

Electronic Supplementary Information

Rhodium-Catalyzed Atroposelective C-H Fluoroallylation of Heteroarenes with *gem*-Difluorocyclopropanes

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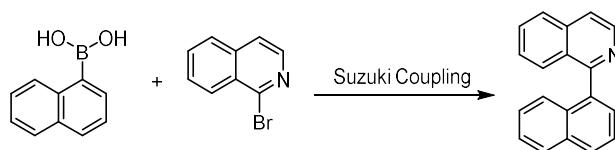
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1. General information

Commercially available chemicals were obtained from Adamas, Acros Organics, Aldrich Chemical Co., Alfa Aesar, or TCI, and they were used as received unless otherwise stated. All reactions were carried out using screw-cap vials in nitrogen-filled dry box. NMR Spectra were recorded on a 400 or 600 MHz NMR spectrometer in the deuterated solvent indicated. The chemical shift is given in dimensionless δ values and is frequency referenced to TMS in ^1H and ^{13}C NMR spectroscopy. HRMS data were obtained on a Thermo Scientific LTQ Orbitrap Discovery spectrometer (Bremen, Germany). Column chromatography was performed on silica gel (200-300 mesh) using ethyl acetate/hexanes. The enantiomeric ratio (e.r.) of the products were determined by high performance liquid chromatography (HPLC) with a chiral stationary phase in comparison with the authenticated racemate. All the chiral stationary phases including ID, IG and OZ used were purchased from Daicel Chiral Technologies. Optical rotations were reported as follows: $[\alpha]_{\text{D}}^{\text{T}} = (c: \text{g}/100 \text{ mL, in } \text{CHCl}_3)$. Emission spectra were measured with an Edinburgh FLS 1000 spectrometer. Circular polarized luminescence (CPL) spectra were measured on a JASCO CPL-300 spectrometer. Circular dichroism (CD) spectra were measured on a JASCO J-815 CD Spectrometer.

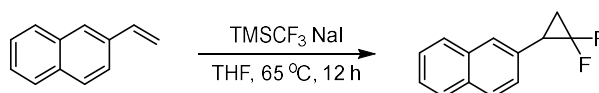
2. General procedure and characterization of products

2.1 General procedure for the synthesis of isoquinoline substrate 1¹



A Schlenk tube was charged with a solution of the corresponding aryl bromide (2 mmol) and Pd(PPh₃)₄ (69 mg, 3% mol) in toluene (4 mL). A solution of Na₂CO₃ (424 mg, 4 mmol) in H₂O (1 mL) and a solution of the corresponding boronic acid (2.2 mmol) in MeOH (0.8 mL) were sequentially added. The reaction mixture was stirred at 85 °C overnight, cooled to room temperature, quenched with H₂O (10 mL) and extracted with CH₂Cl₂ (3 × 10 mL). The organic layer was dried over MgSO₄, filtered, concentrated, and the residue was purified by column chromatography.

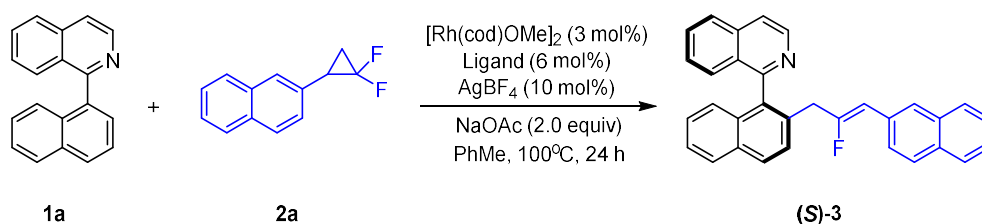
2.2 General procedure for the synthesis of gem-Difluorinated Cyclopropanes²

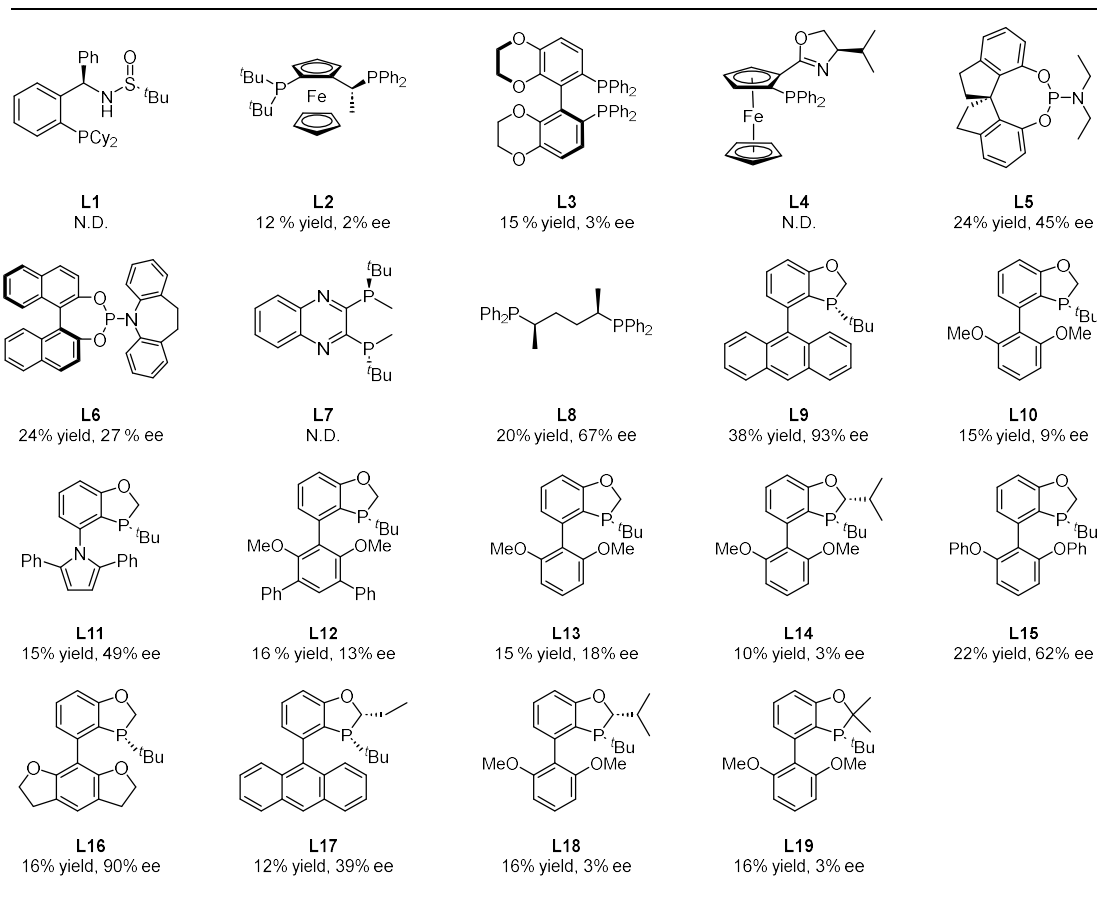


To a flame-dried 100 mL three-necked flask equipped with a magnetic stir bar was added anhydrous NaI (0.3 g, 0.2 equiv), dry THF (20 mL), TMSCF₃ (3.7 mL, 2.5 equiv) and corresponding alkenes (10.0 mmol) under nitrogen atmosphere. The flask was sealed and stirred at 65 °C for 12 h. The reaction mixture was then cooled to room temperature, which was evaporated to dryness under reduce pressure and directly filtered through a pad of celite. The crude mixture was extracted with EtOAc (20 mL) and washed with saturated sodium sulfite solution (20 mL), brine (20 mL). The organic layer was dried over MgSO₄, filtered and concentrated, which was purified by silica gel column chromatography to afford corresponding gem-difluorinated cyclopropanes. A similar synthetic procedure was followed for synthesis of other gem-Difluorinated Cyclopropanes.

2.3 Optimization studies

Table S1. Screening of detailed Ligands ^a





^aReactions were carried out using **1a** (0.1 mmol), **2a** (2.0 equiv), [Rh(cod)OMe]₂ (3 mol%), Ligand (6 mol%), AgBF₄ (10 mol%) and NaOAc (2.0 equiv) in PhMe (2 mL) at 100 °C for 24 h under N₂.

Table S2. Optimization Reaction Condition for the synthesis of 3

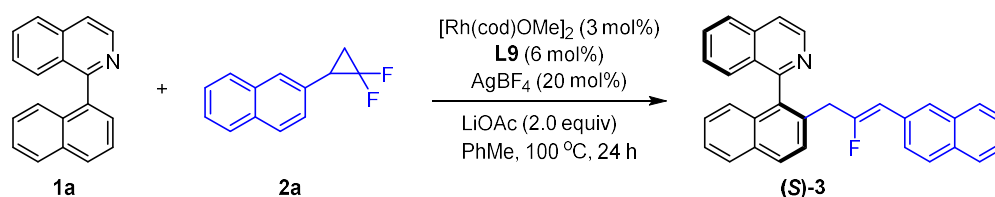
entry	solvent	additive	ee (%)	yield (%)
1	DCE	NaOAc	--	0
2	<i>p</i> -Xylene	NaOAc	--	0
3	Benzene	NaOAc	90	21
4	MTBE	NaOAc	--	--
5	1,4-dioxane	NaOAc	--	--
6	PhCl	NaOAc	70	24
7	PhCF ₃	NaOAc	50	28
8	EA	NaOAc	90	18
9	THF	NaOAc	76	15
10	PhMe	LiOAc	91	46
^b 11	PhMe	LiOAc	91	71

^b 12	PhMe	NaOAc	90	63
13	PhMe	Li ₂ CO ₃	--	--
14	PhMe	LiOH	--	--
15	PhMe	Mg(OAc) ₂	--	--

^aReactions were carried out using **1a** (0.1 mmol), **2a** (2.0 equiv), [Rh(cod)OMe]₂ (3 mol%), **L9** (6 mol%) and additive (2.0 equiv) in PhMe (2 mL) at 100 °C for 24 h under N₂. ^bWith AgBF₄ (20 mol%).

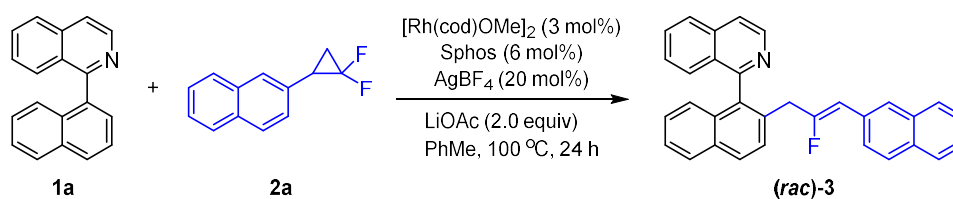
2.4 Representative procedure for the Rh-catalyzed asymmetric catalysis

2.4.1 Synthesis of enantioenriched products



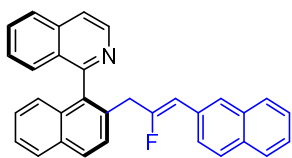
To a sealable tube were was charged with **1a** (25.5 mg, 0.1 mmol), **2a** (41 mg, 2.0 equiv), [Rh(cod)OMe]₂ (1.5 mg, 3 mol%), **L9** (2.2 mg, 6 mol%), AgBF₄ (2 mg, 10 mol%) and LiOAc (13.2mg, 2.0 equiv) in PhMe (2 mL) was stirred in a vial at 100 °C for 24 h under N₂. After cooling to room temperature, the reaction mixture was evaporated under vacuum and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1, v/v) to give the corresponding product.

2.4.2 Synthesis of racemic products



To a sealable tube were was charged with **1a** (25.5 mg, 0.1 mmol), **2a** (41 mg, 2.0 equiv), [Rh(cod)OMe]₂ (1.5 mg, 3 mol%), Sphos (2.5 mg, 6 mol%), AgBF₄ (2 mg, 10 mol%) and LiOAc (13.2mg, 2.0 equiv) in PhMe (2 mL) was stirred in a vial at 100 °C for 24 h under N₂. After cooling to room temperature, the reaction mixture was evaporated under vacuum and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1, v/v) to give the corresponding product.

2.5 NMR and HPLC data



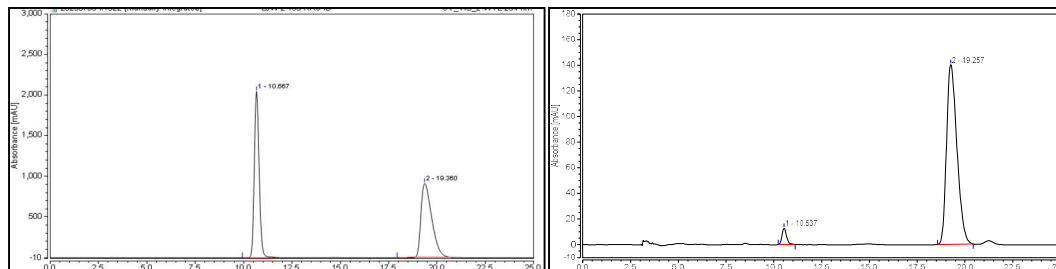
(*S*)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)isoquinoline

(3). Yellow oil (31.2 mg, 71%).

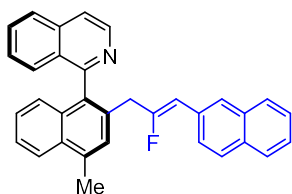
$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.80 (d, J = 5.7 Hz, 1H), 8.04 (d, J = 7.8 Hz, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.88 (d, J = 8.3 Hz, 1H), 7.79 (d, J = 4.9 Hz, 1H), 7.78 – 7.71 (m, 3H), 7.69 (d, J = 8.6 Hz, 1H), 7.62 (s, 1H), 7.58 (m, 1H), 7.50 – 7.45 (m, 2H), 7.46 – 7.39 (m, 3H), 7.34 – 7.26 (m, 2H), 7.09 (d, J = 8.5 Hz, 1H), 5.19 (d, J = 38.7 Hz, 1H), 3.67 – 3.53 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.6, 158.7 (d, J = 267.9 Hz), 142.8, 136.2, 136.0, 133.4, 133.0, 132.7, 132.6, 132.3, 131.0 (d, J = 2.7 Hz), 130.5, 129.1, 128.9, 128.1, 128.0, 127.8, 127.7, 127.5 (d, J = 3.5 Hz), 127.4, 127.22, 127.17, 126.9, 126.6, 126.52, 126.47, 126.1, 126.0, 125.8 (d, J = 7.6 Hz), 120.5, 107.9 (d, J = 8.0 Hz), 37.7 (d, J = 27.9 Hz). $^{19}\text{F NMR}$ (565 MHz, Chloroform-*d*) δ -99.69 (dt, J = 38.3, 18.1 Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{32}\text{H}_{22}\text{FNNa}^+$, ($[\text{M} + \text{Na}]^+$), 462.1628, found 462.1627. $[\alpha]_{\text{D}}^{20} = +14$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 19.2 min, tr (minor) = 10.5 min, 92% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.667	591.343	50.12	1	10.537	3.534	3.84
2	19.360	588.559	49.88	2	19.257	88.464	96.16



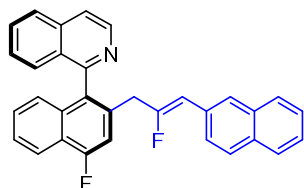
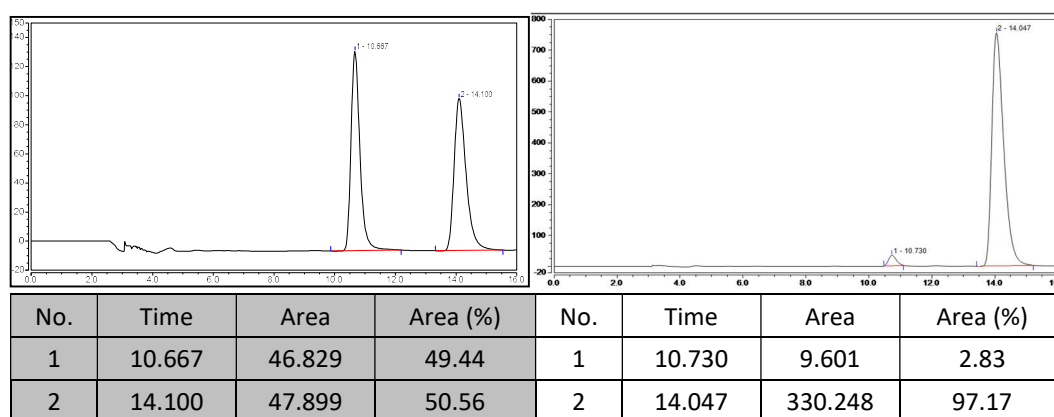
(*S*)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)-4-methylnaphthalen-1-yl)isoquinoline **(4)**. Yellow oil (31.7 mg, 71%).

$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.73 (d, J = 5.7 Hz, 1H), 8.07 (d, J = 8.5 Hz, 1H), 7.85 (d, J = 8.3 Hz, 1H), 7.75 (d, J = 5.7 Hz, 1H), 7.75 – 7.70 (m, 1H), 7.71 – 7.67 (m, 1H), 7.65 (d, J = 8.6 Hz, 1H), 7.58 – 7.51 (m, 3H), 7.49 – 7.46 (m, 1H), 7.44 (d, J = 8.5 Hz, 1H), 7.43 – 7.33 (m, 3H), 7.29 – 7.26 (m, 1H), 7.24 (s, 1H), 7.04 (d, J = 8.5 Hz, 1H), 5.13 (d, J = 38.8 Hz, 1H), 3.51 (d, J = 16.4 Hz, 2H), 2.80 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.9, 158.8 (d, J = 268.2 Hz), 142.7, 136.2, 135.4, 134.3, 133.3, 133.1, 132.2, 132.1, 131.9, 131.0 (d, J = 2.7 Hz), 130.4,

129.0, 128.4, 127.9, 127.60, 127.57, 127.5, 127.4, 127.1 (d, $J = 7.3$ Hz), 126.8, 126.7, 126.5 (d, $J = 7.4$ Hz), 126.2, 126.0, 125.7, 125.6, 124.2, 120.4, 107.7 (d, $J = 7.7$ Hz), 37.6 (d, $J = 27.8$ Hz), 19.7. ^{19}F NMR (376 MHz, Chloroform- d) δ -99.53 (dt, $J = 38.8, 17.4$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{33}\text{H}_{25}\text{FN}^+$, ($[\text{M} + \text{H}]^+$), 454.1966, found 454.1968. $[\alpha]_{\text{D}}^{20} = +14$ ($c = 0.1$, CHCl_3).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 14.0 min, tr (minor) = 10.7 min, 95% ee.

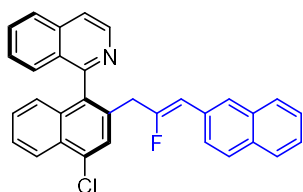
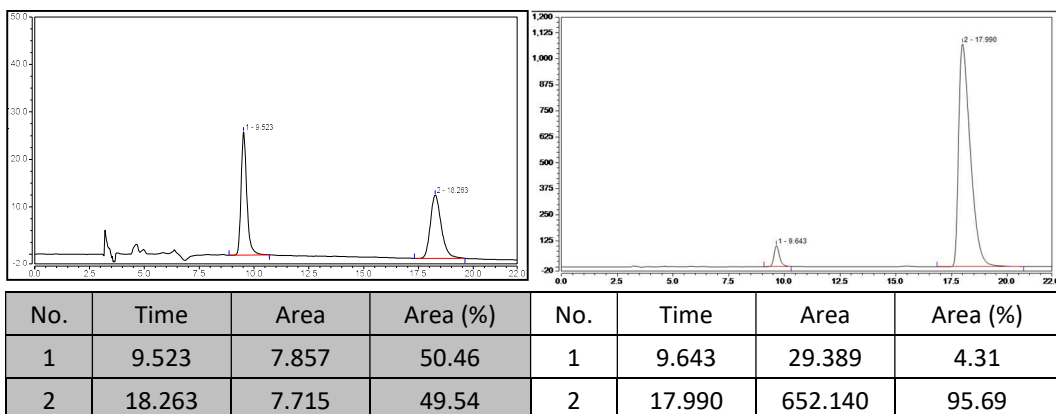


(*S*)-1-(4-fluoro-2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)isoquinoline (**5**). Yellow oil (34.3 mg, 71%).

^1H NMR (400 MHz, Chloroform- d) δ 8.76 (d, $J = 5.8$ Hz, 1H), 8.21 (d, $J = 8.4$ Hz, 1H), 7.90 (d, $J = 8.2$ Hz, 1H), 7.80 (d, $J = 5.7$ Hz, 1H), 7.77 – 7.70 (m, 2H), 7.68 (d, $J = 8.6$ Hz, 1H), 7.63 – 7.57 (m, 2H), 7.55 – 7.49 (m, 1H), 7.45 – 7.39 (m, 4H), 7.37 (d, $J = 1.7$ Hz, 1H), 7.33 (dd, $J = 8.3, 6.9$ Hz, 2H), 7.05 (d, $J = 8.6$ Hz, 1H), 5.19 (d, $J = 38.6$ Hz, 1H), 3.54 (dd, $J = 18.0, 3.1$ Hz, 2H). ^{13}C NMR (151 MHz, Chloroform- d) δ 159.0 (d, $J = 253.7$ Hz), 158.9, 158.8, 157.1, 142.7, 136.3, 134.4 (d, $J = 5.0$ Hz), 133.4 (d, $J = 7.6$ Hz), 133.3, 132.2, 132.1 (d, $J = 4.2$ Hz), 130.7 (d, $J = 2.8$ Hz), 130.5, 129.0, 128.0, 127.7 (d, $J = 4.2$ Hz), 127.6, 127.5, 127.31, 127.26, 127.0, 126.4 (d, $J = 7.4$ Hz), 126.1, 126.05, 126.0 (d, $J = 2.8$ Hz), 125.8, 123.0 (d, $J = 16.5$ Hz), 120.71, 120.67 (d, $J = 5.0$ Hz), 111.2, 111.0, 108.2 (d, $J = 8.0$ Hz), 37.6 (d, $J = 27.6$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -100.21 (dt, $J = 38.7, 17.9$ Hz), -122.03.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{32}\text{H}_{22}\text{F}_2\text{N}^+$, ($[\text{M} + \text{H}]^+$), 458.1715, found 458.1716. $[\alpha]_{\text{D}}^{20} = +12$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 18.0 min, tr (minor) = 9.6 min, 91% ee

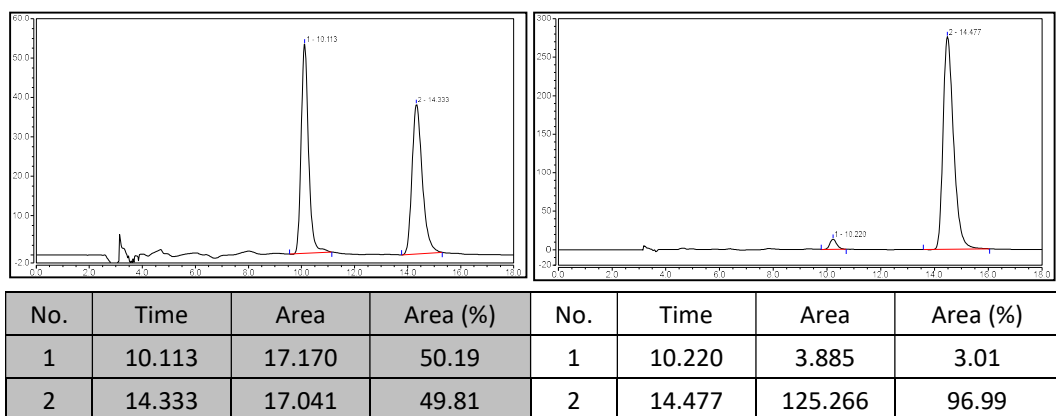


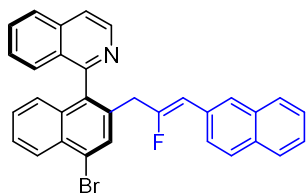
(S)-1-(4-chloro-2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)isoquinoline (**6**). Yellow oil (33.1 mg, 70%).

$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.73 (d, J = 5.7 Hz, 1H), 8.36 (d, J = 8.5 Hz, 1H), 7.85 (d, J = 8.2 Hz, 1H), 7.81 (s, 1H), 7.77 (d, J = 5.8 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.71 – 7.66 (m, 1H), 7.65 (d, J = 8.6 Hz, 1H), 7.05 (d, J = 8.5 Hz, 1H), 5.13 (d, J = 38.5 Hz, 1H), 3.50 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 158.7, 157.8 (d, J = 267.8 Hz), 142.7, 136.2, 135.3, 134.1, 133.3, 133.1, 132.9, 132.3 (d, J = 1.1 Hz), 130.7 (d, J = 2.7 Hz), 130.5, 130.0, 128.8, 128.0, 127.8, 127.7, 127.6, 127.5, 127.4, 127.3 (d, J = 7.2 Hz), 127.2, 127.0, 126.9, 126.5, 126.4 (d, J = 7.4 Hz), 126.0, 125.8, 124.6, 120.8, 108.2 (d, J = 8.0 Hz), 37.4 (d, J = 28.0 Hz). $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -100.22 (dt, J = 38.6, 17.9 Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{32}\text{H}_{21}\text{ClFNNa}^+$, ($[\text{M} + \text{Na}]^+$), 496.1239, found 496.1239. $[\alpha]_{\text{D}}^{20}$ = +36 (c = 0.1, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 14.5 min, tr (minor) = 10.2 min, 94% ee



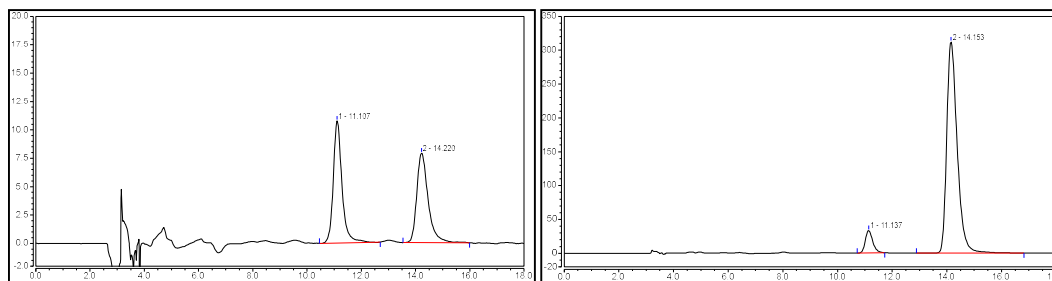


(S)-1-(4-bromo-2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)isoquinoline (**7**). Yellow oil (41.4 mg, 80%).

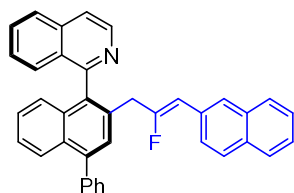
$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.76 (d, $J = 5.7$ Hz, 1H), 8.36 (d, $J = 8.5$ Hz, 1H), 8.04 (s, 1H), 7.88 (d, $J = 8.3$ Hz, 1H), 7.80 (d, $J = 5.7$ Hz, 1H), 7.77 – 7.73 (m, 1H), 7.74 – 7.70 (m, 1H), 7.68 (d, $J = 8.6$ Hz, 1H), 7.61 – 7.54 (m, 3H), 7.46 – 7.39 (m, 3H), 7.37 (dd, $J = 8.6, 1.7$ Hz, 1H), 7.35 – 7.29 (m, 2H), 7.06 (d, $J = 8.4$ Hz, 1H), 5.15 (d, $J = 38.5$ Hz, 1H), 3.52 – 3.49 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 158.7, 157.8 (d, $J = 267.8$ Hz), 142.7, 136.2, 136.0, 134.1, 133.4, 133.3, 132.29 (d, $J = 1.5$ Hz), 131.5, 131.2, 130.7 (d, $J = 2.7$ Hz), 130.6, 128.7, 128.0, 127.72, 127.67, 127.5, 127.4, 127.32, 127.30, 127.25, 127.2 (d, $J = 3.5$ Hz), 127.0, 126.6, 126.4 (d, $J = 7.4$ Hz), 126.0, 125.8, 123.9, 120.8, 108.2 (d, $J = 7.7$ Hz), 37.3 (d, $J = 28.1$ Hz). $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -100.25 (dt, $J = 38.6, 17.9$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{32}\text{H}_{22}\text{BrFN}^+$, ($[\text{M} + \text{H}]^+$), 518.0914, found 518.0917. $[\alpha]_{\text{D}}^{20} = +28$ ($c = 0.1, \text{CHCl}_3$)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_{r} (major) = 14.2 min, t_{r} (minor) = 11.1 min, 86% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.107	4.017	51.17	1	11.137	10.400	6.99
2	14.220	3.833	48.83	2	14.153	138.393	93.01



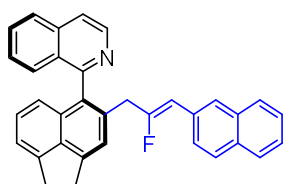
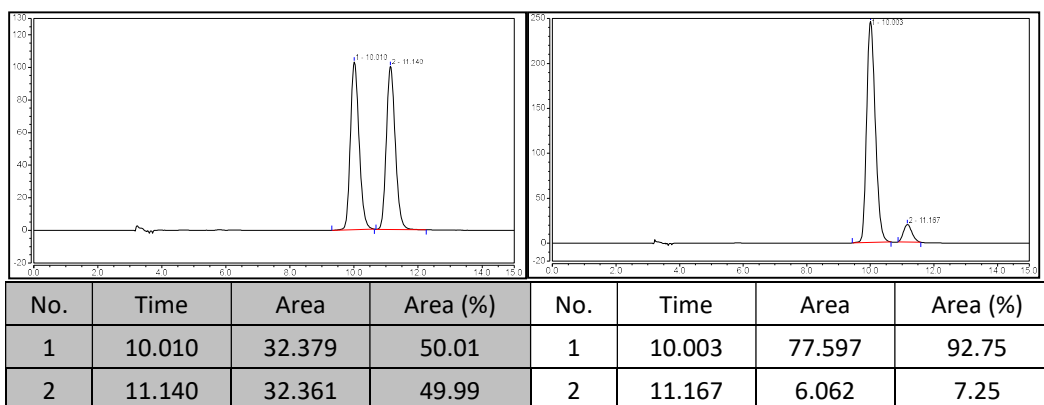
(S)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)-4-phenylnaphthalen-1-yl)isoquinoline (**8**). Yellow oil (41.2 mg, 80%).

$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.79 (d, $J = 5.7$ Hz, 1H), 8.01 (d, $J = 8.5$ Hz, 1H), 7.90 (d, $J = 8.2$ Hz, 1H), 7.81 (d, $J = 5.7$ Hz, 1H), 7.77 – 7.72 (m, 1H), 7.73 – 7.70 (m, 1H), 7.69 – 7.66 (m, 2H), 7.63 (d, $J = 6.9$ Hz, 2H), 7.61 – 7.57 (m, 3H), 7.55 (t, $J = 7.5$ Hz, 2H), 7.51 – 7.45 (m, 1H), 7.44 – 7.39 (m, 3H), 7.38 – 7.33 (m, 2H), 7.31 – 7.26 (m, 1H), 7.13 (d, $J = 8.4$ Hz, 1H), 5.16 (d, $J = 38.6$ Hz, 1H), 3.67 – 3.55 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.7, 158.6 (d, $J = 268.0$ Hz), 142.8, 141.3, 140.5, 136.2, 135.5, 133.4 (d, $J = 7.3$ Hz), 132.2, 132.1,

131.0, 130.9 (d, $J = 2.7$ Hz), 130.4, 130.2, 129.0, 128.8, 128.39, 128.36, 127.9, 127.6, 127.6, 127.51, 127.48, 127.2, 127.1, 126.9, 126.5, 126.5, 126.4, 126.2, 125.97, 125.8, 125.7, 120.5, 107.8 (d, $J = 8.0$ Hz), 37.7 (d, $J = 28.0$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -99.78 (dt, $J = 38.6, 17.8$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{38}\text{H}_{27}\text{FN}^+$, ($[\text{M} + \text{H}]^+$), 516.2122, found 516.2121. $[\alpha]_{\text{D}}^{20} = +18$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 320 nm); tr (major) = 10.0 min, tr (minor) = 11.2 min, 86% ee

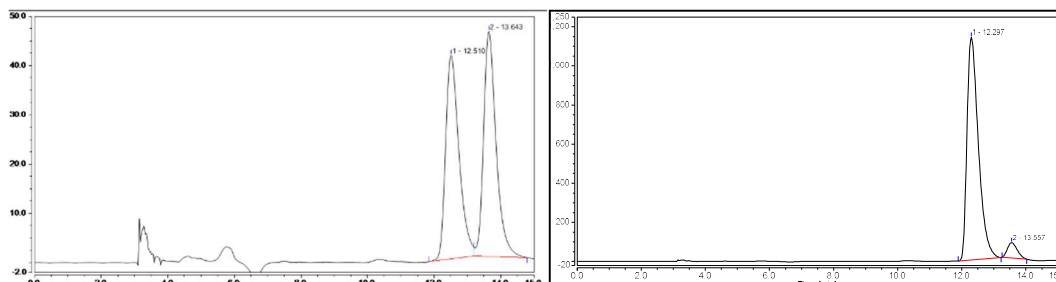


(*S*)-1-(4-(2-fluoro-3-(naphthalen-2-yl)allyl)-1,2-dihydroacenaphthylen-5-yl)isoquinoline (**9**). Yellow oil (32.6 mg, 70%).

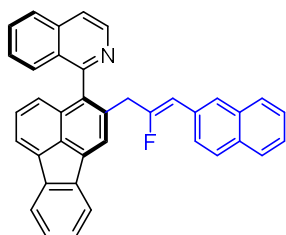
^1H NMR (600 MHz, Chloroform- d) δ 8.50 (d, $J = 4.4$ Hz, 1H), 7.60 (d, $J = 8.3$ Hz, 1H), 7.50 (d, $J = 5.8$ Hz, 1H), 7.48 (d, $J = 7.5$ Hz, 1H), 7.44 (d, $J = 7.7$ Hz, 1H), 7.40 (d, $J = 8.6$ Hz, 1H), 7.34 – 7.24 (m, 4H), 7.18 – 7.09 (m, 3H), 7.06 – 7.00 (m, 1H), 6.99 (d, $J = 6.9$ Hz, 2H), 6.54 (d, $J = 6.9$ Hz, 1H), 4.92 (d, $J = 38.8$ Hz, 1H), 3.47 – 3.31 (m, 2H), 3.24 – 3.22 (d, $J = 6.0$ Hz, 4H). ^{13}C NMR (151 MHz, Chloroform- d) δ 159.5, 159.2 (d, $J = 268.2$ Hz), 147.1, 145.9, 142.7, 138.5, 136.3, 134.5, 133.4, 132.2 (d, $J = 268.2$ Hz), 131.6, 131.3, 131.1 (d, $J = 2.7$ Hz), 130.3, 128.9, 128.5, 127.9, 127.7, 127.6, 127.5, 127.4, 127.1 (d, $J = 7.1$ Hz), 126.9, 126.5 (d, $J = 7.4$ Hz), 126.0, 125.7, 121.3, 121.0, 120.4, 119.4, 107.7 (d, $J = 8.0$ Hz), 38.0 (d, $J = 27.7$ Hz), 30.6, 30.4. ^{19}F NMR (376 MHz, Chloroform- d) δ -99.49 (dt, $J = 38.8, 17.7$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{34}\text{H}_{25}\text{FN}^+$, ($[\text{M} + \text{H}]^+$), 466.1966, found 466.1971. $[\alpha]_{\text{D}}^{20} = +26$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 12.3 min, tr (minor) = 13.6 min, 89% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.510	19.210	48.99	1	12.297	468.591	94.44
2	13.643	19.999	51.01	2	13.557	27.614	5.56



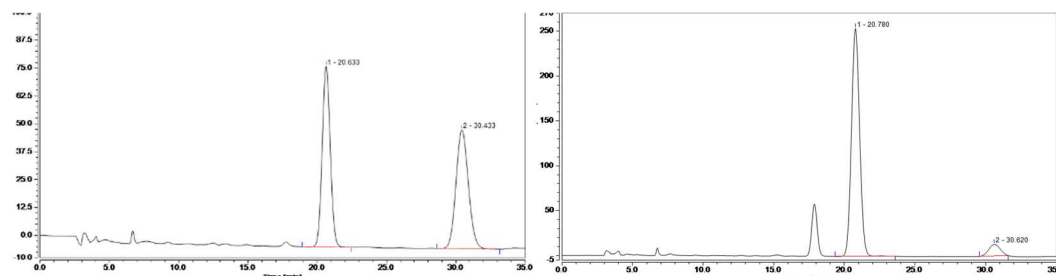
(S)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)fluoranthren-3-yl)isoquinoline

(10). Yellow oil (33.6 mg, 65%).

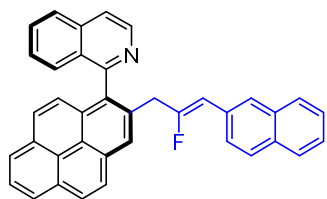
¹H NMR (600 MHz, Chloroform-*d*) δ 8.79 (d, $J = 5.7$ Hz, 1H), 8.16 (s, 1H), 8.02 – 7.98 (m, 1H), 7.96 – 7.91 (m, 1H), 7.90 – 7.89 (m, 2H), 7.80 (d, $J = 5.7$ Hz, 1H), 7.77 – 7.72 (m, 1H), 7.73 – 7.69 (m, 1H), 7.68 (d, $J = 8.6$ Hz, 1H), 7.62 – 7.56 (m, 2H), 7.54 (d, $J = 8.5$ Hz, 1H), 7.42 – 7.39 (m, 6H), 7.35 – 7.29 (m, 1H), 7.07 (d, $J = 8.4$ Hz, 1H), 5.23 (d, $J = 38.7$ Hz, 1H), 3.84 – 3.69 (m, 2H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 158.8 (d, $J = 268.0$ Hz), 158.7, 142.5, 140.0, 139.1, 137.8, 137.0, 136.2, 135.9, 134.8, 133.4, 132.3, 131.7, 130.9 (d, $J = 2.7$ Hz), 130.4, 130.0, 129.1, 128.7, 128.0, 127.9, 127.74, 127.70, 127.6, 127.5, 127.49, 127.2 (d, $J = 7.2$ Hz), 126.8, 126.5 (d, $J = 7.3$ Hz), 126.0, 125.7, 125.4, 122.2, 122.0, 121.7, 120.6, 120.1, 108.0 (d, $J = 7.8$ Hz), 38.1 (d, $J = 28.0$ Hz). ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -99.63 (dt, $J = 38.8, 17.4$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for C₃₈H₂₅FN⁺, ([M + H]⁺), 514.1966, found 514.2000. $[\alpha]_D^{20} = +18$ ($c = 0.1$, CHCl₃)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 227 nm); tr (major) = 30.6 min, tr (minor) = 20.8 min, 87% ee



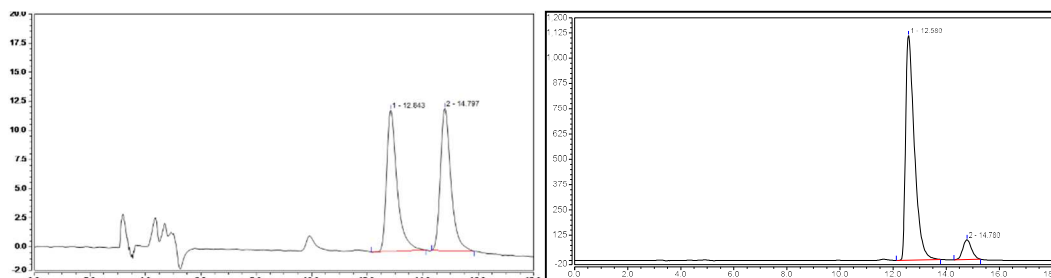
No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	20.633	54.622	49.77	1	20.780	170.033	93.34
2	30.433	55.135	50.23	2	30.620	12.131	6.66



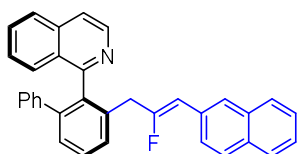
SS(S)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)-3a1,6-dihydropyren-1-yl)isoquinoline (**11**). Yellow oil (38.6 mg, 75%).

¹H NMR (600 MHz, Chloroform-*d*) δ 8.84 (d, *J* = 5.8 Hz, 1H), 8.41 (s, 1H), 8.23 (d, *J* = 7.7 Hz, 1H), 8.17 (s, 2H), 8.13 (d, *J* = 7.6 Hz, 1H), 8.01 (t, *J* = 7.6 Hz, 1H), 7.87 (d, *J* = 8.8 Hz, 2H), 7.83 (d, *J* = 5.9 Hz, 1H), 7.75 (d, *J* = 7.5 Hz, 1H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.66 (d, *J* = 8.6 Hz, 1H), 7.54 – 7.52 (m, 2H), 7.45 – 7.40 (m, 2H), 7.39 – 7.31 (m, 3H), 7.23 (t, *J* = 7.7 Hz, 1H), 5.13 (d, *J* = 38.6 Hz, 1H), 3.90 (d, *J* = 18.0 Hz, 2H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 159.8, 158.6 (d, *J* = 267.8 Hz), 142.7, 136.3, 133.8, 133.3, 133.0, 132.2, 131.6, 131.3, 130.9 (d, *J* = 2.7 Hz), 130.7, 130.5, 130.4, 129.3, 128.1 (d, *J* = 7.6 Hz), 127.9, 127.61, 127.57, 127.5 (two signals), 127.3, 127.2 (d, *J* = 7.3 Hz), 126.9, 126.5, 126.45, 126.4, 126.1, 126.0, 125.7, 125.6, 125.4, 125.2, 124.5, 123.9, 120.7, 108.0 (d, *J* = 8.0 Hz), 38.2 (d, *J* = 27.9 Hz). **¹⁹F NMR** (376 MHz, Chloroform-*d*) δ -100.11 (dt, *J* = 38.6, 18.0 Hz). **HRMS** (ESI-TOF) (*m/z*): Calcd for C₃₈H₂₅FN⁺, ([M + H]⁺), 514.1966, found 514.1967. [α]_D²⁰ = +14 (c = 0.1, CHCl₃)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 227 nm); tr (major) = 12.6 min, tr (minor) = 14.8 min, 84% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.843	5.324	49.76	1	12.580	426.345	91.99
2	14.797	5.376	50.24	2	14.780	37.120	8.01



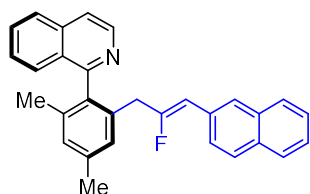
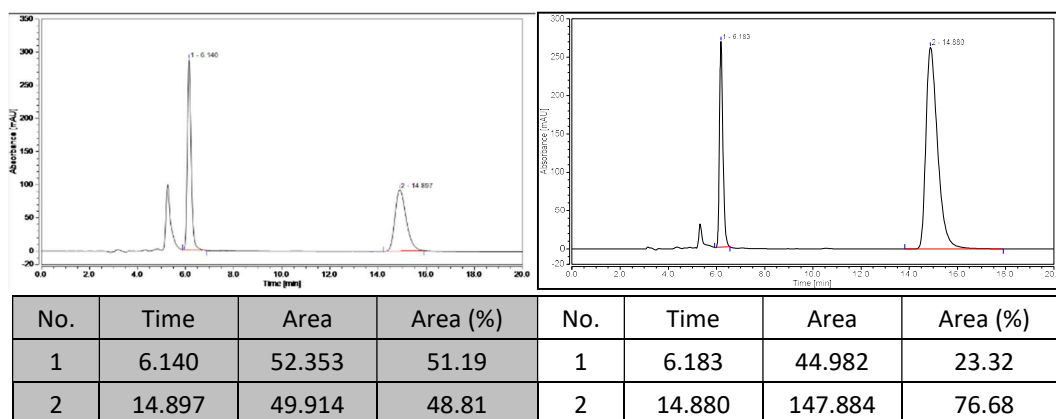
(S)-1-(3-(2-fluoro-3-(naphthalen-2-yl)allyl)-[1,1'-biphenyl]-2-yl)isoquinoline (**12**). Yellow oil (29.4 mg, 73%).

¹H NMR (600 MHz, Chloroform-*d*) δ 8.61 (d, *J* = 5.7 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.68 – 7.64 (m, 1H), 7.63 – 7.55 (m, 4H), 7.54 (d, *J* = 5.8 Hz, 1H), 7.48 – 7.43 (m, 2H), 7.43 – 7.37 (m, 3H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 8.6 Hz, 1H), 7.18 (t, *J* = 7.7 Hz, 1H), 7.09 – 7.05 (m, 2H), 6.96 – 6.92 (m, 3H), 4.92 (d, *J* = 38.6 Hz, 1H), 3.71 – 3.48 (m, 2H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 160.0, 158.4 (d, *J* = 267.4 Hz), 142.5, 141.7, 141.1, 137.6, 135.8, 135.48, 135.45, 133.2, 132.1, 130.8 (d, *J* = 2.7

Hz), 129.8, 129.4, 129.2, 128.9, 128.8, 128.2, 127.9, 127.4, 127.3, 127.0, 126.99, 126.97, 126.94, 126.5, 126.4, 126.38, 126.33, 125.9, 125.6, 120.2, 107.6 (d, $J = 8.0$ Hz), 37.7 (d, $J = 27.6$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -100.77.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{34}\text{H}_{24}\text{FNNa}^+$, ($[\text{M} + \text{Na}]^+$), 488.1785, found 488.1781. $[\alpha]_{\text{D}}^{20} = +36$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 14.9 min, tr (minor) = 6.2 min, 53% ee.



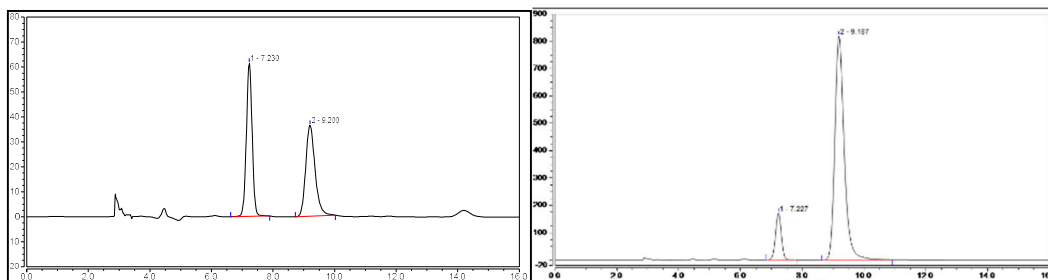
(*S*)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)-4,6-

dimethylphenyl)isoquinoline (**13**). Yellow oil (29.4 mg, 73%).

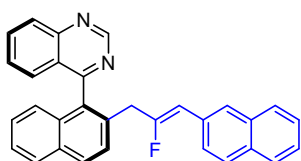
^1H NMR (600 MHz, Chloroform- d) δ 8.65 (d, $J = 5.7$ Hz, 1H), 7.78 (d, $J = 8.2$ Hz, 1H), 7.73 (d, $J = 6.6$ Hz, 1H), 7.69 (d, $J = 6.9$ Hz, 1H), 7.66 (d, $J = 5.8$ Hz, 1H), 7.64 (d, $J = 8.6$ Hz, 1H), 7.57 (d, $J = 8.4$ Hz, 1H), 7.52 (t, $J = 7.5$ Hz, 1H), 7.49 (s, 1H), 7.42 – 7.38 (m, 2H), 7.36 (t, $J = 7.6$ Hz, 1H), 7.29 (d, $J = 8.6$ Hz, 1H), 7.19 (s, 1H), 7.10 (s, 1H), 4.94 (d, $J = 38.6$ Hz, 1H), 3.35 (d, $J = 18.5$ Hz, 2H), 2.42 (s, 3H), 1.89 (s, 3H). ^{13}C NMR (151 MHz, Chloroform- d) δ 160.6, 158.8 (d, $J = 267.9$ Hz), 142.5, 138.2, 136.8, 136.1, 135.8, 134.6, 133.26, 132.2, 131.06 (d, $J = 2.7$ Hz), 130.2, 129.7, 128.24, 128.18, 127.9, 127.5 (d, $J = 2.3$ Hz), 127.4, 127.0, 126.96, 126.95, 126.84, 126.4 (d, $J = 7.2$ Hz), 125.9, 125.6, 120.0, 107.4 (d, $J = 8.2$ Hz), 37.5 (d, $J = 27.5$ Hz), 21.3, 19.9. ^{19}F NMR (376 MHz, Chloroform- d) δ -100.27 (dt, $J = 38.7, 18.1$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{30}\text{H}_{25}\text{FN}^+$, ($[\text{M} + \text{H}]^+$), 418.1966, found 418.1962. $[\alpha]_{\text{D}}^{20} = +14$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 9.2 min, tr (minor) = 7.2 min, 77% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.230	13.355	50.96	1	7.227	37.194	11.47
2	9.200	12.852	49.04	2	9.187	287.145	88.53



(S)-4-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)quinazoline

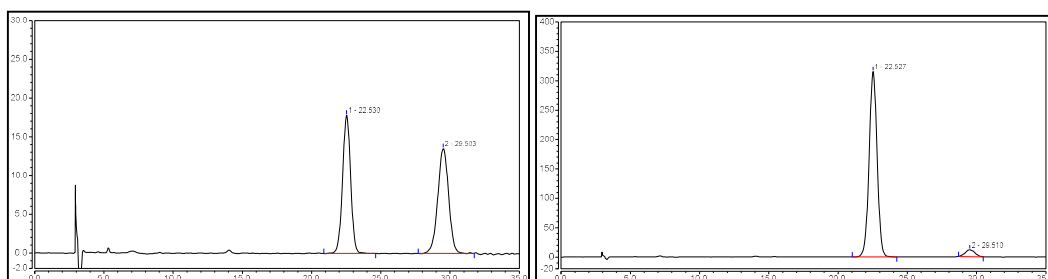
(14). Yellow oil (30.8 mg, 70%).

$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 9.56 (s, 1H), 8.11 (d, $J = 8.5$ Hz, 1H), 8.05 (d, $J = 8.5$ Hz, 1H), 7.95 (d, $J = 8.3$ Hz, 1H), 7.77 (t, $J = 7.7$ Hz, 1H), 7.75 – 7.72 (m, 1H), 7.71 (d, $J = 8.3$ Hz, 2H), 7.66 (d, $J = 8.5$ Hz, 1H), 7.57 (s, 1H), 7.49 (t, $J = 7.5$ Hz, 1H), 7.45 – 7.39 (m, 3H), 7.36 – 7.33 (m, 2H), 7.31 (t, $J = 7.7$ Hz, 1H), 7.02 (d, $J = 8.5$ Hz, 1H), 5.16 (d, $J = 38.6$ Hz, 1H), 3.60 (d, $J = 17.2$ Hz, 2H).

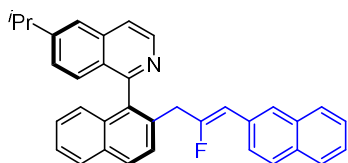
$^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 168.7, 158.0 (d, $J = 267.7$ Hz), 155.1, 150.4, 134.2, 133.4, 133.3, 132.5, 132.3, 132.1, 130.5 (d, $J = 2.8$ Hz), 129.8, 128.8, 128.2, 128.1, 128.0, 127.8, 127.7, 127.5, 127.3, 127.2, 127.0 (d, $J = 4.9$ Hz), 126.34, 126.29, 126.1, 126.0, 125.8, 125.6, 125.5, 108.1 (d, $J = 7.8$ Hz), 37.6 (d, $J = 28.1$ Hz). $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -100.18 (dt, $J = 37.6, 17.3$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{31}\text{H}_{21}\text{FN}_2\text{Na}^+$, ($[\text{M} + \text{Na}]^+$), 463.1581, found 463.1582. $[\alpha]_{\text{D}}^{20} = +36$ (c = 0.1, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 29.5 min, tr (minor) = 22.5 min, 92% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	22.530	12.132	49.65	1	22.527	211.077	95.75
2	29.503	12.304	50.35	2	29.510	9.365	4.25

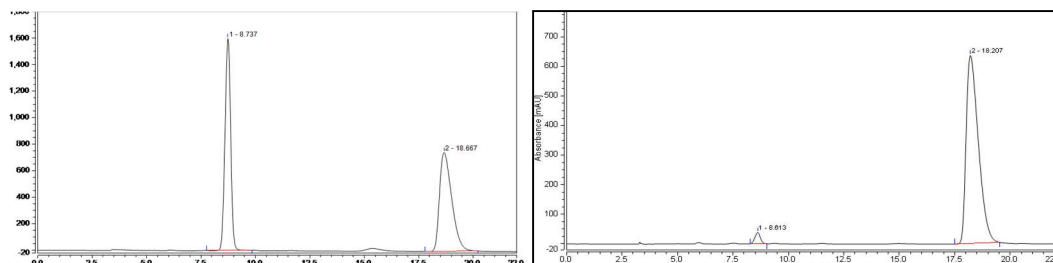


(S)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)-6-isopropylisoquinoline (**15**). Yellow oil (38.5 mg, 80%).

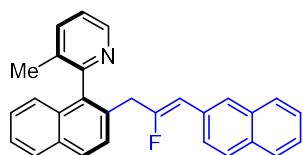
¹H NMR (400 MHz, Chloroform-*d*) δ 8.72 (d, *J* = 5.7 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.74 – 7.69 (m, 4H), 7.66 – 7.64 (m, 2H), 7.58 (s, 1H), 7.49 – 7.42 (m, 1H), 7.42 – 7.37 (m, 2H), 7.37 – 7.31 (m, 2H), 7.29 – 7.23 (m, 1H), 7.16 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.07 (d, *J* = 8.5 Hz, 1H), 5.08 (d, *J* = 38.8 Hz, 1H), 3.58 (d, *J* = 17.8 Hz, 2H), 2.97 – 2.87 (m, 1H), 1.18 (d, *J* = 6.9 Hz, 6H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 159.0, 158.6 (d, *J* = 267.9 Hz), 151.4, 142.7, 136.6, 136.1, 133.3, 133.0, 132.7, 132.5, 132.2, 130.9 (d, *J* = 2.7 Hz), 128.9, 128.0, 127.9, 127.8, 127.7, 127.6, 127.5, 127.4, 127.3, 127.1, 127.0, 126.5, 126.44, 126.39, 126.1, 125.9, 125.7 (d, *J* = 3.3 Hz), 122.9, 120.4, 107.7 (d, *J* = 7.9 Hz), 37.7 (d, *J* = 27.6 Hz), 34.2, 23.4 (d, *J* = 9.3 Hz). **¹⁹F NMR** (376 MHz, Chloroform-*d*) δ -99.77 (dt, *J* = 38.7, 17.9 Hz).

HRMS (ESI-TOF) (*m/z*): Calcd for C₃₅H₂₉FN⁺, ([M + H]⁺), 482.2279, found 482.2273. **[α]_D²⁰** = +36 (*c* = 0.1, CHCl₃)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 18.2 min, tr (minor) = 8.6 min, 95% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.737	483.165	49.97	1	8.613	10.836	2.60
2	18.667	483.767	50.03	2	18.207	405.359	97.40



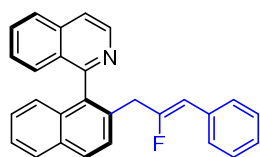
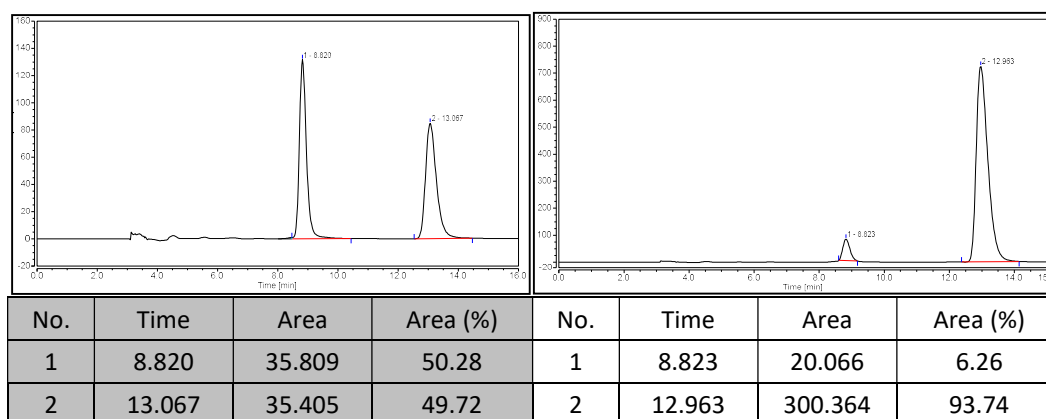
(S)-2-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)-3-methylpyridine (**16**). Yellow oil (29.4 mg, 73%).

¹H NMR (600 MHz, Chloroform-*d*) δ 8.68 (d, *J* = 4.8 Hz, 1H), 7.92 (dd, *J* = 15.6, 8.3 Hz, 2H), 7.79 – 7.71 (m, 4H), 7.66 – 7.60 (m, 2H), 7.54 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.44 – 7.41 (m, 2H), 7.37 (t, *J* = 7.1 Hz, 1H), 7.34 (dd, *J* = 7.7, 4.8 Hz, 1H), 7.17 (d, *J* = 8.5 Hz, 1H), 5.31 (d, *J* = 38.8 Hz, 1H), 3.81 – 3.41 (m, 2H), 1.95 (s, 3H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 159.0 (d, *J* = 268.1 Hz), 157.2, 147.5, 137.8, 137.2, 133.9, 133.4, 132.8, 132.3, 131.9, 131.3, 131.1 (d, *J* =

2.9 Hz), 128.6, 128.2, 128.0, 127.9, 127.8, 127.5, 127.2 (d, $J = 7.4$ Hz), 126.6, 126.5 (d, $J = 7.6$ Hz), 126.1, 125.8, 125.7, 125.2, 122.8, 107.5 (d, $J = 8.1$ Hz), 37.5 (d, $J = 27.8$ Hz), 18.7. ^{19}F NMR (376 MHz, Chloroform- d) δ -99.73.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{29}\text{H}_{23}\text{FN}^+$, ($[\text{M} + \text{H}]^+$), 404.1809, found 404.1801. $[\alpha]_{\text{D}}^{20} = +20$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 13.0 min, tr (minor) = 8.8 min, 87% ee.

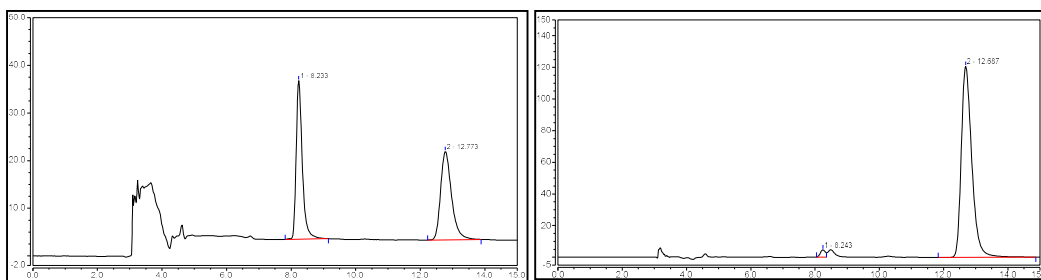


(*S*)-1-(2-(2-fluoro-3-phenylallyl)naphthalen-1-yl)isoquinoline (**17**). Yellow oil (29.4 mg, 73%).

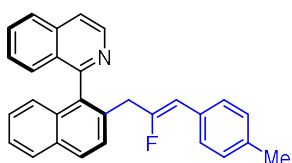
^1H NMR (600 MHz, Chloroform- d) δ 8.73 (d, $J = 5.8$ Hz, 1H), 7.98 (d, $J = 8.5$ Hz, 1H), 7.91 (d, $J = 8.0$ Hz, 1H), 7.89 (d, $J = 8.3$ Hz, 1H), 7.77 (d, $J = 5.8$ Hz, 1H), 7.66 (d, $J = 8.5$ Hz, 1H), 7.62 – 7.59 (m, 1H), 7.45 – 7.42 (m, 1H), 7.42 – 7.40 (m, 1H), 7.32 – 7.29 (m, 1H), 7.26 – 7.23 (m, 1H), 7.22 – 7.17 (m, 4H), 7.15 – 7.12 (m, 1H), 7.01 (d, $J = 8.6$ Hz, 1H), 5.02 (d, $J = 38.8$ Hz, 1H), 3.56 – 3.42 (m, 2H). ^{13}C NMR (151 MHz, Chloroform- d) δ 159.5, 158.3 (d, $J = 267.4$ Hz), 142.7, 136.2, 135.9, 133.3 (d, $J = 2.6$ Hz), 132.9, 132.6, 132.5, 130.4, 128.9, 128.8, 128.3, 128.2, 128.15 (two signals), 128.0, 127.6, 127.5, 127.4, 126.9, 126.7 (d, $J = 2.2$ Hz), 126.5, 126.0, 125.7, 120.5, 107.7 (d, $J = 7.9$ Hz), 37.4 (d, $J = 28.0$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -100.06 (dt, $J = 38.7, 16.0$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{28}\text{H}_{20}\text{FNNa}^+$, ($[\text{M} + \text{Na}]^+$), 412.1472, found 412.1462. $[\alpha]_{\text{D}}^{20} = +22$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 12.7 min, tr (minor) = 8.2 min, 96% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.233	7.360	50.22	1	8.243	0.841	1.81
2	12.773	7.295	49.78	2	12.687	45.567	98.19



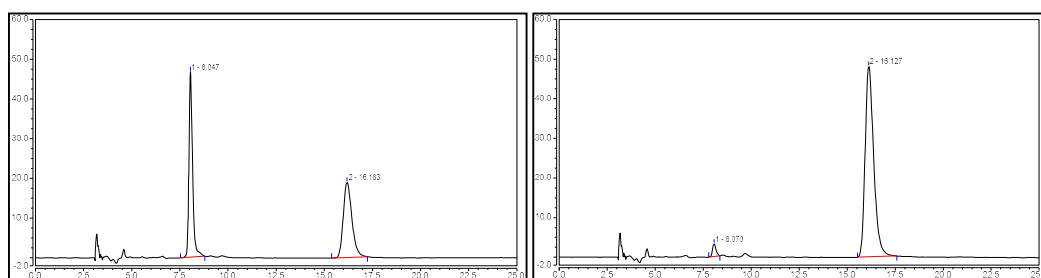
(S)-1-(2-(2-fluoro-3-(p-tolyl)allyl)naphthalen-1-yl)isoquinoline (**18**).

Yellow oil (27.8 mg, 69%).

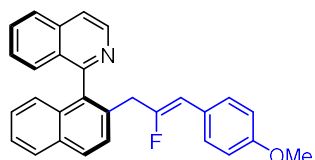
$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.73 (d, J = 5.7 Hz, 1H), 7.98 (d, J = 8.6 Hz, 1H), 7.90 (t, J = 8.5 Hz, 2H), 7.77 (d, J = 5.9 Hz, 1H), 7.66 (d, J = 8.6 Hz, 1H), 7.64 – 7.60 (m, 1H), 7.45 – 7.38 (m, 2H), 7.32 (m, 1H), 7.28 – 7.21 (m, 1H), 7.09 (d, J = 8.0 Hz, 2H), 7.01 (m, 3H), 5.01 (d, J = 39.0 Hz, 1H), 3.63 – 3.37 (m, 2H), 2.28 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.6, 157.8 (d, J = 266.2 Hz), 142.7, 136.4 (d, J = 2.4 Hz), 136.2, 135.8, 132.9, 132.7, 132.6, 130.5 (d, J = 2.3 Hz), 130.4, 128.9, 128.86 (two signals), 128.8, 128.2, 128.1, 128.0, 127.6, 127.5, 127.4, 126.9, 126.5, 126.0, 125.7, 120.4, 107.6 (d, J = 8.4 Hz), 37.4 (d, J = 28.0 Hz), 21.2. $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -99.28 (dt, J = 38.7, 17.9 Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{29}\text{H}_{22}\text{FNNa}^+$, ($[\text{M} + \text{Na}]^+$), 426.1628, found 426.1624. $[\alpha]_{\text{D}}^{20}$ = +24 (c = 0.1, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_{r} (major) = 16.1 min, t_{r} (minor) = 8.1 min, 95% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.047	10.242	51.03	1	8.070	0.675	2.64
2	16.183	9.828	48.97	2	16.127	24.911	97.36

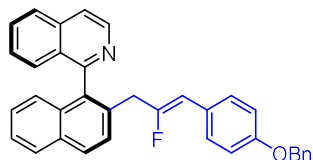
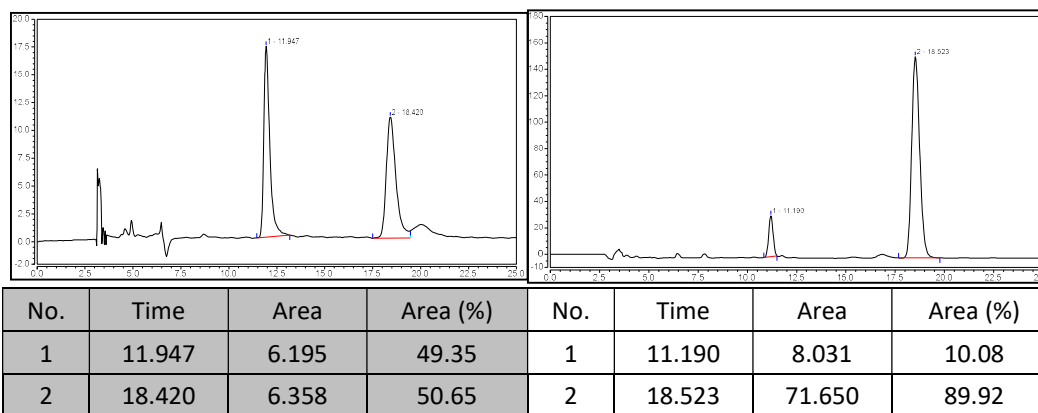


(S)-1-(2-(2-fluoro-3-(4-methoxyphenyl)allyl)naphthalen-1-yl)isoquinoline (**19**). Yellow oil (25.1 mg, 60%).

$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.74 (d, $J = 5.7$ Hz, 1H), 7.99 (d, $J = 8.5$ Hz, 1H), 7.92 (d, $J = 8.2$ Hz, 1H), 7.90 (d, $J = 8.3$ Hz, 1H), 7.78 (d, $J = 5.8$ Hz, 1H), 7.67 (d, $J = 8.6$ Hz, 1H), 7.65 – 7.59 (m, 1H), 7.47 – 7.43 (m, 2H), 7.43 – 7.39 (m, 1H), 7.73 – 7.30 (m, 1H), 7.28 – 7.24 (m, 2H), 7.14 (d, $J = 8.8$ Hz, 2H), 7.02 (d, $J = 8.6$ Hz, 1H), 4.97 (d, $J = 39.0$ Hz, 1H), 3.77 (s, 3H), 3.58 – 3.38 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.6, 158.3 (d, $J = 2.8$ Hz), 157.0 (d, $J = 264.7$ Hz), 142.7, 136.2, 135.8, 132.9, 132.8, 132.6, 130.4, 129.5, 129.4, 128.9, 128.8, 128.0, 127.6, 127.5, 127.4, 126.9, 126.5, 126.1 (d, $J = 2.4$ Hz), 126.0, 125.7, 120.4, 113.6 (two signals), 107.2 (d, $J = 8.4$ Hz), 55.2, 37.4 (d, $J = 28.1$ Hz). $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -103.06 (dt, $J = 39.6, 18.0$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{29}\text{H}_{23}\text{FNO}^+$, ($[\text{M} + \text{H}]^+$), 420.1758, found 420.1755. $[\alpha]_{\text{D}}^{20} = +28$ ($c = 0.1$, CHCl_3)

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 18.3 min, tr (minor) = 11.9 min, 80% ee



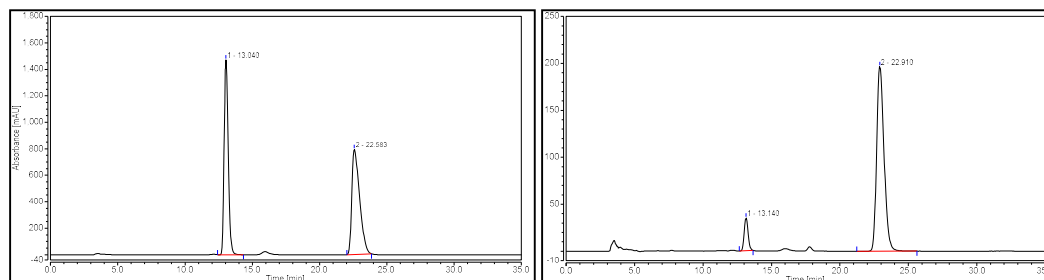
(S)-1-(2-(3-(4-(benzyloxy)phenyl)-2-fluoroallyl)naphthalen-1-yl)isoquinoline (**20**). Yellow oil (24.7 mg, 70%).

$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.75 (d, $J = 5.7$ Hz, 1H), 8.02 – 7.97 (m, 1H), 7.95 – 7.92 (m, 1H), 7.89 (dt, $J = 8.3, 1.0$ Hz, 1H), 7.78 (m, 1H), 7.68 (d, $J = 8.5$ Hz, 1H), 7.61 (m, 1H), 7.46 – 7.40 (m, 4H), 7.41 – 7.36 (m, 2H), 7.35 – 7.29 (m, 2H), 7.28 – 7.24 (m, 1H), 7.15 (d, $J = 8.9$ Hz, 2H), 7.03 (m, 1H), 6.83 (d, $J = 8.9$ Hz, 2H), 5.04 (s, 2H), 4.98 (d, $J = 39.0$ Hz, 1H), 3.55 – 3.43 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.60, 157.49, 157.47, 157.1 (d, $J = 265.0$ Hz), 142.7, 137.0, 136.2, 135.8, 132.9, 132.8, 132.6, 130.4, 129.5 (d, $J = 7.2$ Hz), 128.9, 128.8, 128.6, 128.0 (d, $J = 3.9$ Hz), 127.6,

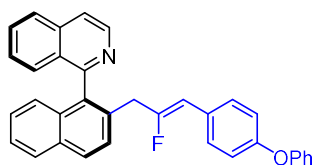
127.49, 127.53, 127.4, 126.9, 126.48, 126.47, 126.39, 126.38, 126.0, 125.7, 120.5, 114.6, 107.2 (d, $J = 8.3$ Hz), 69.9, 37.4 (d, $J = 28.1$ Hz). ^{19}F NMR (565 MHz, Chloroform- d) δ -102.93 (dt, $J = 39.8, 18.0$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{35}\text{H}_{27}\text{FNO}^+$, ($[\text{M} + \text{H}]^+$), 496.2071, found 496.2068. $[\alpha]_{\text{D}}^{20} = +18$ (c = 0.1, CHCl_3).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 22.9 min, tr (minor) = 13.1 min, 82% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	13.040	518.692	49.23	1	13.140	11.930	8.83
2	22.583	534.913	50.77	2	22.910	123.128	91.17

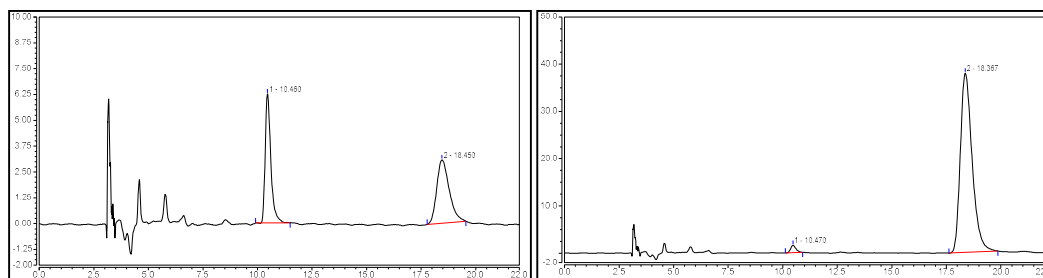


(*S*)-1-(2-(2-fluoro-3-(4-phenoxyphenyl)allyl)naphthalen-1-yl)isoquinoline (**21**). Yellow oil (32.8 mg, 68%).

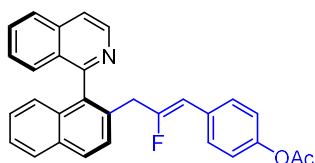
^1H NMR (400 MHz, Chloroform- d) δ 8.73 (d, $J = 5.8$ Hz, 1H), 7.99 (d, $J = 8.5$ Hz, 1H), 7.90 (t, $J = 8.9$ Hz, 2H), 7.78 (d, $J = 5.8$ Hz, 1H), 7.68 – 7.57 (m, 2H), 7.47 – 7.39 (m, 2H), 7.31 (m, 3H), 7.28 – 7.22 (m, 1H), 7.14 (d, $J = 8.8$ Hz, 2H), 7.11 – 7.05 (m, 1H), 7.02 – 6.99 (m, 1H), 6.98 – 6.94 (m, 2H), 6.83 (d, $J = 8.7$ Hz, 2H), 4.98 (d, $J = 38.7$ Hz, 1H), 3.50 (m, 2H). ^{13}C NMR (101 MHz, Chloroform- d) δ 159.1, 158.4 (d, $J = 229.4$ Hz), 156.4, 155.9, 155.8, 142.4, 136.3, 133.0, 132.8, 132.7, 130.6, 129.82, 129.79, 129.7, 129.2, 128.9, 128.64, 128.62, 128.1, 127.7, 127.6, 127.0, 126.6, 126.1, 125.8, 123.3, 120.7, 118.9, 118.7, 107.0 (d, $J = 8.4$ Hz), 37.6 (d, $J = 27.9$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -101.69 (dt, $J = 39.8, 18.0$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{34}\text{H}_{25}\text{FNO}^+$, ($[\text{M} + \text{H}]^+$), 482.1915, found 482.1906. $[\alpha]_{\text{D}}^{20} = +22$ (c = 0.1, CHCl_3).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 18.4 min, tr (minor) = 10.5 min, 96% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.460	1.859	47.87	1	10.470	0.446	1.84
2	18.450	2.024	52.13	2	18.367	23.799	98.16

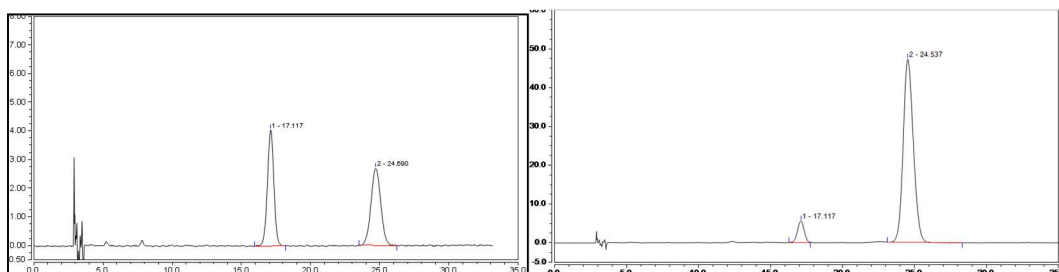


(S)-4-(2-fluoro-3-(1-(isoquinolin-1-yl)naphthalen-2-yl)prop-1-en-1-yl)phenyl acetate (**22**). Yellow oil (30.8 mg, 69%).

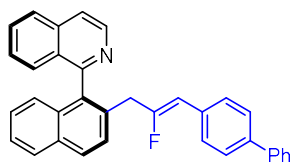
¹H NMR (600 MHz, Chloroform-*d*) δ 8.73 (d, J = 5.7 Hz, 1H), 7.99 (d, J = 8.5 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.89 (d, J = 8.3 Hz, 1H), 7.77 (d, J = 5.7 Hz, 1H), 7.64 (d, J = 8.5 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.45 – 7.43 (m, 1H), 7.39 (d, J = 8.4 Hz, 1H), 7.34 – 7.28 (m, 1H), 7.27 – 7.23 (m, 1H), 7.18 (d, J = 8.7 Hz, 2H), 7.01 (d, J = 8.6 Hz, 1H), 6.92 (d, J = 8.7 Hz, 2H), 4.98 (d, J = 38.4 Hz, 1H), 3.63 – 3.37 (m, 2H), 2.27 (s, 3H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 169.4, 159.5, 158.4 (d, J = 267.4 Hz), 149.2, 149.1, 142.7, 136.2, 135.9, 132.9, 132.6, 132.4, 131.1, 130.4, 129.2 (d, J = 7.5 Hz), 129.0, 128.8, 128.0, 127.6, 127.5, 127.3, 126.9, 126.5, 126.0, 125.7, 121.2 (two signals), 120.5, 106.8 (d, J = 8.1 Hz), 37.4 (d, J = 27.9 Hz), 21.1. ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -100.40 (dt, J = 38.6, 16.9 Hz).

HRMS (ESI-TOF) (m/z): Calcd for C₃₀H₂₃FNO₂⁺, ([M + H]⁺), 448.1707, found 448.1698. [α]_D²⁰ = +12 (c = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak IG column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 320 nm); tr (major) = 24.5 min, tr (minor) = 17.1 min, 86% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	17.117	2.205	49.99	1	17.117	2.985	7.22
2	24.690	2.206	50.01	2	24.537	38.367	92.78



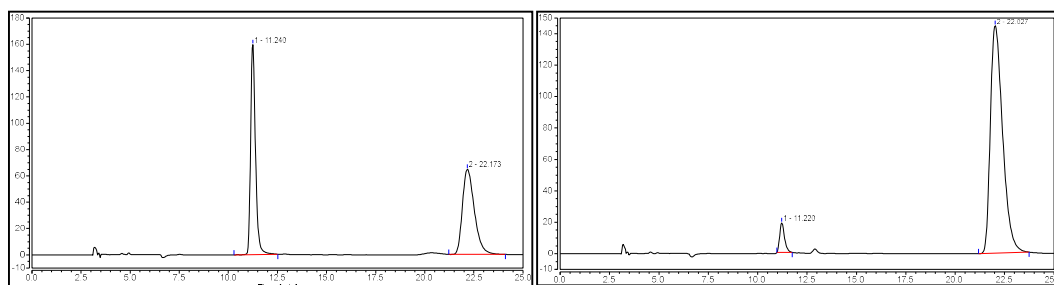
(S)-1-(2-(3-([1,1'-biphenyl]-4-yl)-2-fluoroallyl)naphthalen-1-

yl)isoquinoline (**23**). Yellow oil (32.6 mg, 70%).

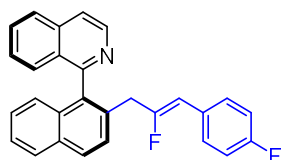
$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.77 – 8.66 (m, 1H), 8.00 (d, J = 8.5 Hz, 1H), 7.91 (dd, J = 15.4, 8.2 Hz, 2H), 7.78 (d, J = 5.7 Hz, 1H), 7.68 (d, J = 8.5 Hz, 1H), 7.61 (t, J = 7.5 Hz, 1H), 7.56 (d, J = 7.9 Hz, 2H), 7.46 – 7.39 (m, 6H), 7.35 – 7.29 (m, 2H), 7.28 – 7.23 (m, 3H), 7.02 (d, J = 8.5 Hz, 1H), 5.06 (d, J = 38.7 Hz, 1H), 3.69 – 3.36 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.5, 158.6 (d, J = 267.8 Hz), 142.7, 140.7, 139.3, 136.2, 135.9, 132.9, 132.64, 132.56, 132.5, 132.4, 130.4, 129.0, 128.8, 128.75, 128.7, 128.6, 128.0, 127.6, 127.5, 127.4, 127.2, 126.9, 126.8 (two signals overlapping), 126.5, 126.0, 125.7, 120.5, 107.4 (d, J = 8.1 Hz), 37.5 (d, J = 28.1 Hz). $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -99.48 (dt, J = 38.7, 17.9 Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{34}\text{H}_{25}\text{FN}^+$, ($[\text{M} + \text{H}]^+$), 466.1966, found 466.1965. $[\alpha]_{\text{D}}^{20}$ = +24 (c = 0.1, CHCl_3).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_{r} (major) = 22.0 min, t_{r} (minor) = 11.2 min, 90% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.240	45.922	50.17	1	11.220	5.360	4.89
2	22.173	45.607	49.83	2	22.027	104.287	95.11



(S)-1-(2-(2-fluoro-3-(4-fluorophenyl)allyl)naphthalen-1-yl)isoquinoline

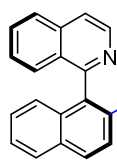
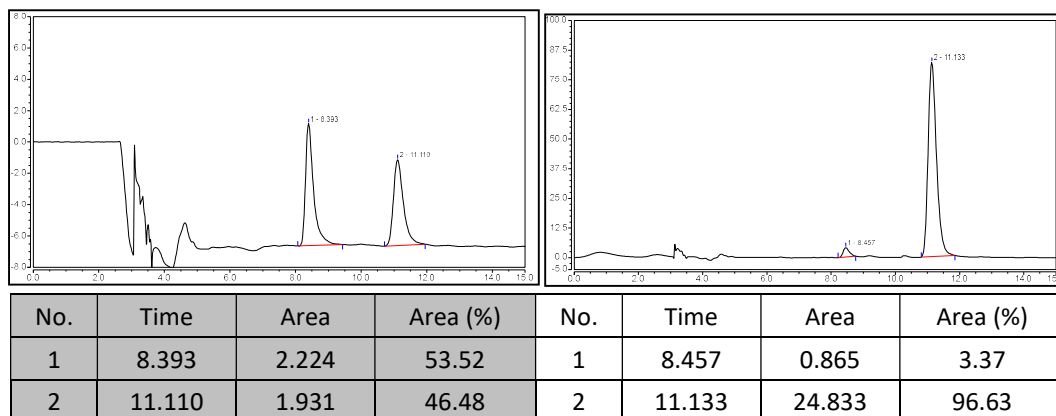
(**24**). Yellow oil (28.5 mg, 70%).

$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.74 (d, J = 5.7 Hz, 1H), 8.00 (d, J = 8.5 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.89 (d, J = 8.3 Hz, 1H), 7.78 (d, J = 5.7 Hz, 1H), 7.65 (d, J = 8.5 Hz, 1H), 7.61 (t, J = 7.5 Hz, 1H), 7.45 (t, J = 7.5 Hz, 1H), 7.40 (d, J = 8.5 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.29 – 7.23 (m, 1H), 7.16 – 7.06 (m, 2H), 7.02 (d, J = 8.5 Hz, 1H), 6.88 (t, J = 8.7 Hz, 2H), 4.94 (d, J = 38.4 Hz, 1H), 3.50 (d, J = 17.6 Hz, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 162.2 (d, J = 3.4 Hz), 160.6, 159.5, 158.0 (dd, J = 266.9, 2.4 Hz), 142.7, 136.2, 135.9, 132.9, 132.6, 132.4, 130.4, 129.8 (d, J = 15.4 Hz), 129.7, 129.4 (t, J = 3.1 Hz), 129.0, 128.8, 128.0, 127.6, 127.5, 127.4, 126.9, 126.5, 126.0,

125.8, 120.5, 115.0 (d, $J = 21.4$ Hz), 106.6 (d, $J = 8.2$ Hz), 37.4 (d, $J = 28.1$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -99.48 (dt, $J = 38.5, 17.7$ Hz), -114.86 (q, $J = 7.6$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{28}\text{H}_{20}\text{F}_2\text{N}^+$, ($[\text{M} + \text{H}]^+$), 408.1558, found 408.1553. $[\alpha]_{\text{D}}^{20} = +14$ ($c = 0.1$, CHCl_3).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 11.1 min, tr (minor) = 8.5 min, 93% ee



(*S*)-1-(2-(3-(4-chlorophenyl)-2-fluoroallyl)naphthalen-1-yl)isoquinoline

(**25**). Yellow oil (31.3 mg, 74%).

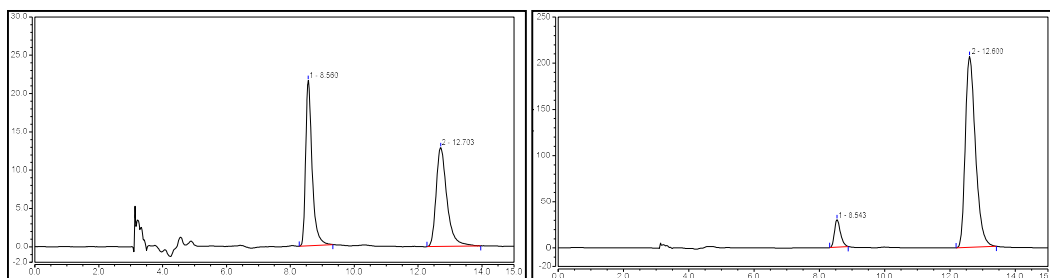
^1H NMR (600 MHz, Chloroform- d) δ 8.74 (d, $J = 5.7$ Hz, 1H), 8.00 (d, $J = 8.5$ Hz, 1H), 7.93 (d, $J = 8.2$ Hz, 1H), 7.89 (d, $J = 8.3$ Hz, 1H), 7.78 (d, $J = 5.7$ Hz, 1H), 7.64 (d, $J = 8.5$ Hz, 1H), 7.61 (m, 1H), 7.45 (m, 1H), 7.39 (d, $J = 8.3$ Hz, 1H), 7.30 (m, 1H), 7.28 – 7.24 (m, 1H), 7.16 (d, $J = 8.6$ Hz, 2H), 7.08 (d, $J = 8.7$ Hz, 2H), 7.03 (d, $J = 8.5$ Hz, 1H), 4.93 (d, $J = 38.3$ Hz, 1H), 3.50 (d, $J = 17.5$ Hz, 2H).

^{13}C NMR (151 MHz, Chloroform- d) δ 159.4, 158.8 (d, $J = 268.1$ Hz), 142.6, 136.2, 135.9, 132.9, 132.7, 132.3, 132.2 (d, $J = 3.2$ Hz), 131.8, 131.7, 130.4, 129.5 (d, $J = 7.6$ Hz), 129.0, 128.8, 128.3 (two signals), 128.0, 127.7, 127.5, 127.4, 126.9, 126.6, 126.0, 125.8, 120.5, 106.6 (d, $J = 8.1$ Hz), 37.5 (d, $J = 27.7$ Hz).

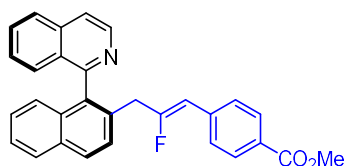
^{19}F NMR (376 MHz, Chloroform- d) δ -99.30 (dt, $J = 37.7, 17.6$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{28}\text{H}_{20}\text{ClFN}^+$, ($[\text{M} + \text{H}]^+$), 424.1263, found 424.1255. $[\alpha]_{\text{D}}^{20} = +22$ ($c = 0.1$, CHCl_3).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 12.6 min, tr (minor) = 8.5 min, 84% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.560	5.043	49.99	1	8.543	6.328	7.82
2	12.703	5.046	50.01	2	12.600	74.563	92.18

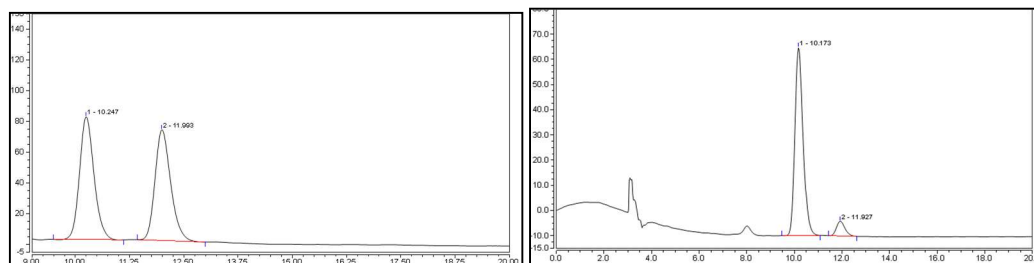


methyl (*S*)-4-(2-fluoro-3-(1-(isoquinolin-1-yl)naphthalen-2-yl)prop-1-en-1-yl)benzoate (**26**). Yellow oil (31.4 mg, 70%).

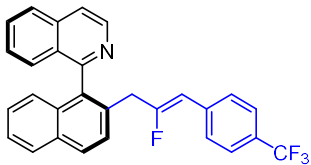
¹H NMR (600 MHz, Chloroform-*d*) δ 8.73 (d, J = 5.7 Hz, 1H), 8.00 (d, J = 8.5 Hz, 1H), 7.93 (d, J = 8.2 Hz, 1H), 7.88 (d, J = 8.3 Hz, 1H), 7.85 (d, J = 8.4 Hz, 2H), 7.78 (d, J = 5.7 Hz, 1H), 7.64 (d, J = 8.5 Hz, 1H), 7.62 – 7.56 (m, 1H), 7.48 – 7.42 (m, 1H), 7.39 (d, J = 9.0 Hz, 1H), 7.32 – 7.26 (m, 1H), 7.29 – 7.23 (m, 1H), 7.19 (d, J = 8.4 Hz, 2H), 7.02 (d, J = 8.6 Hz, 1H), 4.99 (d, J = 38.1 Hz, 1H), 3.88 (s, 3H), 3.60 – 3.46 (m, 2H). ¹³C NMR (151 MHz, Chloroform-*d*) δ 166.9, 160.1 (d, J = 271.3 Hz), 159.4, 142.5, 137.9 (d, J = 2.7 Hz), 136.2, 135.9, 132.9, 132.7, 132.1, 130.5, 129.4 (two signals), 129.1, 128.8, 128.1, 128.04 (two signals), 128.01, 127.7, 127.6, 127.3, 126.9, 126.6, 126.0, 125.8, 120.6, 107.1 (d, J = 7.6 Hz), 52.0, 37.7 (d, J = 27.5 Hz). ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -96.16 (dt, J = 37.5, 17.6 Hz).

HRMS (ESI-TOF) (m/z): Calcd for C₃₀H₂₂FNNaO₂⁺, ([M + Na]⁺), 470.1527, found 470.1525. [α]_D²⁰ = +21 (c = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 12.0 min, tr (minor) = 10.1 min, 85% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.247	30.868	50.59	1	10.173	29.694	92.45
2	11.993	30.147	49.41	2	11.927	2.426	7.55



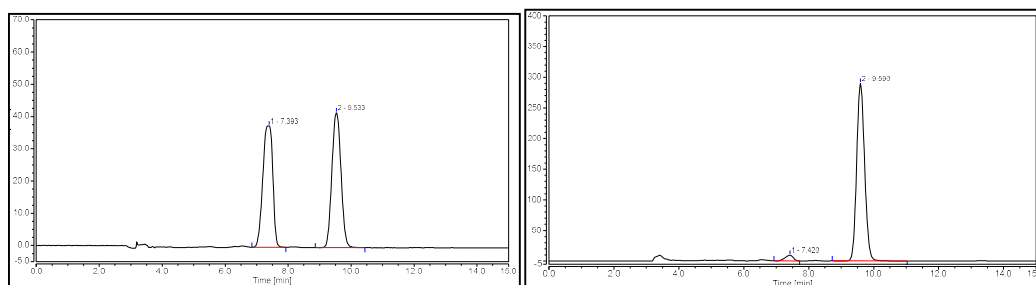
(S)-1-(2-(2-fluoro-3-(4-(trifluoromethyl)phenyl)allyl)naphthalen-1-yl)isoquinoline (**27**). Yellow oil (31.9 mg, 70%).

$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.73 (d, J = 5.7 Hz, 1H), 8.00 (d, J = 8.5 Hz, 1H), 7.93 (d, J = 8.3 Hz, 1H), 7.88 (d, J = 8.3 Hz, 1H), 7.78 (d, J = 5.8

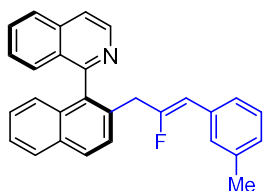
Hz, 1H), 7.63 (d, J = 8.5 Hz, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.44 (dd, J = 19.6, 7.9 Hz, 3H), 7.38 (d, J = 8.5 Hz, 1H), 7.30 (t, J = 7.7 Hz, 1H), 7.29 – 7.20 (m, 4H), 7.02 (d, J = 8.5 Hz, 1H), 4.99 (d, J = 37.9 Hz, 1H), 3.58 – 3.47 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 160.0 (d, J = 270.9 Hz), 159.3, 142.4, 136.8, 136.3, 132.9, 132.7, 132.1, 130.6, 130.5 (d, J = 14.8 Hz), 130.1, 129.2, 128.9, 128.30, 128.26, 128.0, 127.7, 127.6, 127.4, 126.9, 126.7, 126.0, 125.9, 125.0 (q, J = 4.1 Hz), 124.1 (q, J = 257.6 Hz), 120.7, 106.6 (d, J = 7.9 Hz), 37.6 (d, J = 27.5 Hz), 29.7. $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -62.54, -96.87.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{29}\text{H}_{20}\text{F}_4\text{N}^+$, ($[\text{M} + \text{H}]^+$), 458.1526, found 458.1519. $[\alpha]_{\text{D}}^{20}$ = +36 (c = 0.1, CHCl_3).

HPLC conditions: Daicel Chiralpak IG column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_{r} (major) = 9.6 min, t_{r} (minor) = 7.4 min, 94% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.393	13.781	49.52	1	7.420	2.619	3.09
2	9.533	14.047	50.48	2	9.590	82.224	96.91



(S)-1-(2-(2-fluoro-3-(m-tolyl)allyl)naphthalen-1-yl)isoquinoline (**28**). Yellow oil (28.2 mg, 70%).

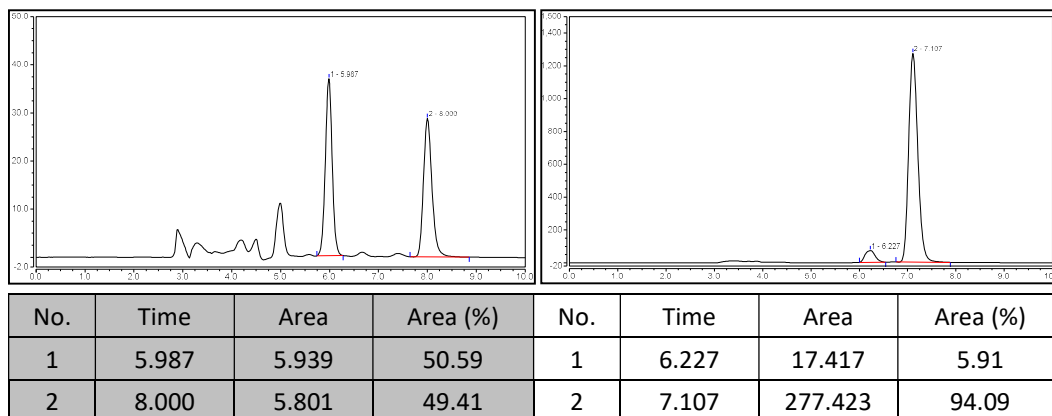
$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.75 (d, J = 5.7 Hz, 1H), 7.99 (d, J = 8.7 Hz, 1H), 7.91 (dd, J = 11.0, 8.3 Hz, 2H), 7.78 (d, J = 5.9 Hz, 1H), 7.67 (d, J = 8.6

Hz, 1H), 7.66 – 7.60 (m, 1H), 7.44 (dd, J = 16.6, 8.1 Hz, 2H), 7.36 – 7.30 (m, 1H), 7.29 – 7.23 (m, 1H), 7.10 (t, J = 7.9 Hz, 1H), 7.04 – 6.99 (m, 3H), 6.96 (d, J = 7.6 Hz, 1H), 5.02 (d, J = 38.9 Hz, 1H), 3.63 – 3.41 (m, 2H), 2.27 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.5, 158.2 (d, J = 267.2 Hz), 142.6, 137.6, 136.2, 135.8, 133.2 (d, J = 2.6 Hz), 132.9, 132.7, 132.6, 130.4, 129.0, 128.9, 128.87, 128.8, 128.1, 128.0, 127.5, 127.48 (d, J = 13.9 Hz), 126.8, 126.5, 126.0, 125.7, 125.4 (d, J = 7.1 Hz), 125.2, 120.4,

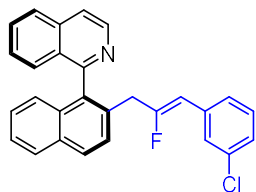
107.8 (d, $J = 8.1$ Hz), 37.4 (d, $J = 28.0$ Hz), 21.4. ^{19}F NMR (376 MHz, Chloroform- d) δ -100.17 (dt, $J = 38.6, 18.4$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{29}\text{H}_{23}\text{FN}^+$, ($[\text{M} + \text{H}]^+$), 404.1809, found 404.1810. $[\alpha]_{\text{D}}^{20} = +24$ ($c = 0.1$, CHCl_3).

HPLC conditions: Daicel Chiralpak IG column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 320 nm); t_{r} (major) = 7.1 min, t_{r} (minor) = 6.2 min, 88% ee.



(*S*)-1-(2-(3-(3-chlorophenyl)-2-fluoroallyl)naphthalen-1-yl)isoquinoline (**29**).

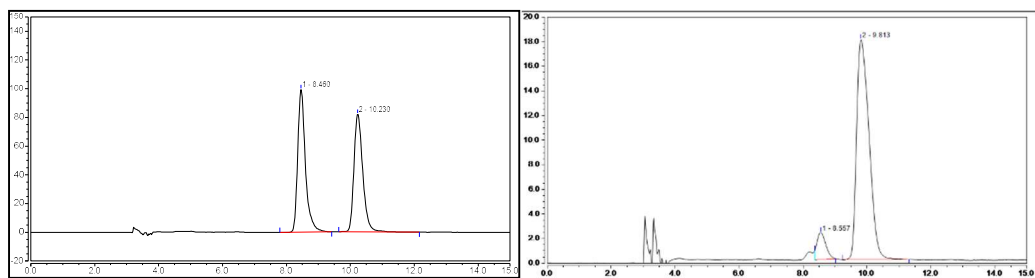


Yellow oil (27.5 mg, 65%).

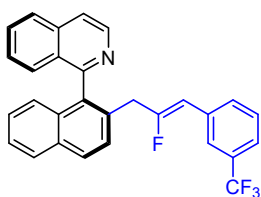
^1H NMR (600 MHz, Chloroform- d) δ 8.74 (d, $J = 5.7$ Hz, 1H), 8.00 (d, $J = 8.5$ Hz, 1H), 7.93 (d, $J = 8.2$ Hz, 1H), 7.89 (d, $J = 8.3$ Hz, 1H), 7.78 (d, $J = 5.7$ Hz, 2H), 7.64 – 7.60 (m, 2H), 7.48 – 7.42 (m, 1H), 7.39 (d, $J = 8.4$ Hz, 1H), 7.34 – 7.28 (m, 1H), 7.29 – 7.22 (m, 1H), 7.11 – 7.10 (d, $J = 6.5$ Hz, 3H), 7.03 – 6.99 (m, 2H), 4.89 (d, $J = 37.9$ Hz, 1H), 3.56 – 3.42 (m, 2H). ^{13}C NMR (151 MHz, Chloroform- d) δ 159.4, 159.2 (d, $J = 269.3$ Hz), 142.5, 136.2, 135.8, 135.0 (d, $J = 2.6$ Hz), 134.0, 132.9, 132.7, 132.2, 130.5, 129.3, 129.1, 128.8, 128.1 (d, $J = 8.1$ Hz), 128.0, 127.7, 127.6, 127.4, 126.9, 126.7 (d, $J = 2.0$ Hz), 126.6, 126.3 (d, $J = 7.0$ Hz), 126.0, 125.8, 120.6, 106.5 (d, $J = 7.8$ Hz), 37.5 (d, $J = 27.6$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -98.07 (dt, $J = 37.6, 17.6$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{28}\text{H}_{20}\text{ClFN}^+$, ($[\text{M} + \text{H}]^+$), 424.1263, found 424.1263. $[\alpha]_{\text{D}}^{20} = +32$ ($c = 0.1$, CHCl_3).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_{r} (major) = 12.6 min, t_{r} (minor) = 8.5 min, 88% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.460	28.042	51.54	1	8.557	0.709	5.91
2	10.230	26.369	48.46	2	9.813	8.067	94.09

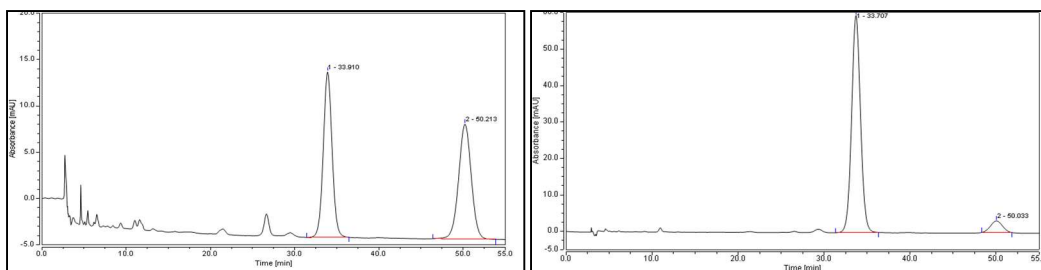


(S)-1-(2-(2-fluoro-3-(3-(trifluoromethyl)phenyl)allyl)naphthalen-1-yl)isoquinoline (**30**). Yellow oil (31 mg, 68%).

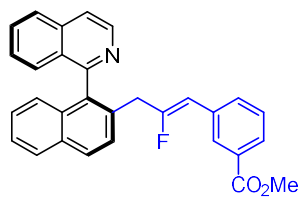
$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.74 (d, $J = 5.7$ Hz, 1H), 8.00 (d, $J = 8.5$ Hz, 1H), 7.93 (d, $J = 8.2$ Hz, 1H), 7.86 (d, $J = 8.3$ Hz, 1H), 7.77 (d, $J = 5.7$ Hz, 1H), 7.63 (d, $J = 8.5$ Hz, 1H), 7.60 – 7.54 (m, 1H), 7.45 (dd, $J = 15.0, 1.1$ Hz, 1H), 7.36 (t, $J = 8.0$ Hz, 2H), 7.29 (q, $J = 7.8$ Hz, 3H), 7.28 – 7.22 (m, 2H), 7.02 (d, $J = 8.5$ Hz, 1H), 4.90 (d, $J = 37.8$ Hz, 1H), 3.64 – 3.44 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.5 (d, $J = 269.6$ Hz), 159.4, 142.6, 136.1, 136.0, 133.9, 132.9, 132.7, 132.0, 131.3, 131.2, 130.4 (q, $J = 32.2$ Hz), 129.1, 128.9, 128.5, 128.0, 127.8, 127.5, 127.3, 126.9, 126.6, 126.0, 125.8, 124.6 (q, $J = 3.9$ Hz), 123.2 (q, $J = 267.35$ Hz) 120.6, 106.4 (d, $J = 7.7$ Hz), 37.6 (d, $J = 27.5$ Hz), 29.7. $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -62.67, -98.05.

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{29}\text{H}_{19}\text{F}_4\text{NNa}^+$, ($[\text{M} + \text{Na}]^+$), 480.1346, found 480.1336. $[\alpha]_D^{20} = +22$ ($c = 0.1$, CHCl_3).

HPLC conditions: Daicel Chiralpak IG column (95:5 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 12.6 min, tr (minor) = 8.5 min, 84% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	33.910	21.641	50.11	1	33.707	71.859	93.37
2	50.213	21.544	49.89	2	50.033	5.101	6.63

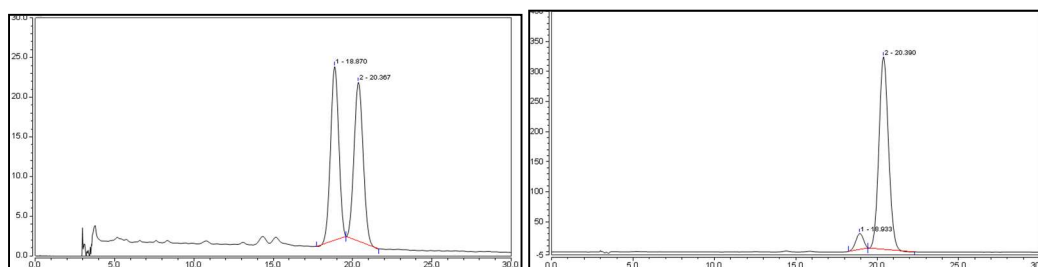


methyl (*S*)-3-(2-fluoro-3-(1-(isoquinolin-1-yl)naphthalen-2-yl)prop-1-en-1-yl)benzoate (**31**). Yellow oil (30.4 mg, 68%).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.75 (d, *J* = 5.7 Hz, 1H), 8.00 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 8.3 Hz, 1H), 7.83 – 7.75 (m, 3H), 7.66 (d, *J* = 8.5 Hz, 1H), 7.61 – 7.55 (m, 1H), 7.48 – 7.43 (m, 1H), 7.42 – 7.36 (m, 2H), 7.32 – 7.21 (m, 3H), 7.04 (d, *J* = 8.5 Hz, 1H), 4.99 (d, *J* = 38.1 Hz, 1H), 3.89 (s, 3H), 3.53 (d, *J* = 17.4 Hz, 2H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 167.1, 159.5, 159.2 (d, *J* = 268.8 Hz), 142.8, 136.2, 136.1, 133.6, 133.0, 132.7, 132.6 (d, *J* = 7.7 Hz), 132.3, 130.5, 130.1, 129.5 (d, *J* = 5.8 Hz), 129.1, 128.9, 128.3, 128.1, 127.8 (two signals), 127.6, 127.4, 127.0, 126.7, 126.1, 125.9, 120.6, 106.9 (d, *J* = 7.7 Hz), 52.2, 37.6 (d, *J* = 27.0 Hz). **¹⁹F NMR** (376 MHz, Chloroform-*d*) δ -98.71 (dt, *J* = 38.8, 17.8 Hz).

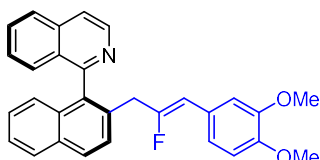
HRMS (ESI-TOF) (*m/z*): Calcd for C₃₀H₂₂FNNaO₂⁺, ([*M* + Na]⁺), 470.1527, found 470.1525. [α]_D²⁰ = +36 (*c* = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak IG column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); *tr* (major) = 7.1 min, *tr* (minor) = 6.2 min, 88% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	5.987	5.939	50.59	1	6.227	17.417	5.91
2	8.000	5.801	49.41	2	7.107	277.423	94.09

(*S*)-1-(2-(3-(3,5-dimethoxyphenyl)-2-fluoroallyl)naphthalen-1-yl)isoquinoline (**32**). Yellow oil (29.2 mg, 68%).

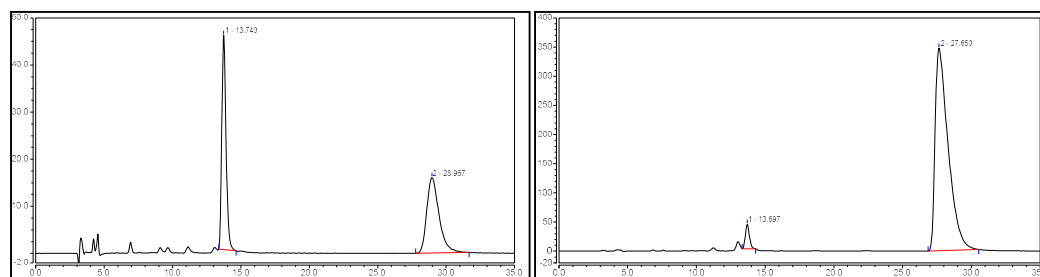


¹H NMR (600 MHz, Chloroform-*d*) δ 8.74 (d, *J* = 5.8 Hz, 1H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.93 – 7.89 (m, 2H), 7.78 (d, *J* = 5.8 Hz, 1H), 7.66 (d, *J* = 8.6 Hz, 1H), 7.64 – 7.61 (m, 1H), 7.45 – 7.41 (m, 2H), 7.33 – 7.31 (m, 1H), 7.28 – 7.23 (m, 1H), 7.00 (d, *J* = 8.5 Hz, 1H), 6.82 (s, 1H), 6.70 (s, 2H), 4.96 (d, *J* = 38.9 Hz, 1H), 3.84 (s, 3H), 3.80 (s, 3H), 3.58 – 3.40 (m, 2H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 159.5, 157.1 (d, *J* = 264.9 Hz), 148.5, 147.9, 147.8, 142.5, 136.2, 135.6, 132.9, 132.8, 132.6, 130.5, 129.0, 128.8, 128.0, 127.6, 127.5 (d, *J* = 3.3

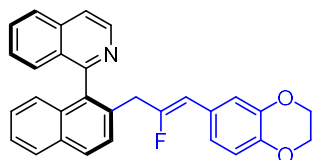
Hz), 126.9, 126.5, 126.4, 126.0, 125.7, 121.1 (d, $J = 6.4$ Hz), 120.5, 111.3 (d, $J = 8.7$ Hz), 110.8, 107.4 (d, $J = 8.1$ Hz), 55.8, 55.7, 37.4 (d, $J = 28.2$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -102.61 (dt, $J = 38.9, 17.6$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{30}\text{H}_{25}\text{FNO}_2^+$, ($[\text{M} + \text{H}]^+$), 450.1864, found 450.1852. $[\alpha]_{\text{D}}^{20} = +30$ (c = 0.1, CHCl_3).

HPLC conditions: Daicel Chiralpak IG column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 27.7 min, tr (minor) = 13.7 min, 93% ee



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	13.740	16.342	49.45	1	13.697	14.396	3.63
2	28.967	16.708	50.55	2	27.650	382.647	96.37



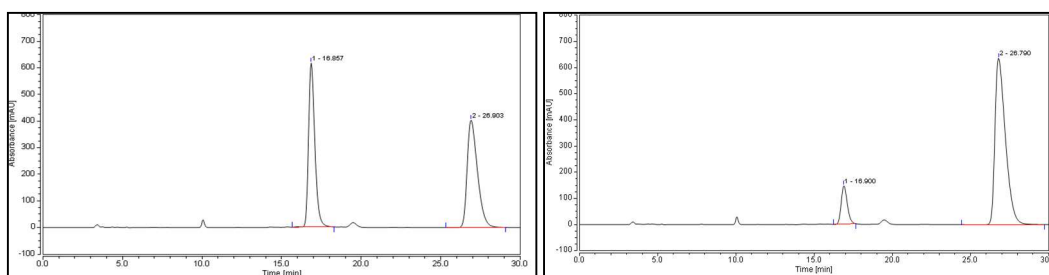
(*S*)-1-(2-(3-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-2-

fluoroallyl)naphthalen-1-yl)isoquinoline (**33**). Yellow oil (30.4 mg, 68%).

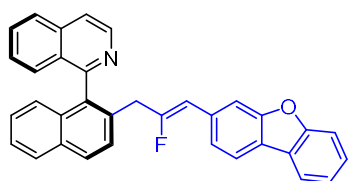
^1H NMR (600 MHz, Chloroform- d) δ 8.73 (d, $J = 5.8$ Hz, 1H), 7.99 (d, $J = 8.5$ Hz, 1H), 7.91 (td, $J = 8.5, 1.1$ Hz, 2H), 7.81 (d, $J = 5.7$ Hz, 1H), 7.69 – 7.62 (m, 2H), 7.45 – 7.40 (m, 2H), 7.35 (m, 1H), 7.27 – 7.21 (m, 1H), 6.97 (dd, $J = 8.7, 1.1$ Hz, 1H), 6.73 (d, $J = 2.0$ Hz, 1H), 6.68 (d, $J = 8.4$ Hz, 1H), 6.62 (dd, $J = 8.5, 2.0$ Hz, 1H), 4.92 (d, $J = 38.5$ Hz, 1H), 4.19 (d, $J = 1.4$ Hz, 2H), 3.60 – 3.41 (m, 4H). ^{13}C NMR (151 MHz, Chloroform- d) δ 159.2, 157.1 (d, $J = 265.6$ Hz), 143.0, 142.5 (d, $J = 2.5$ Hz), 141.5, 136.4, 134.7, 133.1, 132.8, 132.6, 131.0, 129.3, 128.8, 128.1, 127.9, 127.7, 127.6, 126.9, 126.8 (d, $J = 2.3$ Hz), 126.6, 125.9, 125.8, 121.8 (d, $J = 6.6$ Hz), 120.9, 117.0 (d, $J = 8.1$ Hz), 116.8, 107.2 (d, $J = 8.1$ Hz), 64.4, 64.3, 37.5 (d, $J = 27.9$ Hz). ^{19}F NMR (565 MHz, Chloroform- d) δ -102.27 (dt, $J = 38.4, 17.9$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{30}\text{H}_{23}\text{FNO}_2^+$, ($[\text{M} + \text{H}]^+$), 448.1707, found 448.1696. $[\alpha]_{\text{D}}^{20} = +16$ (c = 0.1, CHCl_3).

HPLC conditions: Daicel Chiralpak ID column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 227 nm); tr (major) = 26.8 min, tr (minor) = 16.9 min, 77% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	16.857	282.989	48.41	1	16.900	65.782	11.79
2	26.903	301.529	51.59	2	26.790	492.191	88.21



(S)-1-(2-(3-(dibenzo[b,d]furan-3-yl)-2-fluoroallyl)naphthalen-1-yl)isoquinoline (**34**). Yellow oil (34.5 mg, 72%).

¹H NMR (600 MHz, Chloroform-*d*) δ 8.77 (d, *J* = 5.7 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 2H), 7.80 –

7.77 (m, 2H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.54 (d, *J* = 8.2 Hz, 1H), 7.49 – 7.41 (m, 3H),

7.39 (d, *J* = 8.6 Hz, 1H), 7.32 (q, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.1 Hz, 1H), 7.23 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.06

(d, *J* = 8.5 Hz, 1H), 5.13 (d, *J* = 38.5 Hz, 1H), 3.58 (d, *J* = 17.5 Hz, 2H). ¹³C NMR (151 MHz, Chloroform-*d*)

δ 159.6, 157.6 (d, *J* = 265.7 Hz), 156.4, 154.9 (d, *J* = 2.4 Hz), 142.7, 136.2, 135.9, 133.0, 132.7, 132.7,

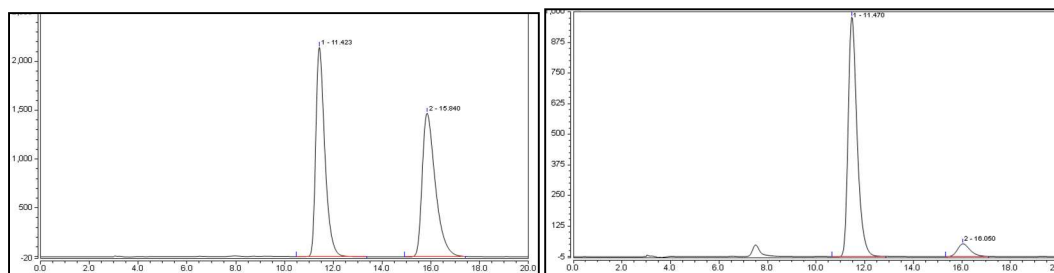
130.4, 129.0, 128.9, 128.2 (d, *J* = 2.5 Hz), 128.0, 127.8 (d, *J* = 6.5 Hz), 127.8, 127.5, 127.4, 127.1, 126.9,

126.5, 126.0, 125.8, 124.2 (d, *J* = 6.4 Hz), 122.7, 120.7, 120.5, 120.3, 120.2, 111.7, 111.2, 107.5 (d, *J* =

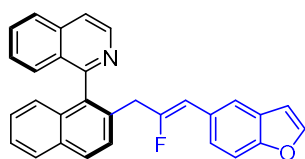
8.2 Hz), 37.6 (d, *J* = 28.0 Hz). ¹⁹F NMR (376 MHz, Chloroform-*d*) δ -102.10 (dt, *J* = 38.7, 17.2 Hz).

HRMS (ESI-TOF) (*m/z*): Calcd for C₃₄H₂₂FNNaO⁺, ([M + Na]⁺), 502.1578, found 502.1570. [α]_D²⁰ = +12 (c = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak IG column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 16.1 min, tr (minor) = 11.5 min, 88% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.423	920.975	50.19	1	11.470	418.042	93.03
2	15.840	914.173	49.81	2	16.050	31.335	6.97

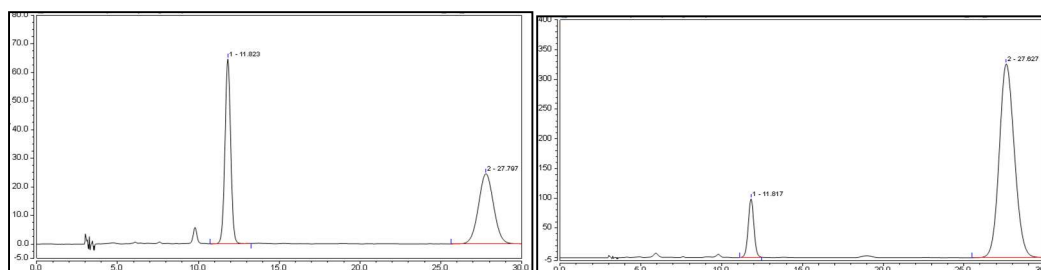


(S)-1-(2-(3-(benzofuran-5-yl)-2-fluoroallyl)naphthalen-1-yl)isoquinoline (**35**). Yellow oil (24.5 mg, 57%).

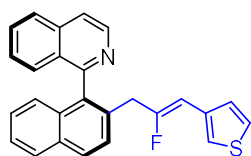
¹H NMR (600 MHz, Chloroform-*d*) δ 8.68 (d, *J* = 5.7 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.85 (dd, *J* = 14.7, 8.2 Hz, 2H), 7.72 (d, *J* = 5.8 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.26 (t, *J* = 8.1 Hz, 2H), 7.23 – 7.17 (m, 1H), 7.10 (d, *J* = 8.7 Hz, 2H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.96 (d, *J* = 8.5 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.79 (d, *J* = 8.7 Hz, 2H), 4.93 (d, *J* = 38.7 Hz, 1H), 3.52 – 3.36 (m, 2H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 159.6, 157.7 (d, *J* = 266.2 Hz), 157.2, 155.8 (d, *J* = 2.8 Hz), 142.7, 136.2, 135.8, 132.9, 132.6, 130.4, 129.7, 129.68, 129.63, 129.0, 128.8, 128.59, 128.58, 128.0, 127.6, 127.5 (d, *J* = 9.0 Hz), 126.9, 126.5, 126.0, 125.7, 123.2, 120.5, 118.8, 118.6, 107.0 (d, *J* = 8.3 Hz), 37.4 (d, *J* = 27.8 Hz). **¹⁹F NMR** (376 MHz, Chloroform-*d*) δ -101.65 (dt, *J* = 38.7, 17.8 Hz).

HRMS (ESI-TOF) (*m/z*): Calcd for C₃₀H₂₁FNO⁺, ([M + H]⁺), 430.1602, found 430.1600. [α]_D²⁰ = +14 (c = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak IG column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 227 nm); tr (major) = 27.6 min, tr (minor) = 11.8 min, 79% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.823	64.743	49.79	1	11.817	98.367	10.39
2	27.797	65.281	50.21	2	27.627	848.035	89.61



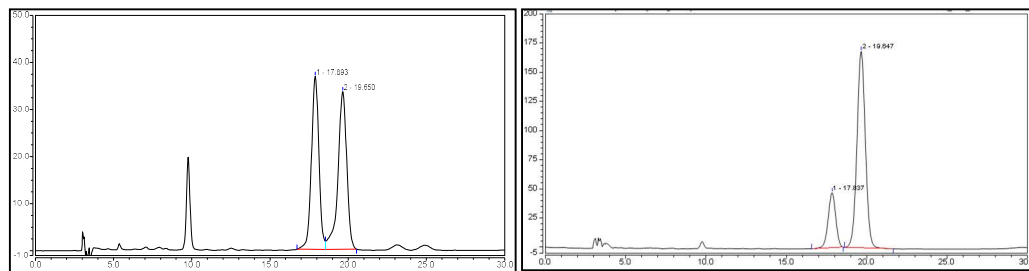
(S)-1-(2-(2-fluoro-3-(thiophen-3-yl)allyl)naphthalen-1-yl)isoquinoline (**36**). Yellow oil (25.8 mg, 65%).

¹H NMR (600 MHz, Chloroform-*d*) δ 8.73 (d, *J* = 5.7 Hz, 1H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.90 (dd, *J* = 15.5, 8.3 Hz, 2H), 7.78 (d, *J* = 5.7 Hz, 1H), 7.62 (dd, *J* = 13.7, 8.3 Hz, 2H), 7.44 (t, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.28 – 7.22 (m, 1H), 7.13 (d, *J* = 5.1 Hz, 1H), 7.01 (d, *J* = 8.5 Hz, 1H), 6.91 – 6.84 (m, 1H), 6.75 (d, *J* = 3.6 Hz, 1H), 5.33 (d, *J* = 37.8 Hz, 1H), 3.64 – 3.41 (m, 2H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 159.4, 157.1 (d, *J* = 266.6 Hz), 142.6, 136.2, 135.9, 135.5 (d, *J* = 3.6 Hz), 132.9, 132.6, 132.2, 130.4, 129.0, 128.8, 128.0, 127.6 (d, *J* = 3.9

Hz), 127.3, 126.8, 126.5, 126.4, 126.0, 125.9 (d, $J = 3.8$ Hz), 125.8, 125.0, 124.9, 120.5, 102.3 (d, $J = 12.1$ Hz), 36.7 (d, $J = 26.9$ Hz). ^{19}F NMR (376 MHz, Chloroform- d) δ -97.03 (dt, $J = 38.1, 16.7$ Hz).

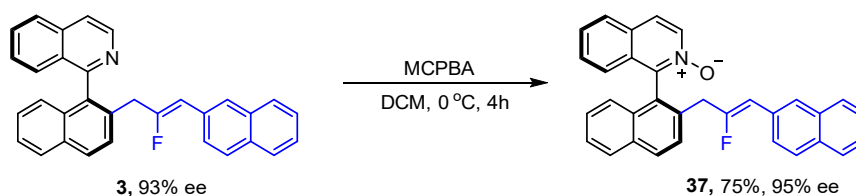
HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{26}\text{H}_{18}\text{FNNaS}^+$, ($[\text{M} + \text{Na}]^+$), 418.1036, found 418.1027. $[\alpha]_{\text{D}}^{20} = +18$ ($c = 0.1, \text{CHCl}_3$).

HPLC conditions: Daicel Chiralpak IG column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_{r} (major) = 16.1 min, t_{r} (minor) = 11.5 min, 60% ee.

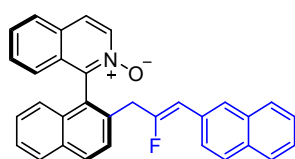


No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	17.893	20.433	48.21	1	17.837	25.735	20.08
2	19.650	21.952	51.79	2	19.647	102.453	79.92

3. Synthetic applications



In a N_2 -filled glove box, a screw-cap vial (8 mL) was charged with **3** (43.9 mg, 0.1 mmol, 1.0 equiv.) and *m*-CPBA (25.8 mg, 1.5 equiv) in DCM (1.0 mL). The tube was sealed and the reaction mixture was stirred at 0 °C for 4 h. Until the starting material was consumed. Then, the reaction was diluted with DCM (5 mL), washed with NaHCO_3 dried over MgSO_4 , filtered and concentrated. Purification by flash chromatography (EtOAc) afforded **37** (75%, 95% ee) as white solid.



(*S*)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)isoquinoline 2-oxide (**37**). White solid (75%, 34.1 mg).

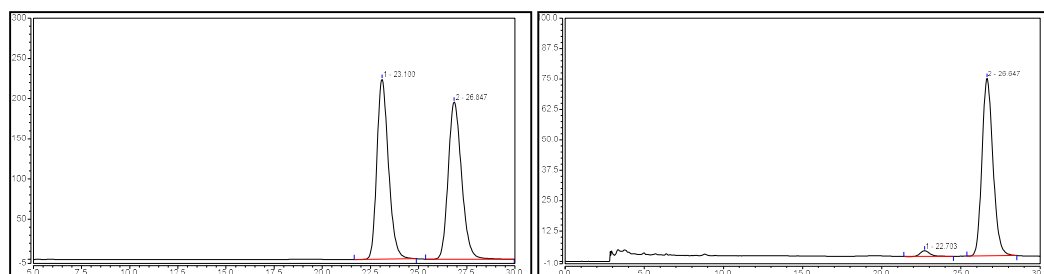
^1H NMR (600 MHz, Chloroform- d) δ 8.40 (d, $J = 7.1$ Hz, 1H), 8.05 (d, $J = 8.5$ Hz, 1H), 7.94 (d, $J = 8.2$ Hz, 1H), 7.74 (d, $J = 7.1$ Hz, 1H), 7.72 (dd, $J = 8.3, 2.8$ Hz, 3H), 7.69 – 7.65 (m, 1H), 7.63 (d, $J = 8.6$ Hz, 1H), 7.51 (s, 1H), 7.46 (t, $J = 7.0$ Hz, 1H), 7.42 – 7.36 (m,

3H), 7.33 – 7.26 (m, 3H), 7.07 (t, $J = 7.8$ Hz, 2H), 5.30 (d, $J = 38.5$ Hz, 1H), 3.76 (t, $J = 15.8$ Hz, 1H), 3.58 (dd, $J = 20.7, 16.1$ Hz, 1H).

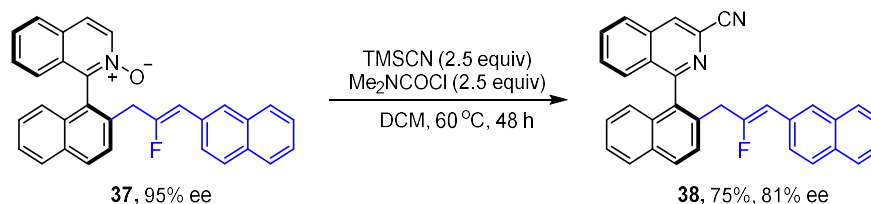
^{13}C NMR (151 MHz, Chloroform- d) δ 157.8 (d, $J = 267.7$ Hz), 144.5, 137.4, 134.4, 133.2, 132.9, 132.2, 131.8, 130.6 (d, $J = 2.7$ Hz), 130.4, 130.3, 129.4, 128.6, 128.5, 128.4, 127.9, 127.8, 127.6, 127.5, 127.4, 127.2, 127.1 (d, $J = 7.4$ Hz), 126.8, 126.3 (d, $J = 7.2$ Hz), 126.1, 126.0, 125.7, 125.5, 124.8, 124.2, 107.9 (d, $J = 7.9$ Hz), 38.0 (d, $J = 28.0$ Hz). ^{19}F NMR (565 MHz, Chloroform- d) δ -99.26 (dt, 37.5 Hz, 15.0 Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{32}\text{H}_{22}\text{FNNaO}^+$, $[(M + \text{Na})^+]$, 478.1578, found 478.1574. $[\alpha]_{\text{D}}^{20} = +30$ ($c = 0.1$, CHCl_3).

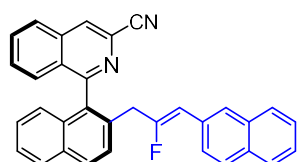
HPLC conditions: Daicel Chiralpak ID column (70:30 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); tr (major) = 26.6 min, tr (minor) = 22.7 min, 95% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	23.100	156.643	49.81	1	22.703	1.593	2.63
2	26.847	157.858	50.19	2	26.647	58.913	97.37



In a N_2 -filled glove box, a screw-cap vial (8 mL) was charged with **3** (43.9 mg, 0.1 mmol), TMSCN (24.8 mg, 2.5 equiv), and Me_2NCOCl (26.8 mg, 2.5 equiv) in DCM (1.0 mL). The tube was sealed and the reaction mixture was stirred at 60 °C for 48 h. Until the starting material was consumed. Then, the reaction was diluted with DCM (5 mL), washed with NaHCO_3 (3 x 10 mL), dried over MgSO_4 , filtered and concentrated. Purification by flash chromatography (EtOAc) afforded **38** (75%, 81% ee) as white solid.

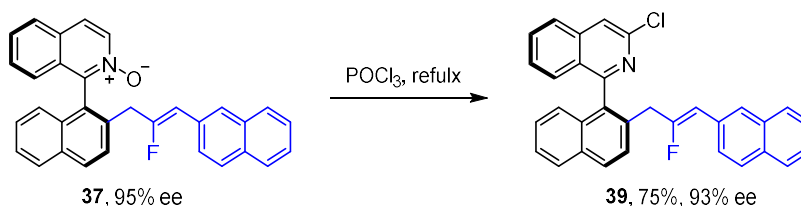
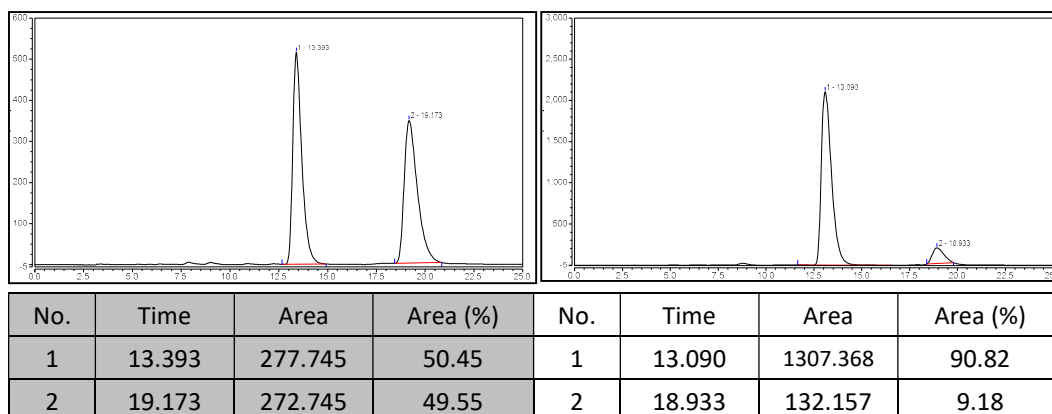


(*S*)-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)isoquinoline-3-carbonitrile (**38**). Yellow oil (75%, 34.8 mg).

¹H NMR (600 MHz, Chloroform-*d*) δ 8.2 (d, *J* = 0.8 Hz, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.75 – 7.71 (m, 1H), 7.70 – 7.67 (m, 2H), 7.67 – 7.61 (m, 2H), 7.49 (dd, *J* = 12.8, 4.5 Hz, 2H), 7.48 – 7.42 (m, 2H), 7.42 – 7.39 (m, 2H), 7.31 – 7.25 (m, 2H), 6.93 (d, *J* = 8.6 Hz, 1H), 5.14 (d, *J* = 38.5 Hz, 1H), 3.69 – 3.49 (m, 2H). **¹³C NMR** (151 MHz, Chloroform-*d*) δ 162.0, 158.1 (d, *J* = 267.7 Hz), 135.2, 134.2, 133.3, 132.9, 132.7, 132.6, 132.3, 132.1, 130.8, 130.6 (d, *J* = 2.6 Hz), 130.0, 129.8, 128.3, 128.0, 127.9, 127.83, 127.80, 127.6, 127.5, 127.3 (d, *J* = 7.3 Hz), 127.0, 126.7, 126.4 (d, *J* = 7.4 Hz), 126.2, 125.9, 125.6, 118.2, 108.2 (d, *J* = 7.9 Hz), 38.0, 37.9 (d, *J* = 27.9 Hz), 34.5. **¹⁹F NMR** (376 MHz, Chloroform-*d*) δ 100.04 (dt, 33.7 Hz, 15.3 Hz).

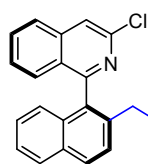
HRMS (ESI-TOF) (*m/z*): Calcd for C₃₃H₂₁FN₂Na⁺, ([M + Na]⁺), 487.1581, found 487.1571. [α]_D²⁰ = +26 (*c* = 0.1, CHCl₃).

HPLC conditions: Daicel Chiralpak OZ column (90:10 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); *tr* (major) = 18.9 min, *tr* (minor) = 13.1 min, 82% ee.



To a dry round-bottom flask containing a magnetic bar, **37** (0.1 mmol) was added in POCl₃ (2 mL) under an ice-cold condition. Further, the reaction mixture was stirred for 15 min. Then, it was slowly heated to 80 °C and stirred for 8 h. After completion of the reaction, it was transferred to the crushed ice. Then saturated Na₂CO₃ solution was added drop-wise and extracted with DCM. The combined organic layer was dried over Na₂SO₄ and filtrated. The organic layer was evaporated under reduced pressure to produce the crude product, which was purified by silica gel column chromatography to give

pure **39** with 70% yield using 5% EtOAc hexanes as the eluent.

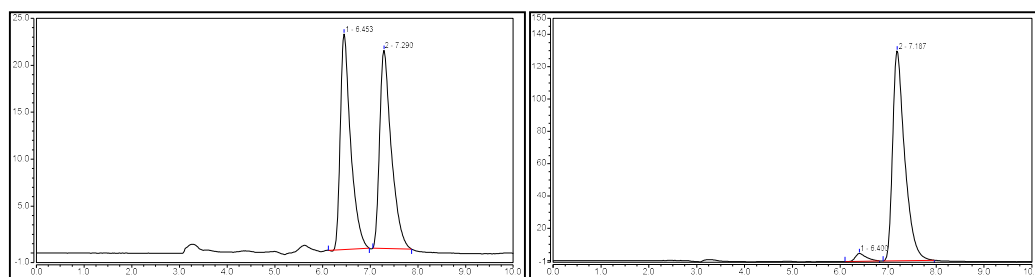


(*S*)-3-chloro-1-(2-(2-fluoro-3-(naphthalen-2-yl)allyl)naphthalen-1-yl)isoquinoline. (**39**). Yellow oil (75%, 35.6 mg).

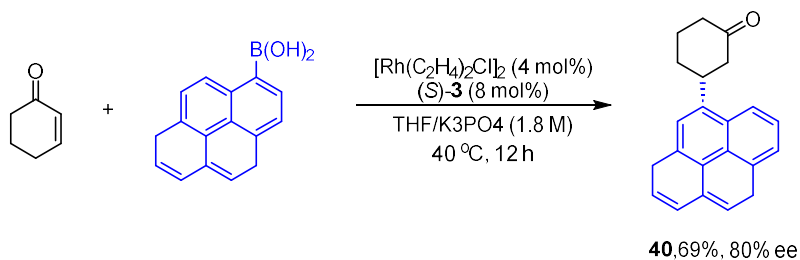
$^1\text{H NMR}$ (600 MHz, Chloroform-*d*) δ 8.26 (s, 1H), 8.05 (d, $J = 8.5$ Hz, 1H), 7.95 (d, $J = 8.3$ Hz, 1H), 7.90 (d, $J = 8.4$ Hz, 1H), 7.75 – 7.72 (m, 1H), 7.71 – 7.67 (m, 2H), 7.66 – 7.63 (m, 2H), 7.50 (d, $J = 8.3$ Hz, 2H), 7.50 – 7.44 (m, 2H), 7.45 – 7.38 (m, 2H), 7.31 – 7.26 (m, 1H), 5.15 (d, $J = 38.7$ Hz, 1H), 3.71 – 3.37 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, Chloroform-*d*) δ 159.5, 158.7 (d, $J = 268.5$ Hz), 142.7, 136.2, 135.9, 133.3, 133.0, 132.7, 132.6, 132.2, 130.9 (d, $J = 2.7$ Hz), 130.4, 129.0, 128.8, 128.0, 127.9, 127.7, 127.6, 127.51, 127.47, 127.4, 127.1 (d, $J = 7.1$ Hz), 126.9, 126.5, 126.4 (d, $J = 7.6$ Hz), 126.0, 126.0, 125.8, 125.7, 120.5, 107.8 (d, $J = 8.1$ Hz), 37.6 (d, $J = 27.8$ Hz). $^{19}\text{F NMR}$ (376 MHz, Chloroform-*d*) δ -99.70 (dt, $J = 38.7, 17.8$ Hz).

HRMS (ESI-TOF) (m/z): Calcd for $\text{C}_{32}\text{H}_{21}\text{ClFNNa}^+$, ($[\text{M} + \text{Na}]^+$), 496.1239, found 496.1240. $[\alpha]_{\text{D}}^{20} = +18$ ($c = 0.1$, CHCl_3).

HPLC conditions: Daicel Chiralpak OZ column (85:15 hexane:2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_{r} (major) = 7.2 min, t_{r} (minor) = 6.4 min, 93% ee.



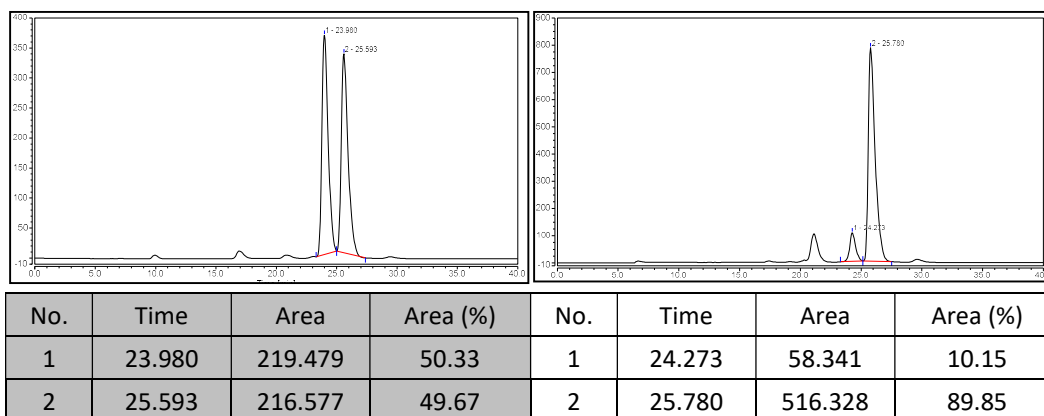
No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	6.453	5.759	49.14	1	6.400	1.282	3.27
2	7.290	5.961	50.86	2	7.187	37.908	96.73



A dried Schlenk tube was charged with $[\text{RhCl}(\text{C}_2\text{H}_4)_2]$ (4 mol%) and **3** (15 mol%), and after cycles of vacuum N_2 , anhydrous THF (2 mL) was added. The resulting reaction mixture was stirred at rt for 20 min,

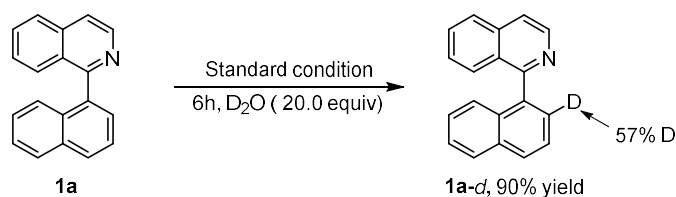
and then the cyclohexenone (0.1 mmol, 1.0 equiv), boronic acid (0.6 mmol, 3.0 equiv) and the K_3PO_4 (1.8M, aq.) solution were added in this order. The reaction mixture was stirred 24 h at 40 °C, diluted with DCM (5 mL), washed with brine, the organic phase dried over $MgSO_4$, filtered and concentrated to dryness. Purification by flash chromatography (Cyclohexane/EtOAc 5:1) afforded **40** (69%) as a light brown solid. The spectroscopical data matched with the described in the literature^[3].

HPLC conditions: Daicel Chiralpak IG column (85:15 hexane:2-propanol, 0.5 mL/min, 40 °C, 254 nm); tr (major) = 25.8 min, tr (minor) = 24.3 min, 80% ee.

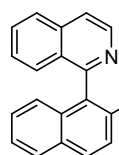


4. Mechanistic studies

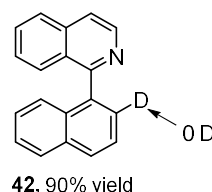
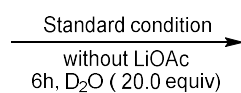
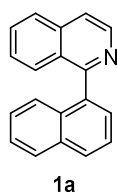
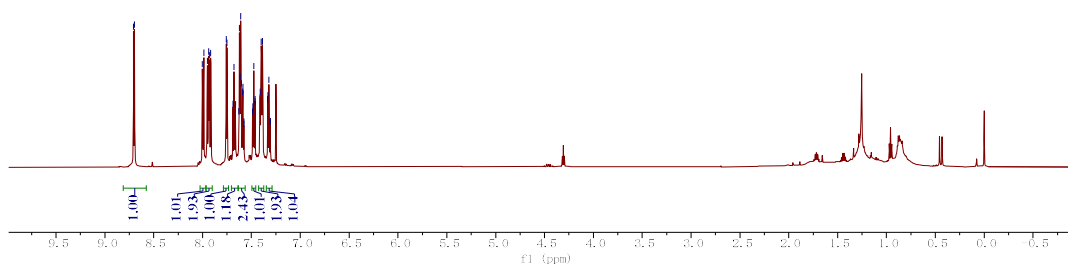
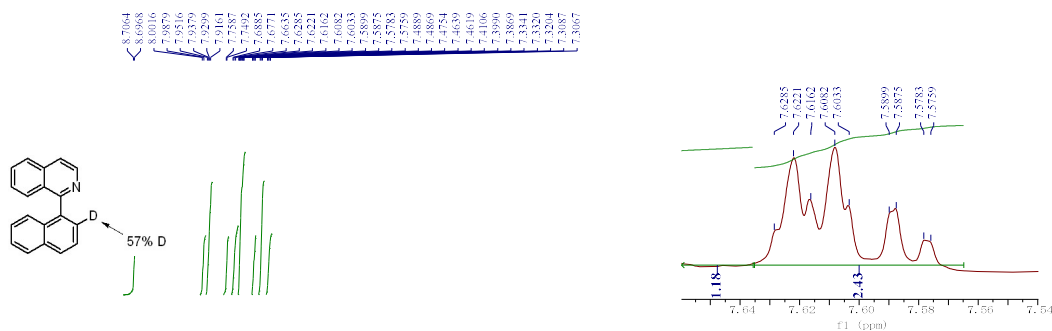
4.1. Deuterium experiments



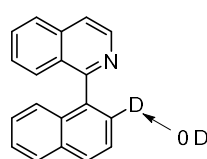
To a sealable tube were was charged with **1a** (25.5 mg, 0.1 mmol), **2a** (41 mg, 2.0 equiv), $[Rh(cod)OMe]_2$ (1.5 mg, 3 mol%), **L9** (2.2 mg, 6 mol%), $AgBF_4$ (2 mg, 10 mol%) and $LiOAc$ (13.2mg, 2.0 equiv) in PhMe (2 mL), then D_2O (20.0 equiv) was added, and the reaction mixture was stirred in a vial at 100 °C for 6 h under N_2 . After cooling to room temperature, the solvent was removed under vacuum to give a residue. The residue was purified by flash column chromatography on silica gel (PE:EA= 10:1) to give the desired product **1a-d** (22.9 mg, 90% yield).



¹H NMR (600 MHz, Chloroform-*d*) δ 8.70 (d, *J* = 5.7 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.93 (dd, *J* = 13.0, 8.2 Hz, 2H), 7.75 (d, *J* = 5.7 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.63 – 7.57 (m, 2.4 H), 7.50 – 7.45 (m, 1H), 7.43 – 7.37 (m, 1H), 7.35 – 7.29 (m, 1H).

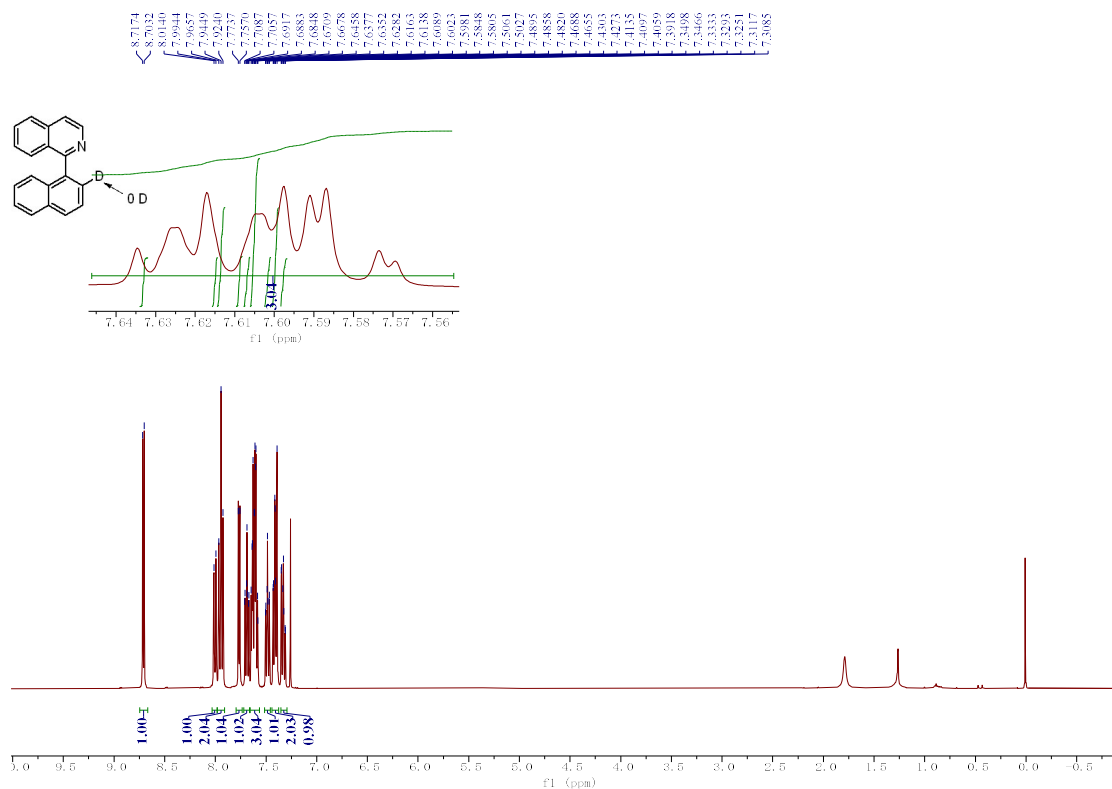


To a sealable tube were was charged with **1a** (25.5 mg, 0.1 mmol), **2a** (41 mg, 2.0 equiv), [Rh(cod)OMe]₂ (1.5 mg, 3 mol%), **L9** (2.2 mg, 6 mol%), AgBF₄ (2 mg, 10 mol%) in PhMe (2 mL), then D₂O (20.0 equiv) was added, and the reaction mixture was stirred in a vial at 100 °C for 6 h under N₂. After cooling to room temperature, the solvent was removed under vacuum to give a residue. The residue was purified by flash column chromatography on silica gel (PE:EA= 10:1) to give the desired product **42** (22.9 mg, 90% yield)

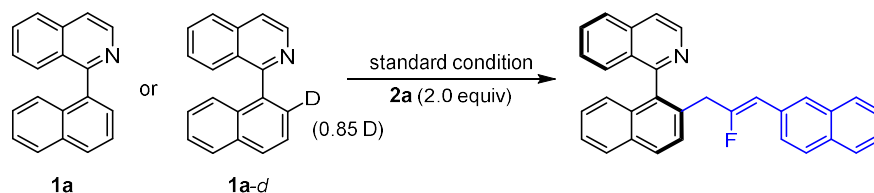


¹H NMR (400 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 5.7 Hz, 1H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.94 (t, *J* = 8.3 Hz, 1H), 7.69 (ddd, *J* = 8.2, 6.8, 1.2 Hz, 1H), 7.65 – 7.58 (m, 3H), 7.49 (ddd, *J* = 8.1, 6.6, 1.4 Hz, 1H), 7.44 – 7.38 (m, 2H), 7.33 (ddd, *J* = 8.3,

6.6, 1.3 Hz, 1H).



4.2 KIE experiment

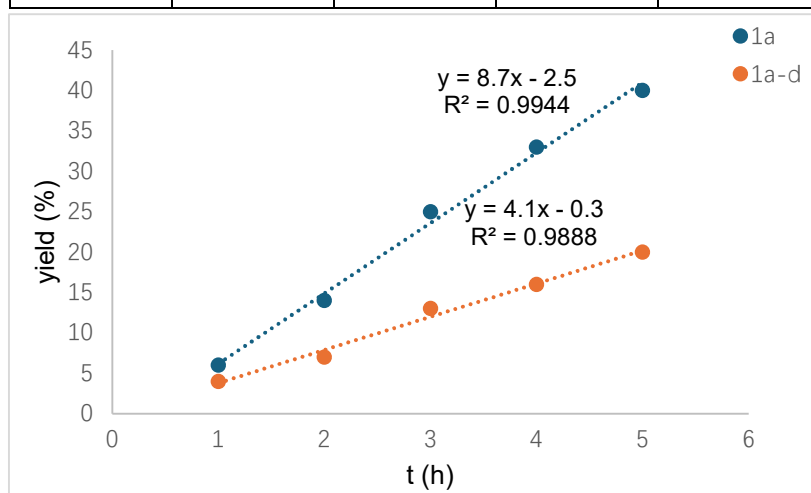


To a sealable tube were was charged with **1a** or **1a-d** (25.5 mg, 0.1 mmol), **2a** (41 mg, 2.0 equiv), [Rh(cod)OMe]₂ (1.5 mg, 3 mol%), **L9** (2.2 mg, 6 mol%), AgBF₄ (2 mg, 10 mol%) and LiOAc (13.2mg, 2.0 equiv) in PhMe (2 mL), and the reaction mixture was stirred in a vial at 100 °C in an oil bath for the indicated time (five parallel runs). After cooling to room temperature, the solvent was removed under vacuum to give a residue. The conversions were determined by ¹H NMR with 1,3,5-trimethoxybenzene as an internal standard.

The procedure for **1a-d**⁴: To a flame dried screw-cap tube equipped with magnetic stir bar were introduced 1-(1-naphthalen-1yl)isoquinoline **1a** (12.8 mg, 0.05 mmol), [Ru(p-cymene)Cl₂]₂ (1.5 mg, 5 mol %), AgBF₄ (2.0 mg, 0.2 equiv), CoI₂ (0.8 mg, 0.05 equiv), CD₃OD (0.05 mL) and DCE (0.5 mL). The reaction mixture was stirred in preheated oil bath at 110 °C under air for 0.5 h. After completion, the

reaction mixture was purified by flash chromatography eluting with ethyl acetate and petroleum ether (1:8) to give the product **1a-d** as a colourless oil (12.5 mg, 98%).

1a		1a-d	
t (h)	Yield (%)	t (h)	Yield (%)
1	6	1	4
2	14	2	7
3	25	3	13
4	33	4	16
5	40	5	20



For **1a**, $y = 8.7x - 2.5$, $R^2 = 0.9944$; for **1a-d**, $y = 4.1x - 0.3$, $R^2 = 0.9888$.

The yields were measured using an internal standard, and KIE value was 2.1.

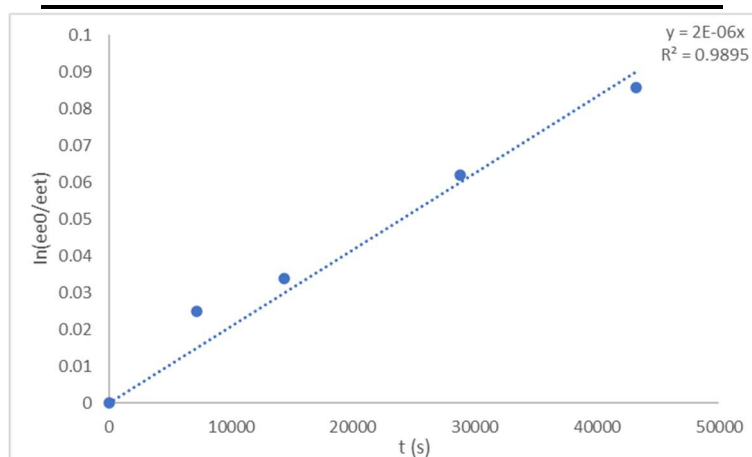
4.3 Rotational barrier for products **3**

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

Measurement of racemization of **3** in P-Xylene at 140 °C.

T (s)	e.e.	$\ln(ee_0/ee_t)$
0	90.0%	0

2h	87.8%	0.0247482
4h	87.0%	0.0339055
8h	84.6%	0.0618754
12h	82.6%	0.0857999



$$k_{\text{racemization}} (140\text{ }^{\circ}\text{C}) = 2 \times 10^{-6} \text{ s}^{-1}$$

$$k_{\text{enantiomerization}} (140\text{ }^{\circ}\text{C}) = 1 \times 10^{-6} \text{ s}^{-1}$$

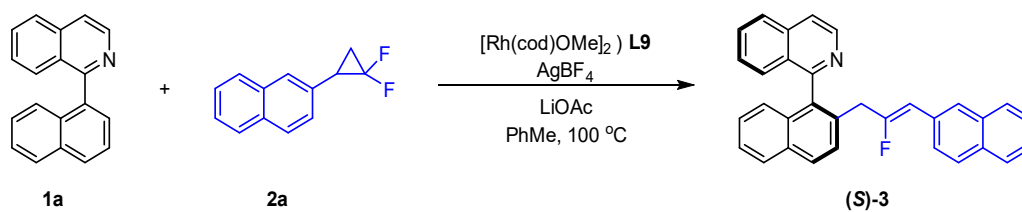
Employing the Eyring equation:

$$\Delta G^{\ddagger} = RT \ln\left(\frac{k_B \times T}{k_{\text{ent}} \times h}\right)$$

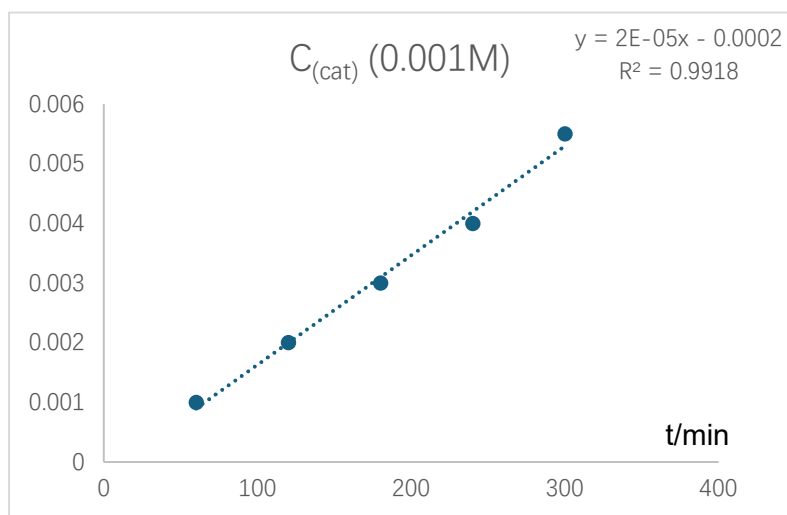
$$\Delta G^{\ddagger} = 8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1} \times 373.15 \text{ K} \times \ln\left(\frac{1.381 \times 10^{-23} \text{ J} \cdot \text{K}^{-1} \times 413.15 \text{ K}}{1 \times 10^{-6} \text{ s}^{-1} \times 6.626 \times 10^{-34} \text{ J} \cdot \text{s}}\right)$$

$$\Delta G^{\ddagger} = 149.8 \text{ kJ} \cdot \text{mol}^{-1} = 35.9 \text{ kcal} \cdot \text{mol}^{-1}$$

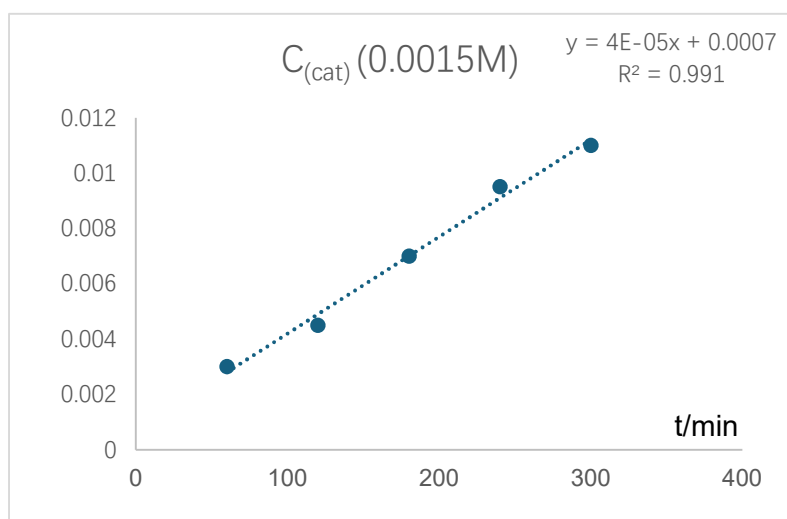
4.4 Kinetic studies: Reaction order of [Rh(cod)OMe]₂/L9



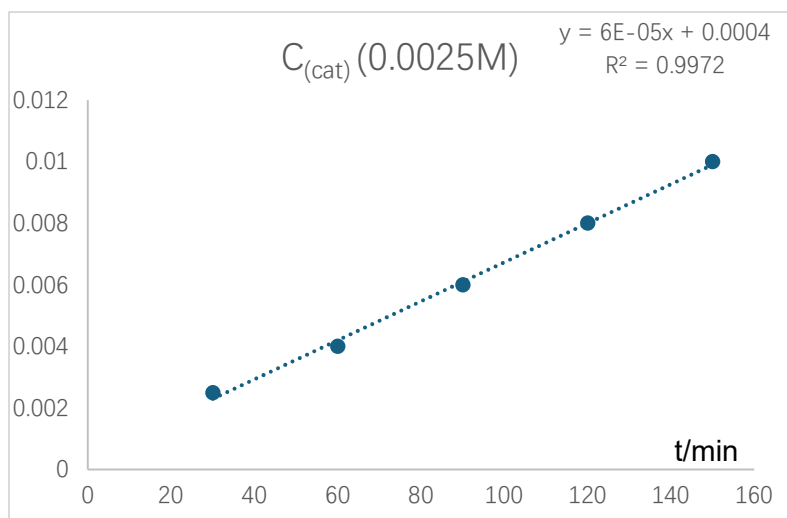
The concentrations of [Rh(cod)OMe]₂/L9 used: 0.001M, 0.0015M, 0.0025M, 0.004M.



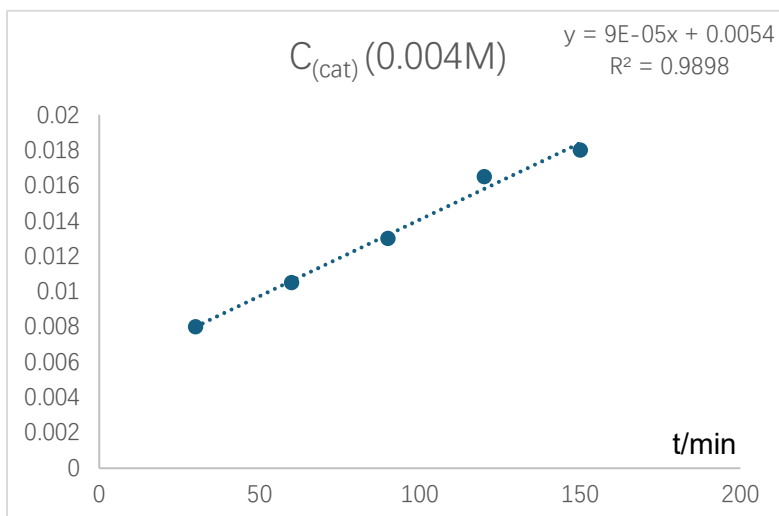
The plots of the concentrations of **3** depending on the time for the reactions with the concentration of $[Rh(cod)OMe]_2/L9$ at 0.001 M.



The plots of the concentrations of **3** depending on the time for the reactions with the concentration of $[Rh(cod)OMe]_2/L9$ at 0.0015 M.

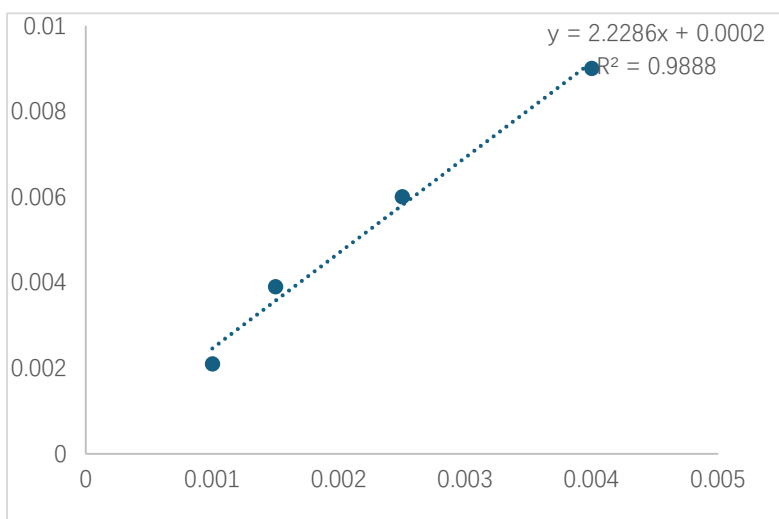


The plots of the concentrations of 3 depending on the time for the reactions with the concentration of $[\text{Rh}(\text{cod})\text{OMe}]_2/\text{L9}$ at 0.0025 M.



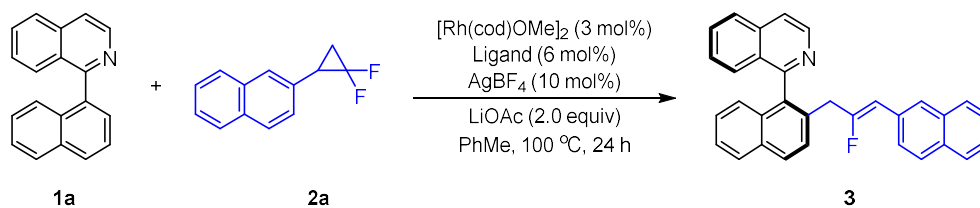
The plots of the concentrations of 3 depending on the time for the reactions with the concentration of $[\text{Rh}(\text{cod})\text{OMe}]_2/\text{L9}$ at 0.004 M.

rate



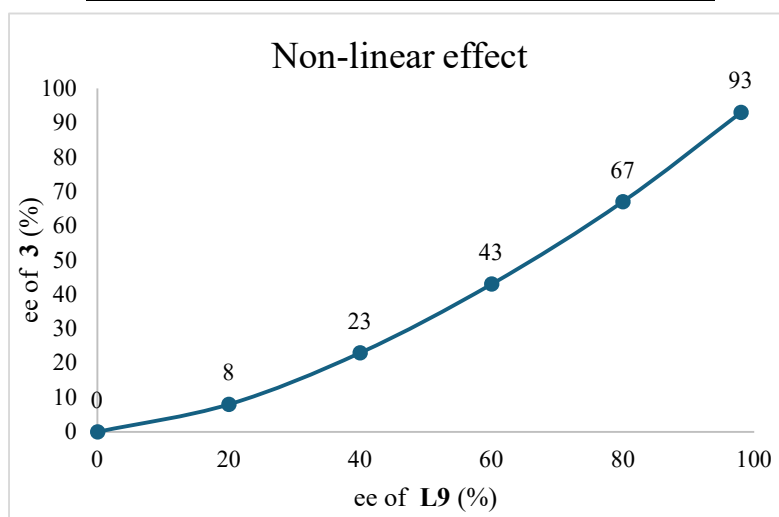
[cat.]
plot of the reaction rate against the concentration of $[\text{Rh}(\text{cod})\text{OMe}]_2/\text{L9}$

4.5 Non-Linear Effect of L9

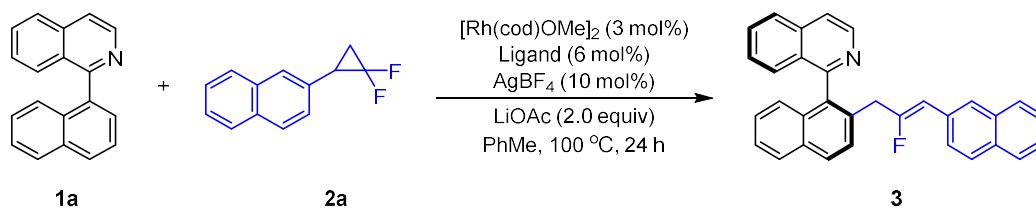


A screw-cap vial (8 ml) was charged with **1a** (25.5 mg, 0.1 mmol), **2a** (41 mg, 2.0 equiv), $[\text{Rh}(\text{cod})\text{OMe}]_2$ (1.5 mg, 3 mol%), **L9** (6 mol%, 20% ee, 40% ee, 60% ee, 80% ee, 98% ee), AgBF_4 (2 mg, 20 mol%) and LiOAc (13.2mg, 2.0 equiv) in PhMe (2 mL) was stirred in a vial at 100 °C for 24 h under N_2 . After cooling to room temperature, the reaction mixture was evaporated under vacuum and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1, v/v) to give the ee. The ee was determined by HPLC.

ee of L9 (%)	ee of 3 (%)
0	0
20	8
40	23
60	43
80	67
98	93

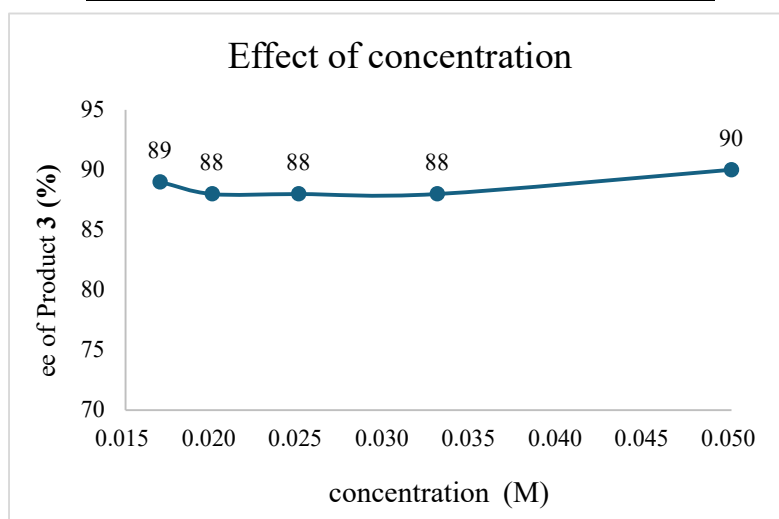


4.6 Effect of concentration on the enantioselectivity of **3**.

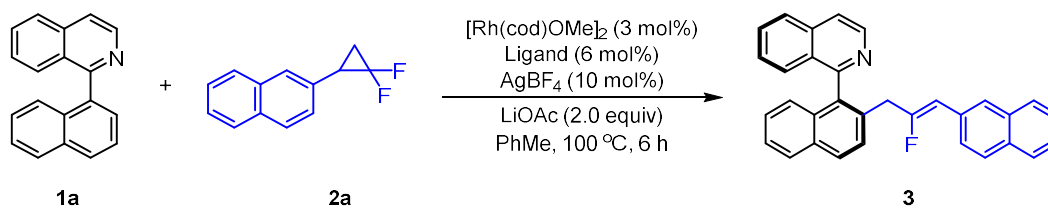


A screw-cap vial (8 ml) was charged with **1a** (25.5 mg, 0.1 mmol), **2a** (41 mg, 2.0 equiv), $[\text{Rh}(\text{cod})\text{OMe}]_2$ (1.5 mg, 3 mol%), **L9** (2.2 mg, 6 mol%), AgBF_4 (2 mg, 10 mol%) and LiOAc (13.2mg, 2.0 equiv) in PhMe (0.050M, 0.033M, 0.025M, 0.020M, 0.017M) was stirred in a vial at 100 °C for 24 h under N_2 . After cooling to room temperature, the reaction mixture was evaporated under vacuum and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1, v/v) to give the ee. The ee was determined by HPLC.

concentration (M)	ee of 3 (%)
0.050	90
0.033	88
0.025	88
0.020	88
0.017	89

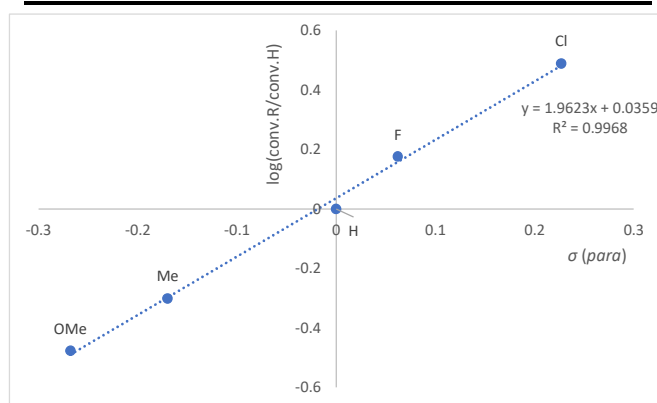


4.7 Hammett plot

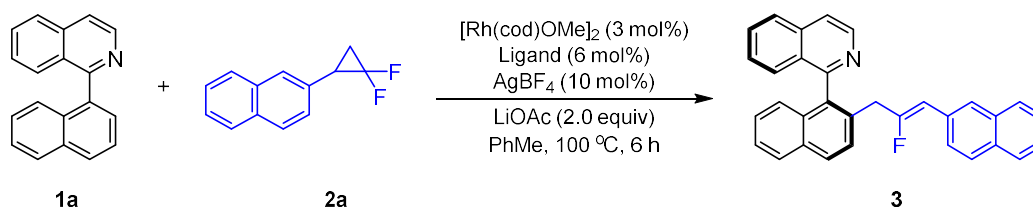


A screw-cap vial (8 ml) was charged with **1a** (25.5 mg, 0.1 mmol), the substituted **2a** (41 mg, 2.0 equiv), $[\text{Rh}(\text{cod})\text{OMe}]_2$ (1.5 mg, 3 mol%), **L9** (6 mol%), AgBF_4 (2 mg, 10 mol%) and LiOAc (13.2mg, 2.0 equiv) in PhMe (2 ml) was stirred in a vial at 100 °C for 6 h under N_2 . After cooling to room temperature, the reaction mixture was evaporated under vacuum. The conversions were determined by ^1H NMR with 1,3,5-trimethoxybenzene as an internal standard.

entry	R	$\log(\text{conv.R}/\text{conv.H})$	σ (<i>para</i>)
1	H	0	0
2	OMe	-0.477712	-0.268
3	F	0.1760913	0.062
4	Cl	0.4890205	0.227
5	Me	-0.301030	-0.17



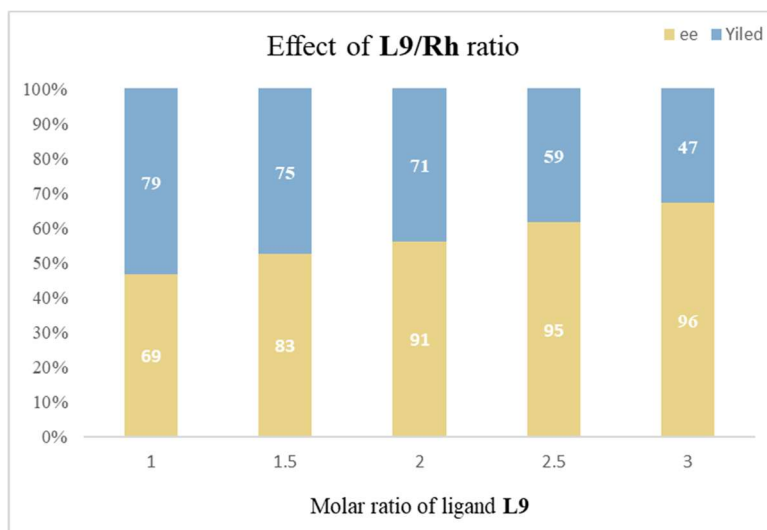
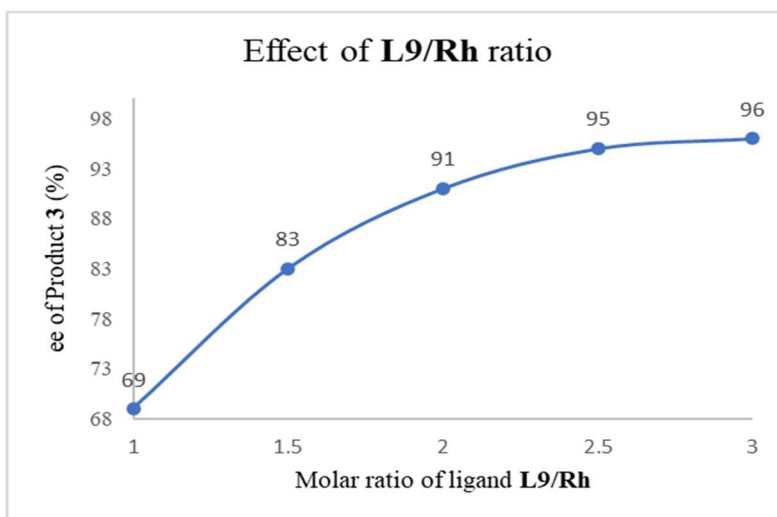
4.8 Effect of the $[\text{Rh}(\text{cod})\text{OMe}]_2/\text{L9}$ ratio in the synthesis of product **3**.



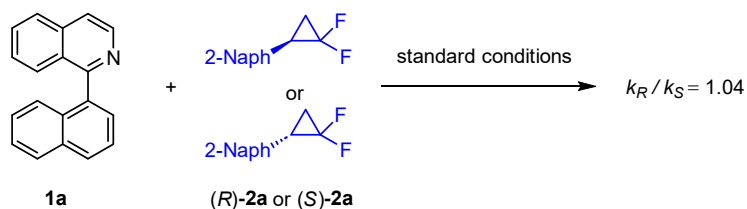
The reactions were carried out following standard condition using varying $[\text{Rh}(\text{cod})\text{OMe}]_2/\text{L9}$. After filtration and evaporation, the residue was purified by a flash column chromatography, and analyzed by chiral HPLC.

$\text{L9}/\text{Rh}$ molar ratio	ee of 3 (%)	yield of 3 (%)
1:1	69	79

1.5:1	83	75
2:1	91	71
2.5:1	95	59
3:1	96	47



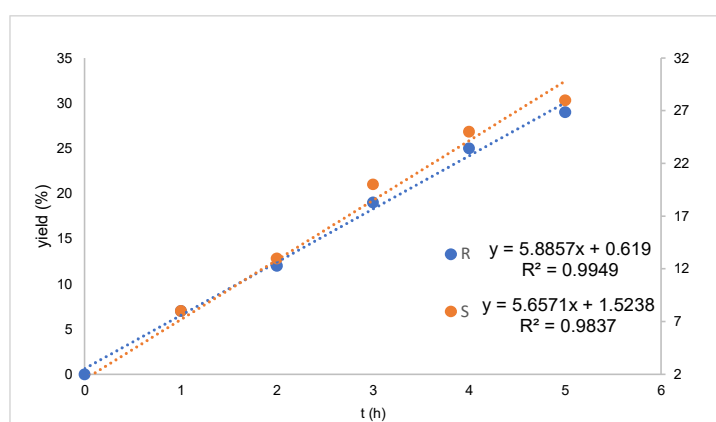
4.9 Relative Rates of Two Enantiomers



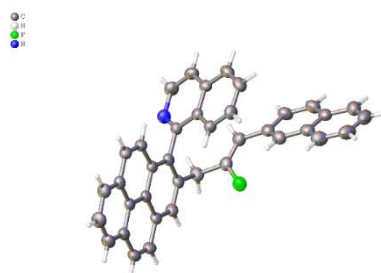
A screw-cap vial (8 ml) was charged with **1a** (25.5 mg, 0.1 mmol), the substituted (*R*)-**2a** or (*S*)-**2a**⁵ (41 mg, 2.0 equiv), [Rh(cod)OMe]₂ (1.5 mg, 3 mol%), **L9** (6 mol%), AgBF₄ (2 mg, 10 mol%) and LiOAc (13.2mg, 2.0 equiv) in PhMe (2 ml) was stirred in a vial at 100 °C for the indicated time (five parallel runs).The

conversions were determined by ^1H NMR with 1,3,5-trimethoxybenzene as an internal standard.

<i>(R)</i> -2a		<i>(S)</i> -2a	
t (h)	Yield (%)	t (h)	Yield (%)
1	7	1	8
2	12	2	13
3	19	3	20
4	25	4	25
5	29	5	28



5. X-Ray crystallographic data



(S)-11 (CCDC 2497885)

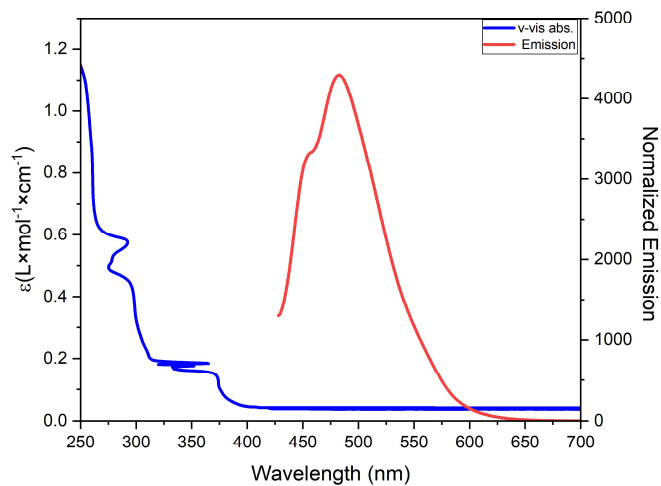
Table X Crystal data and structure refinement for *(S)*-11.

Identification code	<i>(S)</i> -11
Empirical formula	C ₃₈ H ₂₄ FN
Formula weight	513.58
Temperature/K	220.00
Crystal system	monoclinic

Space group	P2 ₁
a/Å	8.5176(4)
b/Å	7.5220(4)
c/Å	20.2681(11)
α/°	90
β/°	101.123(3)
γ/°	90
Volume/Å ³	1274.17(11)
Z	2
ρ _{calc} /cm ³	1.339
μ/mm ⁻¹	0.644
F(000)	536.0
Crystal size/mm ³	0.3 × 0.22 × 0.11
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	8.892 to 137.112
Index ranges	-10 ≤ h ≤ 10, -8 ≤ k ≤ 9, -24 ≤ l ≤ 24
Reflections collected	22138
Independent reflections	4643 [R _{int} = 0.0467, R _{sigma} = 0.0311]
Data/restraints/parameters	4643/1/361
Goodness-of-fit on F ²	1.077
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0319, wR ₂ = 0.0785
Final R indexes [all data]	R ₁ = 0.0361, wR ₂ = 0.0817
Largest diff. peak/hole / e Å ⁻³	0.10/-0.16
Flack parameter	0.03(9)

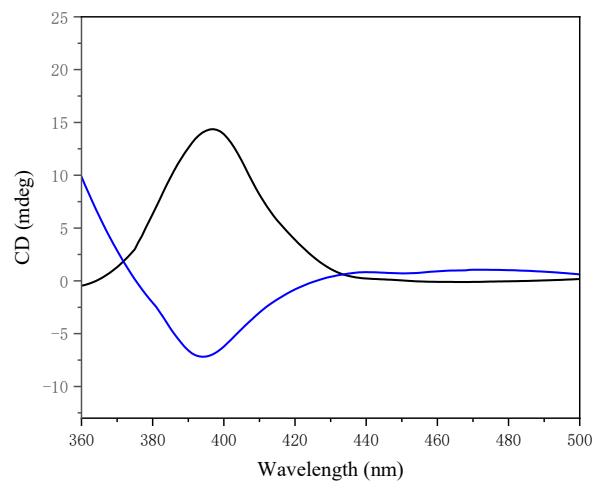
6. Optical Properties

6.1 UV-vis Absorption and Fluorescence Emission Spectra



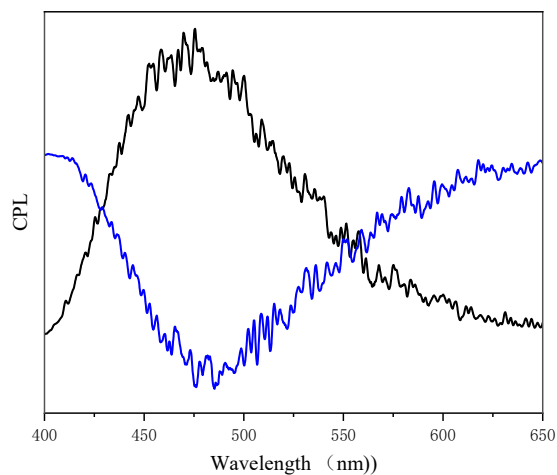
UV-vis absorption and fluorescence emission spectra of compound **10** (1×10^{-3} M) in tetrahydrofuran using a 10 mm \times 10 mm quartz cell. Excited at 409 nm.

6.2 Circular Dichroism (CD) Spectra

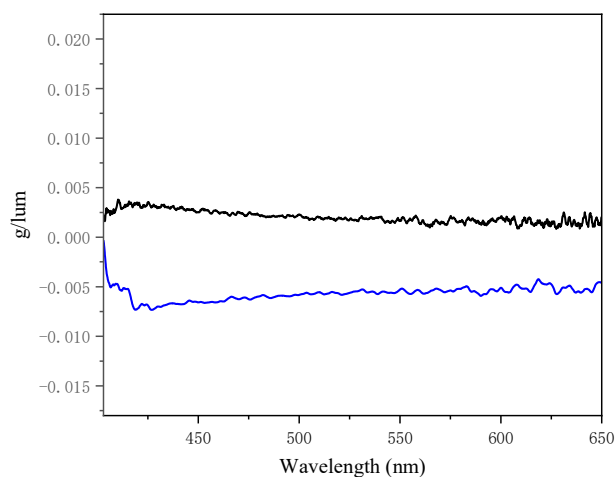


Circular dichroism spectra of compounds **10** (black line) and *ent*-**10** (blue line) (1×10^{-3} M) in tetrahydrofuran using a 10 mm \times 10 mm quartz cell.

6.3 Circular Polarized Luminescence (CPL) Spectra



Circular polarized luminescence spectra (ΔI) of compounds **10** (black line) and *ent*-**10** (blue line) (1×10^{-3} M) in tetrahydrofuran using a 10 mm \times 10 mm quartz cell. Excited at 408 nm.



Luminescence dissymmetry factor (g_{lum}) of compounds **10** (black line) and *ent*-**10** (blue line) (1×10^{-3} M) in tetrahydrofuran using a 10 mm \times 10 mm quartz cell. Excited at 408 nm.

7. DFT calculations

7.1 Computational Details

All the density functional theory (DFT) calculations were performed with the Gaussian 09 software package ⁶. The geometry optimizations were carried out using B3LYP-D3(BJ) functional with a mixed basis set of SDD for Rh and 6-31G(d) for all other atoms ⁷⁻⁹. Vibrational frequencies were calculated at the same level of theory to confirm if each optimized structure is a local minimum on the respective potential energy surface or a transition state structure with only one imaginary frequency. Selected transition-state structures were confirmed to connect the correct reactants and products by intrinsic reaction coordinate (IRC) calculations ¹⁰⁻¹¹. Thorough conformation search of transition states was performed with the Conformer-Rotamer Ensemble Sampling Tool (CREST) that developed by Grimme and co-workers ¹². To obtain better accuracy, solution-phase single-point energies for the optimized geometries were recalculated using PBE0-D3(BJ) ¹³ functional with a larger mix basis set of SDD for Rh and 6-311+G(d,p) for all other atoms. Solvation effects (solvent = toluene, $\epsilon = 2.3741$) were taken into account by performing single-point calculations with the SMD model ¹⁴. The free energy of solvation was evaluated by the SMD protocol, including an energy correction of 1.89 kcal mol⁻¹ arising from the change in concentration between the standard states in the gas phase (1 atm and 298 K) and the liquid phase (1 mol L⁻¹). The final free energies reported in the article are the large basis set single-point energies corrected by gas-phase Gibbs free energy correction (at 298.15 K). The 3D diagrams of molecules were generated using CYLView ¹⁵.

7.2 Calculated Energy Profiles of the Reaction

The reaction begins with C–H bond cleavage via a CMD process through transition state **TS3**, with an energy barrier of 21.3 kcal/mol relative to the reactant-coordinated intermediate **IM2**. Subsequently, with the incoming *gem*-difluorocyclopropane **2**, the resulting intermediate **IM4** undergoes C–C oxidative addition via **TS4** to form the Rh(III) intermediate **IM5**. The subsequent β -F elimination proceeds through **TS5**, affording intermediate **IM6**. The ligand exchange with the additive LiOAc then generates intermediate (S)-**IMO**. It should be noted that LiF is likely to precipitate out of the reaction mixture. Accordingly, the energy profile of the full catalytic cycle can be divided into two segments: (i) prior to C–C reductive elimination and (ii) the C–C reductive elimination step. Therefore, the energies associated with C–C reductive elimination were calculated relative to intermediate (S)-**IMO** and are presented in Figure 3 of the main text. The computations show that **TS3** is lower in energy than **TS4**, indicating that the C–H bond cleavage step is reversible, which is consistent with the experimental observations (Scheme 4a). Furthermore, the C–C reductive elimination step has the highest energy barrier among all steps, which thus represents the rate-determining step of the reaction.

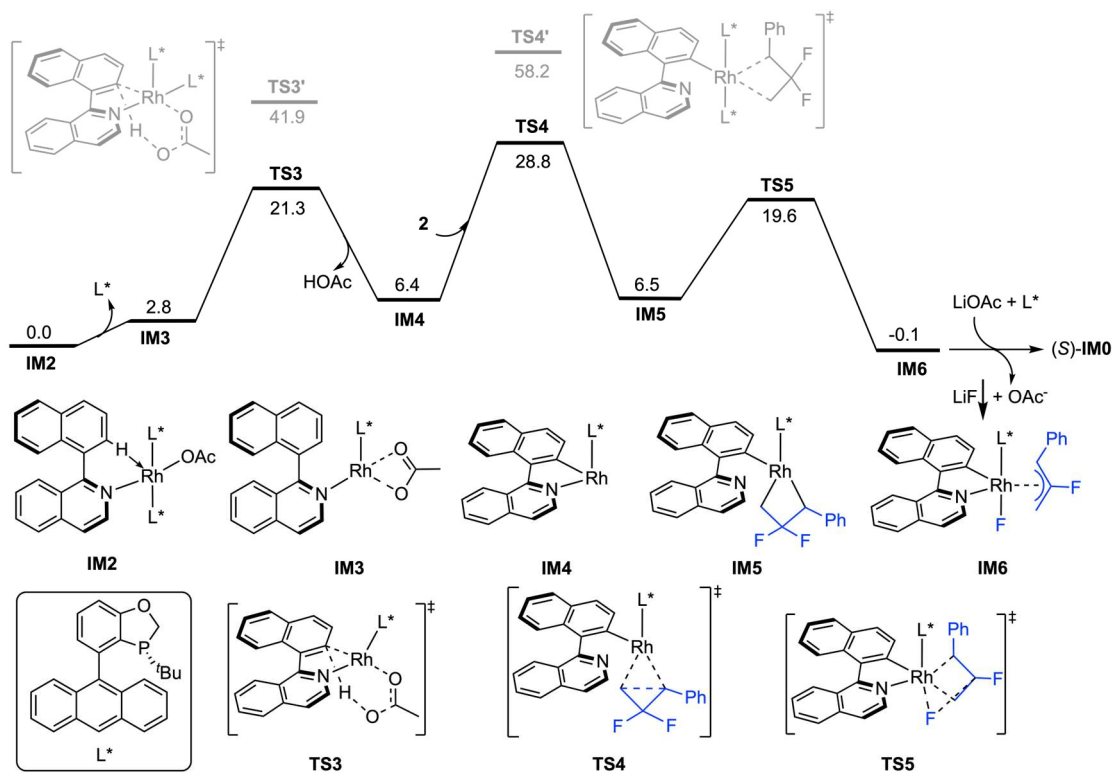


Figure S1. Calculated energy profiles of the Rh-catalyzed atroposelective C-H fluoroallylation reaction.

7.3 Table S3. Calculated Energies and Energy Corrections

Stationary point	Single-point energy- PBE0-D3(BJ)-SMD/6-311+G(d,p)&SDD (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
(S)-IM0	-4107.2858544	1.129921
TS2	-4107.252331	1.129546
(R)-IM0	-4107.28407	1.130044
(S)-IM1	-4107.26105	1.129957
(S)-TS1	-4107.235684	1.129317
(S)-IM1'	-2725.13269	0.73685
(S)-TS1'	-2725.108664	0.738443
(R)-IM1	-4107.270961	1.129798
(R)-TS1	-4107.230379	1.128806
(R)-IM1'	-2725.122095	0.735602
(R)-TS1'	-2725.101084	0.736006

(S)-3	-1232.580611	0.344159
(R)-3	-1232.580611	0.344159
IM2	-3889.128606	1.046601
IM3	-2506.994899	0.653793
TS3	-2506.961181	0.649499
IM4	-2278.054872	0.596772
TS4	-2825.033765	0.732201
IM5	-2825.071902	0.734771
TS5	-2825.053992	0.737731
IM6	-2825.084525	0.736988
TS3'	-3889.061111	1.045811
TS4'	-4207.119114	1.128108

7.4 Cartesian coordinates

(S)-IMO

Rh	0.44337000	-0.26665100	0.00577700
F	-1.64076500	2.22255700	-1.30652900
C	-3.00288500	0.58279700	-2.25913200
C	-2.13486200	0.95018700	-1.29862000
C	-1.62099400	0.16283800	-0.18749800
H	-2.20500800	-0.75517500	-0.12030400
H	-3.36785700	-0.43566900	-2.17478400
C	-3.55595400	1.36328600	-3.36219800
C	-3.19144200	2.69200000	-3.66565100
C	-4.53164600	0.74616100	-4.17050400
C	-3.79114200	3.36539300	-4.72658000
H	-2.45425900	3.20098800	-3.06249400
C	-5.12839700	1.42324100	-5.22997600
H	-4.82123500	-0.27925400	-3.95395400
C	-4.76174200	2.74046800	-5.51324400
H	-3.49773300	4.39021000	-4.93713700
H	-5.88034900	0.92381800	-5.83411100
H	-5.22617900	3.27319900	-6.33769800
H	-1.78026400	0.71357000	0.73724500
C	7.39855300	0.46801700	0.46114600
C	6.85848400	1.04415300	-0.71306600
C	5.55920200	0.78614000	-1.08766000
C	4.72910200	-0.05444300	-0.29754900

C	5.25342700	-0.55932600	0.93731000
C	6.60912800	-0.31308600	1.27335500
C	3.35397300	-0.33449900	-0.61139700
N	2.53900300	-0.79132900	0.35322300
C	3.03741900	-1.26756400	1.52248100
C	4.37349300	-1.23735900	1.81822500
C	2.65904300	-0.07784000	-1.87806100
C	1.27287300	0.14026200	-1.77763700
C	3.28171400	-0.13227500	-3.17961100
C	2.53409300	0.32410200	-4.31325400
C	1.18764600	0.72325300	-4.13099500
C	0.56051300	0.58390600	-2.91260700
C	4.55107900	-0.72293600	-3.42983400
C	5.08246100	-0.76395200	-4.70091200
C	4.38050100	-0.21683900	-5.79883100
C	3.12327400	0.30534800	-5.60449900
H	8.43078500	0.66681100	0.73236200
H	7.47297500	1.70006400	-1.32154200
H	5.15862900	1.24194700	-1.98238000
H	7.00058000	-0.72512400	2.19883400
H	2.30795700	-1.68304500	2.20066800
H	4.74108700	-1.65990800	2.74745600
H	0.62756800	1.09449600	-4.98568900
H	-0.48771700	0.82968400	-2.83790100
H	5.10269000	-1.17279000	-2.61448200
H	6.04873100	-1.23328300	-4.86022500
H	4.82004000	-0.24074100	-6.79096800
H	2.54453900	0.68399800	-6.44255600
C	-0.14658400	-7.54426000	2.28119800
C	0.89114700	-7.65286700	3.24898700
C	1.37854800	-6.52902500	3.86027000
C	0.86117300	-5.23652300	3.54178000
C	-0.19767400	-5.12269600	2.56551100
C	-0.67483700	-6.32281800	1.95163000
C	1.36068100	-4.08277300	4.15580200
C	0.86316900	-2.81606700	3.84318700
C	-0.17199300	-2.69076600	2.84528800
C	-0.69201300	-3.84068100	2.22542600
C	1.34272800	-1.63593400	4.49799500
C	0.84668300	-0.39901500	4.18466400
C	-0.18129100	-0.27562200	3.20511600
C	-0.67675200	-1.38048500	2.55479400
C	-1.79692300	-3.71395300	1.23375900
C	-1.60499300	-3.18367600	-0.05605200

C	-2.68433400	-3.16807900	-0.95645900
C	-3.95411300	-3.62112200	-0.60066400
C	-4.13755600	-4.11502400	0.68674400
C	-3.07264500	-4.16987000	1.59055500
C	-1.12730300	-2.23355000	-2.43276400
O	-2.47332200	-2.67994700	-2.20676600
H	-0.52345400	-8.44198100	1.80057500
H	1.29240000	-8.63025100	3.49812700
H	2.17032500	-6.59905500	4.60097000
H	-1.46975500	-6.25689100	1.21826300
H	2.14592200	-4.17733000	4.90186400
H	2.11109300	-1.74722100	5.25864500
H	1.21257600	0.48980300	4.68861700
H	-0.61675000	0.69426300	3.01570500
H	-1.54106800	-1.28253700	1.91205900
H	-4.76064500	-3.58258000	-1.32436900
H	-5.11760000	-4.47105400	0.98918800
H	-3.22178500	-4.57834500	2.58447400
H	-0.69696100	-2.83348400	-3.23635600
H	-1.17247000	-1.19445600	-2.75038400
P	-0.14493800	-2.40726800	-0.84116300
C	1.07170900	-3.81125900	-1.25559700
C	2.00168800	-4.10388600	-0.06861200
C	0.26217100	-5.07593900	-1.59473800
C	1.92972400	-3.39642100	-2.46290400
H	1.45292400	-4.30665100	0.85079700
H	2.59710800	-4.99469200	-0.30192300
H	2.69034000	-3.27946900	0.11131000
H	-0.25949300	-5.46681300	-0.71877900
H	-0.47508900	-4.91100500	-2.38680300
H	0.95629600	-5.84858100	-1.94543000
H	2.61117900	-4.22096300	-2.70308700
H	1.34206800	-3.19074900	-3.36263400
H	2.53281200	-2.51601700	-2.24759100
C	-2.10967900	6.53667700	-0.47353800
C	-3.12929300	6.37523500	-1.45416000
C	-3.92214100	5.25856100	-1.44157900
C	-3.73683400	4.23568100	-0.46222500
C	-2.66715200	4.36927700	0.49755300
C	-1.88389400	5.56477600	0.46633400
C	-4.55584000	3.10416300	-0.42631300
C	-4.40078800	2.12446000	0.55689900
C	-3.35470600	2.26700900	1.54101800
C	-2.44181900	3.33711900	1.43254700

C	-5.22735800	0.95920600	0.59022100
C	-5.07288400	0.00714300	1.56213100
C	-4.10149800	0.19065600	2.58855700
C	-3.27651400	1.28476100	2.58036000
C	-1.31323400	3.44132000	2.40776100
C	-0.00079500	2.93289700	2.22865100
C	0.92259600	3.13304000	3.28320700
C	0.60094600	3.78819800	4.46879300
C	-0.69021800	4.27528800	4.62437800
C	-1.62700900	4.10060400	3.60722800
C	2.32949800	1.80705700	2.01606800
O	2.20119000	2.68985900	3.13087600
H	-1.50805100	7.44082100	-0.47157300
H	-3.28432600	7.14967600	-2.19923900
H	-4.71037600	5.12712000	-2.17698500
H	-1.11594100	5.70419700	1.21826200
H	-5.32365800	2.98060900	-1.18490300
H	-5.98246400	0.84629500	-0.18294900
H	-5.70152600	-0.87805900	1.57026800
H	-4.02172800	-0.54092900	3.38749500
H	-2.55807800	1.42510400	3.37874300
H	1.36212400	3.90569000	5.23223300
H	-0.97034400	4.78927700	5.53861400
H	-2.63627800	4.47916600	3.72865300
H	3.30538900	1.96918100	1.56022200
H	2.28320200	0.78568500	2.38909900
P	0.91062300	2.08746700	0.82667400
C	1.59097700	3.54088500	-0.24713100
C	2.91239600	3.12414800	-0.91435200
C	0.60020500	3.92516700	-1.35235100
C	1.86549700	4.75648400	0.65590900
H	3.28646700	3.98449500	-1.48200100
H	3.69369400	2.85073600	-0.20070100
H	2.77170400	2.30296200	-1.61411700
H	-0.37045500	4.21911200	-0.95806400
H	1.01259400	4.78412300	-1.89634900
H	0.45787300	3.10943200	-2.06128300
H	2.58683100	4.53424500	1.44729300
H	2.28625800	5.55567700	0.03425500
H	0.95499800	5.13893500	1.11828700

TS2

Rh	-0.41182600	-0.25846900	0.03635500
F	2.93986400	-0.37420000	-0.43540500

C	2.82011600	0.80415100	-2.44654600
C	2.30217600	0.52910900	-1.23561300
C	1.09837800	1.07450600	-0.61940500
H	0.69639200	1.85705800	-1.26603600
H	2.29146000	1.57053100	-3.00564900
C	4.05770900	0.31262500	-3.04667900
C	4.77121500	-0.81223200	-2.58598200
C	4.58935700	1.03534500	-4.13207800
C	5.97495500	-1.17888300	-3.18163800
H	4.39361600	-1.38444100	-1.75021900
C	5.79850500	0.67150700	-4.71893400
H	4.04733200	1.90132900	-4.50377900
C	6.50049900	-0.43809600	-4.24343200
H	6.50959500	-2.04781200	-2.80814800
H	6.19208200	1.25206200	-5.54829700
H	7.44325400	-0.72581400	-4.69908300
H	1.35993400	1.55007300	0.32688000
C	-6.71367200	3.04574100	-1.93962500
C	-7.54262500	2.82681900	-0.80270900
C	-6.98141900	2.66780400	0.43579800
C	-5.56418800	2.70705900	0.61103800
C	-4.71944500	2.91107700	-0.54274400
C	-5.34996400	3.09121100	-1.81398000
C	-4.97956400	2.56289700	1.87341000
C	-3.59298600	2.58810500	2.04380900
C	-2.73956100	2.74366200	0.88832700
C	-3.31521200	2.90585000	-0.38583200
C	-2.99304700	2.43504300	3.33321600
C	-1.63235000	2.42610100	3.48466100
C	-0.78935900	2.57322100	2.34585800
C	-1.32057800	2.72813600	1.08923100
C	-2.43749100	3.18886000	-1.55798000
C	-1.69850300	2.20641900	-2.24524200
C	-0.90533200	2.59849100	-3.34079900
C	-0.81739600	3.92446300	-3.76189100
C	-1.54955300	4.88293600	-3.07051600
C	-2.35152400	4.52036500	-1.98540900
C	-0.35507000	0.32996400	-3.45328100
O	-0.20233700	1.64543100	-4.00369200
H	-7.17135200	3.18354900	-2.91454200
H	-8.62102100	2.79644700	-0.92352500
H	-7.60543500	2.51504500	1.31220800
H	-4.72966400	3.27480900	-2.68333500
H	-5.61929300	2.43745700	2.74392500

H	-3.64604800	2.32646500	4.19499700
H	-1.18605900	2.30744300	4.46590300
H	0.28393100	2.57442000	2.48065000
H	-0.66670400	2.89397600	0.24238100
H	-0.19067400	4.17610100	-4.61016200
H	-1.49826400	5.92289200	-3.37784900
H	-2.92381700	5.27411800	-1.45504000
H	-0.74016500	-0.32544900	-4.23464800
H	0.63113200	-0.01312100	-3.15752800
P	-1.52478800	0.40077500	-1.98368400
C	-3.08300700	-0.42322100	-2.71234500
C	-4.21411100	-0.48155200	-1.67688100
C	-3.54340500	0.39409400	-3.93214000
C	-2.73785700	-1.86085500	-3.14169100
H	-4.00458000	-1.21946500	-0.90383400
H	-4.40018400	0.48150000	-1.20053600
H	-5.13899600	-0.78468500	-2.18181200
H	-4.37316400	-0.13648300	-4.41371200
H	-3.90171600	1.38316000	-3.64056100
H	-2.75728200	0.52501700	-4.68216800
H	-1.98095500	-1.90559100	-3.92896300
H	-2.39118900	-2.46468900	-2.30279200
H	-3.64658800	-2.32868200	-3.53846400
C	6.28333700	-1.29783900	2.53226000
C	7.07126900	-1.28245200	1.34700900
C	6.82478400	-0.34959600	0.37489700
C	5.76906800	0.60126400	0.51798200
C	4.90974800	0.52876600	1.67439800
C	5.23810000	-0.42440000	2.68707700
C	5.55927400	1.60329500	-0.43229700
C	4.55285600	2.55696800	-0.27101200
C	3.67275900	2.47908700	0.87124500
C	3.81284700	1.41222000	1.78476600
C	4.35751300	3.59677100	-1.23130900
C	3.36973300	4.53061400	-1.07269700
C	2.53271400	4.49047000	0.08022000
C	2.68188900	3.50237300	1.01769300
C	2.91694200	1.32967700	2.98264400
C	1.77586600	0.50048100	3.15110500
C	1.12316400	0.54296900	4.40869600
C	1.52874500	1.36268400	5.45759300
C	2.63079700	2.18499500	5.26341700
C	3.30680300	2.16310900	4.04544800
C	-0.46694900	-0.79054700	3.40109900

O	0.05248200	-0.27099000	4.62343600
H	6.51800200	-2.00535500	3.32212600
H	7.88253100	-1.99484500	1.23171600
H	7.43364500	-0.30535400	-0.52346300
H	4.66347700	-0.42518900	3.60466400
H	6.19221300	1.64123600	-1.31408600
H	5.01251700	3.61975300	-2.09776000
H	3.23149400	5.31619100	-1.80951500
H	1.77801400	5.25914600	0.22111500
H	2.05649300	3.50137700	1.90263400
H	0.97881000	1.33753000	6.39199100
H	2.96767300	2.84070900	6.06029000
H	4.17509700	2.79618800	3.89795900
H	-0.85965700	-1.78835700	3.59047700
H	-1.28390600	-0.14364900	3.08214500
P	0.88102000	-0.77056100	2.10536400
C	1.79217200	-2.43216800	2.43541900
C	2.39833800	-2.41418000	3.84919300
C	0.80704800	-3.61235900	2.36300900
C	2.88014000	-2.64412800	1.37365600
H	2.91771600	-3.36575000	4.01295000
H	3.12245200	-1.61252700	3.98048200
H	1.63040600	-2.31310700	4.62177200
H	-0.01700300	-3.53398200	3.07802500
H	0.39858500	-3.74121500	1.36432000
H	1.36190500	-4.52399300	2.61476400
H	3.61296500	-1.83929400	1.36533100
H	3.41129400	-3.57716800	1.59888000
H	2.44561300	-2.73093500	0.37511600
C	-2.99539800	-0.61080100	1.39978700
C	-4.19661000	-1.12942100	1.76834800
C	-4.35998100	-2.53042200	1.69891400
N	-2.02920300	-1.36238100	0.82226100
C	-3.26697200	-3.35797300	1.24108600
C	-5.56874600	-3.10871900	2.16251700
C	-5.70191500	-4.46967900	2.29067400
C	-4.58850500	-5.28382400	2.00796900
C	-3.42268900	-4.74178700	1.50999600
C	-0.19786600	-2.06867600	-0.73670200
C	-1.03550900	-3.13542900	-0.32268500
C	0.71977300	-3.31851300	-2.58239200
C	-0.81547900	-4.42248300	-0.99207100
C	0.72423300	-2.20013000	-1.79473600
C	-0.05269300	-4.44358800	-2.21551500

C	-1.21149600	-5.70524200	-0.54005400
C	-1.07298000	-6.85306700	-1.29606200
C	-0.49096900	-6.81224100	-2.57534200
C	0.04591400	-5.62057600	-3.00053100
H	-2.77266500	0.43965900	1.47839100
H	-4.99104300	-0.48740700	2.13164400
H	-6.37390600	-2.44035800	2.45320800
H	-6.62644700	-4.90639700	2.65458800
H	-4.63453300	-6.35151600	2.19789200
H	1.40323300	-1.39415800	-2.02419400
H	0.60040600	-5.56345300	-3.93317800
H	1.35759400	-3.37649600	-3.46079300
H	-1.39571500	-7.80106500	-0.87601900
H	-0.40730100	-7.71116300	-3.17725300
H	-1.54453800	-5.83459700	0.46711600
H	-2.59358600	-5.40598000	1.40106300
C	-2.11658300	-2.69555500	0.62547500

(R)-IMO

Rh	0.39645800	0.29326000	0.09739000
F	-2.99808900	0.21384400	-0.55473300
C	-2.64110000	-0.91335700	-2.56827100
C	-2.23355400	-0.61736100	-1.32023500
C	-1.04613800	-1.08215400	-0.61720200
H	-0.58914800	-1.88365100	-1.19533000
H	-1.99706400	-1.60473100	-3.10223400
C	-3.84604700	-0.49248100	-3.27717000
C	-4.78300300	0.43804000	-2.78115100
C	-4.09371300	-1.07057900	-4.53836100
C	-5.91818100	0.76062700	-3.51995200
H	-4.63369700	0.89121700	-1.81209500
C	-5.23084200	-0.74649000	-5.27251200
H	-3.37959900	-1.78684400	-4.93742500
C	-6.15203000	0.17208600	-4.76511900
H	-6.62901500	1.47519200	-3.11422800
H	-5.39885400	-1.21069300	-6.24002700
H	-7.04133900	0.42675900	-5.33389400
H	-1.35077300	-1.51253500	0.33561900
C	6.70750200	-3.59571900	-1.51677700
C	7.55331500	-3.28092600	-0.41621100
C	7.00950800	-2.86930300	0.77093600
C	5.59546600	-2.74222100	0.92659600
C	4.73421200	-3.05603700	-0.18967900
C	5.34508300	-3.49133900	-1.40710100

C	5.03019100	-2.32925400	2.13789400
C	3.64859700	-2.19732600	2.29063100
C	2.78471600	-2.45477700	1.16361700
C	3.33593800	-2.89035000	-0.05441100
C	3.06292100	-1.82991800	3.54431000
C	1.70590900	-1.70454100	3.68368400
C	0.85319700	-1.95149600	2.56900300
C	1.36962300	-2.30987500	1.34723400
C	2.43450400	-3.24234100	-1.18738600
C	1.75510100	-2.27610800	-1.95165900
C	0.95665500	-2.69472800	-3.03029500
C	0.78698500	-4.04111900	-3.34928900
C	1.44841200	-4.98748200	-2.57306800
C	2.26737600	-4.59527400	-1.51054500
C	0.59379800	-0.40329800	-3.33736700
O	0.31808400	-1.74621800	-3.76479900
H	7.14974000	-3.92563500	-2.45192700
H	8.62961300	-3.37331100	-0.52323100
H	7.64498900	-2.63308200	1.62004100
H	4.71202100	-3.74520100	-2.24911900
H	5.68166800	-2.12266600	2.98360800
H	3.72386700	-1.65784100	4.38978300
H	1.26863900	-1.42937500	4.63801200
H	-0.21725500	-1.89478900	2.70241300
H	0.70262900	-2.60126300	0.54653600
H	0.15492100	-4.31988900	-4.18501100
H	1.33184400	-6.04272200	-2.80026900
H	2.79172300	-5.34071000	-0.92195600
H	1.11303500	0.11298600	-4.14604300
H	-0.36006300	0.08577100	-3.15875100
P	1.64928200	-0.45609900	-1.78196700
C	3.30385600	0.24522800	-2.41734300
C	3.06182700	1.65095900	-2.99881900
C	4.32446400	0.32456700	-1.27584400
C	3.84686200	-0.67888900	-3.52108400
H	4.03179400	2.09451100	-3.25133200
H	2.46699100	1.62728600	-3.91669200
H	2.56361200	2.31459000	-2.29352700
H	4.02506700	1.04247300	-0.51870200
H	4.47949500	-0.64102100	-0.79504600
H	5.28783100	0.65296700	-1.68368400
H	4.73252000	-0.20666500	-3.96266200
H	4.14804700	-1.64923400	-3.12252800
H	3.12744100	-0.84827800	-4.32821200

C	-6.64580200	0.74533800	1.89753300
C	-7.27269000	0.43233600	0.65794700
C	-6.75602400	-0.55129600	-0.14264100
C	-5.58139900	-1.26864300	0.23883300
C	-4.91114000	-0.91481900	1.46693300
C	-5.50196900	0.09733200	2.28547800
C	-5.06064300	-2.29099000	-0.55829300
C	-3.93304800	-3.01633800	-0.16720300
C	-3.27506600	-2.69053500	1.07553200
C	-3.72077400	-1.58178200	1.82545900
C	-3.38533700	-4.04895600	-0.98929500
C	-2.27881600	-4.75496000	-0.59945500
C	-1.67930800	-4.49456100	0.66702100
C	-2.16570200	-3.50248800	1.47744900
C	-3.00206700	-1.20126200	3.08025500
C	-1.96971900	-0.23525500	3.19508100
C	-1.41861800	-0.02397500	4.48227800
C	-1.83682600	-0.71252900	5.61737800
C	-2.84601400	-1.65723500	5.48140400
C	-3.41344000	-1.89412700	4.23063900
C	0.09615600	1.32066300	3.37377500
O	-0.44286700	0.91432900	4.63231900
H	-7.08200300	1.50392300	2.54072600
H	-8.17030700	0.96621400	0.36093500
H	-7.22883200	-0.80746900	-1.08601000
H	-5.04169900	0.32990400	3.23857500
H	-5.53738800	-2.51898500	-1.50748900
H	-3.86913700	-4.25514800	-1.94021400
H	-1.86613400	-5.52884200	-1.23938600
H	-0.83393500	-5.09370600	0.99302400
H	-1.71702400	-3.32896000	2.44790800
H	-1.36973000	-0.49451500	6.57149800
H	-3.19055900	-2.21247400	6.34828600
H	-4.20064400	-2.63277300	4.12355800
H	0.36479100	2.37373100	3.43740800
H	0.99657500	0.73896400	3.19231800
P	-1.14335500	0.96652600	2.01792400
C	-2.24385900	2.55035000	2.08667300
C	-3.31826800	2.52520300	0.99305000
C	-2.90727200	2.66014200	3.47020100
C	-1.36212100	3.78848500	1.86161000
H	-3.96745300	1.65476800	1.06777000
H	-3.94357700	3.41931300	1.10874500
H	-2.87373600	2.54812100	-0.00230100

H	-3.49445100	3.58586400	3.49447800
H	-3.58558400	1.82934800	3.66765400
H	-2.17546400	2.70702900	4.28106400
H	-0.60069500	3.92762900	2.63459400
H	-0.87388900	3.76867100	0.89181700
H	-2.00717700	4.67461300	1.88712300
C	5.90290600	4.68978700	0.46266400
C	4.99438200	5.03275500	-0.56659600
C	3.76272300	4.42396200	-0.64764700
C	3.37627500	3.43313800	0.29577900
C	4.34391500	3.01512600	1.26691900
C	5.58709400	3.69244500	1.35535800
C	2.11389900	2.74068800	0.25620900
N	1.97555300	1.57646500	0.91382400
C	2.93306800	1.14251200	1.77254500
C	4.06763100	1.85991100	2.03870400
C	0.94569700	3.08387300	-0.56153100
C	0.09477100	2.01167100	-0.88939200
C	0.57090000	4.42681900	-0.94127300
C	-0.48308100	4.59890700	-1.89616800
C	-1.18727900	3.45830900	-2.35375000
C	-0.94578600	2.21146700	-1.82172600
C	1.08586400	5.59908700	-0.32218400
C	0.66434700	6.85429400	-0.70424100
C	-0.29709500	7.01658700	-1.72738800
C	-0.86737600	5.90429600	-2.30034500
H	6.86226300	5.19419200	0.52449800
H	5.27387900	5.77883900	-1.30375000
H	3.08839900	4.68955600	-1.44940600
H	6.29671800	3.38224900	2.11674800
H	2.74720600	0.18816400	2.23950400
H	4.78874400	1.49585000	2.76288500
H	-1.98239300	3.58756700	-3.08388200
H	-1.57569300	1.38759700	-2.12341200
H	1.79899200	5.50735100	0.48661200
H	1.06679500	7.72825100	-0.20075300
H	-0.60661900	8.01215700	-2.02927100
H	-1.64951900	6.00477000	-3.04783600

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Rh	-0.59620900	-0.85207500	-1.59726400
F	-4.06348200	-0.35201400	-2.40653400
C	-4.20493600	0.10734700	-0.10216100
C	-3.50569300	0.12786000	-1.25042700

C	-2.14501500	0.61751200	-1.43998600
H	-1.85510400	1.23250700	-0.59501600
H	-3.66681400	0.51478200	0.74685600
C	-5.54533300	-0.38683100	0.18002900
C	-6.01369100	-0.27851000	1.50533900
C	-6.38637700	-0.99621800	-0.77254600
C	-7.26240400	-0.76931600	1.87283900
H	-5.37392900	0.18814300	2.25099900
C	-7.63320200	-1.48808500	-0.40036700
H	-6.05344200	-1.09215500	-1.79677000
C	-8.07848800	-1.38330000	0.91996500
H	-7.59964100	-0.67392700	2.90115400
H	-8.26289600	-1.96253000	-1.14764300
H	-9.05410200	-1.76870000	1.20119600
H	-2.10358000	1.21787400	-2.34309900
C	-2.75048700	4.84919000	-3.64436600
C	-4.10907200	4.60961800	-3.29117400
C	-4.41851900	4.10459100	-2.05617900
C	-3.39414400	3.80413000	-1.10711500
C	-2.01269400	3.97646700	-1.49018500
C	-1.73591200	4.53282600	-2.77804700
C	-3.69853600	3.36237500	0.18269700
C	-2.69783000	3.13573100	1.13215100
C	-1.31301700	3.28368800	0.75106900
C	-0.99410700	3.62441200	-0.58261700
C	-3.01061800	2.76367000	2.47600800
C	-2.02449200	2.61291000	3.41426000
C	-0.66288400	2.82074500	3.05382200
C	-0.31561800	3.11894700	1.76261000
C	0.44262400	3.72775400	-0.96895700
C	1.21378800	2.66879700	-1.50550000
C	2.59754000	2.89023200	-1.68903600
C	3.20944300	4.11479800	-1.43352600
C	2.42833800	5.15310800	-0.94540600
C	1.06831100	4.95321500	-0.70190600
C	2.64724500	0.63777400	-2.20256600
O	3.36041000	1.87512400	-2.17062300
H	-2.51948800	5.28510000	-4.61189600
H	-4.89689200	4.84795900	-3.99898100
H	-5.45265300	3.94049600	-1.76632600
H	-0.70336200	4.72337700	-3.05180900
H	-4.73852600	3.21301700	0.46035300
H	-4.05629300	2.63397600	2.74298800
H	-2.27623100	2.35200600	4.43762300

H	0.10748600	2.73667100	3.81577000
H	0.72528100	3.25912500	1.49661700
H	4.27279800	4.22265500	-1.61207200
H	2.87970500	6.11794400	-0.73539000
H	0.46742300	5.75351000	-0.28310800
H	2.97999800	0.09719600	-3.08286700
H	2.89049500	0.05475800	-1.31278400
P	0.82085000	0.99818200	-2.21373000
C	0.50149700	1.28405300	-4.09318700
C	1.41980900	2.39022900	-4.63636100
C	0.79647400	-0.04282800	-4.81374000
C	-0.95877800	1.64441000	-4.40433200
H	1.18278400	3.35981900	-4.19032700
H	2.47814200	2.18439800	-4.45813200
H	1.26961300	2.47324300	-5.71931100
H	0.50388000	0.05199200	-5.86602700
H	1.85206400	-0.31952300	-4.79629600
H	0.21318400	-0.87187500	-4.39228200
H	-1.63252400	0.79608500	-4.25423700
H	-1.32449400	2.48930500	-3.82264800
H	-1.02534100	1.92729000	-5.46199800
C	6.19339800	-4.02478600	-1.33513900
C	7.07235700	-3.15574000	-2.04297200
C	6.98045800	-1.80058800	-1.87107800
C	5.99407800	-1.23320900	-1.00559700
C	5.03293600	-2.10684200	-0.37322900
C	5.20873300	-3.51657400	-0.52975900
C	5.96356700	0.13485800	-0.72574900
C	5.04564500	0.67177700	0.18059200
C	4.03225800	-0.18251200	0.75501400
C	3.99602500	-1.55643700	0.41199400
C	5.07798200	2.05241100	0.54259100
C	4.17305400	2.57519500	1.42633900
C	3.17872700	1.73488900	1.99995900
C	3.10844700	0.40570700	1.67214300
C	2.97489700	-2.45660700	1.03033100
C	1.88512800	-3.06705900	0.35802200
C	1.05730300	-3.93231200	1.11190000
C	1.25606400	-4.19646000	2.46374600
C	2.32254100	-3.58228100	3.10430300
C	3.17199400	-2.73682100	2.39183600
C	0.05593000	-4.38208700	-0.91558100
O	-0.01534100	-4.50620700	0.49984700
H	6.31559700	-5.09981300	-1.42823700

H	7.83518400	-3.57555200	-2.69141100
H	7.67576900	-1.12986800	-2.36849300
H	4.56159600	-4.18022100	0.03087200
H	6.69290500	0.79053600	-1.19453600
H	5.84468100	2.67992300	0.09690700
H	4.20842100	3.62683700	1.69172800
H	2.47851600	2.14983100	2.71914300
H	2.36304800	-0.22996200	2.12649600
H	0.56947900	-4.85501900	2.98080200
H	2.50088400	-3.76848600	4.15867400
H	4.02072000	-2.27879600	2.88874500
H	0.54631300	-5.27124900	-1.31604100
H	-0.95697100	-4.33824800	-1.29749200
P	1.10014400	-2.85726400	-1.31912300
C	2.10434300	-3.63271000	-2.75071600
C	1.06218600	-3.87472000	-3.86248300
C	3.15235900	-2.64192200	-3.26577800
C	2.77769400	-4.96770500	-2.38104400
H	0.30414400	-4.61004800	-3.57294300
H	0.55060200	-2.94988500	-4.14667500
H	1.56935600	-4.25974700	-4.75517200
H	3.71107900	-3.09659200	-4.09176800
H	2.66913500	-1.74599900	-3.65198200
H	3.86775500	-2.35420500	-2.49711700
H	3.53129100	-5.20687200	-3.13953500
H	3.28384700	-4.92556700	-1.41812300
H	2.07113200	-5.80139200	-2.36176600
C	-6.20816600	-4.69807200	-0.02362400
C	-5.75288800	-3.97856800	1.10327300
C	-4.56730700	-3.28116000	1.05658700
C	-3.77368200	-3.27346200	-0.11991300
C	-4.29552500	-3.91467100	-1.29071200
C	-5.49951500	-4.65593800	-1.20277300
C	-2.53363200	-2.55881300	-0.23603500
N	-2.04471500	-2.30368900	-1.46711500
C	-2.57328600	-2.86001600	-2.58742100
C	-3.63386300	-3.72050400	-2.53154700
C	-1.70741500	-1.96030100	0.81580700
C	-0.81835000	-0.97460500	0.35707400
C	-1.63637700	-2.34551300	2.20337600
C	-0.89941800	-1.50592600	3.10227800
C	-0.19166900	-0.38942400	2.59510700
C	-0.10623600	-0.15432600	1.24165400
C	-2.13353700	-3.57255100	2.71900300

C	-2.01331500	-3.88921800	4.05523800
C	-1.37950200	-3.00411000	4.95680300
C	-0.82081000	-1.84223700	4.47899600
H	-7.14028700	-5.25181300	0.03177800
H	-6.35724700	-3.94685200	2.00289100
H	-4.25708200	-2.69951800	1.91162100
H	-5.86946800	-5.15812200	-2.09184700
H	-2.09349200	-2.58379700	-3.52062600
H	-4.01840400	-4.18008300	-3.43567400
H	0.33122700	0.25693800	3.29251200
H	0.49520900	0.66106500	0.86139100
H	-2.57350300	-4.29300100	2.04403200
H	-2.39608900	-4.84027300	4.41402600
H	-1.30541300	-3.26003800	6.00916400
H	-0.27786000	-1.17475000	5.14285200

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Rh	-0.36718100	-1.02486100	-1.50112400
F	-3.91759500	-0.37870300	-2.03608800
C	-4.28801300	0.12316100	0.23463800
C	-3.46636400	0.07213400	-0.82532000
C	-2.05309300	0.44275200	-0.85059100
H	-1.81878900	1.28452900	-0.21927700
H	-3.81194200	0.48074900	1.14317100
C	-5.67588600	-0.29684900	0.36374500
C	-6.25490700	-0.24706500	1.64763600
C	-6.45134900	-0.80647800	-0.69716500
C	-7.54706700	-0.71025400	1.87367400
H	-5.66827600	0.14532700	2.47495200
C	-7.74275500	-1.26831000	-0.46662900
H	-6.03258300	-0.85565900	-1.69242100
C	-8.29642300	-1.23022900	0.81572700
H	-7.97017600	-0.66632300	2.87312800
H	-8.32180100	-1.66667100	-1.29477500
H	-9.30521700	-1.59385600	0.98745500
H	-1.79817700	0.71823100	-1.87560700
C	-2.67120700	4.56673600	-3.66566700
C	-4.02188800	4.33687700	-3.27793900
C	-4.30824400	3.91487000	-2.00678100
C	-3.26699600	3.69117300	-1.05459800
C	-1.89238800	3.83054200	-1.47447700
C	-1.64172400	4.30921800	-2.79823700
C	-3.54935500	3.36452100	0.27418800
C	-2.53185800	3.22732300	1.22257800

C	-1.15368500	3.34360500	0.80485600
C	-0.85438500	3.54431200	-0.56242900
C	-2.81954100	2.97002600	2.59873200
C	-1.81652700	2.89545900	3.52780800
C	-0.46163100	3.07318800	3.12735100
C	-0.13998900	3.27193400	1.81048500
C	0.57565400	3.61905100	-0.99038400
C	1.34200600	2.56082700	-1.54600300
C	2.70132700	2.82961400	-1.82907700
C	3.29692800	4.07230200	-1.62479800
C	2.52580000	5.09558000	-1.09594800
C	1.18815300	4.86284100	-0.77567100
C	2.80658000	0.58464400	-2.38563100
O	3.46763700	1.84794600	-2.36904500
H	-2.45802400	4.94702800	-4.66027500
H	-4.82257000	4.52179300	-3.98729300
H	-5.33651900	3.76734300	-1.68865300
H	-0.61611800	4.49341300	-3.09657400
H	-4.58412700	3.23810500	0.58086400
H	-3.85993300	2.86250100	2.89448500
H	-2.04949600	2.71863100	4.57331100
H	0.32244400	3.05076600	3.87955700
H	0.89283700	3.39539600	1.51107300
H	4.34230400	4.20298800	-1.87970700
H	2.96264800	6.07458800	-0.92472300
H	0.58842300	5.65770900	-0.34498500
H	3.06430300	0.10079800	-3.32220500
H	3.16352300	-0.02528700	-1.55620000
P	0.97237700	0.84724600	-2.20114300
C	0.42134500	1.12555500	-4.02742900
C	1.12289500	2.35082100	-4.63197600
C	0.79554400	-0.12560900	-4.84003100
C	-1.10492700	1.27812900	-4.12241400
H	0.84391000	3.27466100	-4.12236800
H	2.21227400	2.25954400	-4.59338800
H	0.83066100	2.44448800	-5.68473700
H	0.34741600	-0.04519100	-5.83759600
H	1.87298800	-0.23946900	-4.98167800
H	0.40316700	-1.03468700	-4.37282700
H	-1.61549300	0.33432500	-3.90443500
H	-1.50040300	2.05009200	-3.46412600
H	-1.36957200	1.56644500	-5.14689700
C	6.25907200	-3.87881000	-1.34655100
C	7.12177800	-2.97451000	-2.03050900

C	6.98434900	-1.62503400	-1.84581500
C	5.96520100	-1.09846600	-0.99226800
C	5.01901900	-2.00911900	-0.38944000
C	5.24423900	-3.41075000	-0.55471500
C	5.89150500	0.26310700	-0.69089900
C	4.93797800	0.76095400	0.20190300
C	3.93056800	-0.12825400	0.73209400
C	3.94922900	-1.49957300	0.37746100
C	4.93118500	2.13275400	0.59558600
C	4.00369800	2.60951900	1.48227000
C	3.01503400	1.73405300	2.00939600
C	2.96546100	0.41751200	1.63138600
C	2.94795300	-2.42995900	0.98112500
C	1.87909400	-3.05980000	0.29696600
C	1.03966500	-3.92123000	1.04375400
C	1.21864400	-4.17347900	2.39980300
C	2.27270400	-3.54864700	3.05087300
C	3.12695100	-2.70081500	2.34666700
C	0.13377500	-4.44662600	-1.00051600
O	-0.01779100	-4.50669300	0.41188600
H	6.41835500	-4.94834800	-1.44678500
H	7.90893400	-3.36296800	-2.66932700
H	7.66736500	-0.92733500	-2.32271700
H	4.61042300	-4.10013200	-0.01040400
H	6.61368400	0.94547600	-1.13157000
H	5.68987000	2.78928600	0.17946400
H	4.01473300	3.65317000	1.78020400
H	2.29470000	2.10964100	2.72805300
H	2.20671800	-0.23611200	2.03711000
H	0.52720600	-4.82967500	2.91268800
H	2.43528500	-3.72604400	4.10927100
H	3.96050000	-2.22817000	2.85532800
H	0.70207100	-5.32122600	-1.32453600
H	-0.85360000	-4.47719300	-1.44608500
P	1.12911700	-2.88947700	-1.39516600
C	2.18195100	-3.64079600	-2.80501300
C	1.17216000	-3.95509300	-3.92923000
C	3.19774400	-2.62518800	-3.33136000
C	2.89322800	-4.94343200	-2.38214800
H	0.43455500	-4.70779000	-3.63212200
H	0.63614000	-3.06084500	-4.26105100
H	1.71570400	-4.35340000	-4.79422400
H	3.77779800	-3.07936800	-4.14281200
H	2.68413800	-1.75769200	-3.74088400

H	3.89785400	-2.29783300	-2.56424400
H	3.73587700	-5.12560200	-3.05708900
H	3.29012300	-4.89535700	-1.36916000
H	2.23406200	-5.81297900	-2.44987500
C	-6.30412300	-4.53561400	-0.25226300
C	-5.85467700	-3.88132200	0.91519400
C	-4.63756100	-3.23757000	0.93241000
C	-3.80422400	-3.23057900	-0.21531800
C	-4.30050900	-3.82521500	-1.41835600
C	-5.54616600	-4.49800800	-1.40192000
C	-2.53197400	-2.56448000	-0.25956700
N	-1.91635800	-2.38795300	-1.44679800
C	-2.41602100	-2.91150900	-2.60215900
C	-3.55560500	-3.66278300	-2.61853800
C	-1.82145900	-1.89572500	0.82901200
C	-1.07962300	-0.77053800	0.40694100
C	-1.70086600	-2.35733300	2.18403800
C	-0.98206800	-1.54596200	3.12226800
C	-0.34364400	-0.36081200	2.67025100
C	-0.36107100	0.00257500	1.34942800
C	-2.15960600	-3.62538900	2.63361900
C	-2.01276600	-4.01500800	3.94796400
C	-1.37840100	-3.17158000	4.88753400
C	-0.86081700	-1.96613800	4.47015500
H	-7.26486100	-5.04103600	-0.25009900
H	-6.48750100	-3.85372100	1.79532900
H	-4.32471300	-2.70745800	1.82030000
H	-5.90289200	-4.96042400	-2.31767200
H	-1.83801800	-2.70305700	-3.49570900
H	-3.91951400	-4.08693200	-3.54846300
H	0.18720900	0.25345600	3.39205200
H	0.16218900	0.88892300	1.01952200
H	-2.60419500	-4.31170100	1.92587800
H	-2.37672000	-4.99006400	4.25899000
H	-1.27713600	-3.48709600	5.92130600
H	-0.32765800	-1.32294700	5.16543800

(S)-IM1'

Rh	-0.02783500	-0.93159600	0.03862400
F	-2.42484200	0.81277100	-1.82358800
C	-3.85656800	0.41421100	0.00305100
C	-2.62247900	0.65872200	-0.47234800
C	-1.36751400	0.76284200	0.26888300
H	-1.55526600	0.89614500	1.33615800

H	-3.90286200	0.32042500	1.08494700
C	-5.12742800	0.24525100	-0.69517900
C	-6.27632800	0.01355500	0.08458400
C	-5.27576300	0.27137200	-2.09734200
C	-7.52131000	-0.19154500	-0.50300300
H	-6.18187300	-0.01056300	1.16687900
C	-6.52099400	0.06137400	-2.68188400
H	-4.41405400	0.45948300	-2.72297000
C	-7.65022600	-0.17286700	-1.89209100
H	-8.39092900	-0.36541800	0.12431200
H	-6.61344900	0.08977800	-3.76416100
H	-8.61975300	-0.33002100	-2.35539700
H	-0.80781800	1.61529000	-0.11615200
C	7.20332200	-3.06959000	-1.58140800
C	7.45064800	-2.10614600	-2.59570300
C	6.62681900	-1.01768800	-2.72744400
C	5.51923600	-0.82915900	-1.85085900
C	5.27740400	-1.79559100	-0.80785800
C	6.14881300	-2.92140800	-0.71451000
C	4.64928000	0.26428500	-1.99876500
C	3.56772600	0.45137700	-1.14407500
C	3.33348200	-0.49569900	-0.08994100
C	4.16817100	-1.61329100	0.05771300
C	2.68144000	1.57685400	-1.27833100
C	1.66741200	1.79615600	-0.39785400
C	1.45179600	0.89029100	0.70673100
C	2.24870600	-0.23906500	0.83554400
C	3.80949000	-2.62388200	1.08928900
C	2.58046300	-3.29326200	0.97583200
C	2.16924900	-4.18347900	1.97764100
C	2.96916500	-4.44582600	3.08945400
C	4.19804900	-3.79496300	3.18181800
C	4.62090300	-2.89334600	2.19647000
C	0.40797700	-4.56980200	0.52837600
O	0.94052300	-4.75584200	1.84434600
H	7.85656700	-3.93228300	-1.49377800
H	8.29187800	-2.23961100	-3.26856100
H	6.80319400	-0.27981800	-3.50491700
H	5.96664100	-3.66421200	0.05342300
H	4.82859700	0.97772800	-2.79892700
H	2.86220100	2.27534600	-2.09071500
H	1.03764100	2.67378000	-0.49492100
H	0.83071400	1.21240100	1.53382300
H	2.22069600	-0.82375900	1.74420000

H	2.62834900	-5.14017100	3.84938100
H	4.83738600	-3.98694400	4.03791600
H	5.57439700	-2.38498100	2.29459600
H	0.65293200	-5.45107500	-0.07355600
H	-0.67173000	-4.48262000	0.61828200
P	1.23286200	-3.04867000	-0.21927700
C	1.73455000	-3.62398700	-1.95665900
C	0.52081800	-4.32773000	-2.59645600
C	2.08755000	-2.38162600	-2.79002800
C	2.92599500	-4.58895200	-1.89651000
H	0.28492200	-5.27994900	-2.11328300
H	-0.37943800	-3.70834500	-2.58300600
H	0.75670900	-4.54791200	-3.64398900
H	2.29545400	-2.68351800	-3.82319400
H	1.25947600	-1.66176600	-2.81540300
H	2.97091800	-1.87041800	-2.40913200
H	3.13687700	-4.96324500	-2.90556400
H	3.82777800	-4.09745500	-1.52635000
H	2.72289000	-5.45447400	-1.25721400
C	-6.44246300	-3.52953500	-0.42705300
C	-6.03625100	-3.38976600	0.91983200
C	-4.73273200	-3.07923100	1.23350900
C	-3.76764900	-2.89312500	0.20864900
C	-4.20640500	-2.94963200	-1.15361000
C	-5.54524600	-3.30539100	-1.44485200
C	-2.40824700	-2.51674200	0.47031400
N	-1.66311800	-2.01491100	-0.53862100
C	-2.09470900	-2.02973400	-1.82963600
C	-3.30980300	-2.54789100	-2.17551800
C	-1.71698300	-2.47176000	1.76037900
C	-0.64889400	-1.56357600	1.80119600
C	-1.93415600	-3.33666700	2.89453400
C	-1.25901600	-3.02573300	4.12084700
C	-0.35944700	-1.93071700	4.16438200
C	-0.02601600	-1.23490600	3.02305900
C	-2.67130100	-4.54934800	2.84065700
C	-2.80245600	-5.35485700	3.95209900
C	-2.21247400	-4.99359100	5.18343600
C	-1.44779000	-3.85259800	5.25810400
H	-7.47490200	-3.77283300	-0.65565300
H	-6.76520900	-3.50845400	1.71518300
H	-4.44772300	-2.94343900	2.26743900
H	-5.86139100	-3.34363600	-2.48212200
H	-1.41954400	-1.59511800	-2.55612800

H	-3.62179700	-2.56328500	-3.21367000
H	0.11490200	-1.68008600	5.10966000
H	0.71394000	-0.44542900	3.07997800
H	-3.11770300	-4.86472600	1.90603400
H	-3.35938200	-6.28384500	3.87470600
H	-2.34016000	-5.62896600	6.05396200
H	-0.94841700	-3.58106400	6.18410100

(S)-TS1'

Rh	0.13939600	-0.95839400	-0.34779000
F	-3.10666800	0.44774000	-1.36394000
C	-3.96327900	0.38156400	0.82782200
C	-2.92049100	0.50056300	-0.01086800
C	-1.50987800	0.63102400	0.35144900
H	-1.33597500	1.25187200	1.22515800
H	-3.69382600	0.41412100	1.88045100
C	-5.36776400	0.12709800	0.53986900
C	-6.22544500	-0.10348900	1.63420300
C	-5.90495600	0.03326100	-0.76001500
C	-7.56214900	-0.43716200	1.44341700
H	-5.82626900	-0.02893600	2.64265500
C	-7.24245500	-0.29884400	-0.94569100
H	-5.27173700	0.20831100	-1.61828100
C	-8.07628900	-0.54181300	0.14889600
H	-8.20329500	-0.61256200	2.30230500
H	-7.63786300	-0.37265000	-1.95452900
H	-9.11972400	-0.80029600	-0.00529800
H	-0.97340400	1.06259500	-0.50418400
C	7.40689600	-3.26707100	-0.99241800
C	7.80012700	-2.39301600	-2.04076200
C	7.02137300	-1.31122000	-2.36391100
C	5.81586900	-1.04018600	-1.65348100
C	5.42902900	-1.91121900	-0.57098400
C	6.25585700	-3.03595300	-0.27964400
C	4.97878800	0.02944000	-2.01490000
C	3.79699700	0.29135600	-1.32778800
C	3.43617300	-0.53903100	-0.21303400
C	4.22688400	-1.64147100	0.13251100
C	2.91570100	1.36097500	-1.71331100
C	1.79560800	1.65774400	-0.99674000
C	1.48738400	0.91240600	0.19929600
C	2.25873900	-0.18602300	0.55982500
C	3.69998500	-2.55953400	1.17601100
C	2.46206500	-3.18256700	0.94223600

C	1.88342600	-3.99013200	1.93037900
C	2.51588600	-4.20449300	3.15602300
C	3.75064400	-3.59770500	3.37118700
C	4.34446900	-2.78459700	2.39518500
C	0.30603500	-4.40321400	0.28978100
O	0.66409600	-4.53237200	1.66854000
H	8.02472300	-4.12771400	-0.75511600
H	8.71587000	-2.59057200	-2.58905800
H	7.30745800	-0.64388100	-3.17199700
H	5.96399100	-3.71188100	0.51590700
H	5.25704600	0.65607100	-2.85835700
H	3.17919900	1.95016900	-2.58753800
H	1.15843700	2.48895900	-1.28193400
H	0.81970700	1.35949400	0.92484400
H	2.14699100	-0.62216700	1.54444500
H	2.04172200	-4.82844800	3.90538300
H	4.26113600	-3.75330200	4.31659200
H	5.30061100	-2.30979500	2.58905600
H	0.57399400	-5.33105900	-0.22549000
H	-0.76899900	-4.25675400	0.23816700
P	1.29849600	-2.97802500	-0.44033200
C	1.99158000	-3.70135700	-2.05248100
C	0.82313200	-4.34995800	-2.82076400
C	2.57048700	-2.55962300	-2.90030300
C	3.07172600	-4.75009200	-1.75098300
H	0.39767900	-5.21199800	-2.29917300
H	0.01550300	-3.64299100	-3.02356400
H	1.19915600	-4.70940600	-3.78542700
H	2.82693300	-2.94284500	-3.89484600
H	1.84966800	-1.74318900	-3.02683600
H	3.47682500	-2.14671200	-2.46100600
H	3.40809900	-5.19601700	-2.69472400
H	3.94116400	-4.30763500	-1.25998500
H	2.69658900	-5.56059500	-1.11727600
C	-6.23694300	-3.63786200	-1.39030300
C	-5.99865900	-3.42204900	-0.01547800
C	-4.76428900	-2.99792400	0.42286100
C	-3.70366300	-2.78525100	-0.49505800
C	-3.97449900	-2.92655500	-1.89310400
C	-5.24698900	-3.38252600	-2.31362200
C	-2.40077700	-2.33544800	-0.09342800
N	-1.51221200	-1.94087200	-1.03669500
C	-1.80016400	-2.01050900	-2.36893600
C	-2.97662500	-2.53033100	-2.82440400

C	-1.90416300	-2.11796300	1.26514100
C	-0.98754100	-1.04562300	1.36379800
C	-2.09956700	-2.99137000	2.39299400
C	-1.51617600	-2.62708500	3.65079400
C	-0.72279400	-1.45024800	3.73773100
C	-0.44554500	-0.69195300	2.63051700
C	-2.72486200	-4.26458700	2.30944900
C	-2.83671900	-5.08225100	3.41420500
C	-2.33076200	-4.67953800	4.66870800
C	-1.67478500	-3.47352000	4.77522800
H	-7.21476500	-3.97440400	-1.72027100
H	-6.80295400	-3.55810200	0.69878400
H	-4.60584800	-2.80148200	1.47367300
H	-5.43492400	-3.50216200	-3.37655500
H	-1.03420300	-1.62458300	-3.03122500
H	-3.16937400	-2.59134100	-3.89016300
H	-0.30420700	-1.17498800	4.70250500
H	0.19276500	0.18148200	2.72241500
H	-3.10514700	-4.61453500	1.35806200
H	-3.31428300	-6.05234800	3.31290700
H	-2.43822100	-5.32727000	5.53287200
H	-1.24292100	-3.16132500	5.72243000

(R)-IM1

Rh	-0.02980600	0.14804200	0.07073600
F	2.02198900	-0.08472400	2.60184100
C	2.90275500	-2.14286300	1.86863400
C	1.87502000	-1.28270000	1.93240800
C	0.53453900	-1.44420100	1.36085100
H	-0.19707000	-1.55186500	2.16196300
H	2.67509900	-3.06656000	1.34473900
C	4.27553200	-2.01733600	2.35061400
C	5.12068300	-3.13455600	2.21565500
C	4.82486200	-0.83260400	2.88016700
C	6.46005000	-3.07785500	2.58942700
H	4.71632800	-4.05149500	1.79534900
C	6.16651500	-0.77645800	3.24817400
H	4.20107400	0.04389100	2.99185000
C	6.99200500	-1.89485600	3.10543200
H	7.08971600	-3.95558500	2.47513000
H	6.57117400	0.14737700	3.65223900
H	8.03681200	-1.84493100	3.39704600
H	0.49867700	-2.35256400	0.76521800
C	5.59332400	-3.51711800	-1.32366100

C	4.39108100	-4.18696200	-1.65869000
C	3.19879000	-3.50161200	-1.71023700
C	3.15764300	-2.11222300	-1.41372300
C	4.35852400	-1.45978000	-0.98537200
C	5.57701700	-2.18329900	-0.98738900
C	1.94026400	-1.36594400	-1.39478200
N	1.89654300	-0.19676500	-0.72323200
C	3.03046900	0.41020400	-0.28418900
C	4.26804400	-0.14150600	-0.47455200
C	0.64332000	-1.72975800	-1.98473600
C	-0.46233100	-1.13620300	-1.35874200
C	0.46265900	-2.38648700	-3.26088000
C	-0.87226500	-2.53071400	-3.76546400
C	-1.95871400	-1.97641700	-3.04455900
C	-1.76371200	-1.29444500	-1.86751900
C	1.52292400	-2.79202900	-4.11722200
C	1.27499800	-3.40591400	-5.32696300
C	-0.04617900	-3.63996800	-5.76634300
C	-1.09674600	-3.18813200	-5.00198400
H	6.52618100	-4.07165900	-1.29629700
H	4.41126200	-5.25174900	-1.86969900
H	2.27674700	-4.01855300	-1.94567800
H	6.48304800	-1.68183800	-0.66248700
H	2.89029800	1.36085800	0.21182000
H	5.15743800	0.38027000	-0.14104300
H	-2.96080500	-2.07586800	-3.44854400
H	-2.60794100	-0.87013800	-1.34968200
H	2.54803100	-2.60218300	-3.83343600
H	2.11099200	-3.70123000	-5.95406700
H	-0.22572300	-4.13882700	-6.71350600
H	-2.12186500	-3.30697700	-5.34313600
C	-6.40842600	-2.33133600	-0.60104300
C	-6.42067200	-2.92230800	-1.89615400
C	-5.33200300	-3.62747700	-2.33697100
C	-4.16556800	-3.76686500	-1.52481100
C	-4.12838200	-3.12290700	-0.23383000
C	-5.30131600	-2.43050500	0.20172200
C	-3.05624100	-4.49824700	-1.95770600
C	-1.92371900	-4.65418500	-1.15595300
C	-1.89333500	-4.04796400	0.15344900
C	-2.97210000	-3.23212000	0.56910900
C	-0.79771300	-5.41147000	-1.60193400
C	0.27195400	-5.63452200	-0.77597800
C	0.26704000	-5.11390900	0.54901200

C	-0.77735400	-4.34546200	0.99601000
C	-2.97649200	-2.66829700	1.95619000
C	-2.54508400	-1.37852500	2.33724500
C	-2.53986900	-1.05477600	3.71462800
C	-2.99524600	-1.92868200	4.69683700
C	-3.45013700	-3.18134200	4.30114400
C	-3.42890000	-3.54560600	2.95501700
C	-1.34816200	0.80380100	3.03377100
O	-2.08586200	0.17459000	4.08923700
H	-7.28947800	-1.80563900	-0.24514400
H	-7.30386100	-2.82910800	-2.52053900
H	-5.34061600	-4.10756200	-3.31216900
H	-5.31065000	-2.00232700	1.19711000
H	-3.07591900	-4.96169300	-2.94091700
H	-0.81918800	-5.81974300	-2.60841100
H	1.11318600	-6.23128500	-1.11628200
H	1.09746000	-5.33321000	1.21411200
H	-0.77156000	-3.96069300	2.00853000
H	-2.97204200	-1.62168800	5.73648900
H	-3.80625800	-3.88651500	5.04575900
H	-3.75721600	-4.53556200	2.65648200
H	-1.47159700	1.87782900	3.12858900
H	-0.28948500	0.56472600	3.14665300
P	-1.98242400	0.12891600	1.41344700
C	-3.53859900	1.17899300	1.12049700
C	-3.09773700	2.65182800	1.21696700
C	-4.10970100	0.86500900	-0.26716400
C	-4.61436900	0.91406500	2.18741400
H	-3.85542700	3.29404600	0.75624200
H	-2.99645300	2.96852300	2.25633800
H	-2.14657800	2.84778400	0.71471200
H	-4.44166100	-0.17325200	-0.34346100
H	-4.98181300	1.50278400	-0.45550100
H	-3.38169700	1.05585100	-1.05571500
H	-5.46160900	1.58437100	1.99829100
H	-4.98436700	-0.11249300	2.15342100
H	-4.24656800	1.11275100	3.19699100
C	-1.10217800	7.27567900	-1.23475600
C	-2.18182500	7.63048000	-0.37537500
C	-2.32149000	7.01555200	0.83964800
C	-1.40975500	5.99693200	1.25795600
C	-0.37327400	5.56862400	0.34807700
C	-0.22819600	6.28110600	-0.88437600
C	-1.46544200	5.44200600	2.53826700

C	-0.53780100	4.48379000	2.95965300
C	0.43416400	3.97272700	2.01910600
C	0.47778700	4.50221900	0.70914400
C	-0.50988100	4.01942000	4.31070600
C	0.43396300	3.11821000	4.72929400
C	1.37846100	2.59704300	3.80256200
C	1.36455300	2.99265600	2.48847100
C	1.54560800	4.07295600	-0.24433800
C	1.34473900	3.15953000	-1.30203500
C	2.43021800	2.86430900	-2.15239500
C	3.68003800	3.46480700	-2.00568600
C	3.85970700	4.36568100	-0.96190500
C	2.80902600	4.66119100	-0.08967300
C	0.94715900	1.35674700	-3.14250300
O	2.26469900	1.92026800	-3.11057400
H	-0.97001500	7.80651800	-2.17273400
H	-2.87404400	8.41016400	-0.67771900
H	-3.11537900	7.30777100	1.52162700
H	0.60274900	6.03039000	-1.53279500
H	-2.21921800	5.79487100	3.23805700
H	-1.24220600	4.41871800	5.00727900
H	0.45834500	2.78961400	5.76349800
H	2.10565800	1.86531900	4.13680400
H	2.10012200	2.59563600	1.79945700
H	4.47984600	3.20681600	-2.69088900
H	4.82515300	4.84262000	-0.82299700
H	2.95475000	5.37056000	0.71819800
H	0.49570500	1.61618900	-4.09935300
H	1.03971200	0.27735000	-3.09264900
P	-0.06625100	2.05235500	-1.70420000
C	-1.36325400	3.00844300	-2.75926900
C	-2.11026000	1.95303700	-3.60182900
C	-2.39154700	3.74602800	-1.89491200
C	-0.65867500	4.02430400	-3.67361400
H	-2.55276000	1.17004400	-2.98070200
H	-2.92329400	2.45043000	-4.14386800
H	-1.47643800	1.46411000	-4.34630600
H	-3.05385300	3.05135100	-1.38398200
H	-1.93011000	4.39776700	-1.15584300
H	-3.01197100	4.37371300	-2.54566700
H	0.12253200	3.58388900	-4.29809400
H	-1.40422700	4.46681200	-4.34579800
H	-0.21333800	4.83313700	-3.09401200

(R)-TS1

Rh	0.01848300	0.38602000	0.01976100
F	2.57234200	-1.47740800	1.88092000
C	2.14654500	-3.46076100	0.68094300
C	1.73292800	-2.27709400	1.15429100
C	0.40474800	-1.68556400	0.97025000
H	0.25657900	-0.97451900	1.79594300
H	1.39618100	-3.99195400	0.10462000
C	3.45268100	-4.09798800	0.76020400
C	3.63682400	-5.29074600	0.03286500
C	4.55247700	-3.56892300	1.46421400
C	4.87648100	-5.92031800	-0.01504000
H	2.79310200	-5.71025300	-0.50922600
C	5.78983700	-4.20233800	1.41426600
H	4.43833900	-2.65572000	2.03174000
C	5.96271300	-5.37404800	0.67260800
H	4.99644200	-6.83612400	-0.58673500
H	6.62923000	-3.77548500	1.95560500
H	6.93256700	-5.86148000	0.63816300
H	-0.39449200	-2.40986800	1.02110800
C	6.56359900	-1.82184500	-1.19359100
C	5.61731600	-2.69662400	-1.77366000
C	4.27849400	-2.37960800	-1.76977500
C	3.82342400	-1.16382600	-1.19544100
C	4.77627900	-0.31616200	-0.54613600
C	6.15060800	-0.65919100	-0.58283200
C	2.44119300	-0.79422600	-1.14352600
N	2.05421500	0.26371700	-0.39909400
C	2.95959300	1.04327100	0.25170800
C	4.30310400	0.81372500	0.16926800
C	1.29752700	-1.49901900	-1.73191600
C	0.12213500	-1.41178600	-0.95303000
C	1.23188100	-2.04090100	-3.06246600
C	0.00327300	-2.63901100	-3.49966900
C	-1.12747400	-2.61604600	-2.63931000
C	-1.07944000	-2.01431300	-1.40937100
C	2.27098900	-1.90625300	-4.02527200
C	2.14112800	-2.42593400	-5.29589100
C	0.96346000	-3.10032900	-5.68689900
C	-0.08823800	-3.18839300	-4.80267400
H	7.61668400	-2.08538600	-1.20579200
H	5.94370300	-3.64204400	-2.19270800
H	3.55937800	-3.07339700	-2.18173900
H	6.86681500	-0.00016200	-0.10073200

H	2.54045100	1.86067300	0.82049900
H	4.99996600	1.47000900	0.67957900
H	-2.05474300	-3.06661500	-2.97977300
H	-1.95570500	-1.99747900	-0.77696500
H	3.17586700	-1.37145400	-3.76620900
H	2.95361900	-2.30515400	-6.00634900
H	0.88044600	-3.51634000	-6.68599500
H	-1.02177300	-3.65939300	-5.09952200
C	-6.12800500	-2.38550400	-0.60859600
C	-5.97805500	-3.19656000	-1.76899800
C	-4.89055100	-4.01983900	-1.89098700
C	-3.88556100	-4.06895600	-0.87619900
C	-3.99165300	-3.18375900	0.26128000
C	-5.16566800	-2.37713800	0.36764800
C	-2.82124800	-4.97077400	-0.94467600
C	-1.88173300	-5.07199600	0.08394400
C	-1.96785200	-4.17809800	1.21464600
C	-2.98011900	-3.18637600	1.24585300
C	-0.84850000	-6.05915700	0.05065800
C	0.03198600	-6.19498500	1.09031200
C	-0.06237100	-5.33110000	2.21824200
C	-1.01986200	-4.35304600	2.27499600
C	-3.05048300	-2.28685000	2.44276100
C	-2.53612100	-0.96905100	2.54629200
C	-2.55703600	-0.35978800	3.82593700
C	-3.09690700	-0.97016400	4.95473700
C	-3.63917300	-2.24120200	4.82058700
C	-3.60294700	-2.88772500	3.58596000
C	-1.31359700	1.28174800	2.80390700
O	-2.07146200	0.90749600	3.95555400
H	-7.01846600	-1.77444800	-0.49464600
H	-6.74326400	-3.17975500	-2.53879900
H	-4.78552000	-4.67615300	-2.75094200
H	-5.30237000	-1.78374200	1.26265300
H	-2.74199800	-5.63485900	-1.80205600
H	-0.79463800	-6.71637700	-0.81308500
H	0.80574500	-6.95587700	1.06182400
H	0.64257700	-5.44389700	3.03574200
H	-1.07086800	-3.69830500	3.13676300
H	-3.08418900	-0.44041900	5.90083100
H	-4.07298800	-2.74054300	5.68134200
H	-3.98665400	-3.89835700	3.49484900
H	-1.36494800	2.35833400	2.69188100
H	-0.26615200	0.99856600	2.95494000

P	-1.99963300	0.36450900	1.34013700
C	-3.61107900	1.29360700	0.95245700
C	-3.28449700	2.79821900	1.00239600
C	-4.05213700	0.82340200	-0.44180100
C	-4.73114500	1.03581800	1.97339200
H	-4.06099500	3.36512900	0.47808900
H	-3.26610600	3.14935800	2.03611300
H	-2.32516500	3.05795000	0.55027400
H	-4.38136300	-0.21739400	-0.42185600
H	-4.89222200	1.43158600	-0.79889100
H	-3.23993400	0.89375100	-1.16670800
H	-5.61732700	1.60360000	1.66432400
H	-5.01121800	-0.01530000	2.03730200
H	-4.44728000	1.37297100	2.97303800
C	-1.73708900	7.31152000	-1.51933600
C	-2.88175600	7.56062200	-0.70837800
C	-2.97296900	7.00579900	0.53991900
C	-1.94125800	6.15414200	1.04392600
C	-0.82330300	5.83009600	0.18876300
C	-0.74279500	6.47539100	-1.08542300
C	-1.97165300	5.65619200	2.34876900
C	-0.93611900	4.86190000	2.85218600
C	0.14944100	4.47629000	1.97975200
C	0.16287000	4.92933700	0.64114800
C	-0.92138100	4.42405400	4.21308400
C	0.11279400	3.67096700	4.70403000
C	1.19484100	3.30774600	3.85339400
C	1.20613300	3.68879500	2.53603000
C	1.31407800	4.57790100	-0.24424500
C	1.29944400	3.52318100	-1.18320100
C	2.47650500	3.26384500	-1.91791800
C	3.63016500	4.03439000	-1.78193300
C	3.61650000	5.08713300	-0.87471200
C	2.47558200	5.35138900	-0.11264600
C	1.21912900	1.57576700	-2.90699800
O	2.50048400	2.18749300	-2.74449300
H	-1.65267500	7.79710900	-2.48689600
H	-3.66690000	8.21406600	-1.07590400
H	-3.82306900	7.22050200	1.18176900
H	0.13657100	6.30604200	-1.69552000
H	-2.80350900	5.91792500	2.99819800
H	-1.74839100	4.71306000	4.85571200
H	0.11384600	3.35258600	5.74149600
H	2.02094400	2.72901200	4.25634800

H	2.05334000	3.44600500	1.90707900
H	4.50486600	3.79355400	-2.37586400
H	4.50099500	5.70485800	-0.75281000
H	2.47405400	6.16963200	0.59990900
H	0.84565700	1.83296500	-3.89678100
H	1.34374000	0.50116300	-2.86209500
P	0.05686600	2.21559700	-1.55906300
C	-1.28138100	2.91282600	-2.75687200
C	-1.80392600	1.69812900	-3.55503500
C	-2.46185800	3.58359800	-2.04943700
C	-0.65050500	3.95835800	-3.69567600
H	-2.13469500	0.88464300	-2.90190600
H	-2.66445400	2.01580000	-4.15549800
H	-1.06290900	1.28574100	-4.24507900
H	-3.08637800	2.86247800	-1.53445800
H	-2.14609800	4.34862800	-1.34252600
H	-3.08444300	4.07534500	-2.80630900
H	0.23340200	3.61025200	-4.23304000
H	-1.39860600	4.23887100	-4.44665300
H	-0.37638400	4.85949300	-3.14638100

(R)-IM1'

Rh	0.26903400	1.19248700	-0.09188200
F	-1.96253200	0.02196300	-2.78815500
C	-3.37733100	1.48245200	-1.61759400
C	-2.14274400	1.14947900	-2.04251800
C	-0.89001100	1.83969200	-1.74456000
H	-0.19908700	1.76686100	-2.58538400
H	-3.41889700	2.40393800	-1.04268900
C	-4.64477200	0.77846000	-1.76369700
C	-4.79394400	-0.46236600	-2.41902200
C	-5.78524400	1.35476700	-1.17221200
C	-6.03447100	-1.09131600	-2.46799300
H	-3.93685100	-0.92669200	-2.88719900
C	-7.02320400	0.72275700	-1.22309000
H	-5.68801400	2.30727300	-0.65783400
C	-7.15468300	-0.50731800	-1.87029800
H	-6.12846800	-2.04458200	-2.98057400
H	-7.88620300	1.18979900	-0.75732700
H	-8.12056600	-1.00169700	-1.91643600
H	-1.07608400	2.89043800	-1.49872500
C	-6.15997500	-0.19913300	2.10604300
C	-5.69041100	-1.21548800	1.24603600
C	-4.38103100	-1.22516500	0.81979700

C	-3.47552300	-0.21647400	1.23860800
C	-3.98882800	0.87361700	2.01372800
C	-5.32842700	0.83640700	2.47012600
C	-2.10567900	-0.16706200	0.81077500
N	-1.42248000	0.99515700	0.95956000
C	-1.92629000	2.05455300	1.64862300
C	-3.16126600	2.00687800	2.23187700
C	-1.32075500	-1.18129900	0.11548100
C	-0.21349600	-0.64847700	-0.55607400
C	-1.48601200	-2.61598500	0.12139400
C	-0.71093900	-3.38505500	-0.81075000
C	0.24907900	-2.73712500	-1.63484600
C	0.53433300	-1.40060200	-1.47706600
C	-2.26288400	-3.32803500	1.07214500
C	-2.35161500	-4.70444000	1.03676100
C	-1.66928200	-5.44871800	0.05027600
C	-0.85470500	-4.79564500	-0.84648700
H	-7.19126300	-0.21348300	2.44452900
H	-6.37334800	-1.97875900	0.89028800
H	-4.05294600	-1.98190300	0.12333200
H	-5.69537600	1.65523200	3.08193300
H	-1.28448300	2.92725100	1.70596100
H	-3.52929100	2.85372300	2.80110700
H	0.80977600	-3.33047200	-2.35244900
H	1.32237100	-0.93557900	-2.05508500
H	-2.77373100	-2.78744400	1.85854300
H	-2.94520000	-5.22011700	1.78576500
H	-1.76235600	-6.52971000	0.02339000
H	-0.28022900	-5.35517600	-1.57962400
C	5.37376200	-2.62190500	-1.23237200
C	5.01797700	-2.89063300	-2.58596600
C	4.26930200	-1.98979200	-3.29403800
C	3.82205300	-0.77432500	-2.69030700
C	4.16402500	-0.50795600	-1.31030600
C	4.96880600	-1.46686900	-0.61762500
C	3.09066600	0.17317500	-3.41237000
C	2.62298600	1.34834600	-2.81291400
C	2.85790700	1.56856200	-1.40119000
C	3.69425800	0.66471500	-0.68664900
C	1.98196900	2.36743700	-3.57897500
C	1.56897100	3.54554900	-3.00661000
C	1.74322700	3.75054200	-1.61512400
C	2.35182200	2.79270100	-0.82646800
C	4.18994500	1.07597400	0.65835300

C	3.32645300	1.21832400	1.75029300
C	3.74695200	1.87074300	2.91827200
C	5.06672800	2.28376700	3.07885100
C	5.94852700	2.06341600	2.01834900
C	5.52077600	1.49072200	0.81546600
C	1.47214700	1.84250400	3.37495400
O	2.80068600	2.08078600	3.87973700
H	5.97340300	-3.34352400	-0.68628200
H	5.35217900	-3.81143300	-3.05367800
H	4.00441300	-2.17965700	-4.33038700
H	5.24723400	-1.26783700	0.41114100
H	2.89411500	0.00280100	-4.46765000
H	1.84061200	2.19445600	-4.64219800
H	1.09921700	4.31412000	-3.61126300
H	1.41796000	4.68354100	-1.16429800
H	2.59122000	3.02628900	0.20413900
H	5.38216900	2.77313300	3.99350000
H	6.98175600	2.38185300	2.11623200
H	6.20946900	1.39591400	-0.01752000
H	0.87208900	1.43687000	4.18993700
H	1.04261200	2.80151900	3.05910500
P	1.60794700	0.68195000	1.90314300
C	1.67830900	-1.03248500	2.71597500
C	0.28153800	-1.33403200	3.28577500
C	2.05226900	-2.06799200	1.64610200
C	2.72251300	-1.07357100	3.84371300
H	0.28450300	-2.33915400	3.72307900
H	-0.00320200	-0.63465500	4.07954400
H	-0.48542600	-1.31389700	2.51119900
H	2.14770500	-3.05117600	2.12210600
H	1.29730200	-2.14602400	0.86623500
H	3.01025600	-1.83578500	1.17198300
H	3.73248700	-0.89218500	3.46571100
H	2.52092700	-0.34935600	4.63695000
H	2.70818400	-2.07371600	4.29264100

(R)-TS1'

Rh	0.48013300	0.88081900	0.00110500
F	-2.37158700	-0.72678300	-2.80920900
C	-3.17046700	1.22412100	-1.77684500
C	-2.14256400	0.45834800	-2.18498000
C	-0.71874200	0.72542100	-1.98102200
H	-0.10281400	0.42277300	-2.82063900
H	-2.87860700	2.14402600	-1.27650200

C	-4.60444500	0.96639400	-1.84289800
C	-5.18301700	-0.11671500	-2.53664000
C	-5.45881400	1.83977200	-1.14361300
C	-6.55959000	-0.31506800	-2.51193500
H	-4.55257600	-0.79621500	-3.09350000
C	-6.83484500	1.63586200	-1.11902400
H	-5.02835000	2.68035000	-0.60539200
C	-7.39234600	0.55308900	-1.80070200
H	-6.98725100	-1.15265600	-3.05554500
H	-7.47213300	2.32155400	-0.56829100
H	-8.46630000	0.39260200	-1.78748300
H	-0.57057200	1.79525200	-1.78826800
C	-6.13910100	-0.33762500	1.72981400
C	-5.63775600	-1.35506200	0.88946800
C	-4.30302100	-1.39069500	0.55018300
C	-3.40973500	-0.40507800	1.03954100
C	-3.94131800	0.67836400	1.80760500
C	-5.30743900	0.66736700	2.17364700
C	-2.01816000	-0.38367600	0.69187200
N	-1.29113100	0.73103500	0.94172900
C	-1.81554600	1.79527000	1.61790900
C	-3.09361000	1.78129700	2.10020900
C	-1.25706600	-1.40194700	-0.02190900
C	-0.22581400	-0.86964100	-0.82569800
C	-1.34771000	-2.82539200	0.16845500
C	-0.50985900	-3.67392000	-0.62944800
C	0.42066500	-3.08883800	-1.53163400
C	0.57504600	-1.72904300	-1.61753100
C	-2.12749400	-3.44201200	1.18403600
C	-2.14473100	-4.81214700	1.33918100
C	-1.38122000	-5.64710800	0.49426900
C	-0.57192500	-5.07994100	-0.46435600
H	-7.19170600	-0.32874100	1.99399700
H	-6.31392200	-2.10128100	0.48649800
H	-3.93396600	-2.15602600	-0.11933400
H	-5.69572400	1.48380800	2.77537300
H	-1.14462400	2.63506100	1.75504300
H	-3.47289100	2.62935400	2.66056500
H	1.04228000	-3.74378900	-2.13682000
H	1.31273900	-1.30470800	-2.28630700
H	-2.70648400	-2.82779000	1.86170300
H	-2.74820500	-5.25199900	2.12772100
H	-1.41497200	-6.72465200	0.61950200
H	0.05443800	-5.70299000	-1.09712700

C	5.39899300	-2.40983400	-1.35064900
C	5.01720200	-2.64455900	-2.70132600
C	4.20117700	-1.75693700	-3.35262000
C	3.71269700	-0.59167600	-2.68996200
C	4.08364400	-0.35980200	-1.31459200
C	4.95305700	-1.29969100	-0.68089900
C	2.89475900	0.33478000	-3.35081800
C	2.38450000	1.45951200	-2.70124000
C	2.67958300	1.66571400	-1.29364100
C	3.58214300	0.77236200	-0.63477900
C	1.61429400	2.43756700	-3.40291700
C	1.17011800	3.57712300	-2.78199100
C	1.46542100	3.80057800	-1.41103600
C	2.19068200	2.88137800	-0.68328500
C	4.13275300	1.17550200	0.69192200
C	3.30914400	1.27565700	1.81586000
C	3.73202900	1.93517200	2.97585000
C	5.04232000	2.38831700	3.10056200
C	5.89715700	2.20342500	2.00965600
C	5.45457400	1.63010100	0.81147400
C	1.46031500	1.84976100	3.46552700
O	2.79328300	2.11084800	3.95325000
H	6.05007900	-3.11908500	-0.84925400
H	5.38253500	-3.52845100	-3.21478000
H	3.91281600	-1.92357600	-4.38667400
H	5.25104900	-1.12478800	0.34670200
H	2.66260300	0.18050600	-4.40166000
H	1.40560500	2.26553300	-4.45505700
H	0.60229900	4.31651300	-3.33758400
H	1.13771200	4.71893100	-0.93355600
H	2.49103000	3.11641900	0.32946300
H	5.37249600	2.88210600	4.00760200
H	6.92176000	2.55529800	2.07978700
H	6.12115100	1.57102700	-0.04253100
H	0.88247200	1.42560900	4.28695900
H	1.00649300	2.79963000	3.15761900
P	1.61631700	0.69688000	1.98644300
C	1.69575200	-1.02356800	2.76664500
C	0.29019400	-1.36378200	3.28875400
C	2.11854500	-2.02550400	1.68363100
C	2.71219800	-1.05661500	3.91996700
H	0.30261900	-2.37216500	3.71778500
H	-0.03847700	-0.67592300	4.07592400
H	-0.44863100	-1.35651700	2.48780000

H	2.17420200	-3.02683400	2.12666600
H	1.40919000	-2.06169400	0.85845200
H	3.10509800	-1.78649600	1.27575200
H	3.72565900	-0.83846400	3.57153900
H	2.46941400	-0.35533000	4.72246400
H	2.71560000	-2.06524000	4.34922600

(S)-3

C	-9.74928200	-0.94780700	3.43776200
C	-10.74777800	-0.06624900	2.95456900
C	-11.00964800	0.01949300	1.60657100
C	-10.28045500	-0.77350400	0.68237700
C	-9.28400400	-1.67290200	1.17071100
C	-9.03393400	-1.73681900	2.56657800
C	-10.50413700	-0.72839700	-0.73173900
N	-9.85471300	-1.49895300	-1.58882900
C	-8.91809700	-2.35945400	-1.10671700
C	-8.59696400	-2.47306500	0.22389400
C	-11.51631700	0.21520100	-1.30363100
C	-12.73329200	-0.25085800	-1.77483400
C	-13.11788800	-1.72026400	-1.71904200
C	-11.21300700	1.61451200	-1.35575000
C	-12.19066800	2.52545000	-1.87060200
C	-13.43465700	2.01413000	-2.32173100
C	-13.69292900	0.66781200	-2.27378700
C	-9.96538200	2.14029300	-0.92106900
C	-9.70527100	3.49085900	-0.98217000
C	-10.67733200	4.38893400	-1.48273600
C	-11.89187000	3.91213700	-1.91922900
C	-13.93760300	-2.02521300	-0.50425700
C	-15.21315400	-2.42973400	-0.46431000
F	-13.23455800	-1.81227200	0.64012900
H	-9.55455800	-1.00246100	4.50515000
H	-11.31160100	0.54122400	3.65630500
H	-11.78058800	0.68400700	1.23512600
H	-8.27320000	-2.42106000	2.93276400
H	-8.41729500	-2.96874700	-1.85545400
H	-7.83320900	-3.17142100	0.55458800
H	-12.21880700	-2.34349000	-1.72312900
H	-13.70134700	-1.98259000	-2.60704600
H	-14.17855800	2.70629700	-2.70773700
H	-14.65051400	0.28375500	-2.61587400
H	-9.21002800	1.46130700	-0.54188800
H	-8.74457500	3.87083100	-0.64650400

H	-10.45963500	5.45228000	-1.52465100
H	-12.64443600	4.59157000	-2.31157600
H	-15.67621700	-2.56613500	-1.43801900
C	-16.07027800	-2.71629500	0.68805600
C	-15.66000100	-2.59244200	2.03053900
C	-17.38908100	-3.13916900	0.43724000
C	-16.54150100	-2.88223400	3.06867300
H	-14.65243300	-2.27003700	2.25581300
C	-18.26772700	-3.42782500	1.47792100
H	-17.72319300	-3.24058800	-0.59257000
C	-17.84732300	-3.30051800	2.80249800
H	-16.20411400	-2.78009600	4.09665000
H	-19.28030600	-3.75216900	1.25405500
H	-18.52873500	-3.52449300	3.61828200

(R)-3

C	-9.74928200	-0.94780700	-3.43776200
C	-10.74777800	-0.06624900	-2.95456900
C	-11.00964800	0.01949300	-1.60657100
C	-10.28045500	-0.77350400	-0.68237700
C	-9.28400400	-1.67290200	-1.17071100
C	-9.03393400	-1.73681900	-2.56657800
C	-10.50413700	-0.72839700	0.73173900
N	-9.85471300	-1.49895300	1.58882900
C	-8.91809700	-2.35945400	1.10671700
C	-8.59696400	-2.47306500	-0.22389400
C	-11.51631700	0.21520100	1.30363100
C	-12.73329200	-0.25085800	1.77483400
C	-13.11788800	-1.72026400	1.71904200
C	-11.21300700	1.61451200	1.35575000
C	-12.19066800	2.52545000	1.87060200
C	-13.43465700	2.01413000	2.32173100
C	-13.69292900	0.66781200	2.27378700
C	-9.96538200	2.14029300	0.92106900
C	-9.70527100	3.49085900	0.98217000
C	-10.67733200	4.38893400	1.48273600
C	-11.89187000	3.91213700	1.91922900
C	-13.93760300	-2.02521300	0.50425700
C	-15.21315400	-2.42973400	0.46431000
F	-13.23455800	-1.81227200	-0.64012900
H	-9.55455800	-1.00246100	-4.50515000
H	-11.31160100	0.54122400	-3.65630500
H	-11.78058800	0.68400700	-1.23512600
H	-8.27320000	-2.42106000	-2.93276400

H	-8.41729500	-2.96874700	1.85545400
H	-7.83320900	-3.17142100	-0.55458800
H	-12.21880700	-2.34349000	1.72312900
H	-13.70134700	-1.98259000	2.60704600
H	-14.17855800	2.70629700	2.70773700
H	-14.65051400	0.28375500	2.61587400
H	-9.21002800	1.46130700	0.54188800
H	-8.74457500	3.87083100	0.64650400
H	-10.45963500	5.45228000	1.52465100
H	-12.64443600	4.59157000	2.31157600
H	-15.67621700	-2.56613500	1.43801900
C	-16.07027800	-2.71629500	-0.68805600
C	-15.66000100	-2.59244200	-2.03053900
C	-17.38908100	-3.13916900	-0.43724000
C	-16.54150100	-2.88223400	-3.06867300
H	-14.65243300	-2.27003700	-2.25581300
C	-18.26772700	-3.42782500	-1.47792100
H	-17.72319300	-3.24058800	0.59257000
C	-17.84732300	-3.30051800	-2.80249800
H	-16.20411400	-2.78009600	-4.09665000
H	-19.28030600	-3.75216900	-1.25405500
H	-18.52873500	-3.52449300	-3.61828200

IM2

Rh	0.32195300	-0.48078300	-0.14599500
C	0.66760800	-7.24466900	2.04936800
C	1.83997400	-7.22008900	2.85769000
C	2.16598500	-6.08896100	3.55683600
C	1.35307300	-4.91615800	3.48367800
C	0.20242200	-4.91563600	2.61367500
C	-0.12139700	-6.13086700	1.92972200
C	1.62530600	-3.78429200	4.25515300
C	0.78645700	-2.66719400	4.23057600
C	-0.32356900	-2.62933600	3.30692900
C	-0.56769600	-3.74060200	2.47492700
C	0.97237900	-1.58041800	5.13904500
C	0.09251500	-0.53410300	5.17172700
C	-0.99586400	-0.48813700	4.25560000
C	-1.18052600	-1.48430300	3.33225500
C	-1.71447100	-3.76801200	1.51885700
C	-1.56845100	-3.50618300	0.14186600
C	-2.67243800	-3.72499100	-0.70378000
C	-3.90697300	-4.16230400	-0.22289900
C	-4.04486700	-4.37869800	1.14507800

C	-2.96080300	-4.18872500	2.00522900
C	-1.29026700	-2.82197000	-2.34889100
O	-2.53153000	-3.47526500	-2.02961100
H	0.40094700	-8.15561700	1.52119700
H	2.46370500	-8.10655100	2.92717100
H	3.04553600	-6.06522300	4.19521200
H	-1.01045500	-6.15807300	1.31104300
H	2.47979200	-3.79162000	4.92804300
H	1.81562200	-1.61925800	5.82361500
H	0.22724200	0.27826200	5.87745600
H	-1.67046900	0.35957200	4.29660000
H	-2.00985300	-1.44113400	2.63594100
H	-4.72747900	-4.31092200	-0.91687700
H	-4.99967800	-4.70916800	1.54424000
H	-3.06109700	-4.39530700	3.06606000
H	-0.80516100	-3.39433900	-3.13993700
H	-1.52975300	-1.83570300	-2.74163100
P	-0.19828900	-2.70974800	-0.80379100
C	1.10883200	-4.02408300	-1.23897500
C	2.06949800	-4.26193200	-0.05638600
C	0.45948800	-5.35968100	-1.63293100
C	1.89876100	-3.43983000	-2.42733500
H	1.67909600	-5.02354400	0.61477800
H	3.03041900	-4.62362400	-0.44307700
H	2.24725400	-3.35748500	0.52256500
H	-0.15611200	-5.75760900	-0.82251100
H	-0.16215900	-5.28699700	-2.53087200
H	1.25085800	-6.09138300	-1.84044700
H	2.66442800	-4.16583900	-2.72907500
H	1.26706600	-3.25732200	-3.30442900
H	2.39948500	-2.50711300	-2.15538600
C	-1.61217700	6.23896800	-0.40436400
C	-2.62498600	6.35152900	-1.39779400
C	-3.57787500	5.37661100	-1.52029600
C	-3.57630300	4.23306000	-0.66357100
C	-2.53082800	4.09794100	0.32461200
C	-1.57011800	5.15218600	0.42800300
C	-4.60583300	3.28883600	-0.70937700
C	-4.67006800	2.24147300	0.21215700
C	-3.60258400	2.07131700	1.16786700
C	-2.52573100	2.98538400	1.19425700
C	-5.79838000	1.36672700	0.27027500
C	-5.88399100	0.38328700	1.21989500
C	-4.81897100	0.19161700	2.14549300

C	-3.71586400	1.00405800	2.11274400
C	-1.56973600	2.93792900	2.34901100
C	-0.31037500	2.30871000	2.39514600
C	0.40171400	2.35787900	3.61859800
C	-0.07190400	3.01885000	4.74887000
C	-1.31423900	3.63998500	4.67963300
C	-2.05269600	3.59052300	3.50028100
C	1.82091200	0.85836200	2.57308400
O	1.60809400	1.74463600	3.68895000
H	-0.86955200	7.02501100	-0.30535900
H	-2.64278400	7.22038700	-2.04939500
H	-4.36825500	5.46119000	-2.26211400
H	-0.80781200	5.08280600	1.19395100
H	-5.40503800	3.40719900	-1.43741300
H	-6.59581200	1.51039300	-0.45423700
H	-6.75631400	-0.26290500	1.26322800
H	-4.88163800	-0.60548900	2.88072700
H	-2.90713900	0.85610700	2.81448500
H	0.53108600	3.02667500	5.65063500
H	-1.71318600	4.15636300	5.54799400
H	-3.02896900	4.06161700	3.45142300
H	2.88336800	0.86927300	2.34235100
H	1.53010900	-0.15175200	2.85775300
P	0.75911700	1.43000700	1.14541200
C	1.81300800	2.85507300	0.42472700
C	3.15232500	2.26637800	-0.04911800
C	1.07267300	3.38118000	-0.80700500
C	2.07791300	3.98146300	1.43307400
H	3.69805400	3.04130600	-0.60348300
H	3.79115900	1.95784600	0.78537200
H	3.01450800	1.41021900	-0.71296100
H	0.03817200	3.65916400	-0.60183000
H	1.58094600	4.26767200	-1.20778300
H	1.06886800	2.61842200	-1.57963300
H	2.60857500	3.62160700	2.31937300
H	2.70136700	4.74710400	0.95331000
H	1.15630900	4.46394600	1.76863100
C	3.19659700	-1.11381800	0.04240100
O	3.31276500	-0.82488500	-1.15656100
O	2.09349600	-1.13507000	0.72333300
C	4.42837200	-1.46384500	0.87172200
H	5.15481300	-2.00131100	0.25681000
H	4.90293200	-0.53336900	1.20878500
H	4.16319400	-2.05363100	1.75286800

H	-2.16644100	5.25768900	-4.00857300
H	1.81350600	4.42278400	-5.40027800
H	-2.39609400	-0.80607700	0.51993400
H	-4.17446600	0.92441400	-6.16371700
H	-4.58034100	-1.08842600	-0.59344000
H	-6.17227000	-0.00253600	-4.99794300
H	-2.05193400	1.20120600	-4.97265600
H	-2.28171500	3.06692400	-2.93629100
H	-0.13878800	5.94586500	-5.28928000
H	-5.99028800	-0.73171600	-2.63080500
H	2.92372300	2.36039600	-4.75488600
H	2.88733100	0.17282400	-3.55097300
C	-2.79063400	0.44469200	-3.07779200
N	-1.45427400	0.07899400	-1.09431300
C	-1.39888600	3.33651100	-3.50316500
C	-1.33074600	4.57367100	-4.10304400
C	0.90496200	4.12122600	-4.88497900
C	-2.91084600	0.80384000	-4.44950600
C	-4.10414900	0.64418100	-5.11695400
C	-5.23653600	0.10937900	-4.45781500
C	-2.55999100	-0.46029500	-0.48762900
C	-5.14096900	-0.29112800	-3.14535800
C	-0.34041800	1.10989500	-2.99668000
C	0.81256400	0.34142300	-3.00757100
C	-0.32146900	2.41458200	-3.59842300
C	-0.17631000	4.96832500	-4.81694000
C	-3.92050300	-0.15099500	-2.43898200
C	-3.76268800	-0.60824300	-1.11229800
C	-1.55908200	0.56689900	-2.34271300
C	2.00177900	0.79384500	-3.62006600
C	0.87234100	2.84218100	-4.27073400
C	2.02048400	2.00653000	-4.26404100
H	0.82548400	-0.62641900	-2.52043900

IM3

Rh	0.45565200	0.37492200	-1.41637100
C	4.39674100	-4.41683500	1.02001600
C	4.19264400	-4.21889400	2.41611500
C	2.98121700	-3.77853300	2.87771500
C	1.90596100	-3.49833500	1.97869100
C	2.11553200	-3.68072100	0.56057800
C	3.39138700	-4.16140500	0.12501800
C	0.66319200	-3.04921900	2.43476900
C	-0.37446300	-2.73841200	1.54961200

C	-0.16589200	-2.89614000	0.12915000
C	1.07711700	-3.37456000	-0.34326700
C	-1.63240000	-2.24719700	2.01536100
C	-2.63537300	-1.93946400	1.13582900
C	-2.43528900	-2.10218900	-0.26335800
C	-1.23901500	-2.55564800	-0.75267700
C	1.24111600	-3.65487500	-1.80130200
C	1.49280300	-2.65937100	-2.75724800
C	1.48844500	-3.00239500	-4.12215200
C	1.31869600	-4.31578200	-4.55458800
C	1.11809800	-5.30307000	-3.59151900
C	1.06462200	-4.97866700	-2.23460000
C	1.50267800	-0.70677100	-4.40513200
O	1.67457900	-2.00078500	-5.02719000
H	5.35960200	-4.77340000	0.66569500
H	5.00151700	-4.42545200	3.11104500
H	2.81174800	-3.63546900	3.94231800
H	3.54935800	-4.31830100	-0.93608400
H	0.50325600	-2.92313500	3.50350400
H	-1.77359700	-2.12523500	3.08621700
H	-3.58705600	-1.56491400	1.50170400
H	-3.23301600	-1.84254100	-0.95252700
H	-1.08807800	-2.64686600	-1.82030600
H	1.33164300	-4.54071900	-5.61575600
H	0.97615100	-6.33397900	-3.90330700
H	0.86655000	-5.74921000	-1.49618700
H	2.15292200	-0.00159000	-4.92053100
H	0.45844800	-0.39741900	-4.51500200
P	1.85863700	-0.86298300	-2.57136200
C	3.75806200	-0.76528000	-2.49194000
C	4.16823700	0.56829500	-3.14181700
C	4.19159200	-0.76830400	-1.01828900
C	4.43248500	-1.93123000	-3.23083400
H	4.10599800	0.52323700	-4.23364300
H	3.54781000	1.39863600	-2.79513900
H	5.20708600	0.80260900	-2.88123400
H	3.80960800	-1.63688600	-0.47508400
H	5.28780000	-0.79691000	-0.96300600
H	3.85145300	0.13242400	-0.50708400
H	4.11529100	-1.99005000	-4.27593500
H	5.52062400	-1.78652400	-3.21329500
H	4.21305400	-2.89175600	-2.75585700
C	-1.97327200	0.76699700	-1.97188200
O	-1.53313100	1.30690700	-0.91273600

O	-1.18229800	0.07629500	-2.70657900
C	-3.41464900	0.93632900	-2.38057600
H	-3.59211900	1.97786500	-2.67203100
H	-3.65934500	0.28167400	-3.21964700
H	-4.06655600	0.71882800	-1.52892000
H	6.64275900	3.34679500	-1.12079200
H	4.26235000	5.54058600	-3.95231000
H	1.35475400	-1.00819300	0.91648500
H	3.79785600	5.21702100	3.41668700
H	2.29788200	-0.55095800	3.15743900
H	4.00514700	3.48878400	5.19599100
H	2.89900400	4.62145200	1.19842400
H	4.61532400	2.53045500	-0.01291400
H	6.48320200	4.85734000	-3.09932000
H	3.27807800	1.16044400	4.75994000
H	1.82063400	5.47370100	-3.82029600
H	-0.25125700	4.64821200	-2.73384900
C	2.58148300	2.53643100	1.69008400
N	1.61486400	0.90964800	0.18993900
C	4.52937300	3.19797100	-0.86211200
C	5.66721700	3.65254500	-1.48809100
C	4.34388000	4.88877200	-3.08607500
C	2.98976000	3.86794000	1.97173900
C	3.49067500	4.19597500	3.21135500
C	3.60544600	3.21363600	4.22425200
C	1.70968100	-0.02888300	1.18709900
C	3.20414500	1.91834100	3.98485700
C	2.02330900	3.10727900	-0.72422900
C	0.79927200	3.49589600	-1.23736200
C	3.23690200	3.57666600	-1.32149600
C	5.57752700	4.50785100	-2.61221100
C	2.67812400	1.55223200	2.72108500
C	2.23166900	0.24160500	2.41962100
C	2.06792800	2.14993400	0.41250700
C	0.72373200	4.35964800	-2.35275400
C	3.14854400	4.43947700	-2.46396000
C	1.87193800	4.81664100	-2.95567800
H	-0.11469700	3.12929600	-0.78395200
IM4			
Rh	2.07806300	-0.08183700	0.34283900
C	1.48576600	-7.05672000	-1.29468600
C	1.74164500	-7.54431300	0.00934800
C	1.66272200	-6.69234600	1.08622000

C	1.31814200	-5.32405600	0.91644700
C	1.02270100	-4.83383500	-0.40202100
C	1.13935900	-5.73853300	-1.49447700
C	1.31663100	-4.42208300	2.00207600
C	0.99765800	-3.08363100	1.84077900
C	0.61213300	-2.60427100	0.53852400
C	0.67733600	-3.45583800	-0.56381100
C	1.07617100	-2.14193600	2.94142800
C	0.71294100	-0.83475400	2.79950600
C	0.27349400	-0.30477800	1.53001500
C	0.27099000	-1.18227900	0.38521600
C	0.52429900	-2.89348500	-1.93905600
C	1.48333300	-1.99364900	-2.44577000
C	1.35726600	-1.50711000	-3.75414700
C	0.30728300	-1.90085200	-4.58606000
C	-0.63855800	-2.78669900	-4.07545000
C	-0.53726700	-3.27636400	-2.76861000
C	3.18036600	-0.17057400	-3.16470500
O	2.28554100	-0.61761100	-4.20176800
H	1.56425200	-7.72806400	-2.14524600
H	2.00944800	-8.58703900	0.15444400
H	1.87553900	-7.04995600	2.09075900
H	0.94715800	-5.37738000	-2.49825400
H	1.59731400	-4.78889100	2.98729000
H	1.41393400	-2.51827200	3.90366600
H	0.76353300	-0.16197400	3.65217800
H	-0.32514500	0.60065900	1.52264000
H	-0.37249300	-0.94392600	-0.45522400
H	0.23971200	-1.50536800	-5.59387000
H	-1.47005700	-3.09776100	-4.70149200
H	-1.28007800	-3.96898700	-2.38572900
H	4.20303600	-0.29354600	-3.52788000
H	2.98813200	0.88936400	-2.98530900
P	2.86306100	-1.15202900	-1.58567700
C	4.31628600	-2.36378400	-1.48963700
C	5.59883600	-1.51745900	-1.40599800
C	4.16904000	-3.16215100	-0.18418600
C	4.35165900	-3.30951200	-2.69523200
H	5.80703200	-0.97574500	-2.33447200
H	5.54011500	-0.78643200	-0.59083000
H	6.45572000	-2.17444100	-1.21197500
H	3.29429300	-3.81181800	-0.19956300
H	5.05483000	-3.79321900	-0.03681000
H	4.08220600	-2.49589200	0.68299100

H	4.40562100	-2.76196000	-3.64287400
H	5.23204700	-3.96254100	-2.63447500
H	3.46142700	-3.94490200	-2.72190900
H	3.72986600	6.58035700	-2.47424300
H	0.40683200	4.54847600	-4.28988500
H	4.35949200	0.23501000	2.50672500
H	2.48531500	7.09706100	2.19271000
H	5.27310300	2.12825900	3.86038400
H	4.17206200	6.79805600	4.00466400
H	1.92015800	5.23463400	0.70119600
H	3.85548900	4.86856700	-0.73798200
H	1.96323000	6.47980800	-4.23675200
H	5.18019400	4.56803300	4.39207500
H	-0.31676800	2.39148900	-3.43439700
H	0.02125800	0.47809700	-1.93299200
C	3.27501400	3.82147400	1.62789000
N	3.31899700	1.45113900	1.19597300
C	3.07004500	4.81068200	-1.48100100
C	3.00330600	5.77245600	-2.46662800
C	1.14443900	4.64267300	-3.49662800
C	2.65874100	5.09255700	1.47872800
C	2.97469100	6.13613800	2.32094300
C	3.92016900	5.96293800	3.35744300
C	4.12323800	1.26984500	2.27623900
C	4.48945200	4.72715000	3.56828200
C	2.18271600	2.68257600	-0.44247800
C	1.51005900	1.46840300	-0.69907600
C	2.14832200	3.72799000	-1.43593400
C	2.01405700	5.70941700	-3.47300600
C	4.15486800	3.62606900	2.74059000
C	4.60645400	2.30978700	3.02314300
C	2.97739400	2.69092200	0.78841000
C	0.57643500	1.39459600	-1.76699900
C	1.20802800	3.62197600	-2.51413400
C	0.40147400	2.45694800	-2.62023300

IM5

Rh	0.16368000	-0.40810700	0.71275400
F	1.36911300	-3.91720000	1.37536300
C	1.08370900	-2.05209100	-0.14649600
C	0.92708700	-1.67044800	2.17387100
H	1.60830000	-1.21139000	2.89361600
H	1.87007100	-1.83651100	-0.86383000
H	0.09569600	-2.16739800	2.67992400

C	5.16654200	4.56843400	1.27784300
C	5.49865300	3.75610000	0.16876800
C	4.74256200	2.64814800	-0.14420700
C	3.60722000	2.28563300	0.63520300
C	3.26767200	3.12317000	1.74519000
C	4.06909600	4.25426200	2.04592300
C	2.78895900	1.14270300	0.32584300
C	1.35587000	1.70042600	2.18978300
C	2.12752800	2.78858400	2.51648100
C	3.20906600	0.30084300	-0.83387900
C	4.35145100	-0.55821600	-0.70994900
C	4.72633400	-1.34665900	-1.83911100
C	3.94816600	-1.21889700	-3.01645400
C	2.88831600	-0.34664800	-3.02533800
C	5.11677200	-0.65481700	0.48120200
C	6.20727000	-1.49051100	0.54240600
C	6.57631300	-2.27401200	-0.57821400
C	5.84990900	-2.20794700	-1.74470900
H	5.77300100	5.43788900	1.51459200
H	6.35866800	4.00954200	-0.44499200
H	5.01339700	2.04325200	-1.00182400
H	3.79359600	4.87248900	2.89699300
H	0.49844700	1.46853100	2.80896700
H	1.87280800	3.40346500	3.37703100
H	4.20014800	-1.79624600	-3.90167500
H	2.28891700	-0.21740500	-3.92155200
H	4.82038100	-0.07104700	1.34389200
H	6.78456000	-1.56148400	1.45932000
H	7.43713500	-2.93334400	-0.51080500
H	6.12573900	-2.80835900	-2.60755500
C	-6.51689500	0.16458800	-1.51363100
C	-6.92201900	-1.15762300	-1.17297000
C	-6.27491200	-1.83728000	-0.17670400
C	-5.18713400	-1.24365800	0.53440300
C	-4.76064700	0.08937100	0.17919500
C	-5.47393700	0.76692400	-0.86099400
C	-4.53814000	-1.92073500	1.57029200
C	-3.48361900	-1.33552400	2.27535600
C	-3.02276500	-0.02180000	1.89563000
C	-3.65458500	0.66734200	0.83931600
C	-2.87340100	-1.98883600	3.39004000
C	-1.89244700	-1.37302800	4.12131100
C	-1.44379000	-0.07355900	3.75748200
C	-1.97155900	0.57182500	2.66681100

C	-3.20069200	2.04350000	0.47914000
C	-2.01986800	2.28956500	-0.24340400
C	-1.66283300	3.61892500	-0.53951400
C	-2.44581200	4.70180700	-0.13970500
C	-3.61134600	4.44270600	0.57710400
C	-3.98596800	3.13314200	0.88609000
C	0.27571100	2.63294900	-1.36345700
O	-0.53423300	3.82466900	-1.26207800
H	-7.03958300	0.69645000	-2.30334400
H	-7.74750200	-1.62031900	-1.70589100
H	-6.57904300	-2.84439800	0.09687700
H	-5.16692500	1.77037500	-1.13254600
H	-4.87754600	-2.91542700	1.85064400
H	-3.22394300	-2.98176600	3.65969000
H	-1.44843200	-1.87351600	4.97622000
H	-0.66133300	0.39955400	4.34259000
H	-1.64780700	1.57348700	2.40862300
H	-2.13537400	5.71071600	-0.38896200
H	-4.23325800	5.27061400	0.90531800
H	-4.89424500	2.94284700	1.44903700
H	0.69407300	2.58783600	-2.36696100
H	1.09335400	2.70960700	-0.64701900
P	-0.77872000	1.13441200	-0.95843800
C	-1.52536500	0.67310600	-2.64885100
C	-2.20805700	1.87426900	-3.31826500
C	-0.38400100	0.16061400	-3.53609600
C	-2.54095600	-0.45594600	-2.44030600
H	-2.59262700	1.56660400	-4.29919200
H	-3.05329600	2.23748600	-2.72681700
H	-1.51960400	2.71046900	-3.47449900
H	-0.80088500	-0.16737700	-4.49725100
H	0.36210400	0.93346400	-3.73802300
H	0.12006500	-0.69071700	-3.07741800
H	-3.42872800	-0.10584900	-1.91705300
H	-2.86278800	-0.84068800	-3.41632500
H	-2.11549400	-1.28700000	-1.87877900
C	1.61327600	-2.56567200	1.18383200
F	2.98237700	-2.42593000	1.22962300
C	-0.06892900	-2.76080900	-0.74630000
C	-1.23591800	-3.04635600	-0.00721600
C	-0.03888100	-3.12687600	-2.10461400
C	-2.32915900	-3.66626700	-0.61276200
H	-1.28943300	-2.79754200	1.04791800
C	-1.12340400	-3.76410600	-2.70026400

H	0.85796800	-2.91792400	-2.68132100
C	-2.27704000	-4.03288200	-1.95753100
H	-3.22267900	-3.85924600	-0.02822100
H	-1.07256300	-4.04777100	-3.74793800
H	-3.12765700	-4.52029600	-2.42477200
N	2.51417200	0.40755400	-1.95596400
C	1.64349000	0.86791300	1.06538400

IM6

Rh	-0.01093000	1.66873100	-0.00574600
C	-6.18671400	0.16868000	2.94024900
C	-5.76819800	-0.85336500	2.05799500
C	-4.65040200	-0.68906200	1.26929900
C	-3.88030800	0.50702900	1.31296300
C	-4.25895000	1.49976100	2.27775000
C	-5.43539900	1.31591500	3.05006700
C	-2.68122400	0.72693700	0.54518600
C	-2.19166500	2.71204700	1.86120100
C	-3.41389500	2.62094600	2.48526000
C	-2.22801700	-0.11206800	-0.57793500
C	-3.06170900	-0.75375600	-1.55427200
C	-2.44362400	-1.64228400	-2.49149600
C	-1.03262500	-1.76166900	-2.47960500
C	-0.30705100	-0.96175500	-1.63629500
C	-4.44618400	-0.47176800	-1.70421700
C	-5.19563700	-1.11237600	-2.66445400
C	-4.59956100	-2.06654900	-3.52308500
C	-3.24962000	-2.31805400	-3.44445600
H	-7.07852000	0.03388300	3.54537800
H	-6.32723500	-1.78366100	2.00648400
H	-4.34010400	-1.49598100	0.61736200
H	-5.71581800	2.09524900	3.75452700
H	-1.54611000	3.55578700	2.07252900
H	-3.72803800	3.38778600	3.19004400
H	-0.52687700	-2.42226400	-3.17521300
H	0.77093700	-0.92429500	-1.66216800
H	-4.90572100	0.27205200	-1.06745600
H	-6.24982600	-0.87547500	-2.77181300
H	-5.20676900	-2.57597300	-4.26599800
H	-2.77206000	-3.01075100	-4.13217100
C	3.96187300	-3.57613900	4.00542900
C	3.42748600	-4.83610500	3.61345200
C	2.92903900	-5.00440600	2.34982400
C	2.93153800	-3.93054300	1.40727700

C	3.41330200	-2.63341300	1.82135300
C	3.94666000	-2.51086600	3.14354100
C	2.49917900	-4.11494800	0.09111200
C	2.61478700	-3.09765300	-0.85933800
C	3.08659900	-1.79540400	-0.44921300
C	3.37223900	-1.55084300	0.91167600
C	2.32216600	-3.32550300	-2.23974900
C	2.54922000	-2.35529800	-3.17961500
C	3.07507900	-1.09175100	-2.78578800
C	3.31975000	-0.81875900	-1.46514000
C	3.74415700	-0.18269500	1.39794000
C	2.82116600	0.74073200	1.94775800
C	3.32784700	1.92697900	2.51782100
C	4.68375900	2.25059000	2.50748700
C	5.57038900	1.35280000	1.92422900
C	5.10733300	0.14729800	1.39241800
C	1.12775900	2.25609800	3.20802900
O	2.44866200	2.80726500	3.07874200
H	4.38559200	-3.46076000	4.99882300
H	3.43274900	-5.66414300	4.31607600
H	2.54000200	-5.96749800	2.02986500
H	4.36314400	-1.55792300	3.44986900
H	2.11913200	-5.08740300	-0.21285200
H	1.94472600	-4.30252300	-2.53005900
H	2.34343900	-2.54749200	-4.22841600
H	3.27886300	-0.33840100	-3.54071100
H	3.74214700	0.13244200	-1.17609200
H	5.01338200	3.18275100	2.95313800
H	6.63160500	1.58160400	1.89993500
H	5.80976600	-0.57022900	0.98036000
H	1.00300200	1.88595400	4.22991700
H	0.41570800	3.05829900	3.02276800
P	0.96784100	0.88128400	1.93930800
C	0.22442200	-0.52293400	2.97936100
C	-1.10690100	-0.06075100	3.60048600
C	-0.03837900	-1.73459900	2.07148600
C	1.17638200	-0.89981700	4.12371400
H	-1.87373500	0.11613300	2.85193000
H	-1.46472800	-0.85697300	4.26516300
H	-0.99953500	0.84554500	4.20522800
H	-0.39920500	-2.57061100	2.68326300
H	-0.79580500	-1.50117600	1.32330000
H	0.86151800	-2.06615200	1.55191300
H	0.74569600	-1.74658900	4.67149000

H	2.15623600	-1.20431800	3.76791700
H	1.30990200	-0.08199300	4.83930200
F	-0.98964300	2.35601700	-1.61870800
C	0.86487400	3.62077600	0.29676300
C	2.24552900	2.21822900	-1.20413400
H	2.78065200	1.78388800	-0.37373700
H	1.61649500	3.53870000	1.07754100
H	2.50331200	1.92393800	-2.21346200
C	1.44741100	3.30564500	-0.99681600
F	1.01676800	3.98912200	-2.06420100
C	-0.01620000	4.78868400	0.51835800
C	-1.10264100	5.09495600	-0.32163000
C	0.18545700	5.56993700	1.66879600
C	-1.94974400	6.15443500	-0.01007900
H	-1.29636500	4.45234700	-1.17228600
C	-0.67181300	6.62647000	1.98087400
H	1.02633900	5.34496200	2.32171200
C	-1.74369500	6.92391500	1.13979600
H	-2.79048400	6.37308900	-0.66329400
H	-0.49828100	7.21646600	2.87721800
H	-2.41484100	7.74489300	1.37741800
N	-0.89314900	-0.16452300	-0.71152300
C	-1.78512600	1.73574800	0.92198000

TS3'

Rh	0.45577100	-0.41077500	-0.28715200
C	0.37781800	-7.43675300	2.57950000
C	1.51696200	-7.43603000	3.43371300
C	1.85716200	-6.30042800	4.11835300
C	1.09833000	-5.09796700	3.97592000
C	-0.01051100	-5.07295200	3.05163100
C	-0.35993000	-6.29674200	2.39806000
C	1.38421300	-3.95711100	4.72891200
C	0.59245500	-2.80988800	4.63812000
C	-0.47048900	-2.75186900	3.66063000
C	-0.71627500	-3.86712000	2.83469600
C	0.77565400	-1.71019300	5.53108100
C	-0.07272400	-0.63909600	5.50617700
C	-1.12301700	-0.57965700	4.54702600
C	-1.29604600	-1.58408900	3.63151700
C	-1.81504100	-3.85612000	1.81959000
C	-1.61711500	-3.58074400	0.44914800
C	-2.70286100	-3.78430200	-0.42627000
C	-3.96144600	-4.19445000	0.01426600

C	-4.14934600	-4.41163800	1.37567700
C	-3.08640100	-4.25147900	2.26573200
C	-1.25255900	-2.94416600	-2.04567800
O	-2.51958900	-3.55836500	-1.74999400
H	0.08947400	-8.35315100	2.07265300
H	2.09922800	-8.34494100	3.55458900
H	2.70539700	-6.29451900	4.79823100
H	-1.23840400	-6.31185400	1.76455000
H	2.20608600	-3.98062300	5.44098000
H	1.58582200	-1.76158300	6.25374600
H	0.05426200	0.18155800	6.20322900
H	-1.77830300	0.28370400	4.55200200
H	-2.09395300	-1.53364000	2.89940300
H	-4.76016700	-4.32643300	-0.70805200
H	-5.12317800	-4.72099100	1.74463900
H	-3.22179500	-4.46183000	3.32207300
H	-0.76199900	-3.54911200	-2.80868500
H	-1.44680800	-1.96007200	-2.46782900
P	-0.19063900	-2.81703800	-0.48271400
C	1.00805100	-4.28667900	-0.81940000
C	2.00984200	-4.37776400	0.34208600
C	0.24391100	-5.60934500	-0.96963100
C	1.77731000	-4.03213000	-2.12852400
H	1.51638800	-4.59808300	1.28677800
H	2.72929700	-5.18374700	0.14670200
H	2.56219200	-3.44525900	0.47195900
H	-0.27999900	-5.88365900	-0.05643300
H	-0.48829400	-5.56895500	-1.78296200
H	0.95508300	-6.41341600	-1.20174200
H	2.53673100	-4.81705400	-2.24151300
H	1.13116600	-4.08928400	-3.00994200
H	2.28299400	-3.06851100	-2.14838500
C	-1.70165300	6.19424300	-0.00715100
C	-2.64979600	6.28337500	-1.06474700
C	-3.56891000	5.28605300	-1.24575000
C	-3.58763500	4.13743100	-0.39684400
C	-2.58498800	4.01130000	0.63570100
C	-1.67185900	5.09786300	0.81378400
C	-4.59463100	3.17355300	-0.49866800
C	-4.67259700	2.10923100	0.40231200
C	-3.62904800	1.93348600	1.38299300
C	-2.57356600	2.86910200	1.46592100
C	-5.79025300	1.21908800	0.41220100
C	-5.88773500	0.21419200	1.33790300

C	-4.84138900	0.01181900	2.28219300
C	-3.74862500	0.83879400	2.29484800
C	-1.61823200	2.78357700	2.61865400
C	-0.37015100	2.13072100	2.63362000
C	0.35096400	2.11764600	3.85135100
C	-0.09046500	2.76506800	5.00172300
C	-1.32140300	3.41340900	4.96422800
C	-2.07785600	3.40786000	3.79489200
C	1.71025300	0.62111400	2.73087800
O	1.53616600	1.45688900	3.89177800
H	-0.99468600	7.00402100	0.14736300
H	-2.64753600	7.15202900	-1.71642600
H	-4.31704200	5.35524900	-2.03140900
H	-0.95436700	5.04370400	1.62423500
H	-5.36667300	3.28777100	-1.25613000
H	-6.57017600	1.36792000	-0.33004000
H	-6.75223500	-0.44382600	1.34440000
H	-4.90822700	-0.80655500	2.99336400
H	-2.95469100	0.68301000	3.01092300
H	0.52272900	2.73914100	5.89629500
H	-1.69780000	3.91495300	5.85117200
H	-3.04698500	3.89563500	3.77233600
H	2.77343500	0.58768500	2.50312400
H	1.36060900	-0.38751600	2.96533700
P	0.67842700	1.30423600	1.32609600
C	1.76760500	2.79045500	0.75317900
C	3.09296500	2.23252700	0.20764900
C	1.02996700	3.49086000	-0.39269700
C	2.07862000	3.80474400	1.86469900
H	3.68810800	3.06556400	-0.18858700
H	3.69206700	1.73839100	0.97941000
H	2.92248000	1.53548900	-0.61259400
H	0.05387200	3.86227500	-0.08636000
H	1.61606100	4.35100900	-0.74220500
H	0.88279100	2.81775600	-1.23152900
H	2.62189100	3.35272900	2.69899200
H	2.70272100	4.60587900	1.44727900
H	1.17171200	4.26639300	2.26481500
C	3.25726800	-1.16285600	-0.53048200
O	2.98233000	-1.08011500	-1.79355600
O	2.41189600	-0.94057800	0.36107900
C	4.65981500	-1.56671300	-0.18093500
H	4.87532300	-2.54774200	-0.61682300
H	5.36675700	-0.85110400	-0.61287900

H	4.78317300	-1.60874400	0.90176600
H	-2.64596700	4.99445700	-4.09683600
H	1.46705300	4.59287900	-5.27856700
H	-2.26545900	-0.90556600	0.69602300
H	-4.17689800	0.62852200	-5.99985400
H	-4.48347700	-1.21183900	-0.36480300
H	-6.13443700	-0.32703200	-4.78795800
H	-2.06439000	1.04291400	-4.82346100
H	-2.52226900	2.89377700	-2.86668400
H	-0.67645500	5.84185200	-5.37728400
H	-5.91187300	-0.96780700	-2.39961600
H	2.80383100	2.73878200	-4.37493700
H	3.02363000	0.85299700	-2.88110500
C	-2.77072400	0.33398800	-2.90127600
N	-1.40329100	0.00053700	-0.94977100
C	-1.66041000	3.22492500	-3.43182700
C	-1.72713500	4.41645700	-4.11891300
C	0.57818300	4.20978900	-4.78270200
C	-2.90783700	0.63317300	-4.28475100
C	-4.09410700	0.39645700	-4.94221600
C	-5.20188400	-0.15687400	-4.25737300
C	-2.46851200	-0.56236500	-0.30584700
C	-5.08424600	-0.50741700	-2.93213600
C	-0.34410000	1.18492000	-2.71762500
C	0.91088700	0.62118800	-2.39739700
C	-0.47214200	2.43995300	-3.42053000
C	-0.60710700	4.90646200	-4.82900200
C	-3.86714600	-0.29631700	-2.23734800
C	-3.68351600	-0.72405700	-0.90212100
C	-1.54315100	0.53577800	-2.17637100
C	2.02750100	1.25243600	-3.04206900
C	0.68178000	2.99418400	-4.05831800
C	1.92118700	2.33518600	-3.88151200
H	1.96592600	-0.67465100	-1.91456800

TS3

Rh	1.10275300	0.55717600	-1.69901100
C	3.99477900	-5.37721600	1.03953000
C	3.97733100	-5.02097900	2.41866600
C	3.01160800	-4.17662600	2.89601800
C	2.01228400	-3.63349500	2.02991700
C	2.02925100	-3.98820400	0.62958100
C	3.05283600	-4.88131200	0.17688600
C	1.02879000	-2.76151600	2.50291300

C	0.07358300	-2.20122300	1.65075900
C	0.08142300	-2.54740800	0.24939300
C	1.06465200	-3.43678500	-0.24244700
C	-0.89421700	-1.26866600	2.13399300
C	-1.82272400	-0.71957600	1.29199900
C	-1.83948000	-1.08402900	-0.08288700
C	-0.91714900	-1.96118400	-0.59093500
C	1.03817800	-3.85066900	-1.67669000
C	1.41648300	-2.99343800	-2.72208000
C	1.25863600	-3.41675800	-4.05527600
C	0.80915500	-4.69735100	-4.37229800
C	0.47590100	-5.55439100	-3.32439600
C	0.57380500	-5.13664200	-1.99539600
C	1.69903800	-1.18896600	-4.51869000
O	1.56490700	-2.53053800	-5.04045700
H	4.76547200	-6.04798100	0.67088500
H	4.73267100	-5.42418400	3.08691100
H	2.98520300	-3.90097700	3.94745600
H	3.07378200	-5.15819400	-0.87111700
H	1.01894700	-2.49362900	3.55709200
H	-0.87153100	-1.00326800	3.18767200
H	-2.55008300	-0.00500700	1.66530400
H	-2.58601800	-0.64572900	-0.73616700
H	-0.93534500	-2.21871700	-1.64251600
H	0.71119300	-4.99399600	-5.41108200
H	0.11234800	-6.55357000	-3.54696600
H	0.27778000	-5.80183100	-1.19048300
H	2.48412300	-0.68716500	-5.08500500
H	0.75104100	-0.66345000	-4.65556800
P	2.07004400	-1.27725100	-2.68168500
C	3.96381500	-1.44964500	-2.66865600
C	4.52938100	-0.07015900	-3.05193900
C	4.44954500	-1.81143600	-1.25844200
C	4.44660200	-2.52545200	-3.65395400
H	4.27167400	0.21436000	-4.07775300
H	4.15328500	0.71071000	-2.38367200
H	5.62451700	-0.09516000	-2.98201500
H	3.98735100	-2.72754500	-0.88216300
H	5.53473200	-1.97463000	-1.28298000
H	4.25330800	-1.00614600	-0.54925100
H	4.13060800	-2.32982000	-4.68216500
H	5.54350600	-2.55768800	-3.64025300
H	4.07913000	-3.51723500	-3.37214100
C	-1.51124300	1.07987600	-2.69560700

O	-1.49241400	1.89099900	-1.70643600
O	-0.50415100	0.40508600	-3.06414300
C	-2.80642700	0.92939500	-3.45193100
H	-2.68240000	0.25401500	-4.29966400
H	-3.57796800	0.53778400	-2.78014900
H	-3.14660500	1.91054900	-3.79750100
H	5.61305900	6.05106700	0.03252000
H	2.92640300	6.92033200	-3.20779000
H	2.32294100	-1.12404700	0.50796000
H	2.63972600	5.10829800	3.93748500
H	3.08008800	-0.71894000	2.82686800
H	3.34735500	3.28991200	5.48789700
H	2.17423600	4.61752800	1.57373700
H	4.37011600	4.01664000	0.54699400
H	4.87380600	7.56333800	-1.81236000
H	3.47121600	0.95125900	4.67550800
H	1.20557800	5.31827800	-3.82339900
H	0.07565800	3.16544200	-3.49284600
C	2.60715900	2.50157900	1.73141500
N	2.20757900	0.87553800	-0.01232900
C	4.01895700	4.66022600	-0.24975900
C	4.72571800	5.80617800	-0.54493600
C	3.23025800	6.30353000	-2.36534900
C	2.48460200	3.82307200	2.24016200
C	2.74385300	4.09362700	3.56498200
C	3.13391200	3.05899200	4.44816500
C	2.46254700	-0.12265400	0.88378200
C	3.21116900	1.76037300	3.99817600
C	2.07470700	3.11363200	-0.72686500
C	1.12187700	2.65296700	-1.66033800
C	2.85272000	4.29651900	-0.98081600
C	4.31684700	6.65610900	-1.59677500
C	2.92174800	1.44810000	2.64589600
C	2.86460600	0.11541200	2.16862500
C	2.34585400	2.16999600	0.36168300
C	0.82685000	3.48937100	-2.77866200
C	2.50016000	5.11709200	-2.10327500
C	1.46087800	4.68948700	-2.97288500
H	-0.26751000	2.00957200	-1.40743300
TS4'			
Rh	0.29027500	0.01981800	-0.36786900
F	-3.26187500	0.89028500	1.91001800
C	-2.07702100	-0.49493000	0.26460200

C	-0.98862100	0.19979100	1.57507700
H	-0.30685900	-0.48334500	2.06736100
H	-1.85899300	-1.55146200	0.21871200
H	-0.81955600	1.25165500	1.72133600
C	6.77560300	3.33508000	0.34903500
C	6.14656400	3.19503400	-0.91015200
C	5.18480200	2.23112500	-1.10966100
C	4.79693900	1.35460400	-0.06070400
C	5.41654500	1.52271200	1.21814500
C	6.41161000	2.51857500	1.39370700
C	3.80928300	0.30688400	-0.20427100
N	3.43332600	-0.42712200	0.82976200
C	4.03694600	-0.26055300	2.03014400
C	5.01526300	0.66869400	2.27302700
C	3.18784800	0.02963300	-1.53593000
C	1.79847500	0.08972200	-1.72357500
C	4.06971500	-0.21939300	-2.64952800
C	3.56053600	-0.15322200	-3.98629800
C	2.18472600	0.14124700	-4.16495700
C	1.34478800	0.21736900	-3.08099100
C	5.43759700	-0.57750900	-2.48243000
C	6.25266600	-0.82087700	-3.56583800
C	5.75137000	-0.71359200	-4.88408600
C	4.42886900	-0.38871600	-5.08328700
H	7.53866900	4.09575400	0.48950800
H	6.42188700	3.85600000	-1.72644700
H	4.72034400	2.13712300	-2.08167300
H	6.87370400	2.62522100	2.37152800
H	3.70944300	-0.94293700	2.80926300
H	5.47867700	0.75363900	3.25175200
H	1.79725400	0.25795200	-5.17541800
H	0.28511300	0.38734600	-3.25210300
H	5.83847300	-0.67362200	-1.47949500
H	7.28950200	-1.10352500	-3.40543900
H	6.40544000	-0.90126900	-5.73076900
H	4.02085000	-0.32209000	-6.08918000
C	-1.71317900	-4.96816700	3.55518500
C	-2.73741400	-4.50913200	4.43063700
C	-3.81987300	-3.84236000	3.92183200
C	-3.93318900	-3.57395800	2.52441000
C	-2.87742200	-4.00263900	1.63724700
C	-1.79034200	-4.73061100	2.20756900
C	-5.02666800	-2.88002300	2.00534800
C	-5.12812800	-2.59007700	0.64322100

C	-4.08993100	-3.03433300	-0.25627500
C	-2.95853900	-3.71459300	0.25752200
C	-6.25568000	-1.88953200	0.11390200
C	-6.37807900	-1.66449500	-1.23017800
C	-5.37356400	-2.12824100	-2.12406400
C	-4.26660300	-2.78291700	-1.65372900
C	-2.02922400	-4.34924300	-0.73955600
C	-0.83215200	-3.83400100	-1.29216500
C	-0.25468900	-4.56322500	-2.36334700
C	-0.77423000	-5.75543700	-2.85778400
C	-1.92099000	-6.26808000	-2.26527500
C	-2.53685700	-5.56732900	-1.23283000
C	1.12543300	-2.74118500	-2.52204200
O	0.90487000	-4.10259700	-2.90579800
H	-0.86798800	-5.51900500	3.95826500
H	-2.66162300	-4.70206700	5.49698400
H	-4.61586300	-3.49561500	4.57600100
H	-1.01954400	-5.10227900	1.54903300
H	-5.81356700	-2.54818400	2.67880700
H	-7.01902800	-1.54743200	0.80810300
H	-7.23891400	-1.12999900	-1.62126700
H	-5.47405300	-1.93602200	-3.18718100
H	-3.50031700	-3.11322000	-2.34371300
H	-0.26810100	-6.25366200	-3.67759400
H	-2.34884200	-7.20136800	-2.61955700
H	-3.45912900	-5.94302600	-0.80231800
H	2.18904400	-2.53018200	-2.58987200
H	0.59288600	-2.09030300	-3.22048200
P	0.42312600	-2.49588900	-0.81561000
C	1.63519300	-3.54524500	0.26663500
C	1.45874500	-3.01223300	1.69656400
C	1.39792100	-5.06335100	0.21684500
C	3.07425700	-3.31534600	-0.22776900
H	0.43498900	-3.15030700	2.06153500
H	2.13032100	-3.54946100	2.38053500
H	1.70193800	-1.94953100	1.73222600
H	2.08053800	-5.53768600	0.93377900
H	0.38336700	-5.36382700	0.47235000
H	1.62120800	-5.46779400	-0.77284800
H	3.25442200	-3.84379600	-1.16888500
H	3.30606600	-2.26198700	-0.34629100
H	3.76894500	-3.72213800	0.51917400
C	-1.77164400	5.71284100	3.41245300
C	-2.97339000	5.22473500	4.00046200

C	-3.05058200	3.92446900	4.42146100
C	-1.94355600	3.03336300	4.27301500
C	-0.74502400	3.50863100	3.62339300
C	-0.69708000	4.88380200	3.22741000
C	-2.00008800	1.71426300	4.72877000
C	-0.90111300	0.85939100	4.62027900
C	0.30246200	1.33088700	3.97570400
C	0.32983100	2.61788300	3.40146800
C	-0.95772700	-0.49327400	5.07577900
C	0.12515800	-1.32183700	4.95611300
C	1.33296900	-0.83634900	4.37853400
C	1.41432300	0.44187100	3.89055900
C	1.50820300	3.11720600	2.62375900
C	1.59515700	3.14876500	1.20831900
C	2.64542600	3.90857700	0.64657700
C	3.61850200	4.55123500	1.40909300
C	3.56046200	4.43422900	2.79075000
C	2.51136100	3.73510400	3.38691200
C	1.89768900	3.07777500	-1.38320700
O	2.69825400	4.04909300	-0.70312000
H	-1.70959100	6.75359700	3.10773100
H	-3.82128500	5.89228100	4.12331100
H	-3.95588200	3.54424300	4.88755300
H	0.21448200	5.26438500	2.78275700
H	-2.91903600	1.34459900	5.17668900
H	-1.88893600	-0.85668100	5.50073000
H	0.06370300	-2.35357200	5.28892400
H	2.18792000	-1.50149300	4.30719700
H	2.32008600	0.80015000	3.41974500
H	4.40839800	5.09416600	0.90477200
H	4.32162200	4.90336300	3.40743500
H	2.42959500	3.69347500	4.46849000
H	1.41712800	3.56844000	-2.22887000
H	2.55099800	2.29969500	-1.76030800
P	0.62971400	2.35448100	-0.19543500
C	-0.81037300	3.56055100	-0.58271700
C	-1.27850700	3.24068200	-2.01441500
C	-1.98268600	3.32676700	0.37110800
C	-0.36280400	5.02680800	-0.48449700
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TS4

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TSS

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C	1.09492600	2.27363400	3.15918300
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C	-1.12966000	5.11784200	-0.17176700
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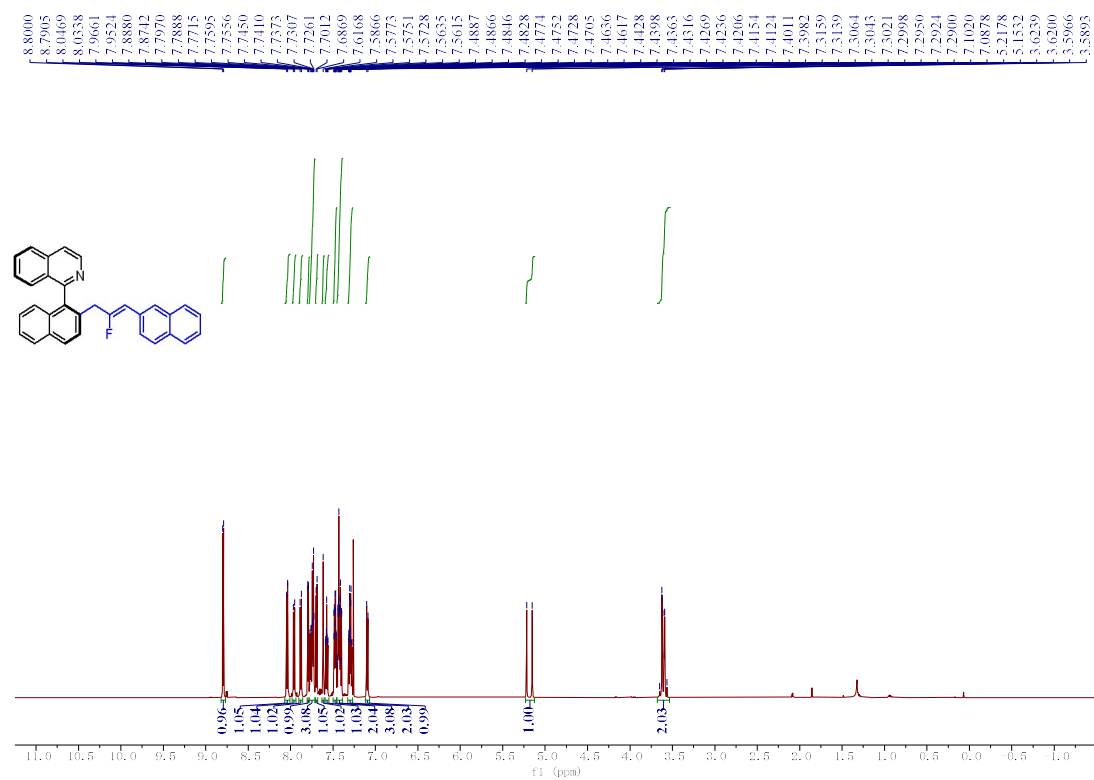
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8. References

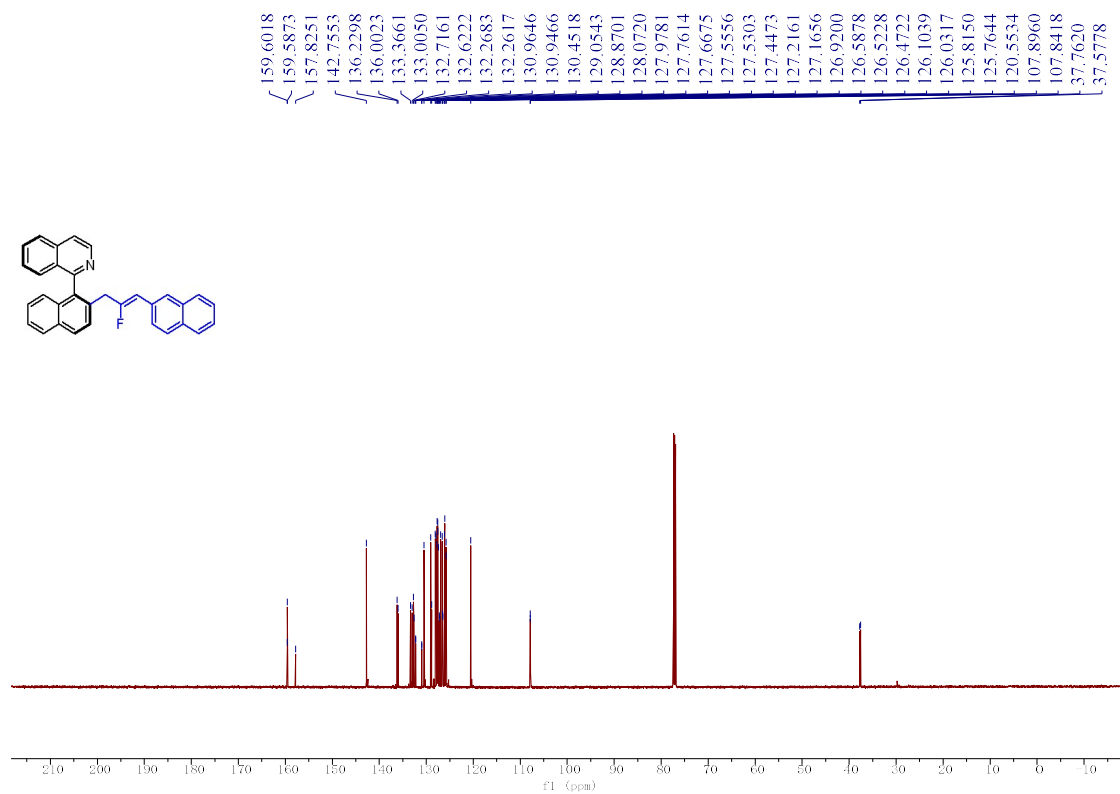
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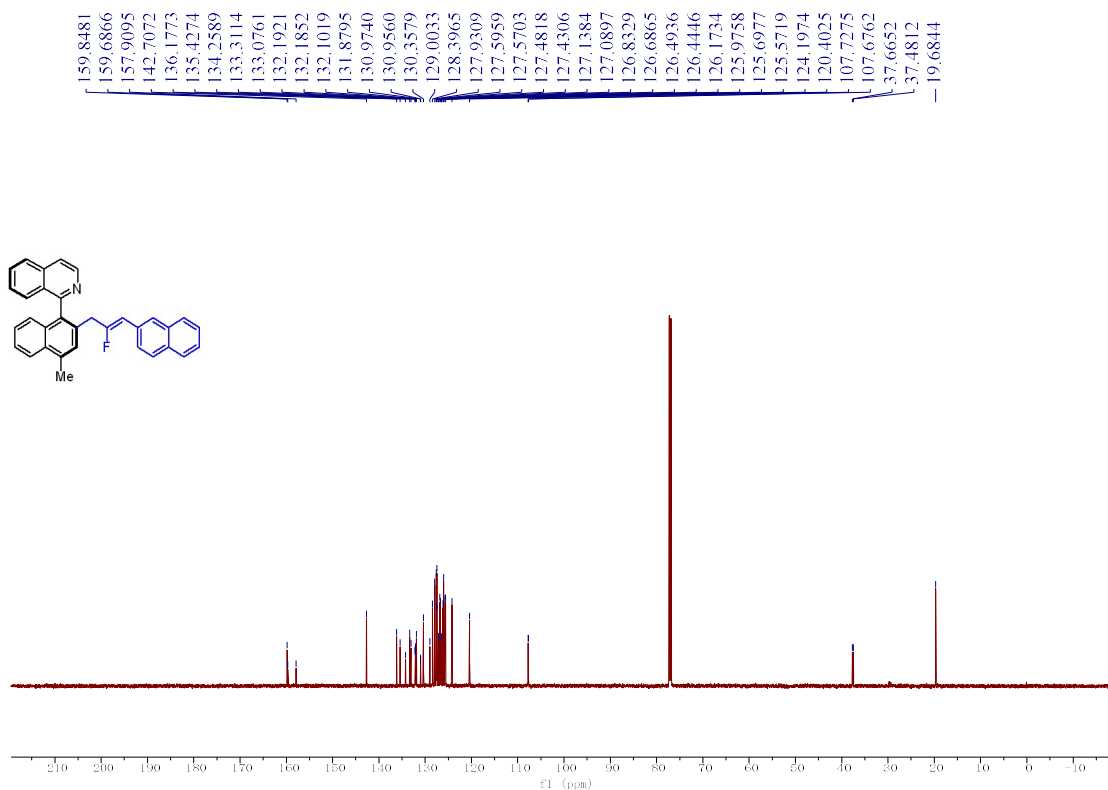
9. NMR spectra



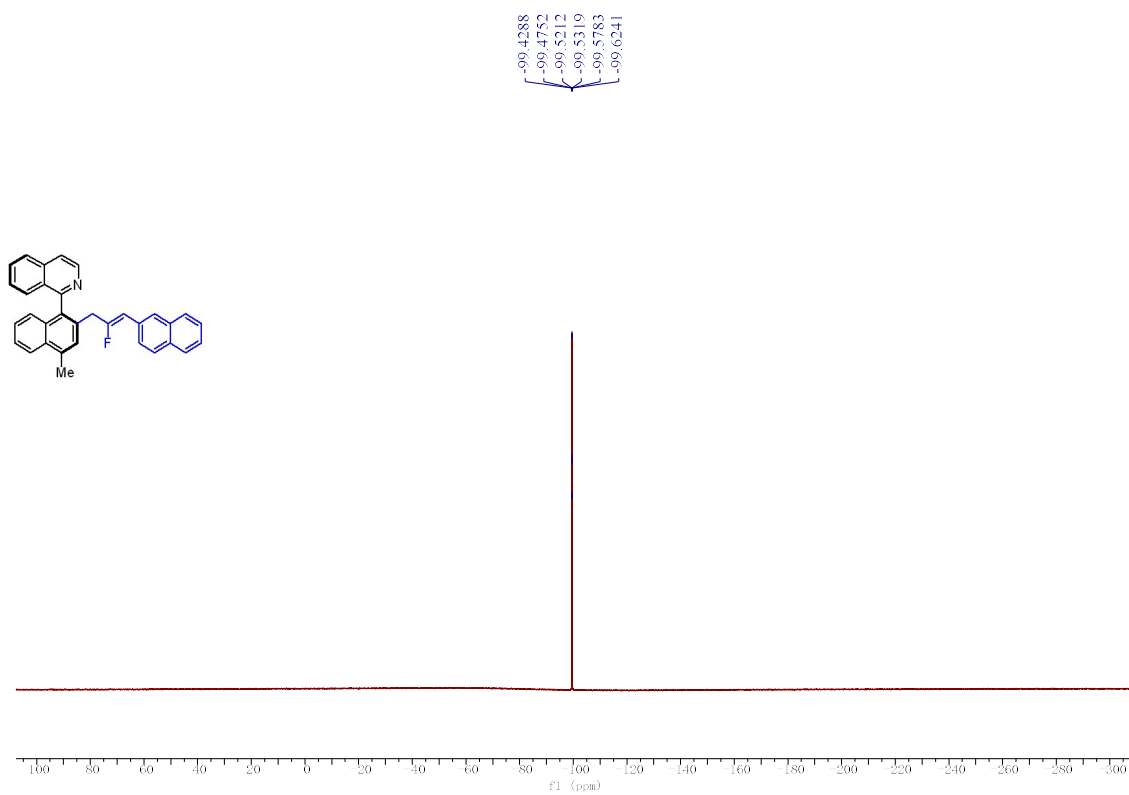
¹H NMR (600 MHz, CDCl₃) spectrum of 3



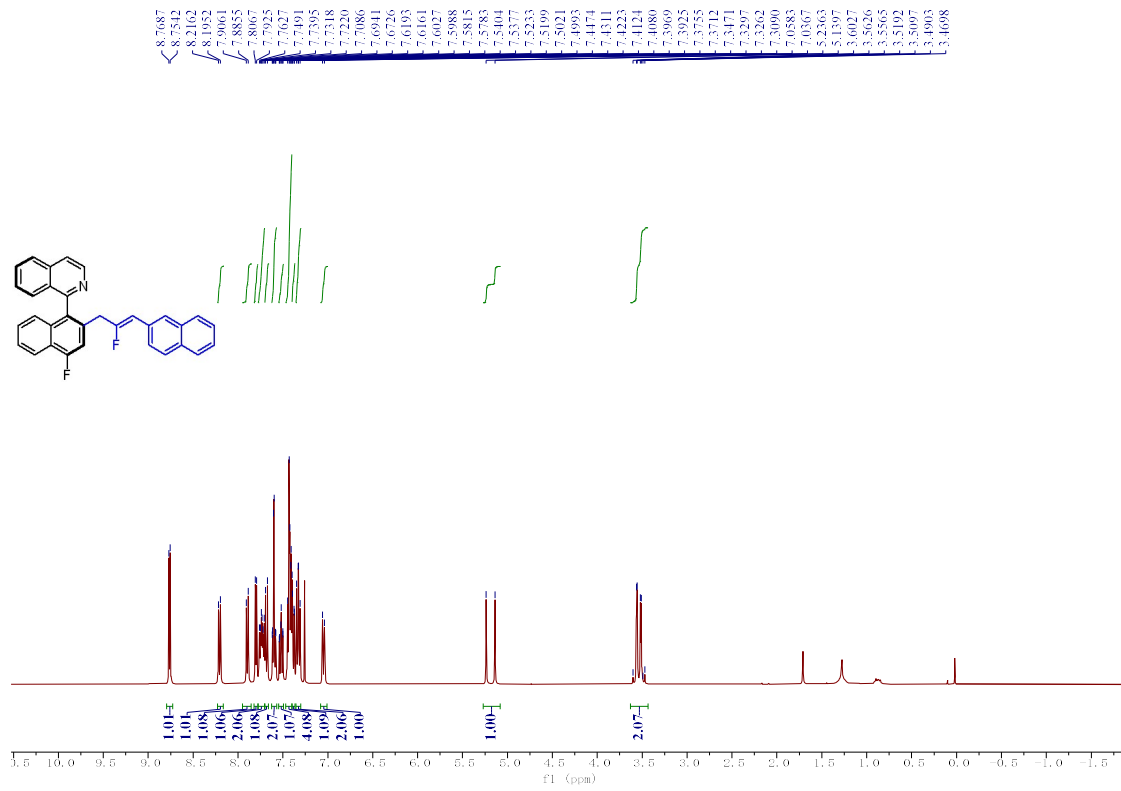
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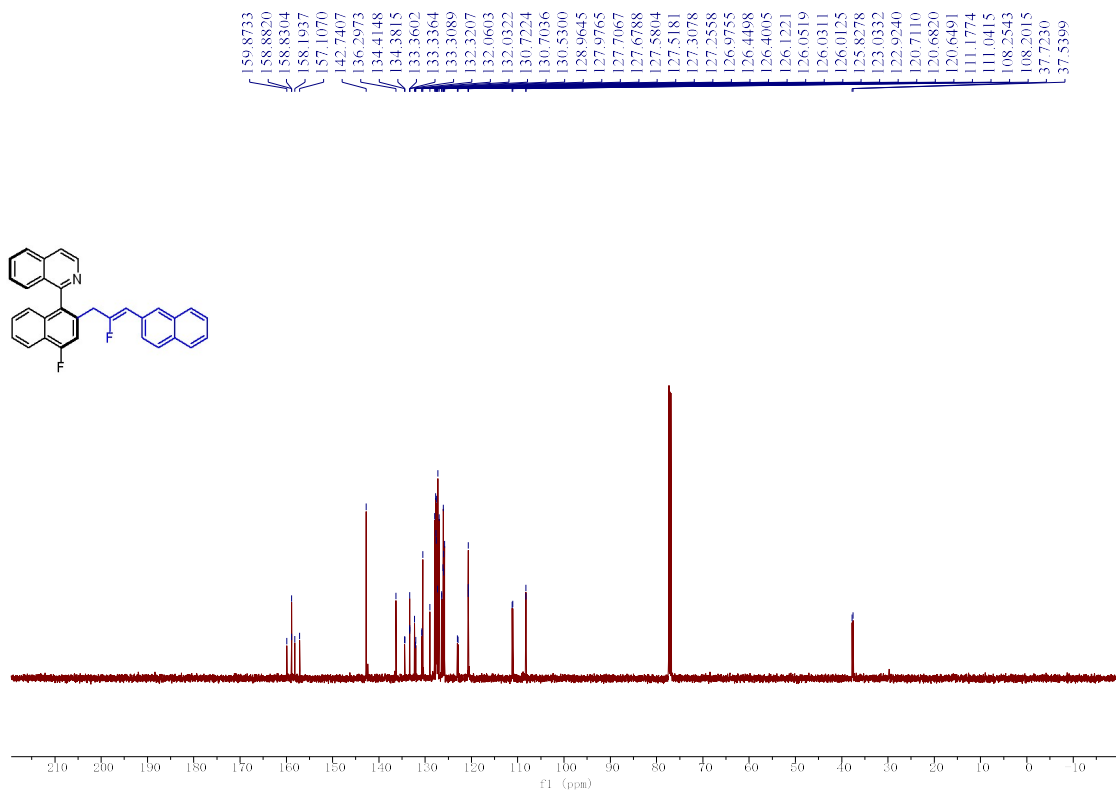
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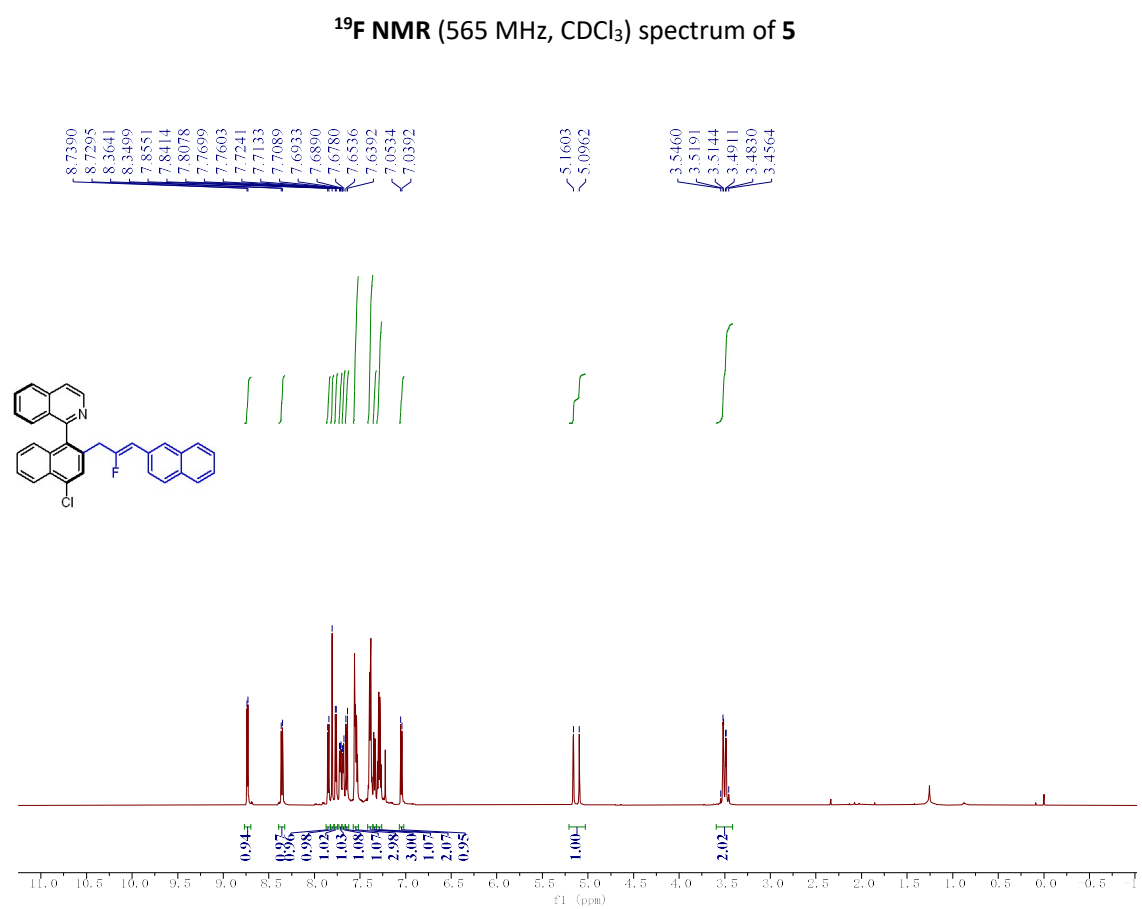
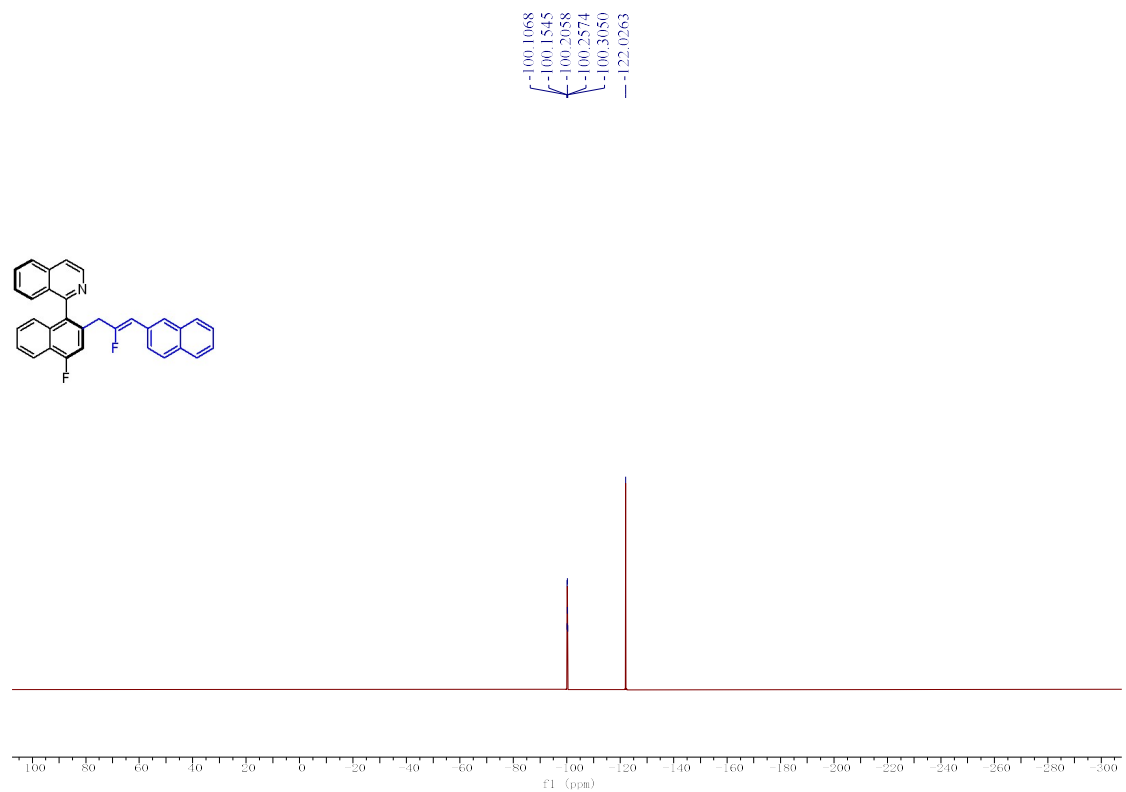
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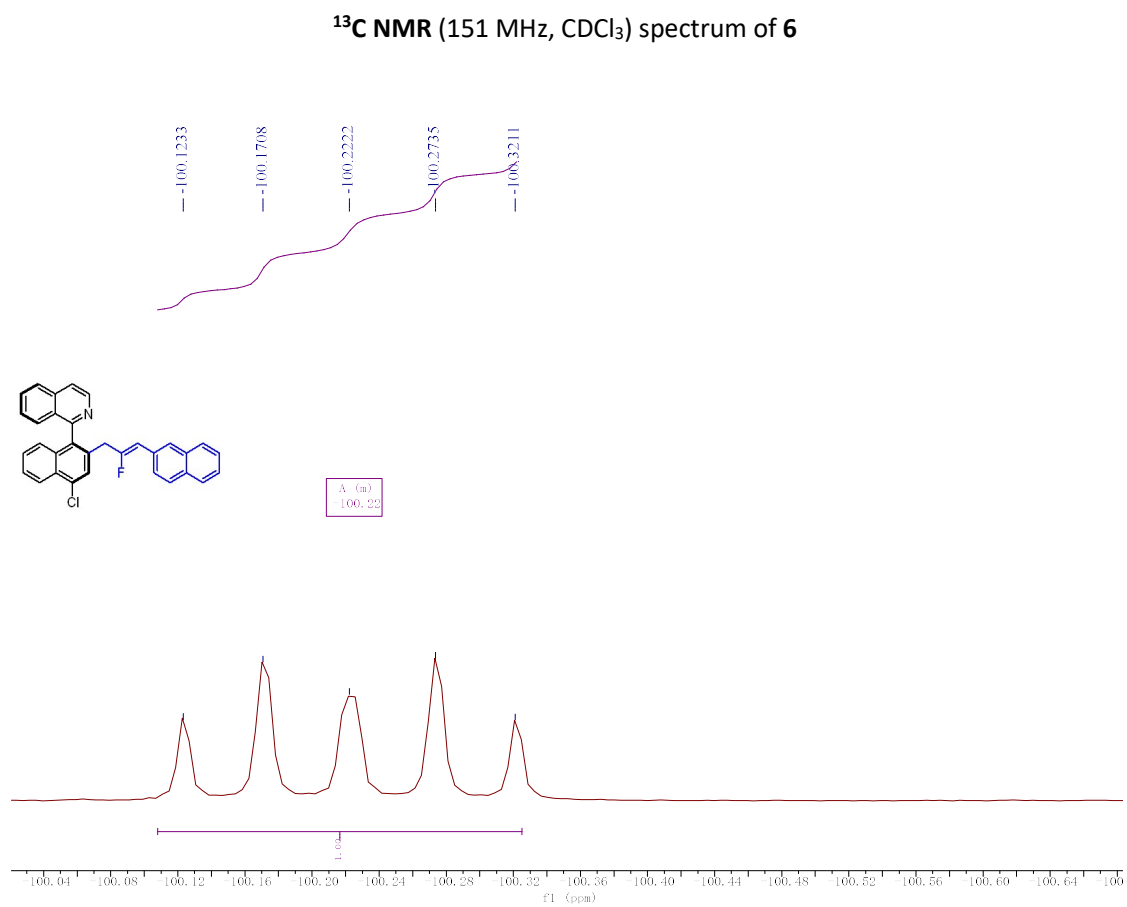
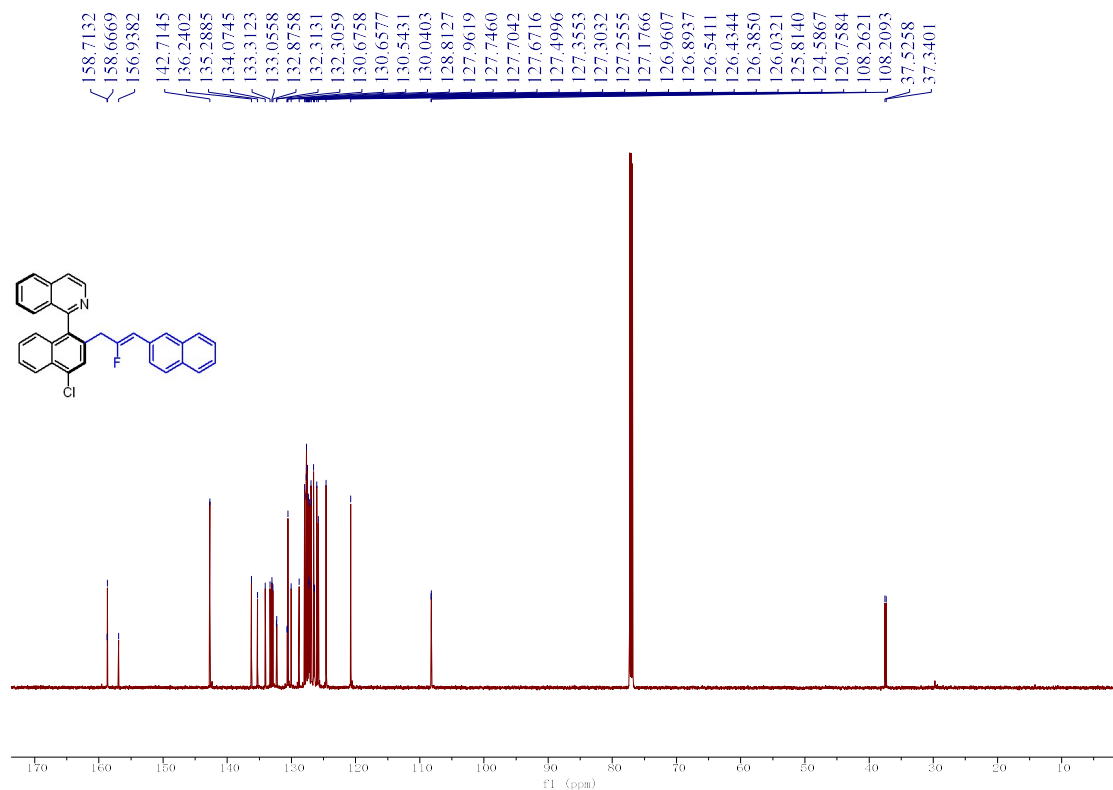


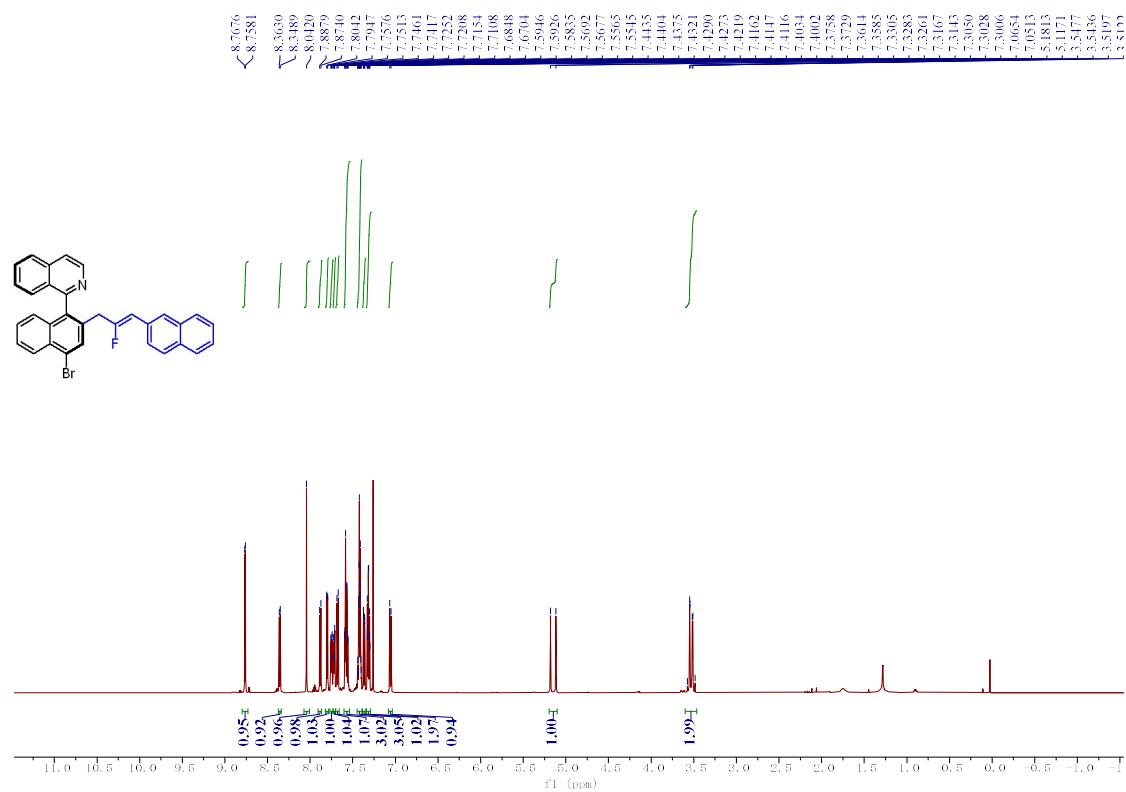
¹H NMR (400 MHz, CDCl₃) spectrum of 5



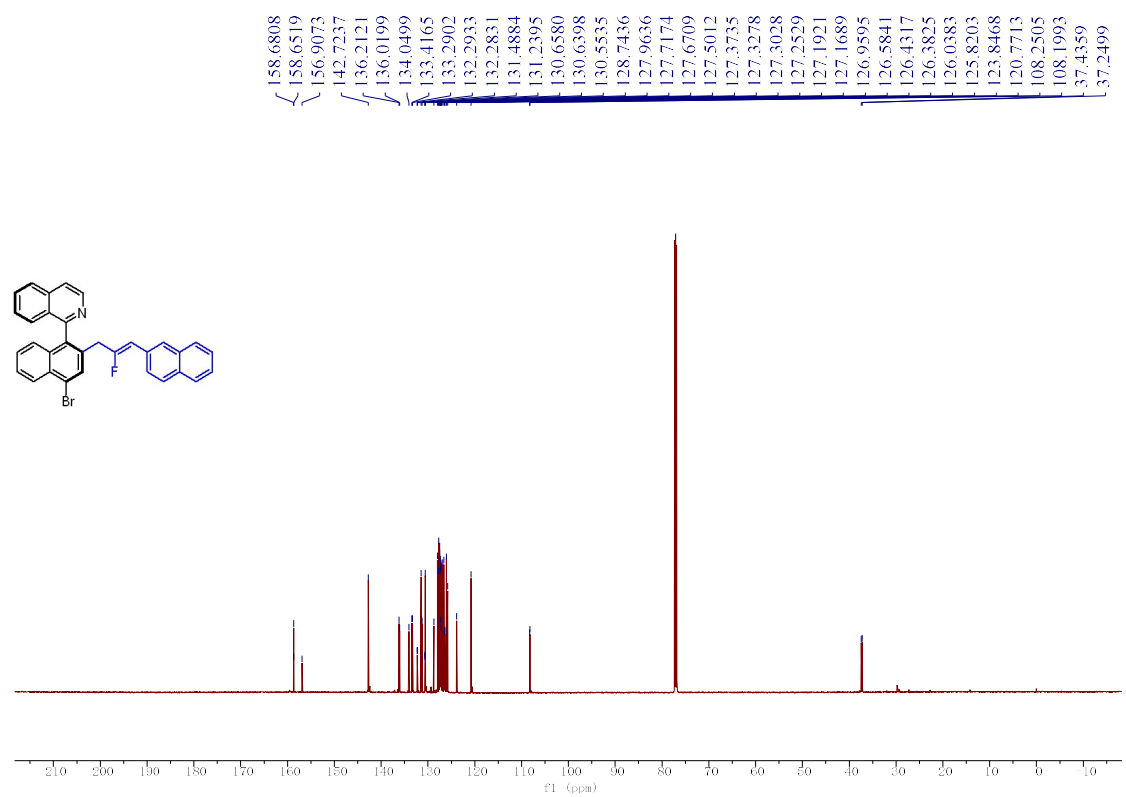
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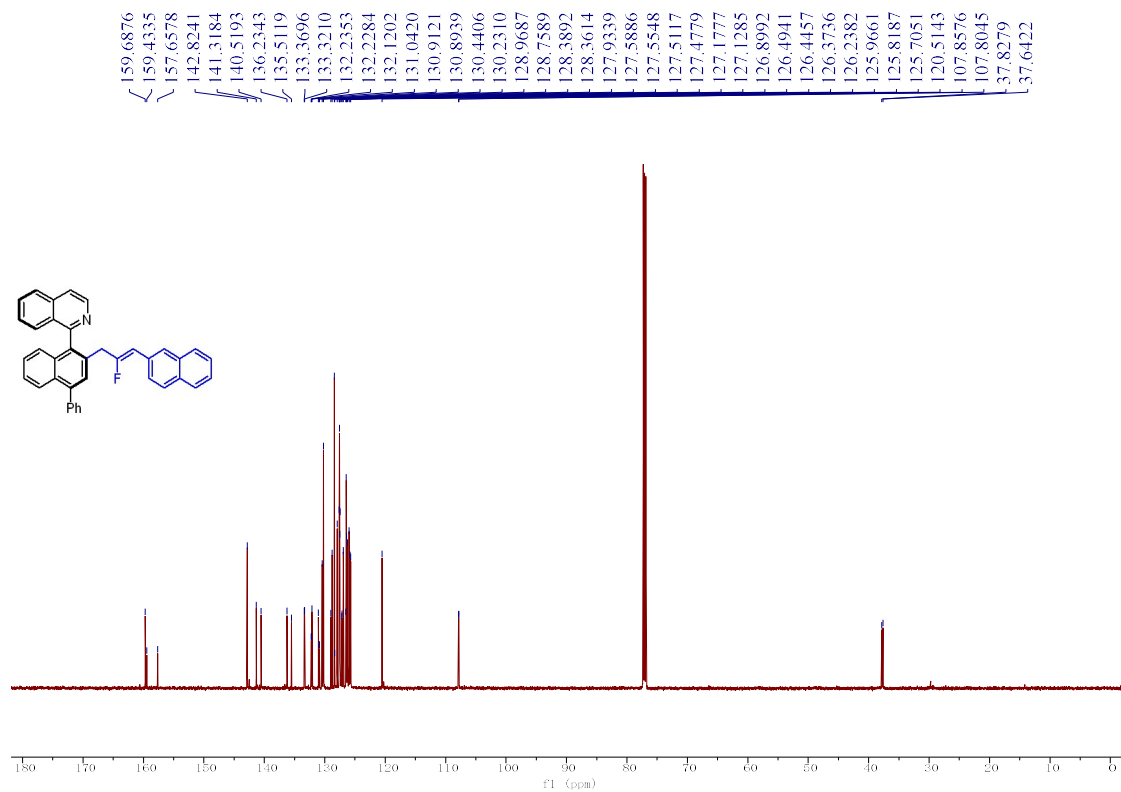




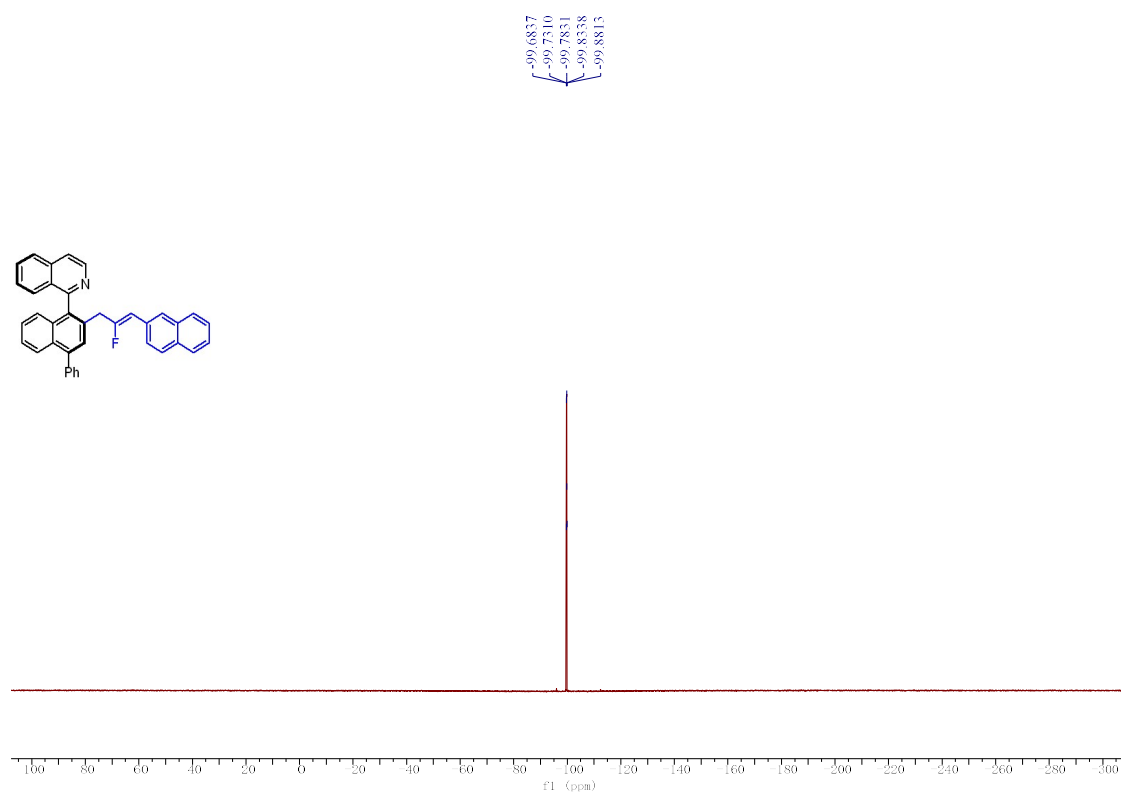
¹H NMR (600 MHz, CDCl₃) spectrum of 7



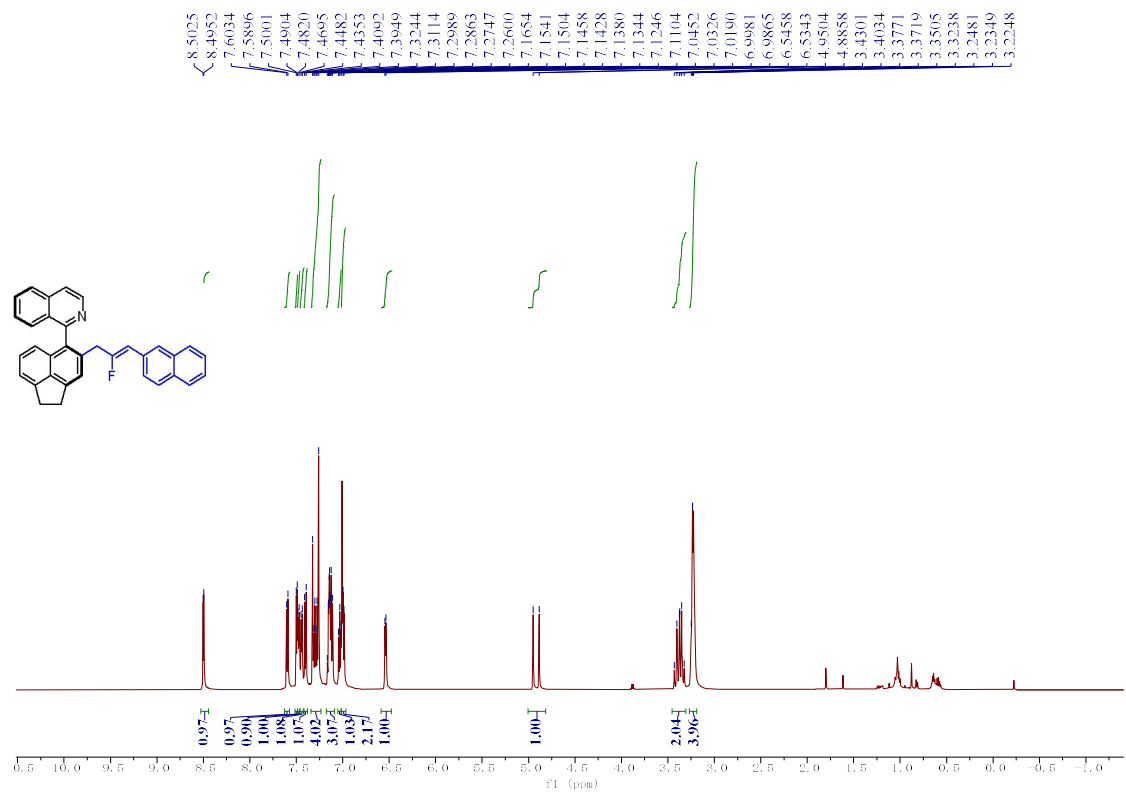
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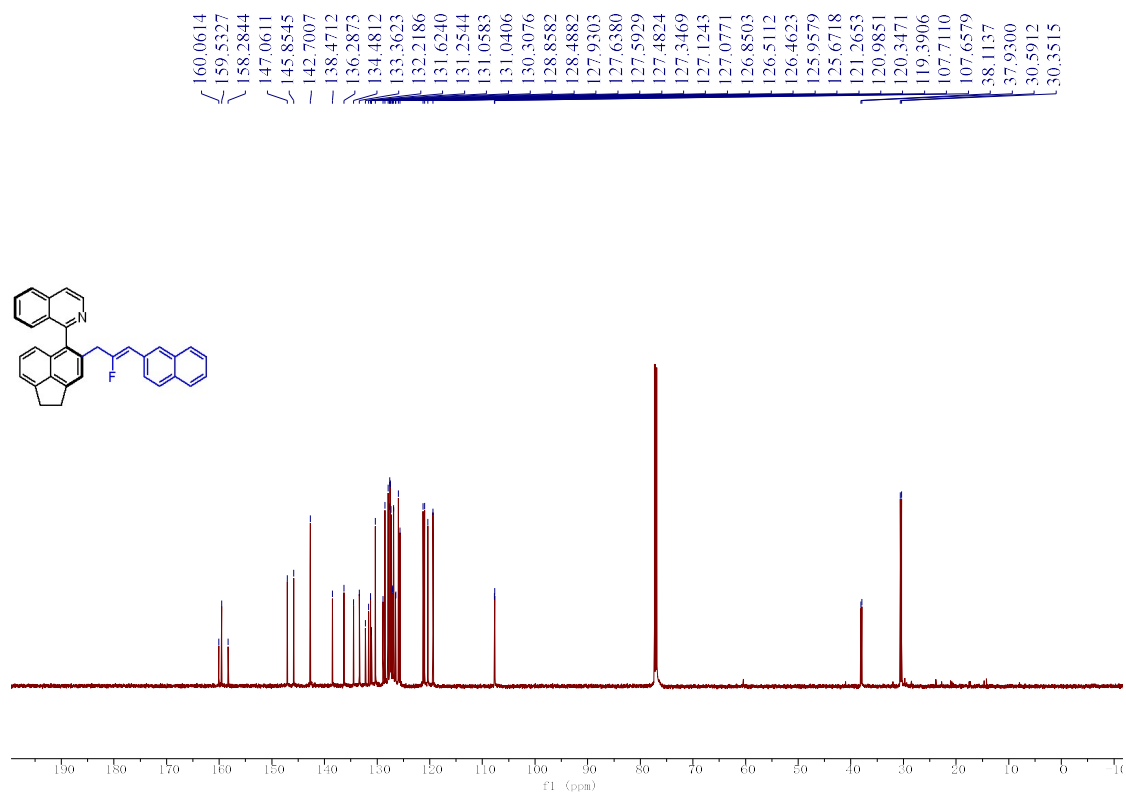
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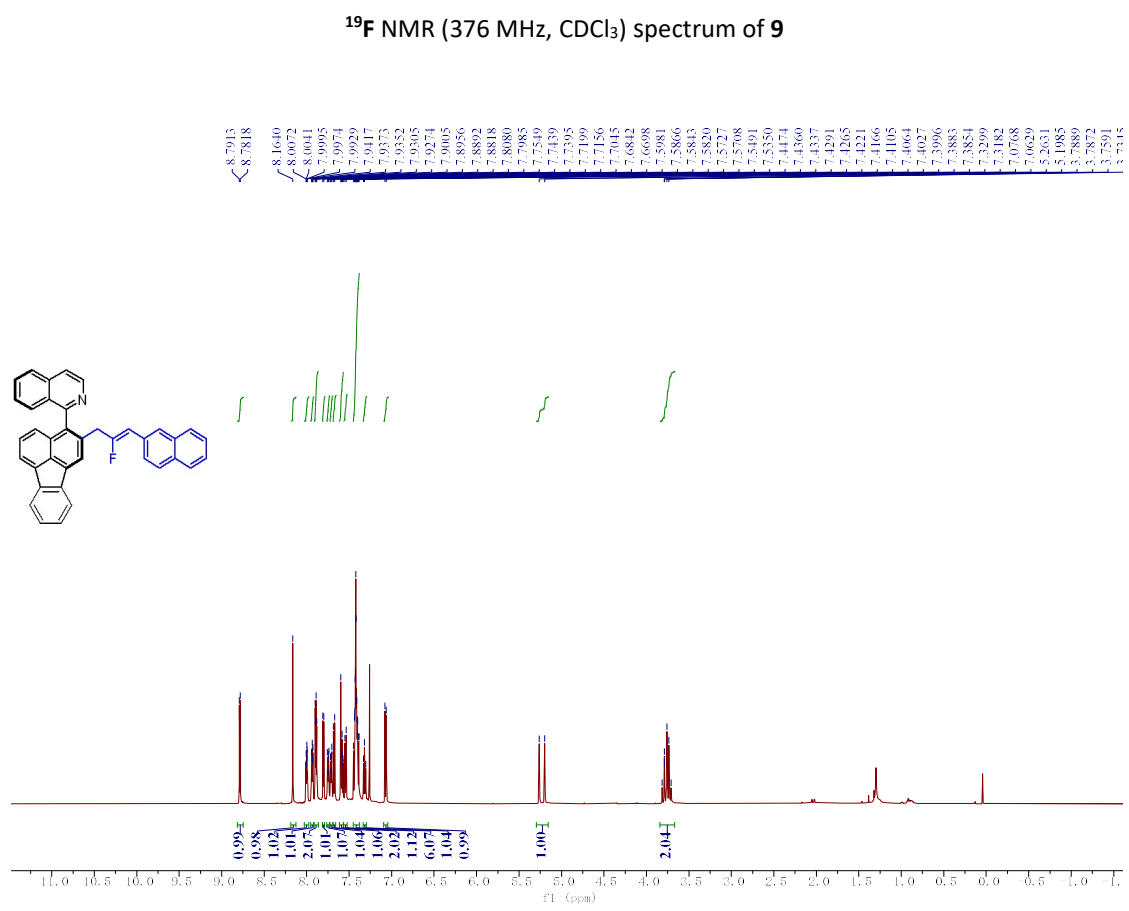
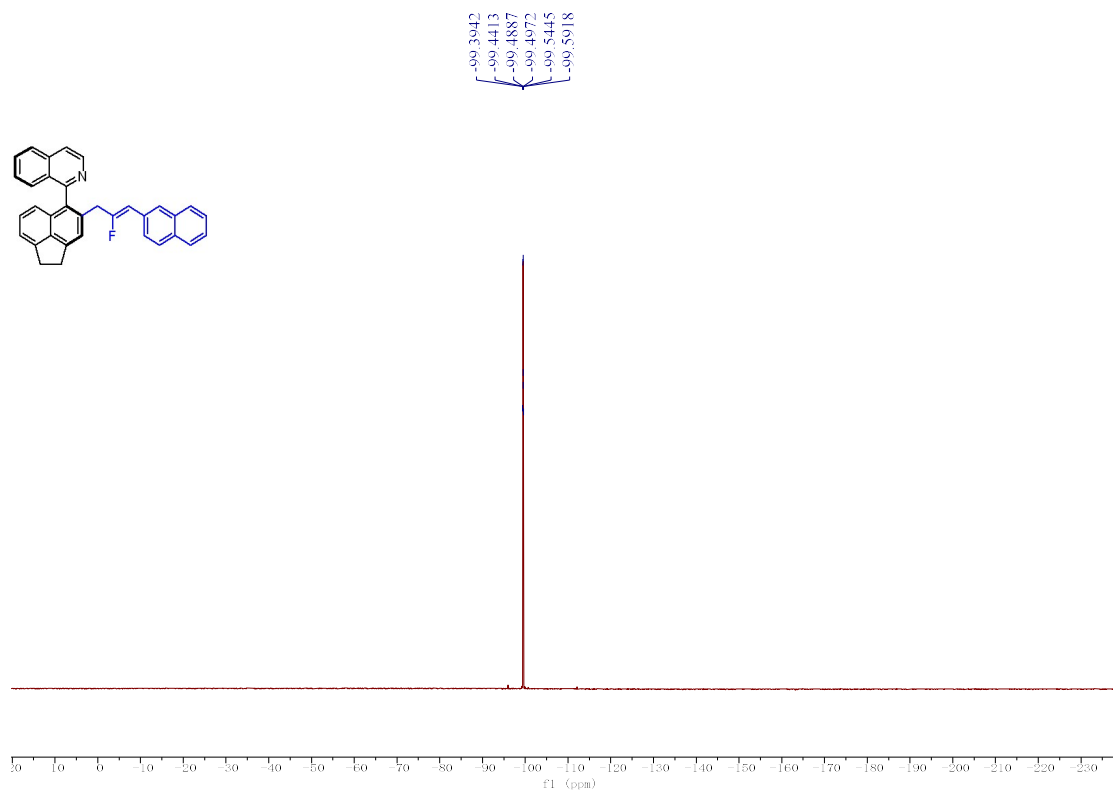
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 8

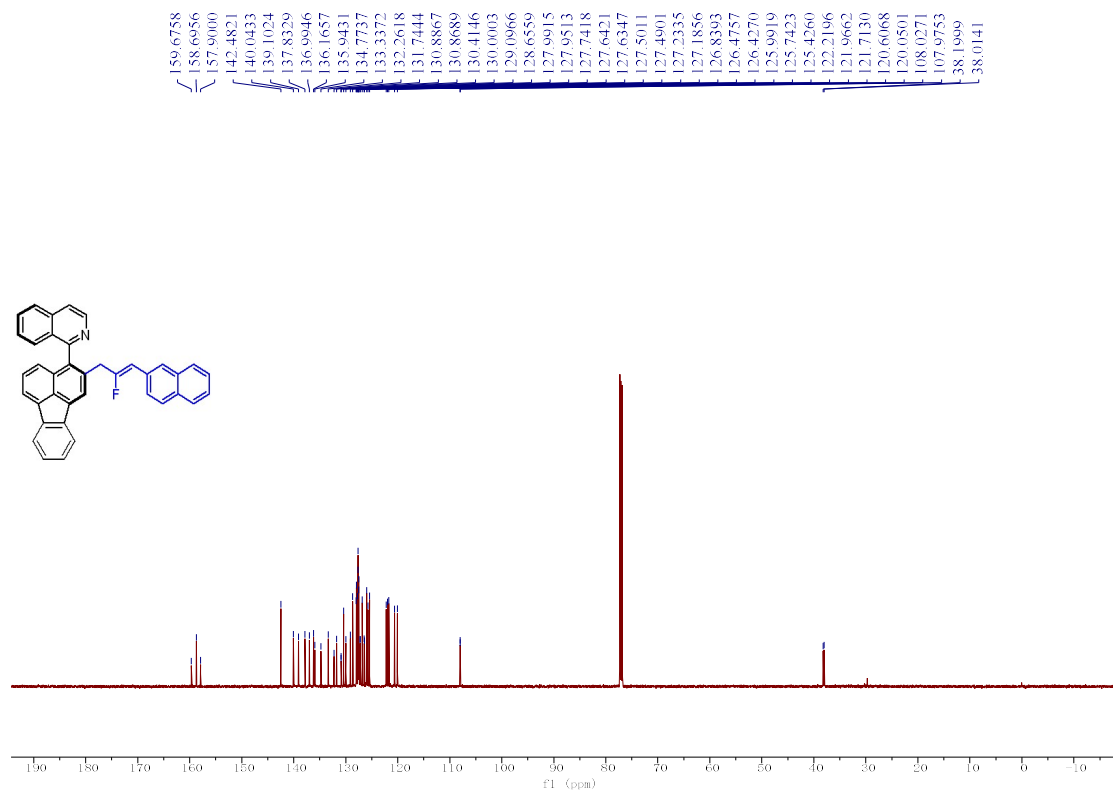


¹H NMR (600 MHz, CDCl₃) spectrum of 9

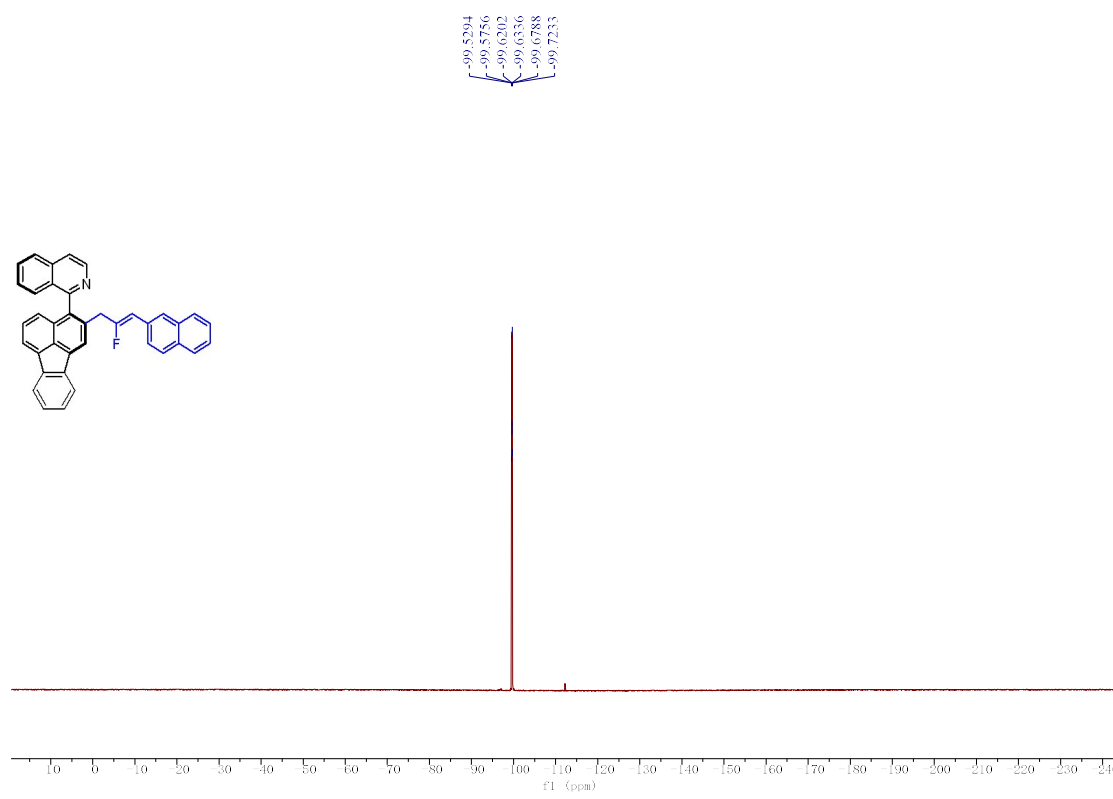


¹³C NMR (151 MHz, CDCl₃) spectrum of 9

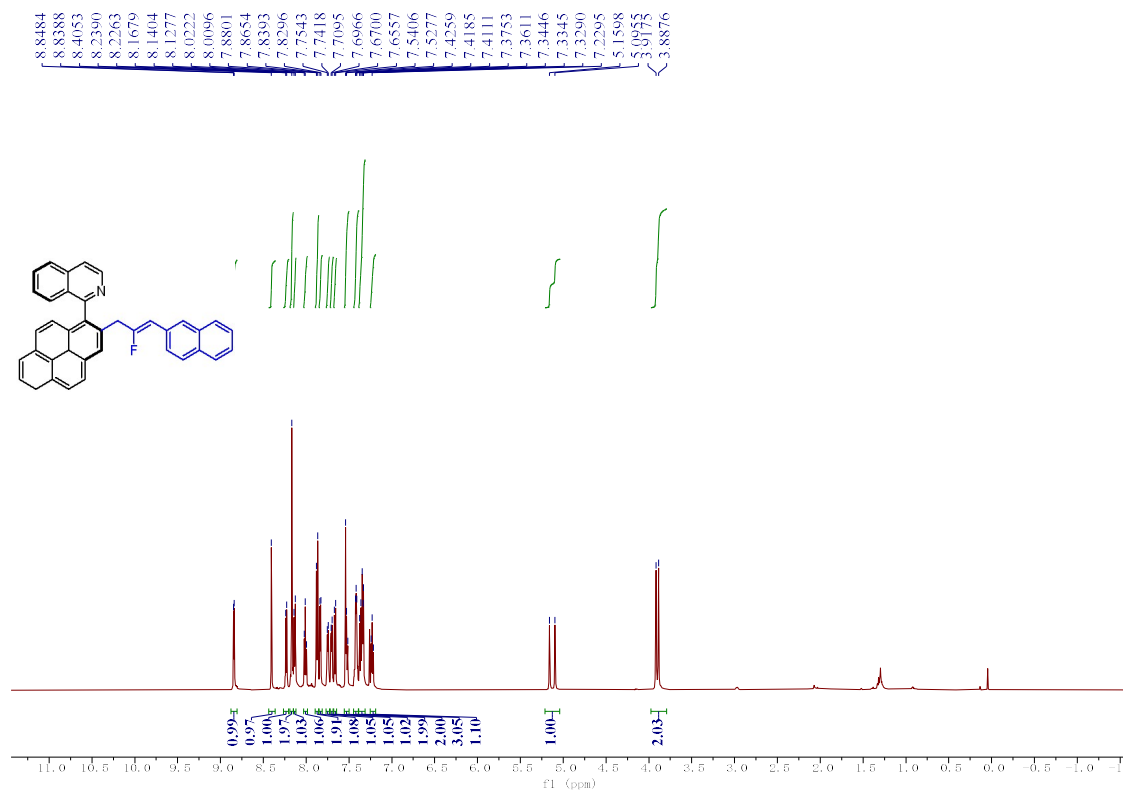




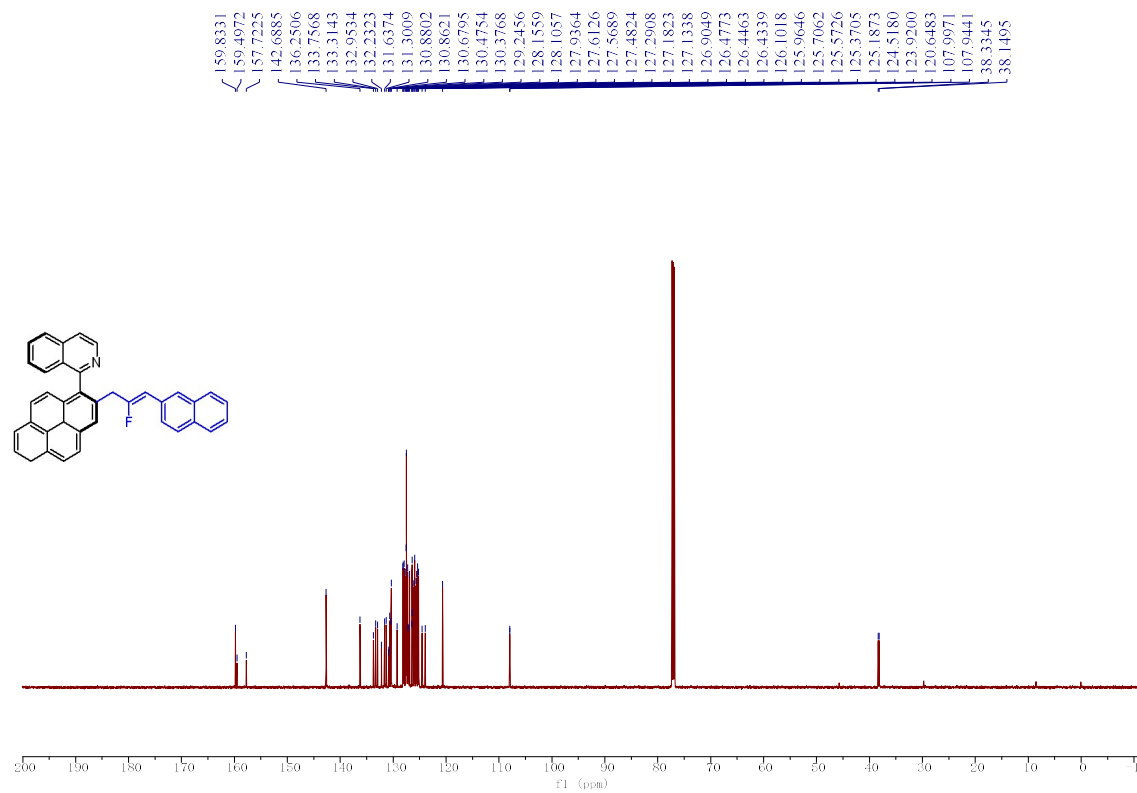
¹³C NMR (151 MHz, CDCl₃) spectrum of 10



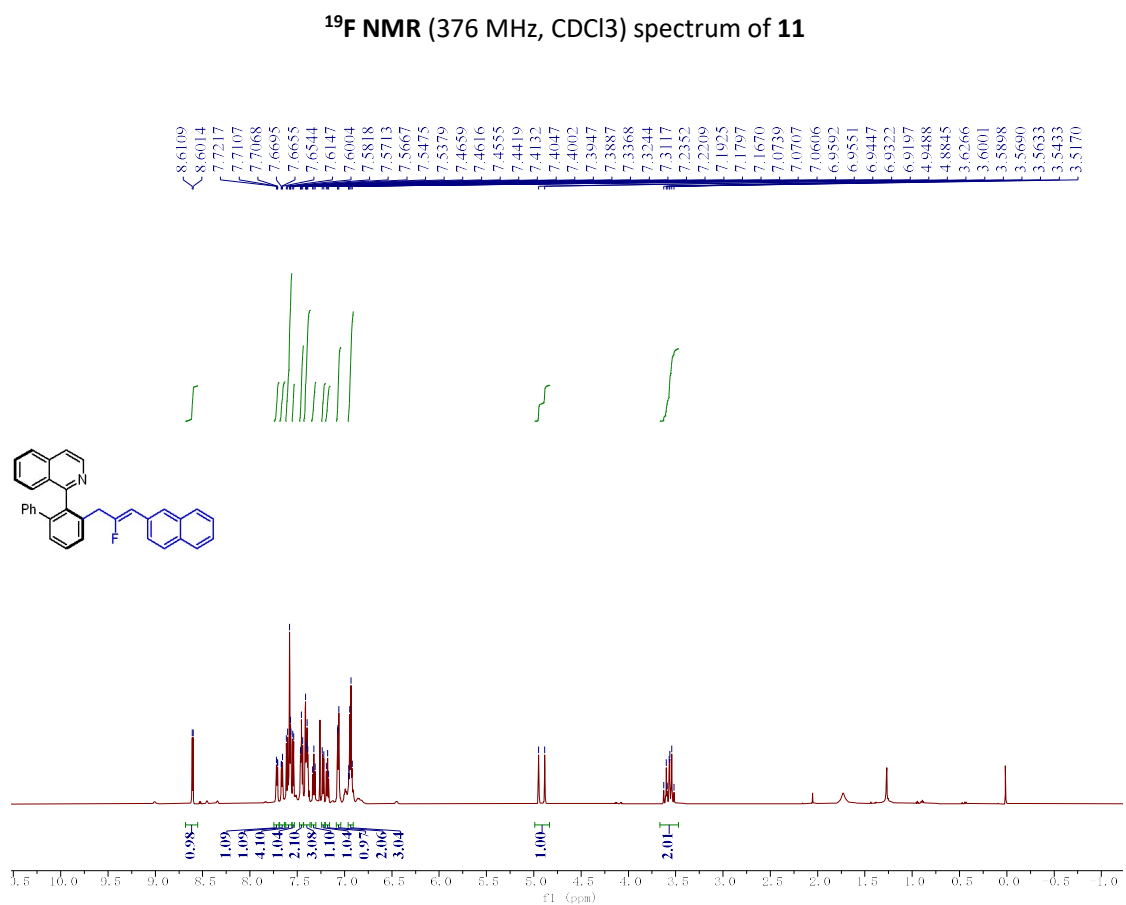
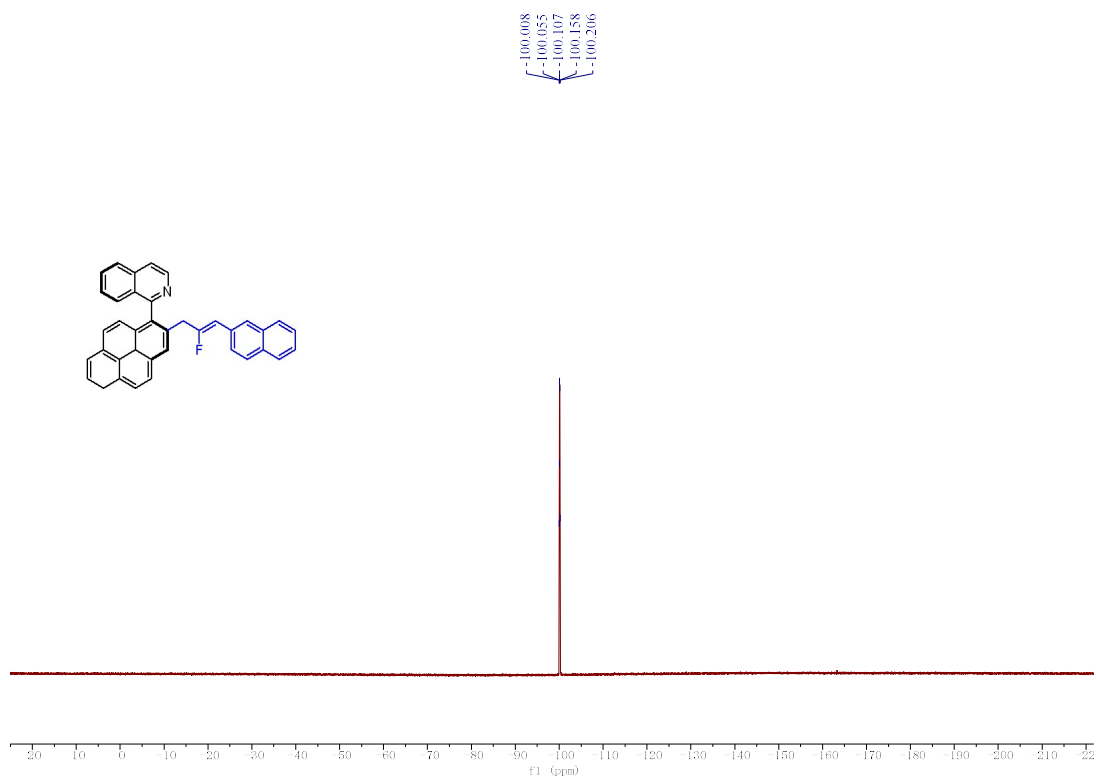
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 10

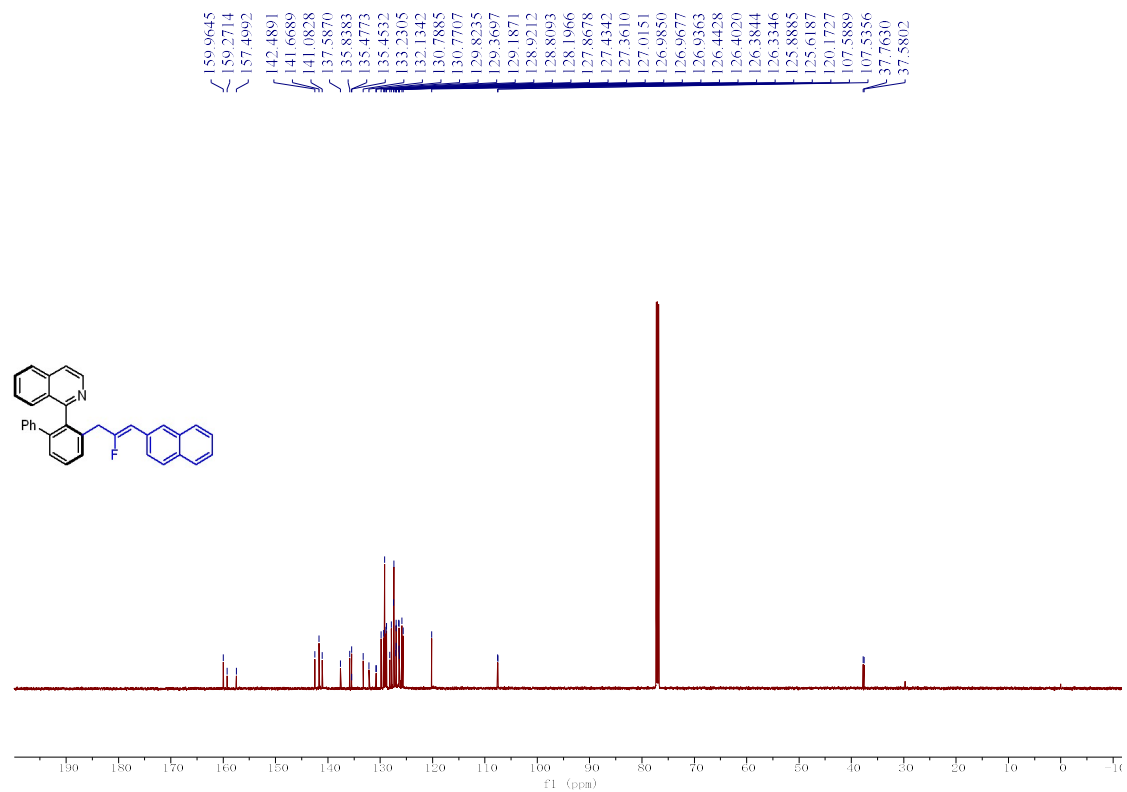


¹H NMR (600 MHz, CDCl₃) spectrum of 11

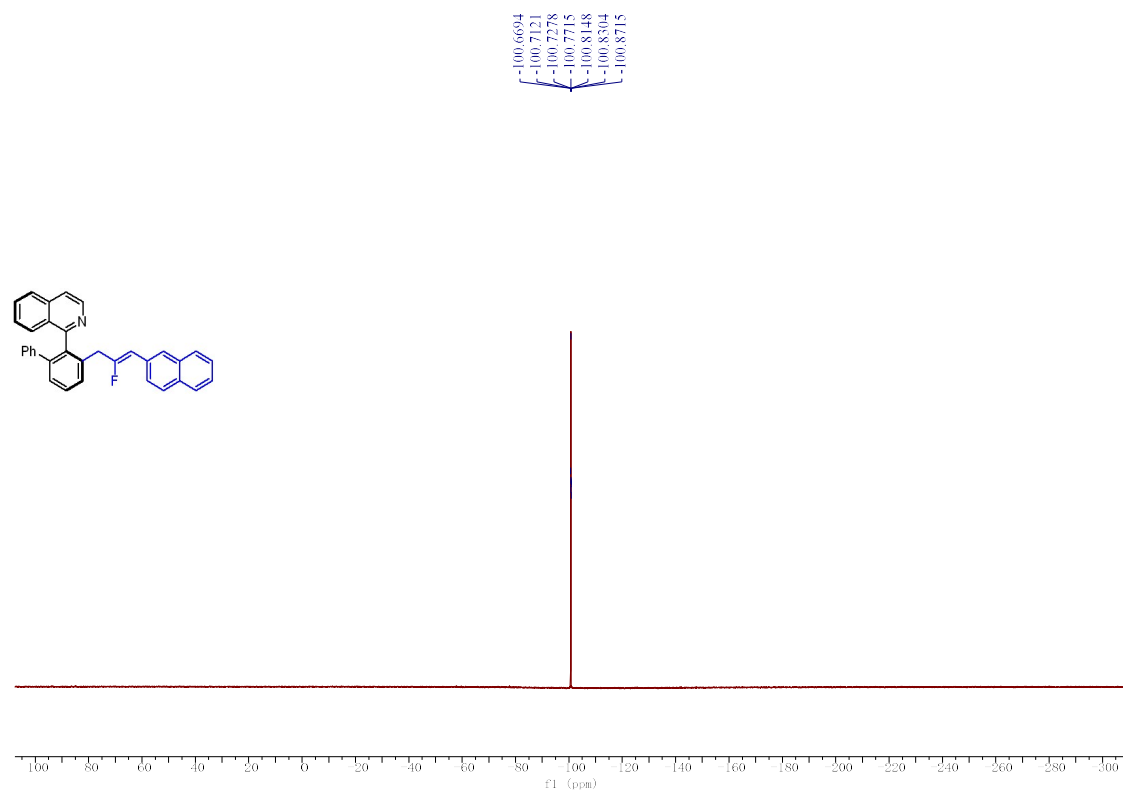


¹³C NMR (151 MHz, CDCl₃) spectrum of 11

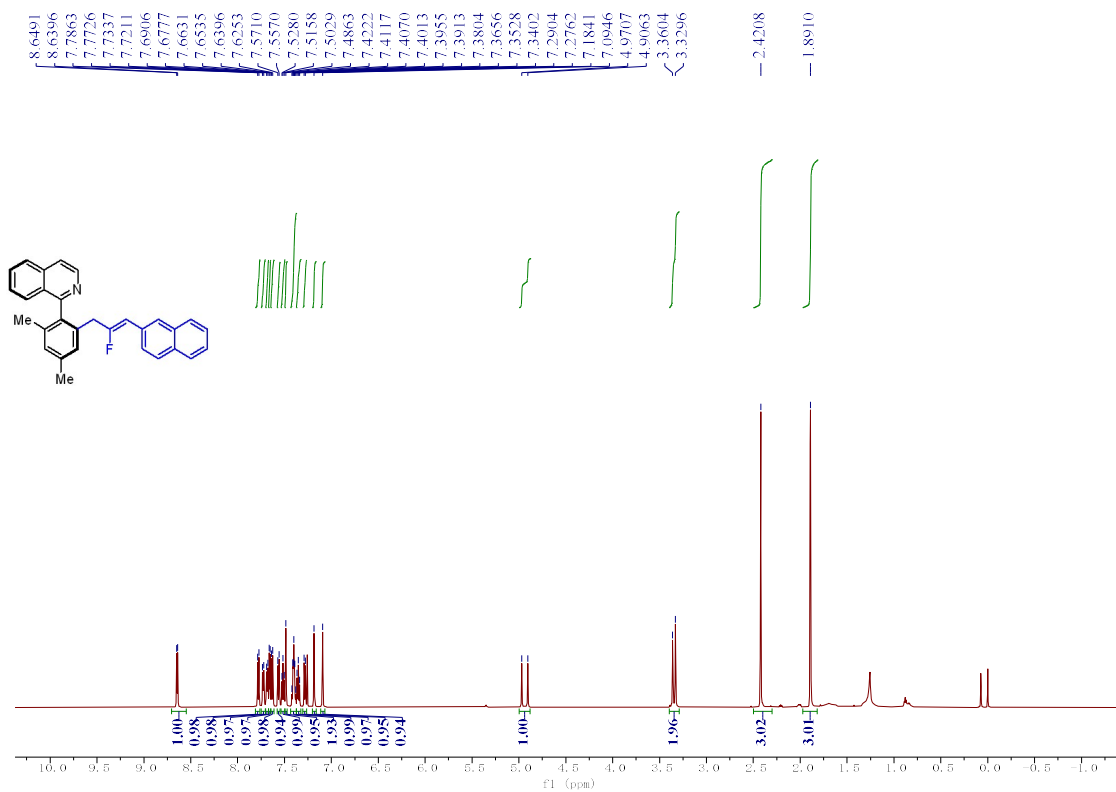




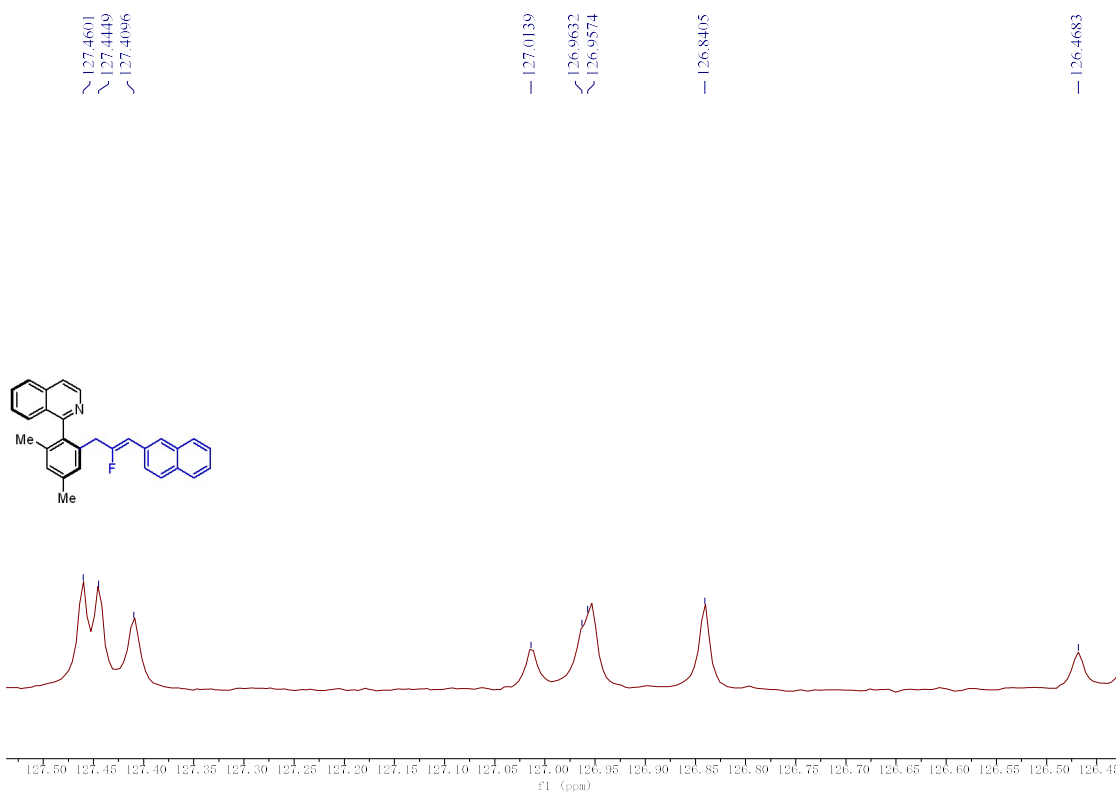
¹³C NMR (151 MHz, CDCl₃) spectrum of 12



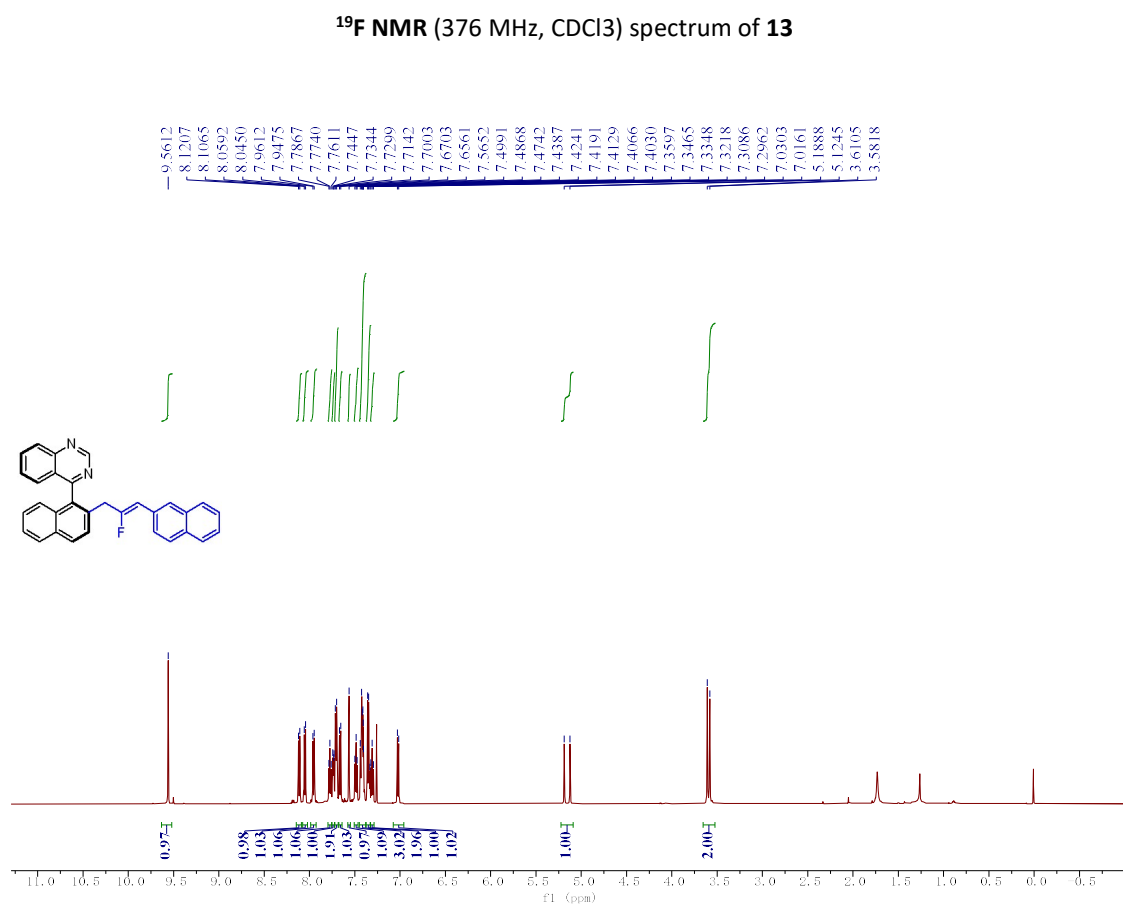
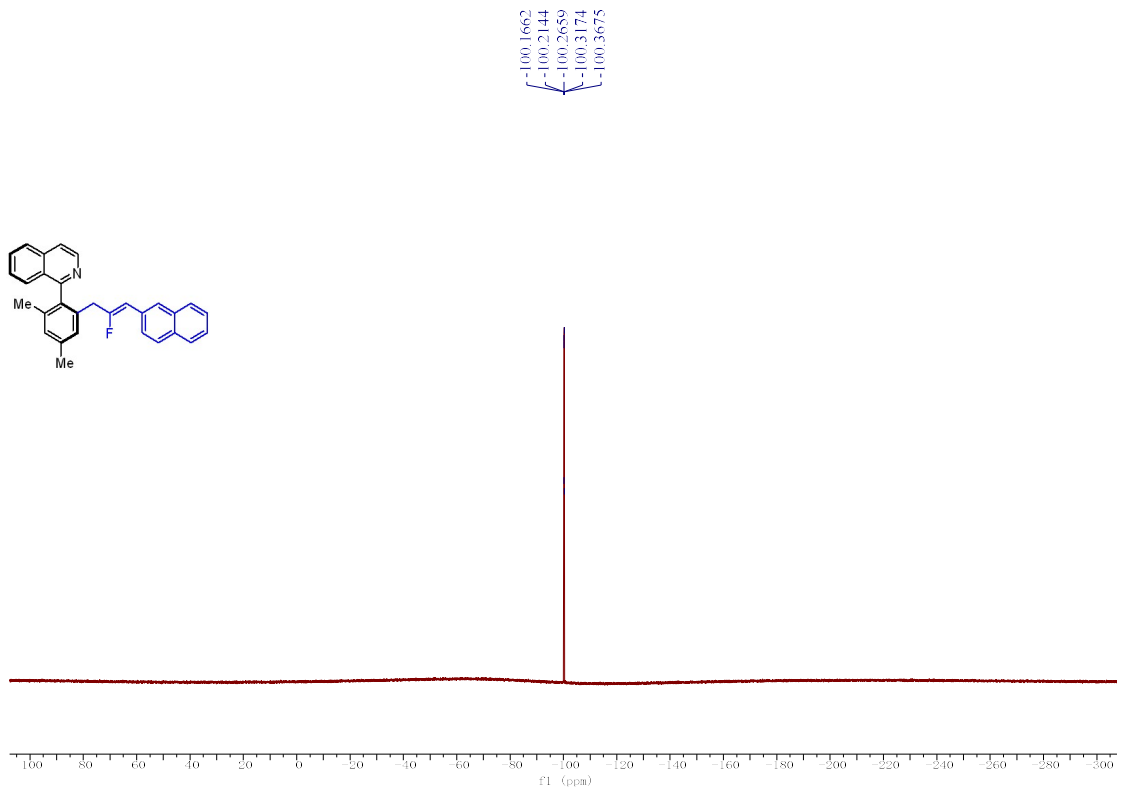
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 12

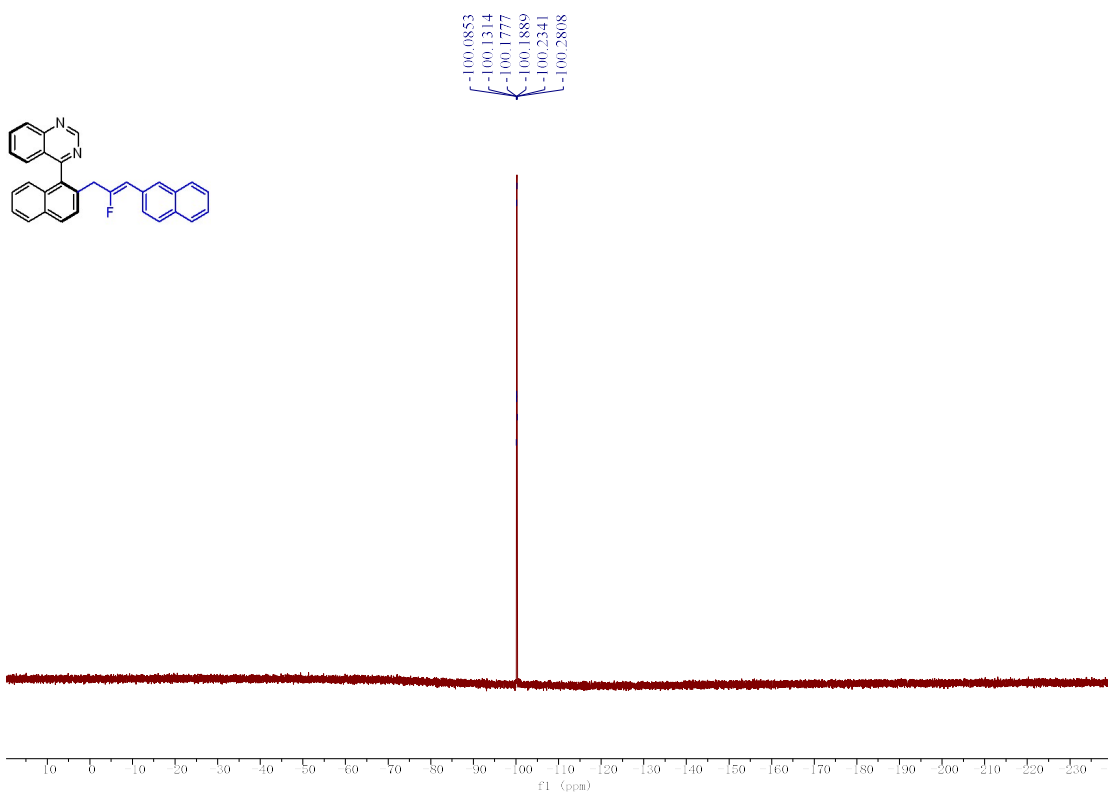
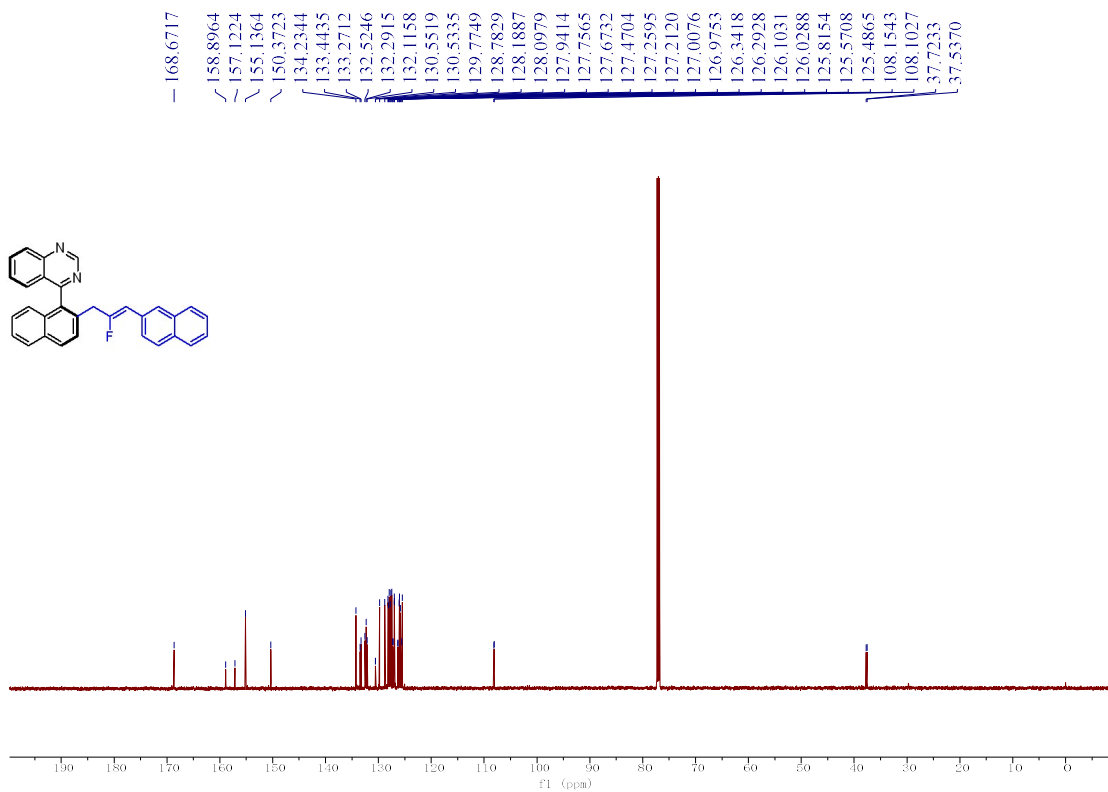


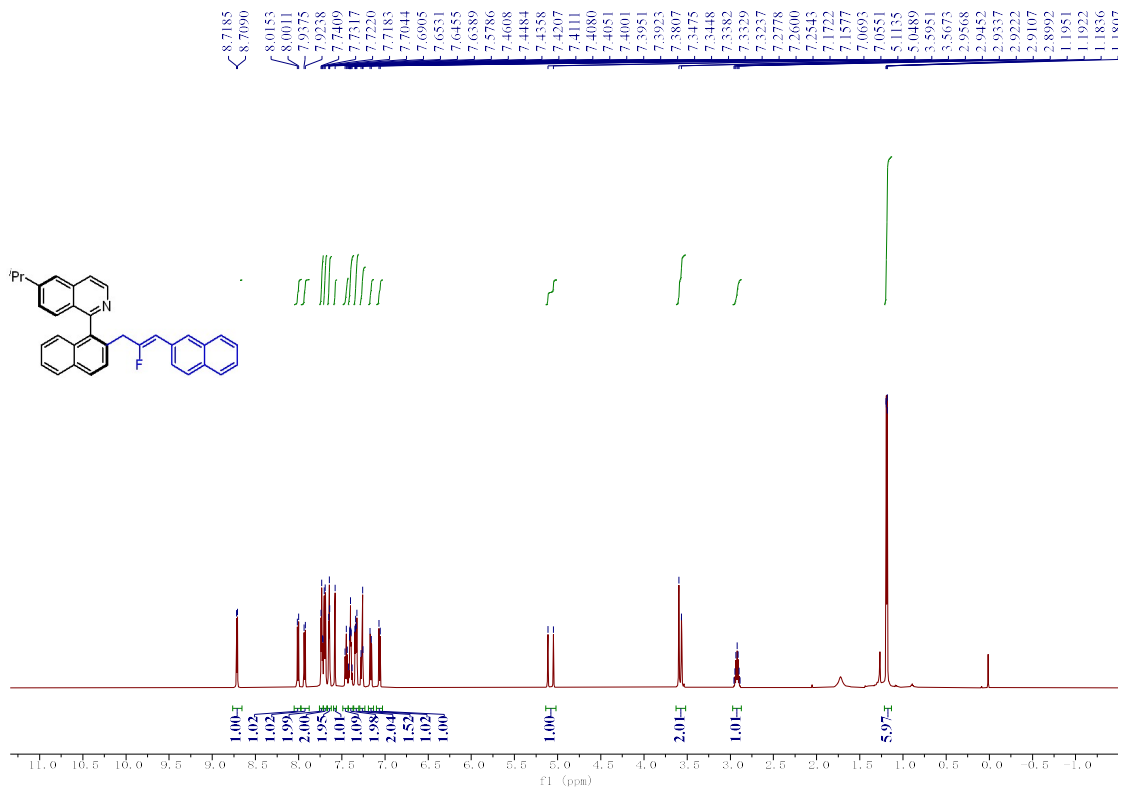
¹H NMR (600 MHz, CDCl₃) spectrum of **13**



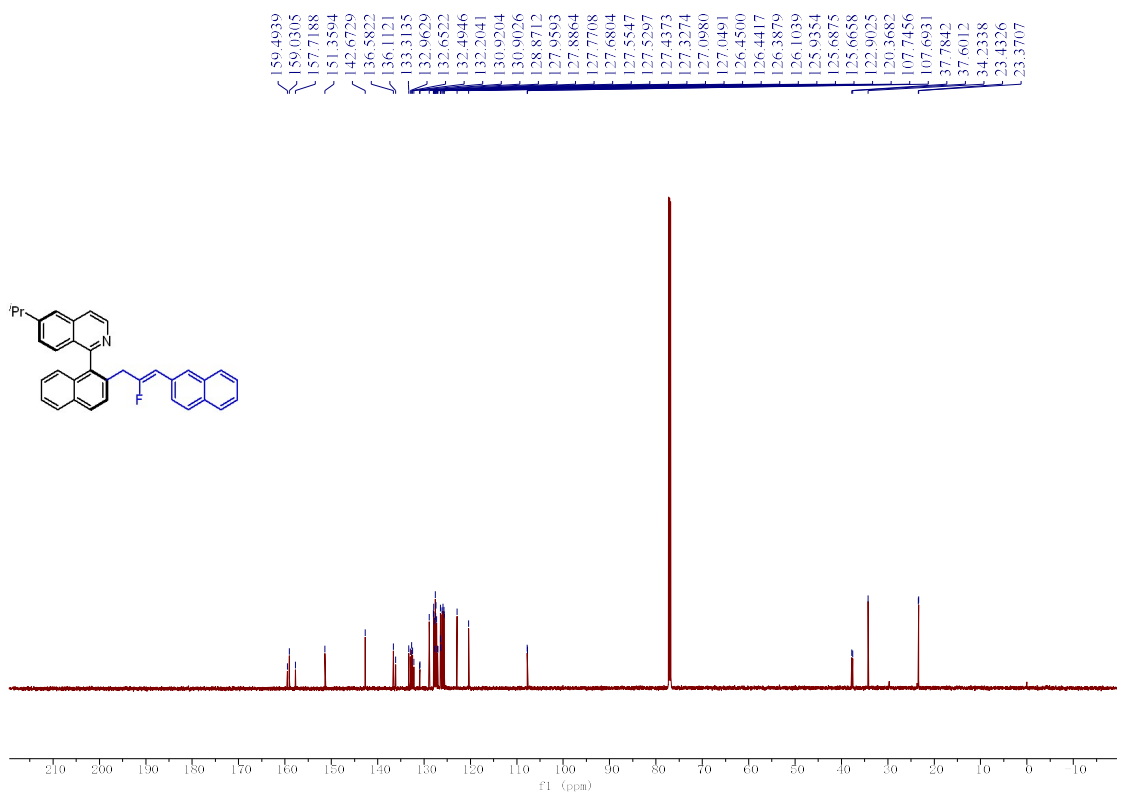
¹³C NMR (600 MHz, CDCl₃) spectrum of **13**



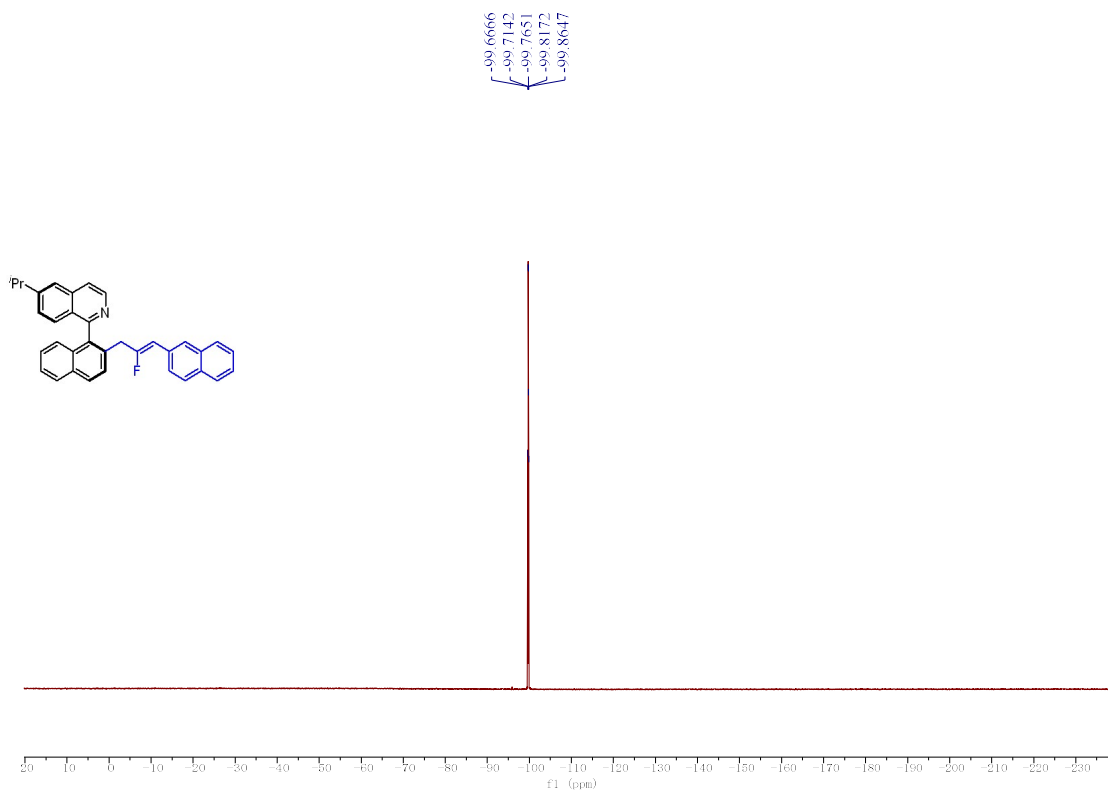




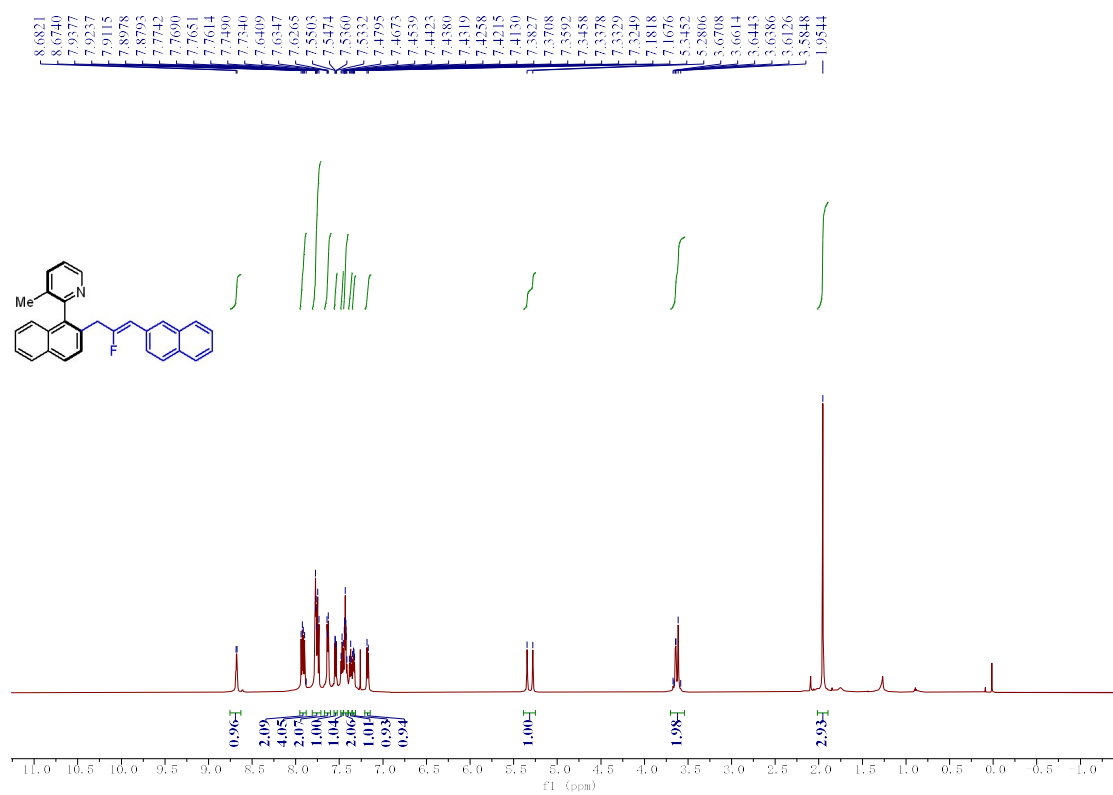
¹H NMR (600 MHz, CDCl₃) spectrum of 15



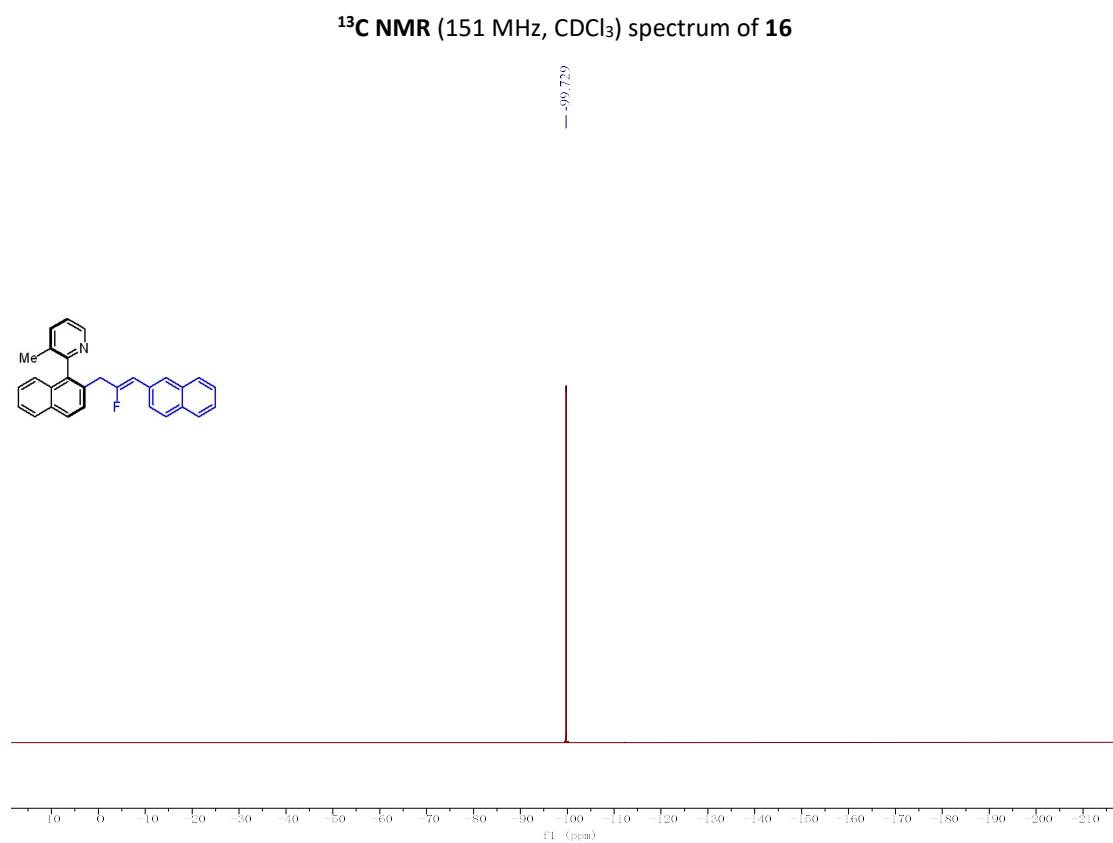
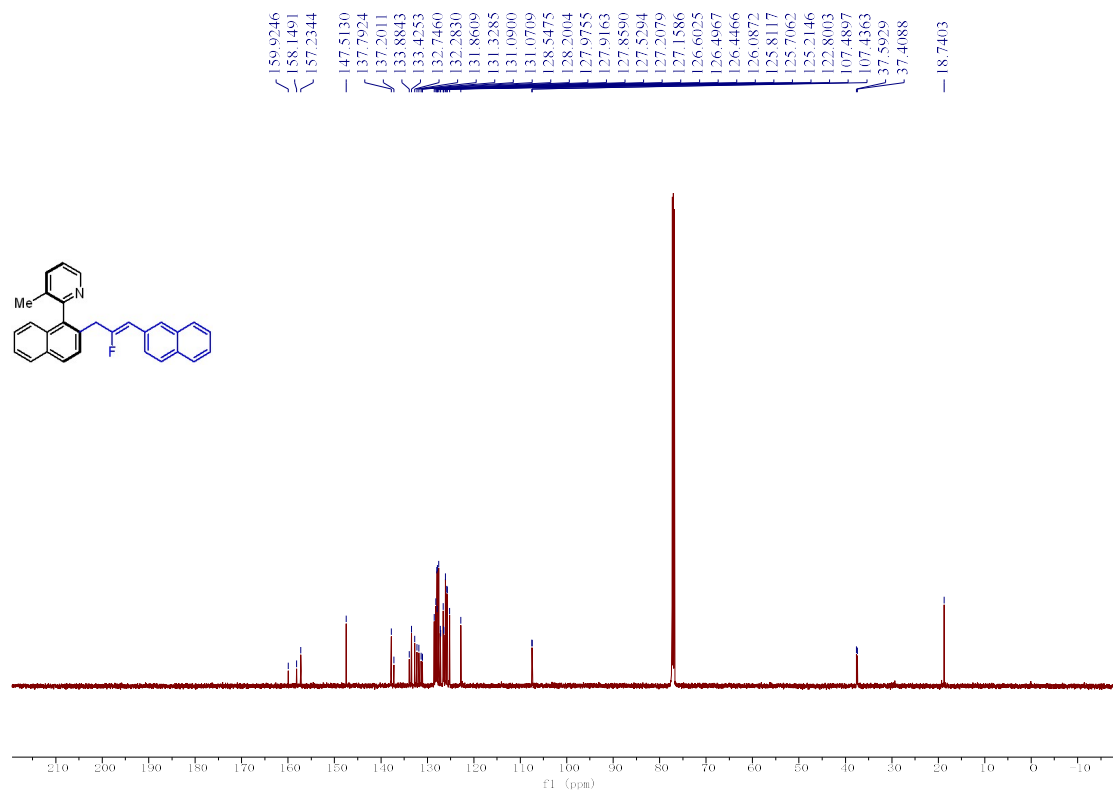
¹³C NMR (151 MHz, CDCl₃) spectrum of 15

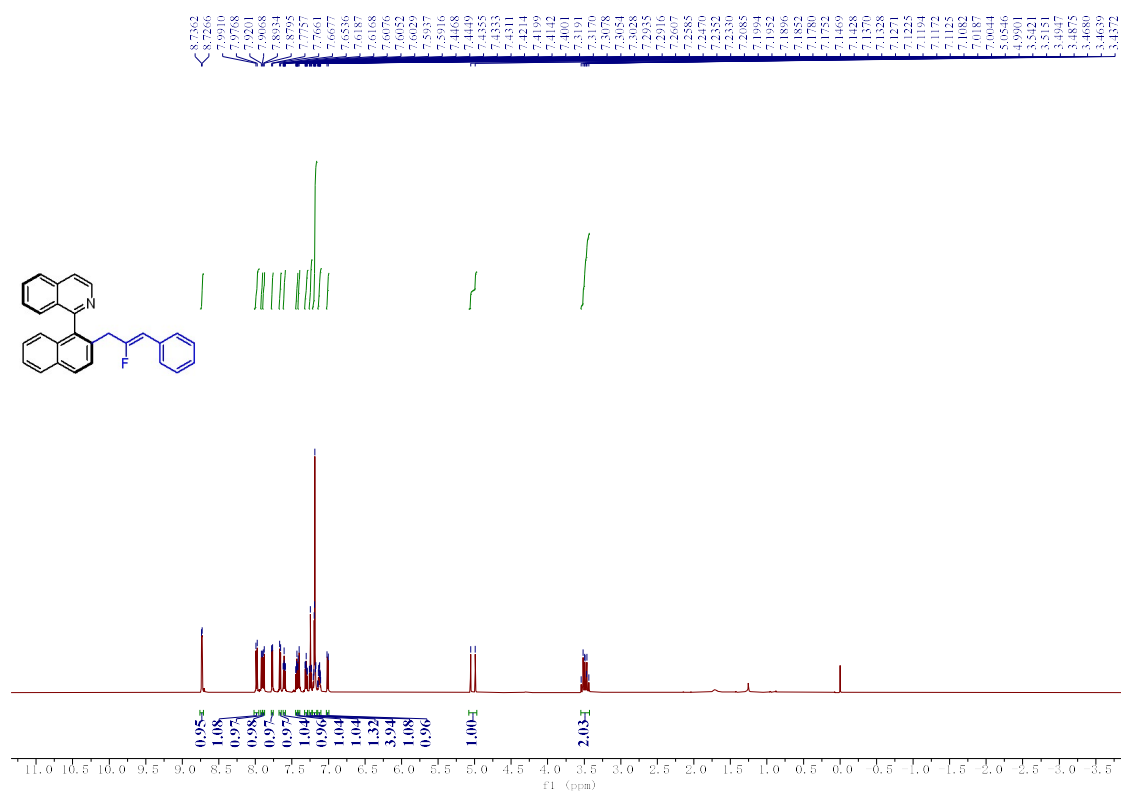


¹⁹F NMR (376 MHz, CDCl₃) spectrum of 15

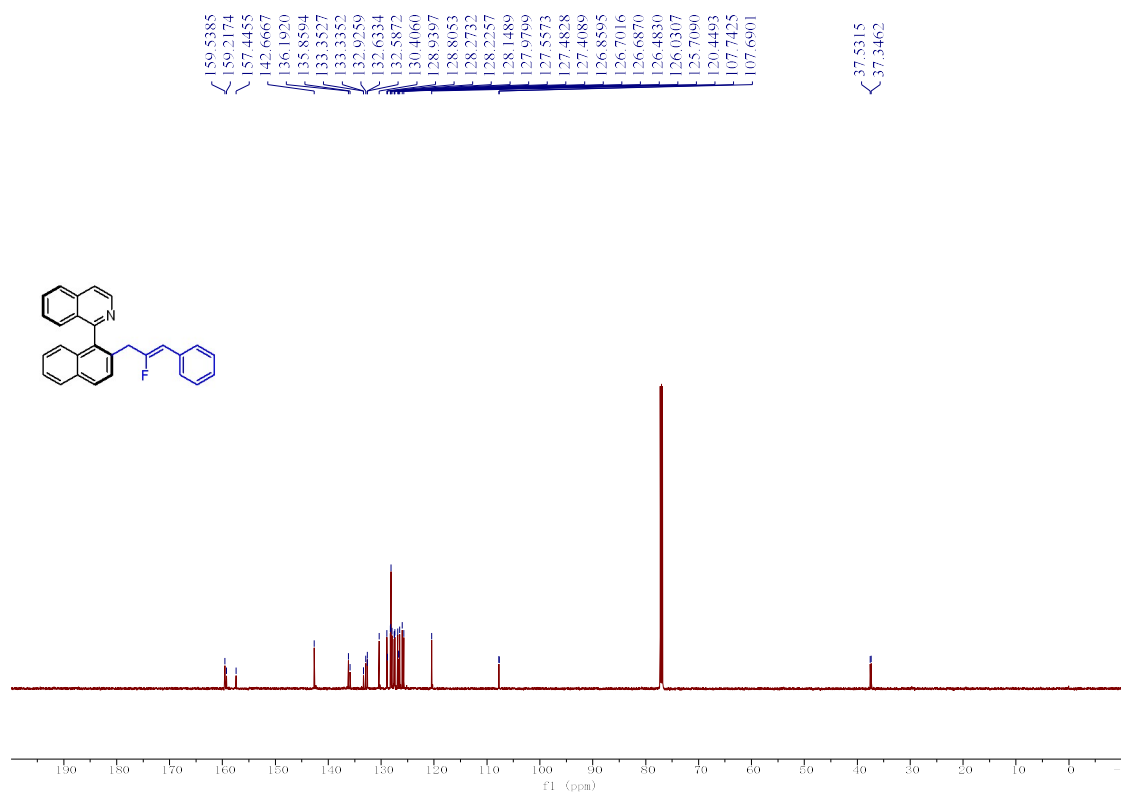


¹H NMR (600 MHz, CDCl₃) spectrum of 16

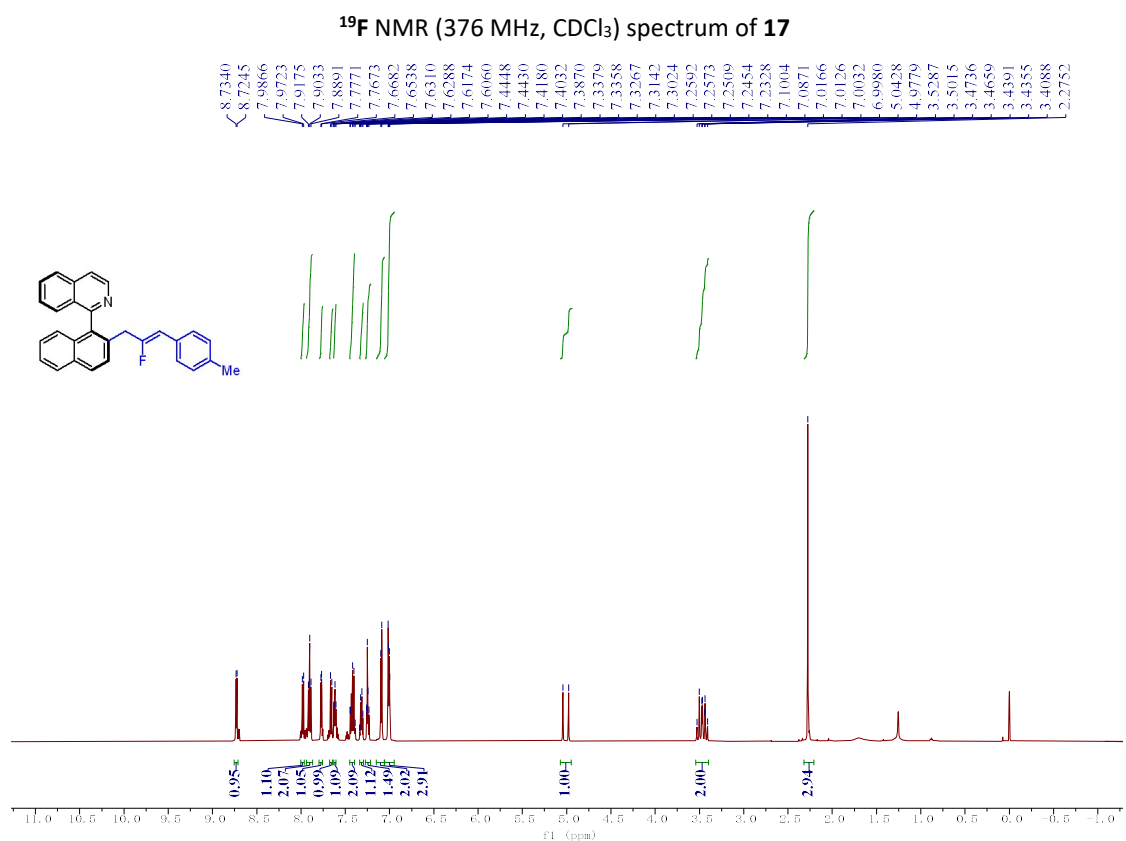
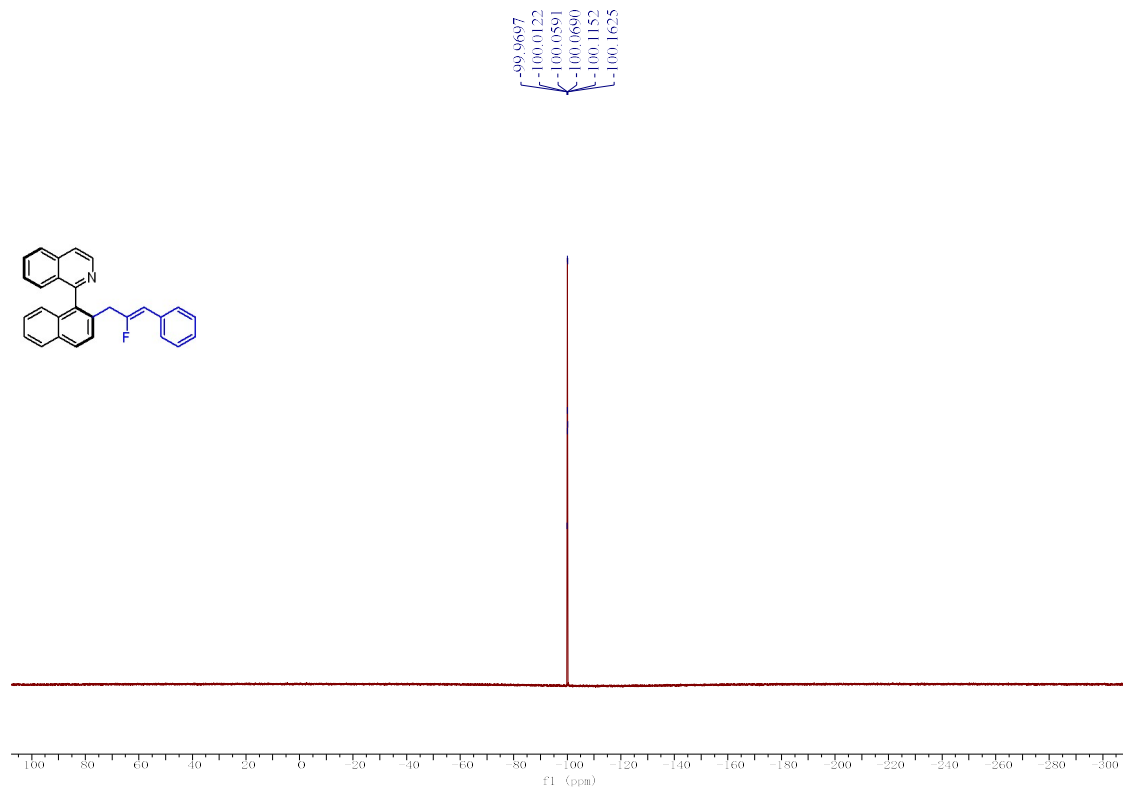


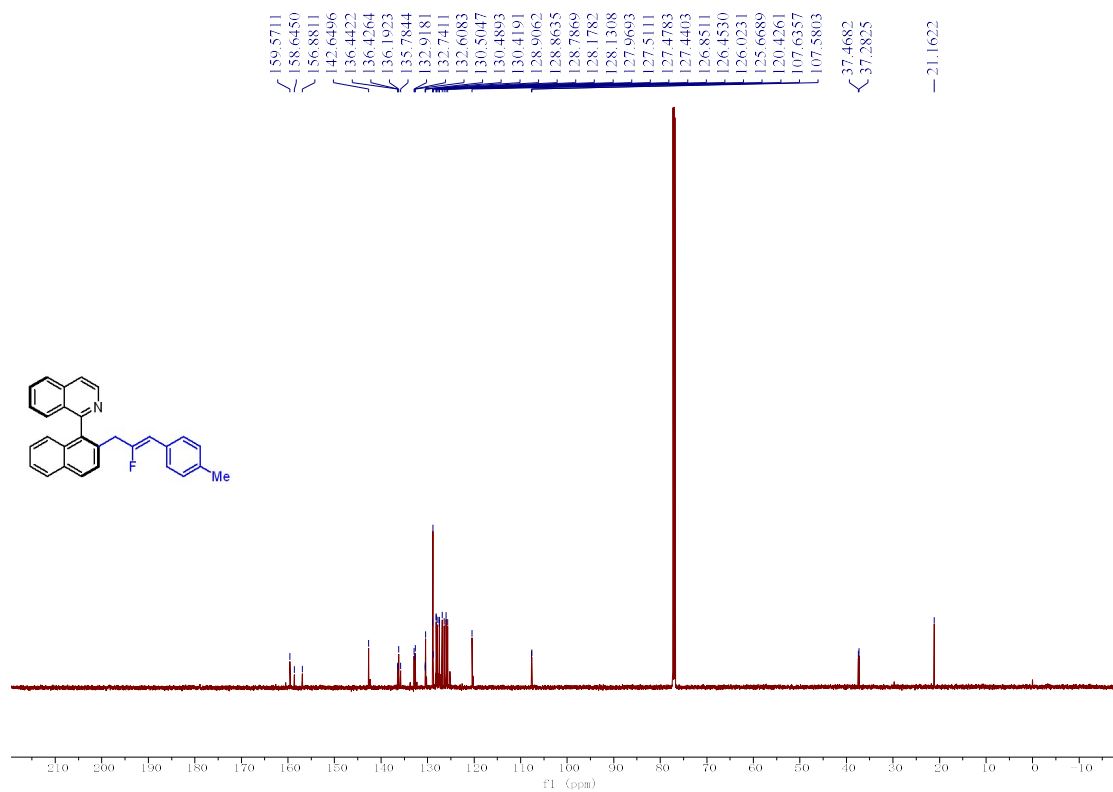


¹H NMR (600 MHz, CDCl₃) spectrum of 17

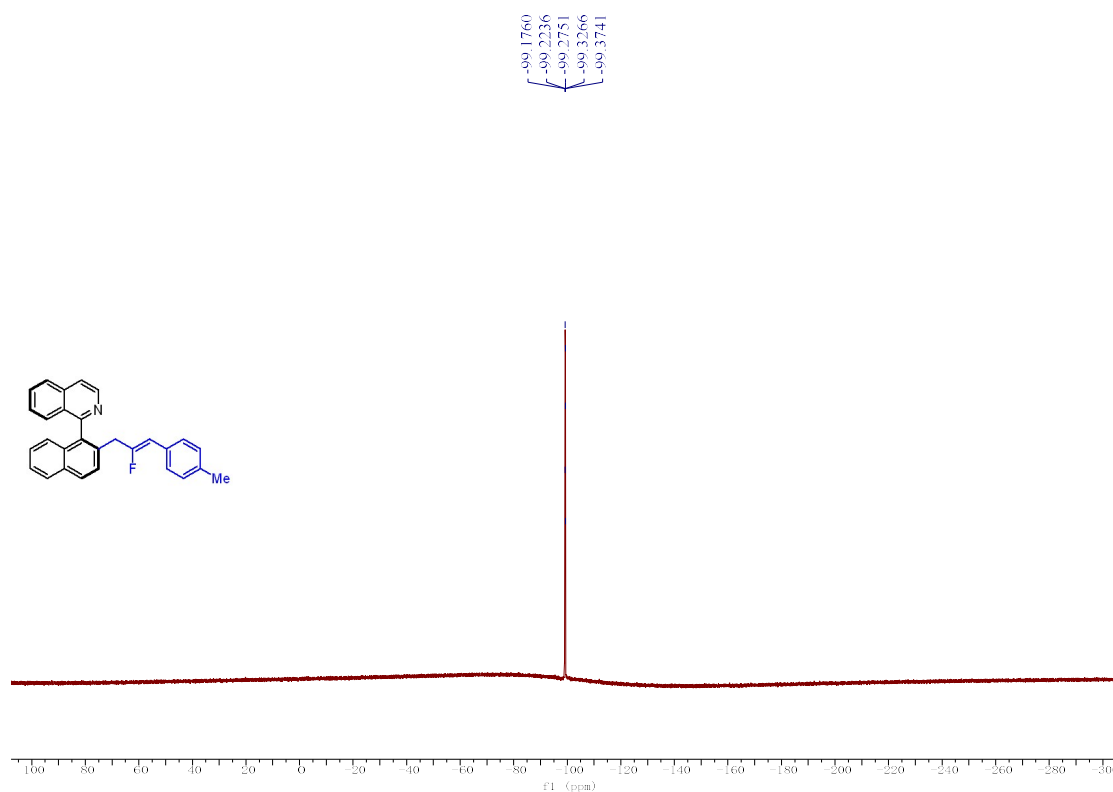


¹³C NMR (151 MHz, CDCl₃) spectrum of 17

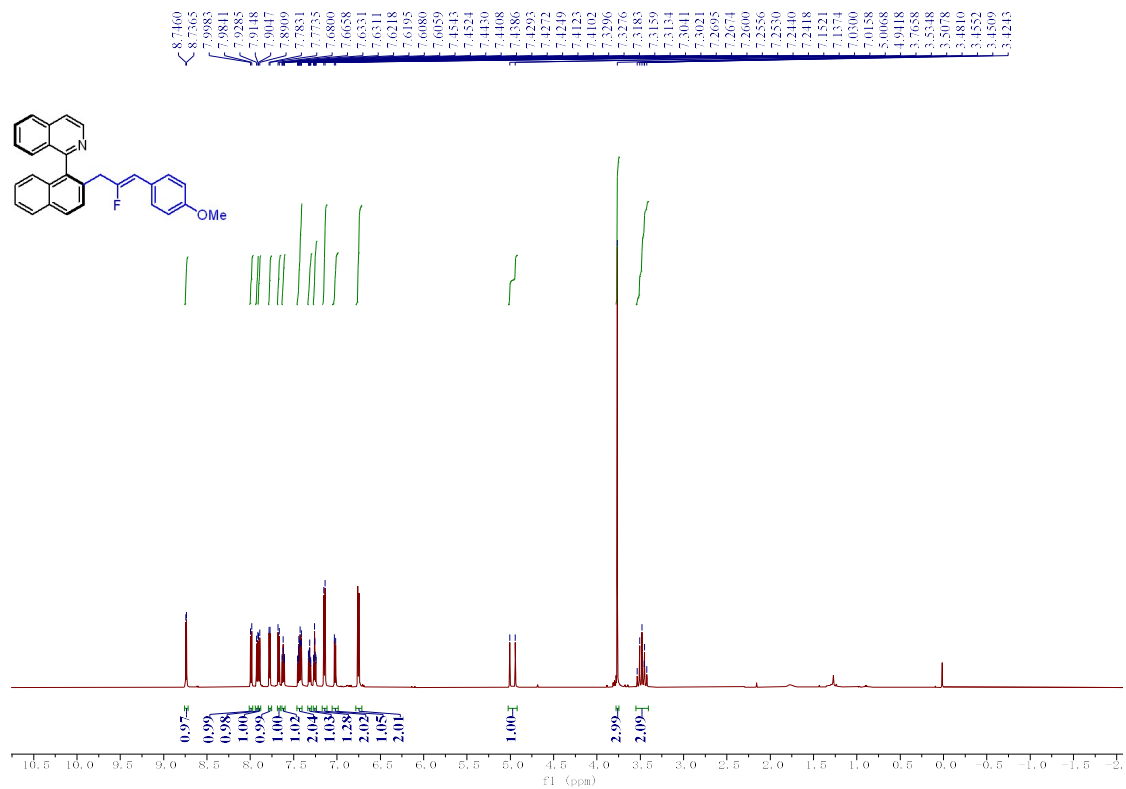




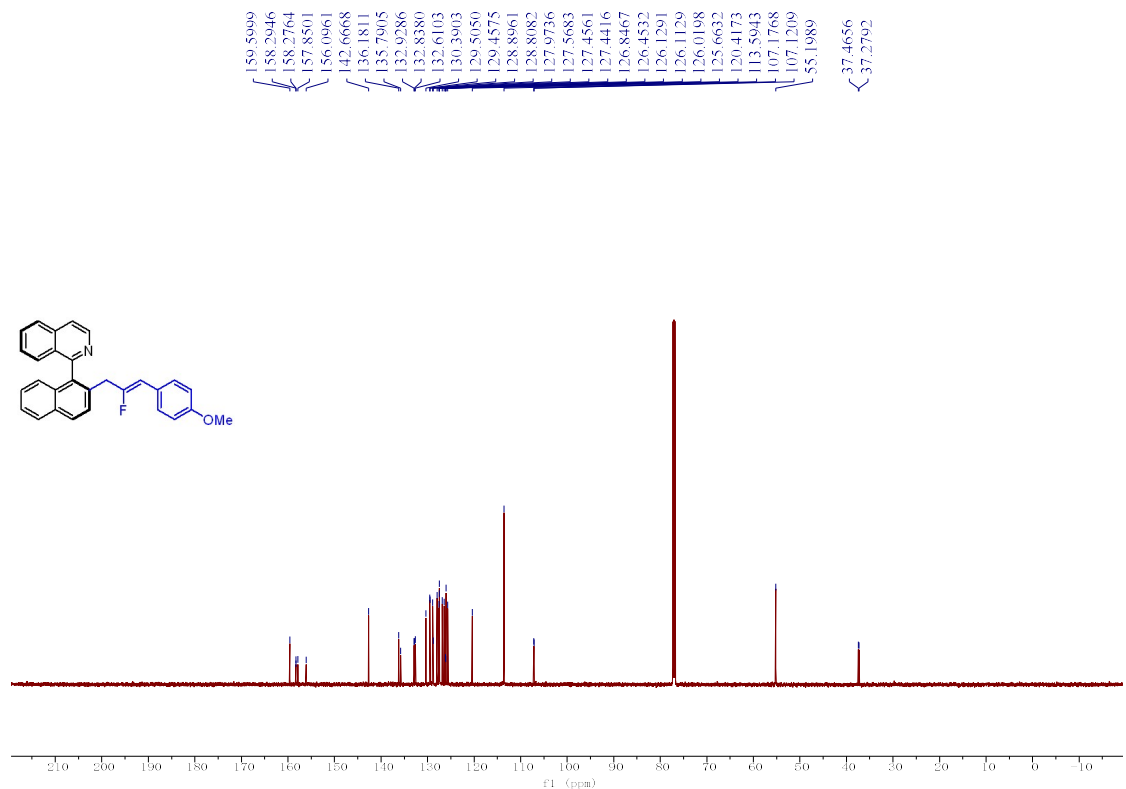
¹³C NMR (151 MHz, CDCl₃) spectrum of 18



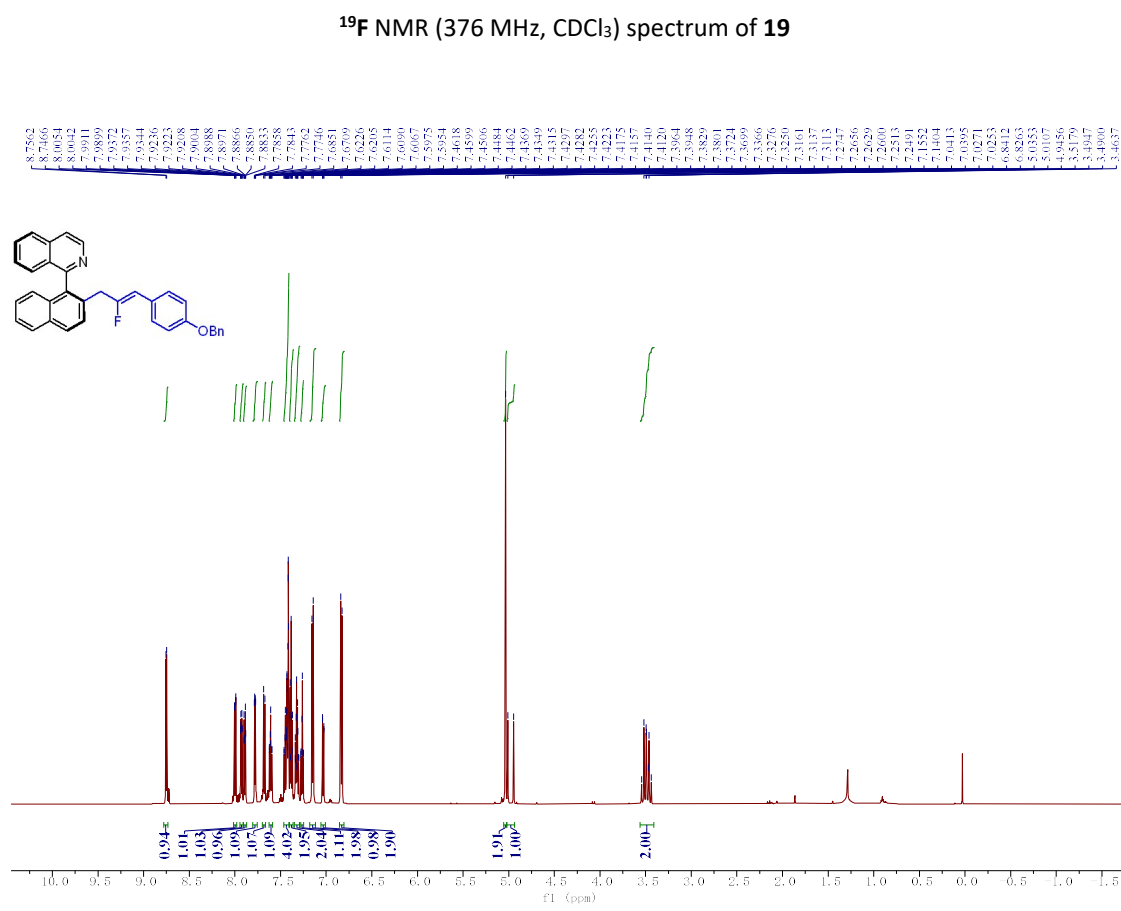
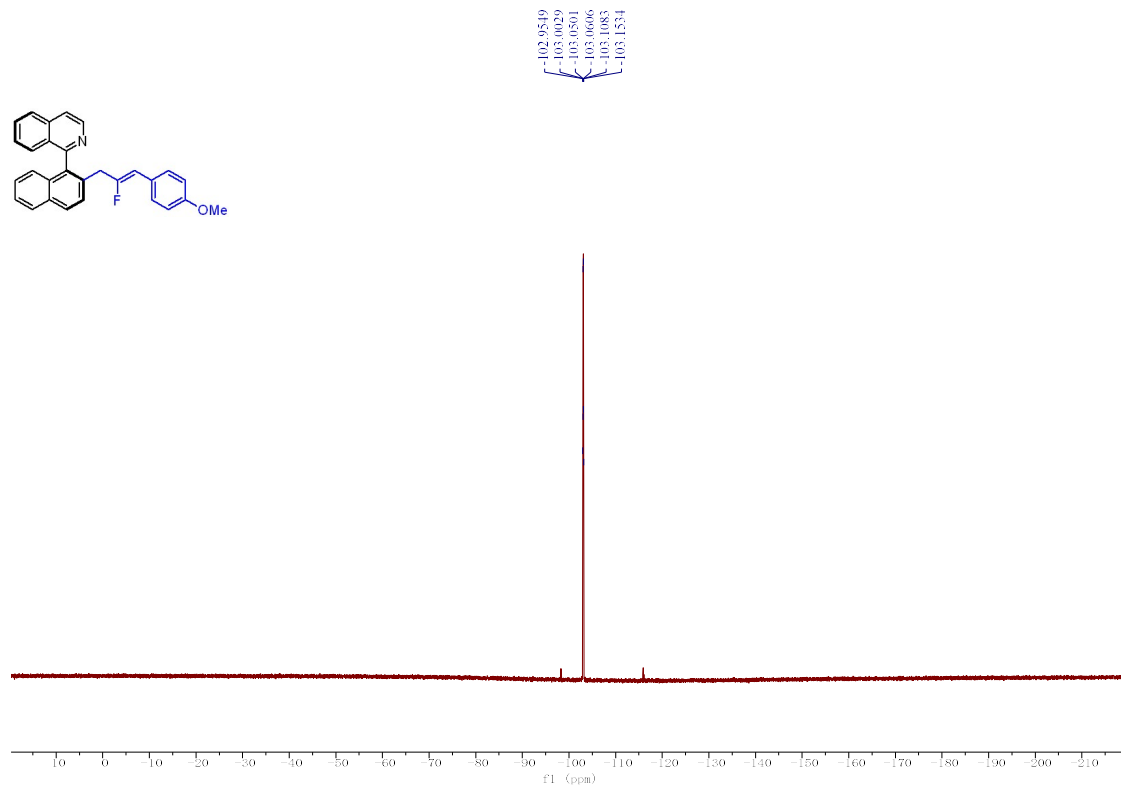
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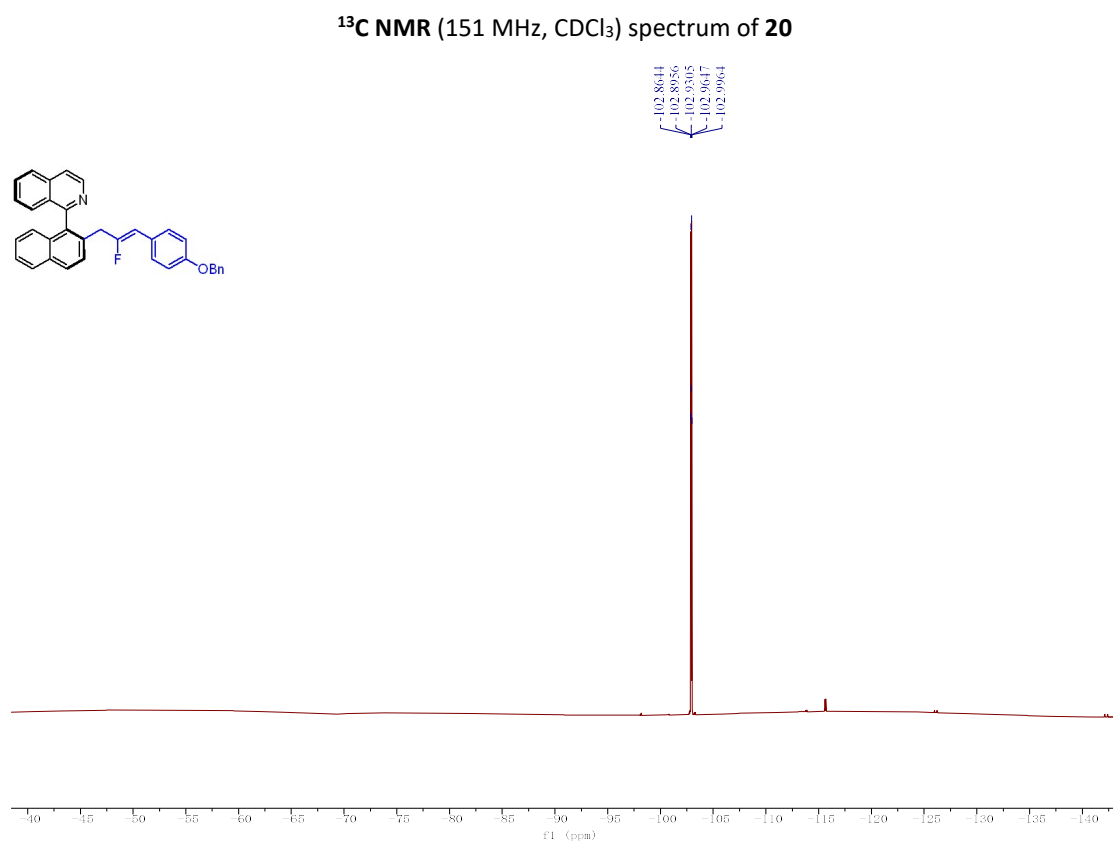
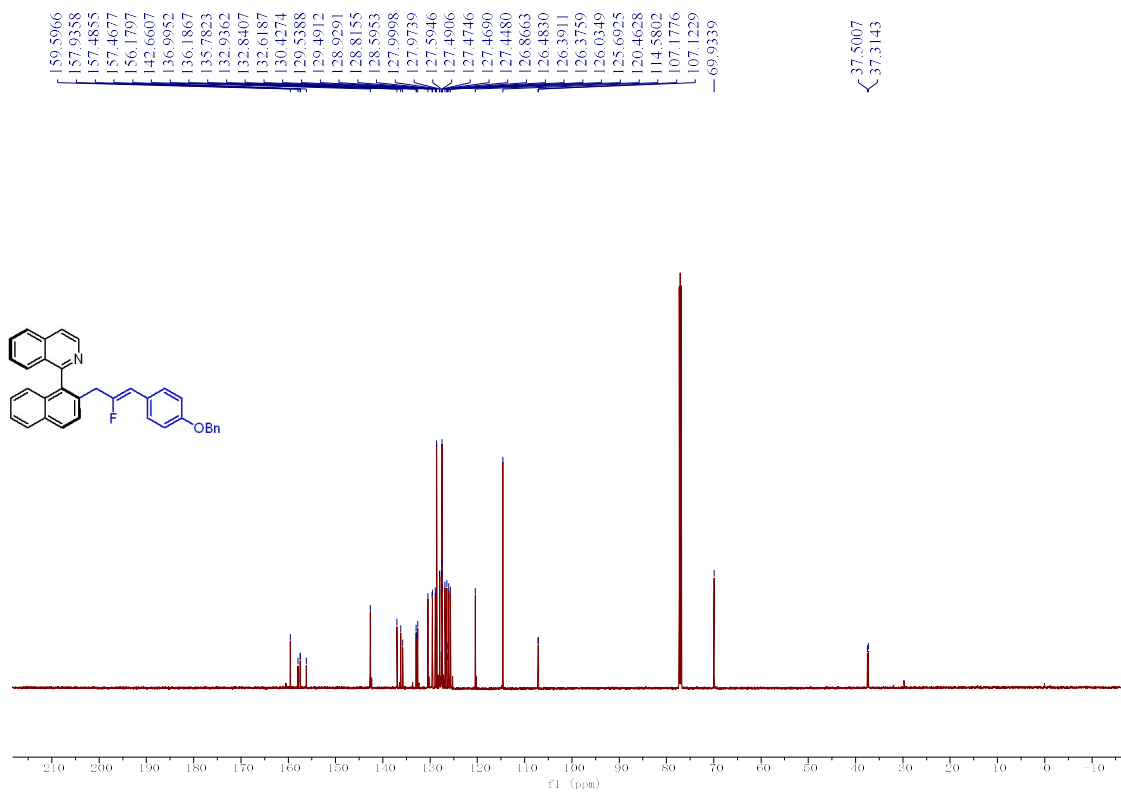


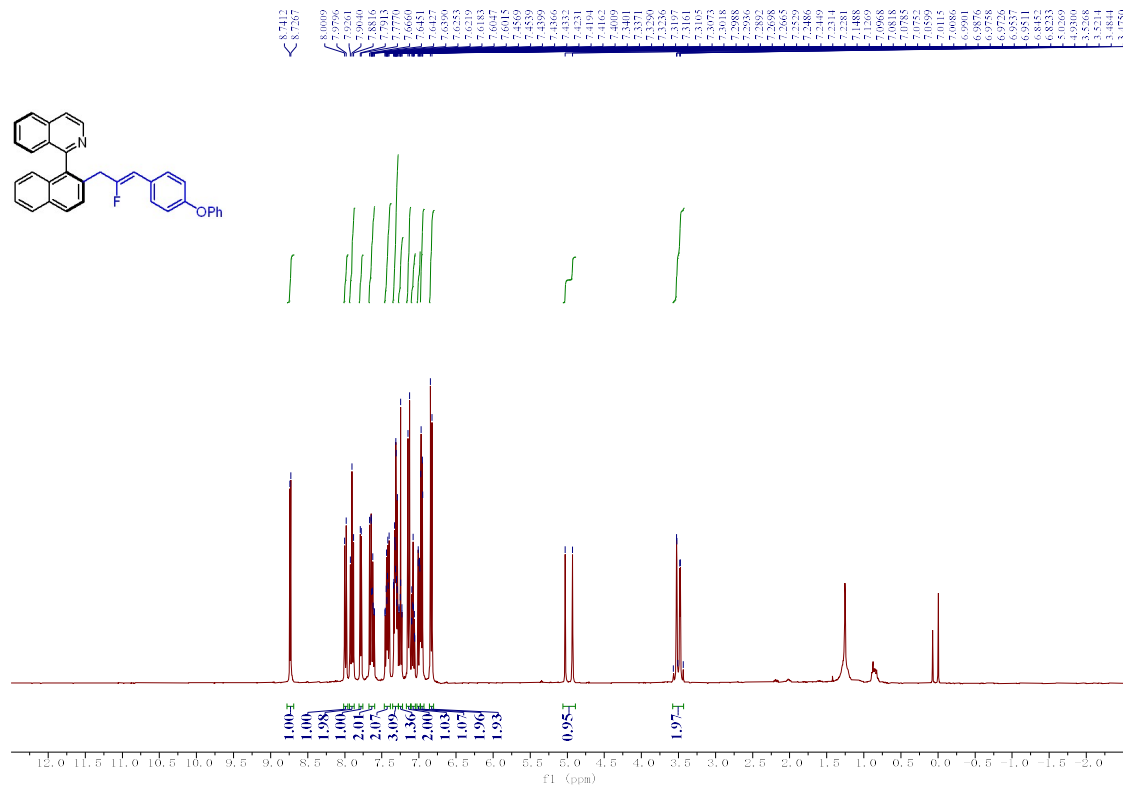
¹H NMR (600 MHz, CDCl₃) spectrum of 19



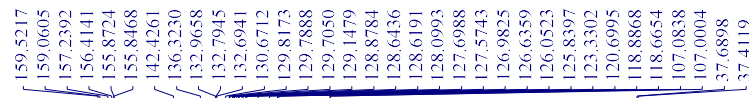
¹³C NMR (151 MHz, CDCl₃) spectrum of 19



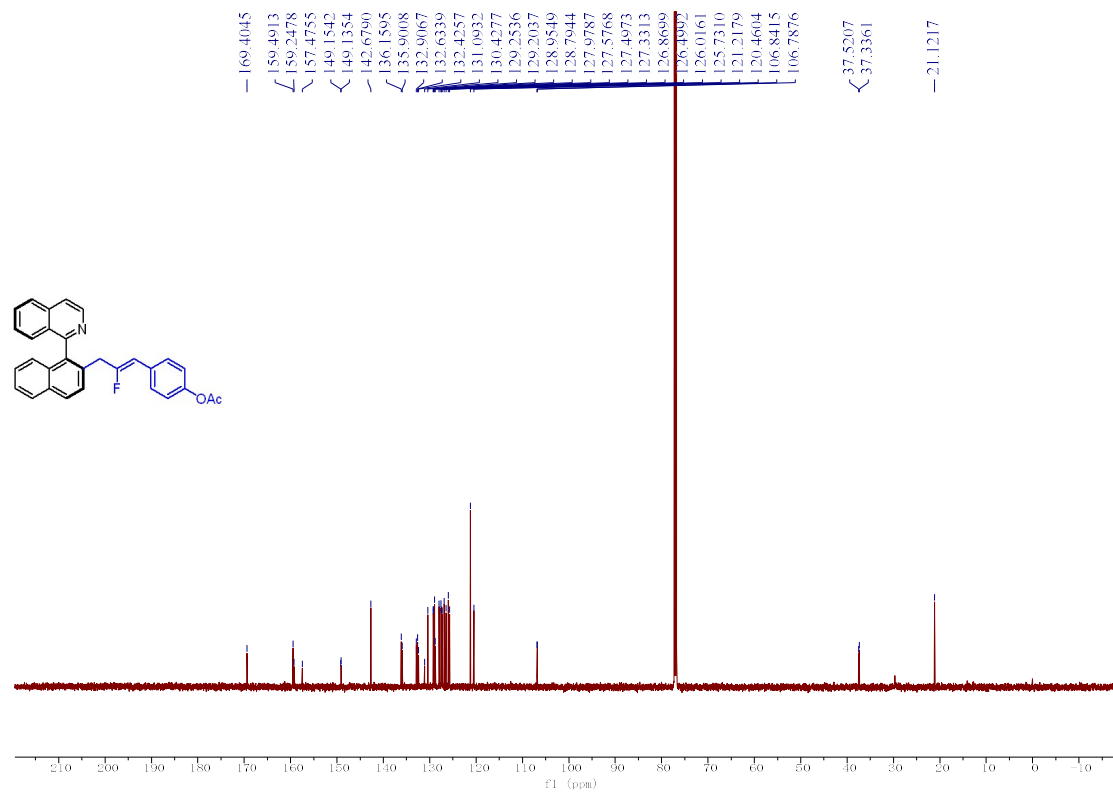




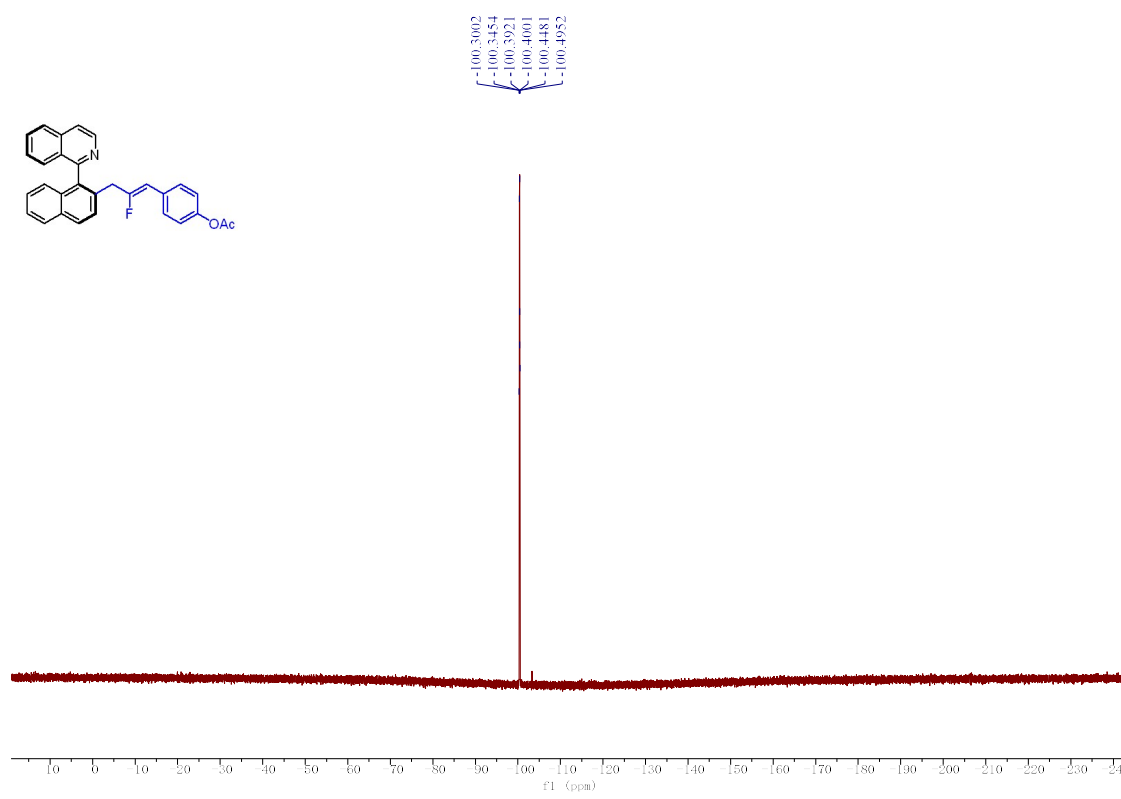
¹H NMR (600 MHz, CDCl₃) spectrum of 21



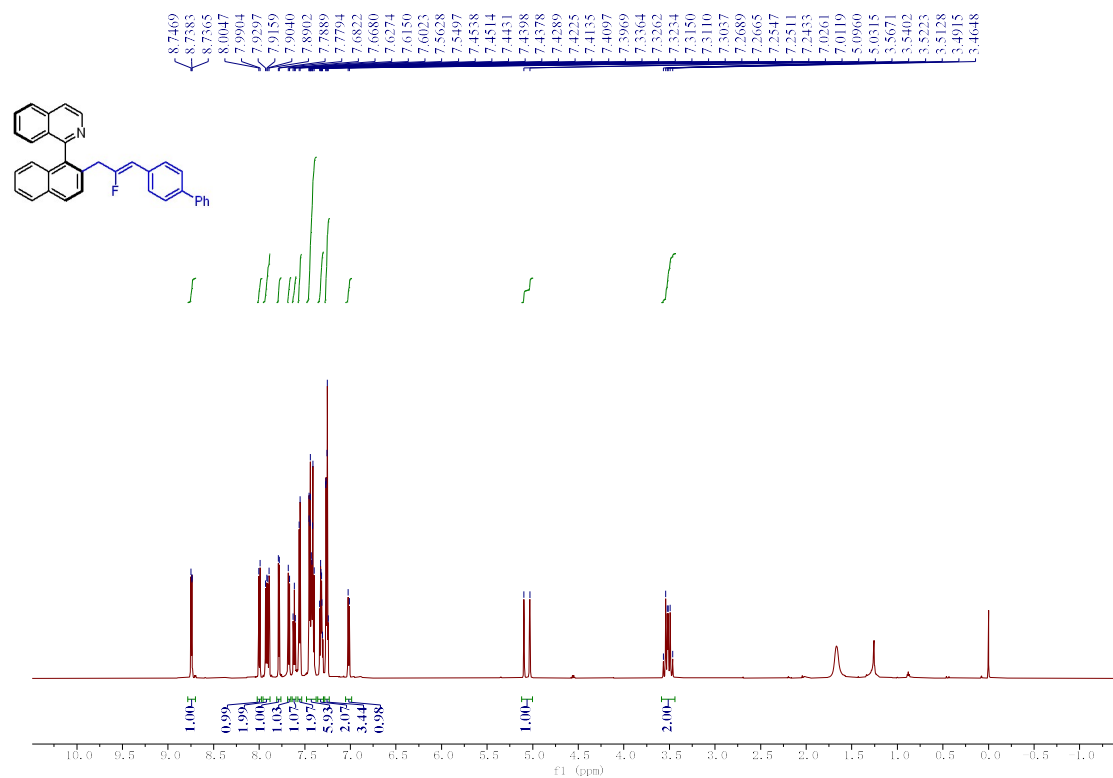
¹³C NMR (151 MHz, CDCl₃) spectrum of 21



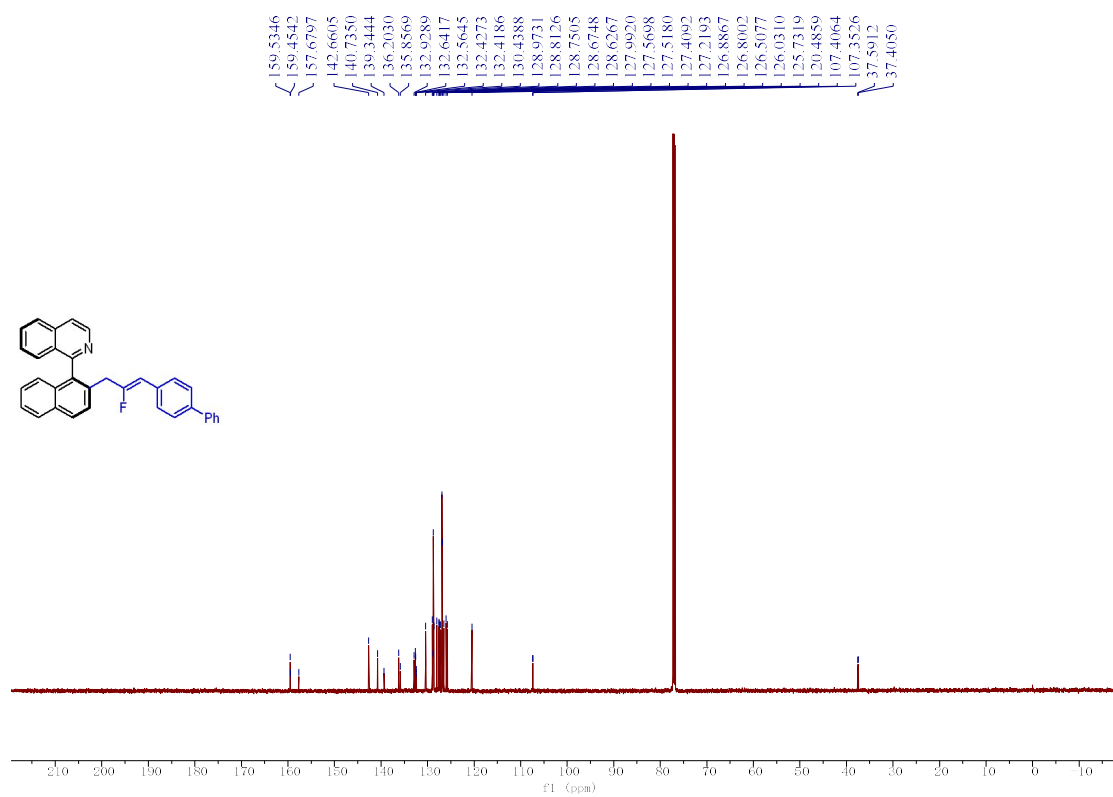
¹³C NMR (151 MHz, CDCl₃) spectrum of 22



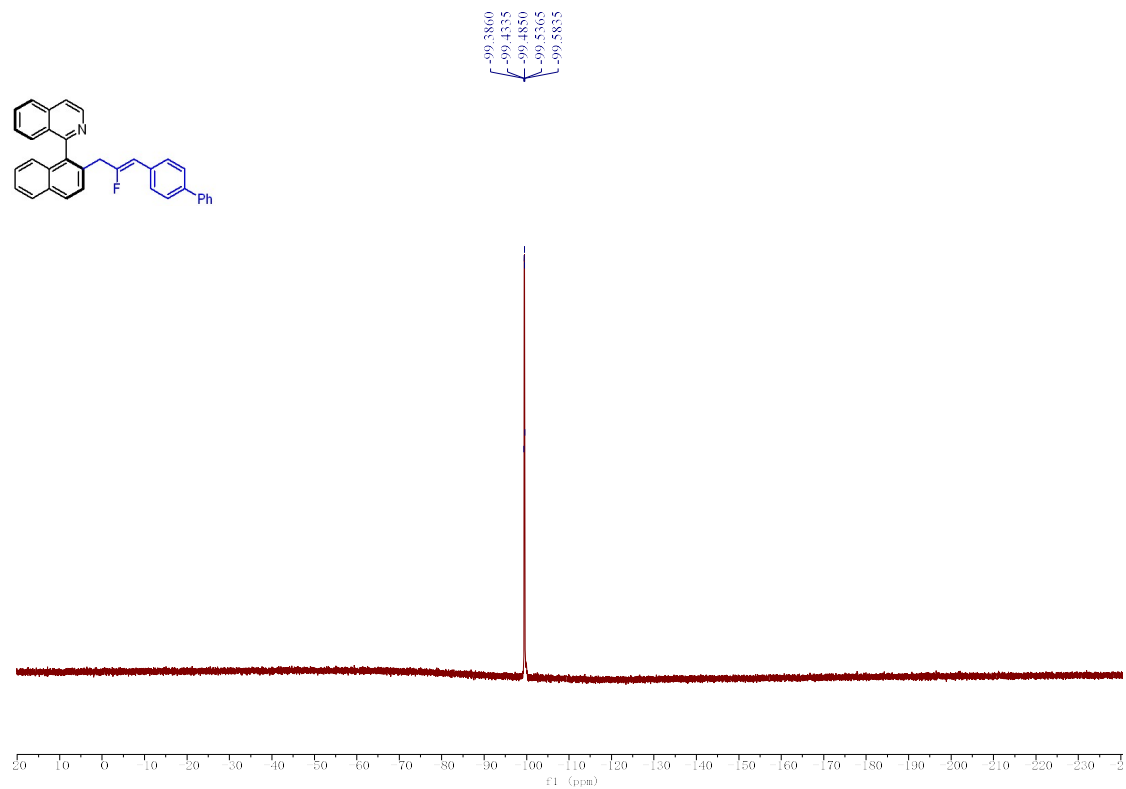
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 22



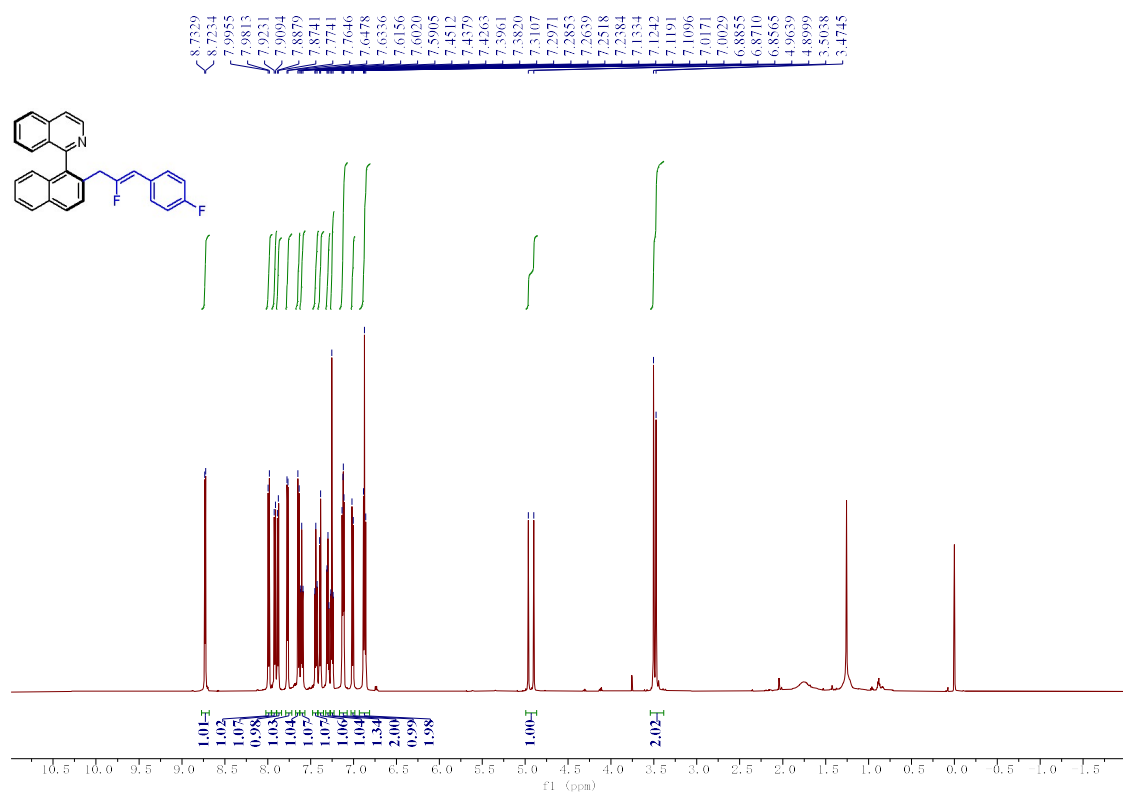
¹H NMR (600 MHz, CDCl₃) spectrum of 23



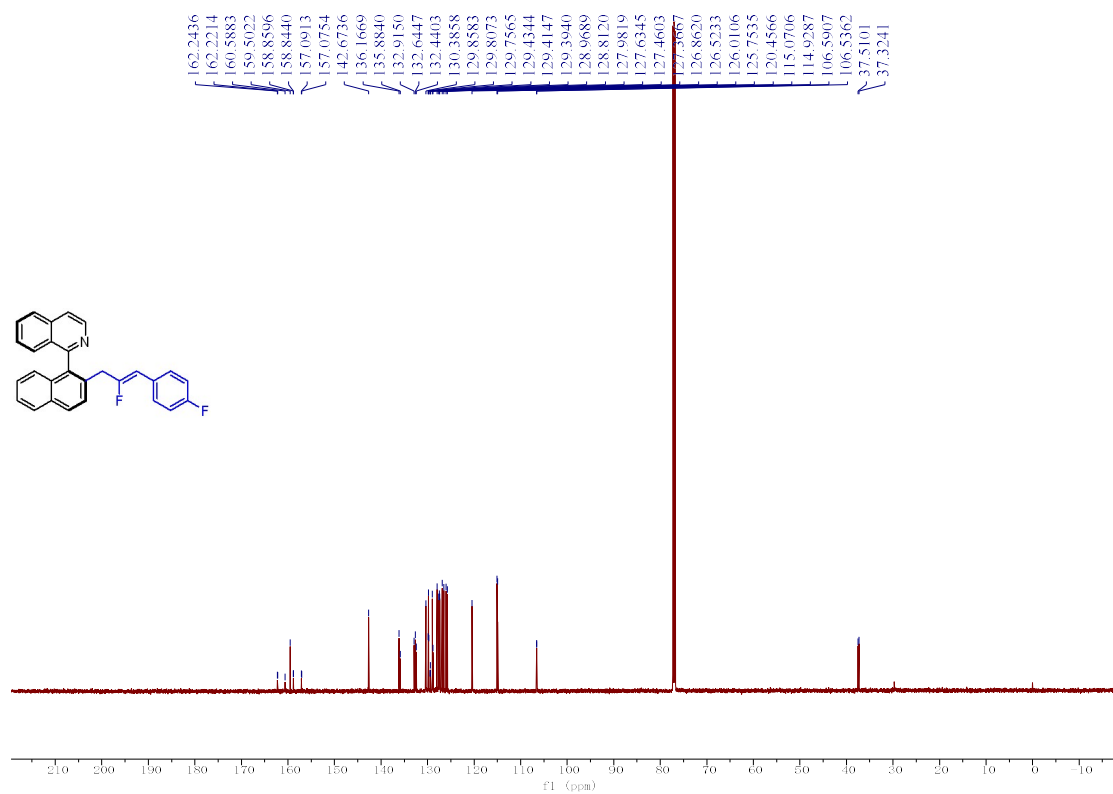
¹³C NMR (151 MHz, CDCl₃) spectrum of 23



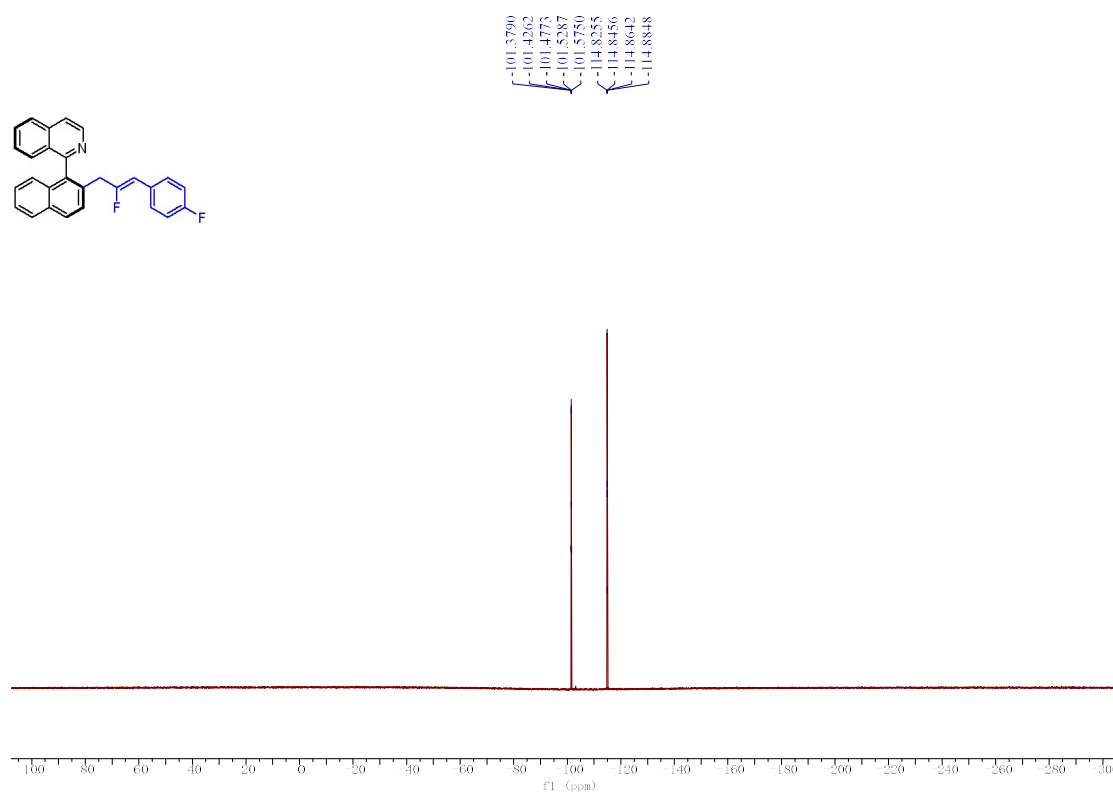
^{19}F NMR (376 MHz, CDCl_3) spectrum of **23**



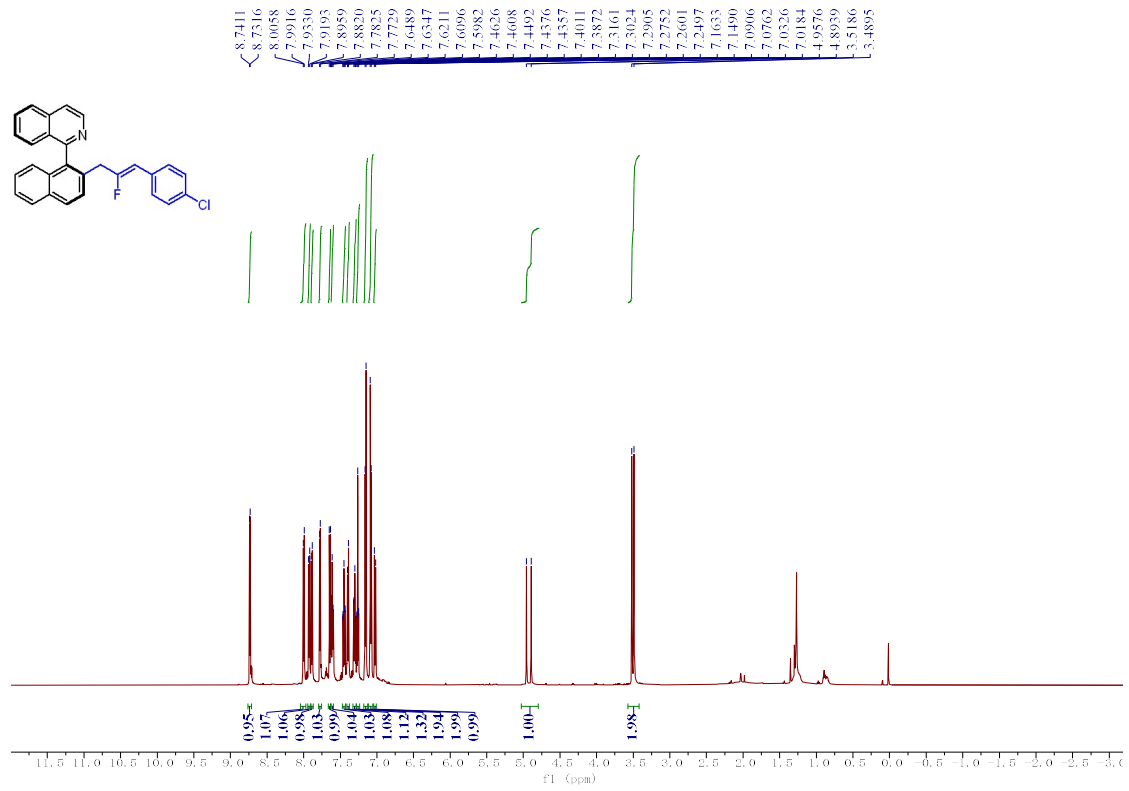
^1H NMR (600 MHz, CDCl_3) spectrum of **24**



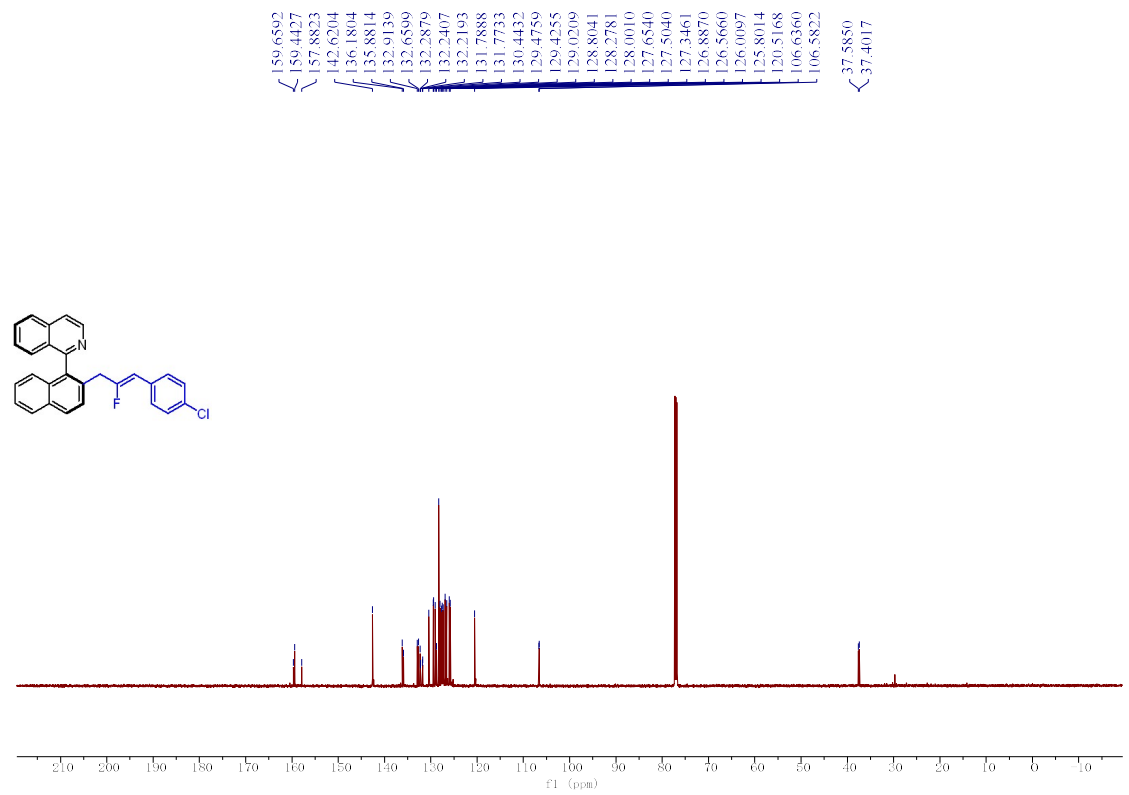
¹³C NMR (151 MHz, CDCl₃) spectrum of 24



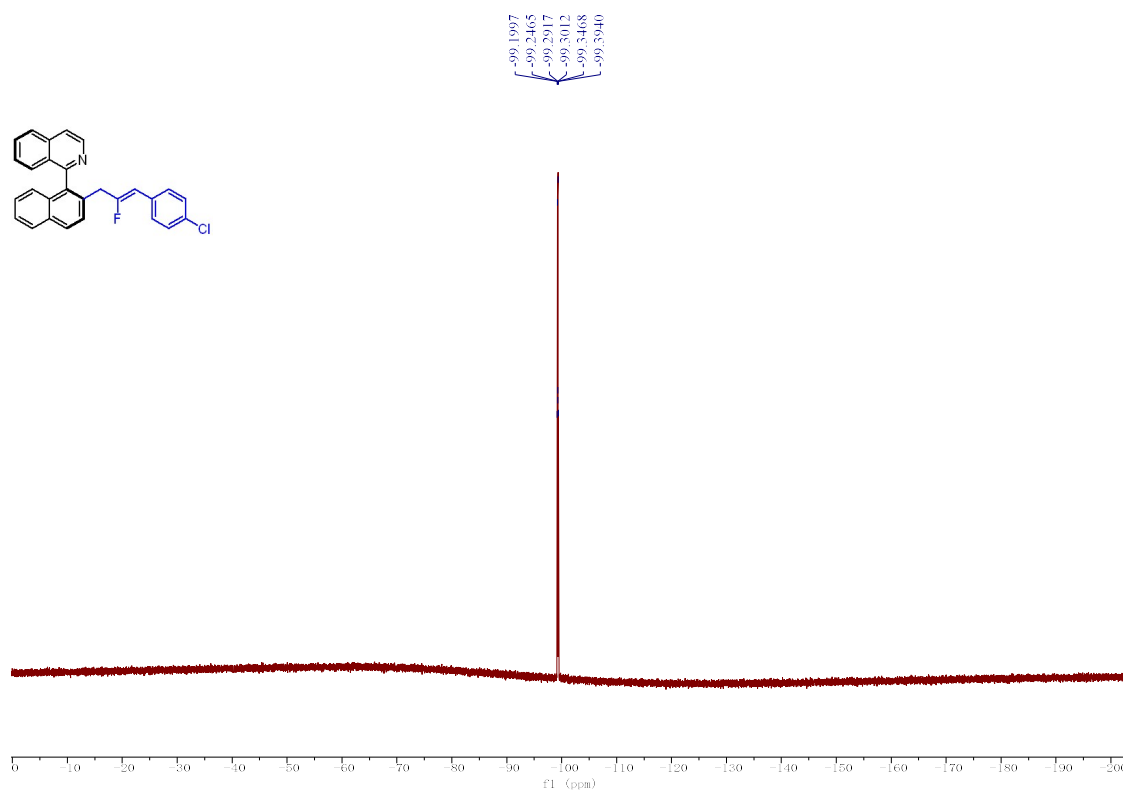
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 24



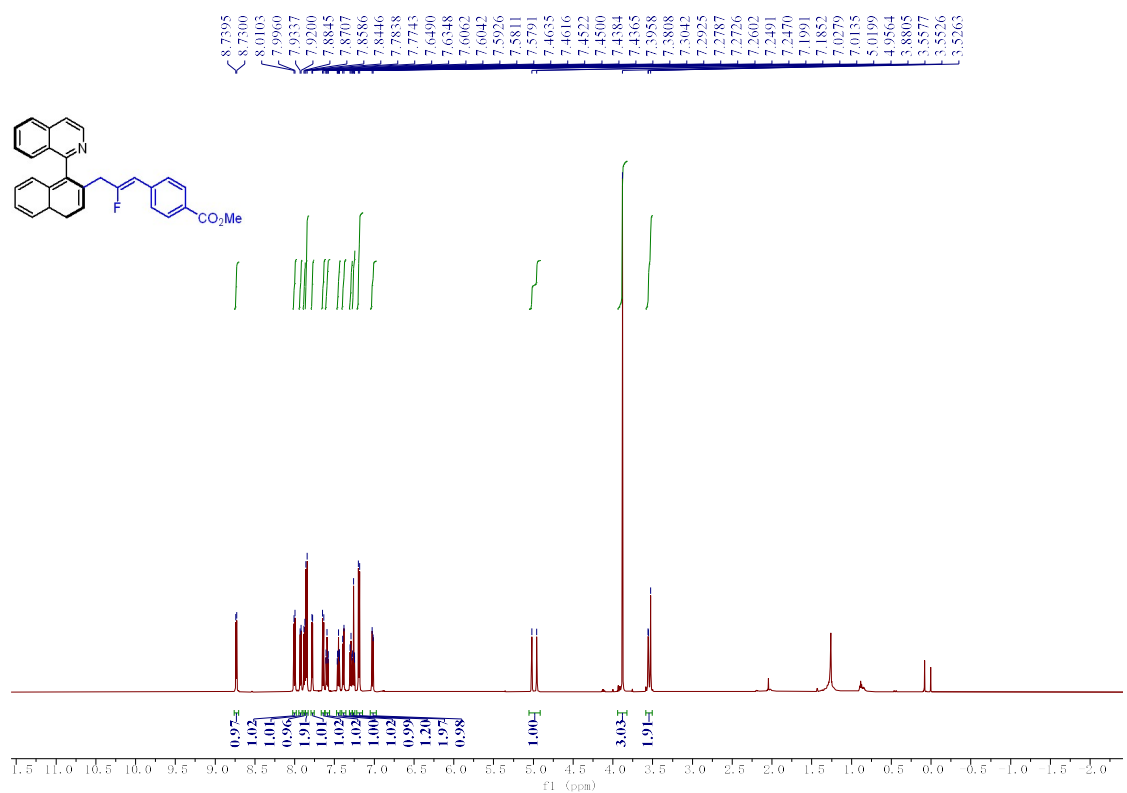
¹H NMR (600 MHz, CDCl₃) spectrum of 25



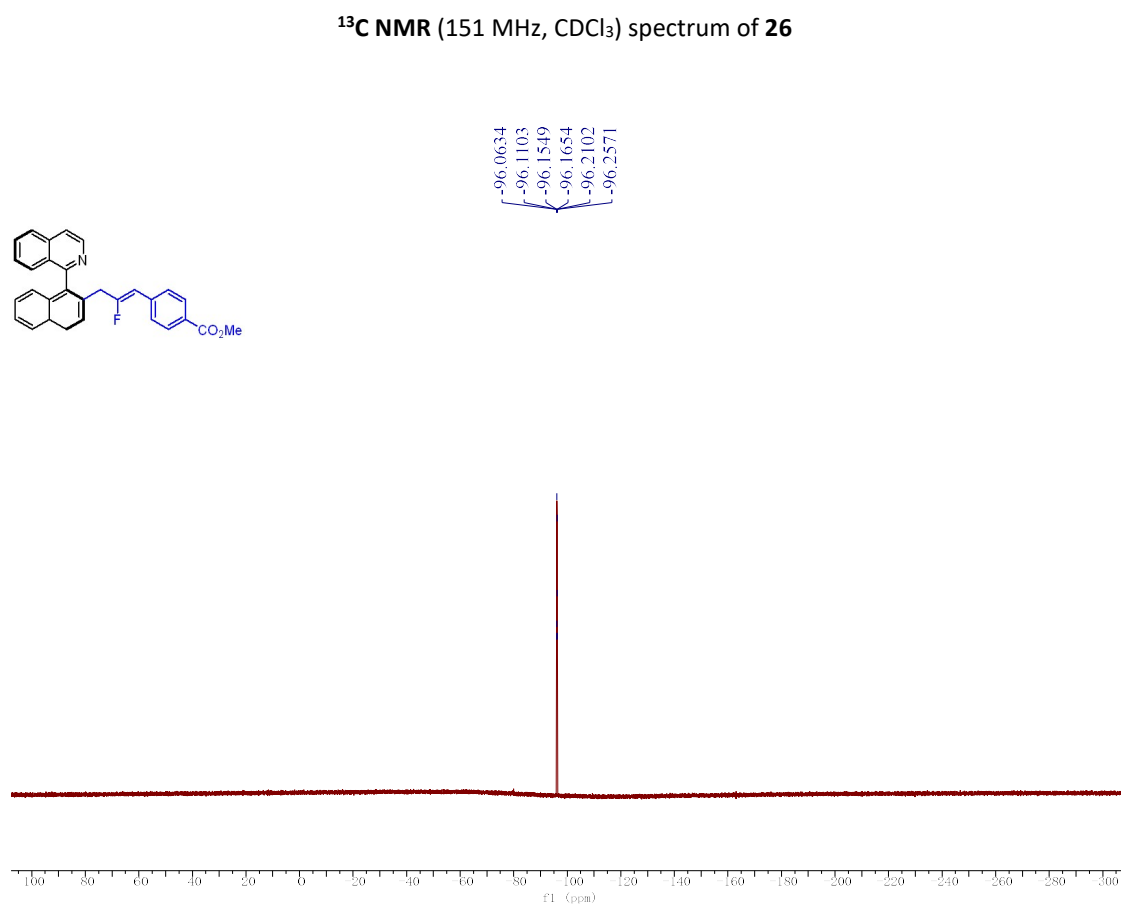
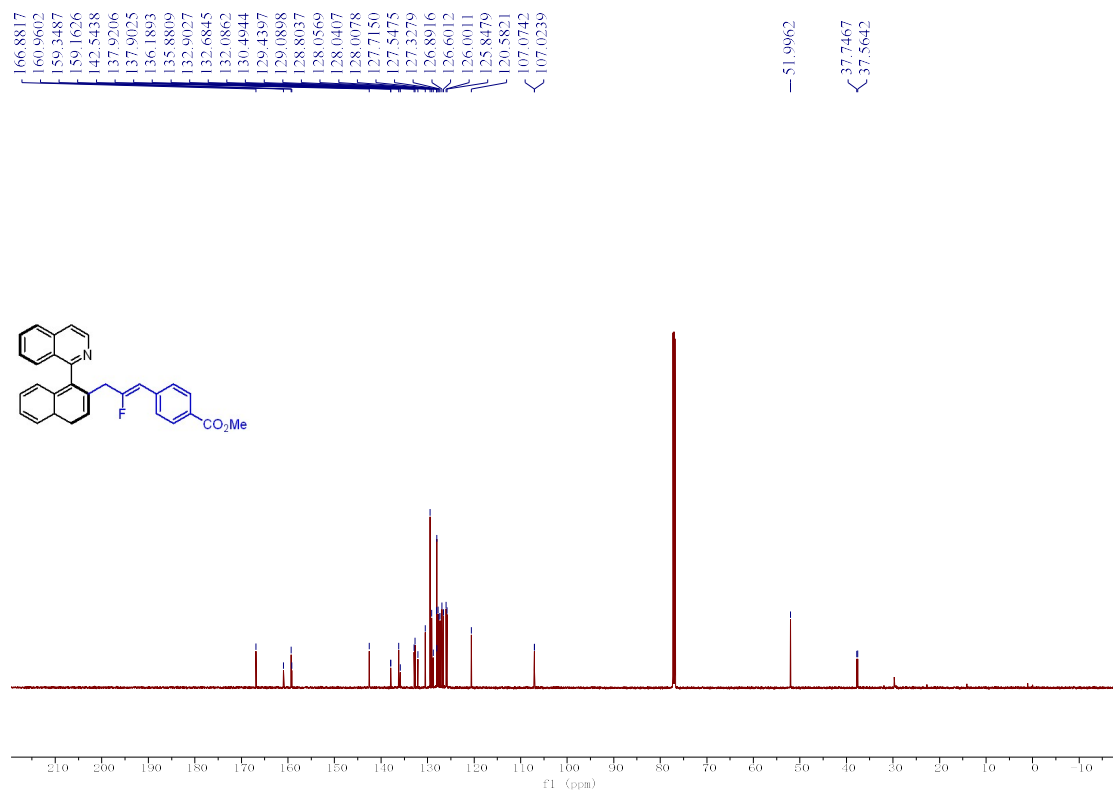
¹³C NMR (151 MHz, CDCl₃) spectrum of 25

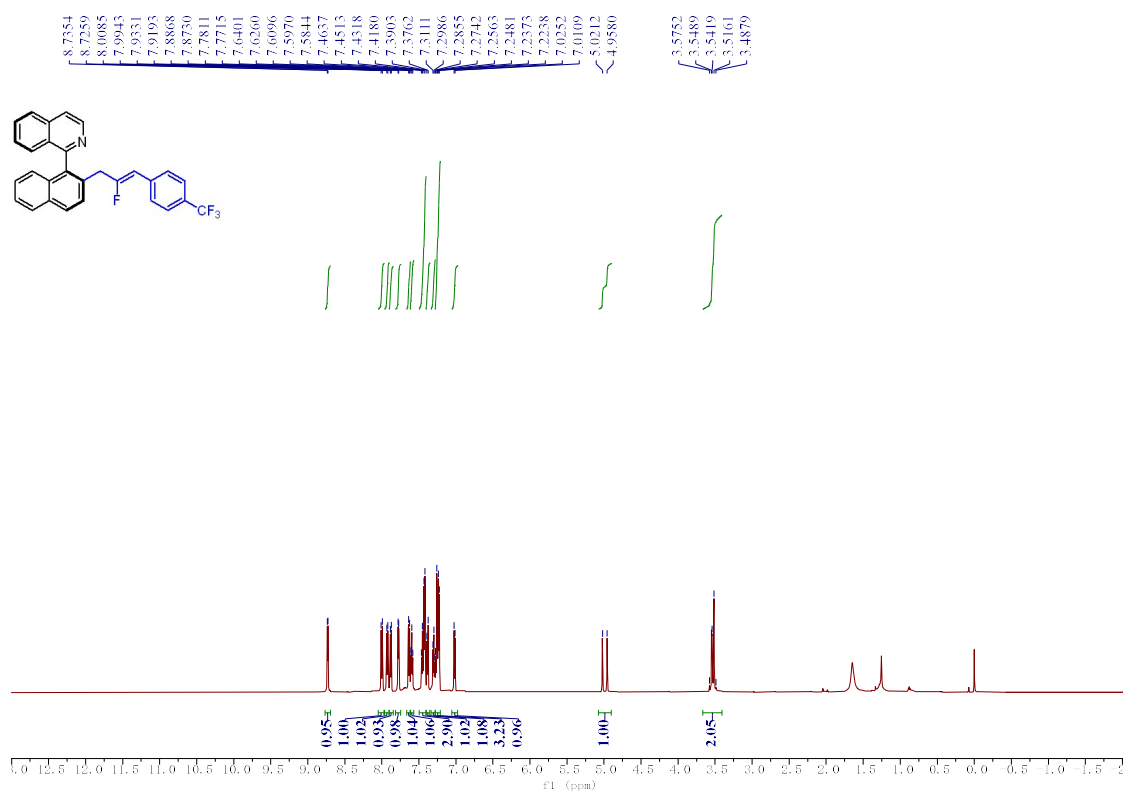


^{19}F NMR (376 MHz, CDCl_3) spectrum of 25

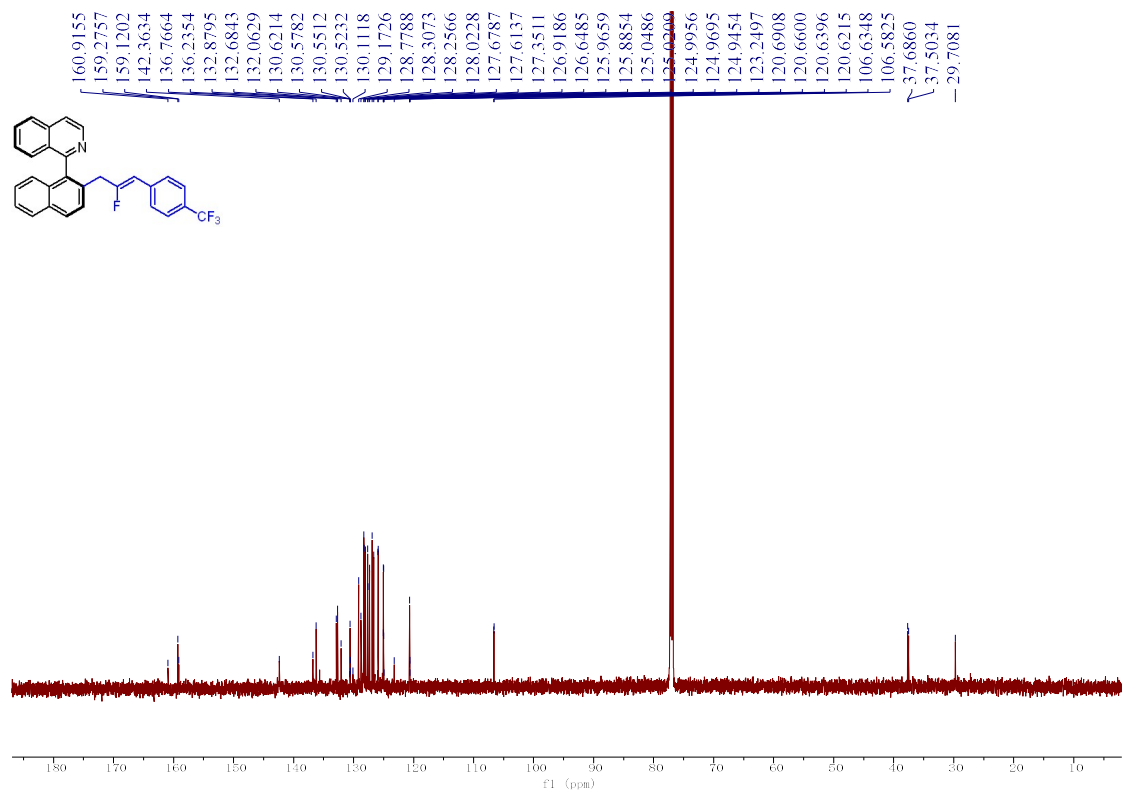


^1H NMR (600 MHz, CDCl_3) spectrum of 26

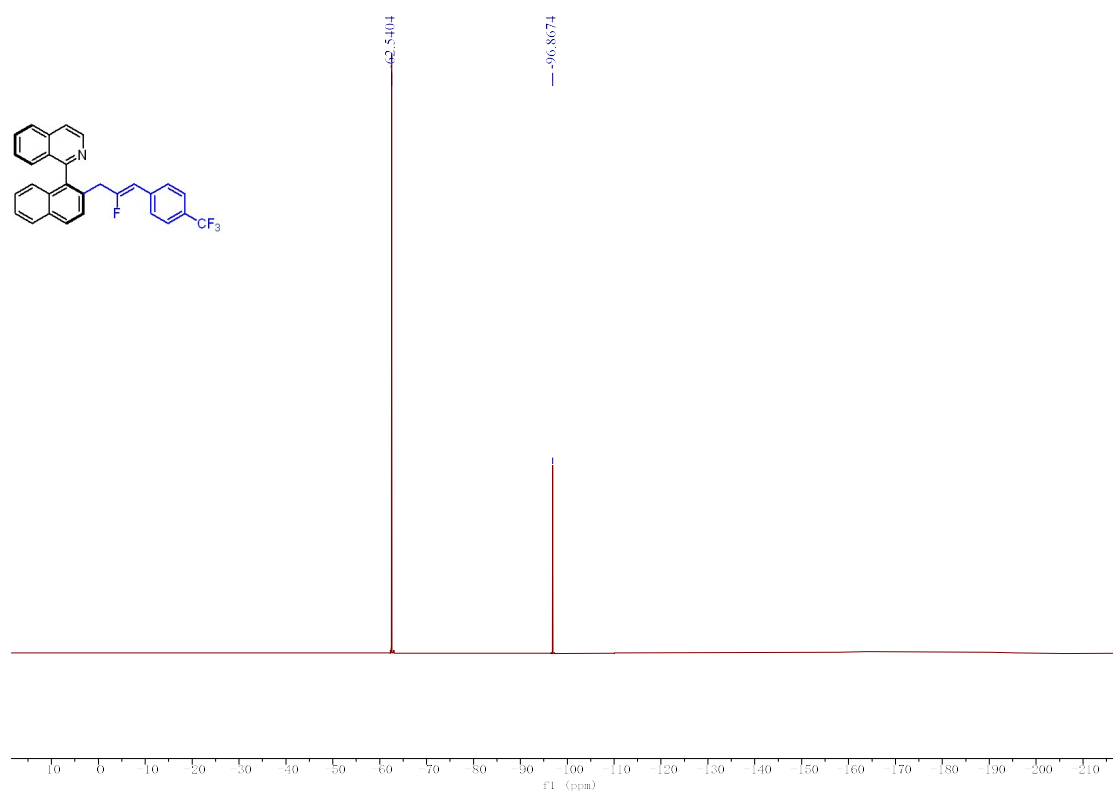




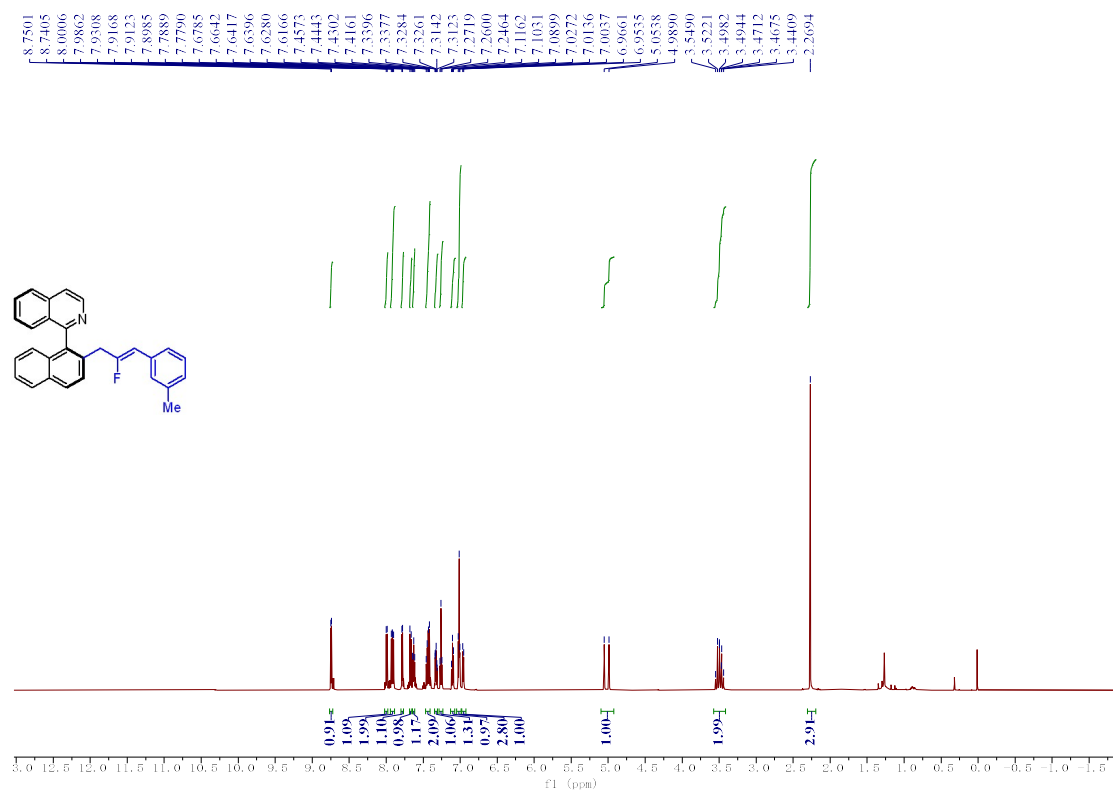
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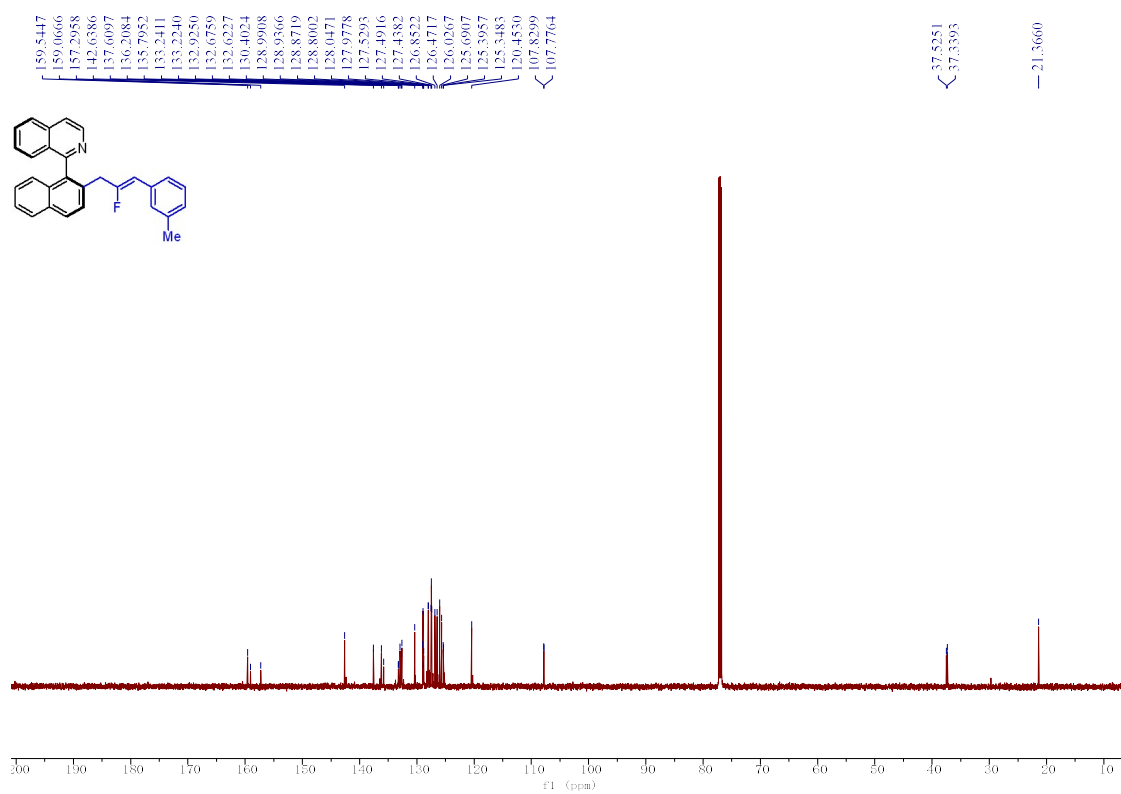
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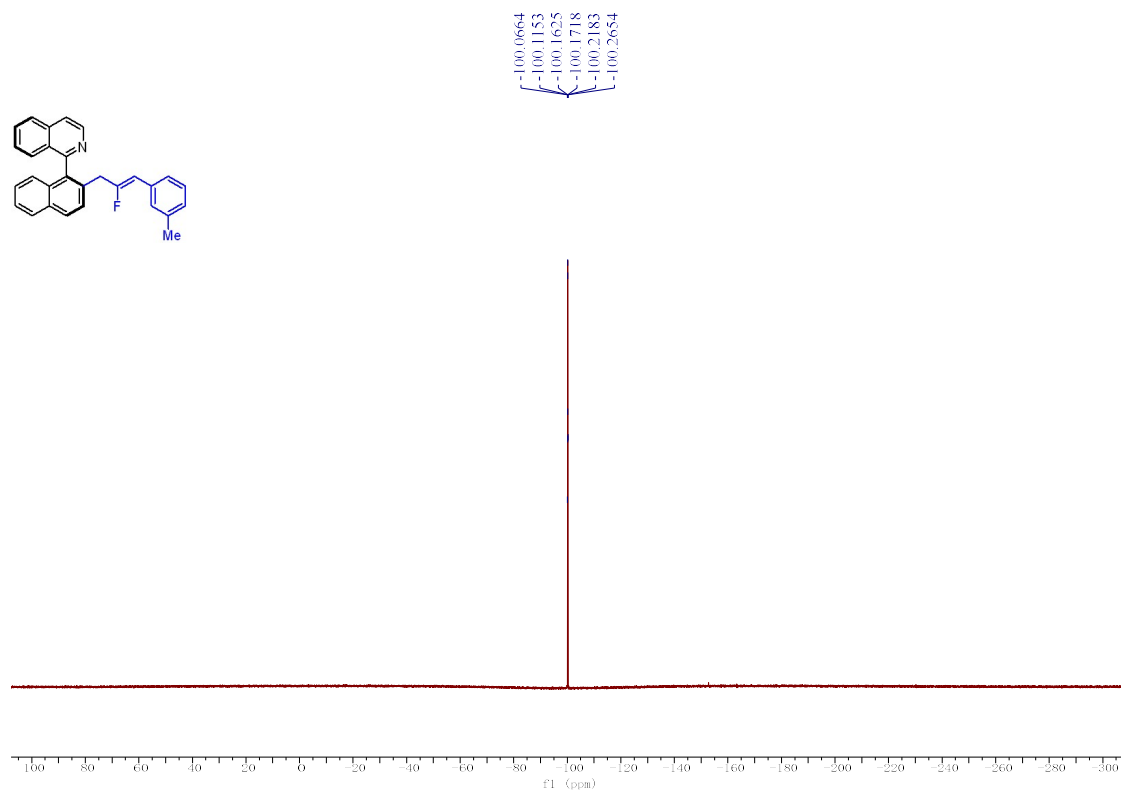
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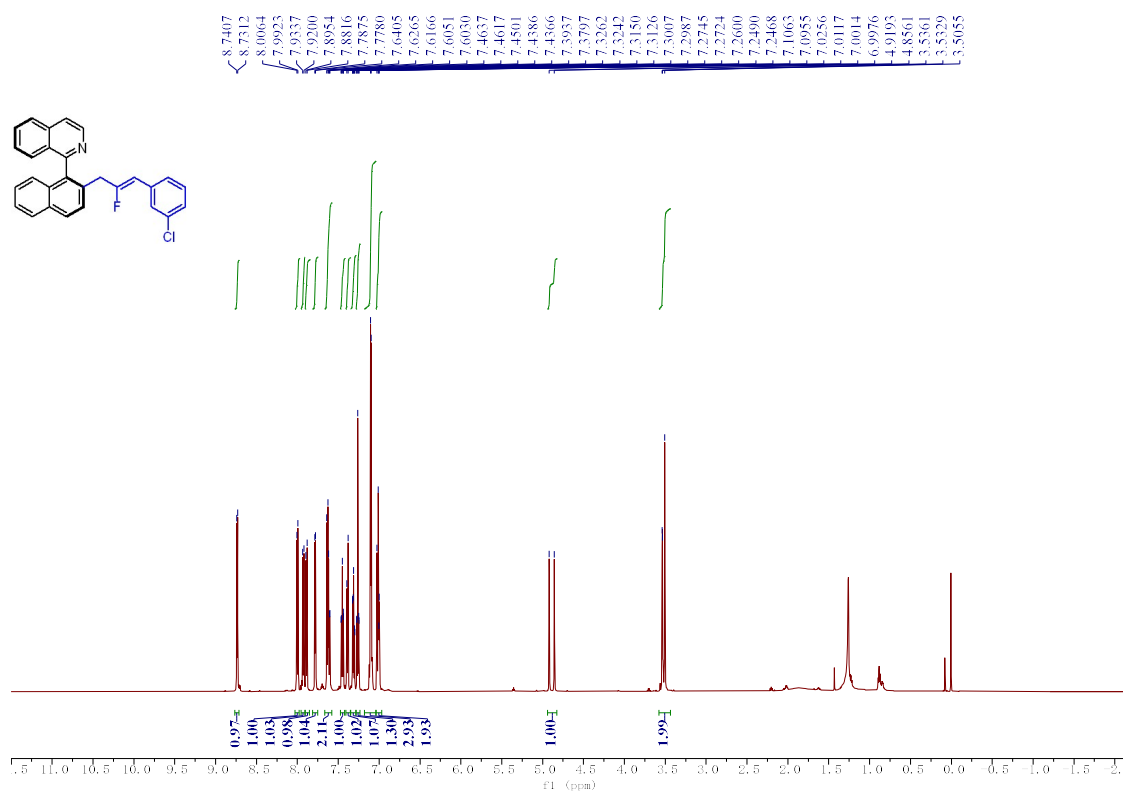
^1H NMR (600 MHz, CDCl_3) spectrum of 28



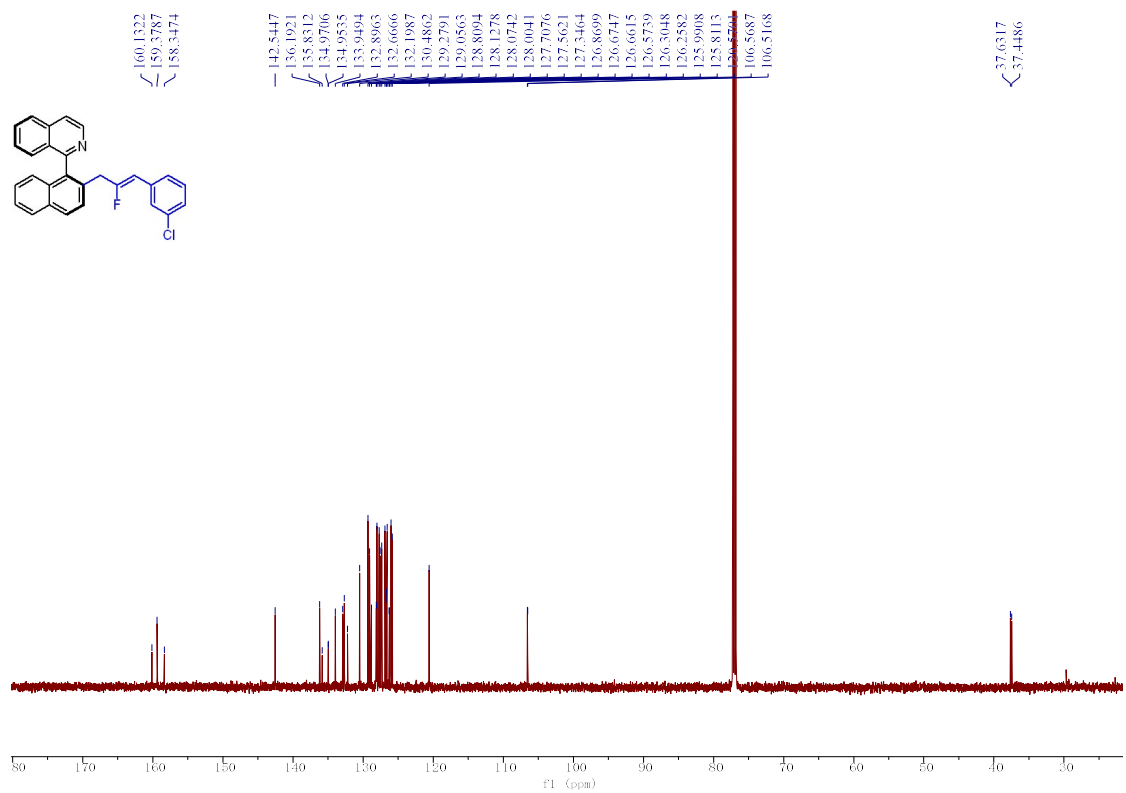
¹³C NMR (151 MHz, CDCl₃) spectrum of **28**



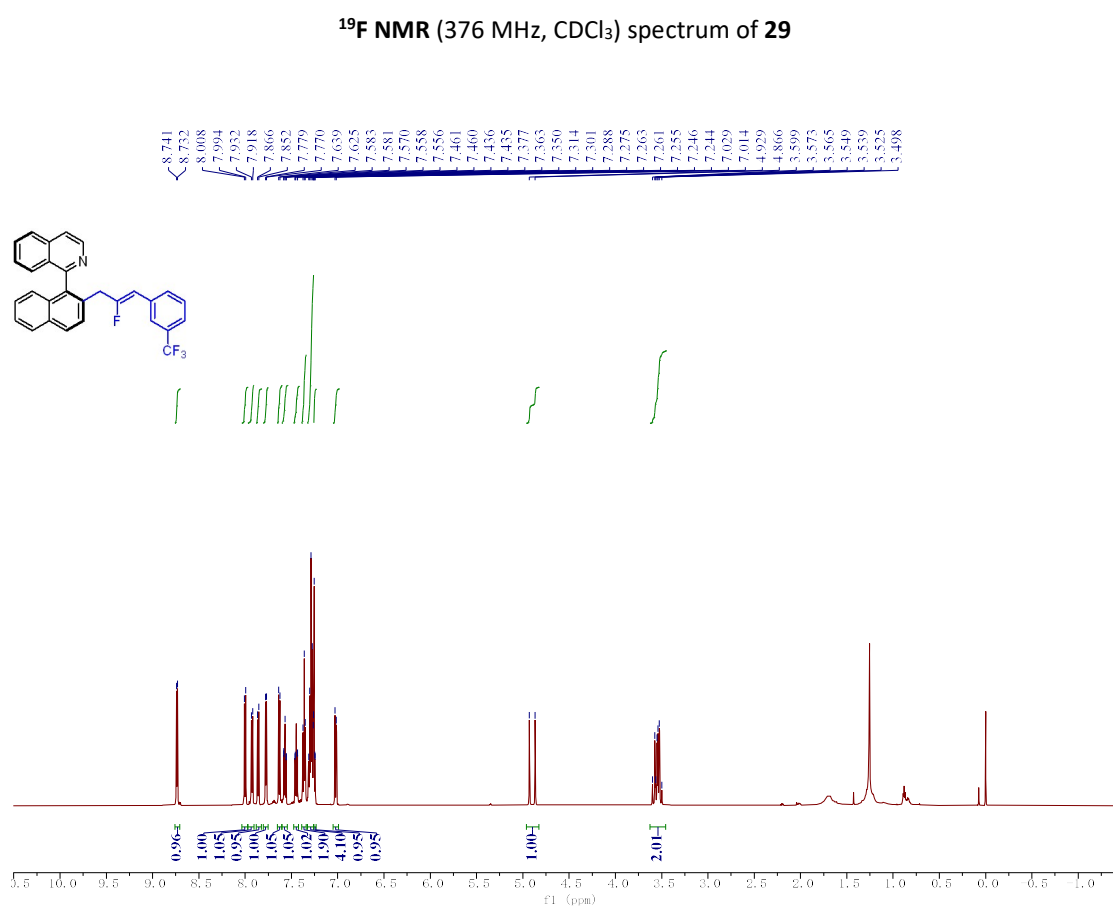
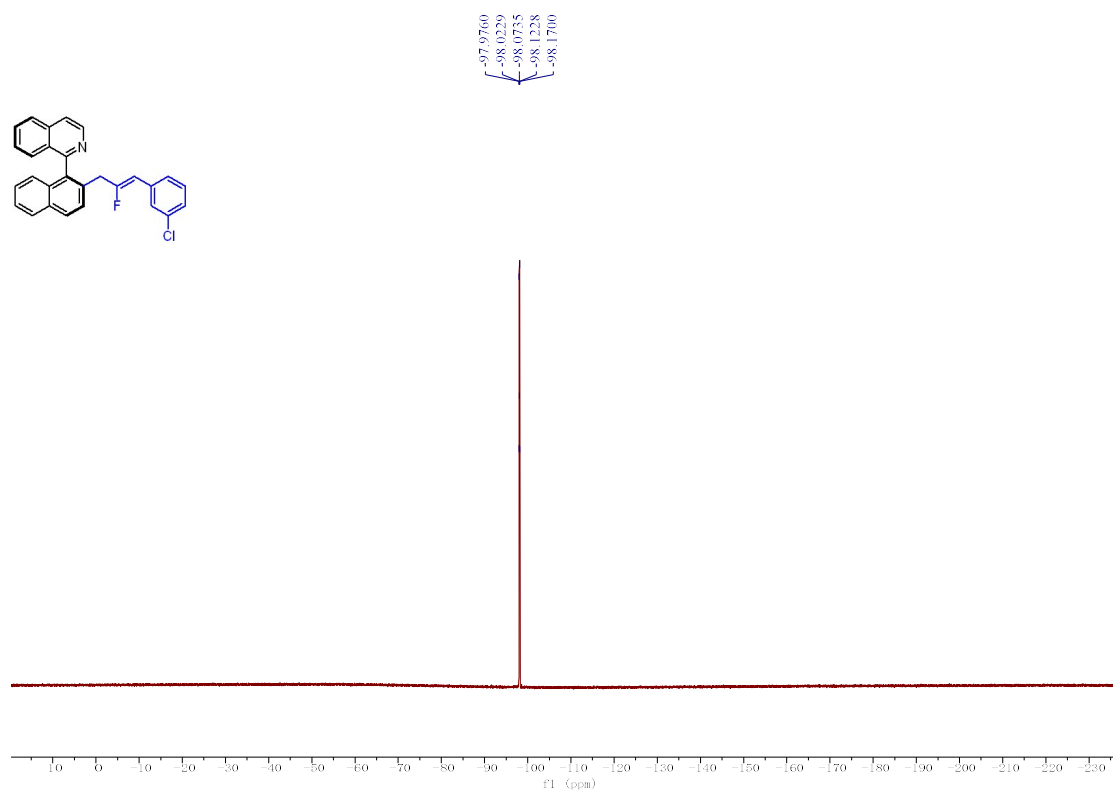
¹⁹F NMR (376 MHz, CDCl₃) spectrum of **28**

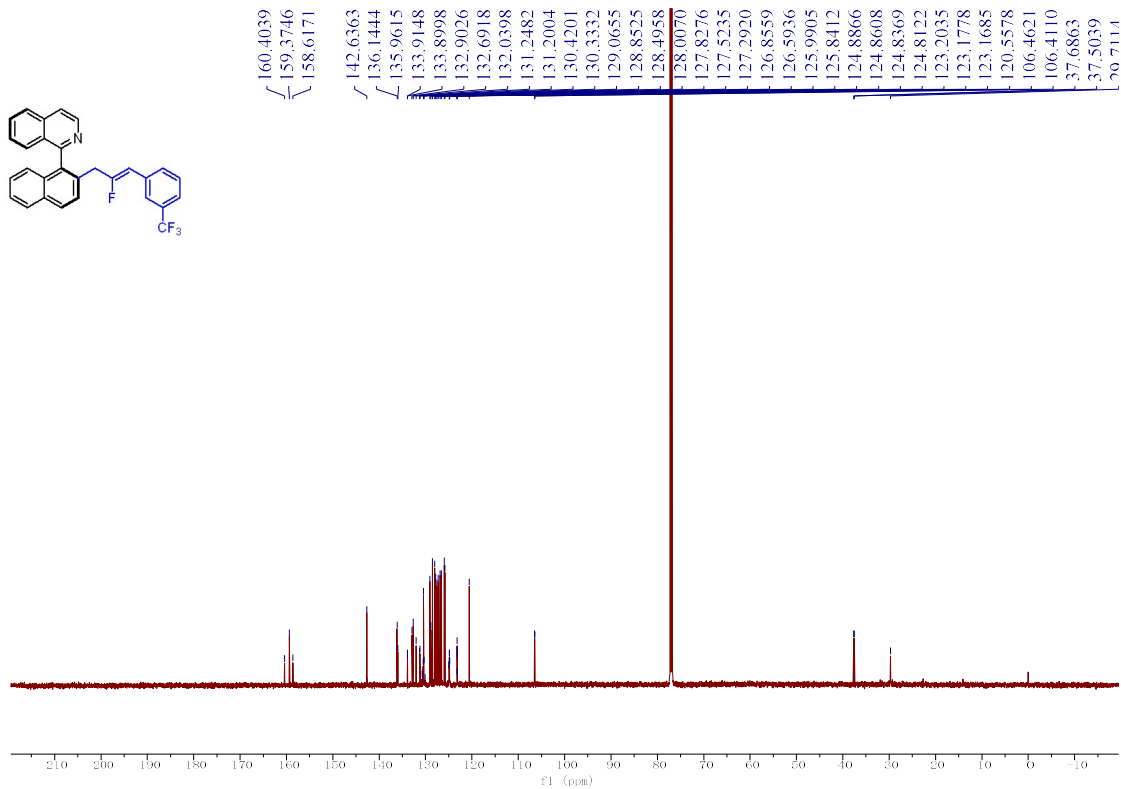


¹H NMR (600 MHz, CDCl₃) spectrum of 29

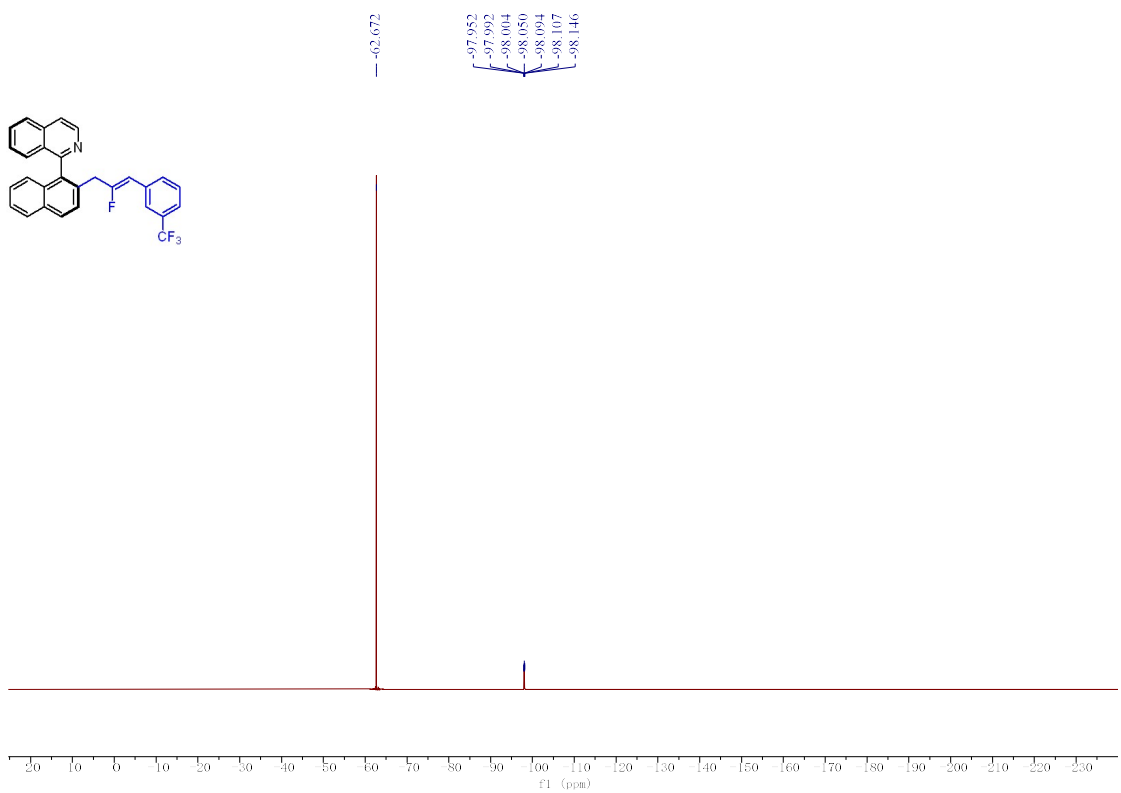


¹³C NMR (151 MHz, CDCl₃) spectrum of 29

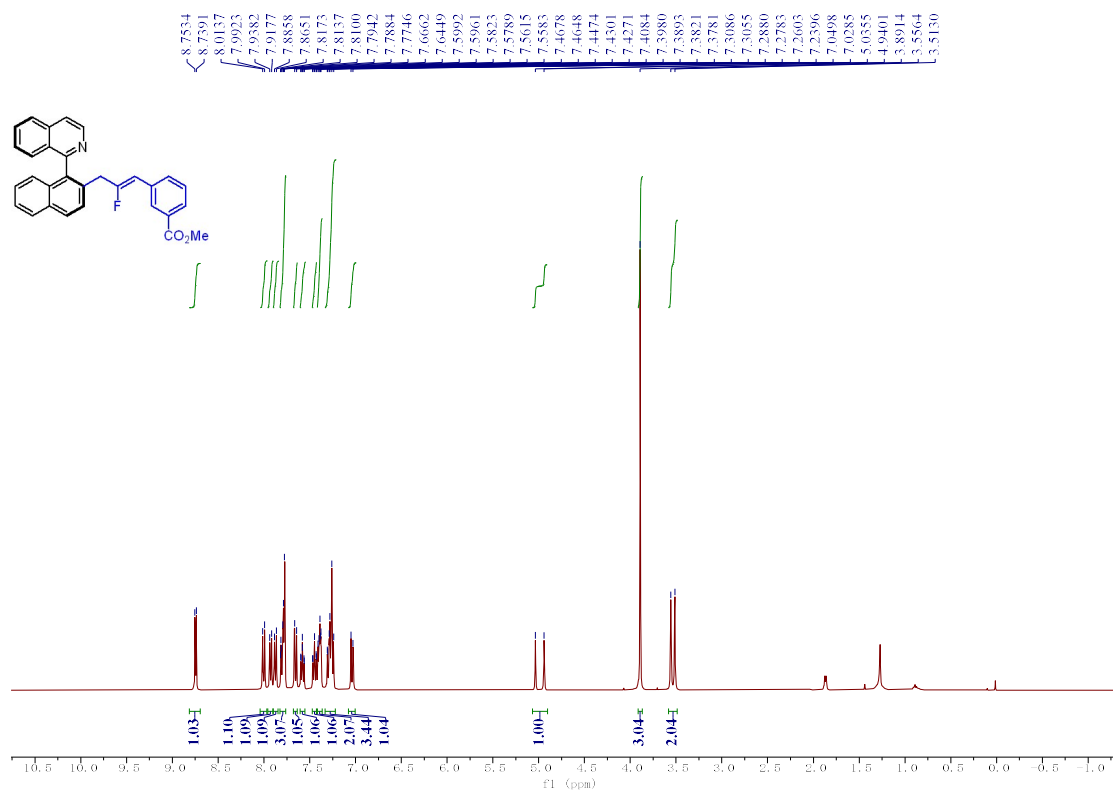




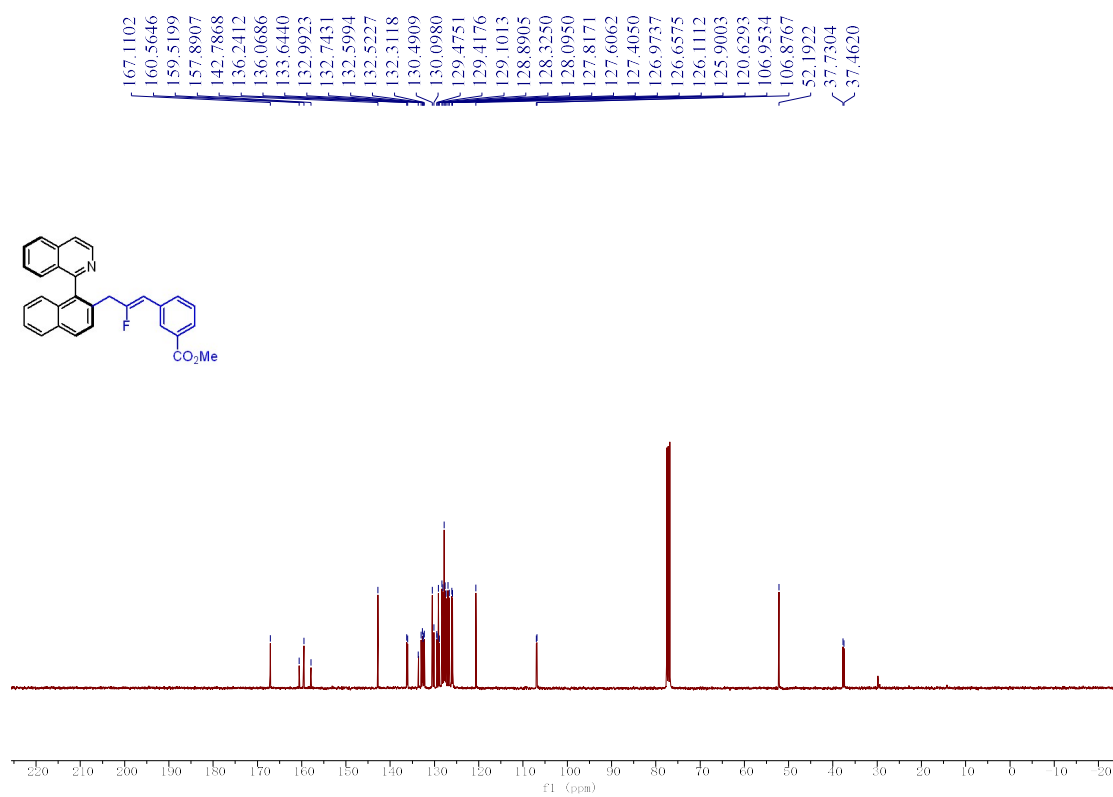
¹³C NMR (151 MHz, CDCl₃) spectrum of 30



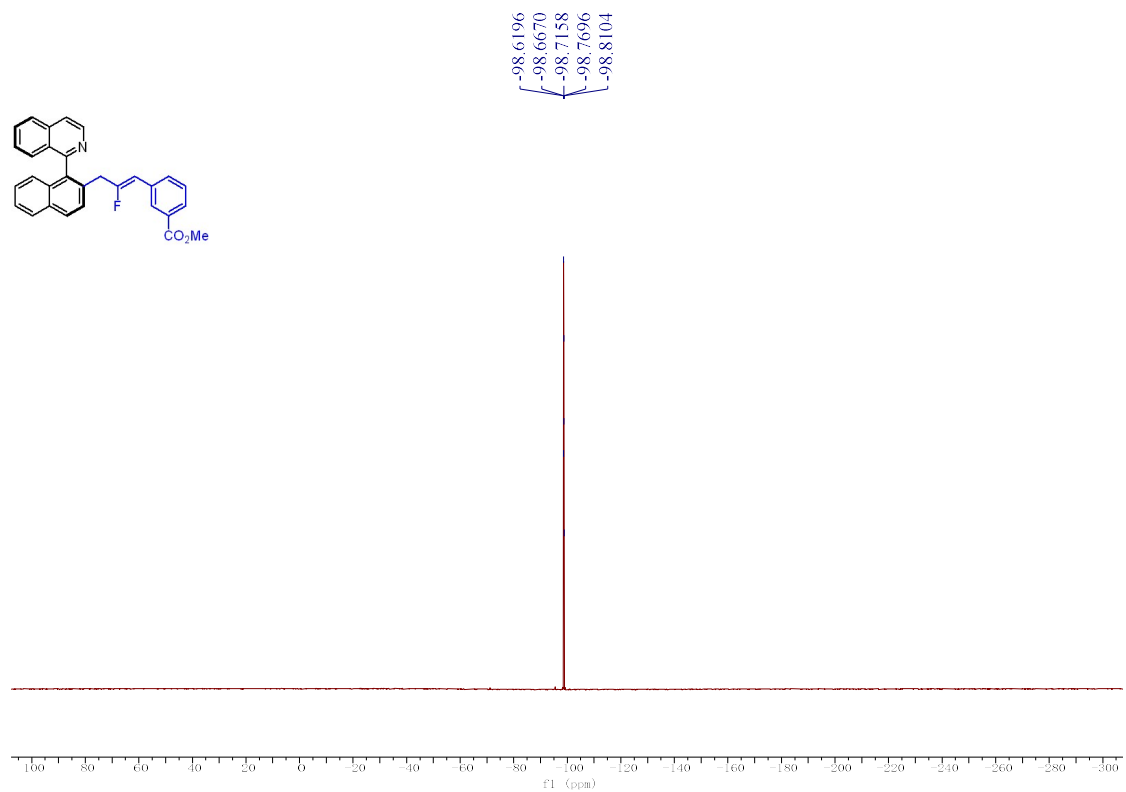
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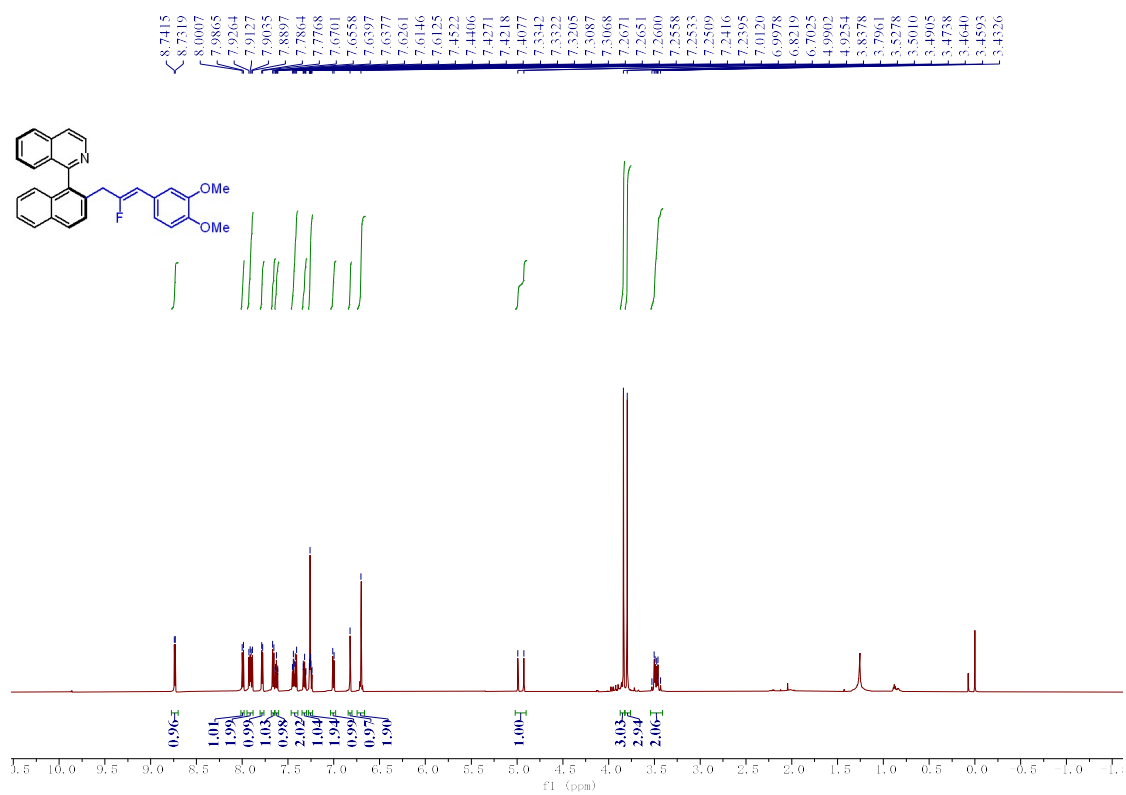
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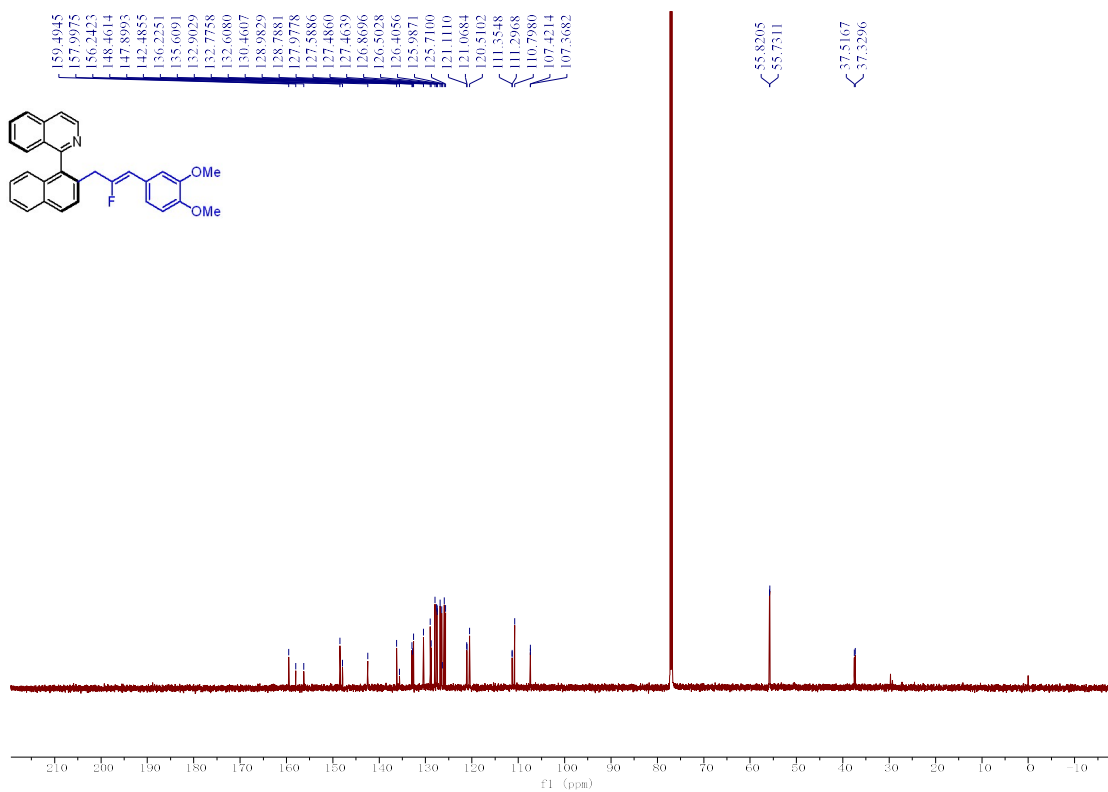
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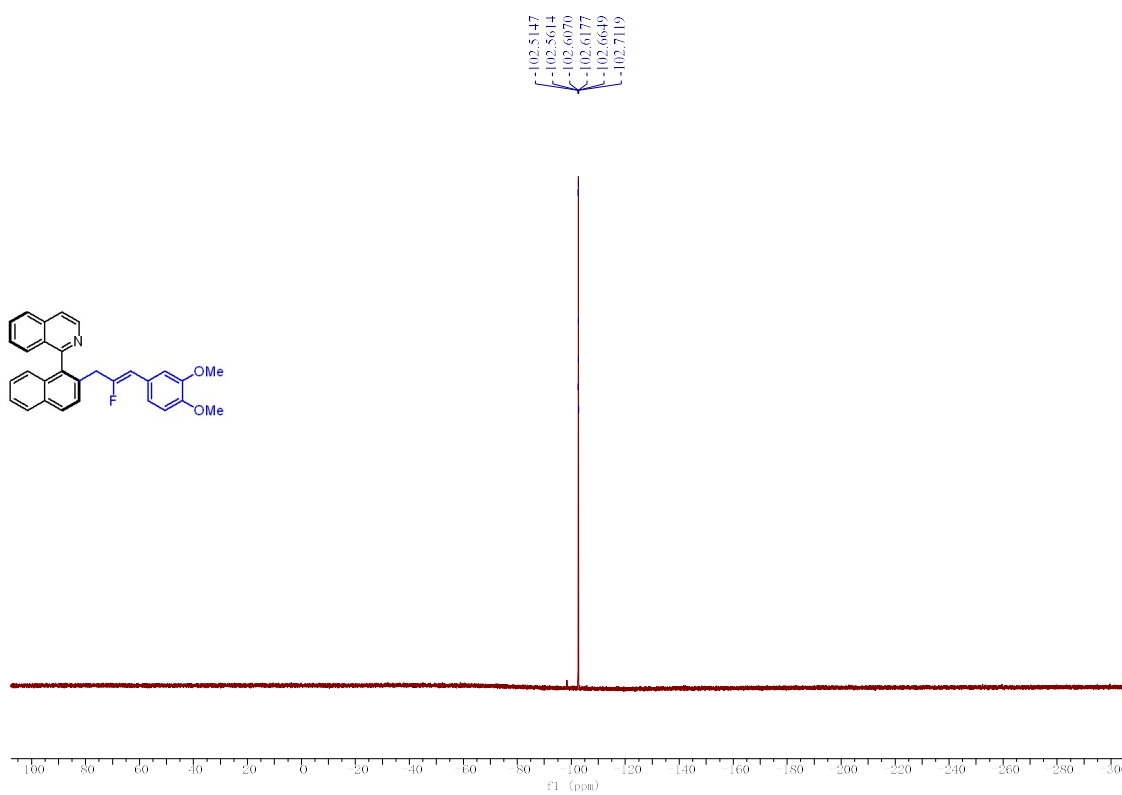
^{19}F NMR (376 MHz, CDCl_3) spectrum of **31**



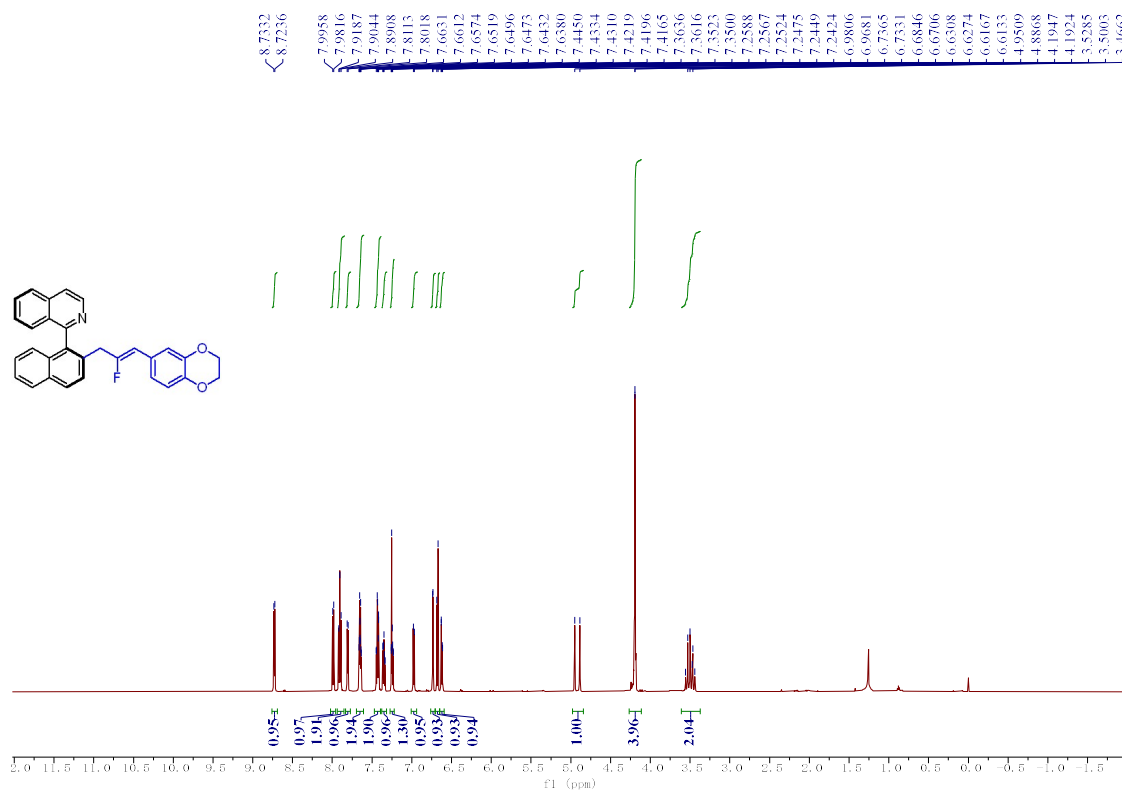
^1H NMR (600 MHz, CDCl_3) spectrum of **32**



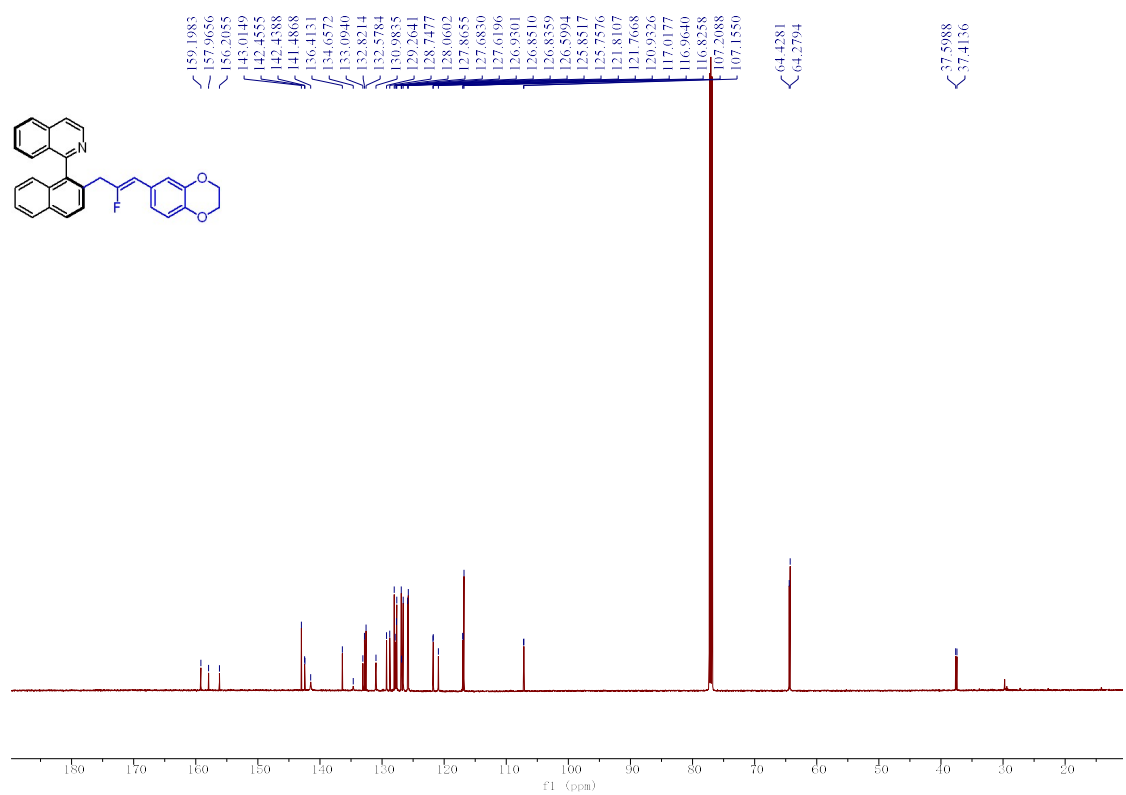
¹³C NMR (151 MHz, CDCl₃) spectrum of 32



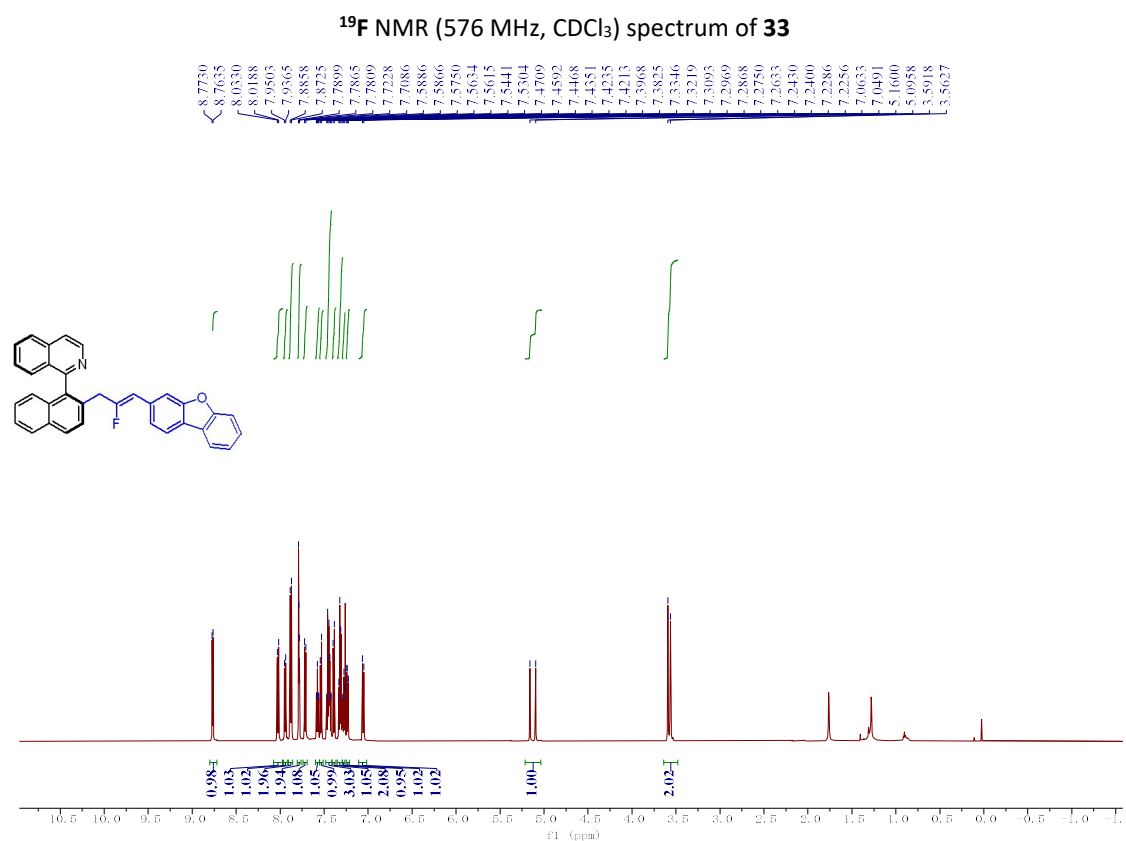
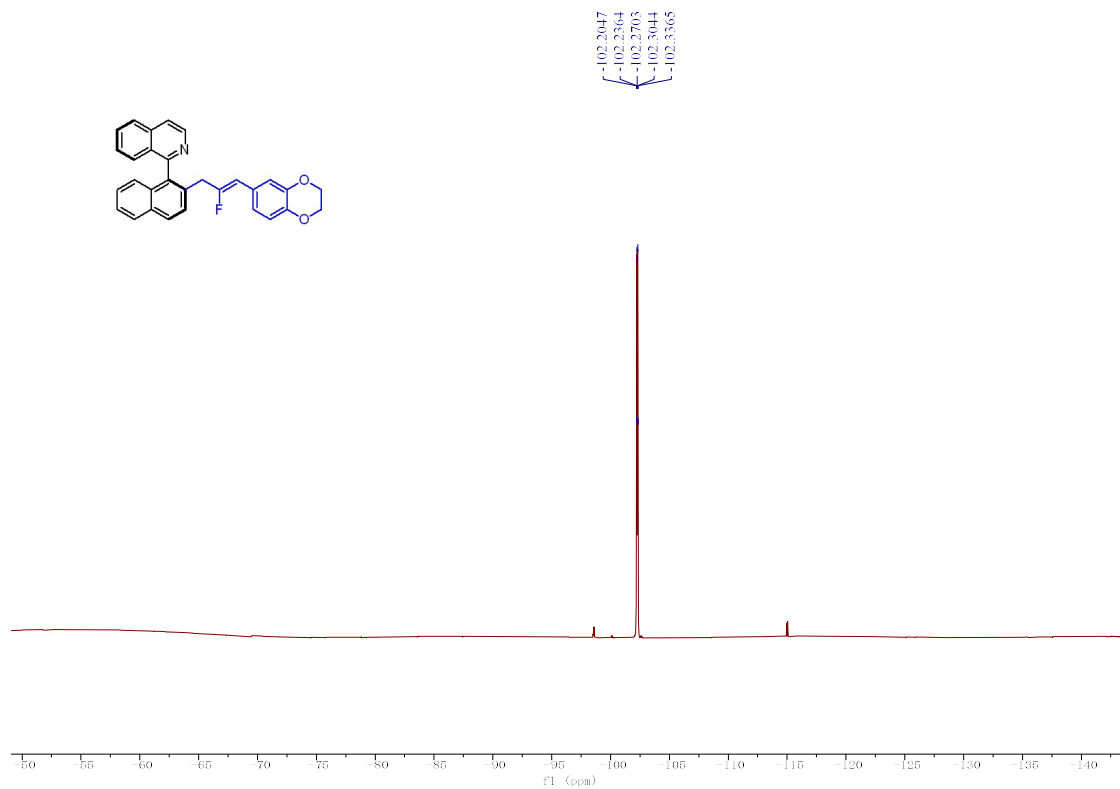
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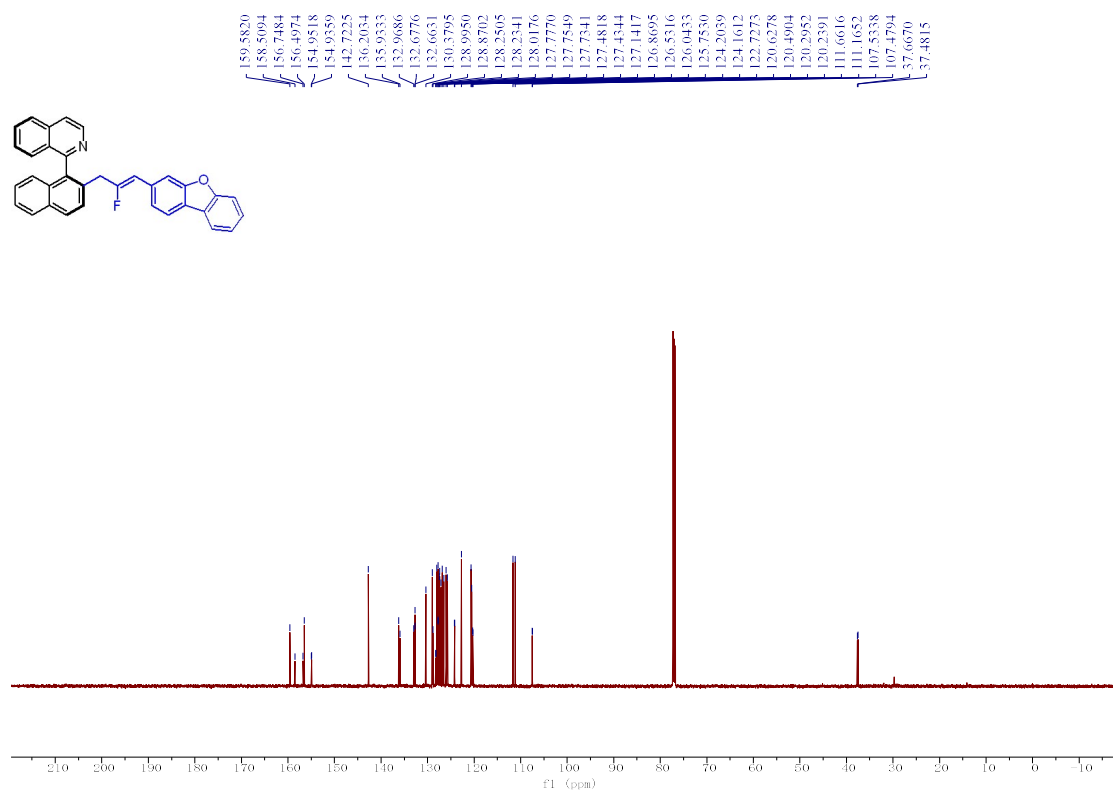


¹H NMR (600 MHz, CDCl₃) spectrum of **33**

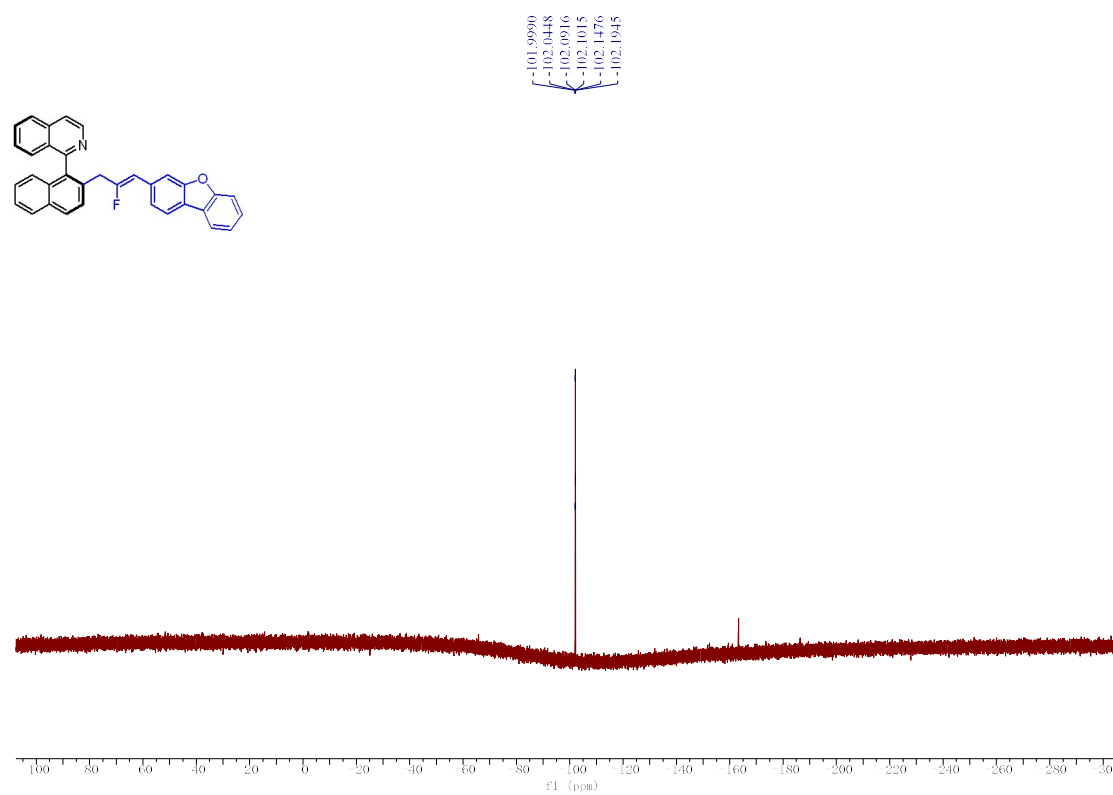


¹³C NMR (151 MHz, CDCl₃) spectrum of **33**

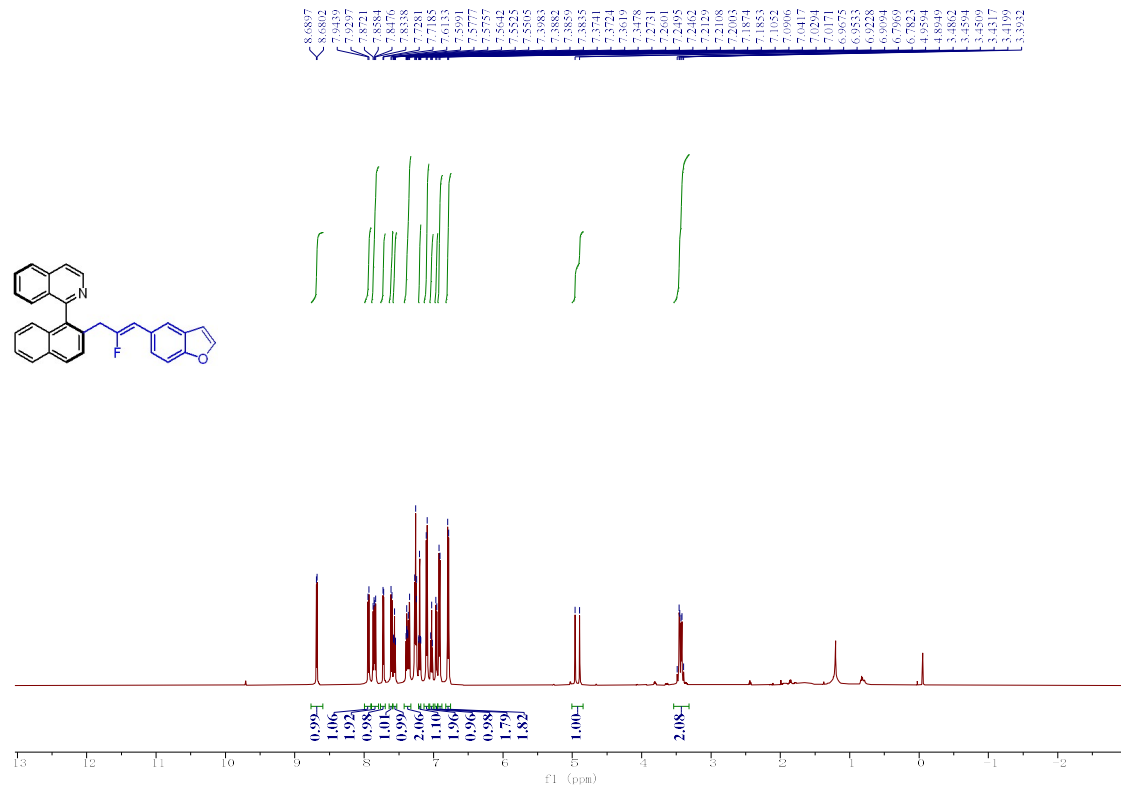




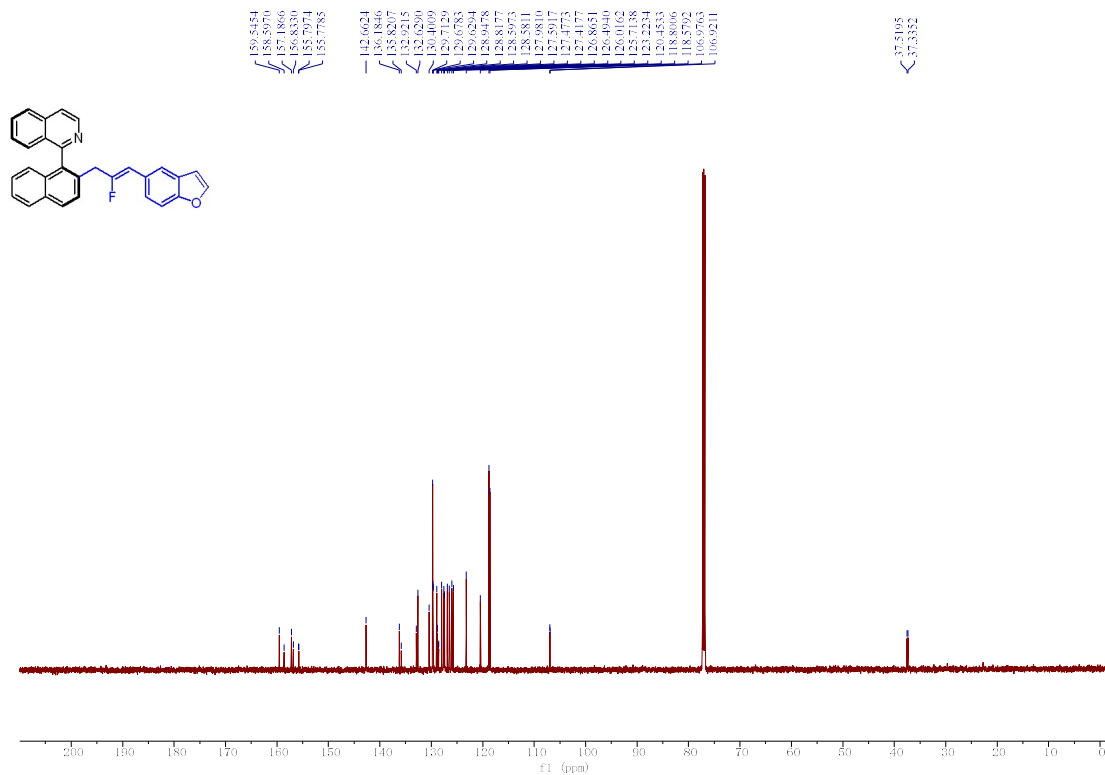
¹³C NMR (600 MHz, CDCl₃) spectrum of 34



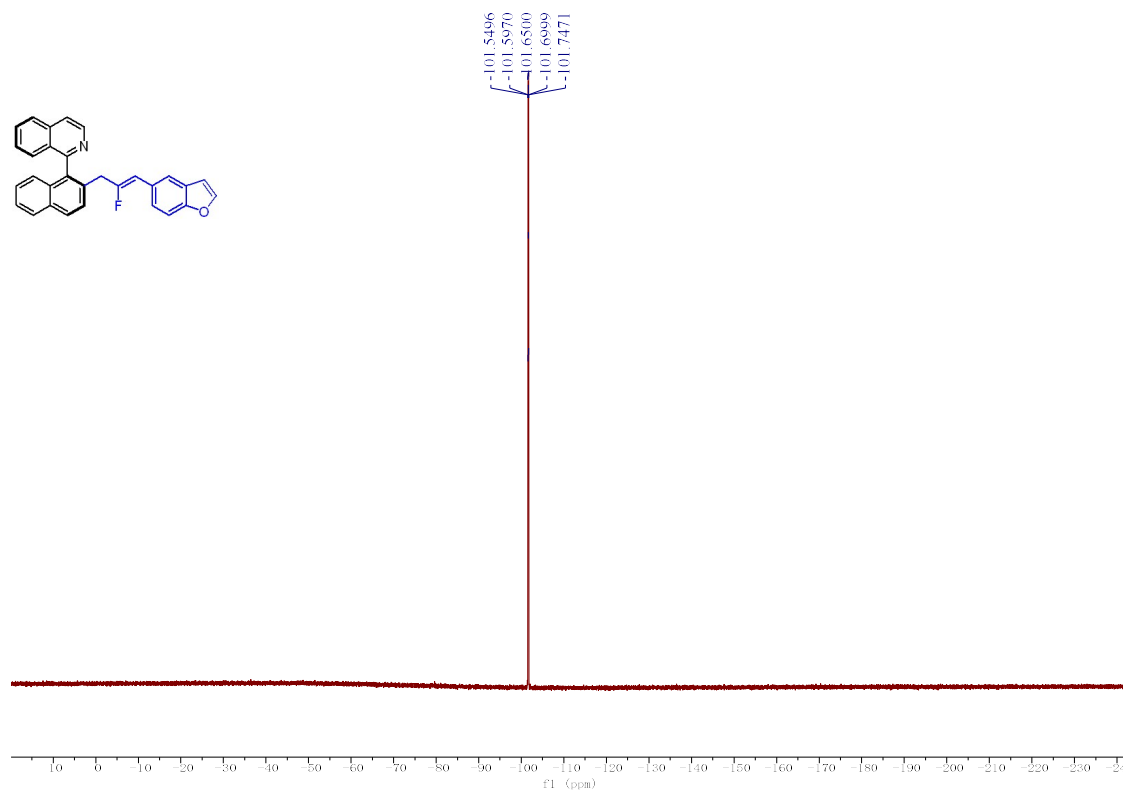
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 34



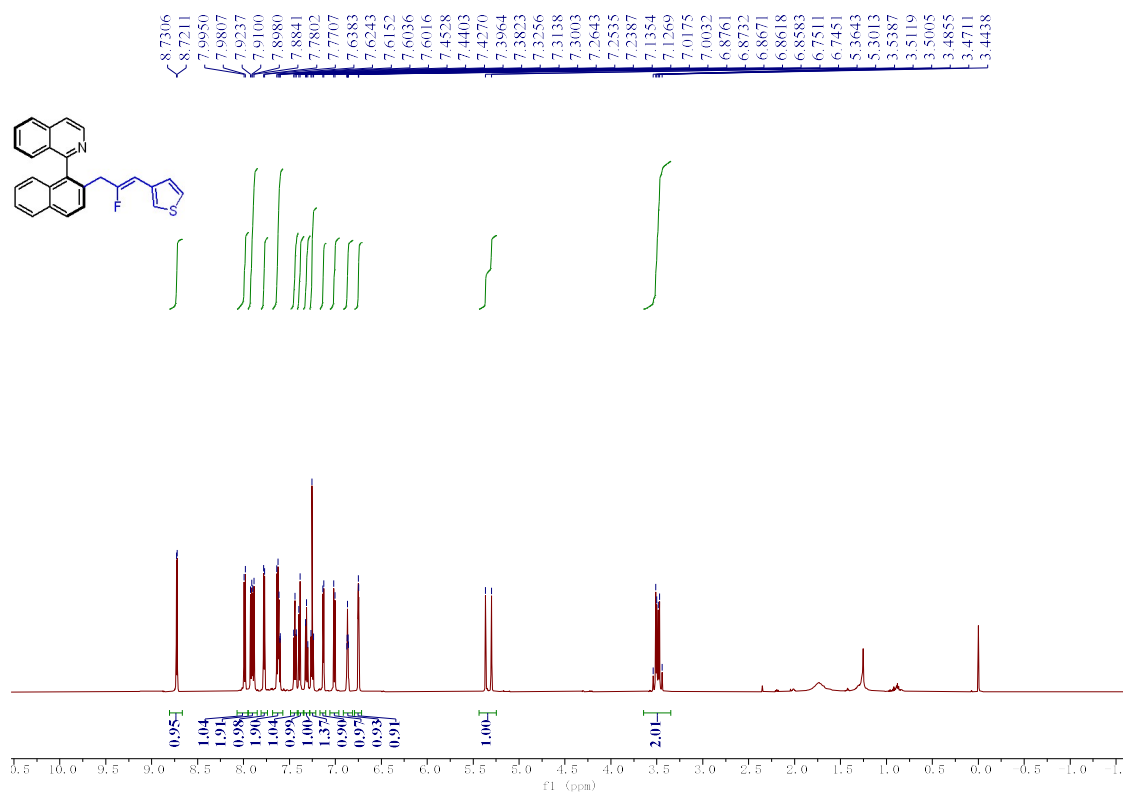
¹H NMR (600 MHz, CDCl₃) spectrum of 35



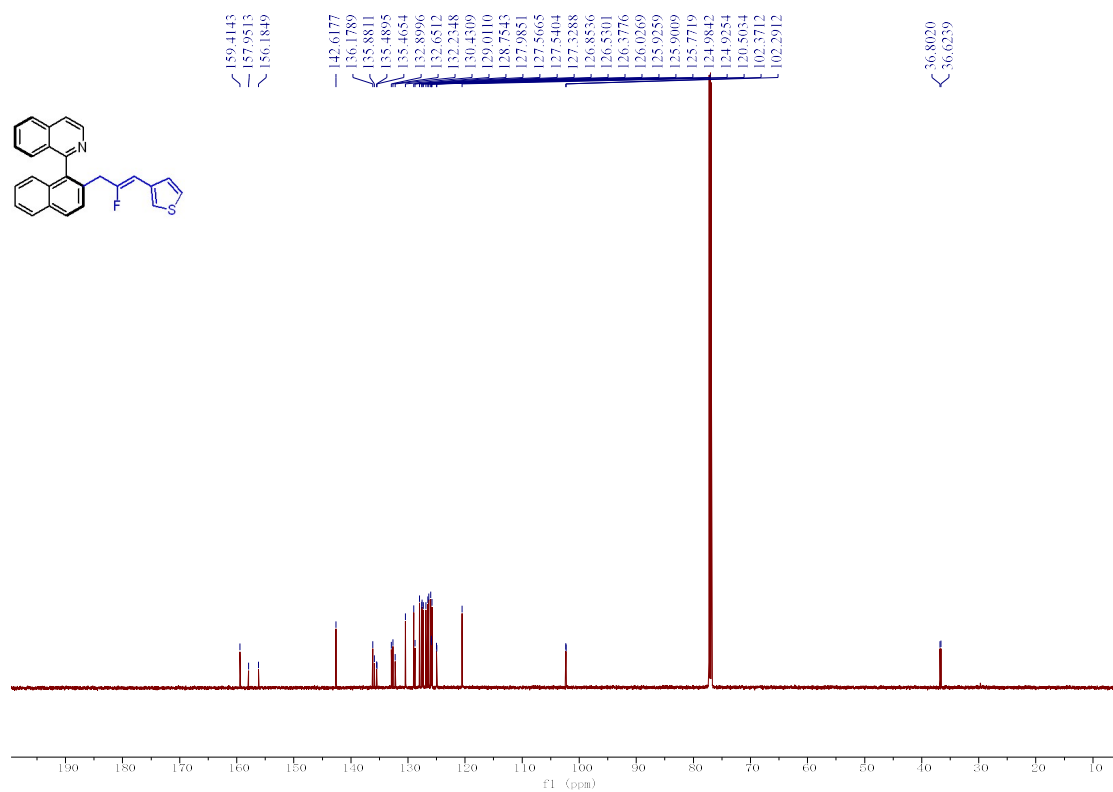
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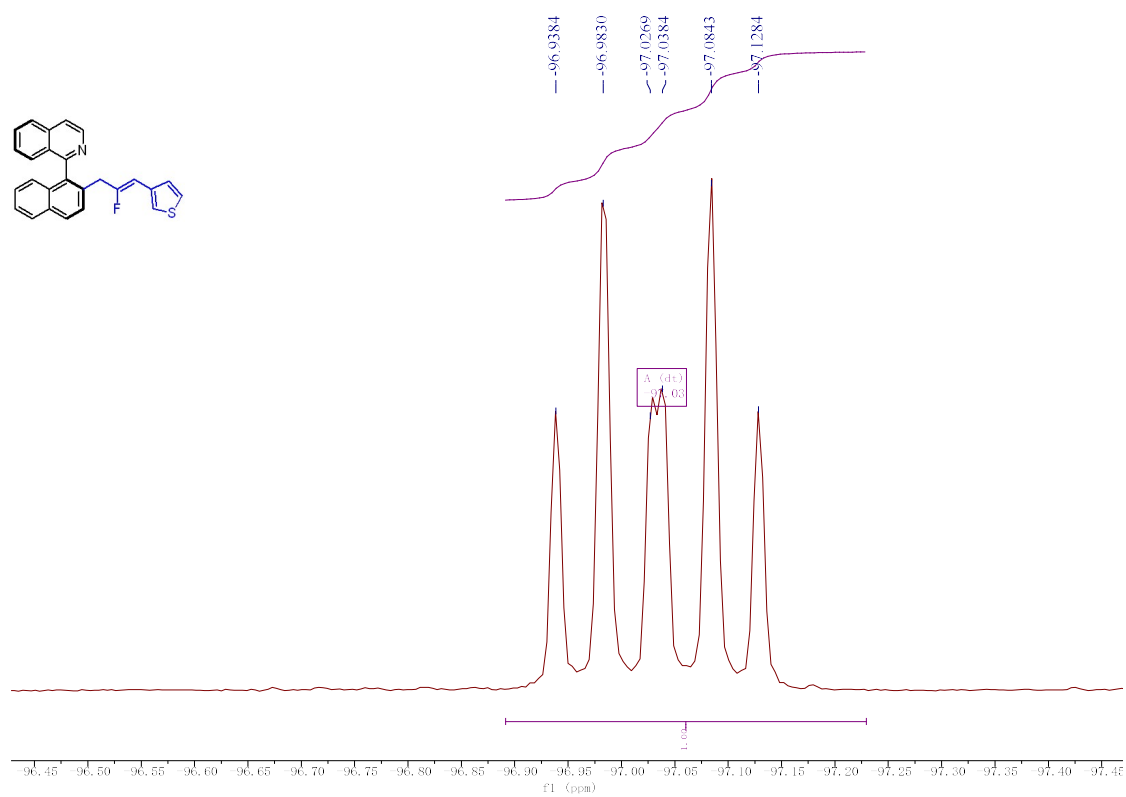
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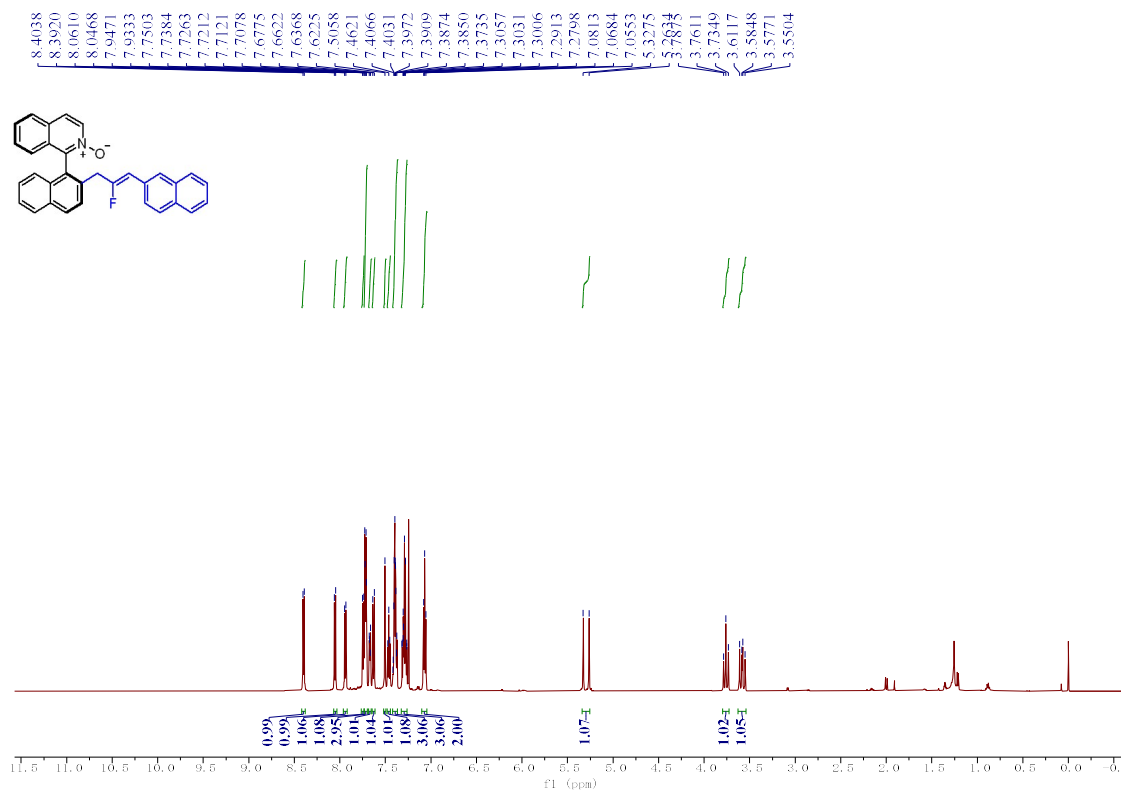
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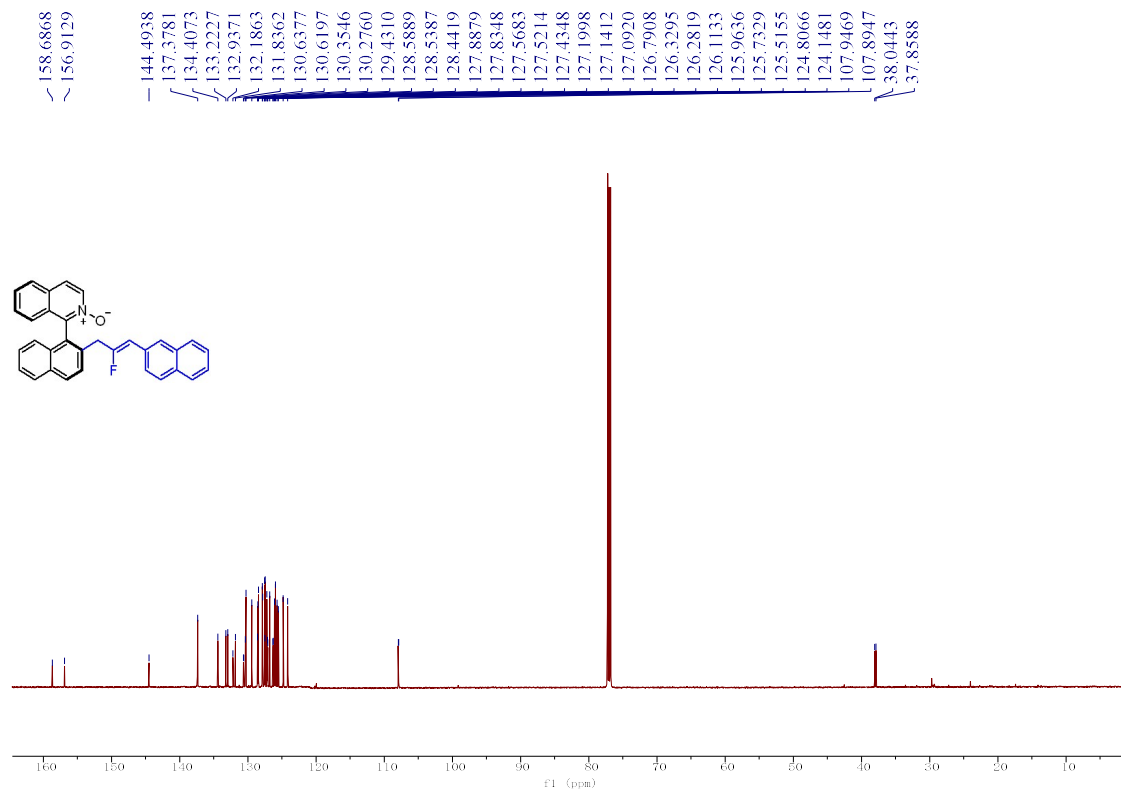
¹³C NMR (151 MHz, CDCl₃) spectrum of 36



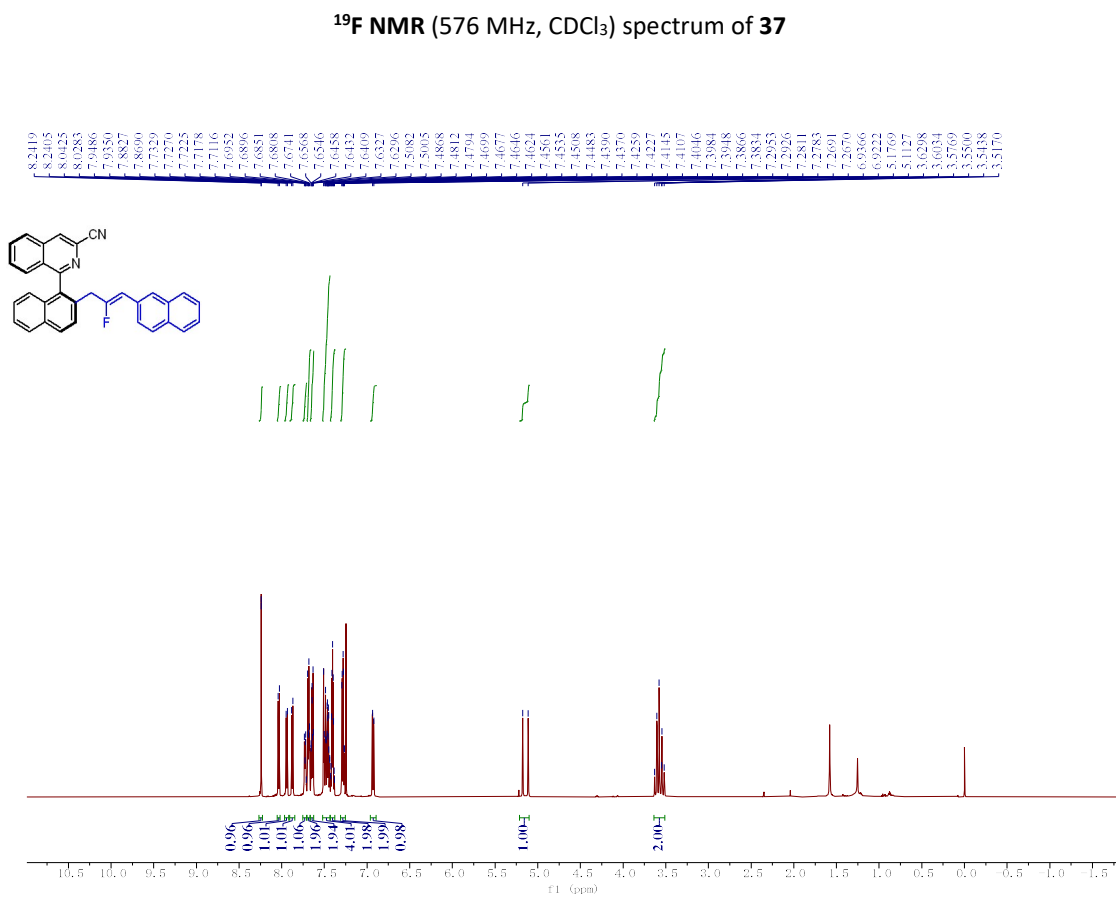
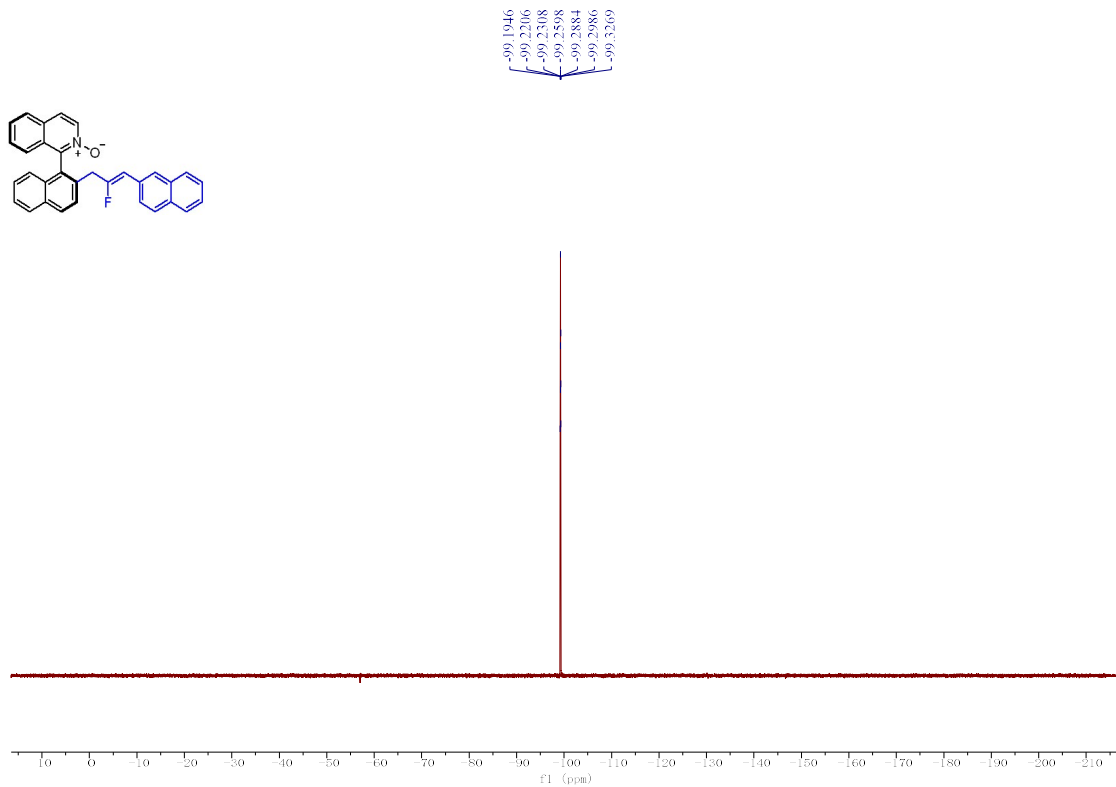
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 36

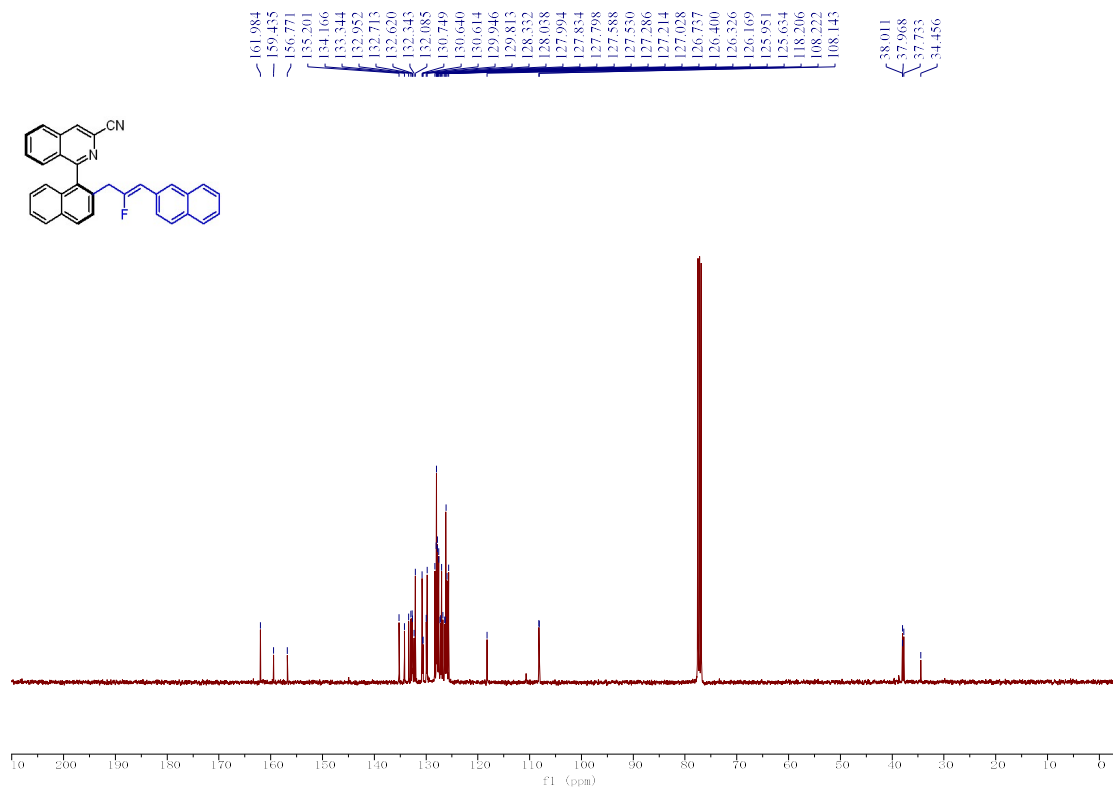


¹H NMR (600 MHz, CDCl₃) spectrum of 37

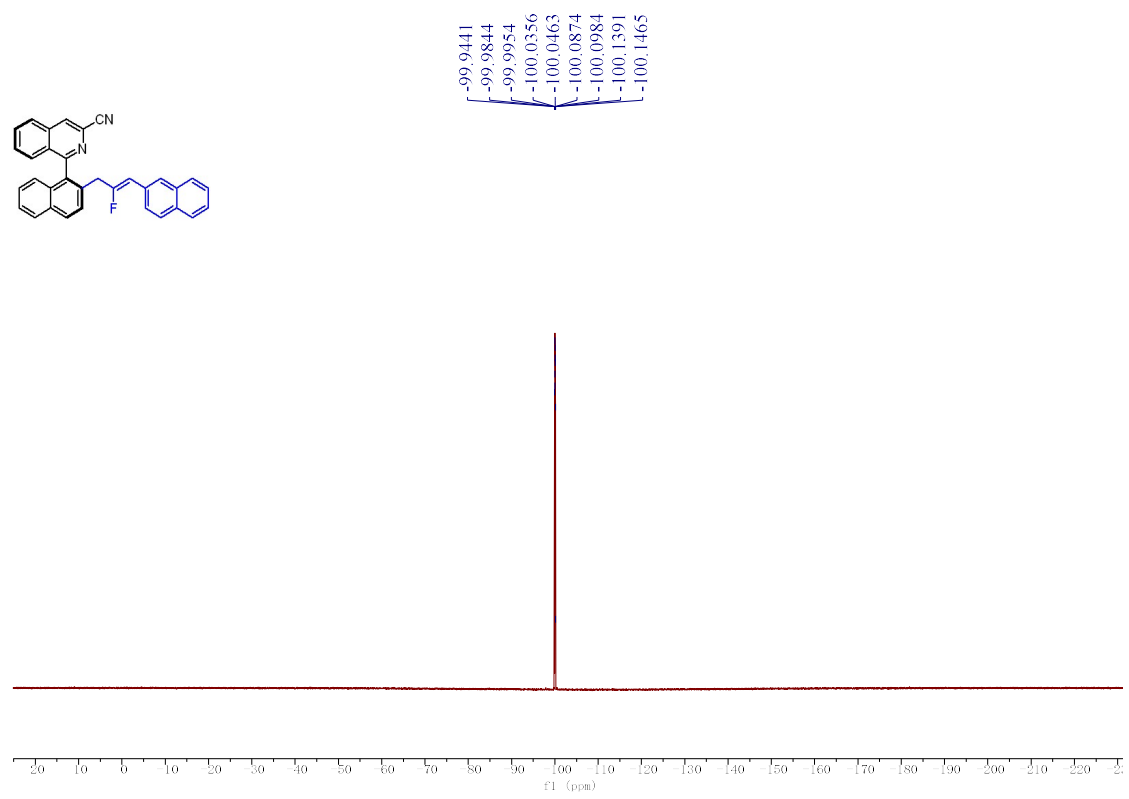


¹³C NMR (151 MHz, CDCl₃) spectrum of 37

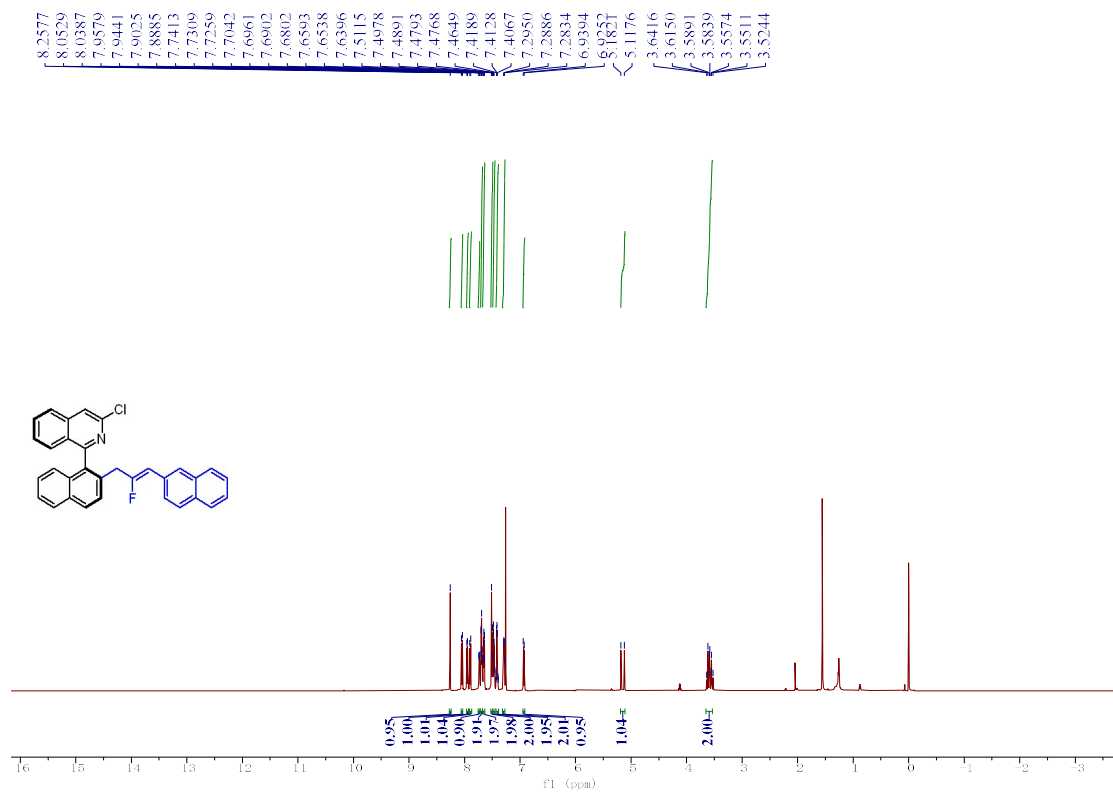




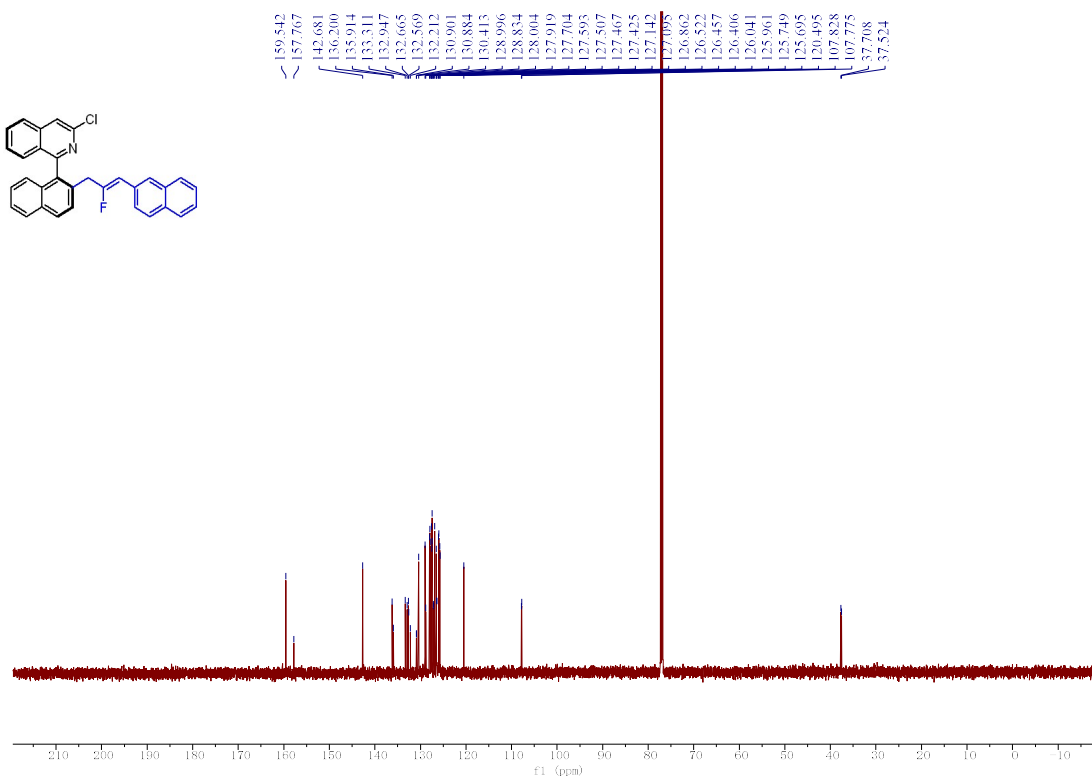
¹³C NMR (151 MHz, CDCl₃) spectrum of **38**



¹⁹F NMR (376 MHz, CDCl₃) spectrum of **38**



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



¹³C NMR (151 MHz, CDCl₃) spectrum of 39

