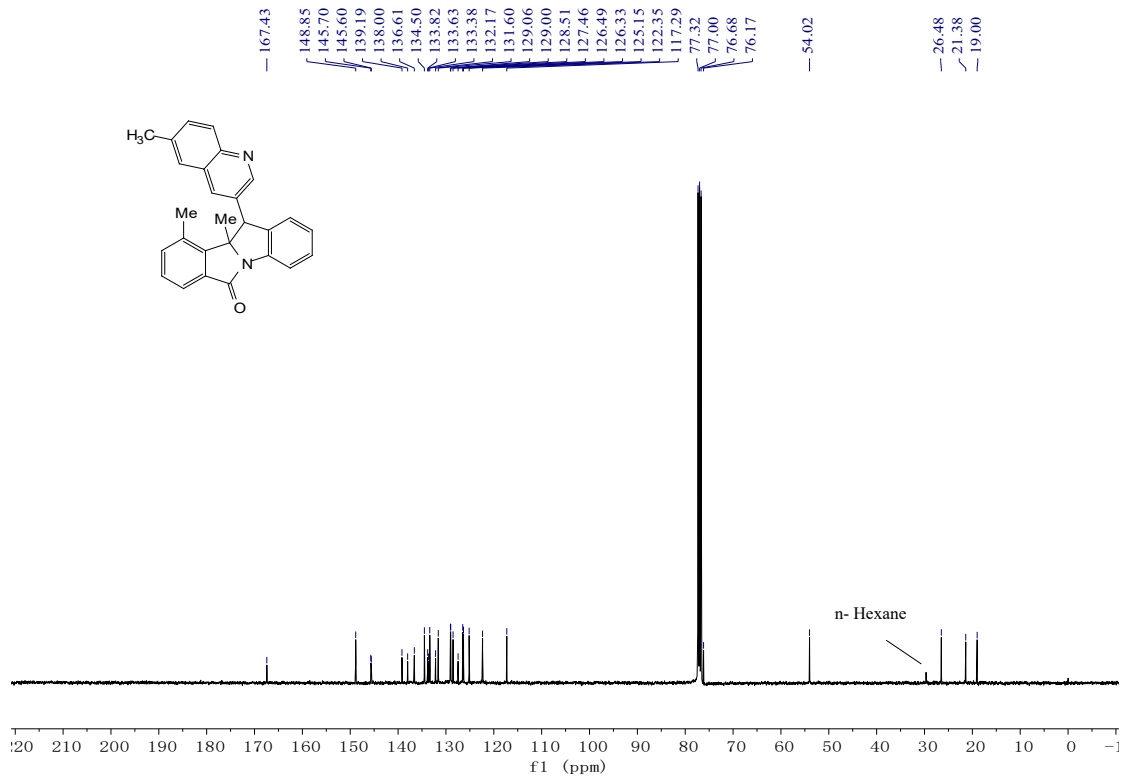
3o-¹H



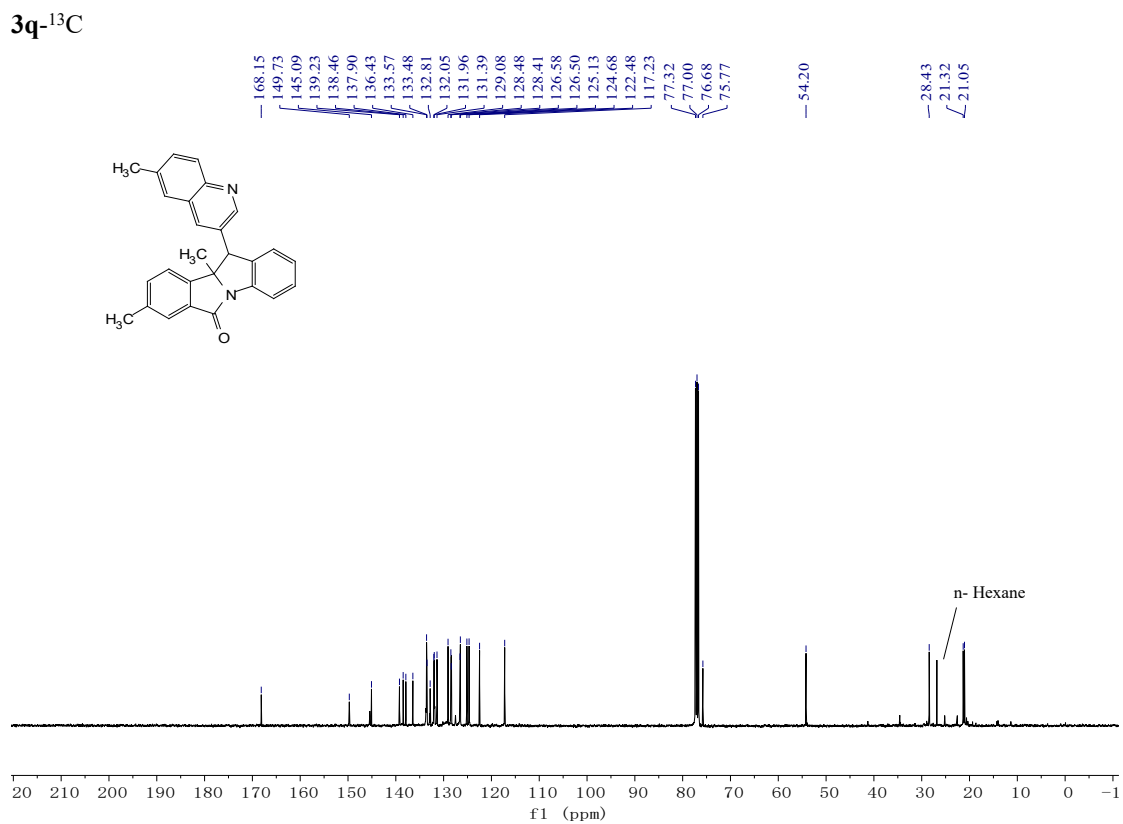
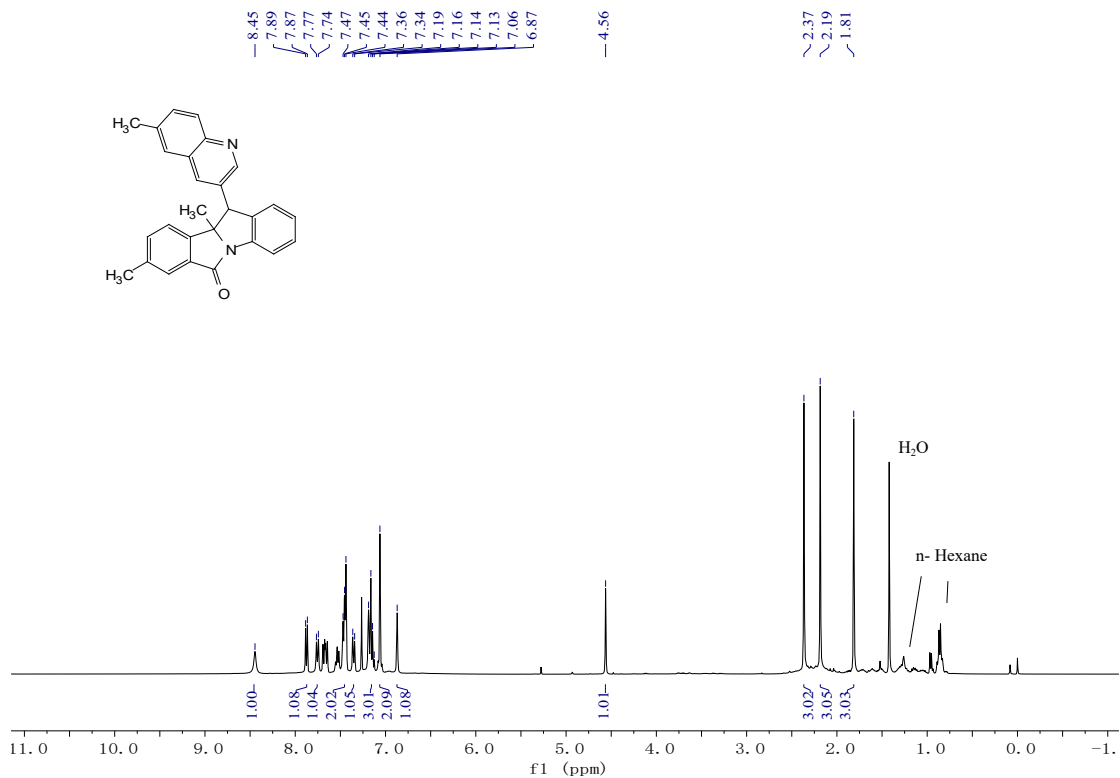
3p-¹H



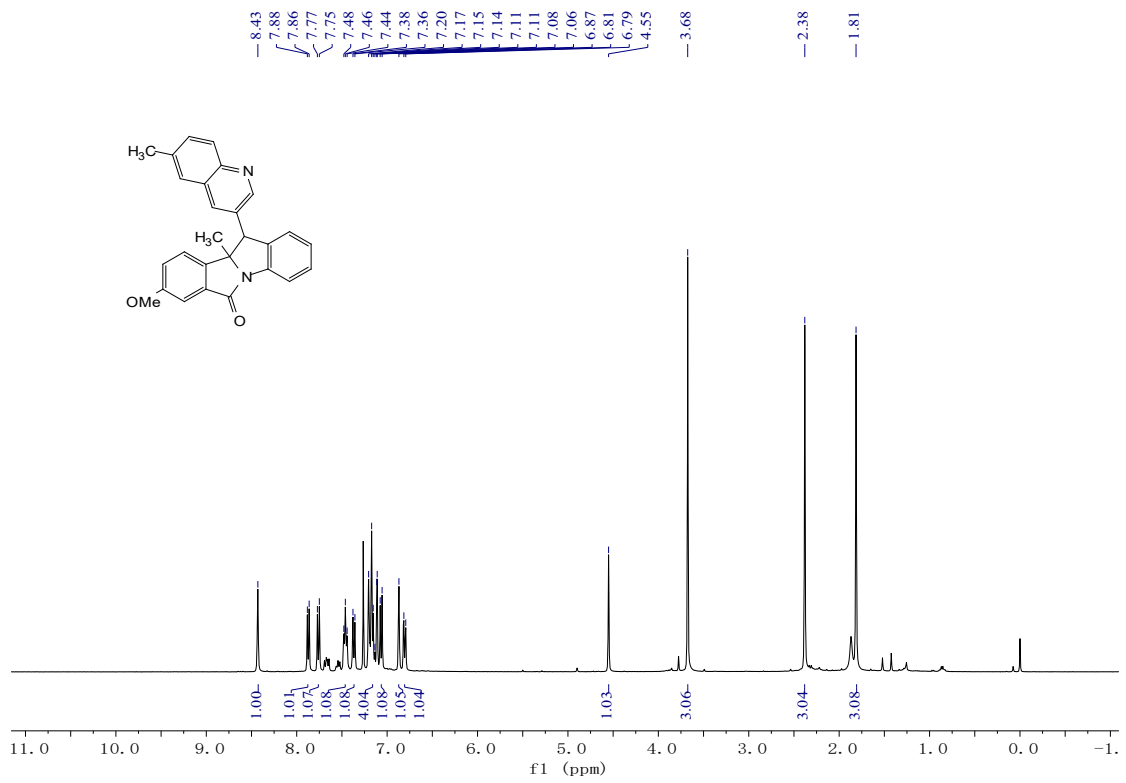
3p-¹³C



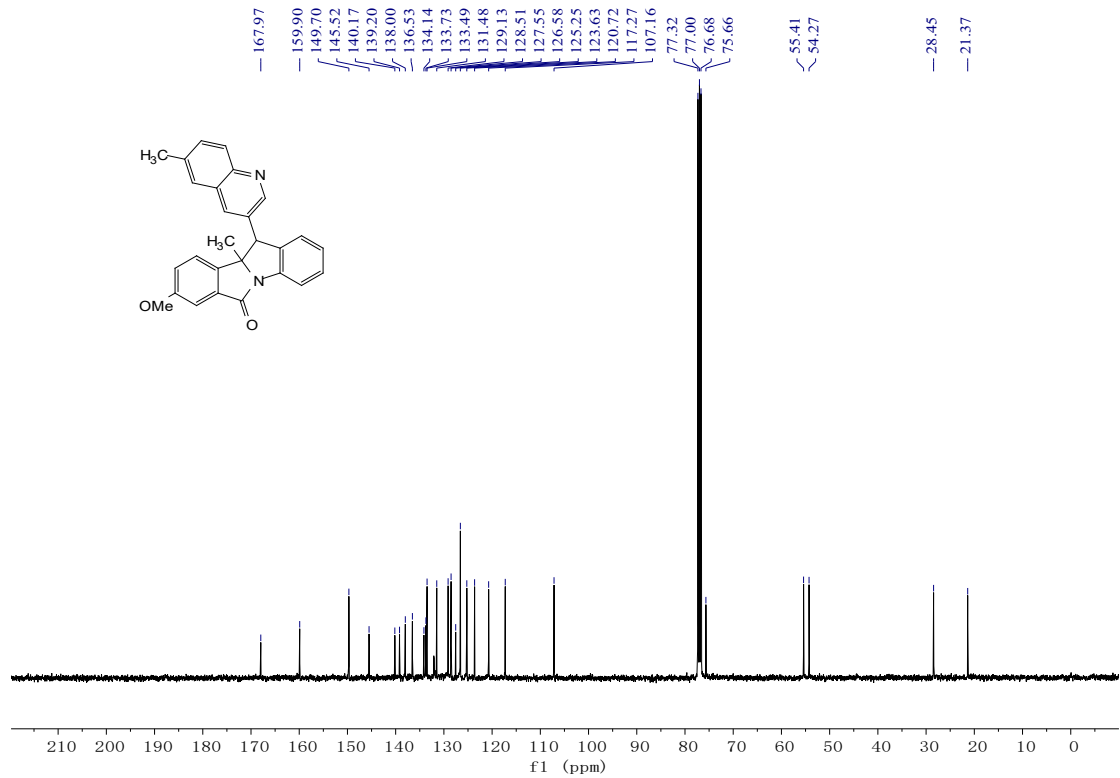
3q-¹H



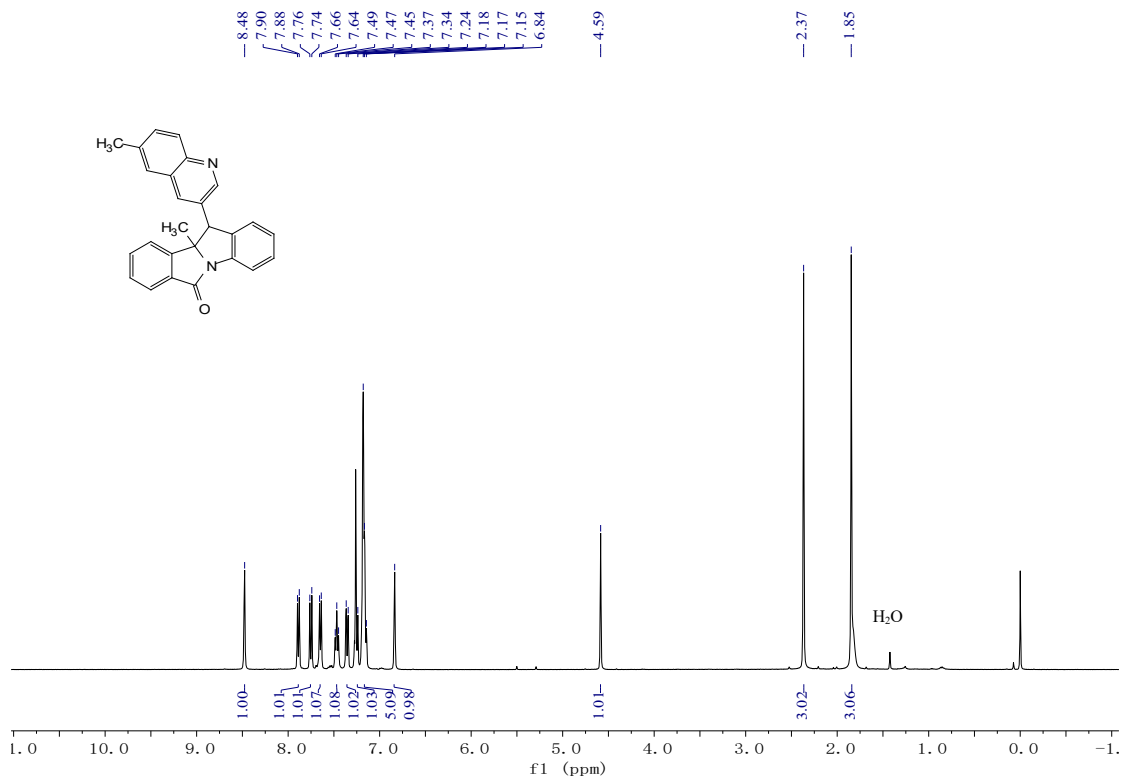
3r-¹H



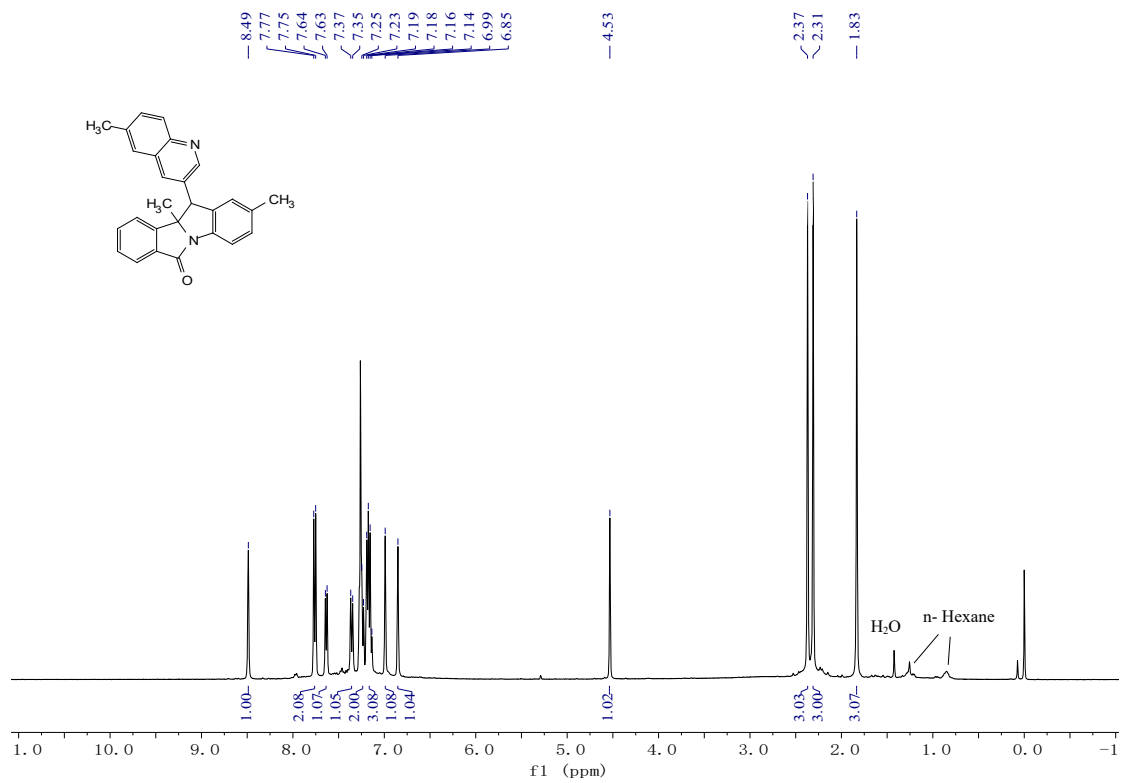
3r-¹³C



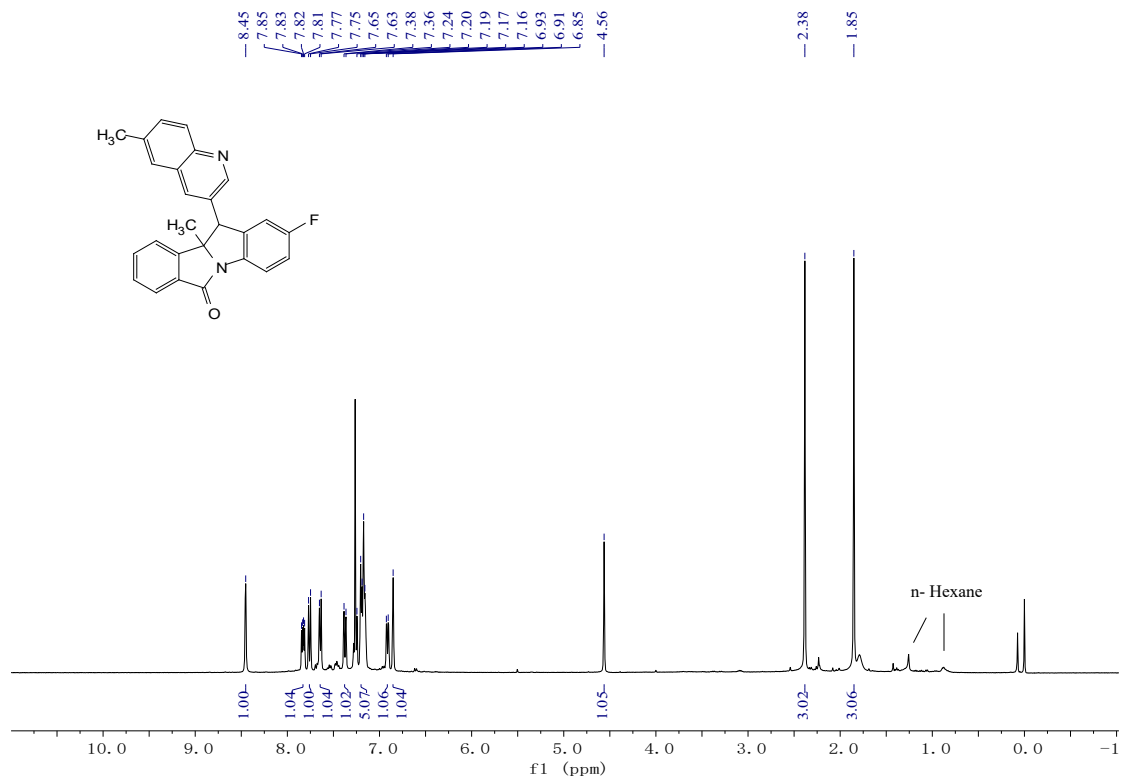
5a-¹H



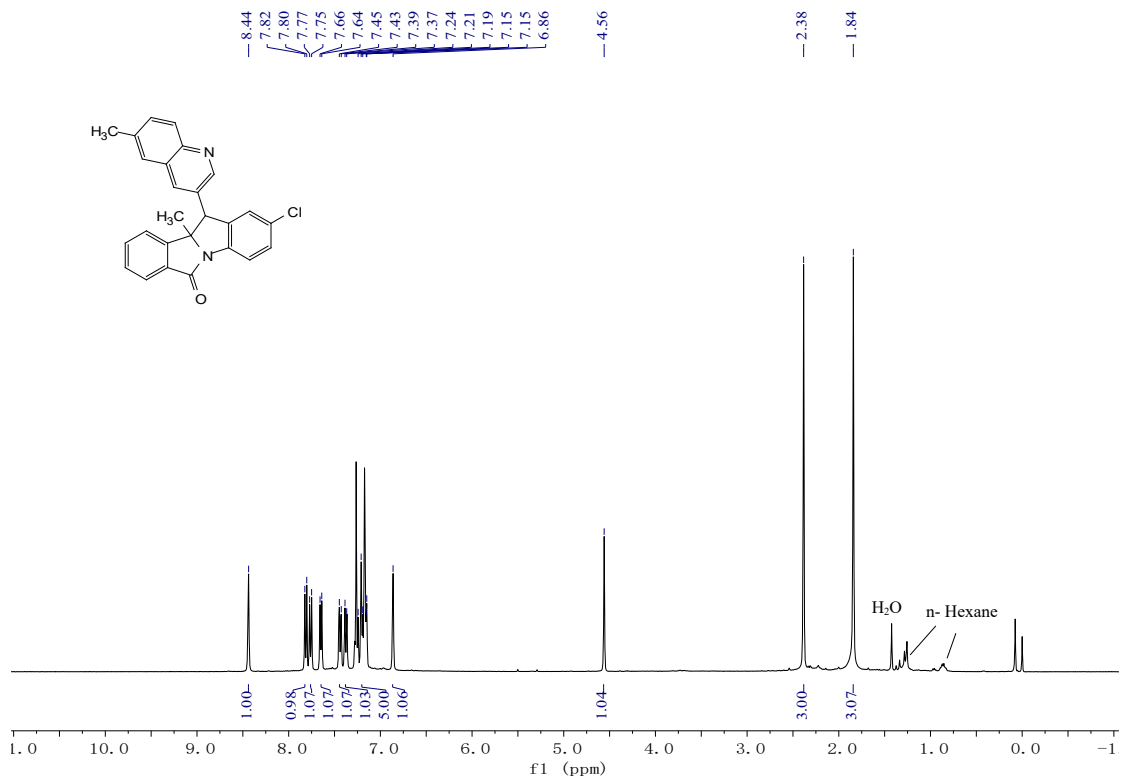
5b-¹H



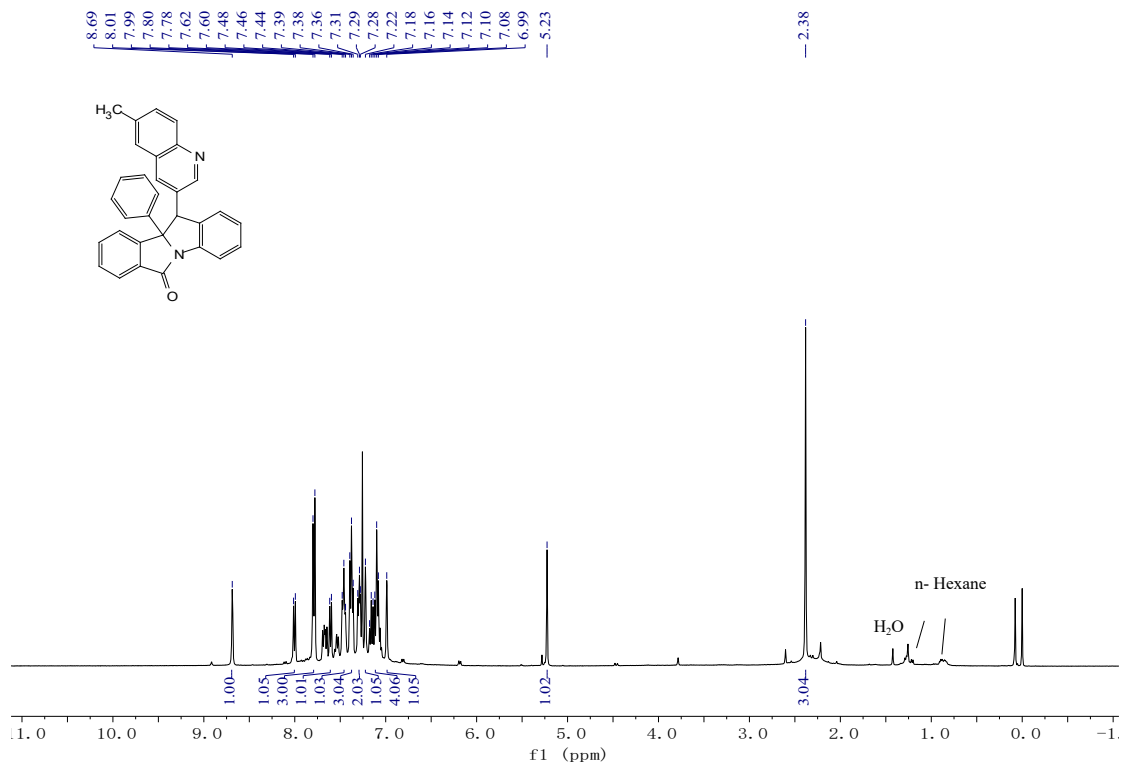
5c-¹H



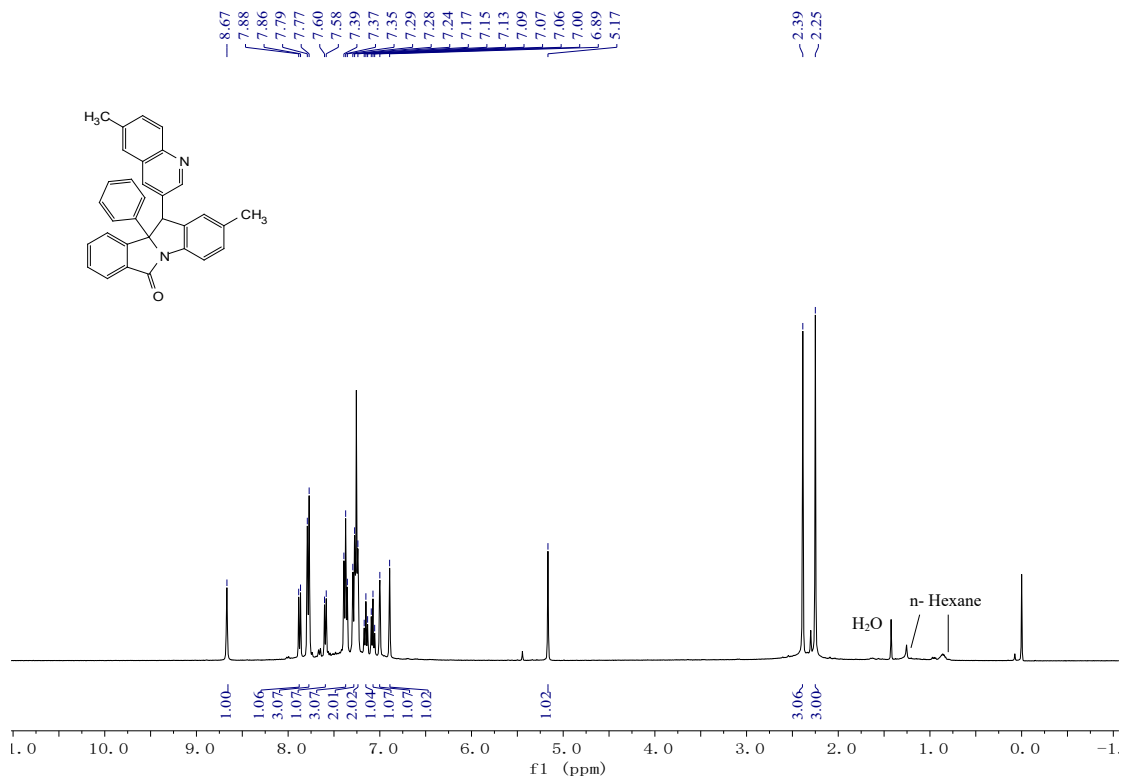
5d-¹H



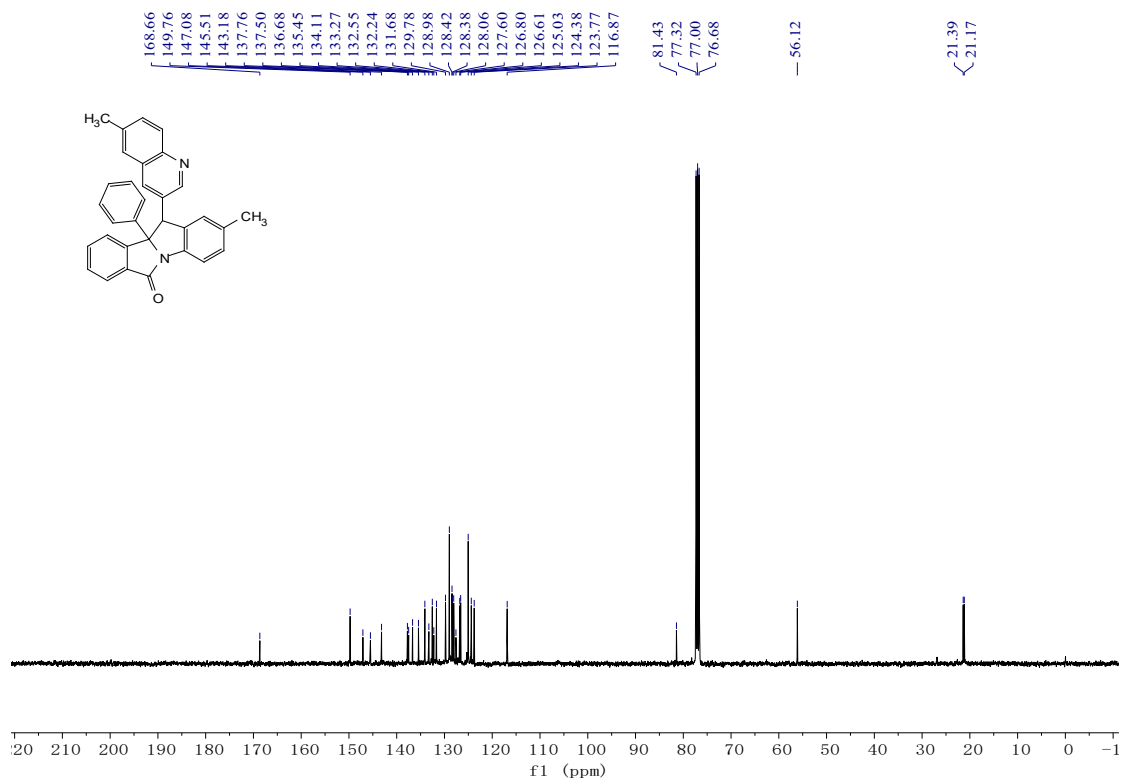
5e-¹H



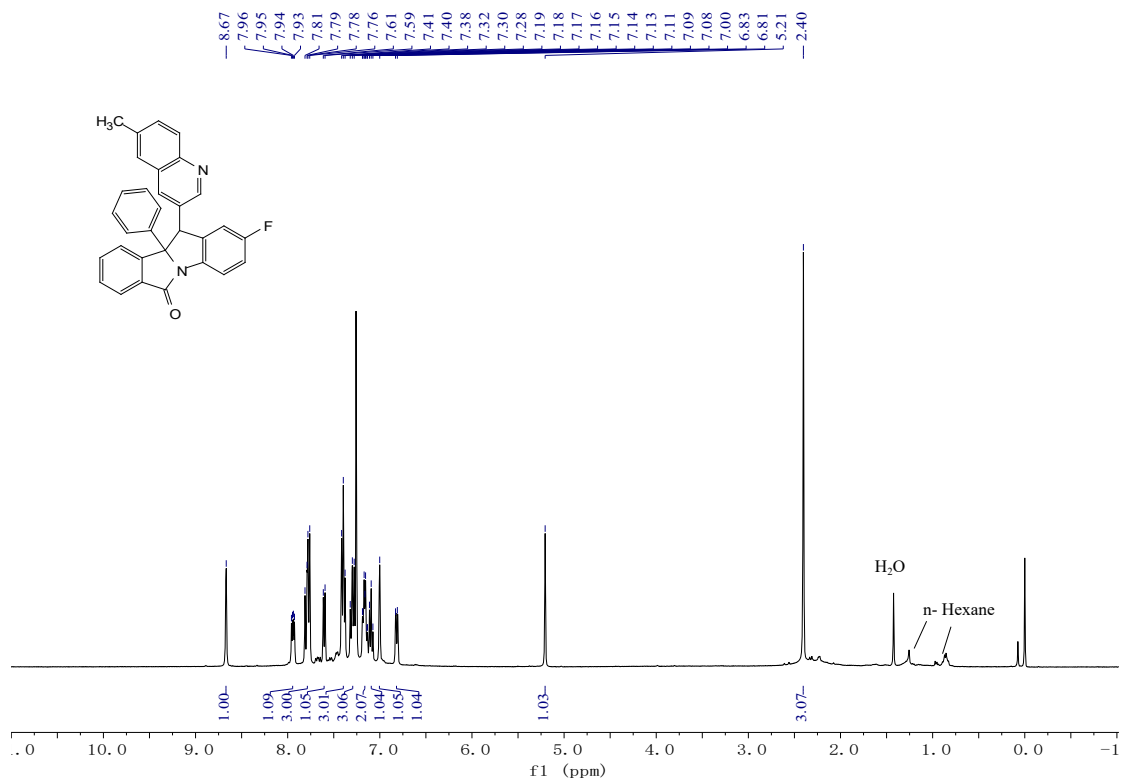
5f-¹H



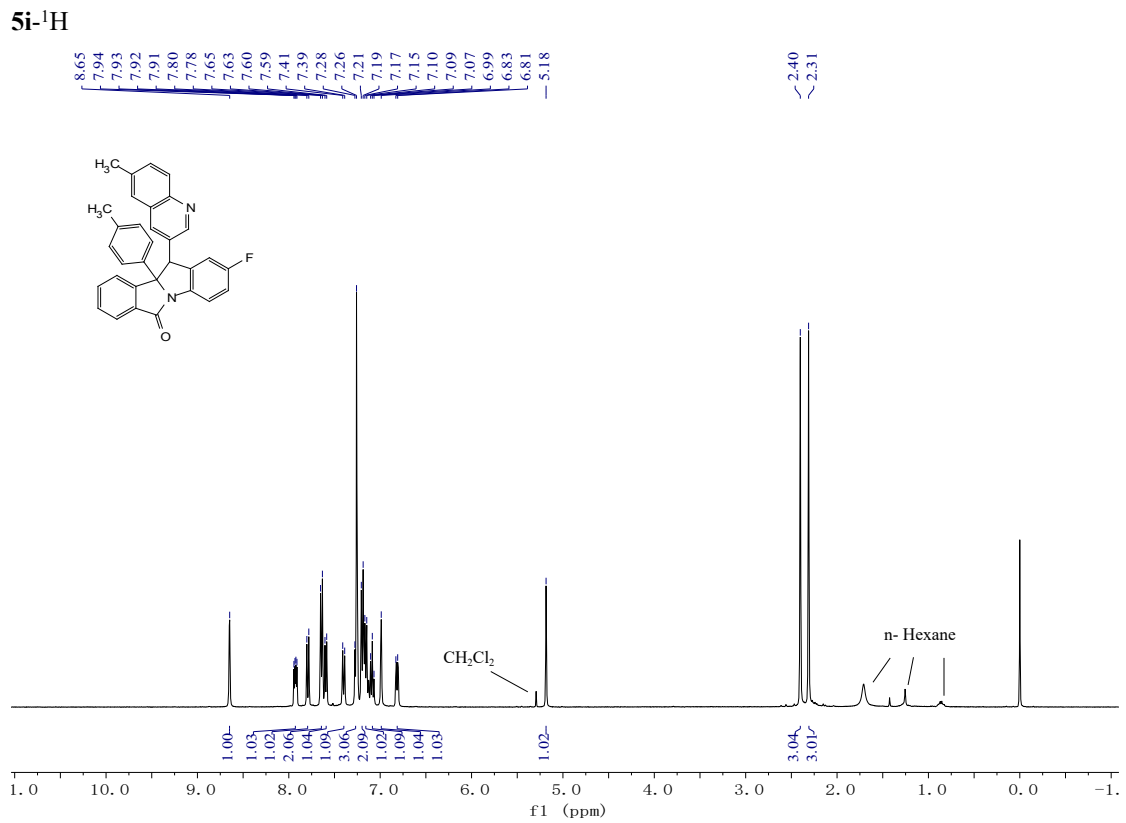
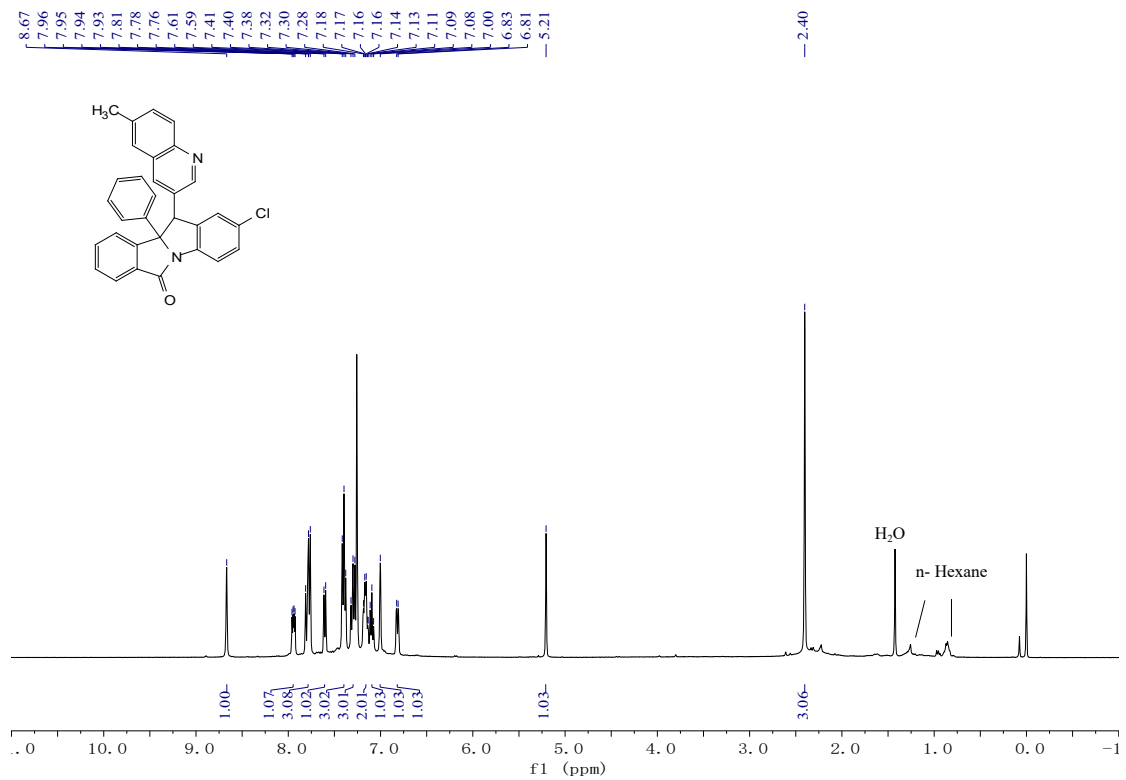
5f-¹³C



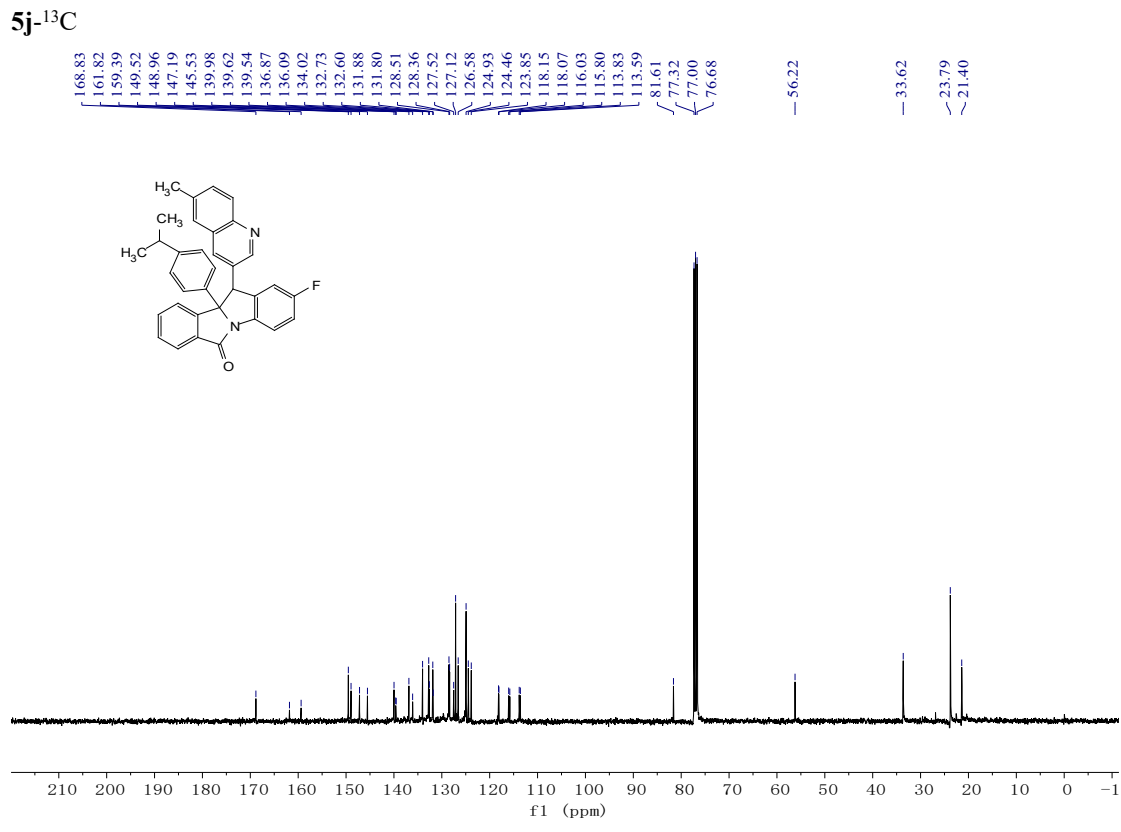
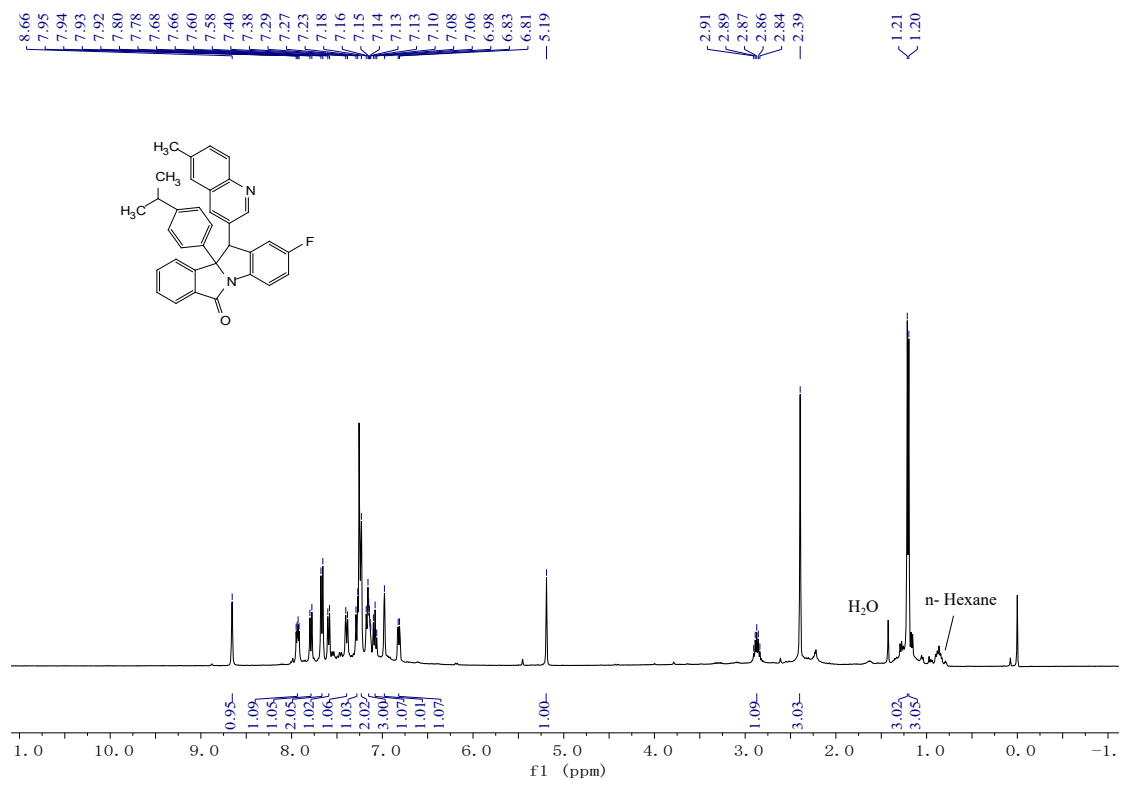
5g-¹H



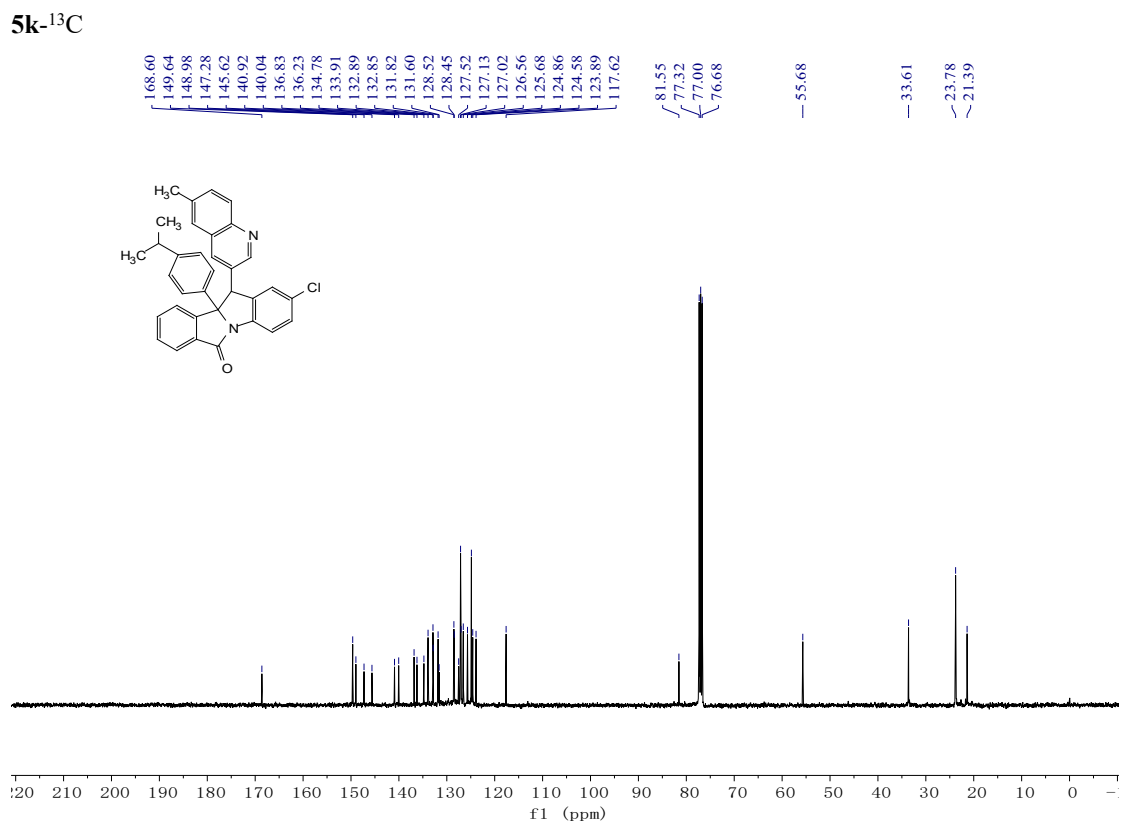
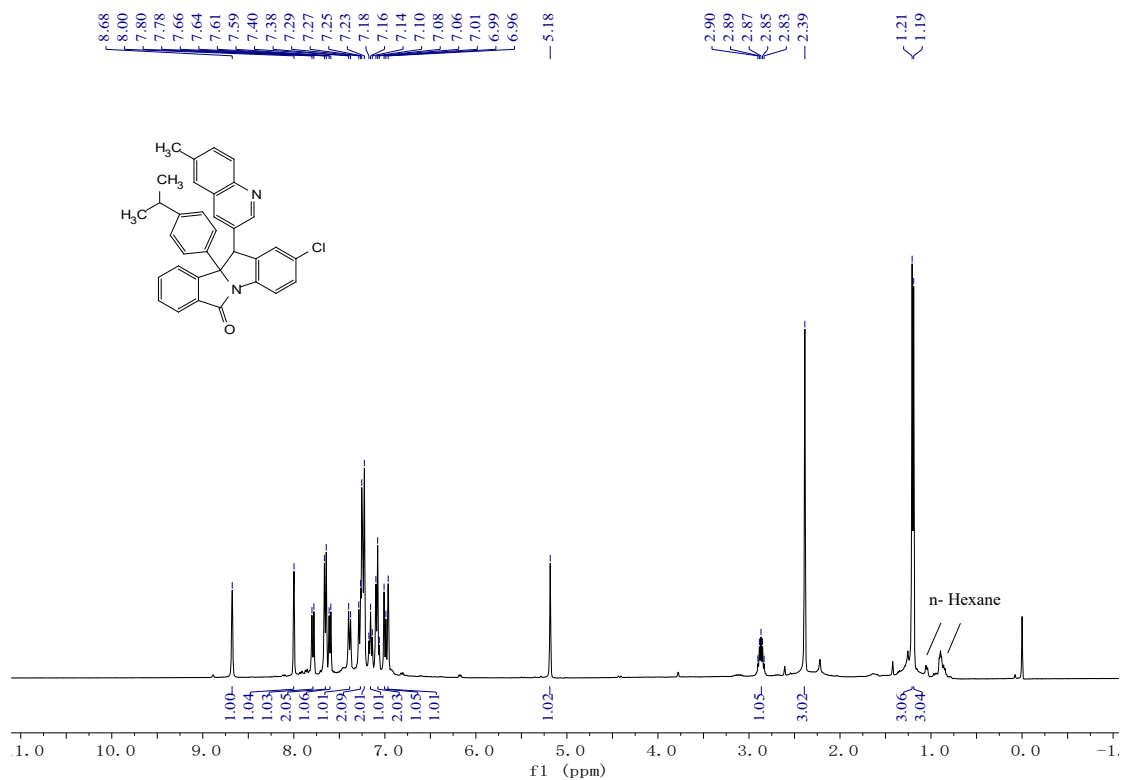
5h-¹H



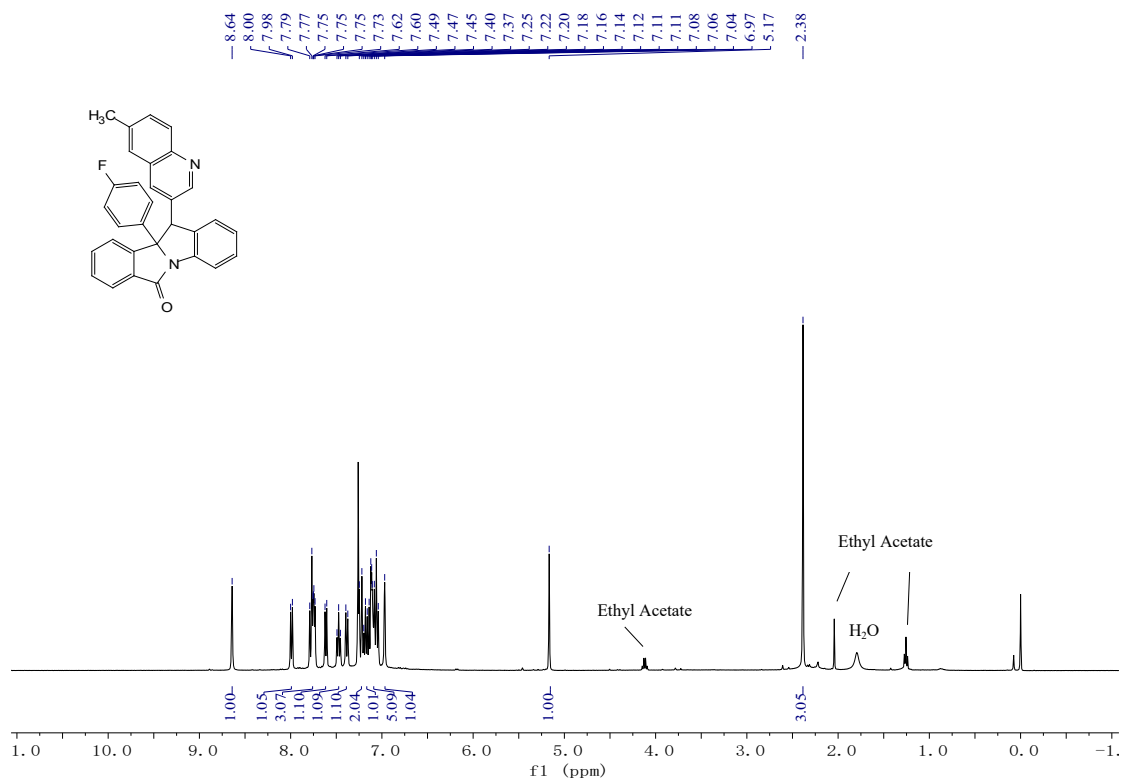
5j-¹H



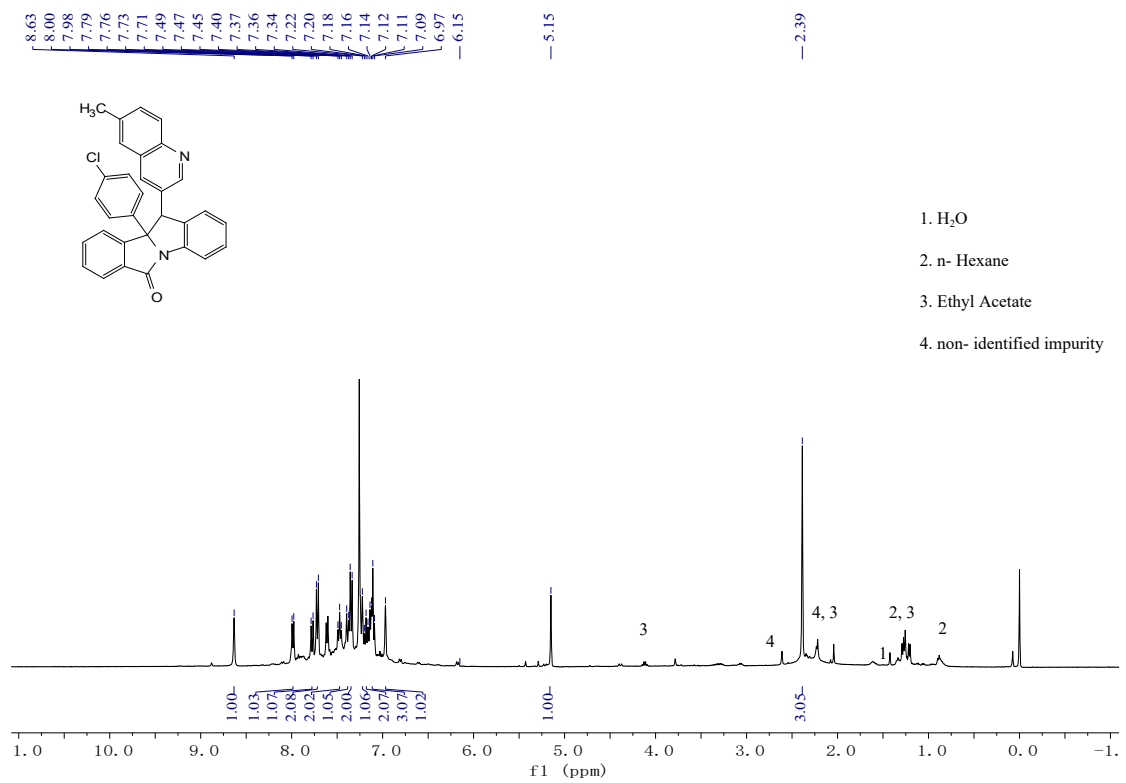
5k-¹H



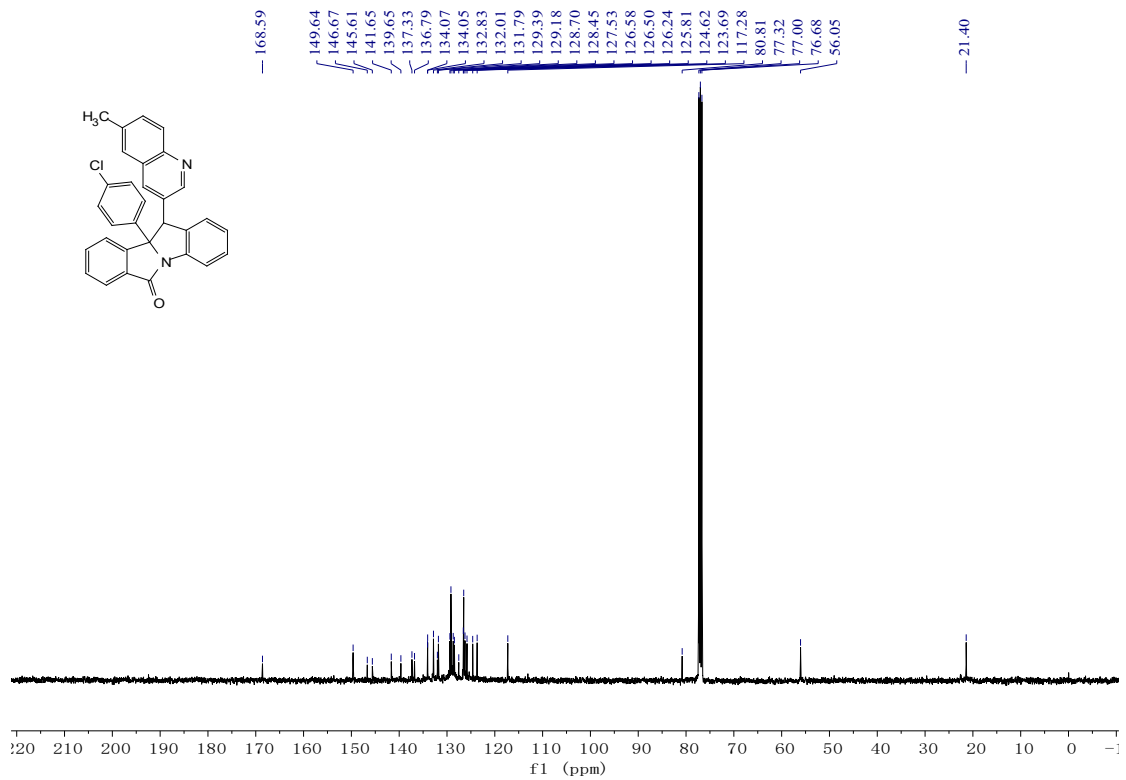
5l-¹H



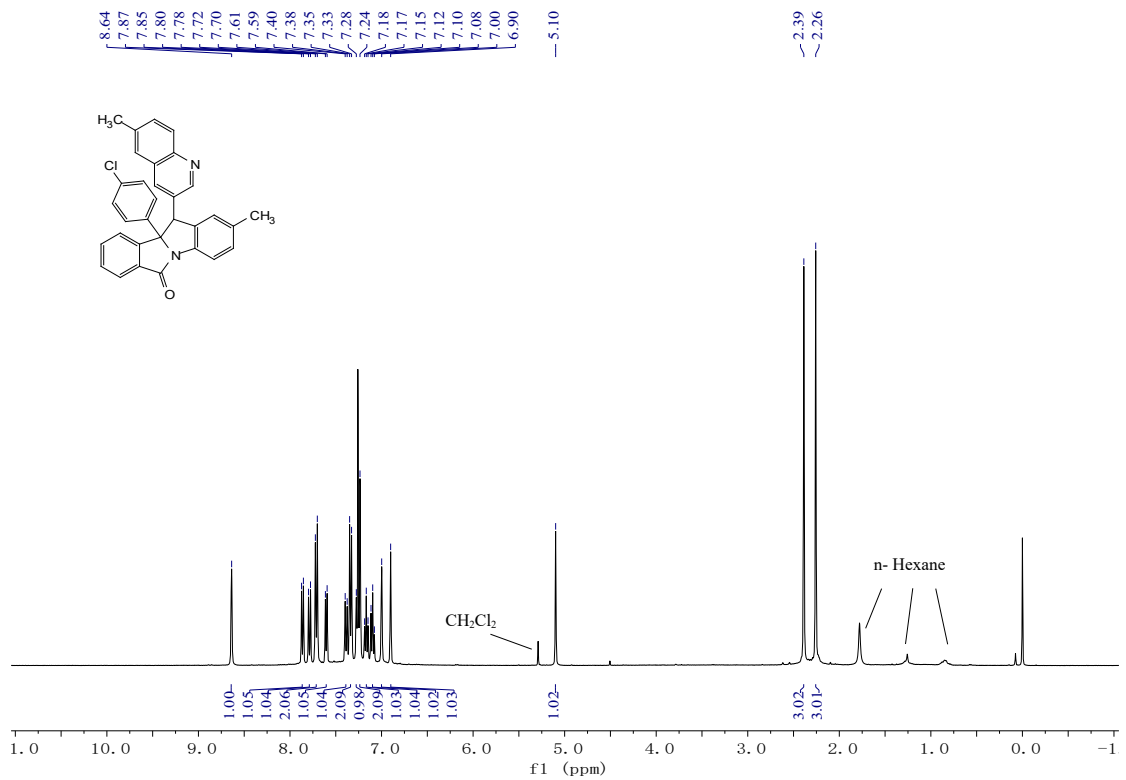
5m-¹H



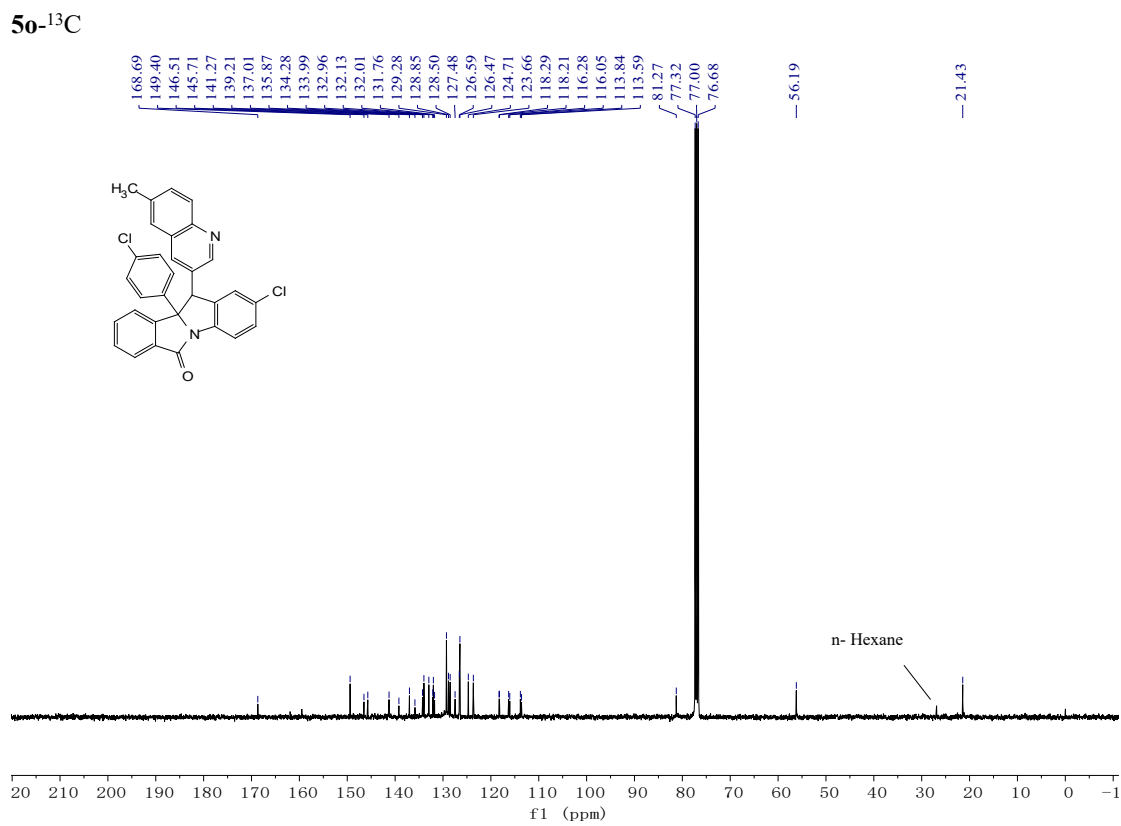
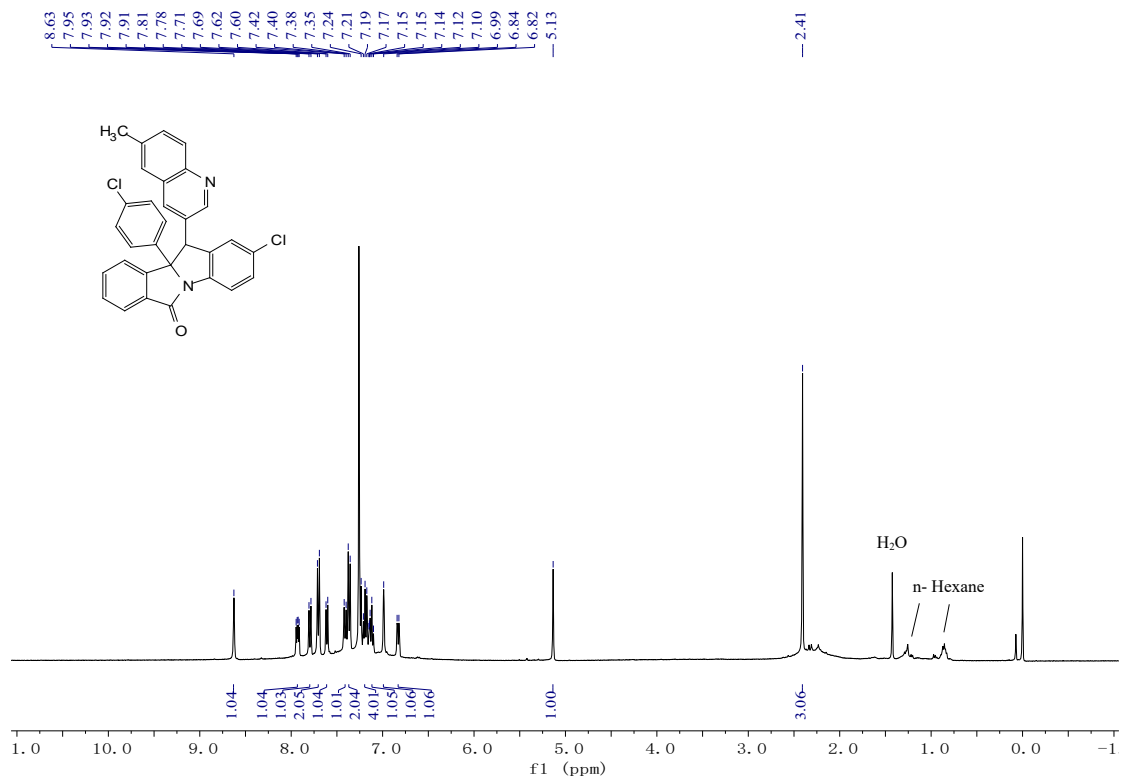
5m-¹³C



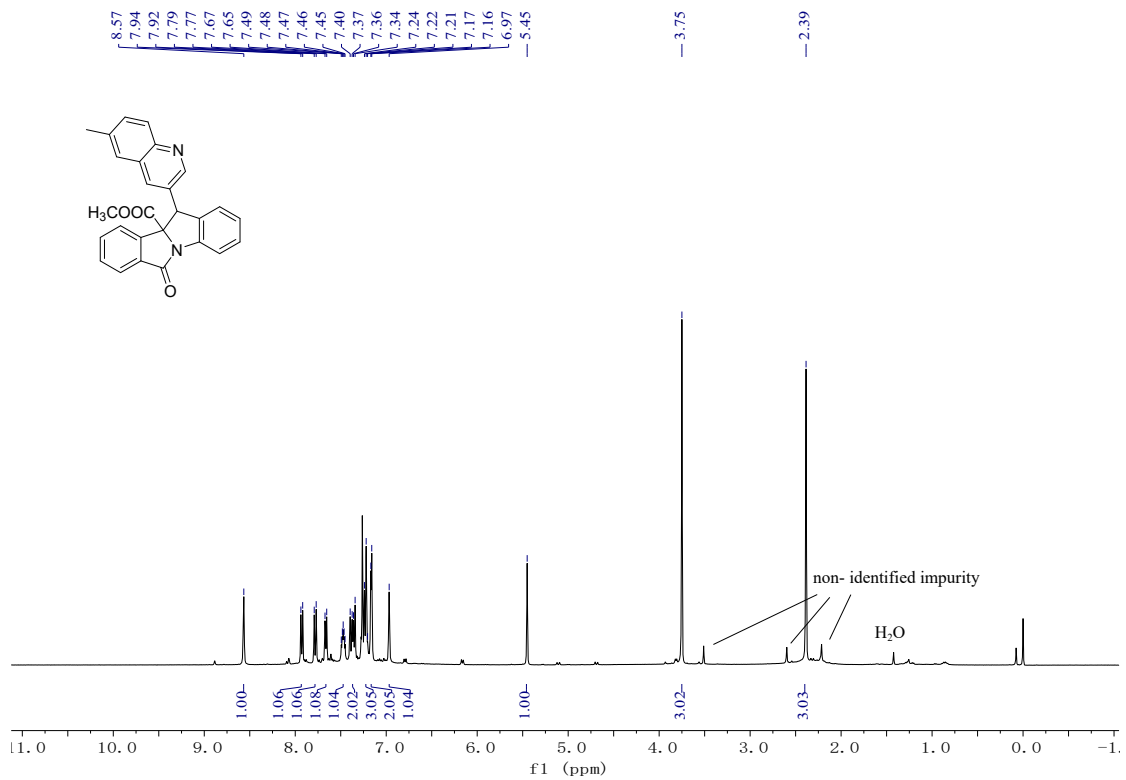
5n- ^1H



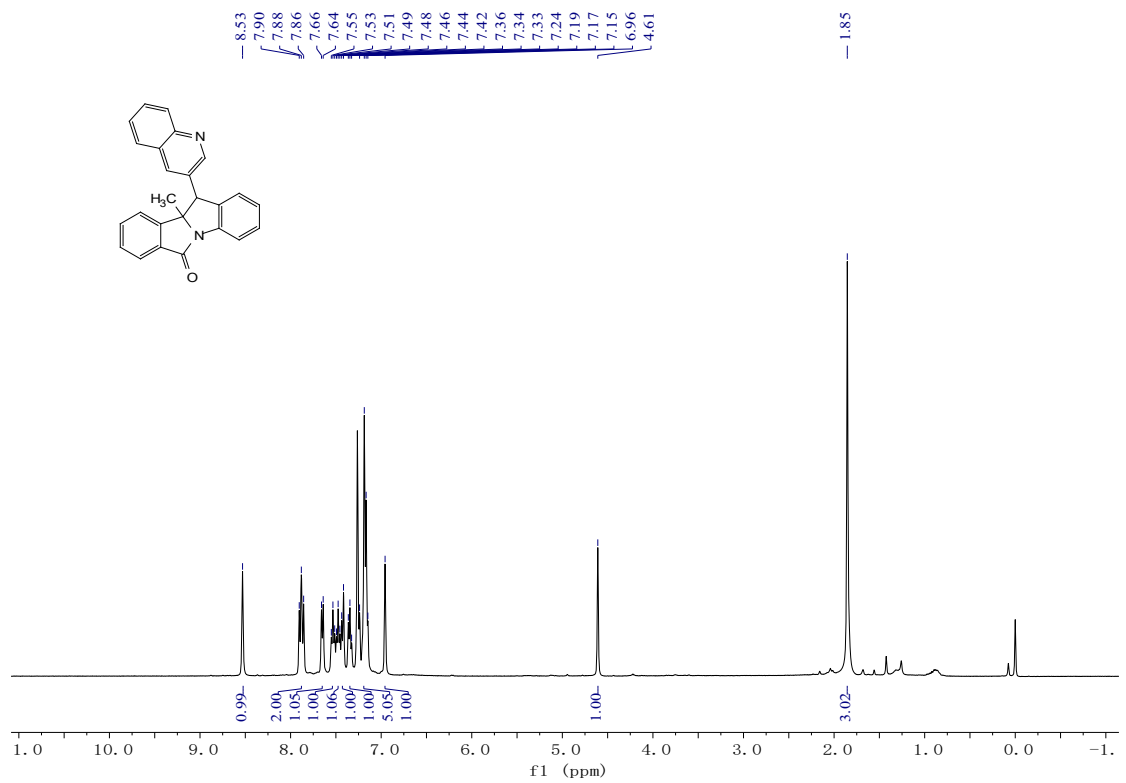
5o- ^1H



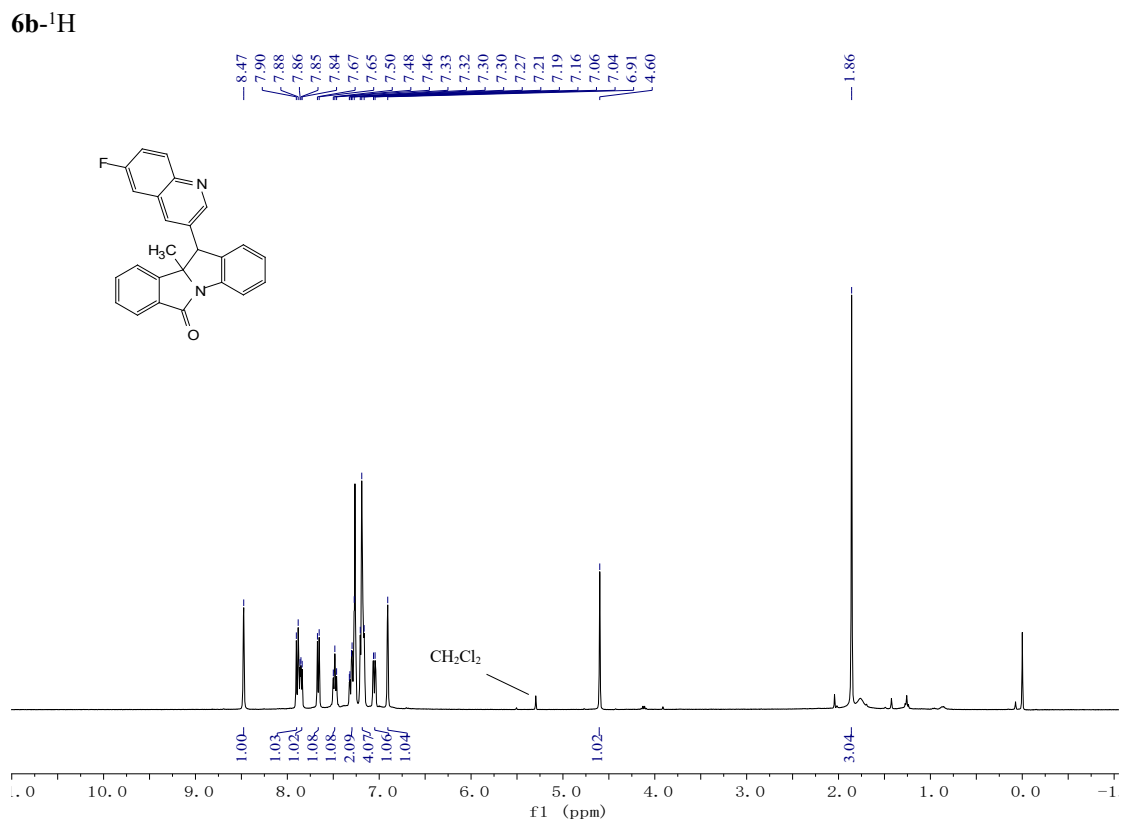
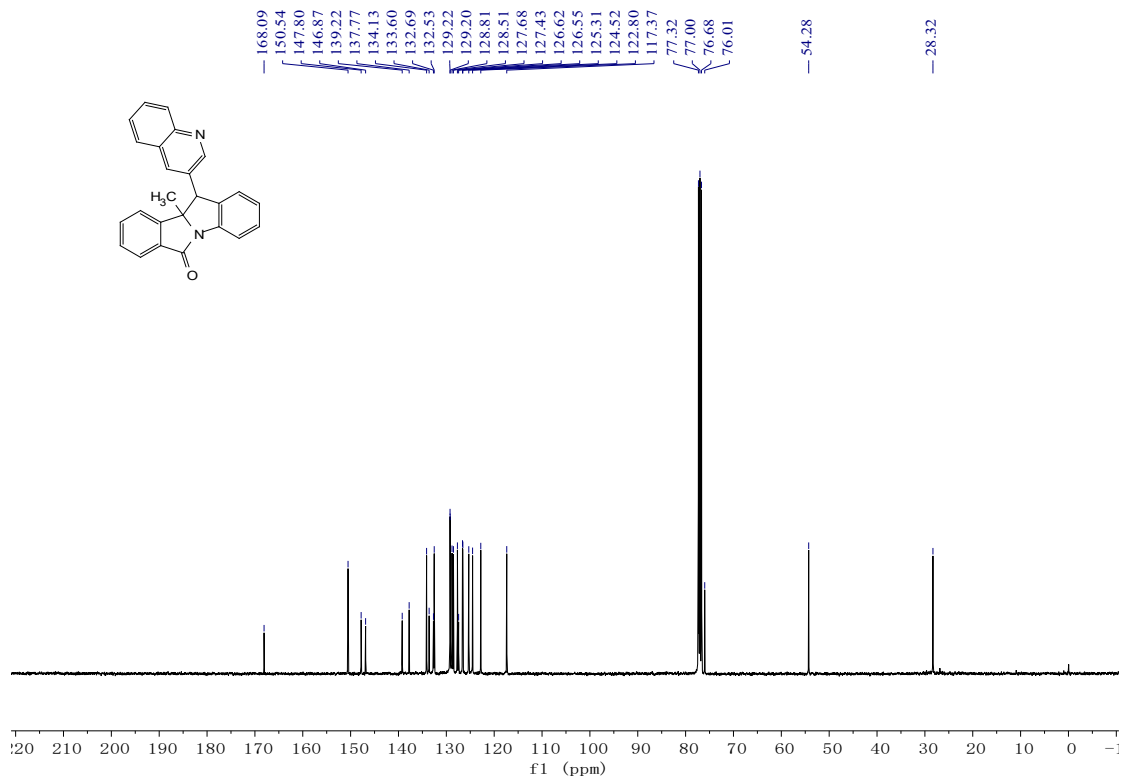
5p-¹H



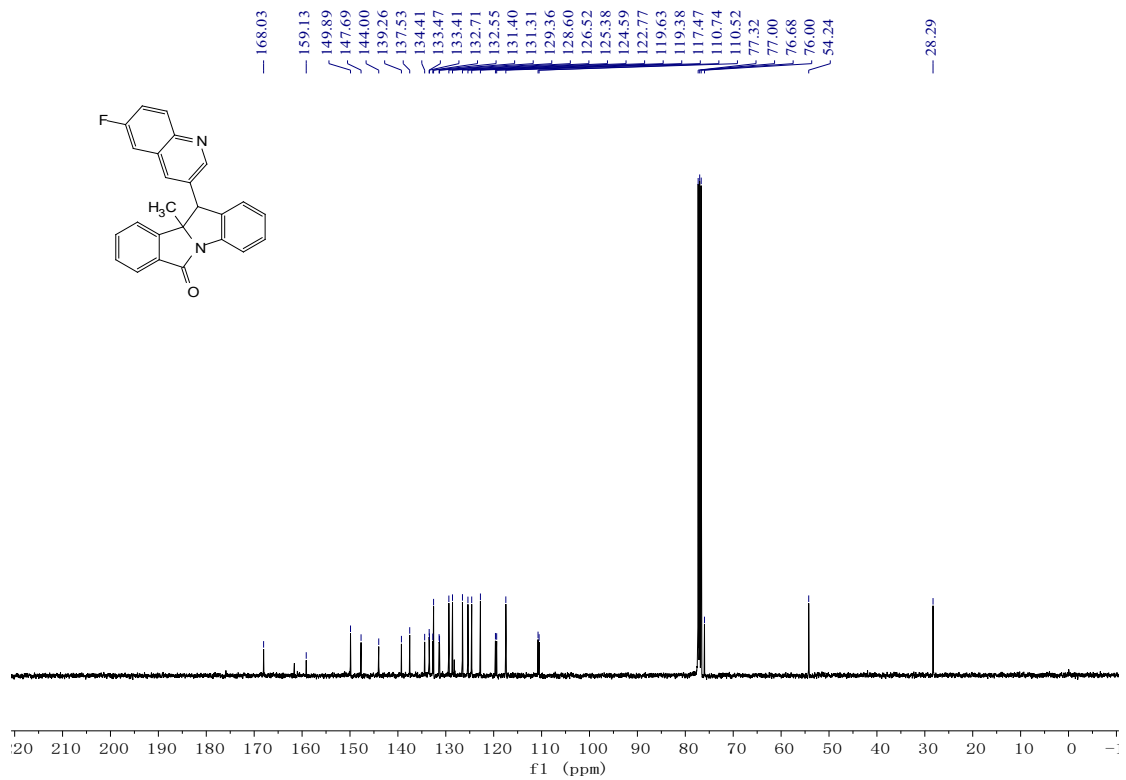
6a-¹H



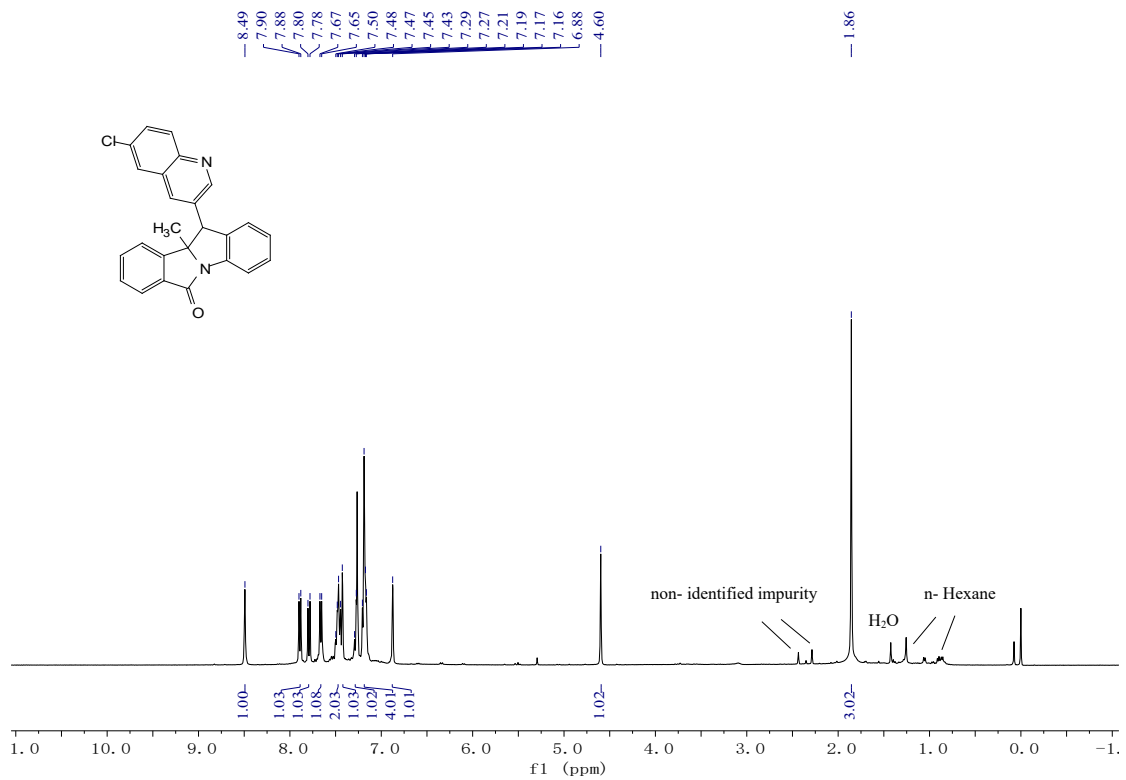
6a-¹³C



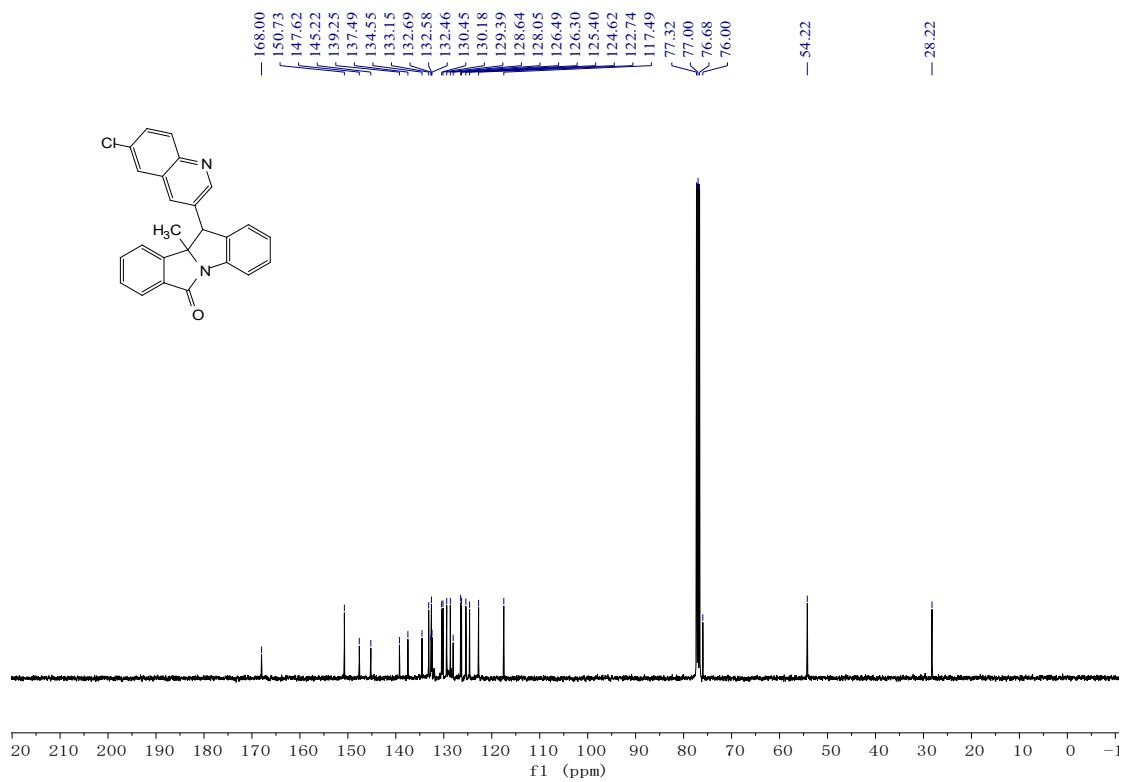
6b-¹³C



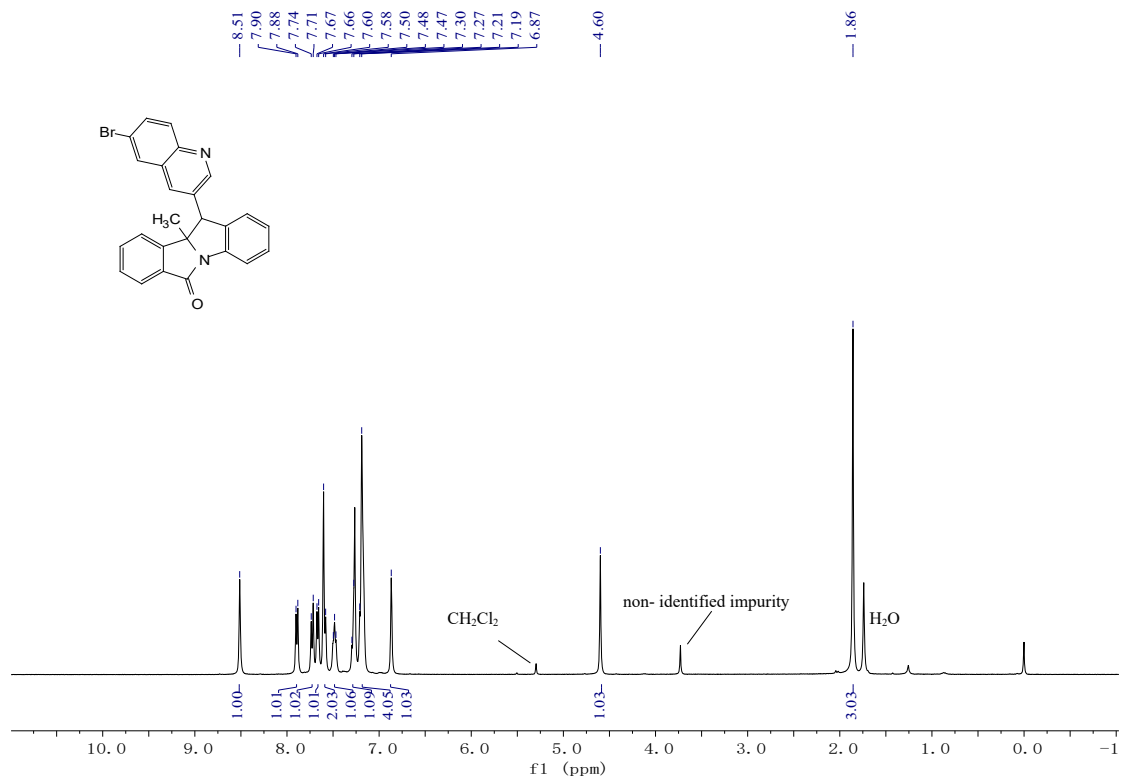
6c-¹H



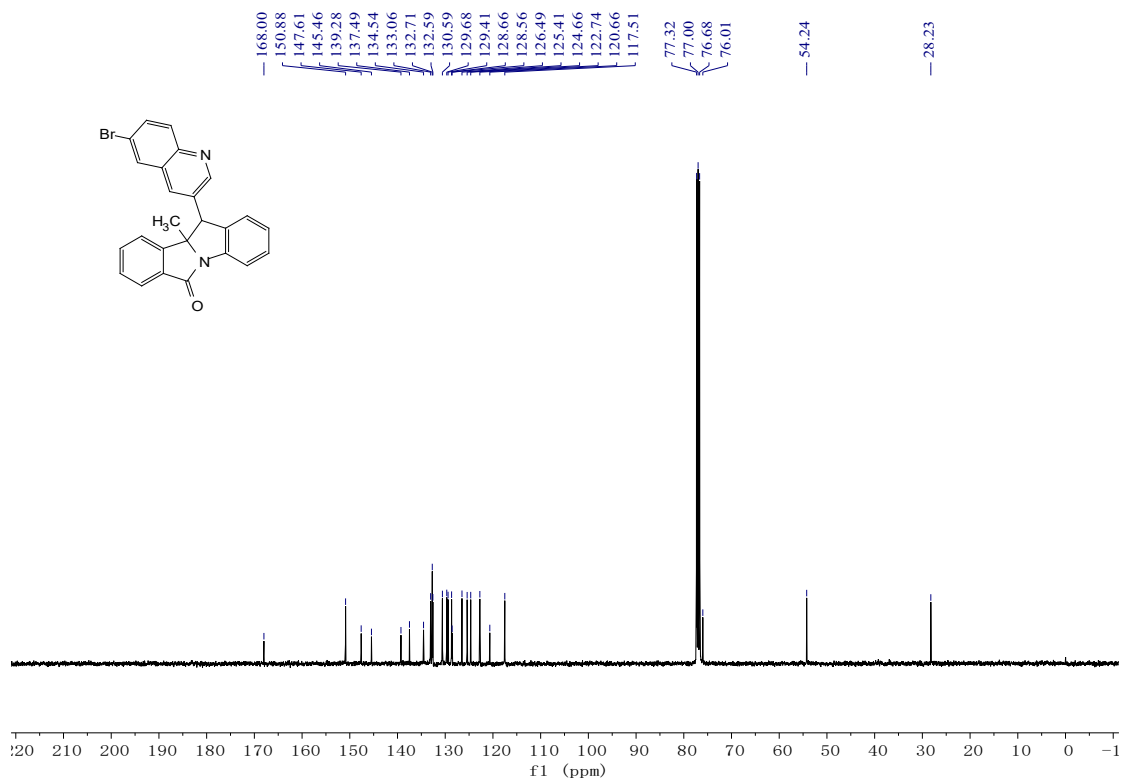
6c-¹³C



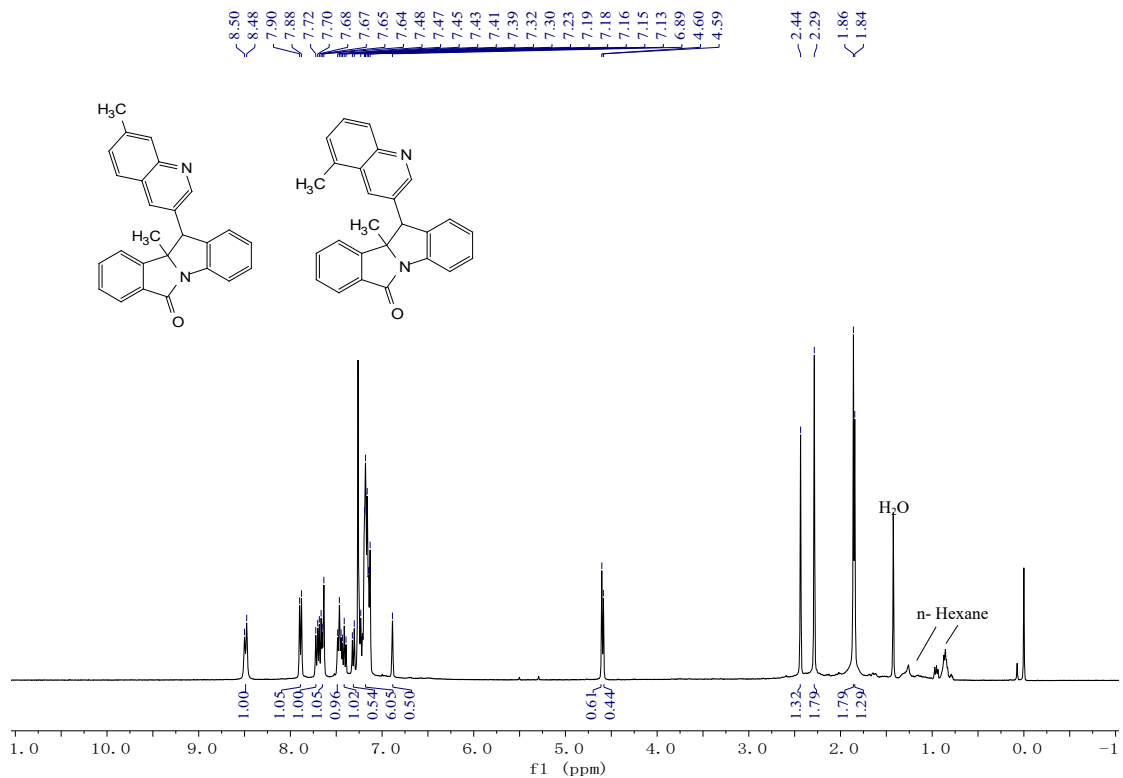
6d-¹H



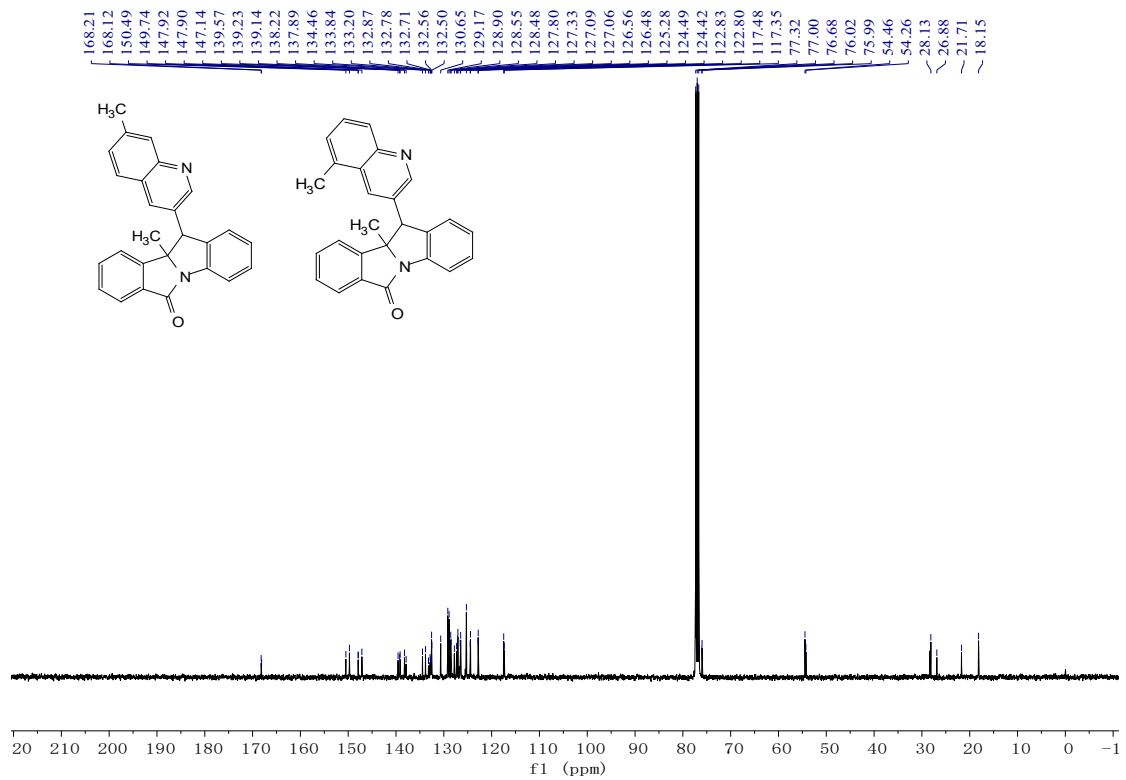
6d-¹³C



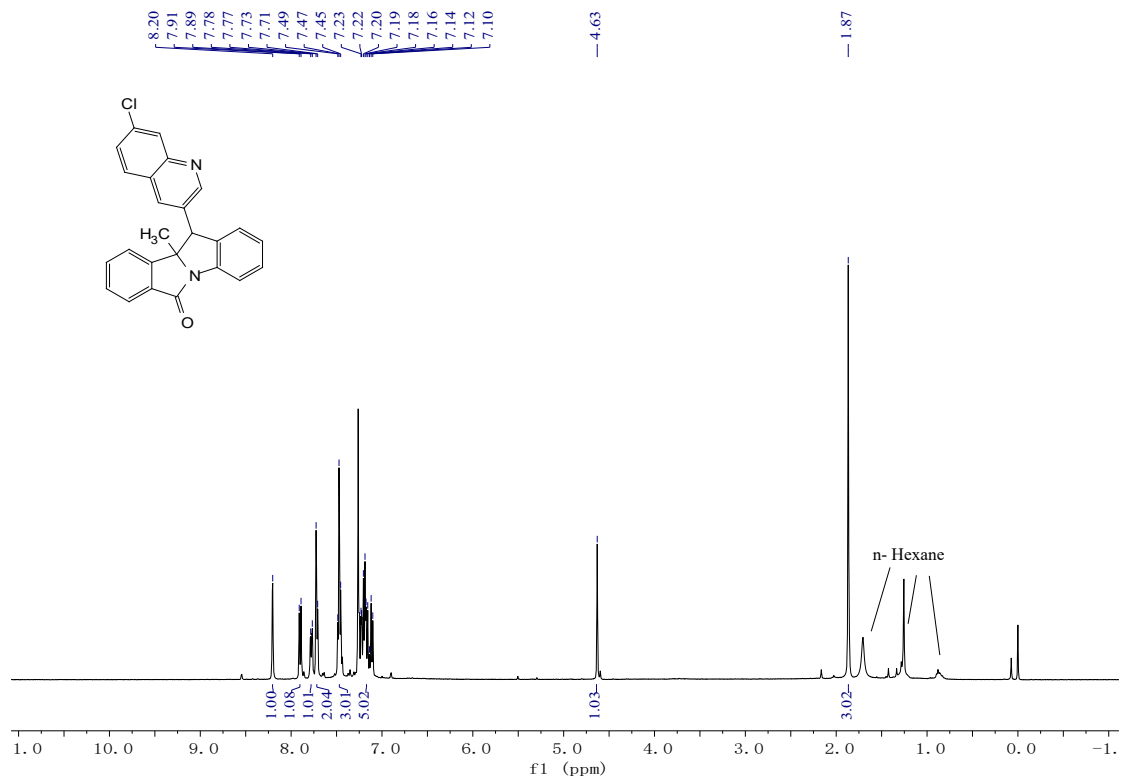
6e-¹H



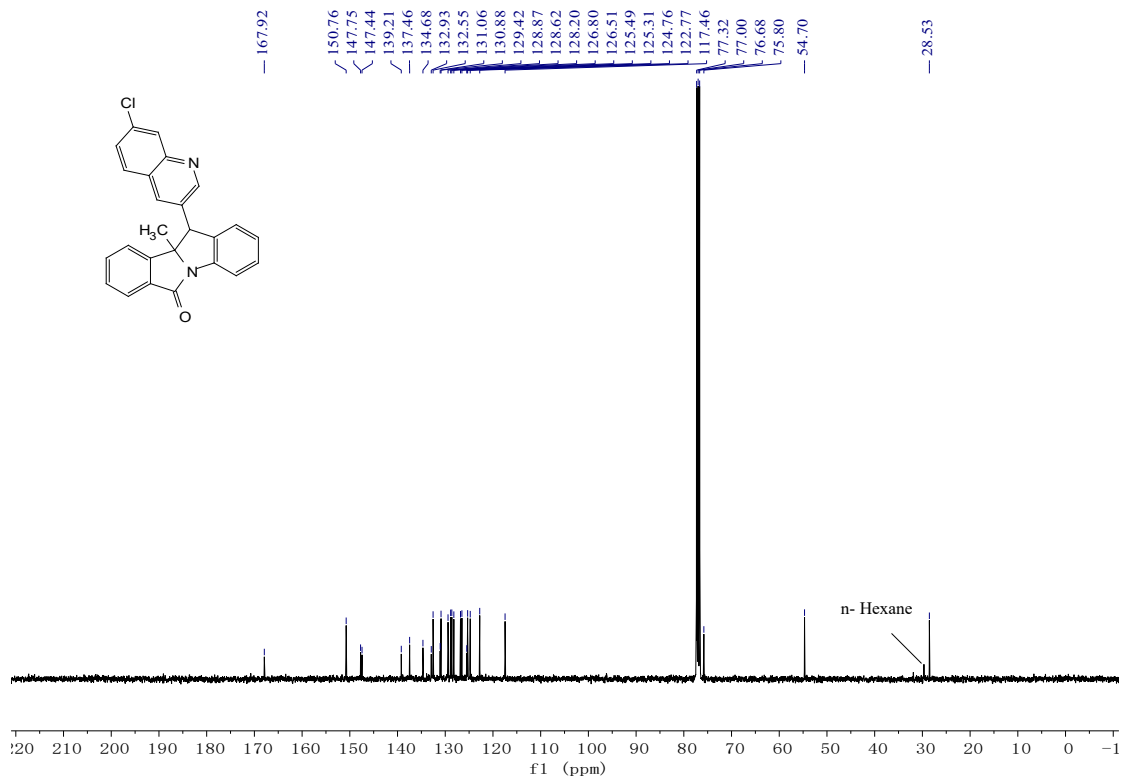
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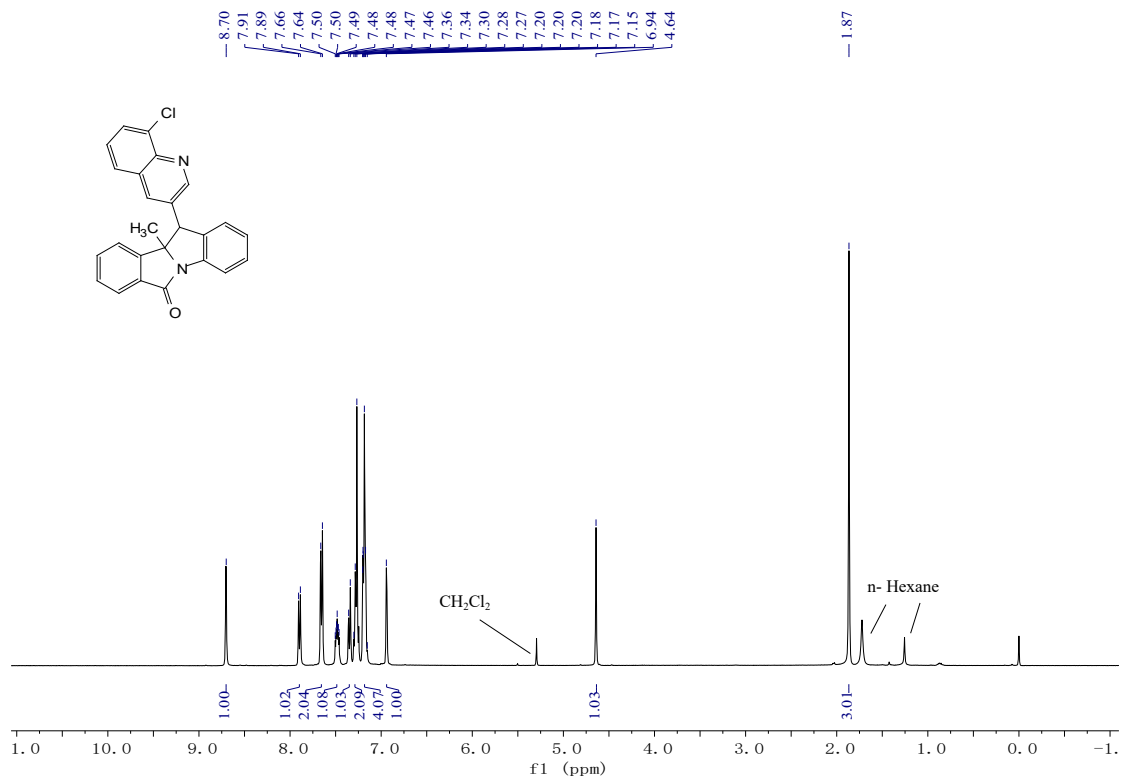
6f-¹H



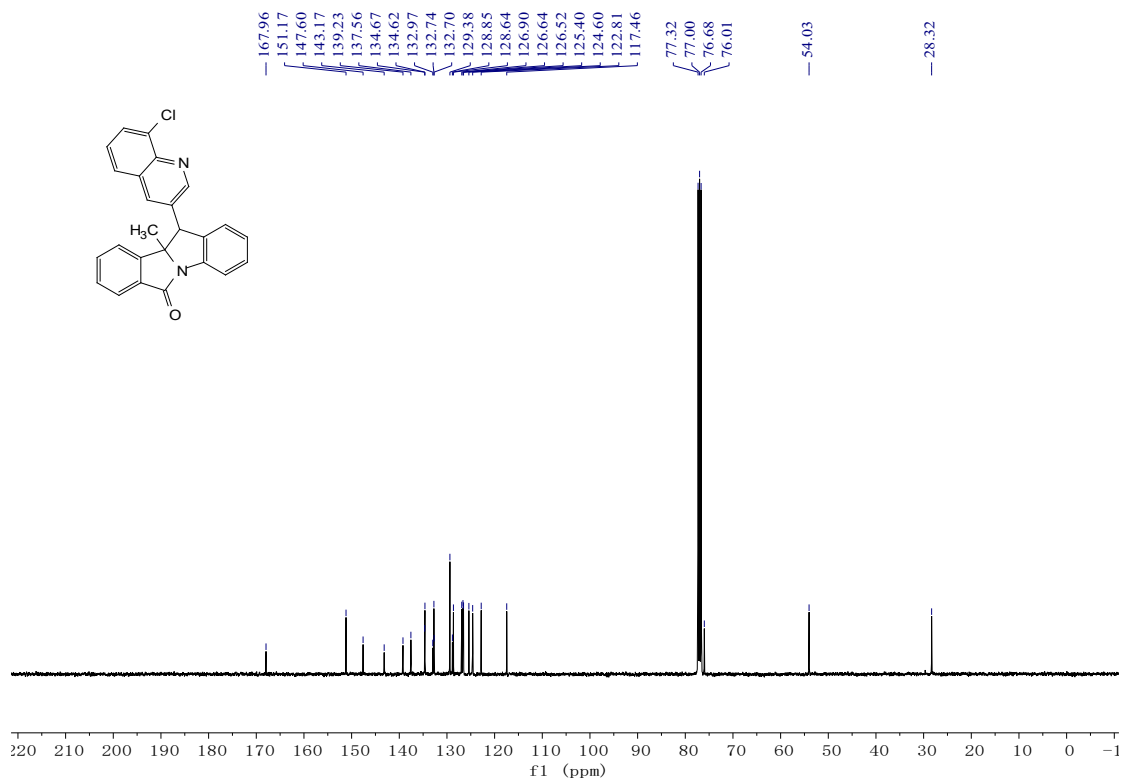
6f-¹³C



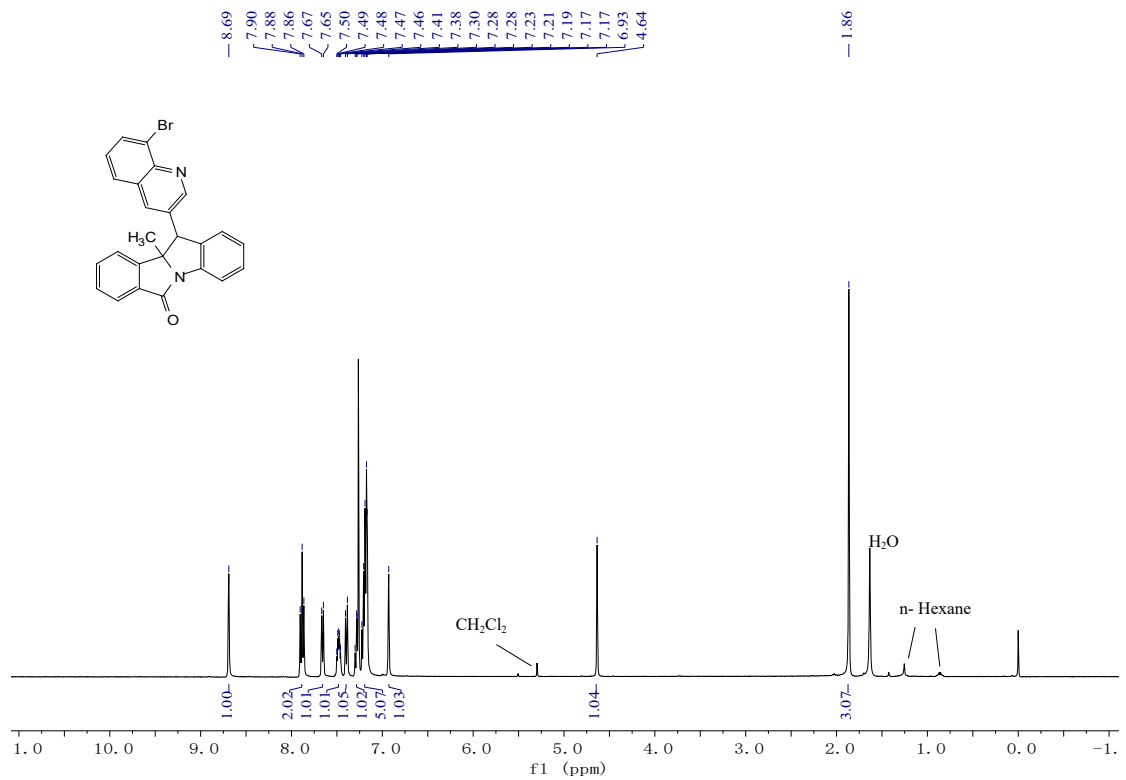
6g-¹H



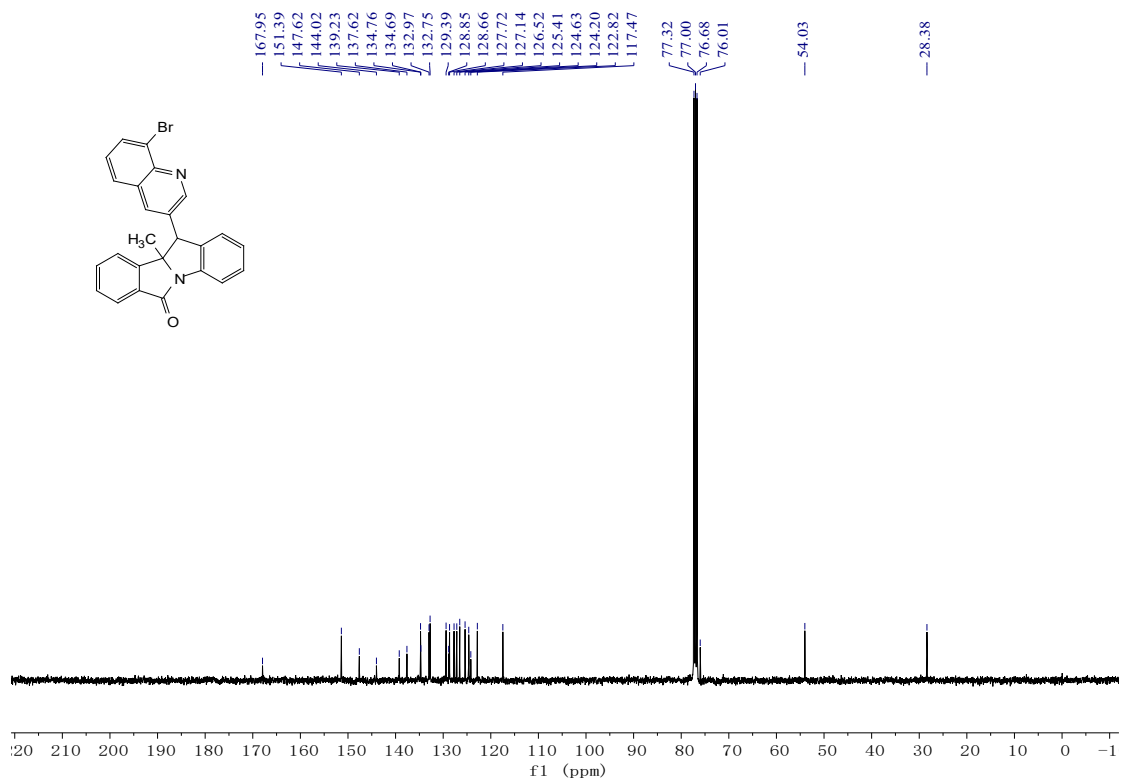
6g-¹³C



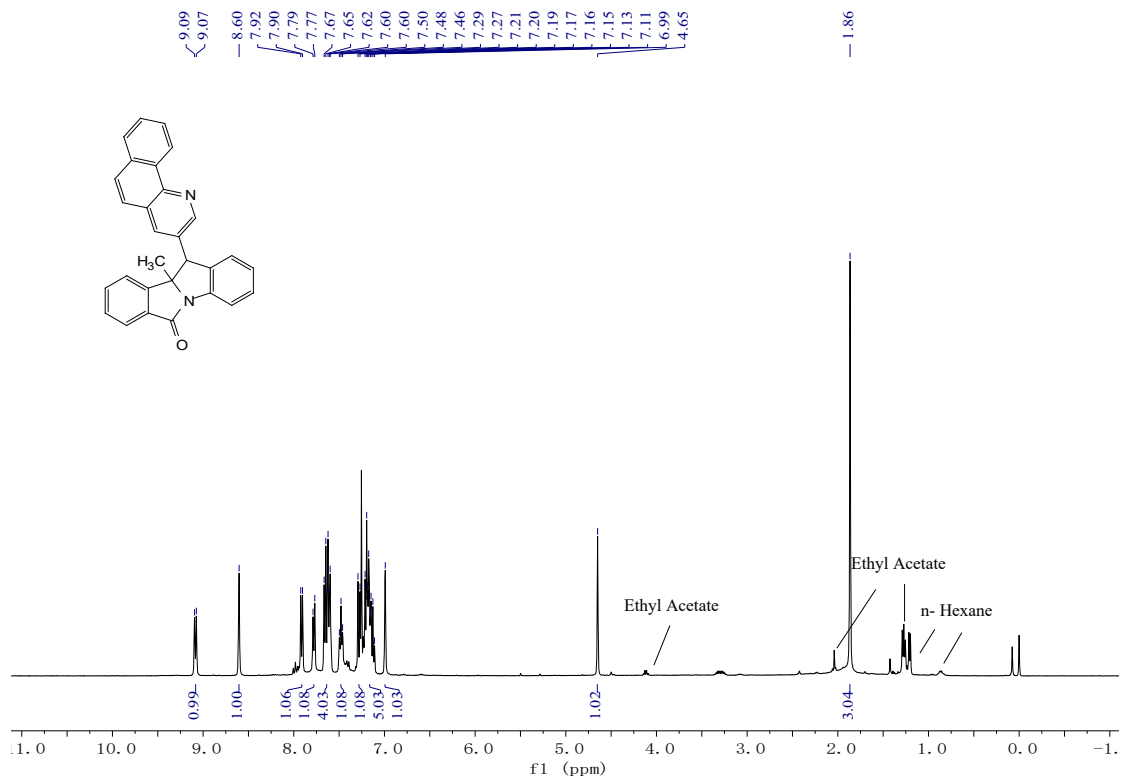
6h-¹H



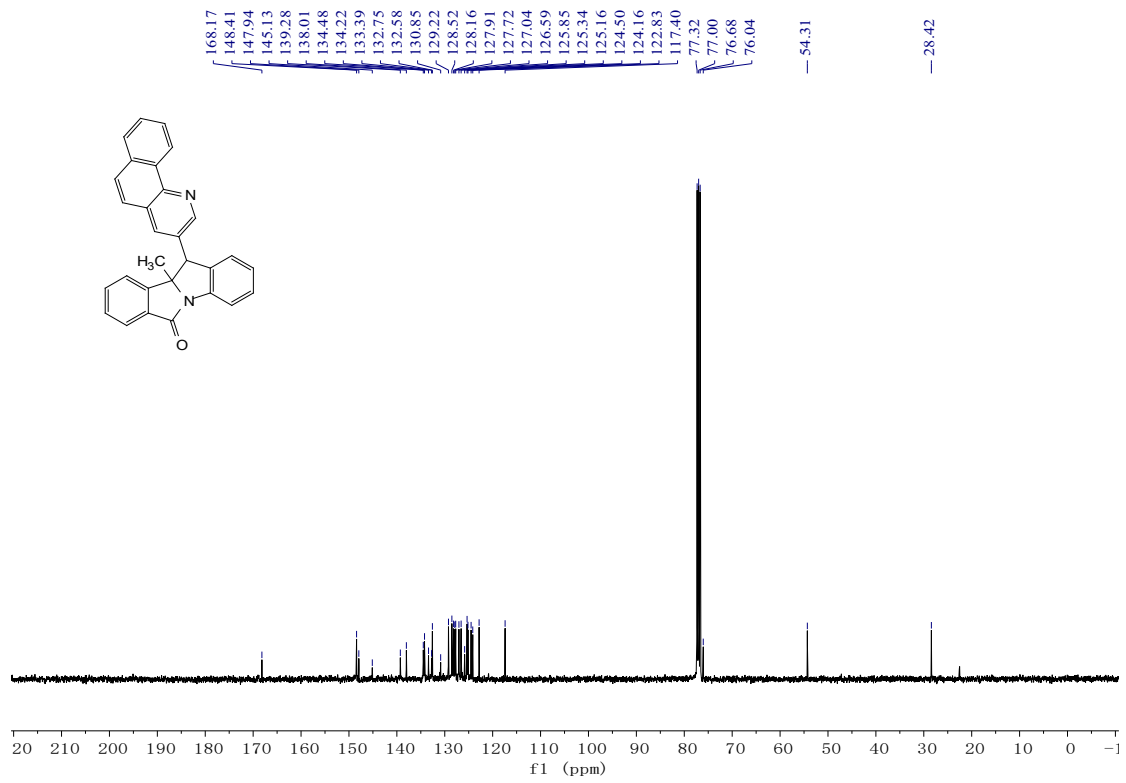
6h-¹³C



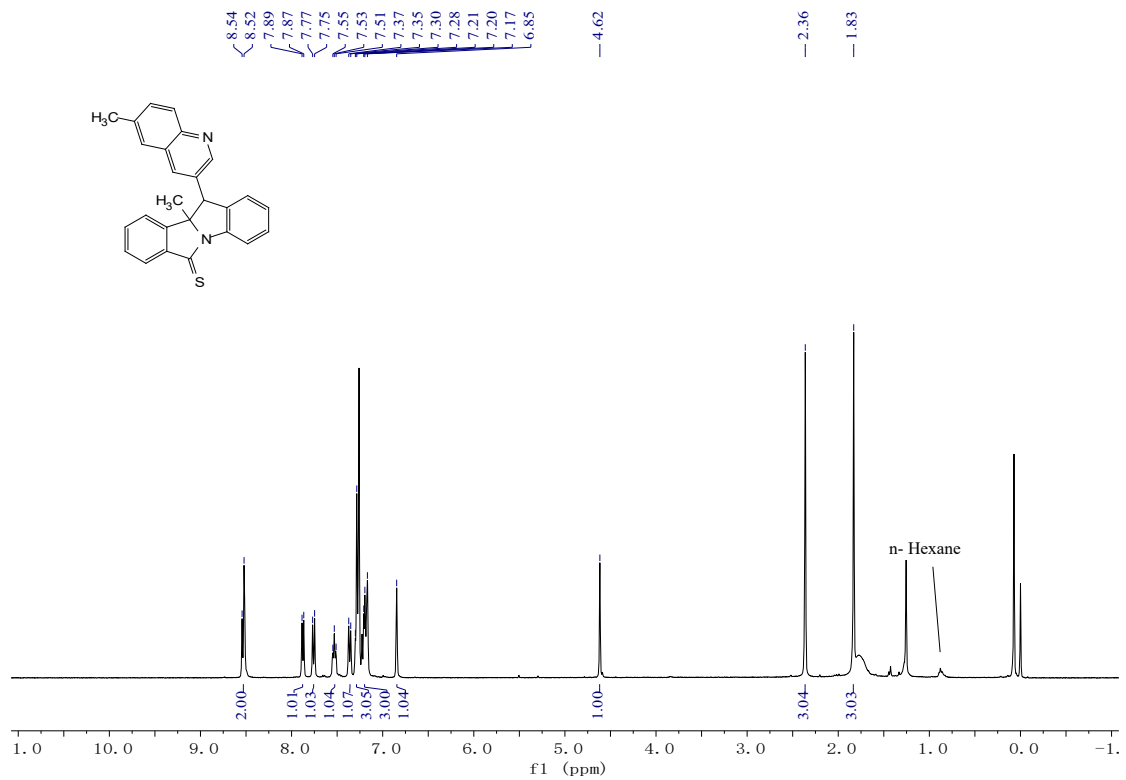
6i-¹H



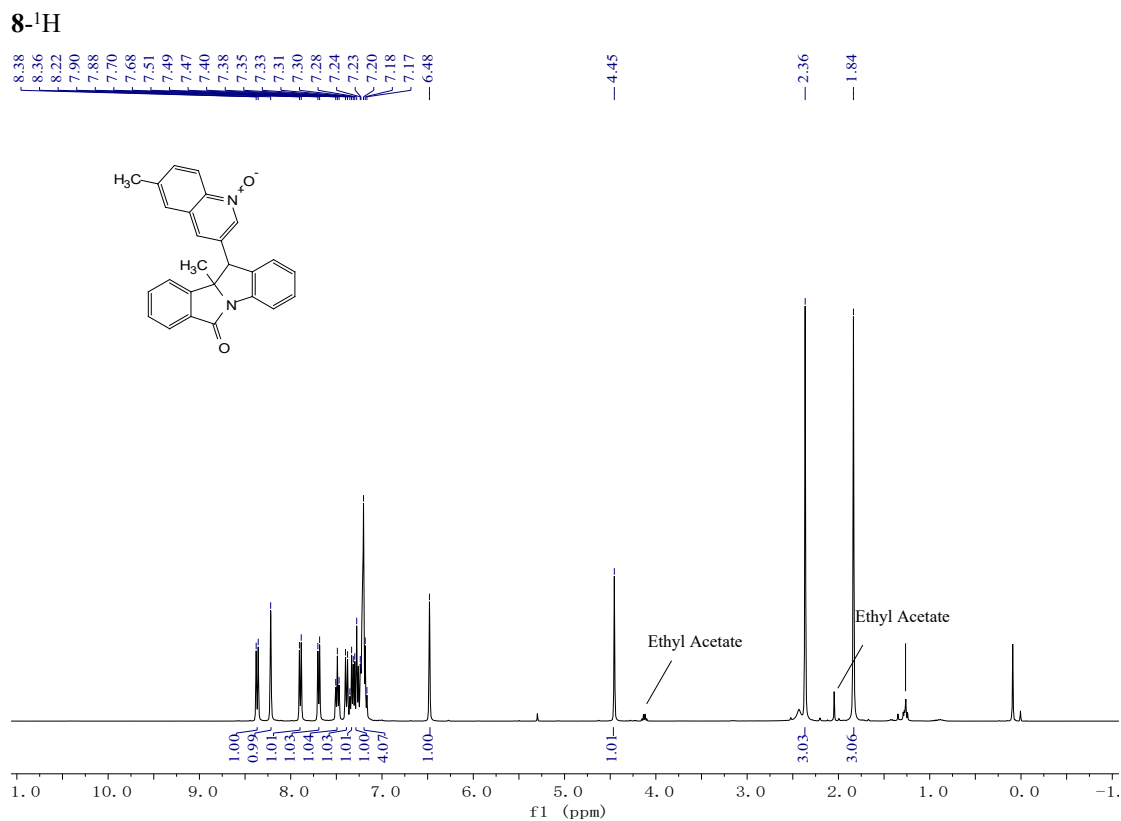
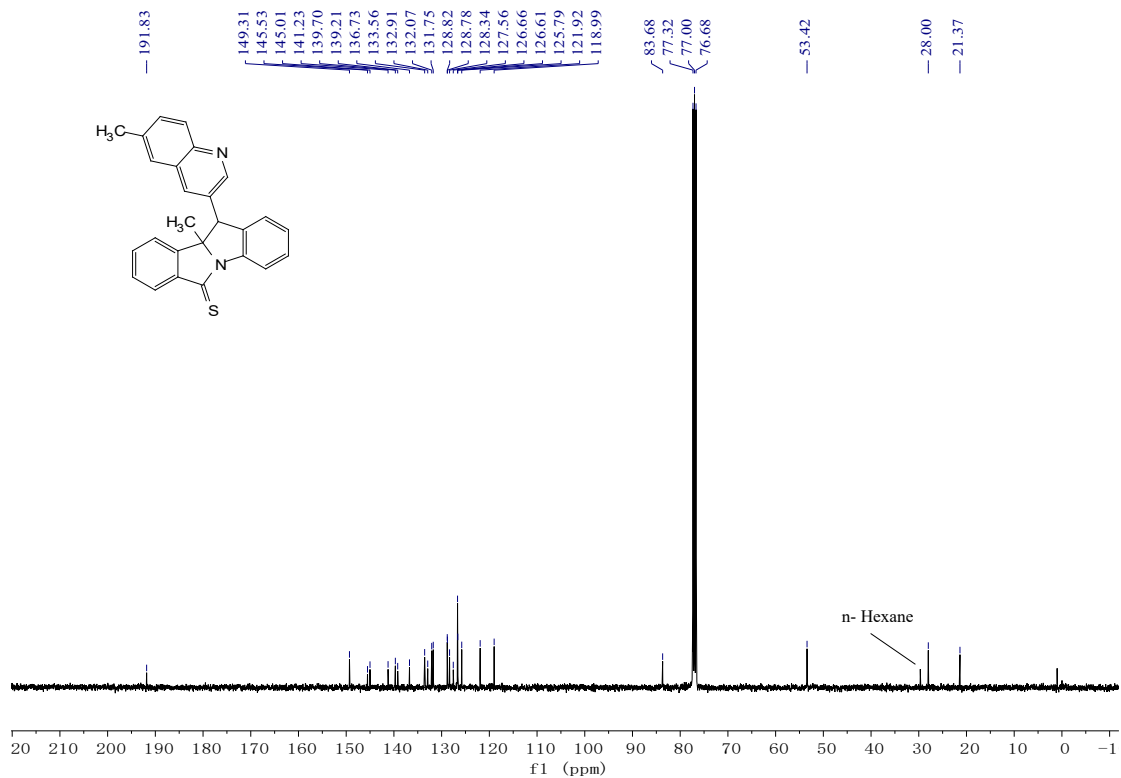
6i-¹³C



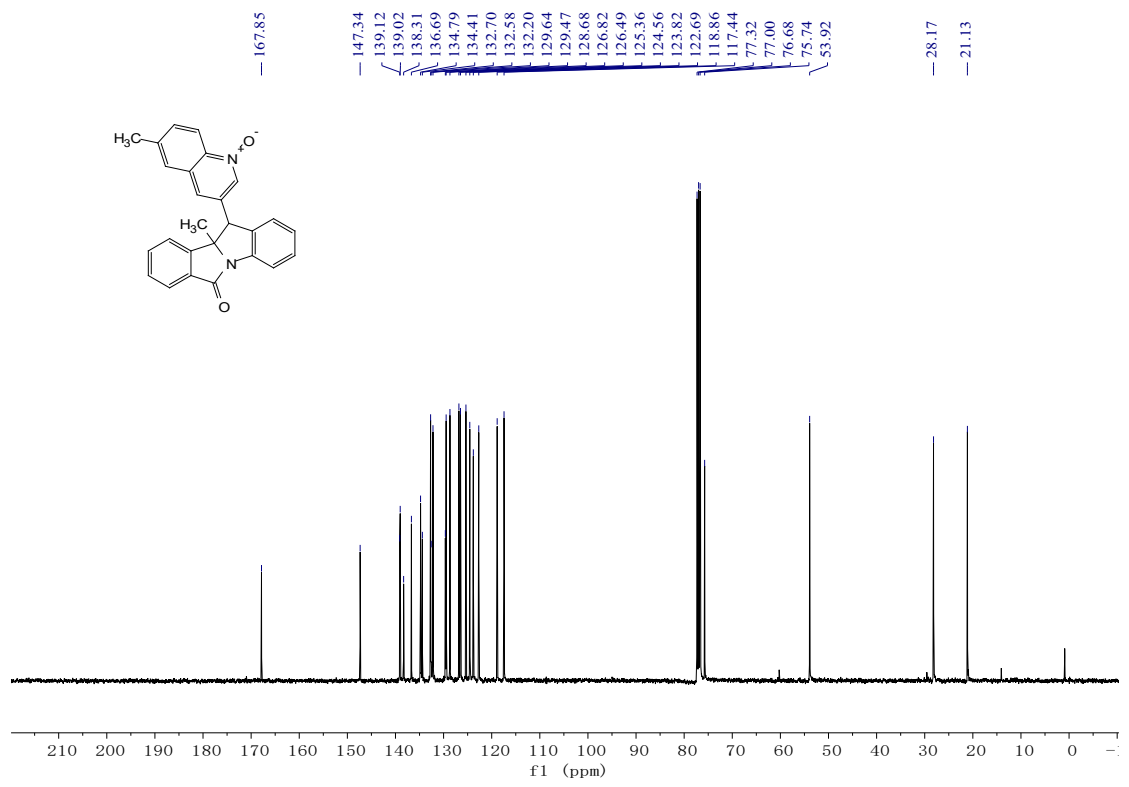
¹H NMR



¹³C



¹³C



8. Computational details

Quantum chemistry calculations were conducted with the Gaussian 09 software package^[3]. The structures were optimized by the density functional theory (DFT)^[4] with B3LYP-D3 functional^[5,6] on basis of def2-SVP^[7] using SMD^[8] continuum solvent model (solvent = dichloroethane). Frequency analyses were performed at the same level of theory to verify the stationary points to be real minima or saddle points and to obtain the thermodynamic energy corrections at 383.15K. All transition states were confirmed by intrinsic reaction coordinate (IRC), and calculations were performed to confirm the connection between two correct minima for a transition state. In order to get more accurate electronic energies, the single point energy were calculated at the M06^[9-10]-D3/def2-TZVP level of theory using SMD continuum solvent model (solvent = dichloroethane).

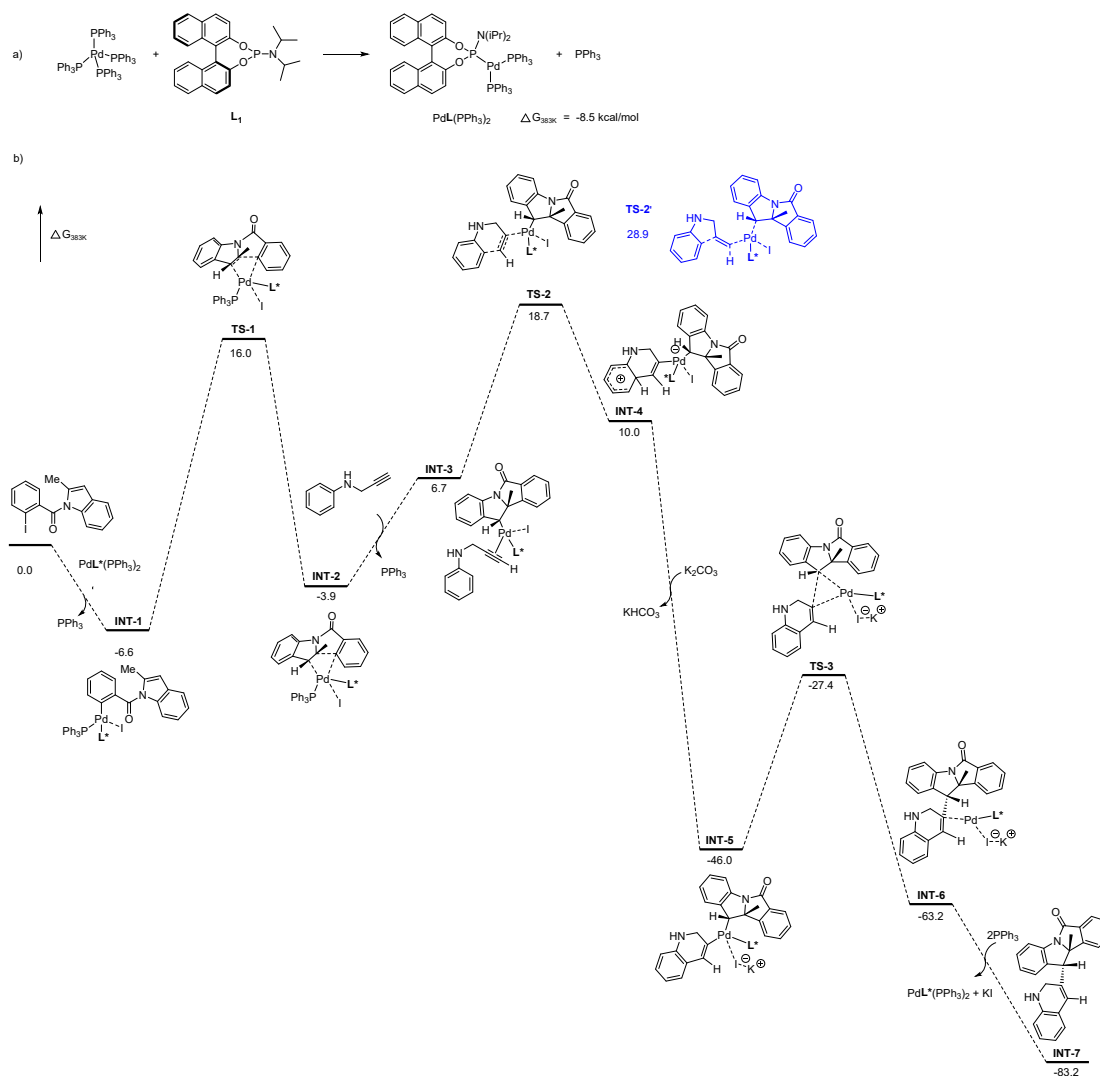


Figure S1 Calculated reaction pathway

Table S1. Calculated energy data and imaginary frequencies for all structure

	Energy (au)	Thermal correction to Enthalpy (au)	Thermal correction to Gibbs Free Energy (au))	Imaginary frequency (cm ⁻¹)
	M06-D3 /def2TZVP/SMD	B3LYP-D3 /def2SVP/SMD	B3LYP-D3 /def2SVP/SMD	B3LYP-D3 / def2SVP//SMD
substrate	-1044.428282	0.264183	0.174116	None
Pd(PPh₃)₄	-4272.14401	1.216526	0.942308	None
L₁	-1552.632762	0.503527	0.380912	None
Catalyst	-3752.735276	1.114176	0.858949	None
INT-1	-3761.177861	1.078905	0.832212	None
PPh₃	-1036.003721	0.300462	0.208347	None
TS-1	-3761.141568	1.077514	0.831978	-236.01
INT-2	-3761.174243	1.079794	0.832935	None
yne	-402.900027	0.170418	0.107278	None
INT-3	-3128.043866	0.947771	0.722068	None
TS-2	-3128.029143	0.946191	0.726437	-344.42
TS-2'	-3128.009342	0.945338	0.722975	-499.68
INT-4	-3128.04608	0.948553	0.729482	None
INT-5	-3727.489101	0.939955	0.710301	None
K₂CO₃	-1463.758711	0.026213	-0.027584	None
KHCO₃	-864.399108	0.036756	-0.01419	None
TS-3	-3727.461788	0.938817	0.712696	-307.95
INT-6	-3727.527657	0.942122	0.721447	None
INT-7	-1149.054173	0.424775	0.314553	None
KI	-897.7785	0.005478	-0.034317	None
Product	-1147.866064	0.400873	0.294911	None
H₂	-1.169854	0.014181	-0.005953	None

Reference:

[3]. Frisch, M. J. *et al. Gaussian 09, Revision D.01* (Gaussian, Inc.: Wallingford, CT, 2009).

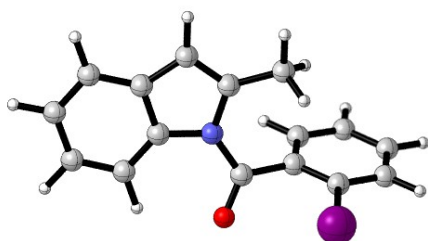
[4]. Hohenberg, P.; Kohn, W. *Phys. Rev.* **1964**, 136(3B), 864

[5]. Becke, A. D. *J. Chem. Phys.* **1993**, 98, 5648

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- [7]. Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, 7, 3297
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- [9]. Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, 41, 157
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Structure and Coordinations

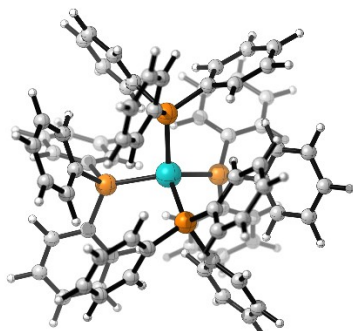
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C	3.23403200	1.38350200	-0.26865100
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N	-1.41876000	0.26734800	0.07594700
C	-1.42652600	0.82770600	1.38453700
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C	-2.70923700	0.81179900	1.85467200
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Pd(PPh₃)₄



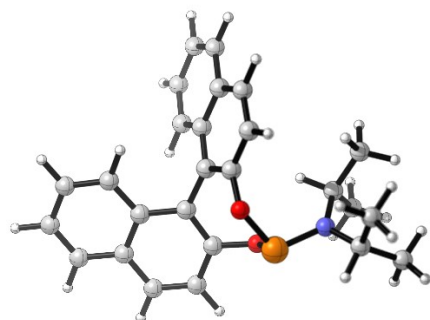
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L₁

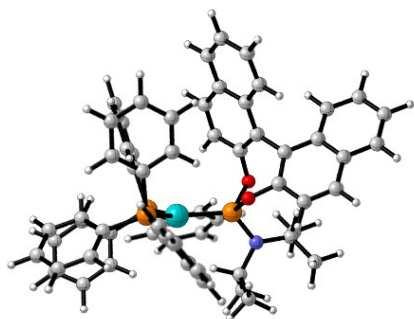


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H	-5.06017700	-2.05966900	1.43530000
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H	-6.35305700	-1.89370300	0.21888000

Catalyst



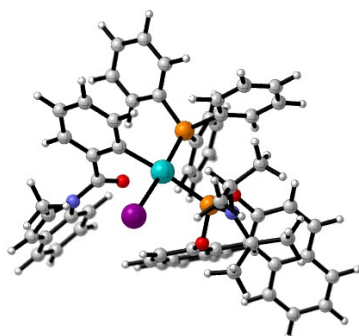
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C	-5.69124200	0.15163400	-2.35418500
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H	-2.13877800	-4.15322100	-0.43734800
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H	-2.00338800	-5.02793100	-1.98815600
H	-3.37440500	-2.10245300	-4.05477600
H	-2.71095200	-3.75539800	-4.19558900
H	-4.30658000	-3.49645900	-3.45949400
C	-0.27001700	-2.43529000	-3.07488200
C	-0.47140300	-1.82434700	-4.47000500
C	0.16845300	-3.89873000	-3.14176200
H	0.57325500	-1.88441800	-2.61851700
H	-0.88092200	-0.80576900	-4.39092700
H	0.49782000	-1.76160600	-4.99165600
H	-1.14684100	-2.41927100	-5.10153000
H	0.35643700	-4.29991500	-2.13458500
H	-0.57819300	-4.53450800	-3.64105200
H	1.10369100	-3.97175300	-3.72046700
P	1.61197300	1.97381700	-1.05289200
C	3.40137800	2.42919100	-1.15289700
C	3.98901300	3.03305400	-2.27658500
C	4.22828900	2.05801900	-0.07473900
C	5.36985100	3.26491600	-2.31744600
H	3.37293400	3.32564100	-3.12919500
C	5.60000800	2.30951300	-0.10811600
H	3.79614100	1.56130100	0.79609900
C	6.17805000	2.90992200	-1.23396200

H	5.81226700	3.73053300	-3.20250100
H	6.22283000	2.01531300	0.73997500
H	7.25527700	3.09345300	-1.26682500
C	0.94629500	3.06461700	0.28838700
C	1.70249500	4.03288000	0.96860400
C	-0.39357800	2.85360400	0.67182200
C	1.13561400	4.76676400	2.01836000
H	2.74134900	4.21832500	0.68915700
C	-0.96024400	3.59965900	1.70707100
H	-0.99263600	2.09252000	0.16404200
C	-0.19480000	4.55264700	2.39036200
H	1.73992000	5.51177900	2.54330900
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C	0.67599200	4.11005000	-2.71649500
C	0.00767600	2.38969500	-4.82086500
H	0.70362400	0.79698400	-3.53259800
C	0.12074100	4.62414800	-3.89217600
H	0.93515500	4.78731500	-1.89866700
C	-0.21284200	3.76565100	-4.94696200
H	-0.25560500	1.71273100	-5.63808300
H	-0.05441600	5.69948900	-3.98476400
H	-0.64959500	4.16984600	-5.86418100
P	2.43832800	-1.48861200	0.83763200
C	2.33746500	-0.96821100	2.61187700
C	2.51081000	-1.85311800	3.68938800
C	2.04124100	0.38063400	2.88194500
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H	2.73053300	-2.90691400	3.50389900
C	1.94347800	0.83967200	4.19776400
H	1.86085900	1.07235900	2.05655400
C	2.12086500	-0.04805300	5.26517600
H	2.53359100	-2.09561100	5.83608500
H	1.70625300	1.89019800	4.38454200
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C	4.23930000	-1.34548300	0.44070800
C	5.25296000	-1.23616900	1.40569800
C	4.58895400	-1.31672700	-0.92121000
C	6.59085300	-1.10626900	1.01446200
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C	5.92514200	-1.20178900	-1.31041600
H	3.80231800	-1.36633800	-1.68058400

C	6.93054200	-1.09283700	-0.34218600
H	7.37051500	-1.01492400	1.77571100
H	6.18119700	-1.17762700	-2.37288900
H	7.97554700	-0.98749300	-0.64546400
C	2.19907800	-3.32660800	0.92499000
C	0.88094600	-3.81476400	0.86429100
C	3.25736900	-4.24588700	1.02229200
C	0.62594800	-5.18762600	0.91251300
H	0.04725500	-3.11656100	0.76556400
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H	4.28965100	-3.89225400	1.06729000
C	1.68673500	-6.09655800	1.00569600
H	-0.40515100	-5.54702800	0.86127400
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H	1.48908300	-7.17155800	1.03026900

INT-1



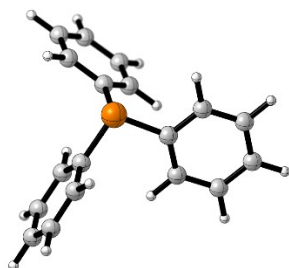
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C	-3.79257600	-0.20006300	-0.30880400
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C	-2.96012000	4.07044700	0.82903100
C	-2.97160200	5.45231000	1.04057100
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C	-4.20606900	5.84314000	-1.02148600
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O	-2.21255900	1.32214200	0.56327300
Pd	-0.92345300	-1.22299600	-0.58901100
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C	6.72114300	3.37250600	-0.46486200
C	5.40665100	2.95719300	-0.39608600
C	5.06551700	1.66118200	0.09069400
C	6.13821600	0.78143400	0.47071300
C	7.48224700	1.24742300	0.40349000
C	3.70389700	1.19942900	0.17503000
C	3.49099800	-0.13833400	0.50323100
C	4.54468700	-1.00696600	0.87525800
C	5.84072800	-0.54798800	0.88213300
C	2.53455200	2.08037400	-0.11346600
C	2.28326200	3.30363800	0.60376700
C	1.12423700	4.08827800	0.27168500
C	0.23881200	3.64273500	-0.74899500
C	0.46236200	2.45090100	-1.39567600
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C	3.10283200	3.74878900	1.68189800
C	2.81054800	4.90705200	2.37341200
C	1.67872100	5.68775500	2.02936300
C	0.85425700	5.28113500	1.00124400
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O	1.77852100	0.48439400	-1.72907800
H	-5.43139400	-3.72332900	-0.31730500
H	-6.85961800	-1.69092200	-0.00757600
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H	3.09219100	-1.95623300	-4.73915100
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C	-3.82774300	-3.59914300	3.77015100
H	-1.92249400	-4.22209000	2.99137800
C	-4.41689900	-1.27642200	3.45060400
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H	-4.06008800	-4.59434500	4.15842000
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C	-0.06075200	-0.41364900	2.80227500
C	0.08855100	-0.70734000	4.17138100
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C	0.51311800	0.27939500	5.06240100
H	-0.13593300	-1.70895200	4.54535000
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C	0.76320700	1.57661100	4.59891500
H	0.63367300	0.03807800	6.12169700
H	0.77813700	2.88877700	2.88368000
H	1.07945500	2.35725800	5.29590500
C	0.31755900	-3.20076300	1.87247700
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C	2.27915400	-4.37790900	2.68668100
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C	1.81097100	-5.56813800	2.12248500
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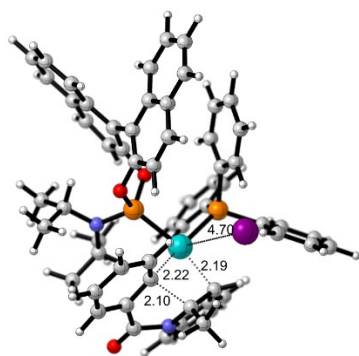
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C	-1.80285100	3.60746100	-0.43892800
H	-0.43000700	2.77416300	-1.88105400
C	-2.60068000	3.36253000	0.68493900
H	-3.25039800	1.88393900	2.12596700
H	-1.77863400	4.60389500	-0.88850700
H	-3.20234000	4.16655800	1.11714600
C	1.64337100	0.26886900	-0.42893900
C	1.84358900	1.08665400	0.69612400
C	2.75186100	-0.38911800	-0.99402100
C	3.12183400	1.23706700	1.24567900
H	0.99923500	1.60874400	1.15164100

C	4.02592800	-0.24815700	-0.43706100
H	2.61624700	-1.02077500	-1.87747300
C	4.21465600	0.56877700	0.68404100
H	3.26218300	1.87791800	2.12054800
H	4.87554800	-0.77060800	-0.88505900
H	5.21213300	0.68719000	1.11568600
C	-0.58742900	-1.55659200	-0.43005900
C	-1.71304900	-2.18567400	-0.99408600
C	0.02042700	-2.13975600	0.69457000
C	-2.22965200	-3.35851700	-0.43680600
H	-2.19240400	-1.75145400	-1.87696500
C	-0.49007900	-3.32108700	1.24459500
H	0.89533100	-1.67031800	1.14969500
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H	-3.10824800	-3.83131400	-0.88412800
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TS-1



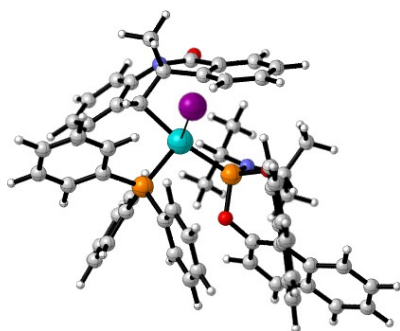
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C	-3.46891200	-2.51317900	-2.38923300
N	-4.08206700	-1.63129300	-1.47720200
C	-3.69913900	-0.25433400	-1.48894000
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C	-4.21617400	-0.90227800	0.69146600
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H	-3.85461100	1.24213700	0.11063800
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H	-5.48795000	-4.29872000	2.08576900
H	-5.21125000	-2.34994100	3.60082500
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H	-4.15083700	0.20288100	-3.56920700
I	-1.54841900	4.10872800	-2.24975200
Pd	-1.51883500	-0.17235700	-0.30647000
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C	2.46064200	-4.58732900	-0.98283300
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H	1.36314600	-2.50331200	-3.56849800
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H	2.61133200	-4.46110500	0.09754700
H	1.81104300	-5.45733000	-1.15240600
H	3.44031800	-4.81403200	-1.43268000
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C	-1.01722600	-0.45916400	3.18617100
C	-0.65157400	-0.13125100	4.50634700
C	-1.35341900	-1.78621300	2.88133500

C	-0.61453700	-1.11924700	5.49247300
H	-0.39501000	0.89680800	4.76829800
C	-1.31982000	-2.77320000	3.87104400
H	-1.64351300	-2.04563700	1.86230600
C	-0.94861400	-2.44205600	5.17681400
H	-0.32510100	-0.85383800	6.51239100
H	-1.58364500	-3.80192200	3.61618500
H	-0.91999900	-3.21324600	5.95103200
C	-2.42537700	1.98703400	2.39499900
C	-2.81548400	2.99515000	1.49438600
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C	-3.79764700	3.92356100	1.84436700
H	-2.37404000	3.05383500	0.49697400
C	-4.04984800	2.84522800	3.99110700
H	-2.80286100	1.13653200	4.36164300
C	-4.41902500	3.85280300	3.09600800
H	-4.08111900	4.69661500	1.12560300
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INT-2



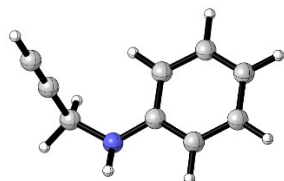
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C	-2.39524700	-0.45238400	-2.73949800
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N	-4.16865000	-1.65379600	-1.82730600
C	-3.64974500	-0.26457800	-1.88131300
C	-4.64909200	-1.93500300	-0.54306200
C	-4.29794900	-0.87548100	0.32983700
C	-3.48409900	0.12459700	-0.39991900
C	-5.33738500	-3.06783300	-0.10721200
C	-5.71462300	-3.11599400	1.24084800

C	-5.42394100	-2.05315900	2.11201900
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O	-3.72546800	-3.73713800	-2.75374100
H	0.21147400	0.81480600	-4.50295500
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H	-1.50706600	-3.15377500	-4.66489500
H	-1.47817100	1.52140800	-2.81066700
H	-3.68796600	1.17520800	-0.18220000
H	-5.57172700	-3.87340900	-0.80274800
H	-6.25833400	-3.98778200	1.61386100
H	-5.74647300	-2.10580700	3.15469500
H	-4.48056800	-0.11872400	2.35050700
H	-4.20642300	1.69060700	-2.62846800
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H	-4.83693000	0.32912600	-3.60856100
I	-1.16078400	4.46421700	-2.10413600
Pd	-1.43736700	-0.29684400	-0.25758900
C	7.88573700	-2.43708000	0.13023300
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C	6.30264200	-0.77235900	-0.66446200
C	5.29038200	-1.28406600	0.19927500
C	5.61083500	-2.42671800	1.01176000
C	6.92632900	-2.97068100	0.96464800
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C	2.99818200	-1.41582800	0.98068200
C	3.31343000	-2.52871100	1.79470900
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C	5.31822200	1.90658000	0.75485800
C	5.94411700	3.11648600	0.97546100
C	5.54876400	4.27564500	0.26239600
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H	8.31715600	-0.92809500	-1.37859700
H	6.07118100	0.07110100	-1.31547900
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H	5.62149800	1.03757300	1.33732600
H	6.74326500	3.18350600	1.71833200
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C	2.50137800	-4.76069800	-0.86564000
H	2.81725900	-2.72703500	-1.35011600
H	1.57505000	-2.64464800	-3.48518300
H	2.85980600	-3.87905000	-3.47381500
H	1.15831400	-4.37281600	-3.32810100
H	2.63395900	-4.64199100	0.21755400
H	1.82253800	-5.60548600	-1.05020300
H	3.48127400	-5.02469700	-1.29416300
C	-0.38411100	-3.67198000	-0.47943100
C	-0.20874300	-4.35050100	0.88637300
C	-0.87257400	-4.65632800	-1.53957200
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H	0.17403700	-3.64202200	1.63511100
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H	-1.03097600	-4.16357000	-2.50471900
H	-0.17189000	-5.49164100	-1.67959100
H	-1.83893800	-5.07456200	-1.22270500
P	-1.27990200	0.68113700	1.84632100
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C	1.33134700	1.10427700	2.90698700
C	1.63843800	3.58333500	1.65293900
H	-0.28107900	3.23661600	0.77008100
C	2.49193000	1.85440900	3.10923300
H	1.24533700	0.12522300	3.37601400
C	2.64375400	3.10104900	2.49506200
H	1.75908600	4.53890500	1.13827100
H	3.28682700	1.45309400	3.74296100
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C	-1.08500200	-0.25463200	4.51867800

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C	-1.18763800	-1.23060800	5.51190000
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H	-1.96374800	-2.14933700	1.81629800
C	-1.56974800	-2.53625600	5.17976900
H	-0.96697300	-0.96978200	6.55000300
H	-2.14432900	-3.88011200	3.58199200
H	-1.64843400	-3.29806600	5.95972900
C	-2.57049200	1.94155500	2.24363800
C	-2.84408900	2.93197200	1.28303600
C	-3.29109800	1.94706800	3.44987700
C	-3.79689700	3.92124700	1.53288200
H	-2.32538100	2.93636600	0.32203800
C	-4.25299500	2.93409100	3.69155700
H	-3.12296000	1.18124900	4.20684600
C	-4.50519300	3.92572700	2.73910100
H	-3.98501600	4.68302700	0.77225800
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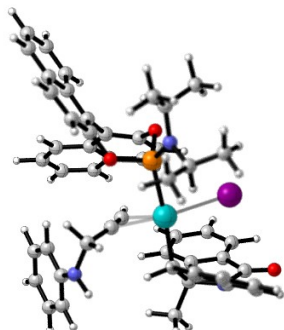
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C	1.70360900	1.39943500	-0.46813300
C	2.77598300	0.73906600	0.13566300
H	3.41024000	-1.10546400	1.07726400
H	1.22641500	-2.23183600	0.80368100
H	-0.36057300	1.33290400	-1.06784500
H	1.82564800	2.42620500	-0.82400200
H	3.74153900	1.23609800	0.25226500
N	-0.92831300	-1.23315000	-0.34443800
H	-1.06016300	-2.01646700	0.28514900
C	-2.15543800	-0.58231800	-0.75456200
H	-1.98306200	-0.04075300	-1.70077200
H	-2.89133300	-1.36746200	-0.99597400
C	-2.74681500	0.34120200	0.23202500

C	-3.21699400	1.08859300	1.06112400
H	-3.63072100	1.75417000	1.79550100

INT-3

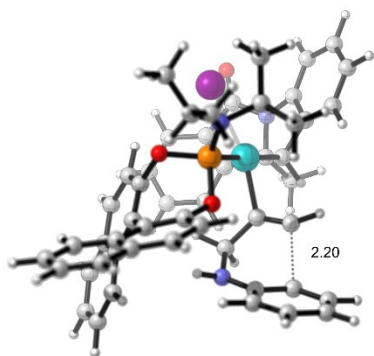


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N	-4.77357500	0.60383400	-0.20424400
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C	-5.75401000	-1.51531400	0.73821800
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C	-4.47088400	-2.45997000	2.59441700
C	-3.54088500	-1.41280500	2.52113800
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O	-5.81558600	-0.10566300	-2.15625400
Pd	-1.11604200	-0.36417200	0.47836800
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C	5.34341800	-0.50415900	-0.37536500
C	6.17121300	-1.22012000	0.55746700
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C	3.92462200	-0.41263300	-0.13988200
C	3.39225100	-1.11173100	0.94004300
C	4.20735100	-1.81963200	1.85775700
C	5.56941100	-1.85722800	1.67932500
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C	1.94852700	-0.30058700	-1.64534600
C	4.12023700	2.56394300	-0.59174700
C	4.21624500	3.92163900	-0.82351400
C	3.37703600	4.55306400	-1.77567900
C	2.44141700	3.81026100	-2.46463900
O	2.04070600	-1.10938300	1.18273100
O	1.66153400	-1.60911000	-1.28470600
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H	-1.23777600	2.27641500	4.03031100
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C	0.07602000	1.04204600	1.72906100
C	0.08996100	1.45448800	0.55891100
H	0.28131800	1.97520000	-0.36692200
P	0.84623300	-1.75450600	0.17498500
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H	1.37314400	-4.22592100	-2.11338400
H	2.73142100	-5.32197100	-1.74426300
H	1.07695300	-5.77282800	-1.27397100
H	2.70476900	-4.62031700	1.99774100
H	1.80660100	-5.97753200	1.25779900
H	3.46013300	-5.60911800	0.72473800
C	-0.37792500	-3.93213200	1.07755200
C	-0.17934800	-4.14883300	2.58357300
C	-0.98729500	-5.14807500	0.38359900
H	-1.12339400	-3.12655900	0.98202400
H	0.29259100	-3.26674200	3.04540600
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H	0.43771800	-5.02899000	2.81277800
H	-1.16717400	-4.93849000	-0.68065400
H	-0.35105100	-6.04121500	0.47199600
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TS-2

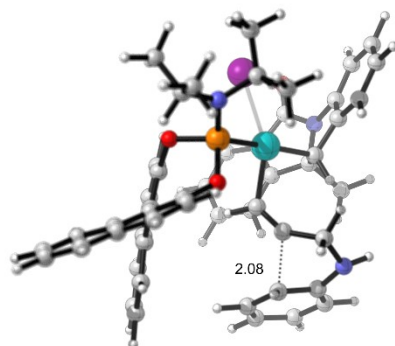


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C	-3.27141800	2.56302000	0.47870200
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C	-4.15819300	-2.30290800	1.52069900
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O	-5.90066000	1.60281700	-1.69773300
Pd	-1.38118800	-0.36723500	0.48644900
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C	7.25665600	-1.16090100	-1.14471800
C	3.71034500	0.06629200	-0.66388900
C	3.21066900	-1.00406700	0.07371100
C	4.02453500	-2.09130600	0.47699400
C	5.34814400	-2.12857200	0.10903100
C	2.80976200	1.21307500	-0.97735000
C	3.11633900	2.56925500	-0.60081100
C	2.21688100	3.62584700	-0.97921300
C	1.02235000	3.30967200	-1.68499200
C	0.69594200	2.00334400	-1.96386200
C	1.58777200	0.96857300	-1.59638400
C	4.25772500	2.91177300	0.18198500
C	4.51181500	4.22003900	0.54206200
C	3.64378600	5.26307900	0.13371500
C	2.51970700	4.96711800	-0.60858500
O	1.89922800	-1.01274600	0.47906200
O	1.20897100	-0.33498800	-1.86109900
H	-1.00434200	5.06034900	0.13594500
H	-2.32418200	5.45594200	-1.92941400

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H	-5.20133500	-4.17313300	1.20756700
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H	5.02209200	1.79277900	-2.35286100
H	7.87489900	-2.00017100	-0.81429100
H	3.57228100	-2.87546400	1.08578600
H	5.98591100	-2.95853500	0.42403000
H	0.34618200	4.11579700	-1.97486700
H	-0.24117000	1.73513700	-2.45454500
H	4.93501400	2.12394000	0.51255600
H	5.39004400	4.45278800	1.14978800
H	3.86172400	6.29564800	0.41778500
H	1.83311800	5.76019700	-0.91732800
C	3.57175000	-1.41583600	4.61527300
C	3.39319900	-0.46423600	3.62742100
C	2.19215900	0.28980000	3.56996500
C	1.17390000	0.04320300	4.54398600
C	1.40646800	-0.91941700	5.56418800
C	2.57259800	-1.66011300	5.58938100
H	4.49824500	-1.99603900	4.63521600
H	4.15925700	-0.29799100	2.86663600
H	0.39323400	0.78869600	4.70745900
H	0.63889700	-1.06596900	6.32859400
H	2.73598500	-2.41494100	6.36185300
N	1.96996000	1.16439500	2.55032600
H	2.65949700	1.12791800	1.80549800
C	0.62140600	1.43964500	2.08960700
H	0.12604800	2.18077900	2.73974600
H	0.68286200	1.87383900	1.08507400
C	-0.23341600	0.18244600	2.12927900
C	-0.24710100	-0.71227500	3.03875900
H	-0.58828900	-1.64192300	3.47269800
P	0.57509800	-1.18872200	-0.56617200
N	0.58897700	-2.73345700	-1.17422200
C	1.64731300	-3.15982500	-2.13291600

C	1.15187500	-3.15597200	-3.58454500
C	2.33325100	-4.47275900	-1.75420800
H	2.42047700	-2.38189500	-2.07204000
H	0.63546500	-2.21160900	-3.81061800
H	2.01132600	-3.25047500	-4.26848700
H	0.46461300	-3.98750800	-3.79492700
H	2.71741300	-4.44040200	-0.72471400
H	1.66342100	-5.33912300	-1.85502800
H	3.18867400	-4.63482400	-2.42940500
C	-0.46169900	-3.63390400	-0.62326900
C	0.02821400	-4.49158500	0.55126700
C	-1.18892700	-4.45389800	-1.68691400
H	-1.21607000	-2.94651600	-0.20553500
H	0.55201900	-3.86897000	1.29422200
H	-0.83641300	-4.95876800	1.05100300
H	0.70613200	-5.29772500	0.23760300
H	-1.58730800	-3.80351300	-2.47867600
H	-0.54208000	-5.21880100	-2.14123600
H	-2.03878500	-4.97388300	-1.21667400
I	-2.60493700	-0.55454000	-2.00637100

TS-2'



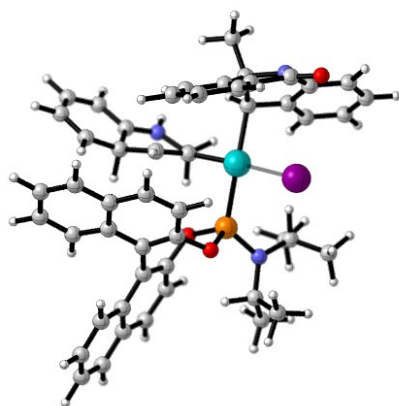
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C	-3.59307800	1.83151700	-2.06663800
C	-2.93078700	2.13662600	-0.86954500
C	-1.91119200	3.08652500	-0.85259500
C	-4.65645400	0.81874500	-1.81008300
N	-4.64267200	0.62309900	-0.43772300
C	-3.60556300	1.41309300	0.27516100
C	-4.91443700	-0.55260300	0.27324600
C	-3.91518700	-0.72651300	1.26028400
C	-2.88486700	0.33994500	1.13346900

C	-5.93952800	-1.47436800	0.08207200
C	-5.97435200	-2.59380300	0.92927900
C	-5.01368400	-2.76901100	1.93554700
C	-3.97850600	-1.83699300	2.10627800
C	-4.27573100	2.44557400	1.20771500
O	-5.38666500	0.25544800	-2.60743000
Pd	-1.10305100	-0.59467200	0.47946500
C	8.20381900	-0.34055500	-0.60208900
C	7.37531800	0.32640700	-1.53848800
C	6.00640100	0.36813500	-1.36401300
C	5.38472900	-0.25451100	-0.24219900
C	6.22656700	-0.95989900	0.68614700
C	7.63567000	-0.97379700	0.48349000
C	3.95974200	-0.22909900	-0.03040100
C	3.43805200	-0.98424300	1.01730800
C	4.26800500	-1.67915500	1.93237500
C	5.63344900	-1.65140400	1.78013500
C	3.03569600	0.53077900	-0.92007100
C	3.13609900	1.95352100	-1.12039700
C	2.24037500	2.59962000	-2.04137000
C	1.25255000	1.82929200	-2.71781200
C	1.11107800	0.48710500	-2.45727200
C	1.99344500	-0.14210100	-1.54847700
C	4.06046200	2.76782900	-0.40291400
C	4.11774800	4.13268700	-0.60453400
C	3.25498200	4.76150500	-1.53700800
C	2.33530100	4.00727600	-2.23575500
O	2.08463200	-1.04859400	1.22983000
O	1.77166700	-1.47635800	-1.25461300
H	-0.73673000	4.42490900	-2.06894200
H	-1.88496800	3.84640200	-4.19547800
H	-3.75828100	2.16405200	-4.19845200
H	-1.40452500	3.35841900	0.07401500
H	-2.57797600	0.75721700	2.09833100
H	-6.67636800	-1.32719900	-0.70789800
H	-6.76631700	-3.33661600	0.80242000
H	-5.06779000	-3.64410200	2.58845100
H	-3.21121400	-1.98984500	2.87052200
H	-3.50104300	3.03915200	1.71761200
H	-4.92424300	3.12732300	0.63610800
H	-4.88415900	1.93418800	1.96993700
H	9.28656000	-0.36130900	-0.74977000
H	7.82377700	0.80789300	-2.41149400
H	5.38790600	0.87741300	-2.10330600

H	8.26031900	-1.50805200	1.20485300
H	3.79100300	-2.22446100	2.74871900
H	6.27899800	-2.17891100	2.48717200
H	0.58030400	2.32463200	-3.41989700
H	0.32214500	-0.11208800	-2.91513400
H	4.72492200	2.30399400	0.32630400
H	4.83041200	4.73444100	-0.03474000
H	3.31381500	5.84188500	-1.69127100
H	1.65449000	4.48077100	-2.94808800
C	-0.94915300	5.68078300	2.06803800
C	-1.39326100	4.81925900	3.05880700
C	-0.64242500	3.65720100	3.35123200
C	0.61531200	3.43460500	2.68993300
C	1.02983300	4.34496500	1.67593700
C	0.24920100	5.43508600	1.34804000
H	-1.55437300	6.55582900	1.81606800
H	-2.34518800	4.98800900	3.56804100
H	1.40551600	2.87392400	3.19959200
H	1.98373100	4.17257900	1.17191100
H	0.56109100	6.12342800	0.55976200
N	-1.12110100	2.60529100	4.07138600
H	-2.10334600	2.60519200	4.33018900
C	-0.51006400	1.34028900	3.68001000
H	0.35841800	1.09114100	4.31406300
H	-1.23002600	0.51208900	3.75605600
C	-0.05473000	1.51545700	2.25757800
C	-0.06553700	1.09000600	1.05285000
H	0.39410300	1.54831200	0.17525200
P	0.94808300	-1.74394900	0.18575100
N	1.07713000	-3.39348800	0.32188200
C	2.32528700	-4.07678100	-0.12040000
C	2.17307600	-4.74066000	-1.49468900
C	2.91321000	-5.02704700	0.92285300
H	3.06124800	-3.27163700	-0.25213900
H	1.71188300	-4.04197600	-2.20790900
H	3.16695700	-5.02096800	-1.88080000
H	1.56223000	-5.65317400	-1.45390100
H	3.04575500	-4.52601900	1.89261700
H	2.28919300	-5.92064300	1.07016500
H	3.90347600	-5.36658300	0.57927600
C	-0.07588700	-4.07415800	0.97168900
C	0.13087800	-4.34073700	2.46877600
C	-0.55509000	-5.31400800	0.21883500
H	-0.89625500	-3.34232600	0.90099100

H	0.50382900	-3.43730300	2.97712800
H	-0.83340800	-4.61435100	2.92788800
H	0.83424900	-5.16243700	2.66428200
H	-0.73303200	-5.08329700	-0.84113200
H	0.15991500	-6.14737400	0.29007500
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I	-2.24147800	-2.05822400	-1.65806300

INT-4

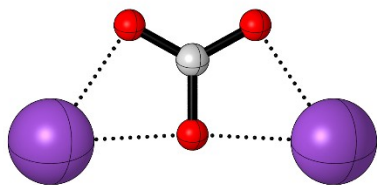


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C	-3.82672800	2.09372800	-2.01142000
C	-3.06108700	2.44481100	-0.89107400
C	-1.96966900	3.29921200	-1.02780800
C	-4.93125400	1.18159100	-1.59718600
N	-4.81536000	1.07725100	-0.22109700
C	-3.69416600	1.86573200	0.35594100
C	-5.07617200	-0.04031900	0.58450600
C	-4.01726300	-0.19141100	1.51109700
C	-2.95660300	0.83209200	1.25820900
C	-6.14329600	-0.93101600	0.51372900
C	-6.16421600	-2.00122000	1.42317000
C	-5.14466100	-2.15299900	2.37235200
C	-4.06847500	-1.25210100	2.42050100
C	-4.25627400	3.01276100	1.22177100
O	-5.75809700	0.61699500	-2.29449300
Pd	-1.28650500	-0.26300000	0.52079200
C	7.91193600	-1.62279400	-1.01379600
C	7.18981300	-0.79591900	-1.91001700
C	5.86973300	-0.47514300	-1.66435000
C	5.19338300	-0.96245200	-0.50760800
C	5.92010900	-1.83005000	0.37995600

C	7.28409900	-2.13100100	0.10416000
C	3.81667400	-0.64834300	-0.22291300
C	3.20450500	-1.28994900	0.85287200
C	3.92335400	-2.14078500	1.72971100
C	5.25650800	-2.39007600	1.50799400
C	3.01704600	0.29200400	-1.05917100
C	3.39352700	1.66599700	-1.26823600
C	2.58194000	2.49678900	-2.11667400
C	1.40142000	1.95972100	-2.70344100
C	1.01019500	0.66902000	-2.43678400
C	1.81937000	-0.14768100	-1.61272600
C	4.52110900	2.26171200	-0.63096300
C	4.85079200	3.58482500	-0.84816900
C	4.06992300	4.39021000	-1.71449000
C	2.95616200	3.85476600	-2.32809500
O	1.87587700	-1.09159900	1.12510300
O	1.37600100	-1.42793500	-1.33651200
H	-0.77667600	4.41759000	-2.43805300
H	-2.10780400	3.74733300	-4.42427200
H	-4.10709200	2.24158400	-4.15146600
H	-1.37969800	3.59796000	-0.15987700
H	-2.62351100	1.32108300	2.18253900
H	-6.92429200	-0.79651400	-0.23513900
H	-6.98773300	-2.71950400	1.38952400
H	-5.18270600	-2.98704200	3.07855700
H	-3.25936100	-1.39658200	3.14217300
H	-3.42643900	3.61347100	1.62549900
H	-4.91220600	3.67011900	0.62947500
H	-4.83449300	2.60474200	2.06563000
H	8.95806400	-1.86474700	-1.21795400
H	7.68082500	-0.41224000	-2.80816300
H	5.33032900	0.15394000	-2.37262600
H	7.82336000	-2.78499700	0.79517300
H	3.38716500	-2.58443700	2.57043200
H	5.81684000	-3.04151500	2.18372500
H	0.78925400	2.59618300	-3.34495500
H	0.08080900	0.25252000	-2.82907400
H	5.12764200	1.66137400	0.04726500
H	5.71779100	4.01714400	-0.34203500
H	4.34404800	5.43475400	-1.88254600
H	2.33425500	4.46961900	-2.98449500
C	1.71288300	5.15878500	3.60749000
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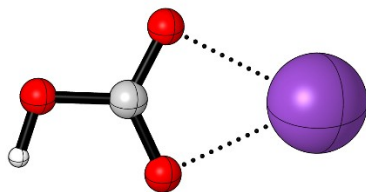
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C	2.12461100	5.16019300	2.22240700
H	1.82763400	6.07955700	4.18615700
H	0.81020500	4.09989500	5.24593100
H	2.42489500	2.11284000	2.15856200
H	2.33232900	4.00279900	0.43973800
H	2.52526700	6.07903300	1.78938300
N	0.32072200	1.83145200	3.93412700
H	-0.05055500	1.88722000	4.88274100
C	-0.02123500	0.64337400	3.14095500
H	0.78458000	-0.10620400	3.25106500
H	-0.93114000	0.21409500	3.58195400
C	-0.17229400	0.96013900	1.67403000
C	0.54292900	1.96933000	1.16760600
H	0.54746000	2.23247700	0.10868400
P	0.58817000	-1.60398000	0.13735500
N	0.51216900	-3.26194400	0.25378600
C	1.60469300	-4.10464700	-0.30646100
C	1.24244900	-4.69738500	-1.67432800
C	2.13235100	-5.16206200	0.66389200
H	2.43695500	-3.41109500	-0.48688200
H	0.82745500	-3.91777800	-2.32942600
H	2.14894500	-5.10343900	-2.15288800
H	0.51017000	-5.51355600	-1.59869100
H	2.42865900	-4.71458500	1.62338200
H	1.39611100	-5.95570300	0.85731400
H	3.02391800	-5.63746300	0.22443200
C	-0.66044500	-3.79235700	1.00164100
C	-0.35936100	-4.08987600	2.47695900
C	-1.35948900	-4.95624100	0.30211000
H	-1.38251700	-2.95989000	0.99898500
H	0.17072000	-3.24399600	2.94324500
H	-1.30616400	-4.23737800	3.02228400
H	0.24795700	-4.99575200	2.61461700
H	-1.61483000	-4.69160900	-0.73363700
H	-0.75012700	-5.87244200	0.30024000
H	-2.29670600	-5.18365000	0.83455600
I	-2.59435200	-1.60032700	-1.63694900

K₂CO₃



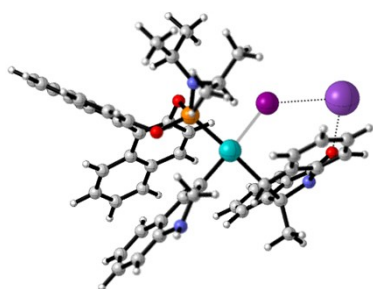
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O	0.00068100	-0.50467800	-0.00000500
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O	-1.12259700	1.44345200	0.00002600
K	-2.52484700	-0.63138600	-0.00000800
K	2.52423400	-0.63165300	0.00001300

KHCO₃



C	-1.02058800	-0.03715900	0.00081600
O	-0.48858100	1.10421900	0.00193400
O	-0.44540000	-1.14786700	0.00172300
O	-2.39515700	-0.08134200	-0.00207900
H	-2.69420100	0.84252100	-0.00253300
K	1.86583300	0.02001900	-0.00078900

INT-5



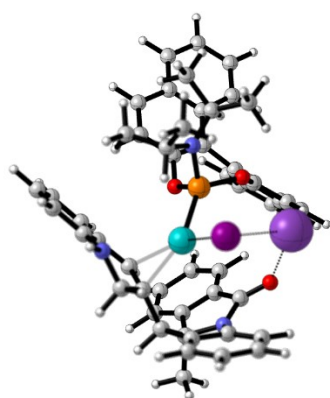
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C	-3.45886300	2.52045600	-1.66226600
C	-2.66700000	2.80670700	-0.54000500
C	-1.51754400	3.58208800	-0.67559000
C	-4.61332700	1.69171800	-1.24352100
N	-4.53229200	1.58932800	0.12063900

C	-3.32574300	2.24875600	0.70259800
C	-4.90275600	0.49236600	0.92114100
C	-3.82184600	0.17810700	1.77639500
C	-2.67120900	1.10093900	1.53575100
C	-6.09716500	-0.22454600	0.91924000
C	-6.20246200	-1.32782700	1.78493500
C	-5.14076700	-1.66415000	2.63579800
C	-3.95633600	-0.91081200	2.64488000
C	-3.75601300	3.40170400	1.62876000
O	-5.46125900	1.14333500	-1.95446800
Pd	-1.09776600	-0.09547200	0.72525800
C	7.83719000	-2.16226600	-1.49821600
C	7.09169300	-1.34172000	-2.38122400
C	5.82627500	-0.90832100	-2.03984100
C	5.23096500	-1.27047500	-0.79591800
C	5.97643000	-2.13344900	0.08015600
C	7.28455200	-2.55146100	-0.29588500
C	3.91255900	-0.83612700	-0.41325400
C	3.35727600	-1.36819500	0.74914100
C	4.09562100	-2.21172100	1.61665100
C	5.38370600	-2.57016000	1.29859800
C	3.11447800	0.12078000	-1.23119000
C	3.57093100	1.44878100	-1.55008400
C	2.73828000	2.30387600	-2.35274100
C	1.46936000	1.83563800	-2.79572400
C	1.01655000	0.58918200	-2.43364800
C	1.84216100	-0.25043200	-1.65013200
C	4.79941500	1.98055600	-1.06109500
C	5.19795600	3.26475600	-1.37261400
C	4.38766500	4.09509500	-2.18616400
C	3.18160500	3.62188900	-2.65972100
O	2.07237600	-1.06622100	1.11893300
O	1.33789300	-1.48136500	-1.26934900
H	-0.24856400	4.61239800	-2.08328300
H	-1.63209100	4.05943300	-4.06988700
H	-3.73755800	2.70744200	-3.80251500
H	-0.90280300	3.83035100	0.18996200
H	-2.28444800	1.51244300	2.47574000
H	-6.93337600	0.08423700	0.28778500
H	-7.12602200	-1.91215300	1.80488700
H	-5.23951300	-2.51962800	3.30943800
H	-3.13201500	-1.18570900	3.30856200
H	-2.86114000	3.89166800	2.04163400
H	-4.35081200	4.15150200	1.08358700

H	-4.35656800	3.01304400	2.46597400
H	8.84085900	-2.49271100	-1.77781600
H	7.52054800	-1.05266900	-3.34437900
H	5.26534300	-0.28587700	-2.73752500
H	7.84091400	-3.19892800	0.38773700
H	3.61102000	-2.55818700	2.53112400
H	5.95956500	-3.21423700	1.96835500
H	0.84222200	2.49270400	-3.40101100
H	0.02718400	0.22673000	-2.71784200
H	5.42695900	1.36771100	-0.41444300
H	6.14066100	3.64945000	-0.97514200
H	4.71375000	5.11070600	-2.42450800
H	2.53798600	4.25715200	-3.27452900
C	3.55080800	4.41734100	3.56514100
C	2.61666800	3.58066200	4.18871700
C	1.75278000	2.77736400	3.42218500
C	1.83533100	2.82550700	2.00007800
C	2.77831500	3.67205000	1.40086900
C	3.64001000	4.46599400	2.16940400
H	4.21557100	5.03034100	4.18083600
H	2.54898500	3.54482100	5.28046000
H	2.83353600	3.70157000	0.30968800
H	4.37198400	5.11407700	1.68046700
N	0.77390700	1.98722800	3.99464200
H	0.82844700	1.89112300	5.00421200
C	0.26464900	0.81138800	3.29114100
H	0.93565200	-0.07091600	3.41074300
H	-0.69801200	0.52954000	3.74636700
C	0.11500300	1.07609400	1.81239900
C	0.89416000	2.01050600	1.22899800
H	0.87892700	2.16313500	0.14646600
P	0.68107900	-1.52996800	0.27670100
N	0.49375000	-3.17299300	0.47811400
C	1.48171700	-4.11748000	-0.11081600
C	0.97441000	-4.75317100	-1.41196900
C	2.01294200	-5.15754500	0.87682600
H	2.34166100	-3.49520600	-0.39306800
H	0.55782300	-3.98056500	-2.07478300
H	1.81083900	-5.24401300	-1.93639500
H	0.20057400	-5.51284600	-1.23330900
H	2.41421000	-4.68090300	1.78265100
H	1.24251500	-5.88409300	1.17351800
H	2.83209500	-5.71873100	0.39937600
C	-0.65346100	-3.58170800	1.33224600

C	-0.26730500	-3.82044300	2.79811500
C	-1.47712500	-4.73043600	0.75079200
H	-1.31923800	-2.70286800	1.33009500
H	0.33273400	-2.98038900	3.18260100
H	-1.17980700	-3.89333500	3.41266300
H	0.30509100	-4.74780000	2.94190800
H	-1.78280500	-4.50774500	-0.28131500
H	-0.93334100	-5.68675700	0.76438100
H	-2.38912500	-4.85745300	1.35608100
I	-2.57763000	-1.45395400	-1.38825000
K	-5.84629000	-1.36847600	-2.36778900

INT-6



C	0.56711100	2.75089700	3.62535000
C	1.33987300	3.02730300	2.48509600
C	0.73724400	3.12220500	1.22845400
C	-0.63972700	2.91172300	1.14162000
C	-1.41195000	2.60366100	2.27177400
C	-0.81702100	2.55280200	3.53219900
C	-1.51550300	2.94444000	-0.05694300
N	-2.79009400	2.79640000	0.41807800
C	-2.86932600	2.49682200	1.87305500
C	-3.94718300	2.32023200	-0.21774900
C	-4.59595800	1.42041400	0.64701200
C	-3.72315600	1.16239300	1.88182400
C	-4.47040200	2.67952000	-1.45731000
C	-5.70444600	2.12345900	-1.82468400
C	-6.38779300	1.26239800	-0.95961900
C	-5.83832100	0.90915800	0.28445200
C	-3.66838000	3.59540400	2.59878100
O	-1.20005500	3.04921400	-1.24512600
Pd	-1.51667900	-0.40028400	0.18079000
C	7.78135400	-1.81180200	-0.32645300
C	7.42332900	-0.64139000	-1.04089300

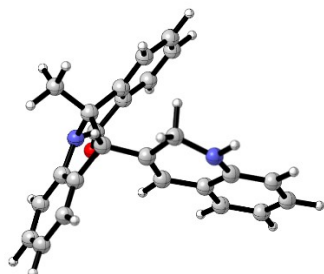
C	6.16221900	-0.09485700	-0.91010200
C	5.18297800	-0.69002500	-0.06215500
C	5.53859600	-1.89918000	0.63157200
C	6.85359400	-2.42628900	0.48830200
C	3.85376800	-0.15528600	0.09201200
C	2.92474800	-0.90823300	0.79651400
C	3.27344300	-2.09128900	1.49153000
C	4.56402700	-2.56155900	1.43034300
C	3.44705200	1.15304100	-0.49617500
C	4.18438900	2.35179100	-0.16745200
C	3.91187100	3.57977200	-0.86045600
C	2.88163600	3.59959300	-1.83932900
C	2.11102700	2.48480200	-2.05357400
C	2.34959100	1.27099800	-1.35316100
C	5.17124000	2.38128300	0.86239300
C	5.85911900	3.53982700	1.16491500
C	5.60941000	4.73807400	0.45107800
C	4.65047500	4.75316900	-0.53975500
O	1.61519500	-0.50644900	0.82330400
O	1.48767100	0.24151400	-1.63686000
H	1.05349700	2.68881600	4.60222800
H	2.41857400	3.17403000	2.58034400
H	1.31807700	3.34912200	0.33586500
H	-1.40776000	2.33408900	4.42453400
H	-4.34879200	1.15859900	2.79185900
H	-3.94758700	3.38721600	-2.10227500
H	-6.14219500	2.38036500	-2.79253800
H	-7.35881300	0.85720700	-1.25449300
H	-6.38248300	0.23955700	0.95388500
H	-3.67433900	3.39201300	3.67994900
H	-3.20862200	4.57989300	2.42736900
H	-4.71012100	3.62536700	2.24562200
H	8.78558100	-2.22994400	-0.43298300
H	8.15109200	-0.16913000	-1.70603400
H	5.90454900	0.80111100	-1.47543900
H	7.10968500	-3.34037700	1.03120100
H	2.49565200	-2.60657100	2.05733100
H	4.84680100	-3.47129600	1.96617000
H	2.68434500	4.52057000	-2.39339000
H	1.29958300	2.52097400	-2.77835400
H	5.37620700	1.47566000	1.43290800
H	6.60129400	3.53240300	1.96755700
H	6.16683100	5.64583500	0.69559700
H	4.43011800	5.67325800	-1.08804900

C	-0.78322900	-4.42043000	3.75126400
C	-1.94600600	-4.20648400	3.00538400
C	-2.28144300	-2.91364700	2.56335400
C	-1.43144500	-1.82211300	2.88961500
C	-0.27409800	-2.06074200	3.64487200
C	0.05917600	-3.34916200	4.07782600
H	-0.53588600	-5.43367400	4.08021600
H	-2.60015900	-5.04420000	2.74620200
H	0.38054200	-1.21588300	3.87755800
H	0.96737500	-3.51580400	4.66248400
N	-3.36988400	-2.66600100	1.75141200
H	-3.99716700	-3.45171600	1.61114100
C	-4.03012500	-1.36795100	1.76883700
H	-4.65006900	-1.30291900	0.86507400
H	-4.71998900	-1.27546900	2.64270700
C	-3.03408200	-0.21404500	1.81657200
C	-1.77945400	-0.48282400	2.39254600
H	-1.16074600	0.32180800	2.77855600
P	0.59771400	-0.73758400	-0.52248400
N	0.96970500	-2.22939400	-1.22002200
C	2.17690600	-2.45342300	-2.06066200
C	1.89426500	-2.28973200	-3.56251300
C	2.91910900	-3.75945800	-1.76700900
H	2.87008200	-1.64908300	-1.79486600
H	1.32602100	-1.36621800	-3.74826000
H	2.84798400	-2.21696200	-4.11142600
H	1.33195000	-3.13469800	-3.98379900
H	3.15917000	-3.85169200	-0.69966700
H	2.35071600	-4.64736200	-2.07976000
H	3.86815200	-3.76088300	-2.32711100
C	-0.05063700	-3.28398500	-0.96992700
C	0.32679900	-4.24298300	0.16556000
C	-0.50920500	-4.02340200	-2.22667600
H	-0.93293300	-2.72447600	-0.61040200
H	0.60724200	-3.68278100	1.06928400
H	-0.54208800	-4.86915700	0.42183900
H	1.15530000	-4.91497700	-0.10001400
H	-0.82975700	-3.31814600	-3.00606400
H	0.26998200	-4.68218700	-2.63836400
H	-1.37606800	-4.65400000	-1.97222300
I	-3.32043800	-1.10127500	-2.36715200
K	-1.13839100	1.35502800	-3.25567600

KI

I	-3.67397559	-4.03195821	0.38096354
K	-7.03397559	-4.03195821	0.38096354

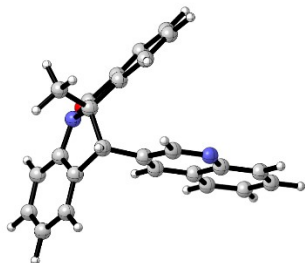
INT-7



C	0.56719500	2.75119100	3.62509700
C	1.33991700	3.02749000	2.48478800
C	0.73724600	3.12223700	1.22815900
C	-0.63973500	2.91178000	1.14140700
C	-1.41191400	2.60380700	2.27160900
C	-0.81693300	2.55306800	3.53201800
C	-1.51553900	2.94443400	-0.05713600
N	-2.79012800	2.79644800	0.41793300
C	-2.86928700	2.49690800	1.87293500
C	-3.94735100	2.32038200	-0.21775100
C	-4.59604700	1.42054200	0.64706500
C	-3.72311800	1.16247100	1.88177600
C	-4.47075100	2.67972800	-1.45722100
C	-5.70481200	2.12362400	-1.82448500
C	-6.38806300	1.26254700	-0.95936900
C	-5.83846400	0.90930000	0.28464700
C	-3.66833000	3.59551500	2.59864600
O	-1.20000300	3.04912200	-1.24531100
H	1.05362200	2.68920000	4.60196100
H	2.41861900	3.17422800	2.57998900
H	1.31804700	3.34908400	0.33552500
H	-1.40764300	2.33442100	4.42438800
H	-4.34864000	1.15868300	2.79189300
H	-3.94804800	3.38745400	-2.10223900
H	-6.14265900	2.38053900	-2.79229300
H	-7.35911000	0.85735600	-1.25415400
H	-6.38255600	0.23971000	0.95415100
H	-3.67453800	3.39197500	3.67978400
H	-3.20836100	4.57994800	2.42747400
H	-4.70998800	3.62569000	2.24526400
C	-0.78313100	-4.42060800	3.75057500

C	-1.94594300	-4.20659100	3.00476700
C	-2.28145600	-2.91369600	2.56297500
C	-1.43143800	-1.82219400	2.88930000
C	-0.27406600	-2.06089200	3.64450100
C	0.05923500	-3.34935900	4.07729500
H	-0.53572700	-5.43389700	4.07934700
H	-2.60004600	-5.04430800	2.74545900
H	0.38059200	-1.21605200	3.87723200
H	0.96745900	-3.51606300	4.66189500
N	-3.36998200	-2.66598900	1.75111400
H	-3.99733700	-3.45165700	1.61091900
C	-4.03016600	-1.36789400	1.76868800
H	-4.65016800	-1.30273600	0.86496800
H	-4.71994200	-1.27546900	2.64262000
C	-3.03411500	-0.21403200	1.81647800
C	-1.77944500	-0.48286800	2.39236100
H	-1.16071300	0.32171900	2.77840300
H ₂			
H	-3.67826486	-5.52976013	0.52693477
H	-4.27826486	-5.52976013	0.52693477

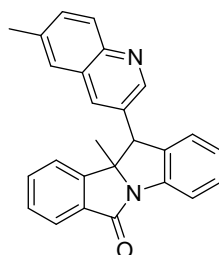
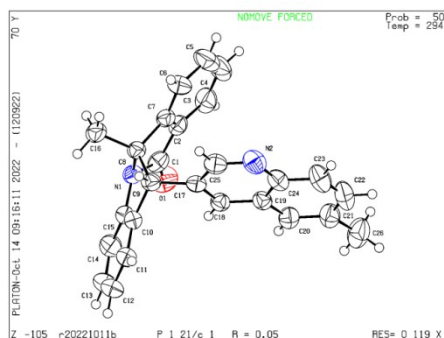
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C	-1.27575700	3.66499400	-0.56469000
C	-1.19778000	3.84515400	0.82653800
C	-0.26713900	3.12687300	1.58346700
C	0.57046900	2.23374300	0.91396300
C	0.49066600	2.04434900	-0.47201600
C	-0.42767000	2.76868600	-1.22971000
C	1.58614900	1.30849200	1.48722500
N	2.15054500	0.66480800	0.39266700
C	1.53491000	1.04064500	-0.90532700
C	2.60412100	-0.66379200	0.33487200
C	2.04889100	-1.29640400	-0.79272500
C	1.06732900	-0.35757900	-1.48101400
C	3.44226200	-1.33673200	1.22320800

C	3.74031700	-2.67836700	0.94267500
C	3.21617500	-3.31437300	-0.19038000
C	2.35784300	-2.62558000	-1.06327500
C	2.57801800	1.67405300	-1.83461500
O	1.85811400	1.09601900	2.65569800
H	-2.01371200	4.23172100	-1.13837000
H	-1.87180900	4.55147100	1.31757600
H	-0.19143900	3.25051700	2.66645700
H	-0.49885100	2.63458900	-2.31130700
H	1.19298800	-0.35868600	-2.57263600
H	3.84258400	-0.82954200	2.10120700
H	4.39757400	-3.23224900	1.61821400
H	3.47032300	-4.35789900	-0.39255500
H	1.92413700	-3.13037900	-1.93043500
H	2.10213200	1.98320300	-2.77754200
H	3.03027900	2.55746700	-1.35987400
H	3.37530900	0.95058000	-2.06625000
C	-4.94005200	-1.61501600	0.76693100
C	-4.48858100	-1.20314400	-0.47069100
C	-3.09657200	-1.02834600	-0.70769700
C	-2.17163900	-1.28795000	0.35736100
C	-2.66730200	-1.71308100	1.62130500
C	-4.02362200	-1.87157300	1.82112100
H	-6.01120400	-1.74526900	0.94230300
H	-5.17755600	-1.00076900	-1.29415200
H	-1.95548800	-1.90746900	2.42831000
H	-4.39941000	-2.19634700	2.79478100
N	-2.67632300	-0.61914400	-1.93908000
C	-1.38777700	-0.45138500	-2.13733600
C	-0.37877000	-0.67435800	-1.15483000
C	-0.79010500	-1.10177100	0.09246800
H	-0.06783600	-1.29714900	0.88925800
H	-1.07879700	-0.11682700	-3.13665400

9. X-ray single crystal diffraction data of 3a



3a

Bond precision:	C-C = 0.0023 Å	Wavelength=0.71073	
Cell:	a=7.1920(5)	b=14.8145(7)	c=18.9231(12)
	alpha=90	beta=96.550(6)	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	2003.0(2)	2003.0(2)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C ₂₆ H ₂₀ N ₂ O	C ₂₆ H ₂₀ N ₂ O	
Sum formula	C ₂₆ H ₂₀ N ₂ O	C ₂₆ H ₂₀ N ₂ O	
Mr	376.44	376.44	
Dx, g cm ⁻³	1.248	1.248	
Z	4	4	
Mu (mm ⁻¹)	0.077	0.077	
F000	792.0	792.0	
F000'	792.30		
h,k,lmax	8,18,23	8,18,23	
Nref	4085	4036	
Tmin,Tmax	0.981,0.985	0.574,1.000	
Tmin'	0.981		
Correction method= # Reported T Limits: Tmin=0.574 Tmax=1.000			
AbsCorr = MULTI-SCAN			
Data completeness=	0.988	Theta(max)= 26.367	
R(reflections)=	0.0465(3060)	wR2(reflections)= 0.1168(4036)	
S =	1.036	Npar= 265	
CCDC: 2286479			