Supporting Information

Synthesis of Axially Chiral Biaryls *via* Pd(II)-Catalysed Direct C(sp^2)-H Arylation

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1. Experimental Section

1.1 Reagent Information

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

1.2 Analytical Information

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

1.3 General procedure for the preparation of 1-arylisoquinolines-*N*-oxides

Quinoline *N*-oxides **1a-h**, were prepared from the reported method.[1] A 50 mL round bottom flask was charged with a solution of 1-chloroisoquinoline (1.0 mmol) and $Pd(PPh_3)_4$ (3.0 mol %) in 1,4-dioxane (6 mL) under an argon atmosphere. A solution of Na_2CO_3 (2.0 equiv.) in H_2O (2 mL) and a solution of corresponding boronic acid (1.1 equiv.) in MeOH (1.6 mL) were sequentially added. The reaction mixture was stirred at 85 °C overnight, cooled to room temperature, quenched with H_2O (10 mL) and extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried over Na_2SO_4, filtrated, evaporated in vacuo. The crude 1-aryl-isoquinoline was purified by flash column chromatography using *n*-hexane/ethyl acetate as eluent.

To a solution of the 1-arylisoquinoline (1.0 mmol) in CH_2Cl_2 (20 mL) was added *m*-chloroperoxybenzoic acid (1.5 equiv.). The reaction mixture was stirred at room temperature for 24 hours. Then the reaction mixture was quenched with saturated Na_2CO_3 aqueous solution and extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were washed with brine, dried over Na_2SO_4 and filtrated. The solvent was removed under reduced pressure and the

residue was purified by flash column chromatography using *n*-hexane/ethyl acetate as eluent to afford 1-arylisoquinoline *N*-oxide.

1.4 General procedure for asymmetric arylation of 1-arylisoquinoline *N*-oxides with iodoarenes

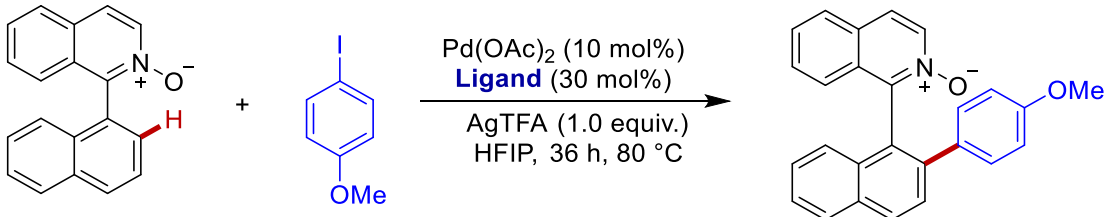
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 1-arylisoquinoline *N*-oxide (0.1 mmol), iodoarene (2.0 equiv.), $Pd(OAc)_2$ (10 mol%), *N*-Ac-Phe-OH (30 mol%), Ag_2CO_3 (3.0 equiv.), and HFIP (0.5 mL) were added. The subsequent mixture was stirred at 60 ˚C for 36 h. After completion, the solvent was evaporated under reduced pressure, and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and EtOAc/*n*-hexane as the eluent.

1.5 General procedure for achiral arylation of 1-arylisoquinoline *N*-oxides with iodoarenes

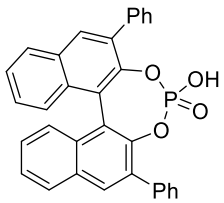
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 1-arylisoquinoline *N*-oxide (0.1 mmol), iodoarene (2.0 equiv.), $Pd(OAc)_2$ (10 mol%), AgTFA (3.0 equiv.) and HFIP (0.5 mL) were added. The subsequent mixture was stirred at 100 ˚C for 24 h. After completion, the solvent was evaporated under reduced pressure, and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and EtOAc/*n*-hexane as the eluent.

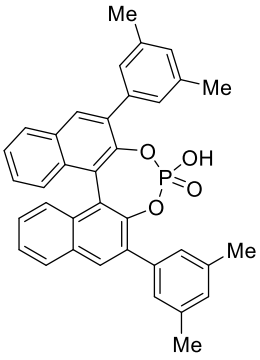
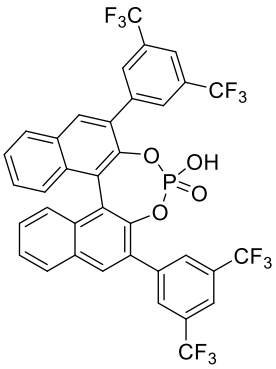
2. Optimization studies

2.1 Ligand screening



1a (0.1 mmol) (*racemic*) + **2a**(2.0 equiv.) → **3a** NMR yield, *ee*

S No.	Ligand	Yield (%)	*ee* (%)
1		98	0

2		98	0
3		97	0
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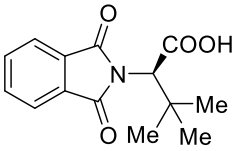
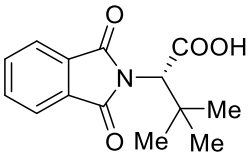
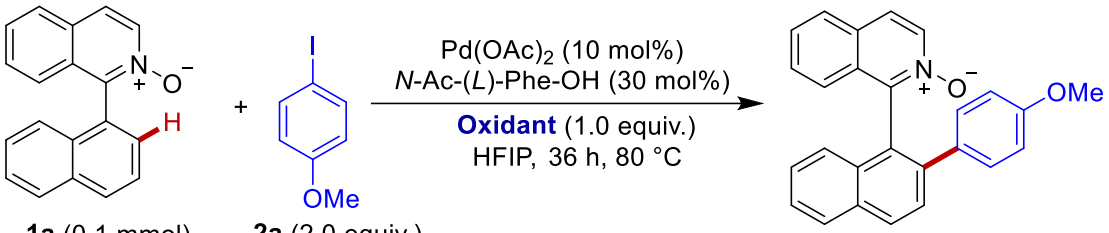
5		96	0
6		98	0
7	*N*-Ac-Gly-OH	96	0
8	*N*-Ac-(*L*)-Leu-OH	98	0
9	*N*-Ac-(*L*)-Val-OH	98	0
10	***N*-Ac-(*L*)-Phe-OH**	**92**	**5**
11	*N*-Boc-(*L*)-Ala-OH	98	0
12	*N*-Boc-(*L*)-PheAla-OH	98	0
13	*N*-Boc-(*L*)-TLE-OH	98	0
14	*N*-Boc-(*L*)-Leu-OH	97	0
15	*N*-Boc-(*L*)-Gly-OH	98	0
16	*N*-Fmoc-(*L*)-Leu-OH	97	0

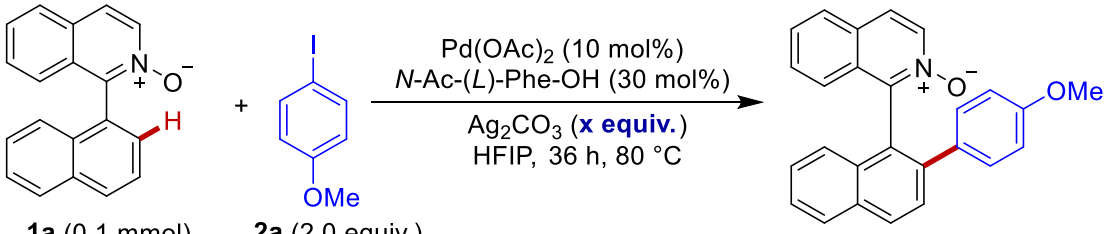
2.2 Oxidant screening



1a (0.1 mmol) (*racemic*) + **2a** (2.0 equiv.) → **3a** NMR yield, *ee*

S No.	Oxidant	Yield (%)	*ee* (%)
1	AgTFA	97	
2	AgOAc	22	27
3	**Ag_2CO_3**	**48**	**88**
4	LiOAc	nr	-
5	NaOAc	20	6
6	KOAc	20	12

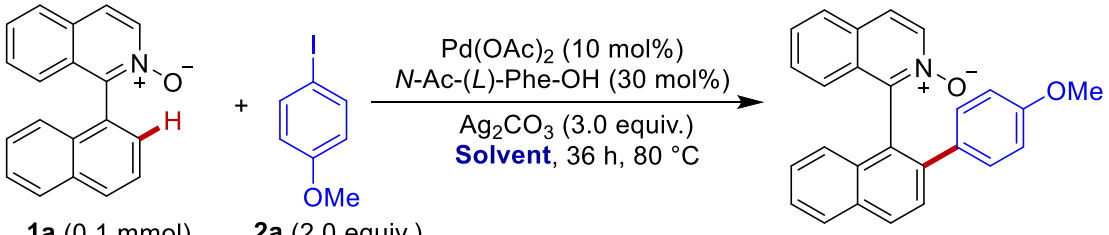
2.3 Oxidant amount screening



1a (0.1 mmol) (*racemic*) + **2a** (2.0 equiv.) → **3a** NMR yield, *ee*

S No.	Ag_2CO_3 (x equiv.)	Yield (%)	*ee* (%)
1	1	56	73
2	2	55	76
3	**3**	**48**	**88**

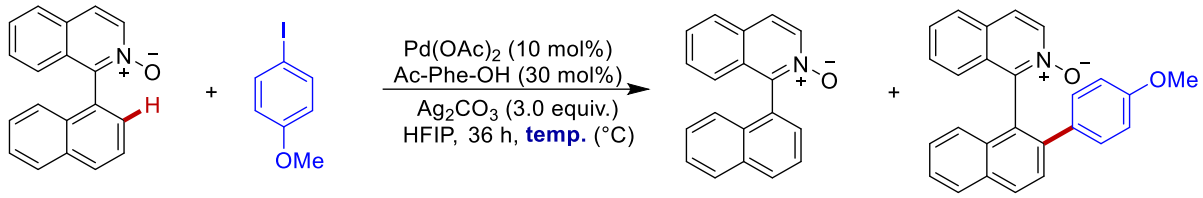
2.4 Solvent screening



1a (0.1 mmol) (*racemic*) + **2a** (2.0 equiv.) → **3a** NMR yield, *ee*

S No.	Solvent	Yield (%)	*ee* (%)
1	**HFIP**	**48**	**88**
2	HFIP:MeCN (1:1)	nr	-
3	HFIP:DME (1:1)	23	62
4	HFIP:THF (1:1)	21	62
5	TFE:DME (1:1)	nr	-

2.5 Temperature screening



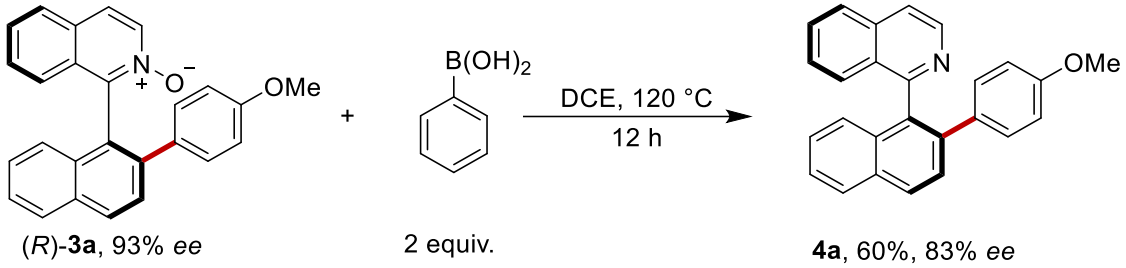
1a (0.1 mmol) (*racemic*) **2a** (2.0 equiv.) **1a**, Recovery yield, *ee* **3a** NMR yield, *ee*

S No.	Temp.	1a, Recovery Yield (%)	*ee* (%)	3h, Isolated Yield (%)	*ee* (%)
1	25	69	30	24	96
2	40	66	42	32	94
3	**60**	**52**	**46**	**45**	**92**
4	70	49	53	48	88
5	80	45	49	48	88
6	100	45	48	48	85

3. Gram scale synthesis

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 1-arylisoquinoline *N*-oxide (5.0 mmol), iodoarene (2.0 equiv.), $Pd(OAc)_2$ (10 mol%), *N*-Ac-Phe-OH (30 mol%), Ag_2CO_3 (3.0 equiv.) and HFIP (25.0 mL) were added. The subsequent mixture was stirred at 60 ˚C for 96 h. After completion, the solvent was evaporated under reduced pressure, and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and EtOAc/*n*-hexane as the eluent.

4. Reduction of product 3a

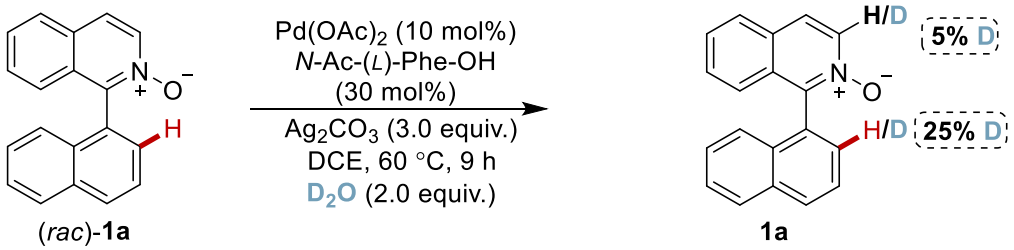


(*R*)-**3a**, 93% *ee* 2 equiv. **4a**, 60%, 83% *ee*

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, product **3a** (0.1 mmol, 93% *ee*), phenyl boronic acid (2 equiv.) and DCE (0.5 mL) were added. The subsequent mixture was stirred at 120 ˚C for 12 h. After completion, the solvent was evaporated under reduced pressure and **4a** was isolated from column chromatography (30% EtOAc/*n*-hexane) as white viscous, yield (60%).

5. Deuterium labelling experiments

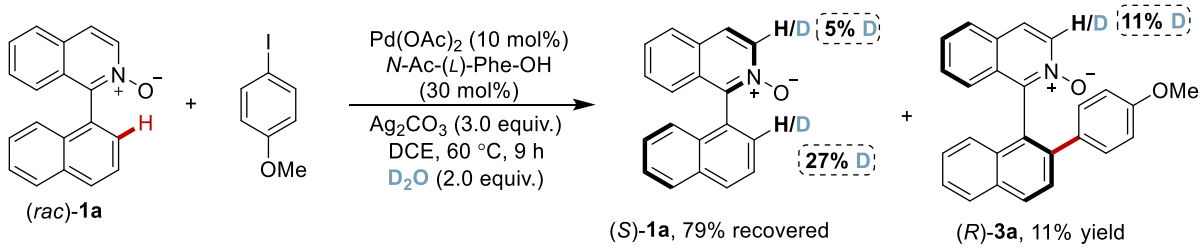
➢ **Deuterium labelling experiments without coupling partner**



(*rac*)-**1a** **1a**

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 1-arylisoquinoline *N*-oxide (0.1 mmol), $Pd(OAc)_2$ (10 mol%), *N*-Ac-Phe-OH (30 mol%), Ag_2CO_3 (3.0 equiv.), and DCE (0.5 mL) were added. The subsequent mixture was stirred at 60 ˚C for 9 h. After completion, the solvent was evaporated under reduced pressure, and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and EtOAc/*n*-hexane as the eluent.

➢ **Deuterium labelling experiments with coupling partner**

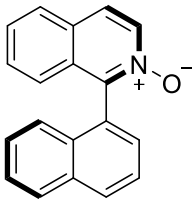


(*rac*)-**1a** (*S*)-**1a**, 79% recovered (*R*)-**3a**, 11% yield

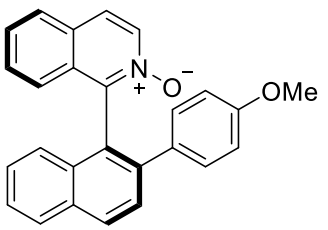
To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar, 1-arylisoquinoline *N*-oxide (0.1 mmol), iodoarene (2.0 equiv.), $Pd(OAc)_2$ (10 mol%), *N*-Ac-Phe-OH (30 mol%), Ag_2CO_3 (3.0 equiv.), and DCE (0.5 mL) were added. The subsequent mixture was stirred at 60 ˚C for 9 h. After completion, the solvent was evaporated under reduced pressure, and the crude mixture was purified by flash chromatography using silica gel (230-400 mesh size) and EtOAc/*n*-hexane as the eluent.

6. Characterization data of synthesised molecules

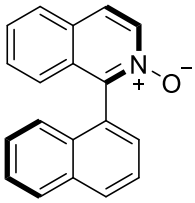
*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (14.1 mg, 52% yield, 46% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +144 (c = 0.10, Acetone, 46% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 20.6 min, t_r (minor) = 27.0 min, 46% *ee*.



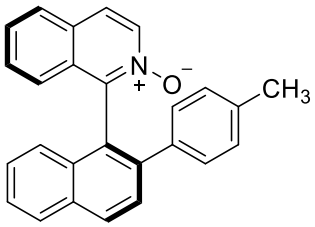
*(R)-1-(2-(4-methoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3a**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 17.0 mg (45%). MP = 154-156 ºC. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.33 (d, *J* = 7.0 Hz, 1H), 8.02 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.63-7.60 (m, 3H), 7.43-7.40 (m, 1H), 7.36-7.25 (m, 4H), 7.20-7.15 (m, 1H), 7.07 (dd, *J* = 8.5 Hz, 1H), 6.87 (d, *J* = 8.5 Hz, 1H), 6.5-6.56 (m, 2H), 3.58 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 159.0, 146.5, 140.6, 136.8, 133.3, 132.8, 131.6, 130.3, 129.6, 129.5, 129.3, 129.1, 128.7, 128.6, 128.0, 127.6, 126.9, 126.3, 126.1, 125.3, 125.0, 124.0, 113.7, 55.1. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{26}H_{20}NO_2^+$ 378.1489; found, 378.1488. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (minor) = 19.4 min, t_r (major) = 26.7 min, 92% *ee*. $[\alpha]_D^{20}$ = -75 (c = 0.10, Acetone).



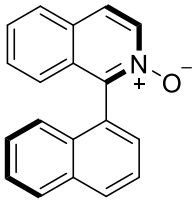
*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (12.7 mg, 47% yield, 54% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +163 (c = 0.10, Acetone, 54% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 21.6 min, t_r (minor) = 26.3 min, 54% *ee*.



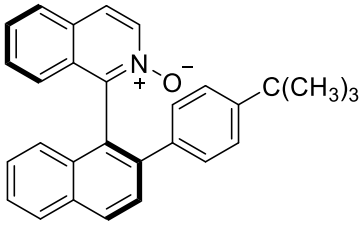
*(R)-1-(2-(p-tolyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3b**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 17.3 mg (48%). MP = 118-120 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.41 (d, J = 7.2 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 8.00 (d, J = 7.8 Hz, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.71-7.69 (m, 2H), 7.51-7.47 (m, 2H), 7.40-7.38 (m, 1H), 7.31-7.28 (m, 1H), 7.20-7.19 (m, 2H), 7.10 (d, J = 8.4 Hz, 1H), 7.01 (d, J = 8.4 Hz, 1H), 6.90-6.89 (m, 2H), 2.15 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 146.9, 141.1, 137.6, 137.5, 136.6, 132.9, 131.0, 130.6, 129.9, 129.7, 129.5, 129.4, 129.1, 129.0, 128.9, 128.3, 127.8, 127.5, 127.0, 126.4, 125.8, 125.4, 124.3, 123.4, 21.14. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{26}H_{20}NO^+$ 362.1539 found, 362.1549. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 274 nm): = t_r (minor) = 14.6 min, t_r (major) = 17.0 min, 95% *ee*. $[\alpha]_D^{20}$ = -93 (c = 0.10, Acetone).



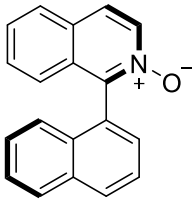
*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (12.5 mg, 46% yield, 58% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +179 (c = 0.10, Acetone, 58% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 20.6 min, t_r (minor) = 26.7 min, 58% *ee*.



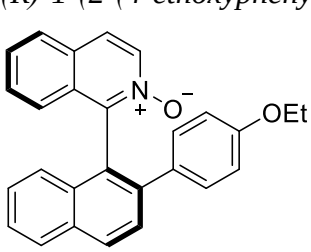
*(R)-1-(2-(4-(tert-butyl)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3c**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 19.3 mg (48%). MP = 164-166 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.42 (d, J = 7.0 Hz, 1H), 8.12 (d, J = 8.5 Hz, 1H), 8.01 (d, J = 8.5 Hz, 1H), 7.78 (d, J = 8.0, 1H), 7.72-7.71 (m, 2H), 7.55-7.49 (m, 2H), 7.40-7.37 (m, 1H), 7.36-7.32 (m, 1H), 7.18-7.16 (m, 2H), 7.12- 7.05 (m, 4H), 1.14 (s, 9H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 150.9, 147.0, 141.0, 137.0, 136.3, 132.7, 130.6, 130.2, 129.9, 129.6, 129.3, 129.1, 128.1, 127.4, 127.2, 126.9, 126.4, 126.1, 124.9, 124.7, 124.3, 122.7, 34.4, 31.0. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{29}H_{26}NO^+$ 404.2009 found, 404.2008. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.7 mL/min, detection at 310 nm): = t_r (minor) = 12.2 min, t_r (major) = 14.8 min, 89% *ee*. $[\alpha]_D^{20}$ = -83 (c = 0.10, Acetone).



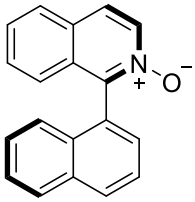
*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (12.7 mg, 47% yield, 58% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +177 (c = 0.10, Acetone, 58% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.3 min, t_r (minor) = 26.9 min, 58% *ee*.



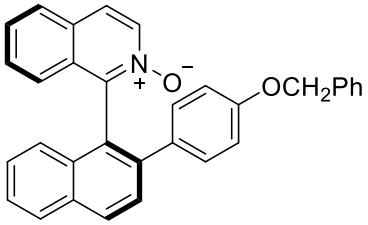
*(R)-1-(2-(4-ethoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3d**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 17.2 mg (44%). MP = 168-170 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.44 (d, *J* = 7.5 Hz, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.70-7.68 (m, 2H), 7.51-7.47 (m, 2H), 7.41-7.37 (m, 1H), 7.31-7.27 (m, 1H), 7.23-7.20 (m, 2H), 7.09 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.00 (dd, *J* = 8.5, 1.0 Hz, 1H), 6.62-6.59 (m, 2H), 3.86-3.82 (m, 2H), 1.29 (t, *J* = 7.0 Hz, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 159.0, 146.5, 140.6, 136.8, 133.3, 132.8, 131.6, 130.3, 129.6, 129.5, 158.6, 147.2, 140.9, 136.4, 132.7, 132.6, 131.0, 130.5, 130.1, 129.8, 129.6, 129.28, 129.26, 129.1, 128.2, 127.5, 127.0, 126.4, 125.8, 125.2, 124.3, 123.25, 123.21, 114.2, 63.4, 14.8. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{27}H_{22}NO_2^+$ 392.1645 found, 392.1645. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.5 mL/min, detection at 274 nm): = t_r (minor) = 27.1 min, t_r (major) = 29.8 min, 92% *ee*. $[\alpha]_D^{20}$ = -87 (c = 0.10, Acetone).



*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (12.2 mg, 45% yield, 43% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +134 (c = 0.10, Acetone, 43% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 20.4 min, t_r (minor) = 26.4 min, 43% *ee*.

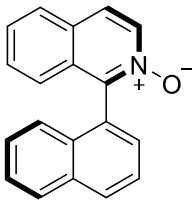


*(R)-1-(2-(4-(benzyloxy)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3e**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 22.2 mg (49%). MP = 106-108 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.44 (d, *J* = 7.2 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.78 (d, J = 7.8 Hz, 1H), 7.73 (d, *J* = 7.2 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.55-7.50 (m, 2H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.34-7.30 (m, 7H), 7.21-7.20 (m, 2H), 7.09 (d, *J* = 7.8 Hz, 1H), 7.04 (d, *J* =

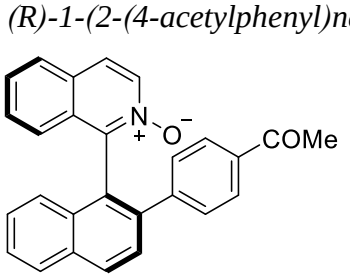


8.4 Hz, 1H), 6.71-6.70 (m, 2H), 4.88 (s, 2H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$, δ): 158.5, 147.3, 140.9, 136.8, 136.4, 132.8, 130.7, 130.4, 130.2, 130.1, 129.8, 129.3, 129.2, 128.8, 128.6, 128.5, 128.3, 128.2, 128.1, 127.8, 127.6, 127.5, 127.1, 126.5, 126.0, 124.8, 124.5, 122.8, 114.7, 69.9. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{32}H_{24}NO_2^+$ 454.1802 found, 454.1802. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.7 mL/min, detection at 310 nm): = t_r (minor) = 26.3 min, t_r (major) = 30.0 min, 89% *ee*. $[\alpha]_D^{20}$ = -84 (c = 0.10, Acetone).

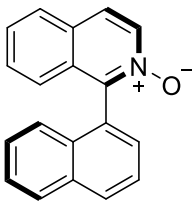
*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (11.1 mg, 41% yield, 48% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +147 (c = 0.10, Acetone, 48% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.2 min, t_r (minor) = 26.9 min, 48% *ee*.



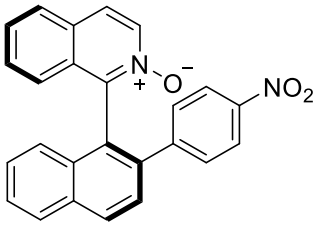
*(R)-1-(2-(4-acetylphenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3f**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 20.2 mg (52%). MP = 244-246 °C. ^1H NMR (500 MHz, $CDCl_3$, δ): 88.36 (d, J = 7.0 Hz, 1H), 8.14 (dd, J = 8.5, 1.0 Hz, 1H), 8.00 (d, J = 7.0 Hz, 1H), 7.72-7.68 (m, 5H), 7.55-752 (m, 1H), 7.50-7.48 (m, 2H), 7.45-7.38 (m, 2H), 7.29-7.25 (m, 1H), 7.16 (dd, J = 8.5, 1.0 Hz, 1H), 6.94 (d, J = 8.5 Hz 1H), 2.46 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, δ): 197.98, 145.81, 145.62, 139.75, 136.85, 136.04, 133.31, 131.39, 130.61, 129.64, 129.60, 129.56, 129.09, 129.00, 128.78, 128.56, 128.30, 127.97, 127.93, 127.41, 127.02, 126.91, 126.57, 125.07, 124.91, 124.89, 124.35, 26.63. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{27}H_{20}NO_2^+$ 390.1489 found, 390.1489. HPLC separation (Lux® 5 μm Amylose-1, *n*-hexane/*i*-PrOH 70:30, 1.0 mL/min, detection at 310 nm): = t_r (minor) = 16.1 min, t_r (major) = 29.2 min, 75% *ee*. $[\alpha]_D^{20}$ = -51 (c = 0.10, Acetone).



*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (16.0 mg, 59% yield, 7% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +15 (c = 0.10, Acetone, 7% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.0 min, t_r (minor) = 26.3 min, 7% *ee*.

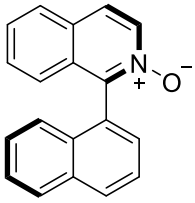


*(R)-1-(2-(4-nitrophenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3g**):* Following



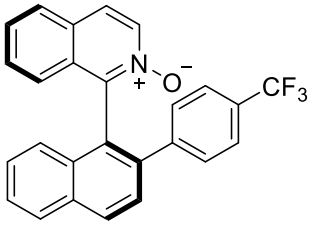
the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 23.1 mg (23%). MP = 122-124 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.47 (d, J = 7.0 Hz, 1H), 8.21 (d, J = 8.0 Hz, 1H), 8.09 (d, J = 8.5 Hz, 1H), 7.94-7.90 (m, 2H), 7.83-7.80 (m, 2H), 7.70 (d, J = 8.5 Hz, 1H), 7.63-7.57 (m, 2H), 7.50-7.47 (m, 1H), 7.45-72 (m, 2H), 7.39-7.36 (m, 1H), 7.14 (d, J = 8.5 Hz, 1H), 7.00 (d, J = 8.5 Hz, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 147.4, 146.5, 146.2, 139.3, 136.3, 133.5, 131.3, 130.7, 130.6, 130.3, 130.1, 129.6, 129.2, 129.0, 128.5, 127.6, 127.6, 127.5, 127.4, 125.4, 125.2, 125.1, 123.6, 122.0. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{25}H_{17}N_2O_3^+$ 393.1234; found, 393.1235. HPLC separation (Lux® 5 μm Amylose-1, *n*-hexane/*i*-PrOH 60:40, 1.0 mL/min, detection at 310 nm): = t_r (major) = 11.2 min, t_r (minor) = 20.2 min, 59% *ee*. $[\alpha]_D^{20}$ = -21 (c = 0.10, Acetone).

*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (11.4 mg, 42% yield,



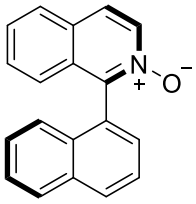
34% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +117 (c = 0.10, Acetone, 34% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 23.4 min, t_r (minor) = 28.0 min, 34% *ee*.

*(R)-1-(2-(4-(trifluoromethyl)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3h**):*

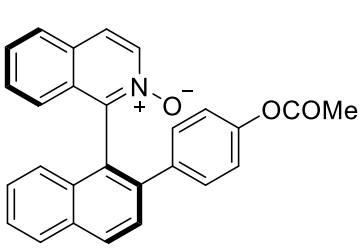


Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 19.5 mg (47%). MP = 130-132 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.45 (d, J = 7.5 Hz, 1H), 8.18 (d, J = 8.5 Hz, 1H), 8.08-8.06 (m, 1H), 7.80 (dd, J = 8.5, 1.0 Hz, 1H), 7.77 (d, J = 7.0 Hz, 1H), 7.69 (d, J = 8.5 Hz, 1H), 7.60-7.54 (m, 2H), 7.48-7.45 (m, 1H), 7.40-7.32 (m, 5H), 7.12 (d, J = 8.5 Hz, 1H), 7.01 (d, J = 8.5 Hz, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 146.5, 143.5, 140.1, 136.3, 133.3, 131.1, 130.5, 130.4, 130.2, 130.1, 130.0, 129.8, 129.5, 129.1, 128.5, 128.3, 127.9, 127.4, 127.1, 125.6, 125.33 (q, J = 3.75 Hz), 125.0, 124.9, 124.0 (q, J = 276.25 Hz), 122.1. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{26}H_{17}F_3NO^+$ 416.1257 found, 416.1257. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 92:8, 0.6 mL/min, detection at 310 nm): = t_r (minor) = 47.4 min, t_r (major) = 53.1 min, 83% *ee*. $[\alpha]_D^{20}$ = -42 (c = 0.10, Acetone).

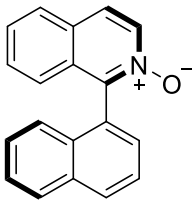
*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (19.8 mg, 73% yield, 12% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +53 (c = 0.10, Acetone, 12% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 28.6 min, t_r (minor) = 28.6 min, 12% *ee*.



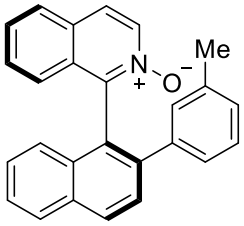
*(R)-1-(2-(4-acetoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3i**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 8.5 mg (21%). MP = 126-128 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.36 (d, *J* = 6.5 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.72-7.70 (m, 1H), 7.67 (d, *J* = 7.0 Hz, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.48-745 (m, 2H), 7.36-7.33 (m, 1H), 7.28-7.25 (m, 1H), 7.22-7.1- (m, 2H), 7.02 (d, *J* = 8.5 Hz, 1H), 6.97-6.95 (m, 1H), 6.77-6.74 (m, 2H), 2.12 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 169.3, 150.3, 147.0, 140.4, 137.8, 136.2, 133.0, 130.9, 130.7, 130.4, 129.9, 129.3, 129.25, 129.20, 128.1, 127.7, 127.2, 126.7, 125.91, 125.90, 125.15, 124.67, 124.64, 122.8, 121.4, 21.2. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{27}H_{20}NO_3^+$ 406.1438 found, 406.1439. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 90:10, 1.0 mL/min, detection at 254 nm): = t_r (minor) = 47.1 min, t_r (major) = 58.4 min, 45% *ee*. $[\alpha]_D^{20}$ = -32 (c = 0.10, Acetone).



*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (11.9 mg, 44% yield, 35% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = + 115 (c = 0.10, Acetone, 35% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.4 min, t_r (minor) = 27.4 min, 35% *ee*.

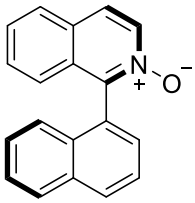


*(R)-1-(2-(m-tolyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3j**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 17.7 mg (49%). MP = 118-120 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.46 (d, *J* = 7.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.74-7.72 (m, 2H), 7.56-7.53 (m, 2H), 7.45-7.41 (m, 1H), 7.36-7.33 (m, 1H), 7.11-7.03 (m, 4H), 6.99-6.960 (m, 1H), 6.89-6.87 (m, 1H), 2.08 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 147.30, 141.37, 139.99, 138.22, 138.18, 136.23, 132.93, 130.79, 130.59, 130.56, 130.49, 130.33, 129.76, 129.49, 129.29, 128.70, 128.65,

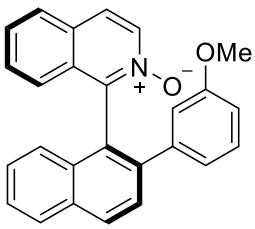


128.62, 128.28, 127.89, 127.50, 127.11, 126.65, 126.60, 126.17, 124.74, 124.67, 124.52, 122.03, 21.23. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{26}H_{20}NO^+$ 362.1539; found, 362.1539. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (minor) = 13.5 min, t_r (major) = 16.7 min, 93% *ee*. $[\alpha]_D^{20}$ = -73 (c = 0.10, Acetone).

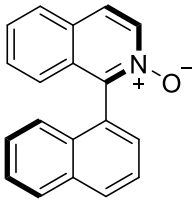
*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (13.3 mg, 49% yield, 33% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = + 114 (c = 0.10, Acetone, 33% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.3 min, t_r (minor) = 27.3 min, 33% *ee*.



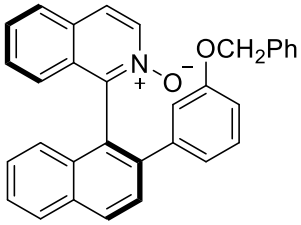
*(R)-1-(2-(3-methoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3k**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 16.2 mg (43%). MP = 104-106 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.48 (d, *J* = 7.0 Hz, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.85-7.81 (m, 2H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.62-7.59 (m, 1H), 7.58-7.55 (m, 1H), 7.44-7.38 (m, 2H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.09-7.03 (m, 2H), 6.91-6.89 (m, 1H), 6.80 (d, *J* = 2.5 Hz, 1H), 6.65-6.6 (m, 1H), 3.53 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 159.6, 141.5, 141.1, 136.0, 133.0, 131.0, 130.8, 130.6, 130.1, 129.4, 129.3, 129.2, 128.2, 127.9, 127.2, 126.8, 126.4, 124.7, 124.6, 123.0, 119.9, 114.3, 113.0, 55.2. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{26}H_{20}NO_2^+$ 378.1489; found, 378.1489. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (minor) = 17.4 min, t_r (major) = 22.3 min, 91% *ee*. $[\alpha]_D^{20}$ = -64 (c = 0.10, Acetone).



*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (14.1 mg, 52% yield, 24% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = + 100 (c = 0.10, Acetone, 24% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 20.8 min, t_r (minor) = 26.8 min, 24% *ee*.

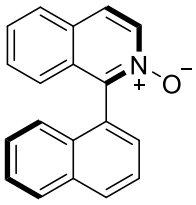


*(R)-1-(2-(3-methoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3l**):*

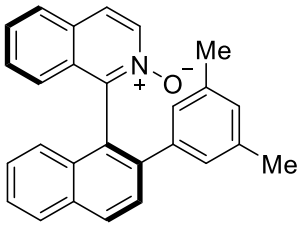


Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 18.6 mg (41%). MP = 98-100 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.35 (d, J = 7.2 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.4 Hz, 1H), 7.73-7.68 (m, 3H), 7.51-7.48 (m, 1H), 7.46-7.43 (m, 1H), 7.38-7.30 (m, 6H), 7.28-7.25 (m, 1H), 7.15 (d, J = 8.4 Hz, 1H), 7.08 (s, 1H), 7.03-7.00 (m, 2H), 6.98 (d, J = 8.4 Hz, 1H), 6.70-.668 (m, 1H), 4.88-4.83 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 158.5, 146.6, 142.2, 140.7, 137.0, 136.7, 133.1, 131.5, 130.4, 129.8, 129.4, 129.3, 129.2, 128.9, 128.6, 128.01, 127.82, 127.76, 127.70, 127.6, 127.5, 126.9, 126.5, 126.2, 125.5, 125.2, 124.1, 121.1, 114.8, 114.1, 69.9. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{32}H_{24}NO_2^+$ 454.1804; found, 454.1804. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 1.0 mL/min, detection at 310 nm): = t_r (minor) = 14.6 min, t_r (major) = 25.5 min, 89% *ee*. $[\alpha]_D^{20}$ = -83 (c = 0.10, Acetone).

*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (12.7 mg, 47% yield, 50% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +150 (c = 0.10, Acetone, 50% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.8 min, t_r (minor) = 28.0 min, 50% *ee*.

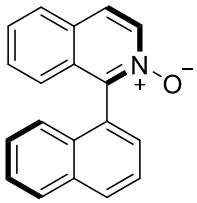


*(R)-1-(2-(3,5-dimethylphenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3m**):*

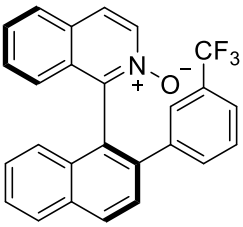


Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 17.6 mg (47%). MP = 104-106 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.46 (d, J = 7.0 Hz, 1H), 8.12 (d, J = 9.0 Hz, 1H), 8.01 (d, J = 8.5 Hz, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 7.5 Hz, 2H), 7.53-7.50 (m, 2H), 7.43-7.40 (m, 1H), 7.34-7.31 (m, 1H), 7.11 (d, J = 8.0 Hz, 1H), 7.05 (d, J = 8.5 Hz, 1H), 6.88 (s, 2H), 6.69 (s, 1H), 2.06 (s, 6H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 147.2, 141.2, 139.9, 137.8, 136.1, 132.8, 130.6, 130.5, 130.1, 129.9, 129.5, 129.2, 128.1, 127.4, 126.9, 126.4, 125.9, 125.6, 124.8, 124.2, 122.3, 21.0. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{27}H_{22}NO^+$ 376.1696; found, 376.1698. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 310 nm): = t_r (minor) = 11.5 min, t_r (major) = 17.5 min, 88% *ee*. $[\alpha]_D^{20}$ = -61 (c = 0.10, Acetone).

*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (mg, 50% yield, 21% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +71 (c = 0.10, Acetone, 21% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.5 min, t_r (minor) = 26.9 min, 21% *ee*.

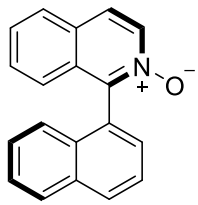


*(R)-1-(2-(3-(trifluoromethyl)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3n**):*

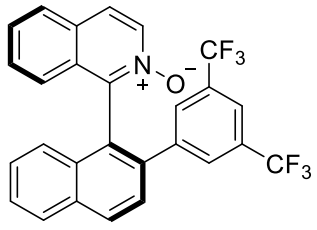


Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 15.3 mg (37%). MP = 112-114 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.47 (d, J = 7.0 Hz, 1H), 8.22 (d, J = 8.5 Hz, 1H), 8.10 (d, J = 8.0 Hz, 1H), 7.82-7.78 (m, 2H), 7.76 (d, J = 8.5 Hz, 1H), 7.63-7.57 (m, 2H), 7.451-7.47 (m, 2H), 7.42 (s, 1H), 7.40-736 (m, 1H), 7.32 (d, J = 7.5 Hz, 1H), 7.23-7.20 (m, 1H), 7.17 (d, J = 8.5 Hz, 1H), 7.03 (d, J = 8.5 Hz, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 146.5, 140.3, 139.9, 136.0, 133.1, 131.3, 131.1, 130.6, 130.5, 130.1, 129.9, 129.5, 128.9, 128.8, 128.2, 127.9, 127.2, 127.0, 125.5, 124.9, 124.8, 124.53, 122.5, 121.6, 120.6, 119.4 (q, J = 287.5 Hz). HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{26}H_{17}F_3NO^+$ 416.1257; found, 416.1259. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 1.0 mL/min, detection at 254 nm): = t_r (minor) = 9.2 min, t_r (major) = 12.9 min, 77% *ee*. $[\alpha]_D^{20}$ = -20 (c = 0.10, Acetone).

*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (16.0 mg, 59% yield, 3% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +4 (c = 0.10, Acetone, 3% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.0 min, t_r (minor) = 26.4 min, 3% *ee*.



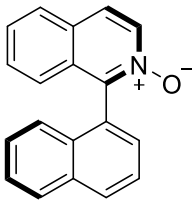
*(R)-1-(2-(3,5-bis(trifluoromethyl)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3o**):*



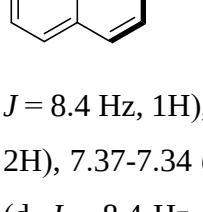
Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 17.4 mg (36%). MP = 78-80 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.48 (d, J = 7.0 Hz, 1H), 8.21 (d, J = 8.5 Hz, 1H), 8.04 (d, J = 8.0 Hz, 1H), 7.83-7.80 (m, 4H), 7.70 (d, J = 8.5 Hz, 1H), 7.61-7.56 (m, 3H), 7.45-7.42 (m, 1H), 7.40-7.37 (m, 1H), 7.19 (d, J = 8.5 Hz, 1H), 7.02 (d, J = 8.5 Hz, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 146.6, 142.5, 137.6, 136.2, 133.4, 131.7, 131.5, 131.4, 131.3, 130.4, 130.3, 130.2, 129.4, 128.7, 128.65, 128.62,

128.3, 127.5, 127.3, 126.7, 125.4, 125.3, 124.8, 123.09 (q, J = 271.25 Hz), 121.3 (q, J = 4.17 Hz). HRMS (ESI TOF) .32(m/z): $[M + H]^+$ calcd for $C_{27}H_{16}F_6NO^+$ 484.1131; found, 484.1131. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 90:10, 1.0 mL/min, detection at 254 nm): = t_r (minor) = 10.8 min, t_r (major) = 30.4 min, 37% *ee*. $[\alpha]_D^{20}$ = -11 (c = 0.10, Acetone).

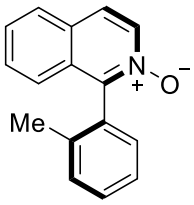
*(S)-1-(Naphthalen-1-yl)isoquinoline-N-oxide (Table 2, Entry **1a**):* Solid (11.6 mg, 43% yield, 50% *ee*). Analytical data for **1a**: $[\alpha]_D^{20}$ = +149 (c = 0.10, Acetone, 50% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (major) = 22.2 min, t_r (minor) = 27.1 min, 50% *ee*.



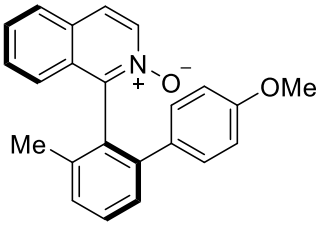
*(R)-1-(2-(9H-fluoren-3-yl)naphthalen-1-yl)isoquinoline 2-oxide (Table 2, Entry **3p**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 21.4 mg (49%). MP = 118-120 °C. ^{1}H NMR (600 MHz, $CDCl_3$, δ): 8.40 (d, J = 7.2 Hz, 1H), 8.13 (d, J = 9.0 Hz, 1H), 8.00 (d, J = 7.8 Hz, 1H), 7.78 (d, J = 8.4 Hz, 1H), 7.65-7.59 (m, 4H), 7.53-7.50 (m, 2H), 7.45 (d, J = 7.8 Hz, 1H), 7.43-7.39 (m, 2H), 7.37-7.34 (m, 1H), 7.30-7.28 (m, 1H), 7.25-7.22 (m, 2H), 7.19 (d, J = 8.4 Hz, 1H), 6.97 (d, J = 8.4 Hz, 1H), 3.74-3.66 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, δ): 146.5, 143.5, 143.3, 141.3, 141.2, 141.0, 139.5, 136.8, 133.0, 131.6, 130.3, 129.6, 129.2, 129.0, 128.7, 128.6, 128.1, 127.7, 127.3, 127.2, 127.0, 126.8, 126.5, 126.4, 125.3, 125.2, 125.1, 125.0, 124.9, 124.0, 119.9, 119.6, 36.9. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{32}H_{22}NO^+$ 436.1696 found, 436.1696. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 310 nm): = t_r (minor) = 18.6 min, t_r (major) = 26.9 min, 88% *ee*. $[\alpha]_D^{20}$ = -110 (c = 0.10, Acetone).



(S)-1-(o-tolyl)isoquinoline 2-oxide (*Table 2, Entry **1b**):* Solid (11.0 mg, 47% yield, 35% *ee*). Analytical data for **1b**: $[\alpha]_D^{20}$ = +36 (c = 0.10, Acetone, 35% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 92:8, 1.0 mL/min, detection at 254 nm): = t_r (major) = 36.5 min, t_r (minor) = 42.6 min, 35% *ee*.

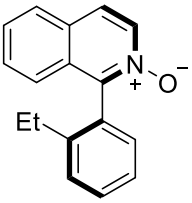


*(R)-1-(4'-methoxy-3-methyl-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (Table 2, Entry **3q**):*

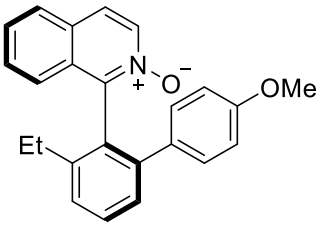


Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 16.4 mg (48%). MP = 106-108 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.41 (d, J = 7.0 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 7.0 Hz, 1H), 7.54-7.47 (m, 2H), 7.39-7.36 (m, 3H), 7.16-7.13 (m, 2H), 7.09 (d, J = 8.5 Hz, 1H), 6.56-6.55 (m, 2H), 3.60 (s, 3H), 2.03 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 158.9, 148.1, 142.5, 138.1, 136.2, 133.0, 133.0, 129.98, 129.94, 129.6, 129.4, 129.1, 129.0, 128.8, 128.7, 127.7, 126.9, 125.6, 123.9, 113.5, 55.1, 19.5. HRMS (ESI TOF) (m/z): [M + H]$^{+}$ calcd for $C_{23}H_{20}NO_2^{+}$ 342.1489 found, 342.1491. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 85:15, 1.0 mL/min, detection at 254 nm): = t_r (minor) = 14.4 min, t_r (major) = 19.1 min, 84% *ee*. $[\alpha]_D^{20}$ = -23 (c = 0.10, Acetone).

(S)-1-(2-ethylphenyl)isoquinoline 2-oxide (*Table 2, Entry **1c**):* Solid (10.4 mg, 42% yield, 23% *ee*). Analytical data for **1c**: $[\alpha]_D^{20}$ = +31 (c = 0.10, Acetone, 23% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 85:15, 0.6 mL/min, detection at 254 nm): = t_r (major) = 21.9 min, t_r (minor) = 25.1 min, 23% *ee*.

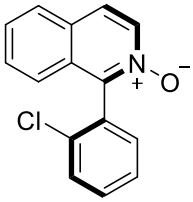


*(R)-1-(3-ethyl-4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (Table 2, Entry **3r**):*

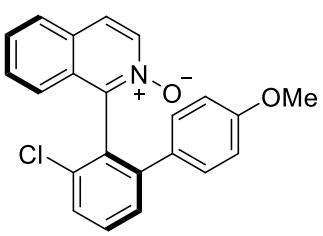


Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 17.0 mg (48%). MP = 98-100 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.37 (d, J = 7.0 Hz, 1H), 7.69 (dd, J = 8.0, 1.0 Hz, 1H), 7.61-7.57 (m, 2H), 7.49-7.45 (m, 2H), 7.39-7.3 (m, 2H), 7.15-7.13 (m, 1H), 7.10 (d, J = 8.5 Hz, 1H), 6.60-6.51 (m, 2H), 3.61 (s, 3H), 2.54-2.46 (m, 1H), 2.22-2.15 (m, 1H), 1.00 (t, J = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 158.9, 143.7, 142.6, 136.2, 133.1, 130.2, 129.5, 129.3, 129.2, 129.1, 127.9, 127.2, 126.9, 125.7, 123.9, 113.5, 55.1, 26.1, 14.2. HRMS (ESI TOF) (m/z): [M + H]$^{+}$ calcd for $C_{24}H_{22}NO_2^{+}$ 356.1645 found, 356.1645. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 1.0 mL/min, detection at 254 nm): = t_r (minor) = 9.1 min, t_r (major) = 12.2 min, 87% *ee*. $[\alpha]_D^{20}$ = -21 (c = 0.10, Acetone).

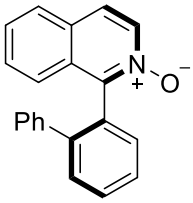
*(S)-1-(2-chlorophenyl)isoquinoline 2-oxide (Table 2, Entry **1d**):* Solid (14.3 mg, 56% yield, 10% *ee*). Analytical data for **1d**: $[\alpha]_D^{20}$ = +17 (c = 0.10, Acetone, 10% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 274 nm): = t_r (major) = 17.7 min, t_r (minor) = 23.5 min, 10% *ee*.



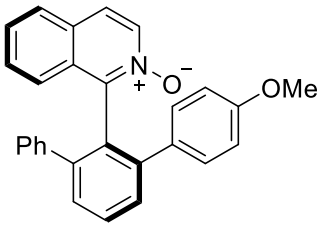
*(R)-1-(3-chloro-4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (Table 3, Entry **3s**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 11.9 mg (33%). MP = 122-124 ºC. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.31 (d, *J* = 7.5 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.58-7.53 (m, 2H), 7.50-7.46 (m, 1H), 7.45 (dd, *J* = 7.0, 2.0 Hz, 1H), 7.42-7.39 (m, 1H), 7.21-7.18 (m, 2H), 7.09 (d, *J* = 8.5 Hz, 1H), 3.63 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 13C 159.3, 145.5, 144.7, 144.6, 136.5, 134.8, 132.0, 131.0, 129.6, 129.3, 129.1, 129.0, 128.9, 128.7, 128.6, 127.1, 124.74, 124.70, 124.25, 113.7, 55.2. HRMS (ESI TOF) (m/z): $[M + H]^+$ calcd for $C_{22}H_{17}ClNO_2^+$ 362.0942 found, 362.0944. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 0.8 mL/min, detection at 254 nm): = t_r (minor) = 14.8 min, t_r (major) = 24.7 min, 91% *ee*. $[\alpha]_D^{20}$ = -31 (c = 0.10, Acetone).



(S)-1-([1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (*Table 2, Entry **1e**):* Solid (18.7 mg, 63% yield, 41% *ee*). Analytical data for **1e**: $[\alpha]_D^{20}$ = +105 (c = 0.10, Acetone, 41% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 70:30, 1.0 mL/min, detection at 254 nm): = t_r (major) = 7.4 min, t_r (minor) = 8.6 min, 41% *ee*.

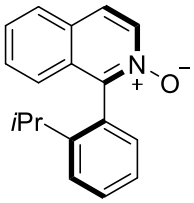


*(R)-1-(4-methoxy-[1,1':3',1''-terphenyl]-2'-yl)isoquinoline 2-oxide (Table 2, Entry **3t**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 11.3 mg (28%). MP = 218-220 ºC. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.06 (d, *J* = 7.0 Hz, 1H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.52-7.50 (m, 3H), 7.38 (d, *J* = 7.0 Hz 1H), 7.35-7.22 (m, 6H), 7.09-7.02 (m, 4H), 6.62-6.59 (m, 2H), 3.65 (s, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 13C 158.9, 147.1, 143.4, 143.0, 140.7, 136.2, 133.1, 129.9, 129.65, 129.61, 129.29, 129.23, 129.03, 128.5, 128.3, 128.1, 127.9, 127.3, 126.7, 125.14, 125.11, 125.09, 123.5, 113.4, 55.1. HRMS (ESI TOF) (m/z): $[M + Na]^+$ calcd for $C_{28}H_{21}NNaO_2^+$ 426.1465 found, 426.1464. HPLC

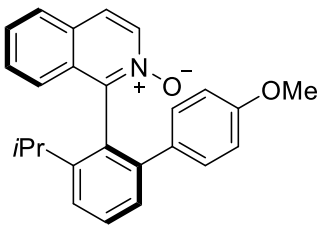


separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 70:30, 1.0 mL/min, detection at 274 nm): = t_r (minor) = 15.7 min, t_r (major) = 18.5 min, 86% *ee*. $[\alpha]_D^{20}$ = -31 (c = 0.10, Acetone).

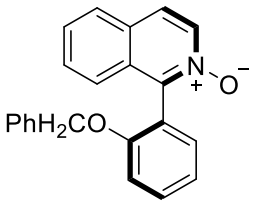
(S)-1-(2-isopropylphenyl)isoquinoline 2-oxide (*Table 2, Entry **1f**):* Solid (14.5 mg, 55% yield, 21% *ee*). Analytical data for **1f**: $[\alpha]_D^{20}$ = +23 (c = 0.10, Acetone, 18% *ee*). The enantiomeric excess was determined by (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 90:10, 1.0 mL/min, detection at 254 nm): = t_r (major) = 14.0 min, t_r (minor) = 17.3 min, 21% *ee*.



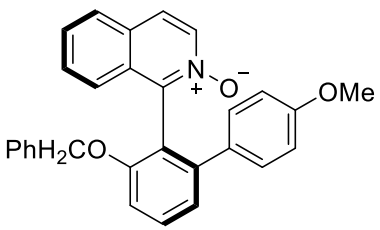
*(R)-1-(3-isopropyl-4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (Table 2, Entry **3u**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 14.8 mg (40%). MP = 204-206 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.21 (d, J = 7.0 Hz, 1H), 7.87 (dd, J = 7.5, 1.0 Hz, 1H), 7.82-7.81 (m, 1H), 7.65-7.62 (m, 1H), 7.57-7.52 (m, 2H), 7.45-7.42 (m, 1H), 7.36 (dd, J = 7.5, 1.5 Hz, 1H), 7.13- 7.09 (m, 2H), 7.08-7.06 (m, 1H), 6.57-6.54 (m, 2H), 3.59 (s, 3H), 2.35-2.26 (m, 1H), 1.33 (d, J = 6.5 Hz, 3H), 0.87 (d, J = 6.5 Hz, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, δ): 160.34, 149.89, 148.97, 143.74, 136.46, 134.58, 131.40, 131.11, 130.67, 130.65, 130.53, 130.10, 129.12, 128.87, 128.14, 126.68, 125.81, 125.69, 114.25, 32.68, 24.63, 23.93, 20.72. HRMS (ESI TOF) (m/z): $[M + Na]^+$ calcd for $C_{25}H_{23}NNaO_2^+$ 392.1621 found, 392.1620. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 80:20, 1.0 mL/min, detection at 254 nm): = t_r (minor) = 6.8 min, t_r (major) = 8.8 min, 83% *ee*. $[\alpha]_D^{20}$ = -40 (c = 0.10, Acetone).



*(S)-1-(2-(benzyloxy)phenyl)isoquinoline 2-oxide (Table 2, Entry **1g**):* Solid (12.4 mg, 38% yield, 83% *ee*). Analytical data for **1g**: $[\alpha]_D^{20}$ = +19 (c = 0.10, Acetone, 83% *ee*). The enantiomeric excess was determined by (Lux® 5 μm Amylose-1, *n*-hexane/*i*-PrOH 70:30, 1.0 mL/min, detection at 274 nm): = t_r (minor) = 13.5 min, t_r (major) = 15.8 min, 83% *ee*.

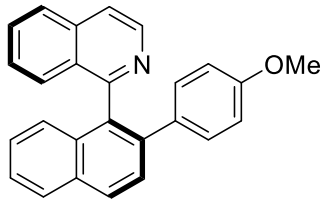


*(R)-1-(3-(benzyloxy)-4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (Table 2, Entry **3v**):* Following the general procedure for arylation, the title compound was isolated from column chromatography (80% EtOAc/*n*-hexane) as brown solid, yield = 24.2 mg (56%). MP = 114-116 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.38 (d, J = 7.0 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.61 (d, J = 7.0 Hz, 1H), 7.52 (dd, J = 8.5, 8.0 Hz, 1H), 7.48-7.45 (m, 1H), 7.37-7.34 (m, 1H), 7.23-7.13 (m, 7H), 7.07 (dd, J



= 8.5, 1.0 Hz, 1H), 7.04-7.00 (m, 2H), 6.62-6.59 (m, 2H), 5.11 (d, *J* = 12.5 Hz, 1H), 5.03 (d, *J* = 12.5 Hz, 1H), 3.63 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, δ): 159.0, 156.7, 146.1, 143.9, 136.9, 136.3, 132.6, 131.2, 129.7, 129.3, 129.2, 129.16, 129.11, 128.4, 127.6, 126.84, 126.81, 126.8, 125.7, 123.7, 122.7, 119.0, 113.6, 111.8, 70.5, 55.1. HRMS (ESI TOF) (m/z): $[M + Na]^+$ calcd for $C_{29}H_{23}NNaO_3^+$ 456.1570 found, 456.1570. HPLC separation (Chiralcel®-ODH, *n*-hexane/*i*-PrOH 70:30, 1.0 mL/min, detection at 274 nm): = t_r (minor) = 38.8 min, t_r (major) = 44.6 min, 82% *ee*. $[\alpha]_D^{20}$ = -25 (c = 0.10, Acetone).

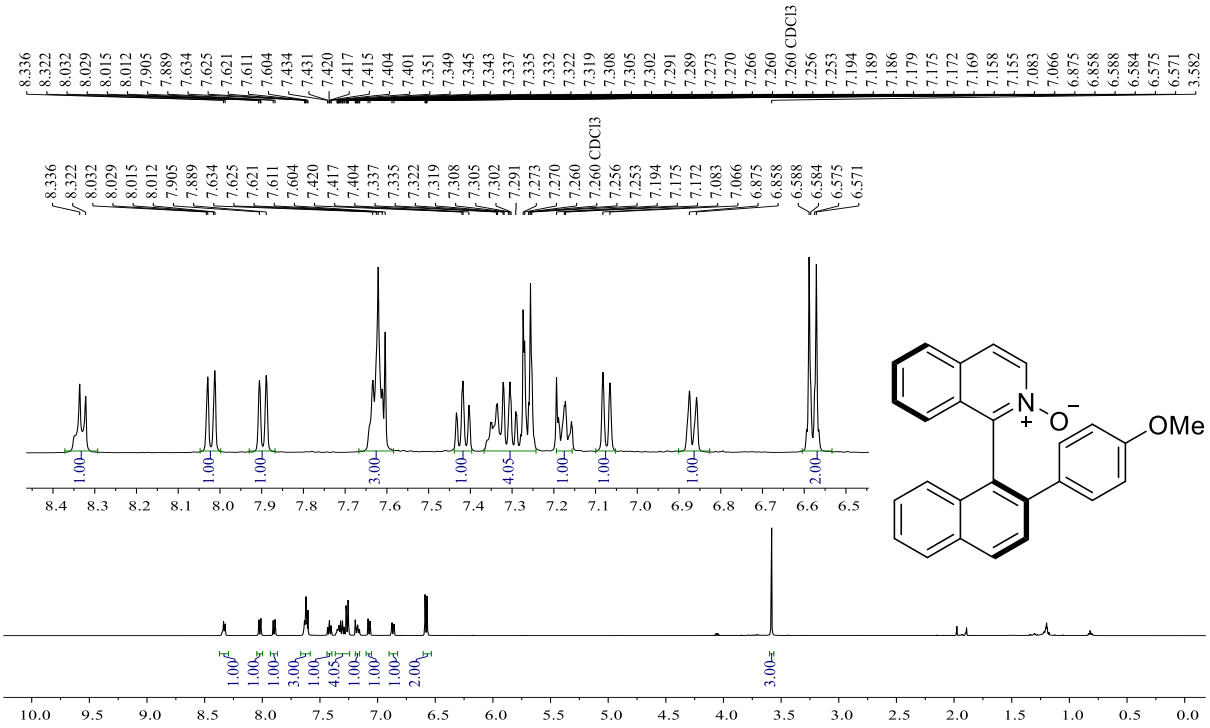
*(R)-1-(2-(4-methoxyphenyl)naphthalen-1-yl)isoquinoline (Scheme 1, **4a**): Yield is 60%),* ^{1}H



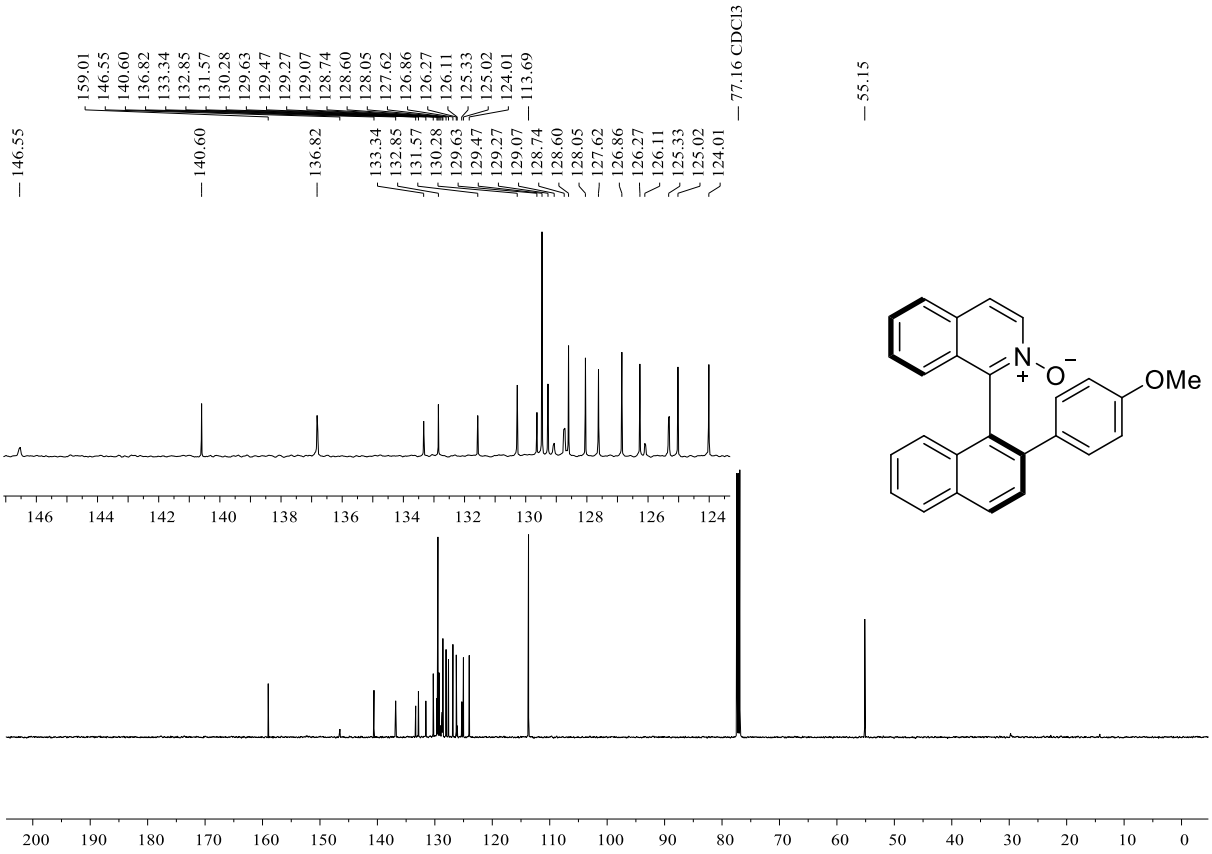
NMR (500 MHz, $CDCl_3$, δ): 8.65 (d, *J* = 5.4 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.65-7.64 (m, 2H), 7.56-7.53 (m, 1H), 7.47-7.44 (m, 1H), 7.40-7.38 (m, 1H), 7.31-7.25 (m, 2H), 7.16 (d, *J* = 7.8 Hz, 1H), 7.12-7.08 (m, 2H), 6.57-6.54 (m, 2H), 3.64 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$, δ): 160.4, 158.3, 142.0, 139.1, 136.2, 134.1, 133.9, 133.7, 133.1, 132.8, 130.6, 130.2, 129.5, 129.0, 128.7, 128.3, 128.2, 128.1, 127.4, 127.2, 126.9, 126.8, 126.7, 126.3, 125.8, 120.2, 120.2, 115.5, 113.2, 55.1. HPLC separation (Lux® 5 µm Amylose-1, *n*-hexane/*i*-PrOH 80:20, 1.0 mL/min, detection at 254 nm): = t_r (minor) = 17.0 min, t_r (major) = 22.3 min, 83% *ee*

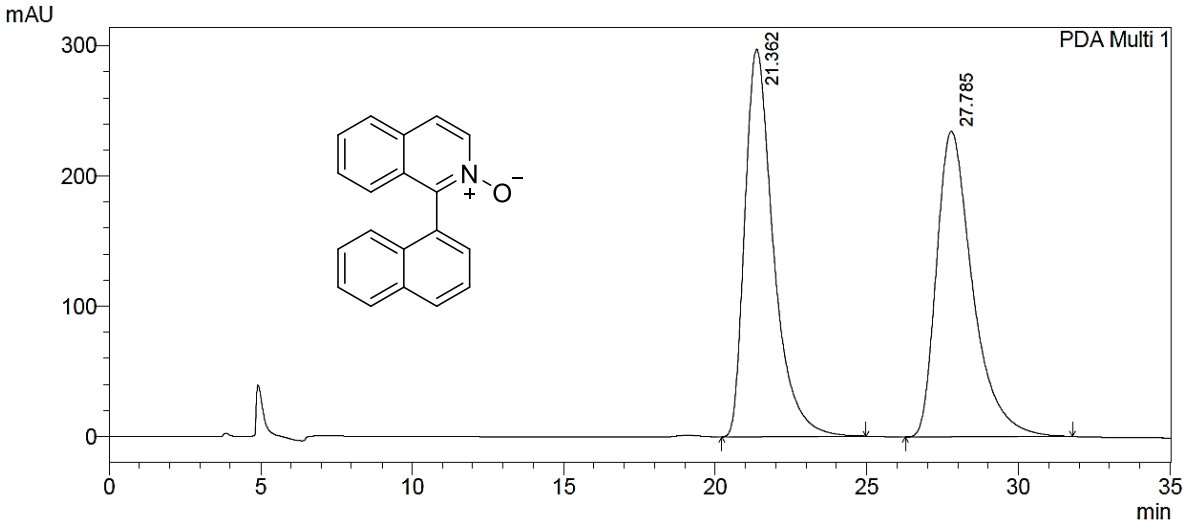
7.0 ^{1}H, ^{13}C and HPLC spectral data

*(R)-1-(2-(4-methoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3a**)*
^{1}H NMR *(*500 MHz*)*



$^{13}C\{^{1}H\}$ NMR *(*125 MHz*)*





PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
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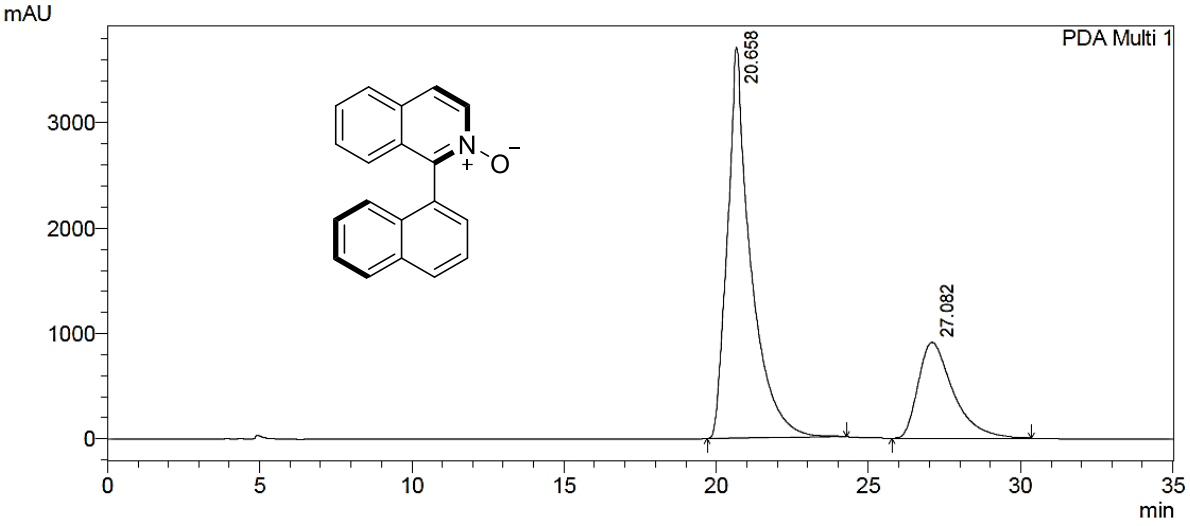
2	27.785	19421622	234536	49.914	44.085
Total		38910399	532004	100.000	100.000



PDA Ch1 254nm 4nm

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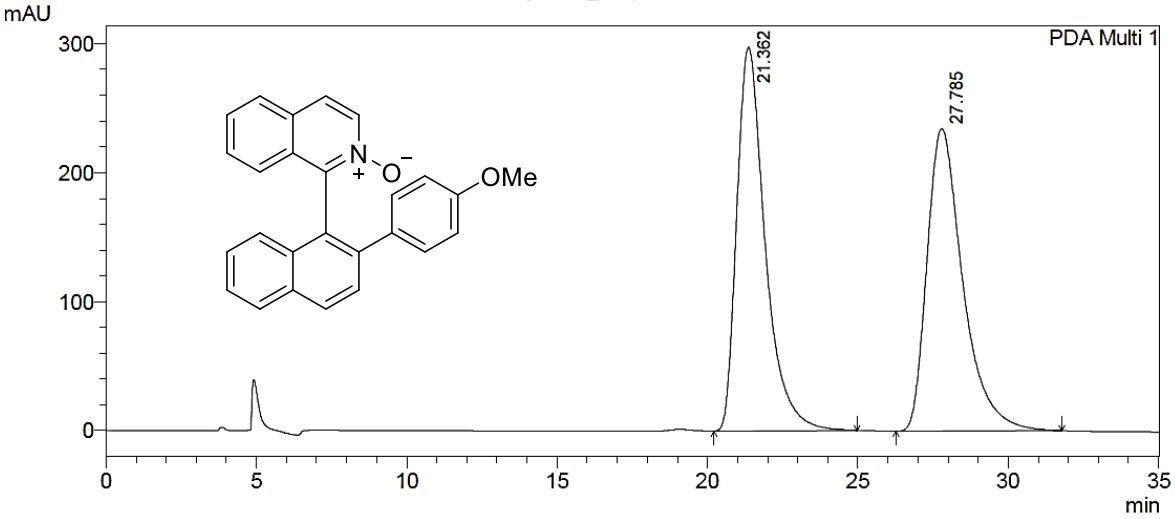
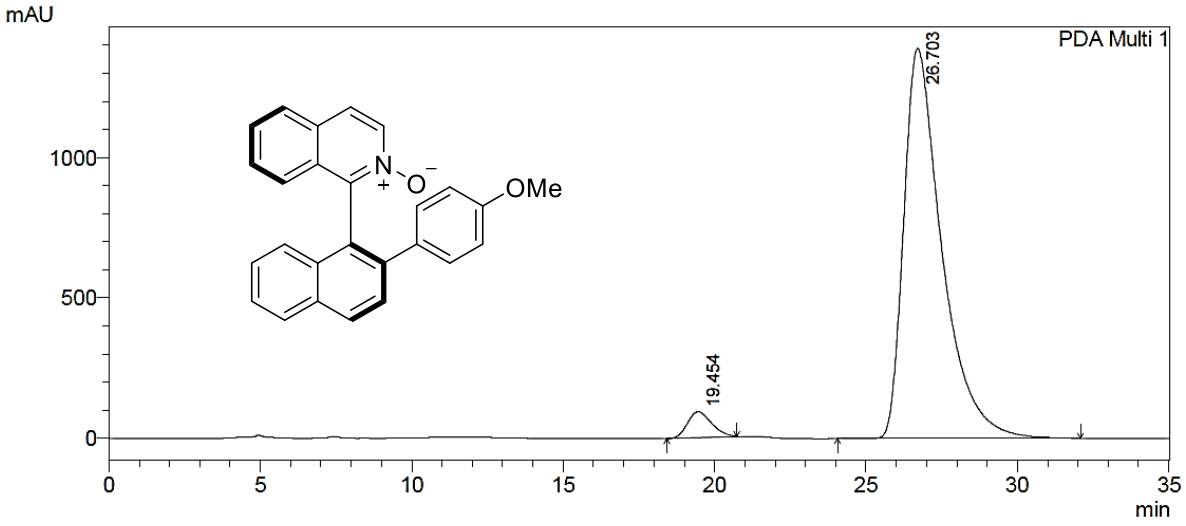
Total		269523057	4613143	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.362	19488777	297468	50.086	55.915
2	27.785	19421622	234536	49.914	44.085
Total		38910399	532004	100.000	100.000

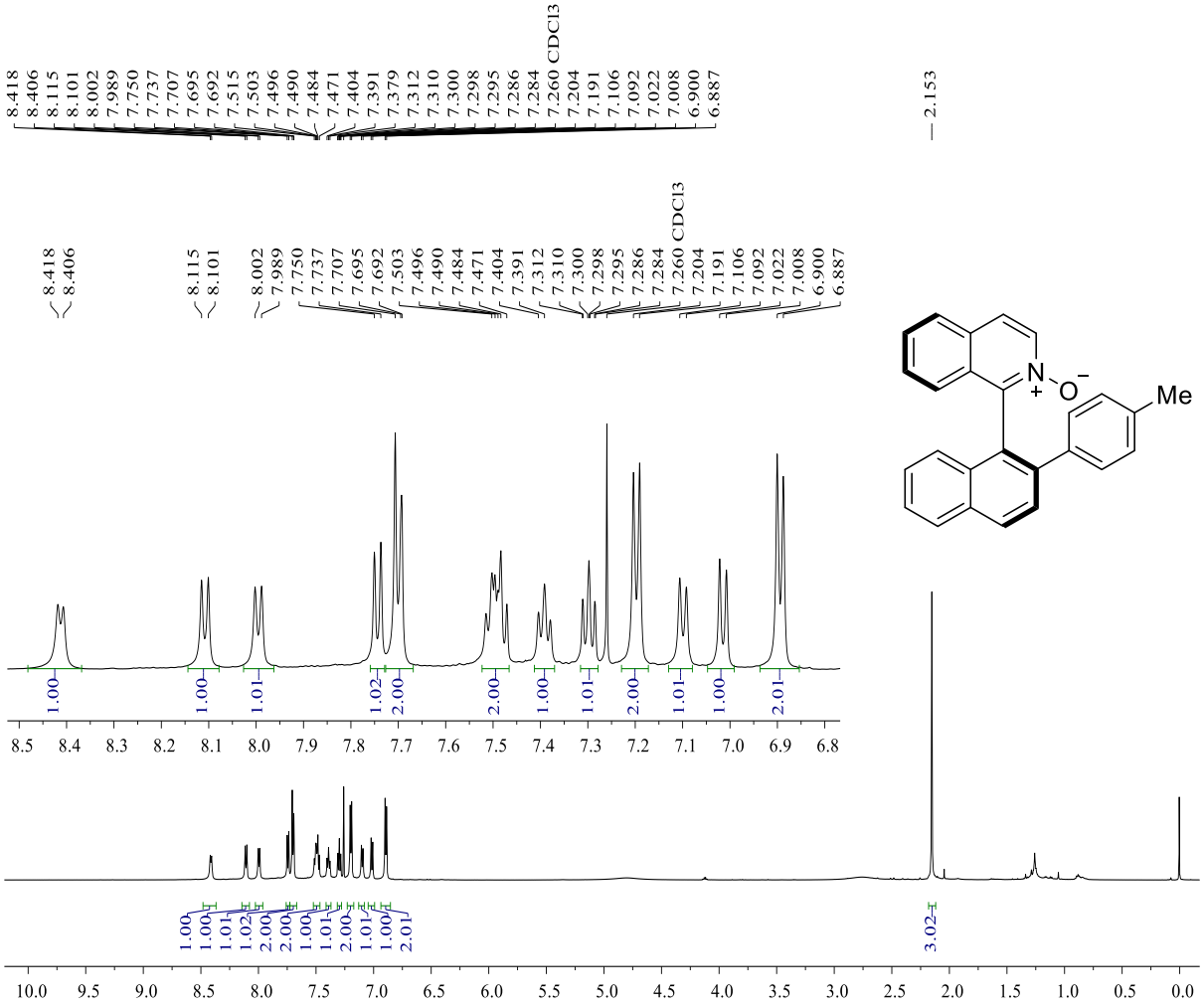


PDA Ch1 254nm 4nm

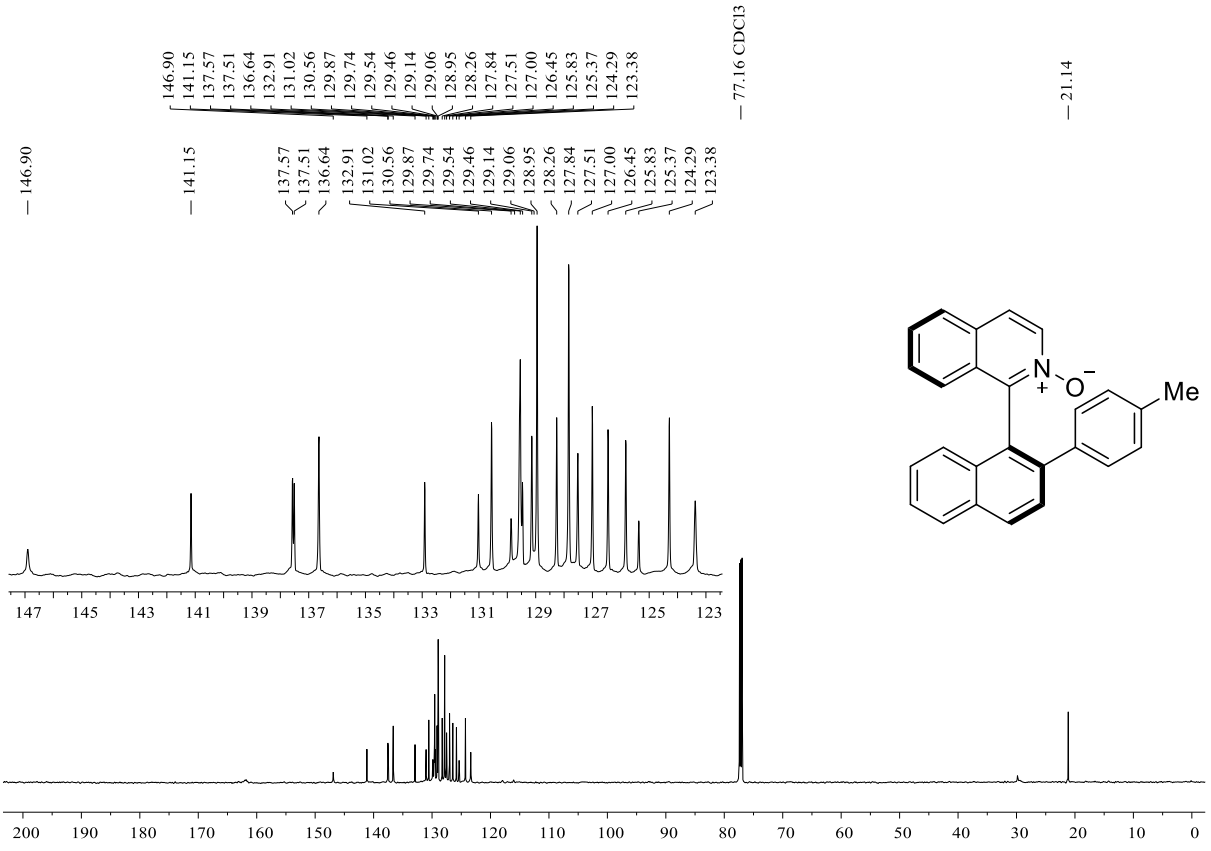
Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.454	5082867	91982	4.013	6.206
2	26.703	121567904	1390062	95.987	93.794
Total		126650770	1482044	100.000	100.000

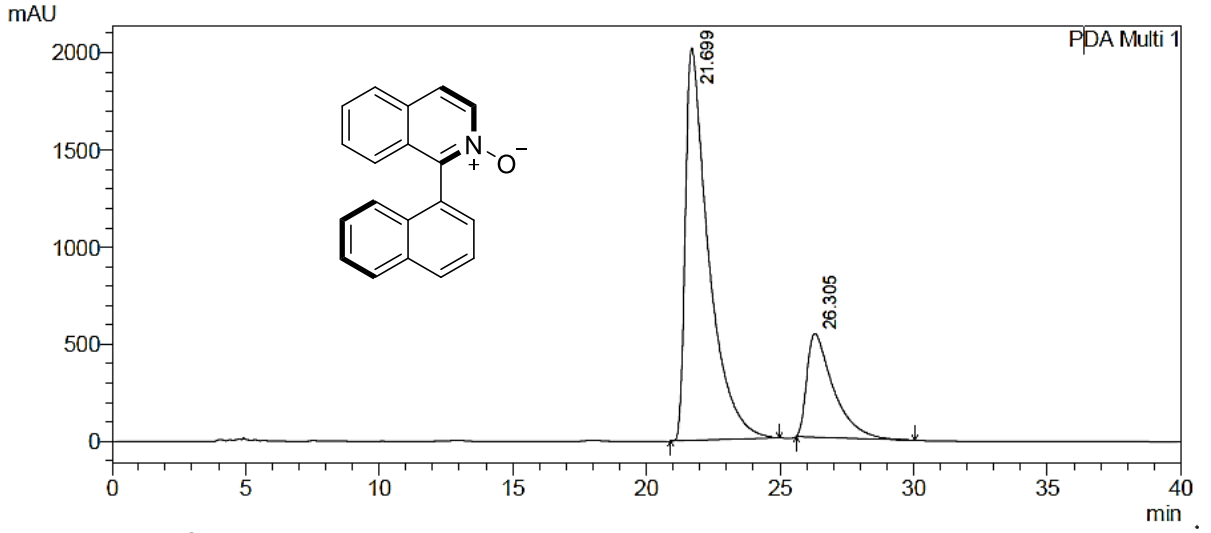
*(R)-1-(2-(p-tolyl)naphthalen-1-yl)isoquinoline 2-oxide (**3b**)*

^{1}H NMR *(*600 MHz*)*



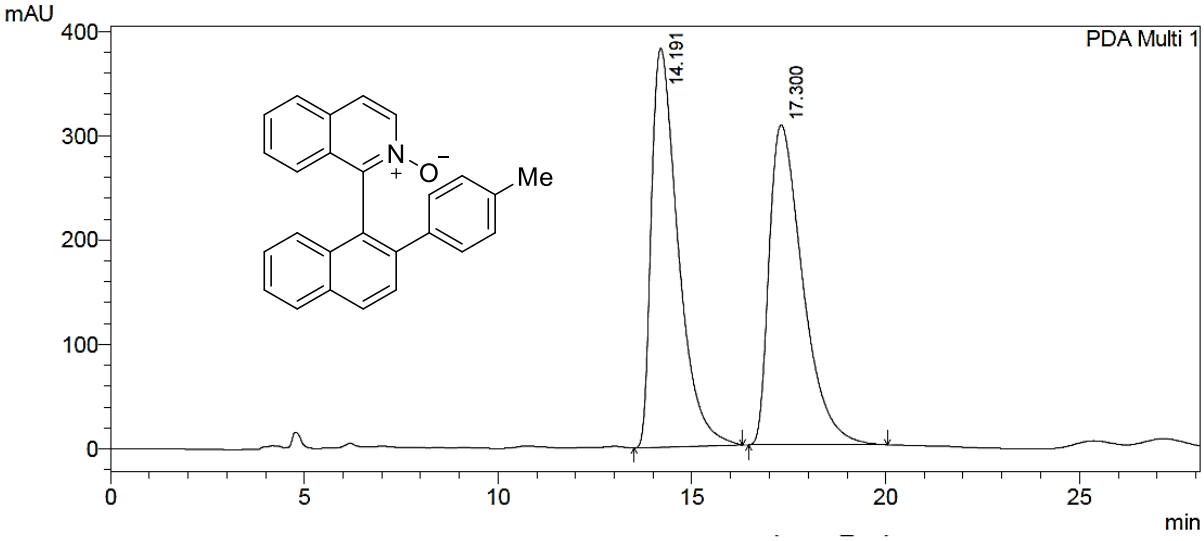
$^{13}C\{^{1}H\}$ NMR *(*125 MHz*)*





PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.699	121412135	2017360	76.834	79.138
2	26.305	36606779	531797	23.166	20.862
Total		158018914	2549157	100.000	100.000



PDA Ch1 274nm 4nm

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1	14.191	18396272	381946	49.901	55.487
2	17.300	18469428	306408	50.099	44.513
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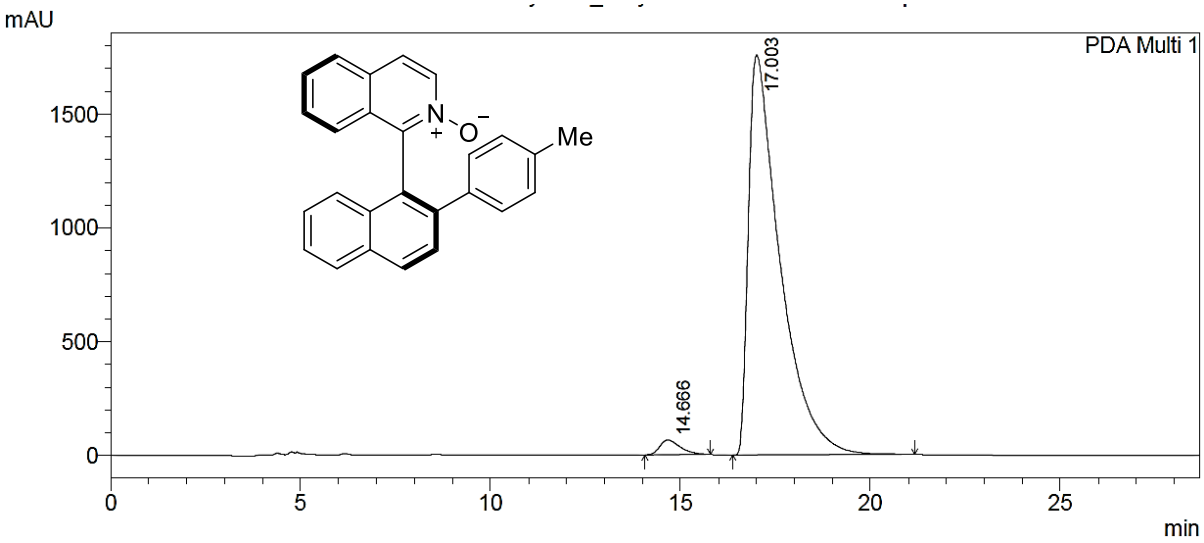
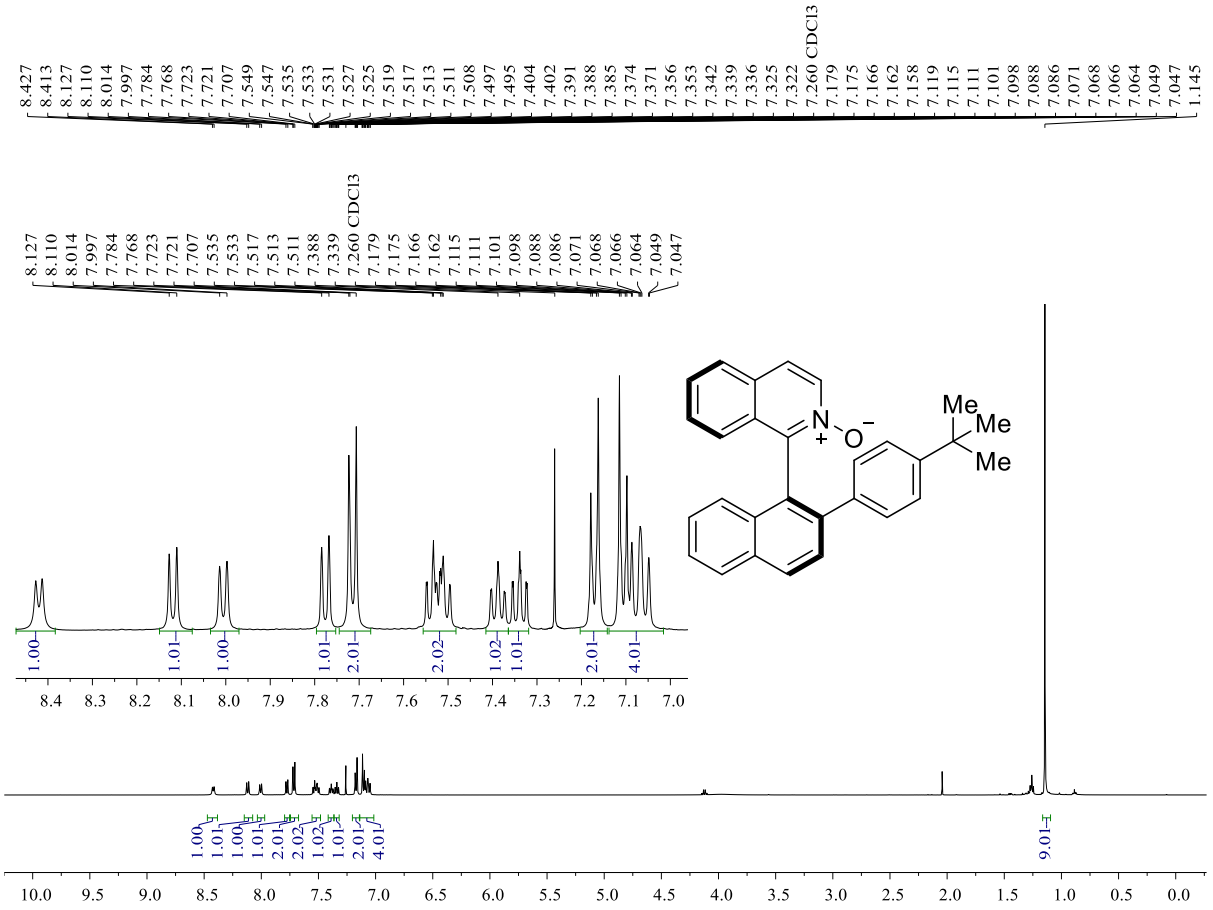


PDA Ch1 274nm 4nm

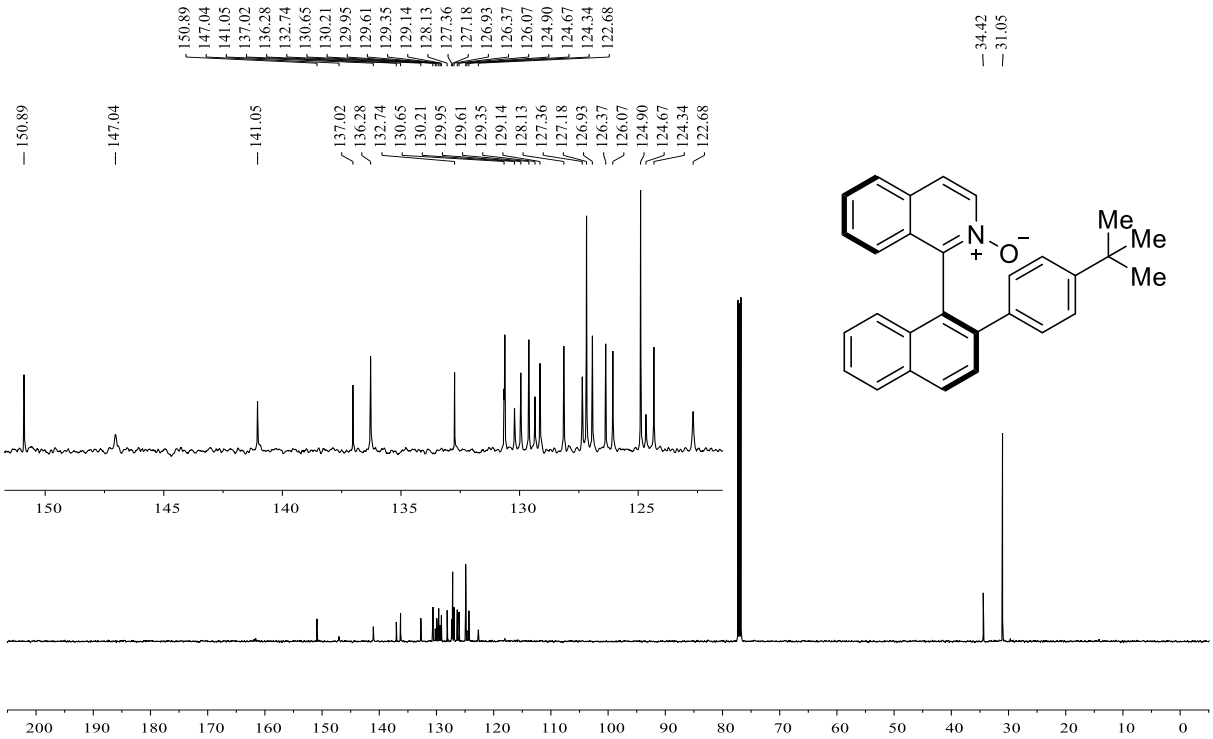
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.666	2452510	64535	2.357	3.544
2	17.003	101593361	1756472	97.643	96.456
Total		104045872	1821006	100.000	100.000

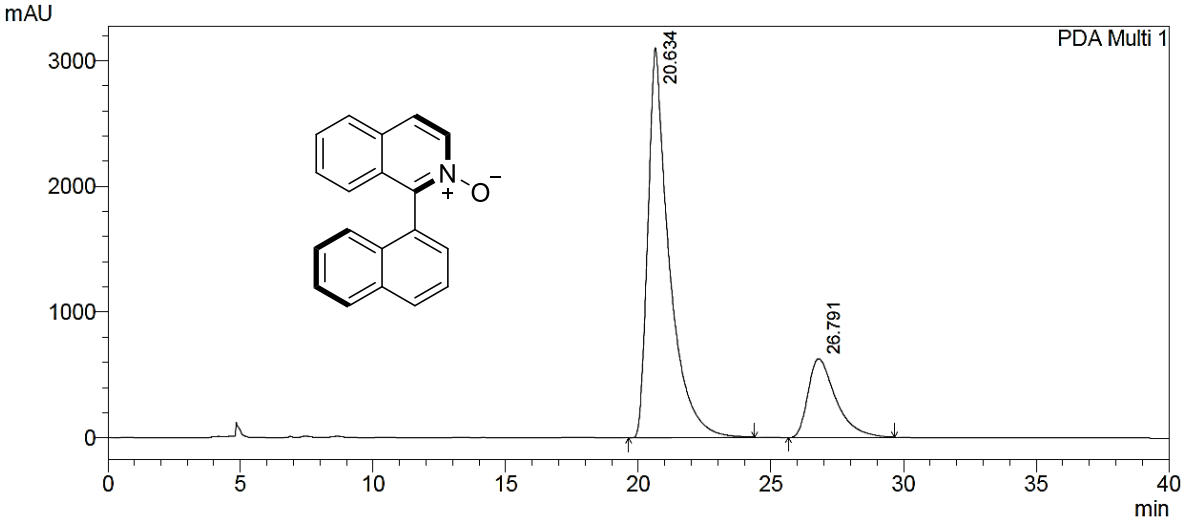
*(R)-1-(2-(4-(tert-butyl)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3c**)*

^{1}H NMR *(*500 MHz*)*



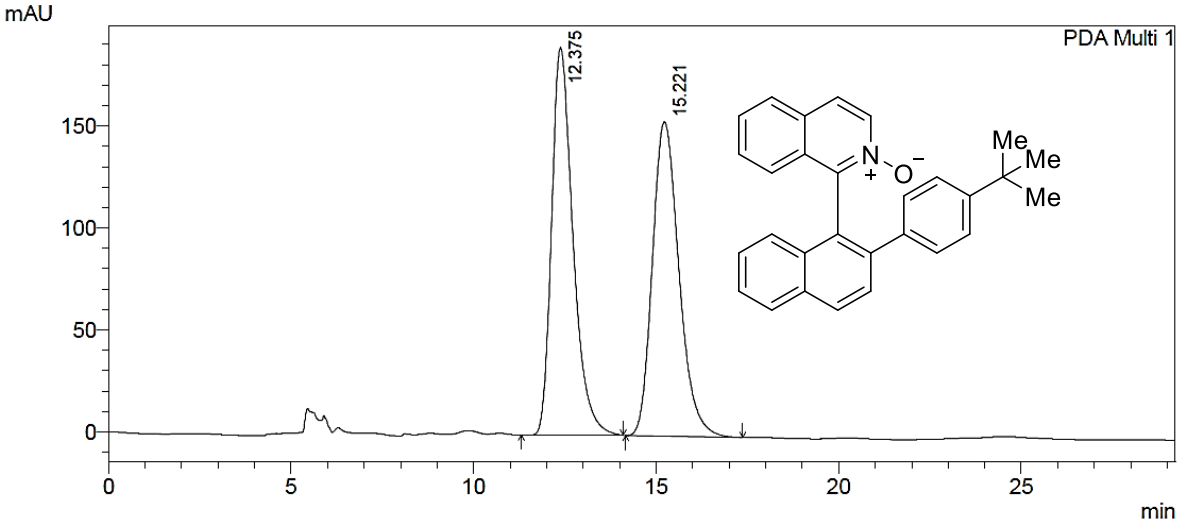
^{13}C{^{1}H} NMR *(*125 MHz*)*





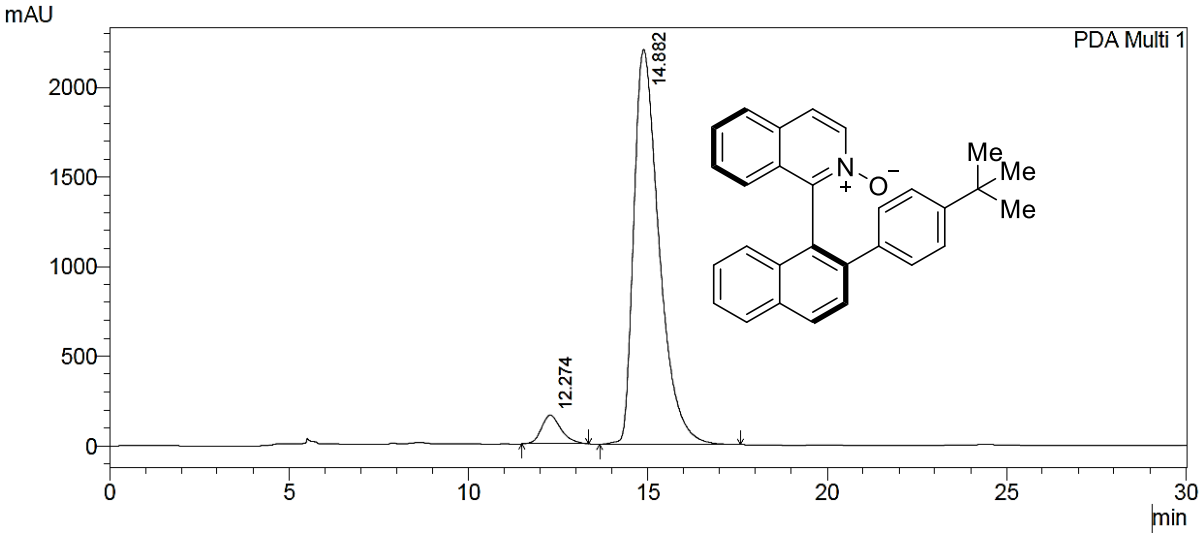
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.634	171455541	3099627	78.986	83.186
2	26.791	45616360	626534	21.014	16.814
Total		217071901	3726161	100.000	100.000



PDA Ch1 310nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.375	7728664	190183	49.745	55.223
2	15.221	7808034	154207	50.255	44.777
Total		15536698	344390	100.000	100.000

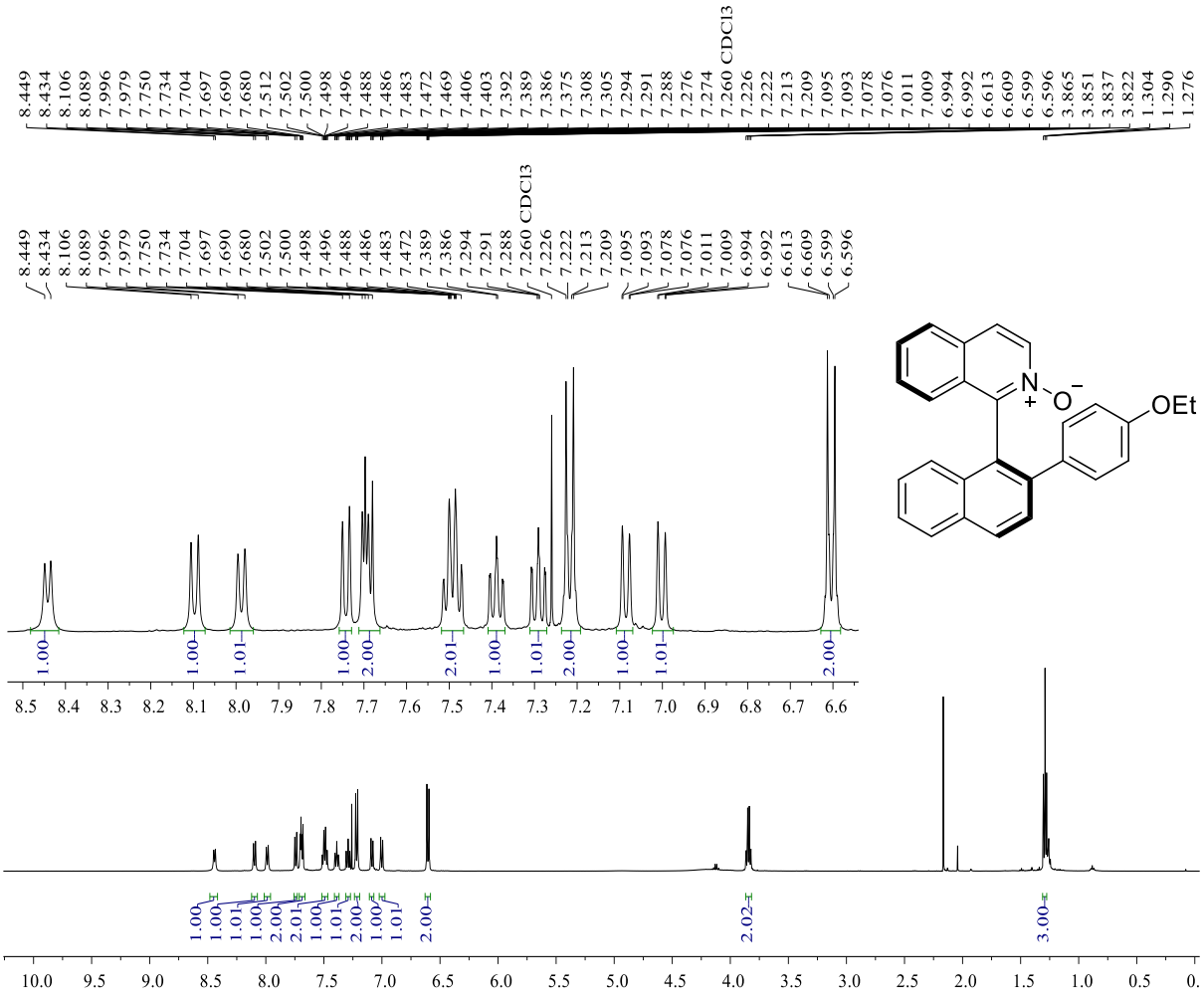


PDA Ch1 310nm 4nm

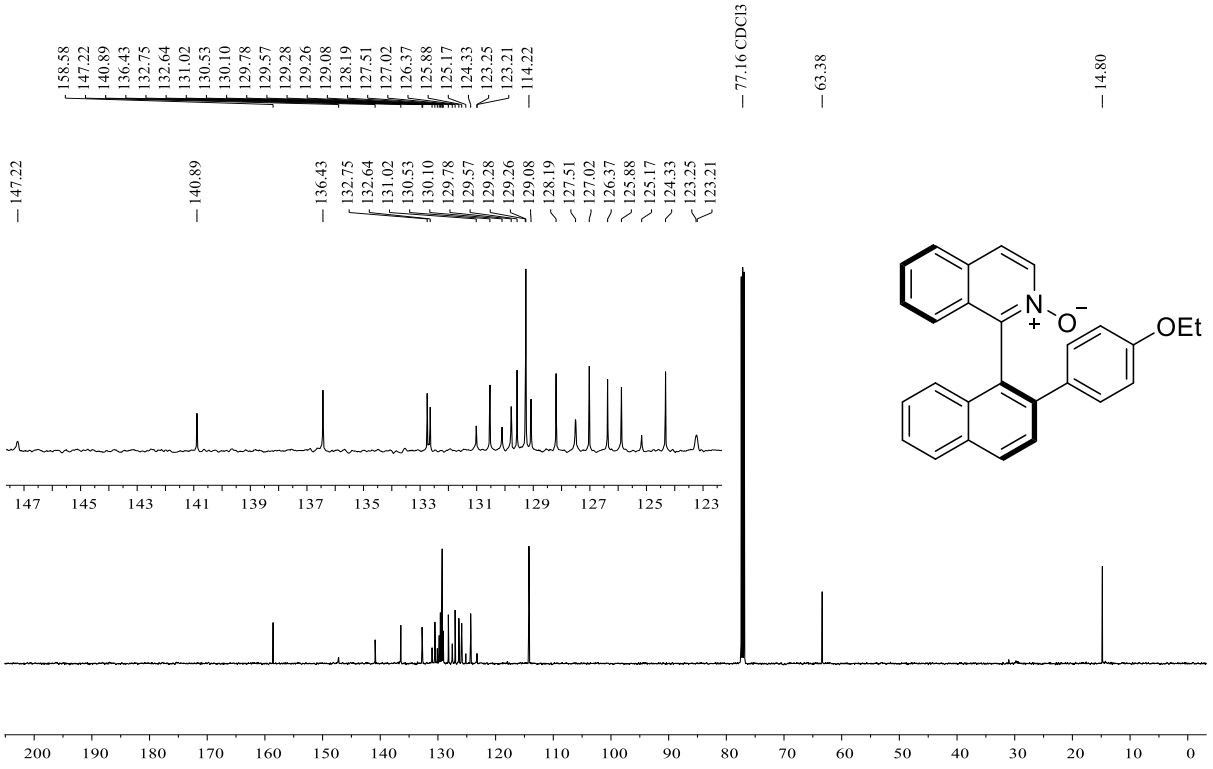
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.274	6195355	161442	5.424	6.828
2	14.882	108027796	2202897	94.576	93.172
Total		114223152	2364339	100.000	100.000

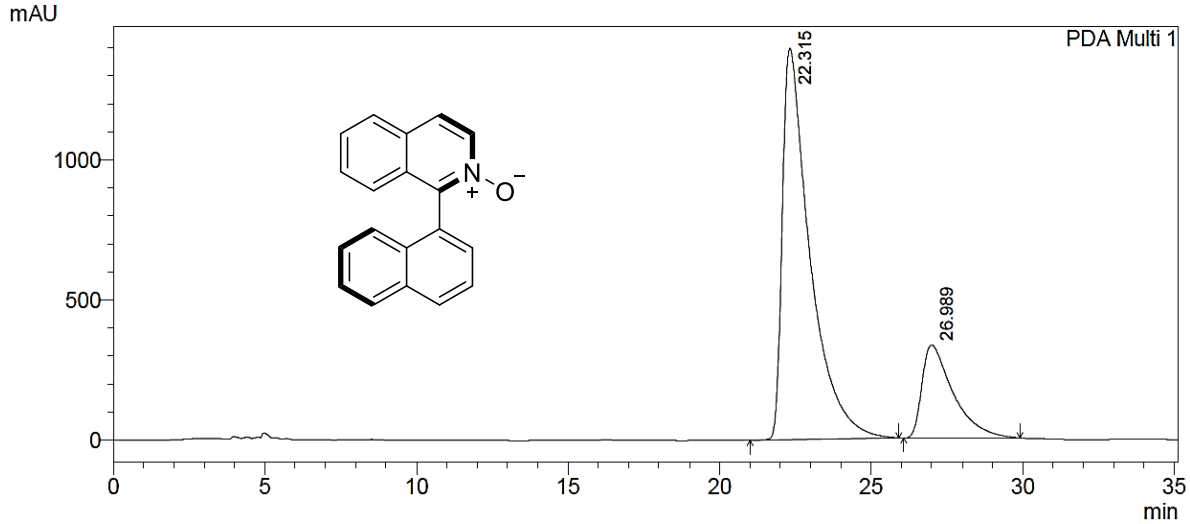
*(R)-1-(2-(4-ethoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3d**)*

^{1}H NMR *(*500 MHz*)*



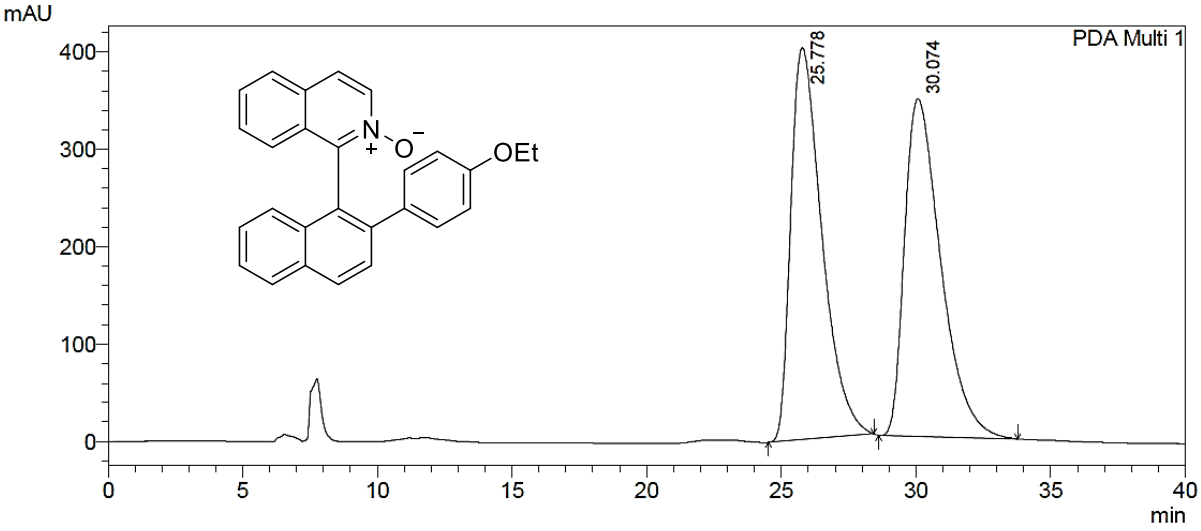
$^{13}C\{^{1}H\}$ NMR *(*125 MHz*)*





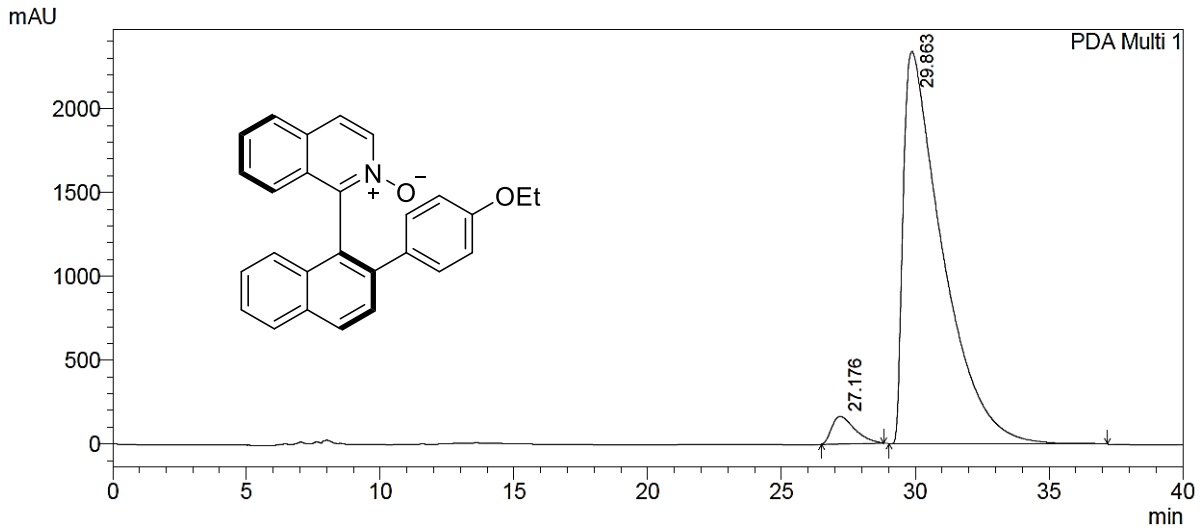
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.315	88494450	1397385	78.842	80.822
2	26.989	23748487	331582	21.158	19.178
Total		112242937	1728968	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	25.778	32305839	402267	49.921	53.715
2	30.074	32408425	346623	50.079	46.285
Total		64714264	748891	100.000	100.000

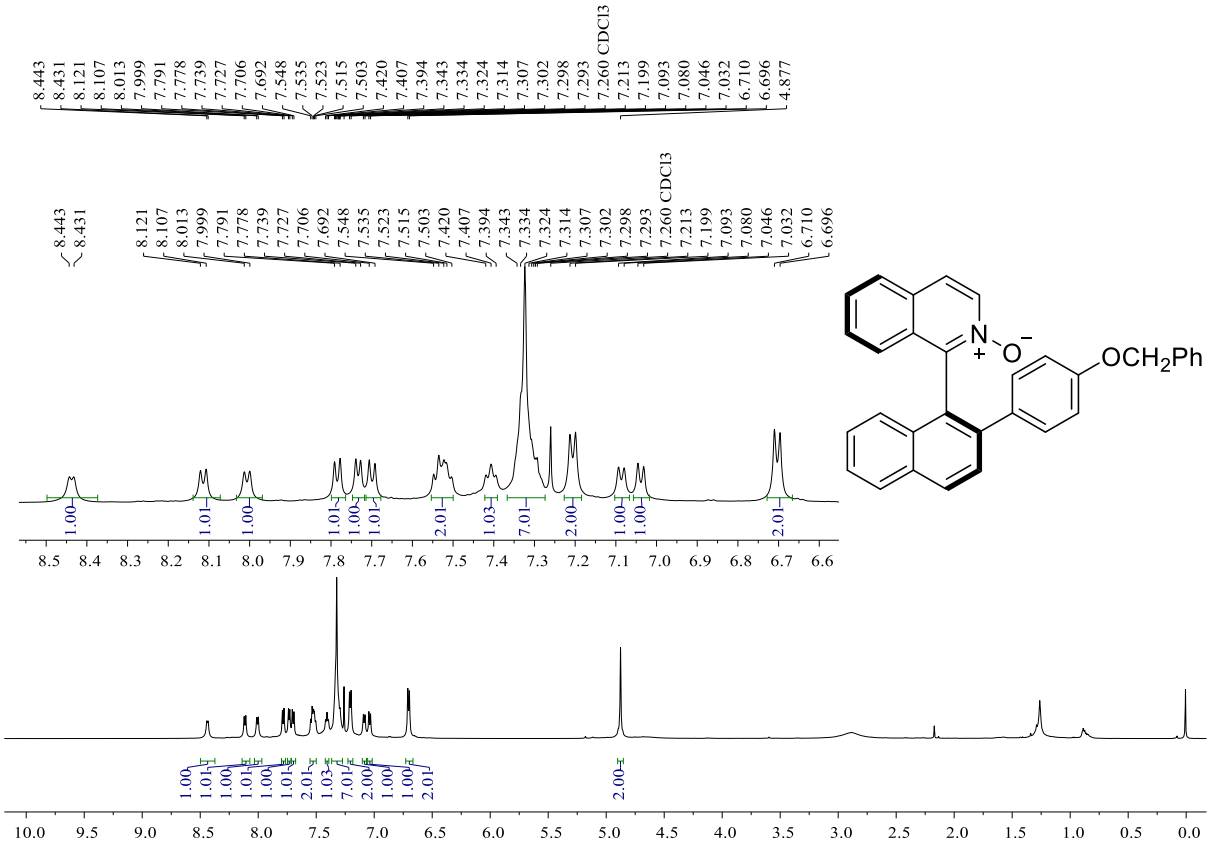


PDA Ch1 274nm 4nm

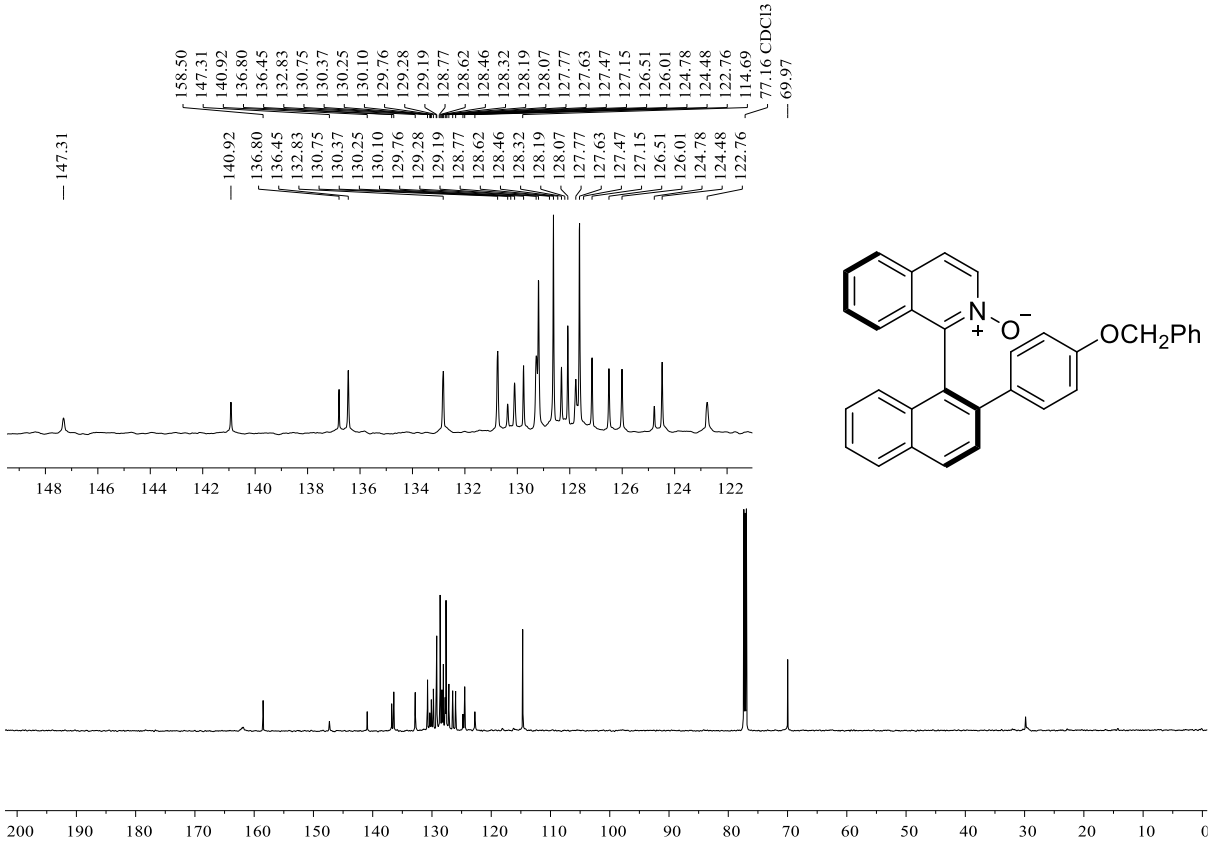
Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.176	9776516	163959	3.935	6.553
2	29.863	238690080	2338189	96.065	93.447
Total		248466595	2502148	100.000	100.000

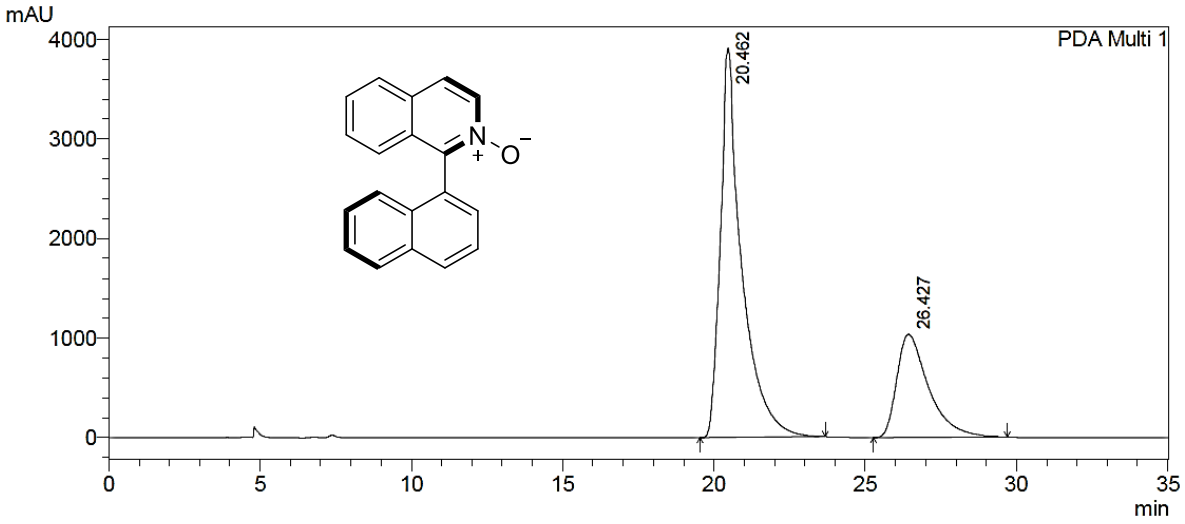
*(R)-1-(2-(4-(benzyloxy)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3e**)*

^{1}H NMR *(*500 MHz*)*



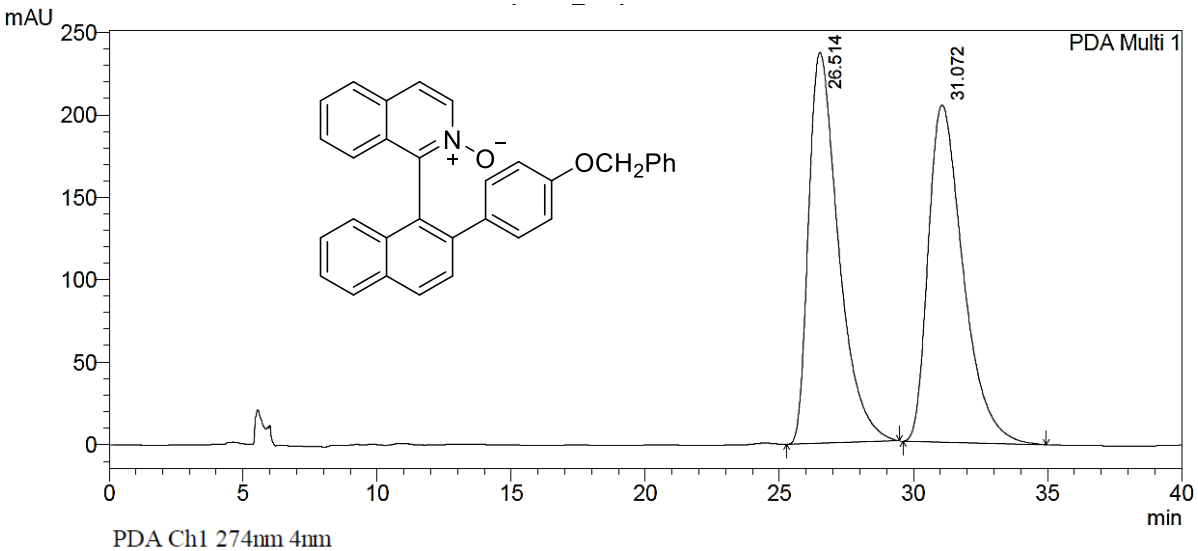
^{13}C{^{1}H} NMR *(*125 MHz*)*





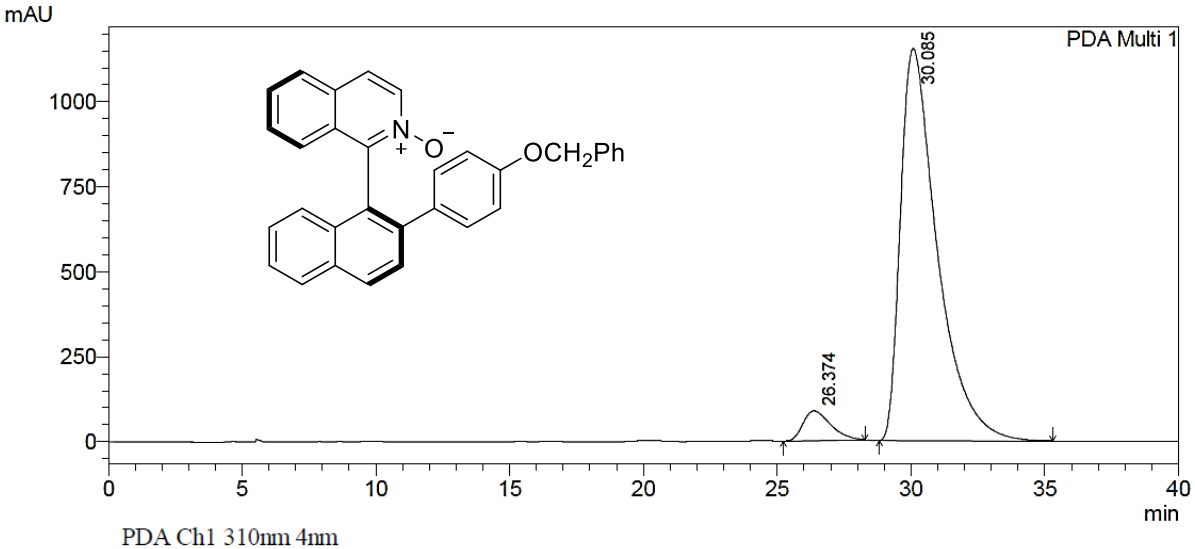
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.462	190885805	3910273	71.559	79.057
2	26.427	75868754	1035857	28.441	20.943
Total		266754559	4946129	100.000	100.000



PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.514	18428864	237139	49.907	53.708
2	31.072	18497324	204395	50.093	46.292
Total		36926188	441534	100.000	100.000

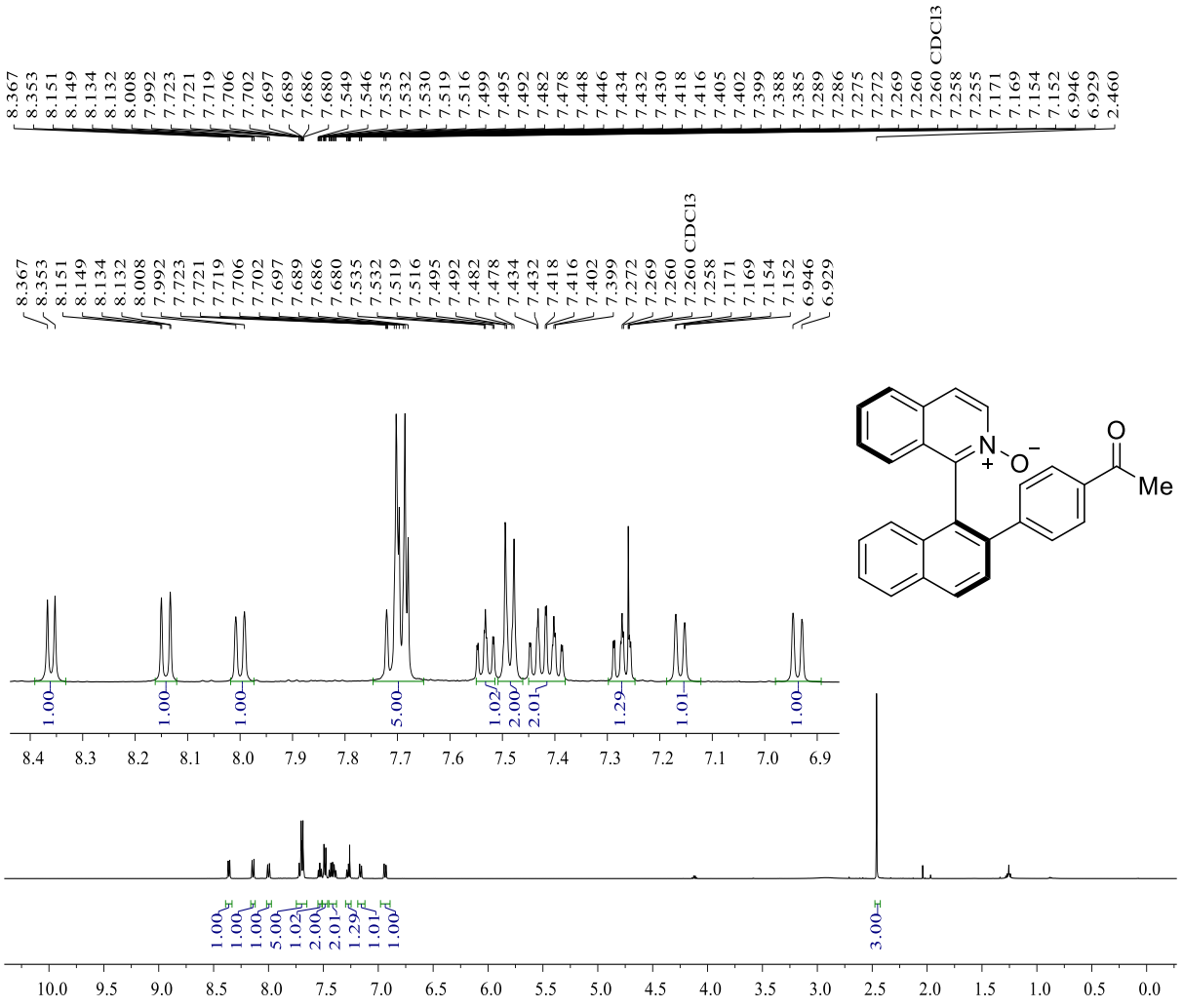


PDA Ch1 310nm 4nm

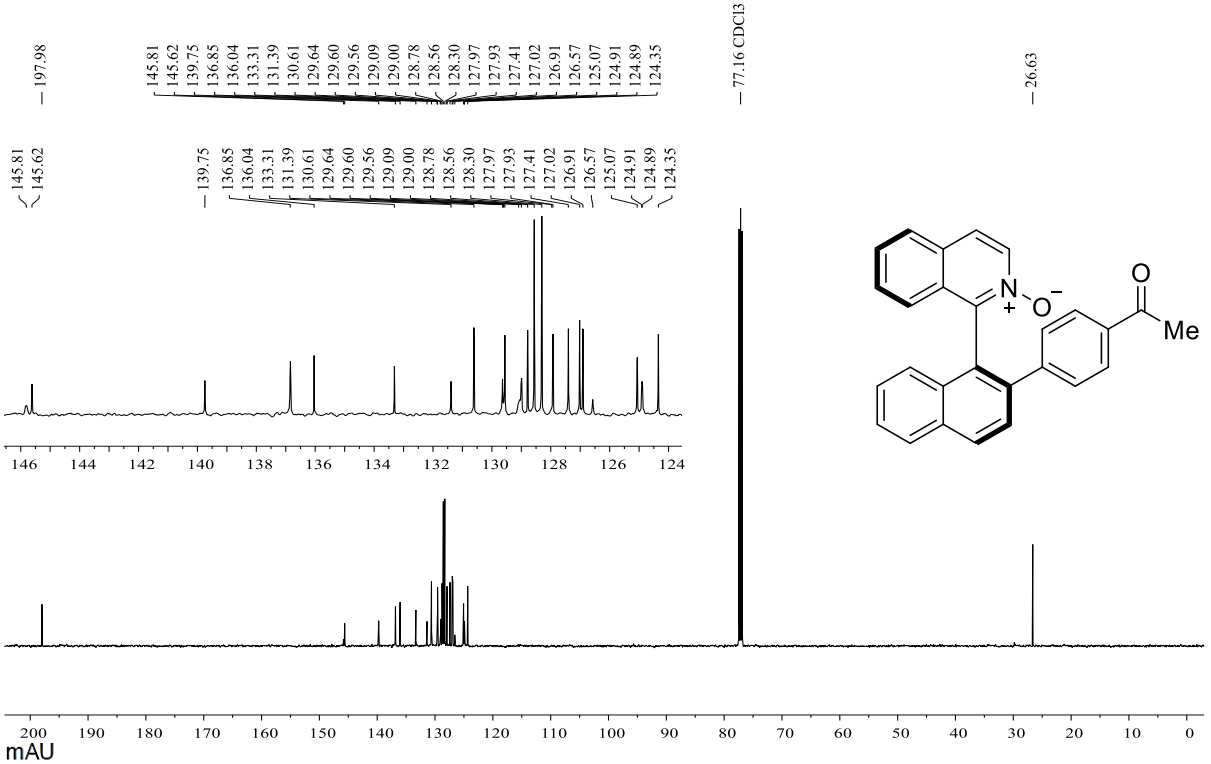
Peak#	Ret. Time	Area	Height	Area %	Height %
1	26.374	6248380	87390	5.349	7.044
2	30.085	110575207	1153324	94.651	92.956
Total		116823588	1240714	100.000	100.000

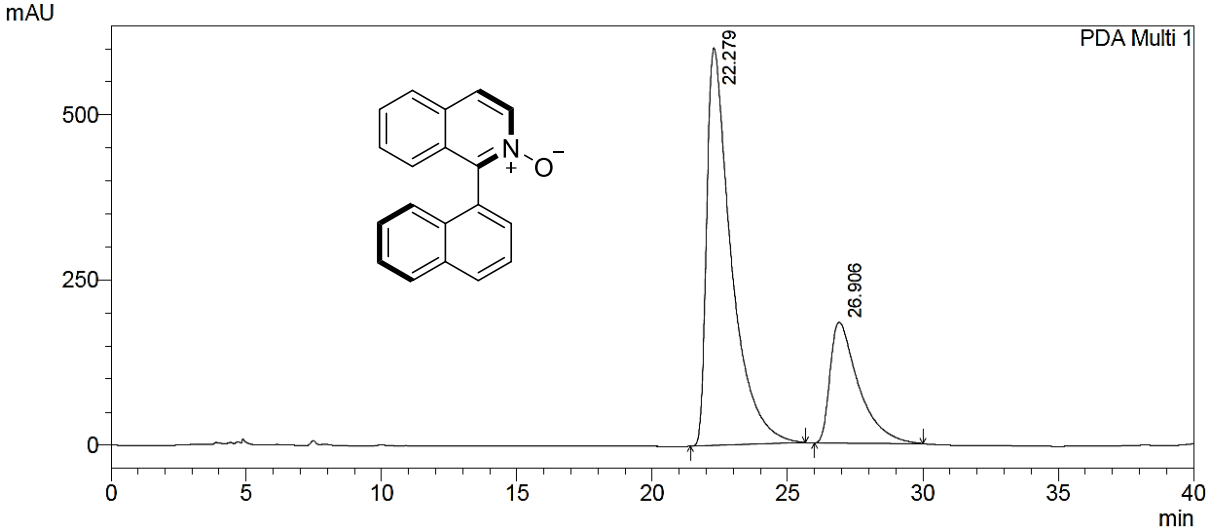
*(R)-1-(2-(4-acetylphenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3f**)*

^{1}H NMR *(*500 MHz*)*



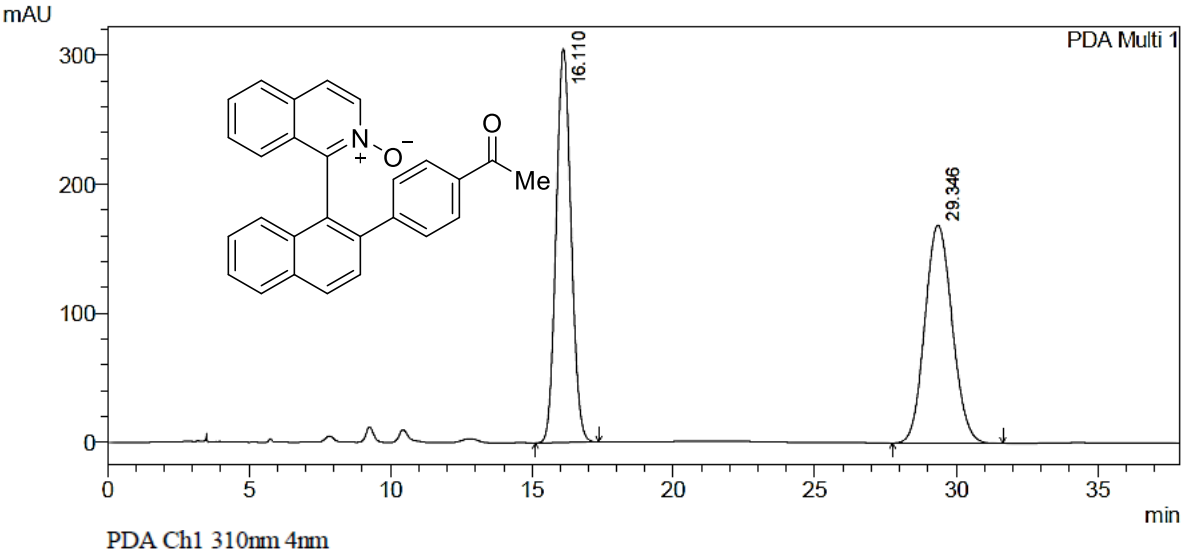
$^{13}C\{^{1}H\}$ NMR *(*125 MHz*)*





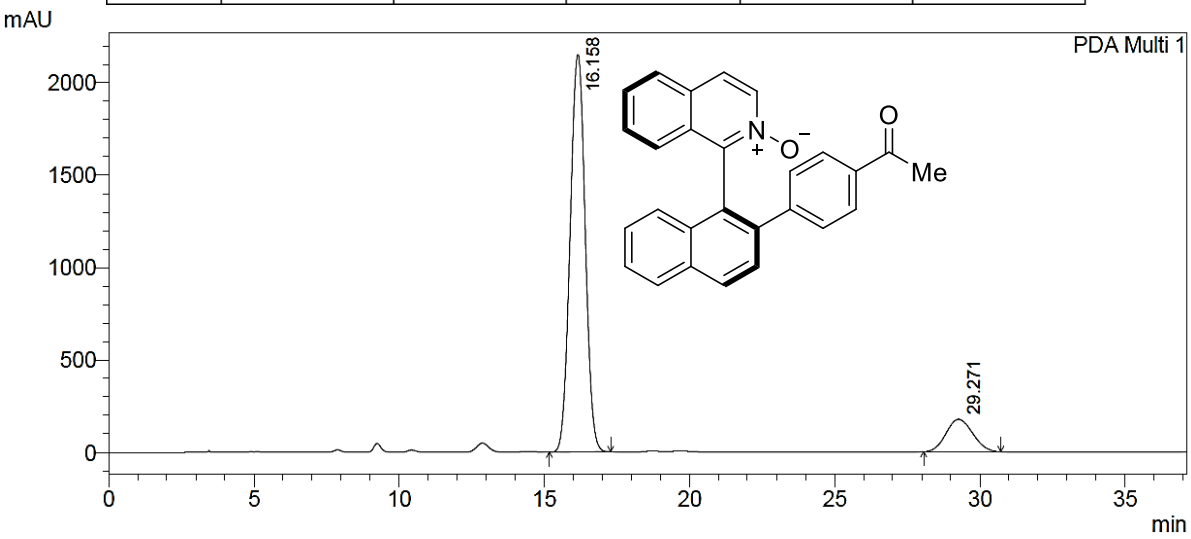
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.279	37913747	601702	73.800	76.639
2	26.906	13460067	183406	26.200	23.361
Total		51373815	785108	100.000	100.000



PDA Ch1 310nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.110	11308354	305305	49.931	64.377
2	29.346	11339760	168941	50.069	35.623
Total		22648114	474246	100.000	100.000

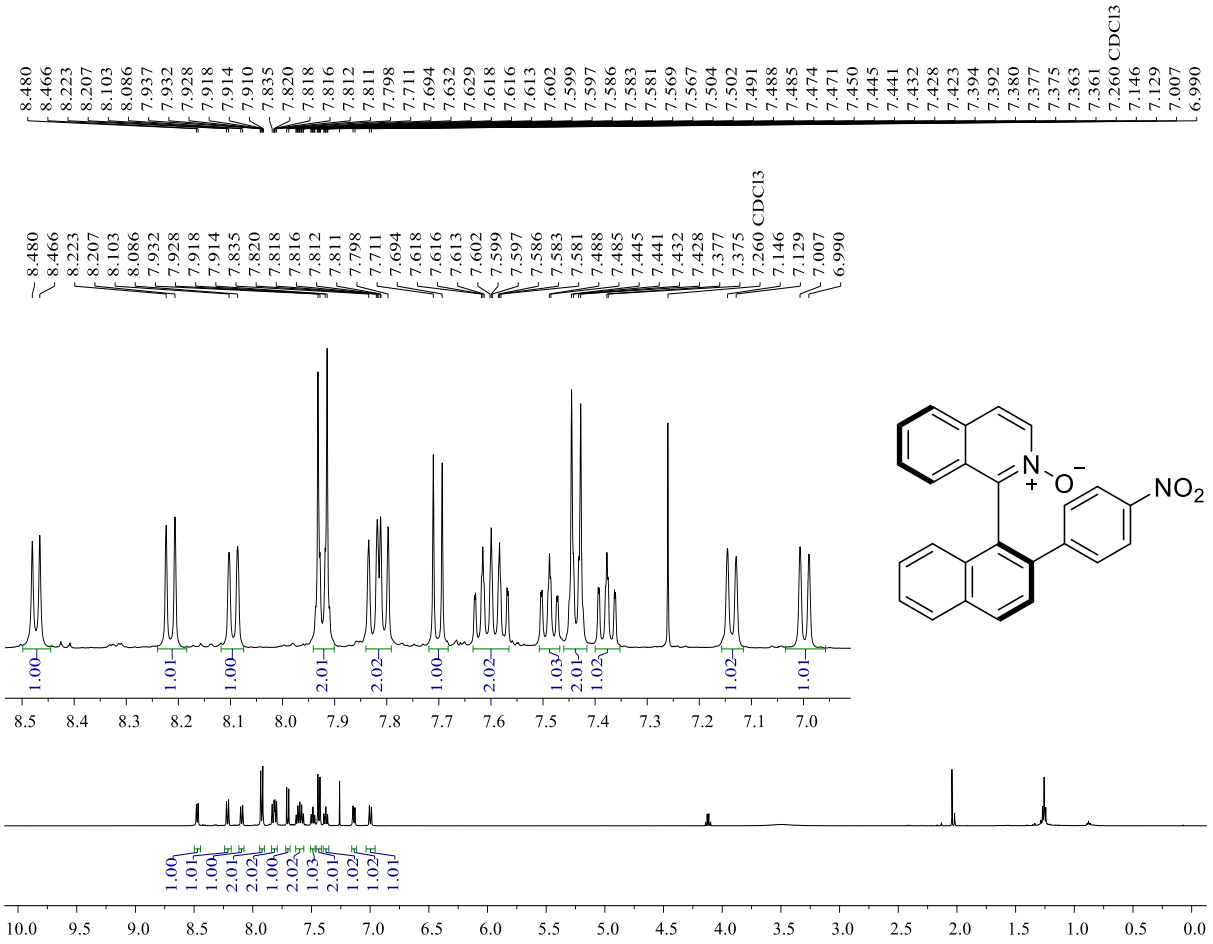


PDA Ch1 310nm 4nm

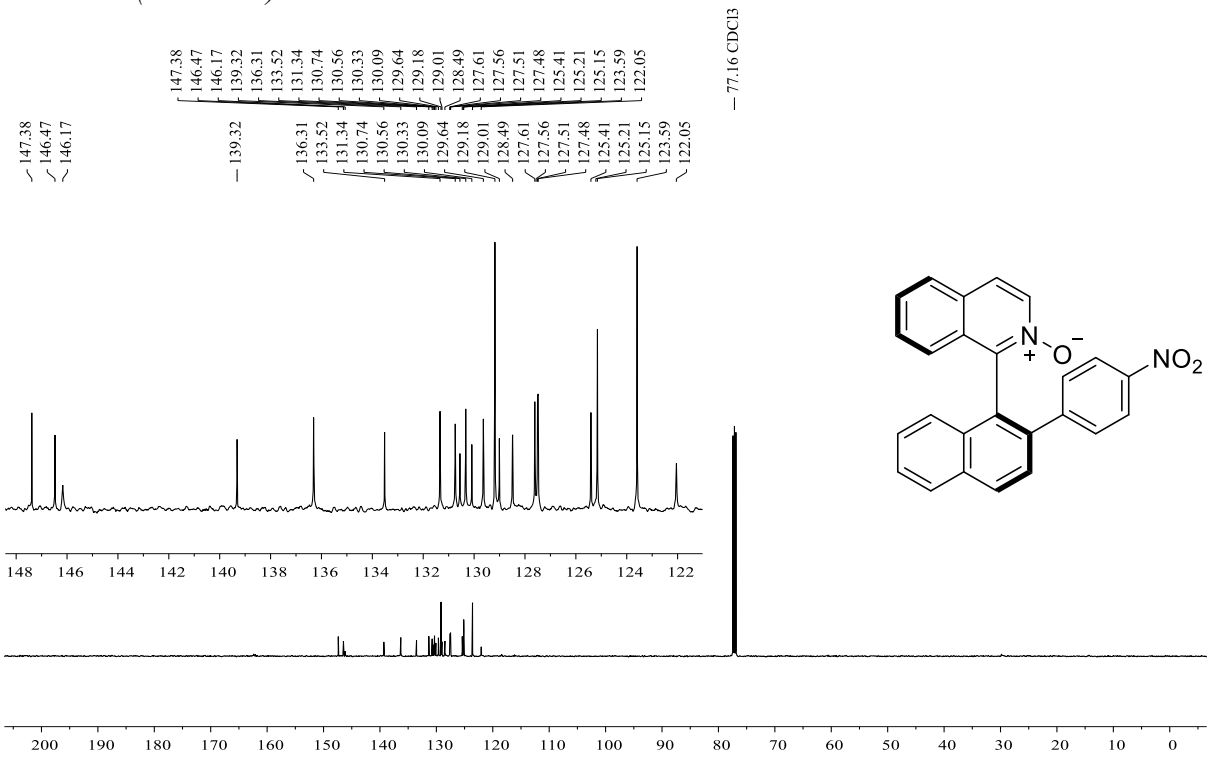
Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.158	77205314	2149194	87.259	92.428
2	29.271	11272989	176078	12.741	7.572
Total		88478303	2325272	100.000	100.000

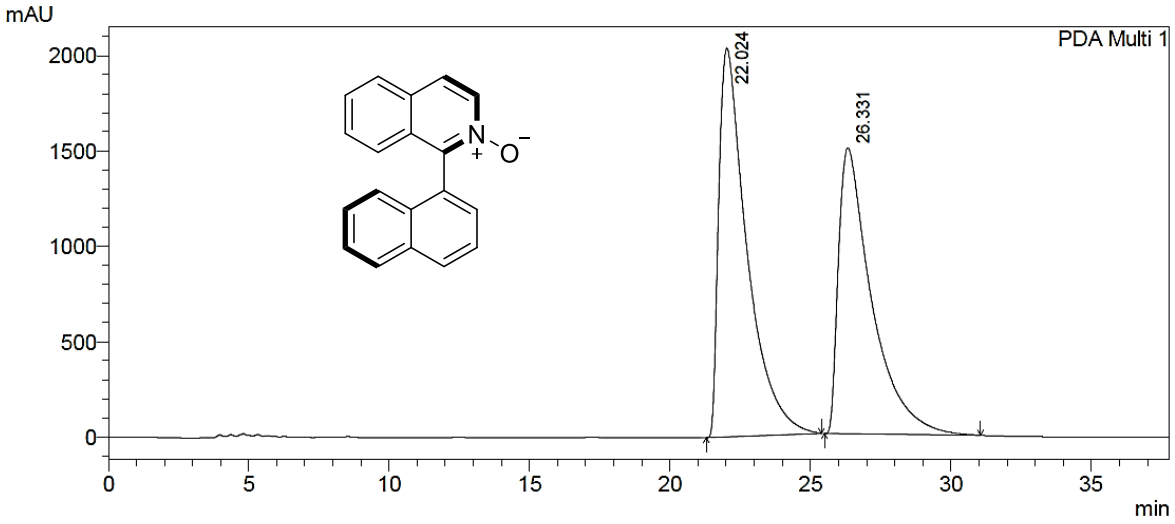
*(R)-1-(2-(4-nitrophenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3g**)*

^{1}H NMR *(*500 MHz*)*



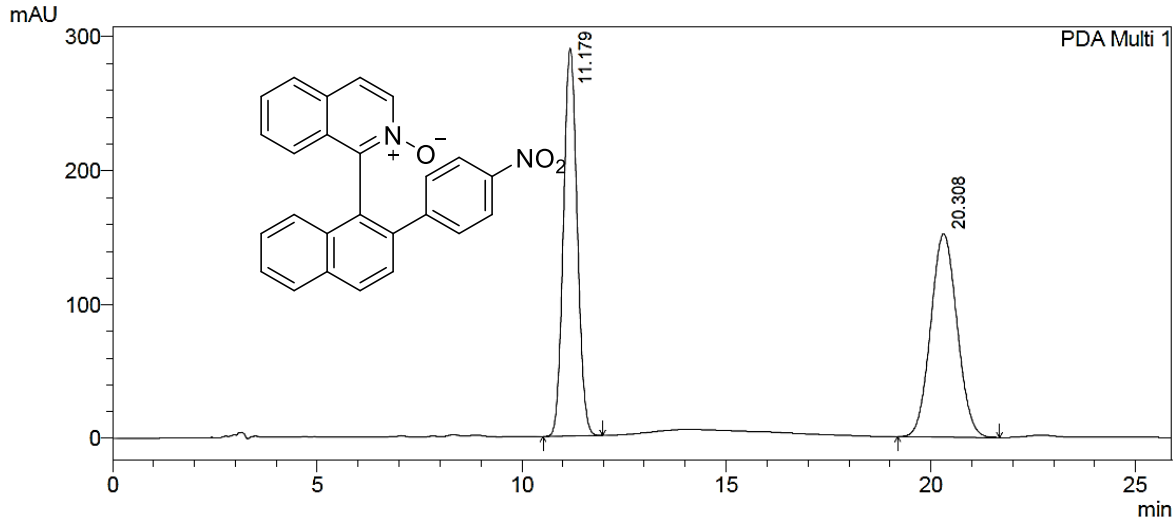
^{13}C NMR *(*125 MHz*)*





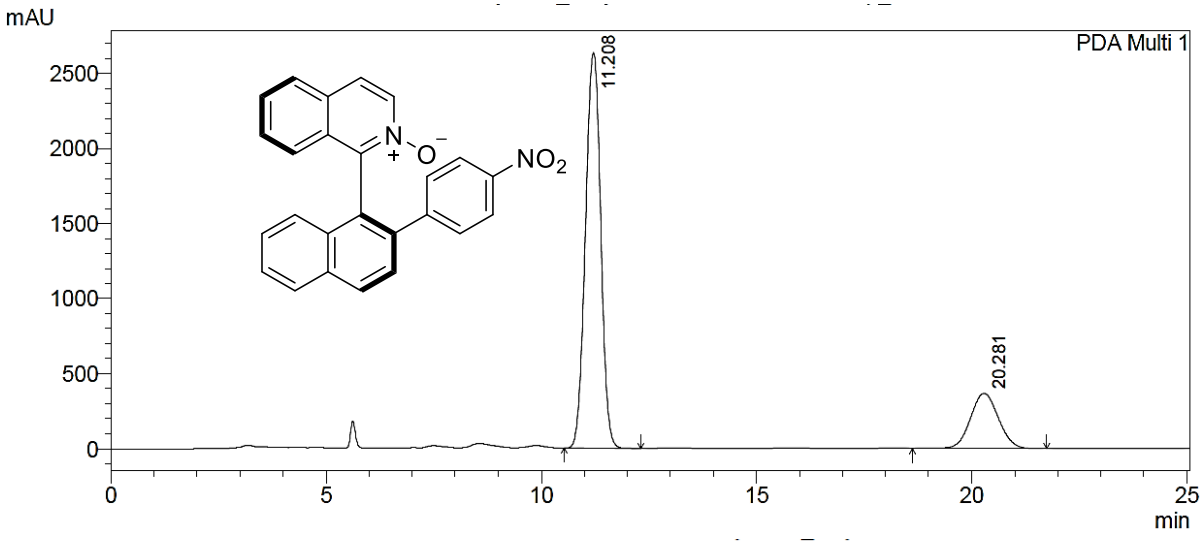
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.024	141404456	2036570	53.375	57.581
2	26.331	123522253	1500294	46.625	42.419
Total		264926709	3536864	100.000	100.000



PDA Ch1 310nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.179	6794856	289502	49.997	65.631
2	20.308	6795716	151607	50.003	34.369
Total		13590572	441109	100.000	100.000

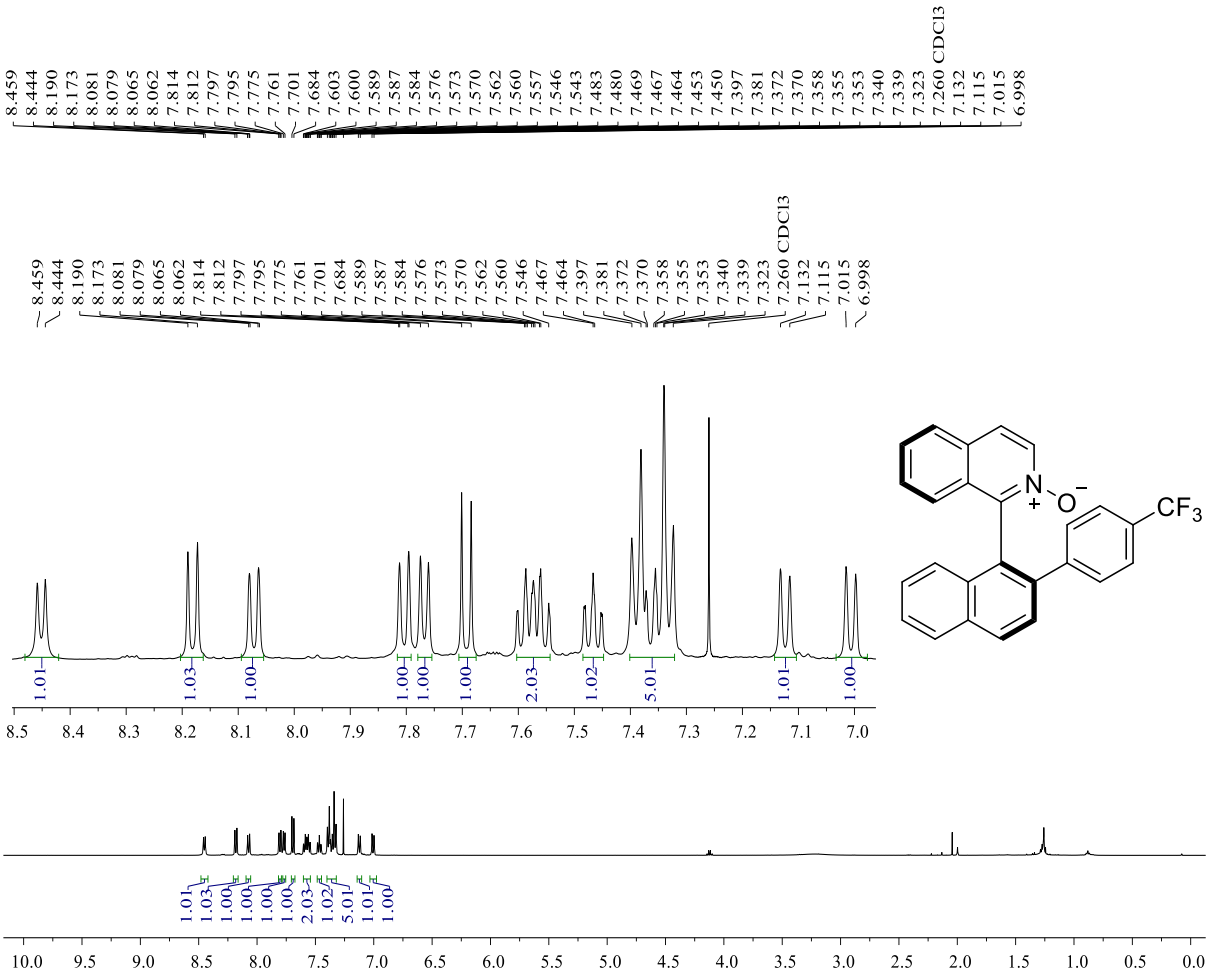


PDA Ch1 310nm 4nm

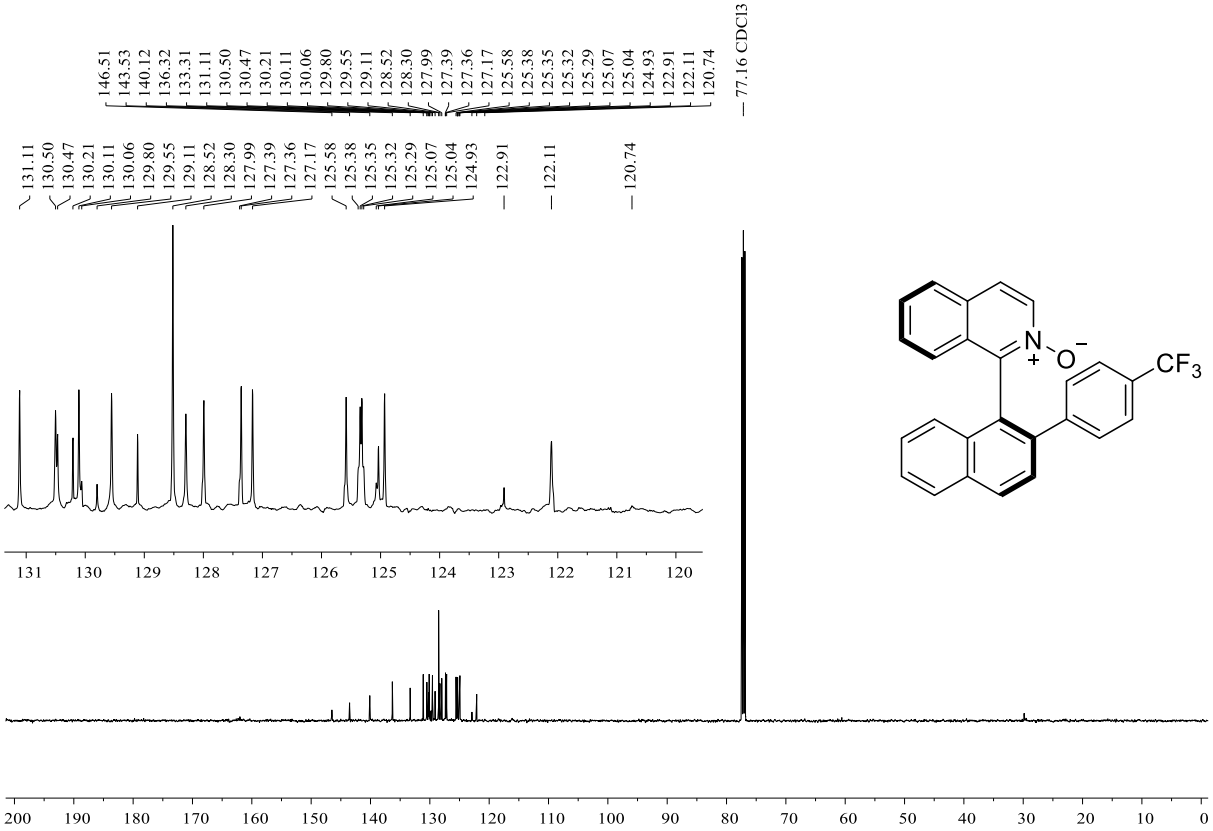
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.208	65121169	2634096	79.629	87.757
2	20.281	16659594	367477	20.371	12.243
Total		81780762	3001572	100.000	100.000

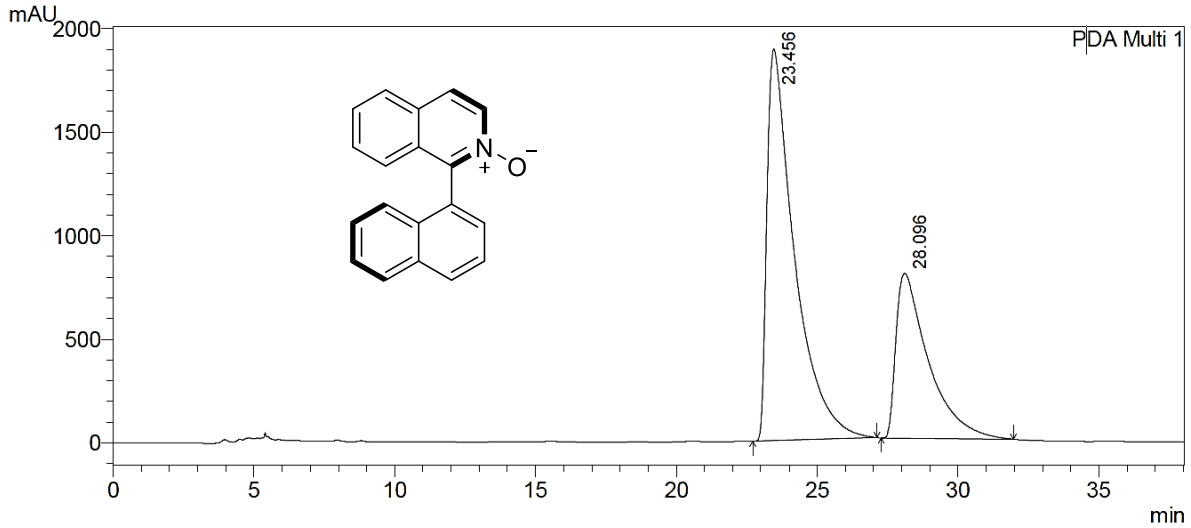
*(R)-1-(2-(4-(trifluoromethyl)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3h**)*

^{1}H NMR *(*500 MHz*)*



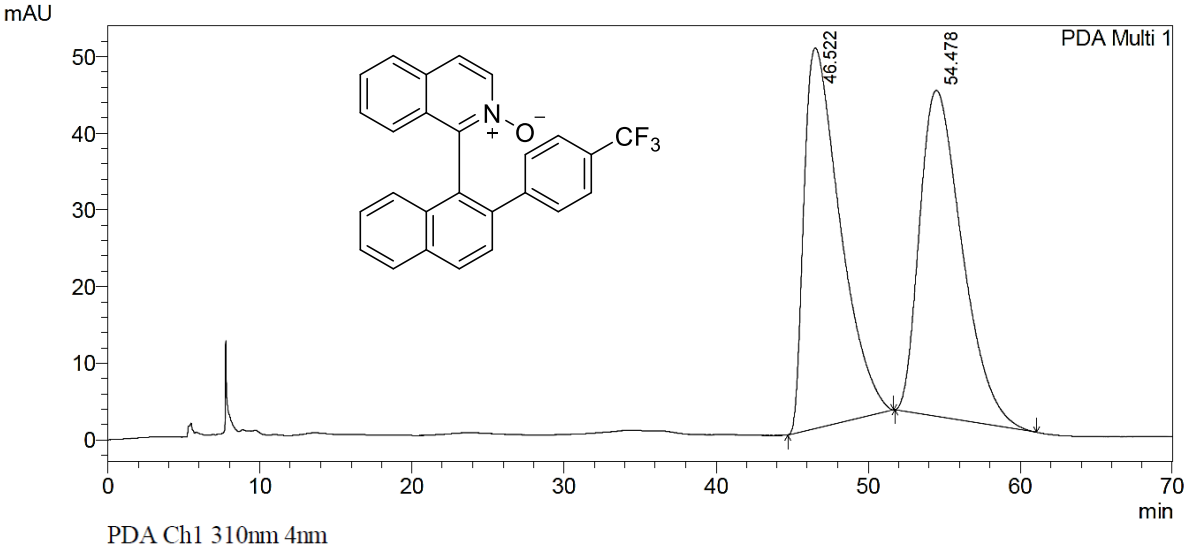
$^{13}C\{^{1}H\}$ NMR *(*125 MHz*)*





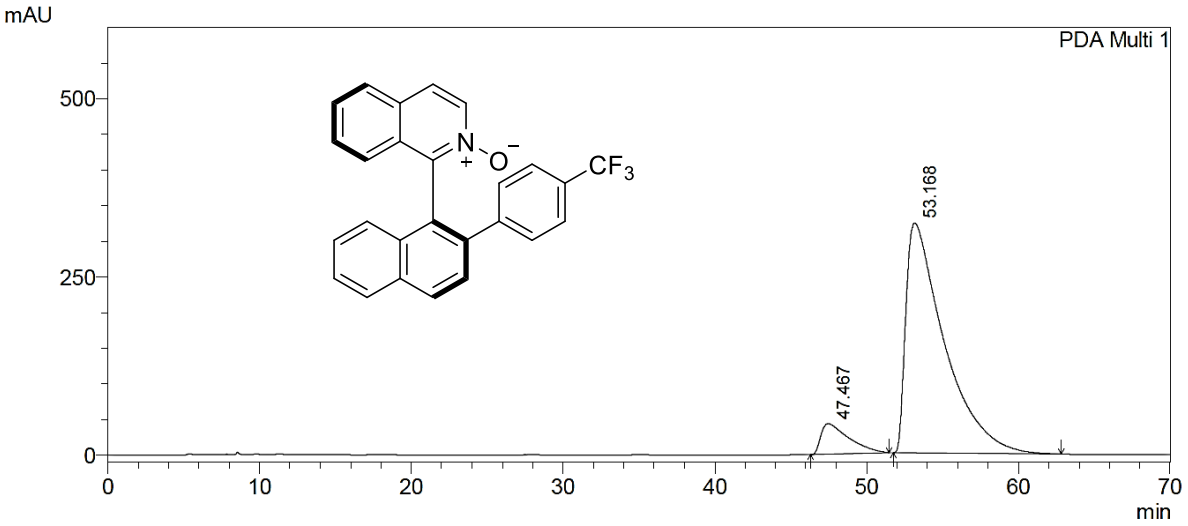
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.456	128401460	1888691	66.883	70.379
2	28.096	63577158	794924	33.117	29.621
Total		191978618	2683615	100.000	100.000



PDA Ch1 310nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	46.522	8209203	49682	49.748	53.840
2	54.478	8292236	42595	50.252	46.160
Total		16501438	92277	100.000	100.000

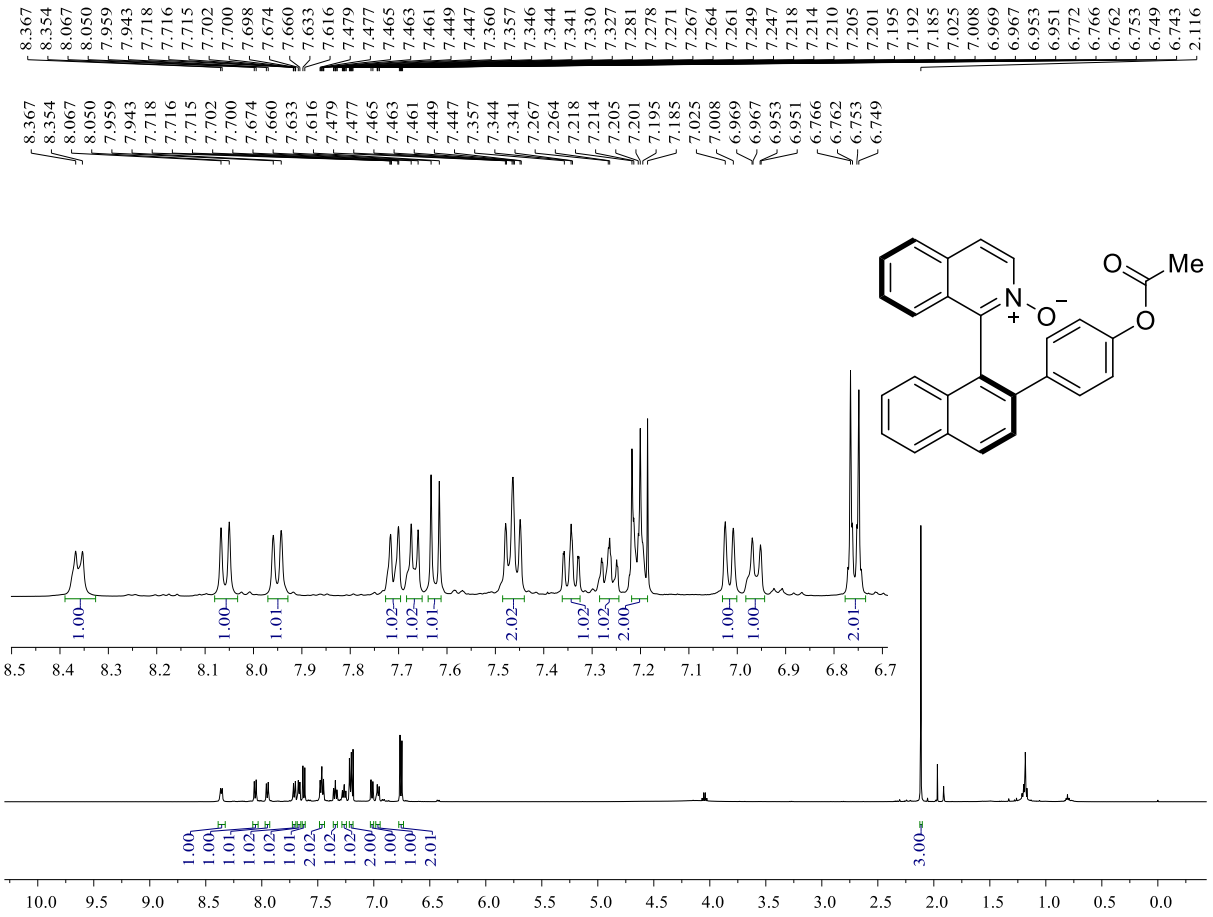


PDA Ch1 310nm 4nm

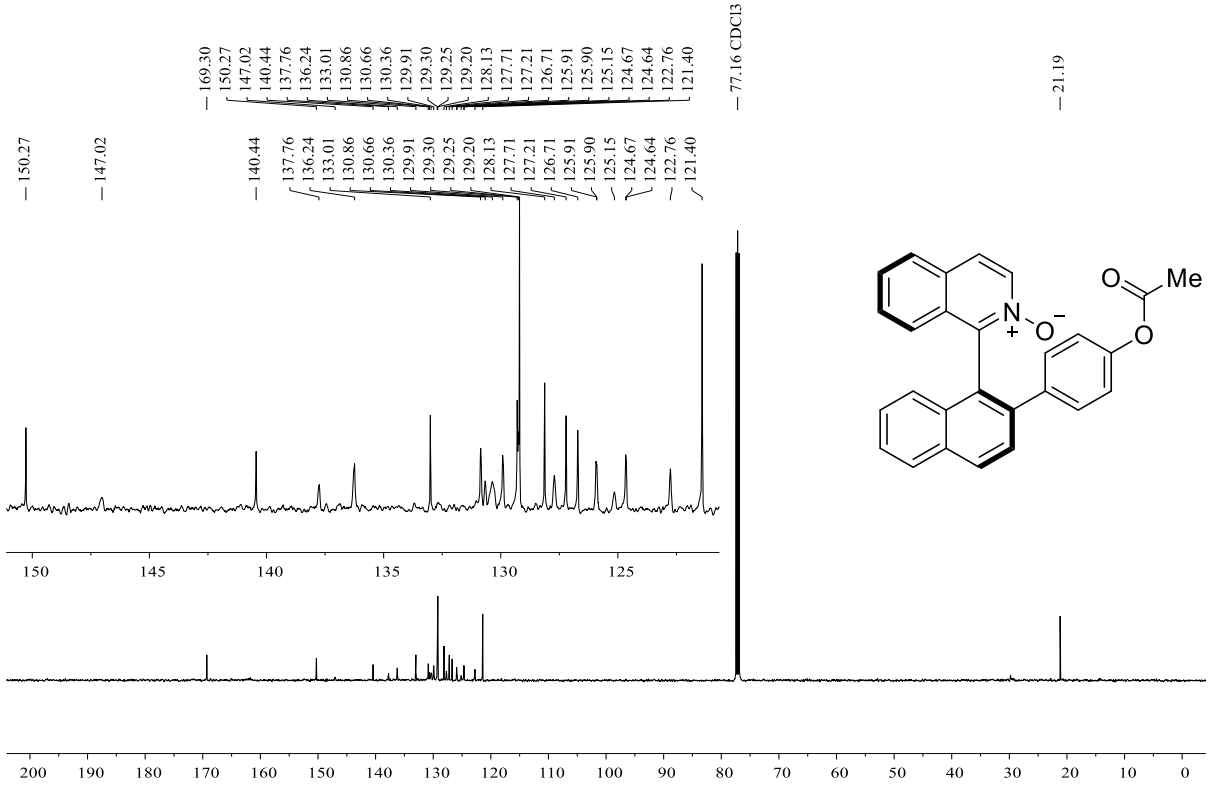
Peak#	Ret. Time	Area	Height	Area %	Height %
1	47.467	5469820	42928	8.798	11.734
2	53.168	56704244	322911	91.202	88.266
Total		62174065	365840	100.000	100.000

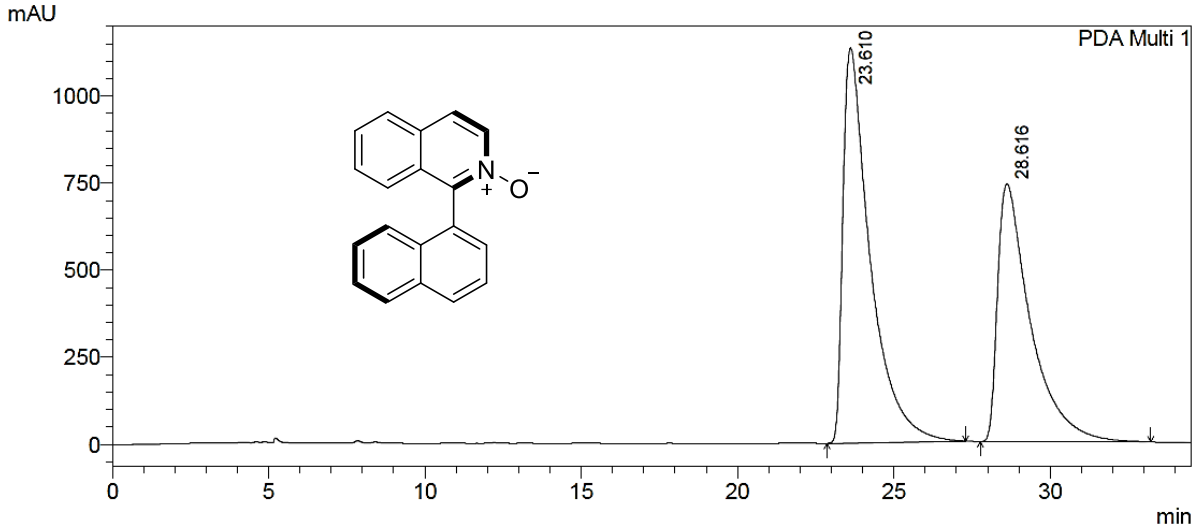
*(R)-1-(2-(4-acetoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3i**)*

^{1}H NMR *(*500 MHz*)*



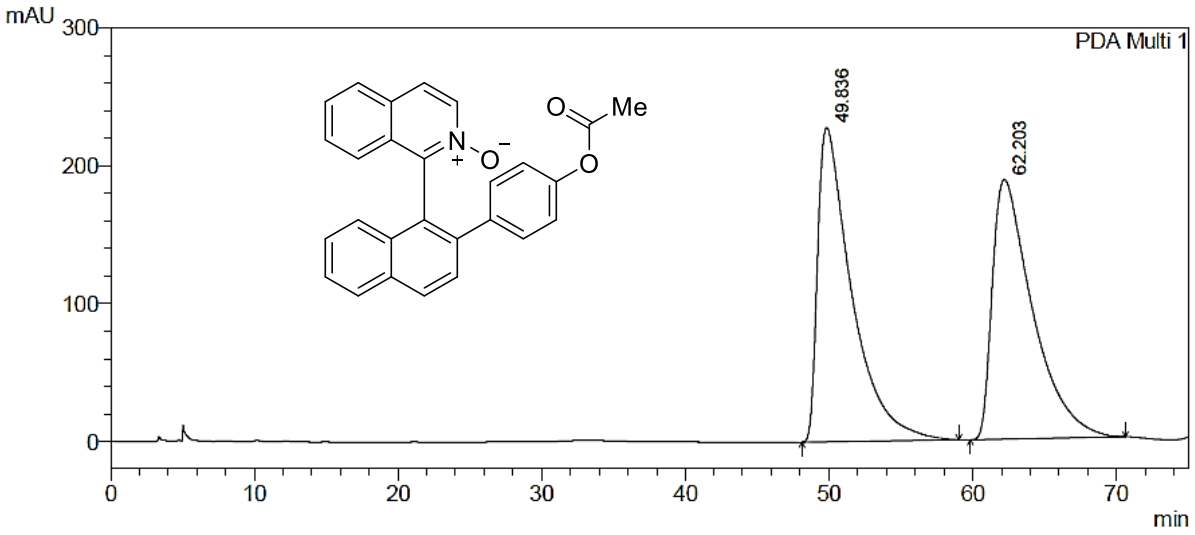
^{13}C{^{1}H} NMR *(*125 MHz*)*





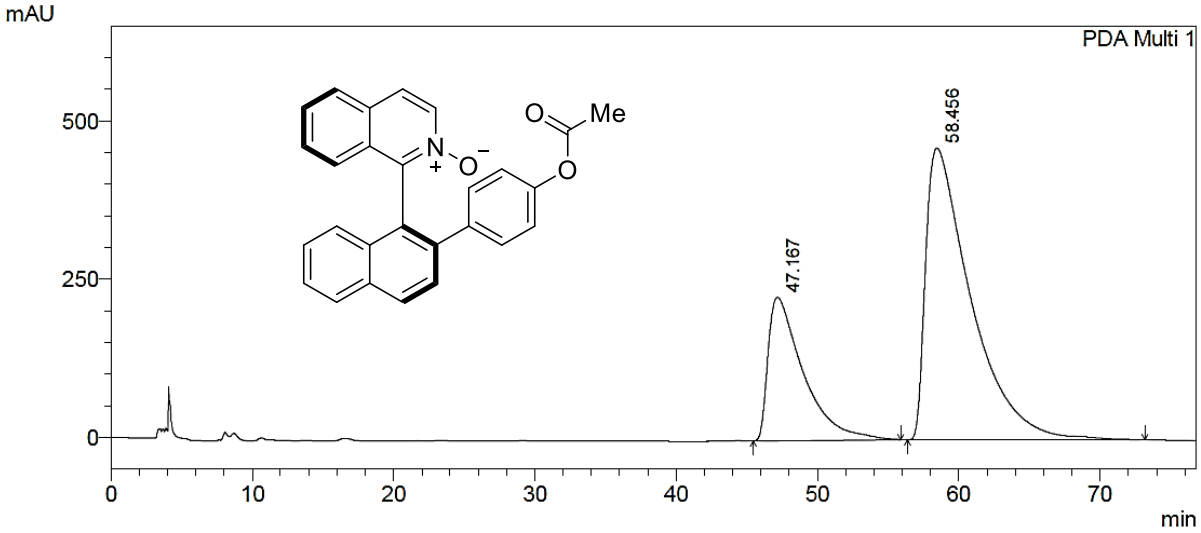
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	23.610	68670185	1133552	56.022	60.507
2	28.616	53906809	739871	43.978	39.493
Total		122576994	1873423	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	49.836	37542546	227970	50.617	54.711
2	62.203	36627683	188710	49.383	45.289
Total		74170229	416681	100.000	100.000

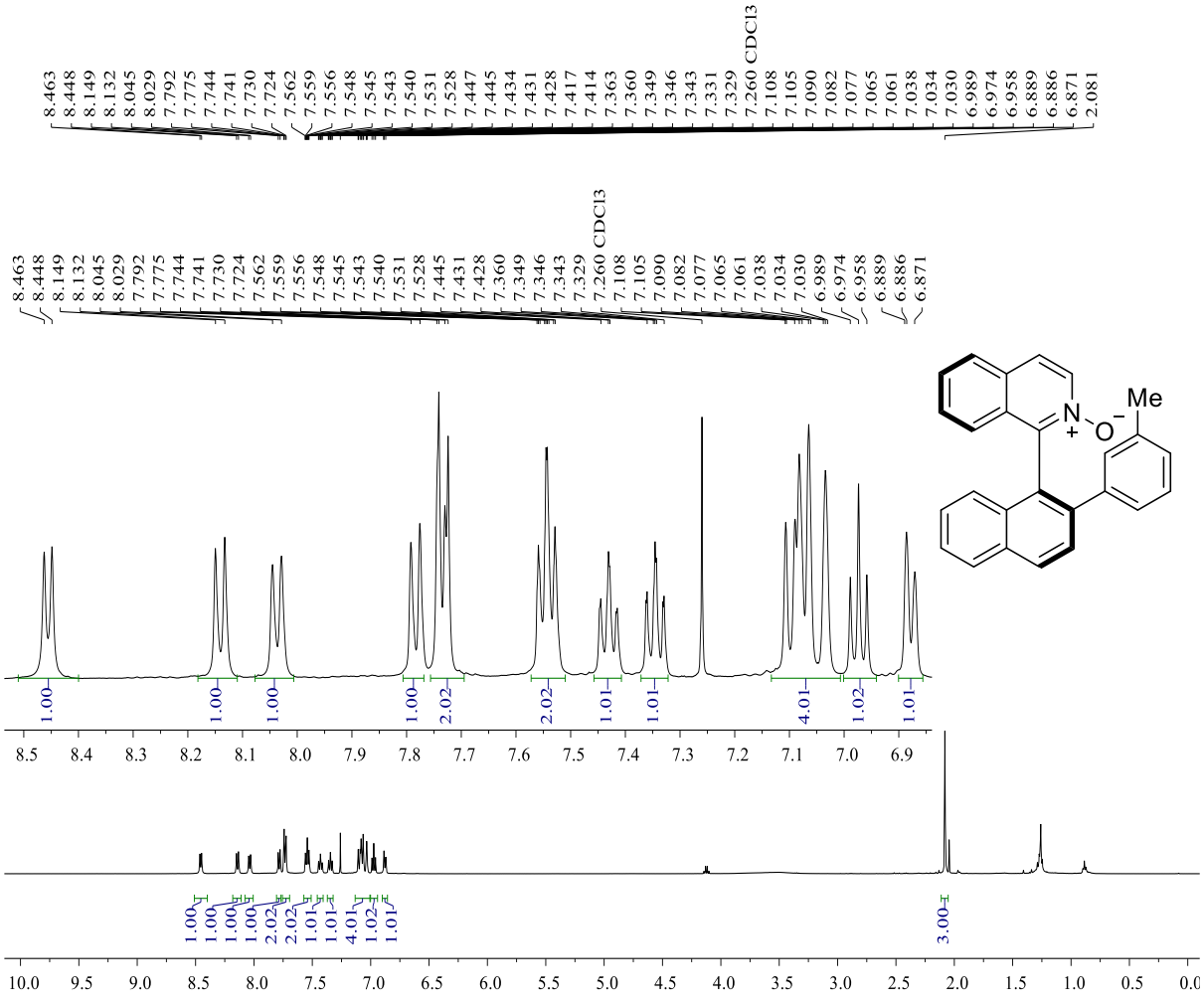


PDA Ch1 254nm 4nm

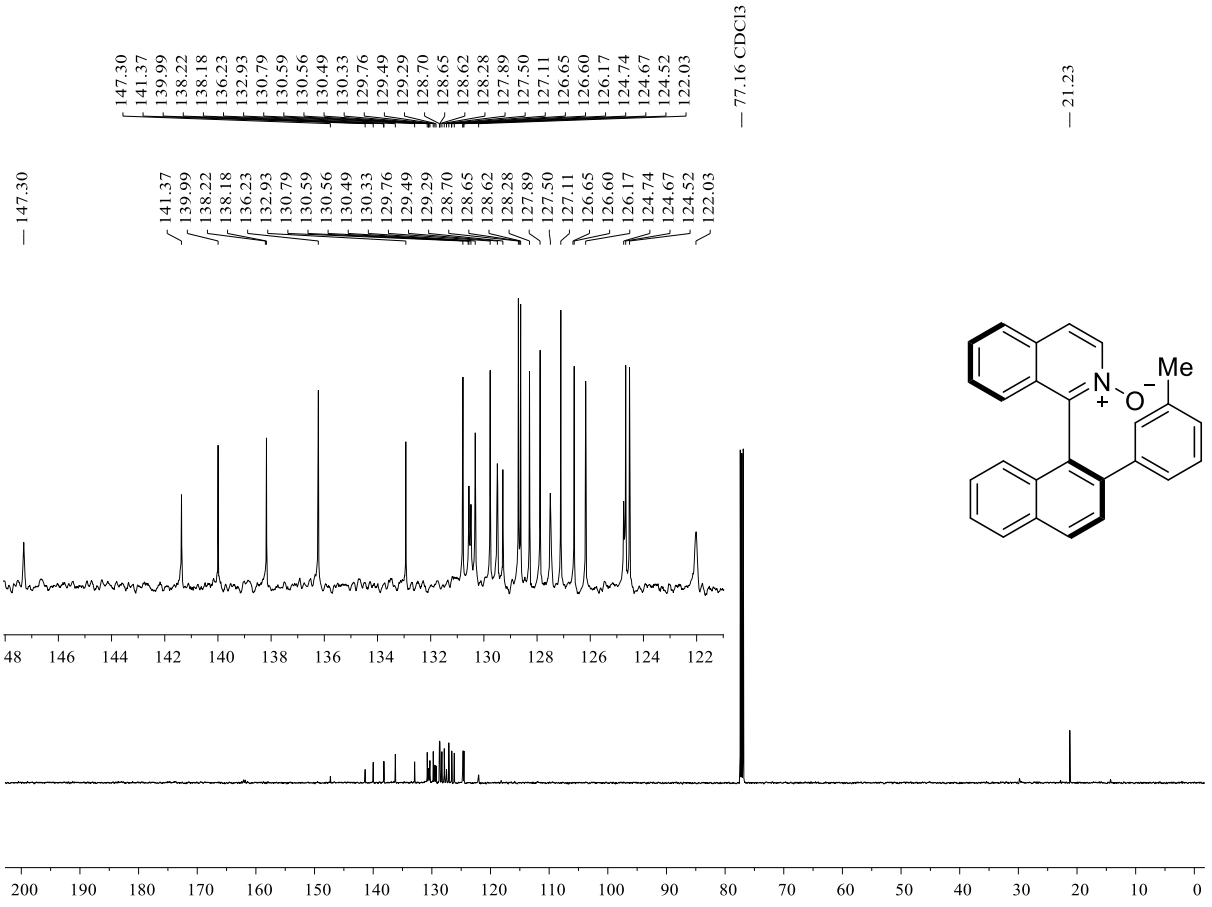
Peak#	Ret. Time	Area	Height	Area %	Height %
1	47.167	39258884	226583	27.696	32.950
2	58.456	102491204	461067	72.304	67.050
Total		141750087	687650	100.000	100.000

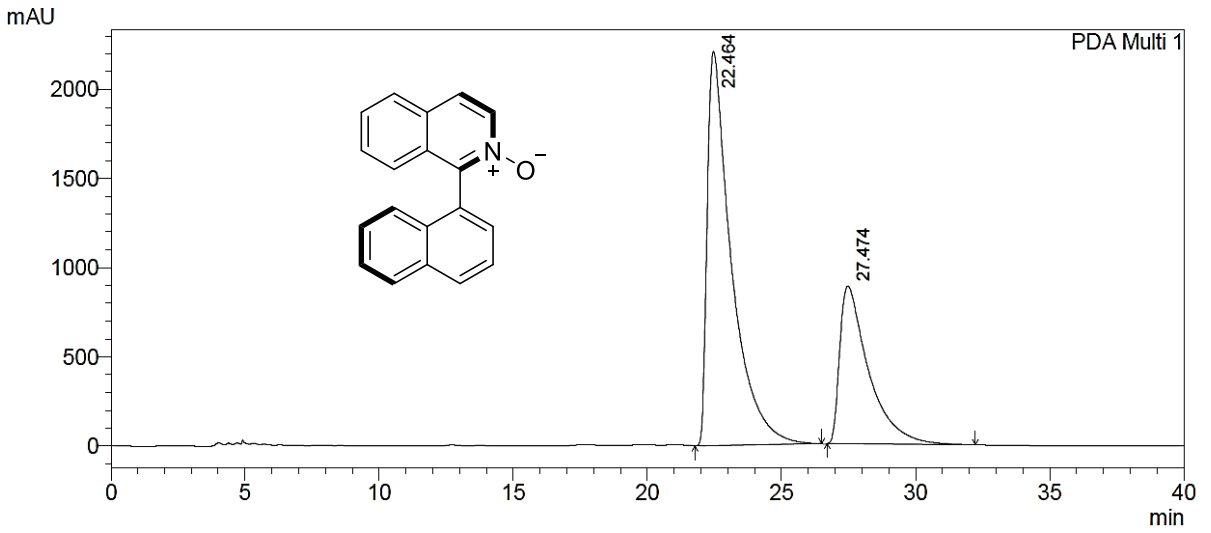
*(R)-1-(2-(m-tolyl)naphthalen-1-yl)isoquinoline 2-oxide (**3j**)*

^{1}H NMR *(*500 MHz*)*



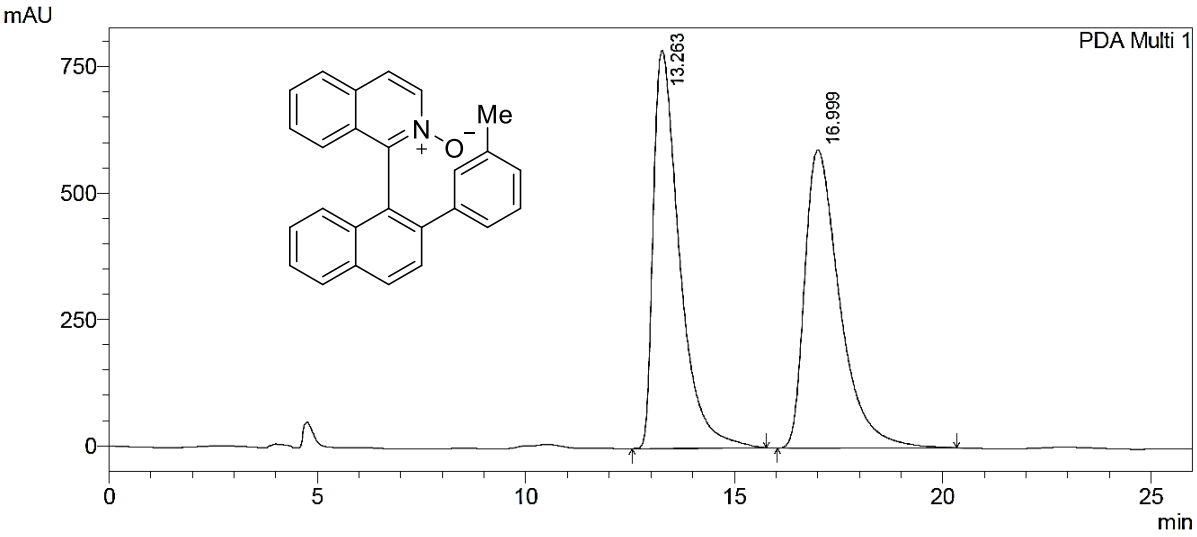
^{13}C NMR *(*125 MHz*)*





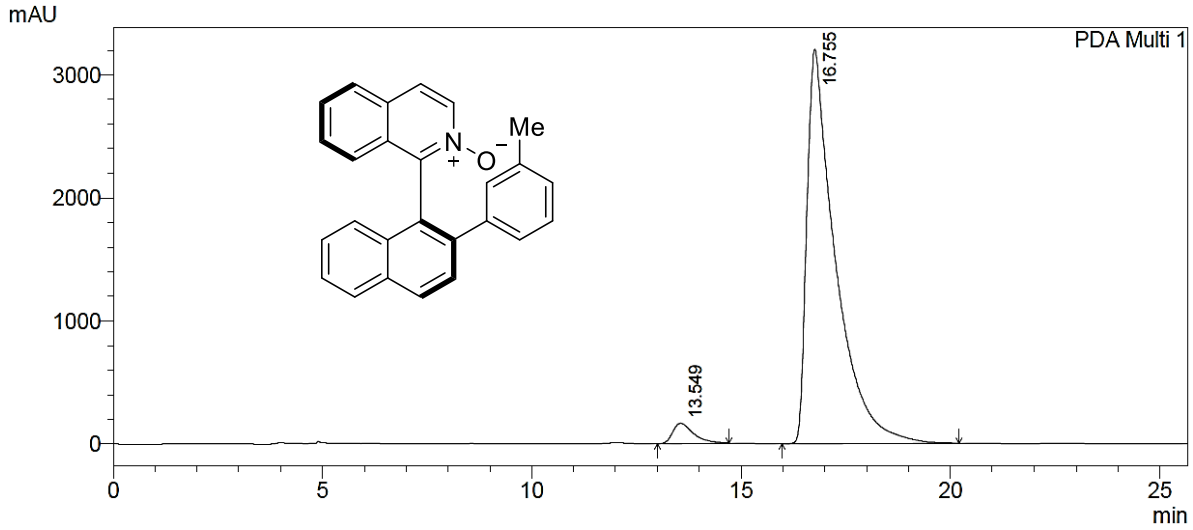
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.464	138092014	2207606	67.605	71.395
2	27.474	66169949	884488	32.395	28.605
Total		204261963	3092094	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.263	34306626	786220	49.898	57.162
2	16.999	34446661	589204	50.102	42.838
Total		68753287	1375425	100.000	100.000

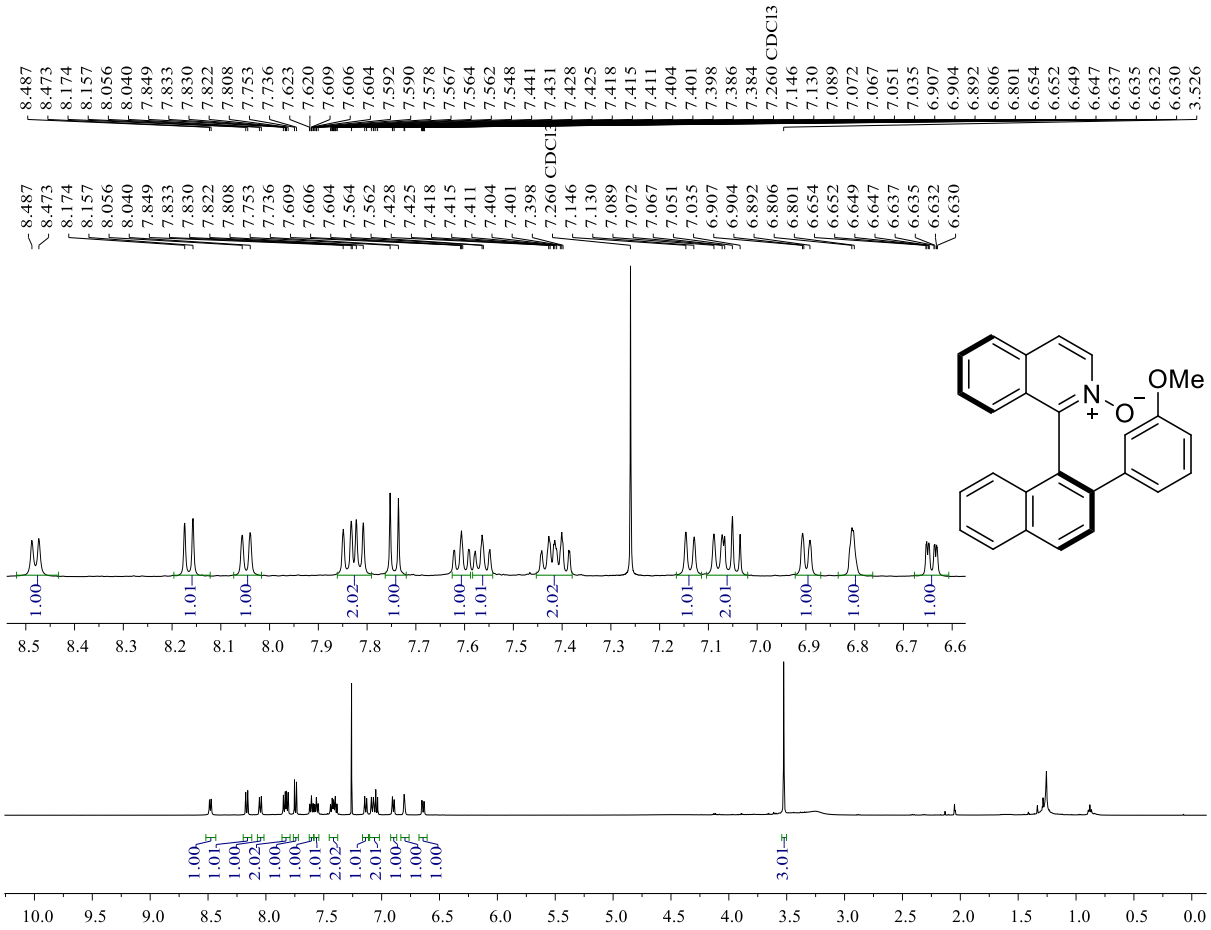


PDA Ch1 254nm 4nm

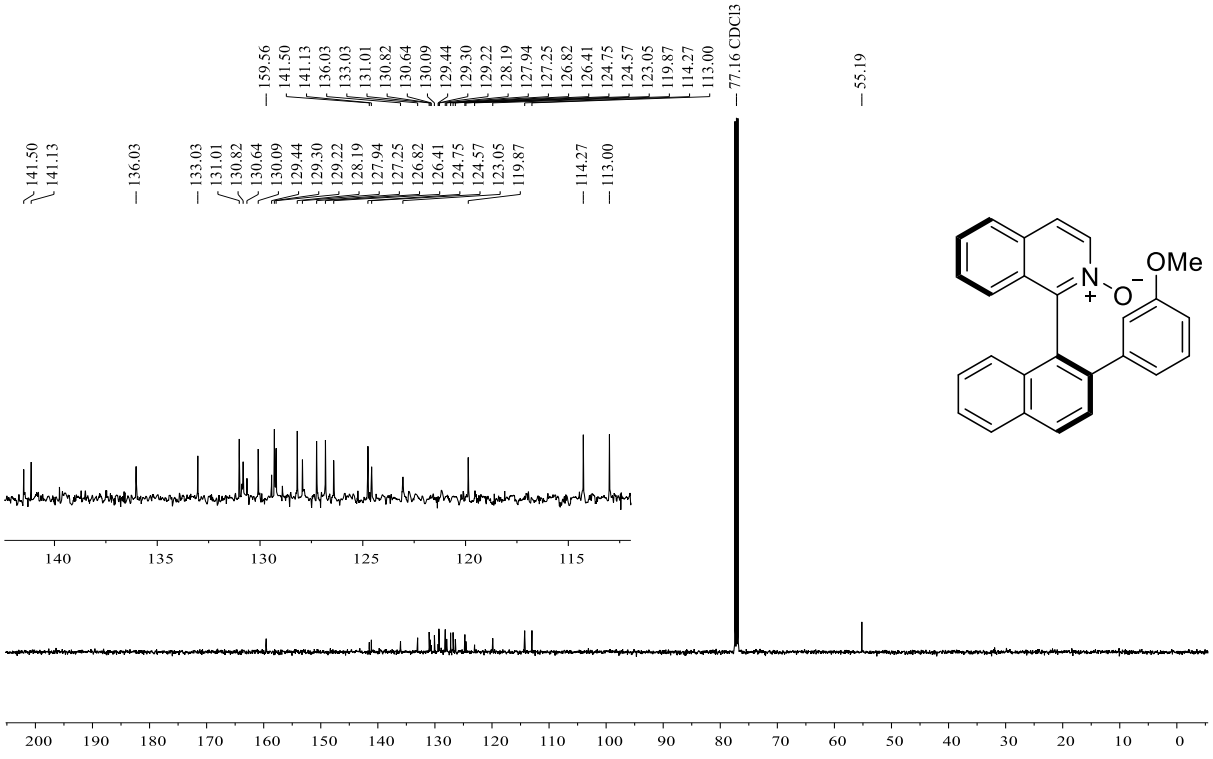
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.549	5634305	163643	3.584	4.863
2	16.755	151575237	3201678	96.416	95.137
Total		157209542	3365322	100.000	100.000

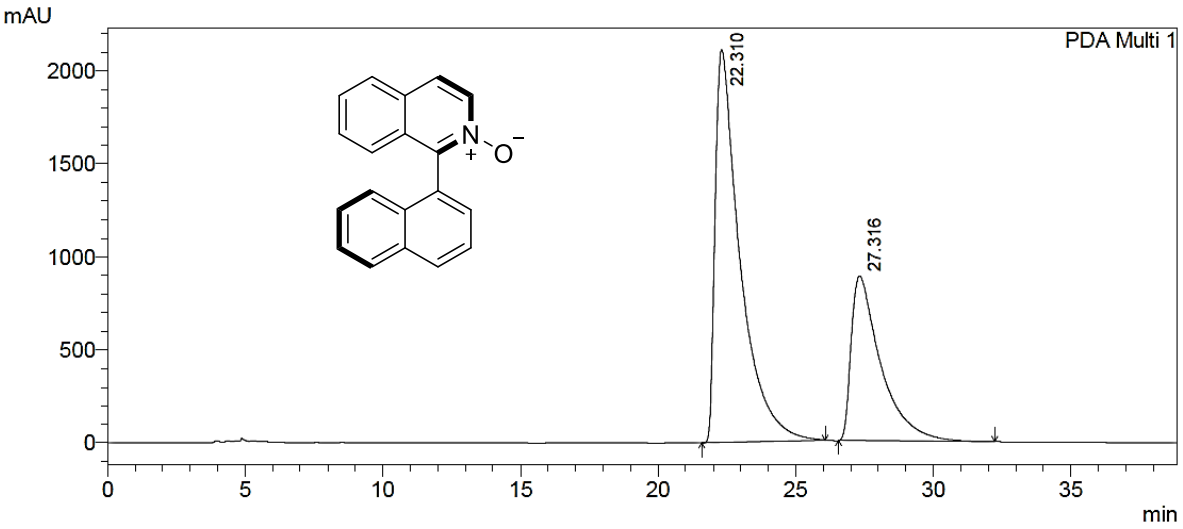
*(R)-1-(2-(3-methoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3k**)*

^{1}H NMR *(*500 MHz*)*



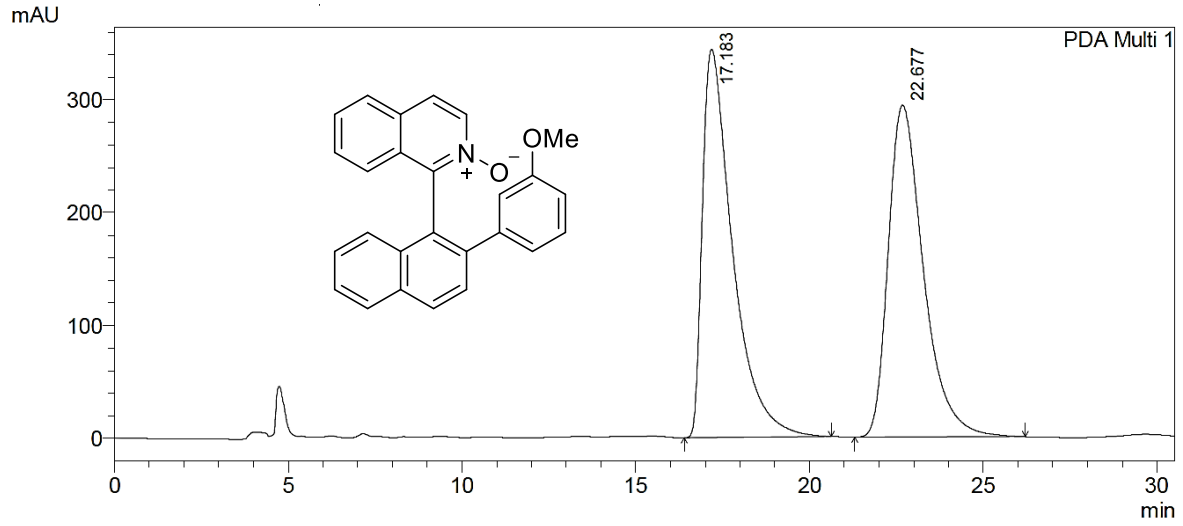
^{13}C NMR *(*125 MHz*)*





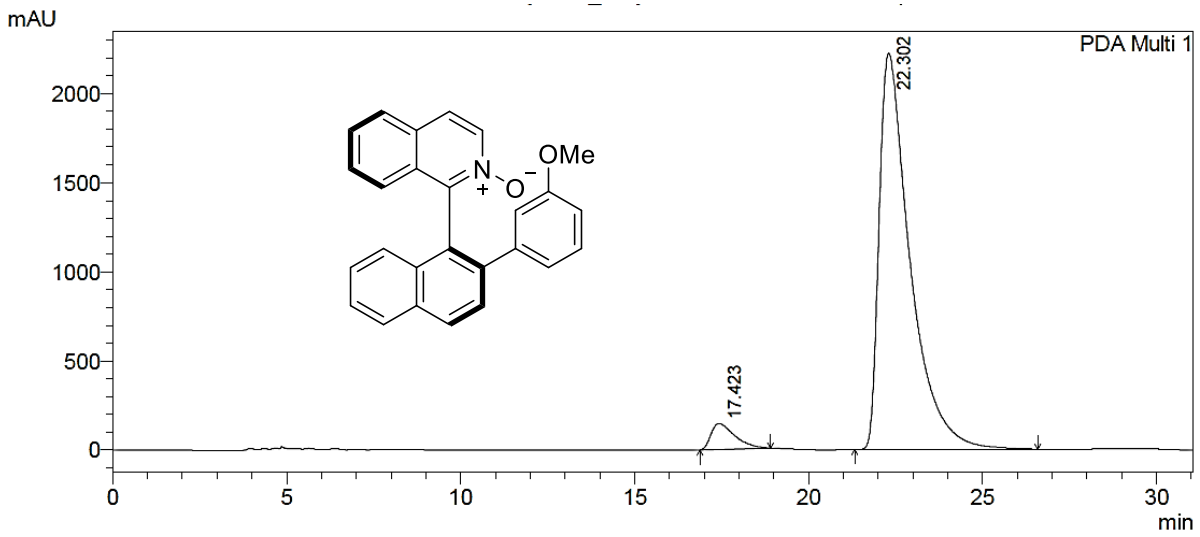
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.310	132418046	2110796	66.658	70.456
2	27.316	66234766	885093	33.342	29.544
Total		198652812	2995889	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.183	20746899	344044	50.018	53.909
2	22.677	20732117	294155	49.982	46.091
Total		41479015	638199	100.000	100.000

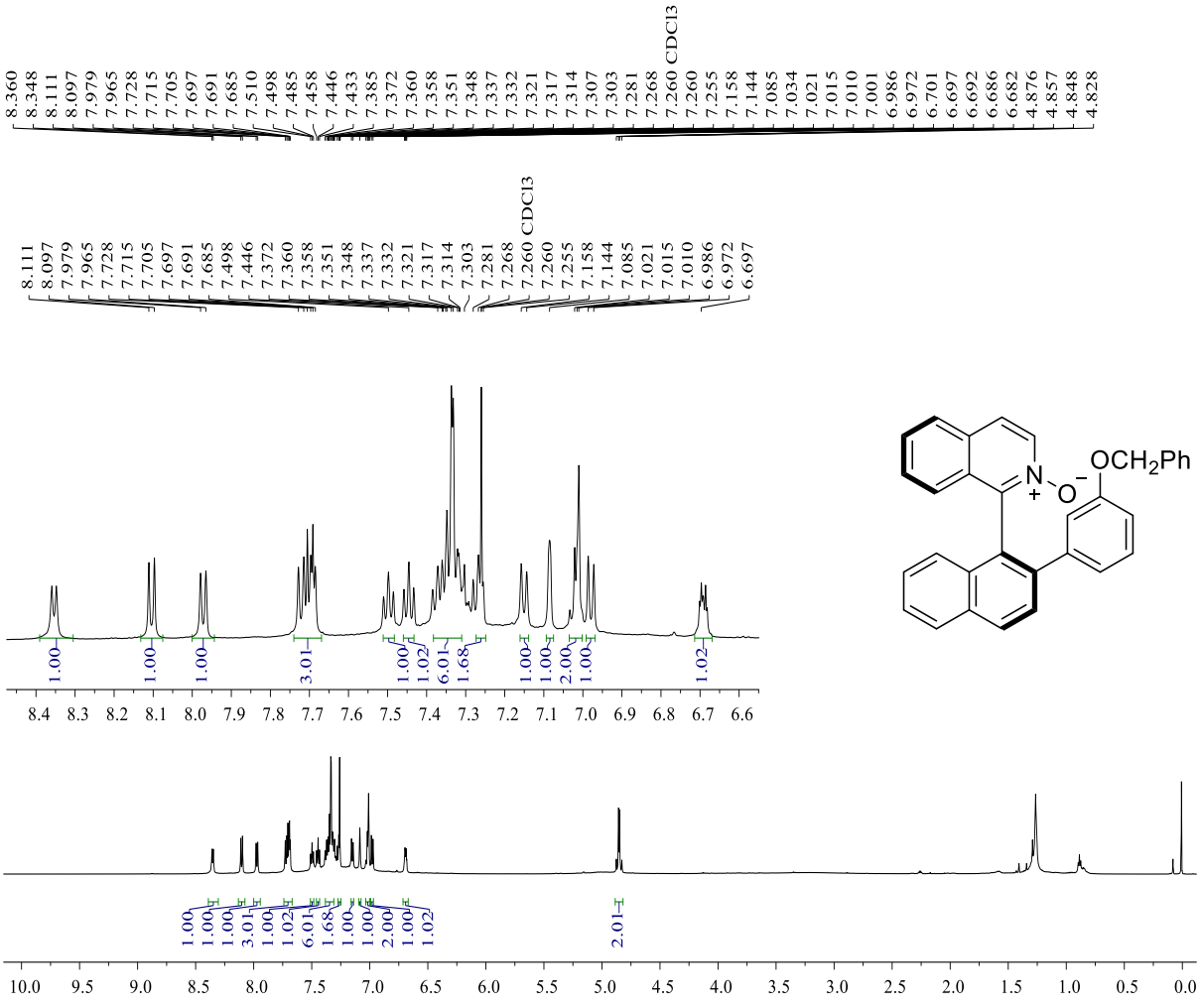


PDA Ch1 254nm 4nm

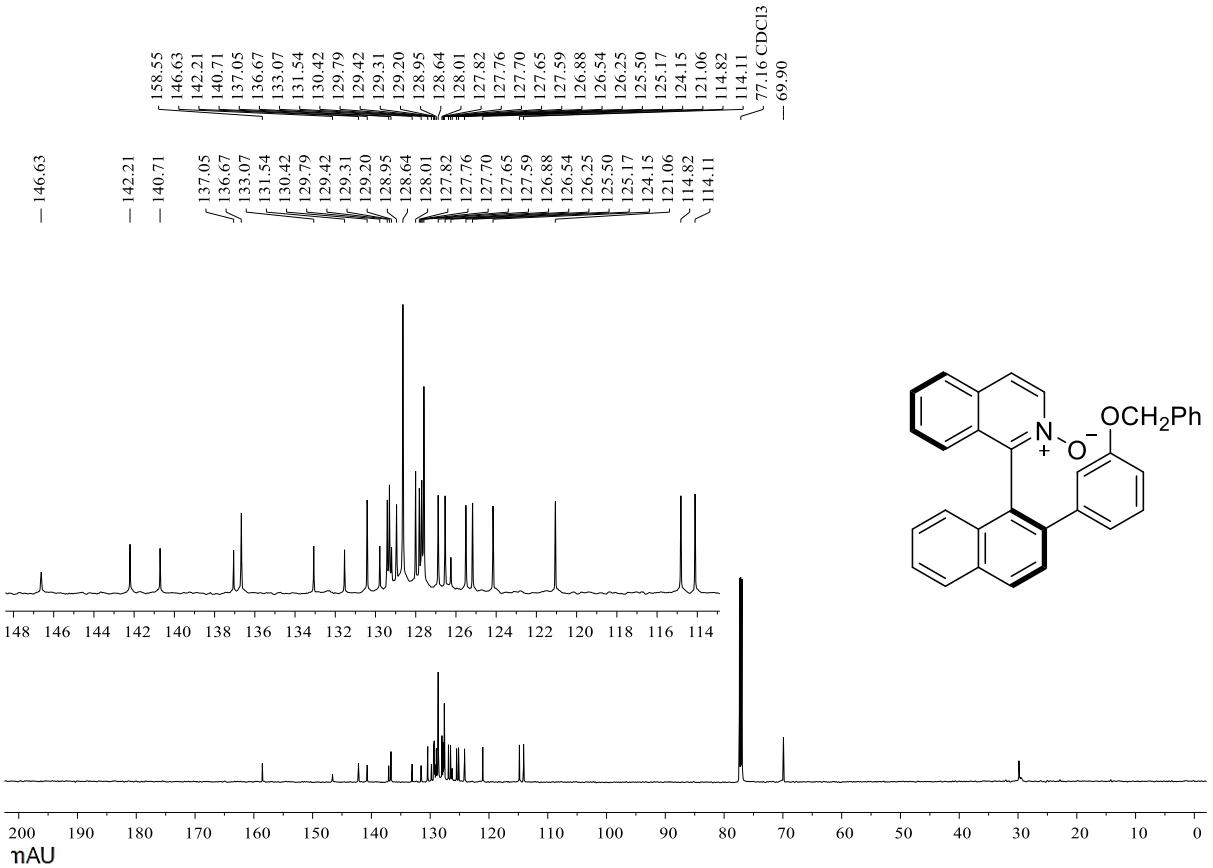
Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.423	6860954	144741	4.763	6.111
2	22.302	137175288	2223928	95.237	93.889
Total		144036241	2368669	100.000	100.000

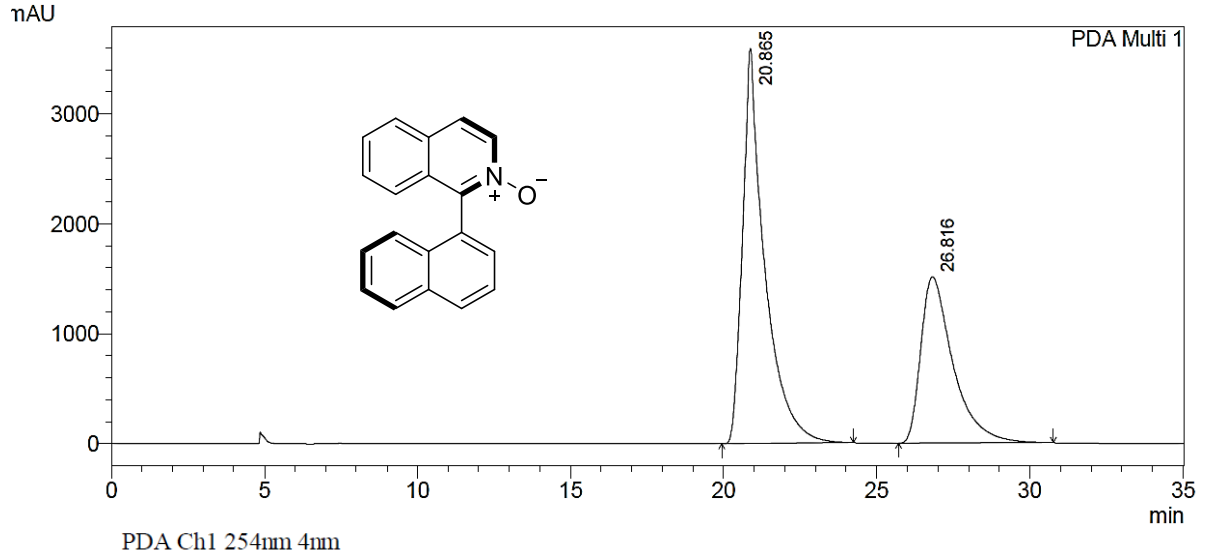
*(R)-1-(2-(3-methoxyphenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3l**)*

^{1}H NMR *(*600 MHz*)*



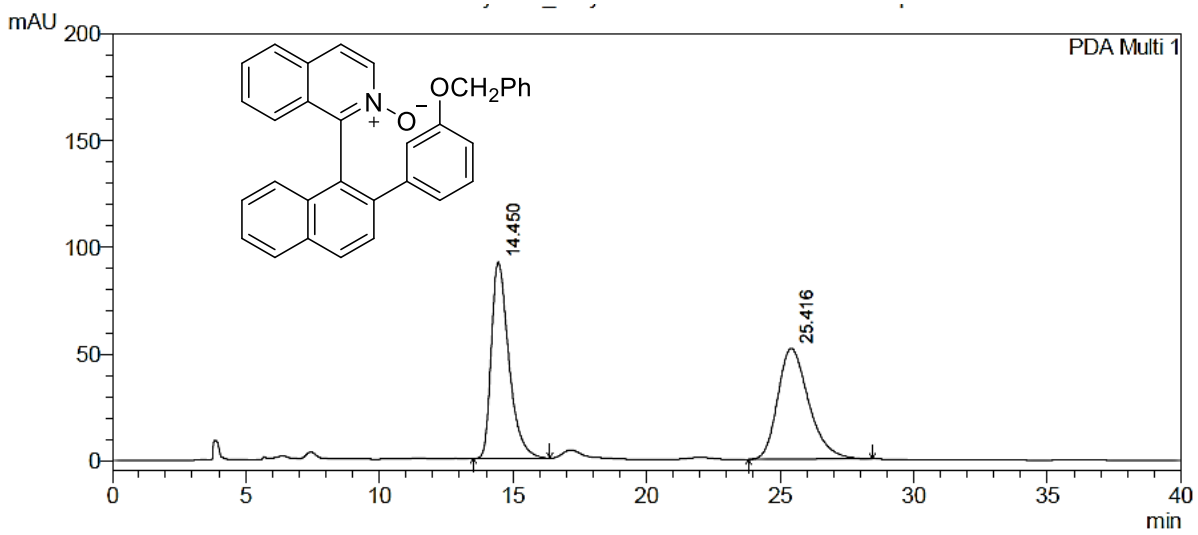
^{13}C NMR *(*150 MHz*)*





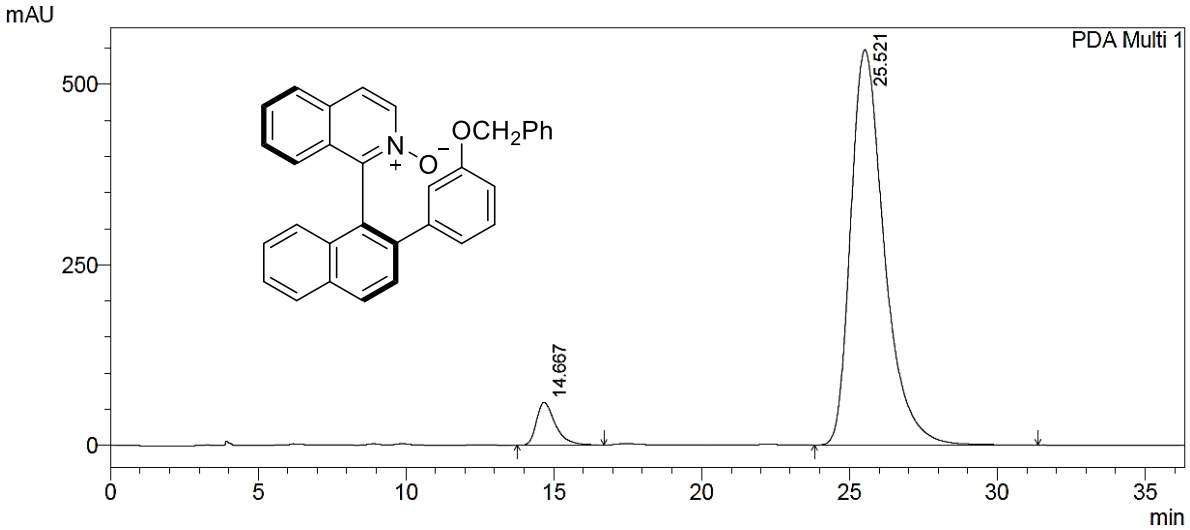
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.865	179922011	3591007	61.846	70.353
2	26.816	110997357	1513229	38.154	29.647
Total		290919368	5104235	100.000	100.000



PDA Ch1 310nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.450	4199431	92073	50.002	63.908
2	25.416	4199174	51997	49.998	36.092
Total		8398605	144070	100.000	100.000

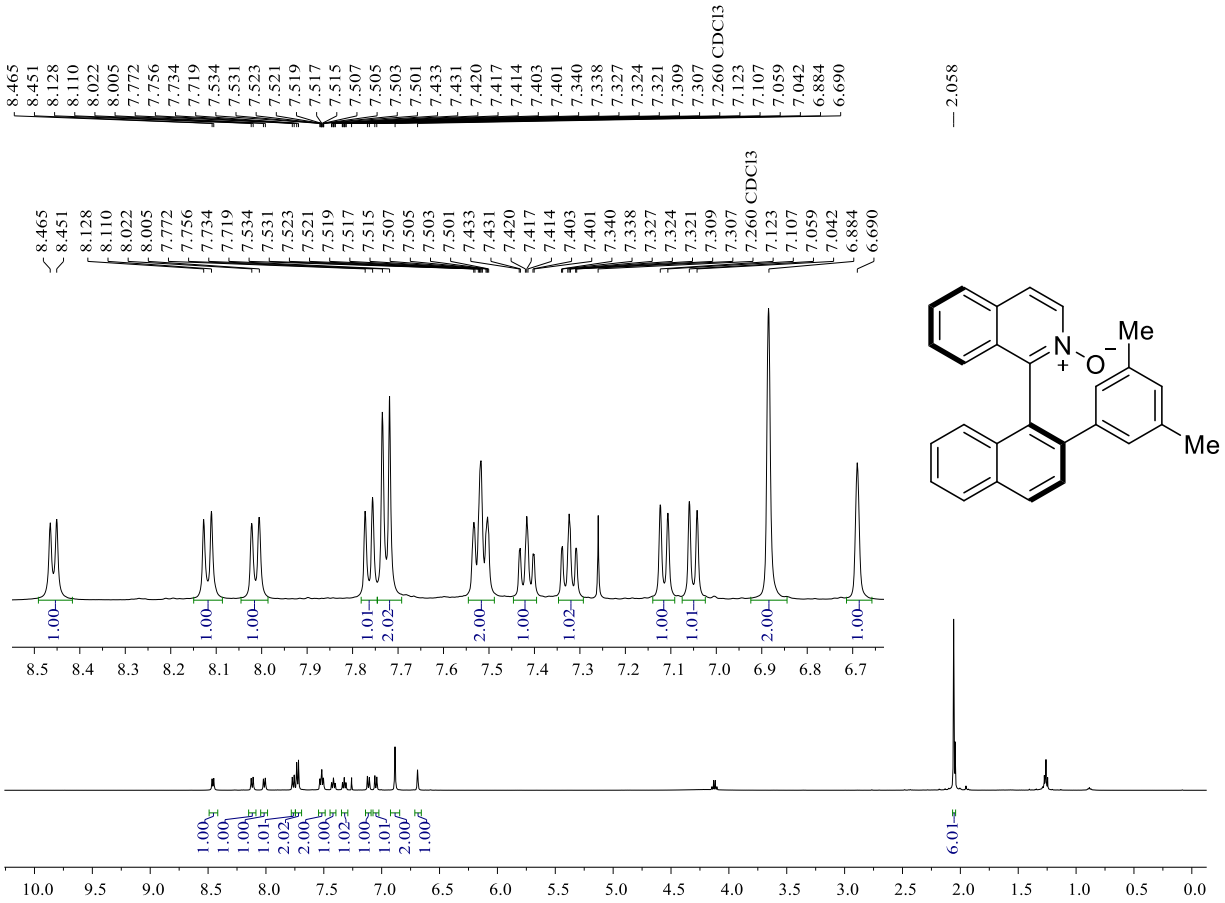


PDA Ch1 310nm 4nm

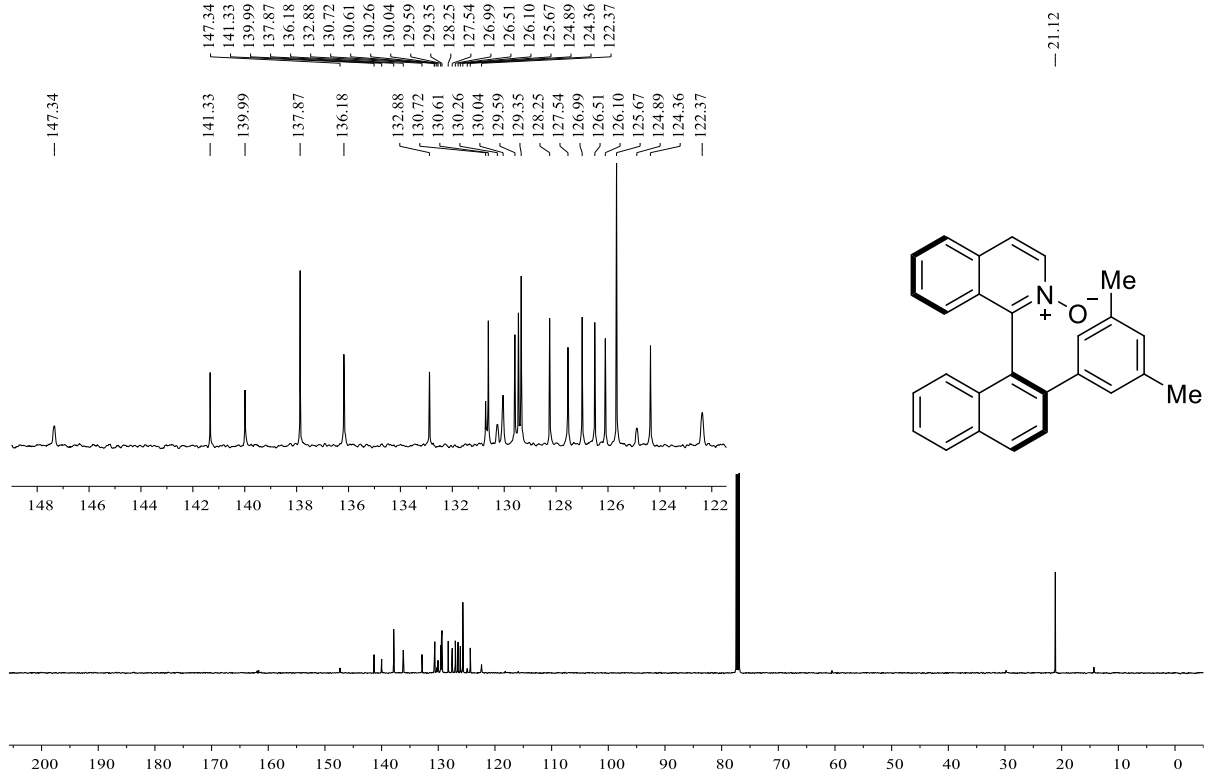
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.667	2607756	58994	5.695	9.744
2	25.521	43185598	546420	94.305	90.256
Total		45793355	605414	100.000	100.000

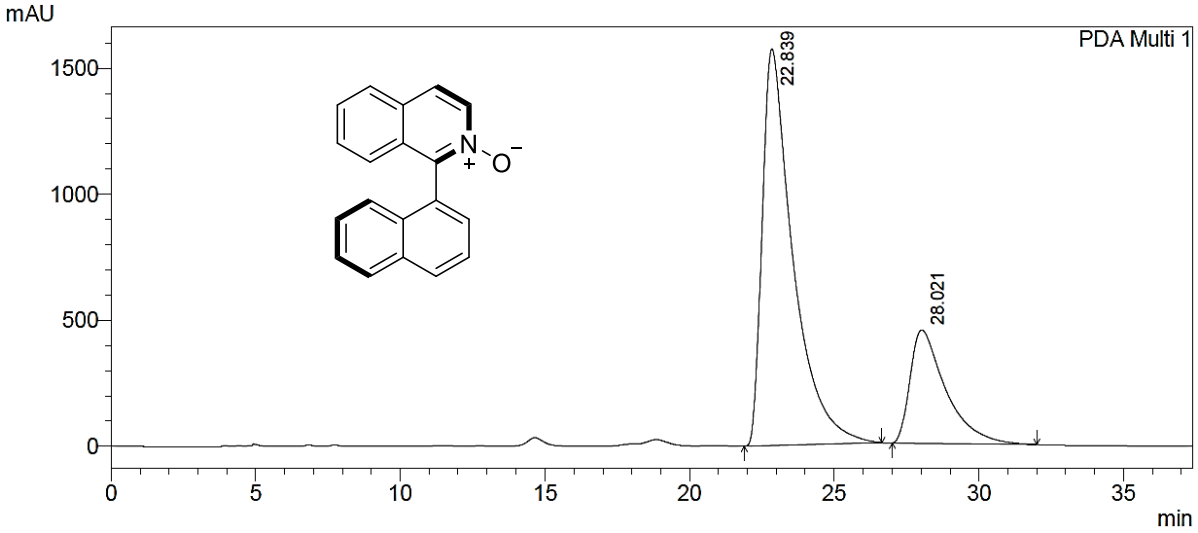
*(R)-1-(2-(3,5-dimethylphenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3m**)*

^{1}H NMR *(*500 MHz*)*



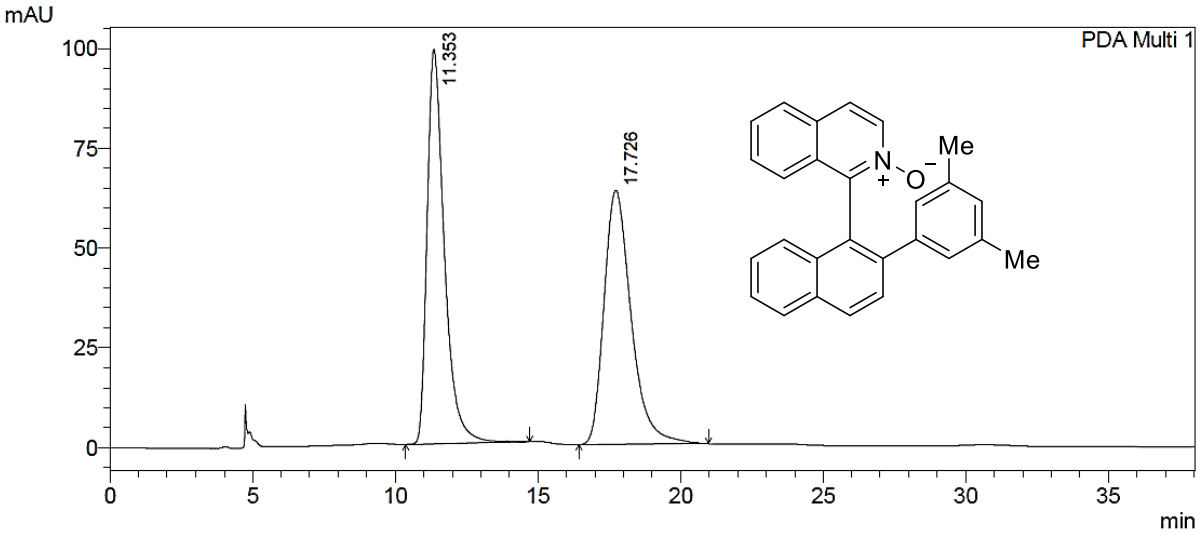
^{13}C NMR *(*125 MHz*)*





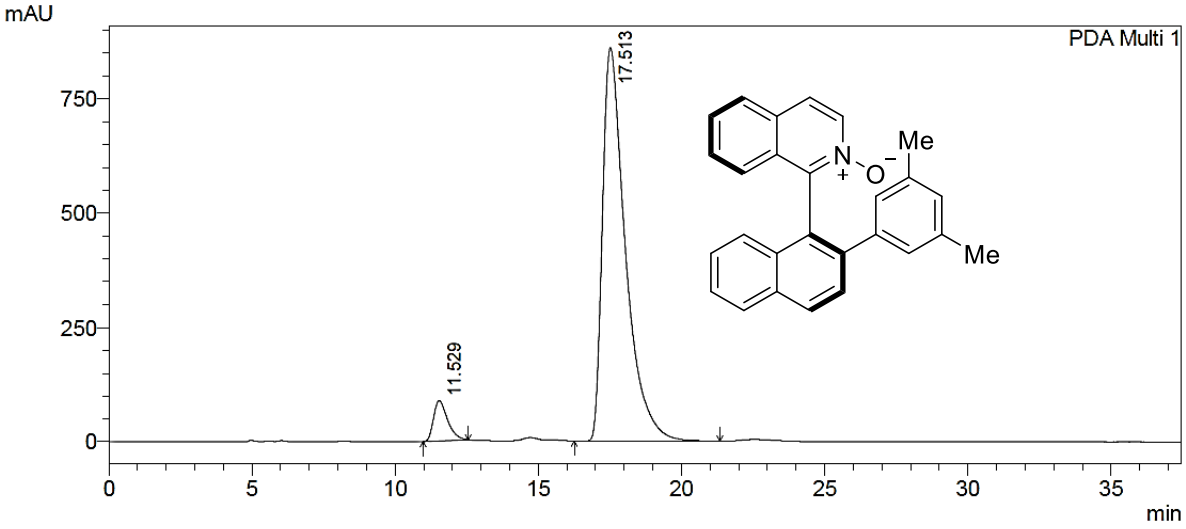
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.839	115989649	1570923	75.027	77.753
2	28.021	38607738	449485	24.973	22.247
Total		154597388	2020407	100.000	100.000



PDA Ch1 310nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.353	4167488	98848	49.721	60.808
2	17.726	4214241	63710	50.279	39.192
Total		8381729	162559	100.000	100.000

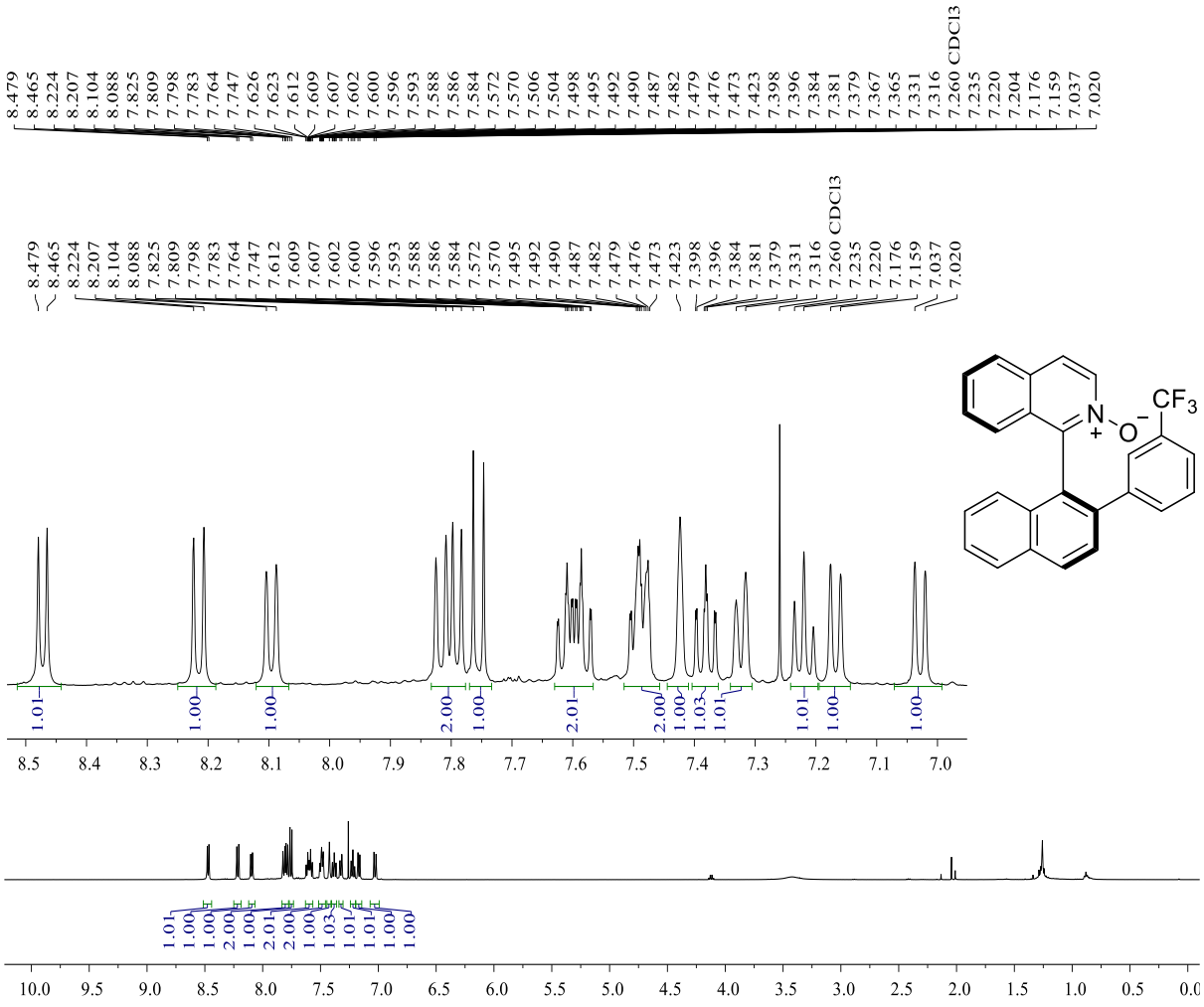


PDA Ch1 310nm 4nm

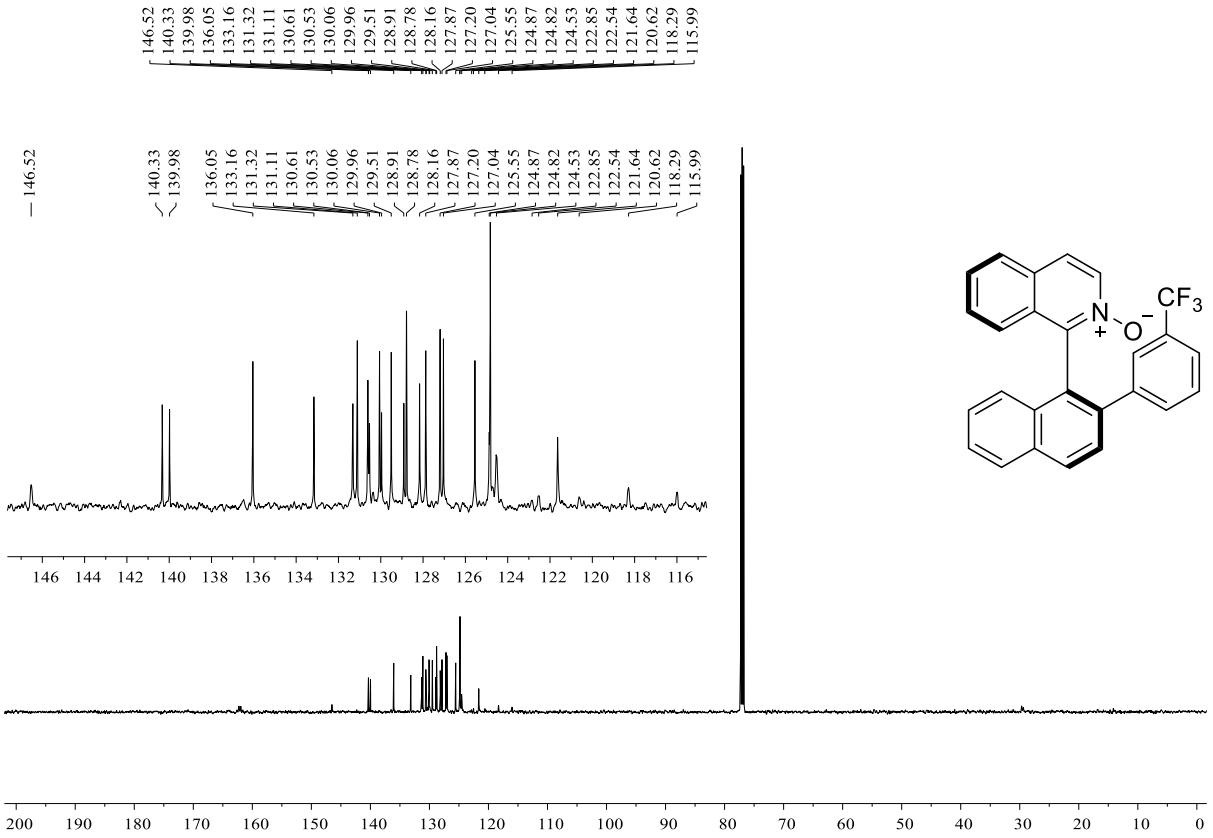
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.529	2997853	87989	5.869	9.283
2	17.513	48085241	859816	94.131	90.717
Total		51083094	947805	100.000	100.000

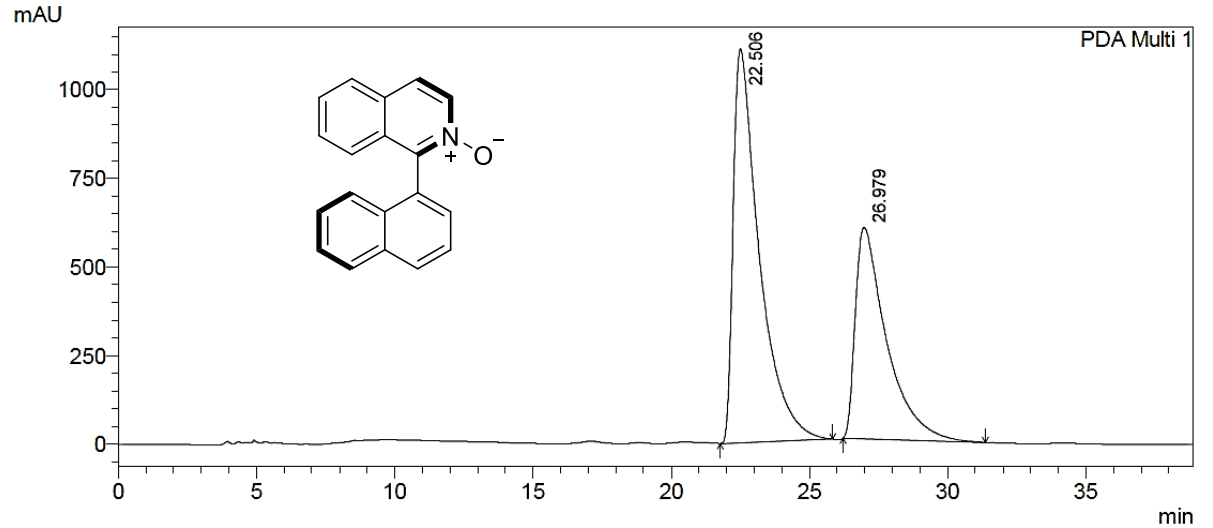
*(R)-1-(2-(3-(trifluoromethyl)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3n**)*

^{1}H NMR *(*500 MHz*)*



^{13}C NMR *(*125 MHz*)*

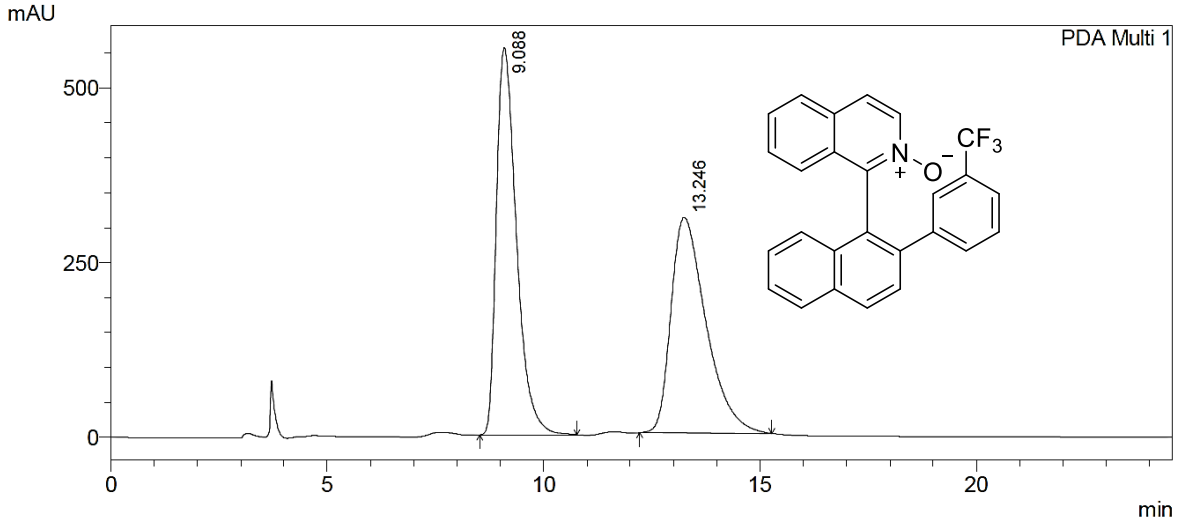




PDA Ch1 254nm 4nm

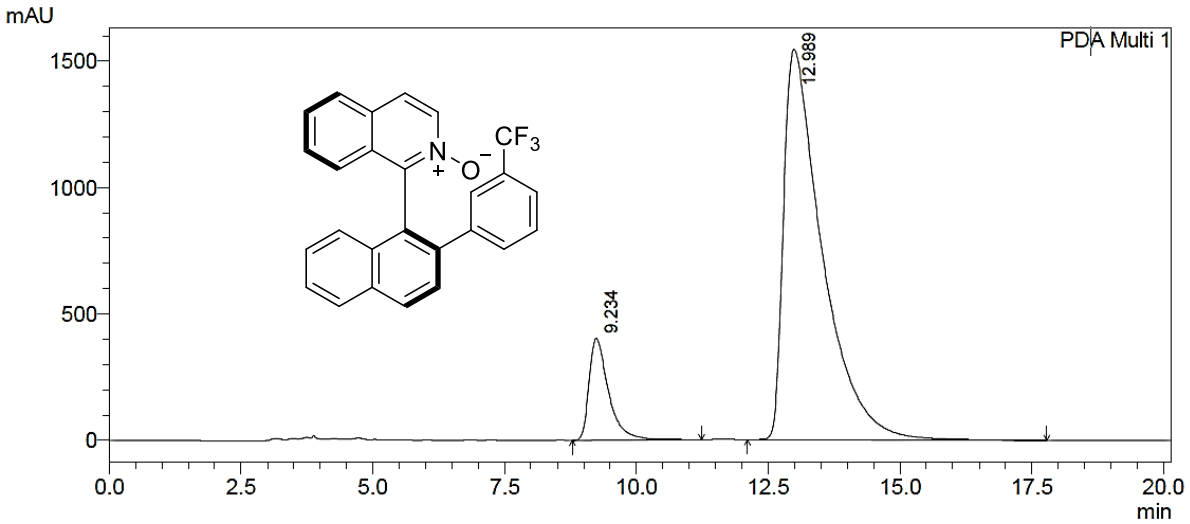
Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.506	72840631	1111765	60.893	65.077
2	26.979	46779754	596626	39.107	34.923
Total		119620385	1708391	100.000	100.000

.



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.088	17791445	553438	50.589	64.224
2	13.246	17377092	308297	49.411	35.776
Total		35168537	861736	100.000	100.000

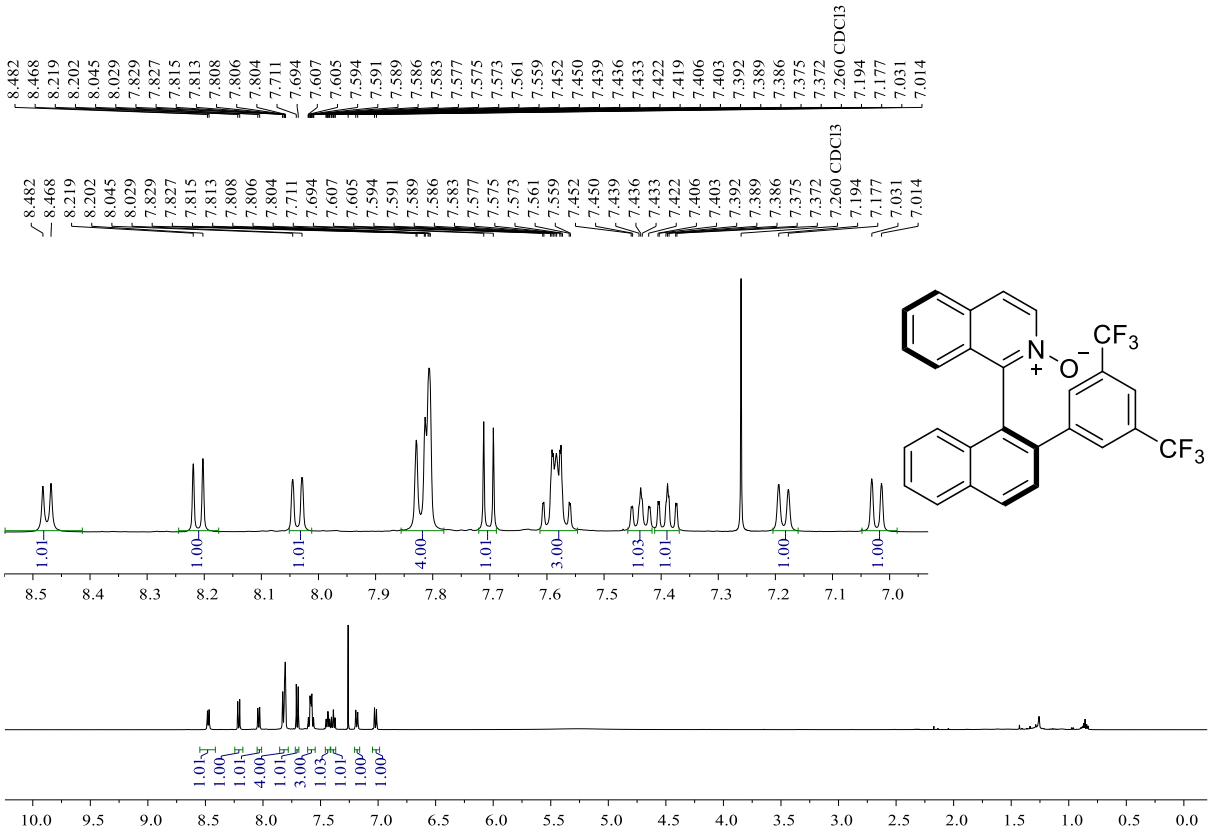


PDA Ch1 254nm 4nm

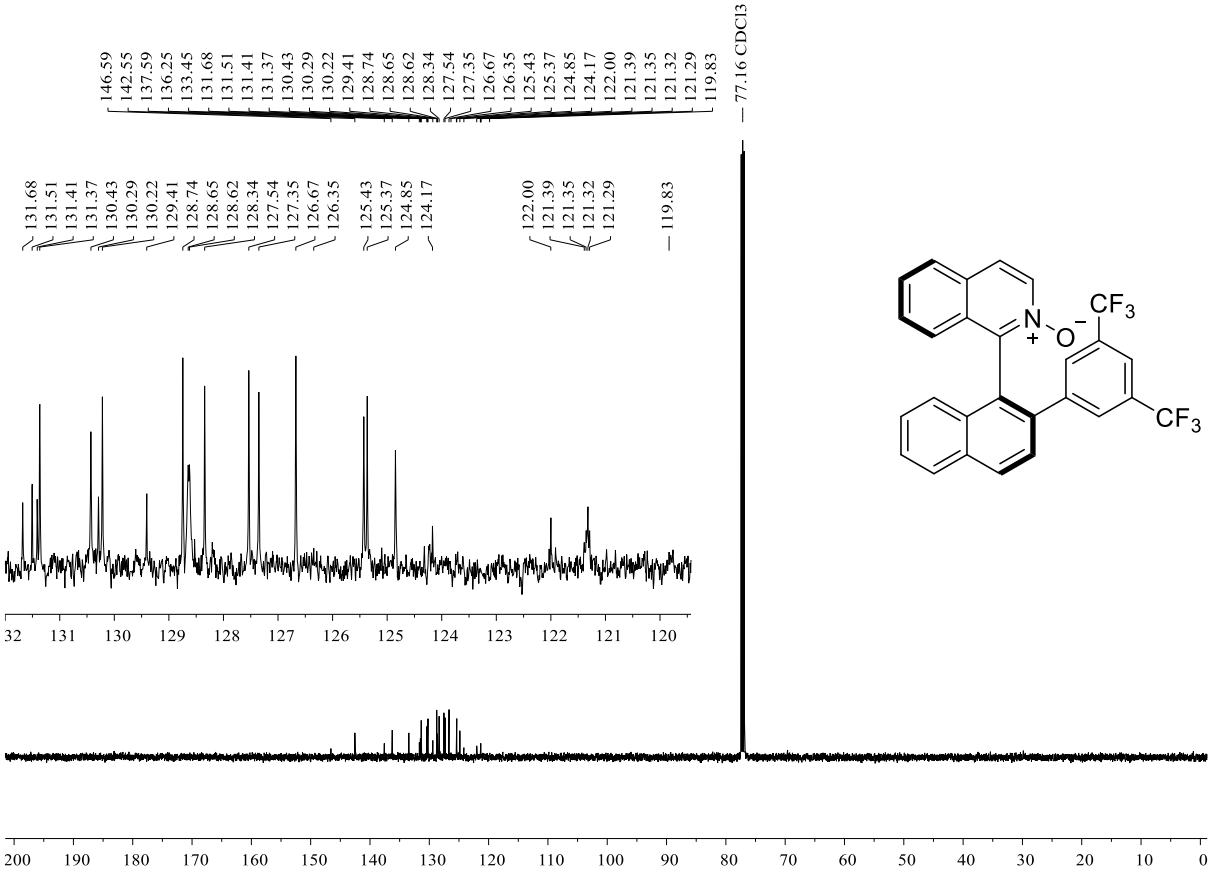
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.234	10423620	402464	11.679	20.694
2	12.989	78826895	1542394	88.321	79.306
Total		89250515	1944858	100.000	100.000

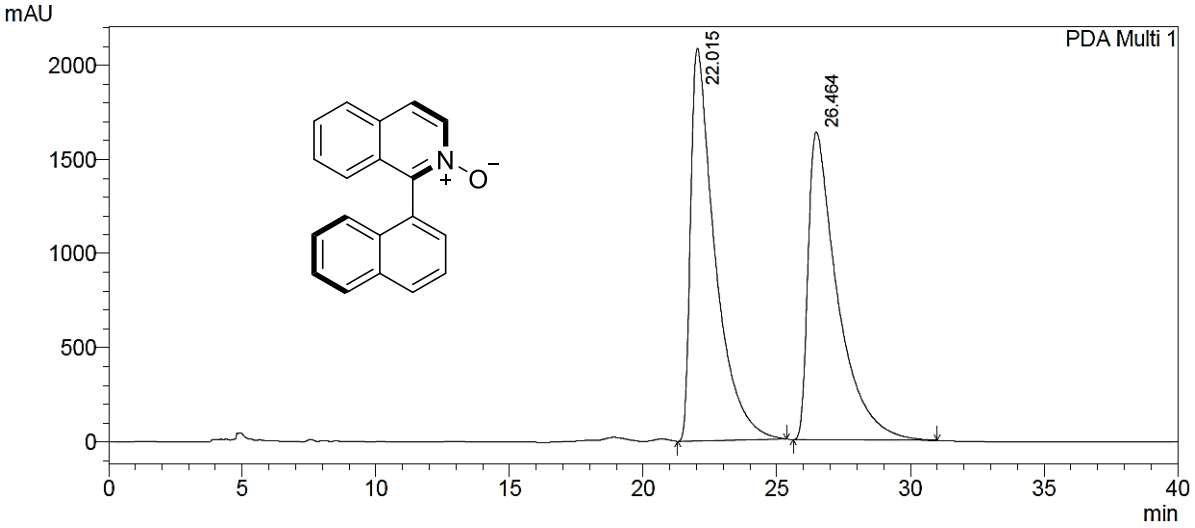
*(R)-1-(2-(3,5-bis(trifluoromethyl)phenyl)naphthalen-1-yl)isoquinoline 2-oxide (**3o**)*

^{1}H NMR *(*500 MHz*)*



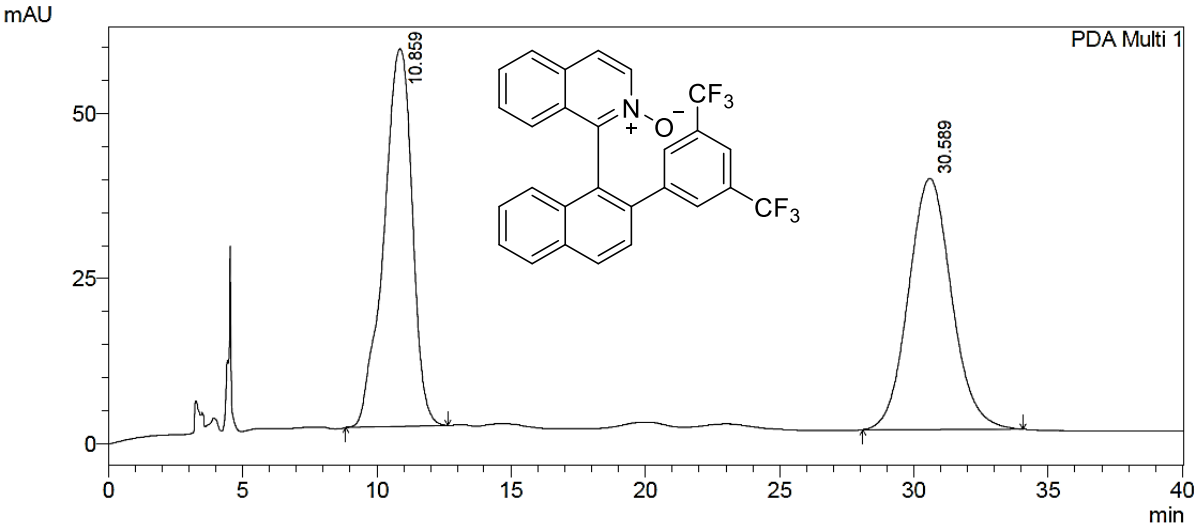
^{13}C NMR *(*125 MHz*)*





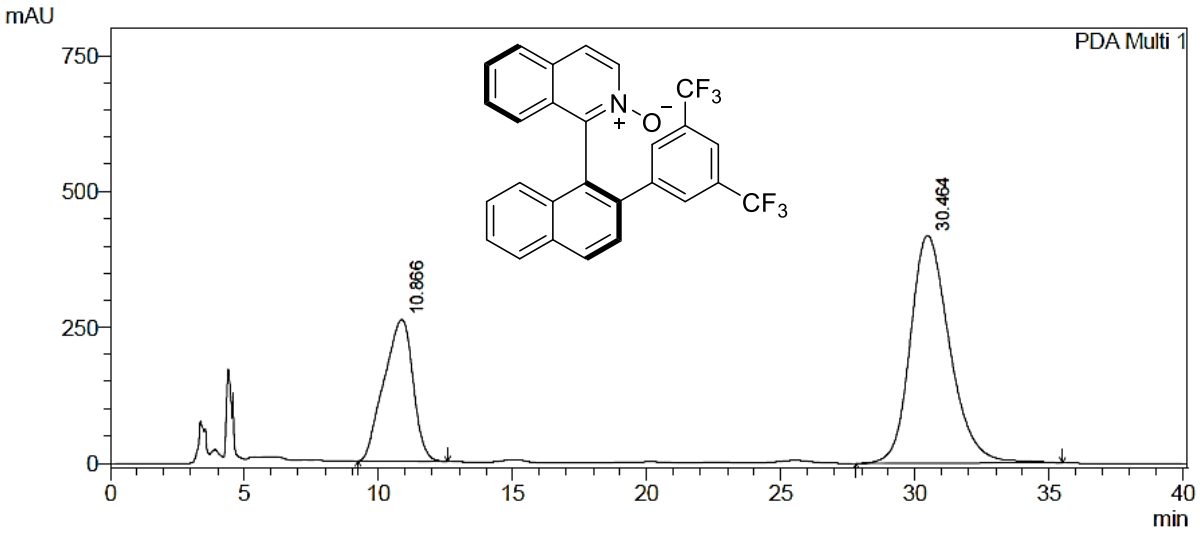
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.015	131965834	2084569	51.366	56.038
2	26.464	124947604	1635338	48.634	43.962
Total		256913438	3719907	100.000	100.000



PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.859	4234787	57225	49.931	60.070
2	30.589	4246500	38039	50.069	39.930
Total		8481287	95264	100.000	100.000

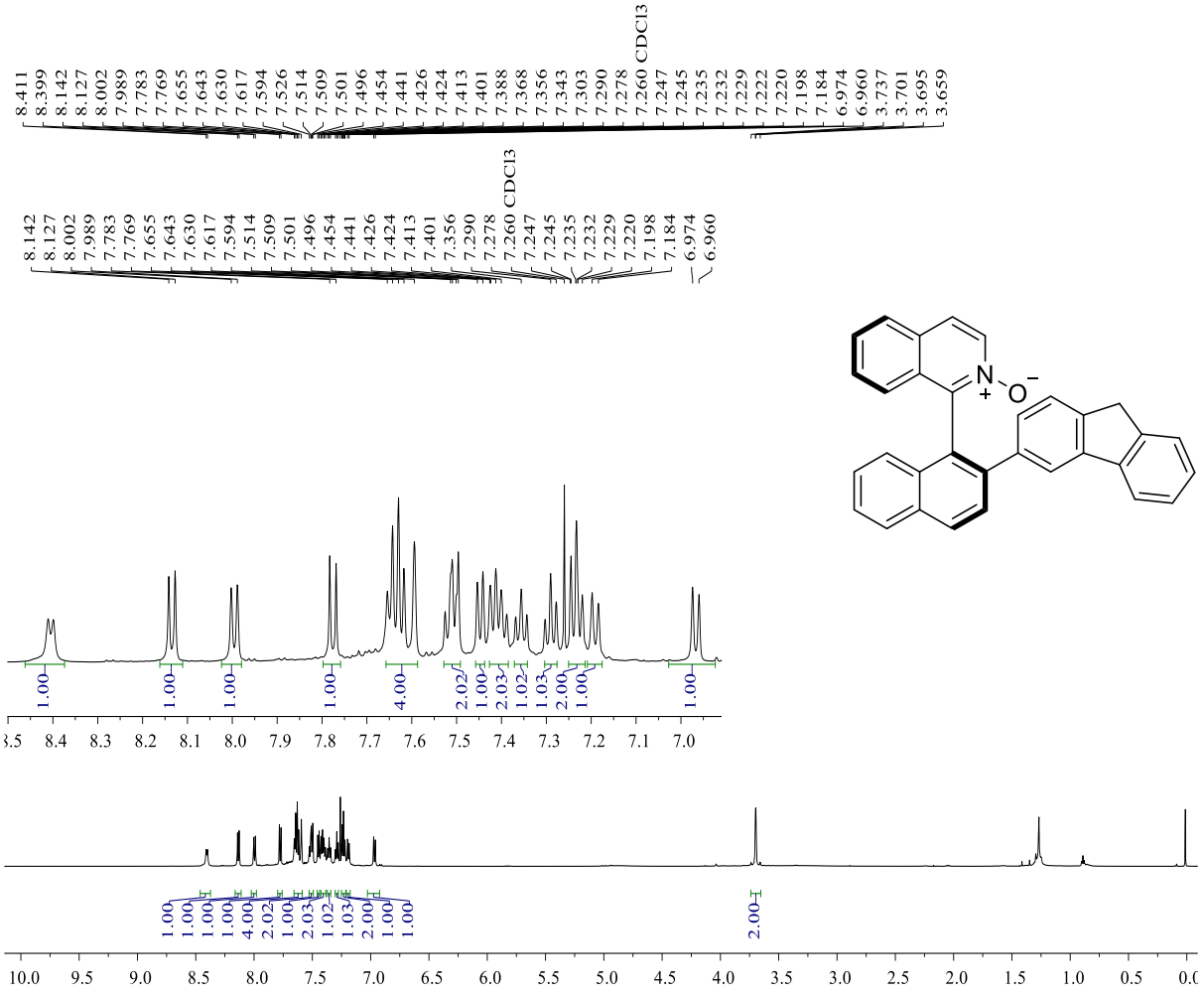


PDA Ch1 254nm 4nm

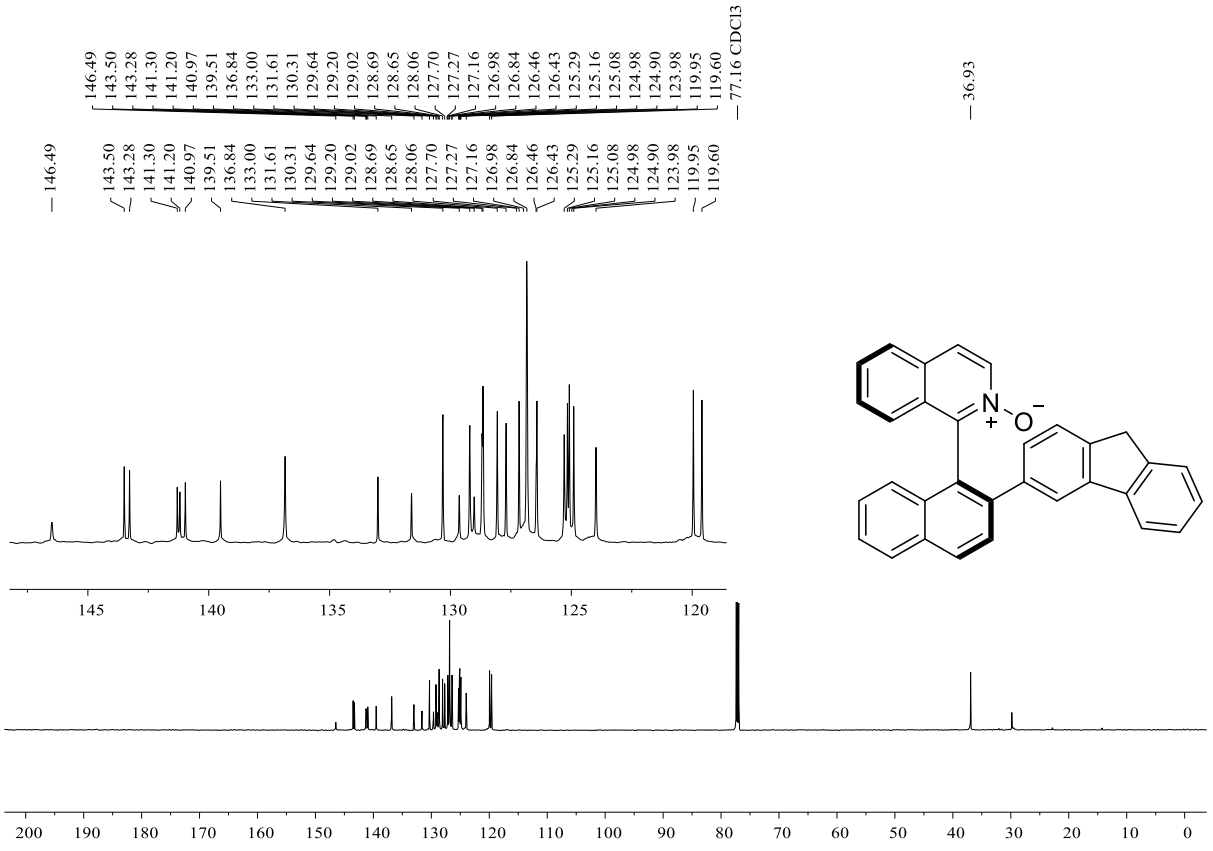
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.866	19681323	260627	31.615	38.350
2	30.464	42571703	418967	68.385	61.650
Total		62253026	679594	100.000	100.000

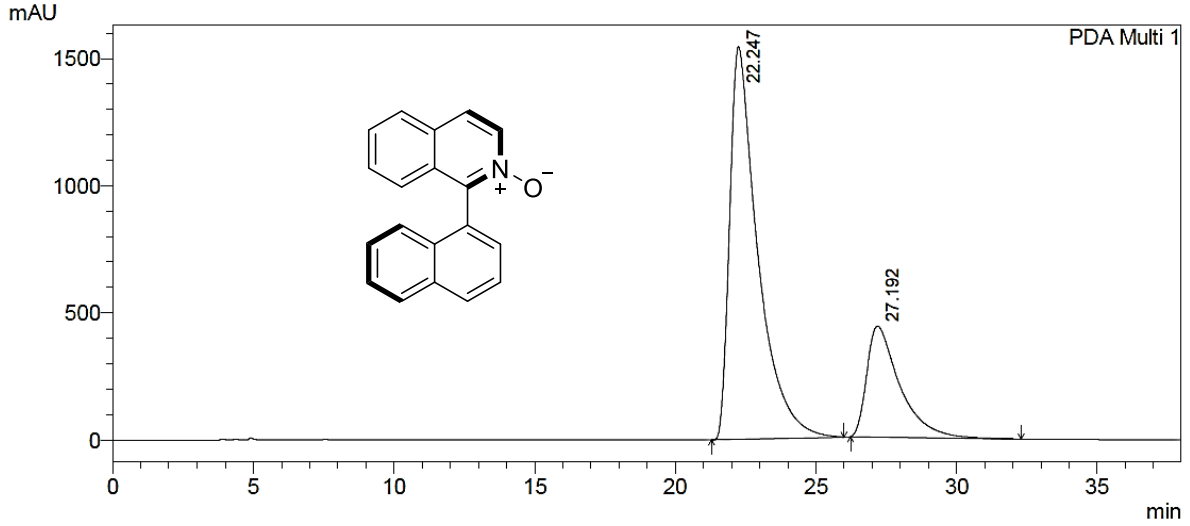
*(R)-1-(2-(9H-fluoren-3-yl)naphthalen-1-yl)isoquinoline 2-oxide (**3p**)*

^{1}H NMR *(*600 MHz*)*



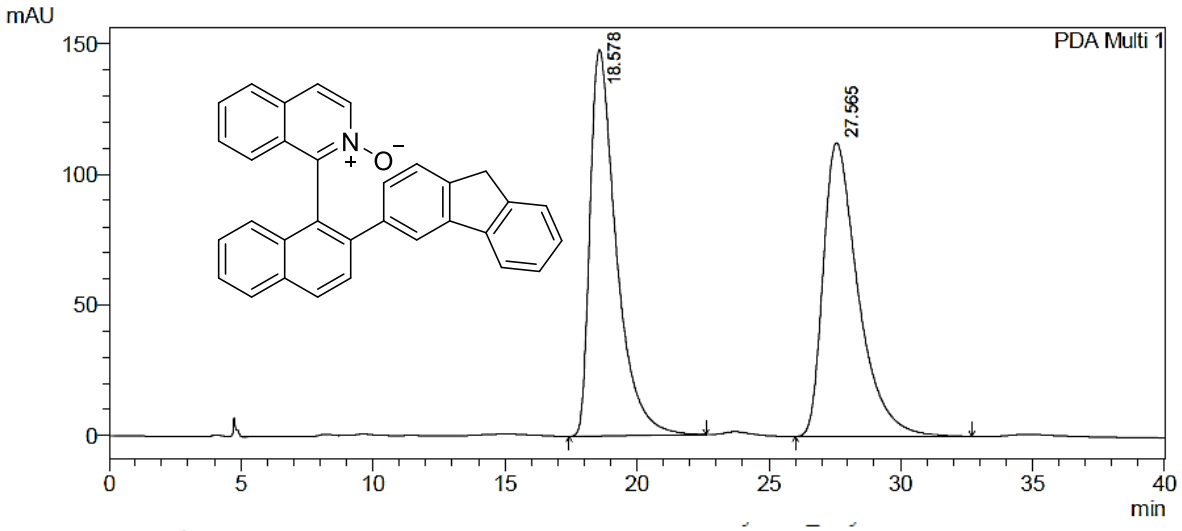
$^{13}C\{^{1}H\}$ NMR *(*150 MHz*)*





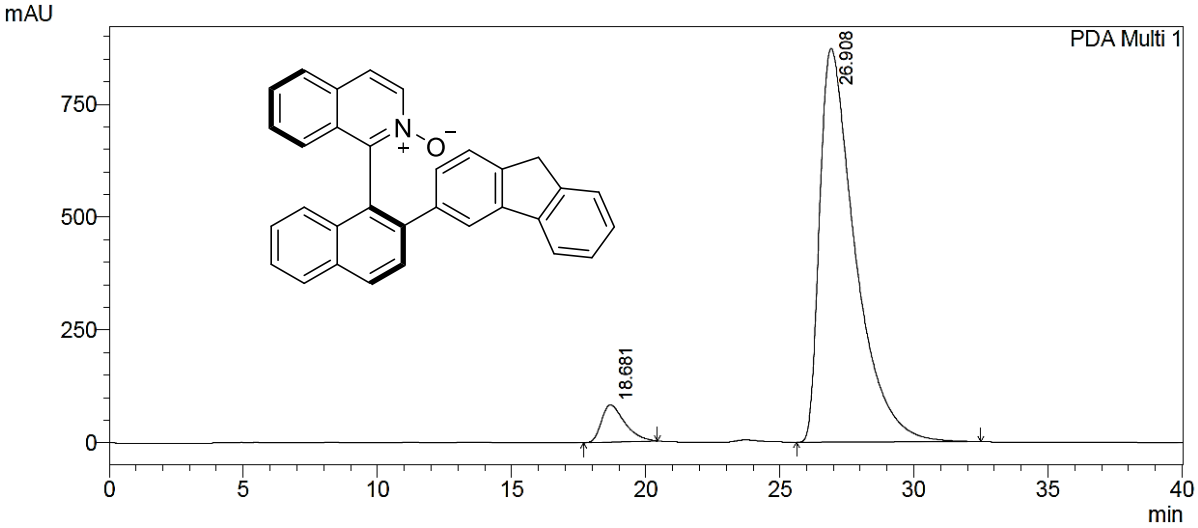
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.247	107291982	1542622	75.125	77.942
2	27.192	35525046	436566	24.875	22.058
Total		142817028	1979188	100.000	100.000



PDA Ch1 310nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.578	10239536	147927	49.700	56.828
2	27.565	10363240	112382	50.300	43.172
Total		20602776	260309	100.000	100.000

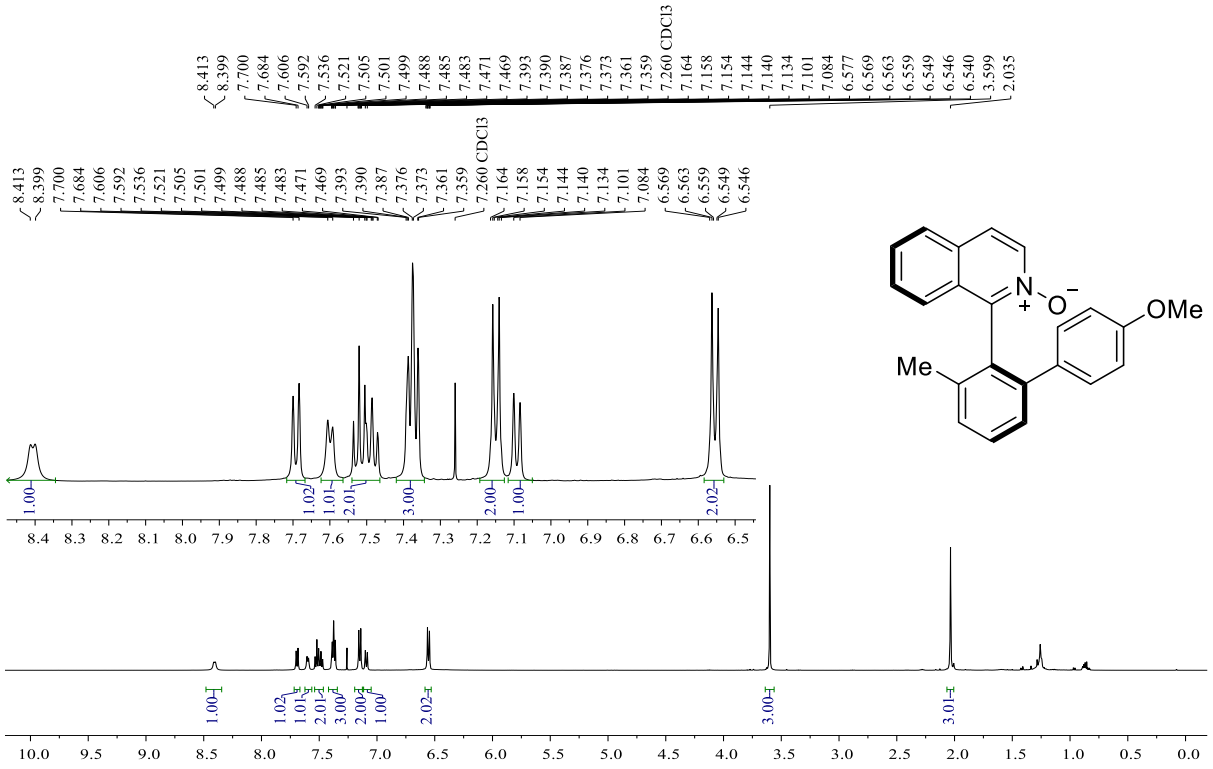


PDA Ch1 310nm 4nm

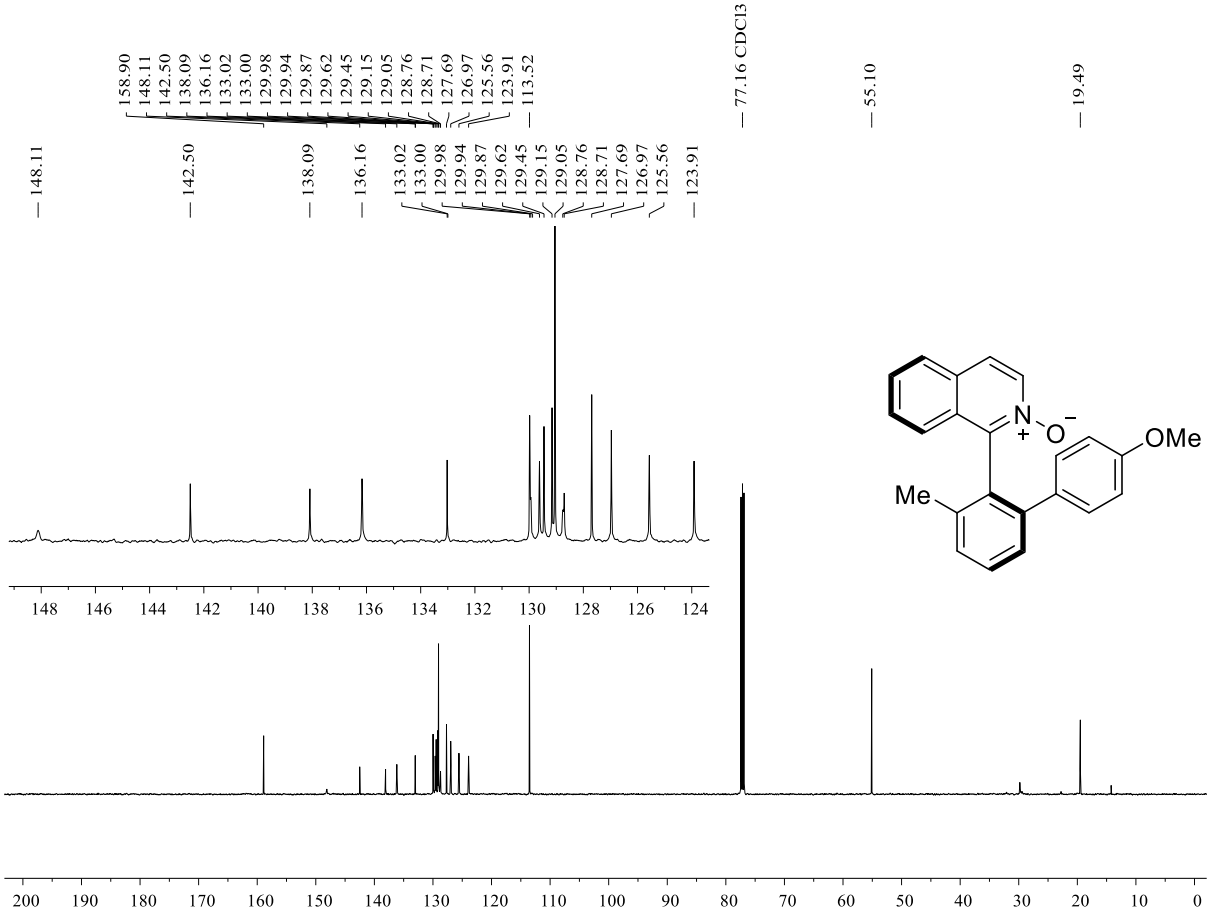
Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.681	4945406	82144	5.809	8.611
2	26.908	80187395	871750	94.191	91.389
Total		85132802	953894	100.000	100.000

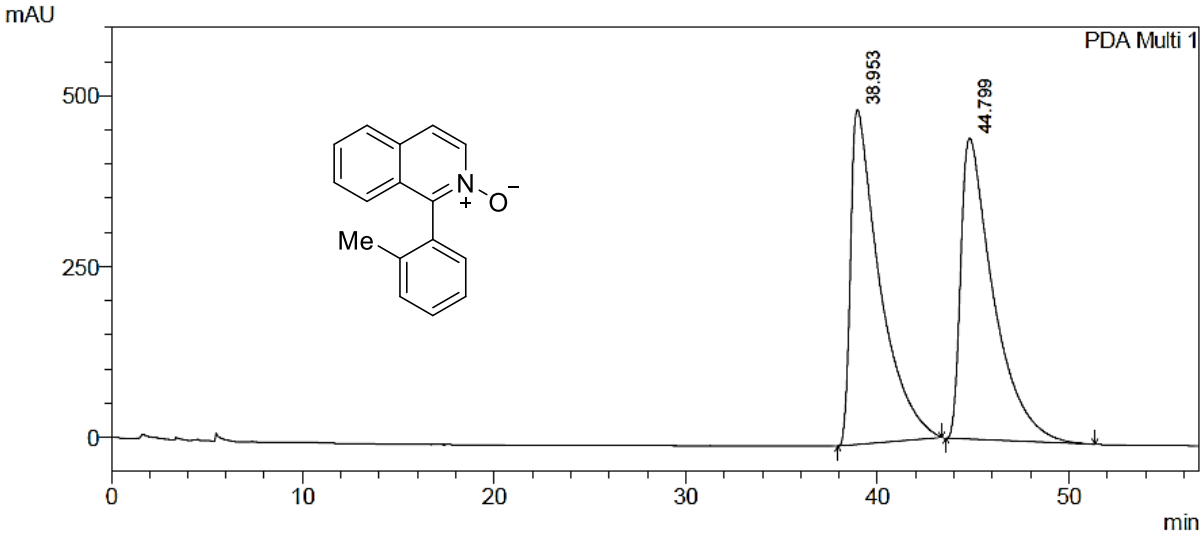
*(R)-1-(4'-methoxy-3-methyl-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (**3q**)*

^{1}H NMR *(*500 MHz*)*



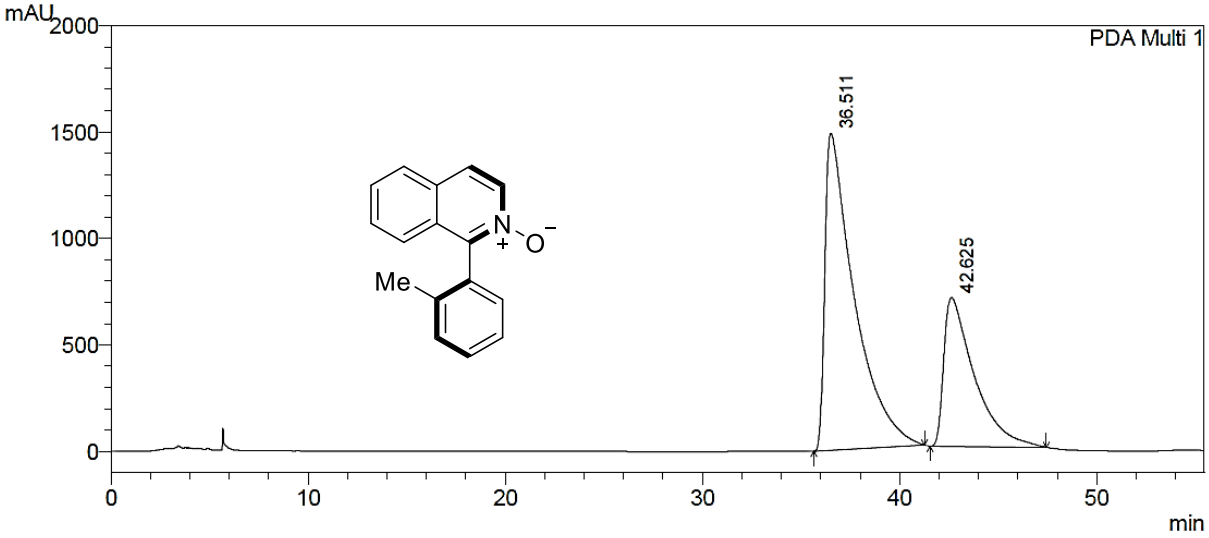
^{13}C{^{1}H} NMR *(*125 MHz*)*





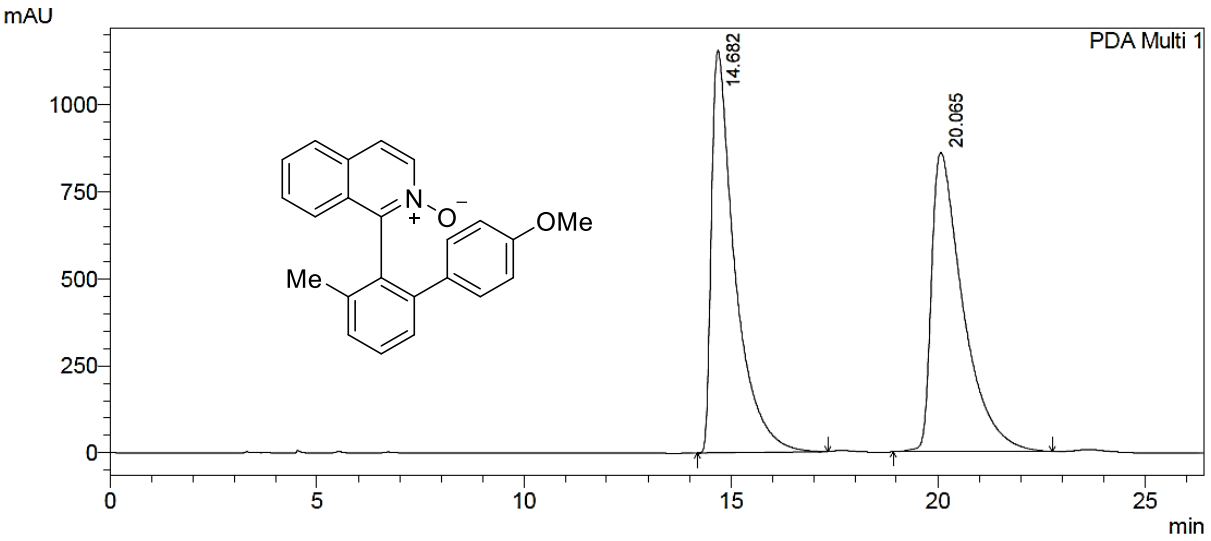
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.953	51618883	489456	49.792	52.650
2	44.799	52050682	440193	50.208	47.350
Total		103669565	929649	100.000	100.000



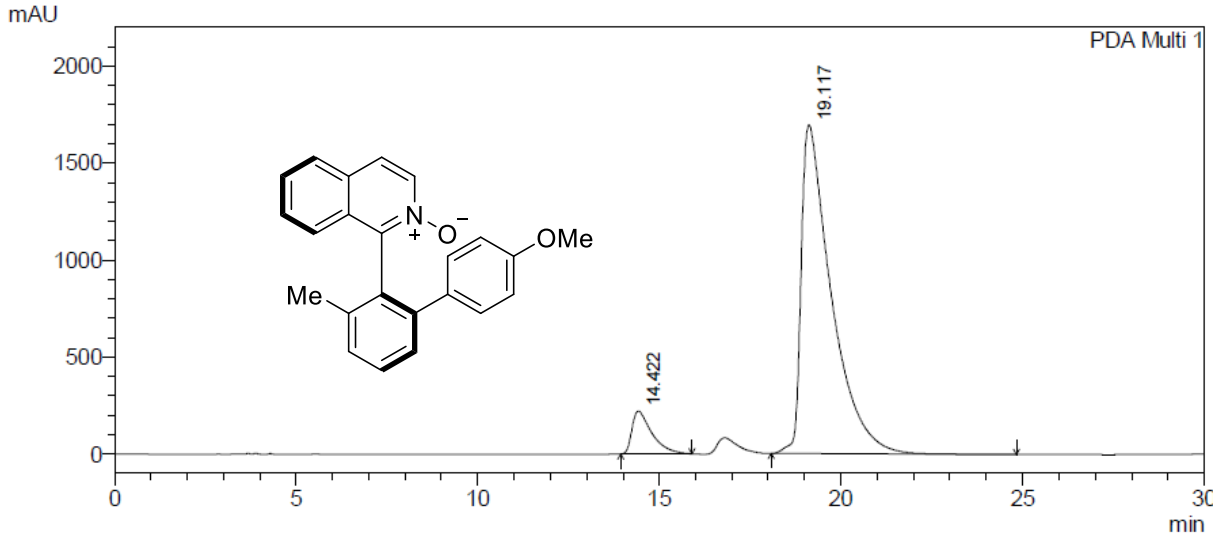
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	36.511	154336306	1489843	67.281	68.075
2	42.625	75055742	698677	32.719	31.925
Total		229392048	2188520	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.682	45501721	1155612	49.952	57.349
2	20.065	45589997	859427	50.048	42.651
Total		91091718	2015039	100.000	100.000

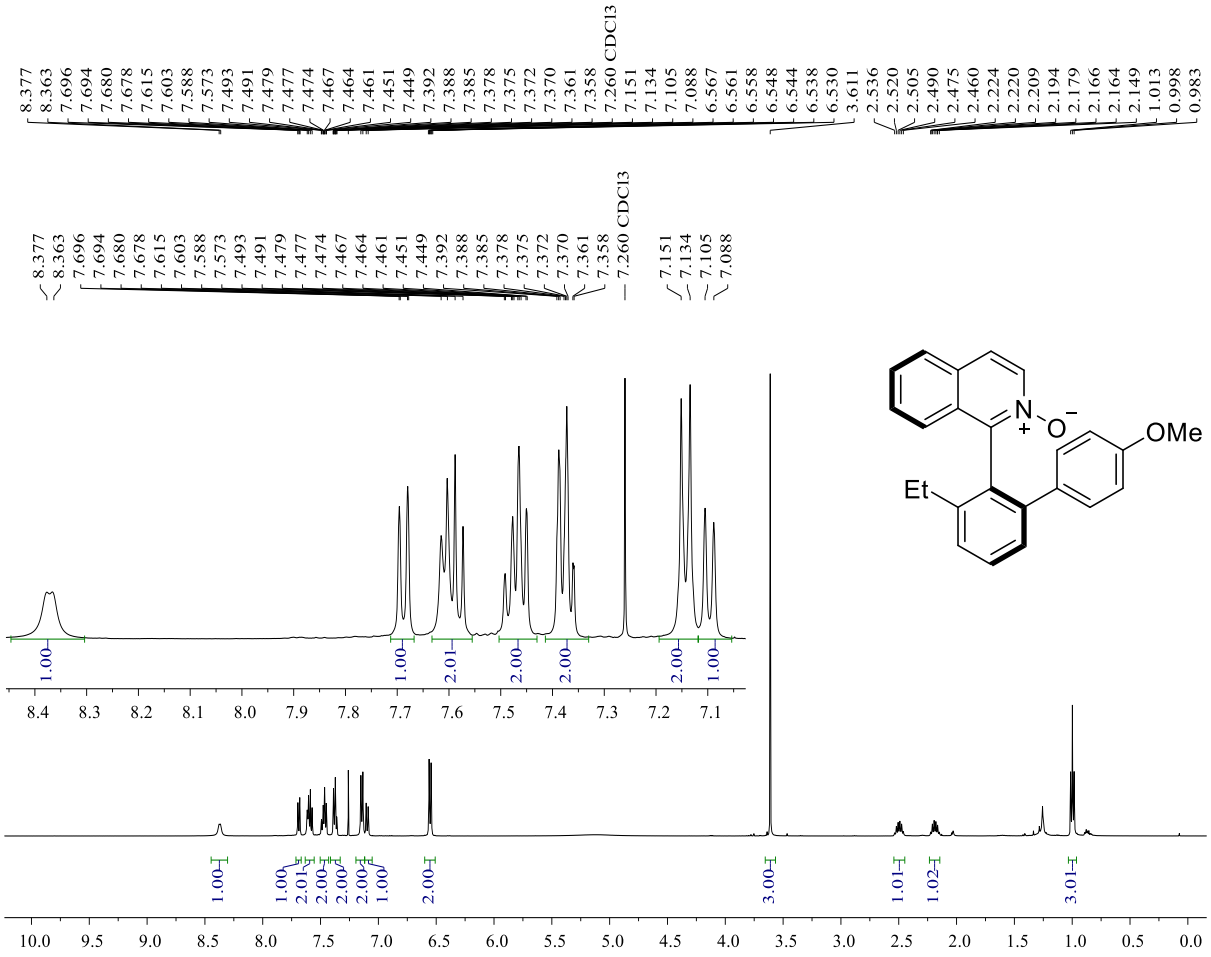


PDA Ch1 254nm 4nm

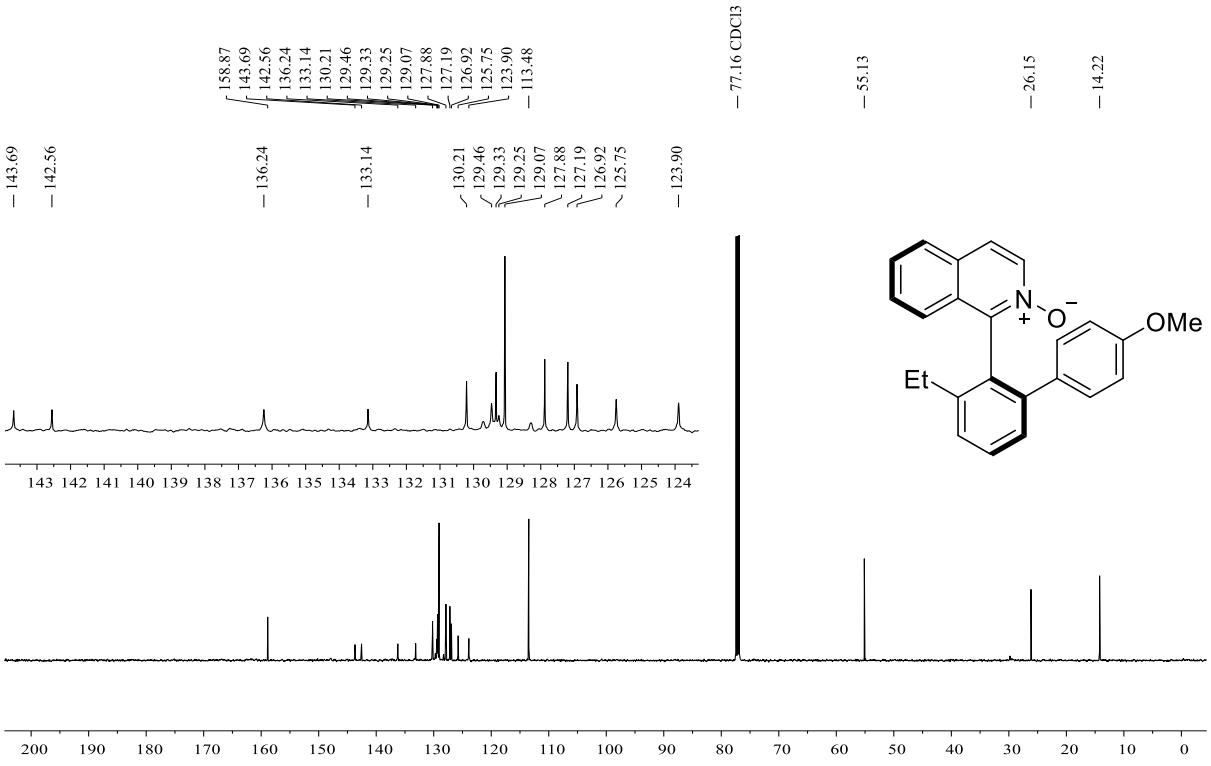
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.422	8376386	220529	7.879	11.523
2	19.117	97938068	1693334	92.121	88.477
Total		106314453	1913863	100.000	100.000

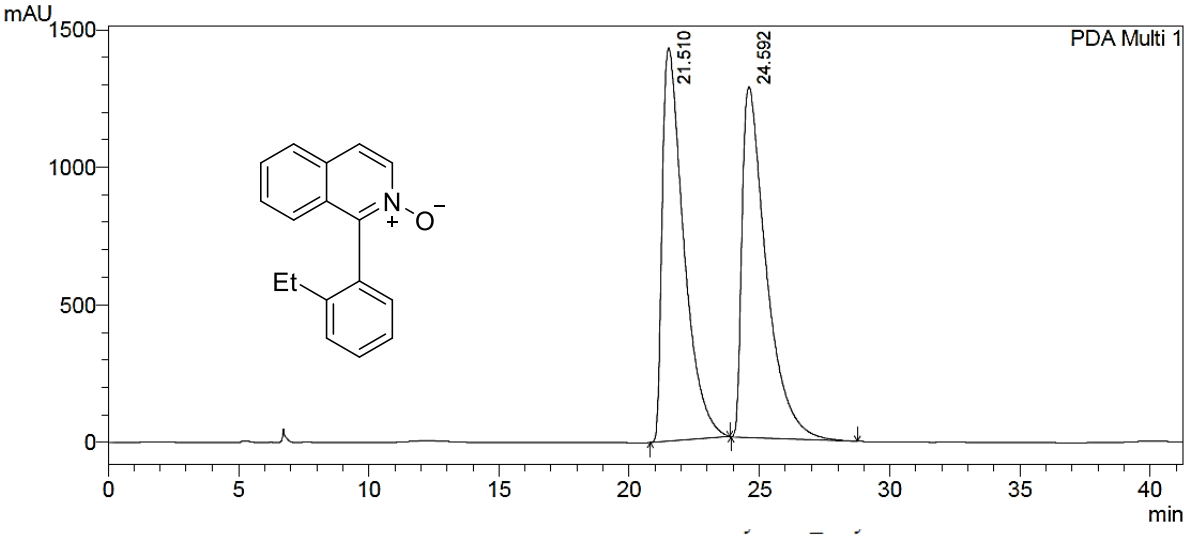
*(R)-1-(3-ethyl-4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (**3r**)*

^{1}H NMR *(*500 MHz*)*



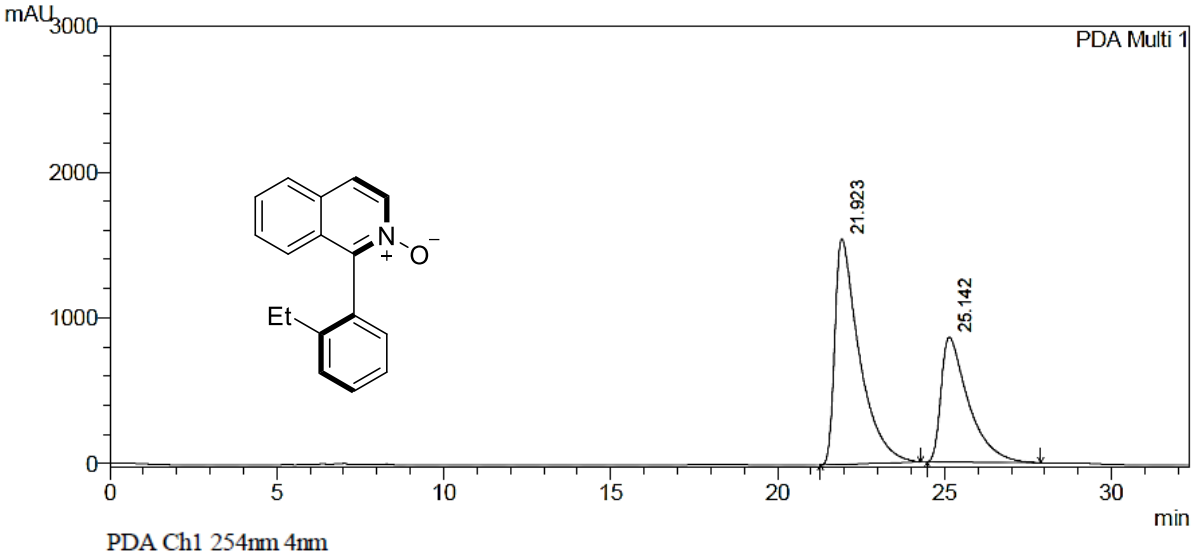
^{13}C{^{1}H} NMR *(*125 MHz*)*





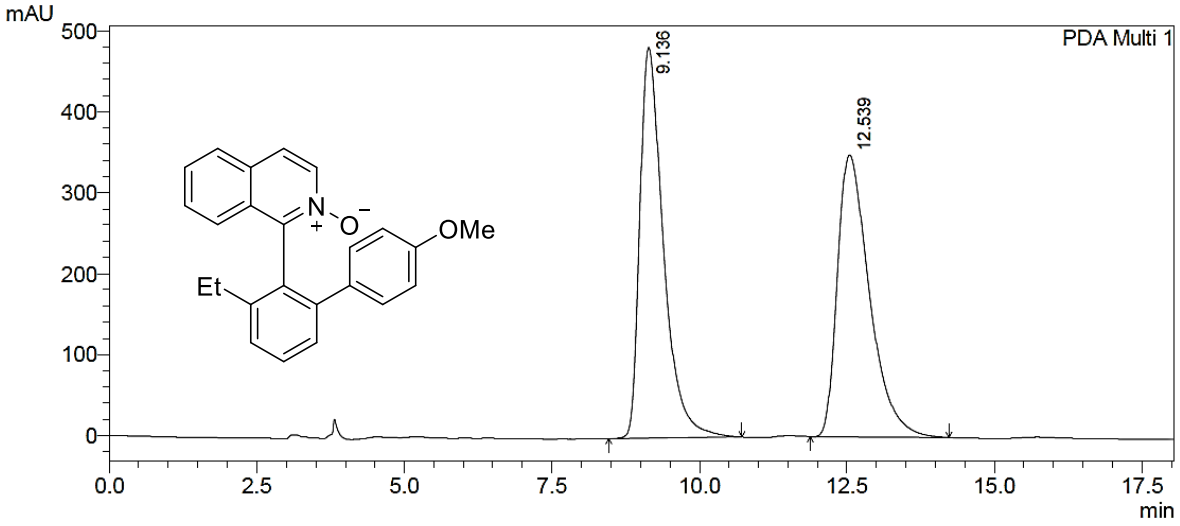
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.510	82199190	1428822	49.966	52.862
2	24.592	82310606	1274092	50.034	47.138
Total		164509796	2702915	100.000	100.000



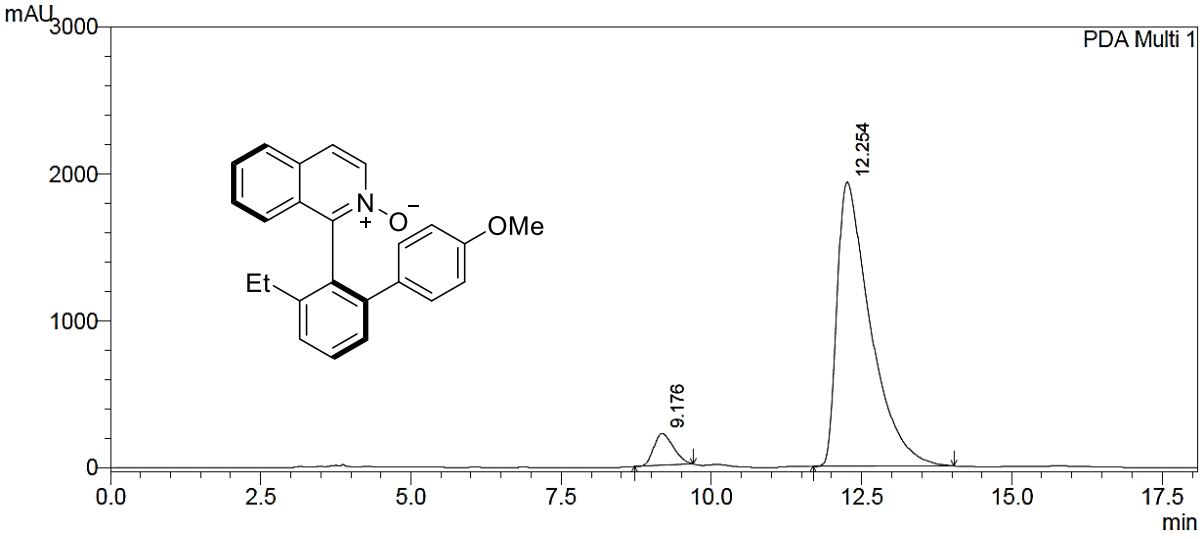
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	21.923	79076722	1547559	61.764	64.351
2	25.142	48954499	857323	38.236	35.649
Total		128031221	2404882	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.136	13420771	482639	50.478	58.083
2	12.539	13166460	348304	49.522	41.917
Total		26587231	830943	100.000	100.000

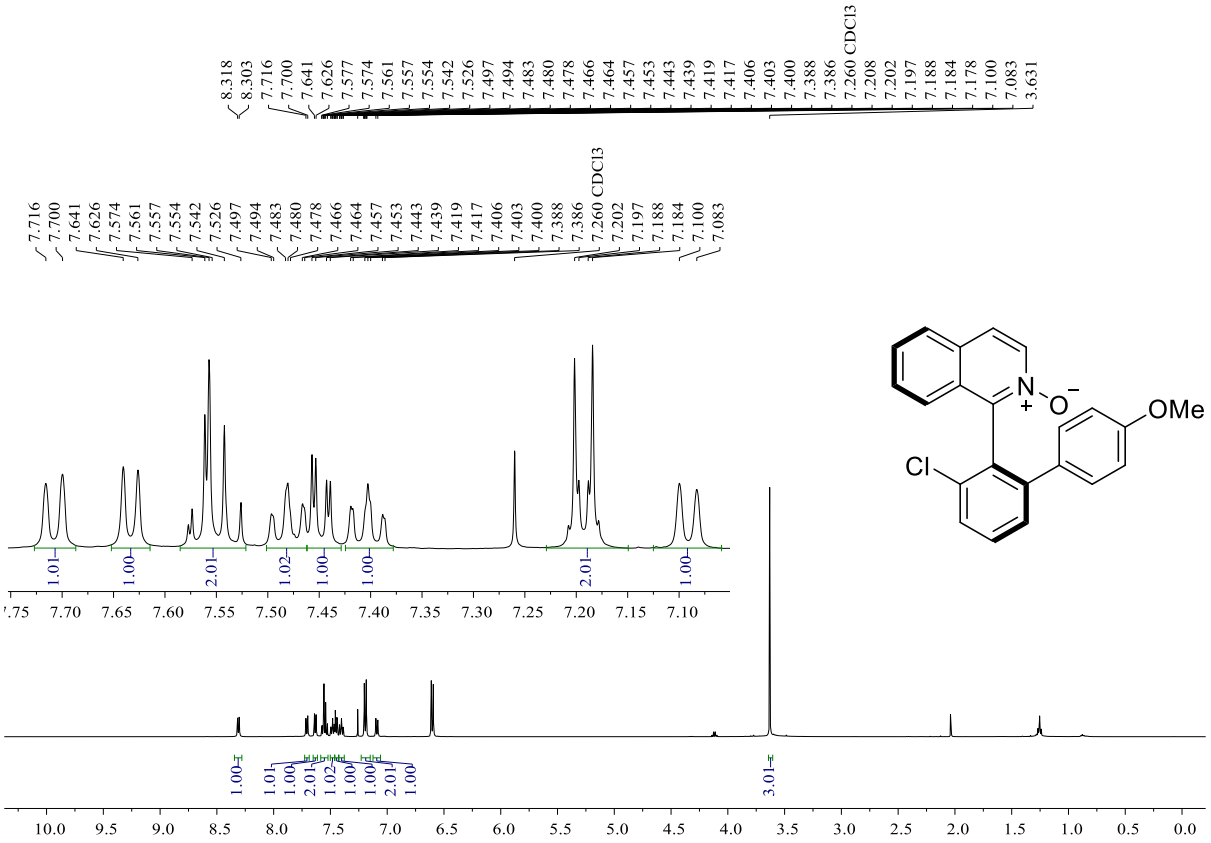


PDA Ch1 254nm 4nm

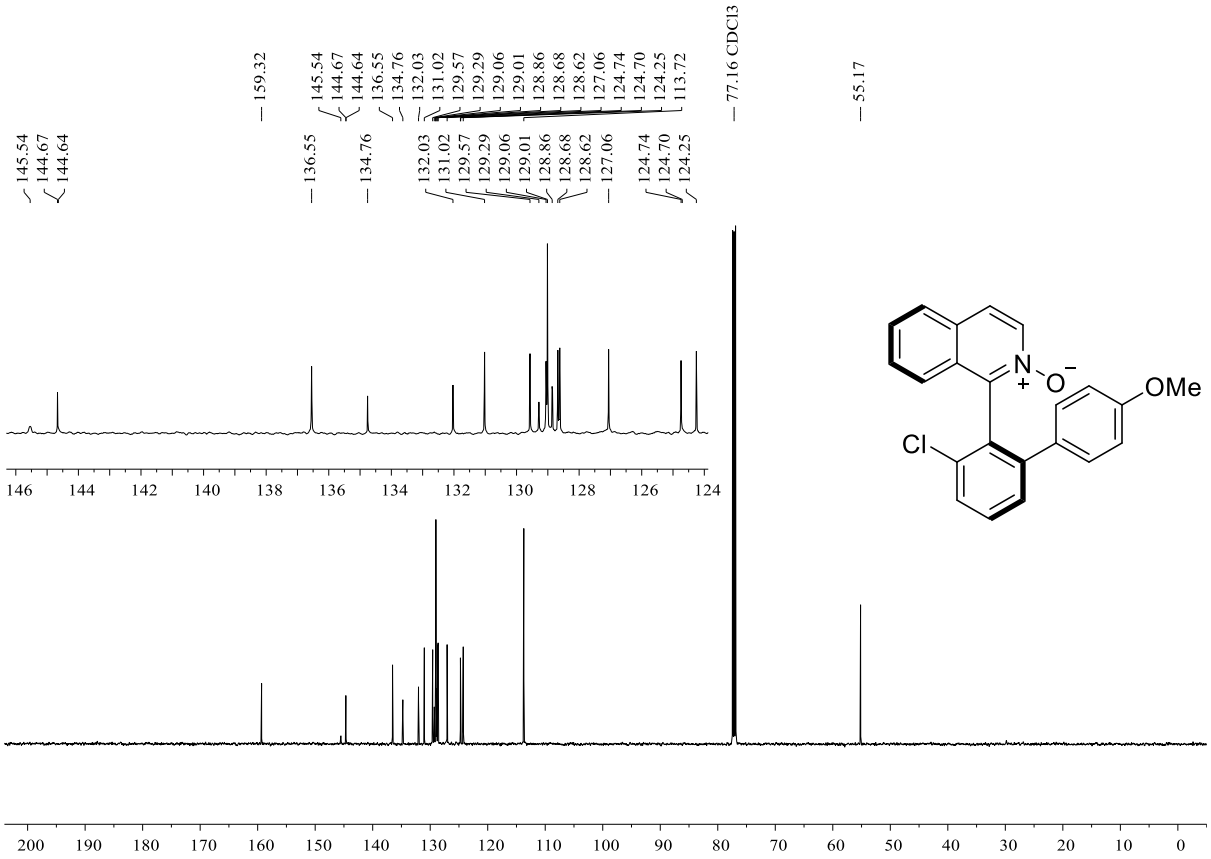
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.176	4959138	217178	6.227	10.104
2	12.254	74676918	1932266	93.773	89.896
Total		79636056	2149444	100.000	100.000

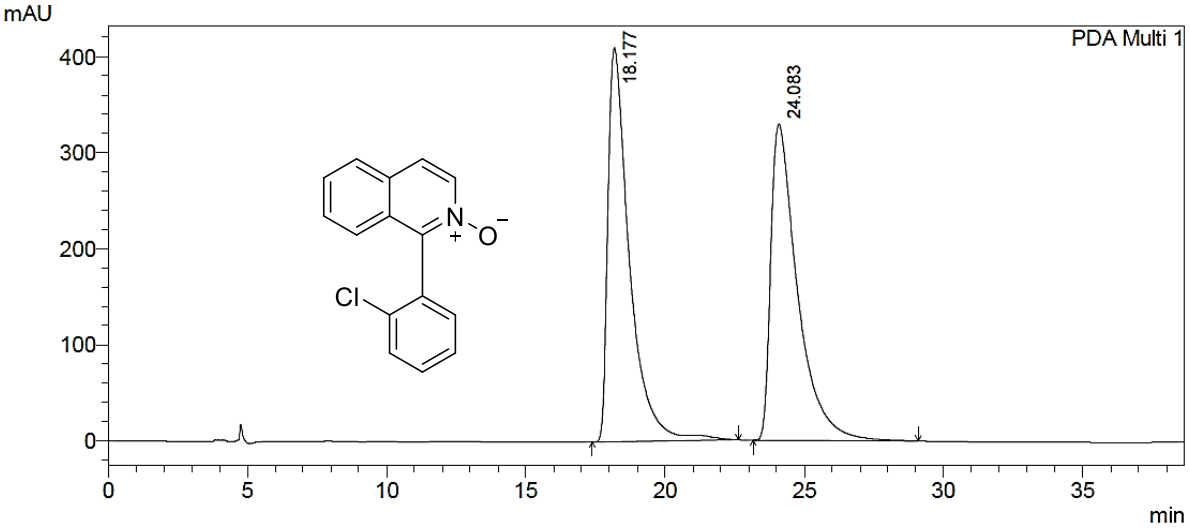
*(R)-1-(3-(benzyloxy)-4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (**3s**)*

^{1}H NMR *(*500 MHz*)*



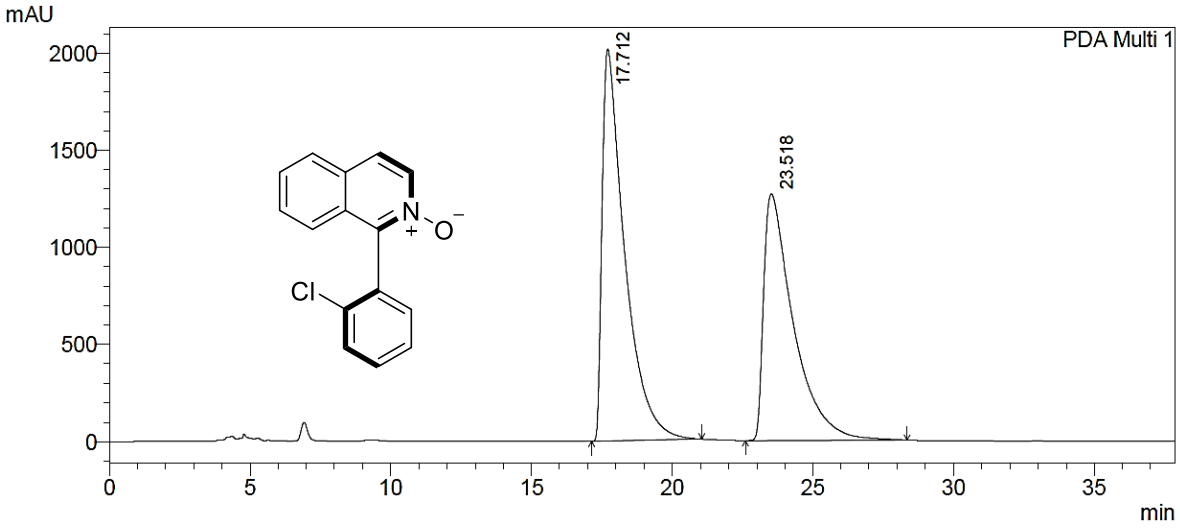
^{13}C{^{1}H} NMR *(*125 MHz*)*





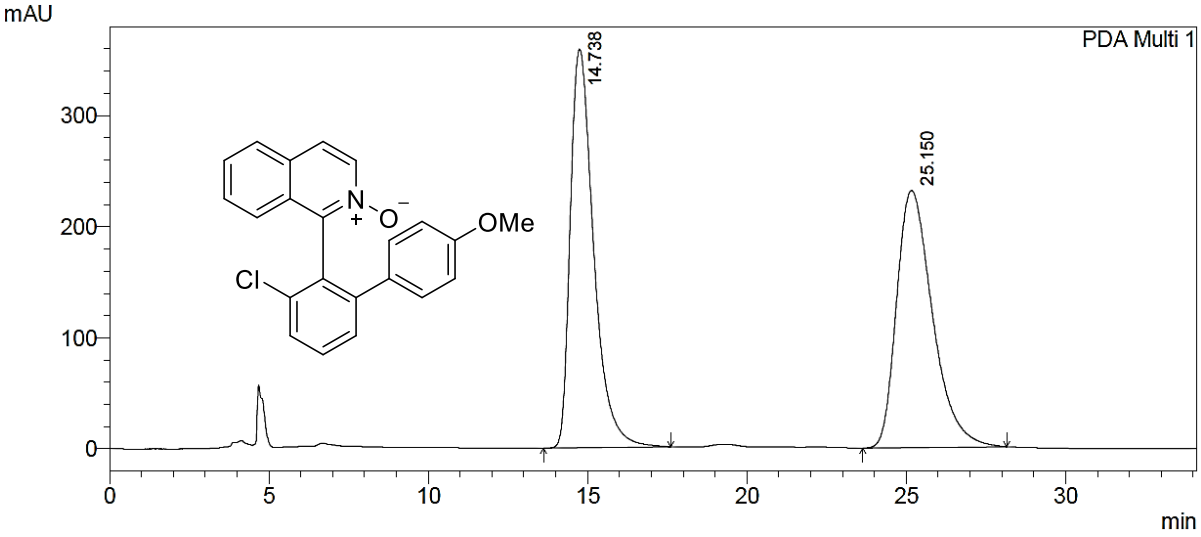
PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.177	22077925	410304	50.091	55.463
2	24.083	21997431	329476	49.909	44.537
Total		44075356	739780	100.000	100.000



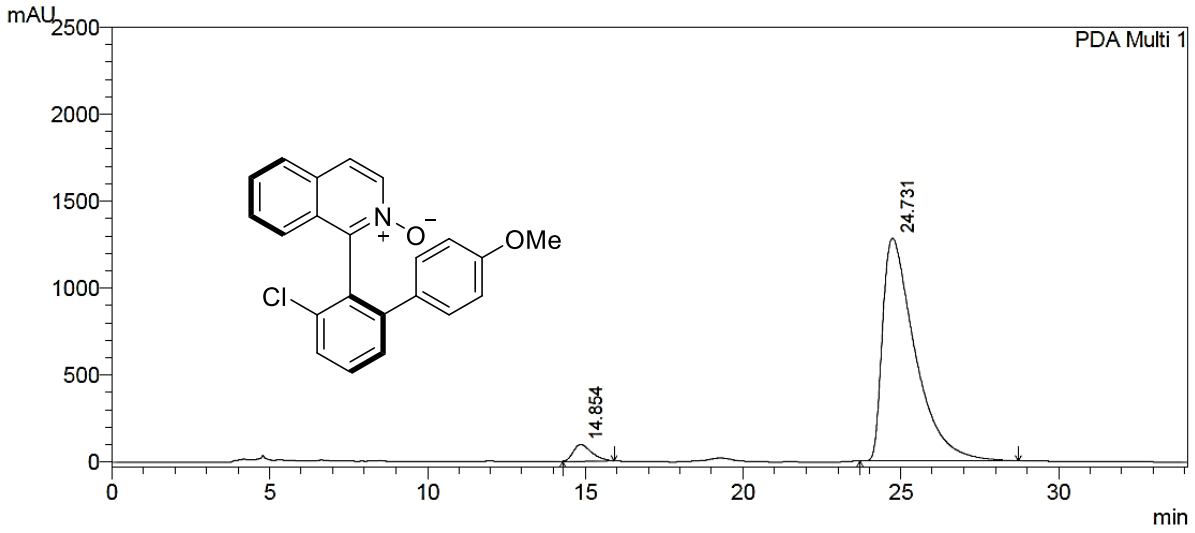
PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.712	112628101	2016241	54.793	61.360
2	23.518	92924575	1269668	45.207	38.640
Total		205552677	3285910	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.738	18272797	358546	50.214	60.791
2	25.150	18117146	231258	49.786	39.209
Total		36389943	589804	100.000	100.000

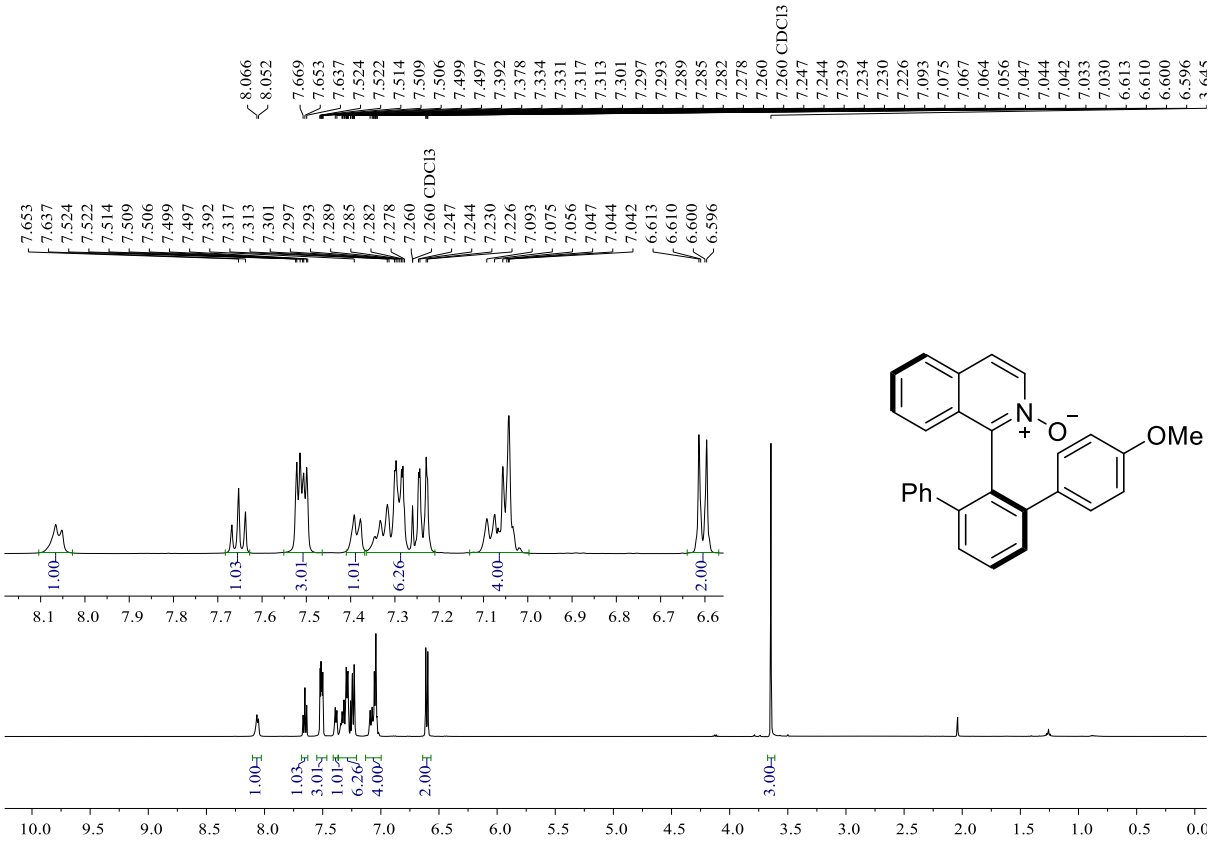


PDA Ch1 254nm 4nm

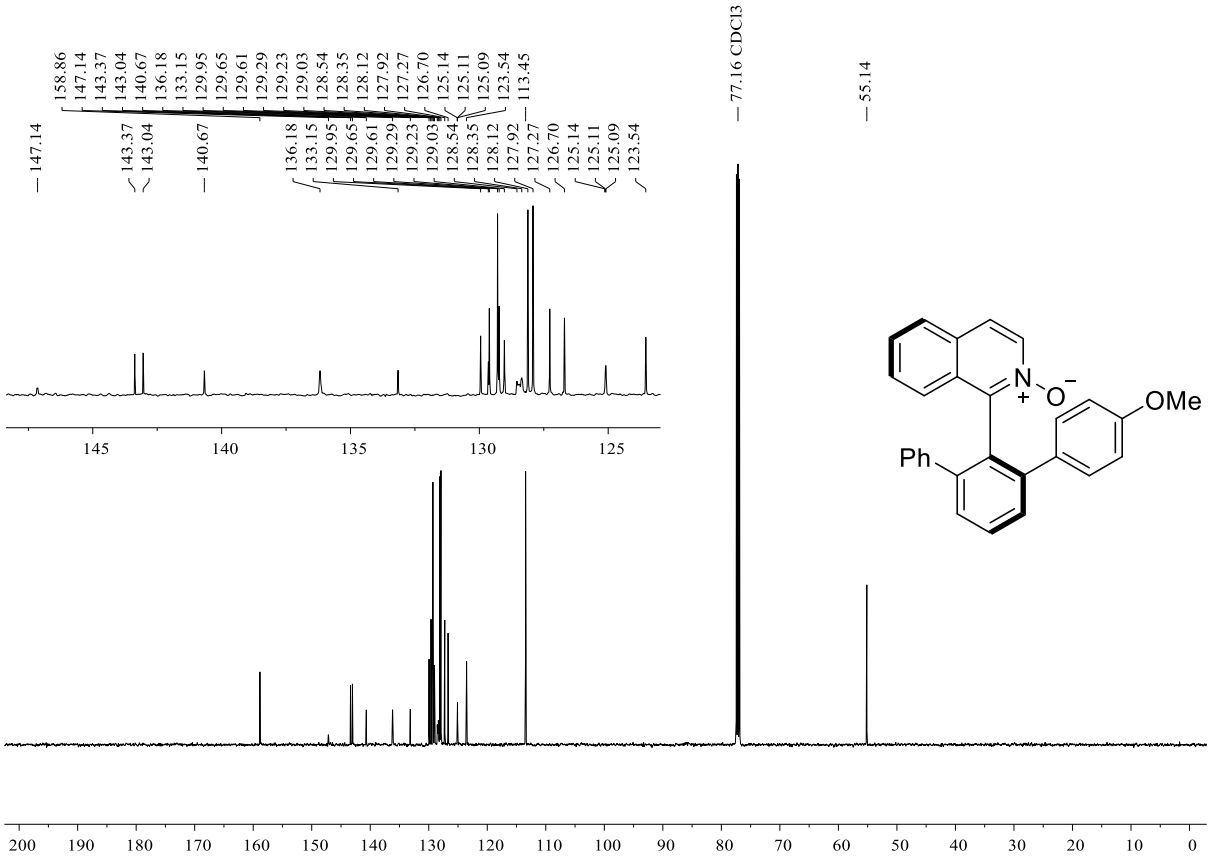
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.854	3874496	95994	4.054	6.979
2	24.731	91705894	1279479	95.946	93.021
Total		95580390	1375473	100.000	100.000

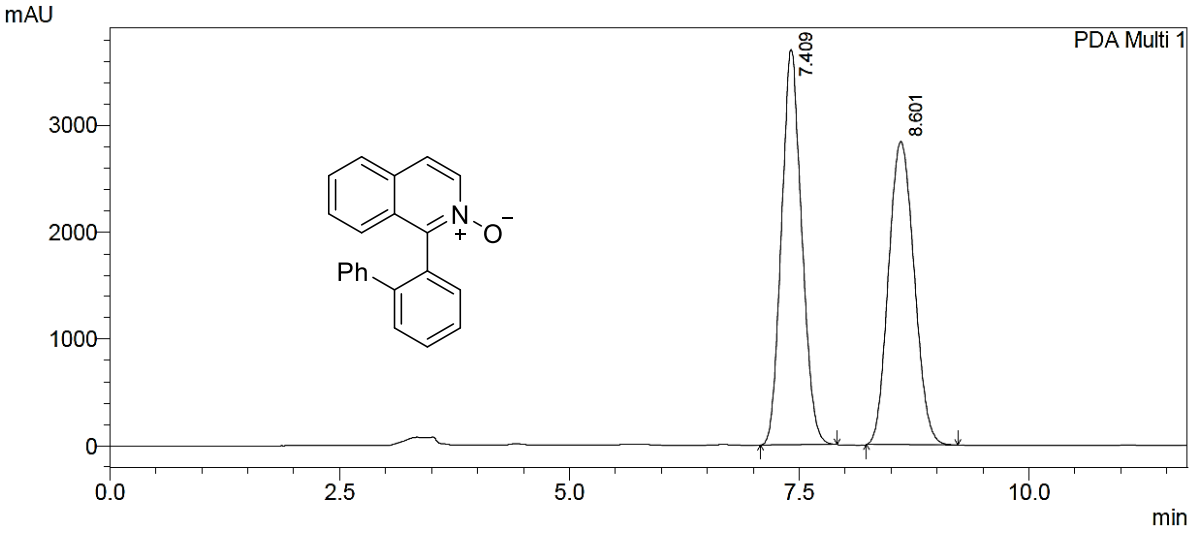
*(R)-1-(4-methoxy-[1,1':3',1''-terphenyl]-2'-yl)isoquinoline 2-oxide (**3t**)*

^{1}H NMR *(*500 MHz*)*



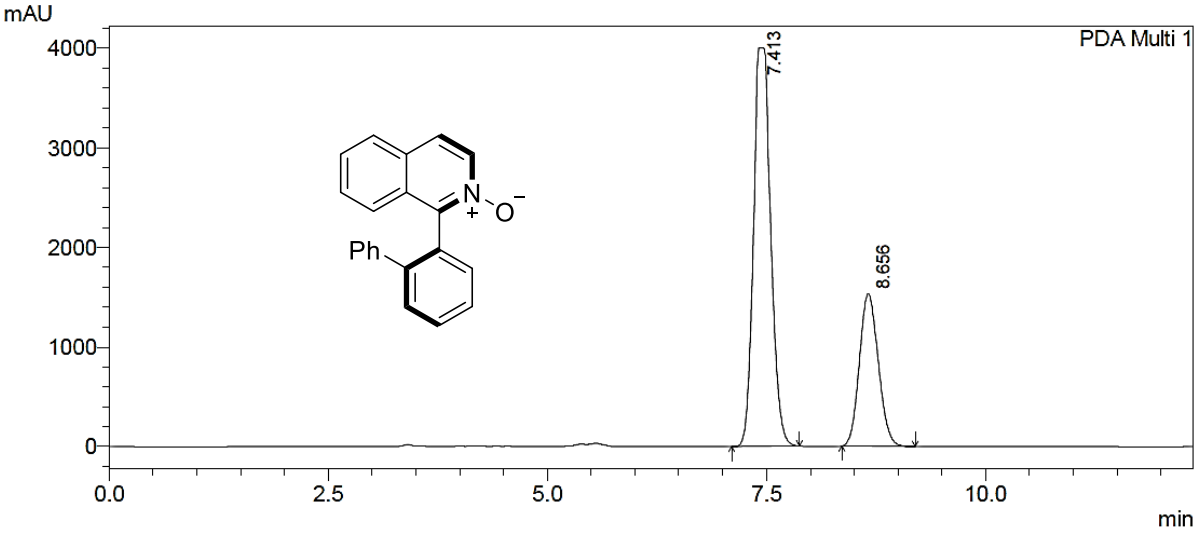
^{13}C{^{1}H} NMR *(*125 MHz*)*





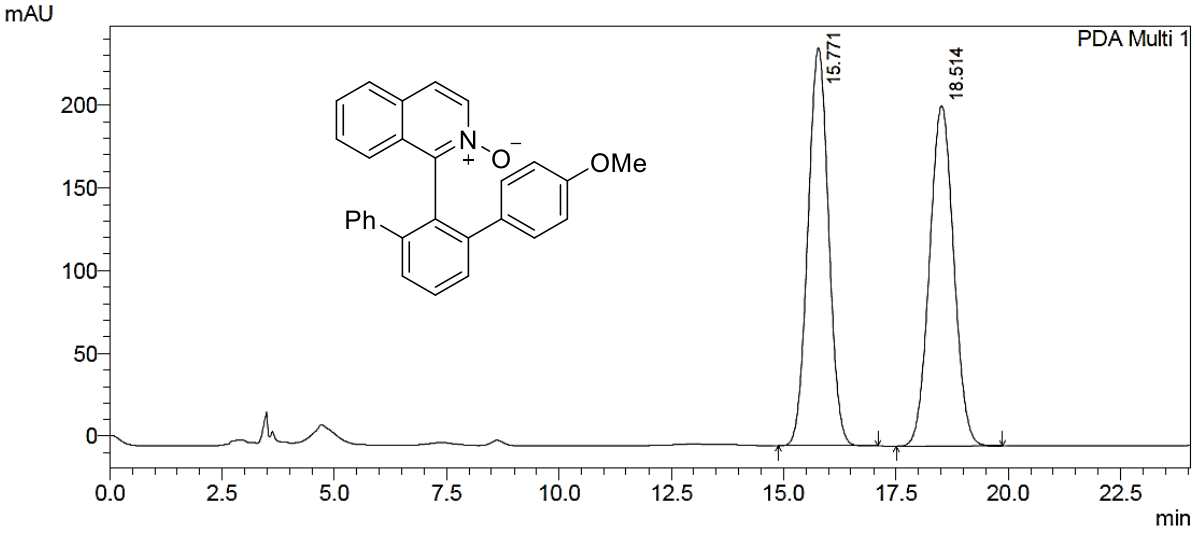
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.409	56721634	3702017	50.647	56.557
2	8.601	55272129	2843585	49.353	43.443
Total		111993763	6545602	100.000	100.000



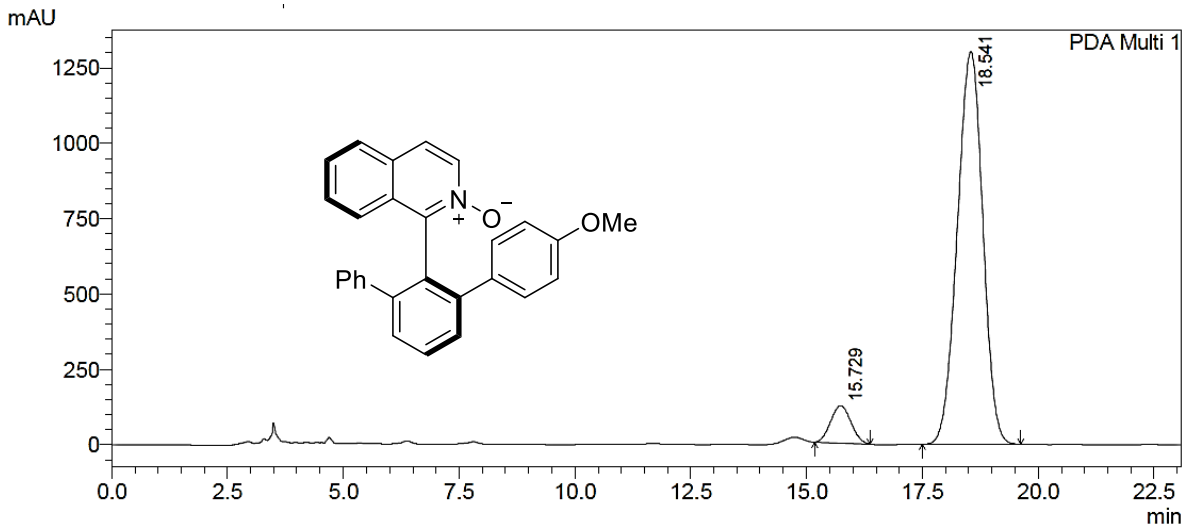
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.413	54709013	3997009	70.474	72.302
2	8.656	22920586	1531240	29.526	27.698
Total		77629599	5528249	100.000	100.000



PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.771	7686236	240414	49.969	53.893
2	18.514	7695635	205681	50.031	46.107
Total		15381872	446095	100.000	100.000

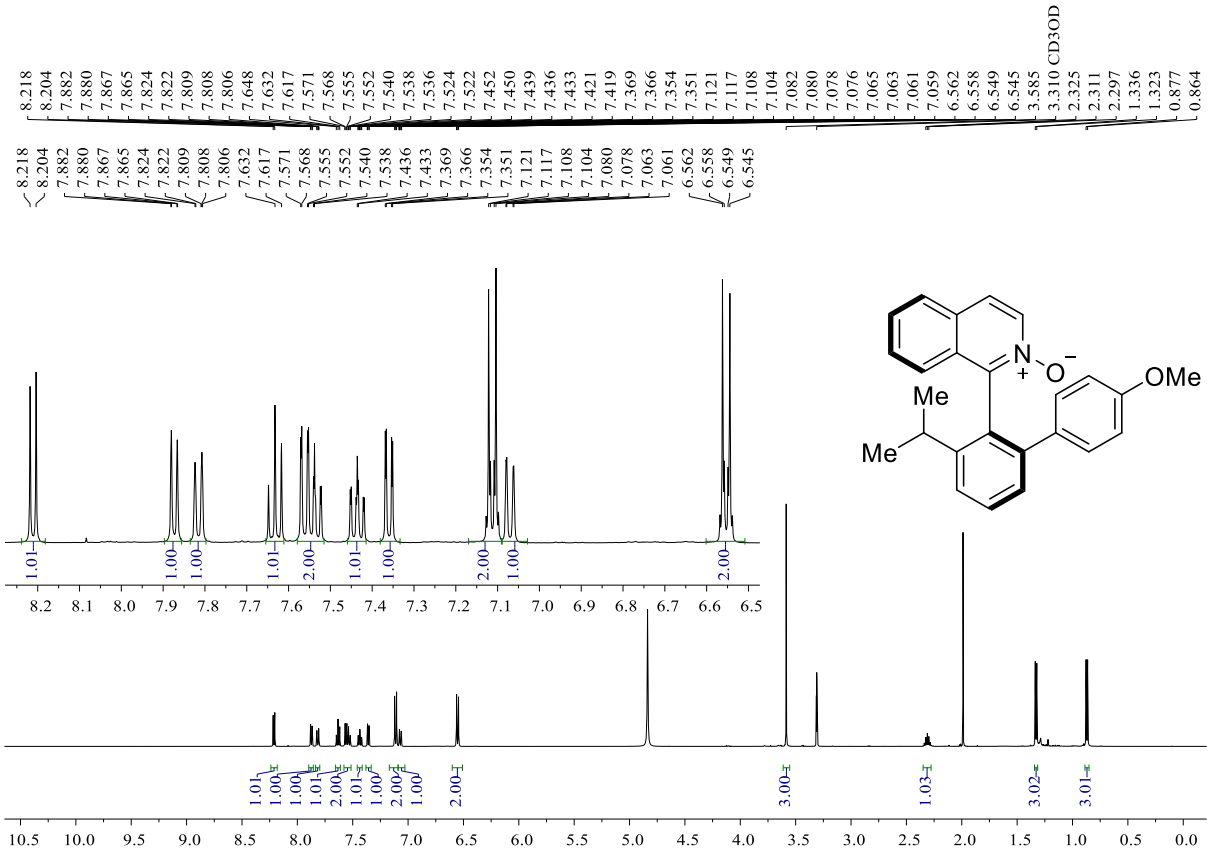


PDA Ch1 274nm 4nm

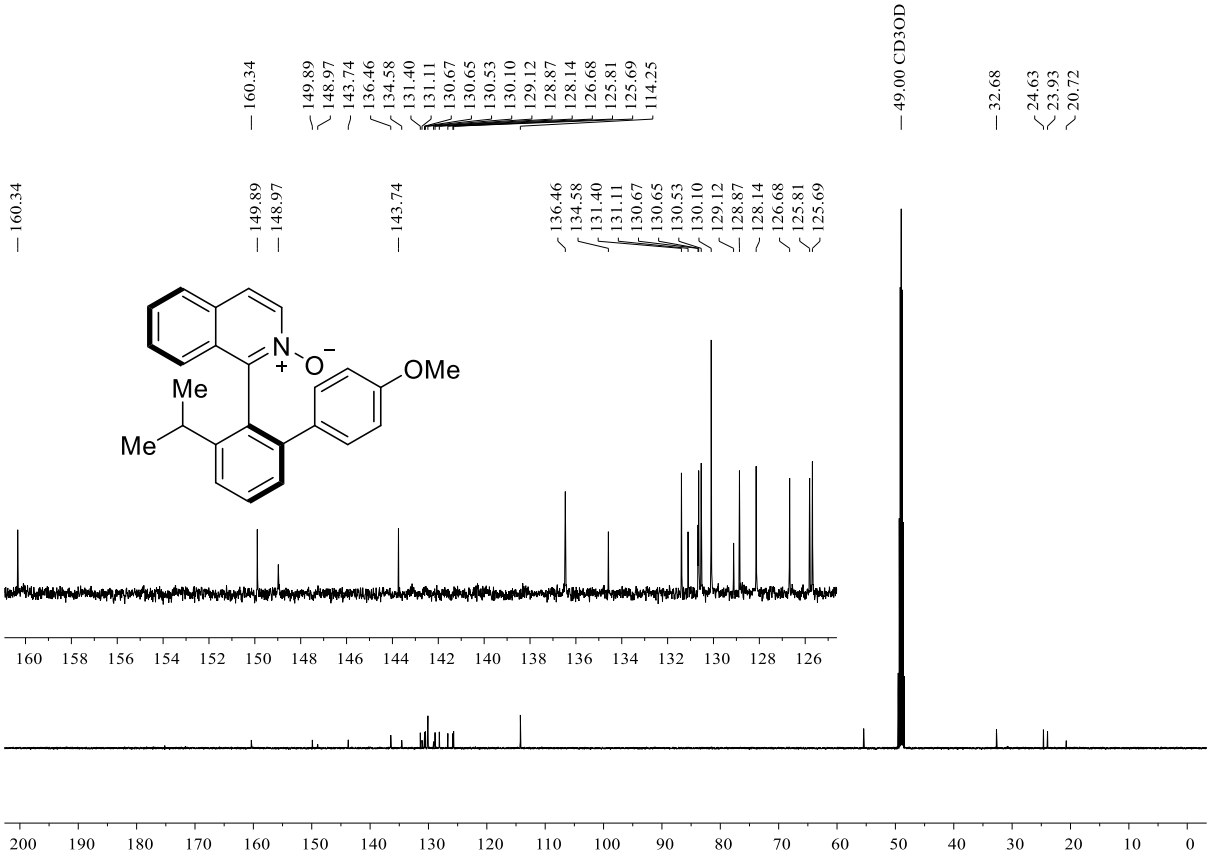
Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.729	3779905	123795	7.035	8.685
2	18.541	49953055	1301567	92.965	91.315
Total		53732960	1425362	100.000	100.000

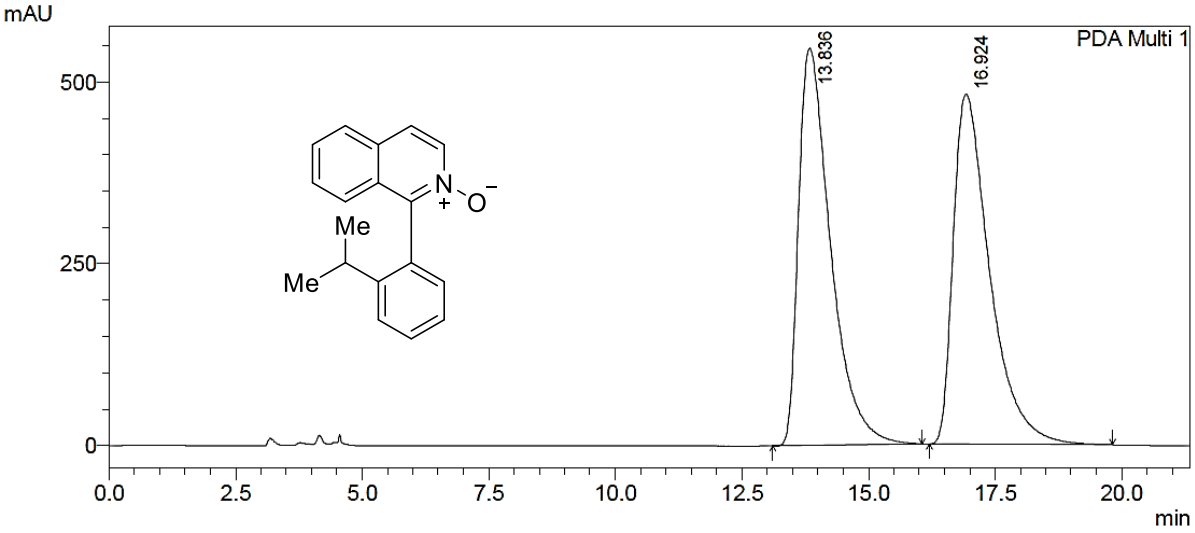
*(R)-1-(3-isopropyl-4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (**3u**)*

^{1}H NMR *(*500 MHz*)*



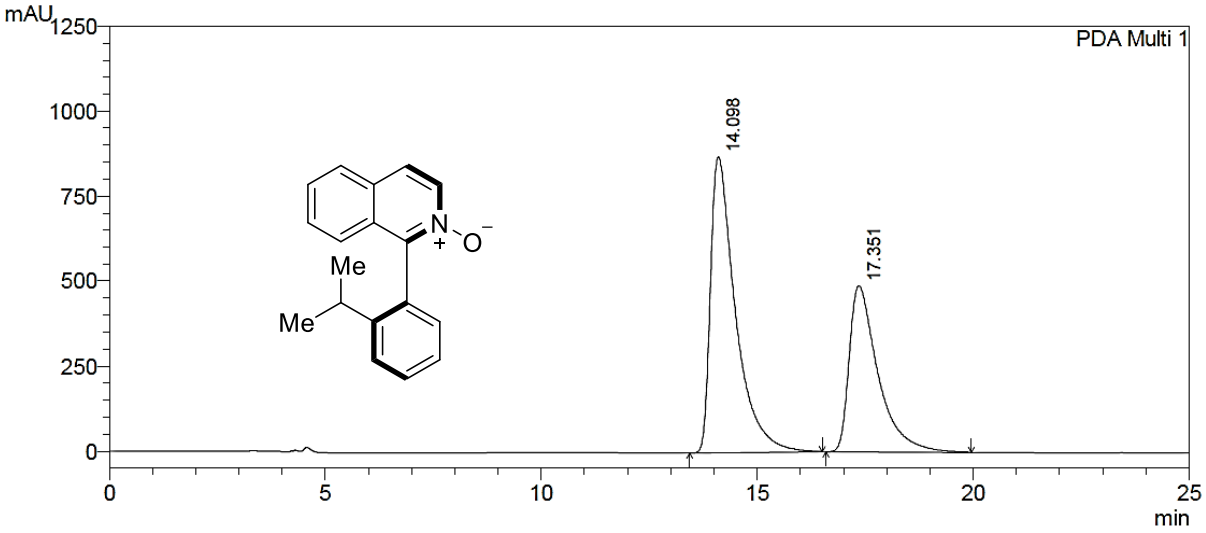
^{13}C{^{1}H} NMR *(*125 MHz*)*





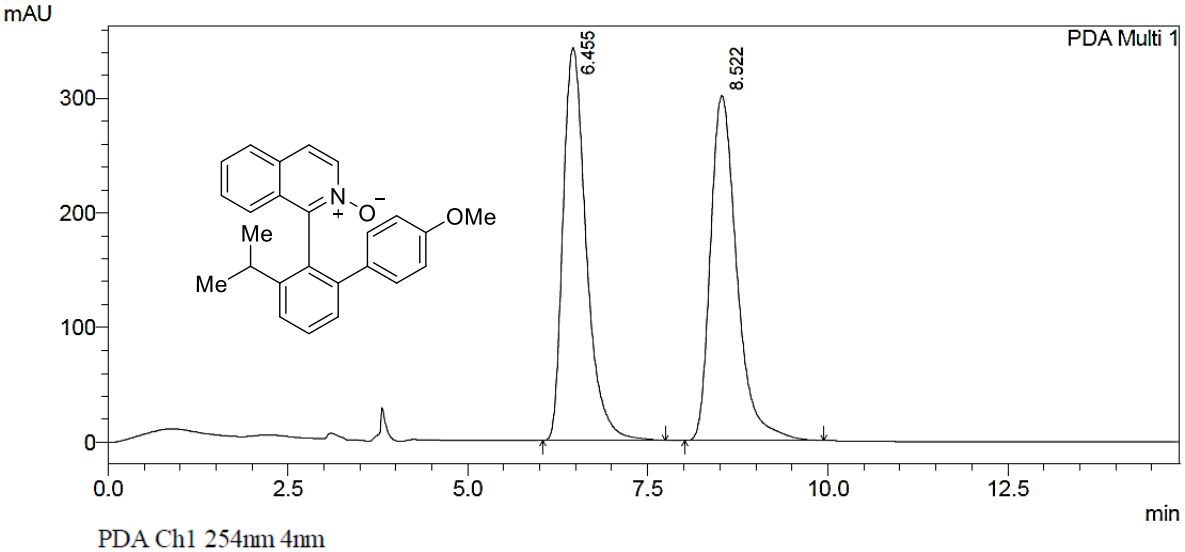
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.836	24115451	546843	49.995	53.148
2	16.924	24120279	482056	50.005	46.852
Total		48235729	1028899	100.000	100.000



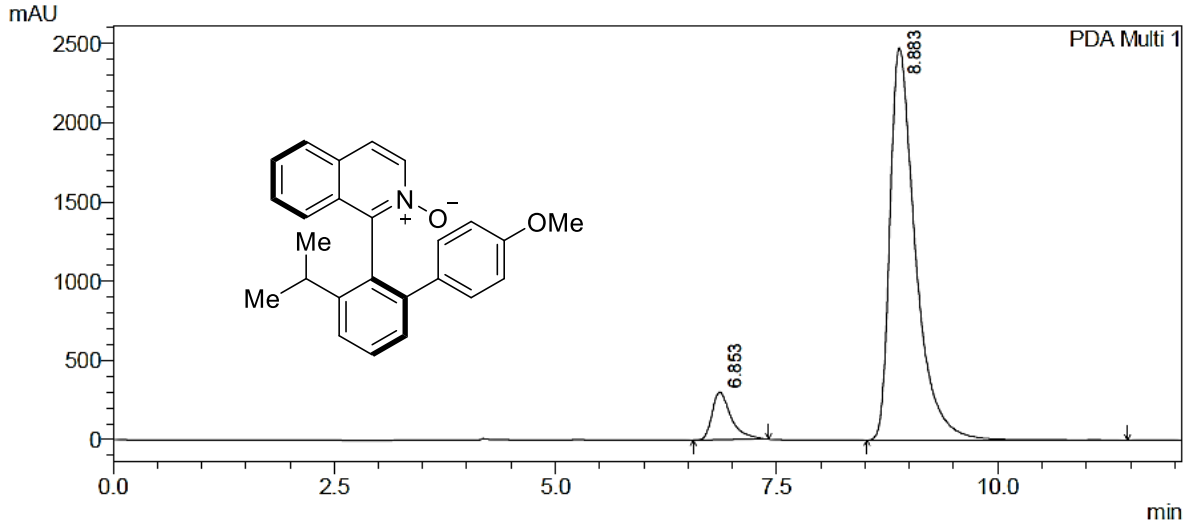
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.098	34973351	870988	60.726	64.070
2	17.351	22618439	488436	39.274	35.930
Total		57591791	1359424	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.455	7664254	342771	49.977	53.254
2	8.522	7671197	300884	50.023	46.746
Total		15335451	643654	100.000	100.000

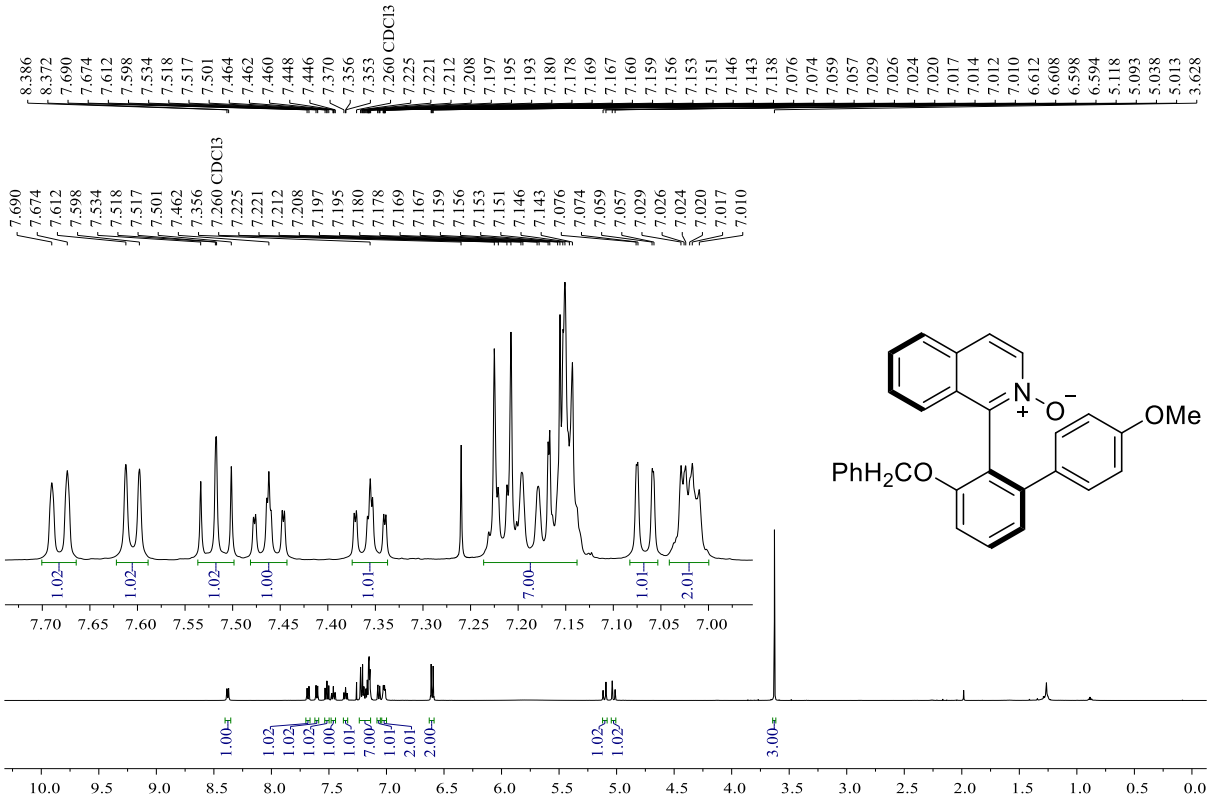


PDA Ch1 254nm 4nm

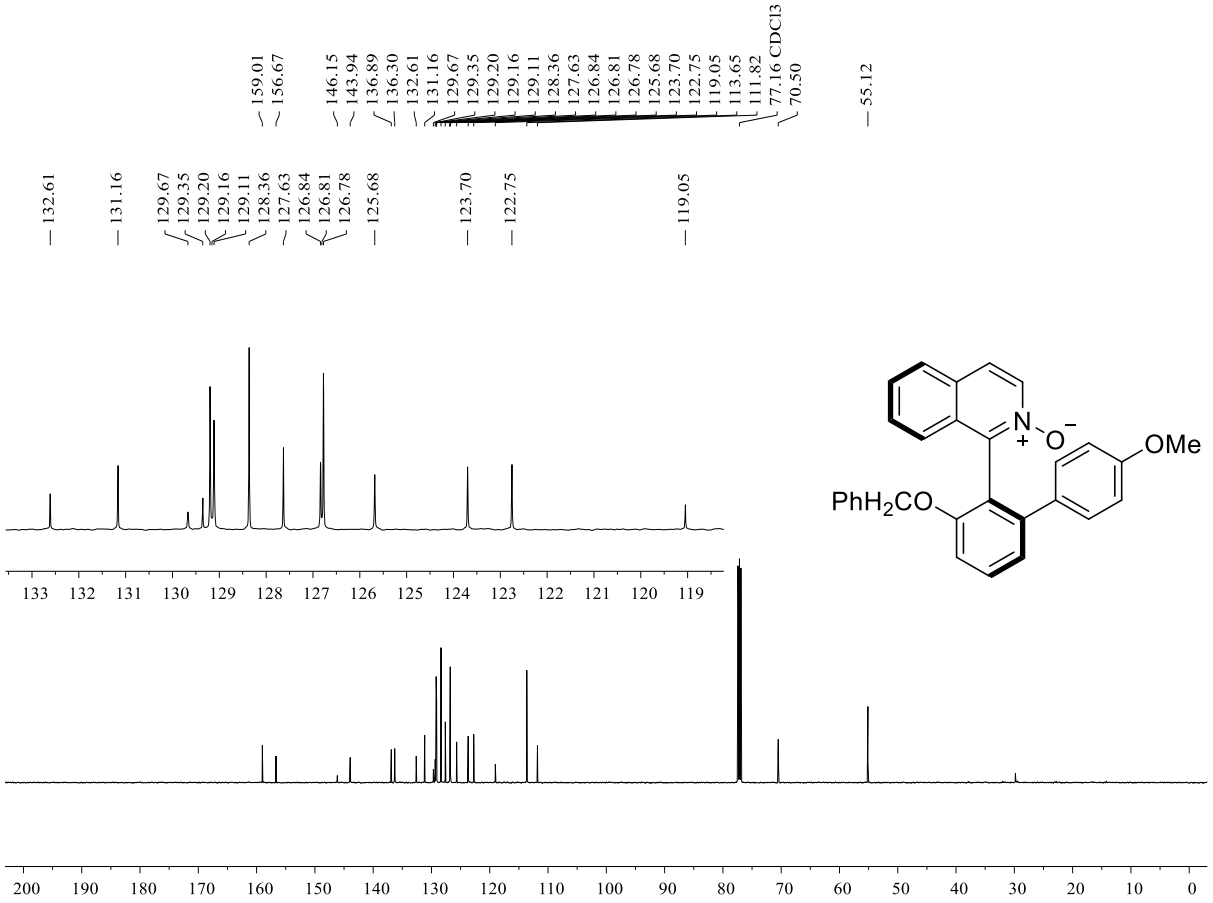
Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.853	4515510	301682	8.315	10.865
2	8.883	49786975	2474944	91.685	89.135
Total		54302485	2776626	100.000	100.000

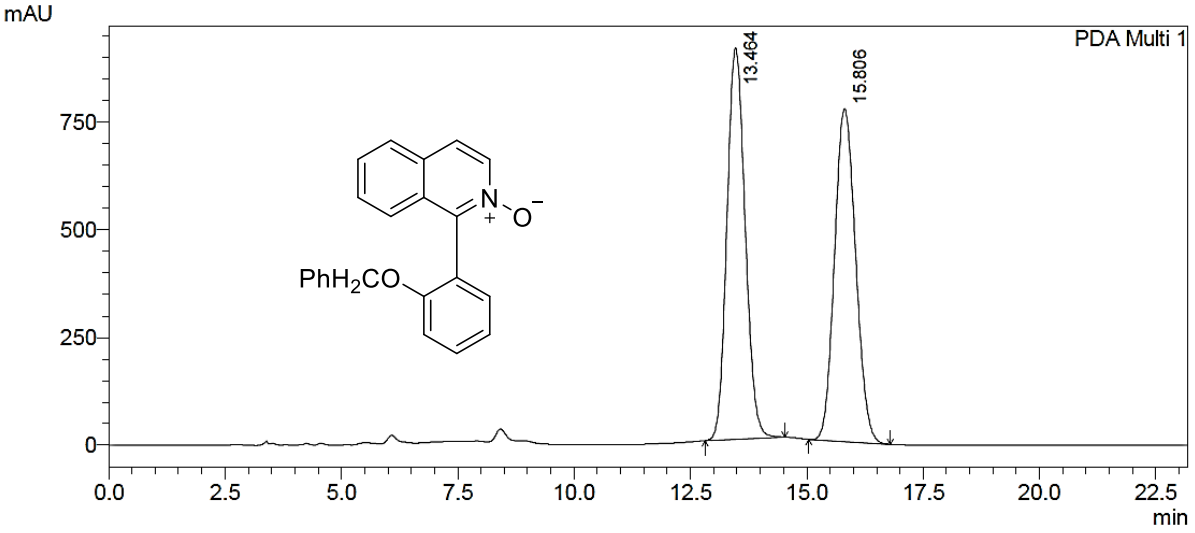
*(R)-1-(3-(benzyloxy)-4'-methoxy-[1,1'-biphenyl]-2-yl)isoquinoline 2-oxide (**3v**)*

^{1}H NMR *(*500 MHz*)*



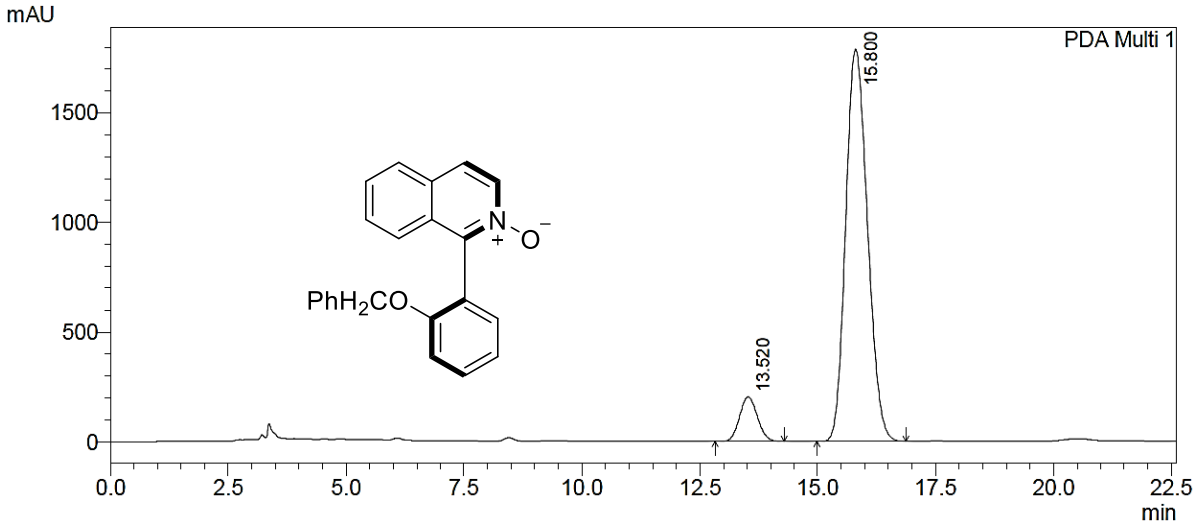
^{13}C{^{1}H} NMR *(*125 MHz*)*





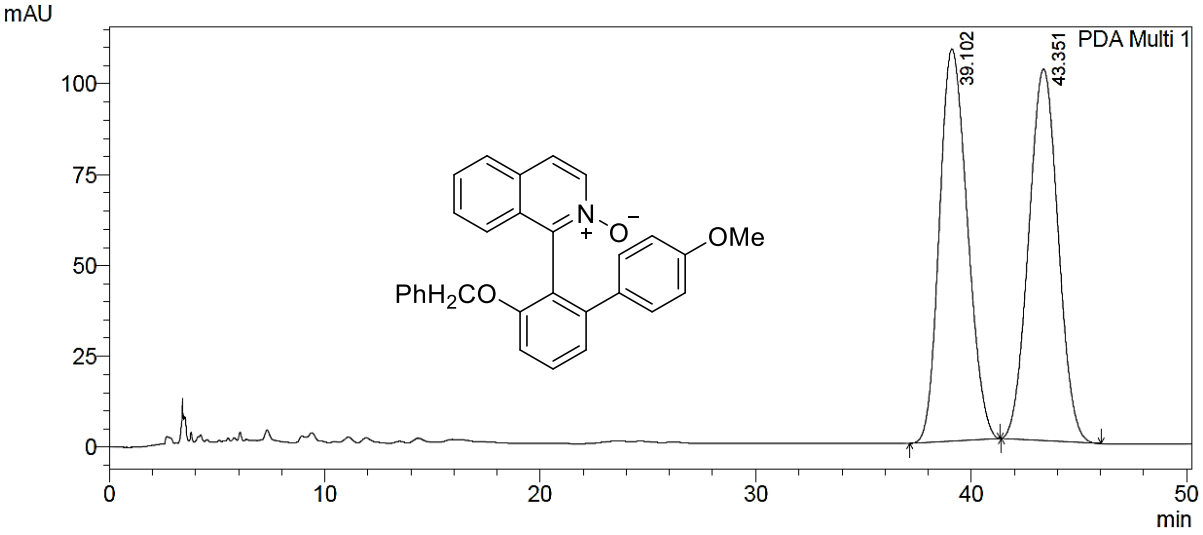
PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.464	24693300	906288	50.330	54.018
2	15.806	24369421	771460	49.670	45.982
Total		49062721	1677748	100.000	100.000



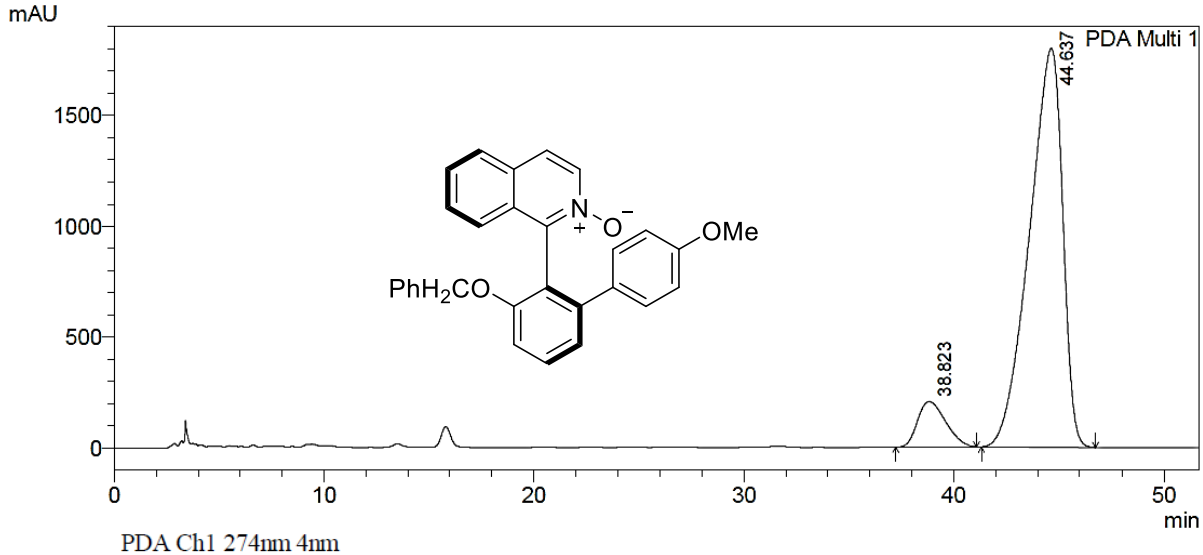
PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.520	5347311	203893	8.498	10.234
2	15.800	57574866	1788384	91.502	89.766
Total		62922177	1992278	100.000	100.000



PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	39.102	9730926	108024	50.020	51.341
2	43.351	9723120	102382	49.980	48.659
Total		19454045	210405	100.000	100.000



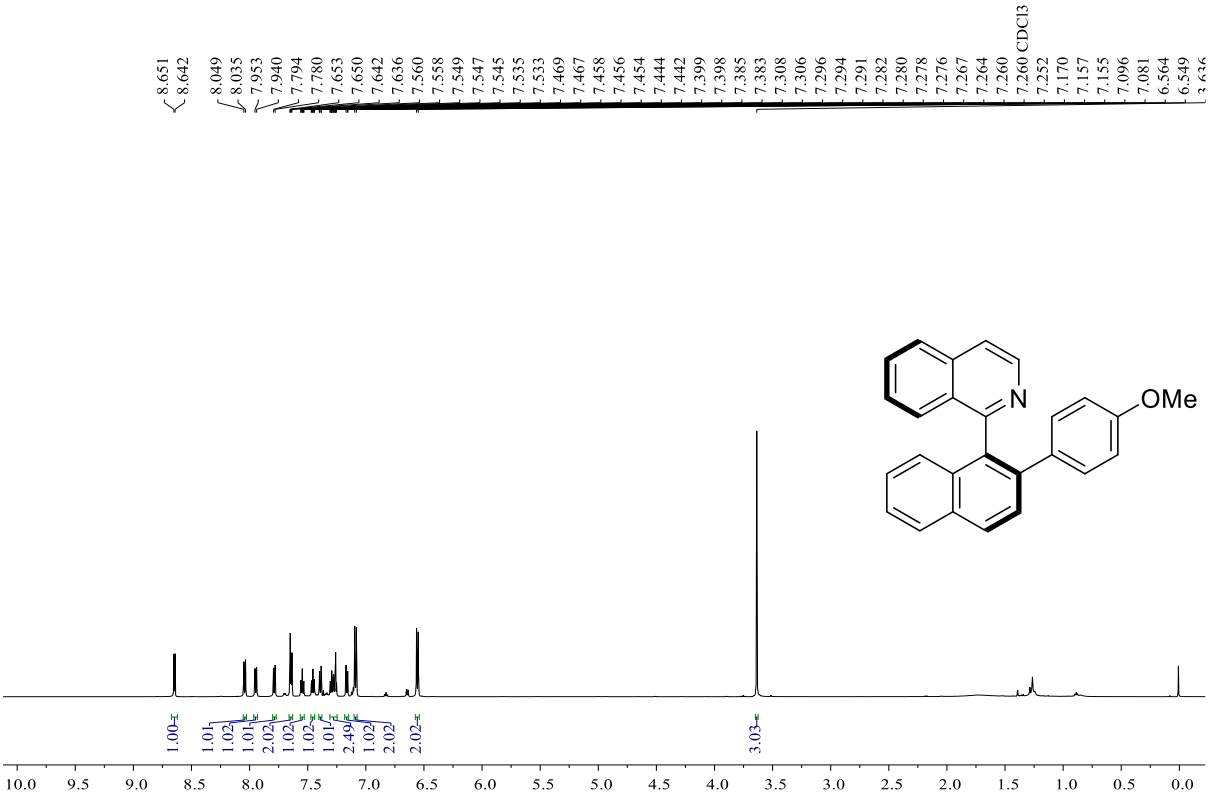
PDA Ch1 274nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	38.823	18989006	205081	8.759	10.235
2	44.637	197810737	1798692	91.241	89.765
Total		216799744	2003773	100.000	100.000

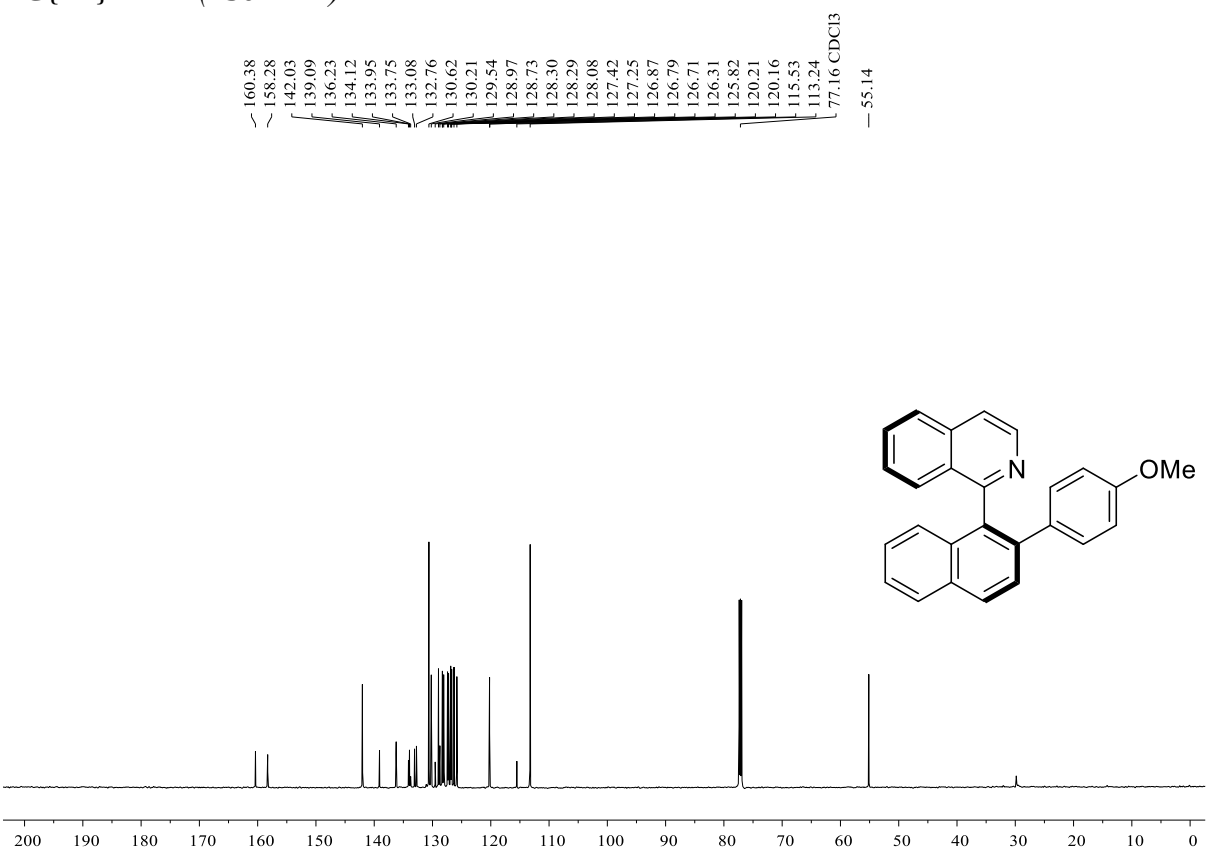
.

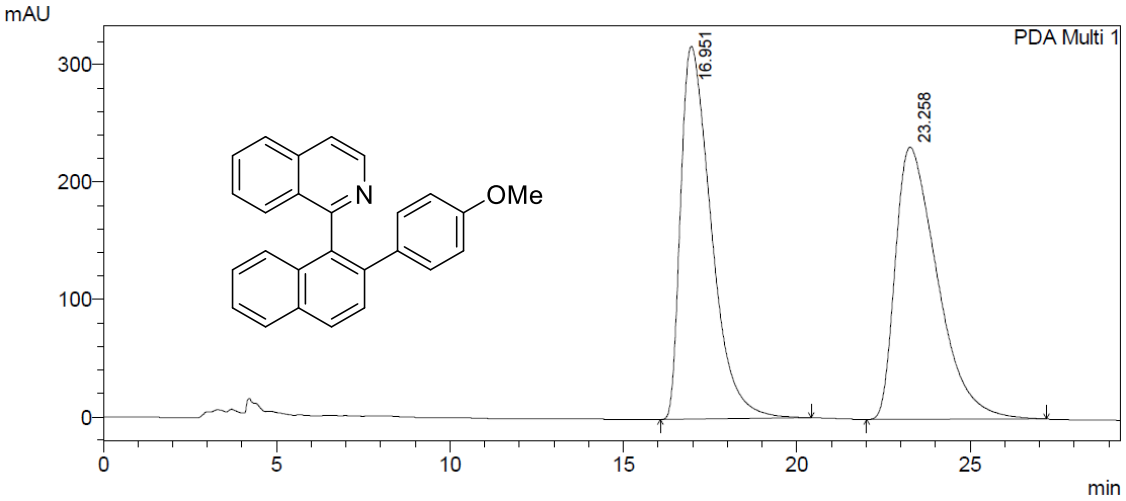
*(R)-1-(2-(4-methoxyphenyl)naphthalen-1-yl)isoquinoline (**4a**)*

^{1}H NMR *(*600 MHz*)*



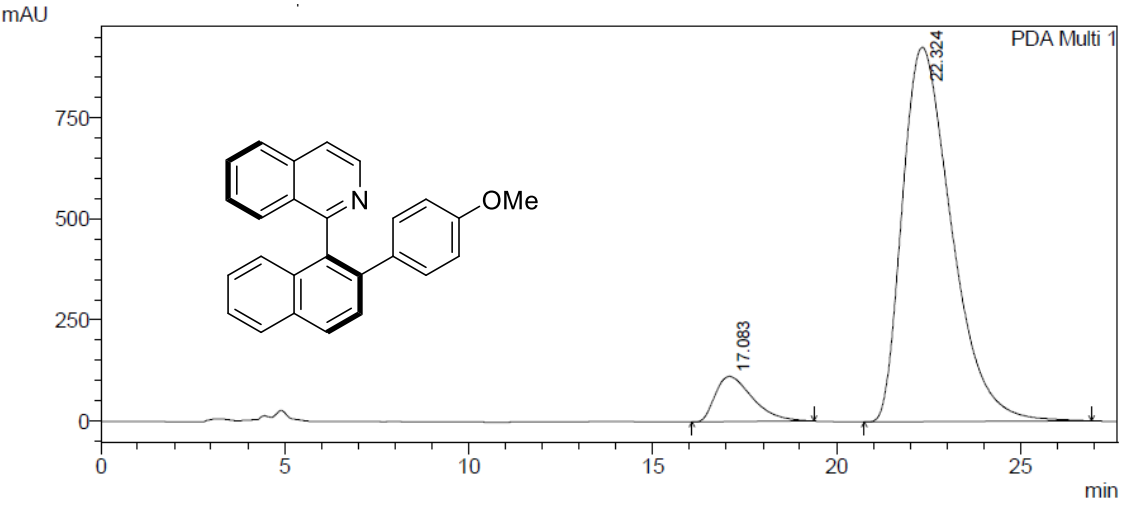
^{13}C{^{1}H} NMR *(*150 MHz*)*





PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	16.951	19489559	317755	49.981	57.812
2	23.258	19504382	231882	50.019	42.188
Total		38993941	549638	100.000	100.000



PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.083	7957897	112287	8.448	10.815
2	22.324	86242815	925936	91.552	89.185
Total		94200712	1038224	100.000	100.000

8. Computational Data

Computational Methods

The DFT calculations were performed using Gaussian 16.A03 program.[2] The geometry optimizations were performed with B3LYP[3] functional with Grimme's D3-dispersion correction including Becke-Johanson damping[4] (B3LYP-D3BJ) was used. The SDD[5] basis set with associated effective core potential (ECP) was used for Pd, whereas 6-31G** basis set[6] were used for all other atoms. The implicit solvation method SMD[7] was used with HFIP as solvent. Hessian calculations were performed to confirm stationary points. The minima have no imaginary frequency and single imaginary frequency for transition states. The energies of stationary points were computed using cc-PVTZ-PP basis set for Pd with ECP28MDF pseudopotentials[8] and 6-311+G** basis set for other atoms. The cc-PVTZPP basis set and ECP28MDF pseudopotentials were downloaded from the Stuttgart/Cologne group website.[9] The energies of stationary points were computed using 6-311+G** basis set. The quasi-harmonic entropy corrections proposed by Grimme[10] with a cutoff of 100 cm^{-1}, correction for standard state of 1 M for all species, and free energy corrections at 333.15 K were computed using GoodVibes v3.0.1 program.[11] Pymol program was used to generate molecular images.[12]

HFIP solvent is not implemented in Gaussian16 program, so we used "Solvent=Generic, Read" options in the SCRF keyword. Following parameters were used for the HFIP solvent,[13]

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

The rate of a reaction (enantiomerizartion, k_{Ent}), rate of racemization (k_{Rac}), and half-life for racemization ($t_{1/2}$) were calculated by using following formula.[14]

$$k_{\mathrm{Ent}} = \kappa \frac{k_{\mathrm{B}}\mathrm{T}}{h} exp \frac{-\Delta G^{\ddagger}}{RT} \quad \text{(Eyring Equation)}$$

$$k_{\mathrm{Rac}} = 2k_{\mathrm{Ent}}$$

$$t_{1/2} = \frac{ln2}{k_{\mathrm{Rac}}}$$

where transmission constant, $\kappa = 1$, Boltzmann constant, $k_B = 1.3806488 \times 10^{-23}$ $J.K^{-1}$, Planck constant, h = $6.62606957 \times 10^{-34}$ J.s, ideal gas constant, R = 8.314462145, temperature, T = 333.15 K, and barrier for enantiomerization ($\Delta G^{\ddagger}$) is calculated using DFT.

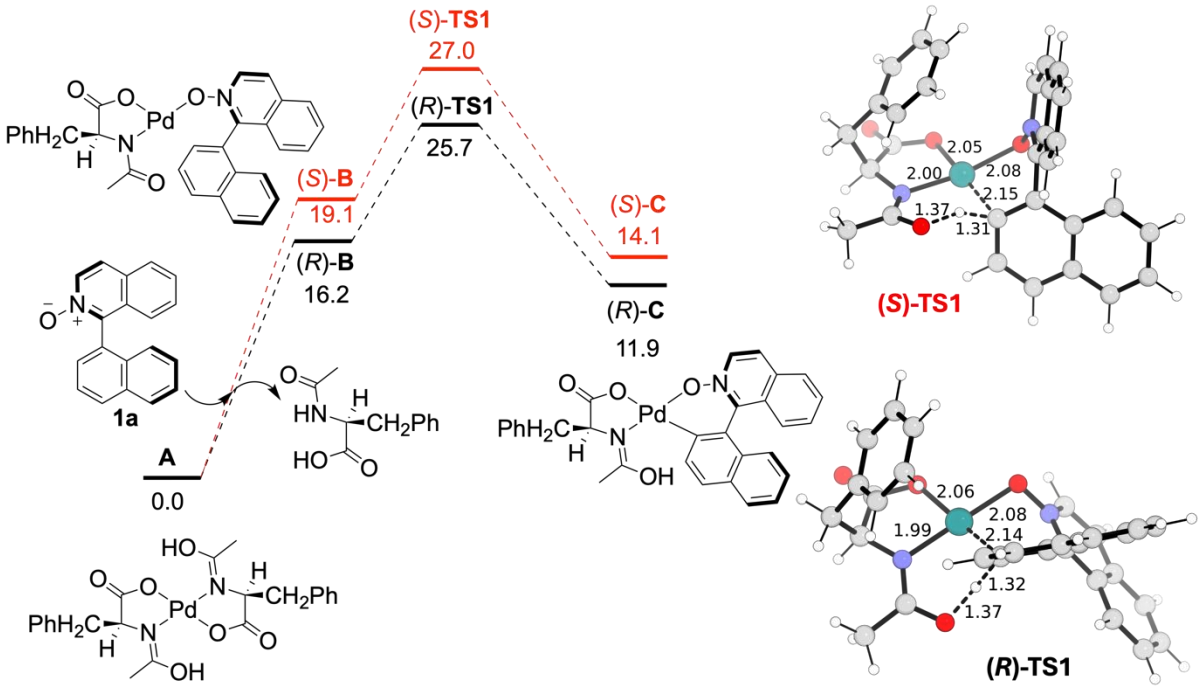


Figure S1. The free energy profile for Pd-catalyzed C-H activation of substrate **1a** enantiomers.

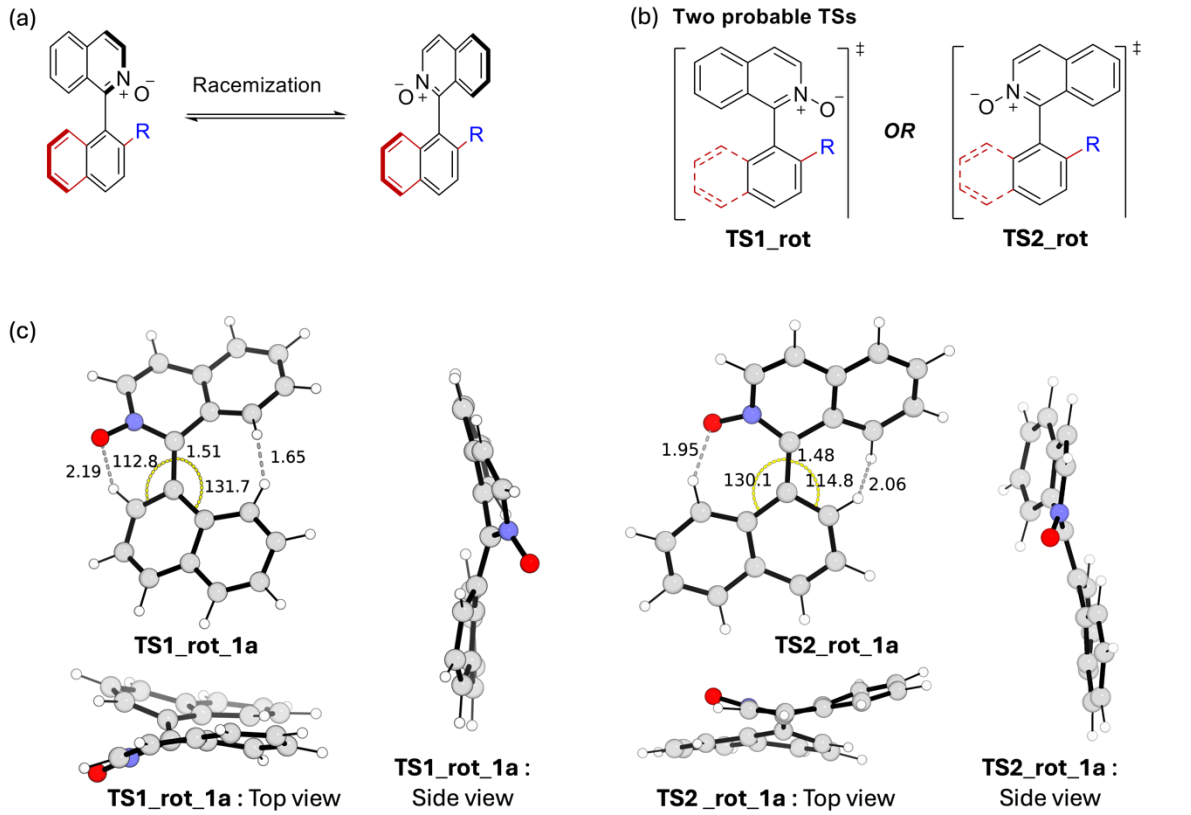
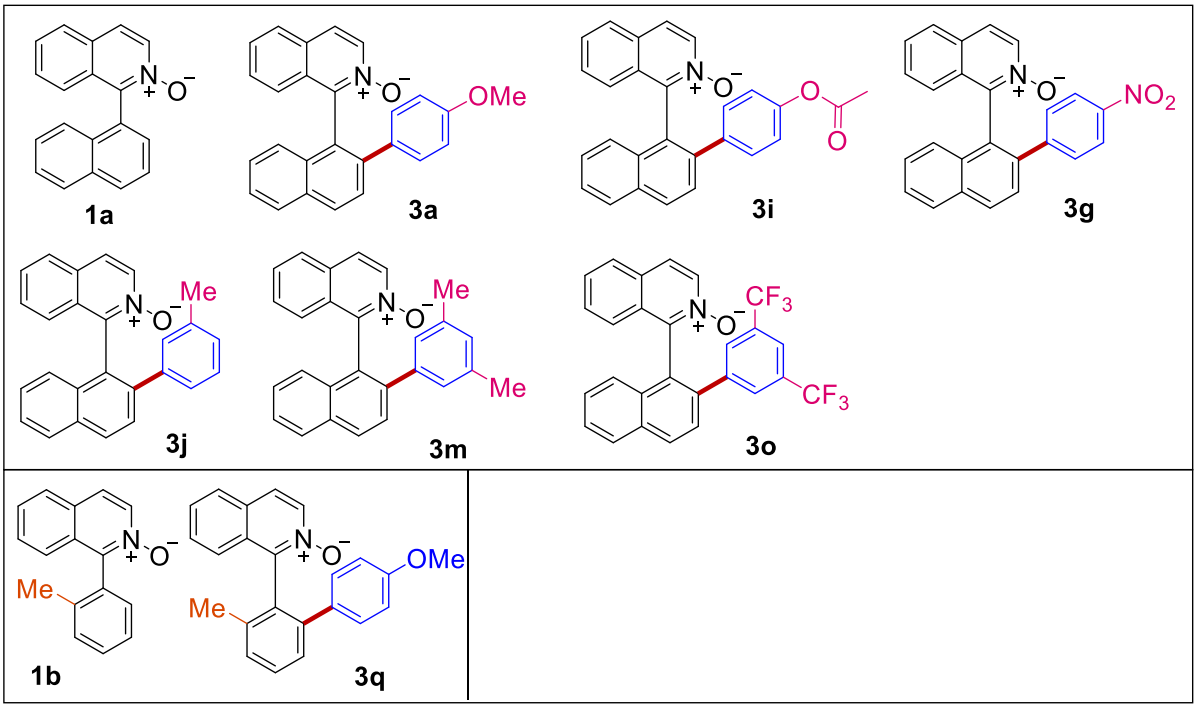


Figure S2. Schematic representation of (a) racemization process and (b) the two probable transition states (TSs). (c) The molecular images of optimized geometry of **TS1_rot** and **TS2_rot** for substrate **1a**. The optimized geometries show the high distortion in the TS even for substrate **1a**. The two aromatic rings are bend in different direction and the atom connecting the rings are slightly pushed out of the plane of the ring.

For substrates **1a** and **1b** (R = H) the **TS2_rot** is lower in energy than **TS1_rot** by around 6 and 4 kcal/mol, respectively (Table S1). The barrier for rotation around C-C bond between aromatic carbons is 32.1 kcal/mol. **TS1_rot** is higher in energy as bulky groups are on the same side, whereas for **TS2_rot**, the bulkier groups of two ring are away from each other leading to less distortion (Figure S1).

For substituted products, the barrier for rotation increases as now both sides of substituted-napthyl ring are bulky leading to higher barrier for rotation (>40 kcal/mol). Also, the difference in energy of two TSs (**TS1_rot** and **TS2_rot**) reduces to around 2 kcal/mol.

Table S1. The DFT computed free energy barrier (kcal/mol) and half-life for racemization for selected substrates and products in HFIP solvent at 333.15 K (60 °C) temperature



	ΔG‡ (TS1_rot)	ΔG‡ (TS2_rot)	$t_{1/2}$ [a]
1a	38.1	**32.1**	665.6 d [b]
3a	42.4	**41.2**	1.6×10^6 y
3i	42.7	**41.5**	2.8×10^6 y
3g	41.8	**41.1**	1.5×10^6 y
3j	42.2	- [c]	8.2×10^6 y
3m	42.6	- [c]	1.4×10^7 y
3o	41.7	- [c]	3.7×10^6 y
1b	36.1	**32.1**	640.8 d [b]
3q	43.8	**42.2**	7.5×10^6 y

[a] Here, s = seconds, h = hours, d = days, y = years. [b] Energies are same, but $t_{1/2}$ values are different as energies are shown only for a single decimal, but $t_{1/2}$ is calculated from barrier computed using energy of stationary points with more decimal points. [c] TS geometry could not be optimized, hence the barrier is calculated using the other TS, although it may not be of lowest energy. As the difference in free energy barrier for two TSs (**TS1_rot** and **TS2_rot**) is smaller (<1.5 kcal/mol) for other products (**3a**, **3i**, and **3g**), the barrier of the **TS2_rot** for products, **3j**, **3m**, **3o** is also expected to >40 kcal/mol. For 40 kcal/mol barrier at 333.15 K temperature, the $t_{1/2}$ for racemization is 2.7×10^5 years.

Table S2. Computed total electronic energies (E_SPC), total electronic energy (E) at the method used for geometry optimization, enthalpy (H_SPC), temperature*entropy (T.S) term, T.S with quasiharmonic correction by Grimme (T.qh-S), and free energy (with quasiharmonic corrections for entropy and correction for solution phase standard state of 1 mole/litre, qh-G_SPC). The E_SPC is at SMD_{HFIP}/B3LYP-D3BJ/6-311+G** level of theory. The E and energy corrections were calaculated at SMD_{HFIP}/B3LYP-D3BJ/6-311+G** level of theory.

Stationary points energies for racemization of **1** and **3** at T = 333.15 K in HFIP solvent						
Structure	**E_SPC**	**E**	**H_SPC**	**T.S**	**T.qh-S**	**qh-G_SPC**
1a	-862.111319	-861.895032	-861.823522	0.065621	0.063437	-861.886959
TS1_rot_1a	-862.051357	-861.835668	-861.764945	0.062461	0.061297	-861.826243
TS2_rot_1a	-862.061342	-861.847631	-861.774978	0.061807	0.060817	-861.835795
3a	-1207.821306	-1207.519174	-1207.410983	0.08791	0.082372	-1207.493355
TS1_rot_3a	-1207.755195	-1207.453459	-1207.346987	0.081848	0.078752	-1207.425739
TS2_rot_3a	-1207.757464	-1207.455359	-1207.349274	0.081294	0.078462	-1207.427737
3i	-1321.214351	-1320.875424	-1320.792645	0.094973	0.087772	-1320.880417
TS1_rot_3i	-1321.147697	-1320.809411	-1320.727992	0.08916	0.084369	-1320.812361
TS2_rot_3i	-1321.149557	-1320.810788	-1320.730085	0.088676	0.084156	-1320.81424
3g	-1297.824614	-1297.487581	-1297.444461	0.08802	0.082263	-1297.526724
TS1_rot_3g	-1297.759162	-1297.42262	-1297.381063	0.082653	0.078989	-1297.460052
TS2_rot_3g	-1297.760433	-1297.423364	-1297.382349	0.082328	0.078863	-1297.461212
3j	-1132.591589	-1132.315321	-1132.187386	0.085069	0.07981	-1132.267195
TS1_rot_3j	-1132.52513	-1132.249333	-1132.123059	0.080097	0.076808	-1132.199867
TS1_rot_3j_c1	-1132.524493	-1132.248506	-1132.122427	0.080334	0.076948	-1132.199375
3m	-1171.925285	-1171.641312	-1171.491432	0.091153	0.08467	-1171.576102
TS1_rot_3m	-1171.858653	-1171.575134	-1171.426897	0.085487	0.081287	-1171.508184
3o	-1767.571939	-1767.069226	-1767.179269	0.102565	0.094347	-1767.273615
TS1_rot_3o	-1767.506258	-1767.004003	-1767.115874	0.097525	0.091245	-1767.207119
1b	-747.747639	-747.558555	-747.480507	0.062144	0.060467	-747.540974
TS1_rot_1b	-747.692281	-747.503885	-747.426058	0.058269	0.057442	-747.4835
TS2_rot_1b	-747.698088	-747.510363	-747.432163	0.058441	0.057688	-747.48985
3q	-1093.457219	-1093.182581	-1093.067452	0.082968	0.078702	-1093.146154
TS1_rot_3q	-1093.388486	-1093.112952	-1093.000924	0.078044	0.075404	-1093.076328
TS2_rot_3q	-1093.390844	-1093.115799	-1093.003413	0.078005	0.075506	-1093.078919
N-Ac-(*L*)-Phe-OH	-707.744395	-707.540606	-707.498126	0.06545	0.061915	-707.560042
A	-1541.888137	-1541.888312	-1541.415572	0.106341	0.099024	-1541.514596
(*R*)-**B**	-1696.227953	-1696.218138	-1695.71334	0.109405	0.102307	-1695.815647
(*R*)-**TS**	-1696.207731	-1696.199314	-1695.699137	0.108684	0.101419	-1695.800557
(*R*)-**C**	-1696.235515	-1696.226593	-1695.720541	0.109323	0.102078	-1695.82262
(*S*)-**B**	-1696.222135	-1696.211946	-1695.707925	0.111214	0.103173	-1695.811098
(*S*)-**TS**	-1696.206417	-1696.19817	-1695.697775	0.107618	0.10079	-1695.798565
(*S*)-**C**	-1696.232164	-1696.223927	-1695.717327	0.108891	0.101771	-1695.819099

Cartesian Coordinates of Stationary points

The Cartesian coordinates of stationary points are given in xyz format, where first line is number of atoms in molecule, second line contain information about molecule, and from third line it is Cartesian coordinate. The information provided in the xyz files are the name of molecule, charge-multiplicity (C,M), electronic energy at the method used for geometry optimization (E), zero-point energy correction (ZPE-Corr), correction for energy at 298.15 K (E-Corr-298), correction for enthalpy at 298.15 K (E-Corr-298), correction for free energy at 298.15 K (G-Corr-298), and number of imaginary frequency (NImag). All energies are in hartree. If NImag=1, then its value in cm^{-1} is also given.

Stationary points for enantiomerization of arylated products in HFIP solvent

34
1a C,M=0,1 E=-861.8950315 ZPE-Corr=0.268171 E-Corr-298=0.283050 H-Corr-298=0.283994 G-Corr-298=0.225736 NImag=0
C -4.0281350314 0.7170177117 -1.6889987783
C -4.1322822676 -0.2710879556 -0.7366867736
C -3.013831624 -0.6322306298 0.0624133596
C -1.7690950292 0.0487327735 -0.1338431145
C -1.6935601602 1.0612524944 -1.1269795498
C -2.7954830205 1.385886878 -1.8863701161
H -4.0525625033 -2.1633317274 1.1845144209
H -4.8890201492 0.9858611915 -2.2941591214
H -5.072488964 -0.793290818 -0.5804694449
C -3.1021857703 -1.6553470906 1.0445717198
C -0.649403879 -0.3200271266 0.6773989253
H -0.752149867 1.5744845697 -1.2922962448
H -2.7212125786 2.1616206181 -2.6430028067
C -0.7746765523 -1.3290199758 1.6129783988
C -2.0065284497 -1.9979903179 1.8019384567
H 0.0843281547 -1.6048376516 2.2169435943
H -2.0781756221 -2.7814911409 2.5501868085
C 0.6637198315 0.346449821 0.5040193997
C 1.7992728855 -0.3108571182 -0.0477327601
C 1.7319952314 -1.6484295745 -0.5241720303
C 3.0421376081 0.3893702735 -0.1450588691
C 1.9604654726 2.3235876505 0.8109435461
C 2.8513701441 -2.2558643168 -1.0503092958
H 0.7916952766 -2.1841827133 -0.4739723848
C 4.1752090924 -0.2629174774 -0.6872223881
C 3.0779139772 1.7340321004 0.3076959636
H 1.904474892 3.3410366987 1.1731276379
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C 2.5993745907 -2.9951000338 0.2250572213
C 2.7595410035 -1.6042583309 -0.1047828941
C 3.9116828118 -1.2821294998 -0.8692876715
C 4.9206177937 -2.1969037807 -1.1007094167
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H -3.5388526202 3.6026244374 0.3344003438
C 2.1627637625 3.3551362953 -0.5081930465
H 2.8809781582 1.8097093586 -1.8455026821
H 1.070113876 4.8256538353 0.617867932
H -1.3806418888 4.7406880822 0.9891128615
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C 2.8554461344 -1.855268862 -1.6179356151
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C 3.432596701 -1.4293453113 -0.4232384724
H 3.4826108144 -2.1916712819 -2.4359727723
H 3.1369134736 -0.6766658497 1.5632277655
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C 5.5445894018 -2.5296342838 -0.3522886085
O 5.0316260668 -3.6163772337 -0.5149632502
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H 7.3385538152 -1.5997401029 -1.0231400535
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46

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C 2.2452008604 -1.3249912031 -0.1062382443
C 3.3110460894 -0.6757319512 -0.7842453234
C 4.5249256877 -1.2945511133 -1.0055763255
H 1.4502384445 -4.6062450581 0.6158316834
H 5.7211419725 -3.0847938889 -0.7162621477
H 3.8142829164 -4.3792317684 0.2156900991
C 1.3035754332 -3.5470323311 0.426530582
C 0.9507181651 -0.7285019754 0.1970391801
H 3.1465154669 0.2961534721 -1.2205025356
H 5.2998277774 -0.7633528782 -1.550711665
C -0.1481631332 -1.6219038105 0.1564944255
C 0.0447711623 -3.0159564162 0.3106826109
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C 2.7361782579 2.0704669786 0.1279142288
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47
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H 4.7593364322 0.9979255591 2.3700155802
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H -0.5500797133 0.1346840991 -3.3484696254
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H -2.2568159445 -4.5149342938 -3.3838223126
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47
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C 3.9807886842 -1.2737969422 -0.7332663567
C 5.034105779 -2.1547416235 -0.8792841023
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C 1.6529293175 -0.7400267062 0.1845854707
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H -1.4292462025 1.6479807593 -3.5645903052
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47
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C 3.9465021703 -1.2785992807 -0.78888857
C 4.9583870725 -2.1995620279 -0.9759042522
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50
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C -0.367875295 2.5600127808 -1.8745502186
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C 2.6311929618 -3.2819117107 0.8137139942
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C -1.511386135 -1.7519027594 1.303205116
C -1.2538372837 -1.0907507056 -0.9986508421
C -2.8728076815 -1.4860635204 1.230783178
H -1.0828533693 -2.0995834917 2.2386948131
C -2.6195709739 -0.8192992964 -1.0866926626
H -0.6302012953 -0.9637055956 -1.8791034661
C -3.4332107477 -1.0125443507 0.035762226
H -3.5202316286 -1.6281990231 2.0906483693
H -3.0332766121 -0.4690989816 -2.0244410238
O -4.7794734917 -0.7724193778 0.0654385893
C -5.3994296584 -0.2805759094 -1.1216575389
H -5.3023988163 -0.9938099311 -1.9485157113
H -6.4551439611 -0.1537937278 -0.8758768579
H -4.9775828032 0.6858931087 -1.4214758776
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TS1_rot_3q C,M=0,1 E=-1093.1129518 ZPE-Corr=0.361671 E-Corr-298=0.381599 H-Corr-298=0.382544 G-Corr-298=0.314315
NImag=1 -34.1017
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C -2.7704414181 2.2861976672 -0.2601606039
H -0.8709607279 5.0228146175 0.5577502648
C -1.1261634205 3.9810995345 0.3880014074
C -1.8681108196 1.2462873119 0.1454858822
C -0.4826184755 1.6472911124 0.2502443655
C -0.1503856682 2.9894438697 0.4368891468
H 0.895702023 3.2595621996 0.5416078721
C -2.2071733944 -0.1741189119 0.3911371482
C -3.4240968055 -0.90312464 0.061724164
C -4.7174264805 -0.3340502555 0.1246620482
C -3.3543098665 -2.3121664673 -0.1787077972
C -1.2068299281 -2.3140549796 0.8606317615
C -5.8428998393 -1.0596830344 -0.2182759935
H -4.8353062075 0.6614465244 0.520768559
C -4.5053560446 -3.0232303648 -0.5899368404
C -2.1483633515 -2.9874592731 0.1560217736
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C -5.7352794338 -2.399759152 -0.6392992389
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H -6.6215703435 -2.9531299739 -0.9341757515
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C -4.0211768887 2.1400511865 -1.1100681625
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H -4.9548702538 2.3134671596 -0.5663615366
H -3.968566994 2.9080816246 -1.8886568467
C 0.6361156862 0.7200153274 -0.0390563608
C 1.8470553622 0.7612327109 0.6786553682

C 0.5517572829 -0.1602880859 -1.1265235257
C 2.9144978305 -0.0532065632 0.3349021462
H 1.9354598257 1.4192482752 1.5374156393
C 1.615994288 -0.9914812982 -1.4828387283
H -0.3561621935 -0.1891602598 -1.7208446599
C 2.8033914355 -0.9412130035 -0.7464067539
H 3.8423238517 -0.0305835115 0.8983533414
H 1.5129977382 -1.6516646712 -2.3355859387
O 3.9081289019 -1.7068753342 -1.0026880029
C 3.842885601 -2.6362473283 -2.0824988666
H 3.685689528 -2.1261458446 -3.0401953755
H 4.8087015851 -3.1441965366 -2.0981357988
H 3.0466493863 -3.3738237059 -1.9275756546
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C -3.5010861983 -1.8623659972 -0.3702791129
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C -2.2961401756 -3.8739915951 0.2851779033
C -2.4001432811 -1.039656742 0.0553545199
C -1.1397170459 -1.7282096596 0.1900751478
C -1.1354876057 -3.1146848519 0.3893113264
H -0.1795274275 -3.6092762224 0.5299558334
C -2.6166105941 0.4118368561 0.247345627
C -1.6498619096 1.5010708253 0.3090618025
C -0.3716071818 1.3858749544 0.903605244
C -2.0438327831 2.809820536 -0.1114185871
C -4.3195294177 2.1121388663 0.0672992202
C 0.5255720454 2.4367499524 0.8950740336
H -0.108964681 0.4811840569 1.4231802214
C -1.094522518 3.8569287629 -0.1712819134
C -3.4293489406 3.058923607 -0.315039206
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C 0.189534404 3.6667750978 0.2961608876
H 1.4921154986 2.3109811461 1.373345984
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H -3.7781244311 4.0273974384 -0.656610234
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C 1.3270017465 -1.4046101298 0.6480017829
C 0.3614093786 -0.4339605872 -1.3299829109
C 2.583601761 -0.9153932636 0.2885772756
H 1.2251001038 -1.9592147527 1.576271268
C 1.6059018614 0.0472234925 -1.7084785945
H -0.4994164825 -0.246912266 -1.9641283737
C 2.7241408883 -0.1788677847 -0.8935729366
H 3.4344801805 -1.1100161517 0.9298677697
H 1.7348388083 0.605835942 -2.6304089654
C 5.068058714 0.1644714768 -0.5368312143
H 5.3111906647 -0.8988470649 -0.4267017221
H 5.8786953626 0.6679900269 -1.0662059617
H 4.9459763263 0.6156941155 0.4548730567
O 3.9031300915 0.3516833654 -1.3389751233
28
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C -2.707034773 -2.2781101336 -0.7241382998
C -2.9349216392 -1.8639442872 0.7154318391
O -3.6907454538 -3.0651735678 -1.1778640238
N -1.7354581197 -1.1956423974 1.1764106841
C -4.2084130265 -0.9742486703 0.8254536597
H -3.1046076722 -2.7663355785 1.3120420679
C -1.5279109795 -0.8985488582 2.4777368528
C -4.0727626177 0.317495554 0.0608936284
H -5.0578907276 -1.5603201901 0.4641203937
H -4.3611209884 -0.7791514466 1.8888504434
O -2.3185912369 -1.249767061 3.3673227399

C -4.3974019693 0.3842281268 -1.301421528
C -3.5574135133 1.4603980502 0.6871572458
C -4.2114670847 1.565612898 -2.0209214736
H -4.8008656985 -0.4946305768 -1.7982270027
C -3.3696275554 2.6430435122 -0.0300237473
H -3.3102333935 1.4201596407 1.7447263799
C -3.6946627019 2.6981617223 -1.3873611619
H -4.4722718977 1.6024443845 -3.075028233
H -2.9717525348 3.5213171569 0.4708889969
H -3.5507782103 3.6184137945 -1.9464103159
C -0.2823880355 -0.1021158526 2.7860947761
H 0.2206768413 -0.5500617995 3.6470477003
H 0.4109279924 -0.0483353178 1.9436603681
H -0.5771661923 0.9151964546 3.0655620666
H -3.5161304682 -3.2713410987 -2.1147779804
H -1.1044038654 -0.849300829 0.4647171511
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C 0.5952449856 -1.9230186161 2.0080938963
C 1.6712281265 -1.557241106 0.9838421049
O 0.8815358518 -2.5216971103 3.0392033251
N 1.0460043406 -1.2763262046 -0.3100127524
C 2.4123983144 -0.3001988603 1.5268564567
H 2.36933602 -2.3932059606 0.9218834838
C 1.6330432576 -1.474816855 -1.4477540847
C 3.4986958744 0.1719233564 0.5984972885
H 1.6692155844 0.4891029408 1.6764395493
H 2.8216111026 -0.5721873187 2.5040941789
O 1.0618524267 -1.0959891051 -2.5875916475
C 3.2035421567 1.0629173533 -0.4427350082
C 4.8037661956 -0.3241919552 0.7129511792
C 4.1890782996 1.4430417265 -1.3550789454
H 2.1973994623 1.4567498681 -0.5370848866
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H 5.0424116009 -1.0165483353 1.5165738466
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H 3.9436837445 2.1334866304 -2.1573382423
H 6.799268644 -0.3385596236 -0.095060597
H 6.2535118257 1.2298035113 -1.9469653752
C 2.9478201957 -2.1463174911 -1.6807344838
H 3.6509615667 -1.4128514704 -2.0858929717
H 3.3742147584 -2.5881066515 -0.7843086523
H 2.7992866743 -2.922372696 -2.4378465872
Pd -0.8403013727 -0.5628662871 -0.0363505061
O -1.073246666 0.3081922424 -1.8356876471
N -2.7509237628 0.0917947877 0.217875829
C -2.1653224211 1.0208607993 -1.9868798512
C -3.1035760146 1.1115688663 -0.7798834448
C -3.5706517057 -0.2642845605 1.1550334908
O -2.4194422825 1.6407818483 -3.0150644294
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H -2.0888254046 2.1489702482 2.3496075146
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H 1.4056353896 4.0250490014 -0.6288613438
H 0.193958716 2.5437924627 3.2238116579
H 1.9552615144 3.4767511184 1.733073586
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61
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C 2.179394043 -0.6629335168 -0.2226948294
C 2.0776740756 -2.2022231702 -2.0430154572
C 3.4069538201 -2.4806068075 -1.9437630318
C 4.2004367881 -1.8544499095 -0.9483334819
H 3.8507141167 -3.1931961707 -2.6300724075
C 1.4466299846 0.3083929443 0.6331472277
C 1.561273368 1.7053564848 0.3538147127
C 0.77934375 -0.137793407 1.776435822
C 1.0164182145 2.6351069896 1.2968320253
C 0.2200316403 0.8071794261 2.6875454949
C 0.3449980542 2.1508810577 2.4554305734
H -0.2882087618 0.4293024934 3.5654890974
H -0.0635527772 2.8721346146 3.1572821886
Pd -1.0093209831 -0.9371384645 0.296377615
H 0.8334152274 -1.1825640942 2.0691691259
N 1.4956726002 -1.2986490943 -1.183421586
O 0.1946596747 -1.0461388613 -1.3861631854
C 4.3328388935 -0.2888305531 0.9460911461
H 3.8560357587 0.4116880671 1.6219763558
C 5.5830353678 -2.118084697 -0.8001534879
C 6.3058759504 -1.4827537743 0.1855850018
H 7.3663437301 -1.6858420894 0.297197627
C 5.676478275 -0.5651014476 1.0611737952
H 6.2616712824 -0.0767921231 1.8338820326
H 6.0562604716 -2.8252428937 -1.4741218389
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H -4.1813063424 1.2569136663 1.4196783129
O -1.2252725931 -1.7996583752 3.3429763433
C -3.39388187 0.8444718056 -1.8714006876
C -2.2323898125 2.1115261082 -0.1819797059
C -2.5104099336 1.319336851 -2.8398245264
H -4.1912330856 0.1644615373 -2.1574516001
C -1.3612204212 2.6078536673 -1.1547299372
H -2.1174653483 2.4191887162 0.8532754126
C -1.4871006636 2.2011191984 -2.4830684907
H -2.6280117467 1.0088712006 -3.8744472951
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H -0.8024992841 2.5810587739 -3.2361985412
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H -4.1552985744 -2.3732999028 3.5194879026
H -3.2073902873 -1.6304439221 4.8200835882
H -4.1934667194 -0.6150524337 3.7366708174
C 2.2071704722 2.1975769451 -0.8101494208
C 2.3229205926 3.5533537057 -1.0243454777
H 2.6091312858 1.4970527445 -1.5345523468
H 2.8177740362 3.9200737105 -1.9181748267
C 1.7976962292 4.4734845154 -0.0866073276
C 1.1549157543 4.0234853384 1.0470175666
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H 0.7402842035 4.7257032546 1.7642990393
61
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C 2.2368573774 -0.4523189704 -0.4351189065
C 2.0783855654 -2.1486784401 -2.1154942931
C 3.2622221703 -2.7053433758 -1.7358742075
C 3.9830190559 -2.1737897176 -0.6357718458
H 3.6369572084 -3.5712889188 -2.2700731212
C 1.6097595988 0.7593696162 0.1383894424
C 2.2854651021 2.0142918012 0.0173102068
C 0.3446381292 0.670073613 0.7327967485
C 1.6613314062 3.1825360269 0.5710982467
C -0.2423564484 1.852954621 1.2691132344
C 0.3953034233 3.0655901369 1.2014881556

H -1.2033396501 1.7703276308 1.7627450603
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C 5.1939335343 -2.7457070152 -0.1768205603
C 5.842181976 -2.2103511326 0.9140520988
H 6.7693522012 -2.6521963835 1.2654570801
C 5.3022439952 -1.0908897787 1.5922235797
H 5.8177578041 -0.6914060179 2.4597544637
H 5.5929557511 -3.6115220458 -0.6958946824
H 1.4480883527 -2.5038989711 -2.9190143726
O -2.2528279402 -1.9048371607 -1.333333732
C -3.357296036 -2.1568020115 -0.6856491522
C -3.4834435934 -1.6124234247 0.7485330076
O -4.307216444 -2.7692537934 -1.1836548011
N -2.1805980573 -1.1251258713 1.1896055259
C -4.5791526155 -0.5140911907 0.7825472861
H -3.8196782357 -2.444444392 1.3749672932
C -1.7184754696 -1.2161657896 2.4181314071
C -4.2157441571 0.7066168056 -0.0266954484
H -5.4979738748 -0.9748483991 0.4057721786
H -4.7489354571 -0.2356958245 1.8264663655
O -0.5057221059 -0.8751699044 2.6881628621
C -4.3315413246 0.7053203039 -1.4252829865
C -3.7007823826 1.8469158708 0.6007799022
C -3.9193965547 1.8072677458 -2.1749407015
H -4.7461306465 -0.1644189015 -1.9270327892
C -3.2910449821 2.9536344587 -0.1455315613
H -3.6165906805 1.8630362027 1.6841814475
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H -4.0162252563 1.7889559605 -3.2569845646
H -2.8912599462 3.828175722 0.3596413795
H -3.0744653301 3.7935242863 -2.1212091871
C -2.5715051481 -1.7303911013 3.5494094589
H -2.7315628814 -2.8080785869 3.4334105025
H -2.0600357264 -1.5502148085 4.4952736001
H -3.5494632211 -1.2433808183 3.5642369747
C 3.5295771869 2.1683711384 -0.6591286831
C 4.1352543147 3.4004011996 -0.7497357684
H 4.0021002036 1.3071925061 -1.1165494889
H 5.082576743 3.4976516855 -1.2713520714
C 3.5318445917 4.544752207 -0.174004108
C 2.3193534809 4.4361006154 0.4672320577
H 4.0250515465 5.5090712348 -0.2510214515
H 1.8395248345 5.310058126 0.8985231322

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C 2.1544620533 -0.3906351278 -0.587450386
C 1.9648453692 -2.0873353503 -2.2743747693
C 3.2329649297 -2.5299822076 -2.0572252287
C 4.0078477659 -1.9700934579 -1.0090755451
H 3.627447014 -3.3379674012 -2.6629293129
C 1.5150068249 0.7662472032 0.067937319
C 2.2447886021 2.0046547351 0.1786721108
C 0.2121666669 0.657316752 0.5703570587
C 1.6826311329 3.0644794666 0.9620211219
C -0.3075803523 1.7270594951 1.3472596816
C 0.4130125933 2.8775685774 1.5647344148
H -1.2966385151 1.6323668599 1.7779493118
H 0.0014657148 3.6768909061 2.1762189745
Pd -0.9698491167 -0.8112555686 -0.0871524305
H -0.1115547236 -0.6928196965 2.3368979873
N 1.4535786814 -1.0543369446 -1.5274517686
O 0.1759160486 -0.719622102 -1.7970000628
C 4.1668981422 -0.4182497485 0.8833537317
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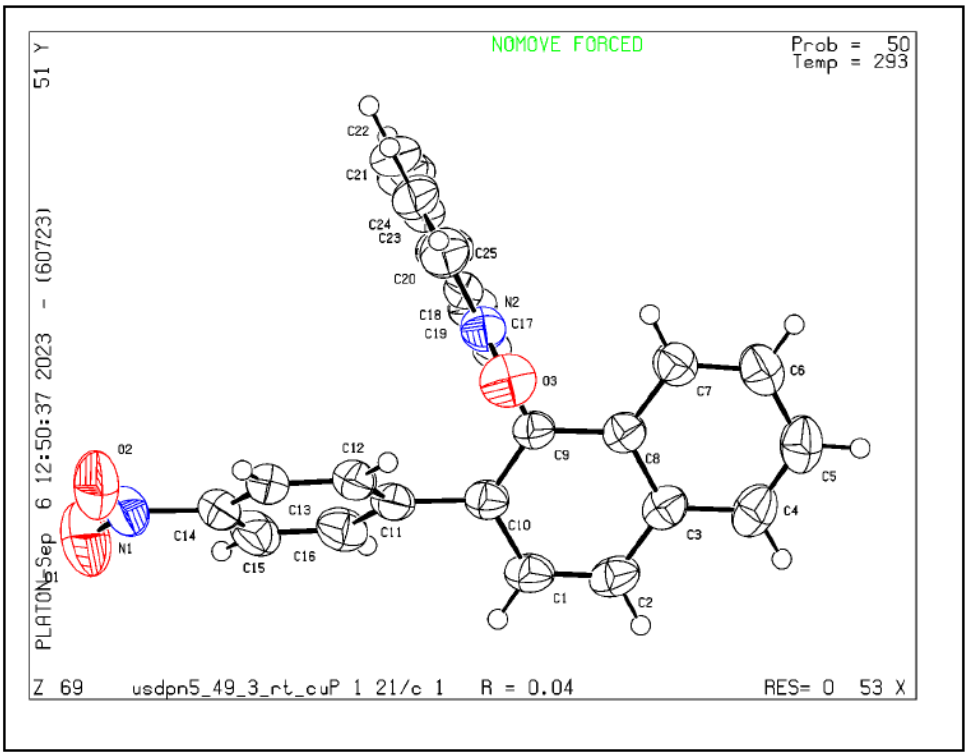
H 5.0147475851 -3.8278453433 0.8275585204

9. XRD data

XRD data for compound 3g



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

Crystal data and structure refinement

Identification code	USDPN5_49_3_Rt_Cu
Empirical formula	C25H16N2O3
Formula weight	392.40
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P21/c
a/Å	11.8307(6)
b/Å	9.9076(4)
c/Å	16.8625(7)
α/°	90
β/°	105.681(5)
γ/°	90
Volume/Å3	1902.95(15)
Z	4
ρcalcg/cm3	1.370
μ/mm-1	0.739
F(000)	816.0
Crystal size/mm3	0.246 × 0.231 × 0.165
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.762 to 138.178
Index ranges	-14 ≤ h ≤ 14, -11 ≤ k ≤ 5, -19 ≤ l ≤ 20
Reflections collected	5509

Independent reflections	3471 [Rint = 0.0208, Rsigma = 0.0300]
Data/restraints/parameters	3471/0/271
Goodness-of-fit on F2	1.037
Final R indexes [I>=2σ (I)]	R1 = 0.0443, wR2 = 0.1200
Final R indexes [all data]	R1 = 0.0550, wR2 = 0.1329
Largest diff. peak/hole / e Å-3	0.15/-0.18

Bond Lengths

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O3	N2	1.304(2)	C3	C2	1.409(3)
N2	C17	1.342(2)	C3	C4	1.414(3)
N2	C25	1.393(2)	C10	C1	1.423(2)
C17	C18	1.423(2)	C12	C13	1.380(2)
C17	C9	1.490(2)	C7	C6	1.363(3)
C18	C23	1.423(2)	C2	C1	1.348(3)
C18	C19	1.406(2)	C13	C14	1.380(3)
C9	C8	1.428(2)	C23	C24	1.408(3)
C9	C10	1.382(2)	C23	C22	1.413(3)
C8	C3	1.426(2)	C19	C20	1.369(3)
C8	C7	1.414(2)	C25	C24	1.341(3)
N1	O2	1.215(3)	C14	C15	1.377(3)
N1	O1	1.208(3)	C4	C5	1.354(3)
N1	C14	1.468(3)	C16	C15	1.374(3)
C11	C10	1.488(2)	C6	C5	1.405(3)
C11	C12	1.396(2)	C20	C21	1.394(3)
C11	C16	1.397(2)	C22	C21	1.353(3)

Bond Angles

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O3	N2	C17	121.59(14)	C9	C10	C1	119.28(15)
O3	N2	C25	117.97(15)	C1	C10	C11	118.90(14)
C17	N2	C25	120.42(16)	C13	C12	C11	121.21(16)
N2	C17	C18	119.89(14)	C6	C7	C8	120.96(17)
N2	C17	C9	118.39(14)	C1	C2	C3	121.27(15)
C18	C17	C9	121.68(14)	C14	C13	C12	118.19(18)
C17	C18	C23	119.69(15)	C24	C23	C18	117.33(17)
C19	C18	C17	121.86(14)	C24	C23	C22	123.76(17)
C19	C18	C23	118.45(16)	C22	C23	C18	118.91(18)
C8	C9	C17	118.61(13)	C20	C19	C18	120.72(17)
C10	C9	C17	120.75(14)	C2	C1	C10	121.20(15)
C10	C9	C8	120.38(14)	C24	C25	N2	121.53(17)
C3	C8	C9	118.87(14)	C13	C14	N1	118.1(2)
C7	C8	C9	122.62(14)	C15	C14	N1	119.67(18)
C7	C8	C3	118.50(15)	C15	C14	C13	122.24(17)
O2	N1	C14	118.8(2)	C5	C4	C3	121.15(18)
O1	N1	O2	123.5(2)	C25	C24	C23	121.12(17)
O1	N1	C14	117.7(3)	C15	C16	C11	120.72(19)
C12	C11	C10	120.41(14)	C7	C6	C5	120.36(18)
C12	C11	C16	118.58(16)	C16	C15	C14	119.02(17)
C16	C11	C10	120.93(16)	C4	C5	C6	120.40(18)

C2	C3	C8	118.97(15)	C19	C20	C21	120.6(2)
C2	C3	C4	122.40(16)	C21	C22	C23	120.91(18)
C4	C3	C8	118.63(16)	C22	C21	C20	120.4(2)
C9	C10	C11	121.76(14)				

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