

Supporting Information

Enantioselectivity Synthesis of Isoquinolin-1-one Derivatives with C–N Axial Chirality via Cobalt-Catalyzed Oxidative Formal (4+2) Cycloaddition: Light or Not

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1. General Information

^1H NMR spectra were recorded on 400 MHz spectrophotometers. Chemical shifts (δ) are reported in ppm from the resonance of tetramethyl silane as the internal standard (TMS: 0.00 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. All NMR spectra were recorded on a Bruker spectrometer at 400 MHz (^1H NMR), 100 MHz (^{13}C NMR), 376 MHz (^{19}F NMR). HRMS was recorded on Waters GCT Premier ESI-TOF. Enantiomeric excesses (ee) values were determined by chiral HPLC with chiral AD-H, AS-H, IA-H, IG-H, OD-H columns with hexane and *i*-PrOH as eluent. Optical rotations were measured with a polarimeter. $[\alpha]_{\text{D}}$ values are reported at a given temperature ($^{\circ}\text{C}$) in degrees cm^2/g with concentration in mg/mL . Unless otherwise noted, all reactions were carried out under an atmosphere of air in oven-dried glassware. The photoreactor used for the reaction is a multi-channel photoreactor (Figure S1) independently developed by us (32 reaction holes, each hole corresponds to a 5 W LED (456 nm or 390 nm), and the light intensity is about $100 \text{ mw}/\text{cm}^2$; Patent No CN201921741216.8).

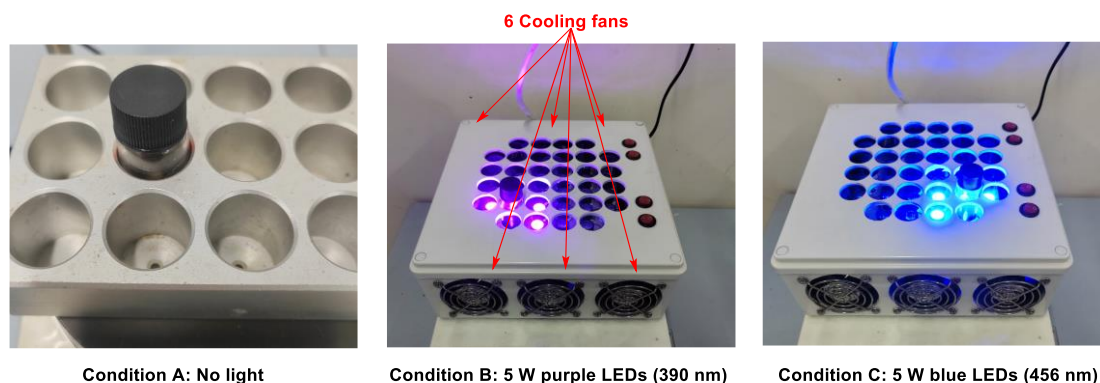
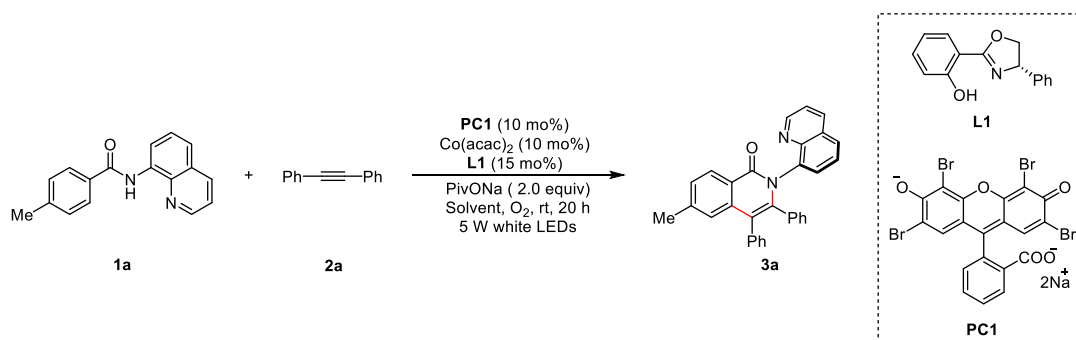


Figure S1. Multi-channel photoreactor and three reaction devices with different conditions

Analytical thin layer chromatography was performed using Qingdao Puke Parting Materials Co. silica gel plates (Silicagel 60 F254). Flash column chromatography was performed using 200-300 mesh silica gel. Reagents, unless otherwise noted, were used as supplied from commercial sources without further purification. Anhydrous solvent (DCM, MeCN, Toluene, MeOH, DMF) were taken from JC-Meyer solvent purification system. Ligands,^[1-2] amides,^[3] alkynes^[4-5] were prepared according to literature.

2. Details for Condition Optimization

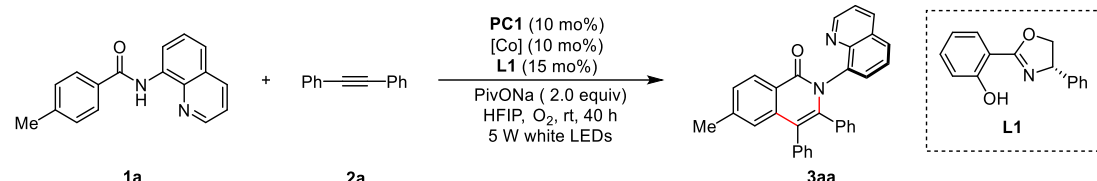
Table S1. The effect of solvent.^a



Entry	Solvent	Yield/%	ee/%
1	TFE	14	78
2	HFIP	11	87
3	MeOH	10	80
4	^t BuOH	trace	67
5	DCE	5	78
6	1,4-dioxane	trace	73
7	MeCN	trace	64
8	DMF	0	0
9	Toluene	trace	65

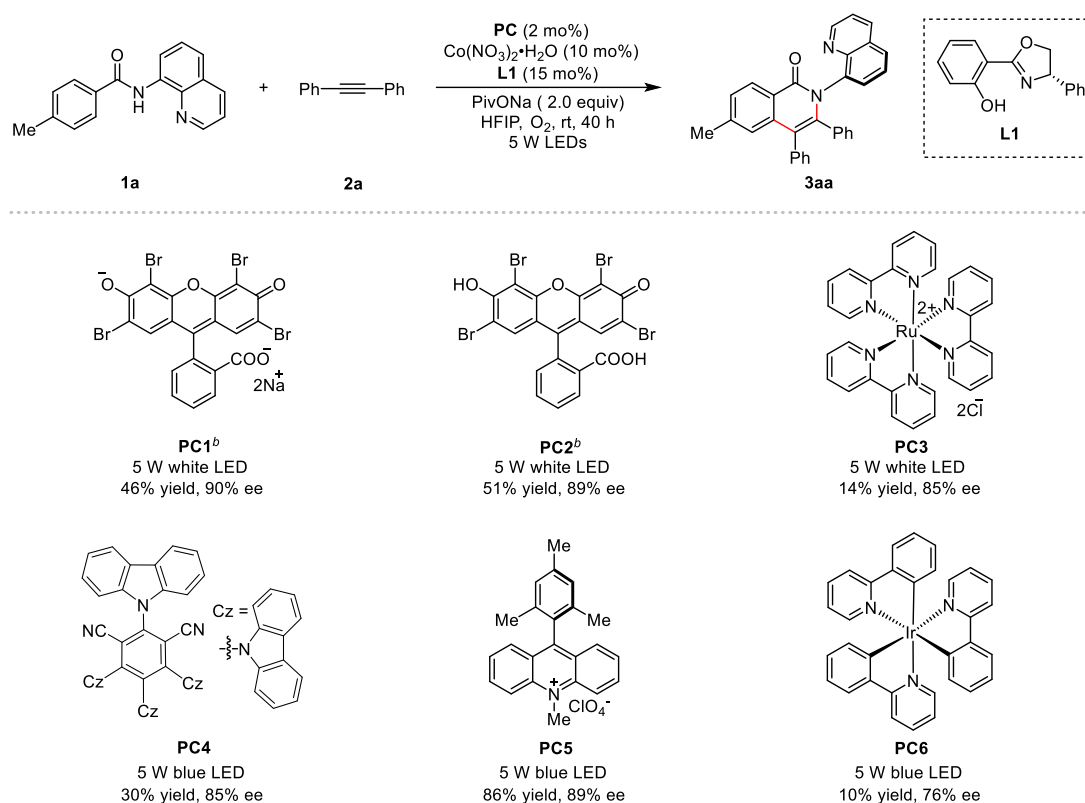
^a **1a** (0.1 mmol), **2a** (0.15 mmol), **PC1** (10 mol%), $\text{Co}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ (10 mol%), **L1** (15 mol%), PivONa (2.0 equiv), solvent (1 mL), O_2 , under 5 W white LEDs at rt for 20 h. Yields was determined using ^1H NMR spectroscopy with 1,3,5-trimethoxybenzene as an internal standard. All the ee values in this work were determined by chiral HPLC analysis of purified products.

Table S2. The effect of cobalt.^a

			
Entry	[Co]	Yield/%	ee/%
1	Co(acac) ₂	16	87
2	Co(acac) ₃	17	87
3	Co(OAc) ₂ •4H ₂ O	23	88
4	Co(ClO ₄) ₂ •6H ₂ O	20	86
5	Co(NO ₃) ₂ •6H ₂ O	46	90
6	Co(BF ₄) ₂ •6H ₂ O	9	90
7	CoBr ₂	9	87

^a **1a** (0.1 mmol), **2a** (0.15 mmol), **PC1** (10 mol%), [Co] (10 mol%), **L1** (15 mol%), PivONa (2.0 equiv), HFIP (1 mL), O₂, under 5 W white LEDs at rt for 40 h. Yields was determined using ¹H NMR spectroscopy with 1,3,5-trimethoxybenzene as an internal standard. All the ee values in this work were determined by chiral HPLC analysis of purified products.

Table S3. The effect of photocatalyst.^a



^a **1a** (0.1 mmol), **2a** (0.15 mmol), **PC** (2 mol%), $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (10 mol%), **L1** (15 mol%), PivONa (2.0 equiv), HFIP (1 mL), O_2 , under 5 W LEDs at rt for 40 h. Yields was determined using ^1H NMR spectroscopy with 1,3,5-trimethoxybenzene as an internal standard. All the ee values in this work were determined by chiral HPLC analysis of purified products. ^b Using **PC** (10 mol%).

Table S4. The effect of oxidant.^a

Reaction scheme showing the conversion of **1a** and **2a** to **3aa** using photocatalyst **PC5** (2 mol%), $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (10 mol%), **L1** (15 mol%), PivONa (2.0 equiv), HFIP, [O], rt, 40 h, 5 W white LEDs.

Entry	oxidant	Yield/%	ee/%
1	O_2	86	89
2	Air	85	89
3	Ar	7	86

^a **1a** (0.1 mmol), **2a** (0.15 mmol), $\text{Acr-Mes}^+\text{ClO}_4^-$ (2 mol%), [Co] (10 mol%), **L1** (15 mol%), PivONa (2.0 equiv), HFIP (1 mL), under 5 W LEDs at rt for 40 h. Yields was determined using ^1H NMR spectroscopy with 1,3,5-trimethoxybenzene as an internal standard. All the ee values in this work were determined by chiral HPLC analysis of purified products.

Table S5. The effect of temperature.^a

Entry	T/°C	Yield/%	ee/%
1	rt	86	89
2	15	83	89
3	0	38	90

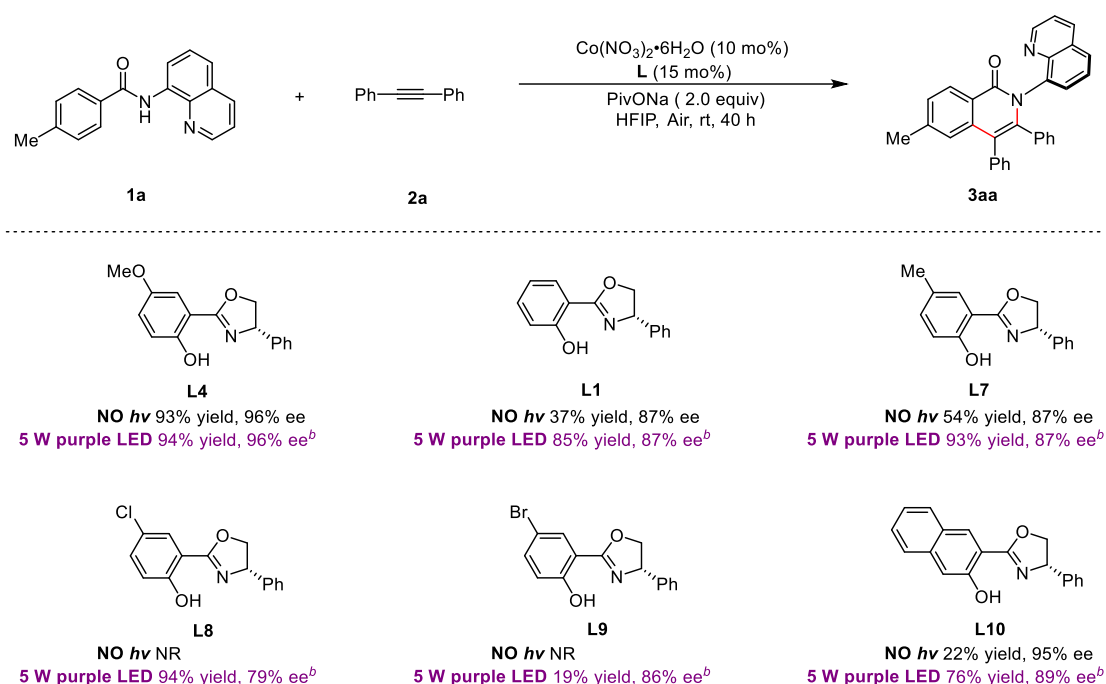
^a **1a** (0.1 mmol), **2a** (0.15 mmol), Acr-Mes⁺ClO₄⁻ (2 mol%), Co(NO₃)₂·6H₂O (10 mol%), **L1** (15 mol%), PivONa (2.0 equiv), HFIP (1 mL), air, under 5 W blue LEDs at T °C for 40 h. Yields was determined using ¹H NMR spectroscopy with 1,3,5-trimethoxybenzene as an internal standard. All the ee values in this work were determined by chiral HPLC analysis of purified products.

Table S6. The effect of ligand.^a

<p>L1 86% yield, 89% ee</p>	<p>L2 95% yield, 61% ee</p>	<p>L3 85% yield, 67% ee</p>	
<p>L4 94% yield, 95% ee</p>	<p>L5 87% yield, 82% ee</p>	<p>L6 67% yield, 75% ee</p>	

^a **1a** (0.1 mmol), **2a** (0.15 mmol), Acr-Mes⁺ClO₄⁻ (2 mol%), Co(NO₃)₂·6H₂O (10 mol%), **L** (15 mol%), PivONa (2.0 equiv), HFIP (1 mL), air, under 5 W blue LEDs at rt for 40 h. Yields was determined using ¹H NMR spectroscopy with 1,3,5-trimethoxybenzene as an internal standard. All the ee values in this work were determined by chiral HPLC analysis of purified products.

Table S7. The effect of ligand under 5 W purple LEDs or not *hν*.^a



^a **1a** (0.1 mmol), **2a** (0.15 mmol), $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (10 mol%), **L** (15 mol%), PivONa (2.0 equiv), HFIP (1 mL), air, under 5 W purple LEDs at rt for 40 h. Yields was determined using ^1H NMR spectroscopy with 1,3,5-trimethoxybenzene as an internal standard. All the ee values in this work were determined by chiral HPLC analysis of purified products. ^b Under 5 W purple LED.

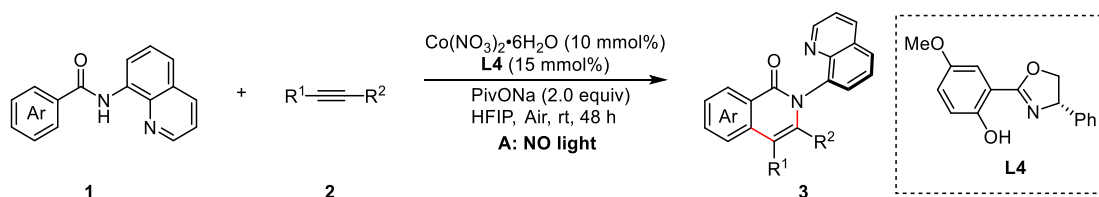
Table S8. Control experiments.^a

Reaction scheme showing the synthesis of **3aa** from **1a** and **2a** under standard conditions. The reaction involves **1a** (4-methyl-N-(quinolin-2-yl)benzamide) and **2a** (diphenylacetylene) reacting with **PC5** (2 mol%), $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (10 mol%), **L4** (15 mol%), PivONa (2.0 equiv), HFIP, Air, rt, 40 h, 5 W blue LEDs to form **3aa** (4-methyl-2-phenyl-3-phenyl-1-quinolin-2-yl-1H-benzimidazole). The structure of **L4** is shown in a dashed box.

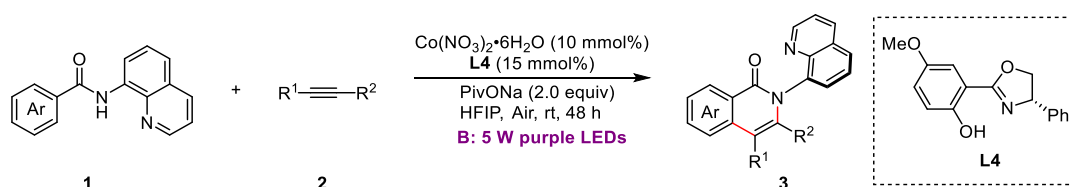
Entry	deviation from standard conditions	Yield/%	ee/%
1	none	94	95
2	no light/ Acr-Mes ⁺ ClO ₄ ⁻	93	96
3	no $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$	0	0
4	no L4	55	0
5	No PivONa	94	89
6	degassed	trace	95

^a **1a** (0.1 mmol), **2a** (0.15 mmol), Acr-Mes⁺ClO₄⁻ (2 mol%), $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (10 mol%), **L4** (15 mol%), PivONa (2.0 equiv), HFIP (1 mL), air, under 5 W blue LEDs at rt for 40 h. Yields was determined using ^1H NMR spectroscopy with 1,3,5-trimethoxybenzene as an internal standard. All the ee values in this work were determined by chiral HPLC analysis of purified products.

3. General Procedures and Characterization Data of Products



Condition A: Under air, Co(NO₃)₂·6H₂O (0.02 mmol, 5.82 mg), **L4** (0.015 mmol, 8.08 mg) and HFIP (2 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, corresponding substrate **1** (0.2 mmol), alkyne **2** (0.3 mmol) and PivONa (49.9 mg, 0.4 mmol) were added to the resulting mixture. The mixture was stirred at room temperature for approximately 48 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent to give corresponding product **3**.



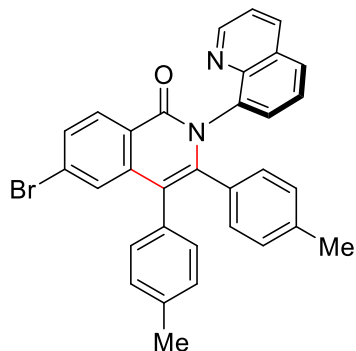
Condition B: Under air, Co(NO₃)₂·6H₂O (0.02 mmol, 5.82 mg), **L4** (0.015 mmol, 8.08 mg) and HFIP (2 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, corresponding substrate **1** (0.2 mmol), alkyne **2** (0.3 mmol) and PivONa (49.9 mg, 0.4 mmol) were added to the resulting mixture. The mixture was stirred at room temperature under 5 W purple LEDs for approximately 48 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent to give corresponding product **3**.



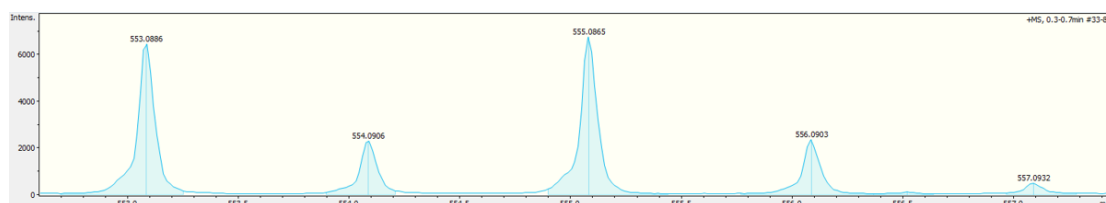
Condition C: Under air, Co(NO₃)₂·6H₂O (0.02 mmol, 5.82 mg), **L4** (0.015 mmol, 8.08 mg) and HFIP (2 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, corresponding substrate **1** (0.2 mmol), alkyne **2** (0.3 mmol), **PC5** (1.64 mg, 0.004 mmol) and PivONa (49.9 mg, 0.4 mmol) were added to the resulting mixture. The mixture was stirred at room temperature under 5 W blue LEDs for approximately 48 h. The concentrated reaction

residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent to give corresponding product **3**.

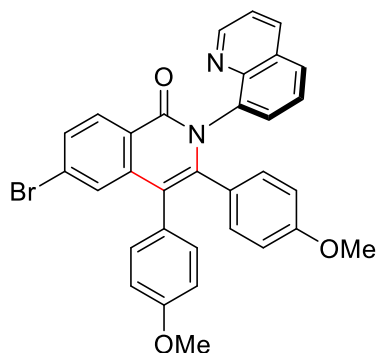
(R)-6-Bromo-2-(quinolin-8-yl)-3,4-di-p-tolylisoquinolin-1(2H)-one (3ab)



Condition C, White solid, mp: 310-311 °C, 103.3 mg, 97% yield, $[\alpha]_D^{25} = +58.0$ ($c = 0.1$ in CHCl_3), 94% ee, determined by HPLC analysis (Chiralpak AZ-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 19.68 min, t_R (major) = 22.82 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.90 (d, $J = 3.5$ Hz, 1H), 8.40 (d, $J = 8.5$ Hz, 1H), 8.00 (d, $J = 8.2$ Hz, 1H), 7.62-7.52 (m, 2H), 7.48-7.29 (m, 4H), 7.10 (d, $J = 7.7$ Hz, 1H), 7.05-6.99 (m, 2H), 6.95 (d, $J = 7.7$ Hz, 1H), 6.83 (d, $J = 7.7$ Hz, 1H), 6.63-6.57 (m, 2H), 6.26 (d, $J = 7.8$ Hz, 1H), 2.24 (s, 3H), 1.90 (s, 3H). **^{13}C NMR** (101 MHz, CDCl_3) δ 162.4, 150.8, 144.7, 143.5, 140.0, 137.6, 136.9, 136.5, 136.1, 132.8, 131.8, 131.43 (d, $J = 17.3$ Hz), 130.7, 130.37 (d, $J = 19.6$ Hz), 129.8, 129.3, 129.1, 128.95-128.50 (m), 128.1, 127.9, 127.5, 127.3, 125.8, 124.2, 121.6, 117.6, 21.3, 21.1. **HRMS** (ESI) for $\text{C}_{32}\text{H}_{23}\text{BrN}_2\text{NaO}$ $[\text{M}+\text{Na}]^+$ calcd: 553.0886 (^{79}Br) and 555.0871 (^{81}Br); found: 553.0886 (^{79}Br) and 555.0865 (^{81}Br).



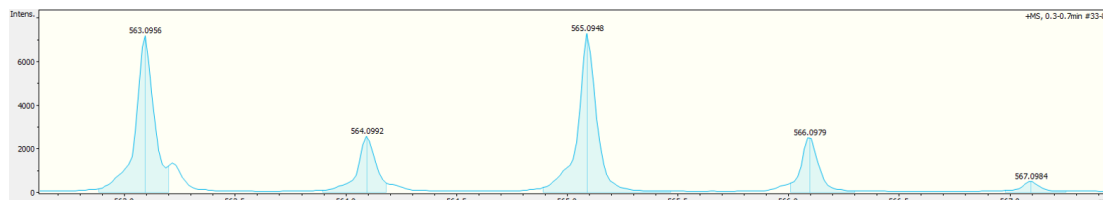
(R)-6-Bromo-3,4-bis(4-methoxyphenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ac)



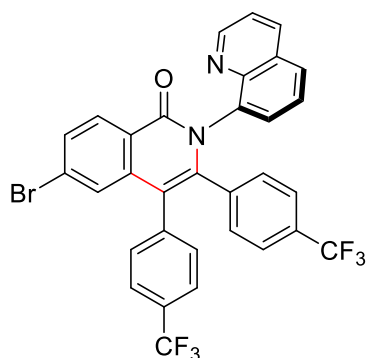
Condition C, White solid, mp: 318-319 °C, 88.0 mg, 78% yield, $[\alpha]_D^{25} = +59.6$ ($c = 0.1$ in CHCl_3), 97% ee, determined by HPLC analysis (Chiralpak AS-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 56.51 min, t_R (major) = 62.96 min.

^1H NMR (400 MHz, CDCl_3) δ 8.89 (s, 1H), 8.39 (d, $J = 8.4$ Hz, 1H), 8.03 (d, $J = 8.0$ Hz, 1H), 7.65 (d, $J = 7.9$ Hz, 1H), 7.58 (d, $J = 8.2$ Hz, 1H), 7.46-7.34 (m, 4H), 7.10 (d, $J = 8.1$ Hz, 1H), 7.05 (d, $J = 8.2$ Hz, 1H), 6.85 (d, $J = 8.1$ Hz, 1H), 6.79 (d, $J = 7.9$ Hz, 1H), 6.72 (d, $J = 7.9$ Hz, 1H), 6.61 (d, $J = 8.1$ Hz, 1H), 6.36 (d, $J = 7.6$ Hz, 1H),

6.01 (d, $J = 7.7$ Hz, 1H), 3.73 (s, 3H), 3.45 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 162.4, 158.3, 158.2, 150.8, 144.6, 143.4, 140.2, 137.6, 136.2, 132.8, 132.6, 131.9, 130.8, 130.7, 130.3, 129.8, 128.8, 128.7, 128.1, 127.9, 127.2, 125.9, 124.2, 121.6, 117.5, 113.7, 113.6, 112.2, 112.0, 55.2, 54.8. **HRMS** (ESI) for $\text{C}_{32}\text{H}_{24}\text{BrN}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ calcd: 563.0965 (^{79}Br) and 565.0950 (^{81}Br); found: 563.0956 (^{79}Br) and 565.0948 (^{81}Br).

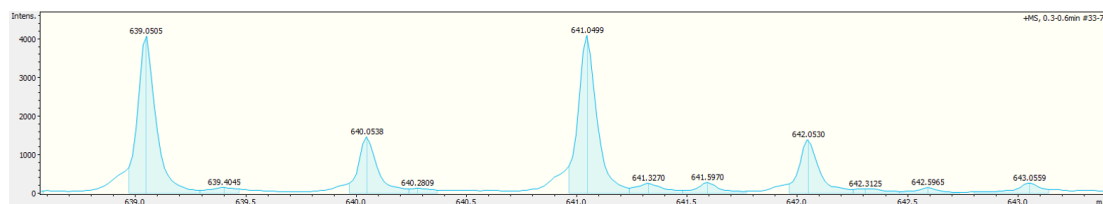


(R)-6-Bromo-2-(quinolin-8-yl)-3,4-bis(4-(trifluoromethyl)phenyl)isoquinolin-1(2H)-one (3ad)

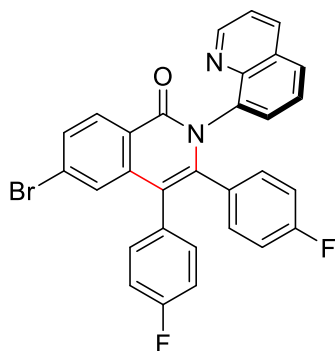


Condition C, White solid, mp: 287-288 °C, 121.5 mg, 95% yield, $[\alpha]_{\text{D}}^{25} = +55.6$ ($c = 0.1$ in CHCl_3), 96% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_{R} (minor) = 5.82 min, t_{R} (major) = 12.49 min. ^1H NMR (400 MHz, CDCl_3) δ 8.90 (d, $J = 3.0$ Hz, 1H), 8.43 (d, $J = 8.5$ Hz,

1H), 8.07 (d, $J = 8.1$ Hz, 1H), 7.78-7.63 (m, 2H), 7.54-7.48 (M, 3H), 7.41-7.31 (m, 5H), 7.14-7.18 (m, 2H), 6.88 (d, $J = 8.1$ Hz, 1H), 6.78 (d, $J = 8.1$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 162.1, 151.1, 144.3, 142.2, 139.3, 138.9, 137.8, 136.7, 136.4, 132.2, 131.9, 130.9, 130.8, 130.8, 130.6, 130.1, 129.8 (q, $J = 32.8$ Hz), 129.7 (q, $J = 32.8$ Hz), 129.4, 129.0, 128.5, 127.8, 125.9, 125.6 (q, $J = 3.5$ Hz), 125.4 (q, $J = 3.6$ Hz), 124.5, 124.0 (q, $J = 3.6$ Hz), 124.0 (q, $J = 273.3$ Hz), 123.8 (q, $J = 3.3$ Hz), 123.4 (q, $J = 273.4$ Hz), 122.0, 116.5. ^{19}F NMR (376 MHz, CDCl_3) δ -62.6, -63.1. **HRMS** (ESI) for $\text{C}_{32}\text{H}_{18}\text{BrF}_6\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 639.0501 (^{79}Br) and 641.0486 (^{81}Br); found: 639.0505 (^{79}Br) and 641.0499 (^{81}Br).

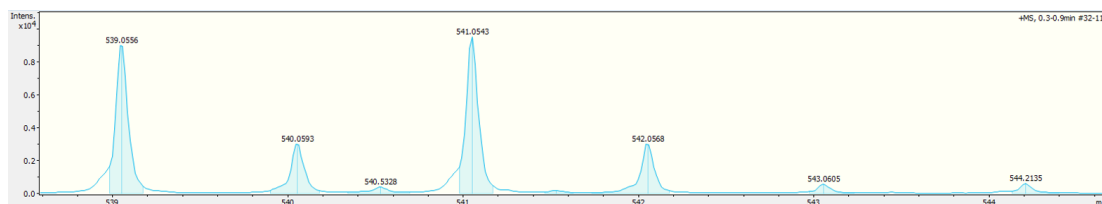


(R)-6-Bromo-3,4-bis(4-fluorophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ae)

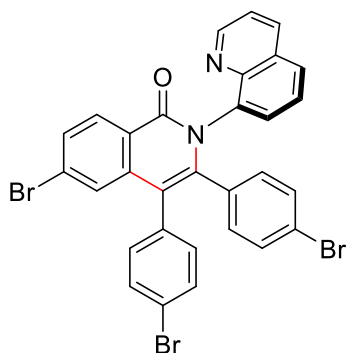


Condition C, White solid, 101.5 mg, mp: 304-305 °C, 94% yield, $[\alpha]_D^{25} = +37.8$ ($c = 0.1$ in CHCl_3), 97% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 15.36 min, t_R (minor) = 17.88 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.90 (d, $J = 3.6$ Hz, 1H), 8.42 (d, $J = 8.5$ Hz, 1H),

8.08 (d, $J = 8.2$ Hz, 1H), 7.70 (d, $J = 8.1$ Hz, 1H), 7.63 (d, $J = 8.5$ Hz, 1H), 7.50 (d, $J = 7.2$ Hz, 1H), 7.46-7.32 (m, 3H), 7.16-7.12 (m, 2H), 6.98-6.90 (m, 3H), 6.72-6.69 (m, 1H), 6.57-6.53 (m, 1H), 6.24-6.19 (m, 1H). **^{13}C NMR** (101 MHz, CDCl_3) δ 162.3, 161.9 (d, $J = 247.7$ Hz), 161.6 (d, $J = 250.0$ Hz), 150.9, 144.5, 142.8, 139.6, 137.2, 136.2, 133.4 (d, $J = 8.0$ Hz), 133.2 (d, $J = 8.0$ Hz), 132.3 (d, $J = 8.2$ Hz), 131.7, 131.6 (d, $J = 8.6$ Hz), 130.8, 130.6, 130.5, 130.3, 129.1, 128.9, 128.2, 128.0, 125.9, 124.5, 121.8, 116.9, 115.6 (d, $J = 13.8$ Hz), 115.4 (d, $J = 13.8$ Hz), 114.1 (d, $J = 22.5$ Hz), 113.9 (d, $J = 23.0$ Hz). **^{19}F NMR** (376 MHz, CDCl_3) δ -112.8, -114.4. **HRMS** (ESI) for $\text{C}_{30}\text{H}_{18}\text{BrF}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 539.0565 (^{79}Br) and 541.0549 (^{81}Br); found: 539.0556 (^{79}Br) and 541.0543 (^{81}Br).



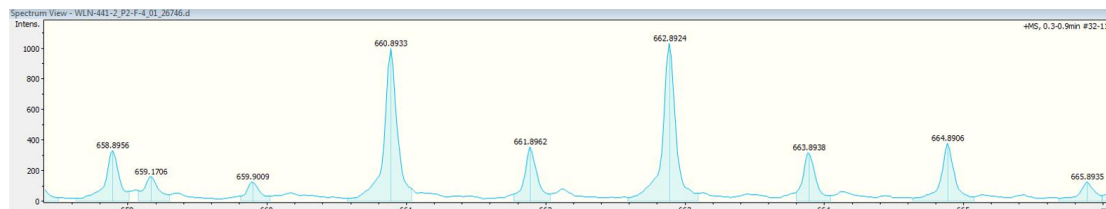
(R)-6-Bromo-3,4-bis(4-bromophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3af)



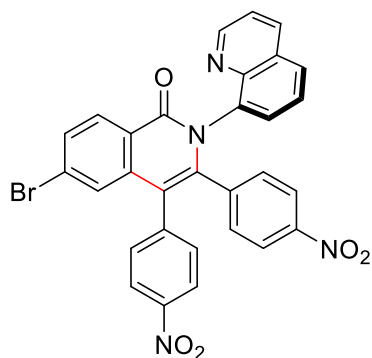
Condition C, White solid, mp: 330-331 °C, 41.1 mg, 31% yield, $[\alpha]_D^{25} = +101.6$ ($c = 0.1$ in CHCl_3), 93% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 15.62 min, t_R (major) = 19.14 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.97-8.85 (m, 1H), 8.40 (d, $J = 8.5$ Hz, 1H),

8.08 (d, $J = 8.3$ Hz, 1H), 7.72 (d, $J = 8.0$ Hz, 1H), 7.63 (dd, $J = 8.5, 1.6$ Hz, 1H), 7.48 (d, $J = 6.8$ Hz, 1H), 7.44-7.34 (m, 5H), 7.09-6.97 (m, 3H), 6.82 (dd, $J = 8.2, 1.8$ Hz, 1H), 6.66 (dd, $J = 8.3, 1.7$ Hz, 1H), 6.60 (dd, $J = 8.3, 1.8$ Hz, 1H). **^{13}C NMR** (101 MHz, CDCl_3) δ 162.2, 151.0, 144.4, 142.4, 139.2, 137.0, 136.3, 134.6, 133.4, 133.3, 133.2, 132.1, 131.9, 131.7,

131.2, 130.8, 130.5, 130.3, 130.1, 129.3, 128.9, 128.3, 127.9, 126.0, 124.4, 122.2, 121.9, 121.7, 116.6. **HRMS** (ESI) for $C_{32}H_{18}Br_3N_2O$ $[M+H]^+$ calcd: 658.8964 (^{79}Br , ^{79}Br , ^{79}Br), 660.8945 (^{79}Br , ^{79}Br , ^{81}Br), 662.8927 (^{79}Br , ^{81}Br , ^{81}Br) and 664.8915 (^{81}Br , ^{81}Br , ^{81}Br); found: 658.8956 (^{79}Br , ^{79}Br , ^{79}Br), 660.8933 (^{79}Br , ^{79}Br , ^{81}Br), 662.8924 (^{79}Br , ^{81}Br , ^{81}Br) and 664.8906 (^{81}Br , ^{81}Br , ^{81}Br).

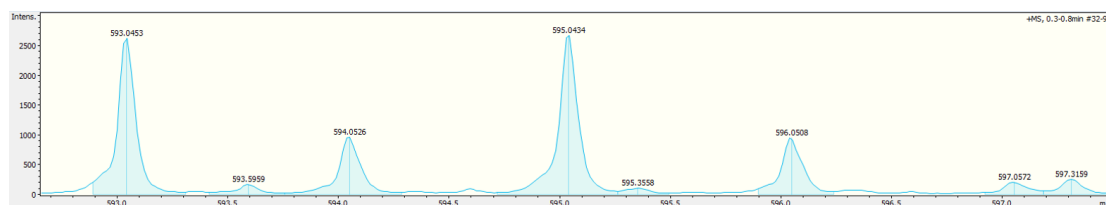


(R)-6-Bromo-3,4-bis(4-nitrophenyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ag)

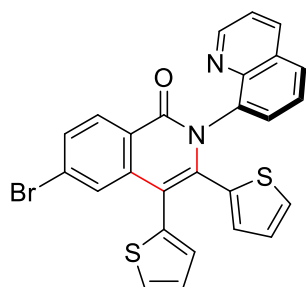


Condition C, White solid, mp: 382-383 °C, 91.2 mg, 77% yield, $[\alpha]_D^{25} = +84.8$ ($c = 0.1$ in $CHCl_3$), 96% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 70:30 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 25.06 min, t_R (major) = 33.45 min.

1H NMR (400 MHz, $CDCl_3$) δ 8.91 (d, $J = 3.2$ Hz, 1H), 8.44 (d, $J = 8.5$ Hz, 1H), 8.24-8.03 (m, 3H), 7.75-7.69 (m, 3H), 7.57 (d, $J = 6.6$ Hz, 1H), 7.45-7.36 (m, 5H), 7.29 (d, $J = 1.4$ Hz, 1H), 7.19 (d, $J = 8.0$ Hz, 1H), 6.98 (d, $J = 8.5$ Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.9, 151.1, 147.3, 146.9, 144.1, 142.2, 141.5, 140.3, 138.2, 136.4, 136.2, 132.7, 132.5, 131.4, 131.2, 130.8, 130.7, 129.7, 129.0, 128.7, 127.6, 125.9, 124.6, 123.9, 123.8, 122.3, 122.1, 115.7. **HRMS** (ESI) for $C_{30}H_{18}BrN_4O_5$ $[M+H]^+$ calcd: 593.0455 (^{79}Br) and 595.0440 (^{81}Br); found: 593.0453 (^{79}Br) and 595.0434 (^{81}Br).

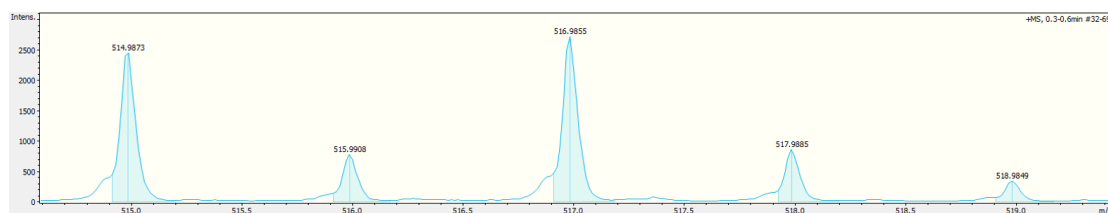


(R)-6-Bromo-2-(quinolin-8-yl)-3,4-di(thiophen-2-yl)isoquinolin-1(2H)-one (3ah)

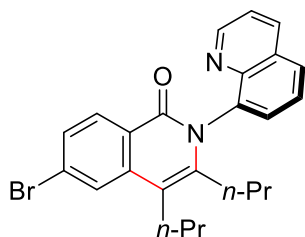


Condition C, White solid, mp: 320-321 °C, 87.4 mg, 85% yield, $[\alpha]_D^{25} = +29.2$ ($c = 0.1$ in $CHCl_3$), 96% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 19.12 min,

t_R (minor) = 30.22 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.91 (d, J = 3.1 Hz, 1H), 8.38 (d, J = 8.4 Hz, 1H), 8.10 (d, J = 8.1 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.64 (d, J = 11.3 Hz, 2H), 7.54 (d, J = 7.1 Hz, 1H), 7.44-7.27 (m, 3H), 6.96 (d, J = 4.4 Hz, 2H), 6.84 (d, J = 4.8 Hz, 1H), 6.45 (d, J = 2.9 Hz, 1H), 6.39-6.29 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.3, 151.1, 144.8, 139.7, 138.7, 137.2, 136.4, 136.2, 134.6, 130.8, 130.7, 130.5, 130.3, 130.2, 129.1, 128.9, 128.4, 127.5, 127.0, 126.8, 125.9, 125.4, 124.6, 121.8, 112.9. **HRMS** (ESI) for $C_{26}H_{16}BrN_2OS_2$ $[M+H]^+$ calcd: 514.9882 (^{79}Br) and 516.9863 (^{81}Br); found: 514.9873 (^{79}Br) and 516.9855 (^{81}Br).

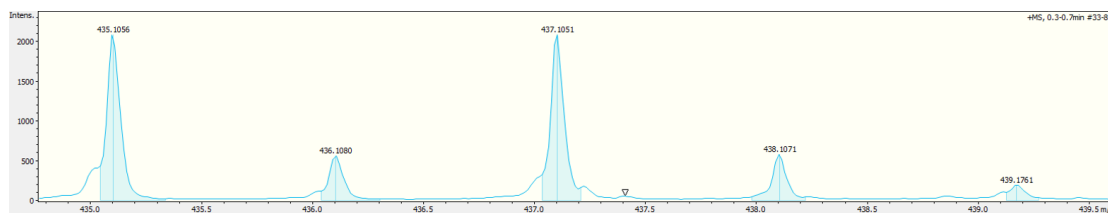


(R)-6-Bromo-3,4-dipropyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ai)

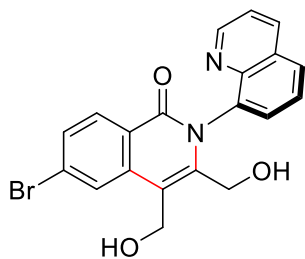


Condition C, White solid, mp: 187-188 °C, 80.2 mg, 93% yield, $[\alpha]_D^{25} = -188.4$ ($c = 0.1$ in $CHCl_3$), 96% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 7.98 min,

t_R (major) = 10.85 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.82 (d, J = 2.7 Hz, 1H), 8.27 (d, J = 8.5 Hz, 1H), 8.22 (d, J = 8.2 Hz, 1H), 7.9-7.86 (m, 2H), 7.71-7.63 (m, 2H), 7.52 (d, J = 8.4 Hz, 1H), 7.43-7.40 (m, 1H), 2.78-2.66 (m, 2H), 2.52-2.40 (m, 1H), 1.98-1.86 (m, 1H), 1.74-1.66 (m, 2H), 1.39-1.25 (m, 2H), 1.11 (t, J = 7.3 Hz, 3H), 0.53 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.9, 151.5, 144.6, 142.7, 139.3, 137.1, 136.4, 130.6, 130.2, 129.4, 129.0, 128.0, 126.2, 125.8, 124.1, 122.0, 113.0, 33.0, 29.9, 23.6, 23.0, 14.6, 14.3. **HRMS** (ESI) for $C_{24}H_{24}BrN_2O$ $[M+H]^+$ calcd: 435.1067 (^{79}Br) and 437.1047 (^{81}Br); found: 435.1056 (^{79}Br) and 437.1051 (^{81}Br).



(R)-6-Bromo-3,4-bis(hydroxymethyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3aj)



Condition C, White solid, mp: 221-222 °C, 76.6 mg, 93% yield,

$[\alpha]_D^{25} = +6.4$ ($c = 0.1$ in CHCl_3), 96% ee, determined by HPLC

analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 70:30 v/v,

flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 8.17 min,

t_R (major) = 11.60 min. **^1H NMR** (400 MHz, DMSO) δ 8.80 (s,

1H), 8.51 (d, $J = 7.9$ Hz, 1H), 8.35-8.05 (m, 3H), 7.96-7.65 (m, 3H), 7.59 (d, $J = 3.5$ Hz, 1H),

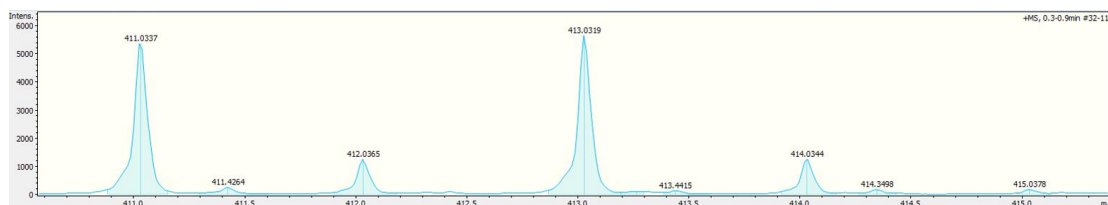
5.21 (s, 1H), 5.01 (s, 1H), 4.79 (s, 2H), 4.49 (d, $J = 12.2$ Hz, 1H), 3.54 (d, $J = 12.2$ Hz, 1H).

^{13}C NMR (101 MHz, DMSO) δ 161.9, 151.6, 144.4, 143.3, 139.2, 137.0, 136.1, 131.5, 130.2,

129.7, 129.0, 127.6, 127.5, 126.8, 124.8, 122.5, 114.1, 57.2, 56.5. **HRMS** (ESI) for

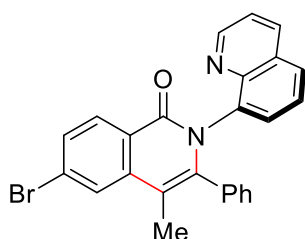
$\text{C}_{20}\text{H}_{16}\text{BrN}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ calcd: 411.0339 (^{79}Br) and 413.0321 (^{81}Br); found: 411.0337 (^{79}Br)

and 413.0319 (^{81}Br).



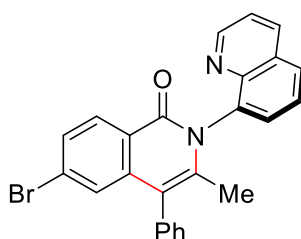
(R)-6-Bromo-4-methyl-3-phenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ak-major)

(R)-6-Bromo-3-methyl-4-phenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ak-minor)



major

and



minor

Condition C, White solid, mp:

226-227 °C, 83.9 mg, 95% yield,

$[\alpha]_D^{25} = -46.5$ ($c = 0.1$ in CHCl_3),

96% ee, 96% ee, determined by

HPLC analysis (Chiralpak AD-H

column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) =

13.07 min for major isomer, t_R (major) = 19.32 min for major isomer, t_R (major) = 23.64 min

for minor isomer, t_R (minor) = 43.31 min for minor isomer. **^1H NMR** (400 MHz, CDCl_3) δ

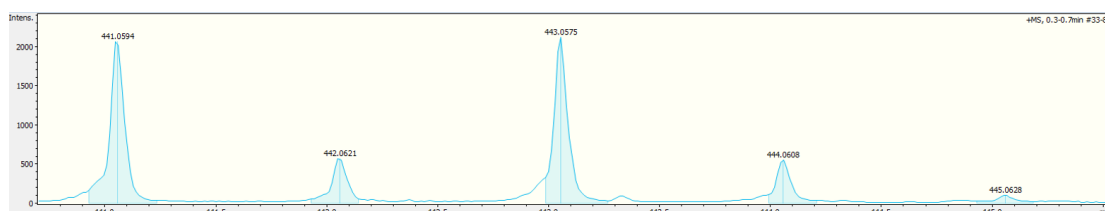
8.88 (s, 1.22H, major + minor), 8.40 (d, $J = 8.8$ Hz, 1H, major), 8.32 (d, $J = 8.4$ Hz, 0.22H,

minor), 8.23 (d, $J = 8.4$ Hz, 0.22H, minor), 8.02 (d, $J = 8.0$ Hz, 1H, major), 7.96 (s, 0.22H,

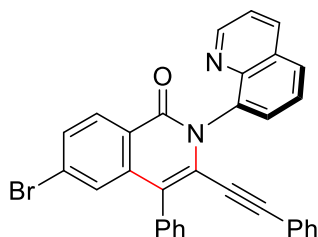
minor), 7.94 (s, 1H, major), 7.74 (d, $J = 7.2$ Hz, 0.22H, minor), 7.68 (d, $J = 7.6$ Hz, 0.22H,

minor), 7.63 (d, $J = 8.4$ Hz, 2.22H, major + minor), 7.52-7.48 (m, 0.66H, minor), 7.43 (d, $J =$

6.8 Hz, 1.22H, major + minor), 7.35-7.32 (m, 2.44H, major + minor), 7.18-7.11 (m, 2.22H, major + minor), 6.99-6.96 (m, 1H, major), 6.82 (d, $J = 7.6$ Hz, 1H, major), 6.74-6.71 (m, 1H, major). ^{13}C NMR (101 MHz, CDCl_3) δ 162.8, 162.2, 151.5, 150.9, 144.6, 142.4, 139.9, 139.8, 139.4, 137.6, 137.3, 136.8, 136.4, 136.1, 135.2, 131.4, 131.1, 130.9, 130.6, 130.2, 130.2, 129.9, 129.8, 129.5, 129.4, 129.2, 129.1, 129.0, 128.8, 128.7, 128.0, 127.9, 127.5, 127.3, 126.5, 126.4, 125.8, 124.7, 123.6, 122.0, 121.6, 116.4, 109.3, 19.2, 14.9. **HRMS** (ESI) for $\text{C}_{25}\text{H}_{18}\text{BrN}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 441.0597 (^{79}Br) and 443.0580 (^{81}Br); found: 441.0594 (^{79}Br) and 443.0574 (^{81}Br).



(R)-6-Bromo-4-phenyl-3-(phenylethynyl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3aI)



Condition C, White solid, mp: 273-274 °C, 99.0 mg, 94% yield,

$[\alpha]_{\text{D}}^{25} = -77.2$ ($c = 0.1$ in CHCl_3), 96% ee, determined by HPLC

analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v,

flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_{R} (minor) = 14.33

min, t_{R} (major) = 16.30 min. ^1H NMR (400 MHz, CDCl_3) δ 8.87 (d, $J = 2.9$ Hz, 1H), 8.40 (d,

$J = 8.5$ Hz, 1H), 8.22 (d, $J = 8.2$ Hz, 1H), 8.00 (d, $J = 8.2$ Hz, 1H), 7.88 (d, $J = 7.2$ Hz, 1H),

7.70 (t, $J = 7.7$ Hz, 1H), 7.63-7.46 (m, 7H), 7.39-7.36 (m, 1H), 7.10-6.97 (m, 3H), 6.31 (d, $J =$

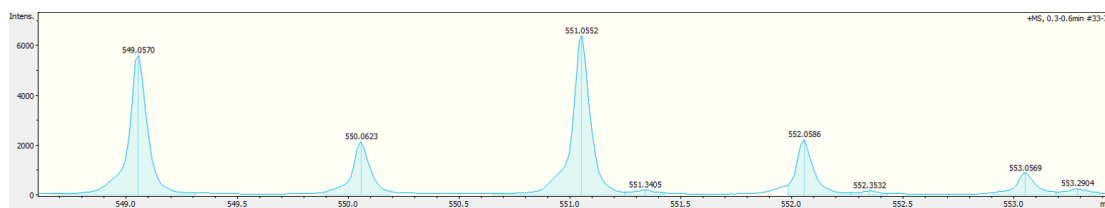
7.6 Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 161.8, 151.3, 144.7, 138.8, 137.7, 136.2, 135.5,

131.5, 131.2, 131.0, 130.6, 130.5, 130.2, 129.4, 129.2, 128.9, 128.128.5, 128.2, 128.1, 128.0,

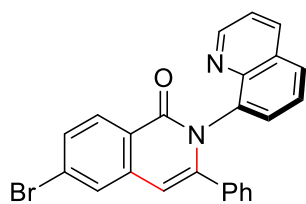
127.0, 126.7, 125.1, 123.4, 121.9, 121.4, 100.0, 83.8. **HRMS** (ESI) for $\text{C}_{32}\text{H}_{19}\text{BrN}_2\text{NaO}$

$[\text{M}+\text{Na}]^+$ calcd: 549.0573 (^{79}Br) and 551.0558 (^{81}Br); found: 549.0570 (^{79}Br) and 551.0552

(^{81}Br).

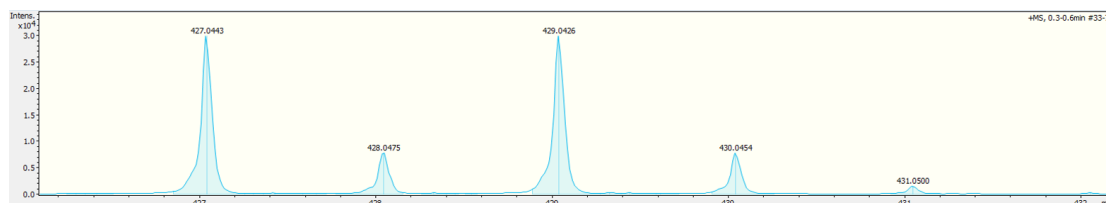


(R)-6-Bromo-3-phenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3am)

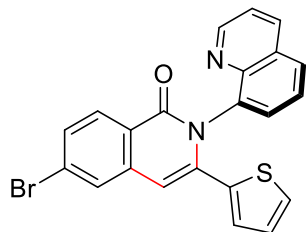


Condition C, White solid, mp: 192-193 °C, 82.2 mg, 96% yield, $[\alpha]_D^{25} = -95.0$ ($c = 0.1$ in CHCl_3), 96% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 46.26 min,

t_R (minor) = 51.41 min. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.87 (d, $J = 2.8$ Hz, 1H), 8.29 (d, $J = 8.6$ Hz, 1H), 8.06 (d, $J = 8.3$ Hz, 1H), 7.74 (s, 1H), 7.70 (d, $J = 8.0$ Hz, 1H), 7.57 (d, $J = 8.5$ Hz, 1H), 7.47 (d, $J = 7.0$ Hz, 1H), 7.41-7.32 (m, 2H), 7.08 (d, $J = 7.5$ Hz, 2H), 7.04-6.92 (m, 3H), 6.54 (s, 1H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 162.9, 151.0, 146.1, 144.6, 138.8, 137.0, 136.2, 136.0, 130.7, 130.4, 130.0, 129.0, 128.9, 128.8, 128.6, 128.3, 127.9, 127.5, 125.9, 124.1, 121.7, 106.4. **HRMS** (ESI) for $\text{C}_{24}\text{H}_{16}\text{BrN}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 427.0441 (^{79}Br) and 429.0423 (^{81}Br); found: 427.0443 (^{79}Br) and 429.0426 (^{81}Br).

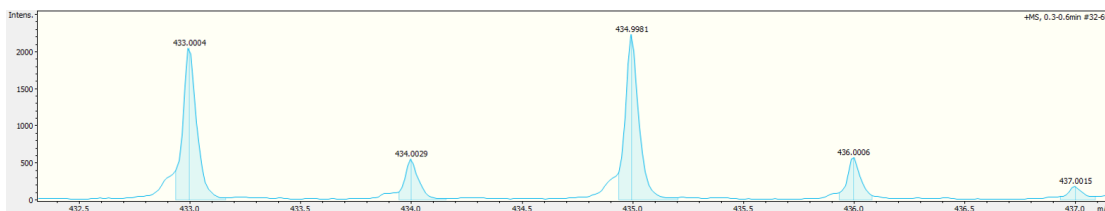


(R)-6-Bromo-2-(quinolin-8-yl)-3-(thiophen-2-yl)isoquinolin-1(2H)-one (3an)

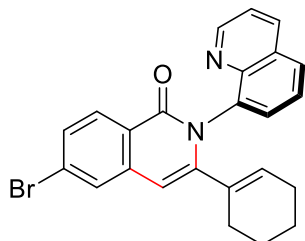


Condition C, White solid, mp: 214-215 °C, 36.5 mg, 42% yield, $[\alpha]_D^{25} = -90.8$ ($c = 0.1$ in CHCl_3), 95% ee, determined by HPLC analysis (Chiralpak AS-H column, hexane/*i*-PrOH, 70:30 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 8.29 min,

t_R (major) = 12.72 min. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.86-8.85 (m, 1H), 8.28 (d, $J = 8.6$ Hz, 1H), 8.14 (dd, $J = 8.3, 1.2$ Hz, 1H), 7.83 (d, $J = 8.1$ Hz, 1H), 7.75 (d, $J = 1.4$ Hz, 1H), 7.60-7.57 (m, 2H), 7.51 (t, $J = 7.7$ Hz, 1H), 7.39-7.36 (m, 1H), 7.01-7.00 (m, 1H), 6.75 (s, 1H), 6.64-6.52 (m, 2H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 162.9, 151.3, 145.1, 139.1, 138.5, 136.9, 136.6, 136.3, 130.6, 130.4, 130.3, 129.4, 129.1, 128.8, 128.7, 127.9, 127.2, 126.3, 126.1, 124.3, 121.9, 107.7. **HRMS** (ESI) for $\text{C}_{22}\text{H}_{14}\text{BrN}_2\text{OS}$ $[\text{M}+\text{H}]^+$ calcd: 433.0005 (^{79}Br) and 434.9986 (^{81}Br); found: 433.0004 (^{79}Br) and 434.9981 (^{81}Br).

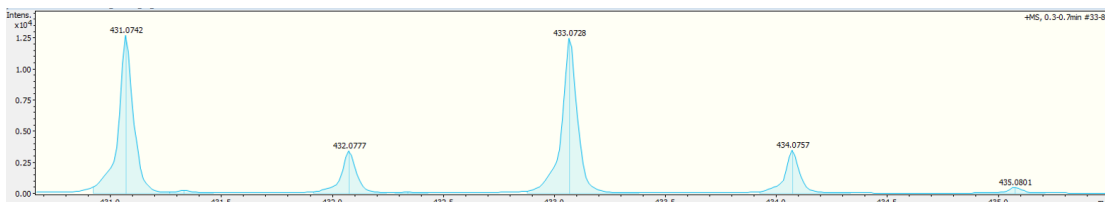


(R)-6-Bromo-3-(cyclohex-1-en-1-yl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ao)



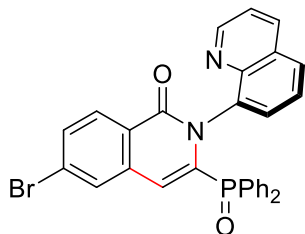
Condition C, White solid, mp: 229-230 °C, 80.9 mg, 94% yield, $[\alpha]_D^{25} = -129.6$ ($c = 0.1$ in CHCl_3), 94% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 70:30 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 15.85 min, t_R (minor) = 39.70 min. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.92-8.81

(m, 1H), 8.25 (d, $J = 8.5$ Hz, 1H), 8.18 (dd, $J = 8.3, 1.2$ Hz, 1H), 7.89 (dd, $J = 7.0, 2.4$ Hz, 1H), 7.69 (d, $J = 1.3$ Hz, 1H), 7.60 (d, $J = 7.3$ Hz, 2H), 7.52 (dd, $J = 8.5, 1.5$ Hz, 1H), 7.40-7.37 (m, 1H), 6.39 (s, 1H), 5.69 (s, 1H), 1.80-1.76 (m, 2H), 1.66-1.58 (m, 1H), 1.49-1.39 (m, 1H), 1.20-1.16 (m, 2H), 1.11-1.00 (m, 2H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 162.9, 151.1, 148.7, 144.9, 139.3, 137.2, 136.2, 134.1, 131.1, 130.4, 130.3, 129.5, 129.0, 128.3, 127.6, 125.8, 124.0, 121.7, 104.1, 28.9, 25.1, 22.2, 21.4. **HRMS** (ESI) for $\text{C}_{24}\text{H}_{20}\text{BrN}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 431.0754 (^{79}Br) and 433.0736 (^{81}Br); found: 431.0742 (^{79}Br) and 433.0728 (^{81}Br).



(R)-6-Bromo-3-(diphenylphosphoryl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one

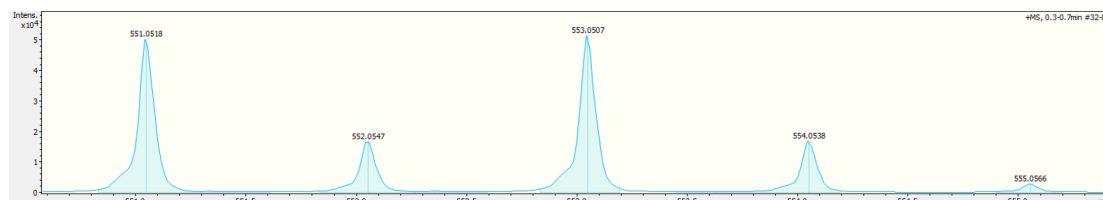
(3ap-major)



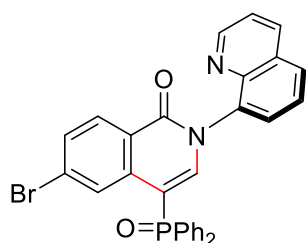
Condition C, White solid, mp: 253-254 °C, 90.2 mg, 82% yield, $[\alpha]_D^{25} = -169.0$ ($c = 0.1$ in CHCl_3), 96% ee, determined by HPLC analysis (Chiralcel OD-H column, hexane/*i*-PrOH, 70:30 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 17.69 min,

t_R (major) = 25.58 min. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.63 (d, $J = 3.2$ Hz, 1H), 8.30 (d, $J = 8.5$ Hz, 1H), 8.01 (d, $J = 7.1$ Hz, 1H), 7.86-7.74 (m, 3H), 7.68 (d, $J = 8.6$ Hz, 1H), 7.65-7.42 (m, 6H), 7.26-7.18 (m, 3H), 6.99-6.83 (m, 3H), 6.59 (d, $J = 12.5$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 162.8 (d, $J = 4.6$ Hz), 150.4, 144.4, 139.9 (d, $J = 106.4$ Hz), 136.6 (d, $J =$

14.3 Hz), 135.8, 135.1 (d, $J = 2.6$ Hz), 132.9, 132.5 (d, $J = 2.7$ Hz), 132.4, 132.2 (d, $J = 9.3$ Hz), 131.1, 131.0 (d, $J = 2.8$ Hz), 130.4 (d, $J = 6.7$ Hz), 130.2, 130.1, 130.0, 129.9, 128.8, 128.7, 128.6, 128.2, 127.9, 127.5, 127.3, 127.2, 126.0, 125.6, 121.3, 116.5 (d, $J = 14.6$ Hz). ^{31}P NMR (162 MHz, CDCl_3) δ 23.3. **HRMS** (ESI) for $\text{C}_{30}\text{H}_{21}\text{BrN}_2\text{O}_2\text{P}$ $[\text{M}+\text{H}]^+$ calcd: 551.0519 (^{79}Br) and 553.0503 (^{81}Br); found: 551.0518 (^{79}Br) and 553.0507 (^{81}Br).



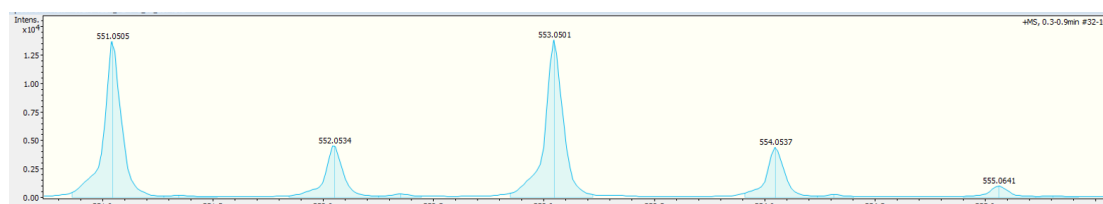
6-Bromo-4-(diphenylphosphoryl)-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ap-minor)



Condition C, Yellow solid, mp: 261-262 °C, 14.3 mg, 13% yield.

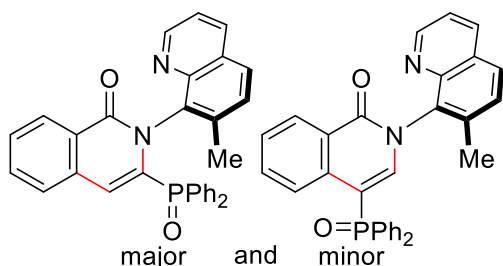
^1H NMR (400 MHz, CDCl_3) δ 8.88 (d, $J = 3.0$ Hz, 1H), 8.35 (d, $J = 8.6$ Hz, 1H), 8.31 (s, 1H), 8.22 (d, $J = 8.2$ Hz, 1H), 7.98-7.71 (m, 6H), 7.66-7.58 (m, 2H), 7.46 (dd, $J = 8.3, 4.2$ Hz, 7H), 7.28

(d, $J = 9.6$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 162.0, 151.0, 144.27 (d, $J = 19.6$ Hz), 143.2, 137.50 (d, $J = 7.0$ Hz), 136.9, 136.4, 132.4 (d, $J = 2.6$ Hz), 132.2, 132.1, 131.0, 130.5, 129.5, 129.5, 129.2 (d, $J = 3.8$ Hz), 128.9, 128.8, 128.6, 126.1, 125.3 (d, $J = 9.2$ Hz), 122.0, 105.5 (d, $J = 111.4$ Hz). ^{31}P NMR (162 MHz, CDCl_3) δ 27.9. **HRMS** (ESI) for $\text{C}_{30}\text{H}_{21}\text{BrN}_2\text{O}_2\text{P}$ $[\text{M}+\text{H}]^+$ calcd: 551.0519 (^{79}Br) and 553.0503 (^{81}Br); found: 551.0505 (^{79}Br) and 553.0501 (^{81}Br).



(R)-3-(Diphenylphosphoryl)-2-(7-methylquinolin-8-yl)isoquinolin-1(2H)-one (3aq-major)

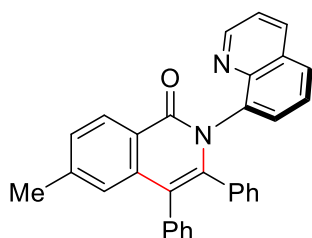
(R)-4-(Diphenylphosphoryl)-2-(7-methylquinolin-8-yl)isoquinolin-1(2H)-one (3aq-minor)



Condition C, White solid, mp: 245-246 °C, 71.8 mg, 74% yield, $[\alpha]_{\text{D}}^{25} = -56.8$ (c = 0.1 in CHCl_3), 91% ee, determined by HPLC analysis (Chiralcel OD-H column, hexane/*i*-PrOH, 90:10 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_{R}

(major) = 46.85 min for major isomer, t_R (minor) = 68.46 min for major isomer. **^1H NMR** (400 MHz, CDCl_3) δ 8.84-8.82 (m, 0.13H, minor), 8.51 (d, J = 8.0 Hz, 0.13H, minor), 8.46 (d, J = 7.6 Hz, 1H, major), 8.44-8.42 (m, 1H, major), 8.14 (d, J = 8.4 Hz, 0.26H, minor), 7.92-7.87 (m, 0.26H, minor), 7.82-7.78 (m, 3H, major), 7.75-7.74 (m, 0.13H, minor), 7.71-7.67 (m, 1.13H, major + minor), 7.62-7.58 (m, 2.26H, major + minor), 7.56-7.54 (m, 1H, major), 7.49-7.44 (m, 4.39H, major + minor), 7.37-7.34 (m, 0.26H, minor), 7.24-7.21 (m, 2H, major), 7.09-7.04 (m, 2.26H, major + minor), 6.95-6.90 (m, 2.26H, major + minor), 6.74-6.71 (m, 1.13H, major + minor), 2.49 (s, 3H, major), 2.37 (s, 0.39H, minor). **^{13}C NMR** (101 MHz, CDCl_3) δ 162.6 (d, J = 5.0 Hz), 161.9, 151.0, 150.3, 145.2, 141.4, 138.8, 137.7, 137.6, 136.1 (d, J = 13.8 Hz), 135.7, 135.4 (d, J = 14.4 Hz), 135.4, 133.5 (d, J = 68.5 Hz), 133.1, 132.8, 132.5, 132.4, 132.3 (d, J = 5.7 Hz), 132.3, 132.1 (d, J = 10.0 Hz), 131.2, 131.1 (d, J = 2.8 Hz), 131.0, 130.9, 129.5, 129.4, 129.3, 129.2, 129.0, 128.8, 128.7 (d, J = 2.9 Hz), 128.6, 128.4, 127.6 (d, J = 3.6 Hz), 127.4, 126.8, 121.2 (d, J = 3.1 Hz), 120.3, 118.1 (d, J = 14.6 Hz), 19.5, 18.7. **^{31}P NMR** (162 MHz, CDCl_3) δ 28.1 (minor), 21.9 (major). **HRMS** (ESI) for $\text{C}_{31}\text{H}_{24}\text{BrN}_2\text{O}_2\text{P}$ $[\text{M}+\text{H}]^+$ calcd: 487.1570; found: 483.1557.

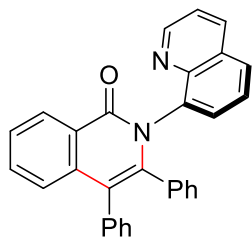
(*R*)-3,4-Diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3aa)



Condition C, White solid, mp: 285-287 °C, 82.3 mg, 94% yield, $[\alpha]_{\text{D}}^{25} = +53.6$ (c = 0.1 in CHCl_3), 95% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, λ = 254 nm, 25 °C), t_R (major) = 12.01 min, t_R (minor) = 25.57 min. **^1H NMR** (400 MHz, CDCl_3) δ

8.96-8.90 (m, 1H), 8.47 (d, J = 8.2 Hz, 1H), 8.03 (d, J = 8.3 Hz, 1H), 7.64 (d, J = 8.1 Hz, 1H), 7.48 (d, J = 7.1 Hz, 1H), 7.39-7.32 (m, 3H), 7.24-7.11 (m, 5H), 7.07 (s, 1H), 6.95 (d, J = 7.6 Hz, 1H), 6.83-6.68 (m, 3H), 6.49-6.45 (m, 1H), 2.38 (s, 3H). **^{13}C NMR** (101 MHz, CDCl_3) δ 162.7, 150.7, 144.7, 143.0, 141.9, 138.2, 137.7, 136.7, 136.1, 135.0, 131.9, 131.7, 131.0, 130.8, 129.8, 128.7, 128.5, 128.4, 128.3, 128.0, 127.7, 127.1, 126.7, 126.6, 126.4, 125.8, 125.3, 123.4, 121.5, 118.4, 22.1. **HRMS** (ESI) for $\text{C}_{31}\text{H}_{23}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 439.1805; found: 439.1801.

(R)-3,4-Diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ba)



Condition C, White solid, mp: 251-253 °C, 83.3 mg, 98% yield,

$[\alpha]_D^{25} = +51.6$ ($c = 0.1$ in CHCl_3), 96% ee, determined by HPLC

analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow

rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 10.39 min, t_R

(minor) = 24.26 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.92 (d, $J = 2.8$ Hz, 1H), 8.58 (d, $J = 7.9$

Hz, 1H), 8.03 (d, $J = 8.1$ Hz, 1H), 7.65-7.48 (m, 4H), 7.41-7.28 (m, 3H), 7.24-7.11 (m, 5H),

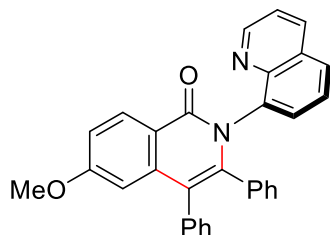
6.97 (d, $J = 7.6$ Hz, 1H), 6.84-6.69 (m, 3H), 6.50-6.46 (m, 1H). **^{13}C NMR** (101 MHz, CDCl_3)

δ 162.8, 150.8, 144.7, 141.9, 138.2, 137.7, 136.6, 136.1, 135.0, 132.6, 131.9, 131.7, 131.0,

130.9, 129.8, 128.8, 128.7, 128.5, 128.1, 127.9, 127.3, 126.8, 126.7, 126.5, 125.9, 125.7, 121.6,

118.6. **HRMS** (ESI) for $\text{C}_{30}\text{H}_{21}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 425.1648; found: 425.1646.

(R)-6-Methoxy-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ca)



Condition C, White solid, mp: 299-301 °C, 74.3 mg, 82%

yield, $[\alpha]_D^{25} = +62.4$ ($c = 0.1$ in CHCl_3), 97% ee, determined by

HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH,

80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major)

= 12.28 min, t_R (minor) = 30.55 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.93 (d, $J = 2.5$ Hz, 1H),

8.51 (d, $J = 8.8$ Hz, 1H), 8.03 (d, $J = 7.8$ Hz, 1H), 7.63 (d, $J = 7.8$ Hz, 1H), 7.49 (d, $J = 7.0$ Hz,

1H), 7.37-7.08 (m, 8H), 6.96 (d, $J = 7.5$ Hz, 1H), 6.83-6.45 (m, 5H), 3.72 (s, 3H). **^{13}C NMR**

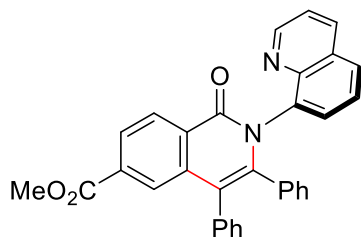
(101 MHz, CDCl_3) δ 163.0, 162.4, 150.7, 144.7, 142.5, 140.3, 137.7, 136.6, 136.1, 135.0,

131.8, 131.6, 131.0, 130.7, 130.6, 129.7, 128.7, 128.5, 128.1, 127.8, 127.2, 126.8, 126.6,

126.4, 125.8, 121.5, 119.5, 118.3, 115.3, 107.6, 55.3. **HRMS** (ESI) for $\text{C}_{31}\text{H}_{23}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$

calcd: 455.1754; found: 455.1745.

(R)-Methyl 1-oxo-3,4-diphenyl-2-(quinolin-8-yl)-1,2-dihydroisoquinoline-6-carboxylate (3da)



Condition C, White solid, mp: 329-330 °C, 88.8 mg, 92%

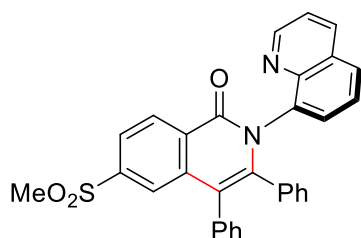
yield, $[\alpha]_D^{25} = +23.75$ ($c = 0.1$ in CHCl_3), 94% ee,

determined by HPLC analysis (Chiralpak AD-H column,

hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm,

25 °C), t_R (major) = 10.06 min, t_R (minor) = 24.57 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.93 (d, J = 3.0 Hz, 1H), 8.64 (d, J = 8.3 Hz, 1H), 8.12 (d, J = 8.3 Hz, 1H), 8.07 (d, J = 8.1 Hz, 1H), 8.03 (s, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.49 (d, J = 6.9 Hz, 1H), 7.41-7.35 (m, 2H), 7.21 (d, J = 29.2 Hz, 5H), 6.96 (d, J = 7.6 Hz, 1H), 6.83 (t, J = 7.6 Hz, 1H), 6.74 (d, J = 7.3 Hz, 2H), 6.49 (t, J = 7.5 Hz, 1H), 3.89 (s, 3H). **^{13}C NMR** (101 MHz, CDCl_3) δ 166.8, 162.3, 150.9, 144.6, 142.9, 138.1, 137.5, 136.2, 135.9, 134.7, 133.6, 131.9, 131.7, 130.9, 130.8, 129.8, 128.9, 128.5, 128.3, 128.1, 127.7, 127.5, 127.2, 126.8, 126.7, 126.6, 125.9, 121.7, 118.8, 52.5. **HRMS** (ESI) for $\text{C}_{32}\text{H}_{23}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ calcd: 483.1703; found: 483.1712.

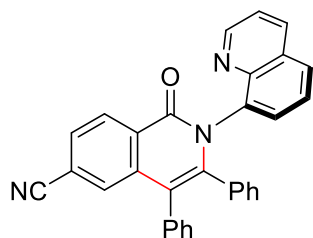
(R)-6-(Methylsulfonyl)-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ea)



Condition C, White solid, mp: 309-310 °C, 96.4 mg, 96% yield, $[\alpha]_D^{25} = +11.6$ (c = 0.1 in CHCl_3), 93% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 75:25 v/v, flow rate 1.0 mL/min, λ = 254 nm, 25 °C), t_R

(major) = 14.79 min, t_R (minor) = 23.53 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.91 (dd, J = 4.0, 1.3 Hz, 1H), 8.76 (d, J = 8.4 Hz, 1H), 8.06 (dd, J = 8.2, 1.1 Hz, 1H), 7.99 (dd, J = 8.4, 1.5 Hz, 1H), 7.94 (s, 1H), 7.68 (d, J = 7.9 Hz, 1H), 7.49 (d, J = 6.9 Hz, 1H), 7.42-7.34 (m, 2H), 7.27-7.15 (m, 5H), 6.96 (d, J = 7.7 Hz, 1H), 6.85 (t, J = 7.5 Hz, 1H), 6.78-6.67 (m, 2H), 6.50 (t, J = 7.6 Hz, 1H), 3.02 (s, 3H). **^{13}C NMR** (101 MHz, CDCl_3) δ 161.8, 151.0, 144.4, 144.3, 144.0, 138.8, 137.1, 136.2, 135.1, 134.3, 131.7, 131.5, 130.7, 130.5, 130.4, 129.5, 129.0, 128.8, 128.5, 128.4, 127.7, 127.5, 126.9, 126.6, 125.8, 125.4, 123.8, 121.8, 118.3, 44.3. **HRMS** (ESI) for $\text{C}_{31}\text{H}_{23}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$ calcd: 503.1424; found: 503.1429.

(R)-1-Oxo-3,4-diphenyl-2-(quinolin-8-yl)-1,2-dihydroisoquinoline-6-carbonitrile (3fa)

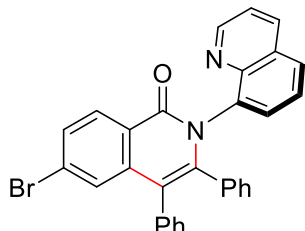


Condition C, White solid, mp: 277-278 °C, 84.4 mg, 94% yield, $[\alpha]_D^{25} = +18.6$ (c = 0.1 in CHCl_3), 93% ee, determined by HPLC analysis (Chiralpak AS-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, λ = 254 nm, 25 °C), t_R (minor) = 11.65

min, t_R (major) = 37.43 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.64 (d, J = 8.2 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.71-7.61 (m, 3H), 7.49 (d, J = 7.2 Hz, 1H), 7.37-7.34 (m, 2H), 7.26-7.10 (m, 5H), 6.97 (d, J = 7.0 Hz, 1H), 6.87-6.70 (m, 3H), 6.49 (t, J = 7.4 Hz, 1H). **^{13}C NMR** (101

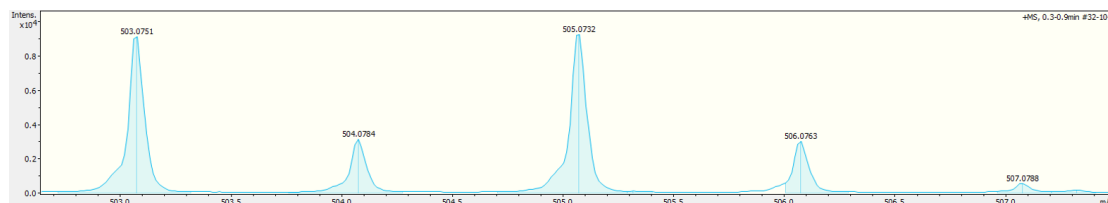
MHz, CDCl₃) δ 161.7, 150.9, 144.3, 144.1, 138.4, 137.0, 136.1, 135.1, 134.1, 131.7, 131.4, 130.6, 130.5, 129.6, 129.4, 129.0, 128.8, 128.5, 128.3, 127.9, 127.7, 127.4, 126.9, 126.6, 125.8, 121.7, 118.5, 117.6, 115.9. **HRMS** (ESI) for C₃₁H₂₀N₃O [M+H]⁺ calcd: 450.1601; found: 450.1609.

(R)-6-Bromo-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ga)

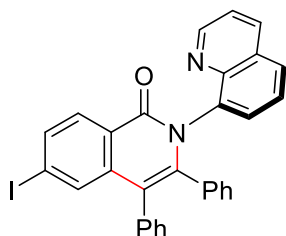


Condition C, White solid, mp: 307-309 °C, 98.7 mg, 98% yield, $[\alpha]_D^{25} = +26.4$ (c = 0.1 in CHCl₃), 95% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, λ = 254 nm, 25 °C), t_R (major) = 12.57 min,

t_R (minor) = 38.87 min. **¹H NMR** (400 MHz, CDCl₃) δ 8.92 (d, J = 2.7 Hz, 1H), 8.42 (d, J = 8.5 Hz, 1H), 8.04 (d, J = 8.2 Hz, 1H), 7.72-7.55 (m, 2H), 7.48 (d, J = 6.7 Hz, 1H), 7.44 (d, J = 1.4 Hz, 1H), 7.39-7.34 (m, 2H), 7.25-7.12 (m, 5H), 6.95 (d, J = 7.6 Hz, 1H), 6.83 (t, J = 7.5 Hz, 1H), 6.72 (t, J = 7.5 Hz, 2H), 6.48 (t, J = 7.5 Hz, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 162.4, 150.94, 144.64, 143.5, 139.8, 137.5, 136.1, 135.9, 134.7, 131.8, 131.6, 130.8, 130.7, 130.4, 130.0, 129.7, 128.8, 128.3, 128.2, 128.1, 128.0, 127.5, 127.2, 126.8, 126.6, 125.8, 124.4, 121.7, 117.7. **HRMS** (ESI) for C₃₀H₂₀BrN₂O [M+H]⁺ calcd: 503.0754 (⁷⁹Br) and 505.0738 (⁸¹Br); found: 503.0751 (⁷⁹Br) and 505.0732 (⁸¹Br).



(R)-6-Iodo-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ha)



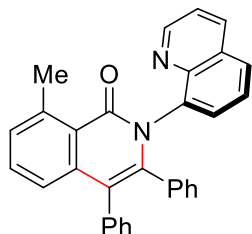
Condition C, White solid, mp: 320-321 °C, 104.6 mg, 95% yield, $[\alpha]_D^{25} = +65.8$ (c = 0.1 in CHCl₃), 96% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, λ = 254 nm, 25 °C), t_R (major) = 14.33 min, t_R

(minor) = 43.58 min. **¹H NMR** (400 MHz, CDCl₃) δ 8.91 (s, 1H), 8.26 (d, J = 8.3 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.72-7.57 (m, 2H), 7.47 (d, J = 7.0 Hz, 1H), 7.38-7.32 (m, 2H), 7.24-7.15 (m, 5H), 6.94 (d, J = 7.3 Hz, 1H), 6.82 (t, J = 7.3 Hz, 1H), 6.70 (d, J = 7.2 Hz, 2H), 6.47 (t, J = 7.4 Hz, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 162.5, 150.9,

144.6, 143.3, 139.7, 137.5, 136.1, 135.8, 134.7, 134.5, 131.8, 131.6, 130.8, 130.7, 130.1, 129.7, 128.8, 128.3, 128.1, 127.5, 127.2, 126.8, 126.6, 125.8, 124.8, 121.6, 117.4, 100.9.

HRMS (ESI) for $C_{30}H_{20}IN_2O$ $[M+H]^+$ calcd: 551.0615; found: 551.0621.

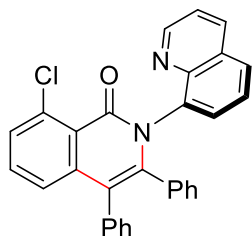
(R)-8-Methyl-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ia)



Condition C, White solid, mp: 279-280 °C, 86.8 mg, 99% yield, $[\alpha]_D^{25} = +7.0$ ($c = 0.1$ in $CHCl_3$), 93% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 5.15 min, t_R (minor)

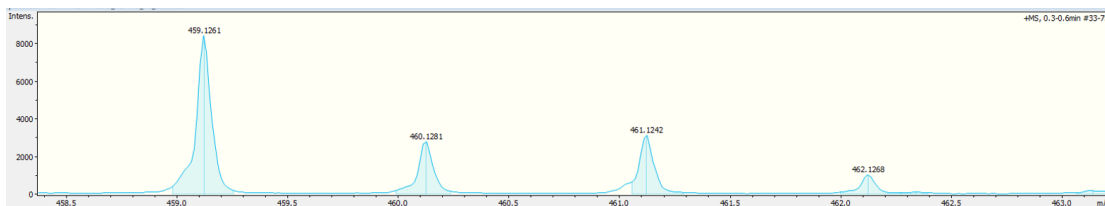
= 9.32 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.94 (d, $J = 2.8$ Hz, 1H), 8.03 (d, $J = 8.3$ Hz, 1H), 7.63 (d, $J = 8.1$ Hz, 1H), 7.52 (d, $J = 7.0$ Hz, 1H), 7.43-7.33 (m, 3H), 7.27 (d, $J = 7.3$ Hz, 1H), 7.22-7.09 (m, 6H), 6.95 (d, $J = 7.7$ Hz, 1H), 6.82-6.66 (m, 3H), 6.46 (t, $J = 7.5$ Hz, 1H), 2.96 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.6, 150.8, 144.9, 142.6, 142.0, 140.1, 138.2, 137.4, 136.1, 135.1, 132.0, 131.9, 131.7, 131.1, 130.8, 130.1, 129.8, 128.9, 128.5, 128.1, 127.9, 127.2, 126.8, 126.6, 126.4, 125.9, 124.2, 121.6, 118.6, 24.5. **HRMS** (ESI) for $C_{31}H_{23}N_2O$ $[M+H]^+$ calcd: 439.1805; found: 439.1806.

(R)-8-Chloro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ja)

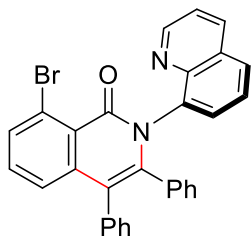


Condition C, White solid, mp: 289-290 °C, 77.1 mg, 84% yield, $[\alpha]_D^{25} = +6.25$ ($c = 0.1$ in $CHCl_3$), 87% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 7.02 min, t_R (minor)

= 13.80 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.97-8.85 (m, 1H), 8.02 (d, $J = 8.3$ Hz, 1H), 7.63 (d, $J = 8.1$ Hz, 1H), 7.51 (d, $J = 7.5$ Hz, 2H), 7.42-7.33 (m, 3H), 7.24-7.12 (m, 6H), 6.95 (d, $J = 7.7$ Hz, 1H), 6.82 (t, $J = 7.5$ Hz, 1H), 6.76-6.66 (m, 2H), 6.47 (t, $J = 7.6$ Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.1, 150.9, 144.7, 143.2, 141.5, 137.7, 136.7, 136.3, 136.1, 134.7, 132.2, 131.8, 131.1, 130.6, 130.0, 129.6, 128.9, 128.7, 128.2, 128.1, 127.4, 127.0, 126.7, 126.5, 125.8, 125.1, 122.2, 121.6, 117.9. **HRMS** (ESI) for $C_{30}H_{20}ClN_2O$ $[M+H]^+$ calcd: 459.1259 (^{35}Cl) and 461.1243 (^{37}Cl); found: 459.1261 (^{35}Cl) and 461.1242 (^{37}Cl).

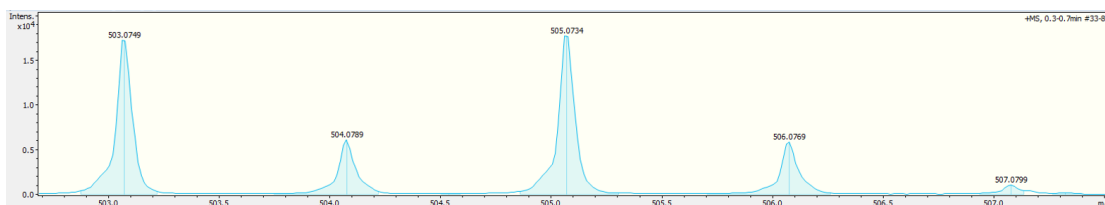


(R)-8-Bromo-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ka)

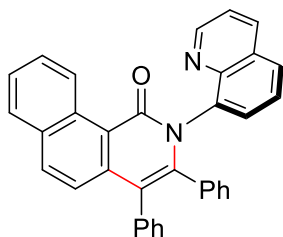


Condition C, White solid, mp: 291-292 °C, 80.6 mg, 80% yield, $[\alpha]_D^{25} = +4.3$ ($c = 0.1$ in CHCl_3), 82% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 7.56 min, t_R (minor)

= 14.53 min. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.97-8.95 (m, k, $J = 8.3, 1.2$ Hz, 1H), 7.81 (d, $J = 7.2$ Hz, 1H), 7.67 (d, $J = 8.0$ Hz, 1H), 7.57 (d, $J = 7.1$ Hz, 1H), 7.43-7.28 (m, 4H), 7.25-7.15 (m, 5H), 6.99 (d, $J = 7.7$ Hz, 1H), 6.86 (t, $J = 7.5$ Hz, 1H), 6.81-6.70 (m, 2H), 6.51 (t, $J = 7.5$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 161.0, 150.8, 144.7, 143.1, 141.4, 137.7, 136.7, 136.1, 134.6, 133.9, 132.2, 131.9, 131.8, 131.1, 130.6, 129.6, 128.9, 128.7, 128.2, 128.1, 127.4, 127.0, 126.7, 126.5, 125.8, 123.9, 123.0, 121.6, 118.0. **HRMS** (ESI) for $\text{C}_{30}\text{H}_{20}\text{BrN}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 503.0754 (^{79}Br) and 505.0738 (^{81}Br); found: 503.0749 (^{79}Br) and 505.0734 (^{81}Br).



(R)-3,4-Diphenyl-2-(quinolin-8-yl)benzo[h]isoquinolin-1(2H)-one (3la)

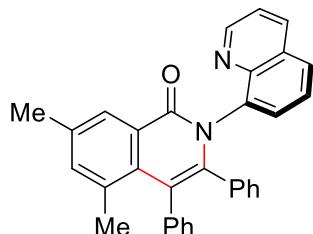


Condition C, White solid, mp: 241-242 °C, 80.7 mg, 85% yield, $[\alpha]_D^{25} = +16.25$ ($c = 0.1$ in CHCl_3), 97% ee, determined by HPLC analysis (Chiralpak IA-H column, hexane/*i*-PrOH, 70:30 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 10.16 min, t_R

(minor) = 29.37 min. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 10.25 (d, $J = 8.7$ Hz, 1H), 8.91 (dd, $J = 4.2, 1.4$ Hz, 1H), 8.06 (dd, $J = 8.3, 1.3$ Hz, 1H), 7.95 (d, $J = 8.9$ Hz, 1H), 7.88 (d, $J = 7.8$ Hz, 1H), 7.69-7.64 (m, 2H), 7.58 (t, $J = 6.9$ Hz, 2H), 7.44-7.35 (m, 3H), 7.26-7.17 (m, 5H), 7.00 (d, $J = 7.7$ Hz, 1H), 6.84 (t, $J = 7.5$ Hz, 1H), 6.78 (d, $J = 7.7$ Hz, 1H), 6.73 (t, $J = 7.5$ Hz, 1H), 6.51 (d, $J = 7.5$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 163.2, 150.9, 144.8, 143.6, 139.7,

138.4, 137.2, 136.1, 135.0, 133.9, 132.4, 132.3, 132.2, 132.0, 130.9, 130.7, 129.6, 128.9, 128.7, 128.4, 128.2, 128.1, 128.0, 127.4, 126.9, 126.7, 126.5, 126.4, 125.9, 123.9, 121.6, 119.1. **HRMS** (ESI) for $C_{34}H_{23}N_2O$ $[M+H]^+$ calcd: 475.1805; found: 475.1809.

(R)-5,7-Dimethyl-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ma)



Condition C, White solid, mp: 280-281 °C, 69.7 mg, 77% yield,

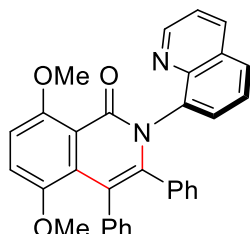
$[\alpha]_D^{25} = +39.25$ ($c = 0.1$ in $CHCl_3$), 90% ee, determined by

HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20

v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 8.55

min, t_R (minor) = 17.52 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.90 (d, $J = 2.9$ Hz, 1H), 8.37 (s, 1H), 8.01 (dd, $J = 8.2, 1.0$ Hz, 1H), 7.61 (d, $J = 8.2$ Hz, 1H), 7.46 (d, $J = 6.9$ Hz, 1H), 7.35-7.31 (m, 2H), 7.25-7.03 (m, 6H), 6.90 (d, $J = 7.6$ Hz, 1H), 6.77 (t, $J = 7.4$ Hz, 1H), 6.66-6.63 (m, 2H), 6.41 (t, $J = 7.5$ Hz, 1H), 2.45 (s, 3H), 1.79 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.0, 150.8, 144.7, 141.5, 140.2, 138.4, 138.0, 136.5, 136.0, 135.4, 135.2, 133.7, 132.3, 132.2, 131.2, 131.0, 130.1, 128.8, 128.5, 127.5, 127.3, 127.1, 127.0, 126.9, 126.5, 126.4, 126.2, 125.8, 121.5, 118.3, 23.9, 21.2. **HRMS** (ESI) for $C_{32}H_{25}N_2O$ $[M+H]^+$ calcd: 453.1961; found: 453.1964.

(R)-5,8-Dimethoxy-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3na)



Condition C, White solid, mp: 195-196 °C, 53.5 mg, 55% yield,

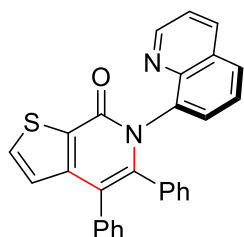
$[\alpha]_D^{25} = +7.4$ ($c = 0.1$ in $CHCl_3$), 73% ee, determined by HPLC

analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 70:30 v/v, flow

rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 5.50 min, t_R (major)

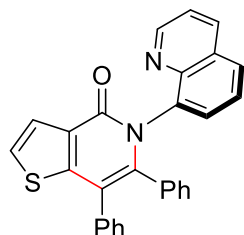
= 6.76 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.89 (d, $J = 3.0$ Hz, 1H), 7.97 (d, $J = 8.1$ Hz, 1H), 7.57 (d, $J = 8.1$ Hz, 1H), 7.45 (d, $J = 7.1$ Hz, 1H), 7.34-7.27 (m, 2H), 7.11-6.89 (m, 8H), 6.76 (t, $J = 7.5$ Hz, 1H), 6.72-6.60 (m, 2H), 6.40 (t, $J = 7.5$ Hz, 1H), 3.90 (s, 3H), 3.22 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.9, 156.2, 150.6, 150.0, 144.8, 143.2, 140.9, 138.1, 135.9, 135.1, 131.2, 131.1, 131.0, 130.8, 130.7, 129.9, 128.7, 128.3, 126.8, 126.5, 126.4, 126.3, 126.1, 125.6, 125.1, 121.3, 118.0, 116.8, 115.5, 109.8, 57.3, 56.9. **HRMS** (ESI) for $C_{32}H_{25}N_2O_3$ $[M+H]^+$ calcd: 485.1860; found: 485.1868.

(R)-4,5-Diphenyl-6-(quinolin-8-yl)thieno[2,3-*c*]pyridin-7(6H)-one (3oa)



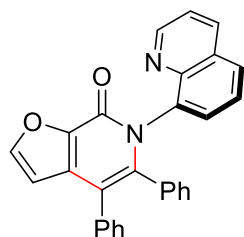
Condition C, White solid, mp: 215-216 °C, 79.3 mg, 92% yield, $[\alpha]_D^{25} = +38.0$ ($c = 0.1$ in CHCl_3), 98% ee, determined by HPLC analysis (Chiralpak AS-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 10.08 min, t_R (minor) = 12.74 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.93 (d, $J = 2.7$ Hz, 1H), 8.04 (d, $J = 8.2$ Hz, 1H), 7.67 (t, $J = 6.3$ Hz, 2H), 7.49 (d, $J = 7.2$ Hz, 1H), 7.42-7.32 (m, 2H), 7.26-7.10 (m, 5H), 7.04 (d, $J = 5.2$ Hz, 1H), 6.95 (d, $J = 7.5$ Hz, 1H), 6.84 (t, $J = 7.5$ Hz, 1H), 6.75 (t, $J = 7.7$ Hz, 2H), 6.52 (t, $J = 7.6$ Hz, 1H). **^{13}C NMR** (101 MHz, CDCl_3) δ 158.7, 150.9, 146.8, 144.8, 143.2, 137.3, 137.1, 136.1, 134.6, 133.3, 131.1, 131.0, 130.9, 130.1, 129.4, 128.8, 128.0, 127.5, 126.9, 126.6, 125.8, 125.2, 121.6, 117.5. **HRMS** (ESI) for $\text{C}_{28}\text{H}_{19}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$ calcd: 431.1213; found: 431.1216.

(R)-6,7-Diphenyl-5-(quinolin-8-yl)thieno[3,2-c]pyridin-4(5H)-one (3pa)



Condition C, White solid, mp: 265-266 °C, 80.2 mg, 93% yield, $[\alpha]_D^{25} = +101.633$ ($c = 0.1$ in CHCl_3), 89% ee, determined by HPLC analysis (Chiralpak AS-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 10.17 min, t_R (major) = 36.26 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.94-8.92 (m, 1H), 8.04 (dd, $J = 8.3, 1.5$ Hz, 1H), 7.78 (d, $J = 5.4$ Hz, 1H), 7.68-7.62 (m, 1H), 7.47 (dd, $J = 7.3, 1.2$ Hz, 1H), 7.39-7.32 (m, 2H), 7.30-7.25 (m, 3H), 7.21-7.13 (m, 3H), 6.96 (d, $J = 7.6$ Hz, 1H), 6.88-6.72 (m, 3H), 6.52 (t, $J = 7.5$ Hz, 1H). **^{13}C NMR** (101 MHz, CDCl_3) δ 159.3, 151.4, 150.9, 144.8, 141.9, 137.5, 137.1, 136.1, 134.3, 130.9, 130.4, 130.0, 129.8, 128.8, 128.3, 127.6, 127.4, 126.9, 126.7, 126.3, 125.8, 124.9, 121.6, 116.5. **HRMS** (ESI) for $\text{C}_{28}\text{H}_{19}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$ calcd: 431.1213; found: 431.1215.

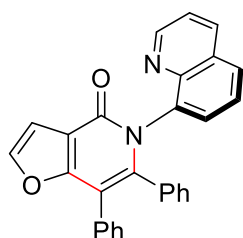
(R)-4,5-Diphenyl-6-(quinolin-8-yl)furo[2,3-c]pyridin-7(6H)-one (3qa)



Condition C, White solid, mp: 269-271 °C, 48.2 mg, 58% yield, $[\alpha]_D^{25} = +303.8$ ($c = 0.1$ in CHCl_3), 93% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 70:30 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor) = 6.03 min, t_R (major) = 10.03 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.93-8.92 (m, 1H), 8.08-8.00 (m, 1H), 7.80 (d, $J = 1.8$ Hz,

1H), 7.67 (d, $J = 8.1$ Hz, 1H), 7.48 (d, $J = 7.3$ Hz, 1H), 7.41-7.31 (m, 2H), 7.17-7.11 (m, 5H), 6.94 (d, $J = 7.7$ Hz, 1H), 6.85 (t, $J = 7.4$ Hz, 1H), 6.80-6.71 (m, 2H), 6.61 (d, $J = 1.8$ Hz, 1H), 6.52 (t, $J = 7.6$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.6, 150.9, 148.4, 144.8, 142.6, 142.4, 137.1, 136.4, 136.2, 134.7, 134.5, 131.2, 130.5, 130.4, 129.0, 128.9, 128.0, 127.6, 126.9, 126.8, 126.7, 125.8, 121.7, 114.8, 107.9. HRMS (ESI) for $\text{C}_{28}\text{H}_{19}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ calcd: 415.1441; found: 415.1451.

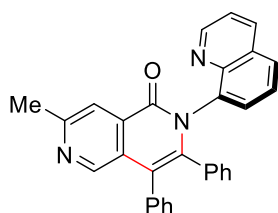
(R)-6,7-Diphenyl-5-(quinolin-8-yl)furo[3,2-c]pyridin-4(5H)-one (3ra)



Condition C, White solid, mp: 291-292 °C, 78.1 mg, 94% yield, $[\alpha]_{\text{D}}^{25} = +280.1$ ($c = 0.1$ in CHCl_3), 95% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 70:30 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_{R} (minor) = 6.52 min, t_{R} (major) = 7.17

min. ^1H NMR (400 MHz, CDCl_3) δ 8.98-8.89 (m, 1H), 8.04 (d, $J = 8.2$ Hz, 1H), 7.66 (d, $J = 8.1$ Hz, 1H), 7.54 (d, $J = 1.9$ Hz, 1H), 7.46 (d, $J = 6.4$ Hz, 1H), 7.39-7.32 (m, 2H), 7.25-7.11 (m, 6H), 6.96 (d, $J = 7.7$ Hz, 1H), 6.87 (t, $J = 7.5$ Hz, 1H), 6.82-6.72 (m, 2H), 6.54 (t, $J = 7.5$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 159.6, 159.2, 150.9, 144.8, 144.2, 143.6, 137.4, 136.2, 134.1, 132.9, 131.1, 131.0, 130.1, 128.8, 127.9, 127.8, 127.2, 127.0, 126.8, 125.8, 121.6, 115.3, 111.1, 108.3. HRMS (ESI) for $\text{C}_{28}\text{H}_{19}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ calcd: 415.1441; found: 415.1439.

(R)-7-Methyl-3,4-diphenyl-2-(quinolin-8-yl)-2,6-naphthyridin-1(2H)-one (3sa)

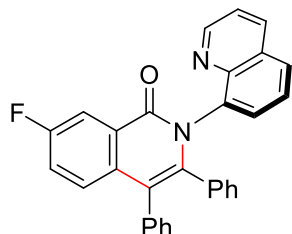


Condition C, White solid, mp: 265-266 °C, 71.2 mg, 81% yield, $[\alpha]_{\text{D}}^{25} = +42.3$ ($c = 0.1$ in CHCl_3), 90% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 70:30 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_{R} (minor) = 6.49 min, t_{R}

(major) = 11.01 min. ^1H NMR (400 MHz, CDCl_3) δ 8.90 (dd, $J = 4.1, 1.7$ Hz, 1H), 8.66 (s, 1H), 8.16 (s, 1H), 8.04 (d, $J = 8.4$ Hz, 1H), 7.65 (dd, $J = 8.2, 1.4$ Hz, 1H), 7.47 (dd, $J = 7.3, 1.5$ Hz, 1H), 7.40 – 7.31 (m, 2H), 7.28 – 7.20 (m, 2H), 7.16 (d, $J = 1.9$ Hz, 3H), 6.96 (d, $J = 7.7$ Hz, 1H), 6.88 – 6.80 (m, 1H), 6.78 – 6.64 (m, 2H), 6.55 – 6.37 (m, 1H), 2.71 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 161.7, 155.5, 150.91, 149.0, 144.5, 142.5, 137.3, 136.1, 135.0, 134.3, 131.7, 131.5, 130.8, 130.7, 130.0, 129.8, 128.9, 128.8, 128.2, 128.0, 127.6, 127.2,

126.6, 125.8, 121.7, 119.0, 116.9, 24.4. **HRMS** (ESI) for $C_{30}H_{22}N_3O$ $[M+H]^+$ calcd: 440.1757; found: 440.1755.

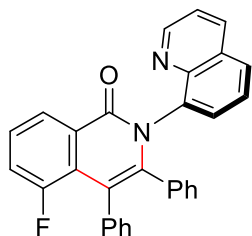
(R)-7-Fluoro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ta-C2)



Condition C, White solid, mp: 200-201 °C, 45.8 mg, 52% yield, $[\alpha]_D^{25} = +56.4$ ($c = 0.1$ in $CHCl_3$), 93% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 65:35 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 6.34 min, t_R

(minor) = 15.31 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.83 (d, $J = 2.6$ Hz, 1H), 8.14 (d, $J = 9.1$ Hz, 1H), 7.94 (d, $J = 8.1$ Hz, 1H), 7.55 (d, $J = 8.0$ Hz, 1H), 7.40 (d, $J = 7.0$ Hz, 1H), 7.28-7.06 (m, 9H), 6.88 (d, $J = 7.5$ Hz, 1H), 6.77-6.60 (m, 3H), 6.39 (t, $J = 7.4$ Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.94 (d, $J = 2.9$ Hz), 161.56 (d, $J = 247.5$ Hz), 150.9, 144.7, 141.3, 137.6, 136.4, 136.1, 134.9, 134.7, 131.8, 131.6, 130.9, 130.8, 129.8, 128.8, 128.3 (d, $J = 7.6$ Hz), 128.2, 128.0, 127.4, 127.3 (d, $J = 8.0$ Hz), 127.0, 126.8, 126.5, 125.8, 121.6, 121.1 (d, $J = 23.3$ Hz), 118.2, 113.4 (d, $J = 22.8$ Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -113.7. **HRMS** (ESI) for $C_{30}H_{20}FN_2O$ $[M+H]^+$ calcd: 443.1552; found: 443.1561.

(R)-5-Fluoro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ta-C6)

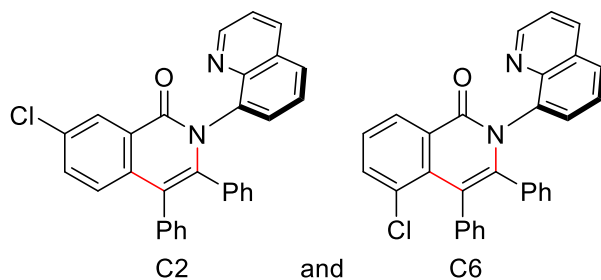


Condition C, White solid, mp: 222-223 °C, 38.1 mg, 43% yield, $[\alpha]_D^{25} = +82.2$ ($c = 0.1$ in $CHCl_3$), 95% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 65:35 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 7.15 min, t_R (minor)

= 17.05 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.92 (d, $J = 2.6$ Hz, 1H), 8.43 (d, $J = 7.9$ Hz, 1H), 8.03 (d, $J = 7.7$ Hz, 1H), 7.64 (d, $J = 8.1$ Hz, 1H), 7.48-7.28 (m, 5H), 7.24-7.07 (m, 5H), 6.93 (d, $J = 7.6$ Hz, 1H), 6.80 (t, $J = 7.5$ Hz, 1H), 6.69 (d, $J = 6.9$ Hz, 2H), 6.45 (t, $J = 7.5$ Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.8, 158.9 (d, $J = 256.0$ Hz), 150.9, 144.6, 143.4, 138.6 (d, $J = 3.4$ Hz), 137.5, 136.1, 134.5, 131.0 (d, $J = 2.8$ Hz), 131.0, 130.9, 129.9, 128.8 (d, $J = 2.6$ Hz), 127.9, 127.4, 127.3, 127.2, 126.9 (d, $J = 9.1$ Hz), 126.6, 126.4 (d, $J = 5.2$ Hz), 125.8, 124.7 (d, $J = 3.7$ Hz), 121.7, 119.6 (d, $J = 22.4$ Hz), 114.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -108.7. **HRMS** (ESI) for $C_{30}H_{20}FN_2O$ $[M+H]^+$ calcd: 443.1554; found: 443.1566.

(R)-7-Chloro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ua-C6)

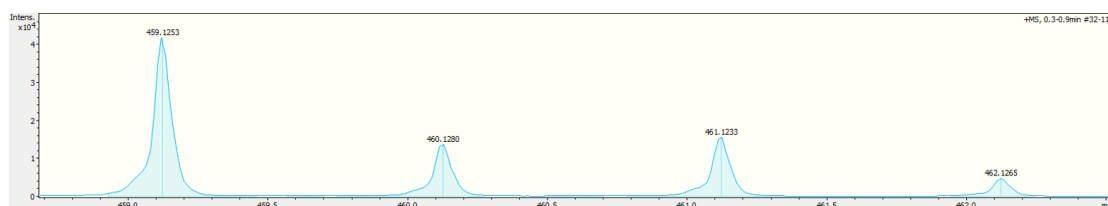
(R)-5-Chloro-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ua-C2)



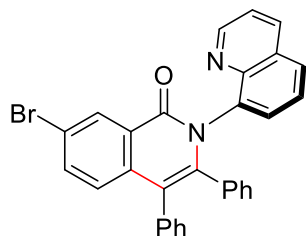
Condition C, White solid, mp: 238-239

°C, 85.5 mg, 93% yield, $[\alpha]_{\text{D}}^{25} = -4.9$ ($c = 0.1$ in CHCl_3), 94% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 65:35 v/v, flow

rate 1.0 mL/min, $\lambda = 220$ nm, 25 °C), t_{R} (major) = 8.68 min for major isomer, t_{R} (minor) = 31.37 min for major isomer. **^1H NMR** (400 MHz, CDCl_3) δ 8.89 (d, $J = 3.2$ Hz, 1.06H, C2 + C6), 8.61 (d, $J = 8.0$ Hz, 0.06H, C6), 8.55 (s, 1H, C2), 7.99 (d, $J = 8.0$ Hz, 1.06H, C2 + C6), 7.60 (d, $J = 8.0$ Hz, 1.06H, C2 + C6), 7.50-7.46 (m, 2.12H, C2 + C6), 7.39 (d, $J = 7.6$ Hz, 0.12H, C6), 7.34-7.30 (m, 2H, C2), 7.25-7.13 (m, 6.36H, C2 + C6), 6.96 (d, $J = 7.6$ Hz, 1.06H, C2 + C6), 6.83-6.67 (m, 3.12H, C2 + C6), 6.62 (d, $J = 7.6$ Hz, 0.06H, C6), 6.48-6.44 (m, 1H, C2), 6.39 (d, $J = 7.6$ Hz, 0.06H, C6). **^{13}C NMR** (101 MHz, CDCl_3) δ 162.0, 161.7, 150.8, 144.5, 143.8, 142.7, 142.3, 138.2, 137.4, 136.6, 136.3, 136.1, 136.0, 135.4, 134.7, 134.6, 132.8, 132.7, 132.3, 132.2, 131.7, 131.5, 130.9, 130.8, 130.7, 129.6, 128.8, 128.2, 128.0, 127.7, 127.5, 127.4, 127.2, 127.1, 127.0, 126.7, 126.6, 126.5, 126.2, 125.7, 121.6, 121.4, 118.0, 117.8. **HRMS** (ESI) for $\text{C}_{30}\text{H}_{20}\text{ClN}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 459.1259 (^{35}Cl) and 461.1243 (^{37}Cl); found: 459.1253 (^{35}Cl) and 461.1233 (^{37}Cl).



(R)-7-Bromo-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3va)

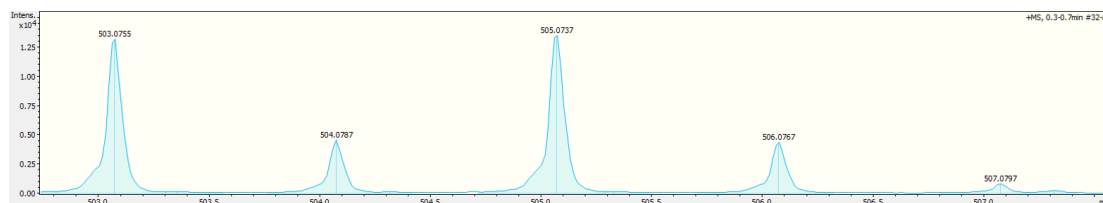


Condition C, White solid, mp: 241-242 °C, 96.8 mg, 96% yield,

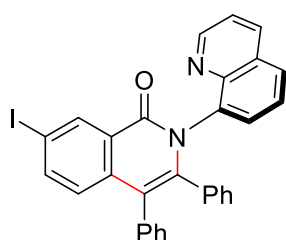
$[\alpha]_{\text{D}}^{25} = -22.23$ ($c = 0.1$ in CHCl_3), 94% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 65:35 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_{R} (major) = 9.86 min,

t_{R} (minor) = 39.44 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.88 (d, $J = 3.1$ Hz, 1H), 8.71 (s, 1H), 7.99 (d, $J = 8.1$ Hz, 1H), 7.62 (t, $J = 9.5$ Hz, 2H), 7.46 (d, $J = 7.1$ Hz, 1H), 7.33-7.30 (m, 2H), 7.24-7.08 (m, 6H), 6.96 (d, $J = 7.5$ Hz, 1H), 6.83-6.67 (m, 3H), 6.47 (d, $J = 7.5$ Hz, 1H). **^{13}C**

NMR (101 MHz, CDCl₃) δ 161.5, 150.8, 144.5, 142.5, 137.4, 136.9, 136.0, 135.5, 134.6, 131.7, 131.5, 130.9, 130.7, 130.6, 129.6, 128.8, 128.2, 128.0, 127.6, 127.4, 127.0, 126.8, 126.5, 125.7, 121.6, 120.6, 118.1. **HRMS** (ESI) for C₃₀H₂₀BrN₂O [M+H]⁺ calcd: 503.0754 (⁷⁹Br) and 505.0738 (⁸¹Br); found: 503.0755 (⁷⁹Br) and 505.0737 (⁸¹Br).



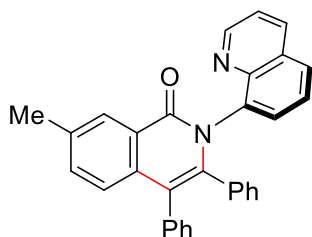
(R)-7-Iodo-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3wa)



Condition C, White solid, mp: 261-262 °C, 104.4 mg, 95% yield, $[\alpha]_D^{25} = -52.2$ (c = 0.1 in CHCl₃), 92% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 65:35 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 10.04 min, t_R

(minor) = 42.16 min. **¹H NMR** (400 MHz, CDCl₃) δ 8.96-8.84 (m, 2H), 8.00 (d, $J = 8.0$ Hz, 1H), 7.82 (d, $J = 7.8$ Hz, 1H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.46 (d, $J = 7.1$ Hz, 1H), 7.35-7.11 (m, 7H), 7.02 (d, $J = 8.6$ Hz, 1H), 6.95 (d, $J = 7.5$ Hz, 1H), 6.86-6.64 (m, 3H), 6.46 (t, $J = 7.5$ Hz, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 161.3, 150.8, 144.5, 142.7, 141.1, 137.4, 137.3, 137.2, 136.1, 136.0, 134.6, 131.7, 131.5, 130.7, 130.6, 129.6, 128.8, 128.7, 128.2, 128.0, 127.5, 127.4, 127.1, 127.0, 126.8, 126.5, 125.7, 121.6, 118.1, 91.8. **HRMS** (ESI) for C₃₀H₂₀IN₂O [M+H]⁺ calcd: 551.0615; found: 551.0619.

(R)-7-Methyl-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3xa)

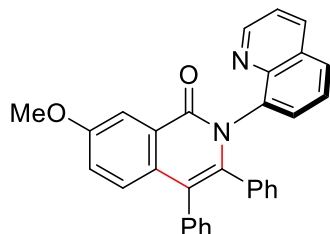


Condition C, White solid, mp: 263-264 °C, 75.4 mg, 86% yield, $[\alpha]_D^{25} = +35.37$ (c = 0.1 in CHCl₃), 96% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 75:25 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 8.47

min, t_R (minor) = 31.48 min. **¹H NMR** (400 MHz, CDCl₃) δ 8.90 (dd, $J = 4.0, 1.4$ Hz, 1H), 8.39 (s, 1H), 8.01 (d, $J = 8.1$ Hz, 1H), 7.62 (d, $J = 8.2$ Hz, 1H), 7.51-7.45 (m, 1H), 7.41 (d, $J = 8.4$ Hz, 1H), 7.36-7.31 (m, 2H), 7.24-7.12 (m, 6H), 6.96 (d, $J = 7.7$ Hz, 1H), 6.81 (t, $J = 7.5$ Hz, 1H), 6.73-6.67 (m, 2H), 6.46 (t, $J = 7.5$ Hz, 1H), 2.49 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃) δ 162.7, 150.8, 144.8, 141.0, 137.9, 136.8, 136.0, 135.9, 135.1, 134.0, 131.9, 139.8,

131.0, 130.9, 129.9, 128.8, 128.6, 128.1, 127.8, 127.2, 126.7, 126.5, 125.8, 125.7, 125.6, 121.5, 118.5, 21.5. **HRMS** (ESI) for $C_{31}H_{23}N_2O$ $[M+H]^+$ calcd: 439.1805; found: 439.1807.

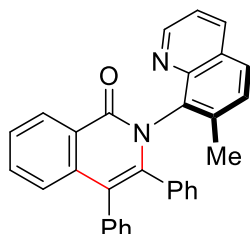
(R)-7-Methoxy-3,4-diphenyl-2-(quinolin-8-yl)isoquinolin-1(2H)-one (3ya)



Condition C, White solid, mp: 281-282 °C, 78.2 mg, 86% yield, $[\alpha]_D^{25} = +11.8$ ($c = 0.1$ in $CHCl_3$), 94% ee, determined by HPLC analysis (Chiralpak AS-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (minor)

= 7.62 min, t_R (major) = 12.02 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.91 (d, $J = 2.8$ Hz, 1H), 8.01 (d, $J = 7.3$ Hz, 2H), 7.61 (d, $J = 8.1$ Hz, 1H), 7.46 (d, $J = 7.1$ Hz, 1H), 7.36-7.11 (m, 9H), 6.96 (d, $J = 7.5$ Hz, 1H), 6.83-6.67 (m, 3H), 6.47 (t, $J = 7.5$ Hz, 1H), 3.90 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.4, 158.7, 150.8, 144.8, 139.6, 137.9, 136.7, 136.0, 135.0, 132.2, 131.8, 131.6, 131.0, 130.8, 129.9, 128.7, 128.6, 128.0, 127.8, 127.5, 127.2, 126.8, 126.7, 126.5, 125.8, 122.8, 121.5, 118.5, 108.2, 55.7. **HRMS** (ESI) for $C_{31}H_{23}N_2O_2$ $[M+H]^+$ calcd: 455.1754; found: 455.1760.

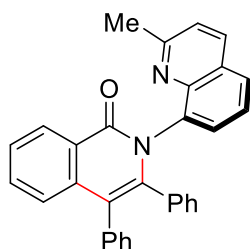
(R)-2-(7-Methylquinolin-8-yl)-3,4-diphenylisoquinolin-1(2H)-one (3za)



Condition C, White solid, mp: 290-291 °C, 37.4 mg, 41% yield, $[\alpha]_D^{25} = +132.25$ ($c = 0.1$ in $CHCl_3$), 93% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 7.39 min, t_R (minor)

= 10.39 min. **1H NMR** (400 MHz, $CDCl_3$) δ 8.89 (d, $J = 3.9$ Hz, 1H), 8.60 (d, $J = 7.9$ Hz, 1H), 7.99 (d, $J = 8.2$ Hz, 1H), 7.62-7.50 (m, 3H), 7.34-7.28 (m, 2H), 7.26-7.13 (m, 6H), 6.95 (d, $J = 7.5$ Hz, 1H), 6.80-6.70 (m, 3H), 6.46 (t, $J = 7.5$ Hz, 1H), 2.38 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.1, 150.7, 145.2, 142.1, 138.4, 137.6, 136.8, 135.9, 135.8, 134.7, 132.5, 132.0, 131.9, 130.0, 129.2, 129.0, 128.6, 128.2, 128.0, 127.8, 127.5, 127.2, 126.8, 126.7, 126.5, 126.3, 125.8, 120.8, 119.0, 19.1. **HRMS** (ESI) for $C_{31}H_{23}N_2O$ $[M+H]^+$ calcd: 439.1805; found: 439.1817.

(R)-2-(2-Methylquinolin-8-yl)-3,4-diphenylisoquinolin-1(2H)-one (3aaa)



Condition C, White solid, mp: 262-263 °C, 30.0 mg, 33% yield,

$[\alpha]_D^{25} = +38.25$ ($c = 0.1$ in CHCl_3), 88% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 8.68 min, t_R (minor) = 28.15 min. **^1H NMR** (400 MHz, CDCl_3) δ 8.59 (d, $J = 7.8$ Hz, 1H), 7.86 (d, $J = 8.4$ Hz, 1H), 7.62-7.49 (m, 4H), 7.30 (t, $J = 8.0$ Hz, 2H), 7.24-7.13 (m, 6H), 6.95 (d, $J = 7.6$ Hz, 1H), 6.79 (t, $J = 7.5$ Hz, 1H), 6.74 (d, $J = 7.7$ Hz, 1H), 6.69 (t, $J = 7.4$ Hz, 1H), 6.48 (t, $J = 7.6$ Hz, 1H), 2.65 (s, 3H). **^{13}C NMR** (101 MHz, CDCl_3) δ 163.0, 159.4, 144.2, 142.4, 138.2, 137.2, 136.8, 135.8, 135.1, 132.4, 132.0, 131.8, 130.8, 130.7, 130.4, 128.5, 128.3, 128.0, 127.2, 127.1, 126.8, 126.6, 126.5, 126.2, 125.8, 125.6, 124.8, 122.4, 118.3, 25.9. **HRMS** (ESI) for $\text{C}_{31}\text{H}_{23}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$ calcd: 439.1805; found: 439.1807.

4. X-Ray Crystallographic Structures of Products

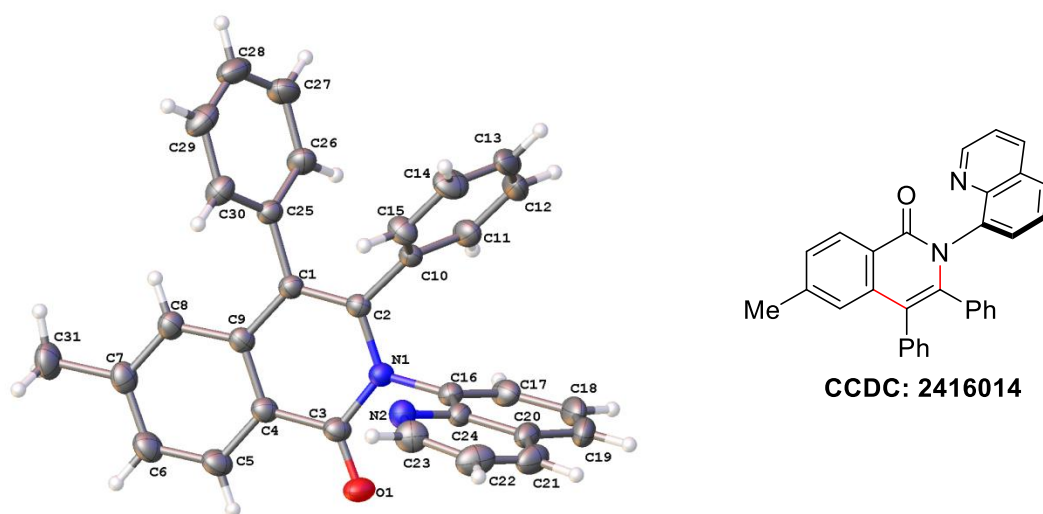


Figure S2. Single-crystal structure of **3aa** (CCDC: 2416014).

Table 9. Crystal data and structure refinement for **3aa**

Identification code	230327c_0m	
Empirical formula	C ₃₁ H ₂₂ N ₂ O	
Formula weight	438.50	
Temperature	200.0 K	
Wavelength	1.34139 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 6.6897(2) Å	= 90°.
	b = 8.5739(3) Å	= 90°.
	c = 40.2002(14) Å	= 90°.
Volume	2305.76(13) Å ³	
Z	4	
Density (calculated)	1.263 Mg/m ³	
Absorption coefficient	0.381 mm ⁻¹	
F(000)	920	
Crystal size	0.3 x 0.2 x 0.2 mm ³	
Theta range for data collection	4.879 to 72.378°.	
Index ranges	-9<=h<=8, -10<=k<=12, -56<=l<=55	
Reflections collected	51497	
Independent reflections	6644 [R(int) = 0.0412]	
Completeness to theta = 53.594°	95.1 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7536 and 0.6360
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6644 / 0 / 309
Goodness-of-fit on F^2	1.164
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0449$, $wR2 = 0.1272$
R indices (all data)	$R1 = 0.0451$, $wR2 = 0.1274$
Absolute structure parameter	0.03(5)
Extinction coefficient	0.011(2)
Largest diff. peak and hole	0.260 and -0.217 e. \AA^{-3}

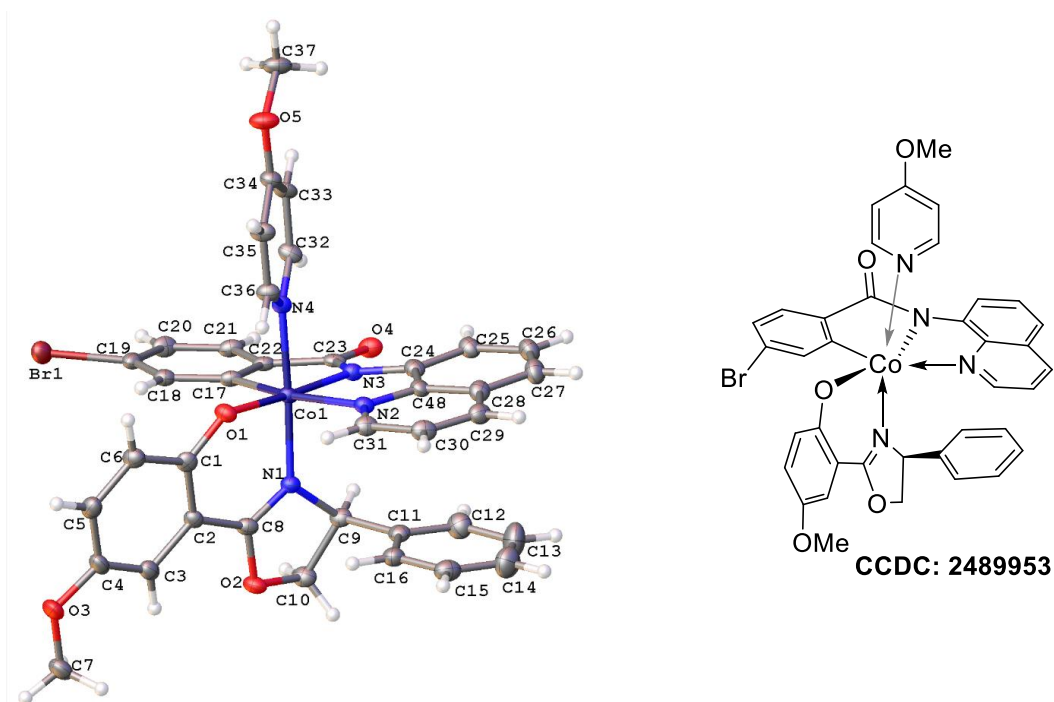


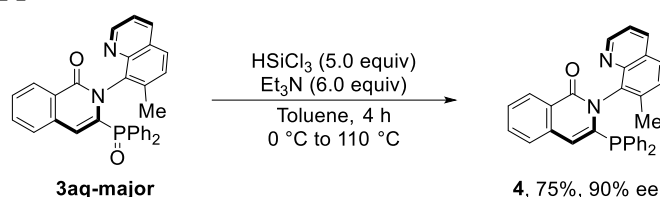
Figure S3. Single-crystal structure of [Co]-1 (CCDC: 2489953).

Table 10. Crystal data and structure refinement for [Co]-1

Identification code	t	
Empirical formula	$C_{41}H_{37}BrCoN_4O_5$	
Formula weight	804.58	
Temperature	100(2) K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	$a = 13.4639(6)$ Å	$a = 90^\circ$.
	$b = 33.6616(14)$ Å	$b =$
	$109.5370(10)^\circ$.	
	$c = 17.1903(7)$ Å	$g = 90^\circ$.
Volume	$7342.4(5)$ Å ³	
Z	8	
Density (calculated)	1.456 Mg/m ³	
Absorption coefficient	3.712 mm ⁻¹	
F(000)	3304	
Crystal size	$0.150 \times 0.120 \times 0.100$ mm ³	

Theta range for data collection	2.284 to 57.142°.
Index ranges	-16<=h<=16, -42<=k<=42, -21<=l<=21
Reflections collected	236844
Independent reflections	29970 [R(int) = 0.0528]
Completeness to theta = 53.594°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7512 and 0.6311
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	29970 / 0 / 1882
Goodness-of-fit on F ²	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0376, wR2 = 0.0981
R indices (all data)	R1 = 0.0389, wR2 = 0.0988
Absolute structure parameter	0.0056(12)
Extinction coefficient	n/a
Largest diff. peak and hole	1.303 and -1.323 e.Å ⁻³

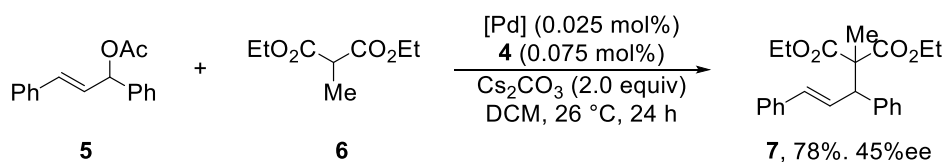
5. Synthetic application



Procedure for synthesis of 4: According to the reported literature,^[6] solution of **3aq-major** (48.6 mg, 0.1 mmol) in toluene (1 mL) was frozen using an EtOH/liquid nitrogen bath, to which trichlorosilane (47.4 mg, 0.5 mmol) and triethylamine (42.5 mg, 0.6 mmol) were added. The mixture was stirred at 110 °C under nitrogen for 4 h. After cooling to room temperature, a saturated aqueous solution of NaHCO₃ (1 mL) was added, and the mixture was stirred for 5 min. The mixture was filtered through a pad of alumina and evaporated in vacuo to give the crude product. Purified by flash chromatography (hexane/EtOAc= 3:1) to afford the desired product **4**.

(*R*)-3-(Diphenylphosphanyl)-2-(7-methylquinolin-8-yl)isoquinolin-1(2*H*)-one (**4**)

Yellow solid, mp: 220-221 °C, 35.3 mg, 75% yield, $[\alpha]_D^{25} = -78.0$ ($c = 0.1$ in CHCl₃), 90% ee, determined by HPLC analysis (Chiralpak AD-H column, hexane/*i*-PrOH, 80:20 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_R (major) = 8.39 min, t_R (minor) = 17.01 min. ¹H NMR (400 MHz, CDCl₃) δ 8.58 (d, $J = 3.0$ Hz, 1H), 8.43 (d, $J = 8.0$ Hz, 1H), 8.05 (d, $J = 7.9$ Hz, 1H), 7.81 (d, $J = 8.4$ Hz, 1H), 7.70-7.60 (m, 1H), 7.51-7.47 (m, 1H), 7.44-7.32 (m, 5H), 7.30-7.26 (m, 1H), 7.25-7.07 (m, 7H), 6.39 (s, 1H), 2.06 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 162.8 (d, $J = 1.7$ Hz), 150.8, 145.8 (d, $J = 11.1$ Hz), 145.1 (d, $J = 2.8$ Hz), 139.4 (d, $J = 3.1$ Hz), 136.3 (d, $J = 140.5$ Hz), 135.1 (d, $J = 4.6$ Hz), 134.7, 134.5, 134.0 (d, $J = 10.8$ Hz), 134.0, 133.8, 133.6 (d, $J = 10.1$ Hz), 132.2, 129.7, 129.0, 129.0, 128.8, 128.8, 128.7, 128.5, 128.3, 128.2, 127.2, 126.7 (d, $J = 115.8$ Hz), 126.4, 120.7, 114.5, 18.56 (d, $J = 4.4$ Hz). ³¹P NMR (162 MHz, CDCl₃) δ -12.2. HRMS (ESI) for C₃₁H₂₄N₂OP [M+H]⁺ calcd: 471.1621; found: 471.1610.



Procedure for synthesis of 7: According to the reported literature^[7], a mixture of [PdCl(η^3 -C₃H₅)]₂ (0.0025 mmol, 0.92 mg), ligand **4** (0.0075 mmol, 3.4 mg), and Cs₂CO₃ (0.2

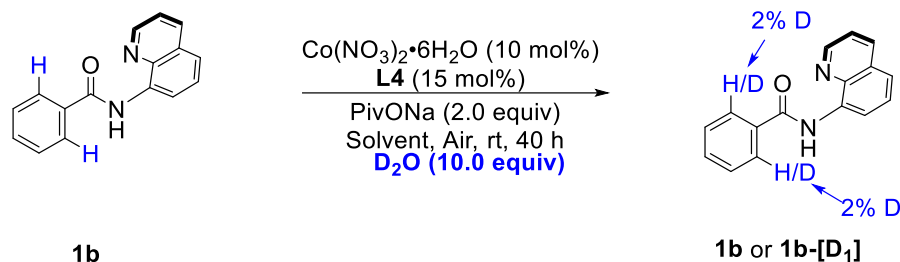
mmol, 65.2 mg) in dichloromethane (0.5 mL) was stirred for 30 min at room temperature. 1,3-Diphenyl-2-propenyl acetate **5** (0.1 mmol, 25.2 mg), diethyl 2-methylmalonate **6** (0.2 mmol, 34 μ l) were added with additional dichloromethane (1.0 mL). The resulting mixture was stirred for 24 h at 26 °C, and passed through a pad of silica gel with EtOAc, and the solvent removed under vacuum. The residue was chromatographed on silica gel with EtOAc/hexane = 1/4 to afford the product **7**.

Diethyl (E)-2-(1,3-diphenylallyl)-2-methylmalonate (7)

colorless oil, 28.6 mg, 78% yield, $[\alpha]_{\text{D}}^{25} = -15.8$ ($c = 0.1$ in CHCl_3), 45% ee, determined by HPLC analysis (Chiralpak IG-H column, hexane/*i*-PrOH, 95:5 v/v, flow rate 1.0 mL/min, $\lambda = 254$ nm, 25 °C), t_{R} (minor) = 11.43 min, t_{R} (major) = 14.50 min. **^1H NMR** (400 MHz, CDCl_3) δ 7.34-7.25 (m, 8H), 7.24-7.19 (m, 2H), 6.70 (dd, $J = 15.7, 8.9$ Hz, 1H), 6.44 (d, $J = 15.7$ Hz, 1H), 4.29 (d, $J = 8.9$ Hz, 1H), 4.22-4.13 (m, 2H), 4.08 (q, $J = 7.1$ Hz, 2H), 1.47 (s, 3H), 1.22 (t, $J = 7.1$ Hz, 3H), 1.16 (t, $J = 7.1$ Hz, 3H). **^{13}C NMR** (101 MHz, CDCl_3) δ 171.3, 171.1, 139.6, 137.5, 132.7, 129.8, 129.0, 128.6, 128.3, 127.4, 127.2, 126.5, 61.5, 61.4, 59.0, 53.9, 18.9, 14.2, 14.1. **HRMS** (ESI) for $\text{C}_{23}\text{H}_{26}\text{NaO}_4$ $[\text{M}+\text{H}]^+$ calcd: 389.1723; found: 389.1713.

6. Mechanistic studies

6.1. H/D exchange experiments



Under air, $\text{Co(NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.01 mmol, 2.91 mg), **L4** (0.015 mmol, 4.04 mg) and HFIP (1 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, **1b** (0.1 mmol), PivONa (24.8 mg, 0.4 mmol) and D_2O (20 mg, 1 mmol) were added to the resulting mixture. The mixture was stirred at room temperature for approximately 40 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (10:1) as eluent. ^1H NMR analysis showed that the D contents in the recovered substrate **1b** was 2%.

6.2. Parallel KIE experiments

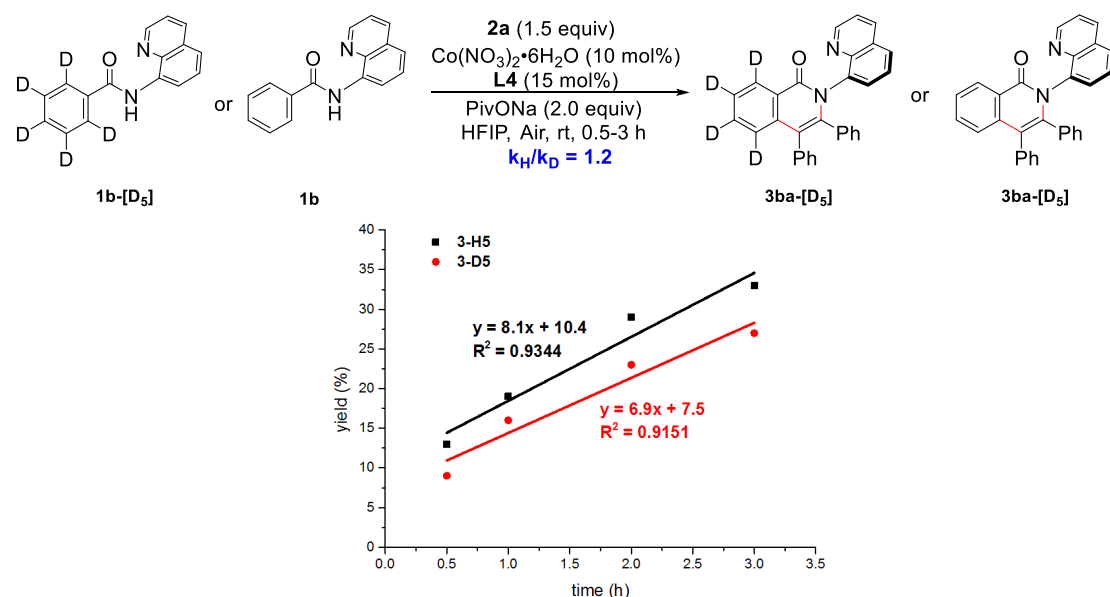
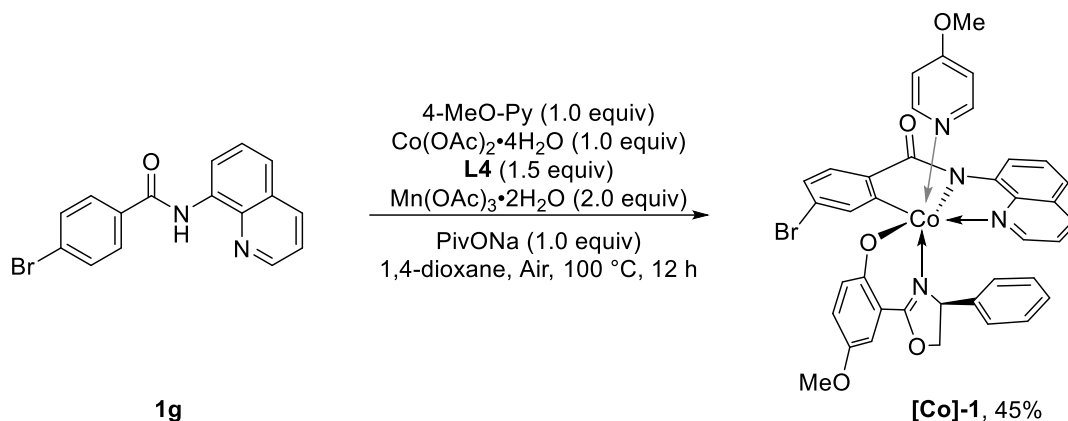


Figure S4 Parallel KIE experiments

Under air, $\text{Co(NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.01 mmol, 2.91 mg), **L4** (0.015 mmol, 4.04 mg) and HFIP (1 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, **1b** (0.1 mmol) or $[\text{D}_5]\text{-1b}$ (0.1 mmol), alkyne **2a** (26.7 mg, 0.15 mmol) and PivONa (24.8 mg, 0.2 mmol) were added to the resulting mixture. The mixture was stirred at room temperature for

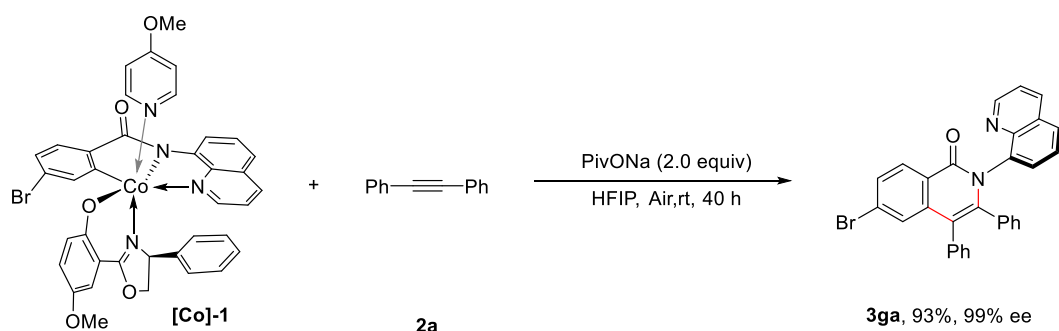
approximately 0.5 h, 1.0 h, 2.0 h, 3.0 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent. The KIE was determined as $k_H/k_D = 8.1/6.9 = 1.2$.

6.3. [Co]-1 via Asymmetric C-H Cleavage



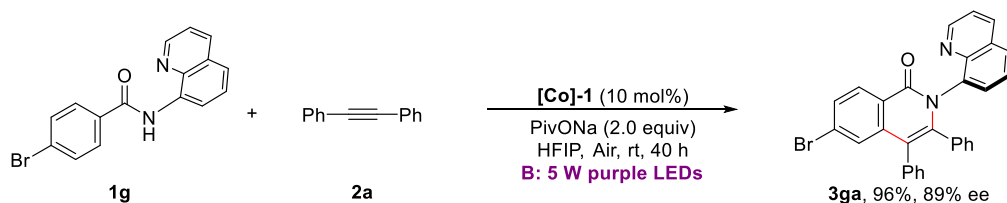
Procedure for synthesis of [Co]-1⁽²⁾: A dried vial equipped with a stirring bar was charged with **1g** (327.0 mg, 1.0 mmol), Co(OAc)₂•4H₂O (249.1 mg, 1.0 equiv), **L4** (404.0 mg, 1.5 equiv), 4-methoxypyridine (109.1 mg, 1.0 equiv), NaOPiv (124.8 mg, 1.0 equiv), Mn(OAc)₃•3H₂O (536.2 mg, 2.0 equiv) and dioxane (15 mL). Then, the vial was instantly placed in a heating block set at 100 °C under air for 12 h. Then, the reaction mixture was cooled to room temperature. The mixture was diluted with DCM and concentrated in vacuo. Then the mixture was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (1:3) as eluent to give the desired **[Co]-1** (343 mg, 45%, yellow solid). **¹H NMR** (400 MHz, CDCl₃) δ 9.24 (dd, *J* = 4.6, 1.3 Hz, 1H), 9.02 (d, *J* = 7.5 Hz, 1H), 7.85 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.75 (dd, *J* = 4.6, 2.6 Hz, 3H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.43 (dd, *J* = 8.3, 4.6 Hz, 1H), 7.36 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.33-7.27 (m, 1H), 7.15 (d, *J* = 9.2 Hz, 1H), 7.07 (dd, *J* = 9.2, 3.2 Hz, 1H), 6.98 (d, *J* = 7.9 Hz, 1H), 6.95 (d, *J* = 3.2 Hz, 1H), 6.63-6.55 (m, 1H), 6.51-6.44 (m, 2H), 6.32 (d, *J* = 7.3 Hz, 2H), 6.22 (d, *J* = 7.3 Hz, 2H), 4.30 (dd, *J* = 9.3, 3.2 Hz, 1H), 4.06-3.98 (m, 1H), 3.80-3.74 (m, 4H), 3.58 (s, 3H). **¹³C NMR** (101 MHz, CDCl₃) δ 175.6, 169.4, 166.2, 165.2, 163.5, 151.5, 148.8, 147.6, 146.8, 146.6, 146.5, 139.4, 137.3, 136.9, 129.2, 128.6, 127.8, 127.4, 127.2, 126.7, 125.0, 124.4, 124.2, 123.7, 121.8, 121.3, 118.4, 109.9, 109.7, 107.6, 74.8, 66.1, 56.1, 55.5. **HRMS** (ESI) for C₂₈H₂₈NO₄ [M+H]⁺ calcd: 761.0804; found: 761.0821.

6.4. Stoichiometric Reaction of [Co]-1



Under air, **[Co]-1** (0.1 mmol, 76.1 mg), alkyne **2a** (0.15 mmol), PivONa (25.0 mg, 0.2 mmol), and HFIP (1 mL) were added to a 10 mL vial. The mixture was stirred at room temperature for approximately 40 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent to give corresponding product **3ga** in 93% isolated yield with 99% ee.

6.5. [Co]-1 as a catalyst



Under air, **[Co]-1** (0.01 mmol, 7.61 mg), substrate **1g** (0.2 mmol), alkyne **2a** (0.15 mmol), PivONa (25.0 mg, 0.2 mmol), and HFIP (1 mL) were added to a 10 mL vial. The mixture was stirred at room temperature under 5 W purple LEDs for approximately 40 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent to give corresponding product **3ga** in 96% isolated yield with 89% ee.

6.6. Probing involvement of singlet oxygen by EPR studies

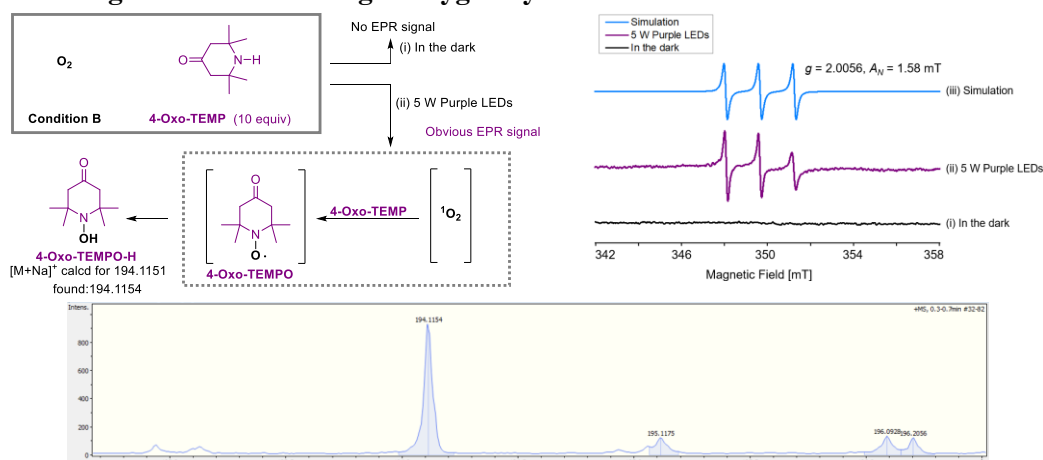
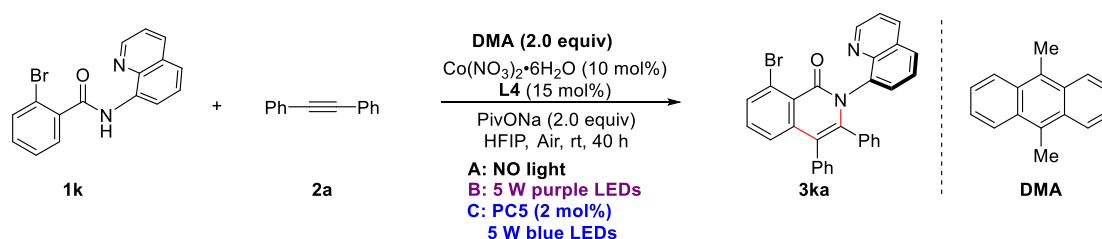


Figure S5 EPR studies and and HRMS spectra

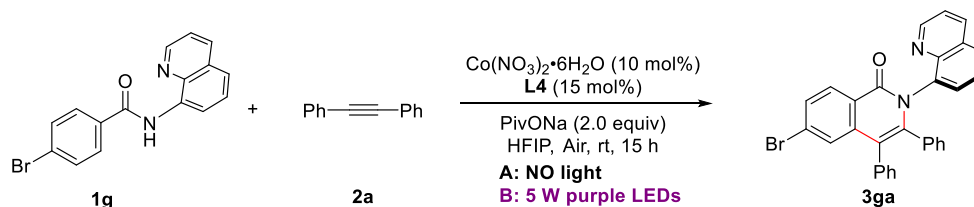
Under air, $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.01 mmol, 2.91 mg), **L4** (0.015 mmol, 4.04 mg) and HFIP (1 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, corresponding substrate **1k** (0.1 mmol), alkyne **2a** (0.15 mmol, 26.7 mg), PivONa (24.8 mg, 0.2 mmol) and 4-Oxo-TEMP (155.2 mg, 1.0 mmol) were added to the resulting mixture. The mixture was stirred at room temperature under 5 W purple LEDs or in dark for 10 min. 20 μL of the mixture was transferred to a capillary tube, the tube was charged into a EPR tube and then the mixture was measured in-situ at rt. As shown in Figure S5, no signal was observed in the dark (black trace). When the mixture was irradiated with 5 W Purple LEDs for 10 min, an obvious triplet signal was recorded (purple trace).

6.7. Singlet oxygen quenching experiments



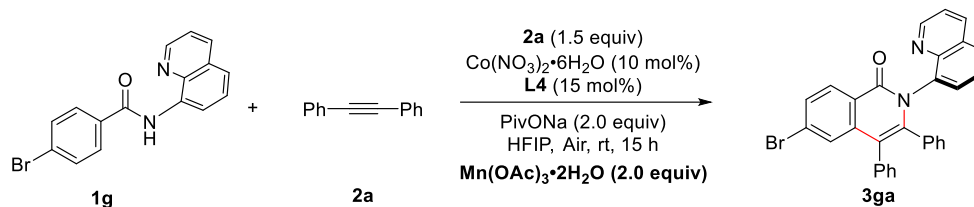
Under air, $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.01 mmol, 2.91 mg), **L4** (0.015 mmol, 4.04 mg) and HFIP (1 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, corresponding substrate **1k** (0.1 mmol), alkyne **2a** (0.15 mmol, 26.7 mg), PivONa (24.8 mg, 0.2 mmol) and DMA (22.4 mg, 0.2 mmol) were added to the resulting mixture. The mixture was stirred at room temperature under the corresponding conditions for approximately 40 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent to give corresponding product **3ka**.

6.8. Oxidant control



Under air, $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.01 mmol, 2.91 mg), **L4** (0.015 mmol, 4.04 mg) and HFIP (1 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, corresponding substrate **1g** (0.1 mmol), alkyne **2a** (0.15 mmol, 26.7 mg), and PivONa (24.8 mg, 0.2 mmol) were added to the resulting mixture. The mixture was stirred at room temperature or under 5

W purple LEDs for approximately 15 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent to give corresponding product **3ga**.



Under air, Co(NO₃)₂•6H₂O (0.01 mmol, 2.91 mg), **L4** (0.015 mmol, 4.04 mg) and HFIP (1 mL) were added to a 10 mL vial. After stirring at room temperature for 2 h, corresponding substrate **1g** (0.1 mmol), alkyne **2a** (0.15 mmol, 26.7 mg), PivONa (24.8 mg, 0.2 mmol) and Mn(OAc)₃•2H₂O (53.6 mg, 0.2 mmol) were added to the resulting mixture. The mixture was stirred at room temperature for approximately 15 h. The concentrated reaction residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (3:1-1.5:1) as eluent to give corresponding product **3ga**.

6.9. UV-Vis Absorption Spectra

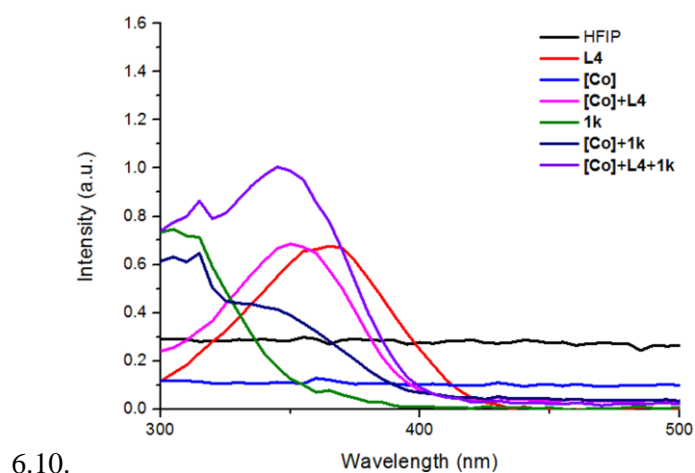


Figure S6 UV-VIS absorption spectra of the related component recorded in HFIP

UV-Vis spectra of the individual component were recorded, including HFIP, **L4**, $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, substrate **1k**, **[Co]+L4** (generated in situ by stirring a 1:1.5 mixture of $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ and **L4**), **[Co]+1k** (generated in situ by stirring a 1:1 mixture of $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ and **1k**), **[Co]+L4+1k** (generated in situ by stirring a 1:1.5:1 mixture of $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, **L4** and substrate **1k**). All of the samples were prepared as a 0.1 mM solution and used freshly for the measurement.

6.10. Luminescence quenching experiments

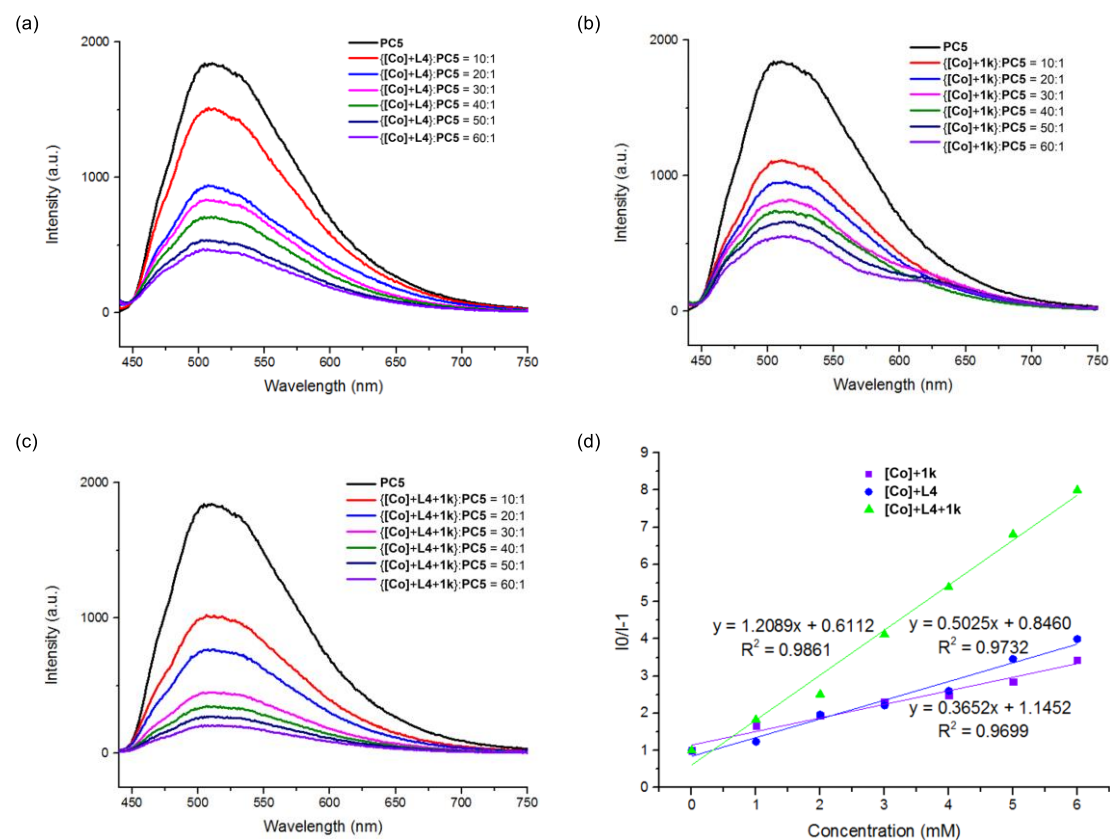
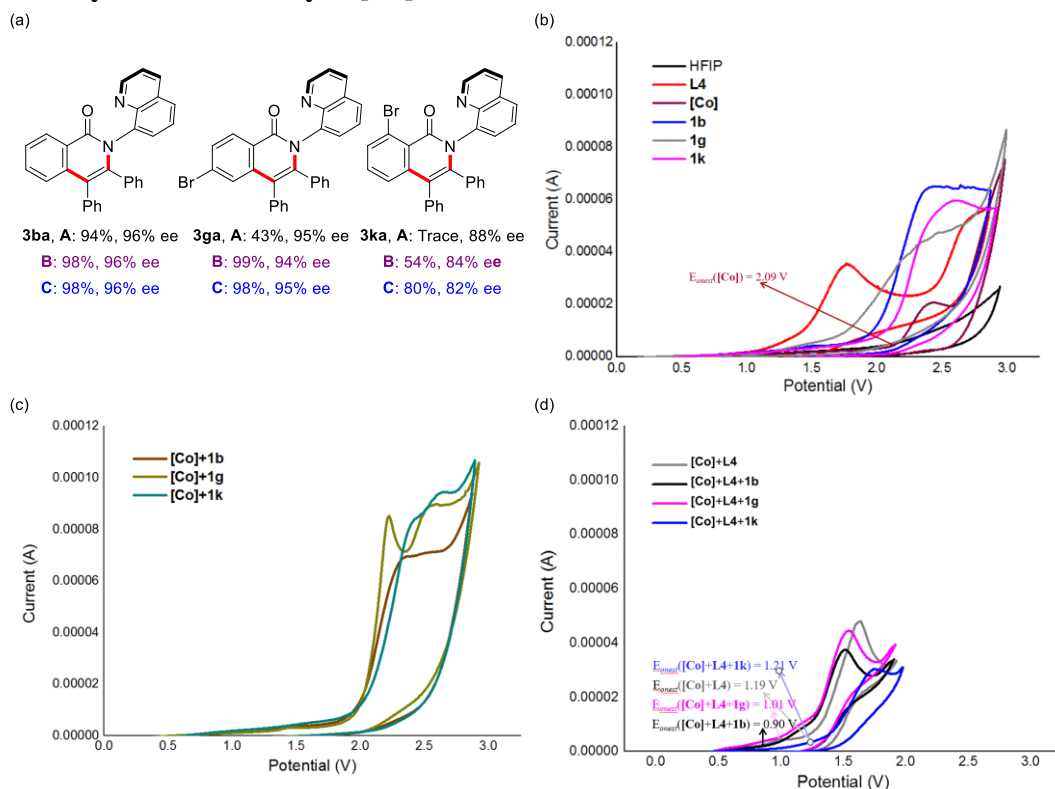


Figure S7 Stern-Volmer plot for the emission quenching of **PC5** by various concentrations of quencher (a) Photocatalyst emission quenching by **[Co]+L4**. (b) Photocatalyst emission quenching by **[Co]+1k**. (c) Photocatalyst emission quenching by **[Co]+L4+1k**. (d) Quenching Efficiency Plot. Fluorescence spectra was collected on Agilent Fluorescence Spectrophotometer G9800AS24 for all experiments. All **PC5** solutions were excited at 426 nm and the emission intensity was collected at 505 nm. In a typical experiment, the emission chromatogram of a 1×10^{-4} M solution of **PC5** in HFIP was collected. **[Co]**, $\text{Co}(\text{NO}_3)_2 \cdot \text{H}_2\text{O}$.

Fluorescence quenching experiments showed that **Co+L4+1k** had a more significant quenching effect on the **PC5** as compared to **Co+ 1k** and **Co+L4**.

6.11. Cyclic Voltammetry of [Co]+L4+1



1.1

Figure S8 Cyclic Voltammetry of [Co]+L4+1

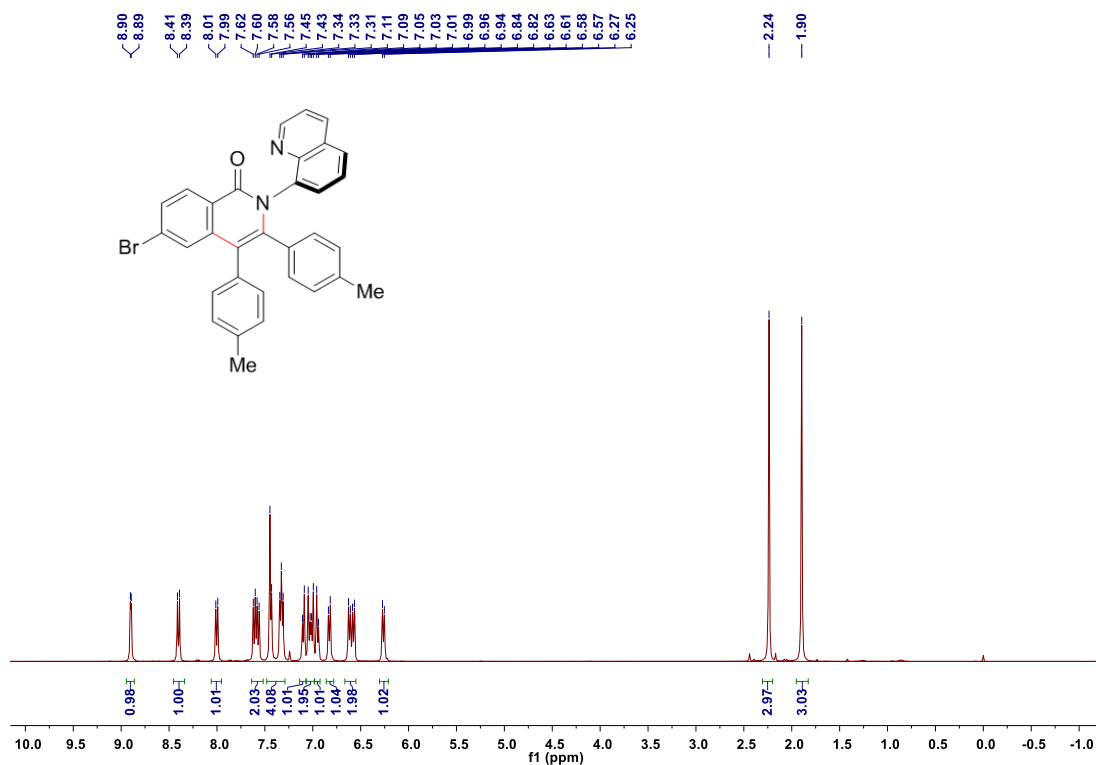
(a) The electrochemical properties of representative substrates were examined by cyclic voltammetry. (b) Cyclic Voltammetry of single component. (c) Cyclic Voltammetry of [Co]+1. (d) Cyclic Voltammetry of [Co]+L4+1. Cyclic voltammetry (CV) was taken using a CHI660D potentiostat. CV measurement was carried out in 0.1 M of $n\text{Bu}_4\text{NPF}_6/\text{HFIP}$ at a scan rate of 100 mV/s. The working electrode is a glassy carbon, the counter electrode is a Pt wire, and the reference electrode is a saturated calomel electrode (SCE).

7. Additional References

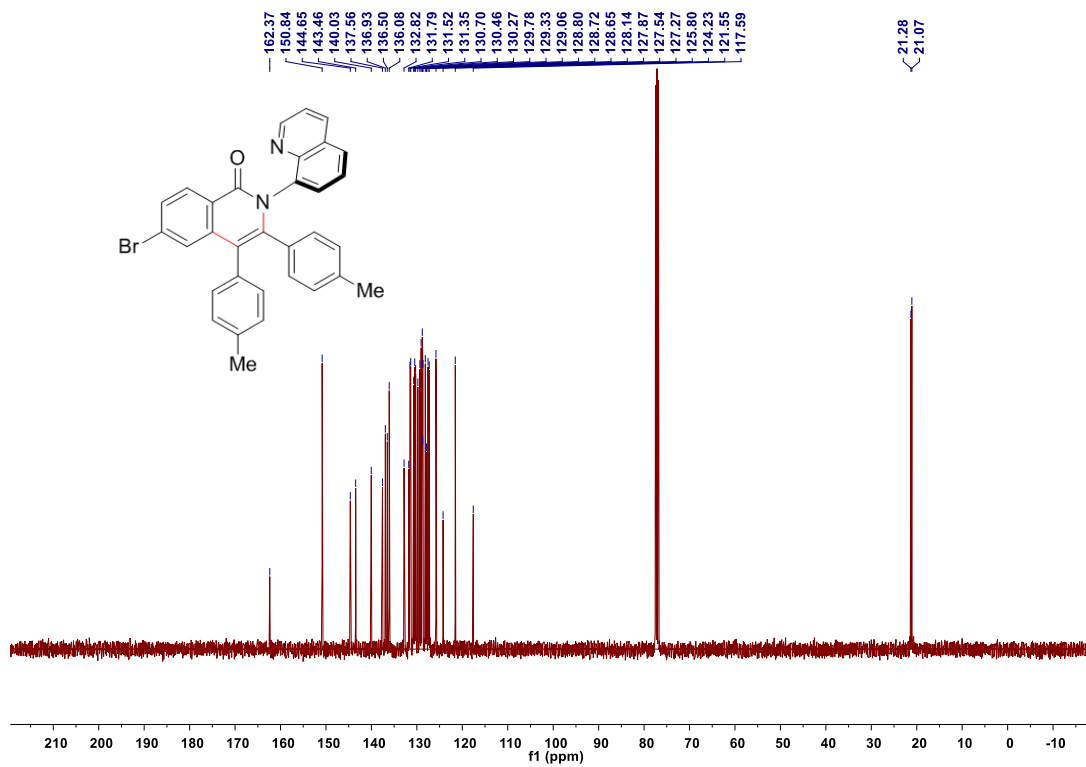
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8. Copies of NMR Spectra

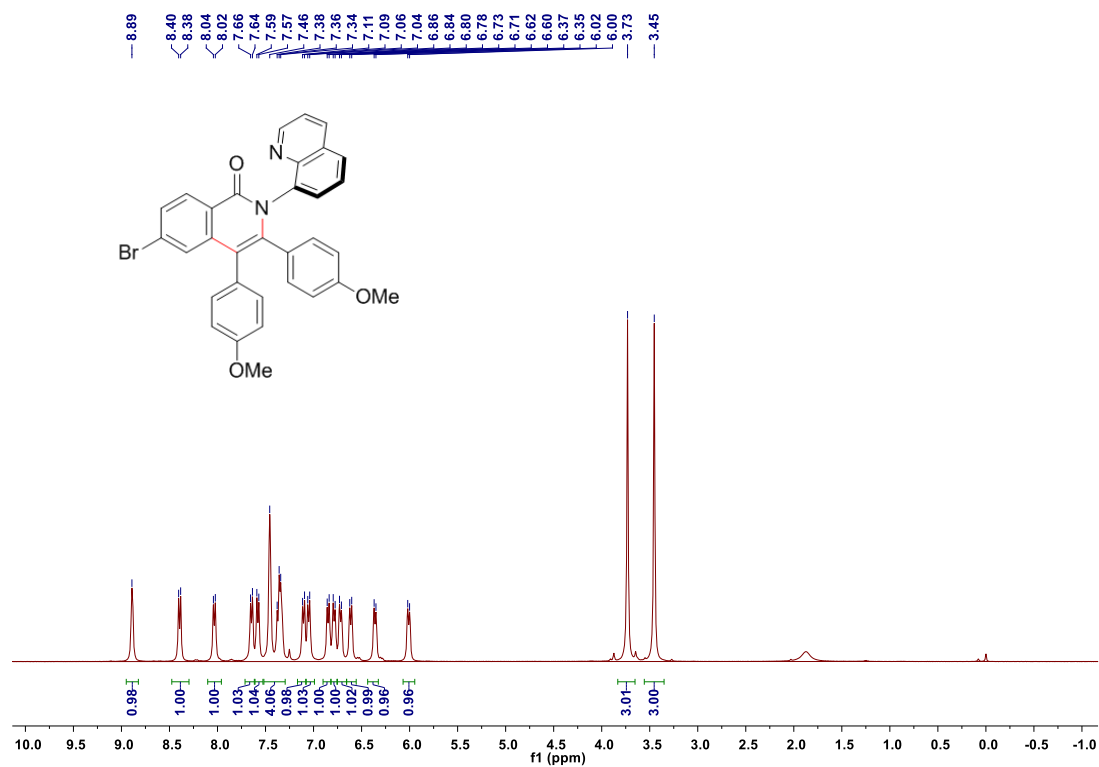
^1H NMR Spectrum of **3ab**



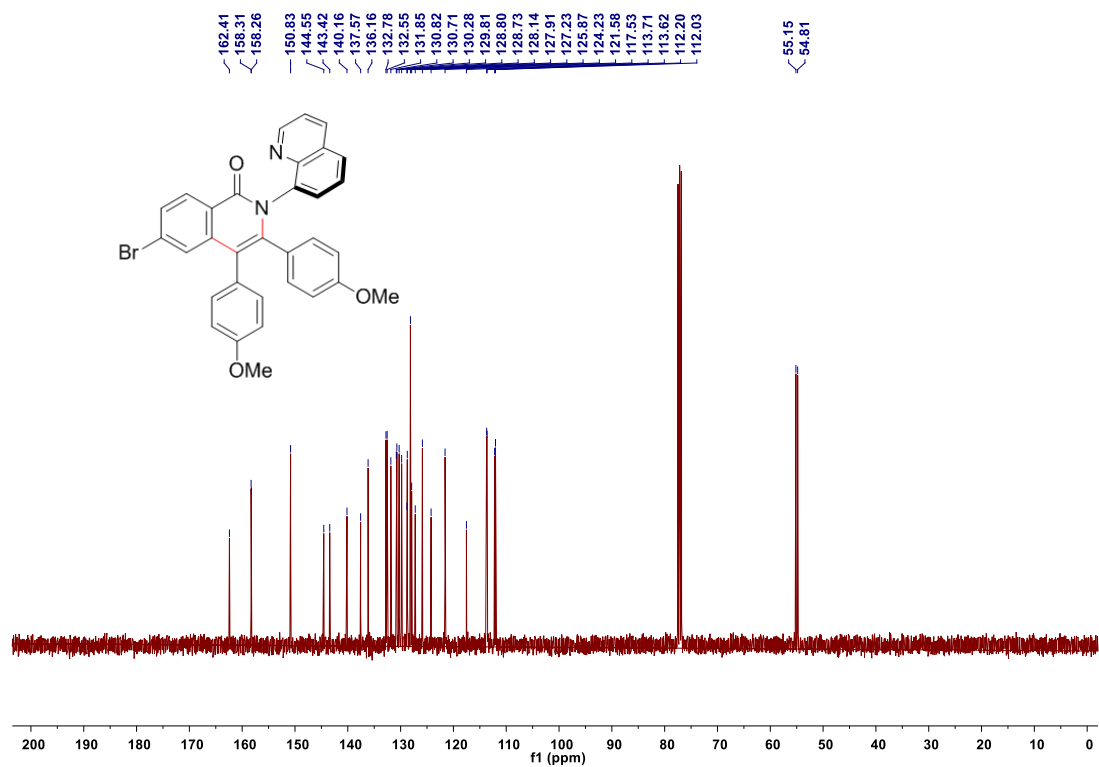
^{13}C NMR Spectrum of **3ab**



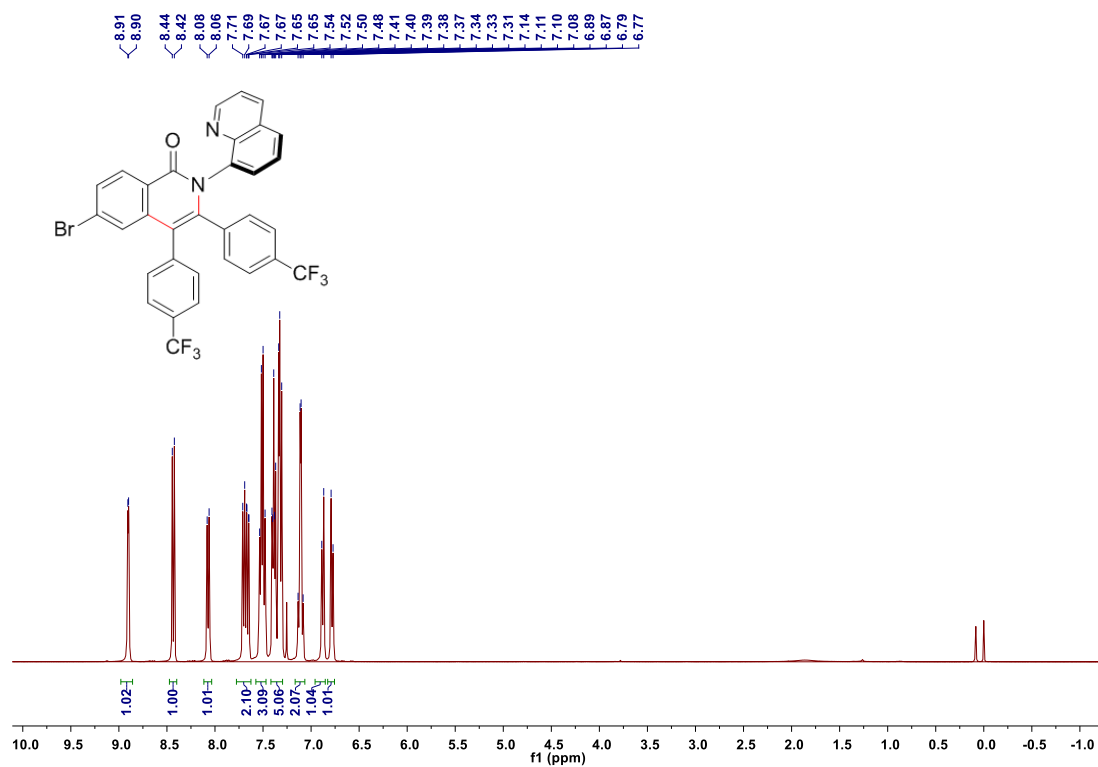
¹H NMR Spectrum of **3ac**



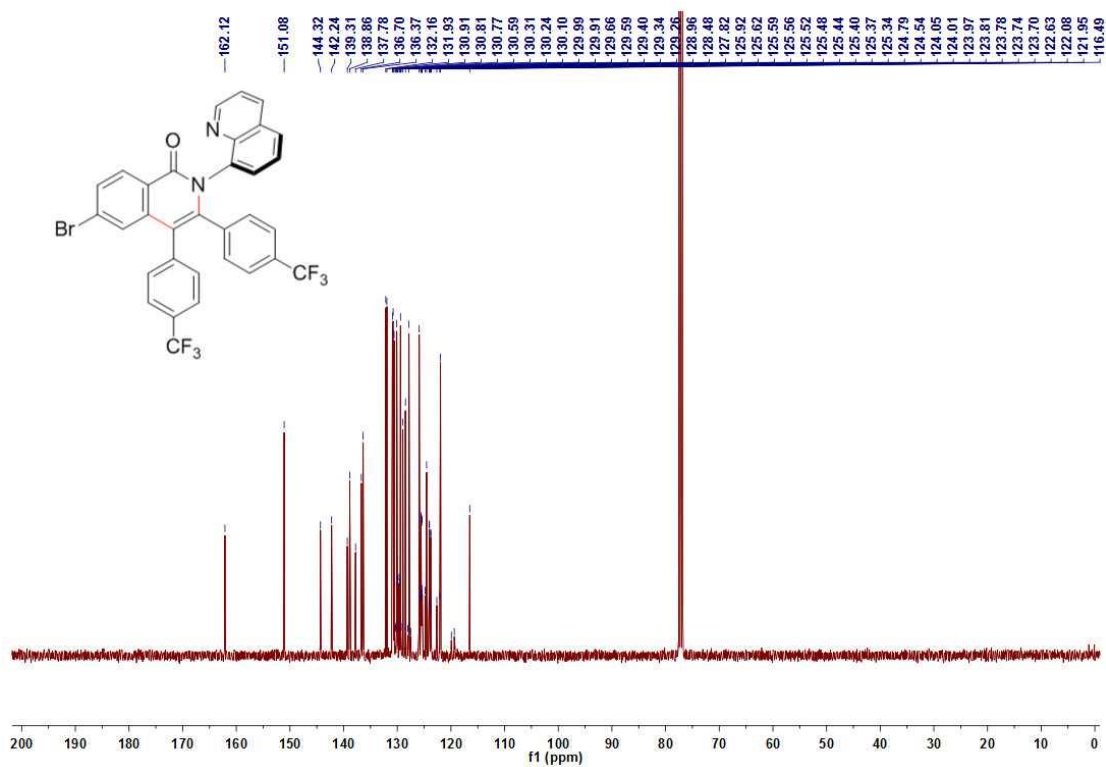
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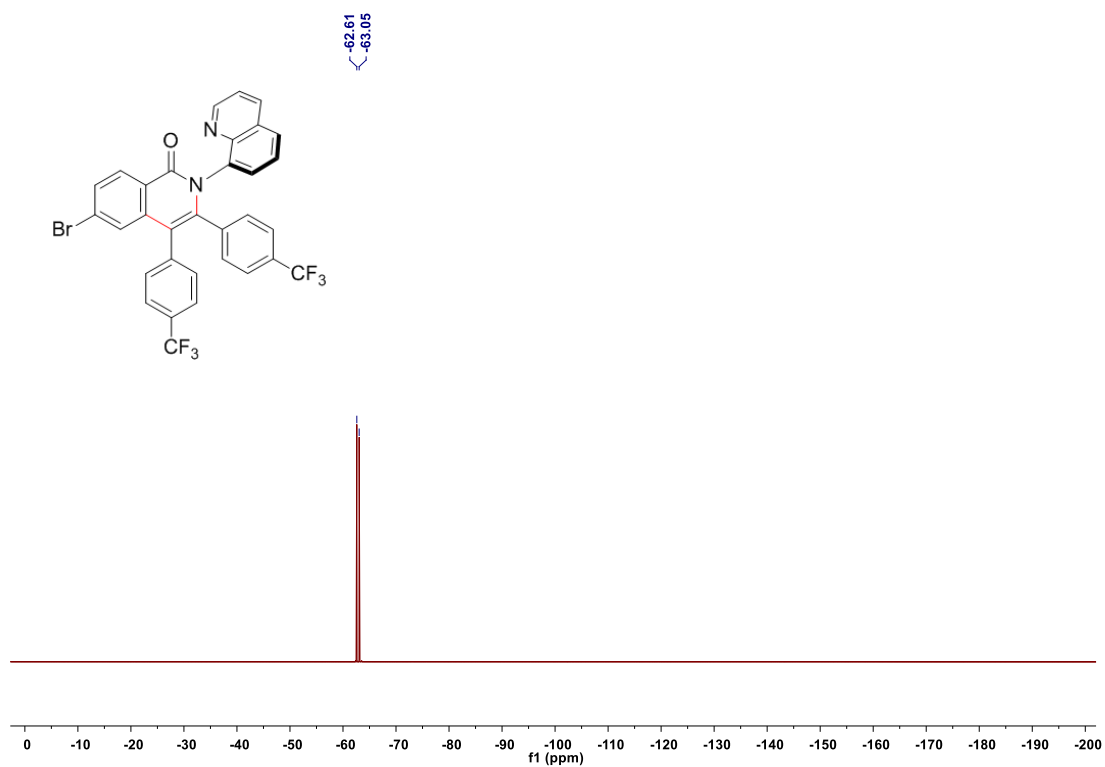
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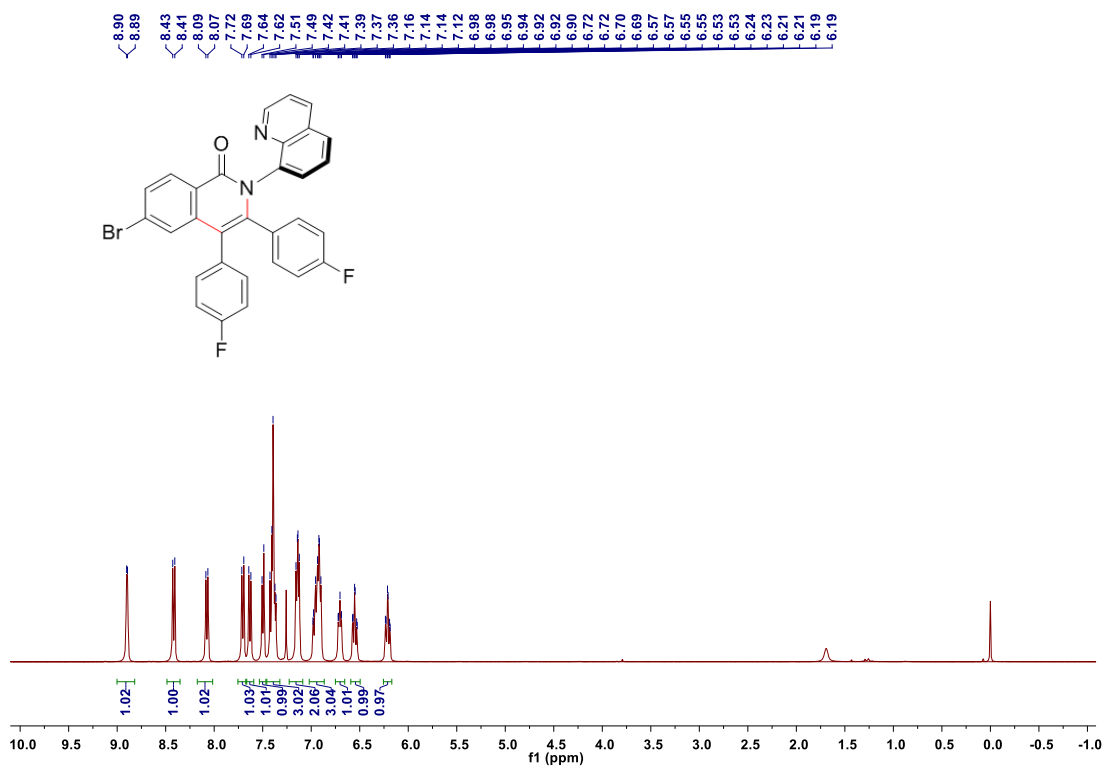
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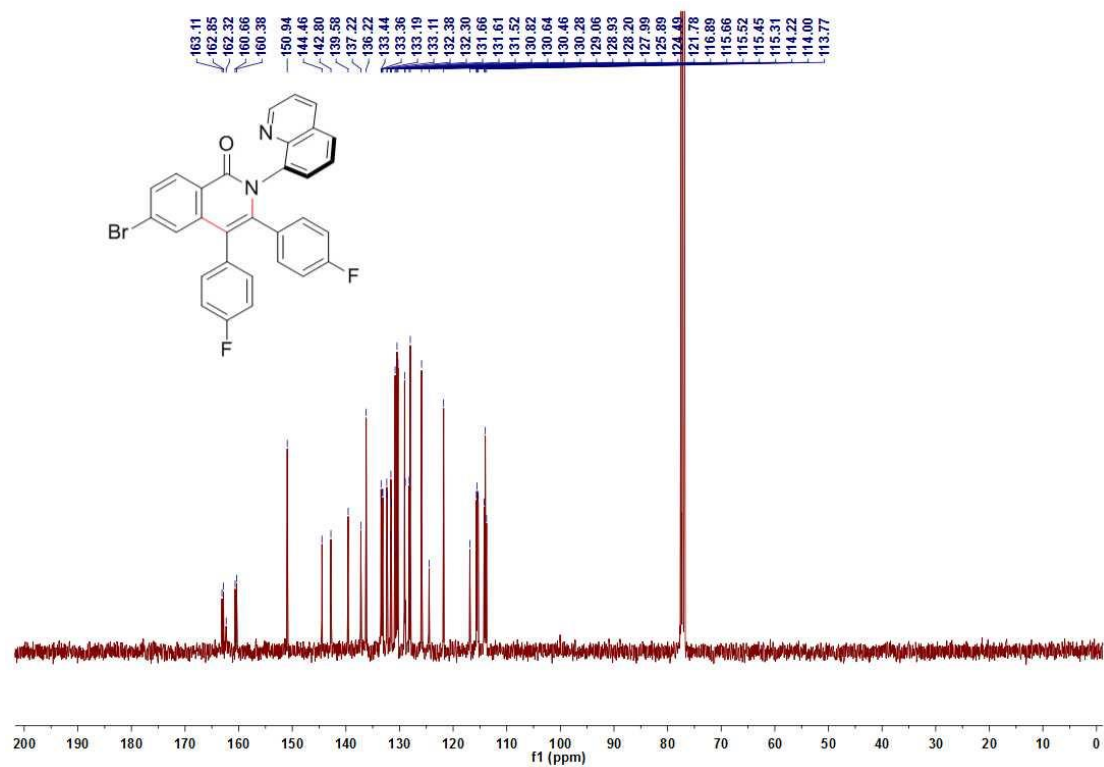
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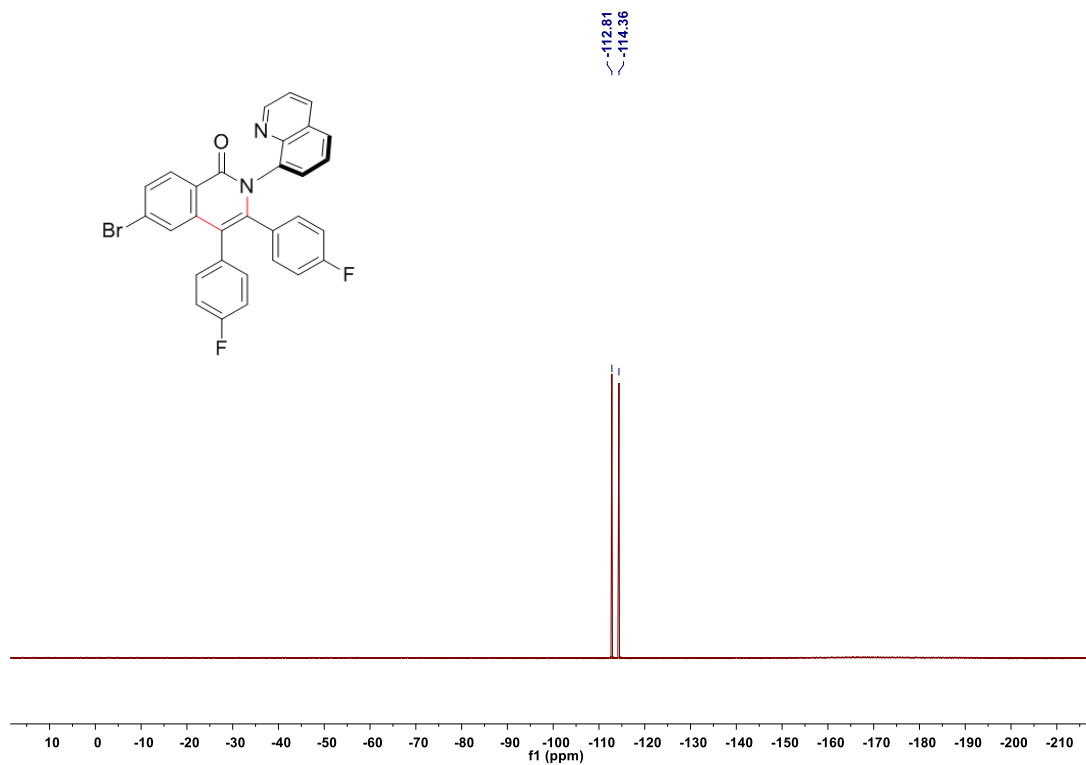
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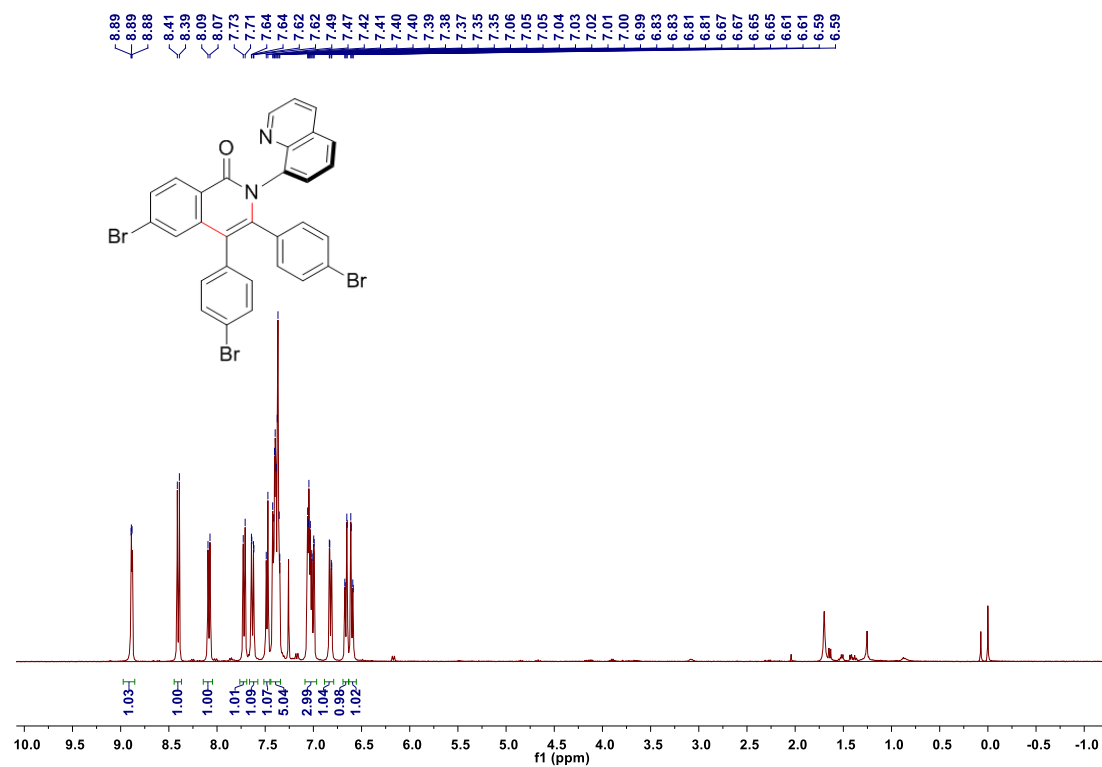
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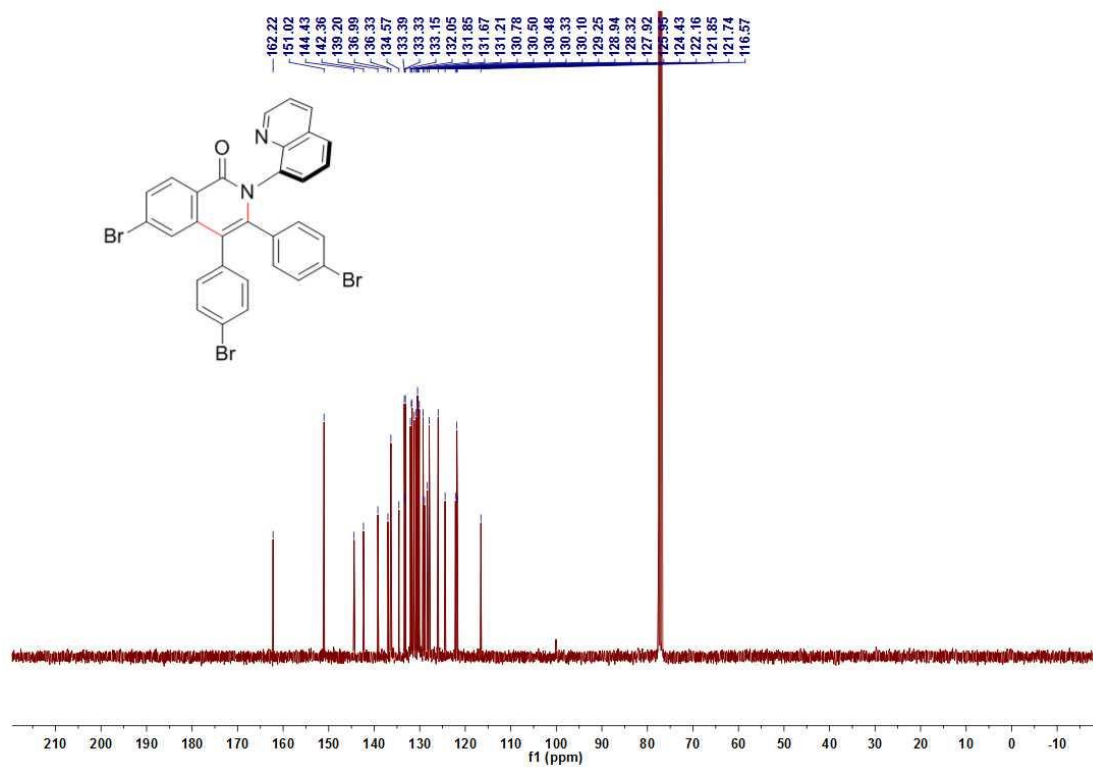
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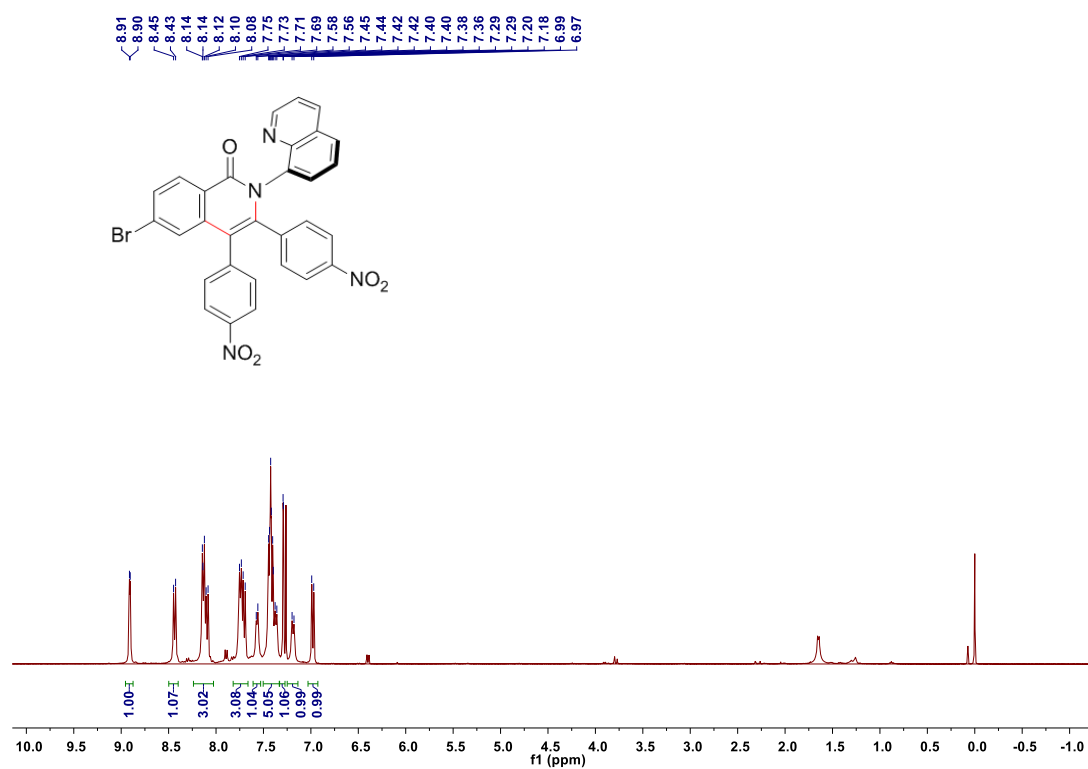
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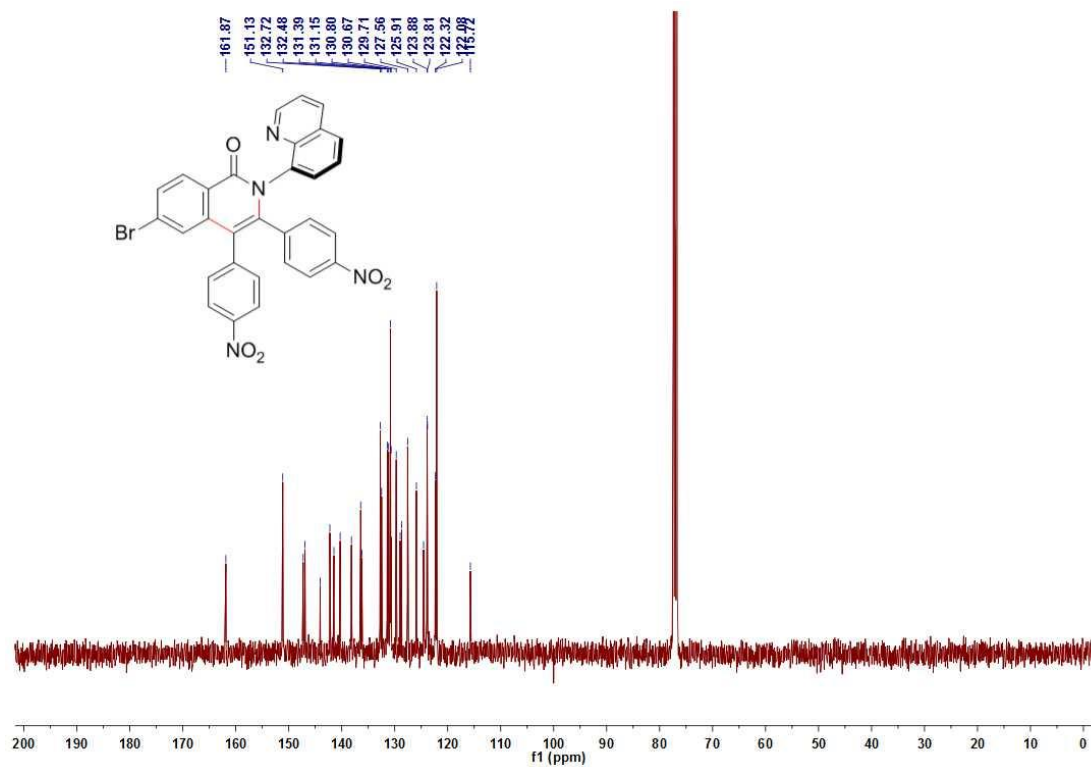
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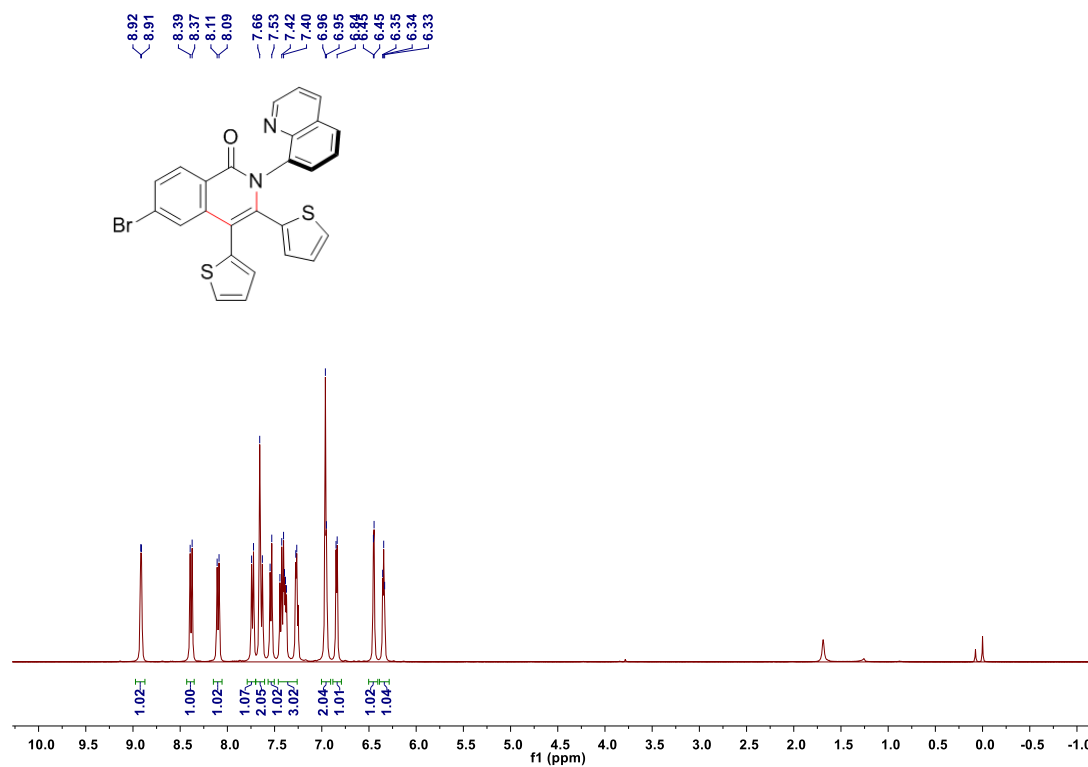
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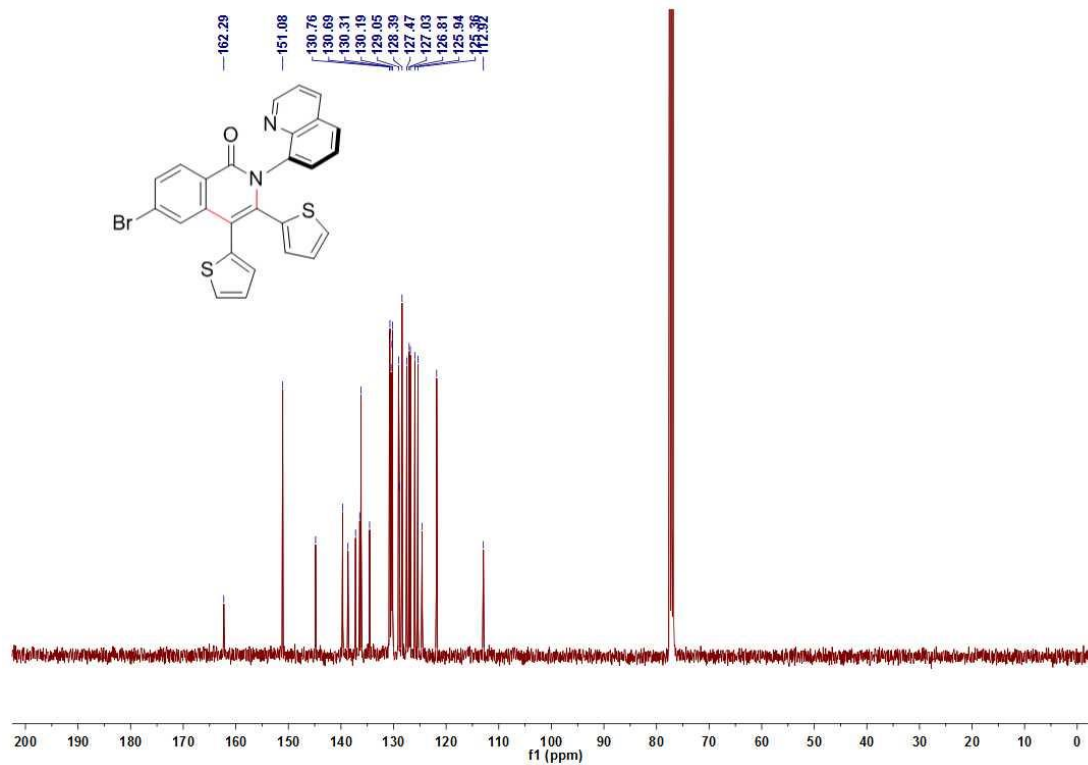
¹³C NMR Spectrum of **3ag**



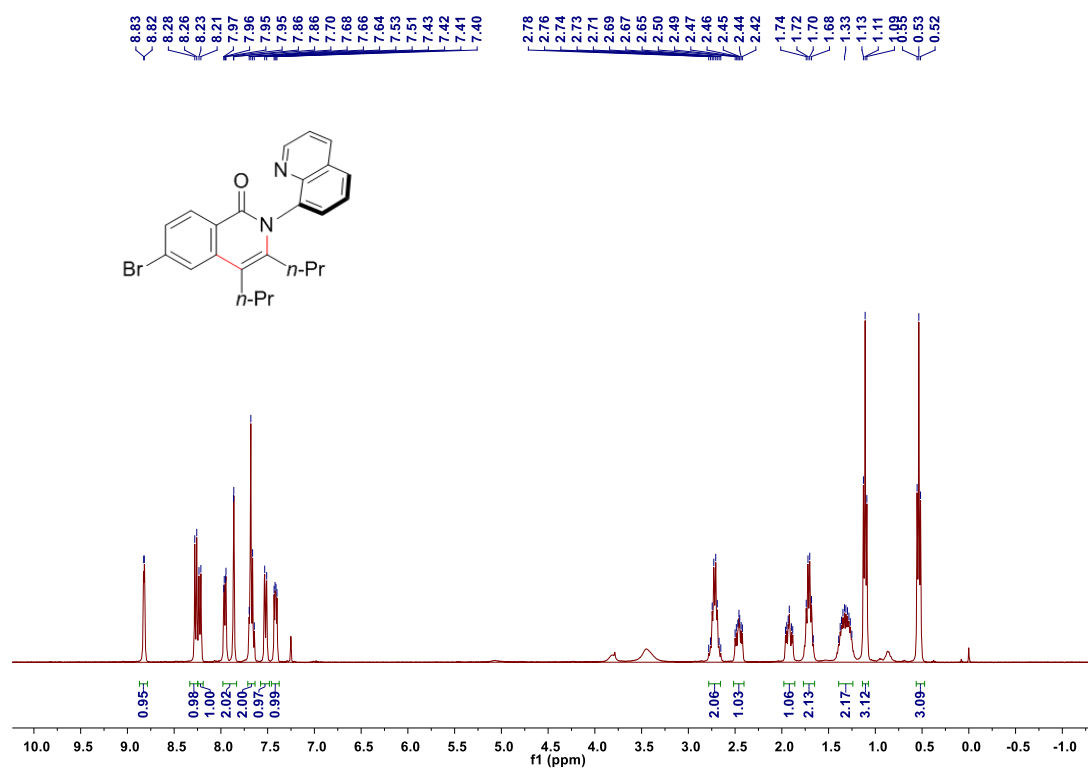
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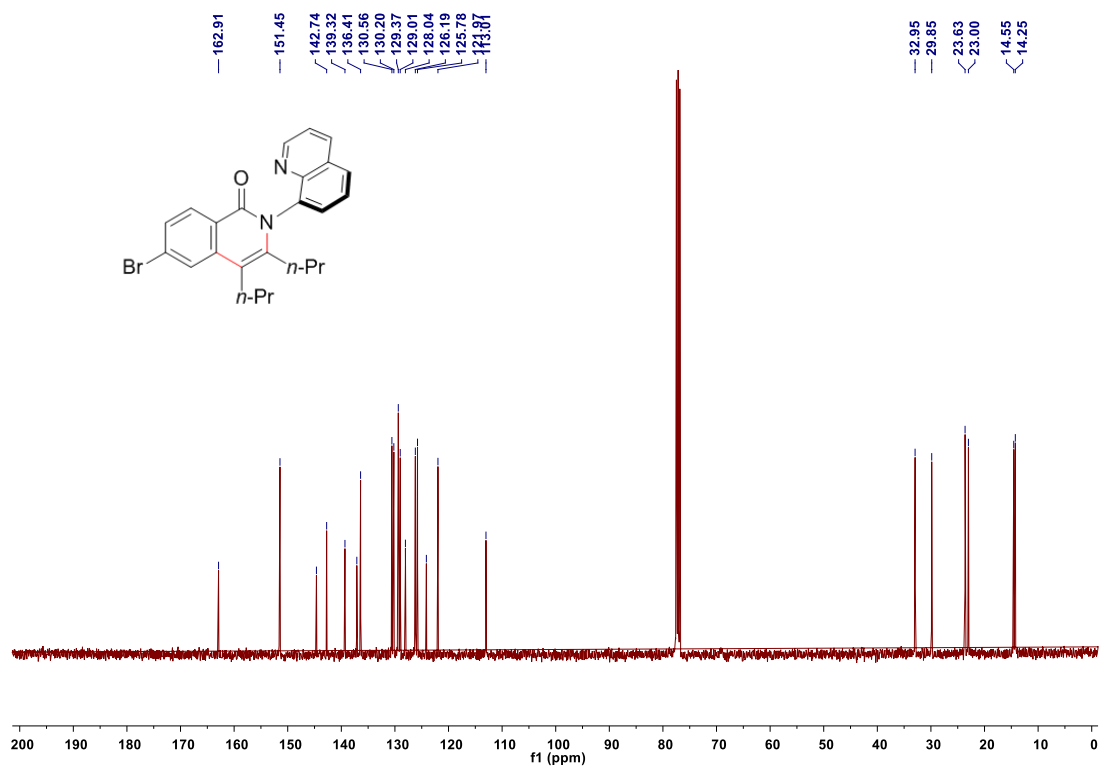
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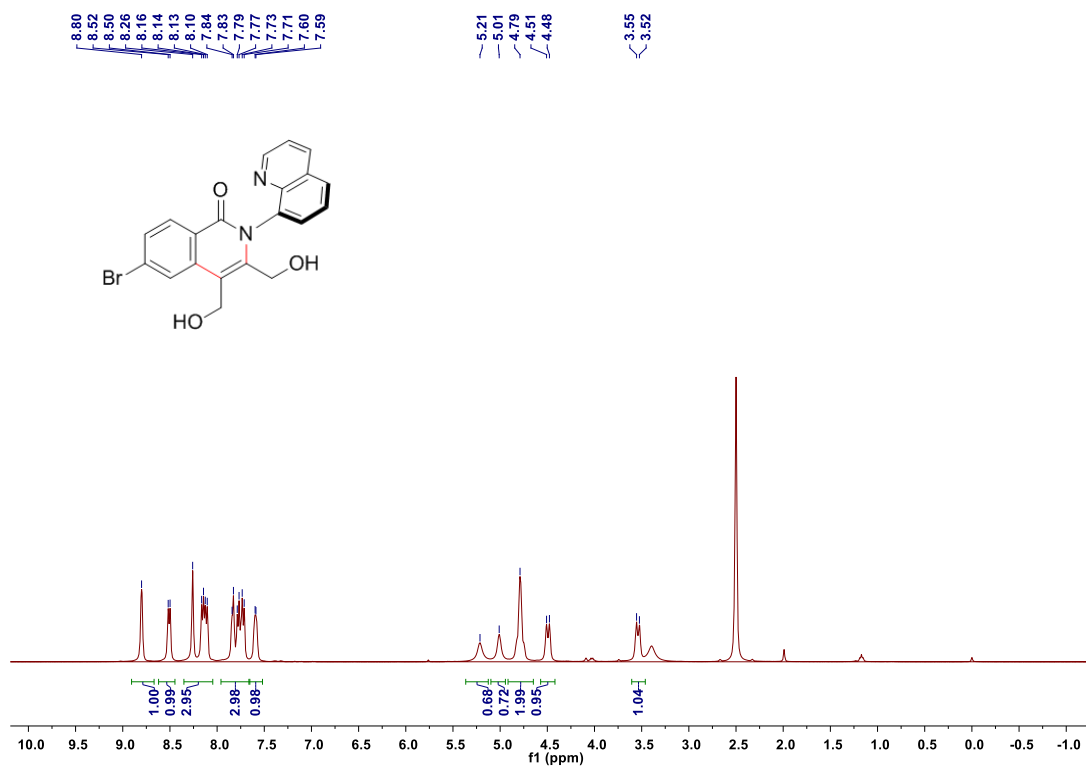
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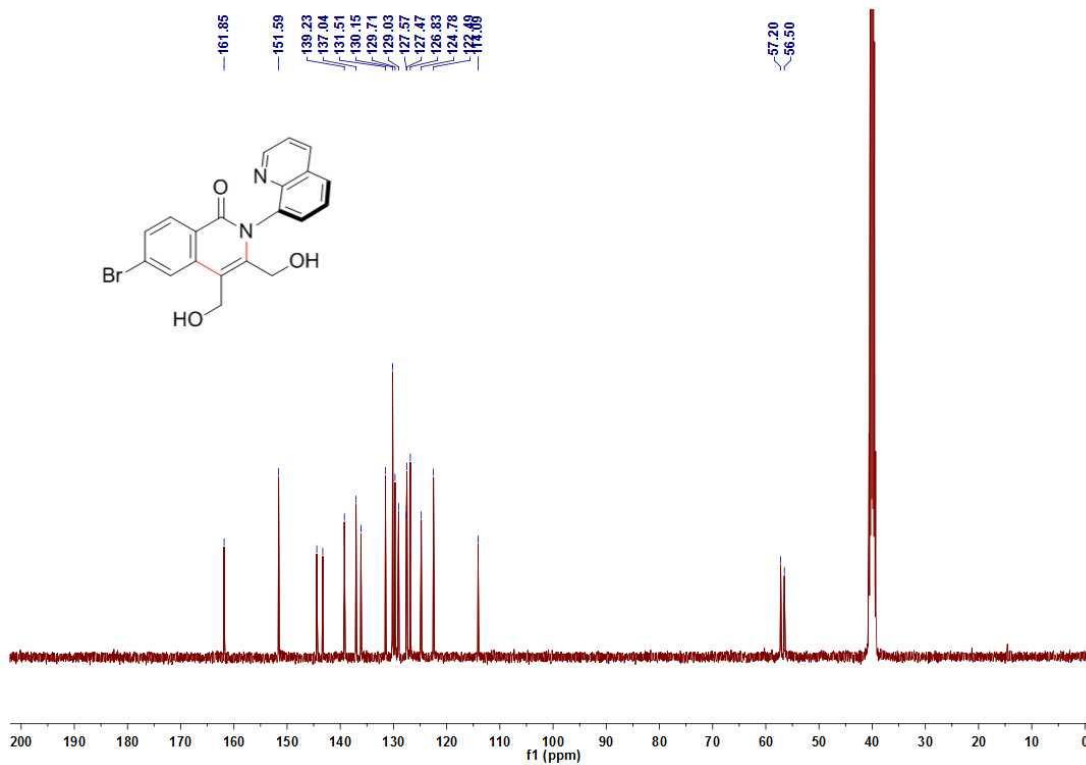
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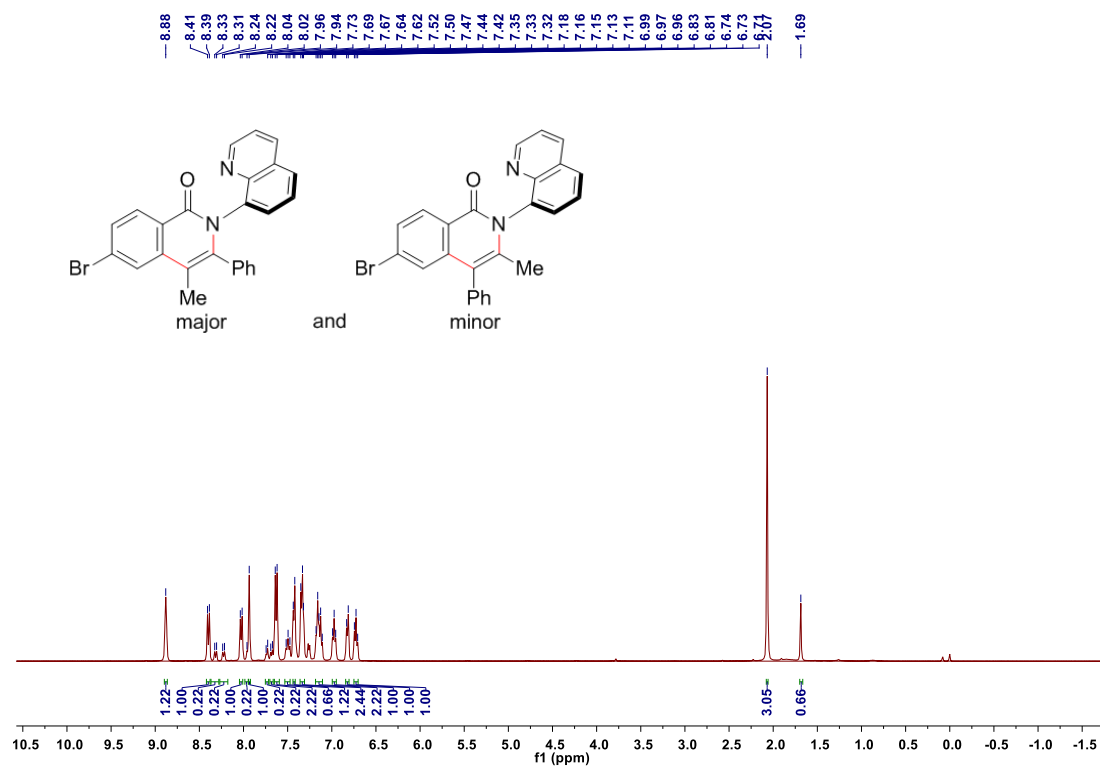
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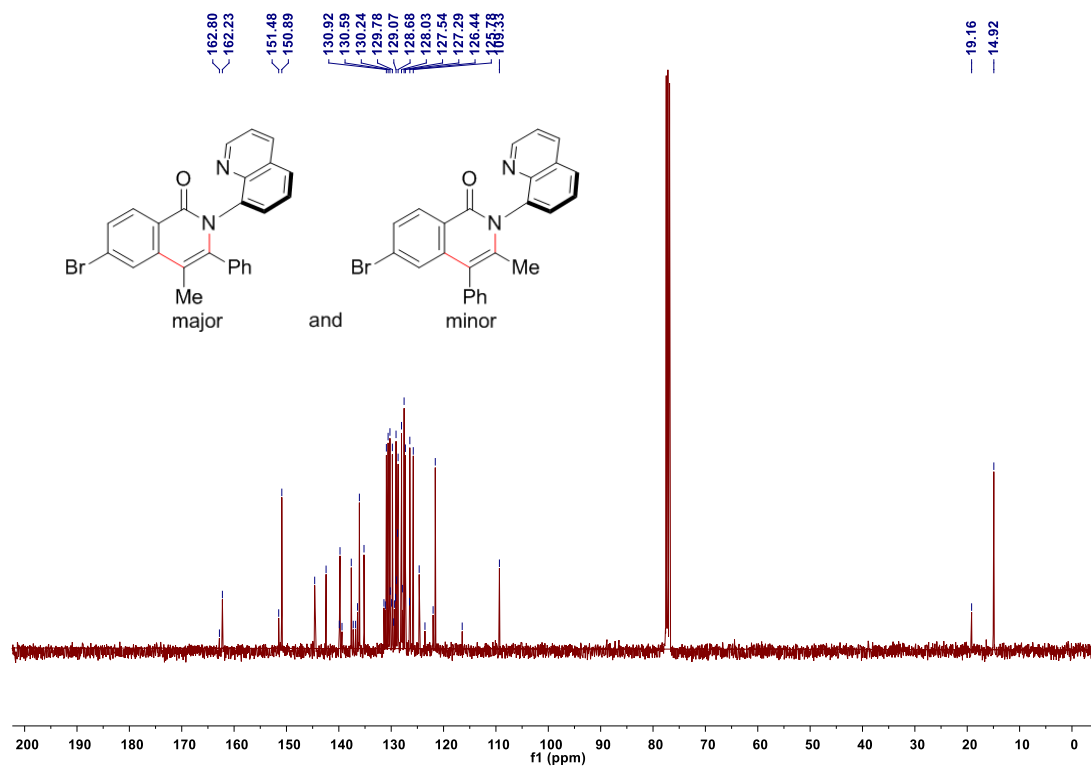
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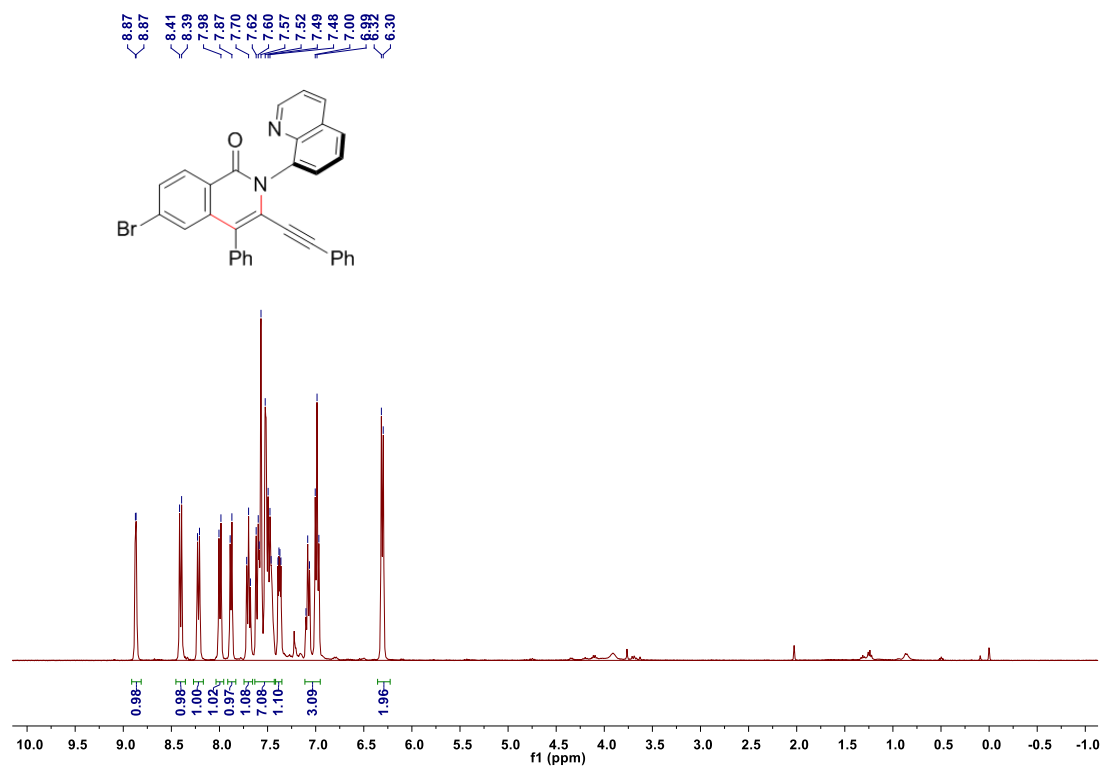
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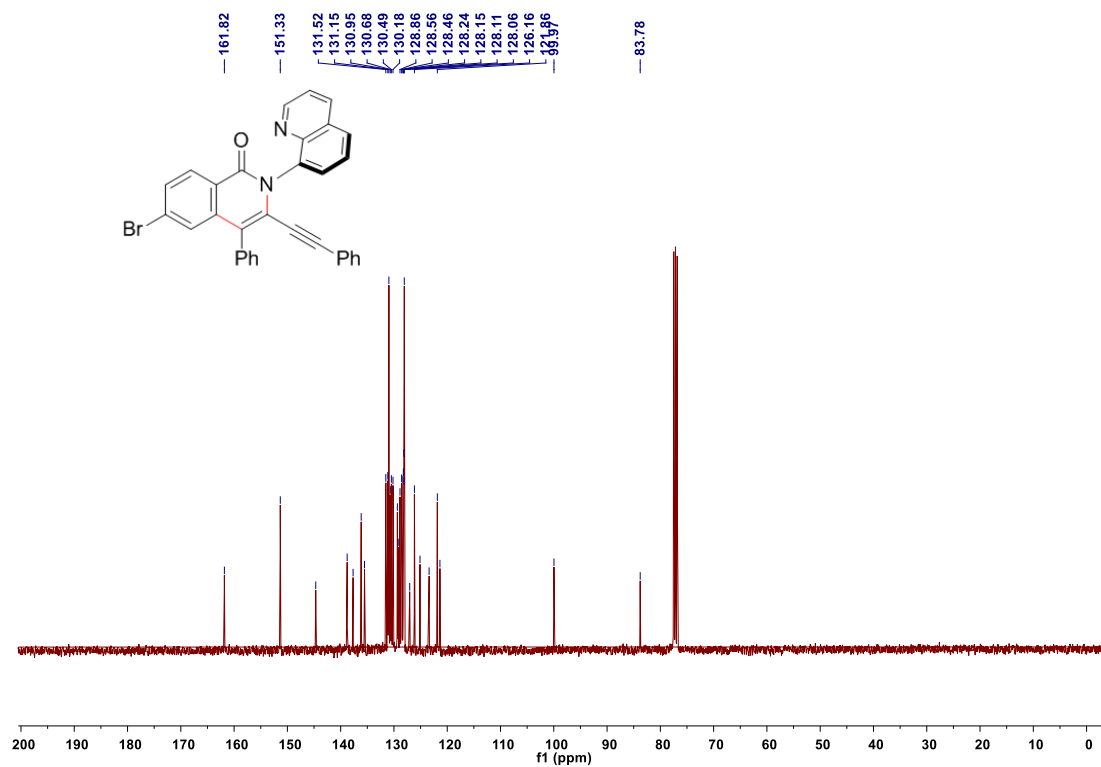
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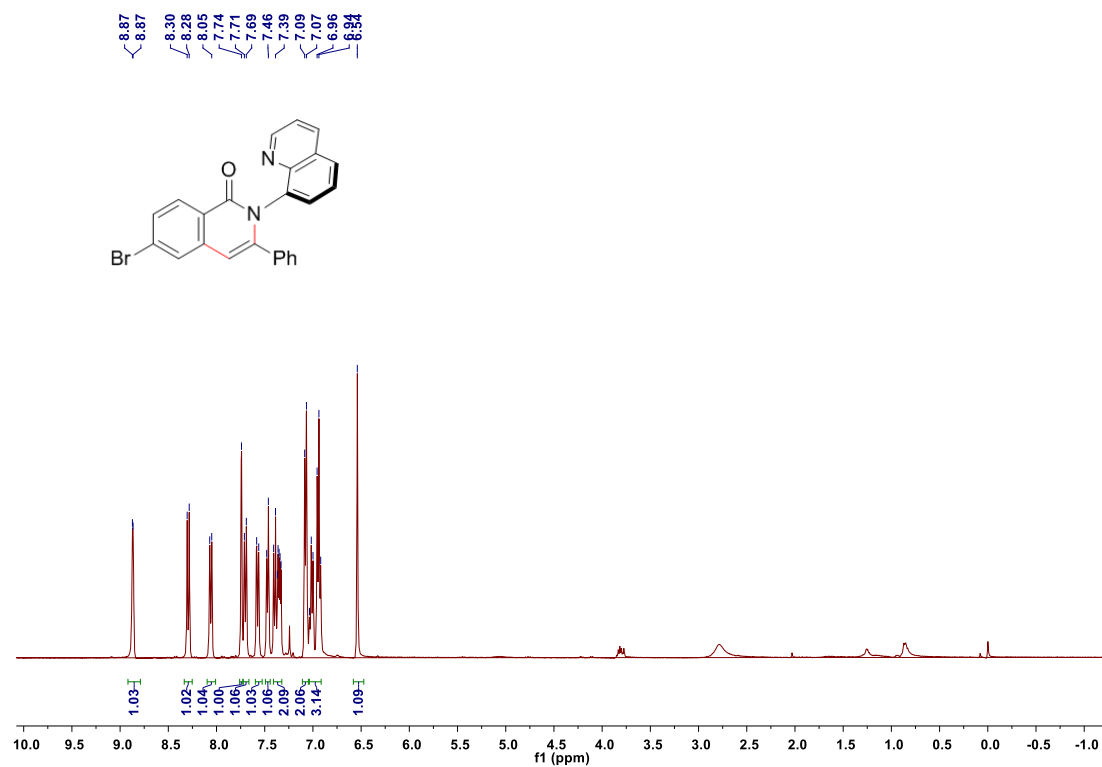
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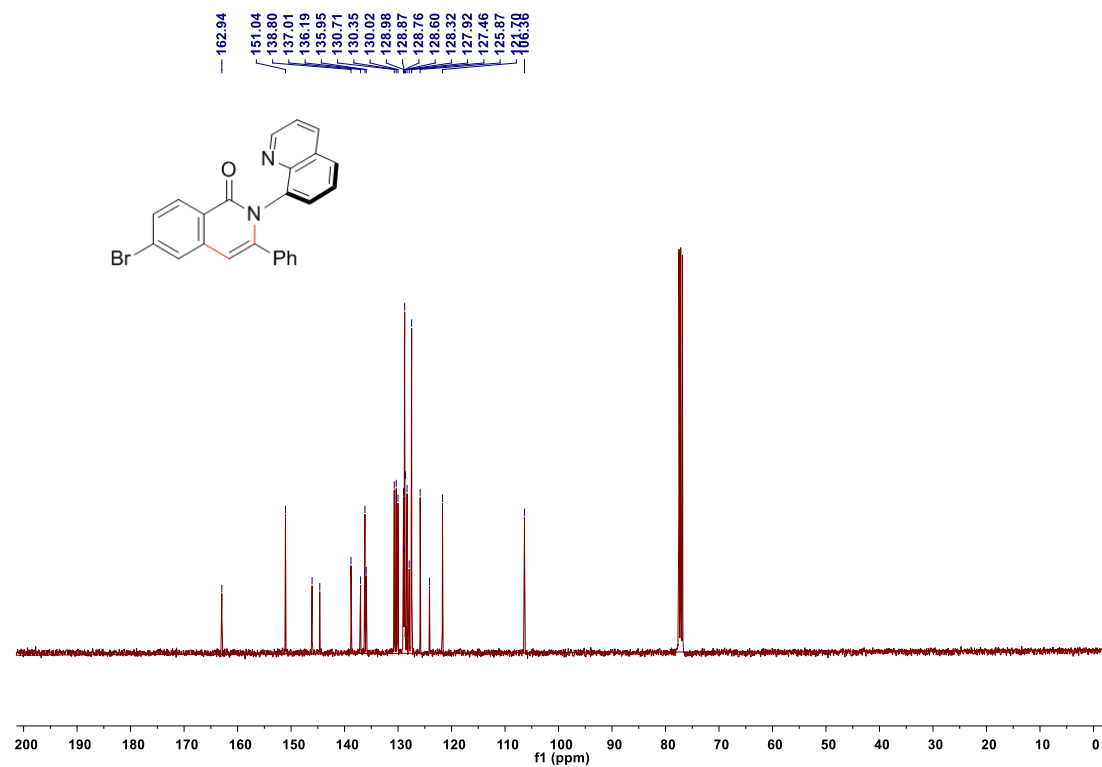
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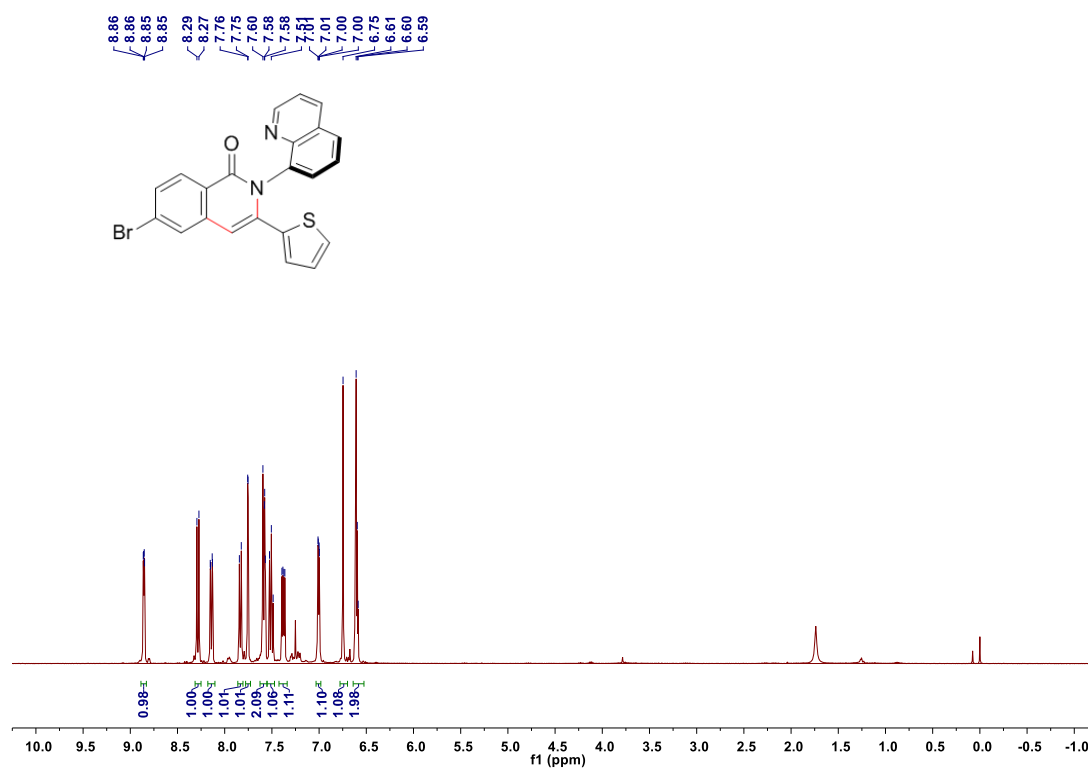
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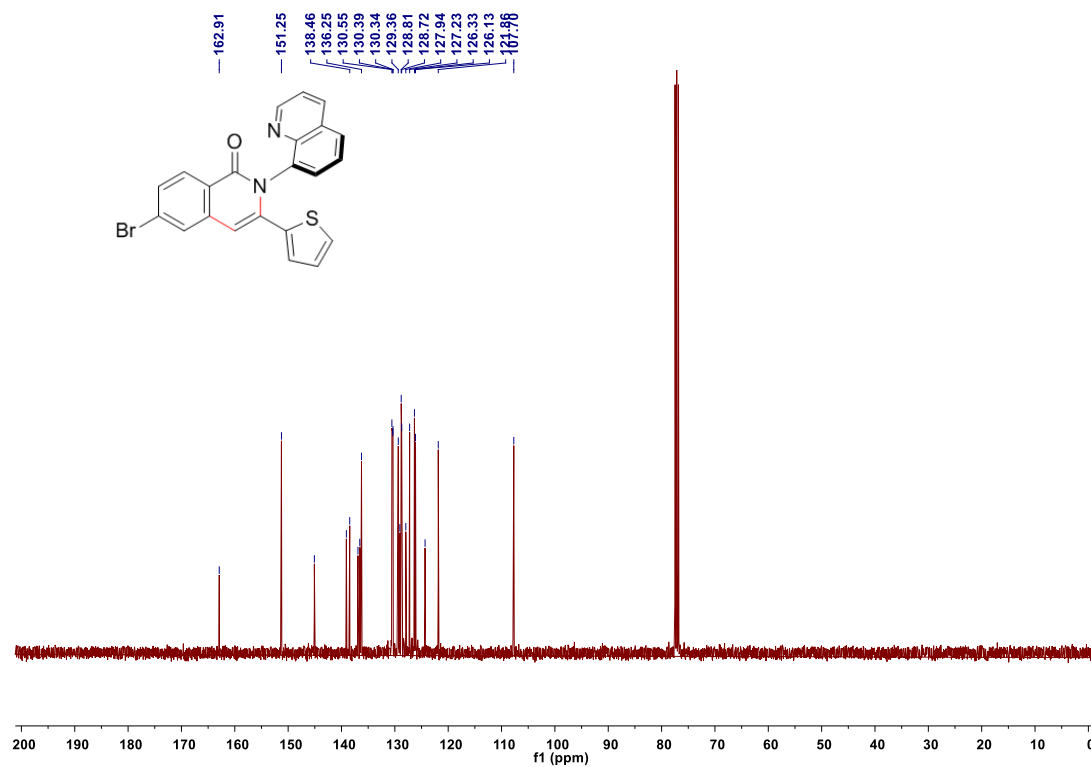
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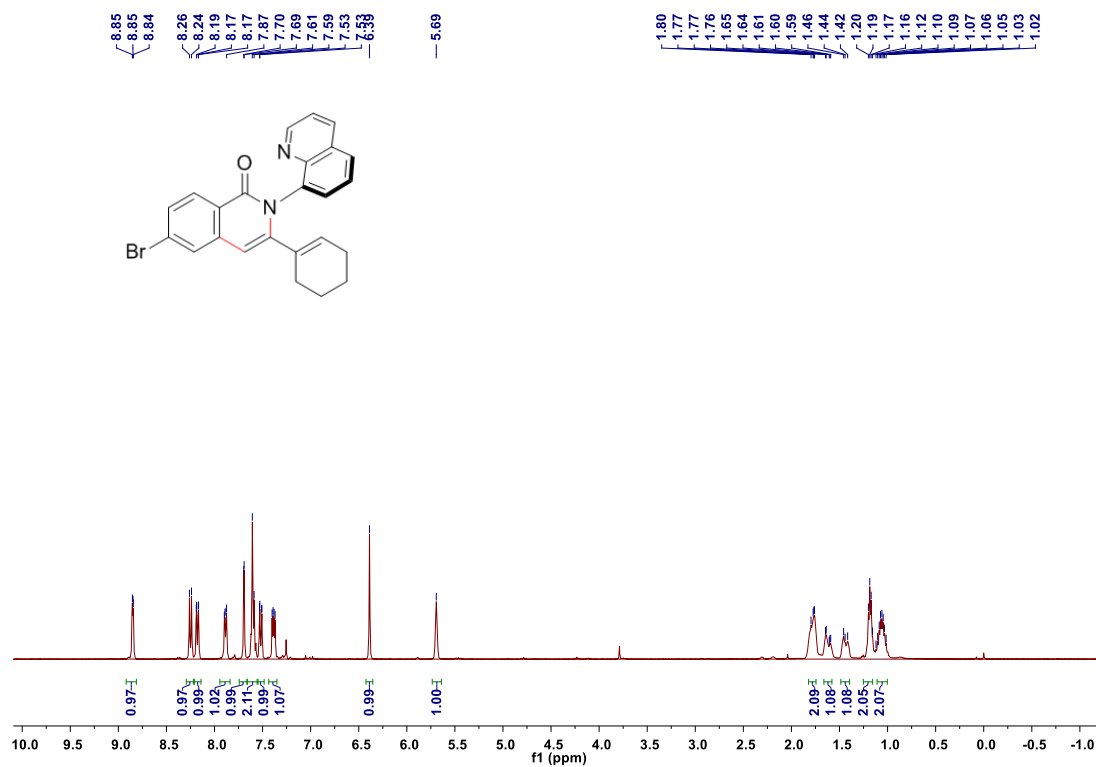
¹H NMR Spectrum of **3an**



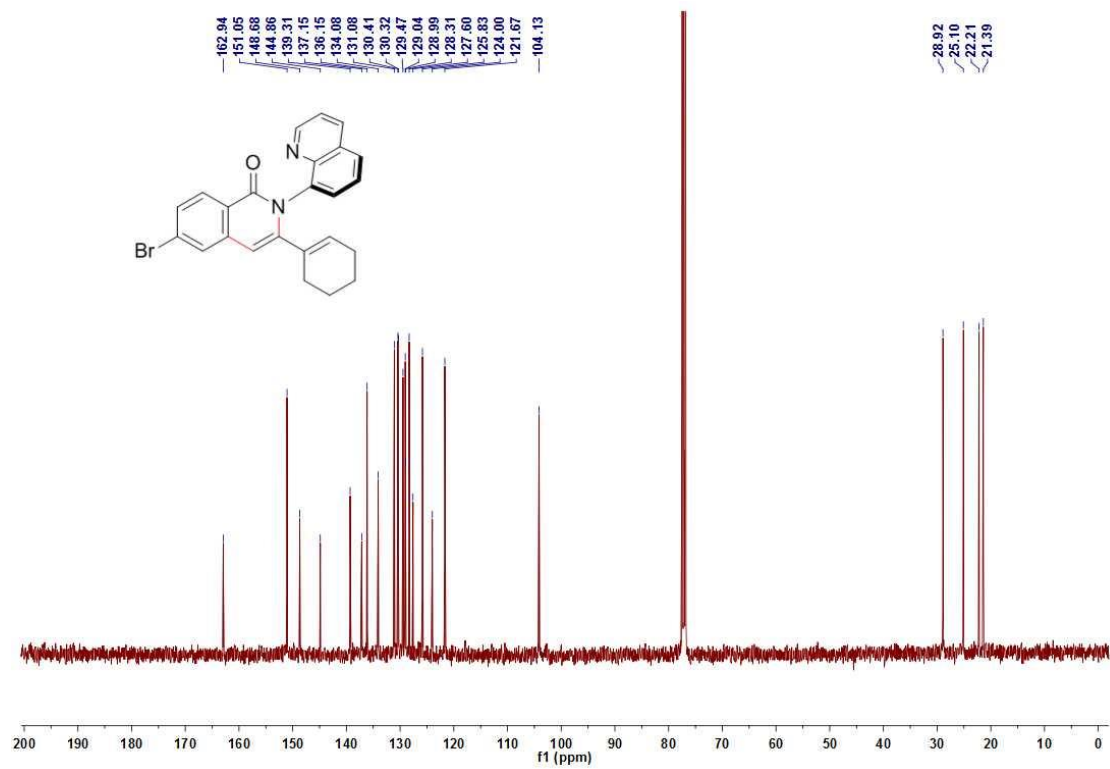
¹³C NMR Spectrum of **3an**



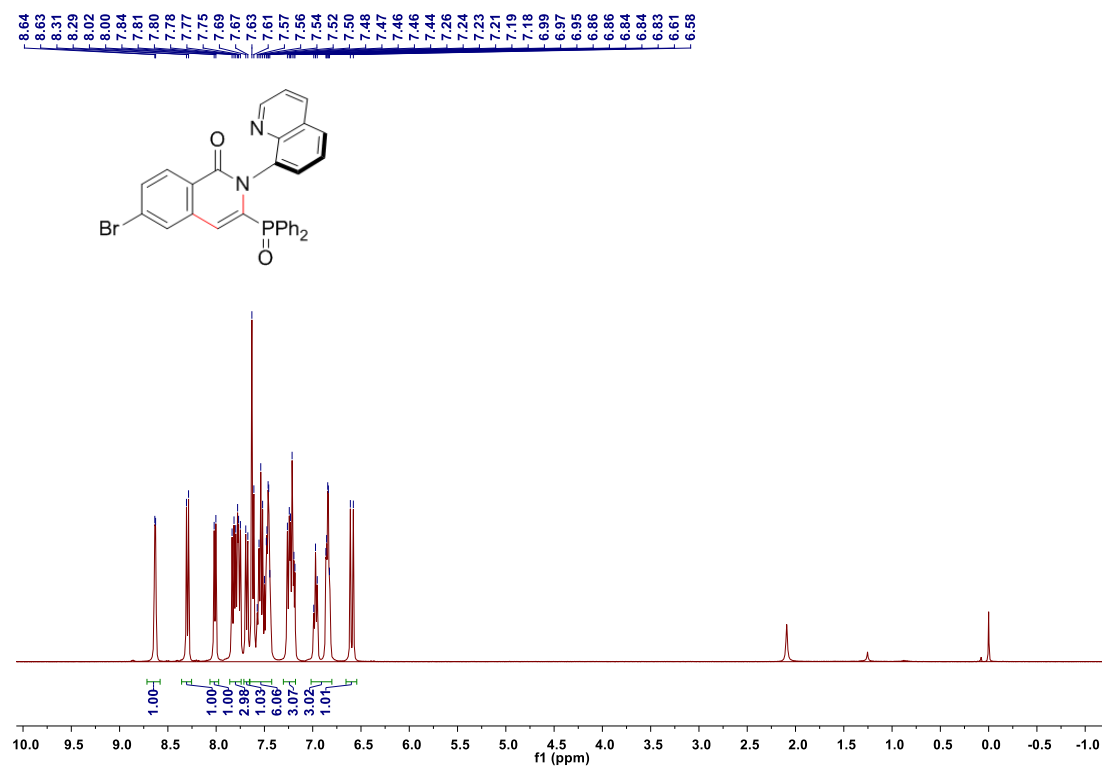
¹H NMR Spectrum of **3ao**



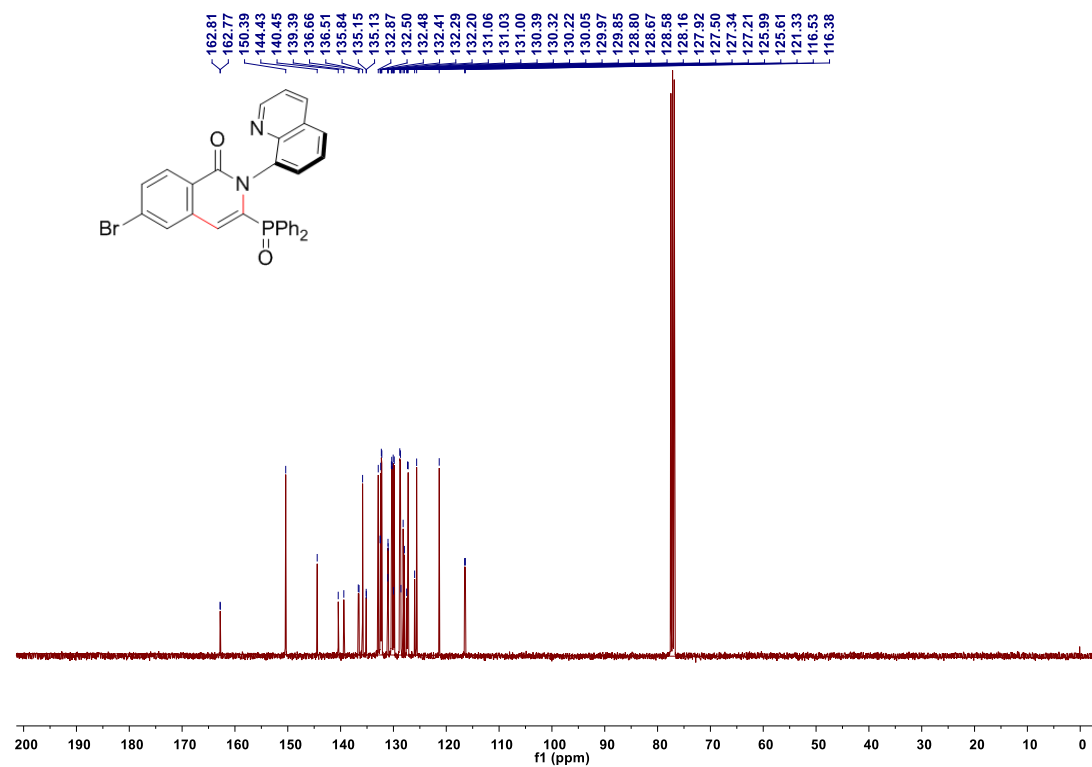
¹³C NMR Spectrum of **3ao**



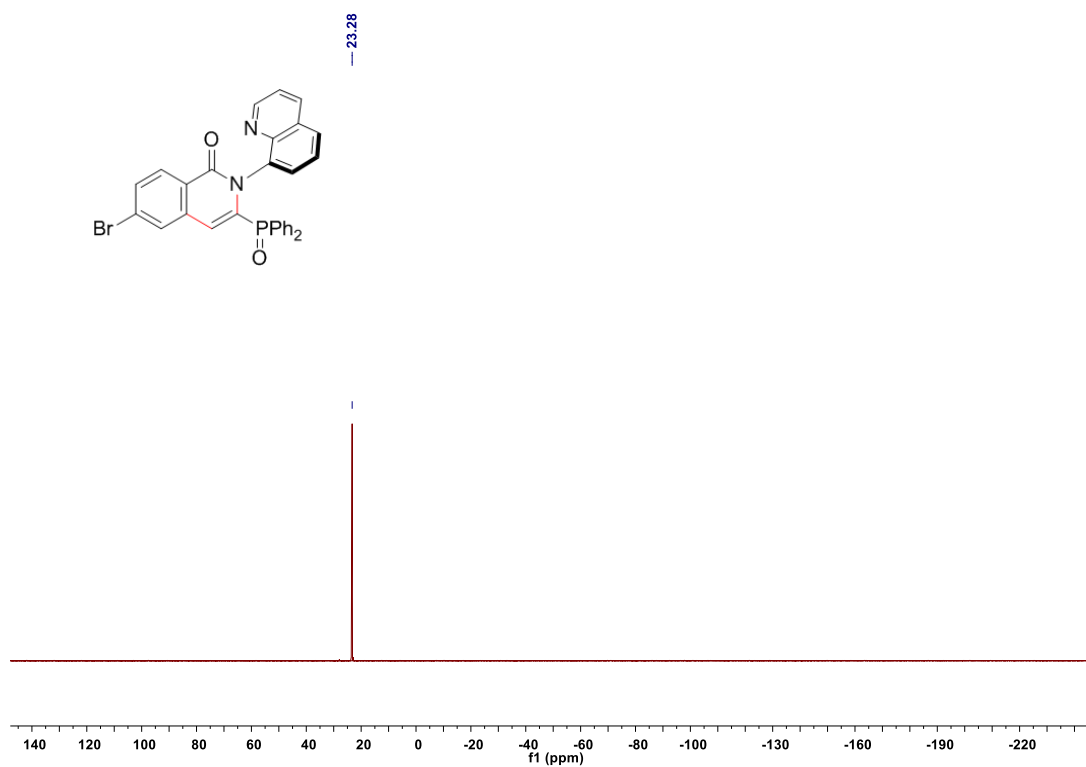
¹H NMR Spectrum of **3ap-major**



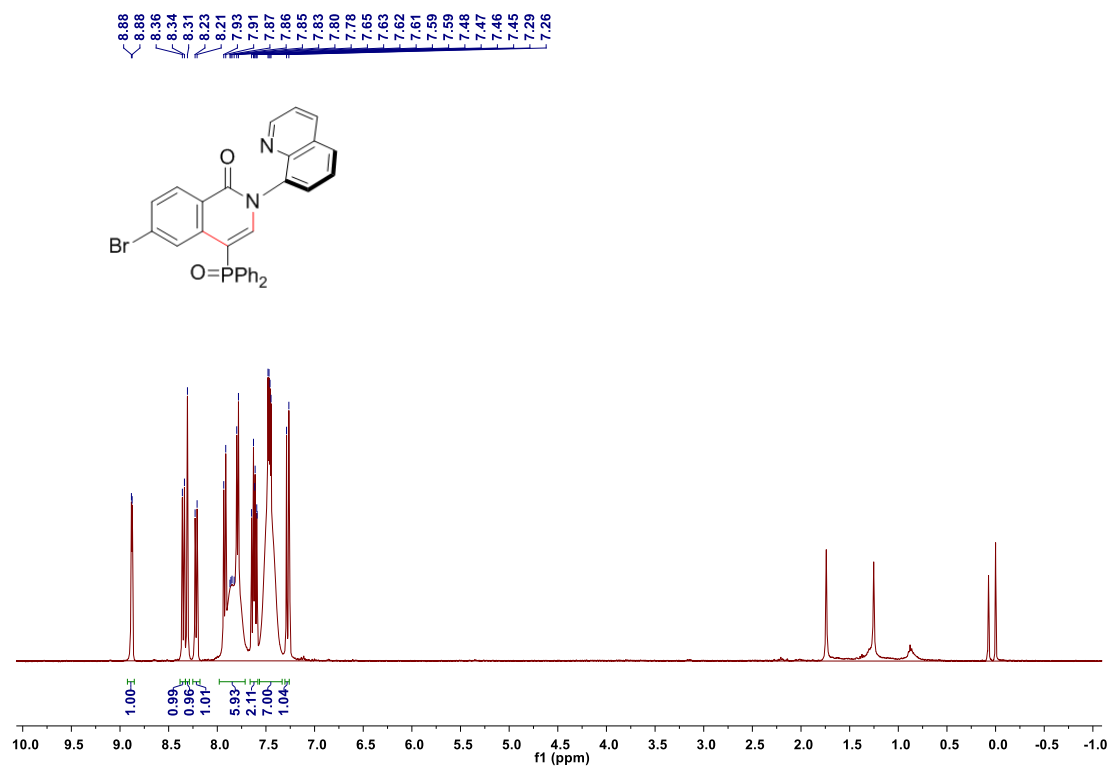
¹³C NMR Spectrum of **3ap-major**



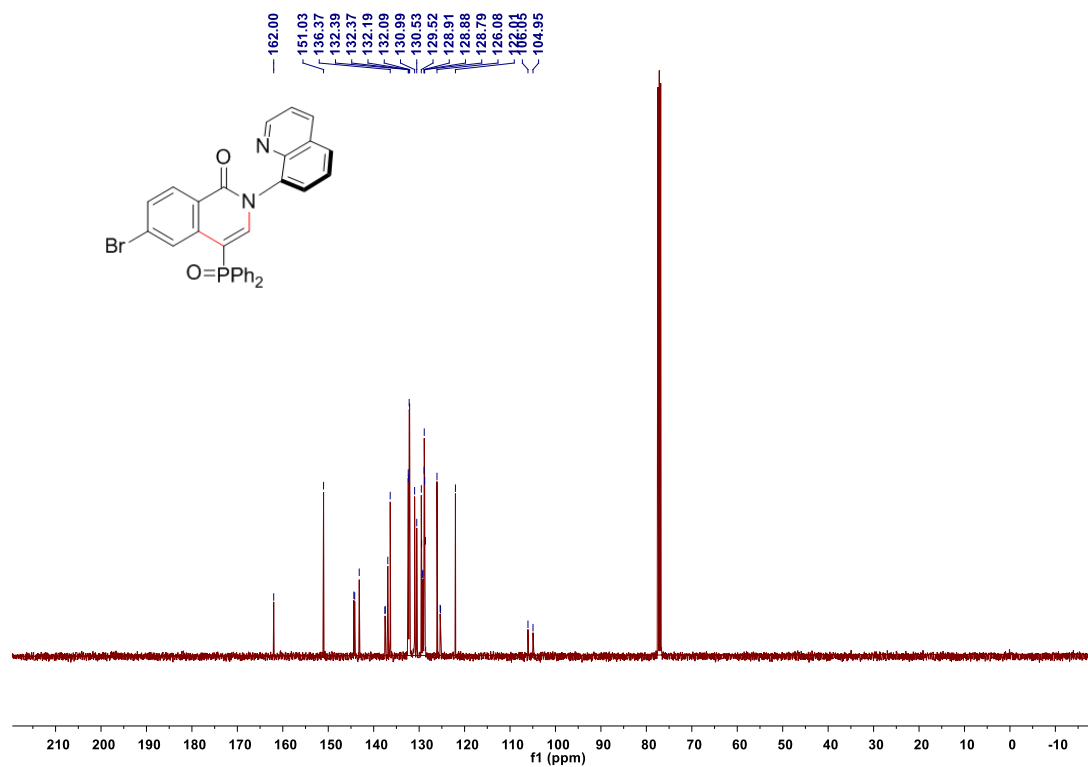
³¹P NMR Spectrum of **3ap-major**



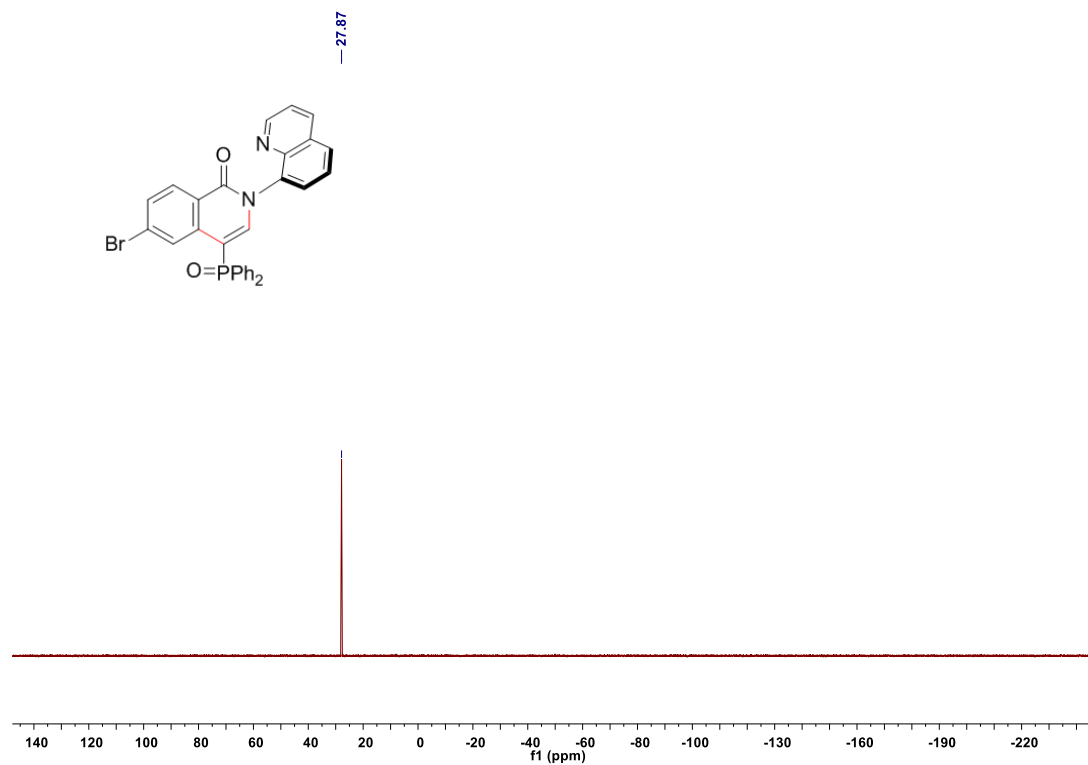
¹H NMR Spectrum of **3ap-minor**



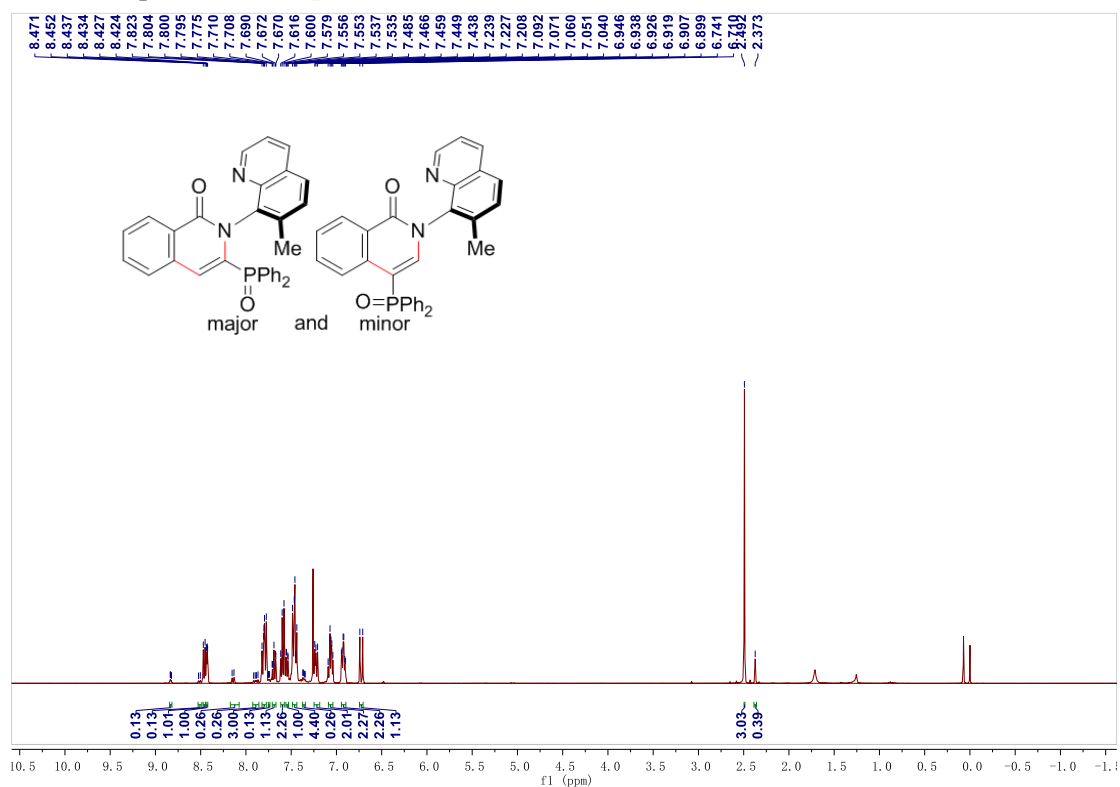
¹³C NMR Spectrum of **3ap-minor**



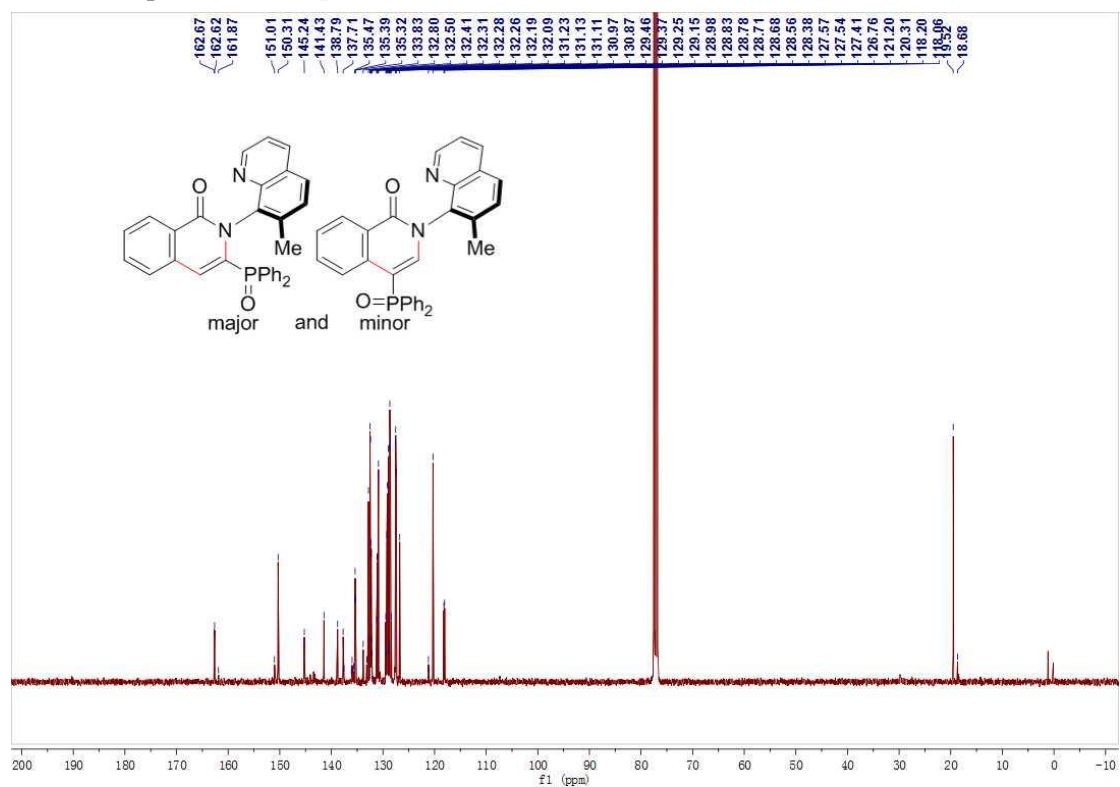
³¹P NMR Spectrum of **3ap-minor**



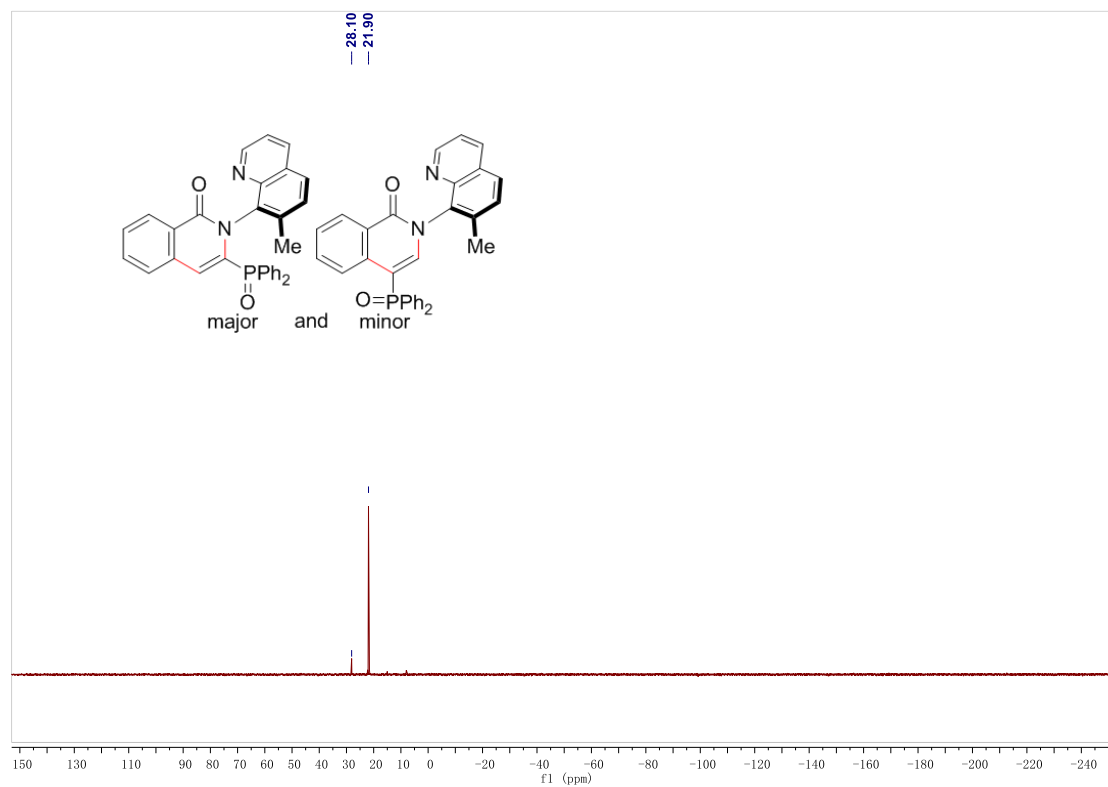
¹H NMR Spectrum of **3aq**



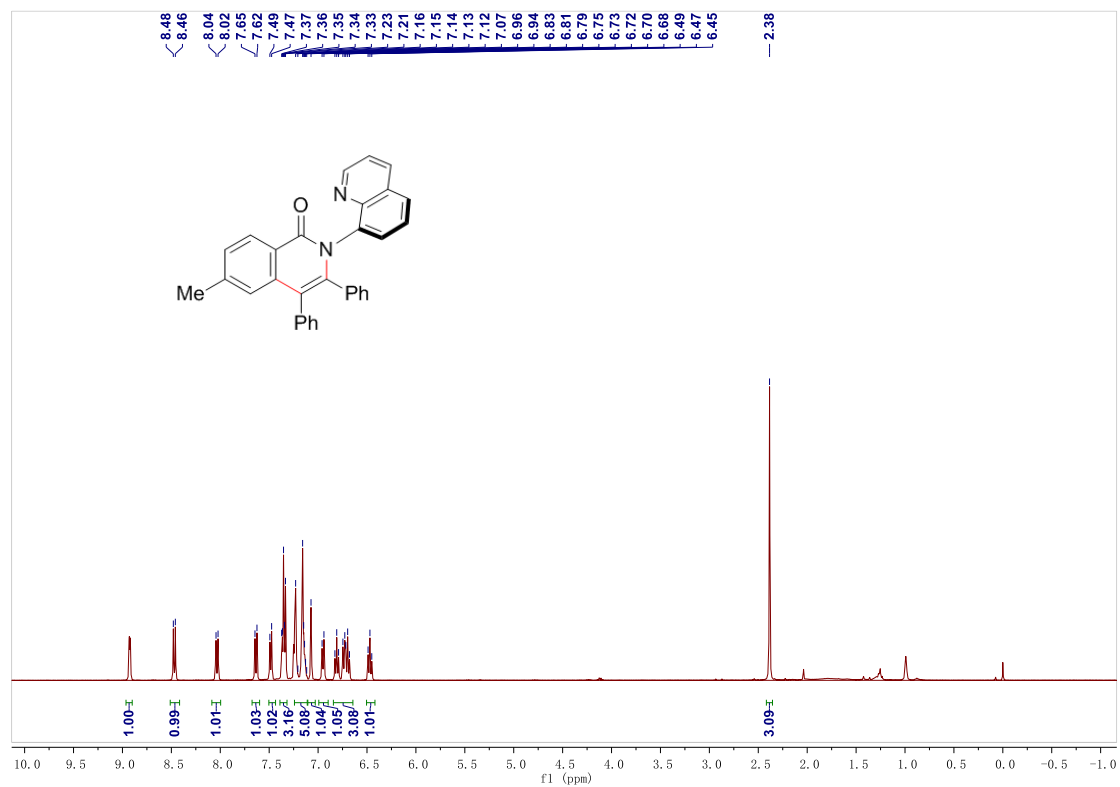
¹³C NMR Spectrum of **3aq**



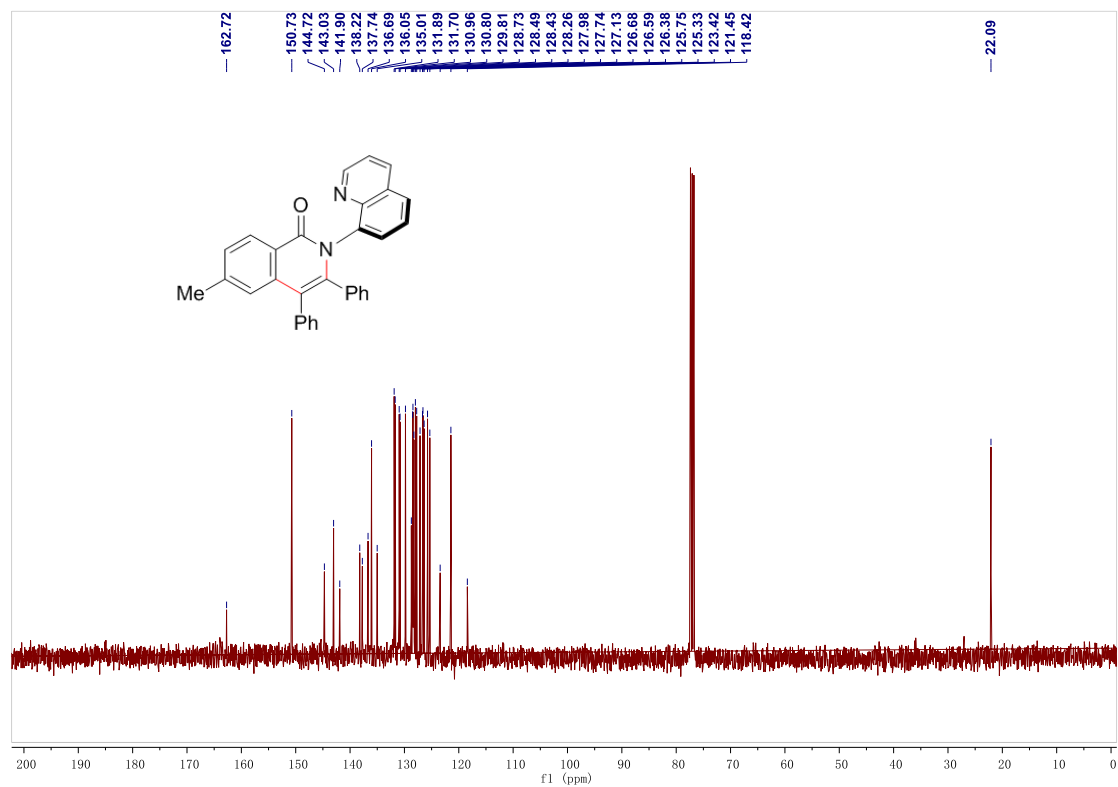
³¹P NMR Spectrum of **3aq**



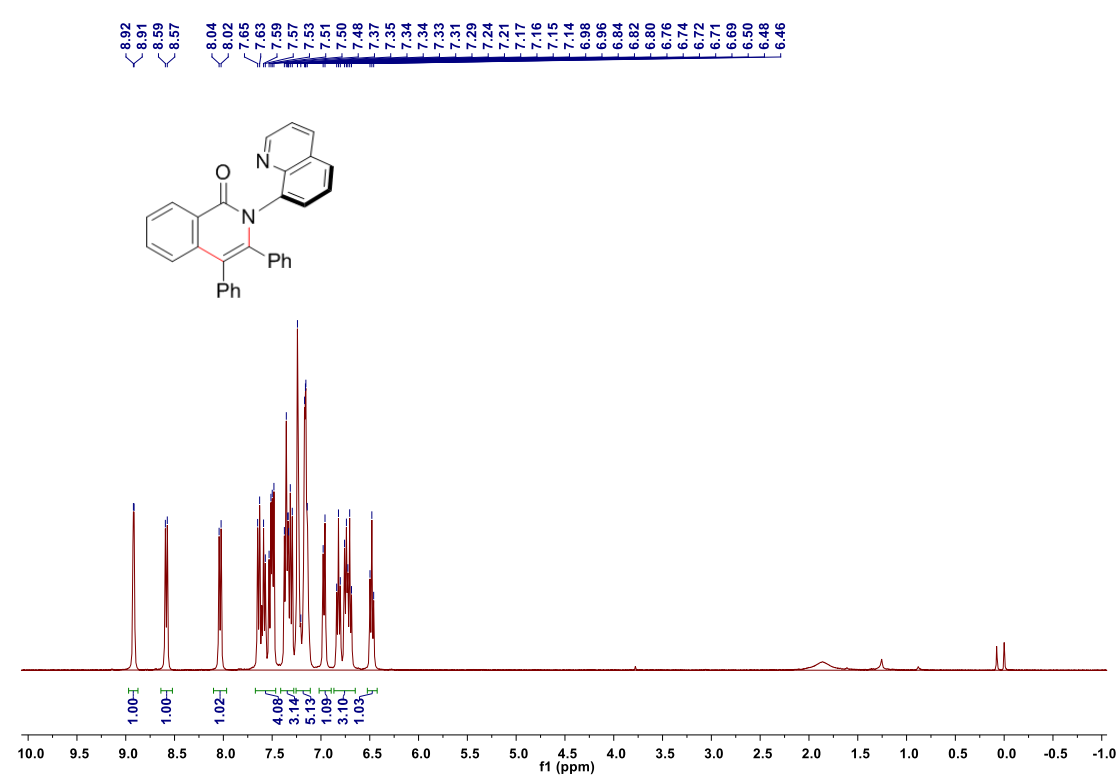
¹H NMR Spectrum of **3aa**



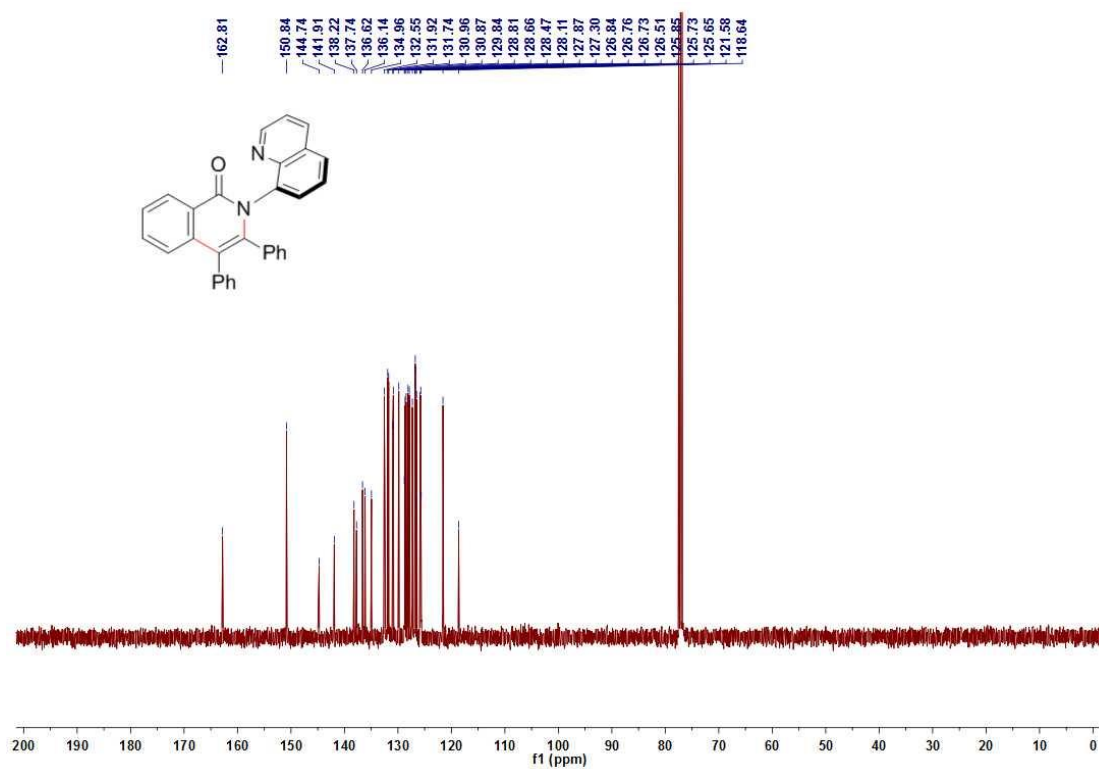
¹³C NMR Spectrum of **3aa**



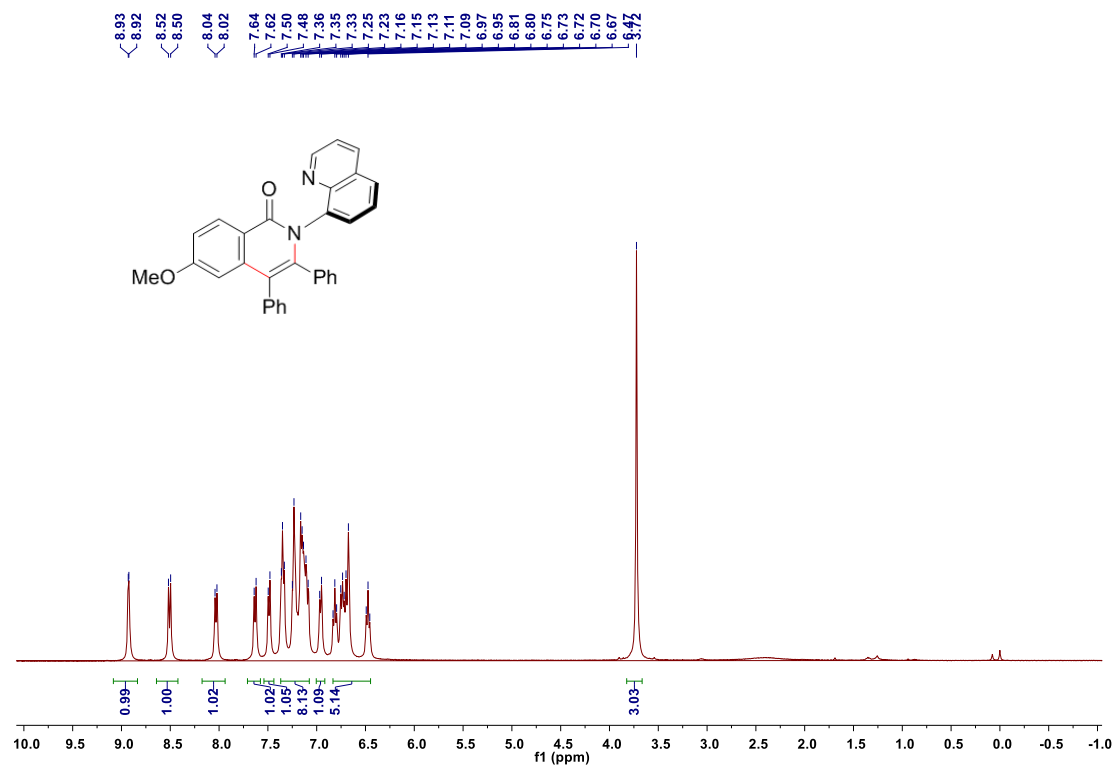
¹H NMR Spectrum of **3ba**



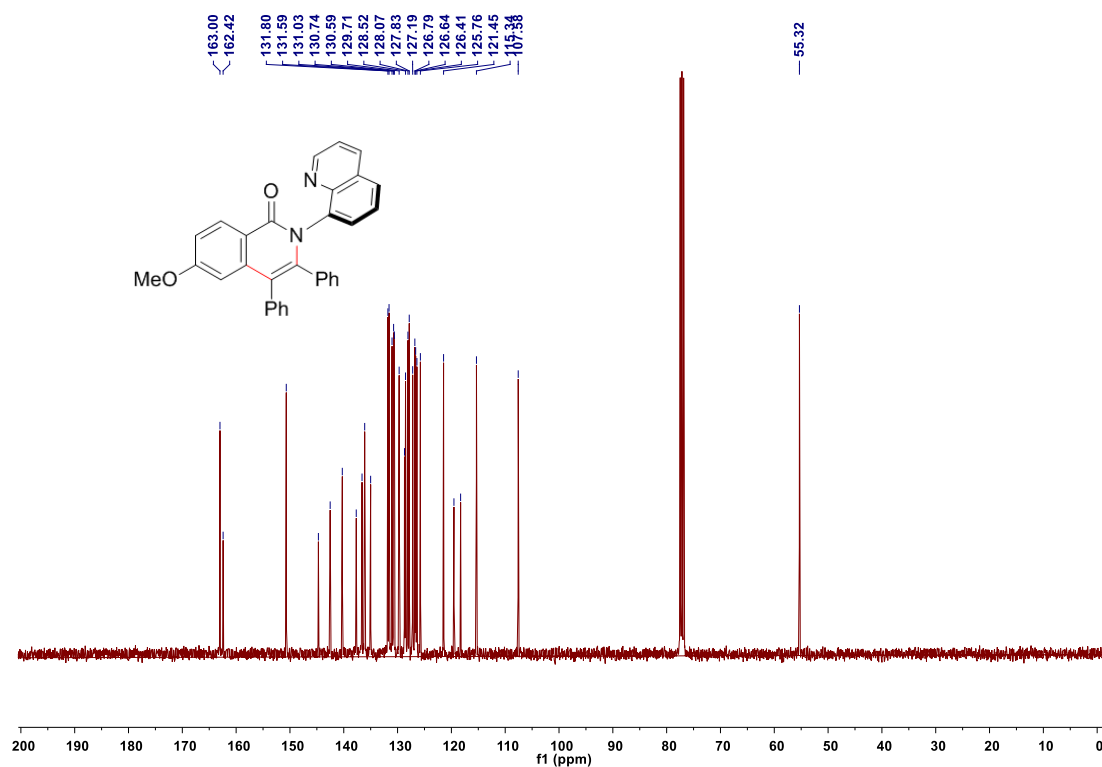
^{13}C NMR Spectrum of **3ba**



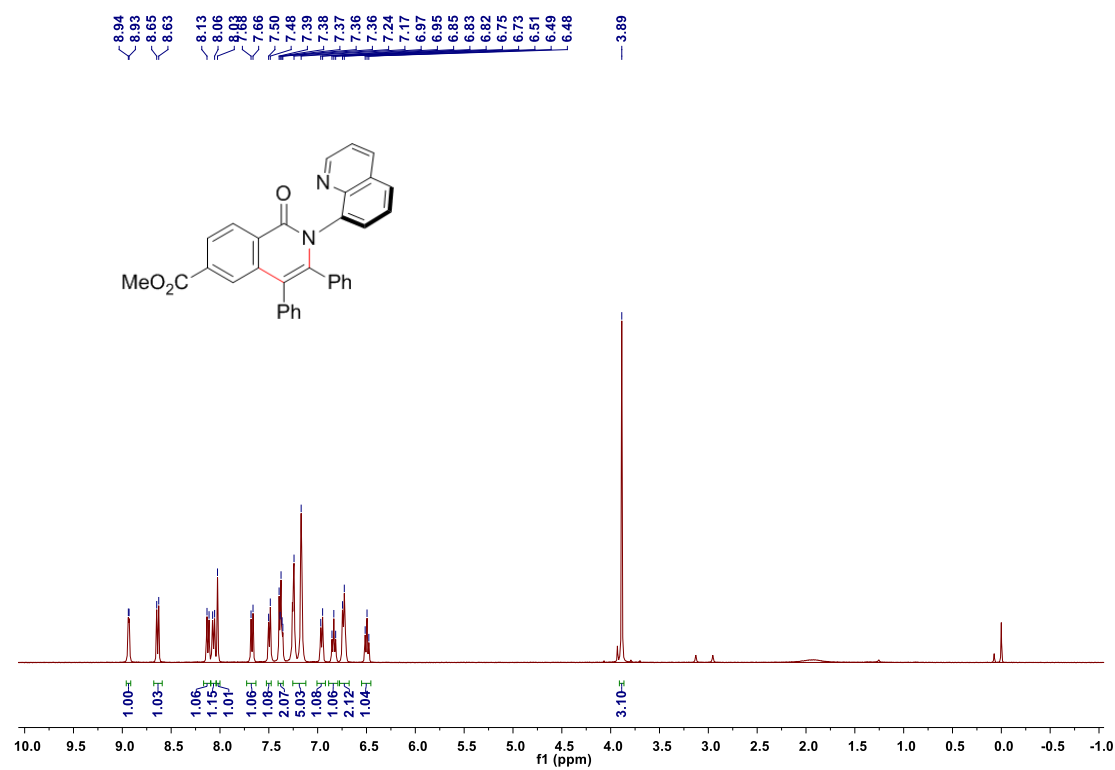
^1H NMR Spectrum of **3ca**



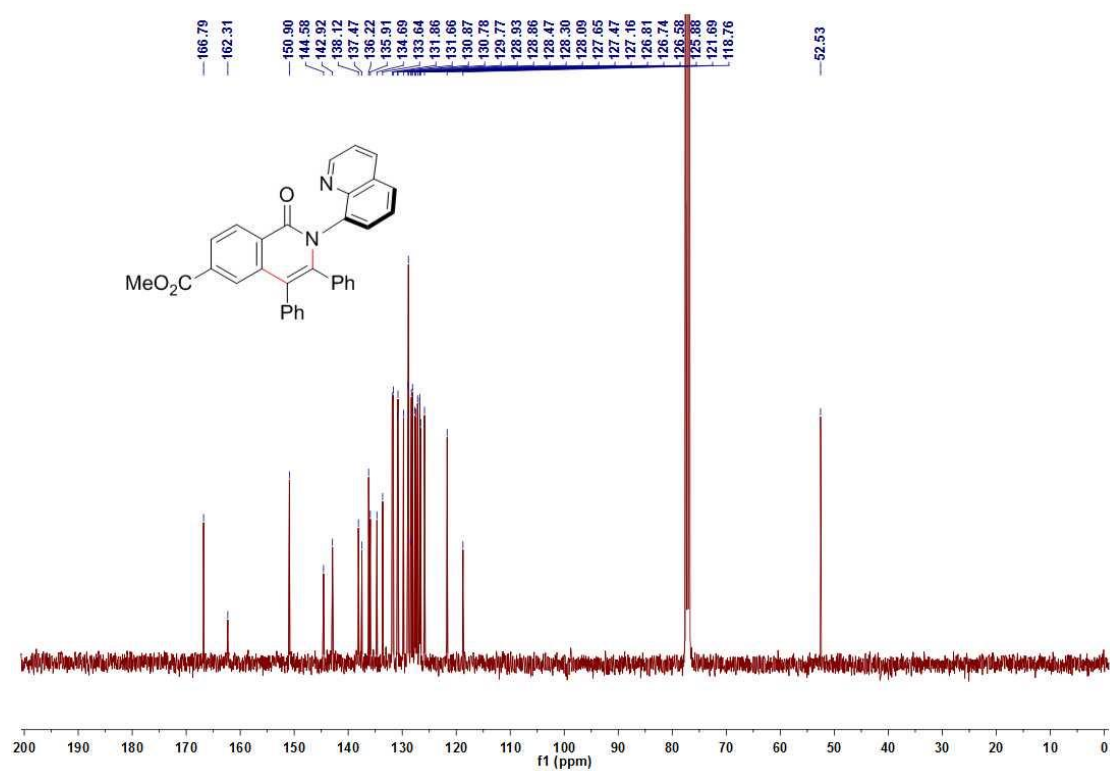
¹³C NMR Spectrum of **3ca**



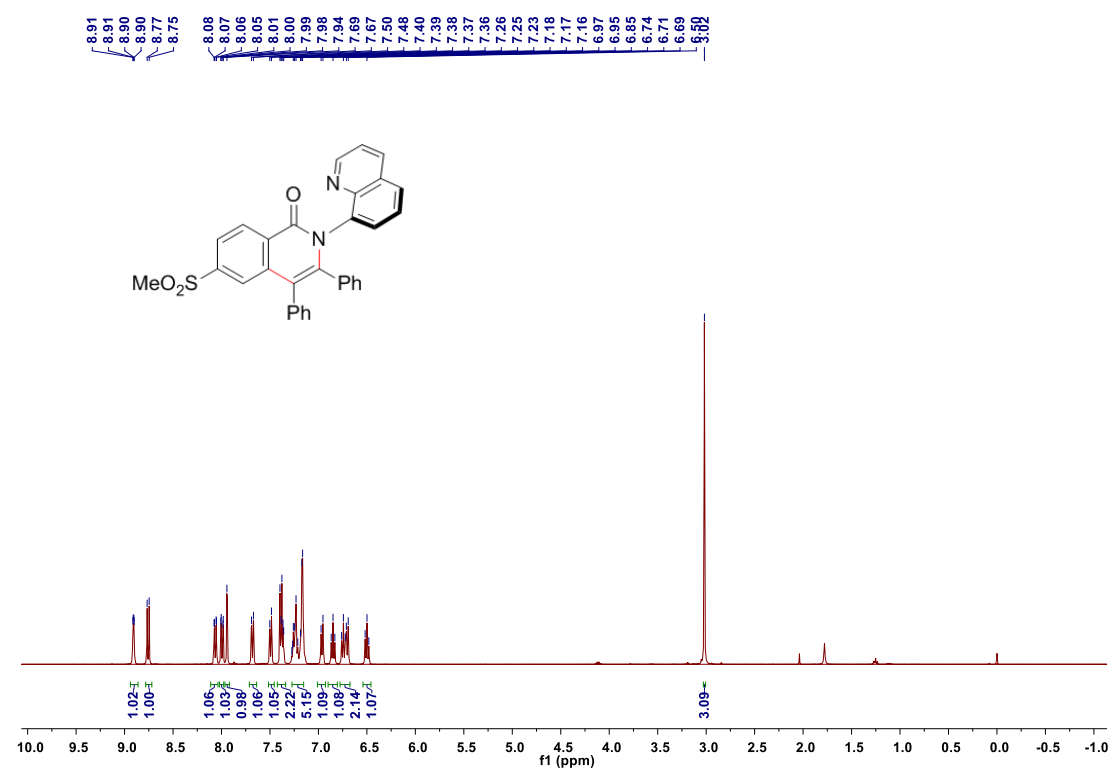
¹H NMR Spectrum of **3da**



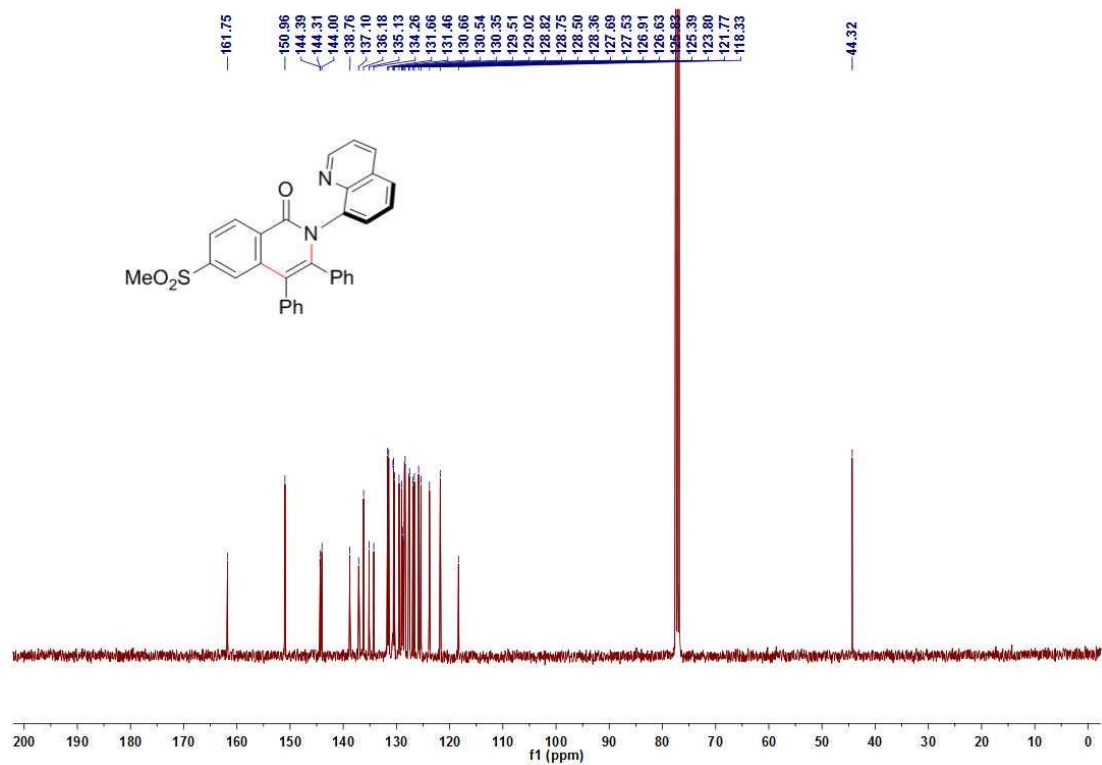
¹³C NMR Spectrum of **3da**



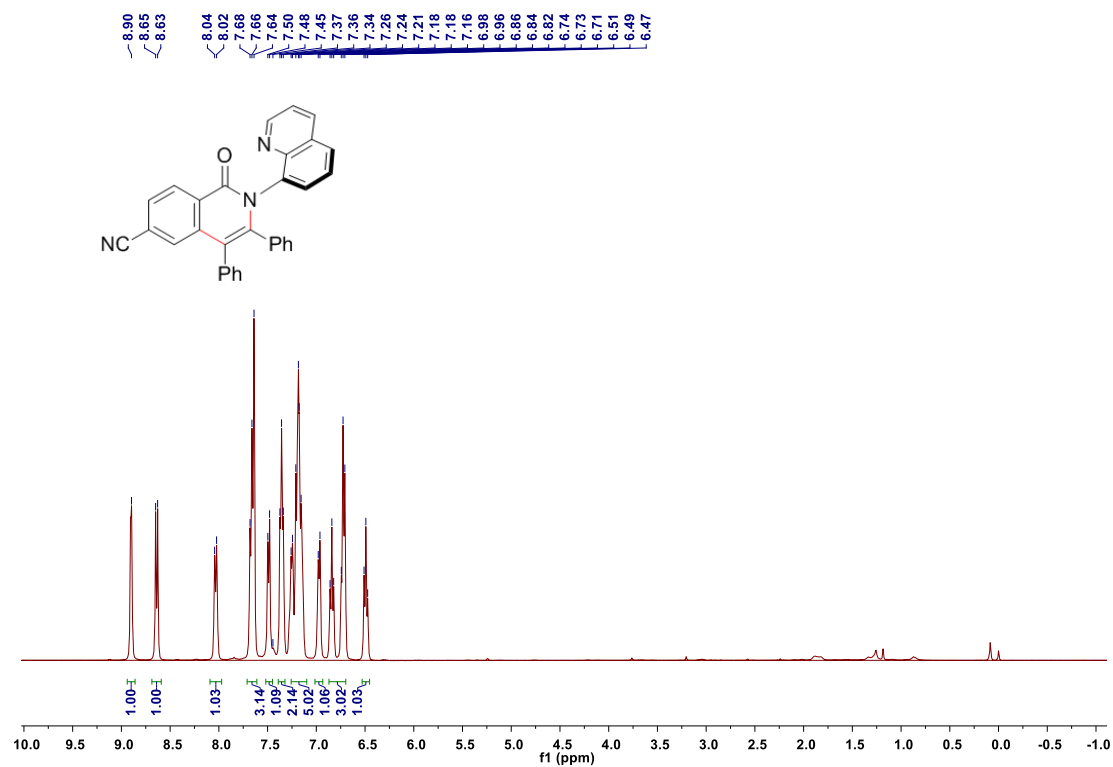
¹H NMR Spectrum of **3ea**



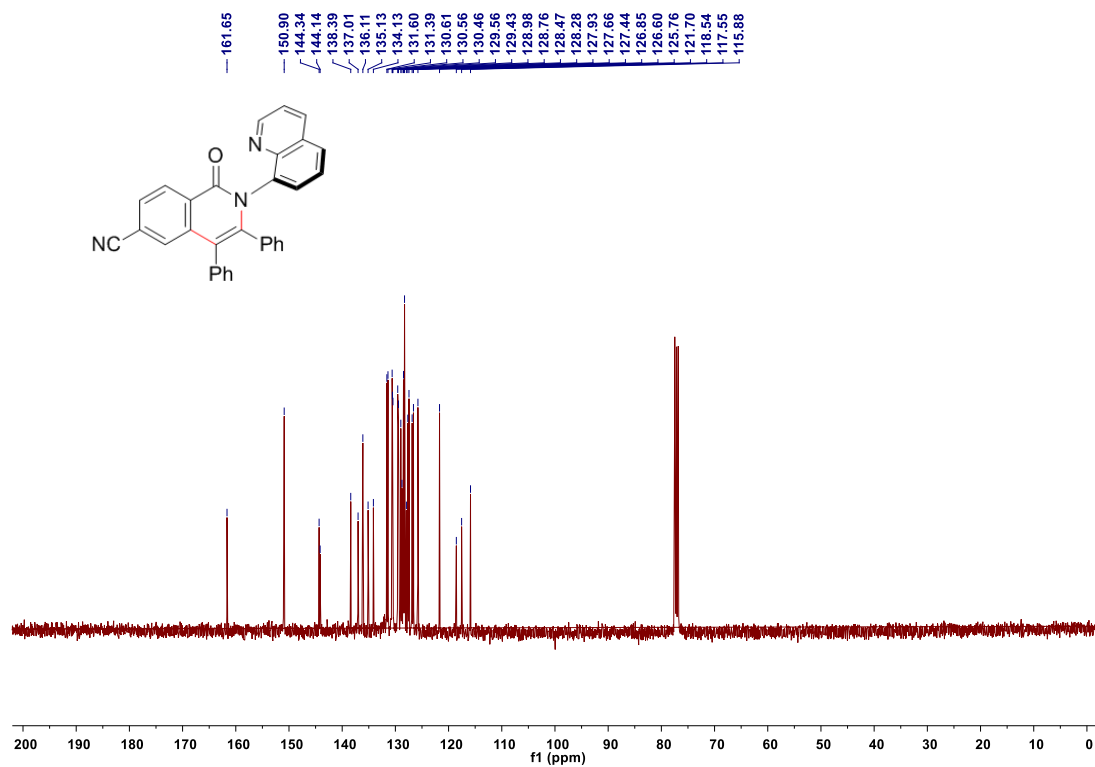
¹³C NMR Spectrum of **3ea**



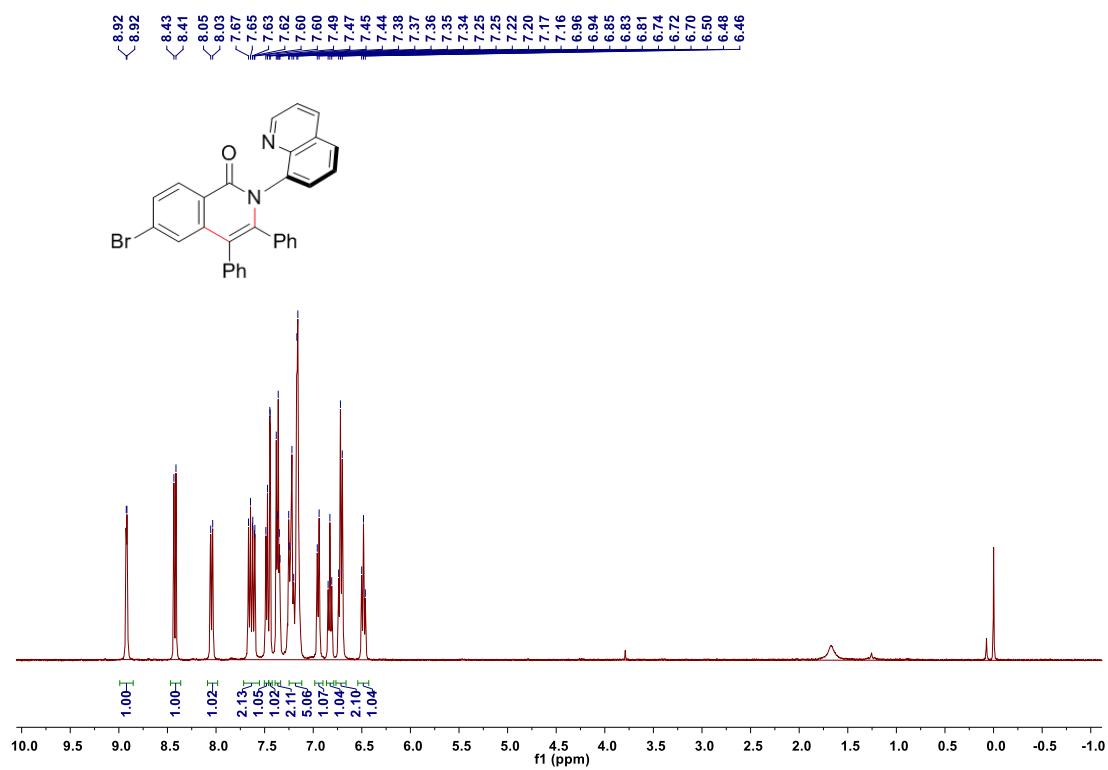
¹H NMR Spectrum of **3fa**



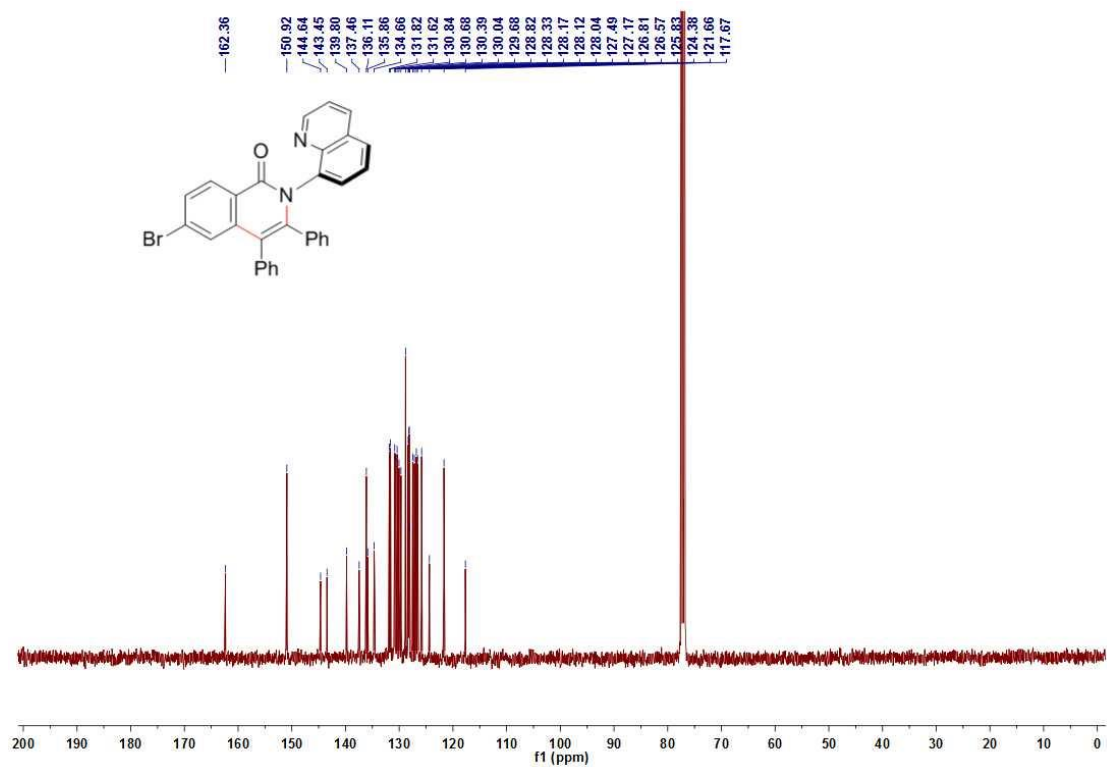
¹³C NMR Spectrum of **3fa**



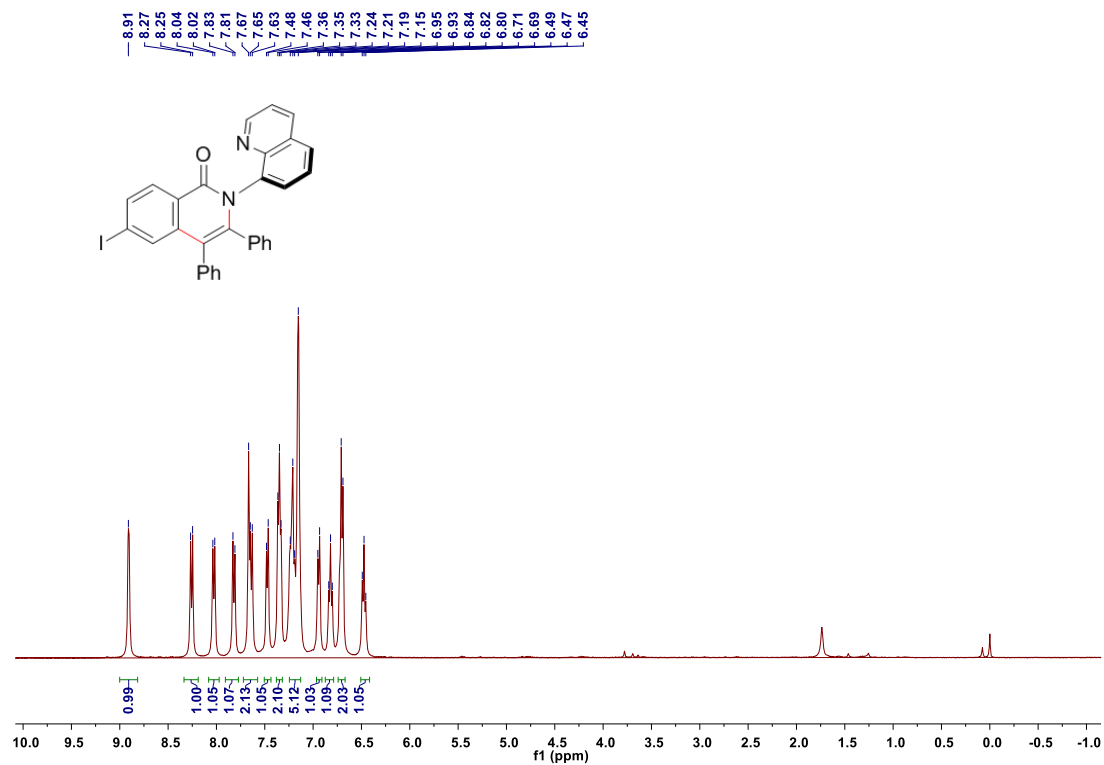
¹H NMR Spectrum of **3ga**



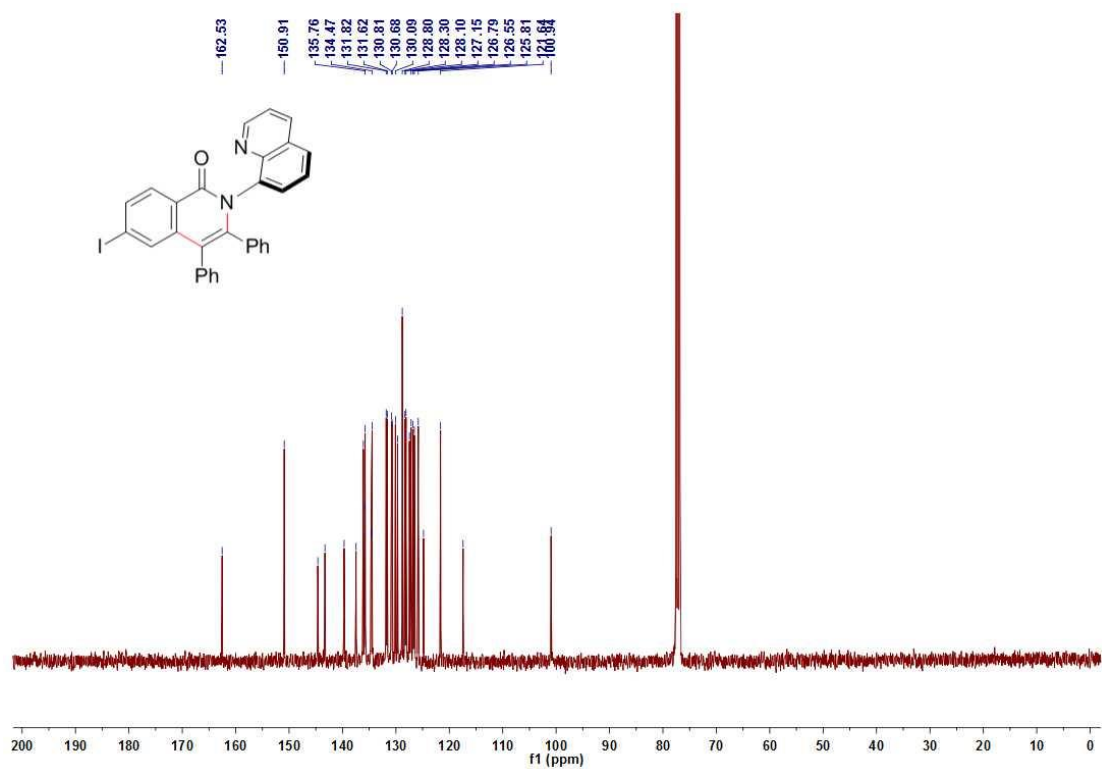
¹³C NMR Spectrum of **3ga**



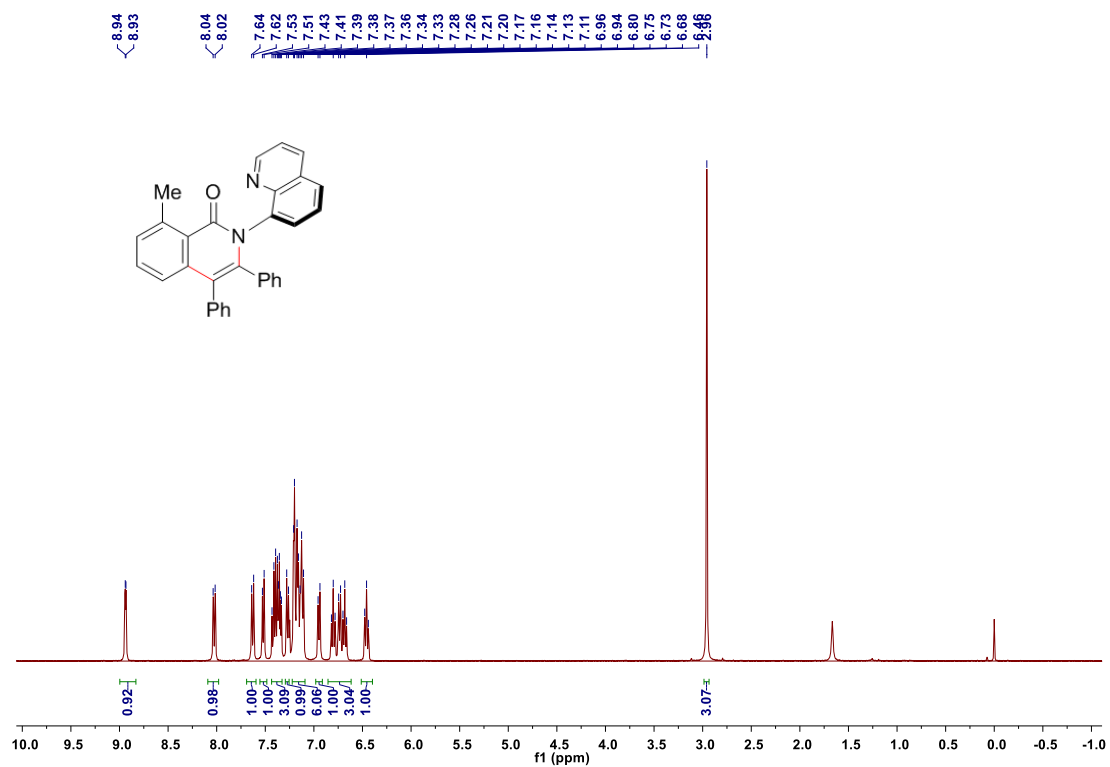
¹H NMR Spectrum of **3ha**



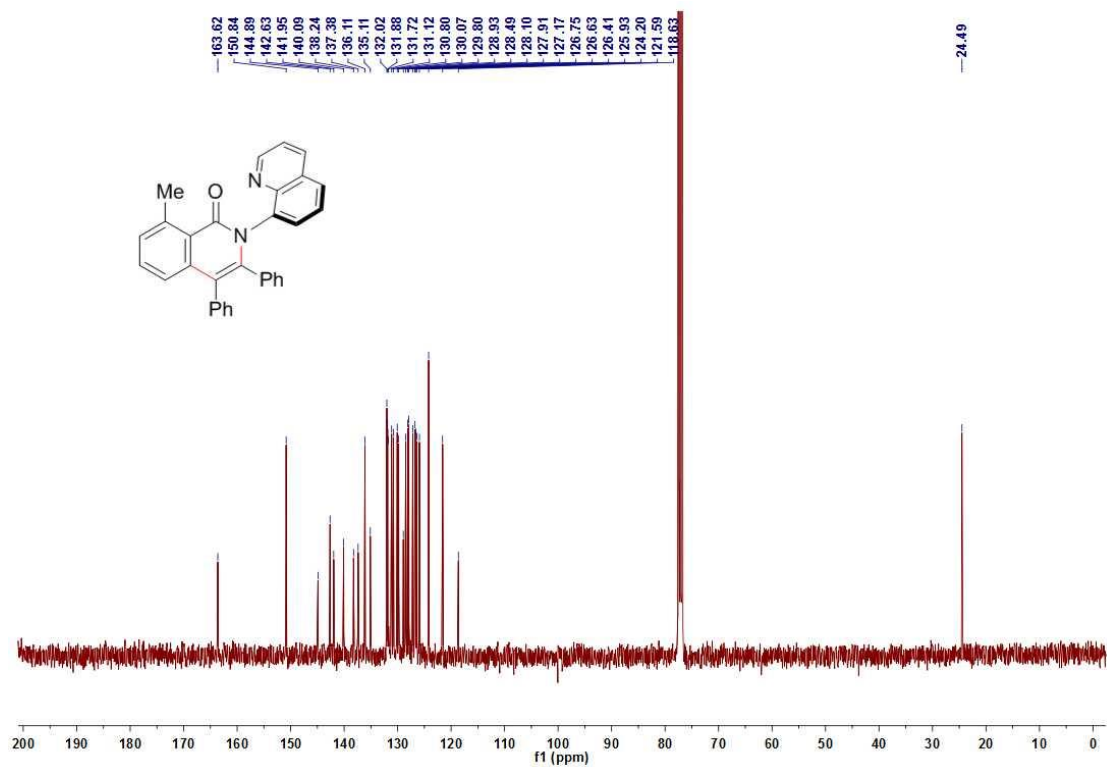
¹³C NMR Spectrum of **3ha**



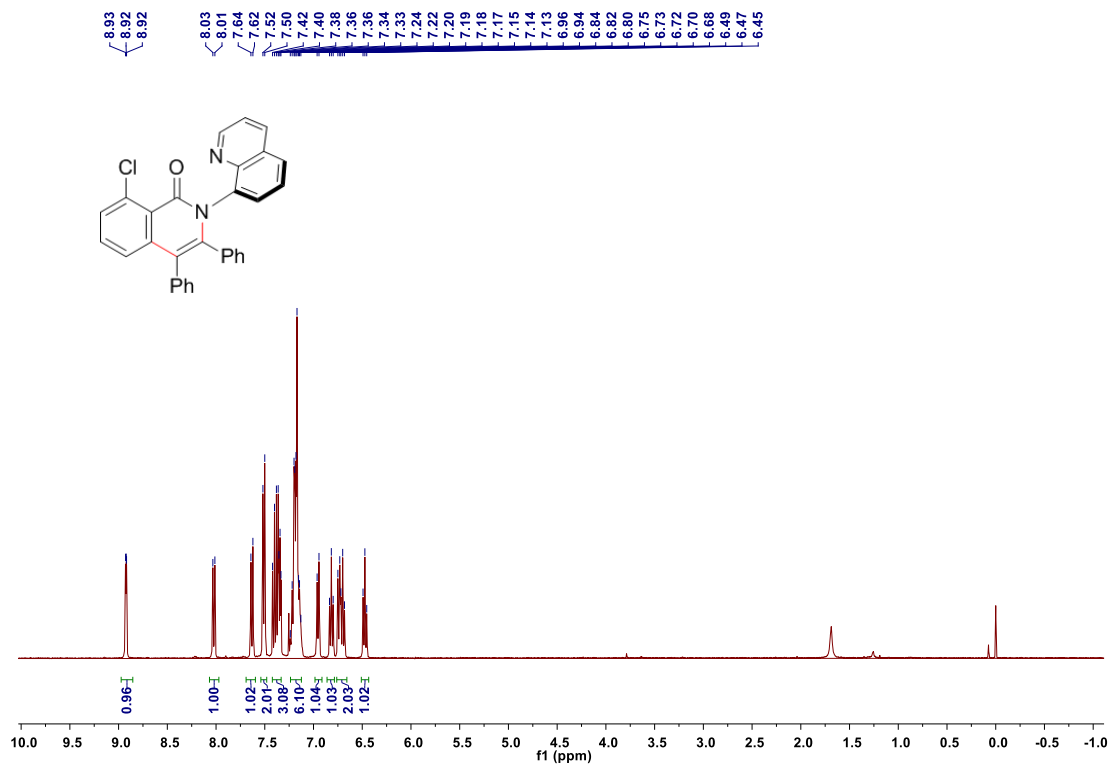
¹H NMR Spectrum of **3ia**



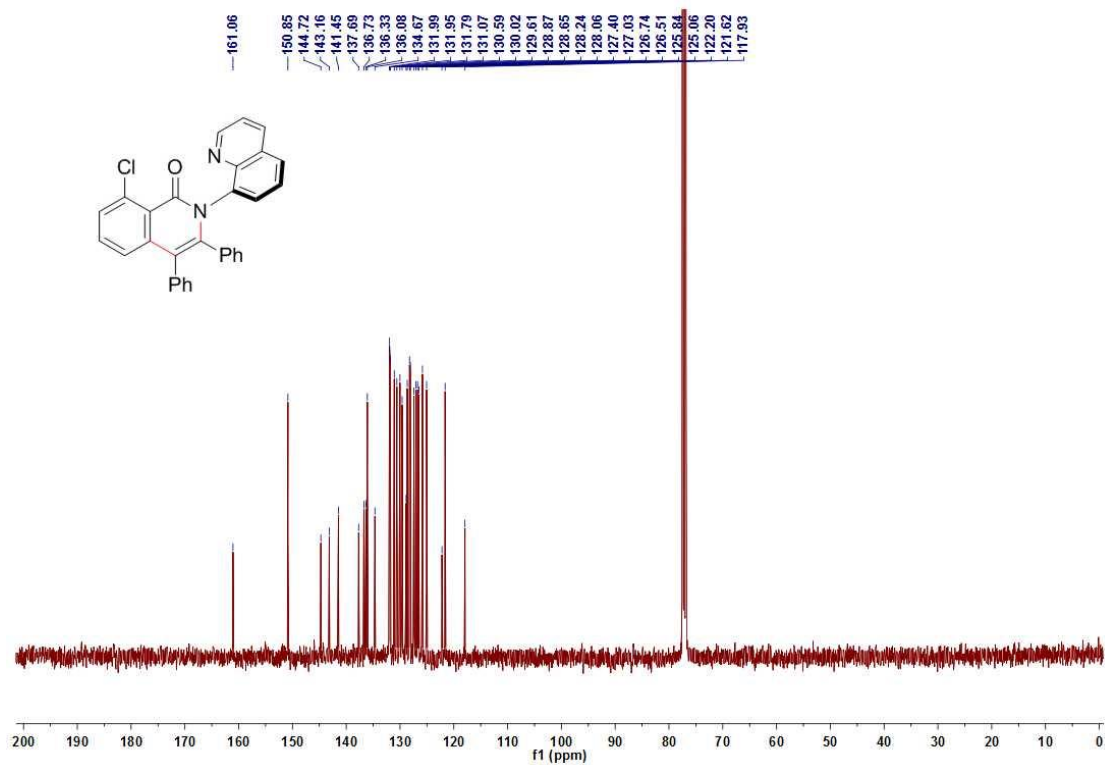
¹³C NMR Spectrum of **3ia**



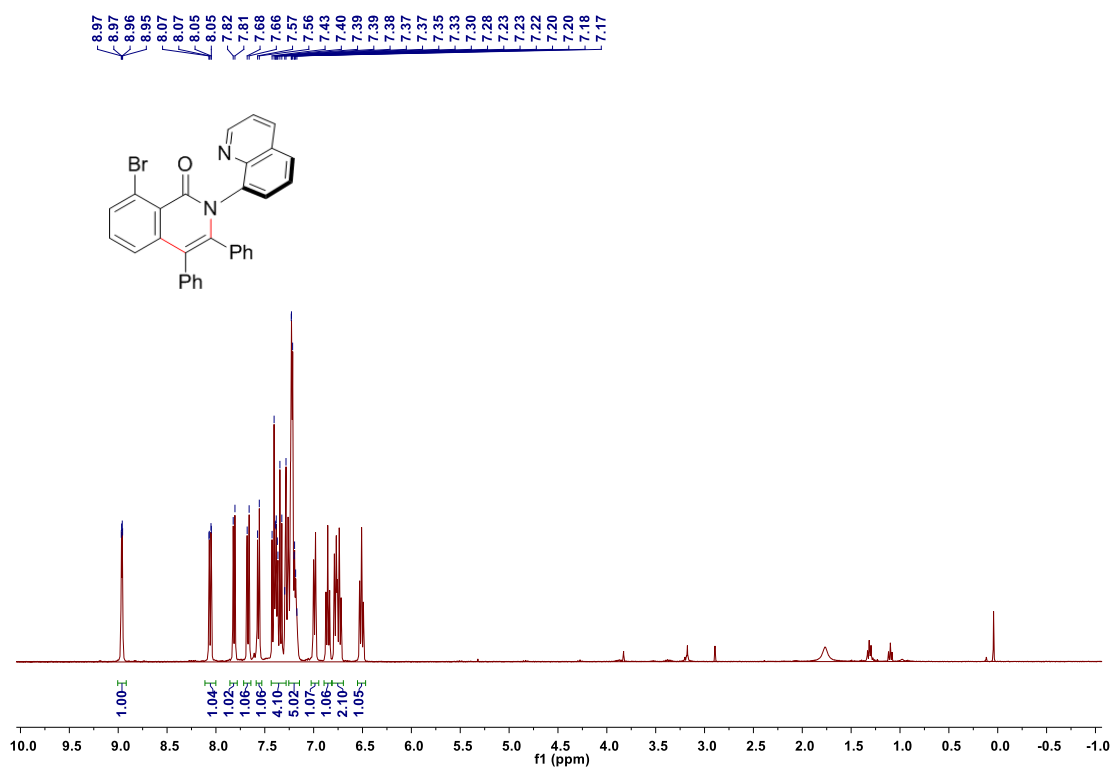
¹H NMR Spectrum of 3ja



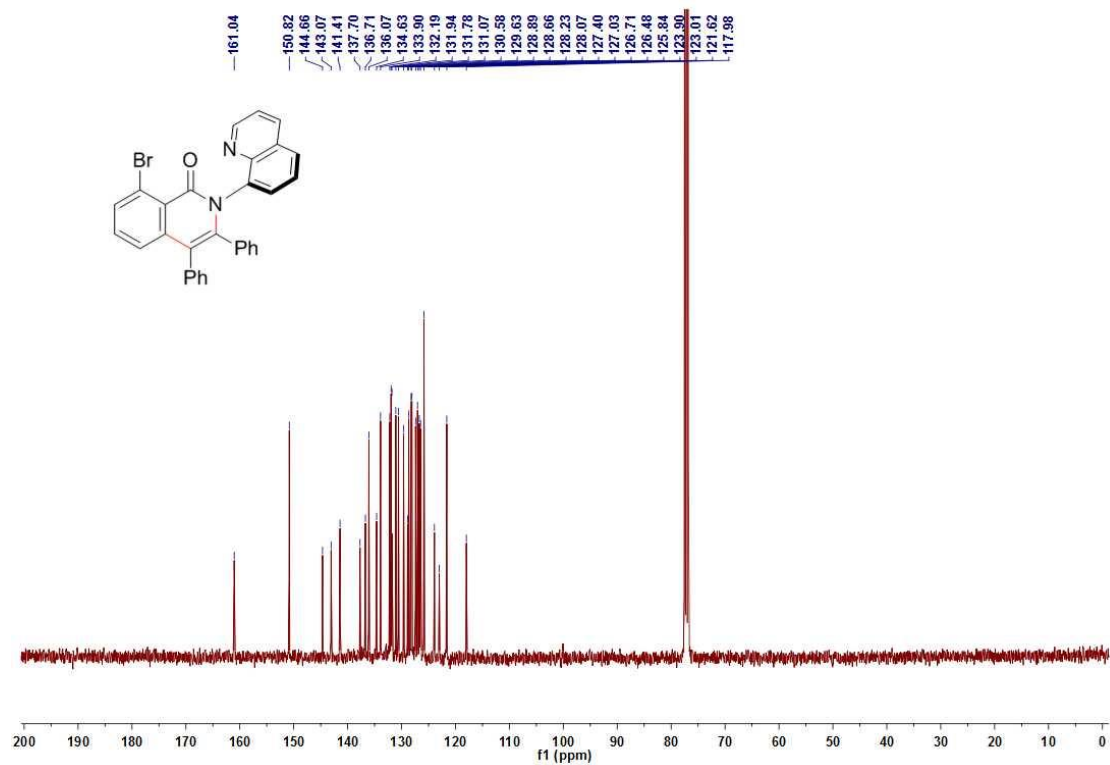
¹³C NMR Spectrum of 3ja



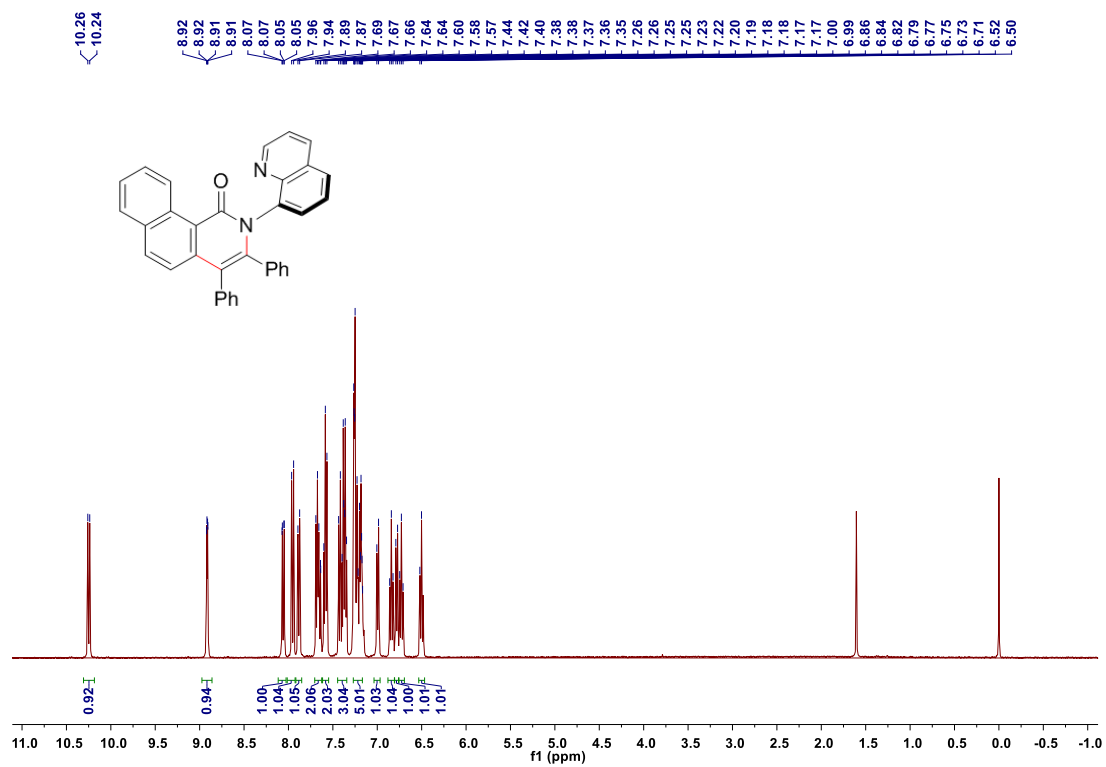
¹H NMR Spectrum of **3ka**



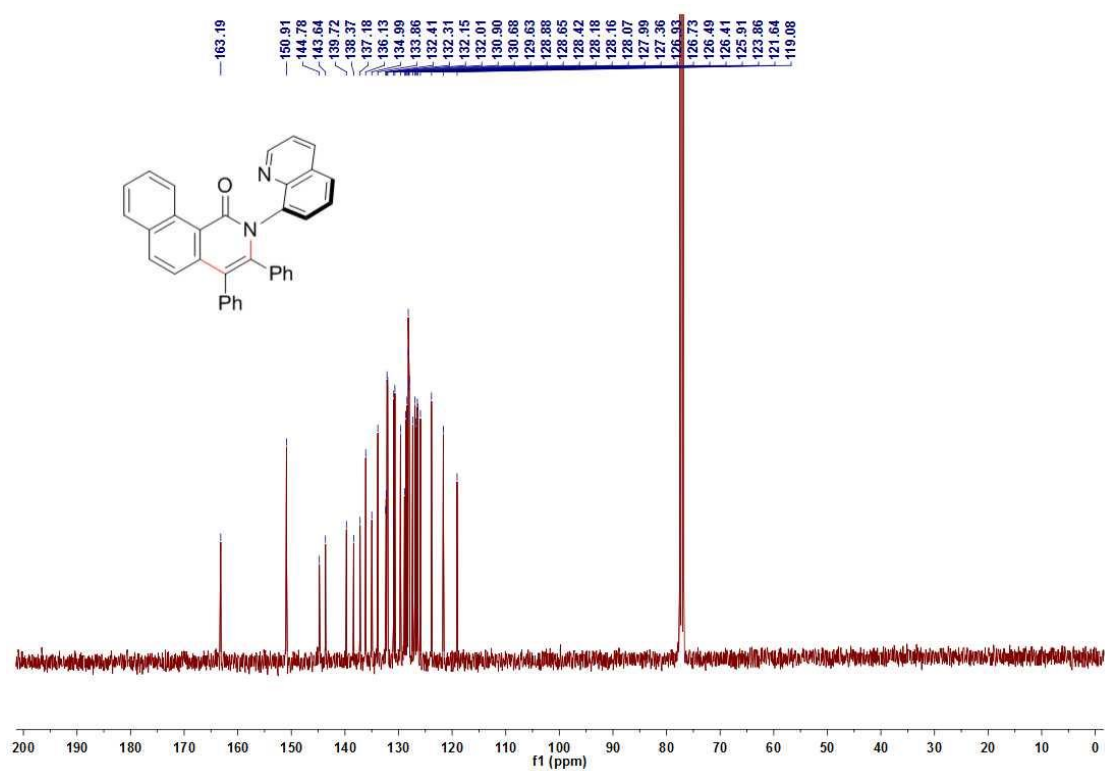
¹³C NMR Spectrum of **3ka**



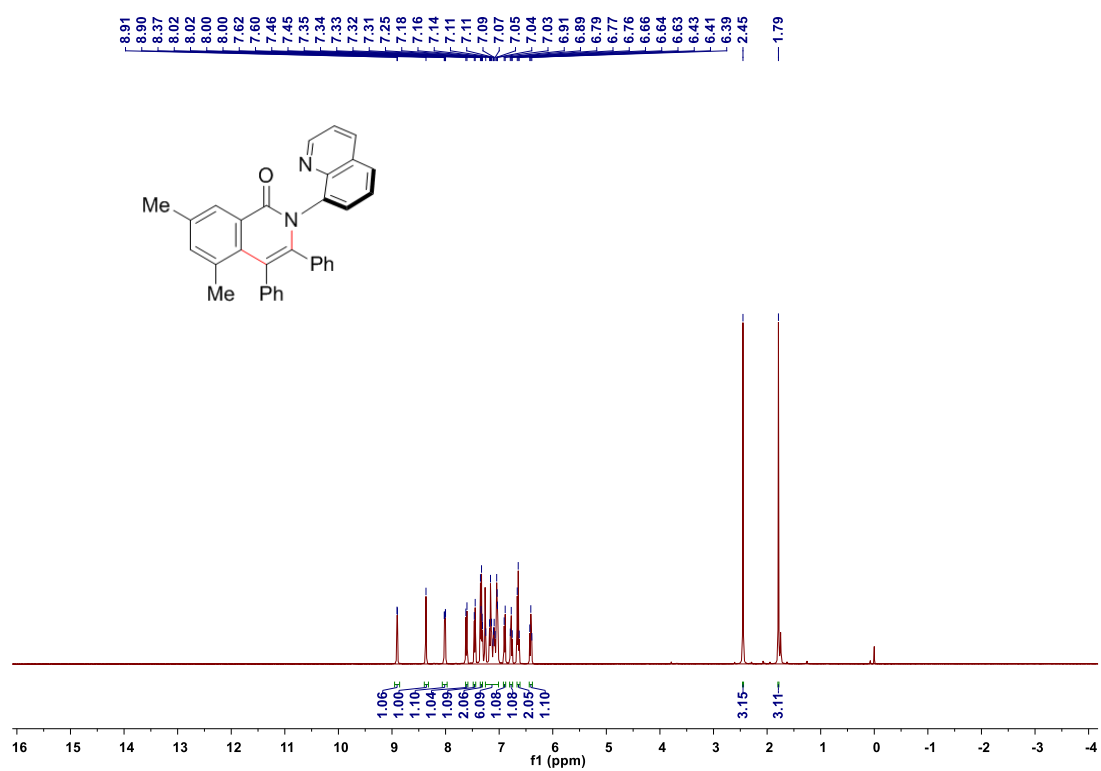
¹H NMR Spectrum of **3la**



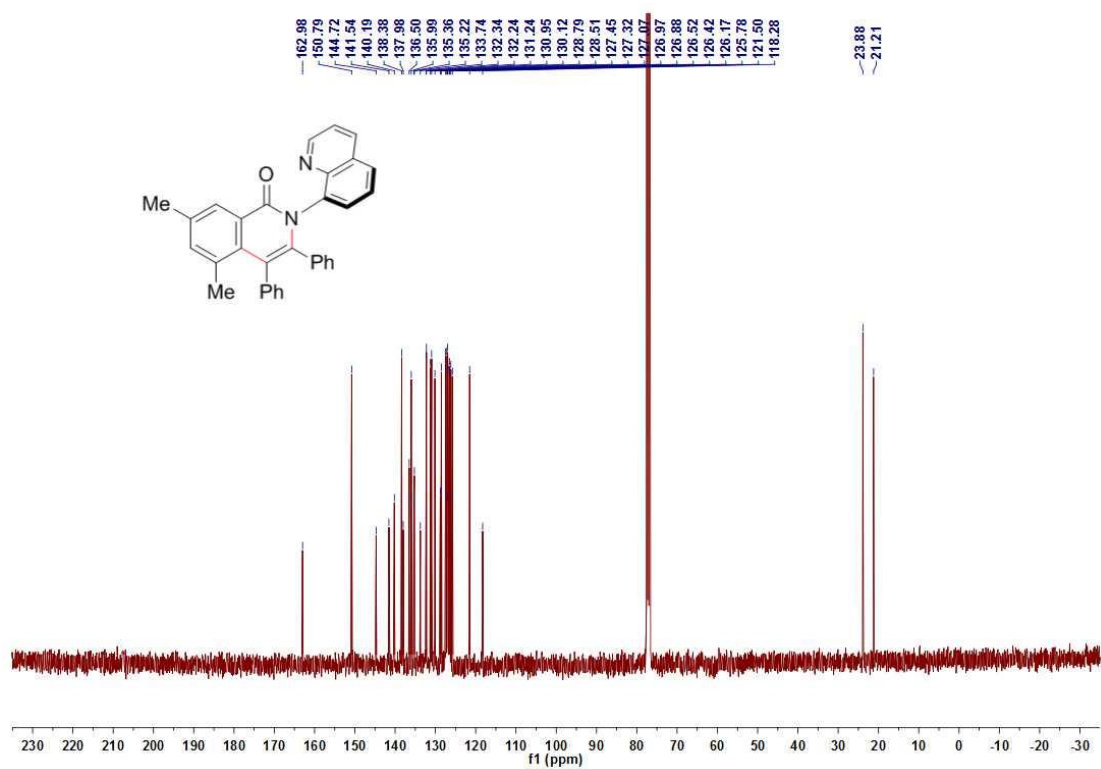
¹³C NMR Spectrum of **3la**



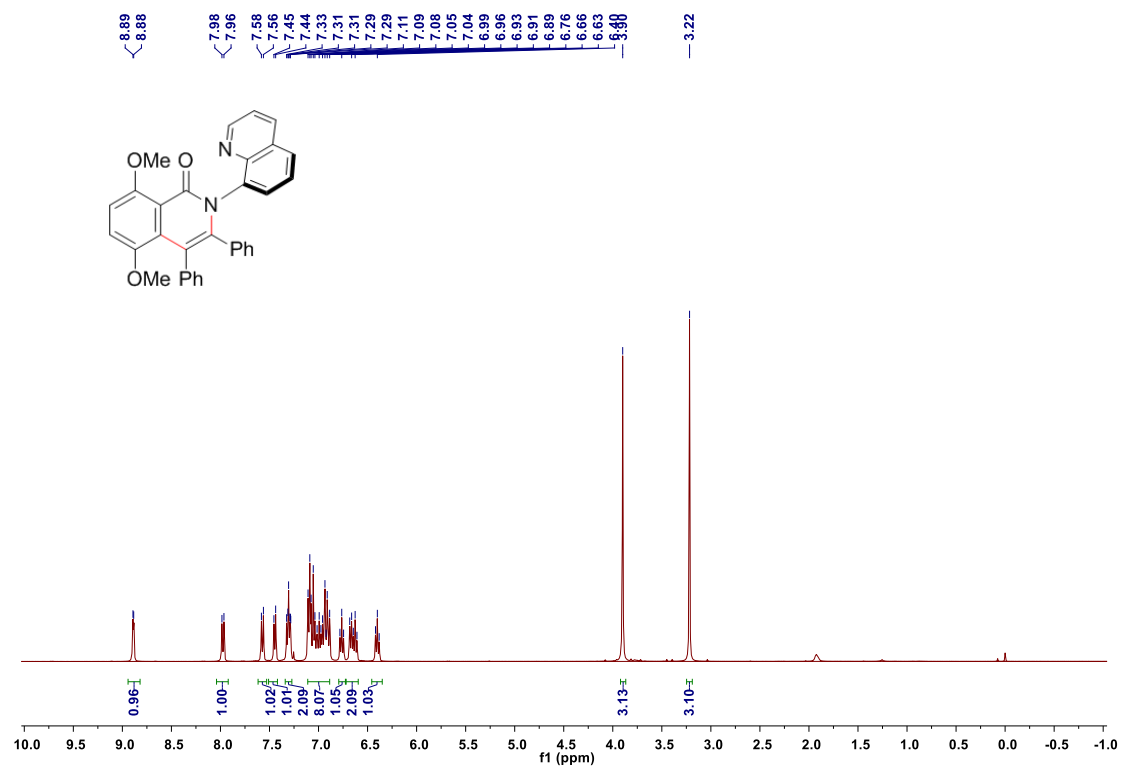
¹H NMR Spectrum of **3ma**



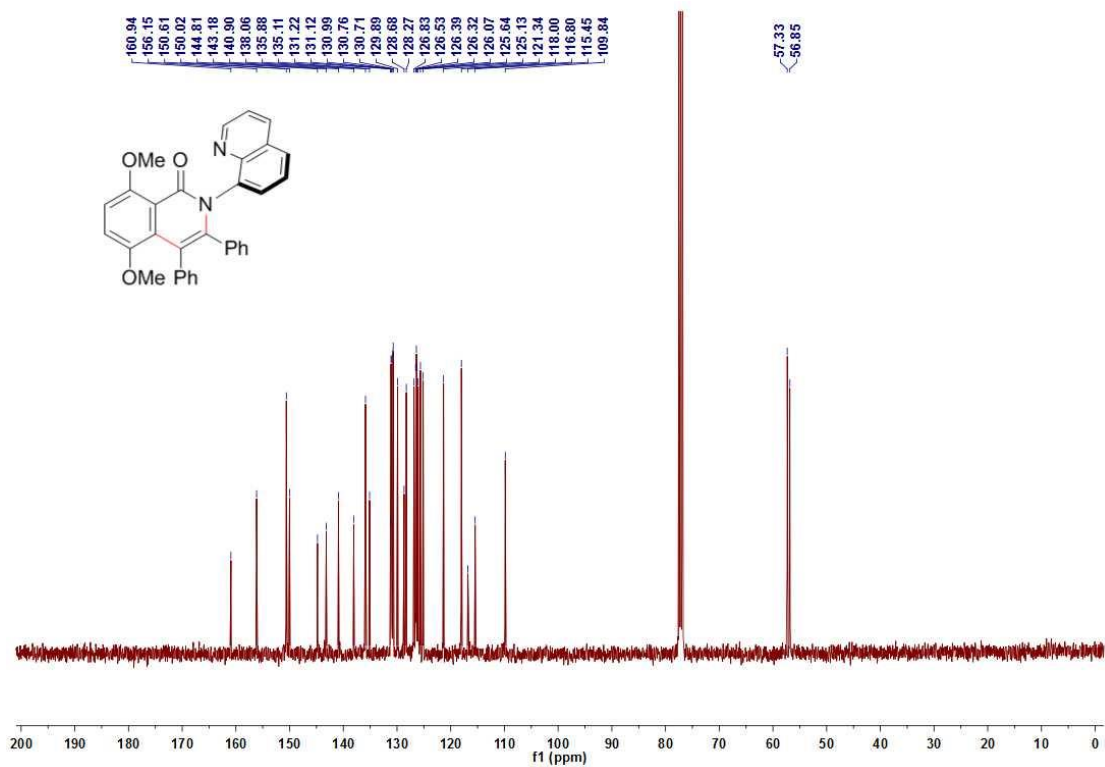
¹³C NMR Spectrum of **3ma**



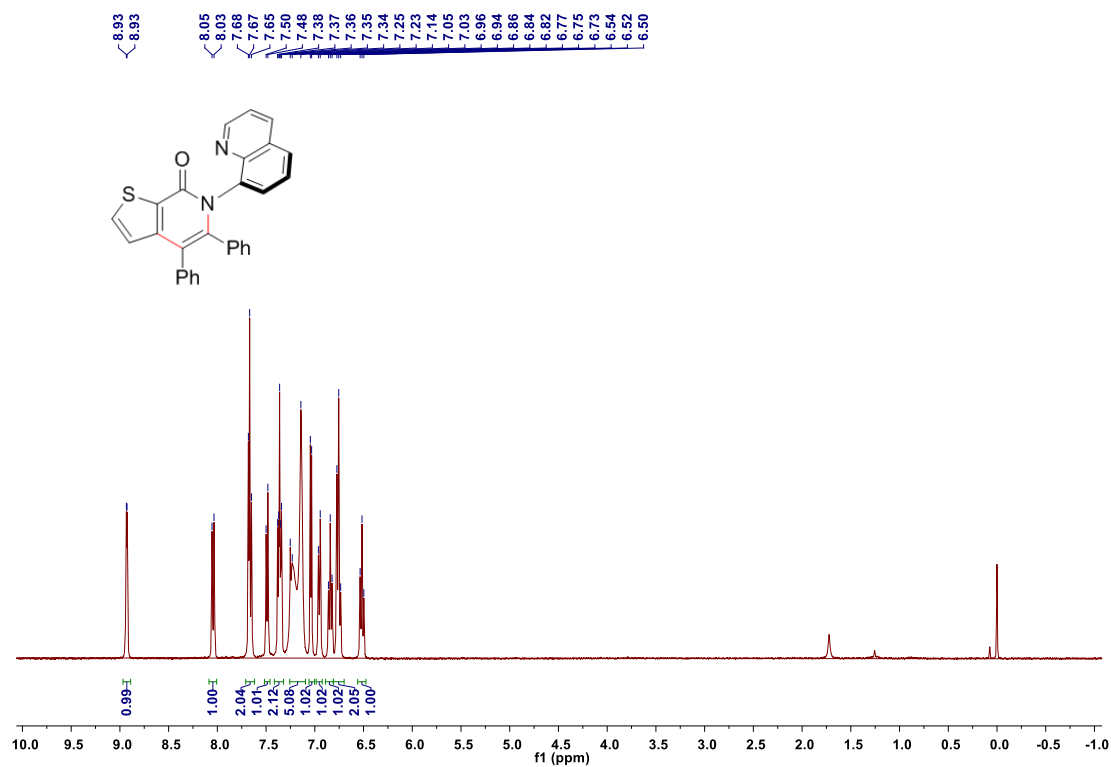
¹H NMR Spectrum of **3na**



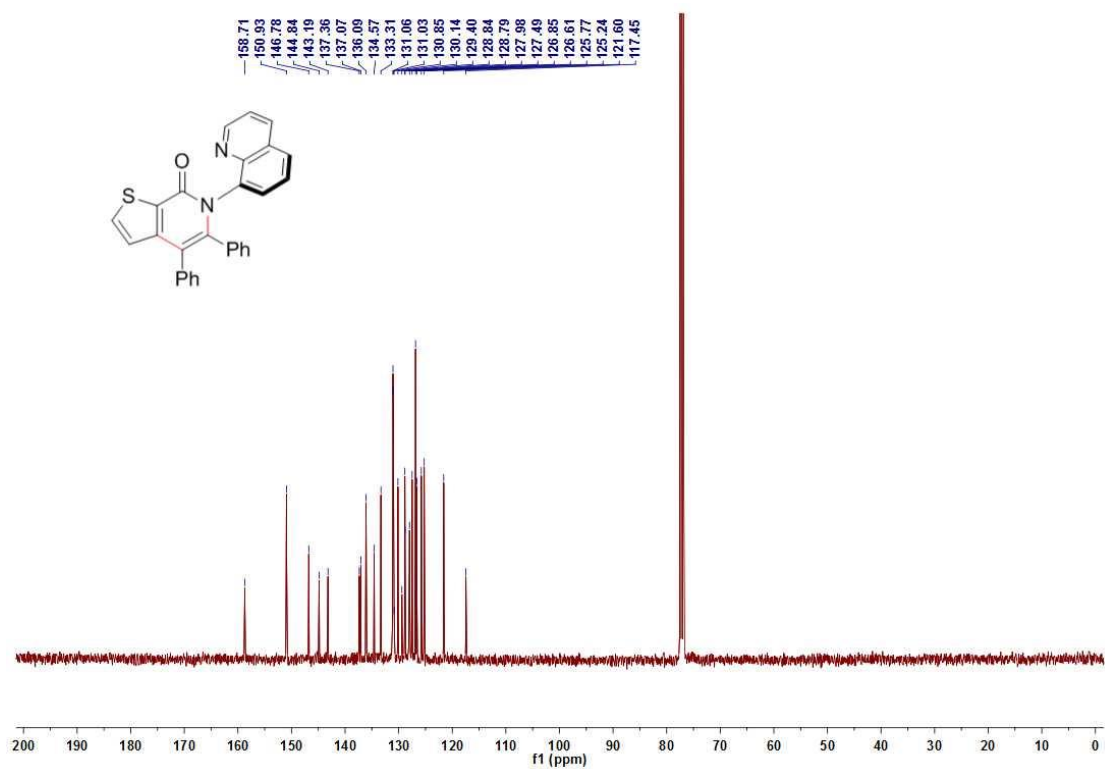
¹³C NMR Spectrum of **3na**



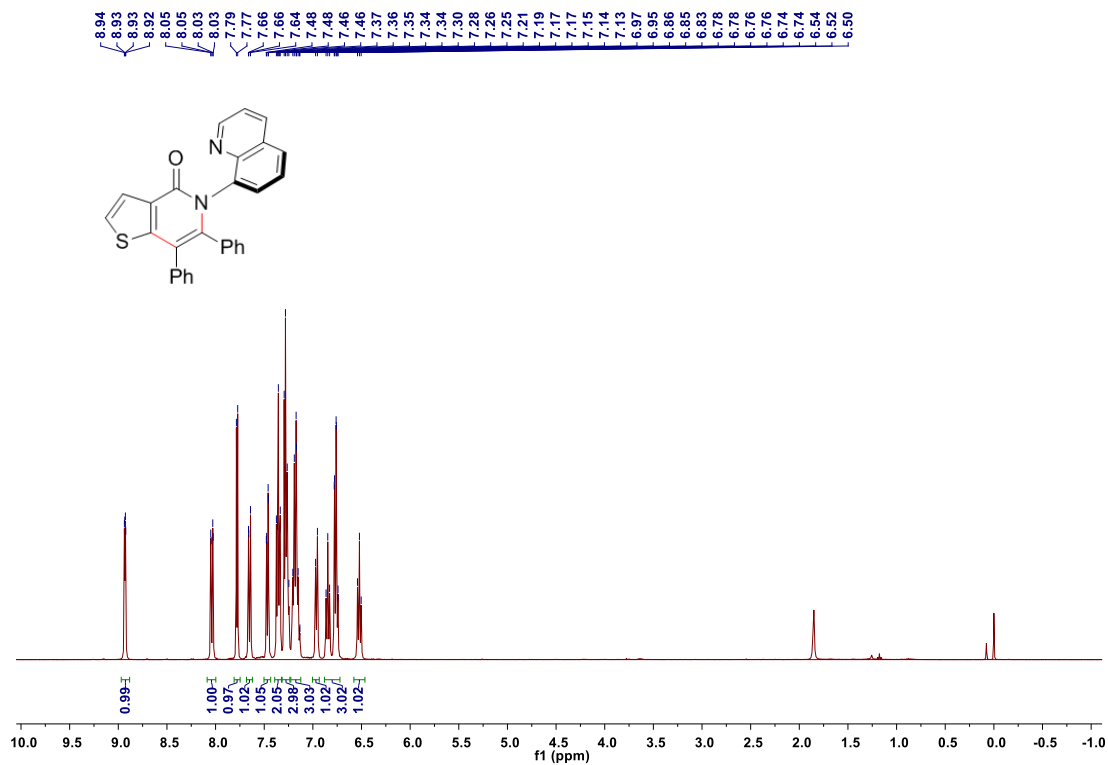
¹H NMR Spectrum of **30a**



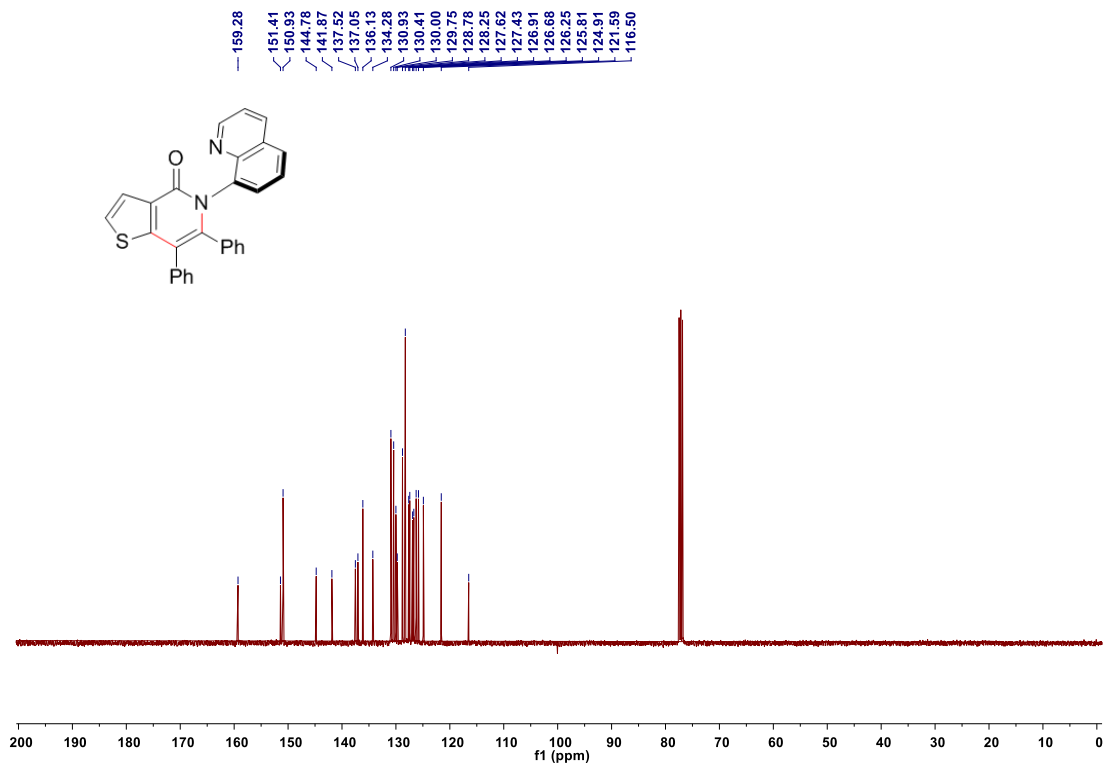
¹³C NMR Spectrum of **30a**



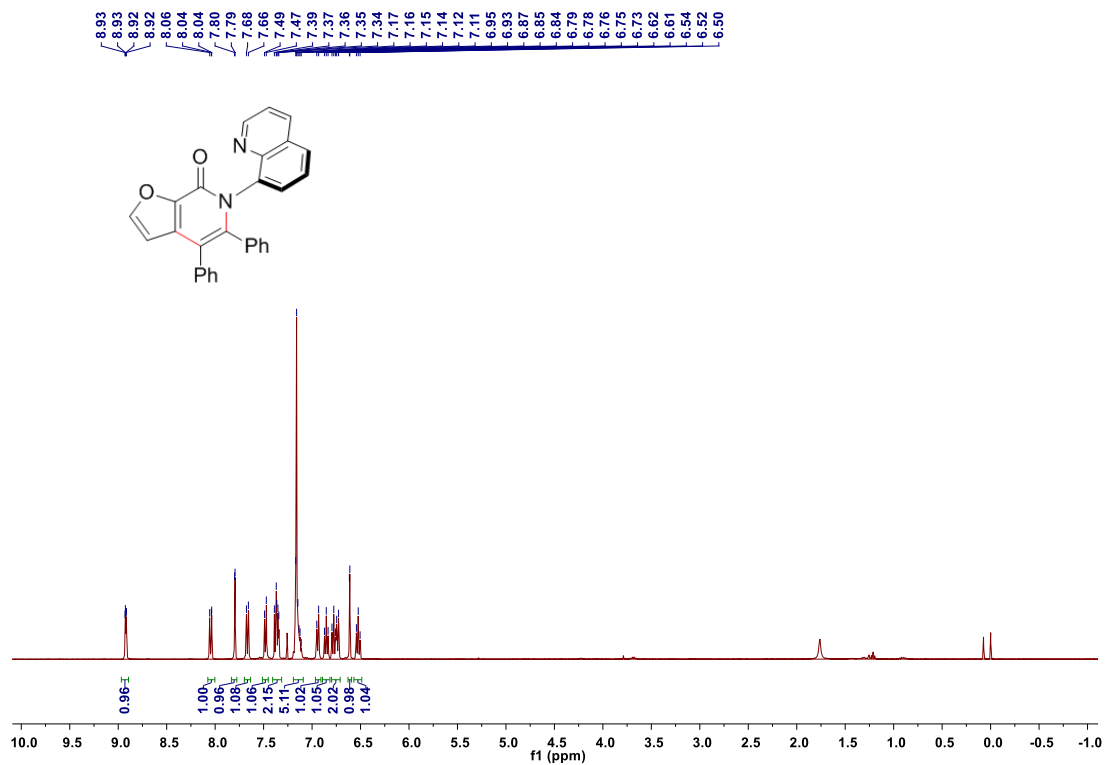
¹H NMR Spectrum of **3pa**



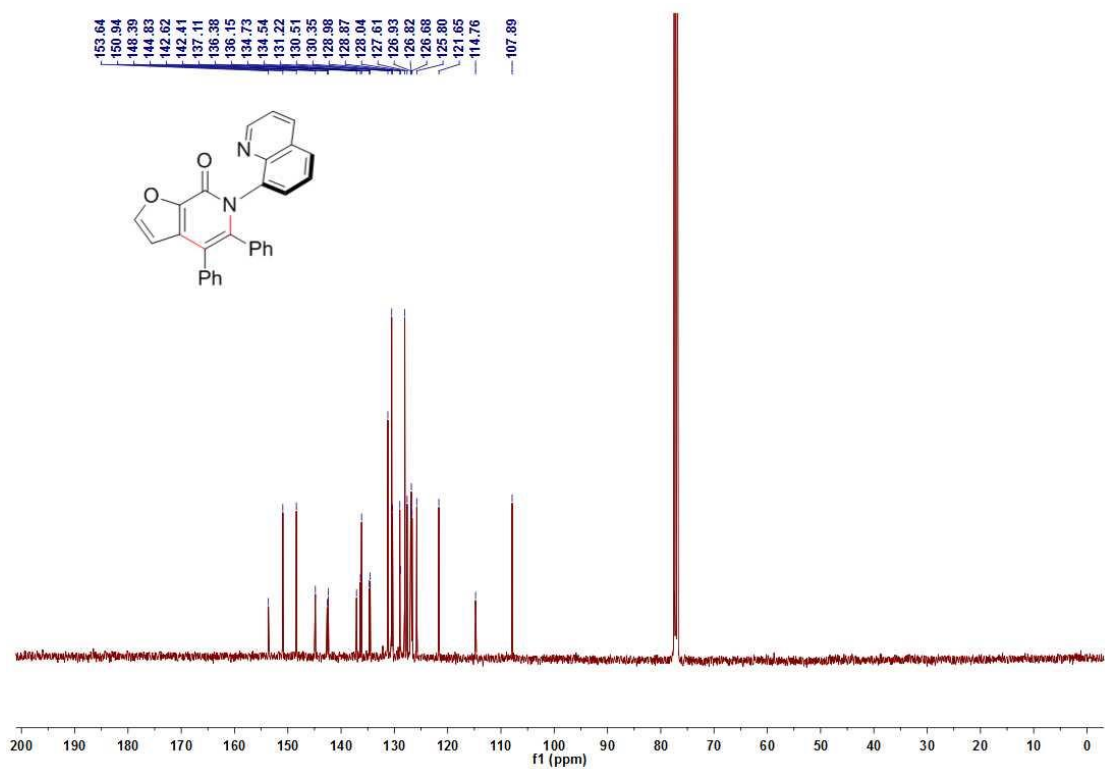
¹³C NMR Spectrum of **3pa**



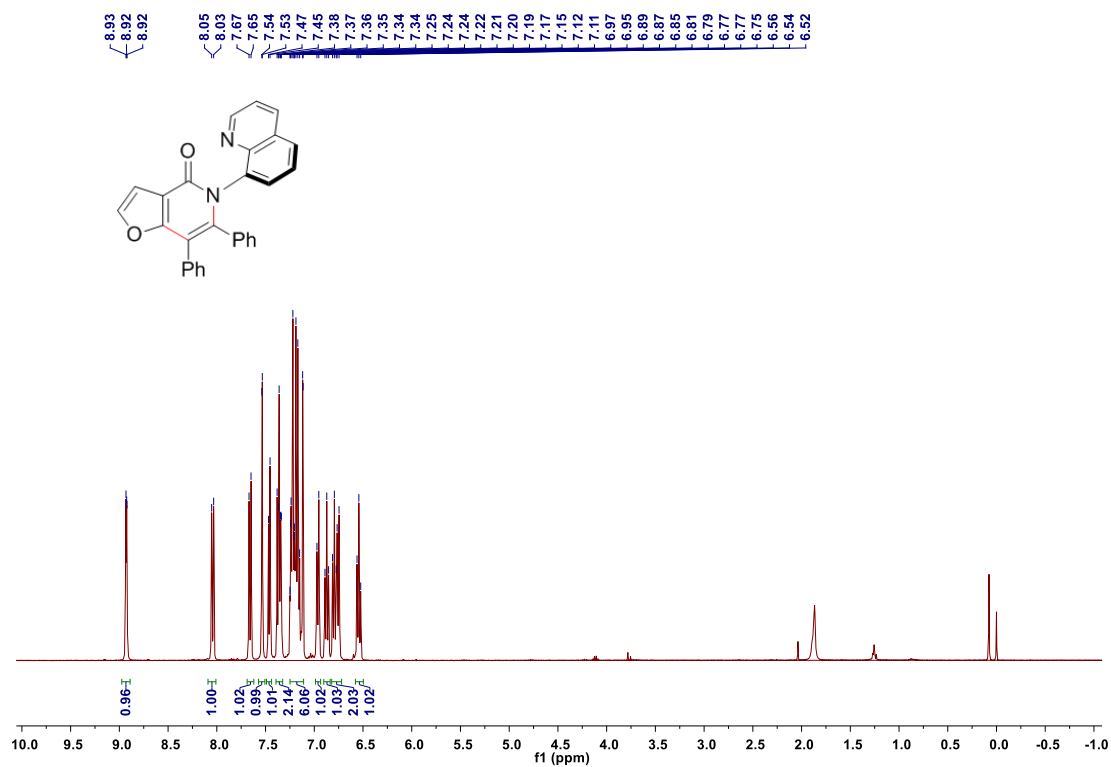
¹H NMR Spectrum of **3qa**



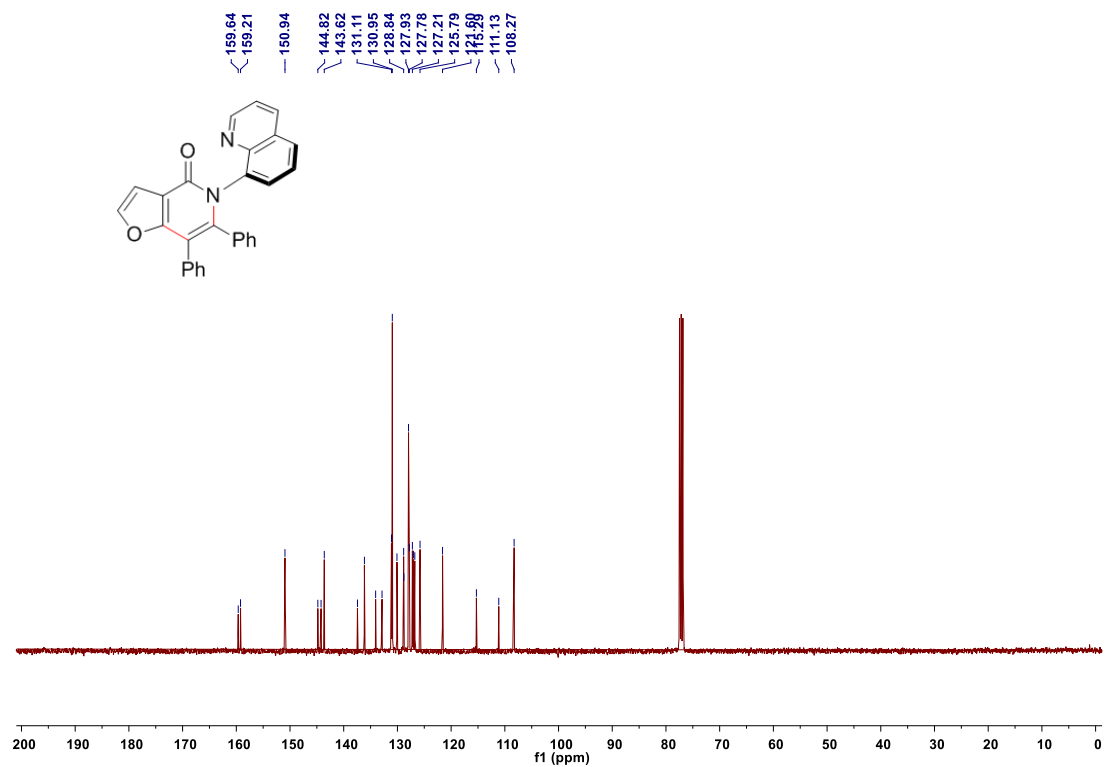
¹³C NMR Spectrum of **3qa**



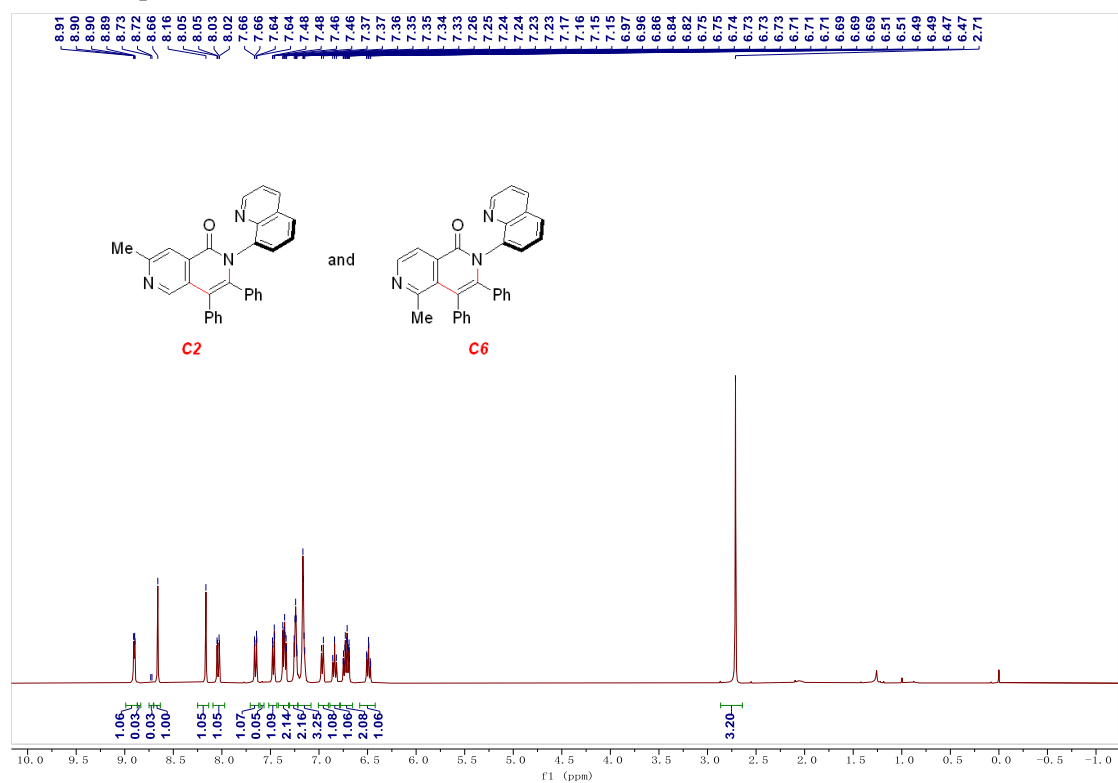
¹H NMR Spectrum of **3ra**



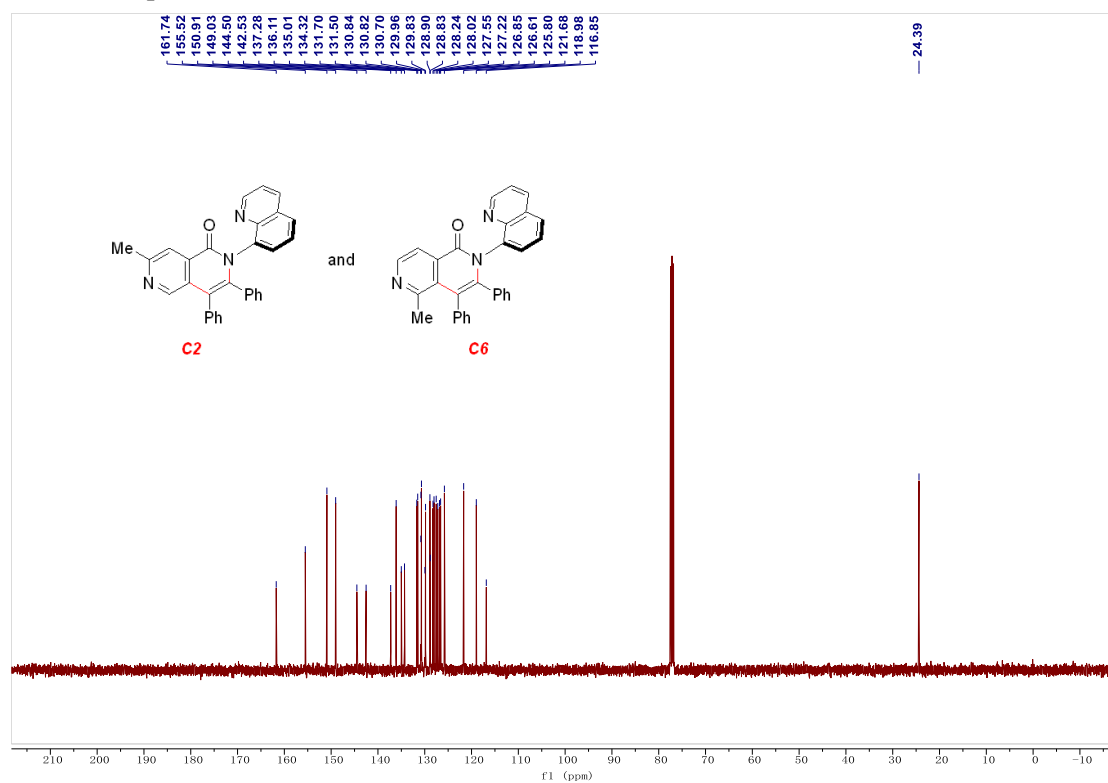
¹³C NMR Spectrum of **3ra**



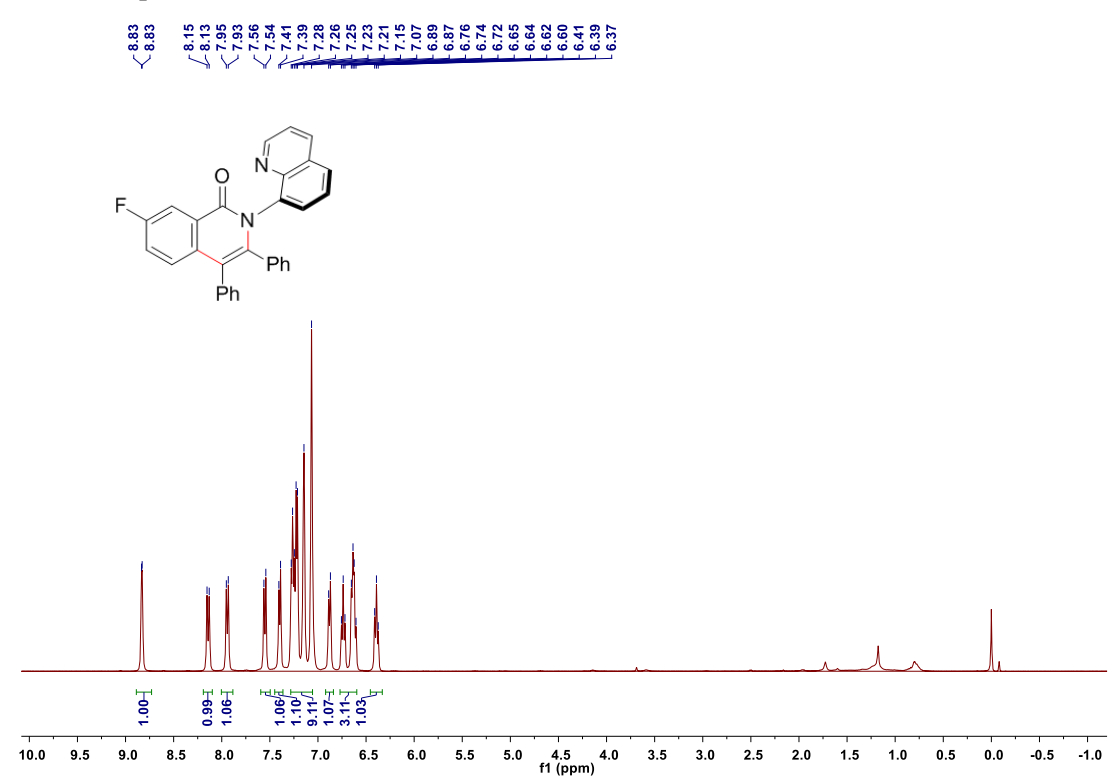
¹H NMR Spectrum of 3sa



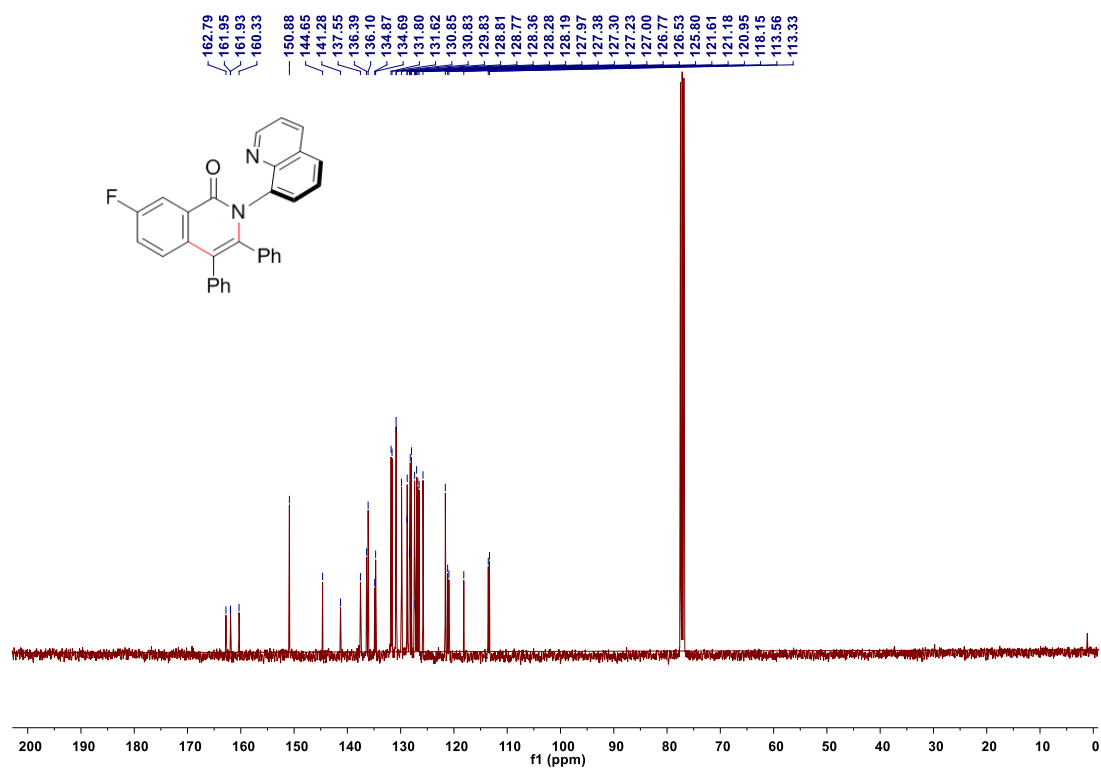
¹³C NMR Spectrum of **3sa**



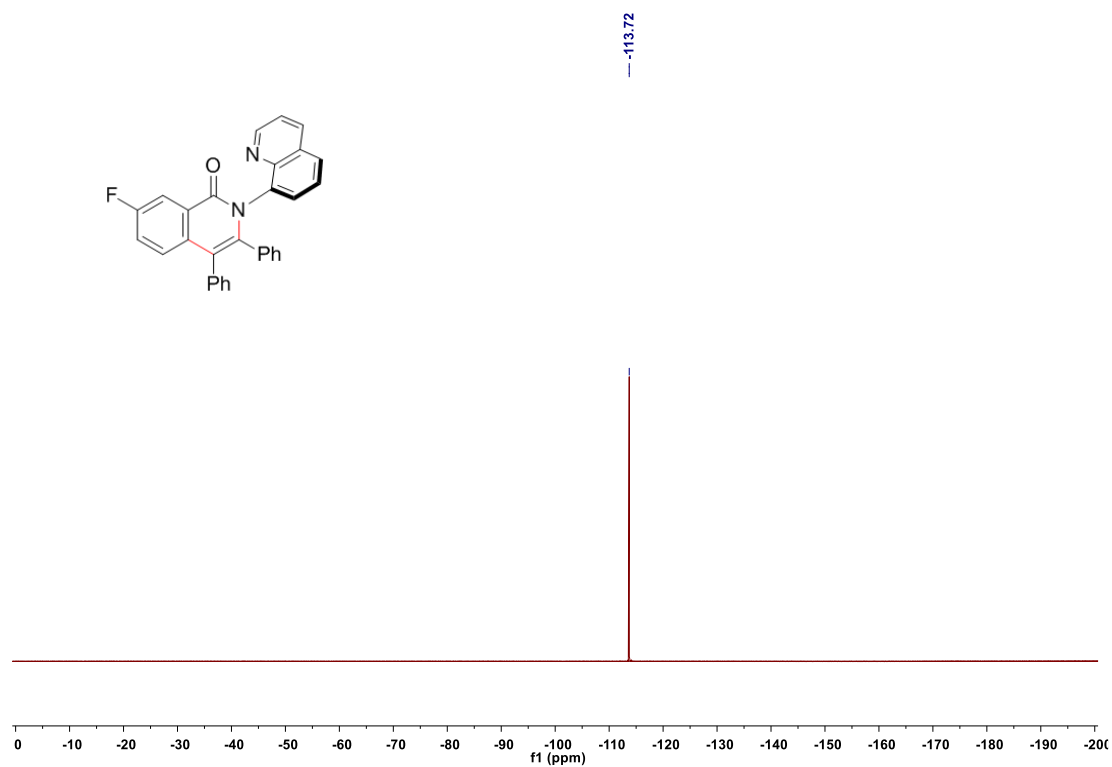
¹H NMR Spectrum of **3ta-C2**



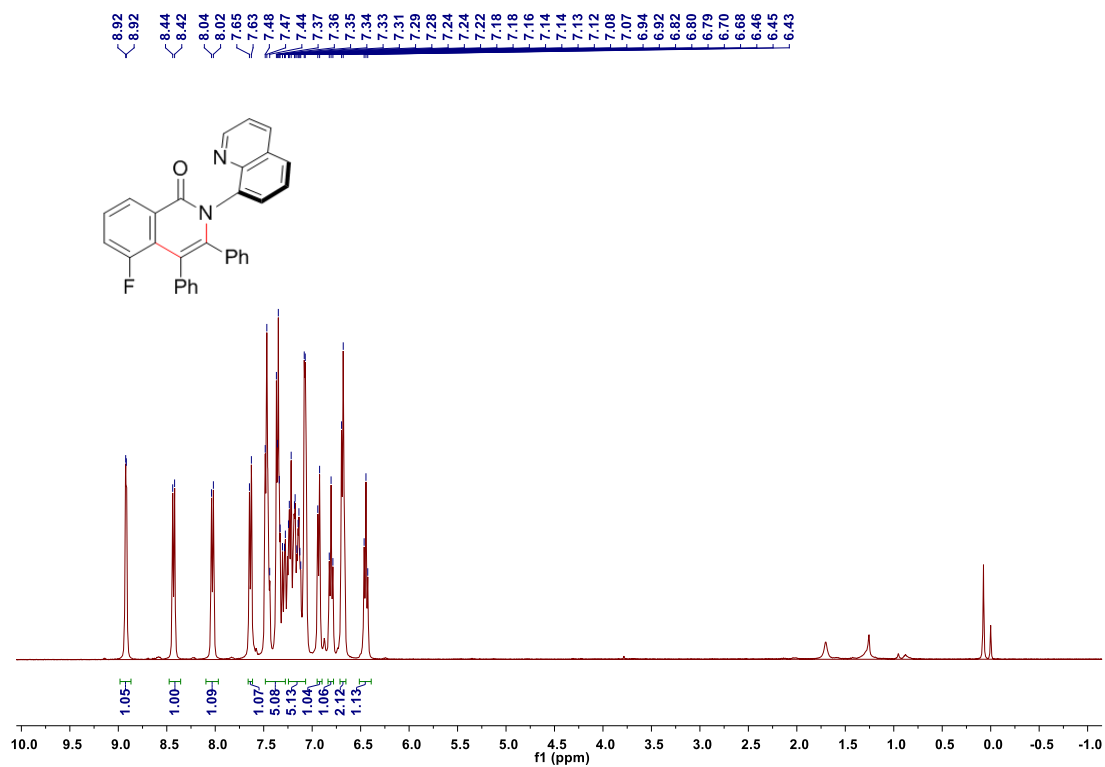
¹³C NMR Spectrum of **3ta-C2**



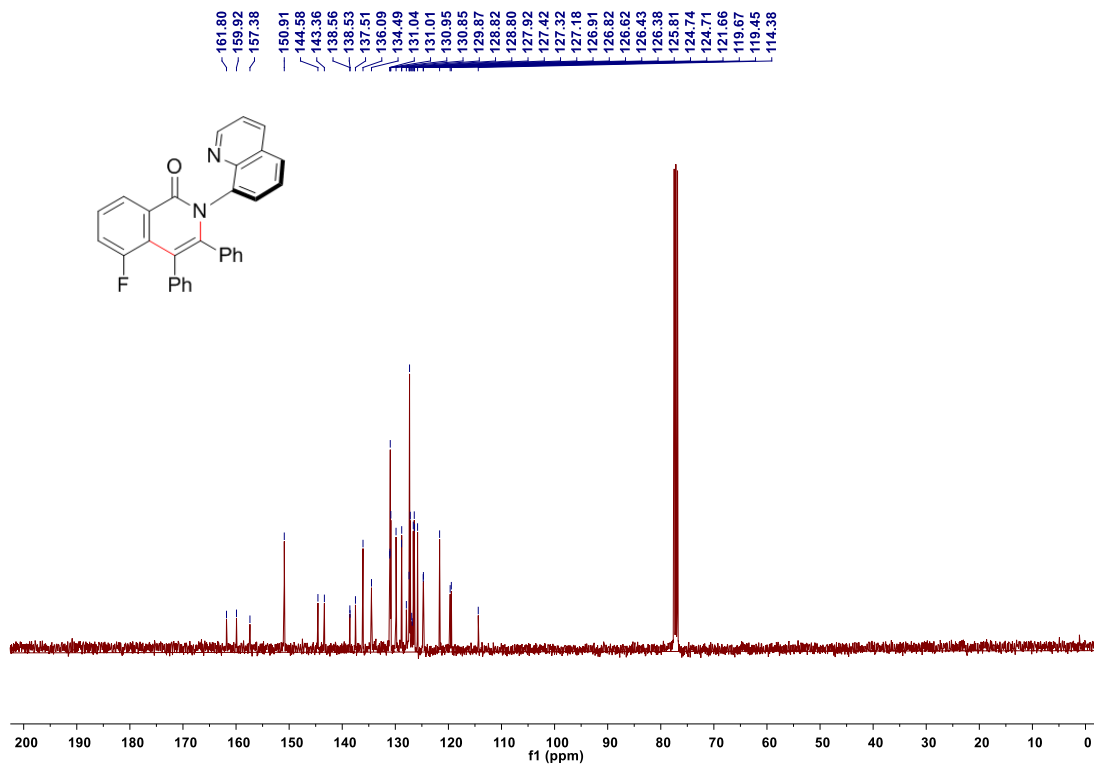
¹⁹F NMR Spectrum of **3ta-C2**



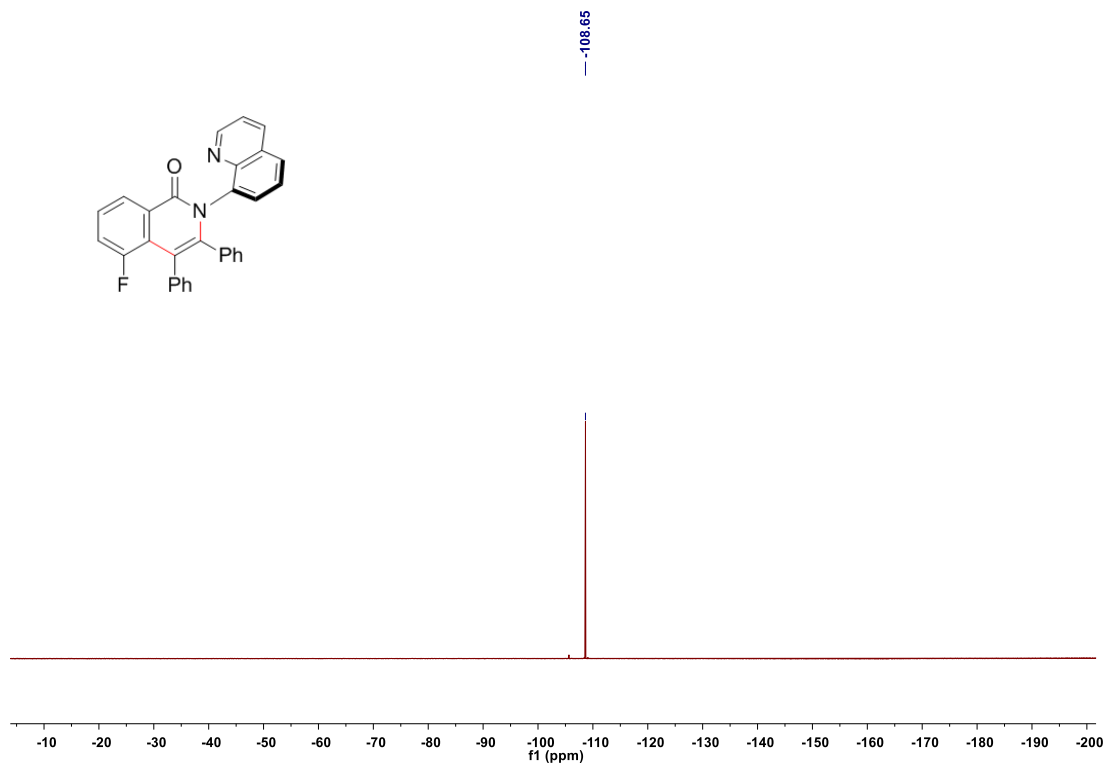
¹H NMR Spectrum of **3ta-C6**



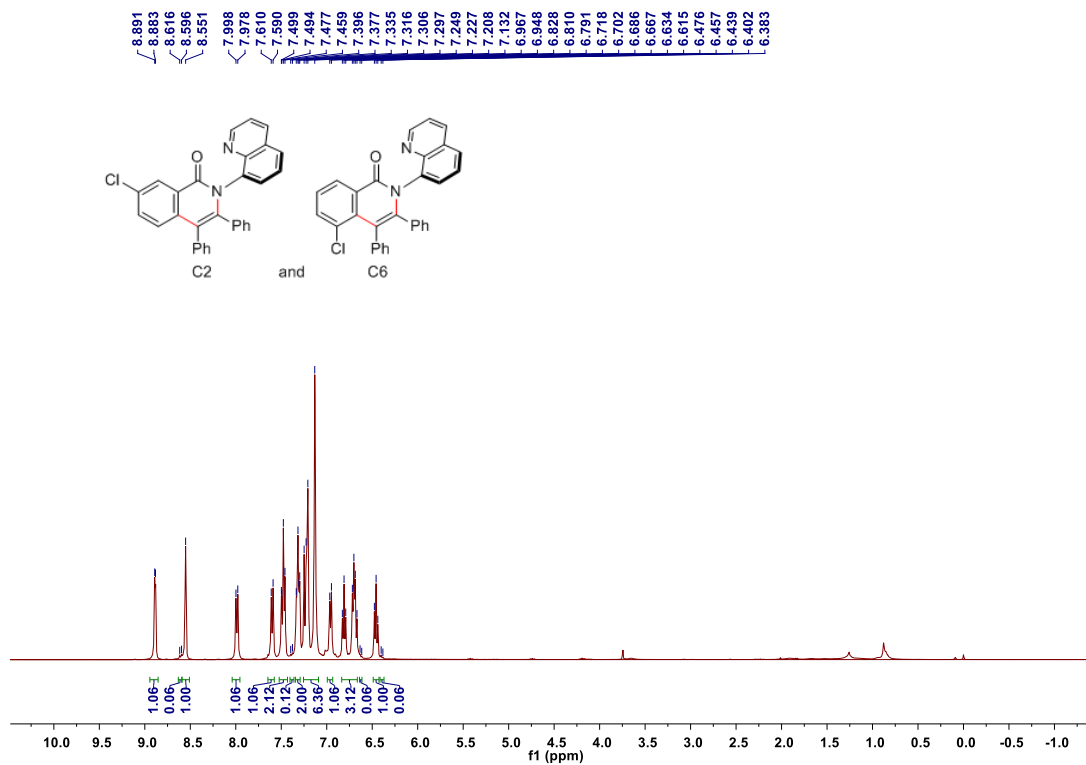
¹³C NMR Spectrum of **3ta-C6**



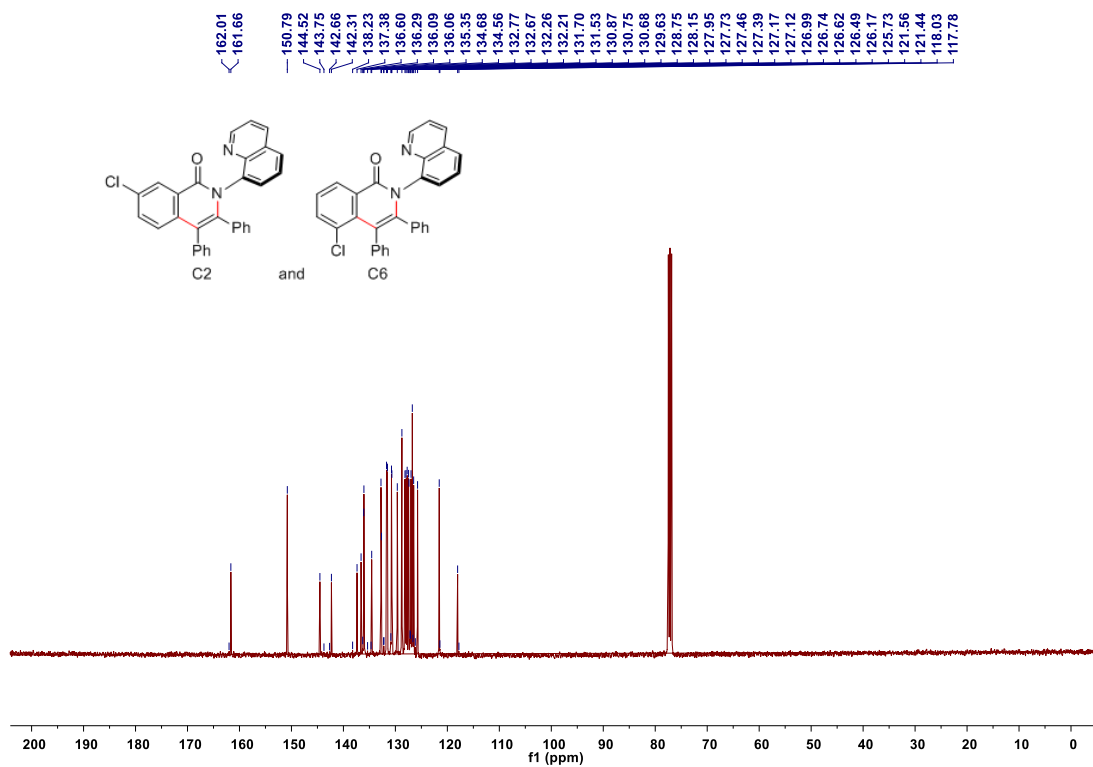
¹⁹F NMR Spectrum of **3ta-C6**



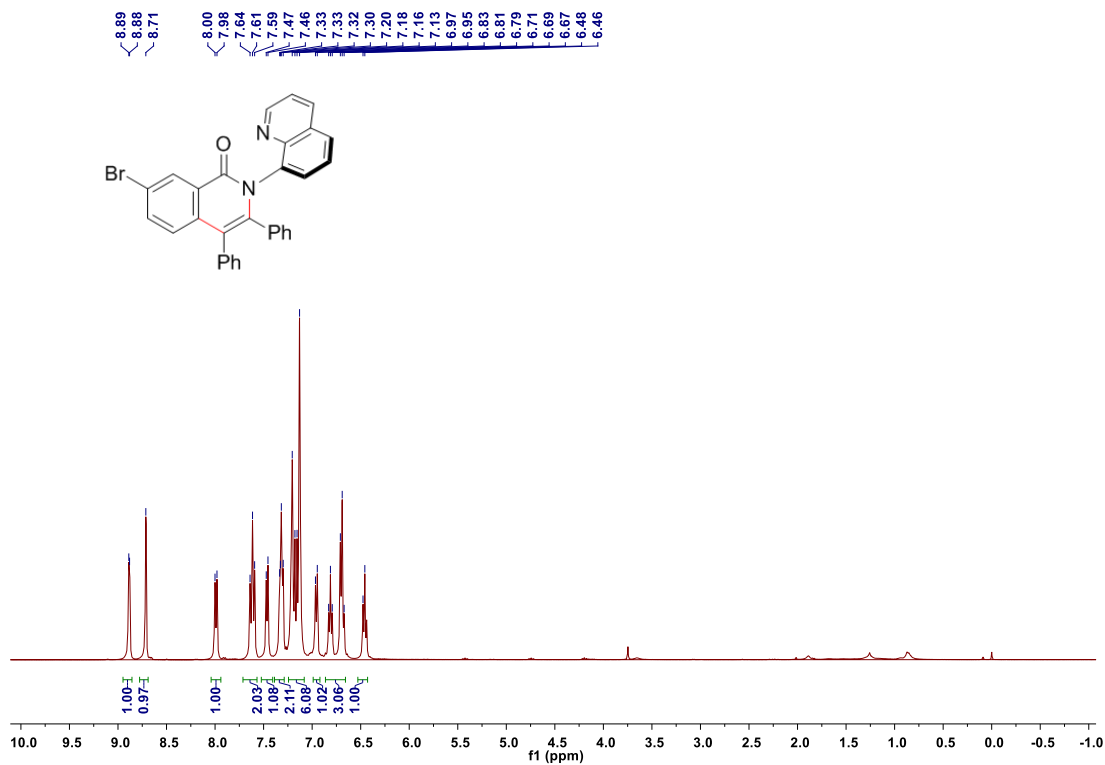
¹H NMR Spectrum of **3ua**



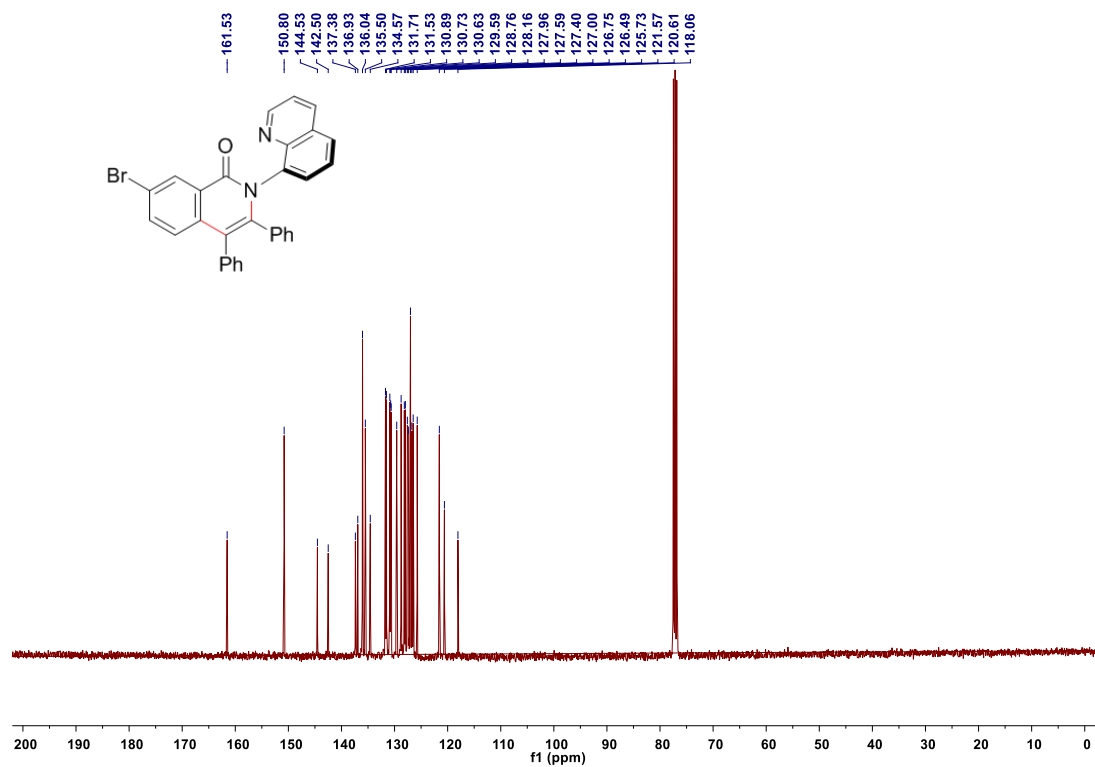
¹³C NMR Spectrum of **3ua**



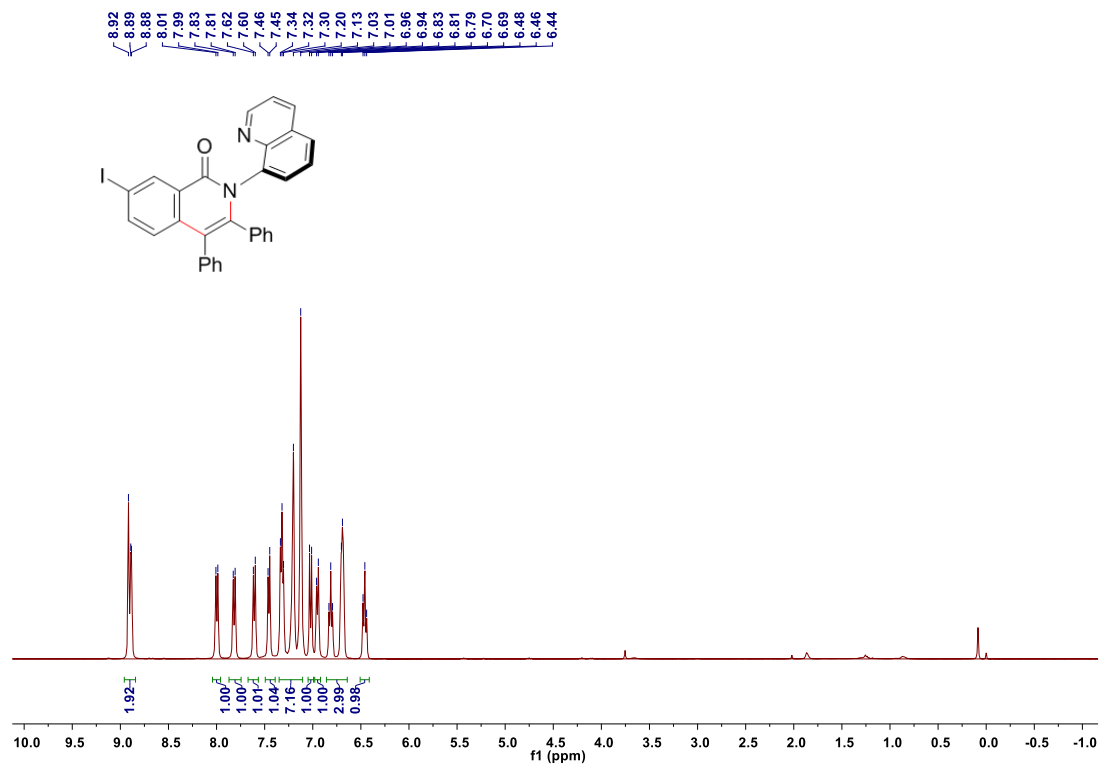
¹H NMR Spectrum of **3va**



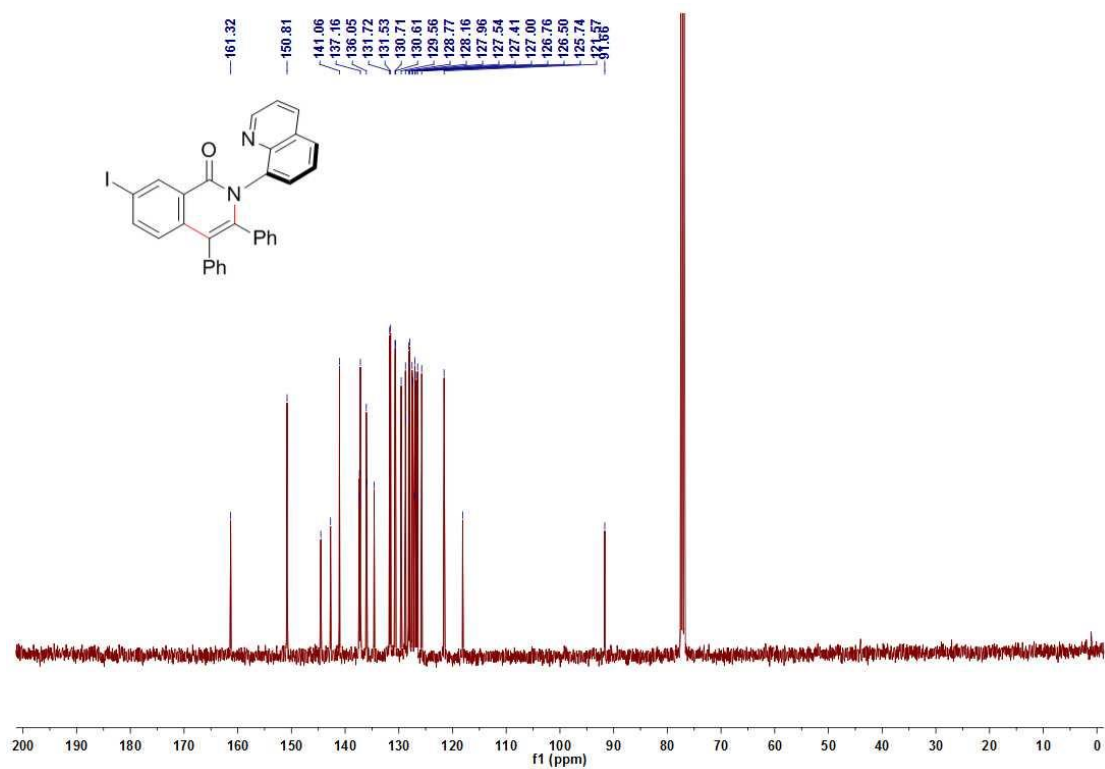
¹³C NMR Spectrum of **3va**



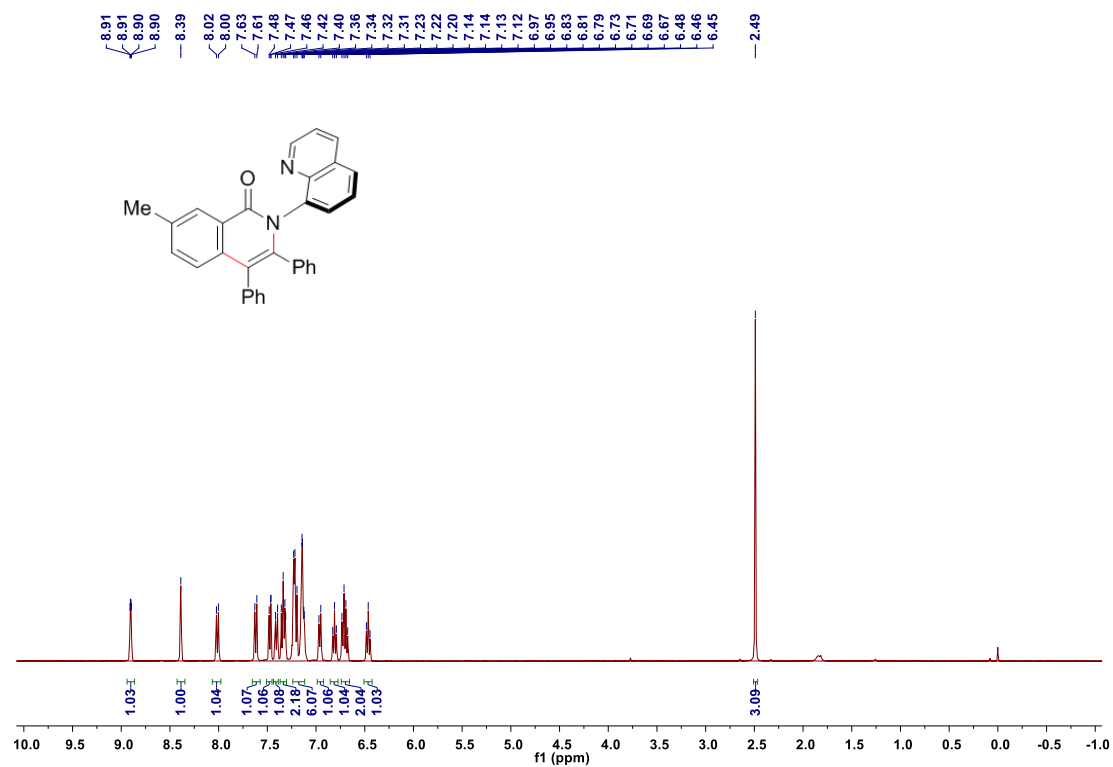
¹H NMR Spectrum of **3wa**



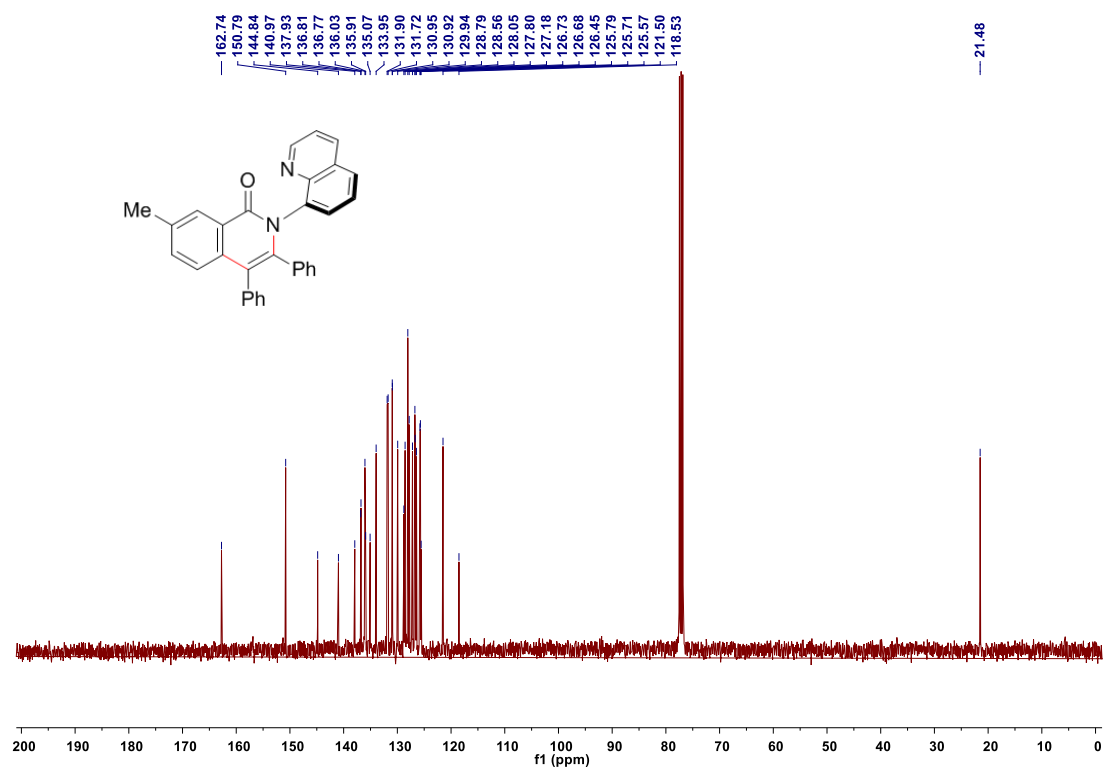
¹³C NMR Spectrum of **3wa**



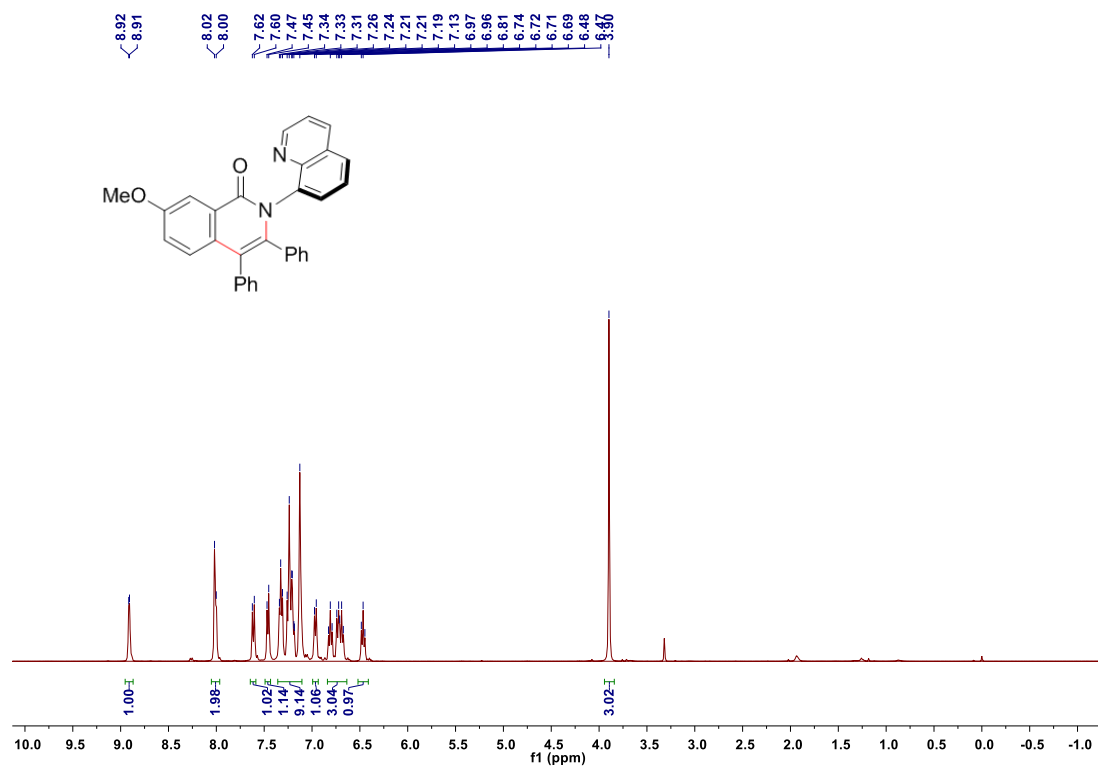
¹H NMR Spectrum of **3xa**



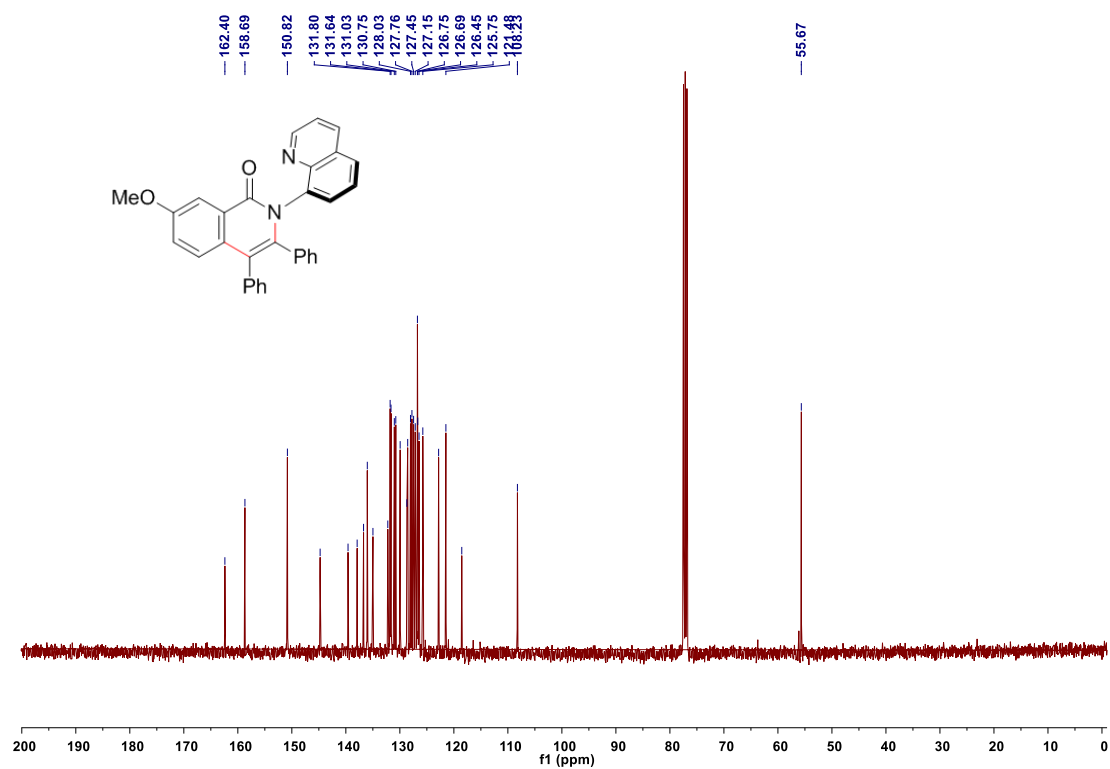
¹³C NMR Spectrum of **3xa**



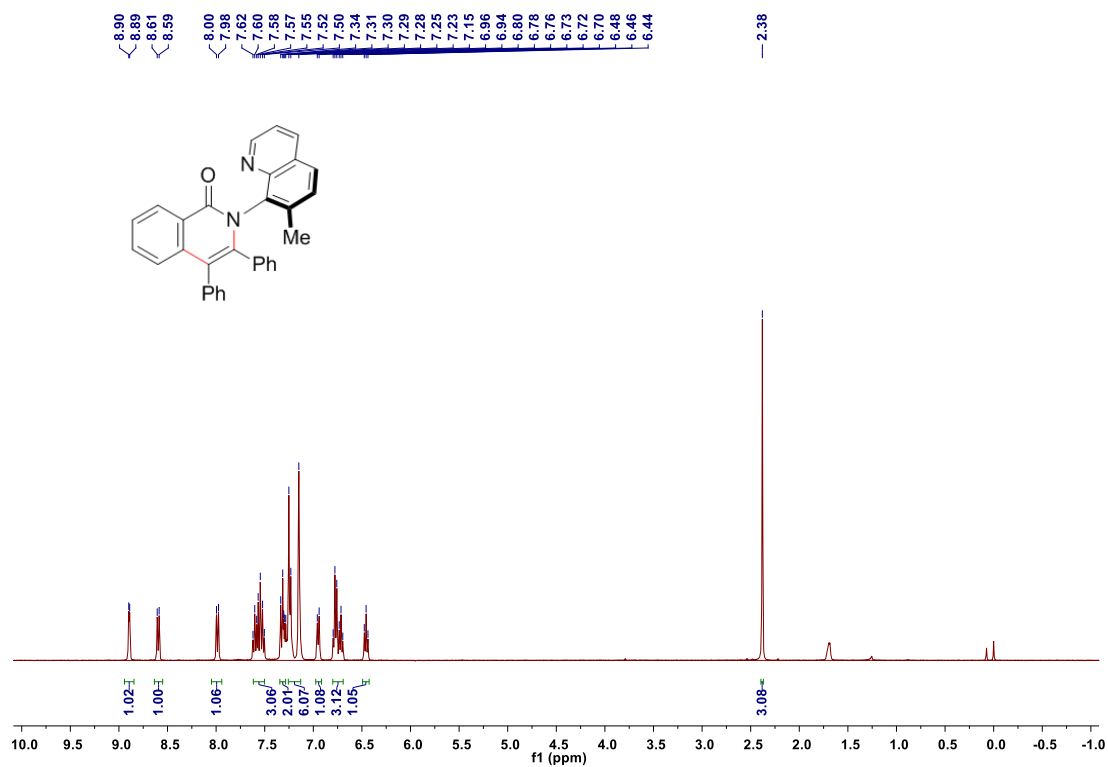
¹H NMR Spectrum of 3ya



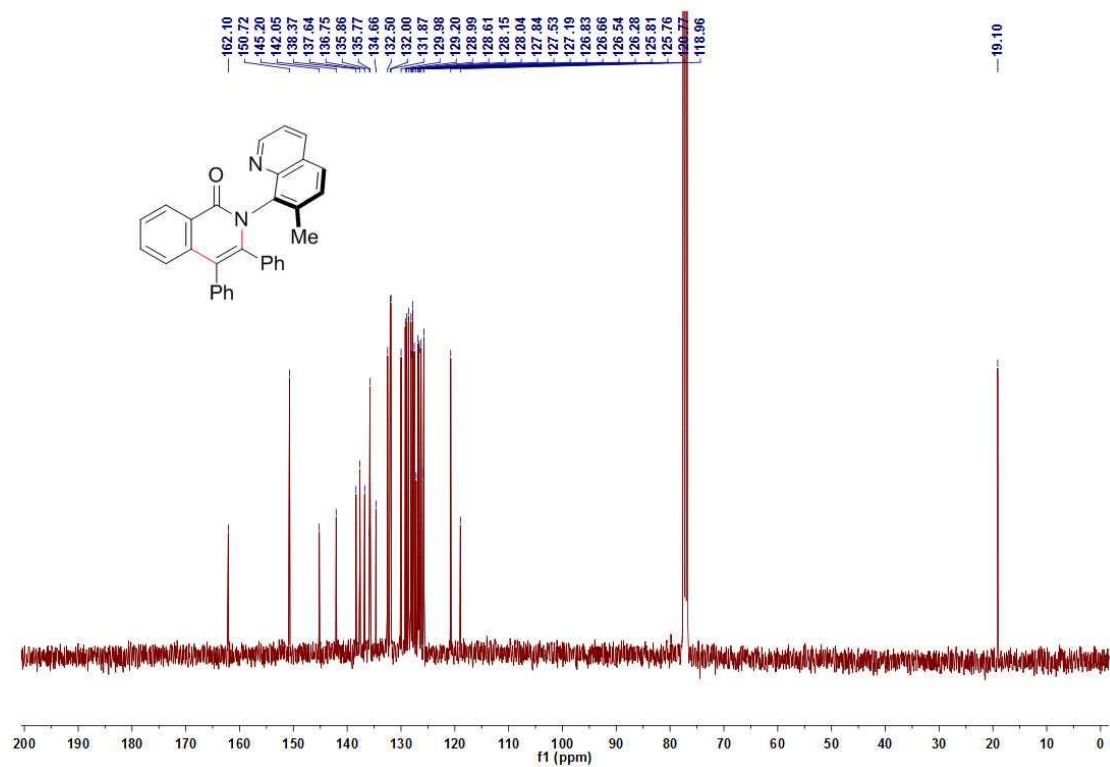
¹³C NMR Spectrum of 3ya



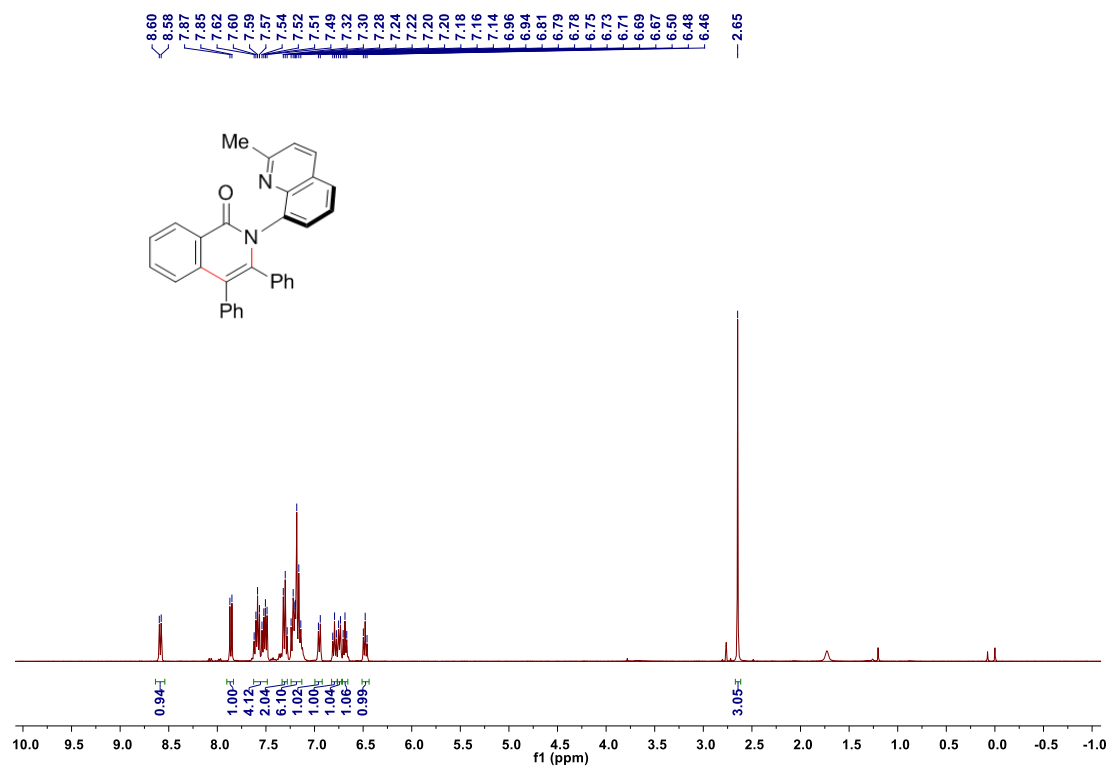
¹H NMR Spectrum of **3za**



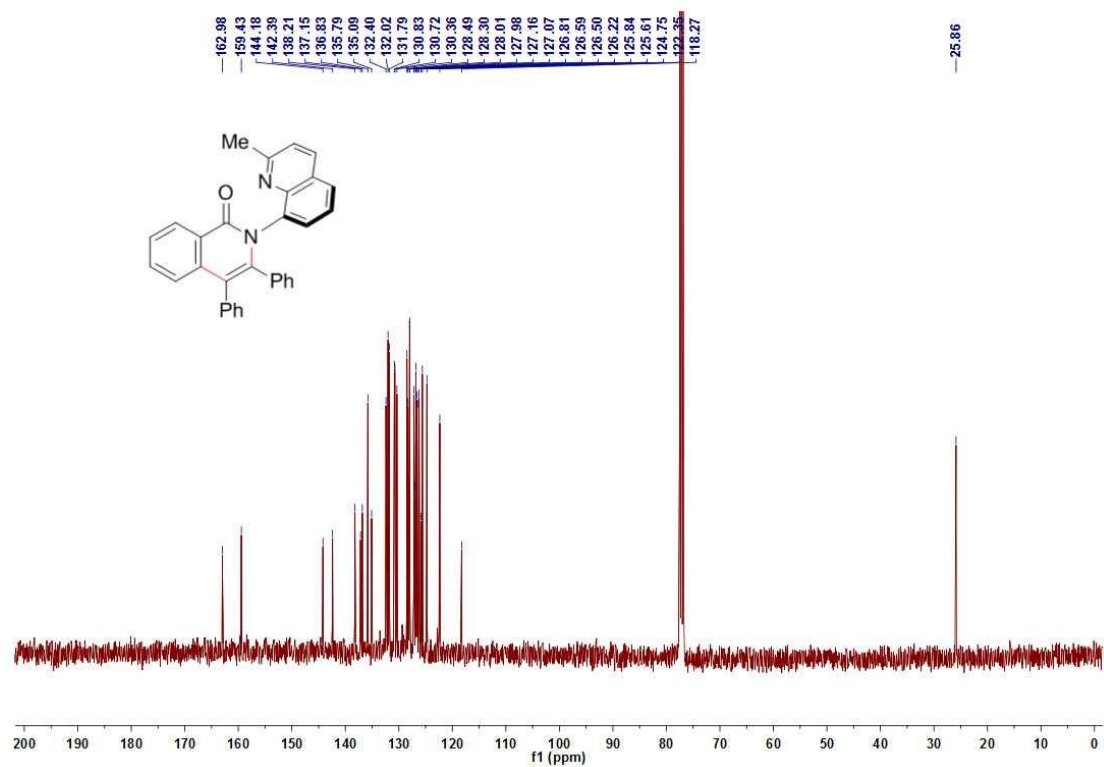
¹³C NMR Spectrum of **3za**



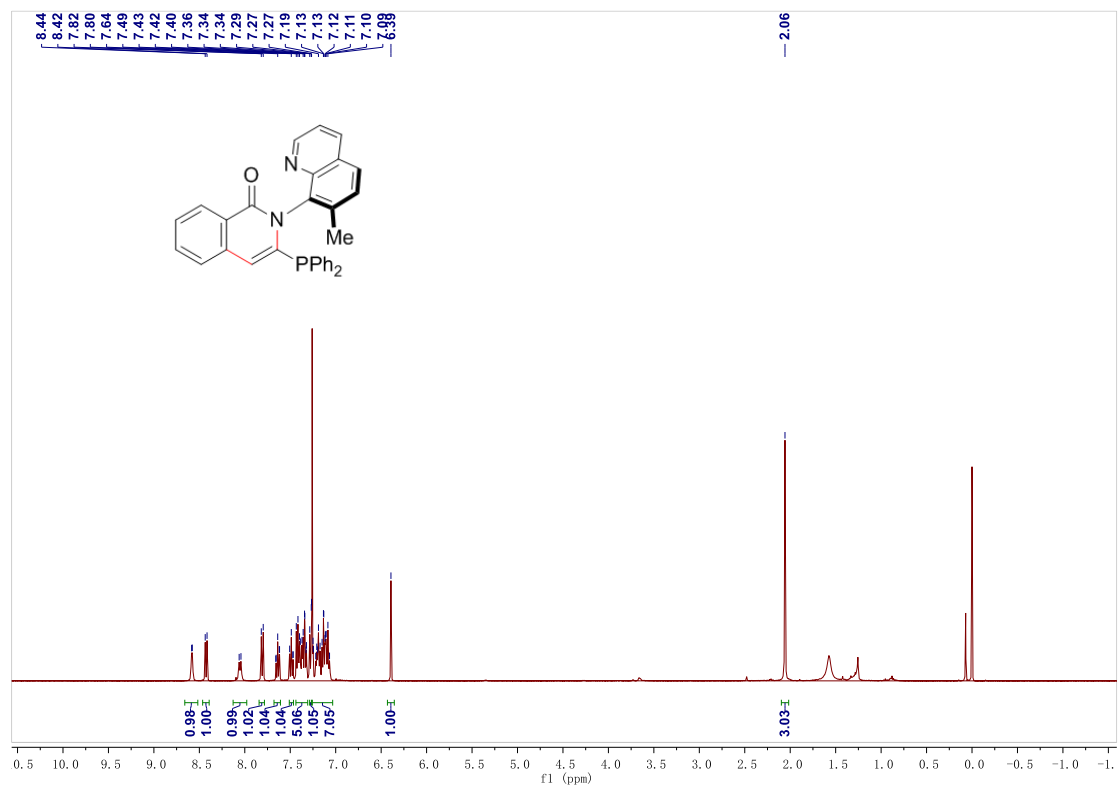
¹H NMR Spectrum of 3aaa



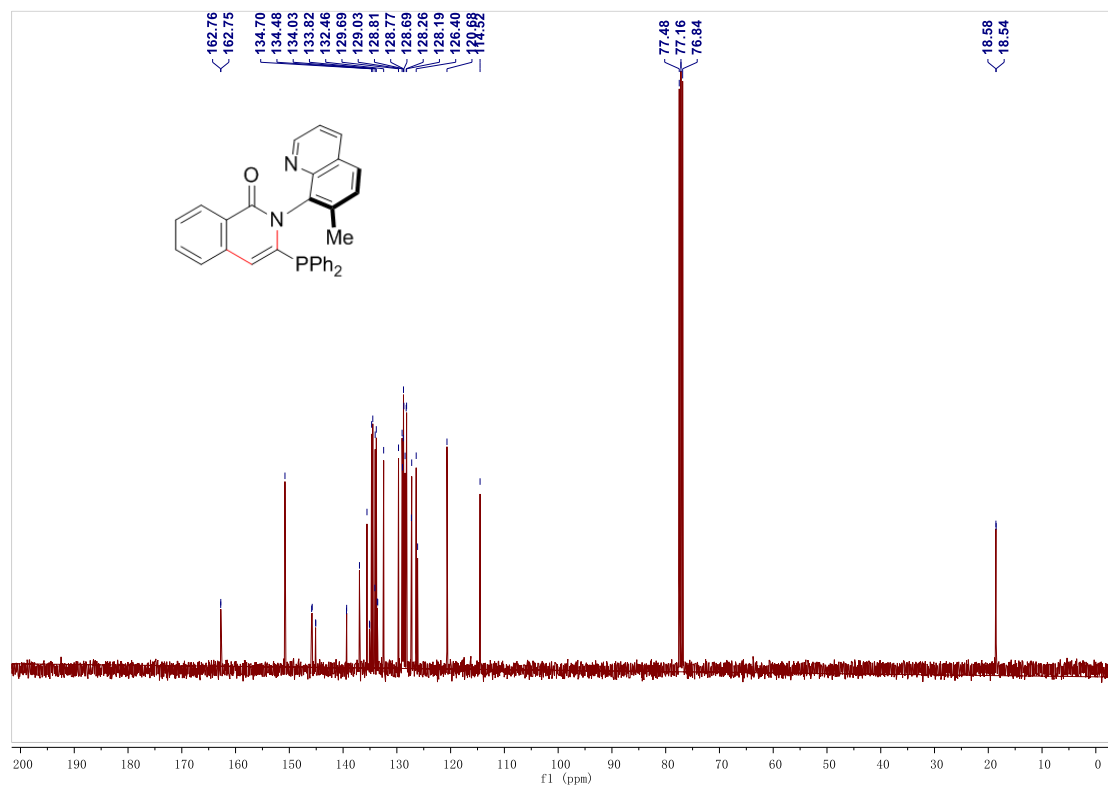
¹³C NMR Spectrum of 3aaa



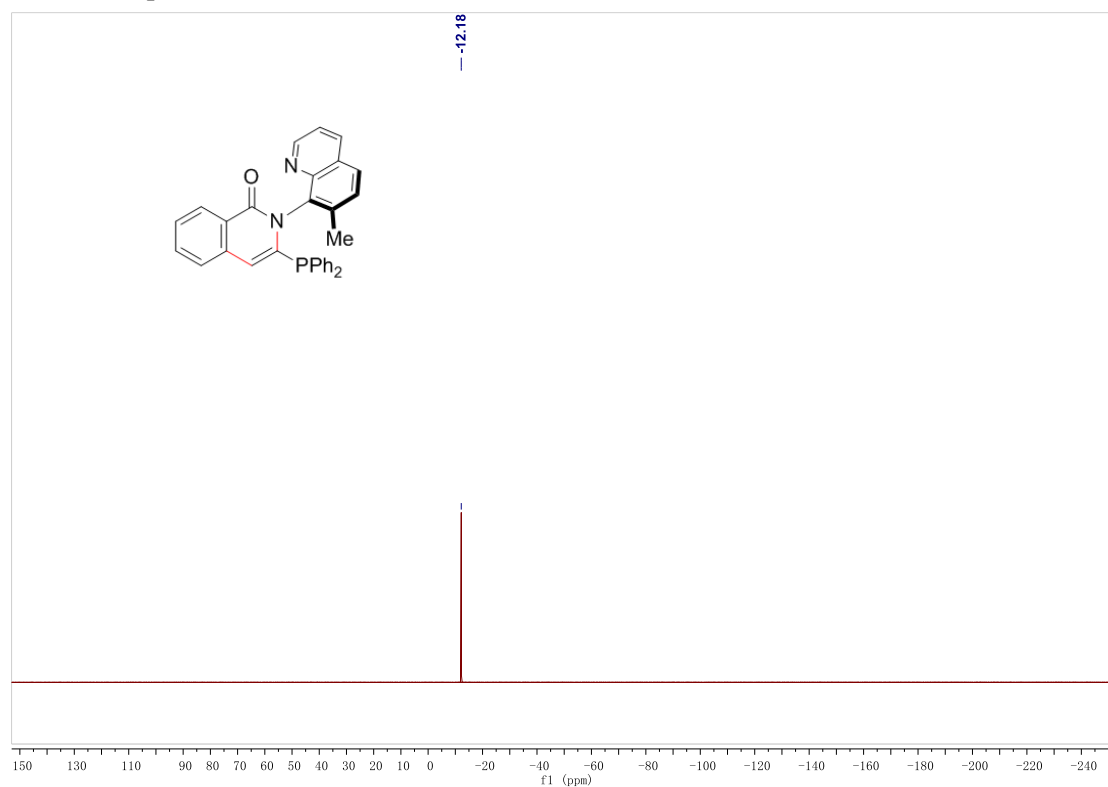
¹H NMR Spectrum of 4



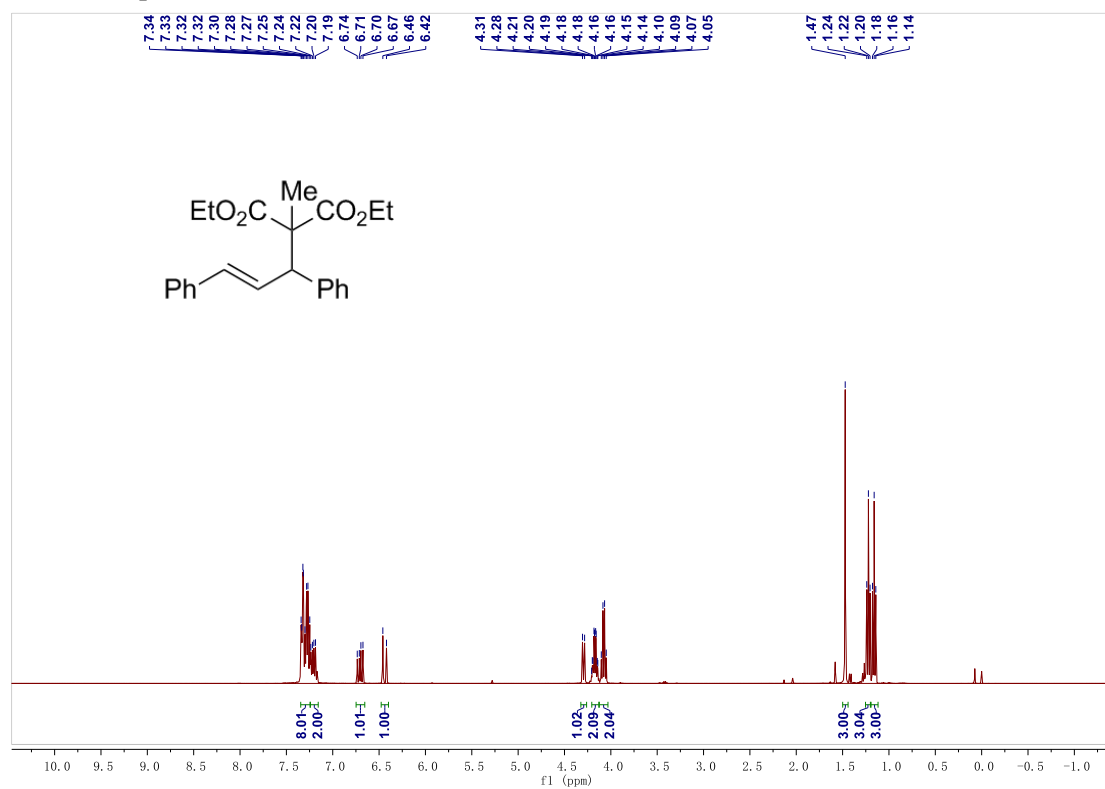
¹³C NMR Spectrum of **4**



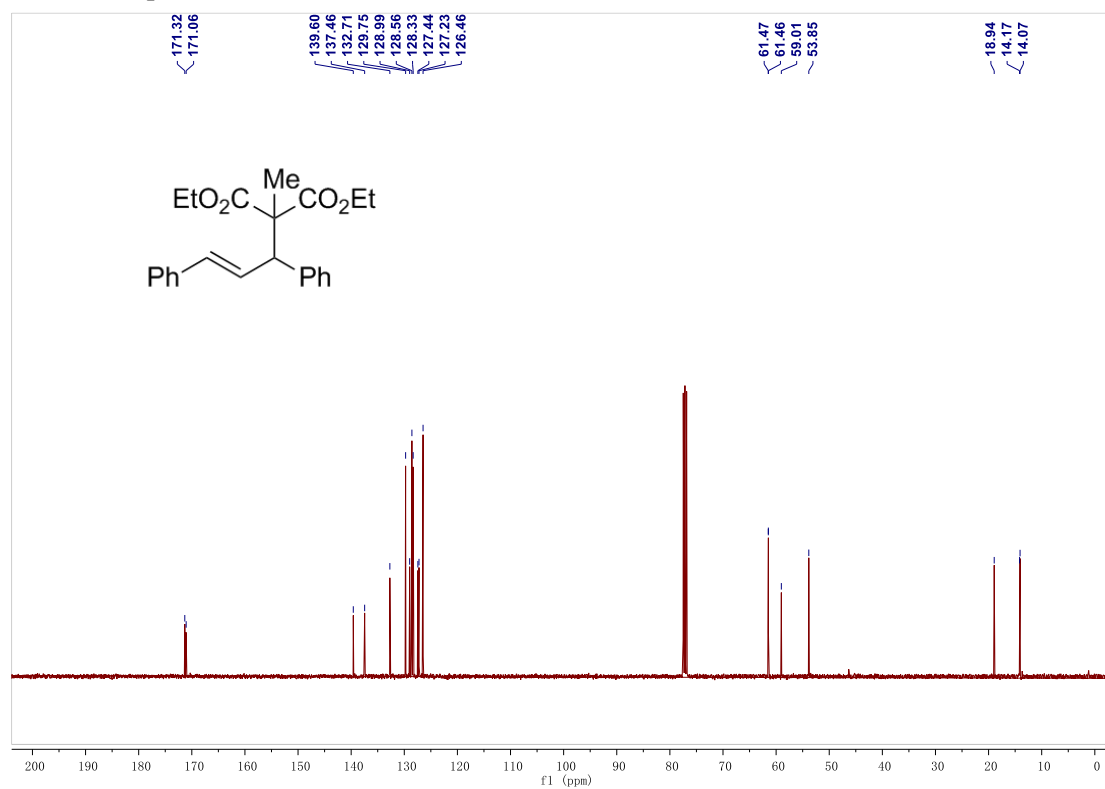
¹⁹C NMR Spectrum of **4**



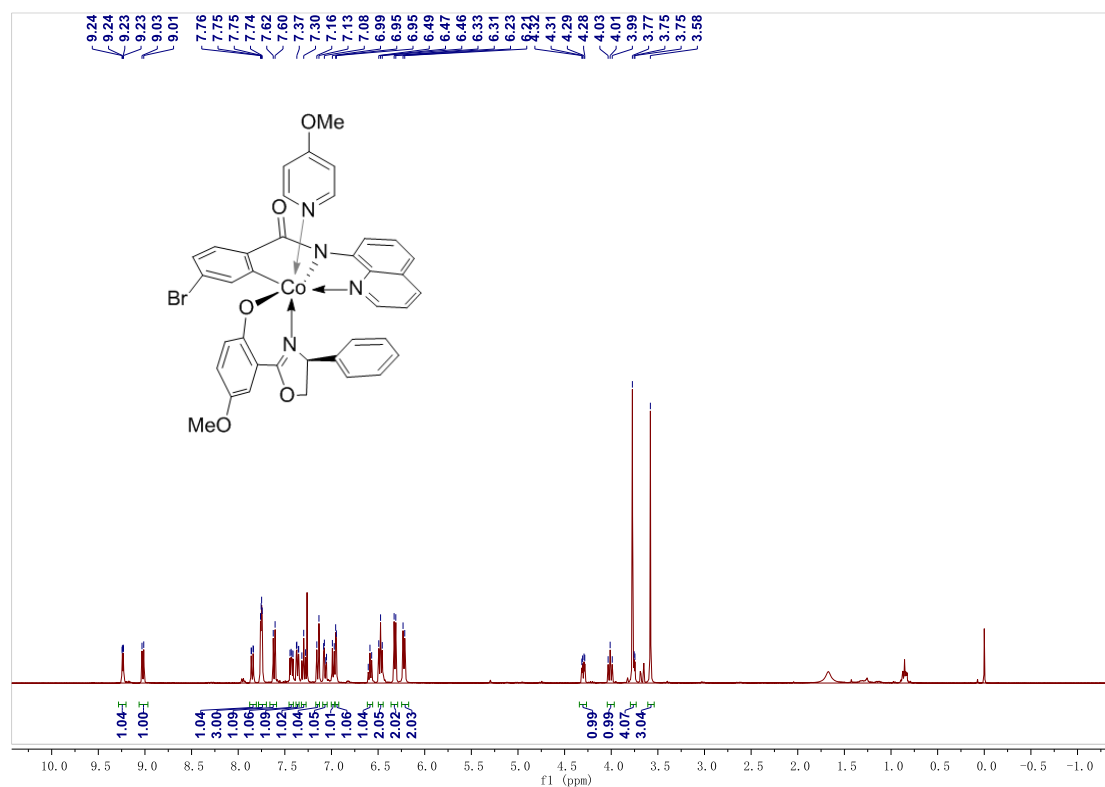
¹H NMR Spectrum of **7**



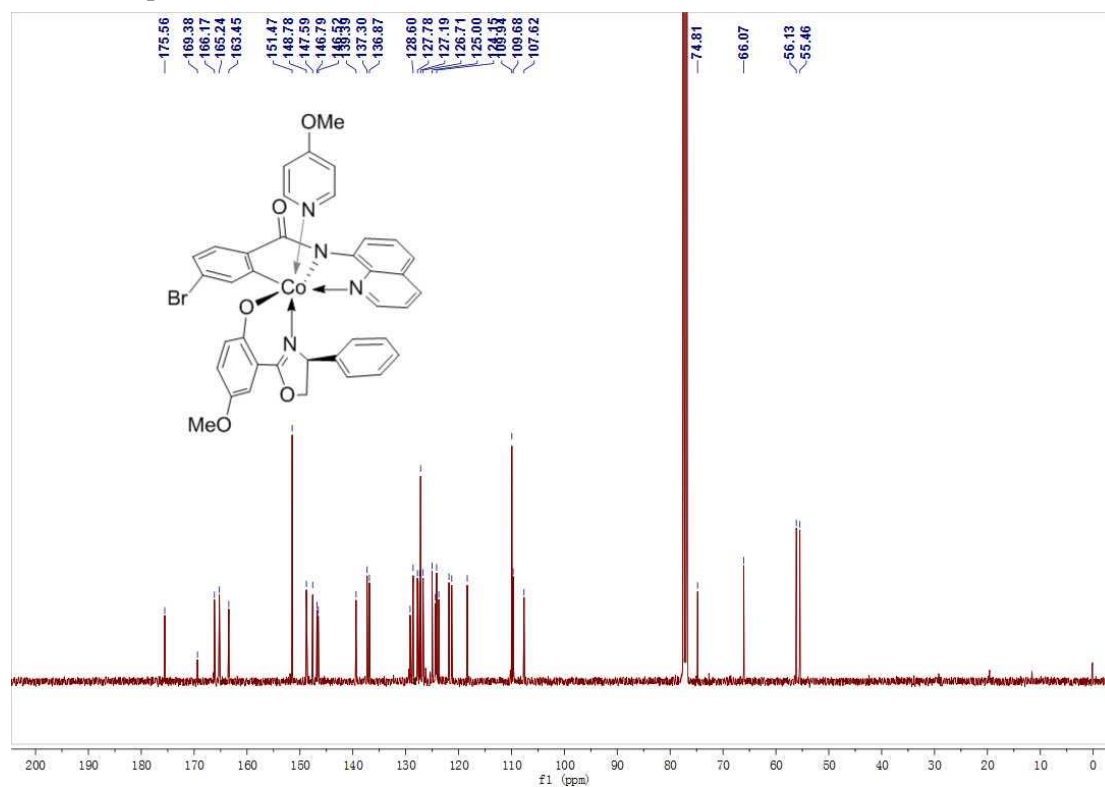
¹³C NMR Spectrum of **7**



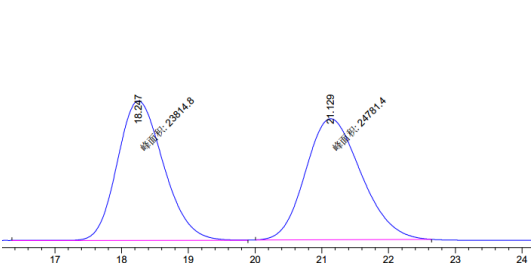
¹H NMR Spectrum of **[Co]-1**



¹³C NMR Spectrum of [Co]-1



9. Copies of HPLC Spectra

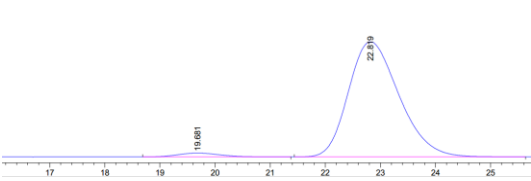


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	18.247	MM	0.8048	2.38148e4	493.19608	49.0055
2	21.129	MM	0.9654	2.47814e4	427.83908	50.9945

Cc1ccc(cc1)C2=C(C(=O)N2c3ccc(Br)cc3)c4ccc(C)cc4

Rac-3ab

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	18.247	MM	0.8048	2.38148e4	493.19608	49.0055
2	21.129	MM	0.9654	2.47814e4	427.83908	50.9945

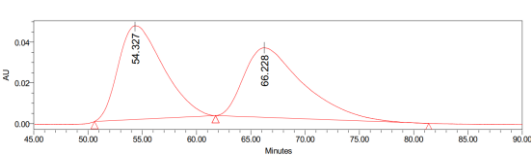


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	19.681	BB	0.6985	815.39612	15.33174	2.7084
2	22.819	BB	0.9802	2.92911e4	459.17862	97.2916

Cc1ccc(cc1)C2=C(C(=O)N2c3ccc(Br)cc3)c4ccncc4

3ab

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	19.681	BB	0.6985	815.39612	15.33174	2.7084
2	22.819	BB	0.9802	2.92911e4	459.17862	97.2916

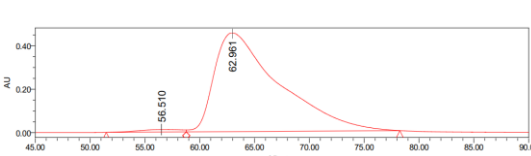


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COc1ccc(cc1)C2=C(C(=O)N2c3ccc(Br)cc3)c4ccc(OC)cc4

Rac-3ac

Name	RT	Area	Height	Amount	Units	% Area
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2	66.228	13028799	34142			49.55

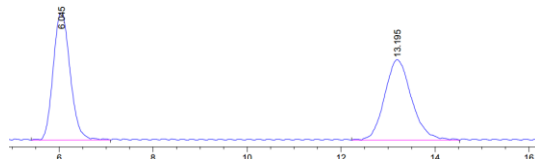
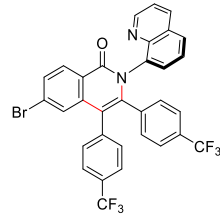
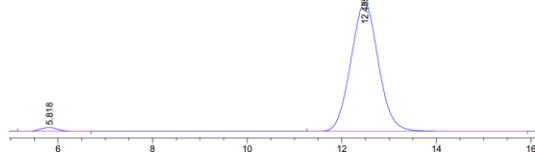
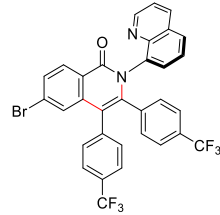
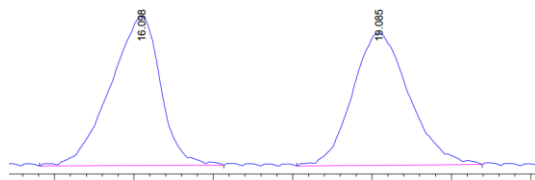
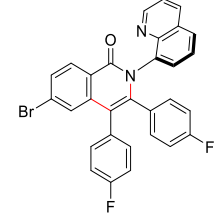
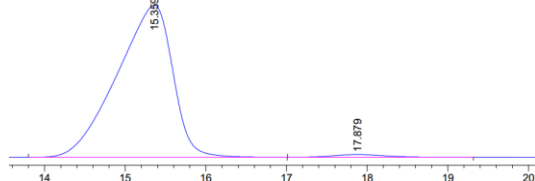
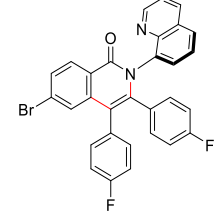


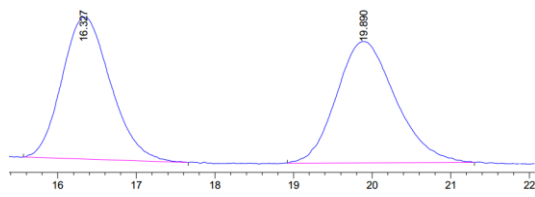
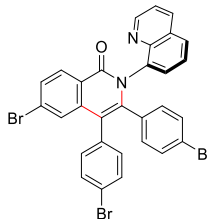
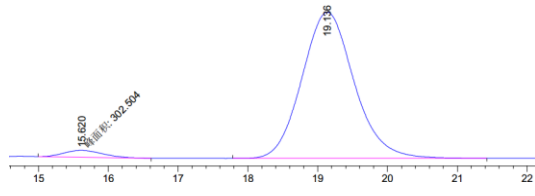
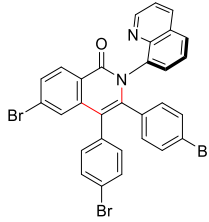
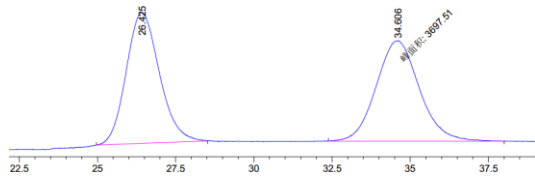
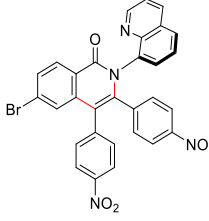
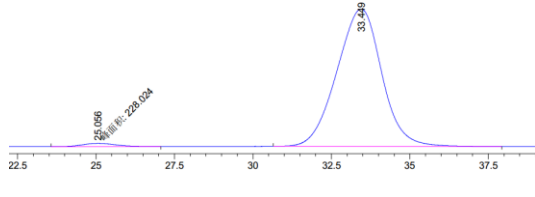
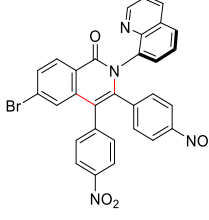
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	56.510	BB	0.6985	815.39612	15.33174	2.7084
2	62.961	BB	0.9802	2.92911e4	459.17862	97.2916

COc1ccc(cc1)C2=C(C(=O)N2c3ccc(Br)cc3)c4ccncc4

3ac

Name	RT	Area	Height	Amount	Units	% Area
1	56.510	3013896	11449			1.59
2	62.961	186743361	455499			98.41

	<div></div> <p>Rac-3ad</p> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>6.045</td><td>VV R</td><td>0.3952</td><td>1.77591e4</td><td>704.95428</td><td>49.9638</td></tr><tr><td>2</td><td>13.195</td><td>VV R</td><td>0.5183</td><td>1.77849e4</td><td>444.44052</td><td>50.0362</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	6.045	VV R	0.3952	1.77591e4	704.95428	49.9638	2	13.195	VV R	0.5183	1.77849e4	444.44052	50.0362
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
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2	13.195	VV R	0.5183	1.77849e4	444.44052	50.0362																
	<div></div> <p>3ad</p> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>5.818</td><td>BB</td><td>0.4067</td><td>933.51129</td><td>36.21332</td><td>1.8746</td></tr><tr><td>2</td><td>12.485</td><td>BB</td><td>0.6244</td><td>4.88640e4</td><td>1206.87207</td><td>98.1254</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	5.818	BB	0.4067	933.51129	36.21332	1.8746	2	12.485	BB	0.6244	4.88640e4	1206.87207	98.1254
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2	12.485	BB	0.6244	4.88640e4	1206.87207	98.1254																
	<div></div> <p>Rac-3ae</p> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>16.098</td><td>VV R</td><td>0.5722</td><td>1.85359e4</td><td>420.55746</td><td>50.0197</td></tr><tr><td>2</td><td>19.085</td><td>VV R</td><td>0.6371</td><td>1.85213e4</td><td>373.18677</td><td>49.9803</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	16.098	VV R	0.5722	1.85359e4	420.55746	50.0197	2	19.085	VV R	0.6371	1.85213e4	373.18677	49.9803
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
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2	19.085	VV R	0.6371	1.85213e4	373.18677	49.9803																
	<div></div> <p>3ae</p> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>15.359</td><td>BB</td><td>0.7340</td><td>3.20145e4</td><td>664.55322</td><td>98.3021</td></tr><tr><td>2</td><td>17.879</td><td>BB</td><td>0.6954</td><td>552.97864</td><td>11.82943</td><td>1.6979</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	15.359	BB	0.7340	3.20145e4	664.55322	98.3021	2	17.879	BB	0.6954	552.97864	11.82943	1.6979
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
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2	17.879	BB	0.6954	552.97864	11.82943	1.6979																

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Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %																		
1	16.327	BB	0.5491	860.44141		19.95296	49.1550																		
2	19.890	BB	0.6314	890.02478		17.04029	50.8450																		
	<div></div> <p>3af</p> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Area *s</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>15.620</td><td>MM</td><td>0.6544</td><td>302.50357</td><td></td><td>7.70408</td><td>3.4688</td></tr><tr><td>2</td><td>19.136</td><td>BB</td><td>0.7964</td><td>8418.31543</td><td></td><td>161.96645</td><td>96.5312</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %	1	15.620	MM	0.6544	302.50357		7.70408	3.4688	2	19.136	BB	0.7964	8418.31543		161.96645	96.5312
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %																		
1	15.620	MM	0.6544	302.50357		7.70408	3.4688																		
2	19.136	BB	0.7964	8418.31543		161.96645	96.5312																		
	<div></div> <p>Rac-3ag</p> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Area *s</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>26.425</td><td>BB</td><td>0.8954</td><td>3706.46069</td><td></td><td>50.31774</td><td>50.0604</td></tr><tr><td>2</td><td>34.606</td><td>MM</td><td>1.5974</td><td>3697.51367</td><td></td><td>38.57820</td><td>49.9396</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %	1	26.425	BB	0.8954	3706.46069		50.31774	50.0604	2	34.606	MM	1.5974	3697.51367		38.57820	49.9396
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %																		
1	26.425	BB	0.8954	3706.46069		50.31774	50.0604																		
2	34.606	MM	1.5974	3697.51367		38.57820	49.9396																		
	<div></div> <p>3ag</p> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Area *s</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>25.056</td><td>MM</td><td>1.2582</td><td>228.02400</td><td></td><td>3.02060</td><td>1.8086</td></tr><tr><td>2</td><td>33.449</td><td>BB</td><td>1.4798</td><td>1.23798e4</td><td></td><td>124.52622</td><td>98.1914</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %	1	25.056	MM	1.2582	228.02400		3.02060	1.8086	2	33.449	BB	1.4798	1.23798e4		124.52622	98.1914
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2	33.449	BB	1.4798	1.23798e4		124.52622	98.1914																		

Chromatogram of Rac-3ah showing two peaks. The x-axis represents time in minutes, ranging from 20 to 36. The y-axis represents intensity. The first peak is at 20.647 minutes, and the second peak is at 32.898 minutes.

Brc1ccc2c(c1)c3c(c2)nc4c3sc5ccccc45

Rac-3ah

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	20.647	BB	0.7560	7634.36133	153.56555	49.6648	
2	32.898	BB	0.9425	7737.41748	98.28225	50.3352	

Chromatogram of 3ah showing two peaks. The x-axis represents time in minutes, ranging from 18 to 32. The y-axis represents intensity. The first peak is at 19.122 minutes, and the second peak is at 30.217 minutes.

Brc1ccc2c(c1)c3c(c2)nc4c3sc5ccccc45

3ah

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	19.122	BB	0.7533	2.47551e4	503.73279	97.8391	
2	30.217	MM	1.1677	546.75055	7.80394	2.1609	

Chromatogram of Rac-3ai showing two peaks. The x-axis represents time in minutes, ranging from 7 to 13. The y-axis represents intensity. The first peak is at 8.122 minutes, and the second peak is at 11.086 minutes.

CCc1c2c(c3c1c4c(c2)nc5c4sc6ccccc56)cc(Br)cc3

Rac-3ai

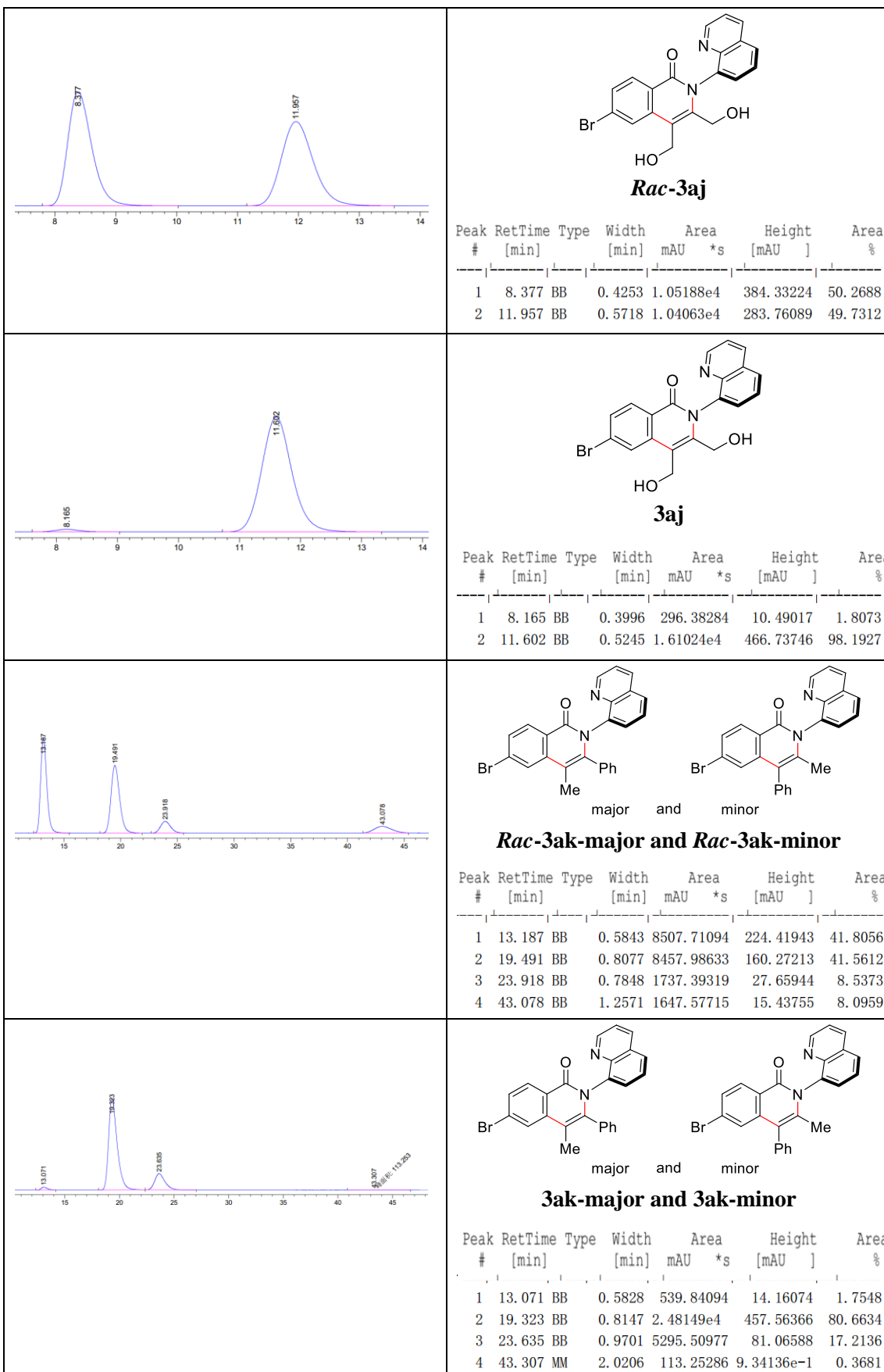
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	8.122	BB	0.4046	9270.40234	362.19122	50.1873	
2	11.086	BB	0.5077	9201.22363	282.70105	49.8127	

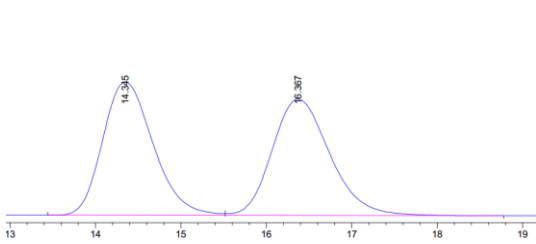
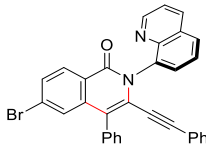
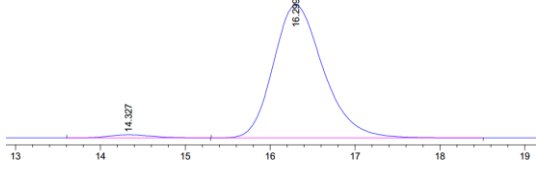
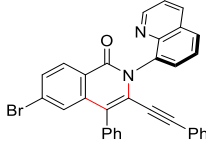
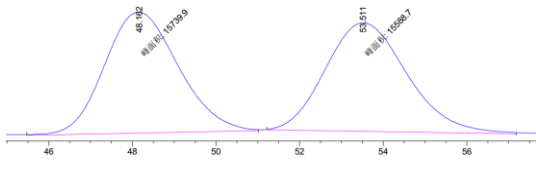
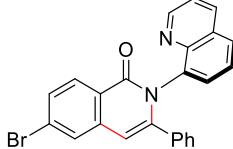
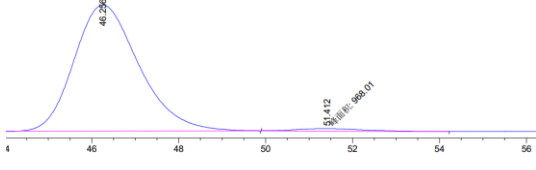
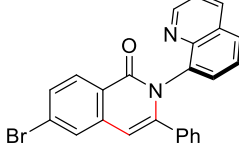
Chromatogram of 3ai showing two peaks. The x-axis represents time in minutes, ranging from 7 to 13. The y-axis represents intensity. The first peak is at 7.977 minutes, and the second peak is at 10.847 minutes.

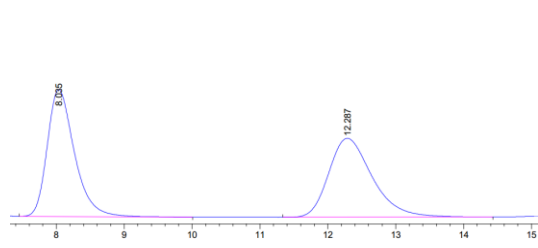
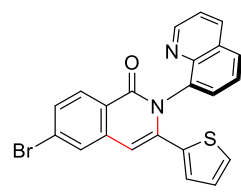
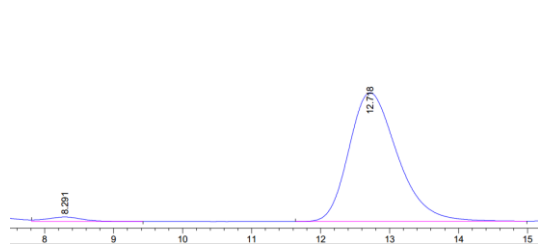
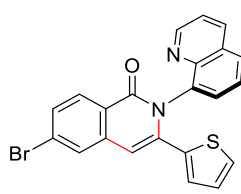
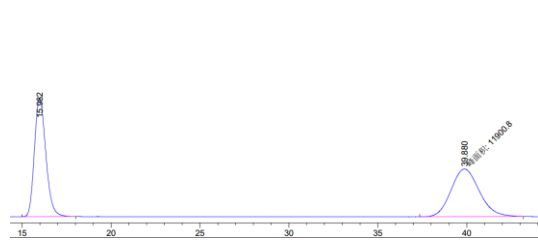
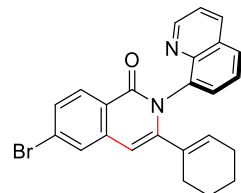
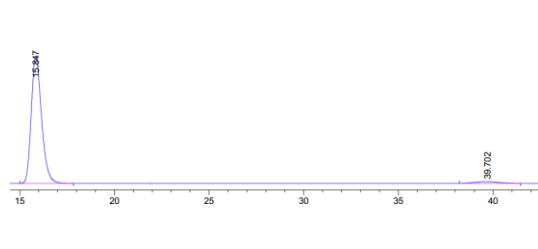
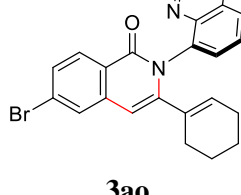
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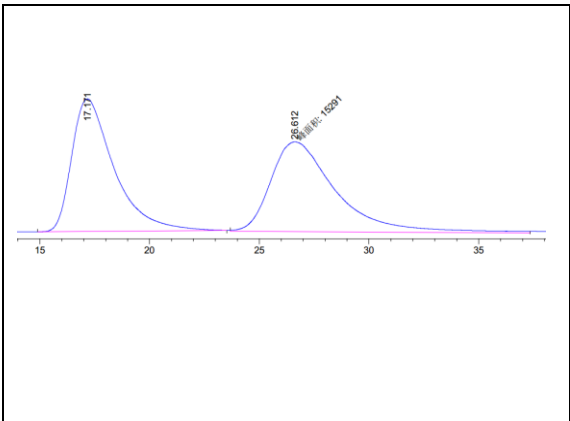
3ai

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	7.977	BB	0.3454	347.92865	14.95374	1.7800	
2	10.847	BB	0.4256	1.91991e4	687.95673	98.2200	



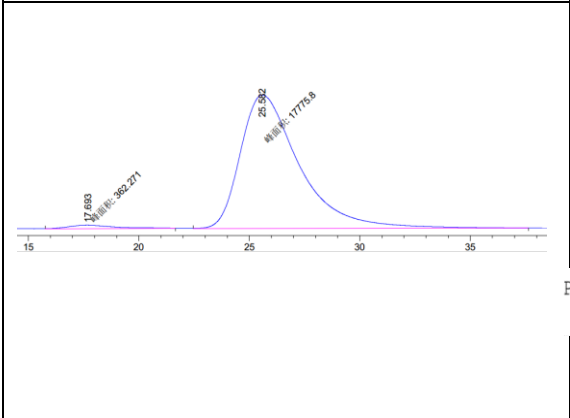
	<div><p><i>Rac-3al</i></p><table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>14.345</td><td>BV</td><td>0.6408</td><td>1.58115e4</td><td>385.26675</td><td>50.0401</td></tr><tr><td>2</td><td>16.367</td><td>VB</td><td>0.7201</td><td>1.57862e4</td><td>336.03943</td><td>49.9599</td></tr></table></div>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	14.345	BV	0.6408	1.58115e4	385.26675	50.0401	2	16.367	VB	0.7201	1.57862e4	336.03943	49.9599
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	<div><p>3al</p><table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>14.327</td><td>BB</td><td>0.5127</td><td>765.95532</td><td>21.34326</td><td>2.0431</td></tr><tr><td>2</td><td>16.299</td><td>BB</td><td>0.6240</td><td>3.67244e4</td><td>896.25427</td><td>97.9569</td></tr></table></div>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	14.327	BB	0.5127	765.95532	21.34326	2.0431	2	16.299	BB	0.6240	3.67244e4	896.25427	97.9569
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	14.327	BB	0.5127	765.95532	21.34326	2.0431																
2	16.299	BB	0.6240	3.67244e4	896.25427	97.9569																
	<div><p><i>Rac-3am</i></p><table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>48.162</td><td>MM</td><td>2.0478</td><td>1.57399e4</td><td>128.10672</td><td>50.2414</td></tr><tr><td>2</td><td>53.511</td><td>MM</td><td>2.2576</td><td>1.55887e4</td><td>115.08096</td><td>49.7586</td></tr></table></div>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	48.162	MM	2.0478	1.57399e4	128.10672	50.2414	2	53.511	MM	2.2576	1.55887e4	115.08096	49.7586
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	<div><p><i>Rac-3an</i></p><table><thead><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr></thead><tbody><tr><td>1</td><td>8.035</td><td>BB</td><td>0.4237</td><td>7385.69531</td><td>264.53314</td><td>50.1792</td></tr><tr><td>2</td><td>12.287</td><td>BB</td><td>0.6848</td><td>7332.94678</td><td>164.27812</td><td>49.8208</td></tr></tbody></table></div>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	8.035	BB	0.4237	7385.69531	264.53314	50.1792	2	12.287	BB	0.6848	7332.94678	164.27812	49.8208
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	<div><p><i>Rac-3ao</i></p><table><thead><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr></thead><tbody><tr><td>1</td><td>15.982</td><td>BB</td><td>0.6937</td><td>1.19046e4</td><td>267.24329</td><td>50.0080</td></tr><tr><td>2</td><td>39.880</td><td>MM</td><td>1.8474</td><td>1.19008e4</td><td>107.36781</td><td>49.9920</td></tr></tbody></table></div>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	15.982	BB	0.6937	1.19046e4	267.24329	50.0080	2	39.880	MM	1.8474	1.19008e4	107.36781	49.9920
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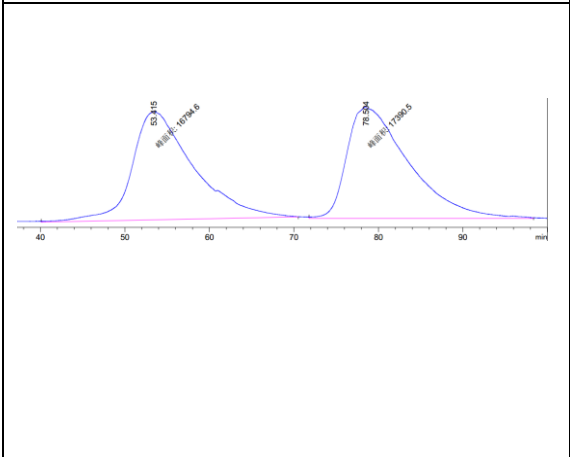
Rac-3ap-major

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	17.171	BB	1.9057	1.46966e4	109.93509	49.0090
2	26.612	MM	3.4277	1.52910e4	74.35004	50.9910



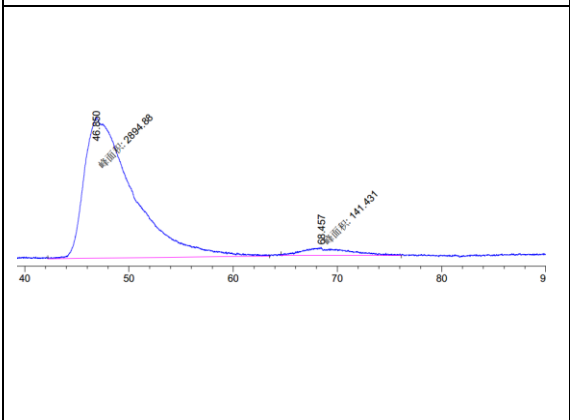
3ap-major

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	17.693	MM	2.4410	362.27130	2.47355	1.9973
2	25.582	MM	3.0910	1.77758e4	95.84570	98.0027



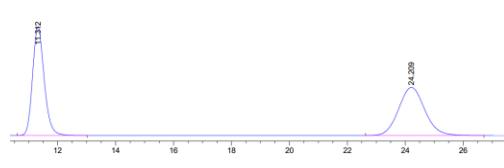
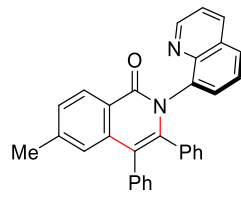
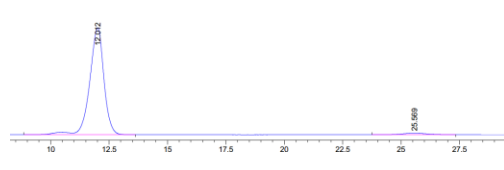
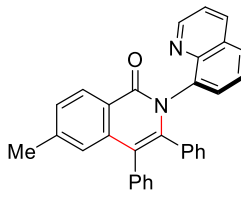
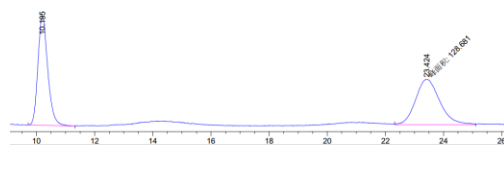
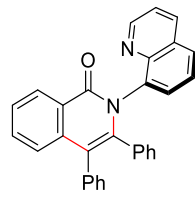
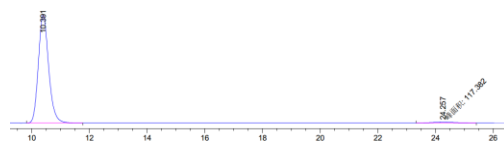
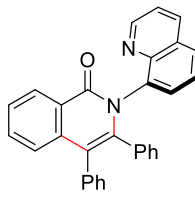
Rac-3aq-major

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	53.415	MM	8.4158	1.67946e4	33.25992	49.1283
2	78.504	MM	8.4434	1.73905e4	34.32754	50.8717



3aq-major

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	46.850	MM	5.4281	2894.88330	8.88857	95.3420
2	68.457	MM	4.8405	141.43098	4.86975e-1	4.6580

	<div><p>Rac-3aa</p><table><thead><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr></thead><tbody><tr><td>1</td><td>11.312</td><td>BB</td><td>0.4265</td><td>4150.40820</td><td>149.21095</td><td>49.9726</td></tr><tr><td>2</td><td>24.209</td><td>BB</td><td>0.9602</td><td>4154.96533</td><td>66.02279</td><td>50.0274</td></tr></tbody></table></div>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	11.312	BB	0.4265	4150.40820	149.21095	49.9726	2	24.209	BB	0.9602	4154.96533	66.02279	50.0274
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2	24.257	MM	0.9483	117.38180	2.06312	1.8589																

Chromatogram of Rac-3ca showing two peaks. The first peak is at 12.254 minutes with an area of 50.1921%. The second peak is at 29.961 minutes with an area of 49.8079%.

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	12.254	BB	0.4496	1.05024e4	358.65424	50.1921
2	29.961	BB	1.1386	1.04220e4	138.38376	49.8079

COc1ccc2c(c1)c(c3ccccc3n2C(=O)N4C5=CC=CC=C5N=C6C=CC=CC=C64)c7ccccc7

Rac-3ca

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	12.254	BB	0.4496	1.05024e4	358.65424	50.1921
2	29.961	BB	1.1386	1.04220e4	138.38376	49.8079

Chromatogram of 3ca showing two peaks. The first peak is at 12.279 minutes with an area of 98.3434%. The second peak is at 30.547 minutes with an area of 1.6566%.

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	12.279	BB	0.4696	7304.82031	238.33360	98.3434
2	30.547	MM	1.2498	123.04949	1.64097	1.6566

COc1ccc2c(c1)c(c3ccccc3n2C(=O)N4C5=CC=CC=C5N=C6C=CC=CC=C64)c7ccccc7

3ca

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	12.279	BB	0.4696	7304.82031	238.33360	98.3434
2	30.547	MM	1.2498	123.04949	1.64097	1.6566

Chromatogram of Rac-3da showing two peaks. The first peak is at 10.017 minutes with an area of 50.0424%. The second peak is at 24.319 minutes with an area of 49.9576%.

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	10.017	BB	0.3703	574.88300	23.75918	50.0424
2	24.319	BB	0.8467	573.90881	9.55517	49.9576

COC(=O)c1ccc2c(c1)c(c3ccccc3n2C(=O)N4C5=CC=CC=C5N=C6C=CC=CC=C64)c7ccccc7

Rac-3da

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	10.017	BB	0.3703	574.88300	23.75918	50.0424
2	24.319	BB	0.8467	573.90881	9.55517	49.9576

Chromatogram of 3da showing two peaks. The first peak is at 10.056 minutes with an area of 97.1118%. The second peak is at 24.569 minutes with an area of 2.8882%.

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	10.056	BB	0.3994	8447.14844	326.95456	97.1118
2	24.569	MM	1.0280	251.23070	4.07296	2.8882

COC(=O)c1ccc2c(c1)c(c3ccccc3n2C(=O)N4C5=CC=CC=C5N=C6C=CC=CC=C64)c7ccccc7

3da

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	10.056	BB	0.3994	8447.14844	326.95456	97.1118
2	24.569	MM	1.0280	251.23070	4.07296	2.8882

Chromatogram of Rac-3ea showing two peaks. The x-axis represents time in minutes, ranging from 12 to 22. The y-axis represents intensity. The first peak is at 12.871 minutes, and the second peak is at 19.940 minutes.

COs(=O)c1ccc2c(c1)c(c3ccccc3n2C(=O)N4C5=CC=CC=C5C6=CC=CC=C64)c7ccccc7

Rac-3ea

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	12.871	BB	0.5507	3360.53394		93.64193	49.5894
2	19.940	BB	0.8266	3416.18213		62.41036	50.4106

Chromatogram of 3ea showing two peaks. The x-axis represents time in minutes, ranging from 14 to 24. The y-axis represents intensity. The first peak is at 14.787 minutes, and the second peak is at 23.525 minutes.

COs(=O)c1ccc2c(c1)c(c3ccccc3n2C(=O)N4C5=CC=CC=C5C6=CC=CC=C64)c7ccccc7

3ea

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	14.787	MM	0.5460	7823.03467		238.78339	96.7357
2	23.525	BB	0.6735	263.98373		5.08641	3.2643

Chromatogram of Rac-3fa showing two peaks. The x-axis represents time in minutes, ranging from 10 to 45. The y-axis represents intensity. The first peak is at 11.814 minutes, and the second peak is at 38.638 minutes.

N#Cc1ccc2c(c1)c(c3ccccc3n2C(=O)N4C5=CC=CC=C5C6=CC=CC=C64)c7ccccc7

Rac-3fa

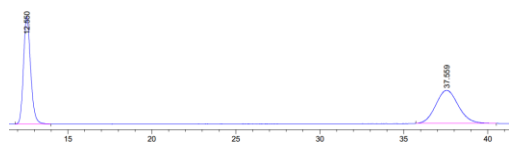
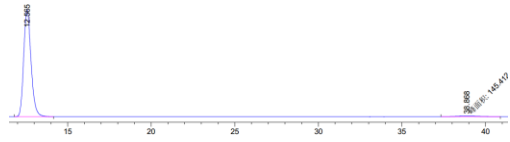
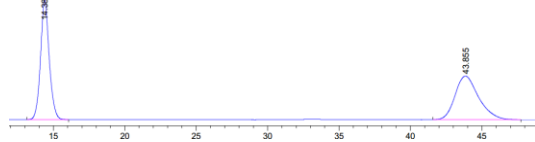

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	11.814	BB	1.2323	1.52099e4		188.70953	50.7110
2	38.638	BB	3.1968	1.47834e4		54.15517	49.2890

Chromatogram of 3fa showing two peaks. The x-axis represents time in minutes, ranging from 10 to 40. The y-axis represents intensity. The first peak is at 11.652 minutes, and the second peak is at 37.433 minutes.

N#Cc1ccc2c(c1)c(c3ccccc3n2C(=O)N4C5=CC=CC=C5C6=CC=CC=C64)c7ccccc7

3fa

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	11.652	BB	0.8011	492.94778		7.63638	3.2552
2	37.433	BB	3.0050	1.46505e4		57.26081	96.7448

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Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	12.550	BB	0.4492	860.42078	29.25014	50.5137																
2	37.559	BB	1.1086	842.92181	9.00039	49.4863																
	<div data-bbox="962 622 1195 808" data-label="Chemical-Block"></div> <p data-bbox="1053 824 1106 857">3ga</p> <table data-bbox="802 880 1361 1014"><thead><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr></thead><tbody><tr><td>1</td><td>12.565</td><td>BB</td><td>0.4697</td><td>5821.27588</td><td>190.90700</td><td>97.5629</td></tr><tr><td>2</td><td>38.868</td><td>MM</td><td>1.6096</td><td>145.41203</td><td>1.50567</td><td>2.4371</td></tr></tbody></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	12.565	BB	0.4697	5821.27588	190.90700	97.5629	2	38.868	MM	1.6096	145.41203	1.50567	2.4371
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	12.565	BB	0.4697	5821.27588	190.90700	97.5629																
2	38.868	MM	1.6096	145.41203	1.50567	2.4371																
	<div data-bbox="973 1043 1185 1229" data-label="Chemical-Block"></div> <p data-bbox="1024 1245 1133 1279">Rac-3ha</p> <table data-bbox="802 1301 1361 1435"><thead><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr></thead><tbody><tr><td>1</td><td>14.387</td><td>BB</td><td>0.6316</td><td>1.20857e4</td><td>285.65054</td><td>50.3425</td></tr><tr><td>2</td><td>43.855</td><td>BB</td><td>1.6529</td><td>1.19213e4</td><td>104.03642</td><td>49.6575</td></tr></tbody></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	14.387	BB	0.6316	1.20857e4	285.65054	50.3425	2	43.855	BB	1.6529	1.19213e4	104.03642	49.6575
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	14.387	BB	0.6316	1.20857e4	285.65054	50.3425																
2	43.855	BB	1.6529	1.19213e4	104.03642	49.6575																
	<div data-bbox="962 1464 1185 1650" data-label="Chemical-Block"></div> <p data-bbox="1053 1666 1106 1700">3ha</p> <table data-bbox="802 1722 1361 1850"><thead><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr></thead><tbody><tr><td>1</td><td>14.328</td><td>BB</td><td>0.6254</td><td>3.29366e4</td><td>781.99872</td><td>97.8211</td></tr><tr><td>2</td><td>43.580</td><td>MM</td><td>1.9059</td><td>733.62506</td><td>6.41524</td><td>2.1789</td></tr></tbody></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	14.328	BB	0.6254	3.29366e4	781.99872	97.8211	2	43.580	MM	1.9059	733.62506	6.41524	2.1789
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	14.328	BB	0.6254	3.29366e4	781.99872	97.8211																
2	43.580	MM	1.9059	733.62506	6.41524	2.1789																

Chromatogram of *Rac-3ia* showing two peaks. The x-axis represents time in minutes, ranging from approximately 4 to 10. The y-axis represents detector response. Peak 1 is at 5.083 minutes and Peak 2 is at 8.996 minutes.

Chemical structure of *Rac-3ia*: A quinazolinone derivative with a methyl group at position 6, a phenyl group at position 4, and a 2-quinolineyl group at position 2.

Rac-3ia

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	5.083	BB	0.3960	6596.25879		256.48309	50.1989
2	8.996	BB	0.4411	6543.99121		226.46921	49.8011

Chromatogram of **3ia** showing two peaks. The x-axis represents time in minutes, ranging from approximately 4 to 10. The y-axis represents detector response. Peak 1 is at 5.154 minutes and Peak 2 is at 9.322 minutes.

Chemical structure of **3ia**: A quinazolinone derivative with a methyl group at position 6, a phenyl group at position 4, and a 2-quinolineyl group at position 2.

3ia

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	5.154	BB	0.1949	6018.07520		471.43573	96.6998
2	9.322	BB	0.3613	205.38449		8.51952	3.3002

Chromatogram of *Rac-3ja* showing two peaks. The x-axis represents time in minutes, ranging from approximately 6 to 14. The y-axis represents detector response. Peak 1 is at 6.947 minutes and Peak 2 is at 13.312 minutes.

Chemical structure of *Rac-3ja*: A quinazolinone derivative with a chlorine atom at position 6, a phenyl group at position 4, and a 2-quinolineyl group at position 2.

Rac-3ja

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	6.947	BB	0.4046	1.57125e4		582.61871	50.3225
2	13.312	BB	0.6111	1.55111e4		390.75006	49.6775

Chromatogram of **3ja** showing two peaks. The x-axis represents time in minutes, ranging from approximately 6 to 14. The y-axis represents detector response. Peak 1 is at 7.016 minutes and Peak 2 is at 13.802 minutes.

Chemical structure of **3ja**: A quinazolinone derivative with a chlorine atom at position 6, a phenyl group at position 4, and a 2-quinolineyl group at position 2.

3ja

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	7.016	BB	0.2762	6708.27100		372.35162	93.6434
2	13.802	BB	0.5423	455.36288		12.34616	6.3566

Chromatogram of Rac-3ka showing two peaks. The x-axis represents time in minutes (8 to 18), and the y-axis represents AU (0 to 0.30). The first peak is at 7.524 minutes (BB) and the second peak is at 14.373 minutes (BB).

O=C1C(=C(C(=C1)C2=CC=CC=C2)N3C4=CC=CC=C4c5cccnc53)C6=CC=CC=C6Br

Rac-3ka

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	7.524	BB	0.4010	1.33040e4	495.89404	50.2851
2	14.373	BB	0.6500	1.31531e4	306.88925	49.7149

Chromatogram of 3ka showing two peaks. The x-axis represents time in minutes (8 to 18), and the y-axis represents AU (0 to 0.30). The first peak is at 7.560 minutes (BB) and the second peak is at 14.529 minutes (MM).

O=C1C(=C(C(=C1)C2=CC=CC=C2)N3C4=CC=CC=C4c5cccnc53)C6=CC=CC=C6Br

3ka

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	7.560	BB	0.2912	5522.03174	291.18604	91.0442
2	14.529	MM	0.6961	543.18622	13.00598	8.9558

Chromatogram of Rac-3la showing two peaks. The x-axis represents time in minutes (8.00 to 34.00), and the y-axis represents AU (0.00 to 0.30). The first peak is at 10.220 minutes and the second peak is at 29.130 minutes.

O=C1C(=C(C(=C1)C2=CC=CC=C2)N3C4=CC=CC=C4c5cccnc53)C6=CC=CC=C6

Rac-3la

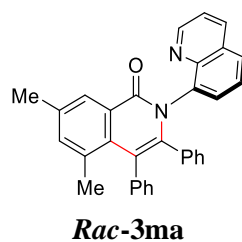
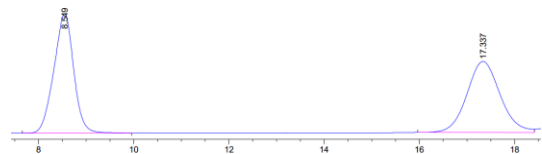
Name	RT	Area	Height	Amount	Units	% Area
1	10.220	6624540	299754			49.18
2	29.130	6844272	113358			50.82

Chromatogram of 3la showing two peaks. The x-axis represents time in minutes (8.00 to 34.00), and the y-axis represents AU (0.00 to 1.50). The first peak is at 10.162 minutes and the second peak is at 29.370 minutes.

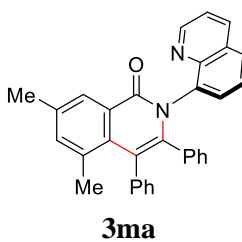
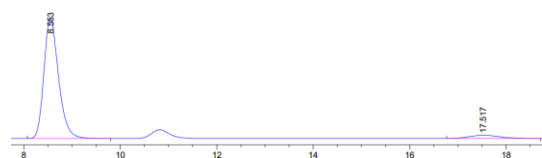
O=C1C(=C(C(=C1)C2=CC=CC=C2)N3C4=CC=CC=C4c5cccnc53)C6=CC=CC=C6

3la

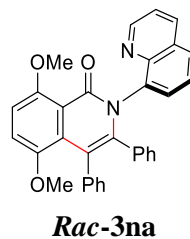
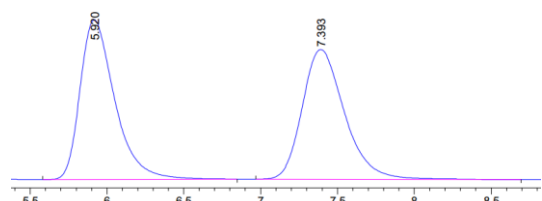
Name	RT	Area	Height	Amount	Units	% Area
1	10.162	32806109	1545837			98.60
2	29.370	464636	8674			1.40



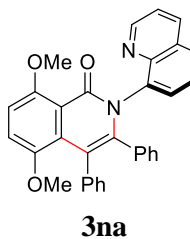
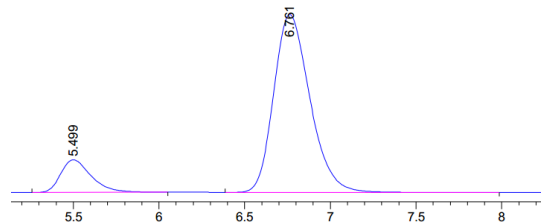
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	8.549	BB	0.4325	6919.75049		239.92329	49.9211
2	17.337	BV	0.7393	6941.62793		142.75163	50.0789



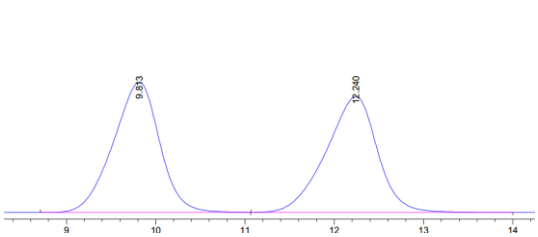
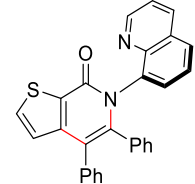

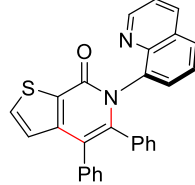
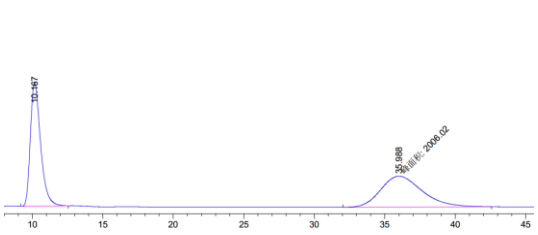
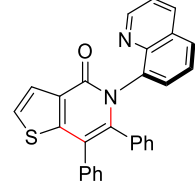
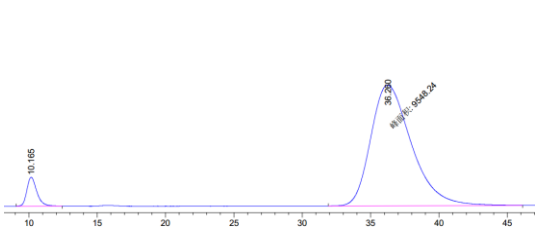
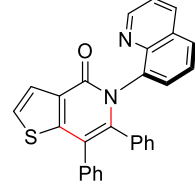
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.553	BB	0.3234	3761.54224	178.80400	94.8451
2	17.517	BB	0.5361	204.44304	4.62169	5.1549



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.920	BB	0.2389	2816.35596	179.62920	50.1516
2	7.393	BB	0.2936	2799.32690	146.03270	49.8484



Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	5.499	BB	0.1908	383.30219		30.88238	13.3726
2	6.761	BB	0.2271	2483.02026		169.28778	86.6274

	<div><p>Rac-30a</p></div> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>9.813</td><td>BB</td><td>0.5463</td><td>1.66228e4</td><td>459.27887</td><td>50.4410</td></tr><tr><td>2</td><td>12.240</td><td>BB</td><td>0.5970</td><td>1.63322e4</td><td>408.01407</td><td>49.5590</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	9.813	BB	0.5463	1.66228e4	459.27887	50.4410	2	12.240	BB	0.5970	1.63322e4	408.01407	49.5590
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	9.813	BB	0.5463	1.66228e4	459.27887	50.4410																
2	12.240	BB	0.5970	1.63322e4	408.01407	49.5590																
	<div><p>30a</p></div> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>10.080</td><td>BB</td><td>0.3758</td><td>4811.84668</td><td>196.40164</td><td>98.7755</td></tr><tr><td>2</td><td>12.739</td><td>BB</td><td>0.3740</td><td>59.65347</td><td>1.95495</td><td>1.2245</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	10.080	BB	0.3758	4811.84668	196.40164	98.7755	2	12.739	BB	0.3740	59.65347	1.95495	1.2245
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	10.080	BB	0.3758	4811.84668	196.40164	98.7755																
2	12.739	BB	0.3740	59.65347	1.95495	1.2245																
	<div><p>Rac-3pa</p></div> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>10.167</td><td>BB</td><td>0.7634</td><td>1964.50269</td><td>39.02128</td><td>49.4771</td></tr><tr><td>2</td><td>35.988</td><td>MM</td><td>3.4259</td><td>2006.02441</td><td>9.75899</td><td>50.5229</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	10.167	BB	0.7634	1964.50269	39.02128	49.4771	2	35.988	MM	3.4259	2006.02441	9.75899	50.5229
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	10.167	BB	0.7634	1964.50269	39.02128	49.4771																
2	35.988	MM	3.4259	2006.02441	9.75899	50.5229																
	<div><p>3pa</p></div> <table><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr><tr><td>1</td><td>10.165</td><td>BB</td><td>0.7299</td><td>557.89508</td><td>11.07052</td><td>5.5204</td></tr><tr><td>2</td><td>36.260</td><td>MM</td><td>3.4490</td><td>9548.23926</td><td>46.13993</td><td>94.4796</td></tr></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	10.165	BB	0.7299	557.89508	11.07052	5.5204	2	36.260	MM	3.4490	9548.23926	46.13993	94.4796
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %																
1	10.165	BB	0.7299	557.89508	11.07052	5.5204																
2	36.260	MM	3.4490	9548.23926	46.13993	94.4796																

Chromatogram of Rac-3qa showing two peaks. The first peak is at 6.012 minutes with an area of 50.1963%. The second peak is at 9.990 minutes with an area of 49.8037%.

c1ccc2c(c1)c3cc4c(c2)oc5ccccc5c3n2C(=O)c6cccnc6

Rac-3qa

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.012	BB	0.2307	1697.42749	112.06480	50.1963
2	9.990	BB	0.3782	1684.15076	68.16767	49.8037

Chromatogram of 3qa showing two peaks. The first peak is at 6.030 minutes with an area of 3.4901%. The second peak is at 10.029 minutes with an area of 96.5099%.

c1ccc2c(c1)c3cc4c(c2)oc5ccccc5c3n2C(=O)c6cccnc6

3qa

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.030	BB	0.2771	105.80864	5.73976	3.4901
2	10.029	BB	0.4314	2925.84570	104.88694	96.5099

Chromatogram of Rac-3ra showing two peaks. The first peak is at 7.142 minutes with an area of 50.0665%. The second peak is at 7.954 minutes with an area of 49.9335%.

c1ccc2c(c1)c3cc4c(c2)oc5ccccc5c3n2C(=O)c6cccnc6

Rac-3ra

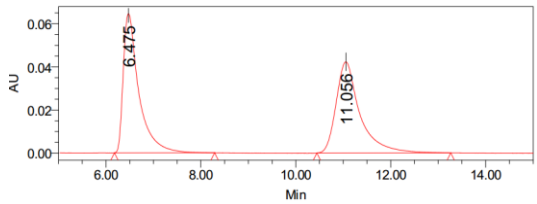
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	7.142	BV	0.2546	2876.23218	172.47978	50.0665
2	7.954	VB	0.2886	2868.58740	151.68057	49.9335

Chromatogram of 3ra showing two peaks. The first peak is at 6.521 minutes with an area of 2.4914%. The second peak is at 7.186 minutes with an area of 97.5086%.

c1ccc2c(c1)c3cc4c(c2)oc5ccccc5c3n2C(=O)c6cccnc6

3ra

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.521	BB	0.1847	40.82689	3.38463	2.4914
2	7.186	BB	0.2060	1597.85828	119.49137	97.5086



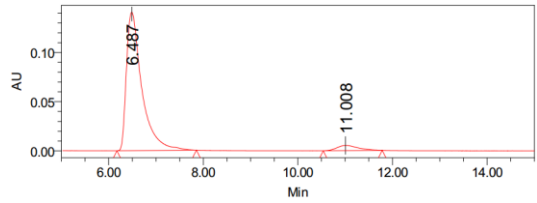
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.475	BB	0.2879	4699.35645	249.36087	50.5861
2	11.056	BB	0.6635	4590.45557	105.10640	49.4139

Cc1cc(C(=O)N(c2ccccc2)c3ccncc3)c(Cc4ccccc4)c5ccncc15

Rac-3ra

Peak Results

	Name	RT	Area	Height	Amount	Units	% Area
1		6.475	1470247	64562			50.04
2		11.056	1467969	42242			49.96



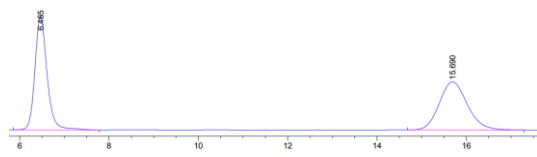
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.487	BB	0.2879	4699.35645	249.36087	50.5861
2	11.008	BB	0.6635	4590.45557	105.10640	49.4139

Cc1cc(C(=O)N(c2ccccc2)c3ccncc3)c(Cc4ccccc4)c5ccncc15

3sa

Peak Results

	Name	RT	Area	Height	Amount	Units	% Area
1		6.487	3173646	140671			95.18
2		11.008	160717	5251			4.82

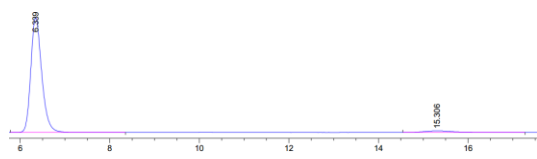


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.465	BB	0.2879	4699.35645	249.36087	50.5861
2	15.690	BB	0.6635	4590.45557	105.10640	49.4139

Fc1ccc(C(=O)N(c2ccccc2)c3ccncc3)c(Cc4ccccc4)c13

Rac-3ta-C2

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.465	BB	0.2879	4699.35645	249.36087	50.5861
2	15.690	BB	0.6635	4590.45557	105.10640	49.4139

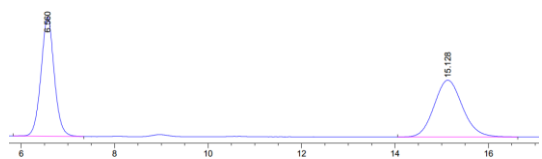
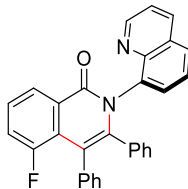
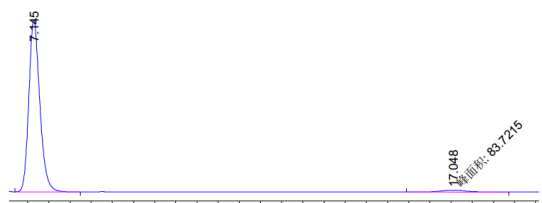
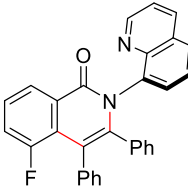
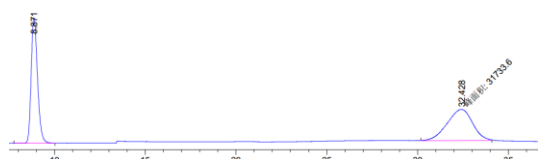
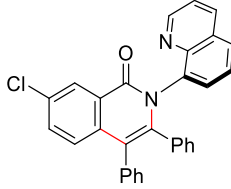
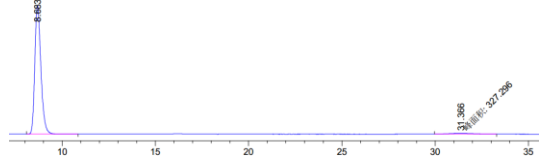
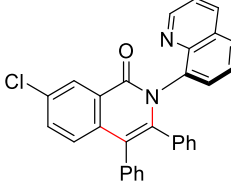


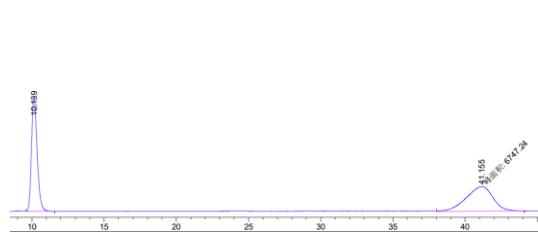
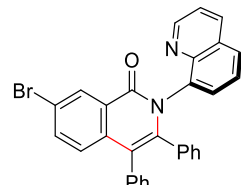
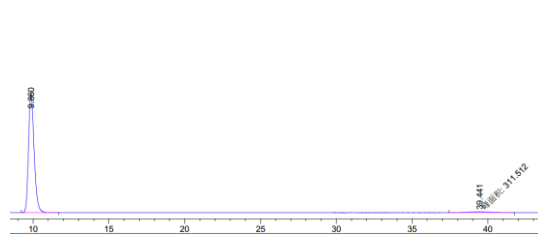
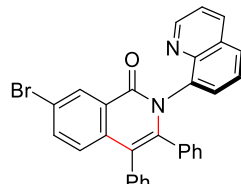
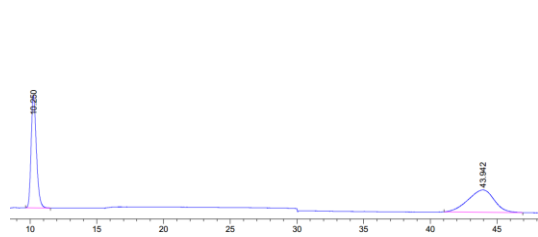
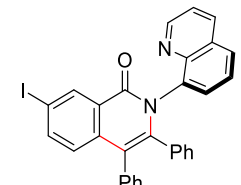
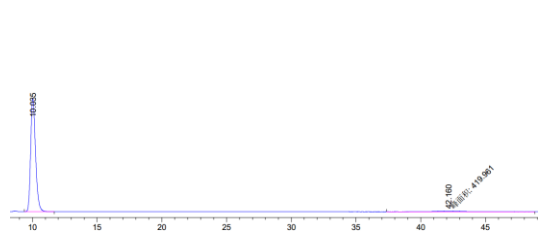
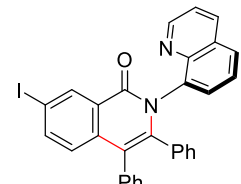
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.339	BB	0.2596	5861.12256	346.05618	96.3553
2	15.306	BB	0.6319	221.70181	4.89921	3.6447

Fc1ccc(C(=O)N(c2ccccc2)c3ccncc3)c(Cc4ccccc4)c13

3ta-C2

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	6.339	BB	0.2596	5861.12256	346.05618	96.3553
2	15.306	BB	0.6319	221.70181	4.89921	3.6447

	<div></div> <p>Rac-3ta-C6</p> <table><thead><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU</th><th>Height [mAU]</th><th>Area %</th></tr></thead><tbody><tr><td>1</td><td>6.560</td><td>BB</td><td>0.2987</td><td>5359.47607</td><td>271.00064</td><td>49.6125</td></tr><tr><td>2</td><td>15.128</td><td>BB</td><td>0.6480</td><td>5443.19727</td><td>129.06407</td><td>50.3875</td></tr></tbody></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %	1	6.560	BB	0.2987	5359.47607	271.00064	49.6125	2	15.128	BB	0.6480	5443.19727	129.06407	50.3875
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Chromatogram of Rac-3xa showing two peaks. The first peak is at 8.455 minutes with a height of 185.36739 mAU. The second peak is at 31.836 minutes with a height of 43.33953 mAU.

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	8.455	BB	0.3294	3993.71484	185.36739	50.6229
2	31.836	BB	1.0886	3895.43506	43.33953	49.3771

Cc1ccc2c(c1)c(c3ccccc3n2C(=O)c4cccnc4)c5ccccc5

Rac-3xa

Chromatogram of 3xa showing two peaks. The first peak is at 8.472 minutes with a height of 307.54611 mAU. The second peak is at 31.478 minutes with a height of 1.82678 mAU.

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	8.472	BB	0.3268	6558.32373	307.54611	97.8327
2	31.478	MM	1.3255	145.28601	1.82678	2.1673

Cc1ccc2c(c1)c(c3ccccc3n2C(=O)c4cccnc4)c5ccccc5

3xa

Chromatogram of Rac-3ya showing two peaks. The first peak is at 7.630 minutes with a height of 133.80492 mAU. The second peak is at 12.157 minutes with a height of 74.17764 mAU.

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	7.630	BB	0.8363	7343.65967	133.80492	50.3630
2	12.157	BB	1.4024	7237.80713	74.17764	49.6370

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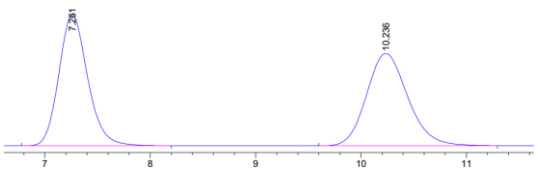
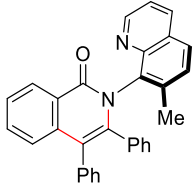
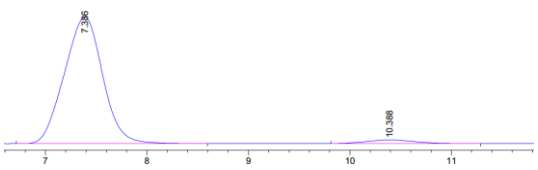
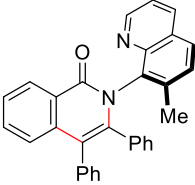
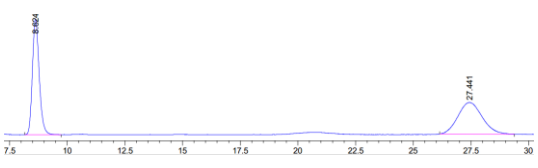
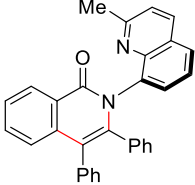
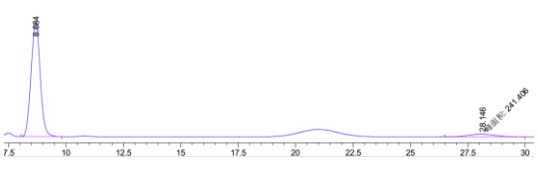
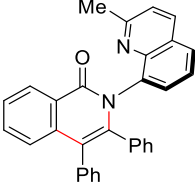
Rac-3ya

Chromatogram of 3ya showing two peaks. The first peak is at 7.622 minutes with a height of 4.04656 mAU. The second peak is at 12.019 minutes with a height of 69.43001 mAU.

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	7.622	BB	0.6267	211.11412	4.04656	3.1284
2	12.019	BB	1.3965	6537.30029	69.43001	96.8716

COc1ccc2c(c1)c(c3ccccc3n2C(=O)c4cccnc4)c5ccccc5

3ya

	<div><p><i>Rac-3za</i></p></div> <table><thead><tr><th>Peak #</th><th>RetTime [min]</th><th>Type</th><th>Width [min]</th><th>Area mAU *s</th><th>Height [mAU]</th><th>Area %</th></tr></thead><tbody><tr><td>1</td><td>7.261</td><td>BB</td><td>0.2891</td><td>1662.65674</td><td>87.73969</td><td>49.7377</td></tr><tr><td>2</td><td>10.236</td><td>BB</td><td>0.4176</td><td>1680.19409</td><td>61.71933</td><td>50.2623</td></tr></tbody></table>	Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %	1	7.261	BB	0.2891	1662.65674	87.73969	49.7377	2	10.236	BB	0.4176	1680.19409	61.71933	50.2623
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %																
1	7.261	BB	0.2891	1662.65674	87.73969	49.7377																
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2	28.146	MM	1.3222	241.40619	3.04290	6.2204																

Chromatogram for **Rac-4** showing two peaks. The x-axis represents time in minutes, ranging from 8 to 22. The y-axis represents intensity. Peak 1 is at 9.165 minutes and Peak 2 is at 18.826 minutes.

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.165	BB	0.4760	9402.06934	296.44104	49.6025
2	18.826	BB	0.8722	9552.75195	158.71529	50.3975

Chemical structure of **Rac-4**: A benzimidazole derivative with a diphenylphosphino group (PPh₂) and a methyl group (Me).

Rac-4

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.165	BB	0.4760	9402.06934	296.44104	49.6025
2	18.826	BB	0.8722	9552.75195	158.71529	50.3975

Chromatogram for **4** showing two peaks. The x-axis represents time in minutes, ranging from 8 to 20. The y-axis represents intensity. Peak 1 is at 8.394 minutes and Peak 2 is at 17.014 minutes.

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.394	BB	0.4054	5672.18555	208.48030	94.9655
2	17.014	BB	0.5915	300.70673	6.05383	5.0345

Chemical structure of **4**: A benzimidazole derivative with a diphenylphosphino group (PPh₂) and a methyl group (Me).

4

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.394	BB	0.4054	5672.18555	208.48030	94.9655
2	17.014	BB	0.5915	300.70673	6.05383	5.0345

Chromatogram for **Rac-7** showing two peaks. The x-axis represents time in minutes, ranging from 10 to 16. The y-axis represents intensity. Peak 1 is at 11.061 minutes and Peak 2 is at 14.029 minutes.

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.061	VB	0.7684	2.82923e4	553.49164	49.8718
2	14.029	BB	0.6899	2.84377e4	648.08789	50.1282

Chemical structure of **Rac-7**: A chiral molecule with two ester groups (EtO₂C and CO₂Et) and two phenyl groups (Ph).

Rac-7

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.061	VB	0.7684	2.82923e4	553.49164	49.8718
2	14.029	BB	0.6899	2.84377e4	648.08789	50.1282

Chromatogram for **7** showing two peaks. The x-axis represents time in minutes, ranging from 10 to 16. The y-axis represents intensity. Peak 1 is at 11.433 minutes and Peak 2 is at 14.499 minutes.

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.433	BB	0.5314	2012.85864	57.92440	27.3068
2	14.499	BB	0.5299	5358.40771	156.33768	72.6932

Chemical structure of **7**: A chiral molecule with two ester groups (EtO₂C and CO₂Et) and two phenyl groups (Ph).

7

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	11.433	BB	0.5314	2012.85864	57.92440	27.3068
2	14.499	BB	0.5299	5358.40771	156.33768	72.6932