Supporting Information

Organocatalytic asymmetric cascade bicyclization: Access to chiral polycyclic bisindoles from 2-indolylmethanols and propargylic alcohols

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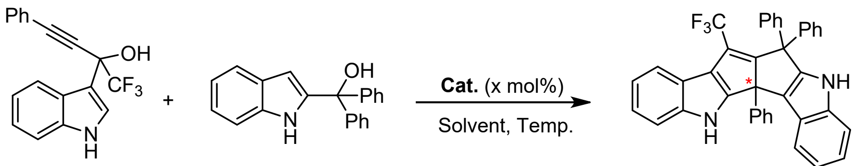
1. General Information

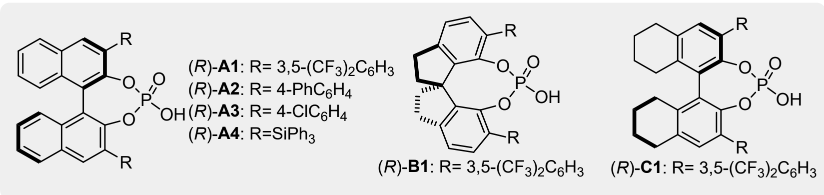
All reactions were carried out in oven-dried reaction vessel unless otherwise noted and solvents were dried according to established procedures. Reactions were monitored by thin layer chromatography (TLC). Purification of reaction product was carried out by flash chromatography using Qing Dao Sea Chemical Reagent silica gel (200-300 mesh). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on Bruker 400 MHz or 500 MHz spectrometer in $CDCl_3$ unless otherwise noted. Chemical shifts in ^{1}H NMR spectra are reported in parts per million (ppm, δ) downfield from the internal standard Me_4Si (TMS, δ = 0 ppm). Chemical shifts in ^{13}C NMR spectra are reported relative to the central line of the chloroform signal (δ = 77.0 ppm). Data are presented as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet) and coupling constant in Hertz (Hz). HPLC analyses were conducted on an Agilent instrument using Daicel Chiralpak IA, IB, AD-H or Chiralcel OD-H columns. High resolution mass spectra were obtained with a Shimadzu LCMS-IT-TOF mass spectrometer. The single crystal X-ray diffraction studies were carried out on a Xcalibur Onyx Nova diffractometer equipped with CuK/α radiation.

Substrates **1** and **2** were synthesized according to the literature method.[1]

2. Screening of Catalysts and Condition Optimization

Table S1. Screening of catalysts and optimization of reaction conditions[a]





Entry	Catalyst (x mol%)	Solvent (x mL)	**1a**: **2a**	Temperature (°C)	Additive (x mg)	Time	Yield[b] (%)	*er*[c]
1	**DPP** (10)	DCM (1)	1:1	RT	--	12h	89	50:50
2	(*R*)-**A1** (10)	DCM (1)	1:1	RT	--	36h	60	90:10
3	(*R*)-**A2** (10)	DCM (1)	1:1	RT	--	12h	86	57:43
4	(*R*)-**A3** (10)	DCM (1)	1:1	RT	--	12h	78	52:48
5	(*R*)-**A4** (10)	DCM (1)	1:1	RT	--	96h	30	40:60
6	(*R*)-**B1** (10)	DCM (1)	1:1	RT	--	96h	25	93:7
7	(*R*)-**C1** (10)	DCM (1)	1:1	RT	--	48h	56	93:7
8	(*R*)-**C1** (10)	Tol (1)	1:1	RT	--	48h	80	88:12
9	(*R*)-**C1** (10)	DCE (1)	1:1	RT	--	72h	65	93:7
10	(*R*)-**C1** (10)	$CHCl_3$ (1)	1:1	RT	--	72h	46	61:19

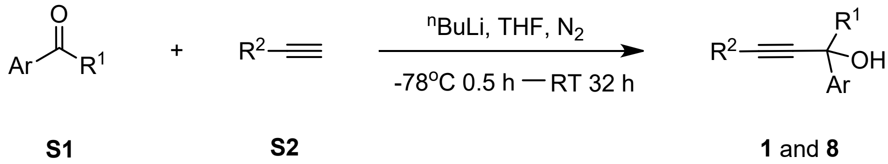
11	(*R*)-**C1** (10)	CCl_4 (1)	1:1	RT	--	72h	86	89:11
12	(*R*)-**C1** (10)	Mesitylene (1)	1:1	RT	--	24h	65	78:22
13	(*R*)-**C1** (10)	$PhCF_3$ (1)	1:1	RT	--	24h	86	85:15
14	(*R*)-**C1** (10)	PhCl (1)	1:1	RT	--	48h	85	90:10
15	(*R*)-**C1** (10)	$CHCl_2CHCl_2$ (1)	1:1	RT	--	72h	45	86:14
16	(*R*)-**C1** (10)	DCM (1)	1:1	10	--	5d	30	90:10
17	(*R*)-**C1** (10)	DCM (1)	1:1	20	--	5d	40	92:8
18	(*R*)-**C1** (10)	DCM (1)	1:1.2	RT	--	36h	60	95:5
19	(*R*)-**C1** (10)	DCM (1)	1:1	RT	$B(C_6F_5)_3$ (5 mol%)	36h	55	73:27
20	(*R*)-**C1** (10)	DCM (1)	1:1	RT	HFIP (60 mol%)	48h	56	87:13
21	(*R*)-**C1** (10)	DCM/Tol=1:1 (1)	1:1	RT	--	48h	75	93:7
22	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	--	5d	72	93:7
23	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	$MgSO_4$ (25)	3d	75	93:7
24	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	Na_2SO_4 (25)	3d	60	93:7
25	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	3Å MS (25)	5d	trace	--
26	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	4Å MS (25)	5d	trace	--
27	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	5Å MS (25)	5d	45	97:3
28	(*R*)-**C1** (10)	DCM/PhCl=3:1 (1)	1:1	RT	--	3d	75	93:7
29	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	--	4.5d	72	93:7
30	(*R*)-**C1** (10)	DCM/CCl_4=3:1 (1)	1:1	RT	--	4.5d	80	90:10
31	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	RT	--	6d	85	94:6
32	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	RT	--	4.5d	86	93.5:6.5
33	(*R*)-**C1** (10)	DCE/CCl_4=1:1 (1)	1:1	RT	--	4.5d	89	93.5:6.5
34	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	RT	--	3d	85	93:7
35	(*R*)-**C1** (10)	DCM:Tol=3:1 (1)	1:1	RT	--	3d	90	90:10
36	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	--	3d	90	90:10
37	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	5Å MS (30)	5d	45	97:3
38	(*R*)-**C1** (10)	DCM/Tol=3:1 (1)	1:1	RT	5Å MS (15)	5d	43	97:3
39	(*R*)-**C1** (10)	DCM/CCl_4=3:1 (1)	1:1	RT	5Å MS (15)	9d	34	96:4

40	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	RT	5Å MS (15)	12d	<5	--
41	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	30	5Å MS (15)	10d	40	97.5:2.5
42	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	40	5Å MS (15)	3d	45	97.5:2.5
43	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	50	5Å MS (15)	3d	40	97.5:2.5
44	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	40	5Å MS (3)	3d	82	96:4
45	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	40	5Å MS (1)	3d	90	96:4
46	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	30	$MgSO_4$ (30)	4.5d	85	96.5:3.5
47	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	30	Na_2SO_4 (30)	4.5d	85	96:4
48	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (0.6)	1:1	40	5Å MS (1)	3d	87	95:5
49	**(*R*)-C1 (10)**	**DCE/CCl_4=1:1 (1)**	**1:1**	**40**	**5Å MS (1)**	**2d**	**83**	**96:4**
50	(*R*)-**C1** (10)	DCE/CCl_4=1:1 (0.6)	1:1	40	5Å MS (1)	2d	86	95:5
51	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1.2	40	5Å MS (1)	3d	78	96:4
52	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1.2:1	40	5Å MS (1)	3d	77	96:4
53	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (0.6)	1:1	30	$MgSO_4$ (30)	69h	78	95:5
54	**(*R*)-C1 (10)**	**DCE/CCl_4=1:1 (1)**	**1:1**	**30**	**$MgSO_4$ (30)**	**91h**	**82**	**96:4**
55	(*R*)-**C1** (10)	DCE/CCl_4=1:1 (0.6)	1:1	30	$MgSO_4$ (30)	69h	86	94:6
56	(*R*)-**C1** (10)	DCE/CCl_4=3:1 (1)	1:1	40	$MgSO_4$ (30)	45h	80	96:4

[a] Unless otherwise specified, all reactions were carried out with catalyst (x mol%), **1a** (0.05 mmol) and **2a** (0.05 mmol) in the indicated solvent (x mL) at room temperature. [b] Isolated yield of **3a**. [c] Determined by chiral-phase HPLC analysis.

3. Experimental Procedure and Characterization of Substrates

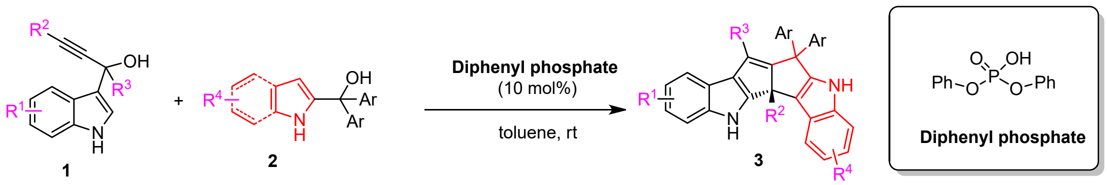
a. General Procedure to Prepare Substrates 1 and 8



At -78 °C, under N_2, to a flame-dried flask charged with a solution of the terminal alkyne **S2** (6 mmol, 3 equiv.) in dry THF (15 mL) was added ⁿBuLi (6 mmol, 2.5 mL, 2.4 M in hexane) dropwise. The reaction was stirred for 0.5 h at the same temperature and then a solution of the corresponding ketones **S1** (2 mmol, 1.0 equiv.) in THF (5 mL) was added via syringe. The reaction mixture was then slowly warmed up to room temperature and stirred for 32 h. Upon completion, the reaction mixture was cooled to 0 °C and a saturated aqueous NH_4Cl solution (7 mL) was added dropwise. The organic layer was separated. The aqueous layer was extracted with ethyl acetate (3×10 mL). The combined organic layers were washed with brine (30 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated. The crude product was purified directly by flash column chromatography on silica gel (petroleum ether/ ethyl acetate = 10:1~5:1) or recrystallization to give the desired propargylic alcohols **1** and **8**.

4. Experimental Procedure and Characterization of Products

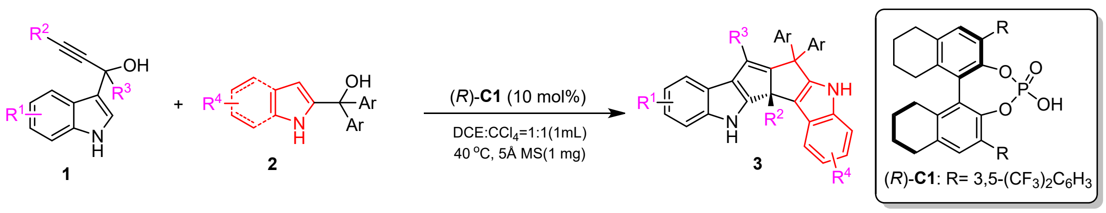
a. General Procedure to Prepare Racemic Products 3a-3w, 5, 7, 9



To a solution of *α*-indolyl propargylic alcohol **1** (0.10 mmol, 1.0 equiv.), and catalyst diphenyl phosphate (0.01 mmol, 10 mol%) in toluene (1 mL) was added 2-indolylmethanol **2** (0.01 mmol, 1.0 equiv.). The mixture was stirred at room temperature until the reaction was completed (monitored by TLC analysis). The crude product was purified directly by flash column chromatography on silica gel (petroleum ether/ ethyl acetate =30:1~20:1) to give the desired racemic products **3a-3w, 5, 7, 9**.

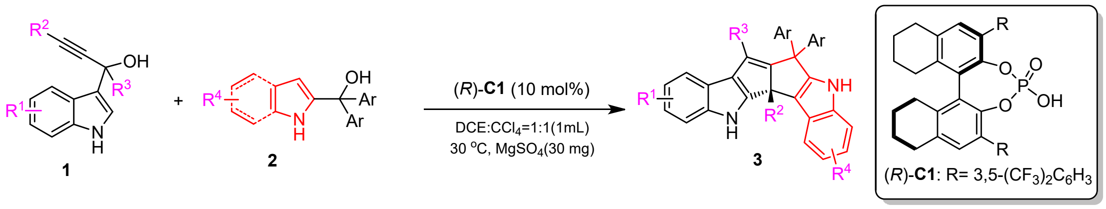
b. General Procedure to Prepare Chiral Products 3a-3w, 5, 7, 9

Conditions A:



To a solution of α-indolyl propargylic alcohol **1** (0.10 mmol, 1.0 equiv.), 1 mg 5Å MS and catalyst (*R*)-**C1** (0.01 mmol, 10 mol%) in DCE:CCl_4 (1 mL, v/v=1:1) was added 2-indolylmethanol **2** (0.01 mmol, 1.0 equiv.). The mixture was stirred at 40 °C until the reaction was completed (monitored by TLC analysis). The crude product was purified directly by flash column chromatography on silica gel (petroleum ether/ ethyl acetate =30:1~20:1) to give the desired racemic products **3a**, **3c**, **3e**, **3i-3o, 3q-3w, 5, 7, 9**.

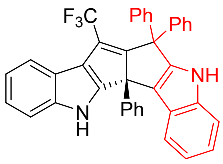
Conditions B:



To a solution of α-indolyl propargylic alcohol **1** (0.10 mmol, 1.0 equiv.), 30 mg $MgSO_4$ and catalyst (*R*)-**C1** (0.01 mmol, 10 mol%) in DCE:CCl_4(1 mL, v/v=1:1) was added 2-indolylmethanols **2** (0.01 mmol, 1.0 equiv.). The mixture was stirred at 30 ℃ until the reaction was completed (monitored by TLC analysis). The crude product was purified directly by flash column chromatography on silica gel (petroleum ether/ ethyl acetate =30:1~20:1) to give the desired racemic products **3b, 3d, 3f-3h, 3p**.

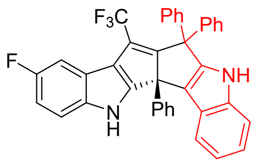
c. Analytical Data for Products 3a-3w, 5, 7, 9

(*R*)-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3a**)



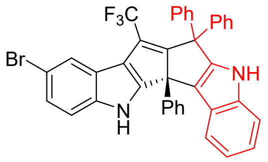
White foam, 48 h, 83% yield, 96:4 *er*, $[\alpha]_D^{20}$ = +49.60 (c = 0.25, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.97 (s, 1H), 7.74 (dd, J = 33.9, 7.1 Hz, 2H), 7.35 (dd, J = 19.6, 7.5 Hz, 2H), 7.27–7.13 (m, 9H), 7.06–6.93 (m, 4H), 6.84 (t, J = 7.2 Hz, 1H), 6.80–6.66 (m, 3H), 6.45 (d, J = 7.7 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.4 (q, J = 4.7 Hz), 149.8, 149.2, 143.6, 141.2, 139.9, 139.7, 139.6, 129.7, 129.5, 128.3, 128.0, 128.0, 127.6, 127.3, 126.8, 126.6, 126.4, 124.0, 123.1 (q, J = 36.5 Hz), 122.7 (q, J = 270.5 Hz), 122.5, 122.4, 121.3, 121.2, 121.1, 121.0, 120.2, 119.2, 112.7, 112.4, 110.3, 63.1, 60.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.70. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{25}N_2F_3$ $[M-H]^-$: 577.1897; found: 577.1904. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 10.7 min, t_{minor} = 13.9 min.

(*R*)-2-fluoro-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3b**)



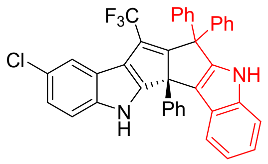
Light yellow foam, 4 d, 84% yield, 97:3 *er*, $[\alpha]_D^{20}$ = +68.24 (c = 0.17, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.00 (s, 1H), 7.68 (d, J = 7.9 Hz, 1H), 7.51–7.32 (m, 2H), 7.32–7.11 (m, 8H), 7.10–6.88 (m, 5H), 6.88–6.83 (m, 1H), 6.75 (t, J = 7.7 Hz, 3H), 6.50–6.39 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.4 (q, J = 5.1 Hz), 159.6, 157.8, 150.9, 149.8, 143.4, 139.7, 139.6, 139.5, 137.6, 129.6, 129.5, 128.3, 128.1, 128.0, 127.7, 127.4, 126.9, 126.6, 126.4, 124.8 (q, J = 270.4 Hz), 124.0, 122.7 (q, J = 36.5 Hz), 122.5, 121.5, 121.5, 121.2, 120.9, 119.1, 112.9, 112.8, 112.7, 110.8, 110.6, 110.2, 105.5 (d, J = 1.2 Hz), 105.3 (d, J = 1.3 Hz), 63.2, 60.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.67 (d, J = 5.6 Hz), -122.48 (d, J = 11.0 Hz). **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_4$ $[M-H]^-$: 595.1803; found: 595.1811. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 16.2 min, t_{minor} = 9.8 min.

(*R*)-2-bromo-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3c**)



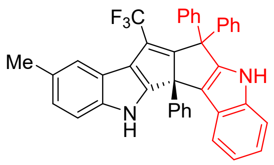
White foam, 72 h, 78% yield, 96:4 *er*, $[\alpha]_D^{20}$ = +66.15 (c = 0.13, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.03 (s, 1H), 7.88 (s, 1H), 7.76–7.61 (m, 1H), 7.45–7.34 (m, 1H), 7.32–7.09 (m, 9H), 7.06–6.93 (m, 4H), 6.86 (t, J = 7.3 Hz, 1H), 6.75 (t, J = 7.8 Hz, 3H), 6.45 (d, J = 7.5 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.8 (q, J = 5.0 Hz), 150.3, 149.8, 143.3, 139.7, 139.6, 139.5, 139.5, 129.6, 129.5, 128.3, 128.1, 128.0, 127.7, 127.4, 127.0, 126.7, 126.3, 125.3, 123.9, 123.0 (q, J = 36.6 Hz), 122.7, 122.6 (q, J = 270.5 Hz), 122.5, 121.2, 120.4, 120.3, 119.1, 114.5, 113.7, 112.7, 110.0, 63.1, 60.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.63. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_3Br$ $[M]^-$: 656.1080; found: 656.1041. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 245 nm): t_{major} = 13.5 min, t_{minor} = 20.4 min.

(*R*)-2-chloro-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3d**)



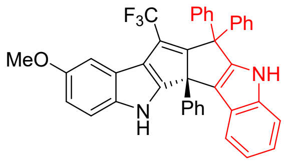
White foam, 42 h, 85% yield, 96.5:3.5 *er*, $[\alpha]_D^{20}$ = +70.00 (c = 0.15, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.03 (s, 1H), 7.72 (s, 1H), 7.71–7.62 (m, 1H), 7.38 (dd, J = 6.1, 2.7 Hz, 1H), 7.30–7.09 (m, 9H), 7.05–6.93 (m, 4H), 6.85 (t, J = 7.3 Hz, 1H), 6.74 (dd, J = 10.6, 4.8 Hz, 3H), 6.54–6.35 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.8 (q, J = 5.2 Hz), 150.5, 149.8, 143.3, 139.6, 139.5, 139.5, 139.4, 129.6, 129.5, 128.3, 128.1, 128.0, 127.7, 127.4, 127.0, 126.9, 126.7, 126.3, 123.9, 123.0 (q, J = 36.8 Hz), 122.8, 122.6 (q, J = 270.6 Hz), 122.5, 122.1, 121.2, 120.5, 120.5, 119.7, 119.8, 119.1, 113.3, 112.7, 110.1, 63.2, 60.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.61. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_3Cl$ $[M-H]^-$: 611.1507; found: 611.1489. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 12.3 min, t_{minor} = 17.0 min.

(*R*)-2-methyl-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3e**)



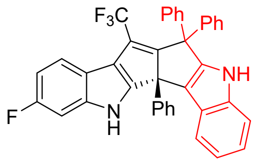
White solid, 66 h, 88% yield, 97:3 *er*, $[\alpha]_D^{20}$ = +66.67 (c = 0.24, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.34 (d, J = 7.4 Hz, 1H), 8.02 (s, 1H), 7.70 (dd, J = 6.4, 2.0 Hz, 1H), 7.55 (s, 1H), 7.41 (d, J = 6.9 Hz, 1H), 7.21 (ddd, J = 16.3, 8.3, 3.1 Hz, 8H), 7.08–6.95 (m, 5H), 6.85 (t, J = 7.3 Hz, 1H), 6.75 (dd, J = 12.7, 4.9 Hz, 3H), 6.46 (d, J = 7.4 Hz, 2H), 2.47 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.1 (q, J = 5.4 Hz), 149.8, 149.4, 143.7, 140.1, 139.8, 139.6, 139.5, 130.6, 129.8, 129.5, 128.3, 128.0, 128.0, 127.6, 127.3, 126.8, 126.6, 126.4, 124.1, 124.0, 123.2 (q, J = 36.3 Hz), 122.8 (q, J = 270.2 Hz), 122.4, 121.4, 121.1, 120.5, 120.5, 119.8, 119.2, 112.6, 112.0, 110.4, 63.0, 60.2, 21.7. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.72**. HRMS** (ESI): *m/z* calcd. for $C_{40}H_{27}N_2F_3$ $[M-H]^-$: 591.2054; found: 591.2054. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 245 nm): t_{major} = 9.7 min, t_{minor} = 24.5 min.

(*R*)-2-methoxy-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3f**)



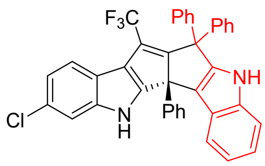
White foam, 18 h, 40% yield, 96:4 *er*, $[\alpha]_D^{20}$ = +44.00 (c = 0.10, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.05 (s, 1H), 7.69 (d, J = 7.2 Hz, 1H), 7.40 (d, J = 7.3 Hz, 1H), 7.22 (dt, J = 19.6, 8.3 Hz, 9H), 7.04 (d, J = 7.9 Hz, 2H), 6.98 (s, 2H), 6.87–6.81 (m, 2H), 6.75 (t, J = 7.7 Hz, 3H), 6.44 (t, J = 20.2 Hz, 2H), 3.85 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.0 (q, J = 4.8 Hz), 155.1, 150.0, 149.8, 143.6, 140.0, 139.7, 139.6, 136.2, 129.7, 129.5, 128.3, 128.0, 128.0, 127.6, 127.3, 126.8, 126.6, 126.4, 124.9 (q, J = 270.5 Hz), 124.0, 123.1 (q, J = 36.6 Hz), 122.4, 121.7, 121.1, 120.8, 120.7, 119.2, 113.0, 112.6, 112.3, 110.5, 102.3, 63.0, 60.2, 56.0. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.62. **HRMS** (ESI): *m/z* calcd. for $C_{40}H_{27}N_2OF_3$ $[M-H]^-$: 607.2003; found: 607.2009. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak AD-H column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 9.8 min, t_{minor} = 7.7 min.

(*R*)-3-fluoro-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3g**)



White foam, 4 d, 75% yield, 96:4 *er*, $[\alpha]_D^{20}$ = +61.43 (c = 0.14, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.42 (s, 1H), 8.02 (s, 1H), 7.80–7.62 (m, 2H), 7.39 (dd, J = 6.3, 2.4 Hz, 1H), 7.31–7.10 (m, 7H), 7.04 (dt, J = 11.0, 5.6 Hz, 3H), 6.99–6.92 (m, 3H), 6.85 (t, J = 7.3 Hz, 1H), 6.75 (dd, J = 9.6, 6.0 Hz, 3H), 6.44 (d, J = 7.4 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.8 (q, J = 5.2 Hz), 160.9, 159.0, 149.7, 149.3 (d, J = 3.2 Hz), 143.5, 141.2, 141.1, 139.7, 139.6, 129.7, 129.5, 128.3, 128.1, 128.0, 127.7, 127.4, 126.9, 126.6, 126.4, 124.0, 122.8 (q, J = 36.4 Hz), 122.7 (q, J = 270.6 Hz), 122.5, 121.2, 121.0, 121.0, 120.9, 119.1, 117.9, 112.7, 110.2, 109.9, 109.7, 99.0, 98.8, 63.3, 60.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.68, -119.83. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_4$ $[M-H]^-$: 595.1803; found: 595.1807. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak AD-H column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 7.7 min, t_{minor} = 6.2 min.

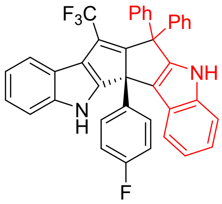
(*R*)-3-chloro-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3h**)



White foam, 3 d, 78% yield, 96.5:3.5 *er*, $[\alpha]_D^{20}$ = +60.77 (c = 0.26, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.05 (s, 1H), 7.66 (t, J = 8.4 Hz, 2H), 7.45–7.31 (m, 2H), 7.29–7.10 (m,8H), 7.06–6.93 (m, 4H), 6.85 (t, J = 7.3 Hz, 1H), 6.75 (t, J = 7.7 Hz, 3H), 6.43 (d, J = 7.5 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.9 (q, J = 5.2 Hz), 149.8, 149.7, 143.4, 141.4, 139.6, 139.5, 129.7, 129.5, 128.3, 128.2, 128.1, 128.0, 127.7, 127.4, 126.9, 126.6, 126.3, 123.9, 122.7 (q, J = 36.2 Hz), 122.6 (q, J = 270.6 Hz), 122.5, 121.9, 121.2, 121.0, 119.8, 119.1, 112.7, 112.3, 110.1, 63.2, 60.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.66. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_3Cl$ $[M-H]^-$: 611.1507; found: 611.1491. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak AD-H column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 6.9 min, t_{minor} = 6.0

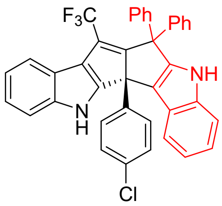
min.

(*R*)-5b-(4-fluorophenyl)-11,11-diphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3i**)



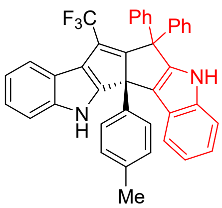
White foam, 88 h, 98% yield, 96:4 *er*, $[\alpha]_D^{20}$ = +61.43 (c = 0.21, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.42 (s, 1H), 8.05 (s, 1H), 7.80–7.74 (m, 1H), 7.67 (dd, J = 7.7, 5.9 Hz, 1H), 7.47–7.35 (m, 2H), 7.30–7.11 (m, 9H), 7.03 (dd, J = 12.6, 7.6 Hz, 4H), 6.77 (d, J = 7.1 Hz, 1H), 6.55 – 6.21 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.3 (q, J = 5.3 Hz), 162.7, 160.7, 149.9, 148.8, 143.4, 141.2, 139.7, 139.6, 135.6, 135.6, 129.7, 129.5, 128.3, 128.2, 128.1, 128.1, 127.7, 127.4, 126.8, 123.8, 123.0 (q, J = 36.6 Hz), 122.7 (q, J = 271.0 Hz), 122.6, 122.5, 121.3, 121.2, 121.2, 120.9, 120.2, 119.1, 114.8, 114.6, 112.7, 112.4, 110.1, 62.4, 60.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.73, -116.04. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_4$ $[M-H]^-$: 595.1803; found: 595.1799. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 245 nm): t_{major} = 11.5 min, t_{minor} = 16.2 min.

(*R*)-5b-(4-chlorophenyl)-11,11-diphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3j**)



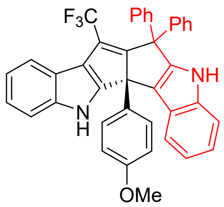
White foam, 24 h, 70% yield, 97:3 *er*, $[\alpha]_D^{20}$ = +44.35 (c = 0.23, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.01 (s, 1H), 7.86–7.71 (m, 1H), 7.69–7.59 (m, 1H), 7.46–7.32 (m, 2H), 7.27–7.07 (m, 9H), 7.02 (d, J = 7.4 Hz, 4H), 6.78 (d, J = 7.3 Hz, 1H), 6.68 (d, J = 8.6 Hz, 2H), 6.35 (d, J = 8.6 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.2 (q, J = 4.9 Hz), 149.9, 148.6, 143.3, 141.2, 139.6, 139.6, 138.6, 132.5, 129.6, 129.5, 128.3, 128.1, 128.0, 127.9, 127.7, 127.4, 126.8, 123.8, 123.2 (q, J = 36.6 Hz), 122.7, 122.7 (q, J = 270.7 Hz), 122.6, 121.3, 121.2, 121.2, 121.1, 120.2, 119.0, 112.7, 112.4, 109.8, 62.5, 60.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.73. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_3Cl$ $[M-H]^-$: 611.1507; found: 611.1489. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 245 nm): t_{major} = 11.9 min, t_{minor} = 16.1 min.

(*R*)-11,11-diphenyl-5b-(p-tolyl)-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3k**)



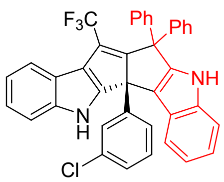
White foam, 88 h, 91% yield, 97:3 *er*, $[\alpha]_D^{20}$ = +57.39 (c = 0.23, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.01 (s, 1H), 7.84 (t, J = 6.1 Hz, 1H), 7.78–7.70 (m, 1H), 7.42 (ddd, J = 9.1, 5.5, 3.2 Hz, 2H), 7.31–7.17 (m, 9H), 7.12–7.01 (m, 4H), 6.84 (d, J = 7.2 Hz, 1H), 6.60 (d, J = 8.1 Hz, 2H), 6.39 (d, J = 8.2 Hz, 2H), 2.11 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.5 (q, J = 5.1 Hz), 149.7, 149.3, 143.7, 141.2, 139.8, 139.6, 136.8, 136.4, 132.6, 130.2, 129.7, 129.5, 128.6, 128.4, 128.3, 127.9, 127.6, 127.3, 126.4, 126.3, 124.0, 123.1 (q, J = 36.3 Hz), 122.8 (q, J = 270.3 Hz), 122.4, 122.4, 121.3, 121.1, 121.1, 120.9 (d, J = 1.7 Hz), 120.1, 119.2, 112.6, 112.3, 110.5, 62.9, 60.2, 20.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.71**.** **HRMS** (ESI): *m/z* calcd. for $C_{40}H_{27}N_2F_3$ [M-H]$^-$: 591.2054; found: 591.2043. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 10.1 min, t_{minor} = 13.1 min.

(*R*)-5b-(4-methoxyphenyl)-11,11-diphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3l**)



White foam, 24 h, 99% yield, 98:2 *er*, $[\alpha]_D^{20}$ = +48.75 (c = 0.24, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.99 (s, 1H), 7.83–7.72 (m, 1H), 7.63 (d, J = 7.2 Hz, 1H), 7.37 (t, J = 7.1 Hz, 1H), 7.31 (dt, J = 6.5, 2.9 Hz, 1H), 7.26–7.10 (m, 9H), 7.00 (d, J = 6.6 Hz, 4H), 6.76 (d, J = 7.2 Hz, 1H), 6.52–6.10 (m, 4H), 3.52 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.5 (q, J = 5.4 Hz), 158.4, 149.8, 149.2, 143.7, 141.1, 139.8, 139.6, 131.9, 129.7, 129.5, 128.3, 128.0, 127.7, 127.6, 127.3, 126.6, 123.9, 122.9 (q, J = 36.9 Hz), 122.8 (q, J = 270.6 Hz), 122.4, 122.4, 121.3, 121.1, 121.1, 120.8, 120.1, 119.2, 113.4, 112.6, 112.3, 110.6, 62.5, 60.2, 55.3. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.72. **HRMS** (ESI): *m/z* calcd. for $C_{40}H_{27}N_2OF_3$ [M-H]$^-$: 607.2003; found: 607.2003. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 15.4 min, t_{minor} = 20.0 min.

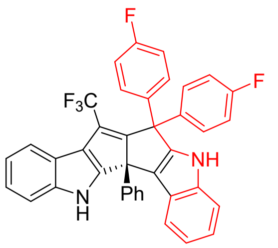
(*R*)-5b-(3-chlorophenyl)-11,11-diphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3m**)



White foam, 48 h, 92% yield, 96:4 *er*, $[\alpha]_D^{20}$ = +85.45 (c = 0.11, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.94 (s, 1H), 7.76 (d, J = 7.1 Hz, 1H), 7.73–7.61 (m, 1H), 7.40 (dd, J = 6.8, 1.6 Hz, 1H), 7.35 (dt, J = 6.7, 2.7 Hz, 1H), 7.30–7.09 (m, 7H), 7.04 (d, J = 15.0 Hz, 3H), 6.97–6.86 (m, 3H), 6.77 (t, J = 7.8 Hz, 2H), 6.70–6.63 (m, 1H), 6.42 (dd, J = 12.2, 4.9 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.8 (q, J = 5.2 Hz), 149.9, 148.3, 143.2, 142.2, 141.1, 139.6, 139.5, 133.9, 129.6, 129.5, 129.3, 128.3, 128.1, 127.7, 127.4, 127.1, 126.9, 126.7, 124.5, 123.7, 123.1 (q, J = 36.7 Hz), 122.7, 122.6 (q, J = 269.9 Hz), 122.6, 121.3, 121.3, 121.2, 121.0 (d, J = 1.6 Hz), 120.2, 119.0, 112.7, 112.4, 109.7, 62.6, 60.2. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.68. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_3Cl$ [M-H]$^-$: 611.1507; found: 611.1503. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 12.2 min, t_{minor} = 15.0 min.

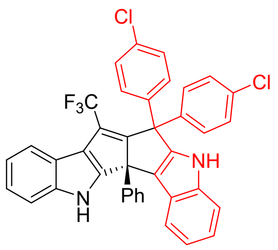
(*R*)-11,11-bis(4-fluorophenyl)-5b-phenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-

b']diindole (**3n**)



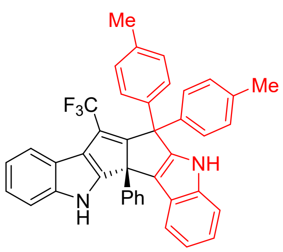
White foam, 88 h, 95% yield, 97:3 *er*, $[\alpha]_D^{20}$ = +122.00 (c = 0.10, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.95 (s, 1H), 7.76 (d, J = 7.4 Hz, 1H), 7.68 (d, J = 7.4 Hz, 1H), 7.43–7.30 (m, 2H), 7.29–7.15 (m, 4H), 7.12 (d, J = 16.4 Hz, 2H), 6.97 (dd, J = 9.3, 5.5 Hz, 1H), 6.94 – 6.84 (m, 3H), 6.80–6.56 (m, 5H), 6.42 (d, J = 7.7 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.9 (q, J = 5.2 Hz), 163.1, 162.4, 161.1, 160.5, 149.1, 141.1, 139.6, 139.6, 139.1, 135.6 (d, J = 3.0 Hz), 131.3 (d, J = 8.1 Hz), 131.0 (d, J = 8.0 Hz), 128.1, 127.0, 126.4, 123.9, 123.2 (q, J = 36.7 Hz), 122.7, 122.7 (q, J = 270.6 Hz), 122.6, 121.3, 121.3, 121.2, 120.8, 120.2, 119.3, 115.7, 115.5, 115.0, 114.8, 114.3, 114.1, 112.7, 112.4, 110.5, 62.9, 59.0. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.52, -115.14, -115.83. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{23}N_2F_5$ $[M-H]^-$: 613.1709; found: 613.1702. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 14.5 min, t_{minor} = 9.4 min.

(*R*)-11,11-bis(4-chlorophenyl)-5b-phenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3o**)



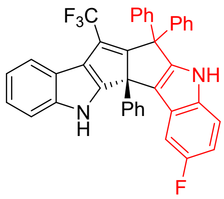
White foam, 4 d, 83% yield, 96.5:3.5 *er*, $[\alpha]_D^{20}$ = +72.86 (c = 0.28, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.94 (s, 1H), 7.76 (d, J = 7.1 Hz, 1H), 7.73–7.65 (m, 1H), 7.46–7.37 (m, 1H), 7.35 (dt, J = 6.7, 2.7 Hz, 1H), 7.29–7.12 (m, 7H), 7.12–7.02 (m, 2H), 6.98–6.88 (m, 3H), 6.76 (dd, J = 16.5, 8.9 Hz, 2H), 6.71–6.64 (m, 1H), 6.50–6.26 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.2 (q, J = 5.2 Hz), 149.1, 148.7, 141.6, 141.2, 139.6, 139.4, 138.1, 133.5, 132.7, 131.0, 130.6, 128.7, 128.2, 127.8, 127.1, 126.3, 123.9, 123.5 (q, J = 36.7 Hz), 122.8, 122.7, 122.6 (q, J = 270.7 Hz), 121.4, 121.4, 121.2, 120.8, 120.8, 120.2, 119.3, 112.7, 112.4, 110.7, 62.9, 59.1. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -58.46**.** **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{23}N_2F_3Cl_2$ $[M-H]^-$: 645.1118; found: 645.1117. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 13.8 min, t_{minor} = 12.5 min.

(*R*)-5b-phenyl-11,11-di-p-tolyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3p**)



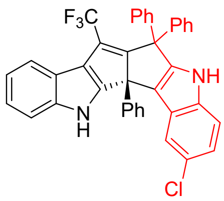
White foam, 48 h, 40% yield, 96:4 *er*, $[\alpha]_D^{20}$ = +95.00 (c = 0.08, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 8.35 (s, 1H), 7.91 (s, 1H), 7.77 (d, J = 7.4 Hz, 1H), 7.72 – 7.63 (m, 1H), 7.32 (d, J = 7.9 Hz, 2H), 7.25 – 7.10 (m, 4H), 6.97 (dd, J = 15.9, 7.9 Hz, 4H), 6.84 (dd, J = 11.3, 4.4 Hz, 2H), 6.79 – 6.59 (m, 5H), 6.45 (d, J = 8.2 Hz, 2H), 2.29 (s, 3H), 2.14 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.8 (q, J = 5.2 Hz), 150.2, 149.2, 141.1, 140.8, 140.0, 139.5, 136.8, 136.8, 135.9, 129.6, 129.4, 129.0, 128.5, 128.1, 128.0, 126.6, 126.5, 124.1, 122.9 (q, J = 36.3 Hz), 122.8 (q, J = 270.5 Hz), 122.4, 122.3, 121.3, 121.1, 121.0, 120.2, 119.1, 112.6, 112.3, 110.1, 63.1, 59.6, 21.1, 21.0. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.53. **HRMS** (ESI): *m/z* calcd. for $C_{41}H_{29}N_2F_3$ [M-H]$^-$: 605.2210; found: 605.2195. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 245 nm): t_{major} = 8.5 min, t_{minor} = 6.9 min.

(*R*)-7-fluoro-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3q**)



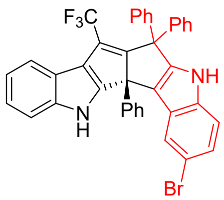
White foam, 4 d, 85% yield, 93:7 *er*, $[\alpha]_D^{20}$ = +55.65 (c = 0.23, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.03 (s, 1H), 7.81–7.73 (m, 1H), 7.42–7.32 (m, 2H), 7.29 (dd, J = 8.8, 4.3 Hz, 1H), 7.26–7.09 (m, 8H), 6.98 (ddd, J = 12.6, 11.5, 5.2 Hz, 4H), 6.85 (t, J = 7.3 Hz, 1H), 6.75 (t, J = 7.6 Hz, 3H), 6.42 (d, J = 7.7 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.0 (q, J = 4.9 Hz), 159.6, 157.7, 151.7, 149.0, 143.4, 141.2, 139.6, 139.4, 136.0, 129.6, 129.5, 128.3, 128.1, 128.0, 127.7, 127.4, 126.9, 126.7, 126.3, 124.3, 124.3, 123.4 (q, J = 36.4 Hz), 122.7 (q, J = 270.5 Hz), 122.6, 121.3, 121.2, 121.0 (d, J = 1.6 Hz), 120.2, 113.3, 113.3, 112.4, 110.7, 110.6 (d, J = 4.4 Hz), 110.5, 104.4, 104.2, 62.9, 60.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.74, -122.44. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_4$ [M-H]$^-$: 595.1803; found: 595.1796. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 280 nm): t_{major} = 12.1 min, t_{minor} = 8.1 min.

(*R*)-7-chloro-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3r**)



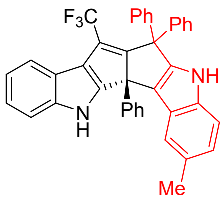
White foam, 4 d, 71% yield, 89:11 *er*, $[\alpha]_D^{20}$ = +22.50 (c = 0.20, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.02 (s, 1H), 7.77 (dd, J = 5.6, 3.0 Hz, 1H), 7.67 (d, J = 1.8 Hz, 1H), 7.41–7.29 (m, 1H), 7.30–7.08 (m, 10H), 7.03–6.94 (m, 3H), 6.85 (t, J = 7.3 Hz, 1H), 6.75 (dt, J = 13.8, 4.4 Hz, 3H), 6.43–6.36 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.9 (q, J = 5.1 Hz), 151.3, 148.9, 143.4, 141.2, 139.5, 139.3, 137.8, 129.6, 129.5, 128.4, 128.1, 128.1, 127.7, 127.4, 126.9, 126.8, 126.7, 126.3, 125.0, 123.5 (q, J = 36.8 Hz), 122.7, 122.7 (q, J = 270.4 Hz), 122.6, 121.3, 121.2, 121.0 (d, J = 1.5 Hz), 120.2, 118.6, 113.6, 112.5, 110.2, 62.9, 60.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.73**. HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_3Cl$ [M-H]$^-$: 611.1507; found: 611.1496. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 11.6 min, t_{minor} = 7.5 min.

(*R*)-7-bromo-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3s**)



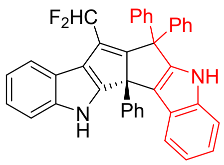
White foam, 4 d, 83% yield, 88:12 *er*, $[\alpha]_D^{20}$ = +7.50 (c = 0.24 MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.98 (s, 1H), 7.83 (d, J = 1.2 Hz, 1H), 7.77 (dd, J = 5.5, 3.0 Hz, 1H), 7.35 (dd, J = 6.1, 3.1 Hz, 1H), 7.30 (dd, J = 8.7, 1.7 Hz, 1H), 7.28–7.09 (m, 9H), 6.98 (d, J = 7.0 Hz, 3H), 6.85 (t, J = 7.3 Hz, 1H), 6.74 (dd, J = 13.8, 6.1 Hz, 3H), 6.38 (d, J = 7.5 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.9 (q, J = 5.1 Hz), 151.1, 148.8, 143.4, 141.2, 139.5, 139.3, 138.1, 129.6, 128.4, 128.1, 128.1, 127.7, 127.4, 126.9, 126.7, 126.3, 125.6, 125.3, 123.5 (q, J = 36.6 Hz), 122.7, 122.6 (q, J = 270.3 Hz), 121.7, 121.3, 121.2, 121.1 (d, J = 1.4 Hz), 120.2, 114.3, 114.1, 112.5, 110.1, 62.9, 60.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.74. **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{24}N_2F_3Br$ $[M-H]^-$: 655.1002; found: 655.0988. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 10.9 min, t_{minor} = 7.4 min.

(*R*)-7-methyl-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3t**)



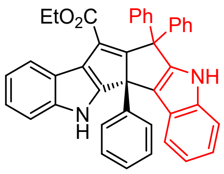
White foam, 3 d, 73% yield, 90:10 *er*, $[\alpha]_D^{20}$ = +41.00 (c = 0.20, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.86 (s, 1H), 7.77 (d, J = 5.8 Hz, 1H), 7.49 (s, 1H), 7.37 (d, J = 5.8 Hz, 1H), 7.20 (ddd, J = 20.3, 17.8, 7.6 Hz, 8H), 7.09–6.91 (m, 5H), 6.84 (t, J = 7.0 Hz, 1H), 6.74 (t, J = 7.6 Hz, 3H), 6.45 (d, J = 7.7 Hz, 2H), 2.49 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.4 (q, J = 5.3 Hz), 149.9, 149.2, 143.7, 141.2, 139.9, 139.7, 137.9, 130.5, 129.7, 129.5, 128.3, 128.0, 127.9, 127.6, 127.2, 126.8, 126.5, 126.5, 124.2, 123.9, 123.0 (q, J = 36.6 Hz), 122.8 (q, J = 270.6 Hz), 122.4, 121.3, 121.2, 121.0, 120.2, 118.9, 112.4, 112.3, 109.8, 63.1, 60.2, 21.7. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.70. **HRMS** (ESI): *m/z* calcd. for $C_{40}H_{27}N_2F_3$ $[M-H]^-$: 591.2054; found: 591.2042. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak AD-H column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 6.4 min, t_{minor} = 5.3 min.

(*R*)-12-(difluoromethyl)-5b,11,11-triphenyl-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3u**)



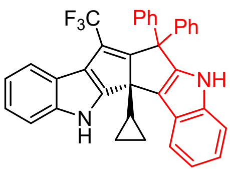
White foam, 3 d, 73% yield, 88:12 *er*, $[\alpha]_D^{20}$ = +108.00 (c = 0.25, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.07 (s, 1H), 7.81 (d, J = 7.4 Hz, 1H), 7.68 (dd, J = 5.9, 2.7 Hz, 1H), 7.43–7.35 (m, 1H), 7.34–7.10 (m, 12H), 7.06 (d, J = 7.3 Hz, 1H), 6.96 (t, J = 7.0 Hz, 1H), 6.85 (t, J = 7.3 Hz, 1H), 6.79 (d, J = 7.7 Hz, 1H), 6.74 (t, J = 7.7 Hz, 2H), 6.45 (d, J = 7.4 Hz, 2H), 5.71–5.08 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.7 (t, J = 12.4 Hz), 149.7, 148.8, 143.6, 141.2, 140.1, 139.9, 139.4, 132.6, 130.2, 129.6, 129.3, 129.1, 128.4, 128.3, 128.0, 127.9, 126.7, 126.5, 124.2, 122.4, 122.2, 121.8, 121.8, 121.1, 121.0, 120.9, 120.9, 119.2, 113.0, 112.6, 112.2, 111.6, 111.2, 111.1, 109.3, 62.5, 59.8. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -110.03 (d, J = 313.4 Hz), -113.79 (d, J = 313.4 Hz). **HRMS** (ESI): *m/z* calcd. for $C_{39}H_{26}N_2F_2$ $[M-H]^-$: 559.1991; found: 559.1985. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 19.6 min, t_{minor} = 12.8 min.

ethyl (*R*)-5b,11,11-triphenyl-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole-12-carboxylate (**3v**)



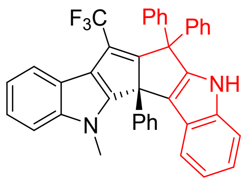
Light yellow foam, 24 h, 75% yield, 93:7 *er*, $[\alpha]_D^{20}$ = +4.75 (c = 0.18, MeOH). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.05 (s, 1H), 7.95–7.90 (m, 1H), 7.79–7.70 (m, 1H), 7.39–7.33 (m, 4H), 7.25–7.16 (m, 8H), 7.06–6.99 (m, 3H), 6.86 (t, *J* = 7.3 Hz, 2H), 6.77 (t, *J* = 7.5 Hz, 2H), 6.55 (d, *J* = 7.3 Hz, 2H), 3.95 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.46 (dd, *J* = 10.8, 7.2 Hz, 1H), 1.12 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.2, 165.3, 149.5, 149.3, 145.4, 144.2, 141.4, 140.4, 140.2, 139.6, 128.3, 127.9, 127.9, 127.3, 127.1, 126.8, 126.6, 126.6, 126.5, 124.2, 122.3, 122.2, 122.2, 121.8, 121.0, 120.9, 120.8, 120.0, 119.2, 112.5, 112.2, 111.2, 110.8, 103.3, 62.7, 60.8, 60.2, 14.1. **HRMS** (ESI): *m/z* calcd. for $C_{41}H_{30}N_2O_2$ $[M+H]^+$: 583.2380; found: 583.2373. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IC column (hexane/*i*-PrOH = 90/10, flow rate 0.8 mL·min^{-1}, λ = 245 nm): t_{major} = 6.2 min, t_{minor} = 6.8 min.

(*R*)-5b-cyclopropyl-11,11-diphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**3w**)



Yellow foam, 24 h, 70% yield, 85:15 *er*, $[\alpha]_D^{20}$ = +26.33 (c = 0.25, MeOH). **^{1}H NMR (**400 MHz, $CDCl_3$) δ 8.74 (s, 1H), 8.07 (s, 1H), 7.87–7.80 (m, 1H), 7.68–7.64 (m, 1H), 7.51 (d, J = 7.9 Hz, 1H), 7.46–7.37 (m, 3H), 7.36–7.32 (m, 3H), 7.24–7.20 (m, 3H), 7.18 (s, 1H), 7.18–7.16 (m, 2H), 0.74–0.69 (m, 1H), 0.43–0.39 (m, 1H), 0.36–0.29 (m, 1H), -0.42 – -0.47 (m, 1H), -0.48 – -0.55 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.0 (q, J = 5.0 Hz), 150.1, 149.1, 144.3, 140.8, 140.7, 139.3, 130.0, 129.7, 129.5, 128.7, 128.5, 128.2, 127.5, 127.1, 127.1, 123.2 (q, J = 36.4 Hz), 122.2 (q, J = 277.2 Hz), 122.1, 122.1, 121.5, 121.0, 120.8, 119.9, 119.0, 112.5, 112.1, 109.5, 61.5, 60.1, 21.1, 2.5, 2.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.85. **HRMS** (ESI): *m/z* calcd. for $C_{36}H_{26}N_2F_3$ $[M+H]^+$: 543.2043; found: 543.2041. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak AD-H column (hexane/*i*-PrOH = 90/10, flow rate 0.8 mL·min^{-1}, λ = 280 nm): t_{major} = 7.8 min, t_{minor} = 6.1 min.

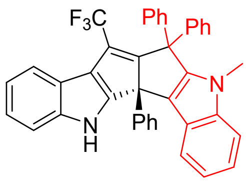
(*R*)-5-methyl-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**5**)



White foam, 48 h, 43% yield, 57:43 *er*, $[\alpha]_D^{20}$ = +8.52 (c = 0.13, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.90–7.70 (m, 2H), 7.39 (dd, J = 11.2, 4.9 Hz, 1H), 7.34 (d, J = 8.1 Hz, 1H), 7.29–7.13 (m, 9H), 7.09 (d, J

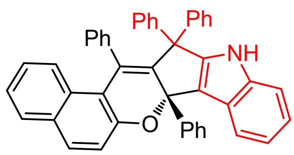
= 7.1 Hz, 1H), 6.96 (t, J = 6.8 Hz, 3H), 6.83 (t, J = 7.3 Hz, 1H), 6.79–6.69 (m, 3H), 6.41 (d, J = 7.7 Hz, 2H), 3.81 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.5 (q, J = 5.0 Hz), 150.9, 150.4, 143.8, 141.6, 139.6, 139.5, 138.8, 129.7, 129.5, 128.3, 128.0, 127.9, 127.6, 127.3, 126.7, 126.5, 126.5, 124.0, 123.1 (q, J = 36.4 Hz), 122.8 (q, J = 270.5 Hz), 122.3, 121.9, 121.1, 120.8, 120.3, 119.6, 119.3, 112.7, 110.3, 110.3, 63.4, 59.5, 32.2. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -58.61. **HRMS** (ESI): *m/z* calcd. for $C_{27}H_{19}N_2F_3$ [M-H]$^-$: 591.2054; found: 591.2081. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 5.6 min, t_{minor} = 6.2 min.

(*R*)-10-methyl-5b,11,11-triphenyl-12-(trifluoromethyl)-5,5b,10,11-tetrahydropentaleno[1,2-b:5,6-b']diindole (**7**)



White foam, 48 h, 79% yield, 97:3 *er*, $[\alpha]_D^{20}$ = +102.73 (c = 0.17, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.45–7.35 (m, 2H), 7.34–7.17 (m, 9H), 7.11 (d, *J* = 6.6 Hz, 1H), 7.00 (dt, *J* = 22.8, 7.0 Hz, 3H), 6.88 (d, *J* = 6.4 Hz, 1H), 6.81 (t, *J* = 7.2 Hz, 1H), 6.72 (t, *J* = 7.6 Hz, 2H), 6.50 (d, *J* = 7.7 Hz, 2H), 3.17 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.4 (q, *J* = 4.5 Hz), 150.2, 149.6, 143.5, 141.1, 140.5 (d, *J* = 4.2 Hz), 140.0, 139.7, 129.6, 128.5, 128.2, 127.9, 127.8, 127.2, 126.7, 126.6, 126.3, 123.7, 122.8 (q, *J* = 270.7 Hz), 122.4, 122.0 (q, *J* = 36.4 Hz), 121.8, 121.4, 121.1, 120.7, 120.5 (d, *J* = 1.4 Hz), 120.1, 119.1, 112.3, 110.5, 109.0, 62.7, 60.3, 31.1. **^{19}F NMR** (470 MHz, $CDCl_3$) δ -58.62. IR (ATR) ν_{max}: 3410, 2923, 1454, 1171, 895, 739 cm^{-1}. **HRMS** (ESI): *m/z* calcd. for $C_{27}H_{19}N_2F_3$ [M-H]$^-$: 591.2054; found: 591.2067. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IA column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 6.6 min, t_{minor} = 5.3 min.

(*R*)-7a,13,13,14-tetraphenyl-12,13-dihydro-7aH-benzo[5',6']chromeno[2',3':3,4]cyclopenta[1,2-b]indole (**9**)



White foam, 48 h, 85% yield, 63:37 *er*, $[\alpha]_D^{20}$ = +12.54 (c = 0.13, MeOH). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79–7.70 (m, 5H), 7.65 (d, *J* = 7.4 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 2H), 7.45 (d, *J* = 8.8 Hz, 1H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.21 (dd, *J* = 5.8, 3.1 Hz, 1H), 7.12 (dd, *J* = 5.9, 3.1 Hz, 2H), 7.10–7.02 (m, 5H), 7.00 (d, *J* = 8.8 Hz, 1H), 6.96 (t, *J* = 7.4 Hz, 1H), 6.89–6.74 (m, 6H), 6.49 (t, *J* = 7.4 Hz, 1H), 5.77 (d, *J* = 7.7 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ: 154.0, 149.9, 143.8, 143.4, 142.1, 142.1, 141.0, 139.7, 136.1, 131.2, 131.0, 130.8, 130.3, 130.3, 129.6, 129.1, 128.2, 128.1, 127.8, 127.6, 127.4, 127.2, 127.2, 127.1, 126.9, 126.6, 126.1, 125.5, 125.1, 122.8, 122.5, 122.4, 120.8, 120.7, 120.0, 119.7, 118.2, 112.0, 86.4, 62.0. **HRMS** (ESI): *m/z* calcd. for $C_{27}H_{19}N_2F_3$ [M-H]$^-$: 612.2474; found: 612.2469. **HPLC analysis:** The enantiomeric excess was determined by HPLC with Chiralpak IB column (hexane/*i*-PrOH = 95/5, flow rate 1 mL·min^{-1}, λ = 254 nm): t_{major} = 8.2 min, t_{minor} = 7.3 min.

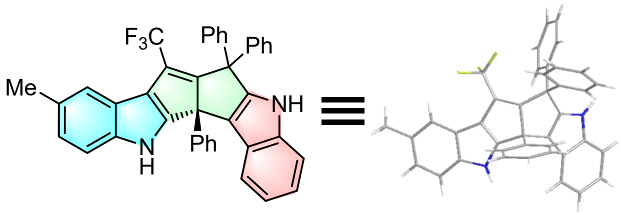
5. References

[1] a) Zhu, W.-R.; Su, Q.; Deng, X.-Y.; Liu, J.-S.; Zhong, T.; Meng, S.-S;. Yi, J.-T.; Weng, J.; Lu, G., *Chem. Sci.*, **2022**, *13*, 170–177; b) Zhu, W.-R.; Su, Q.; Diao, H.-J.; Wang, E.-X.; Wu, F.; Zhao, Y.-L.; Weng, J.; Lu,

G., *Org. Lett.,* **2022**, *22*, 6873–6878; c) Li, T.-Z.; Liu, S.-J.; Sun, Y.-W.; Deng, S.; Tan, W.; Jiao, Y.; Zhang Y.-C.; Shi, F., *Angew. Chem., Int. Ed.***,** **2021**, *60*, 2355–2363.

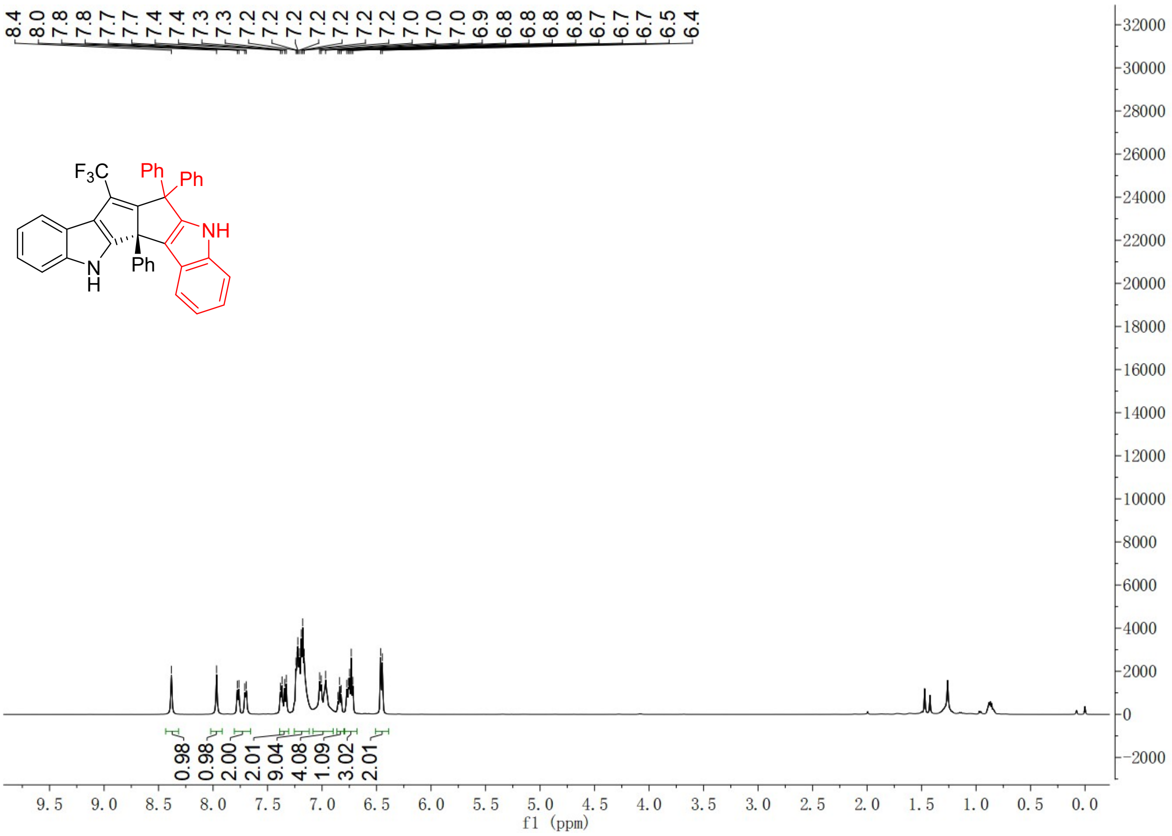
6. Data for X-Ray Crystal Structure of 3e

Table 1 Crystal data and structure refinement for 3e.

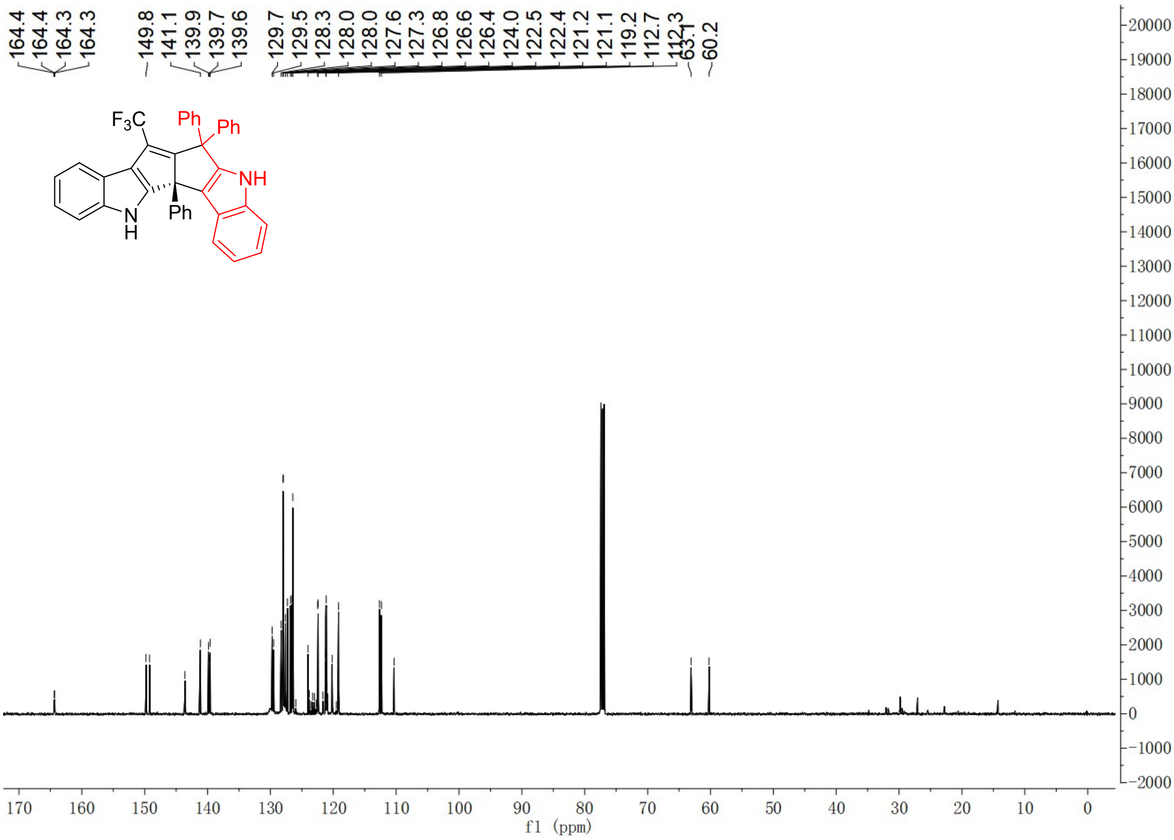
Compound	
Empirical formula	$C_{40}H_{27}F_3N_2$
Formula weight	592.63
Temperature/K	99.99(10)
Crystal system	hexagonal
Space group	P65
a/Å	19.97510(10)
b/Å	19.97510(10)
c/Å	13.78270(10)
α/°	90
β/°	90
γ/°	120
Volume/Å3	4762.58(6)
Z	6
ρcalcg/cm3	1.240
μ/mm-1	0.687
F(000)	1848.0
Crystal size/mm3	0.25 × 0.2 × 0.2
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.108 to 157.992
Index ranges	-25 ≤ h ≤ 25, -25 ≤ k ≤ 23, -17 ≤ l ≤ 17
Reflections collected	65556
Independent reflections	6834 [Rint = 0.0528, Rsigma = 0.0228]
Data/restraints/parameters	6834/1/407
Goodness-of-fit on F2	1.064
Final R indexes [I>=2σ (I)]	R1 = 0.0273, wR2 = 0.0712
Final R indexes [all data]	R1 = 0.0276, wR2 = 0.0715
Largest diff. peak/hole / e Å-3	0.13/-0.18
Flack parameter	-0.01(4)

7. Copies of NMR Spectra

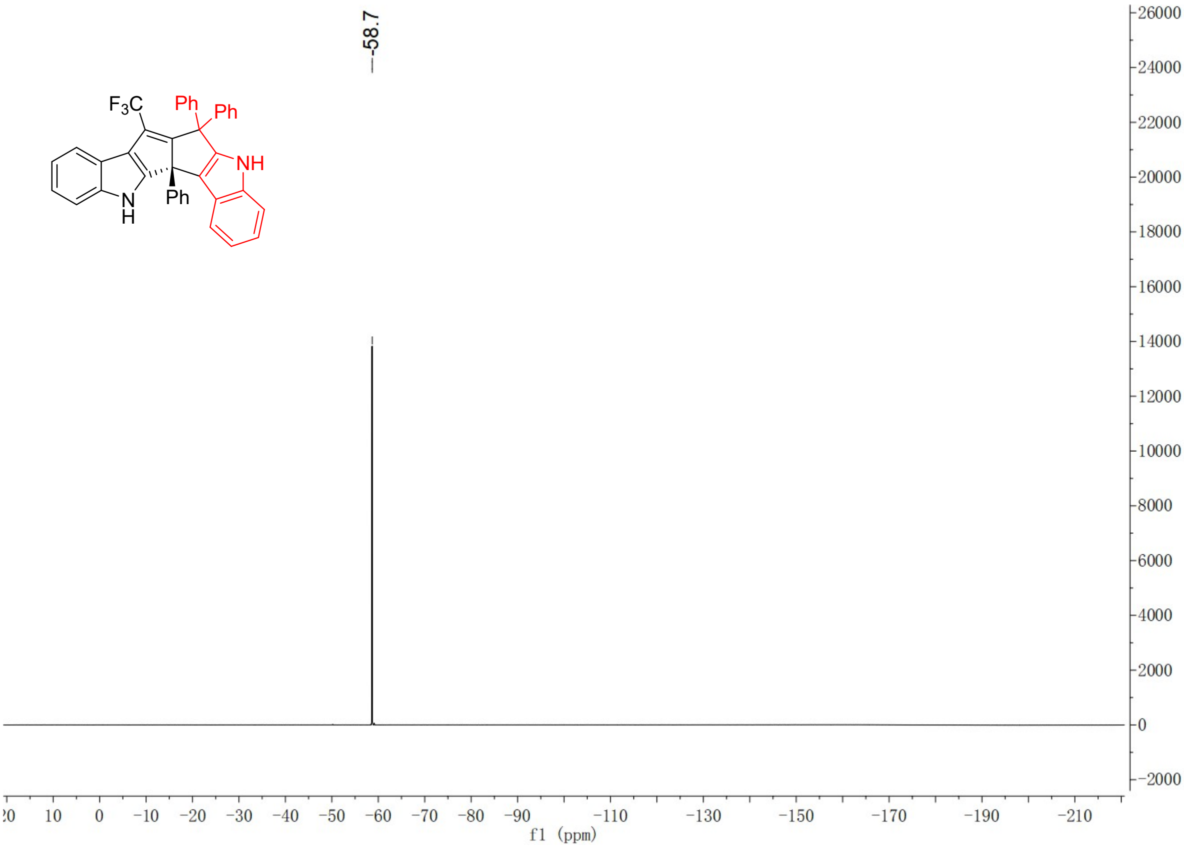
^{1}H NMR of compound 3a (in $CDCl_3$)



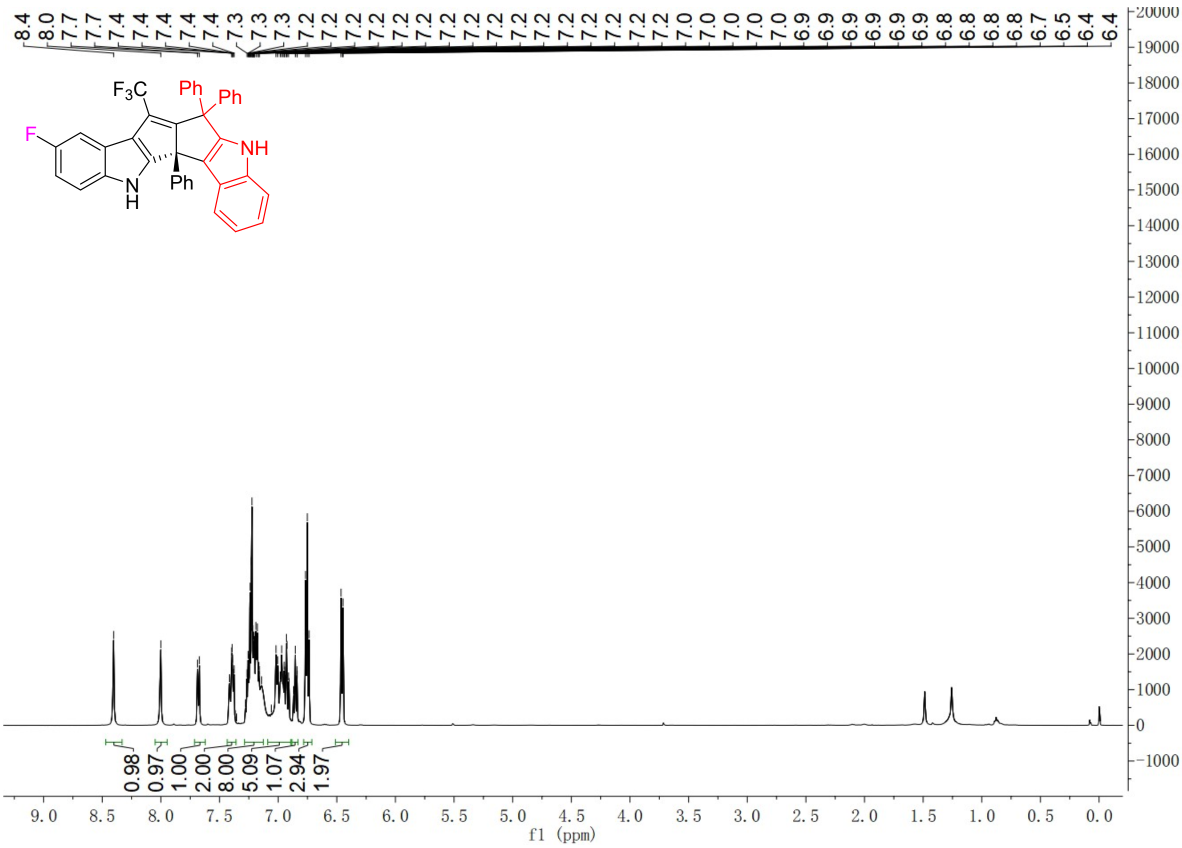
^{13}C NMR of compound 3a (in $CDCl_3$)



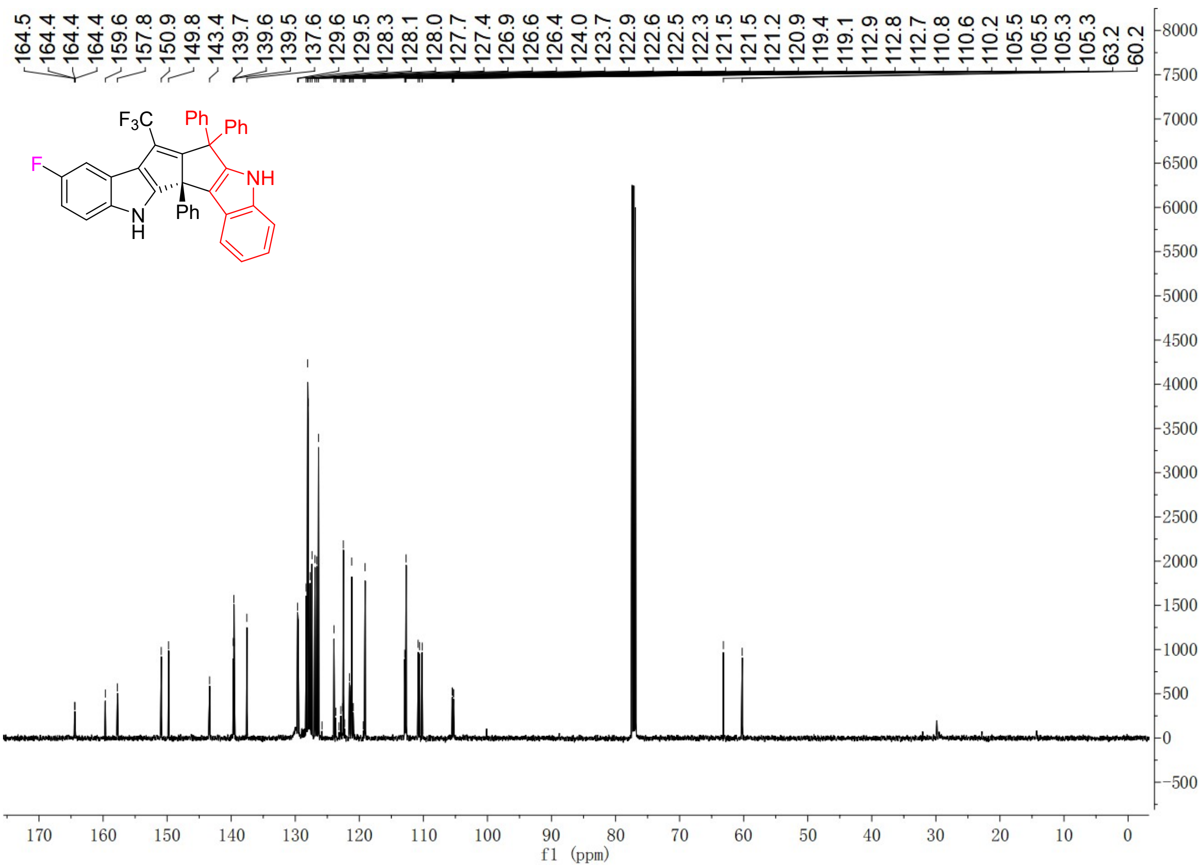
^{19}F NMR of compound 3a (in $CDCl_3$)



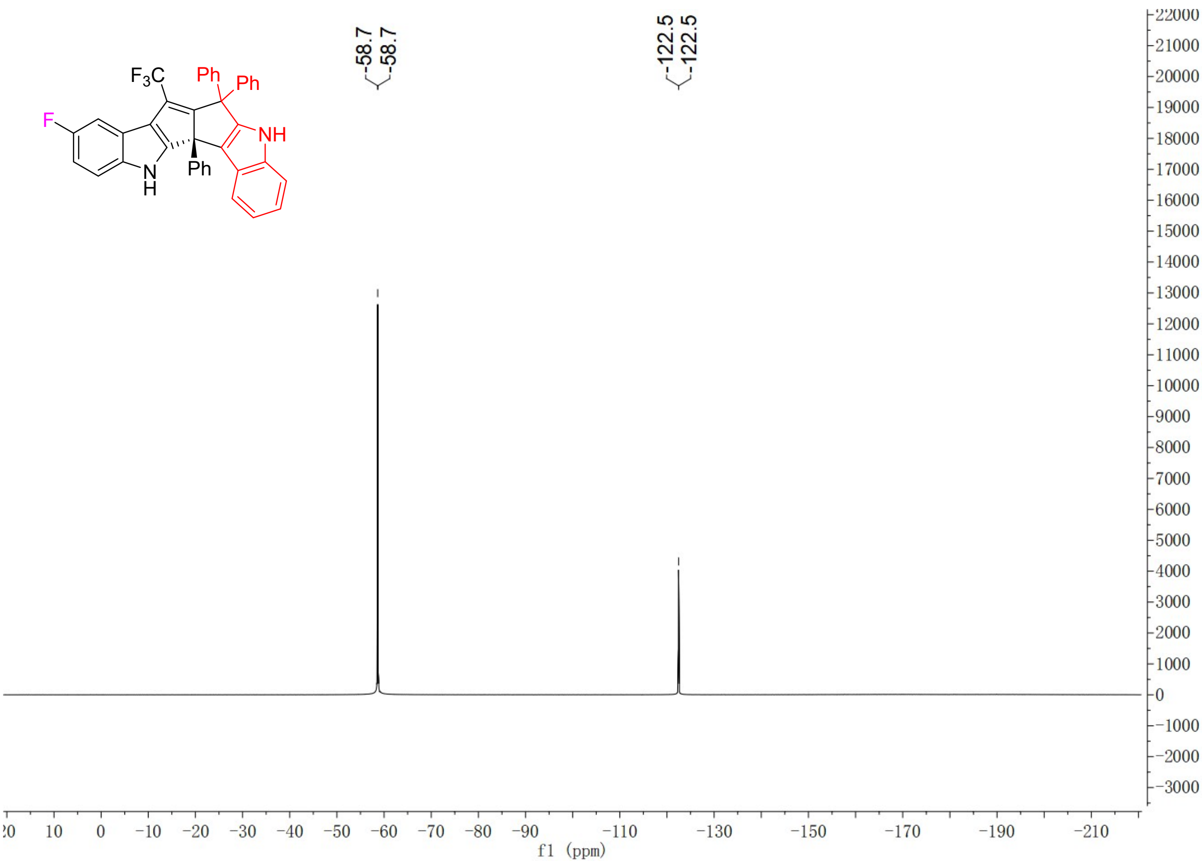
^{1}H NMR of compound 3b (in $CDCl_3$)



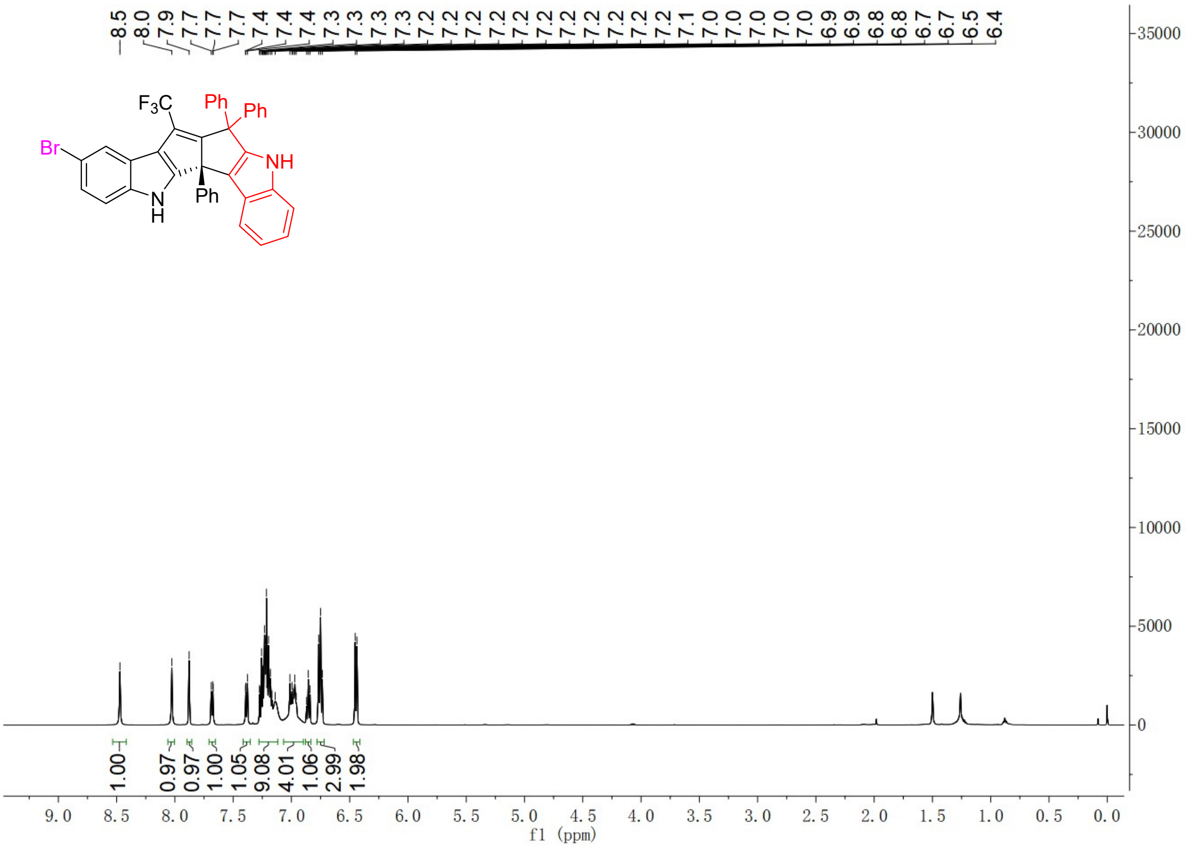
^{13}C NMR of compound 3b (in $CDCl_3$)



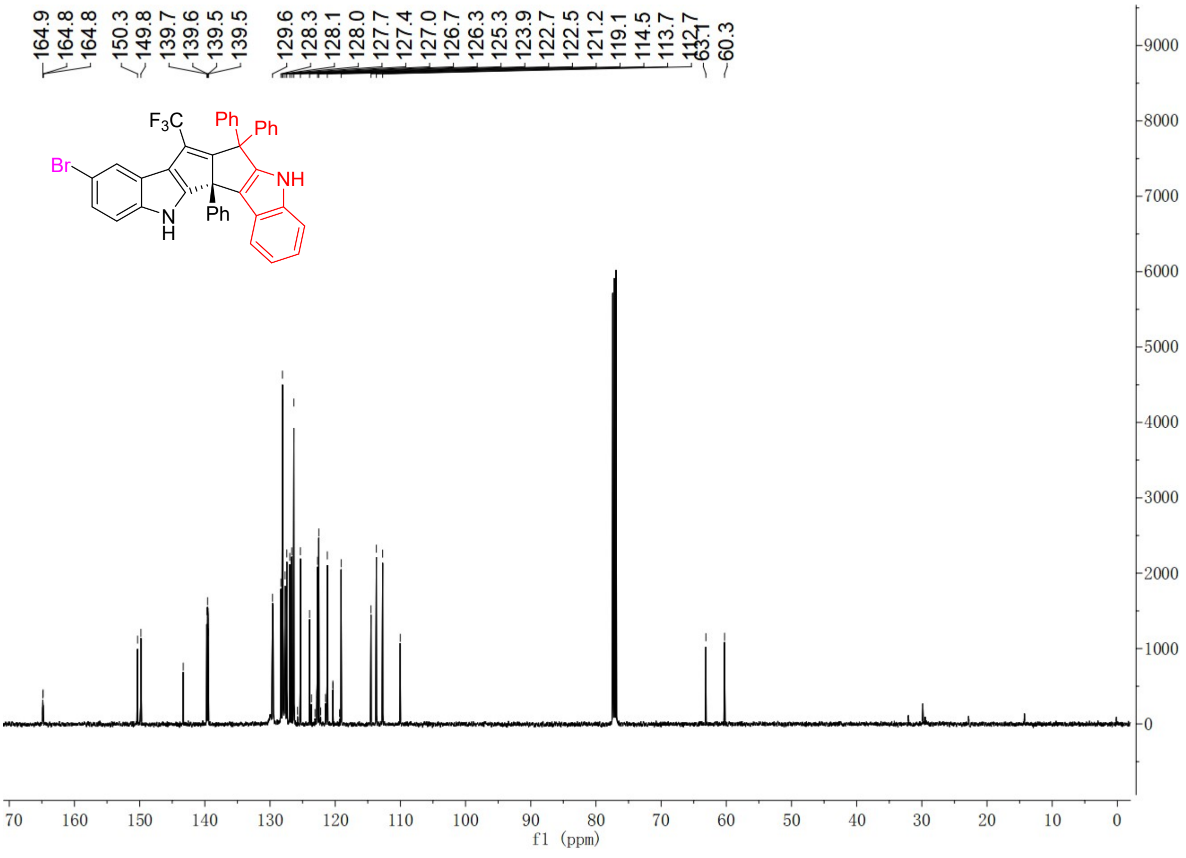
^{19}F NMR of compound 3b (in $CDCl_3$)



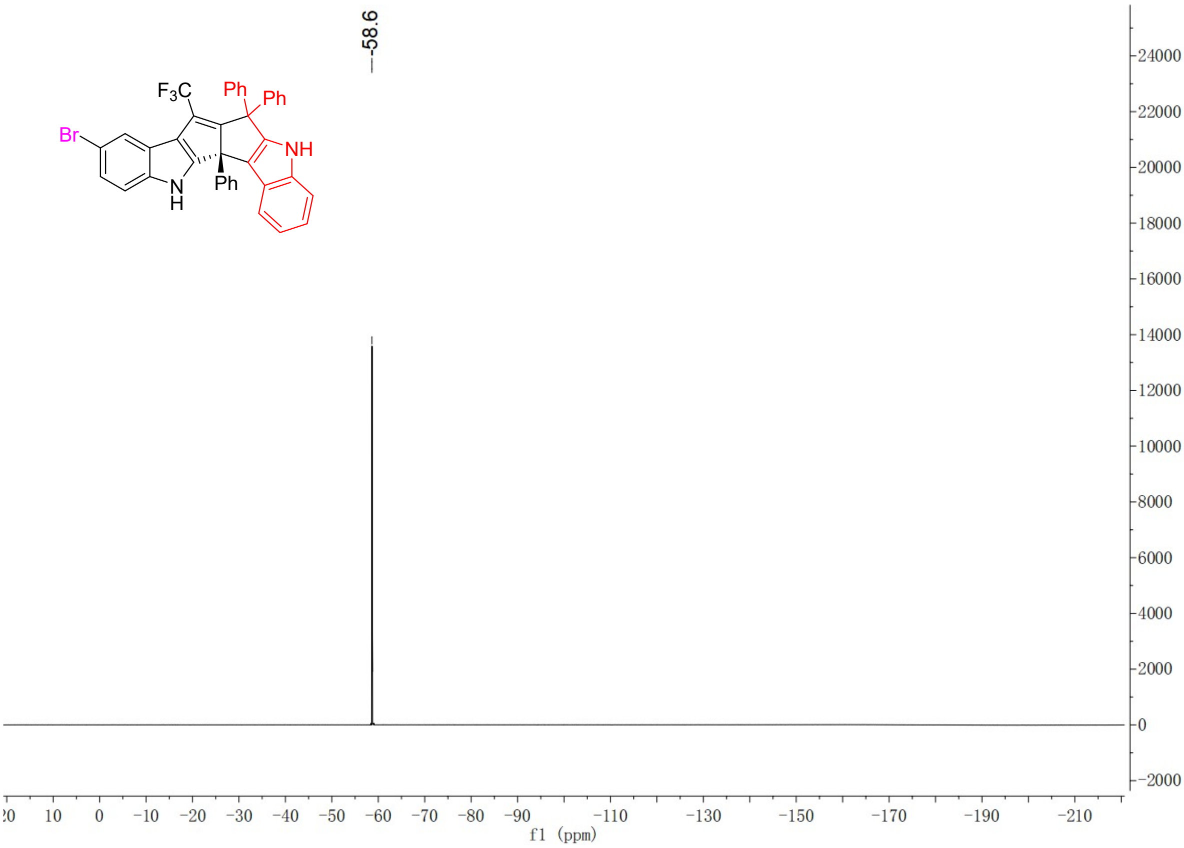
[1]H NMR of compound 3c (in $CDCl_3$)



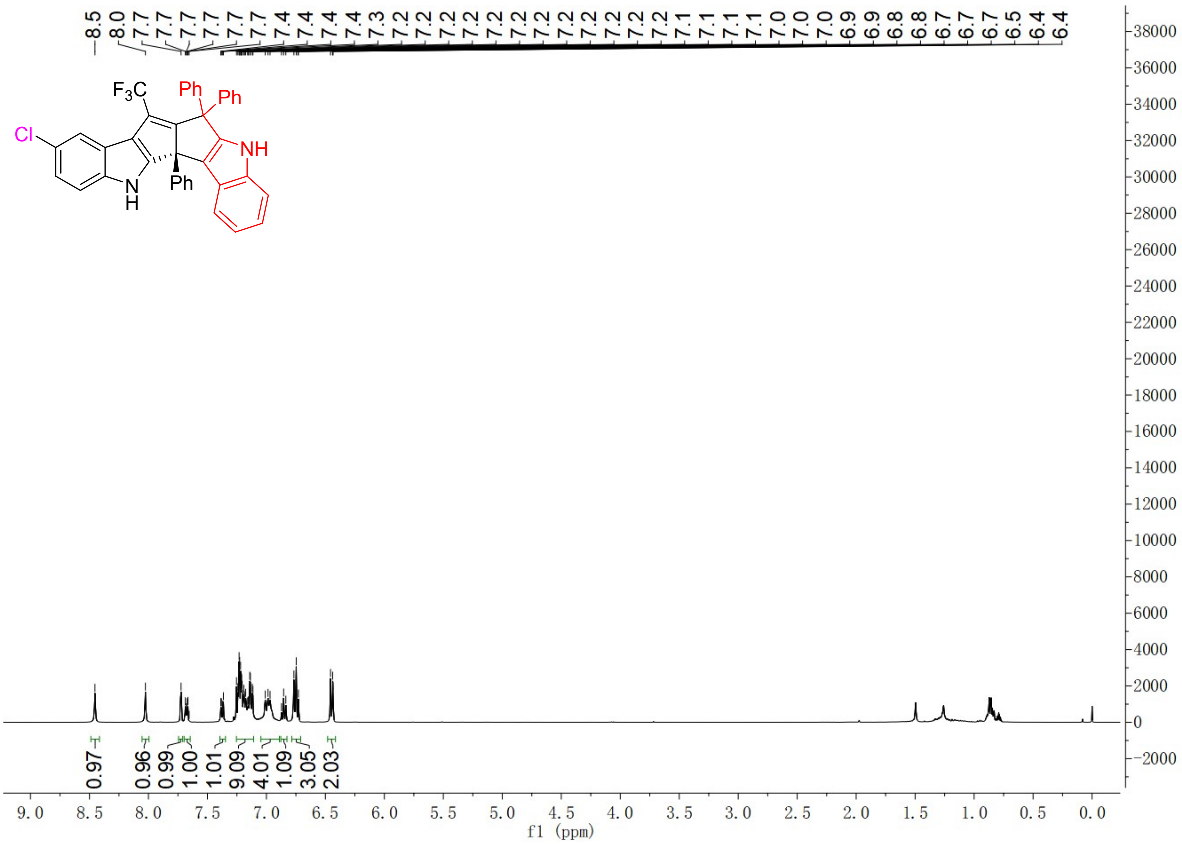
[13]C NMR of compound 3c (in $CDCl_3$)



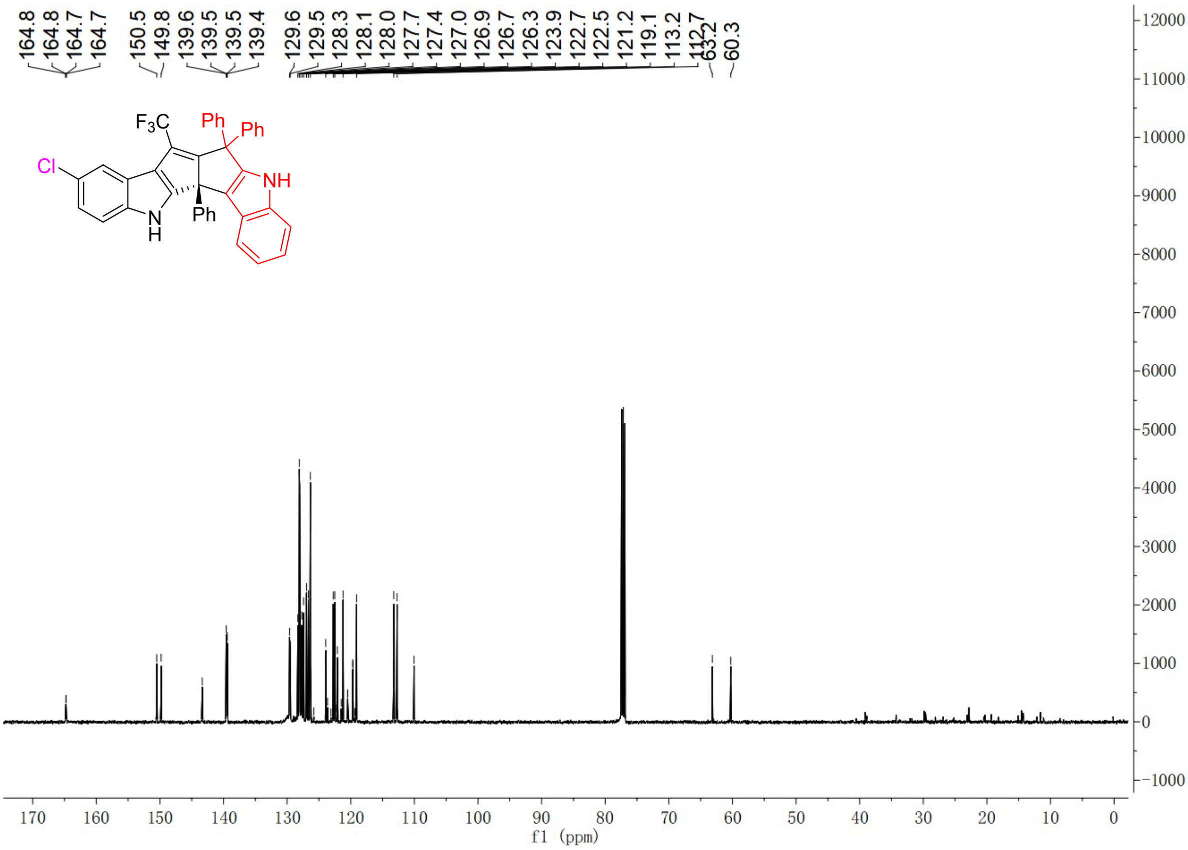
^{19}F NMR of compound 3c (in $CDCl_3$)



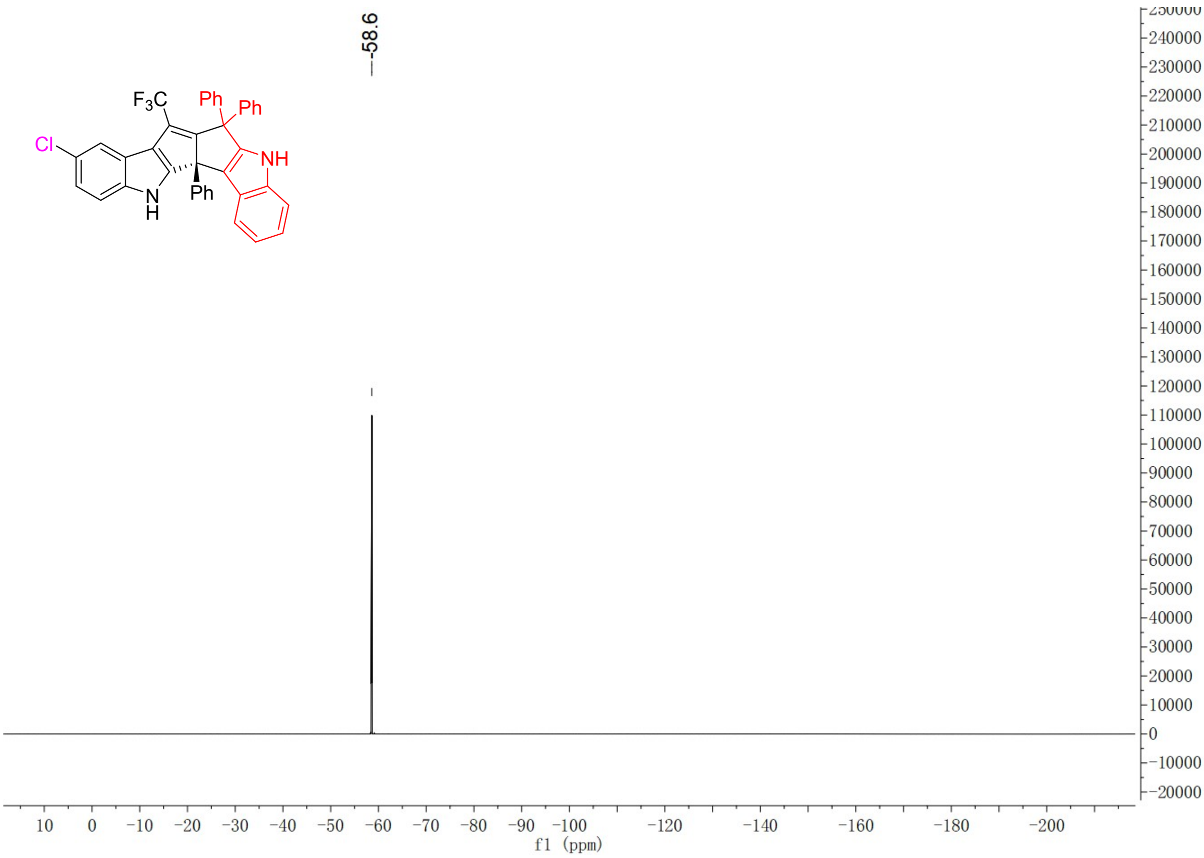
^{1}H NMR of compound 3d (in $CDCl_3$)



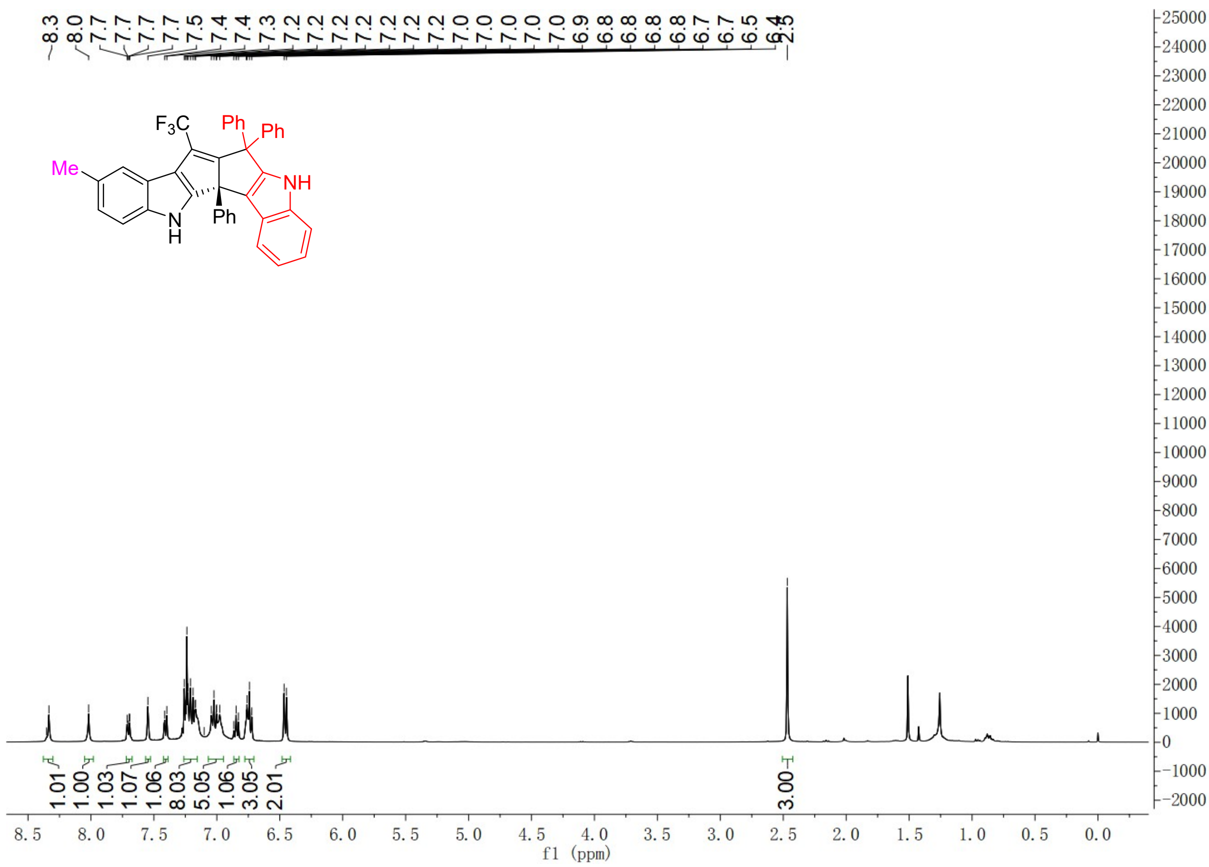
^{13}C NMR of compound 3d (in $CDCl_3$)



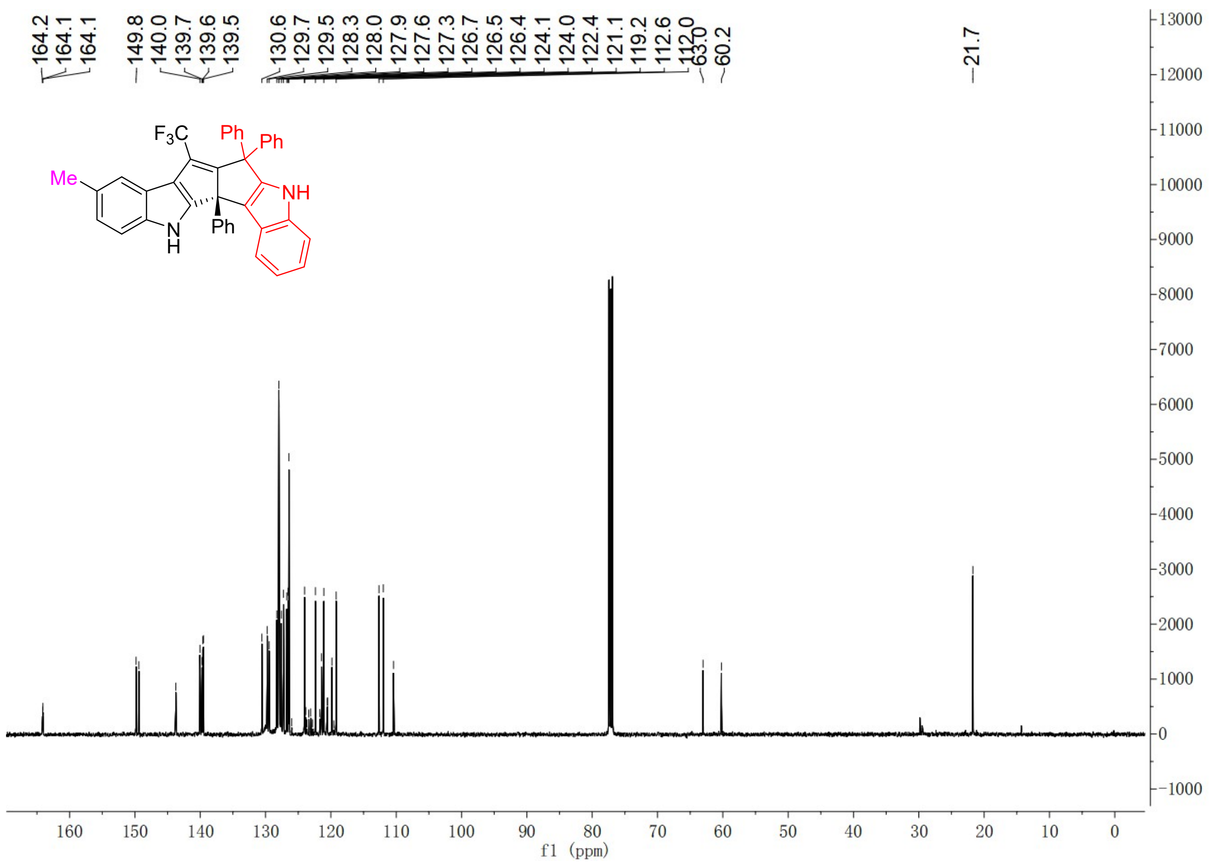
^{19}F NMR of compound 3d (in $CDCl_3$)



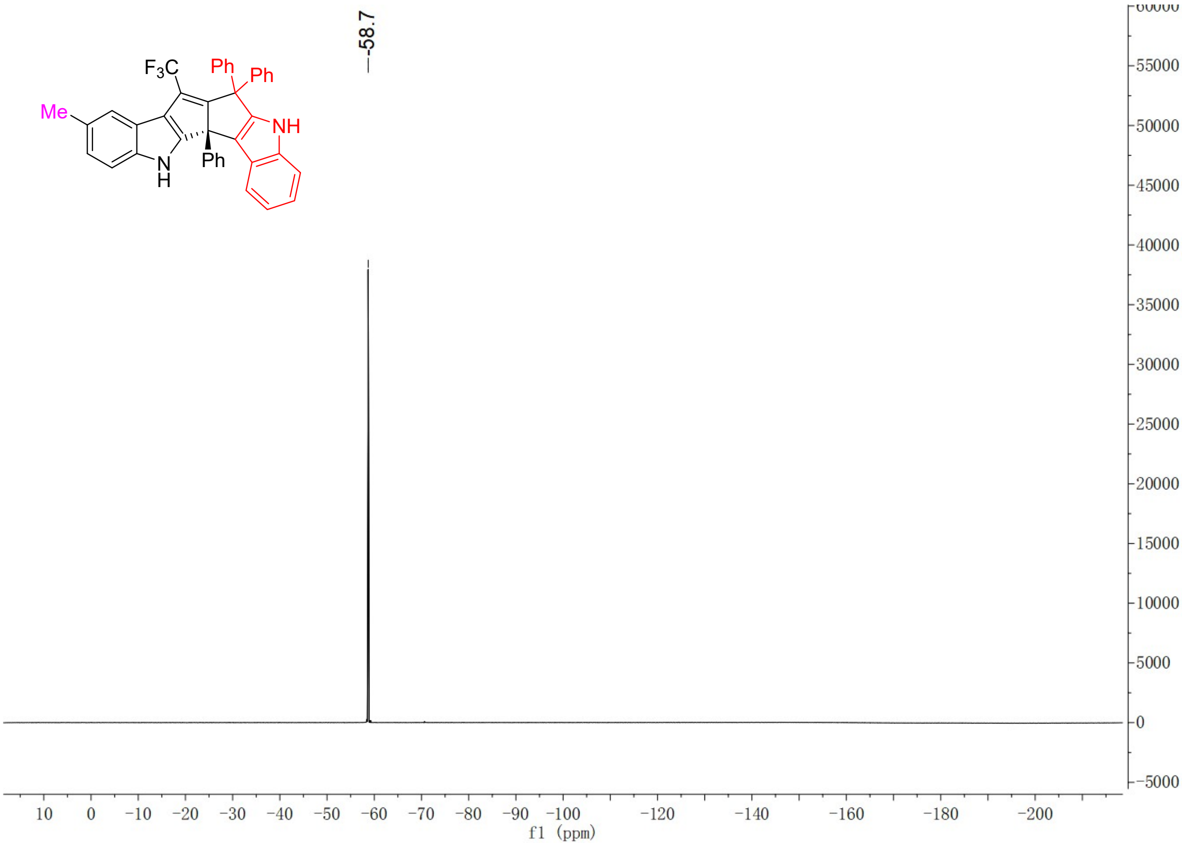
^{1}H NMR of compound 3e (in $CDCl_3$)



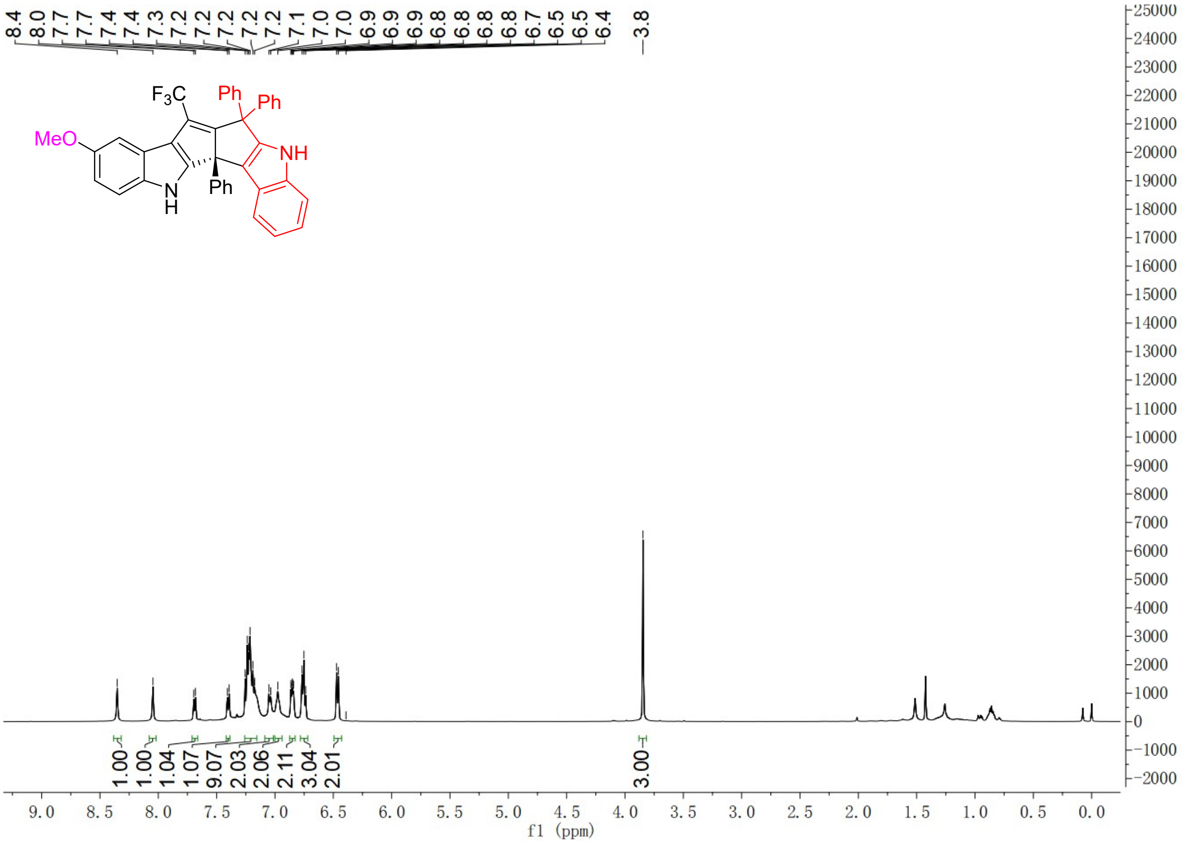
^{13}C NMR of compound 3e (in $CDCl_3$)



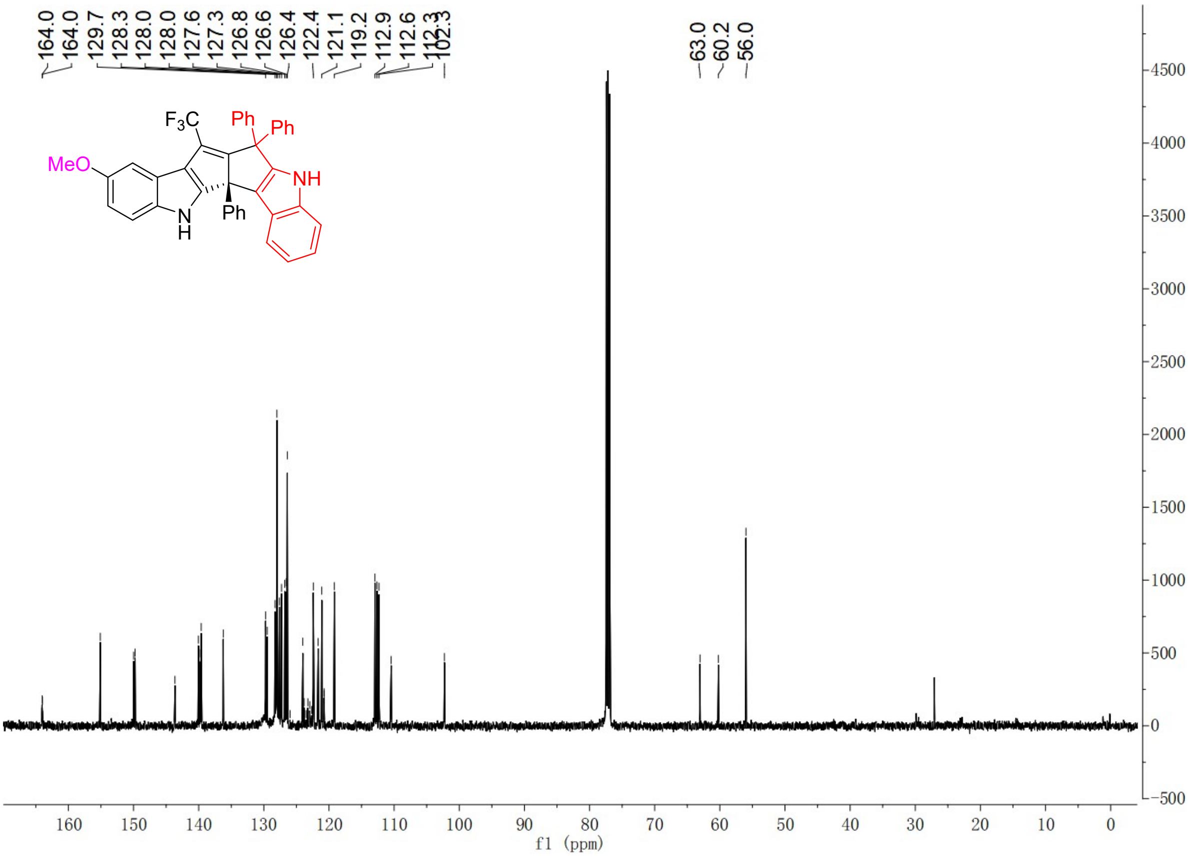
^{19}F NMR of compound 3e (in $CDCl_3$)



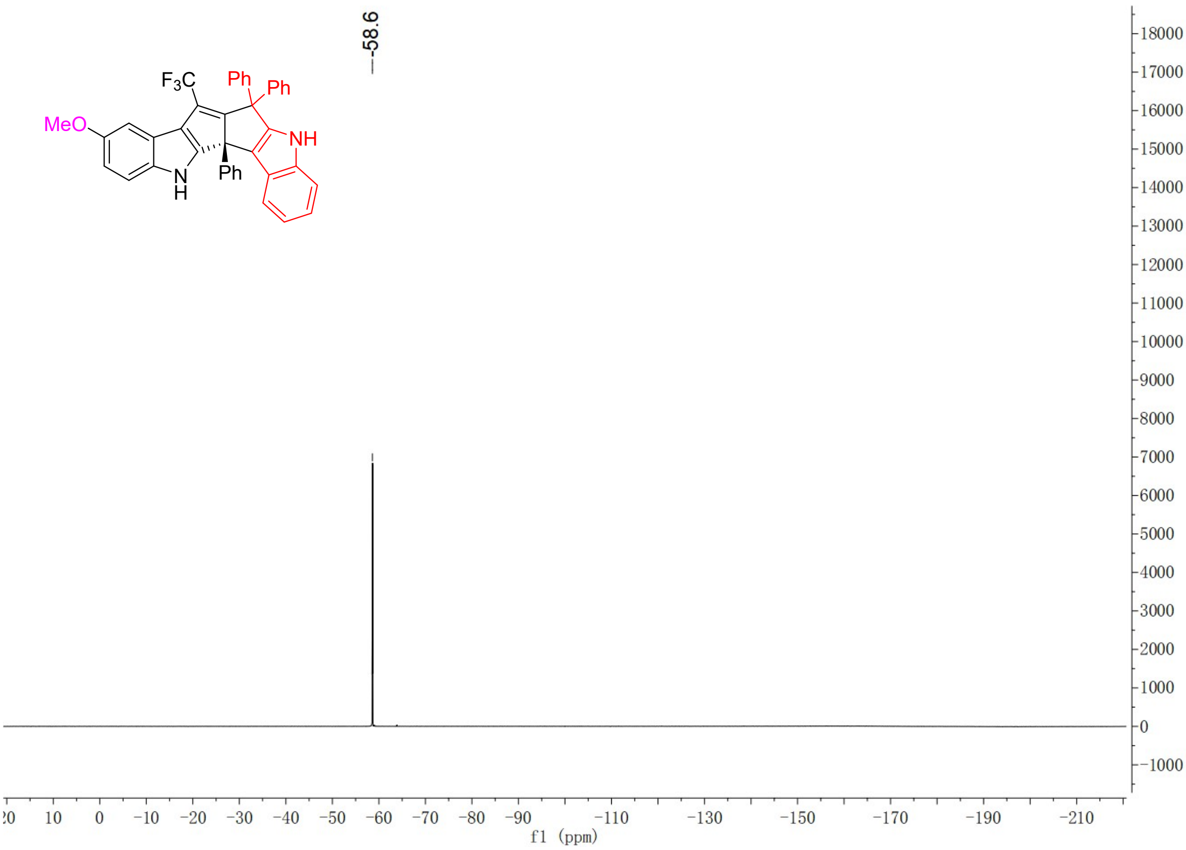
^{1}H NMR of compound 3f (in $CDCl_3$)



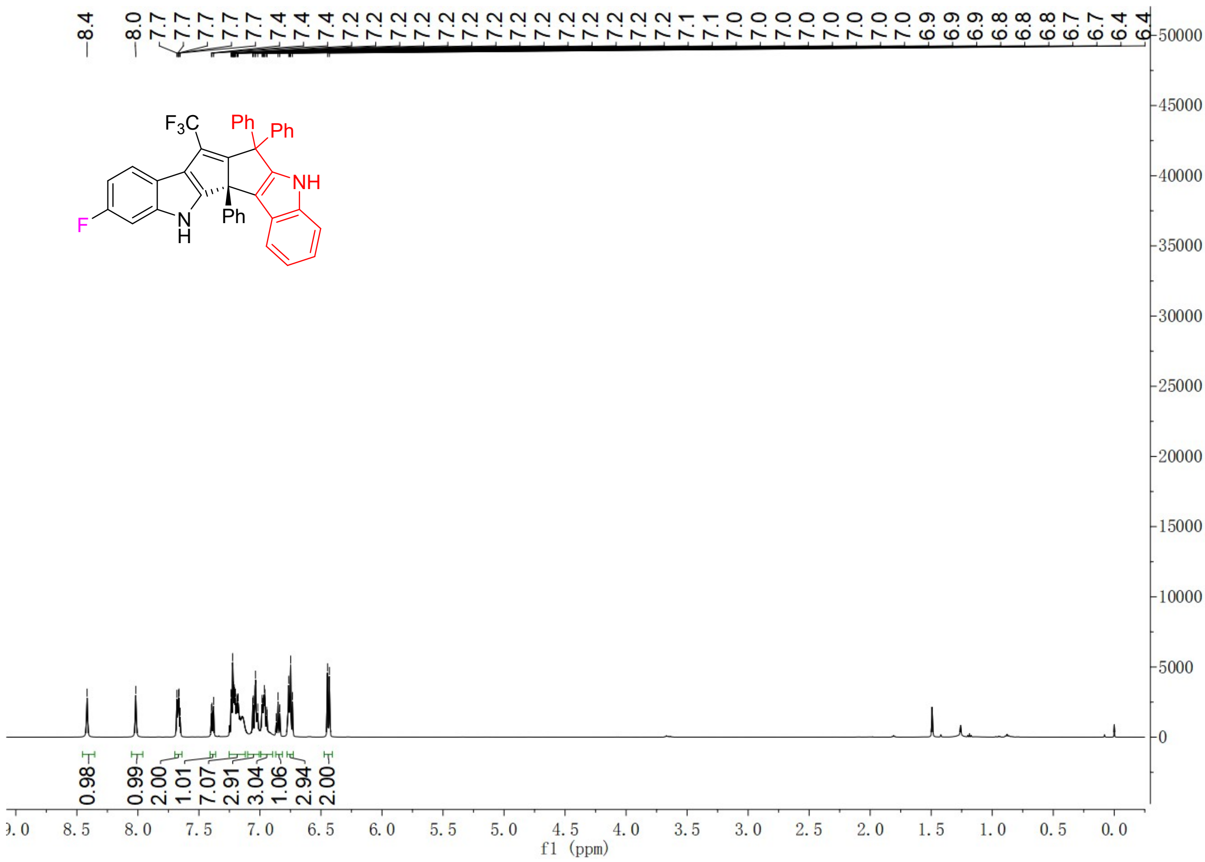
^{13}C NMR of compound 3f (in $CDCl_3$)



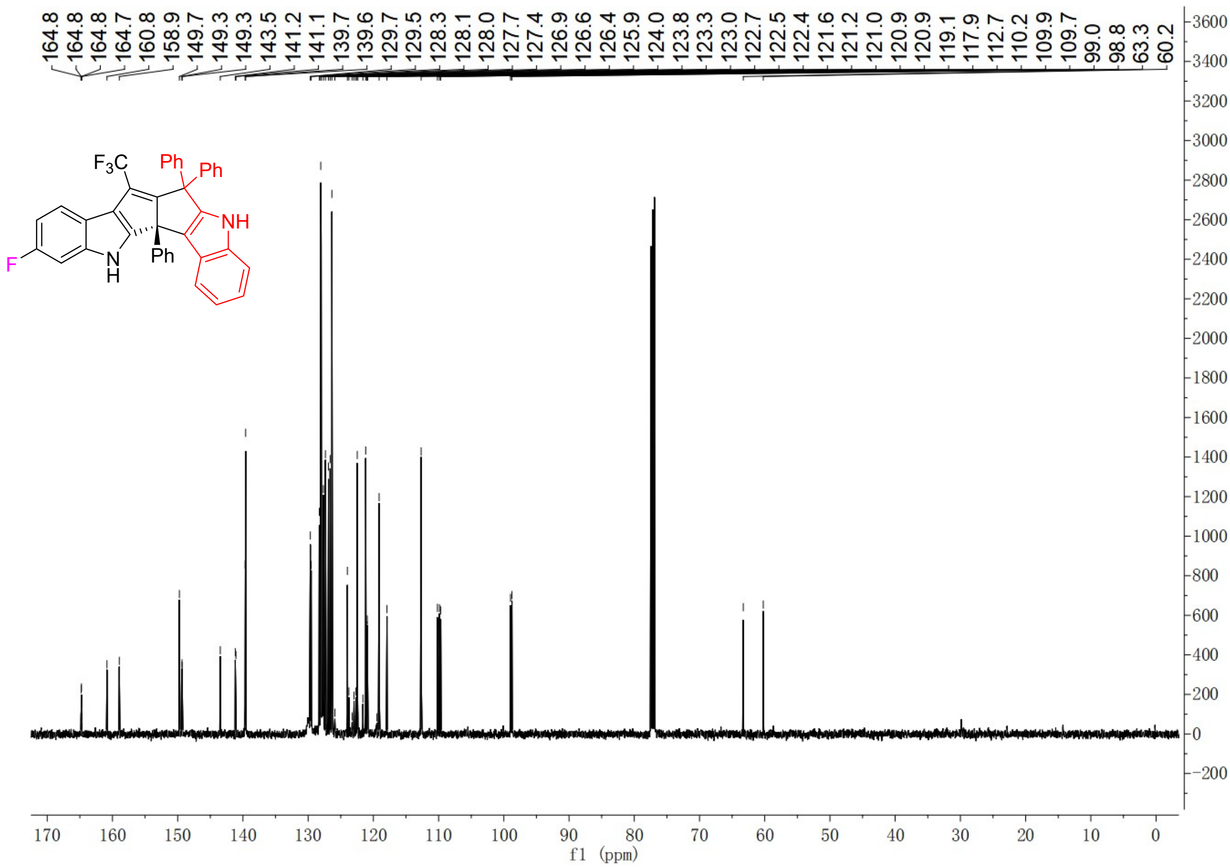
^{19}F NMR of compound 3f (in $CDCl_3$)



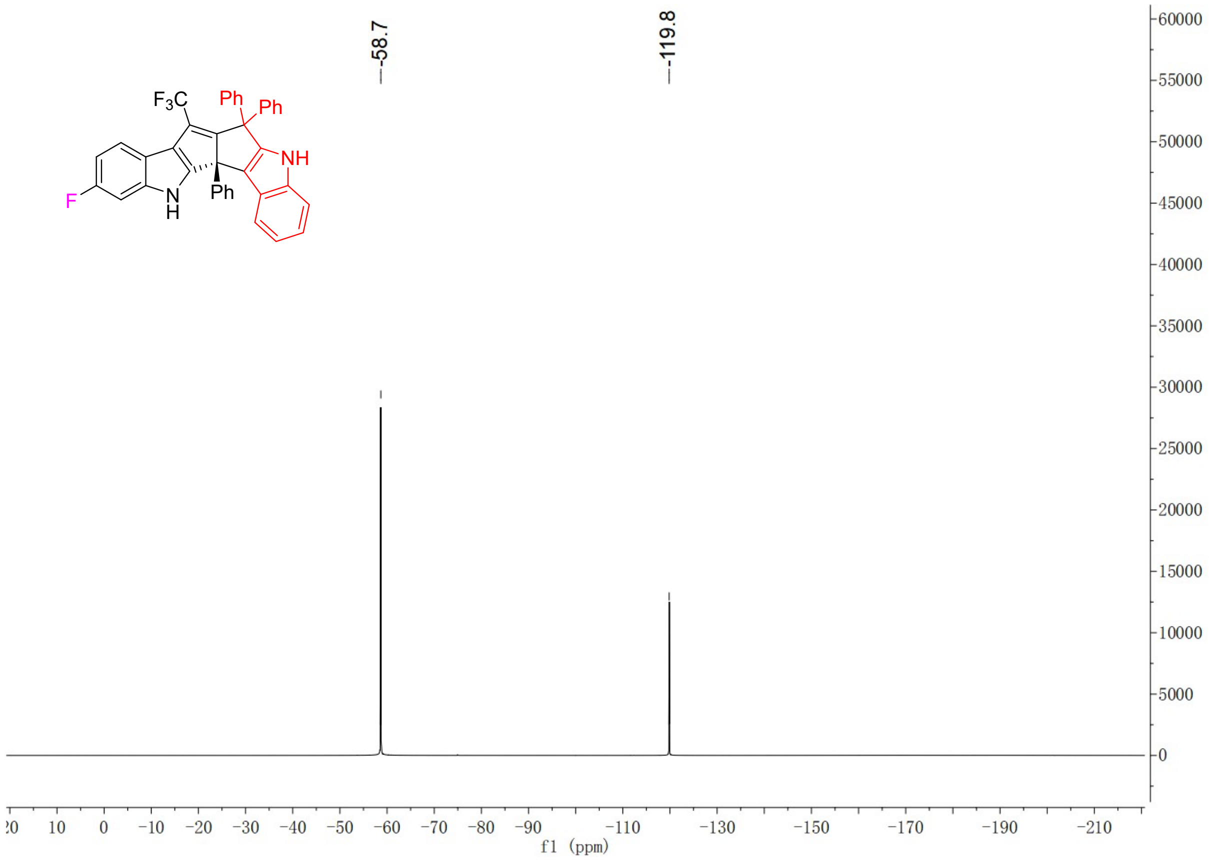
[1]H NMR of compound 3g (in $CDCl_3$)



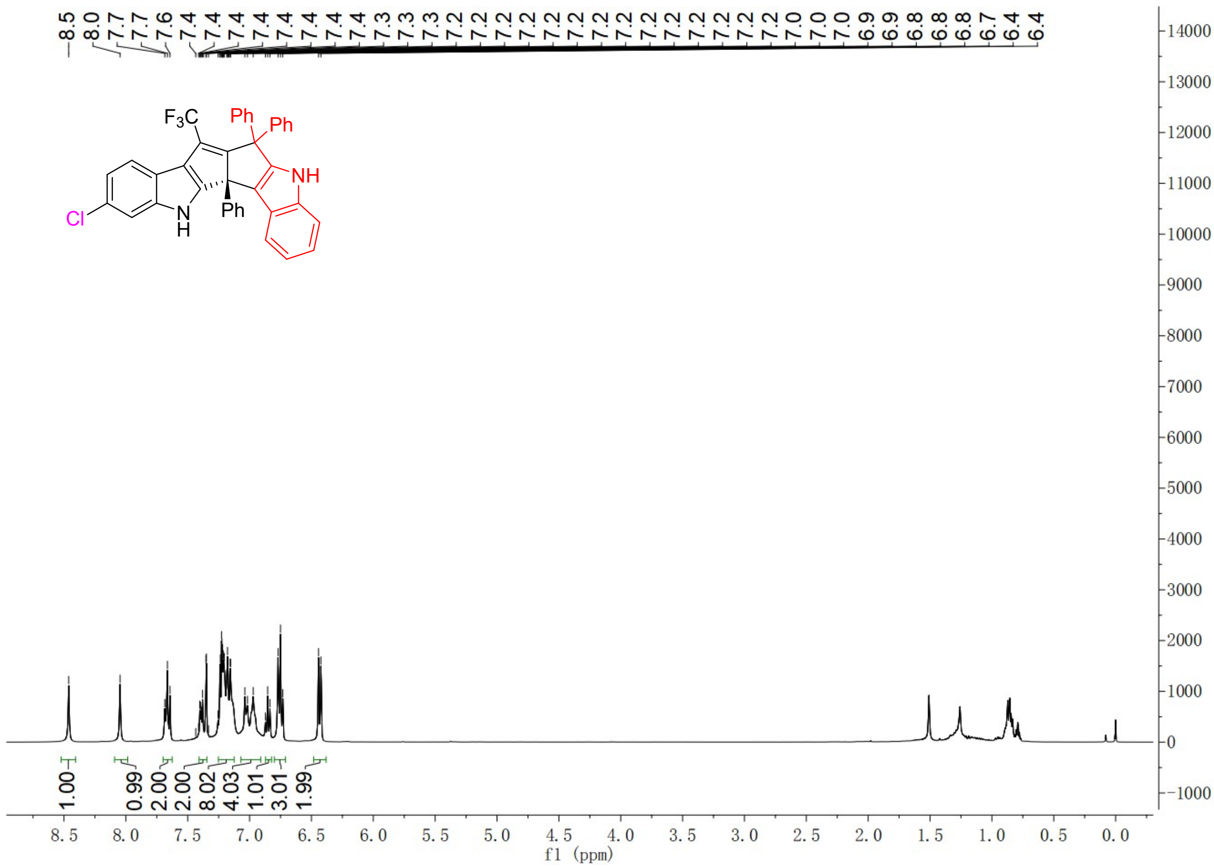
[13]C NMR of compound 3g (in $CDCl_3$)



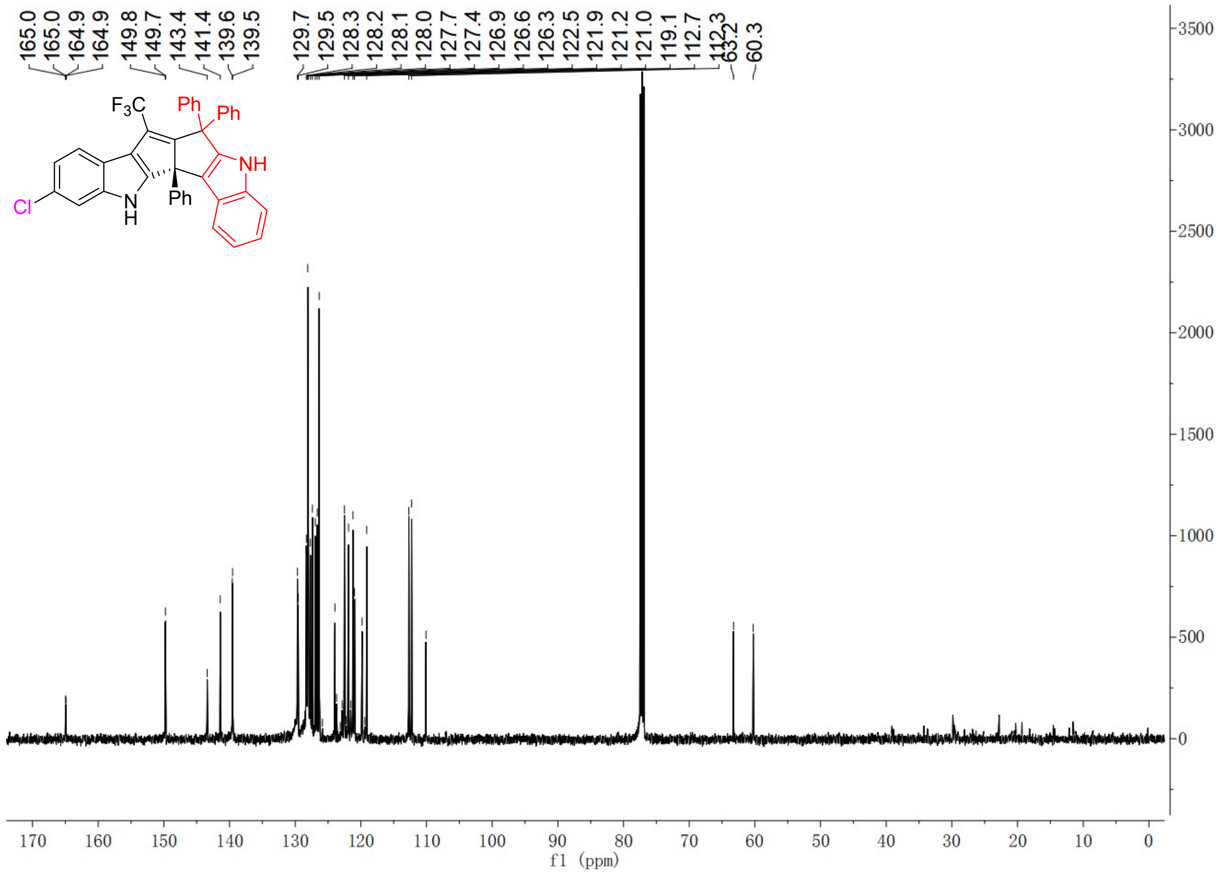
^{19}F NMR of compound 3g (in $CDCl_3$)



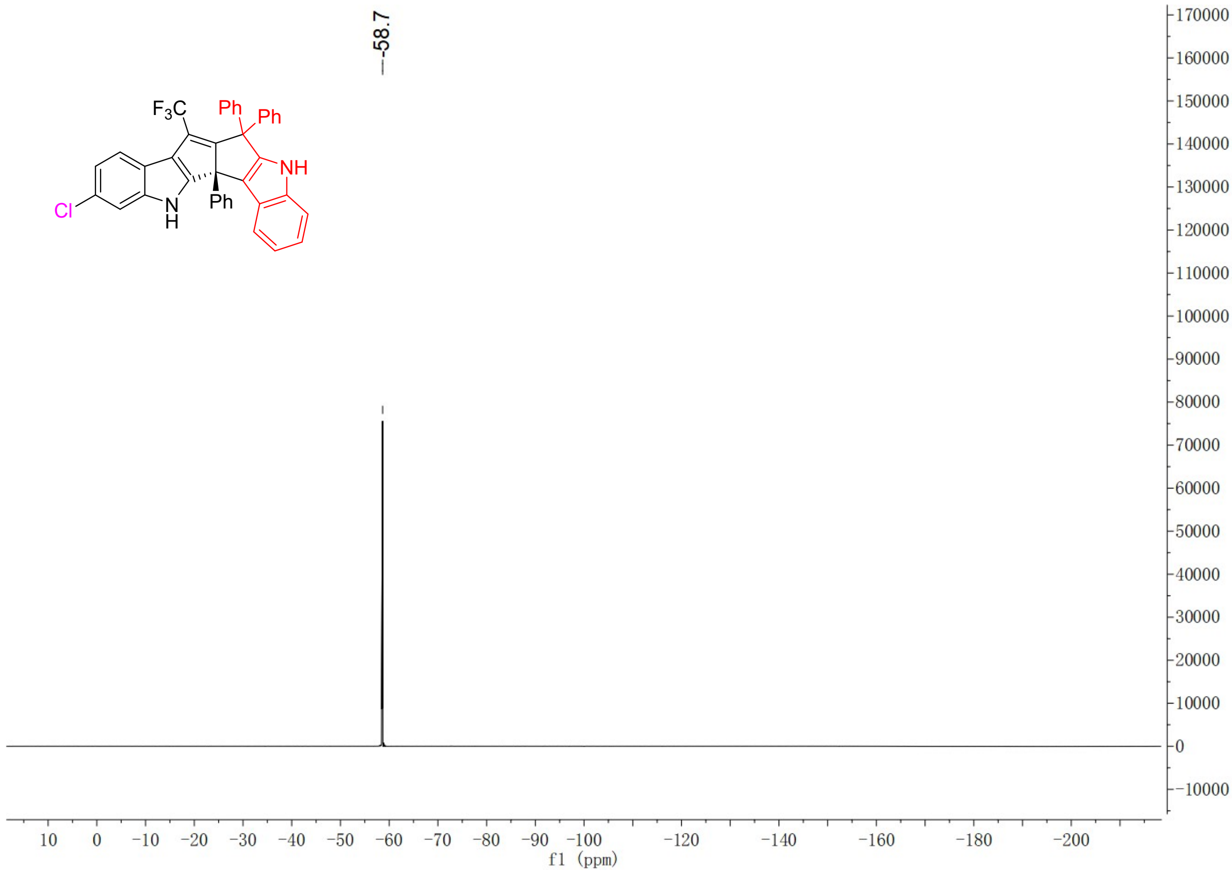
^{1}H NMR of compound 3h (in $CDCl_3$)



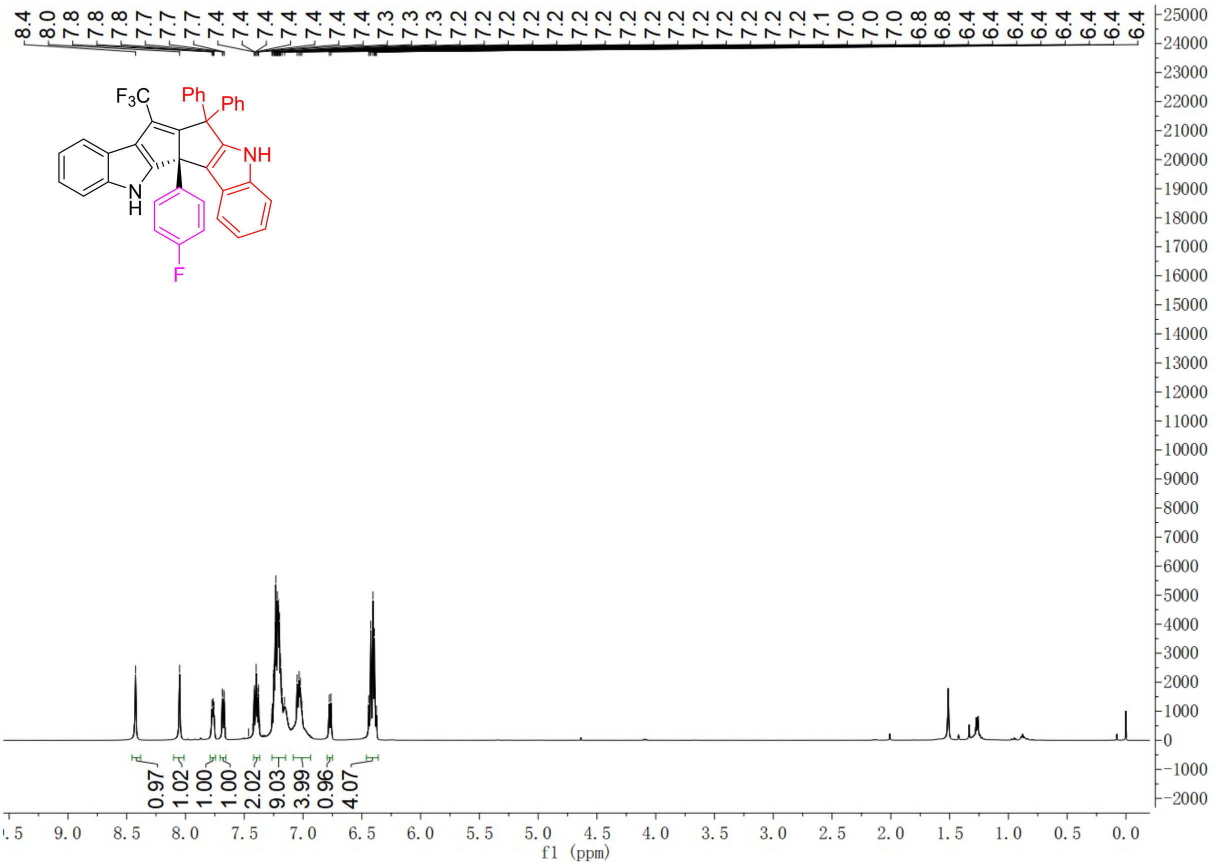
^{13}C NMR of compound 3h (in $CDCl_3$)



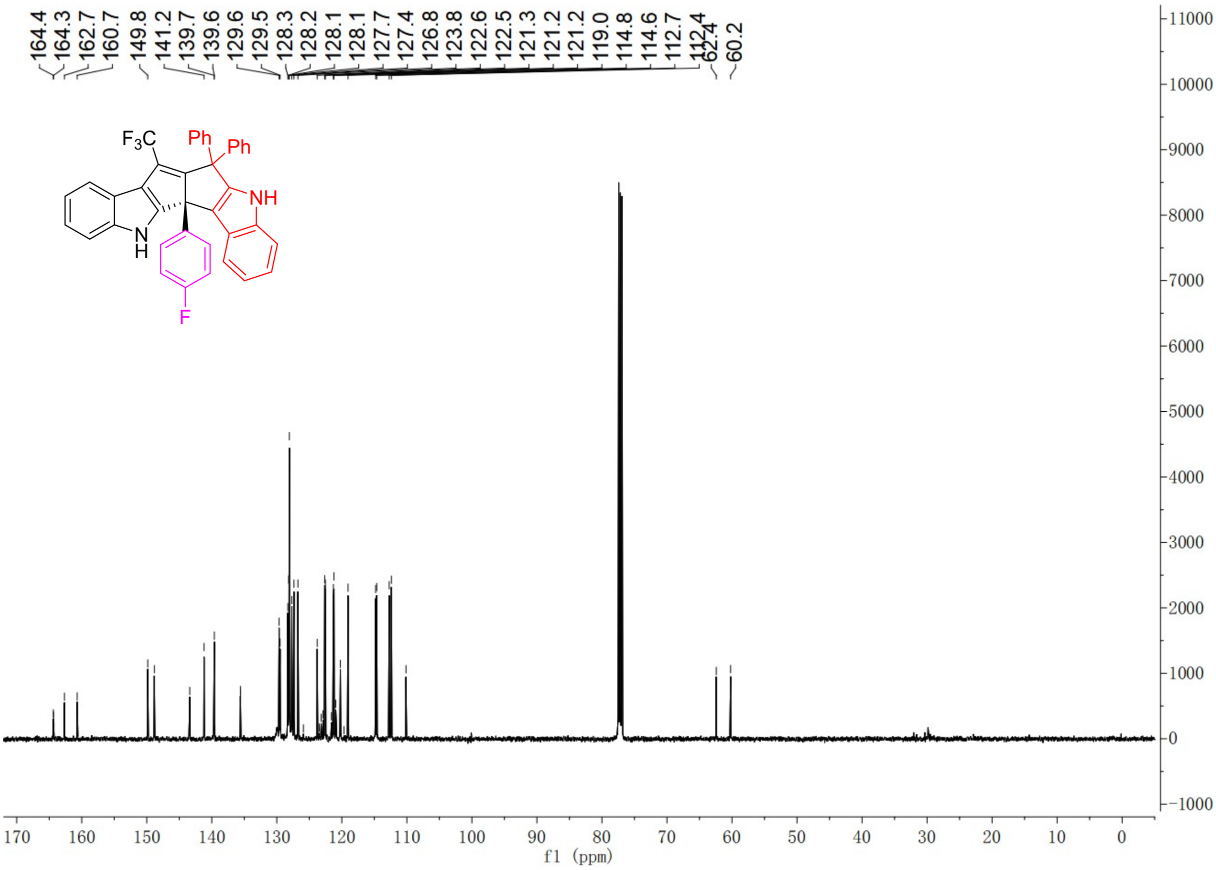
^{19}F NMR of compound 3h (in $CDCl_3$)



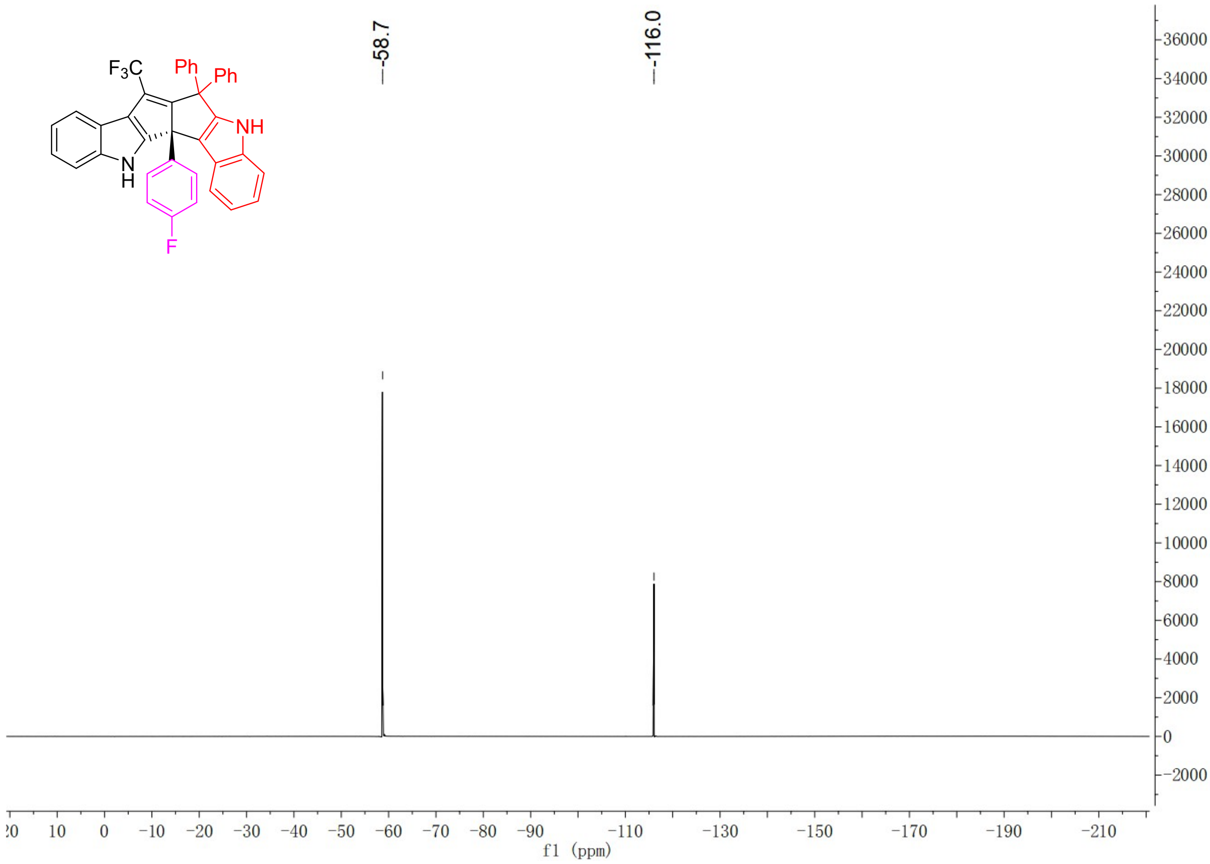
^{1}H NMR of compound 3i (in $CDCl_3$)



^{13}C NMR of compound 3i (in $CDCl_3$)



^{19}F NMR of compound 3i (in $CDCl_3$)



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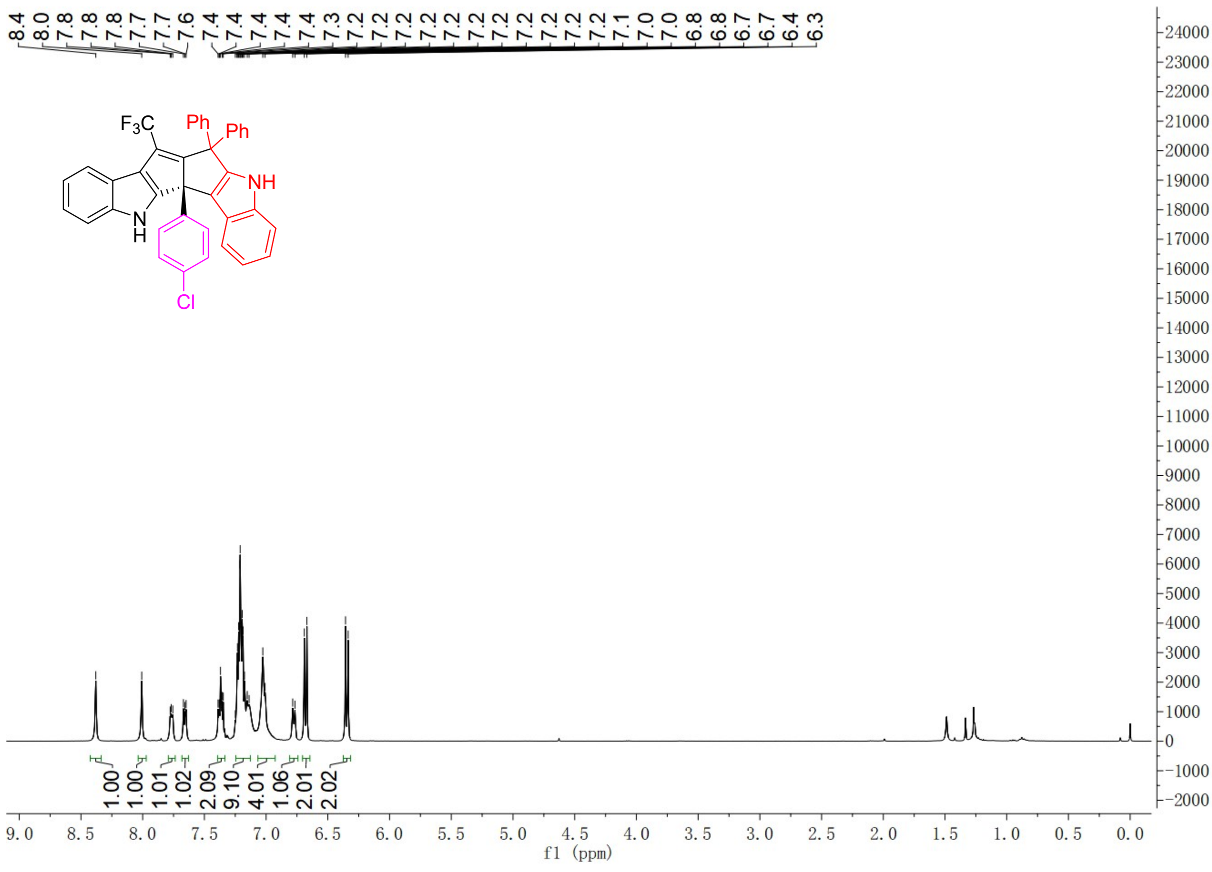

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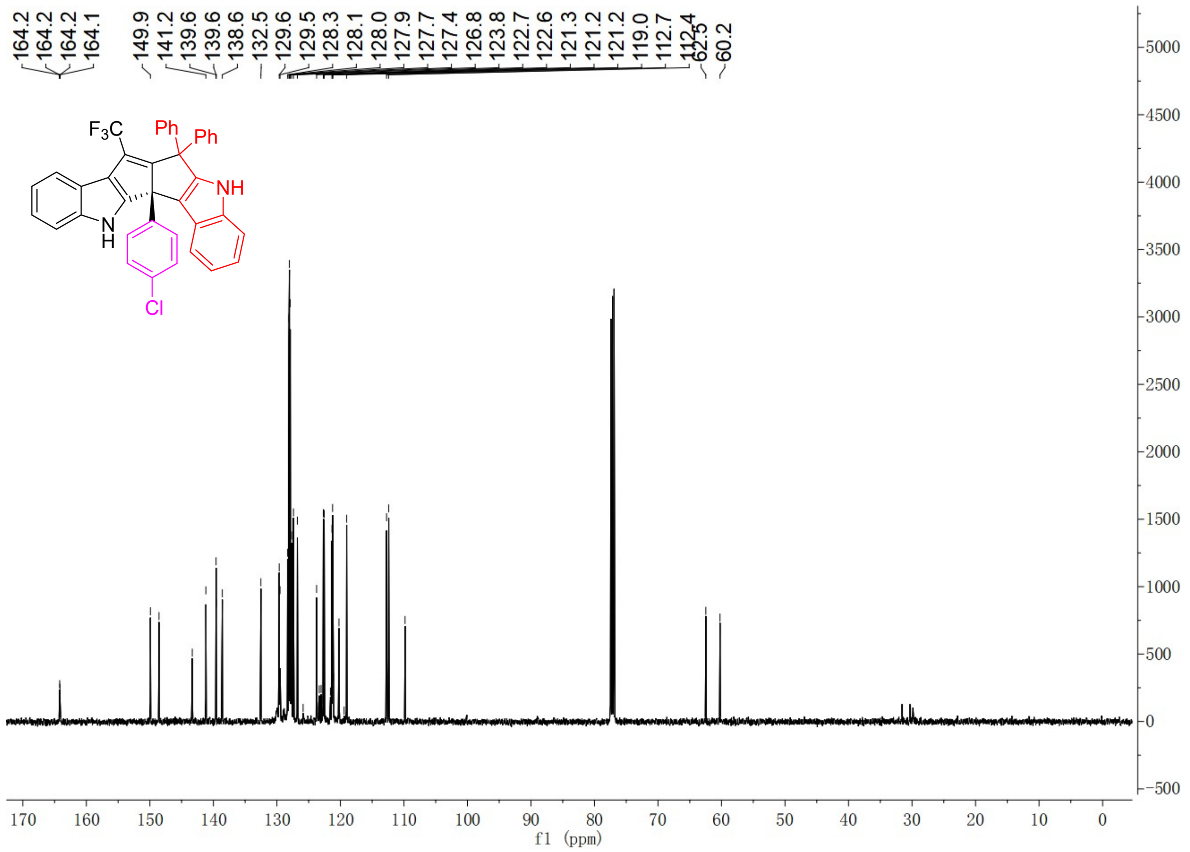

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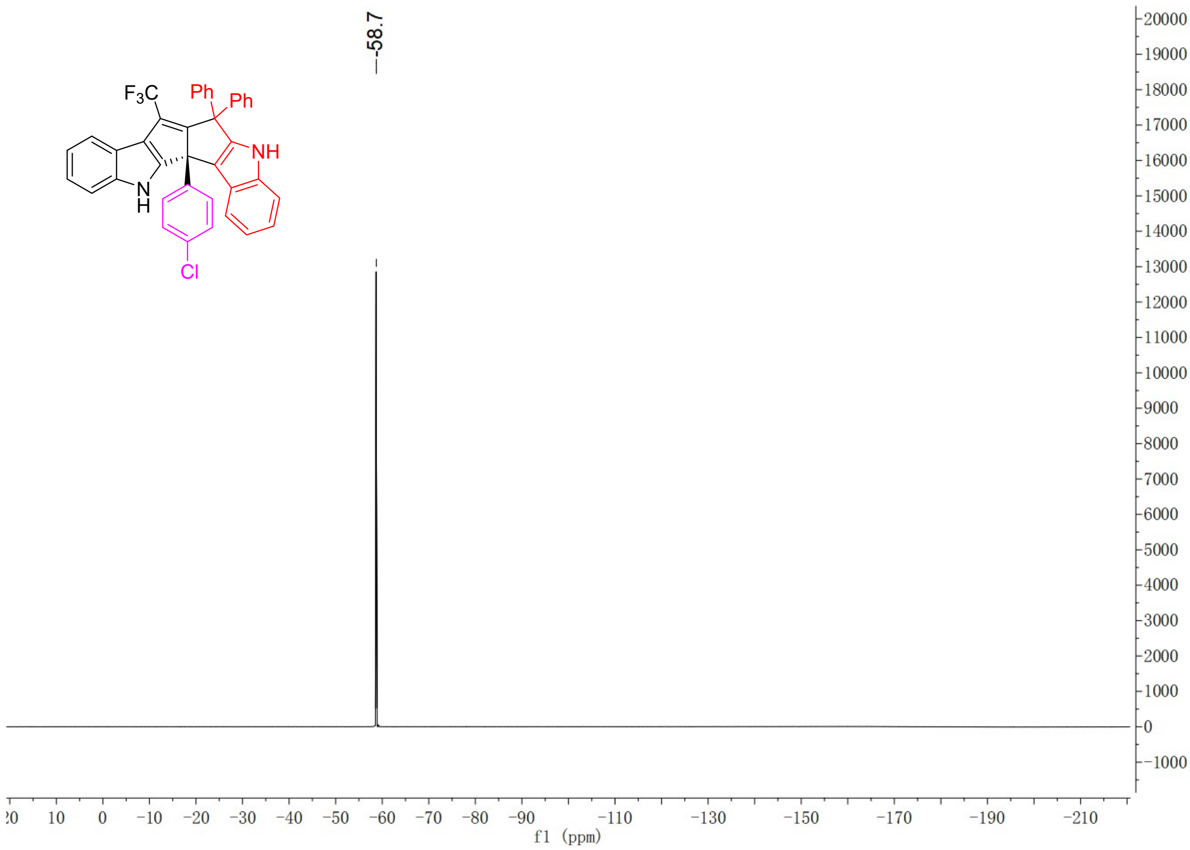
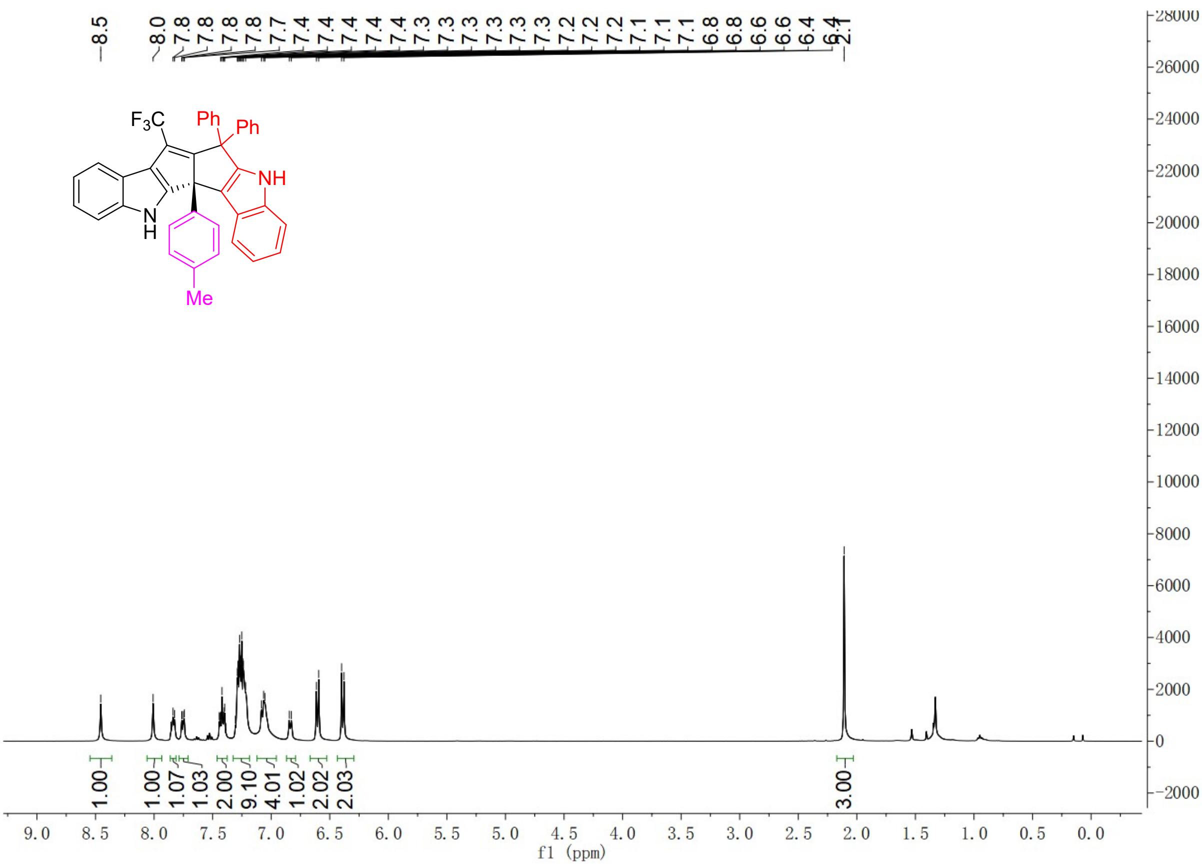


^{1}H NMR of compound 3k (in $CDCl_3$)



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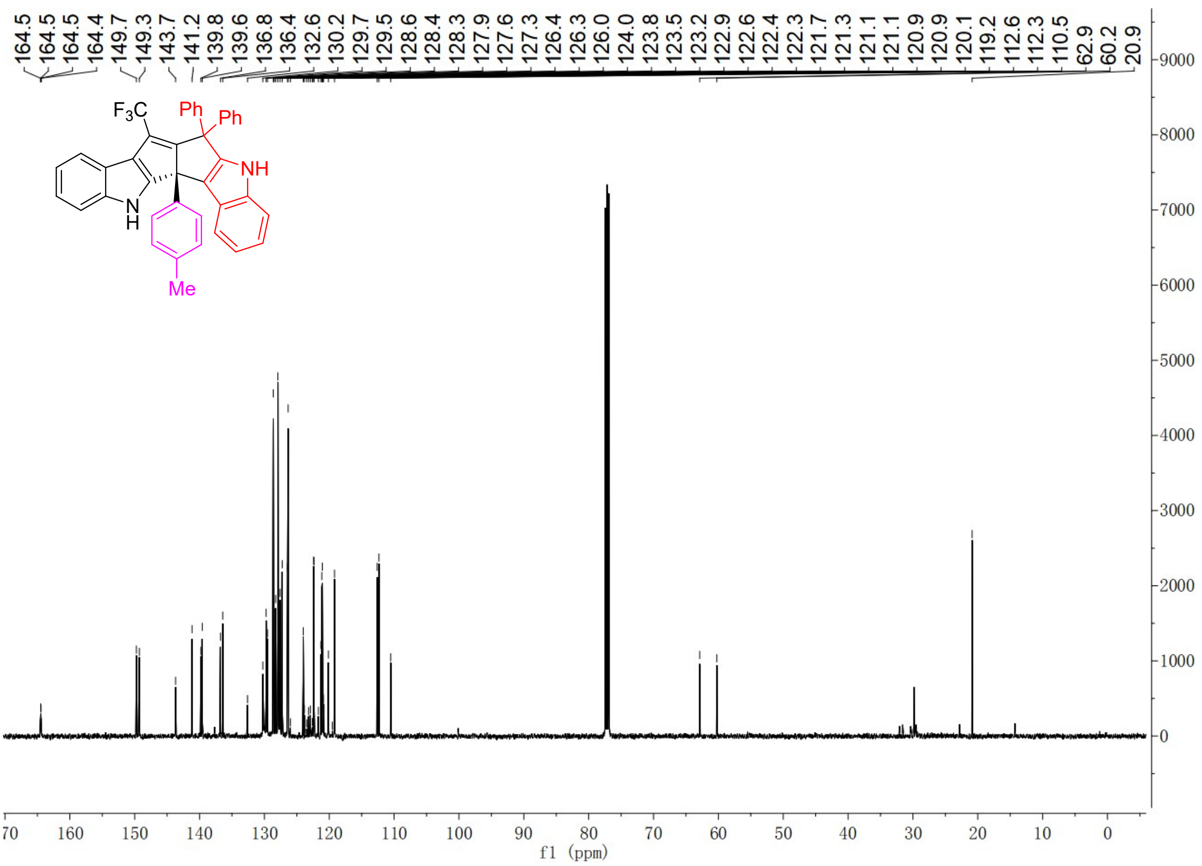
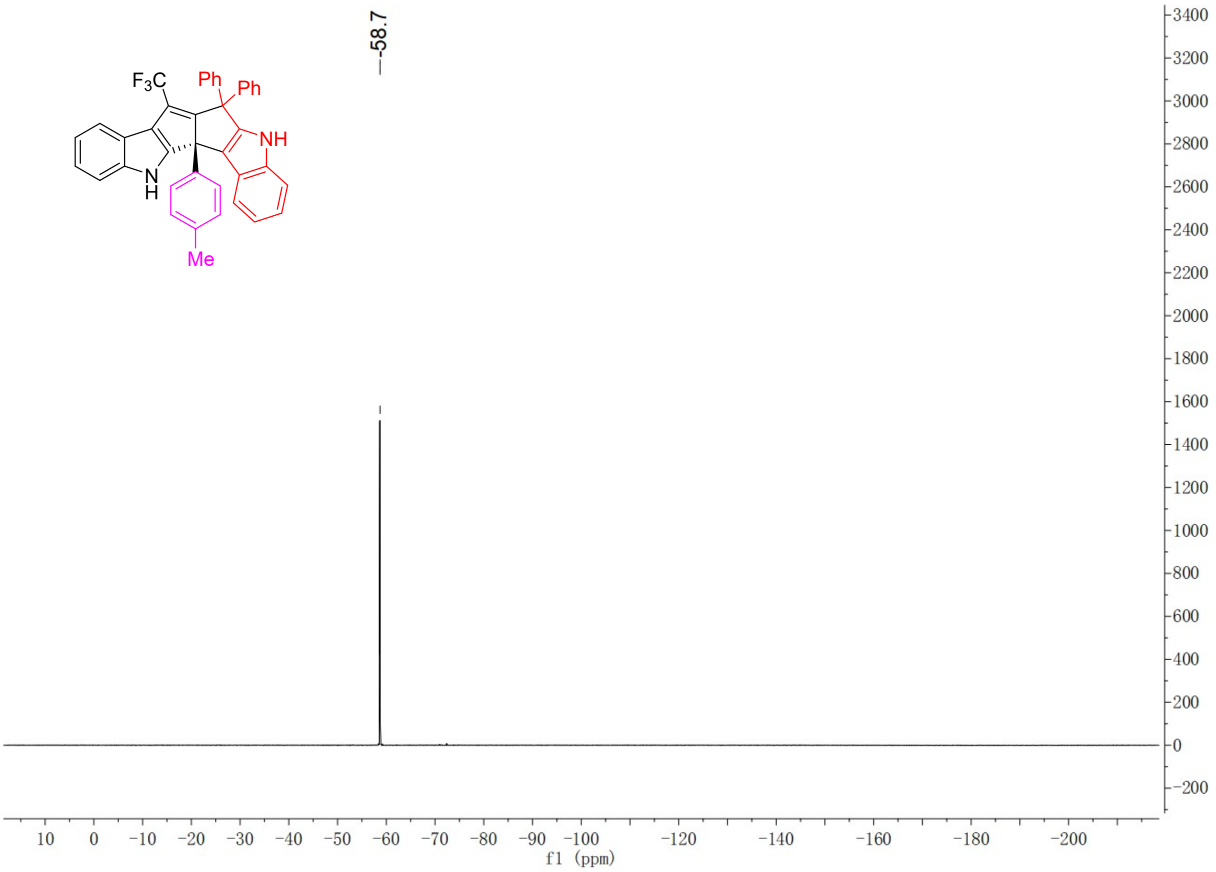


^{19}F NMR of compound 3k (in $CDCl_3$)



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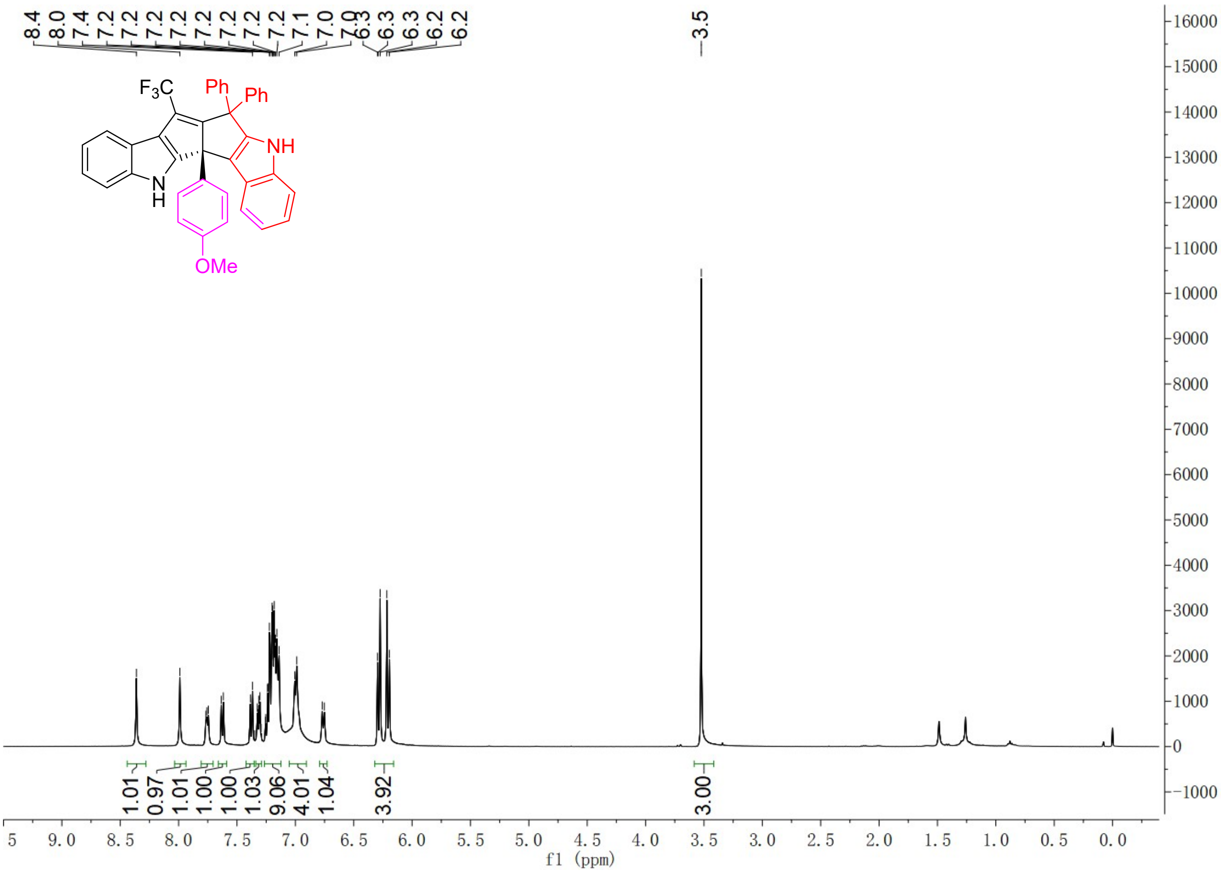
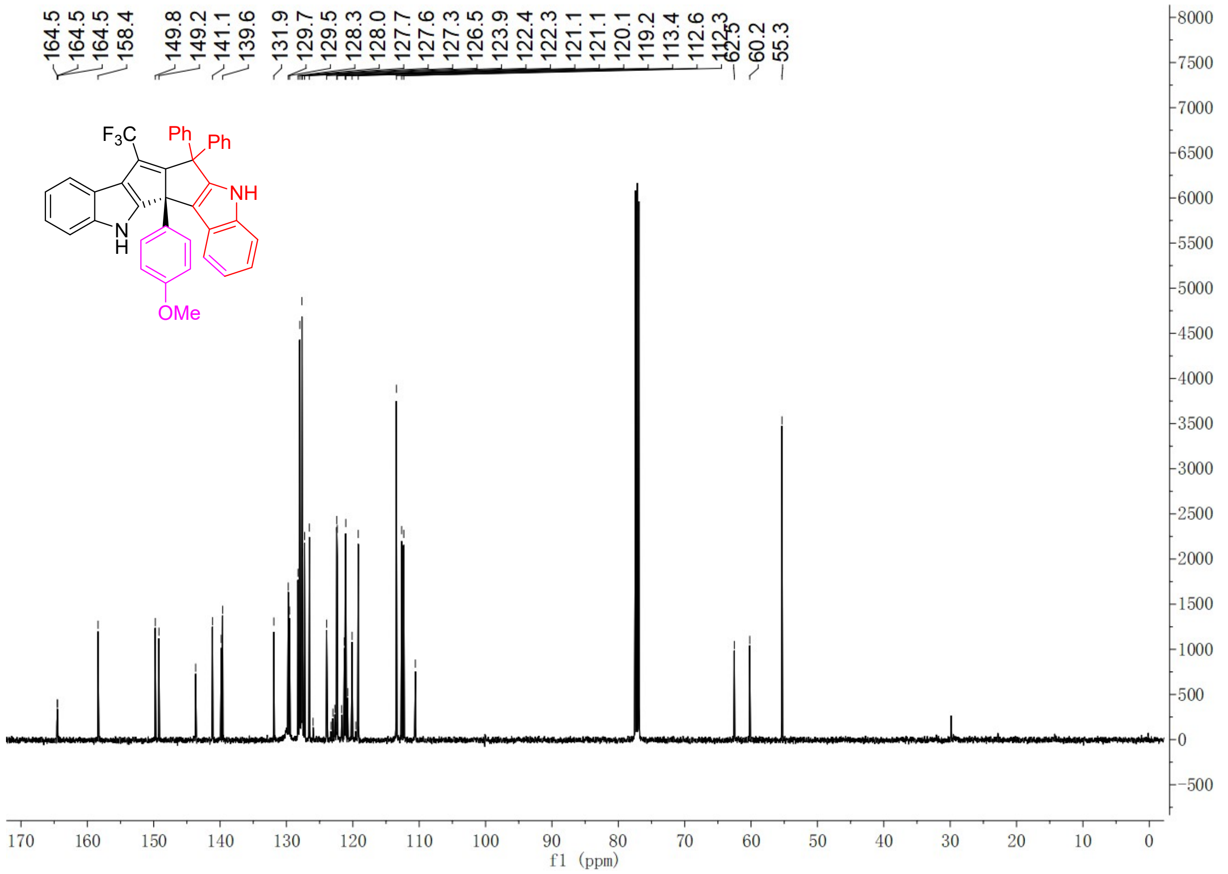


^{13}C NMR of compound 3l (in $CDCl_3$)



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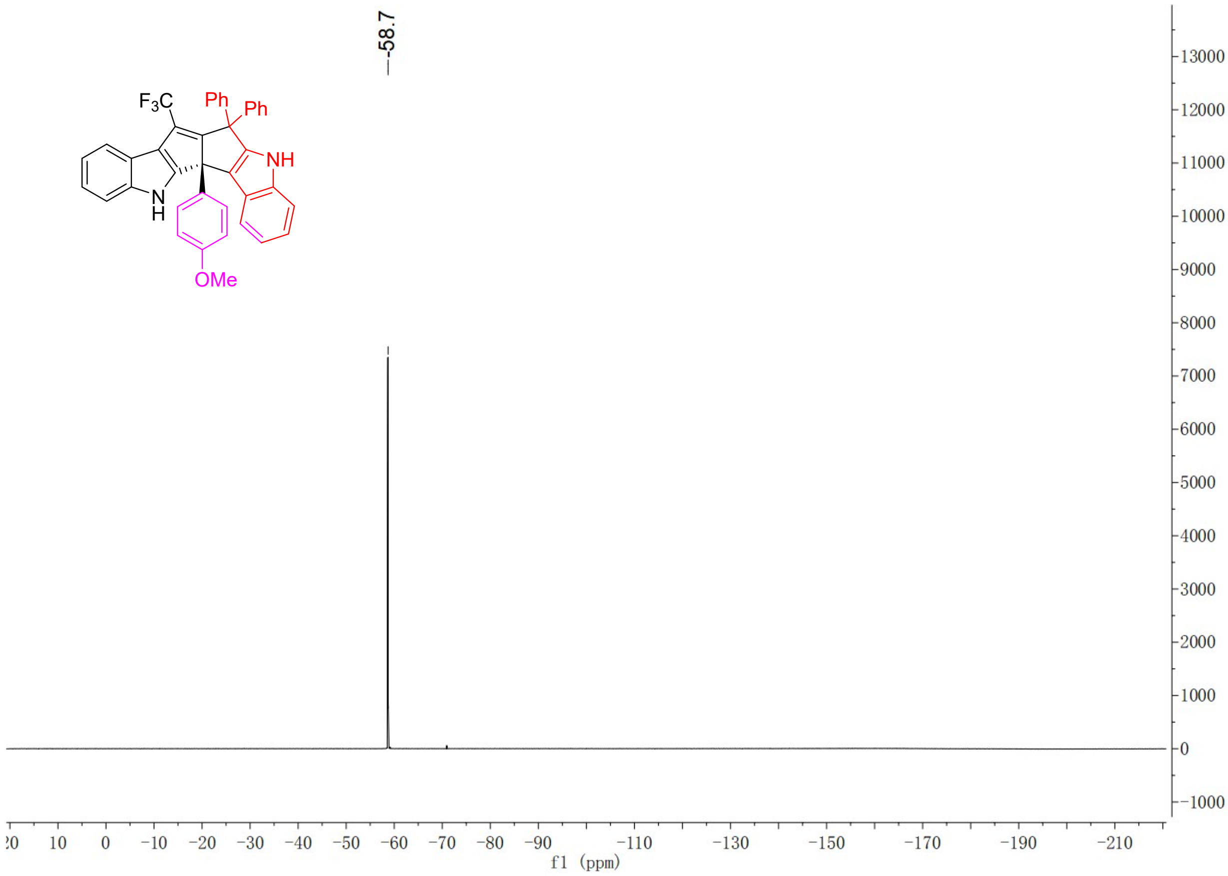
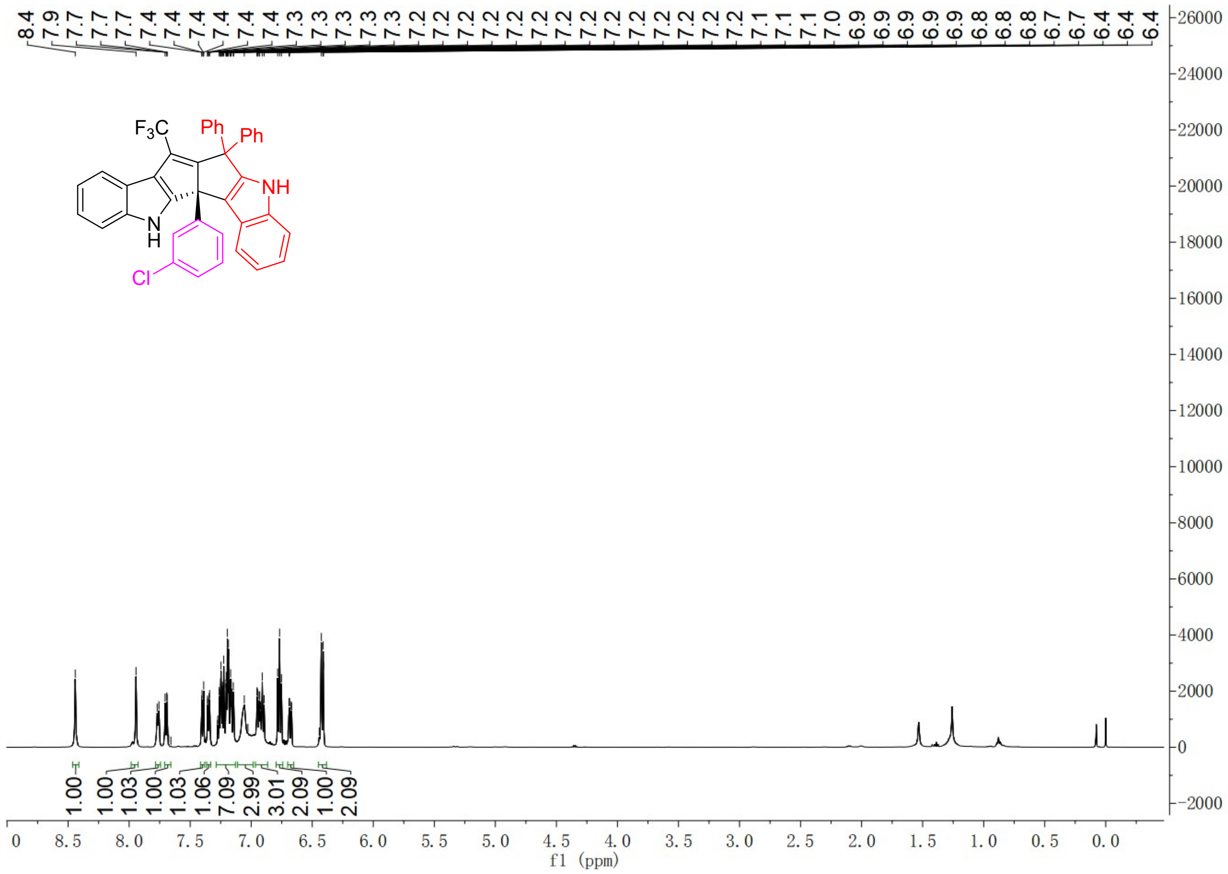
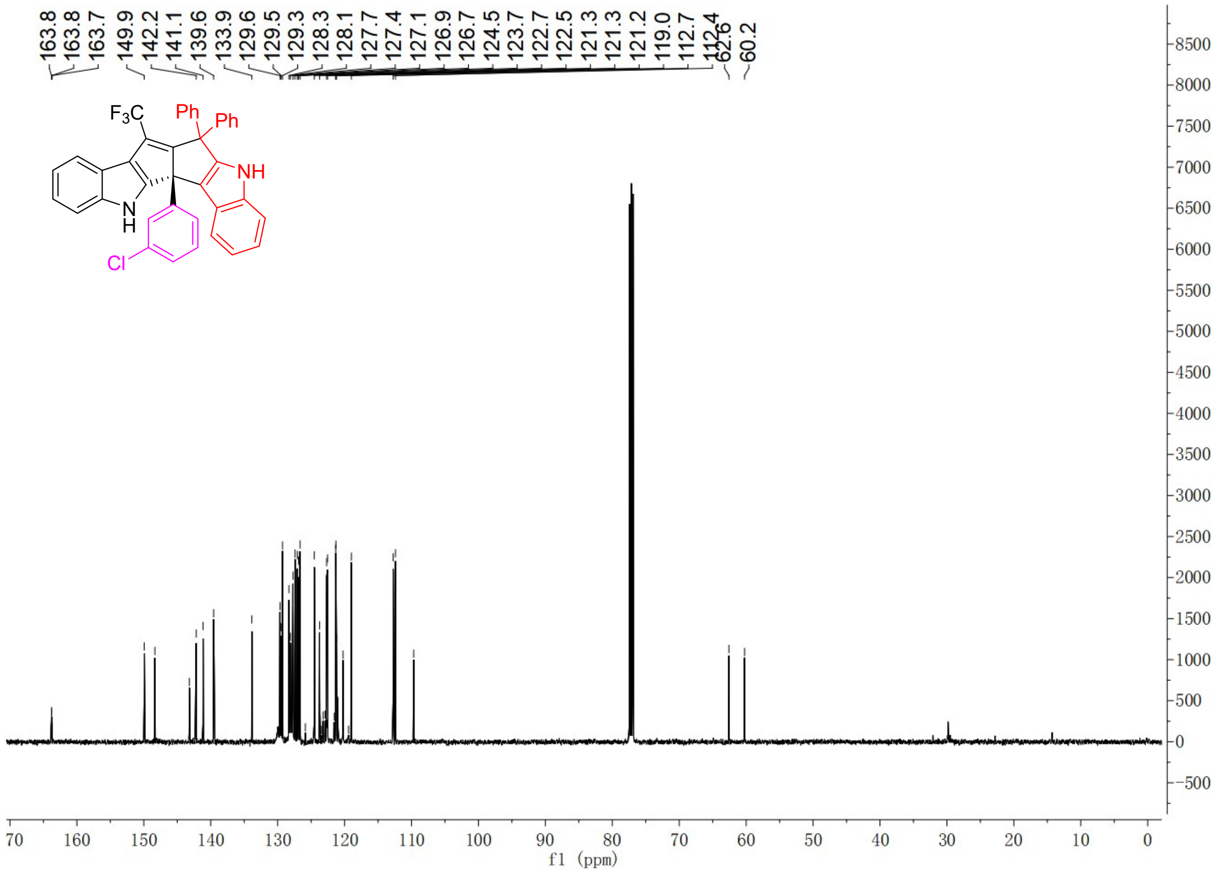


^{1}H NMR of compound 3m (in CDCl$_3$)



^{13}C NMR of compound 3m (in CDCl$_3$)



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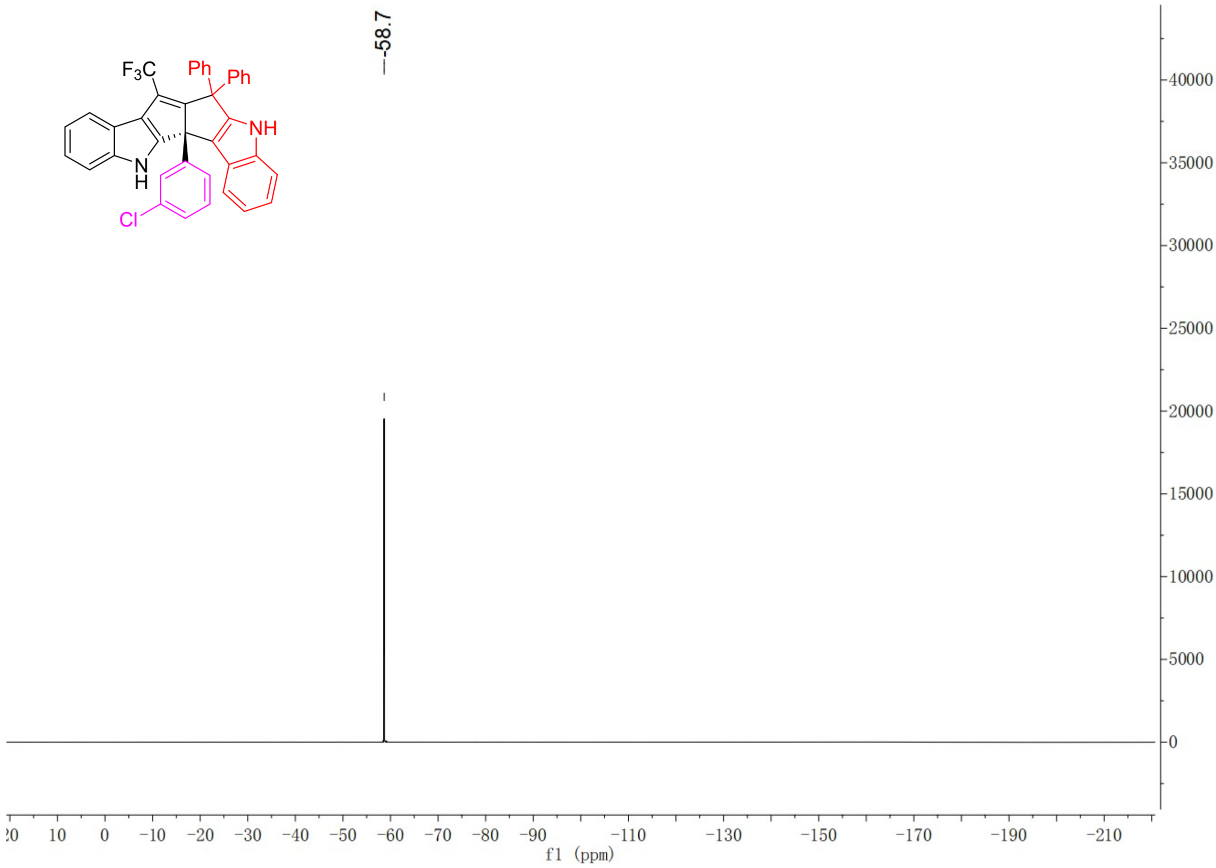
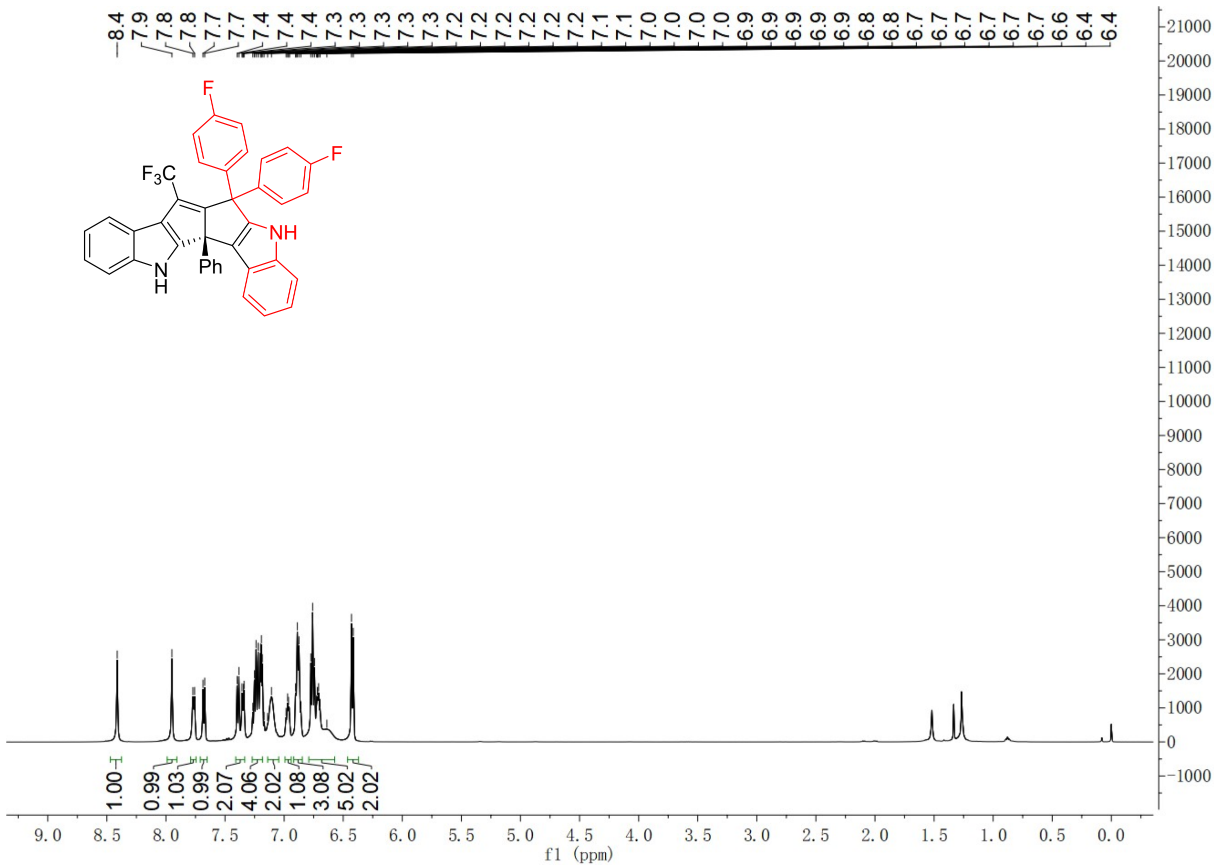


^{1}H NMR of compound 3n (in $CDCl_3$)



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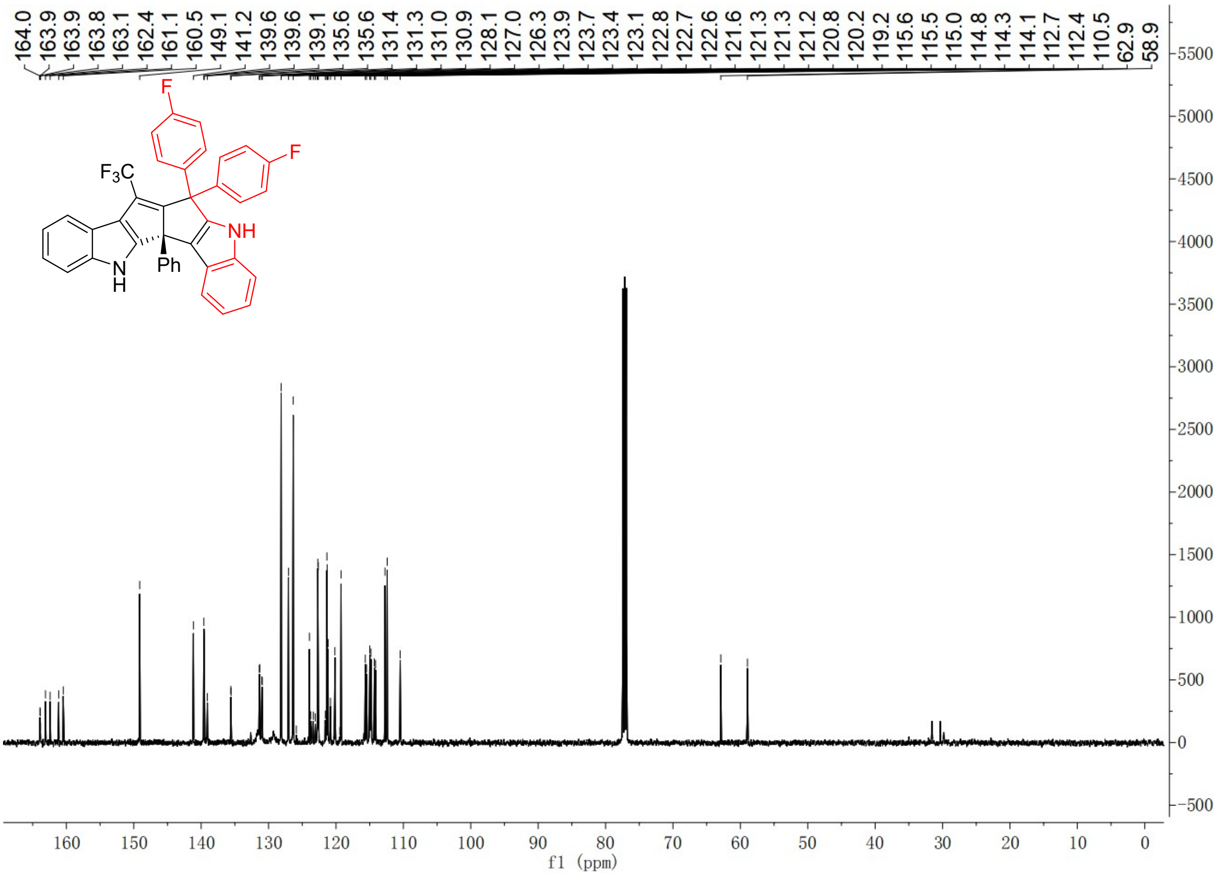

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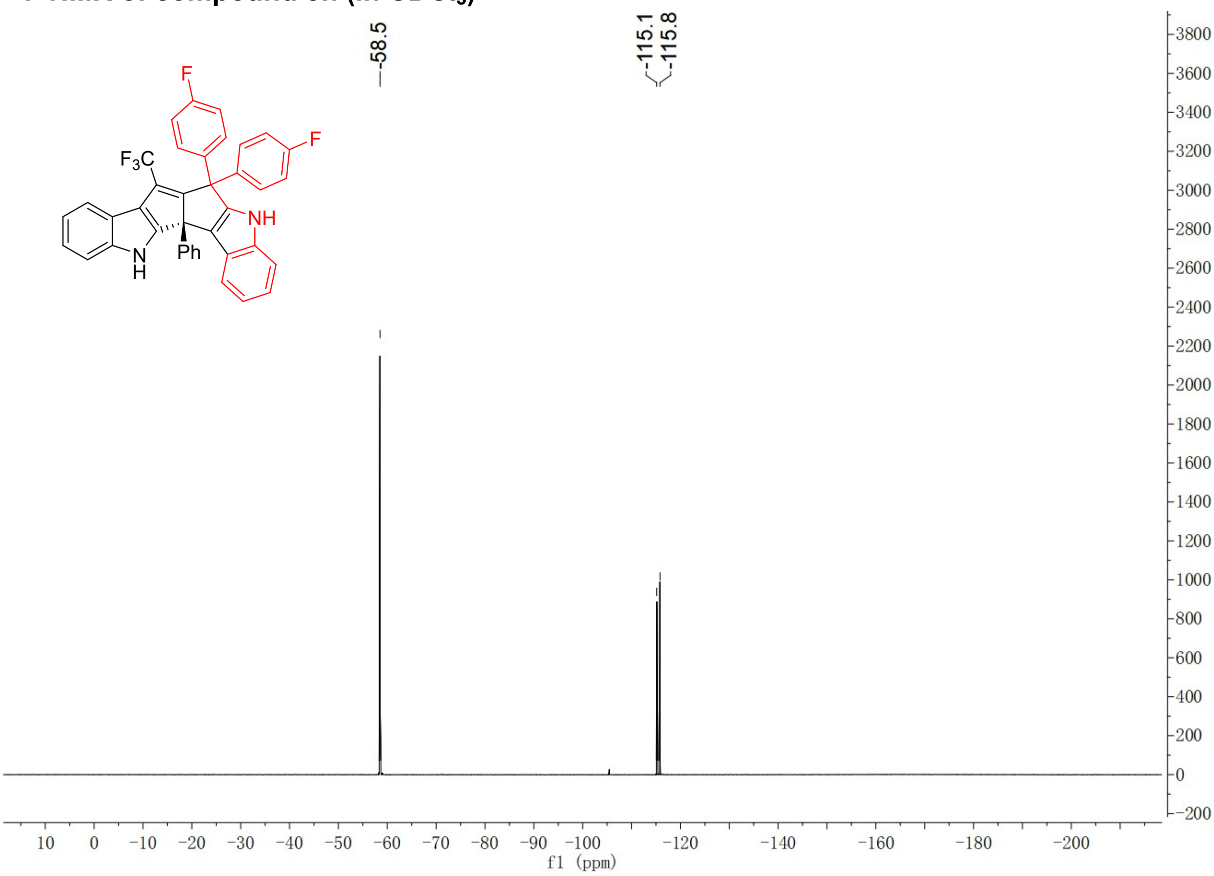
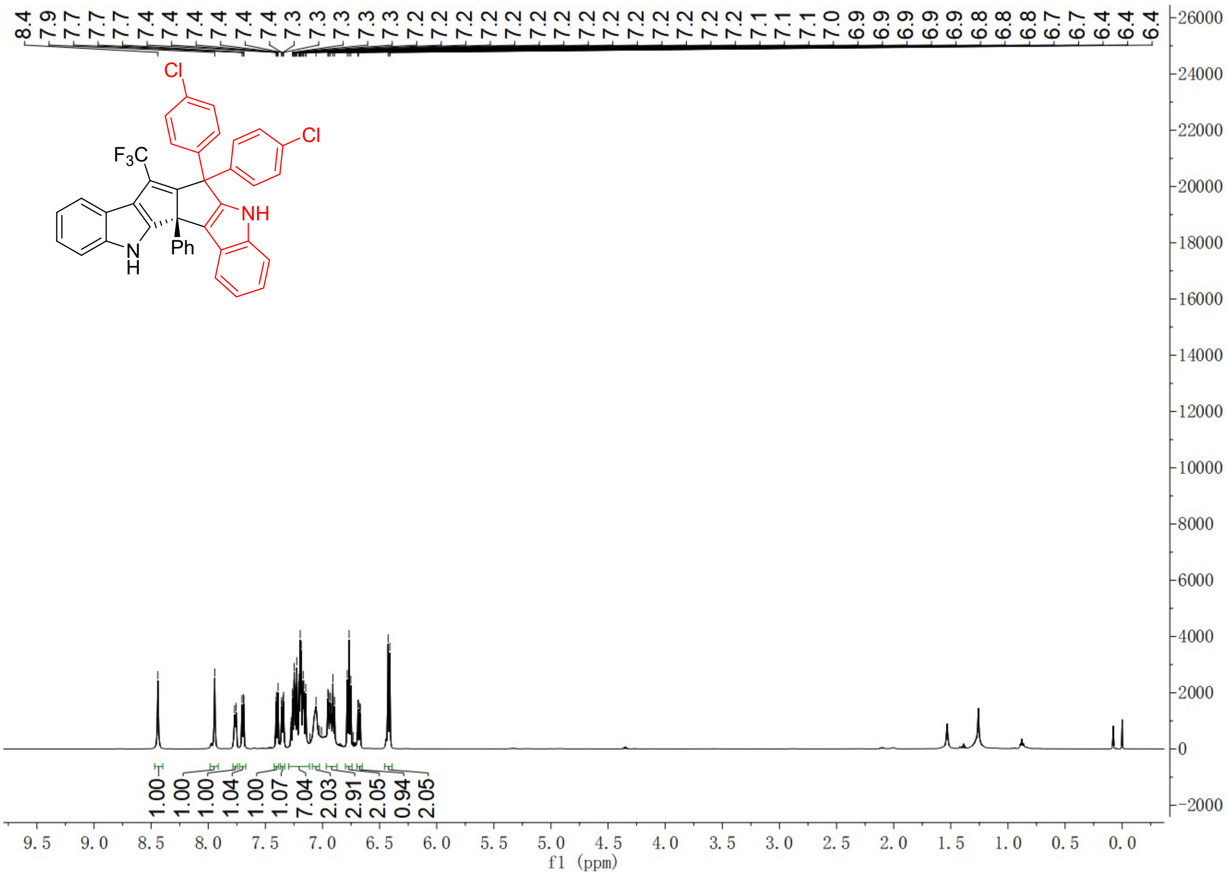
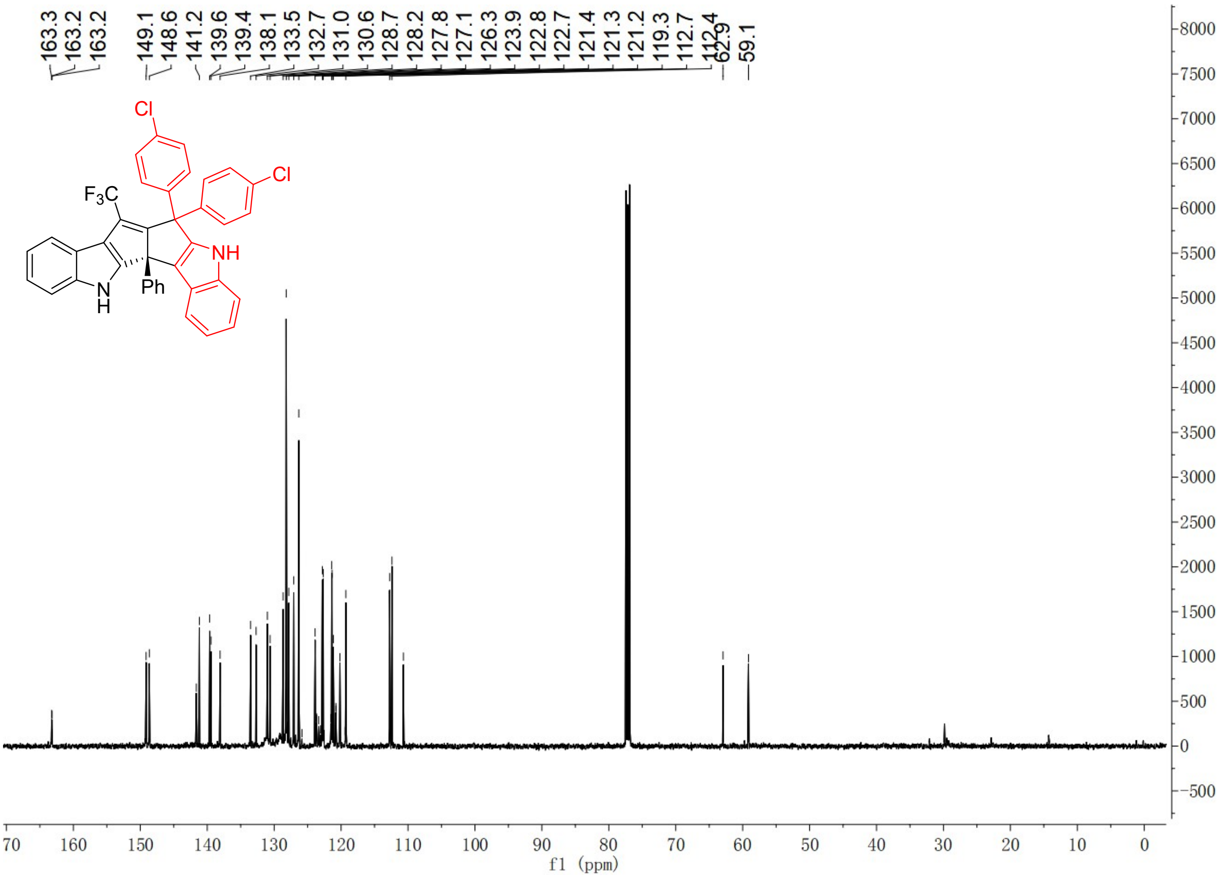


^{1}H NMR of compound 3o (in $CDCl_3$)



^{13}C NMR of compound 3o (in $CDCl_3$)



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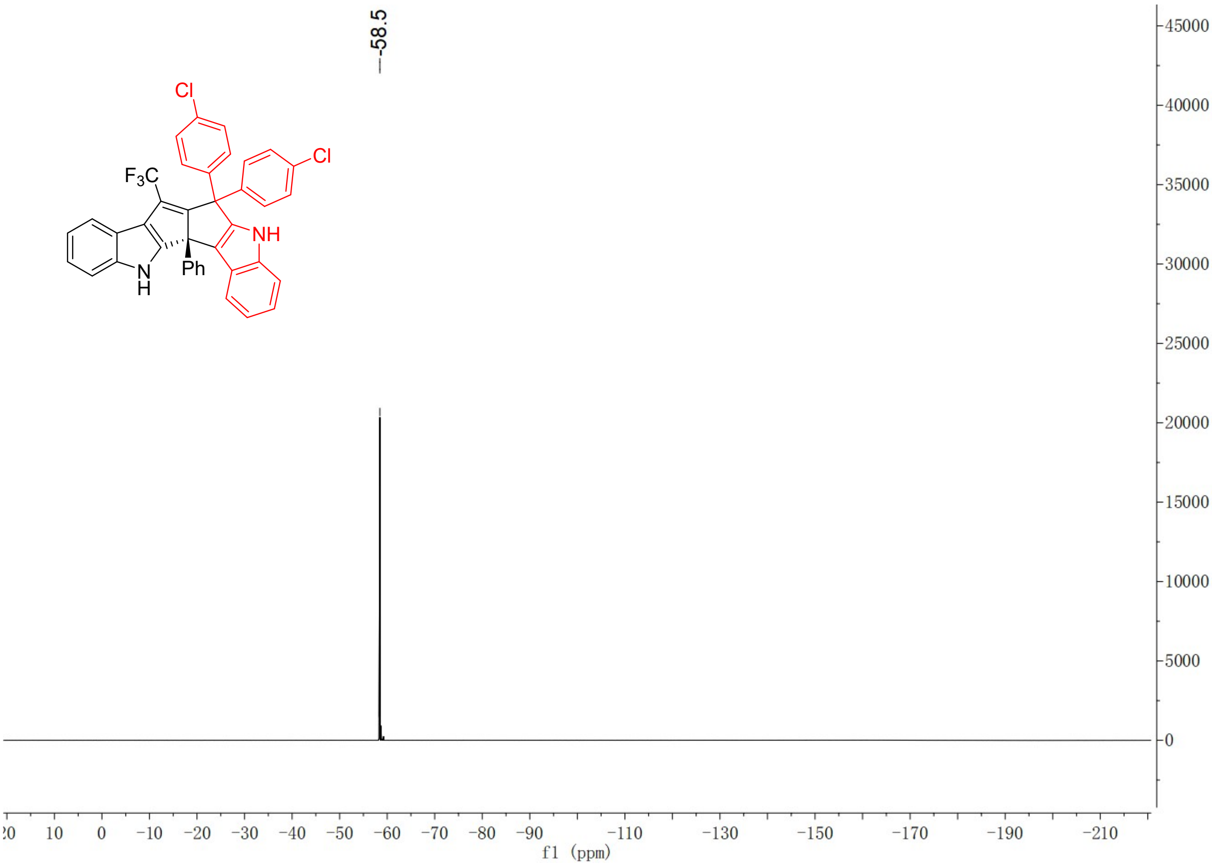
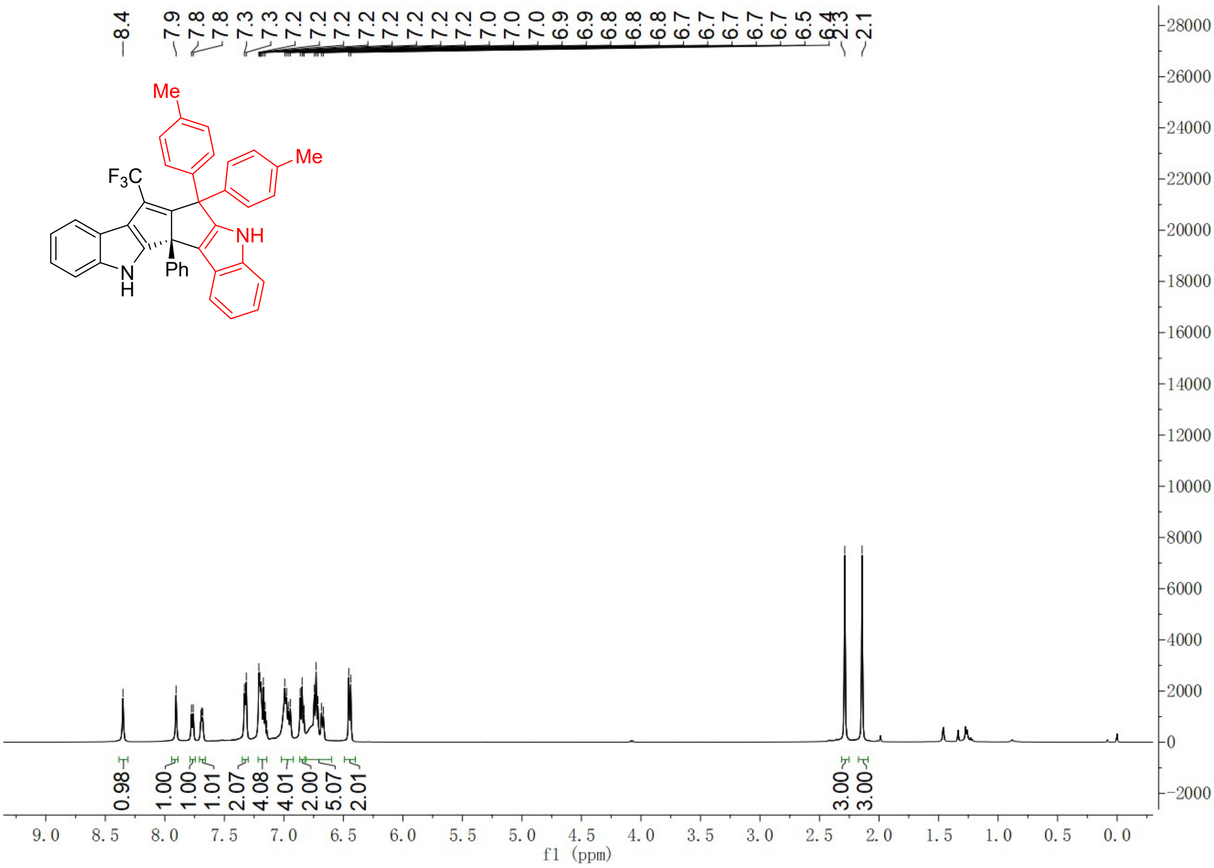
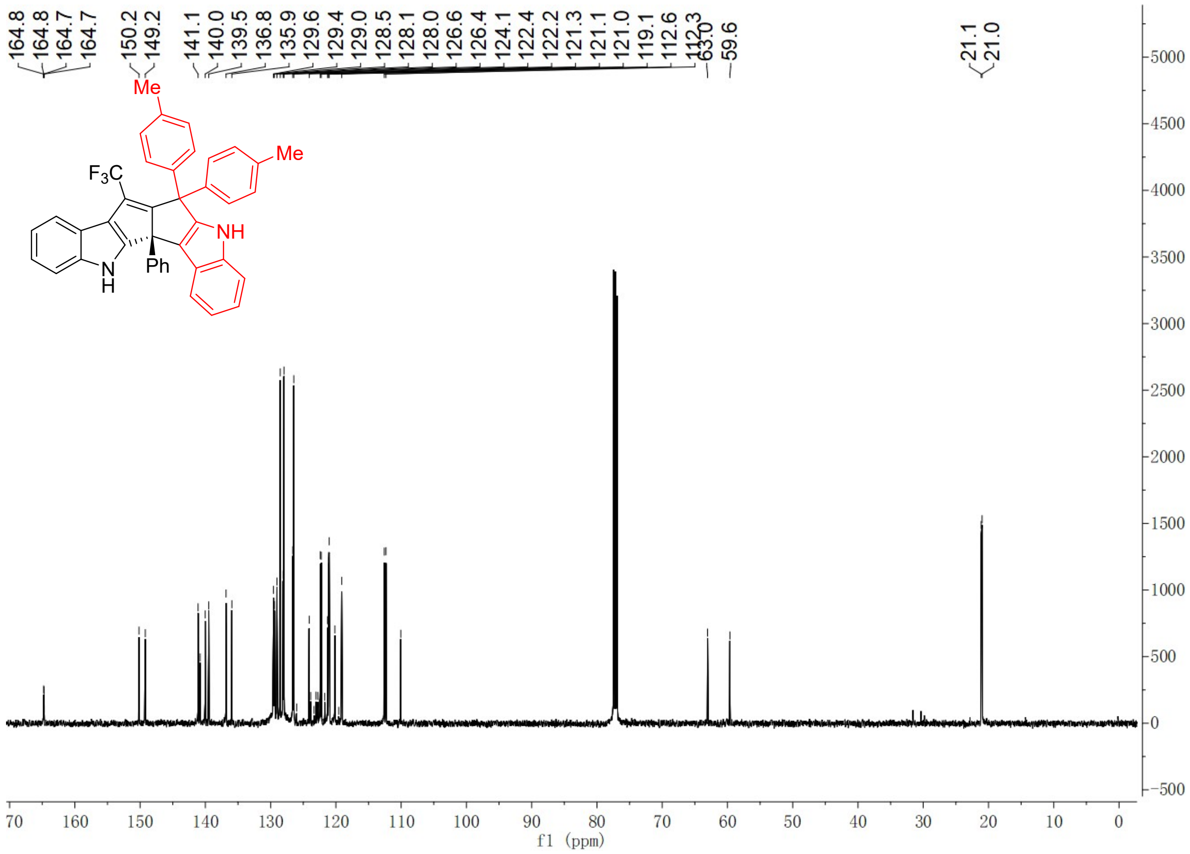


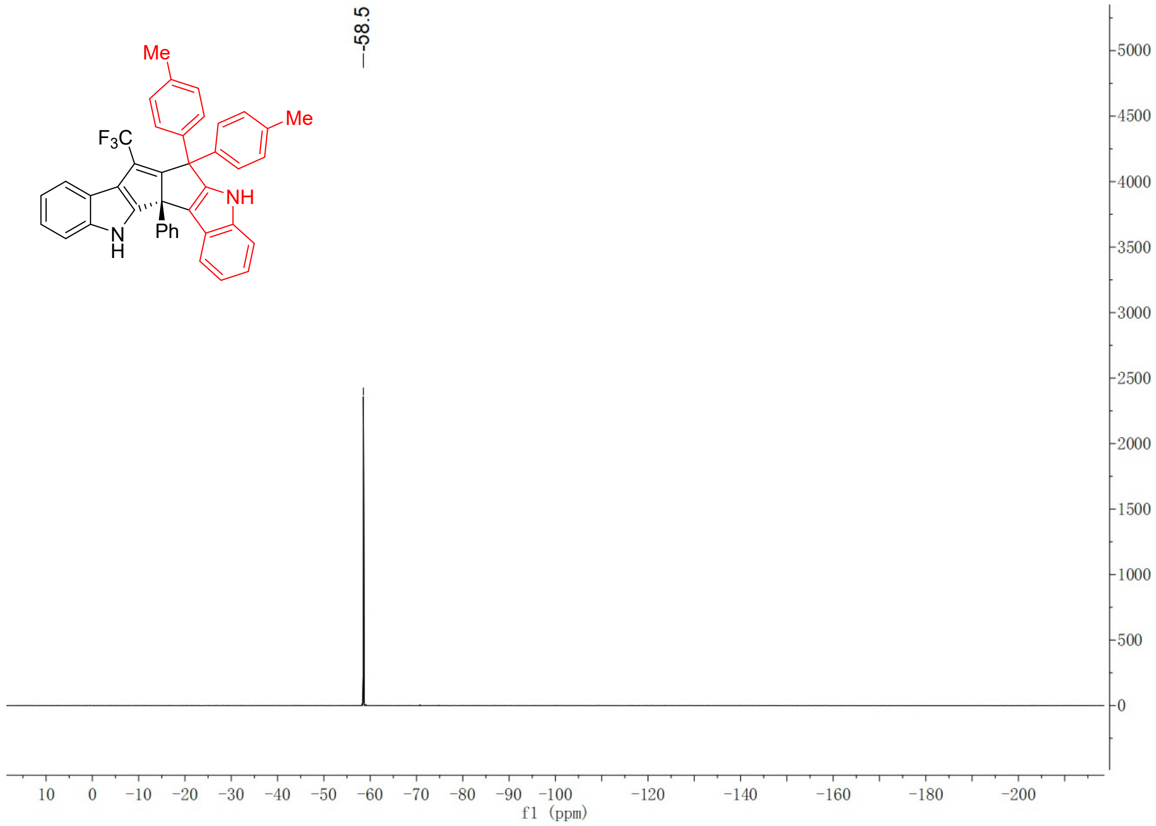
[1]H NMR of compound 3p (in $CDCl_3$)



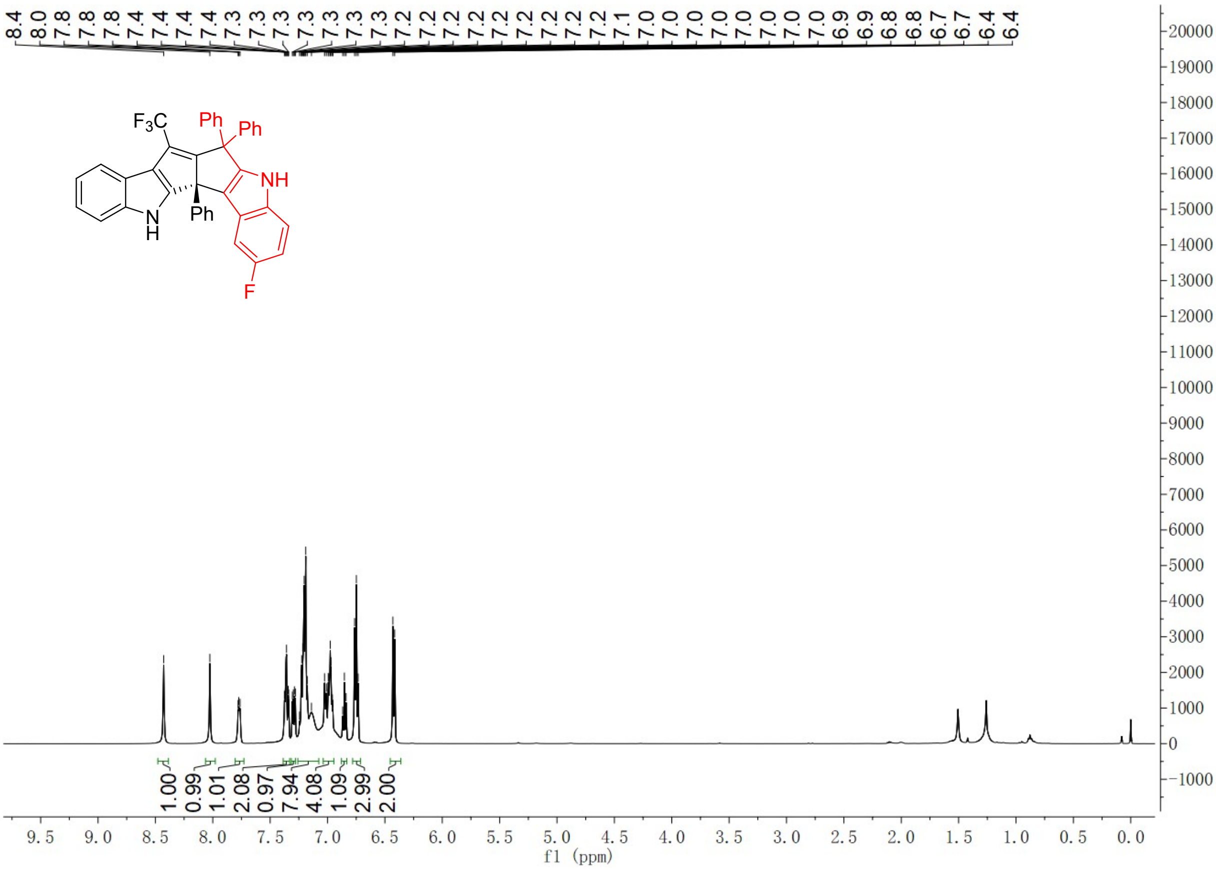
^{13}C NMR of compound 3p (in $CDCl_3$)



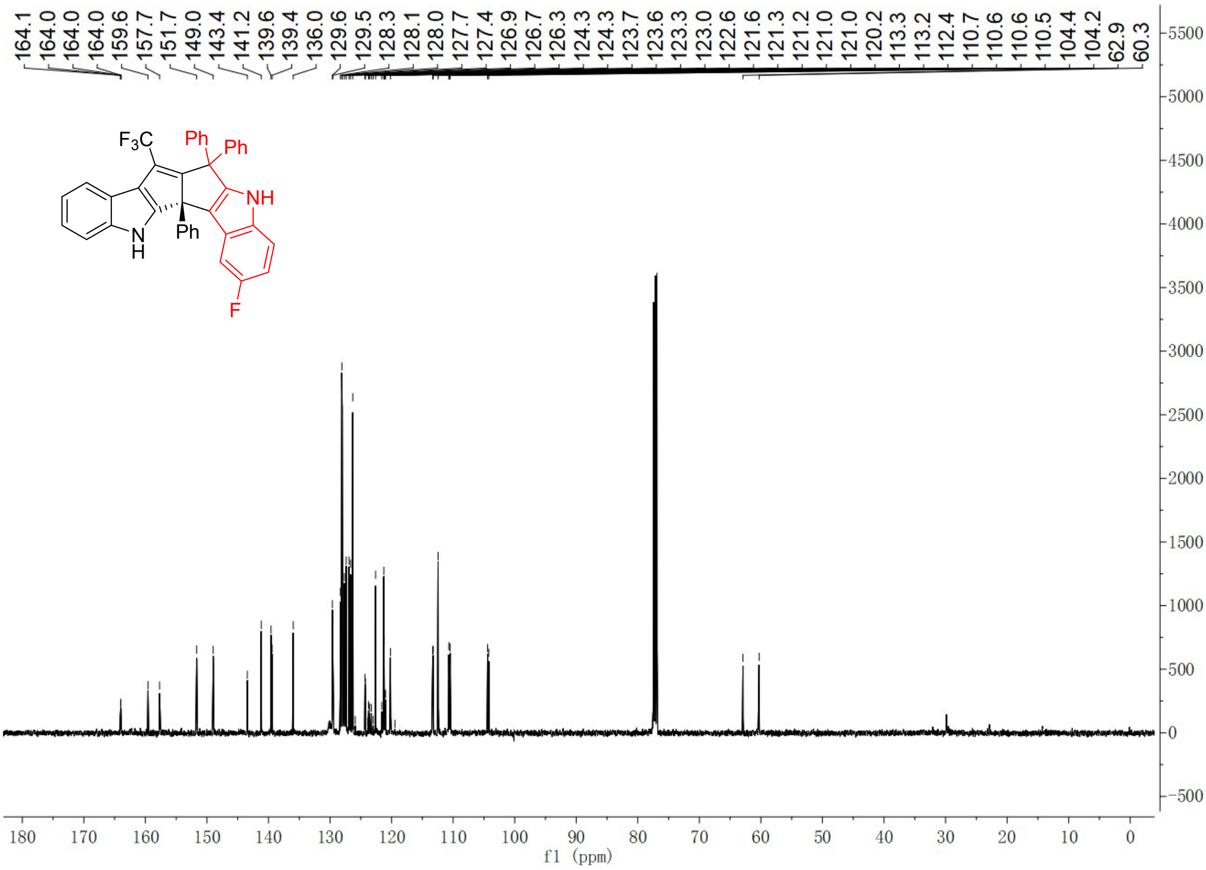
^{19}F NMR of compound 3p (in $CDCl_3$)



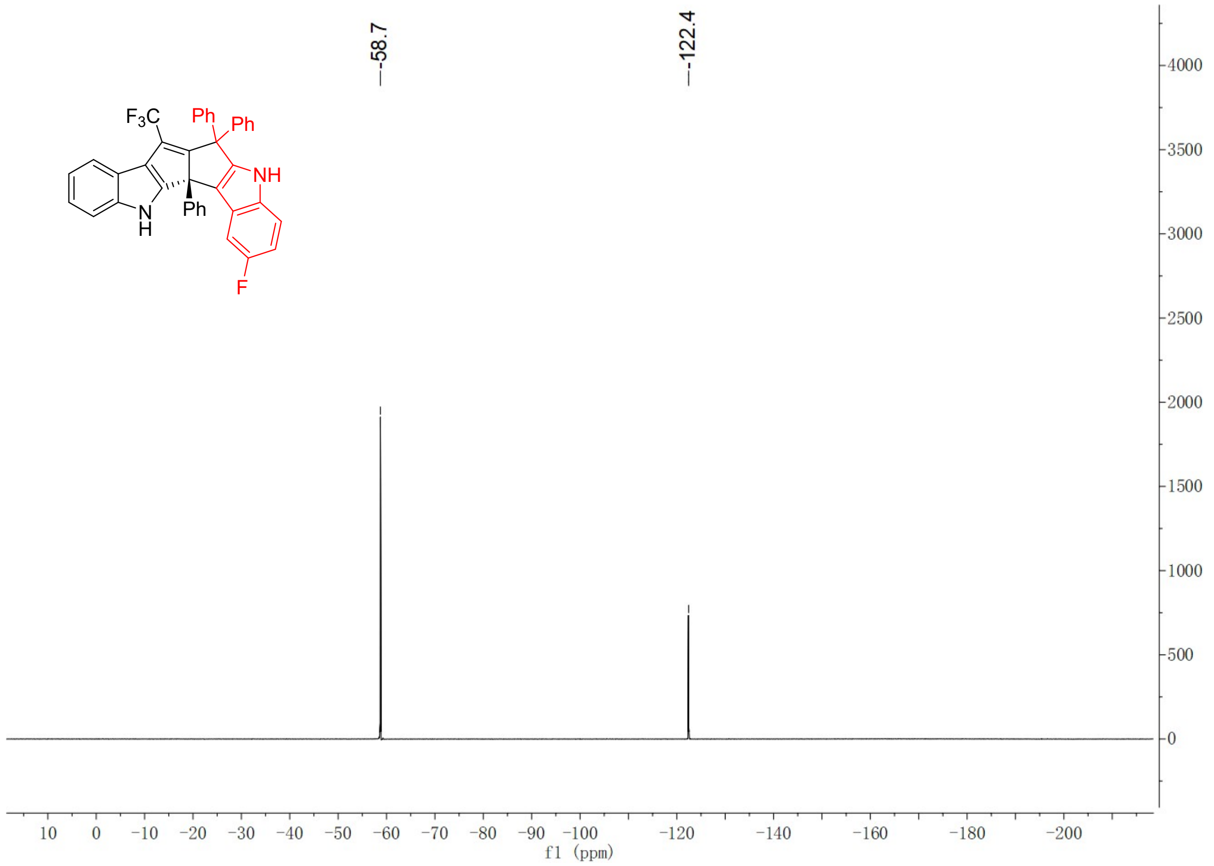
^{1}H NMR of compound 3q (in $CDCl_3$)



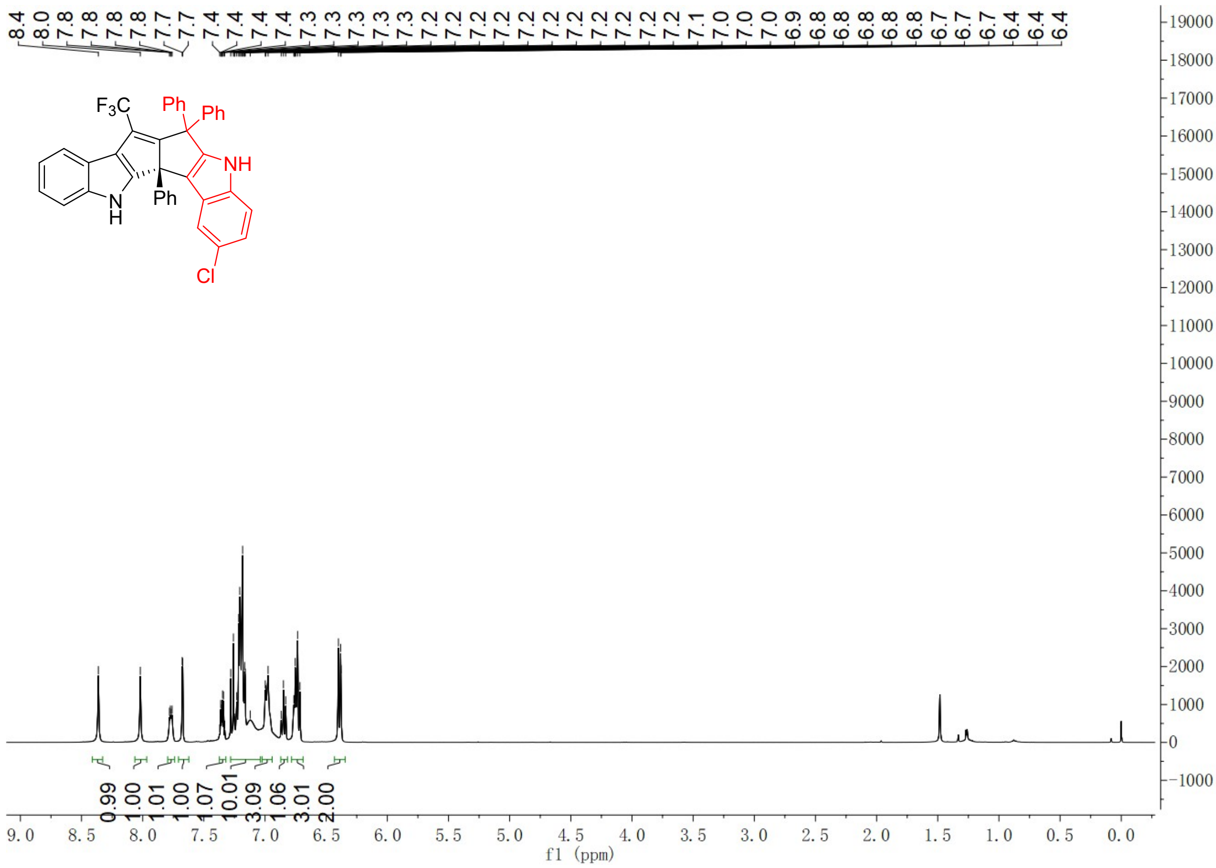
^{13}C NMR of compound 3q (in $CDCl_3$)



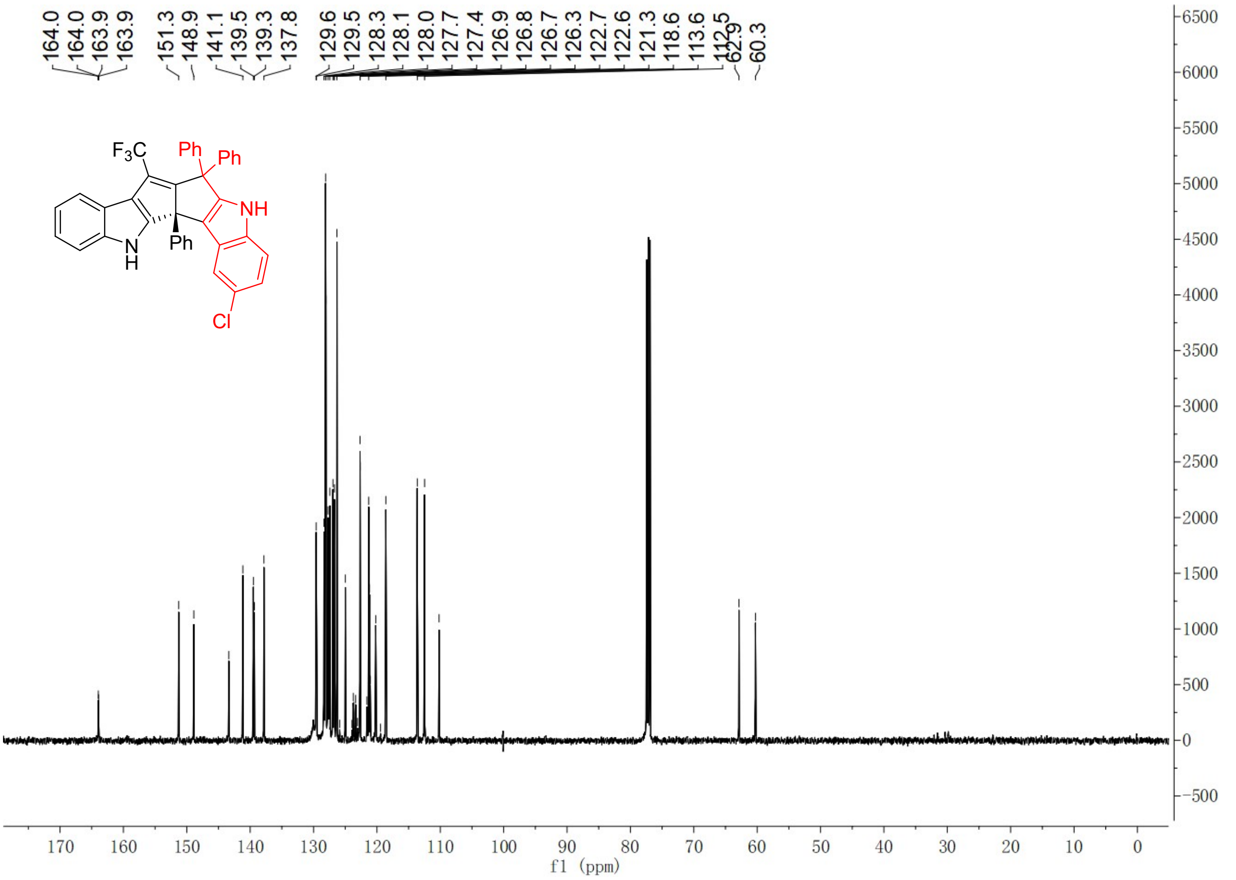
^{19}F NMR of compound 3q (in CDCl$_3$)



^{1}H NMR of compound 3r (in CDCl$_3$)



^{13}C NMR of compound 3r (in $CDCl_3$)



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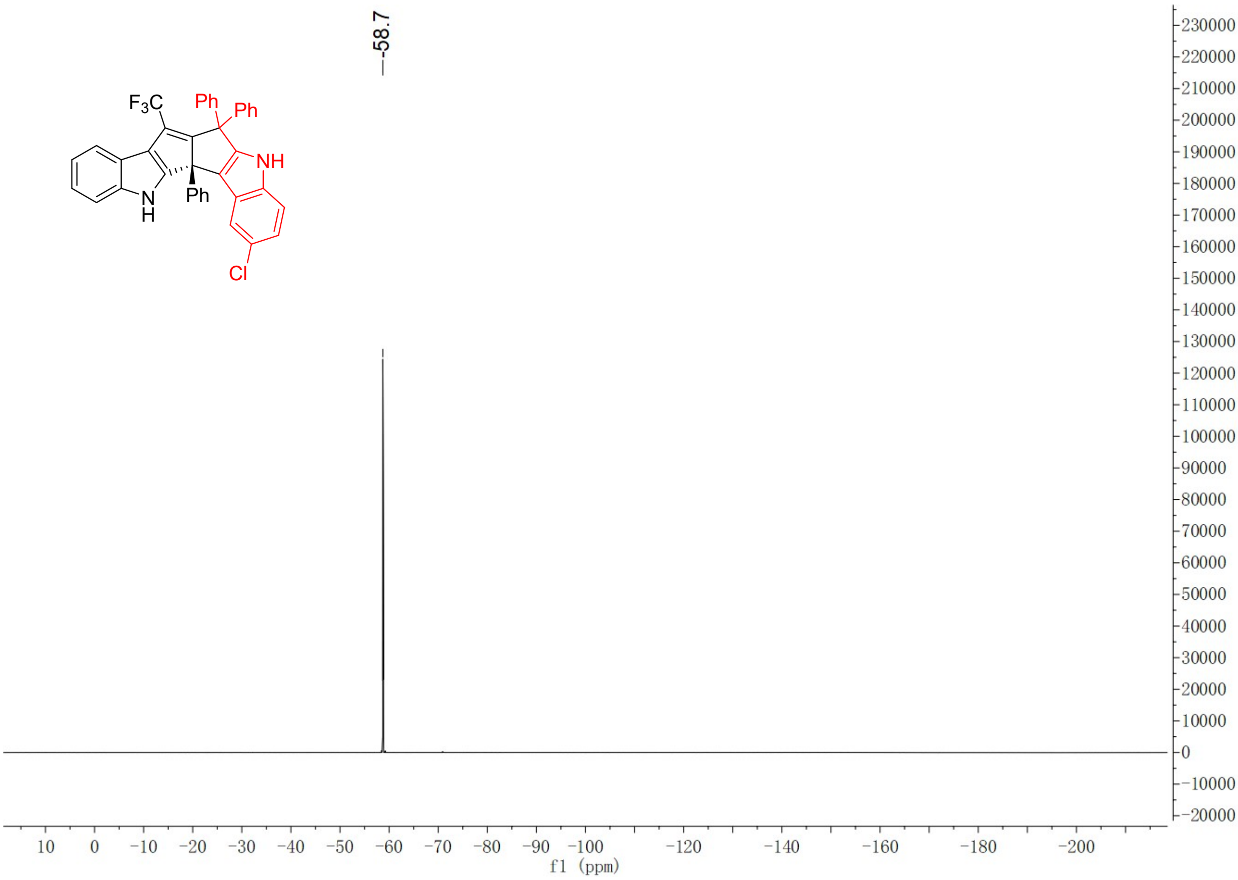
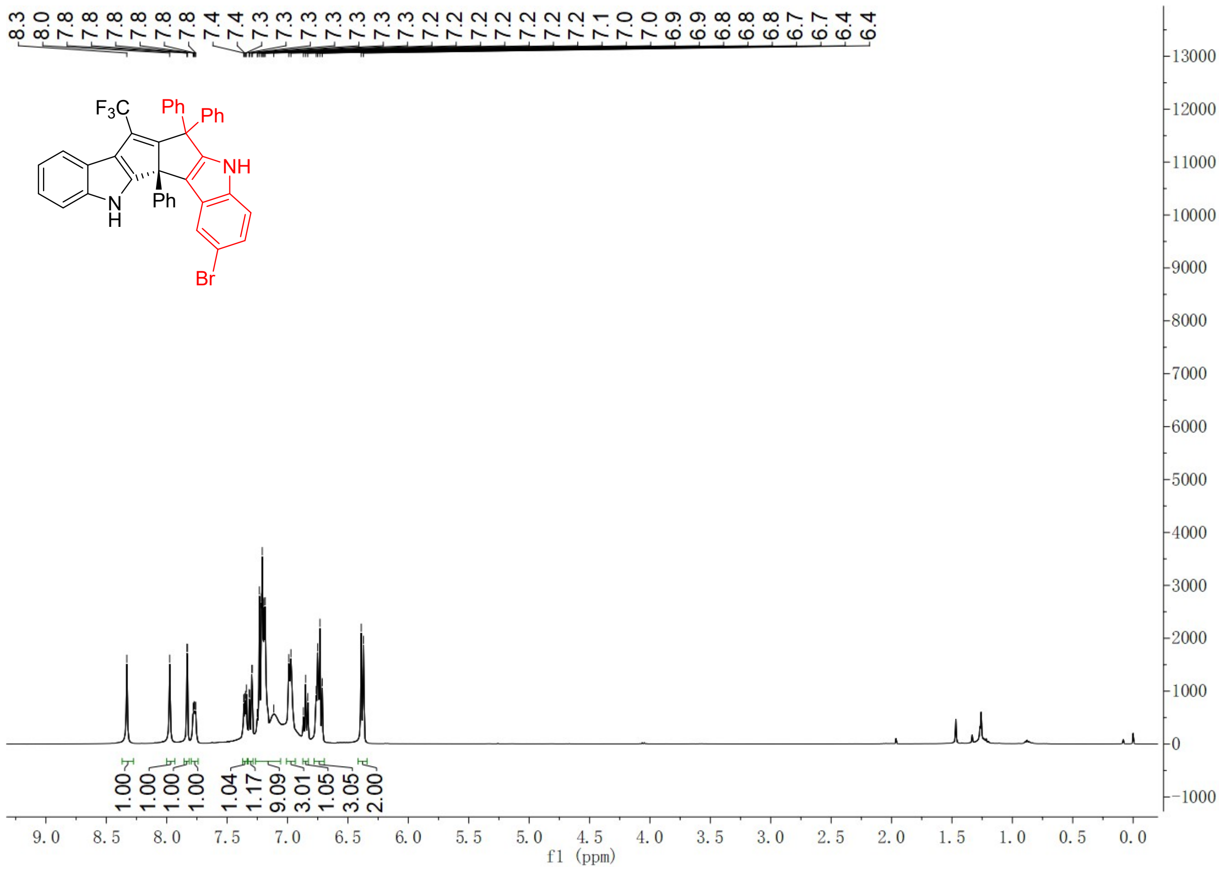
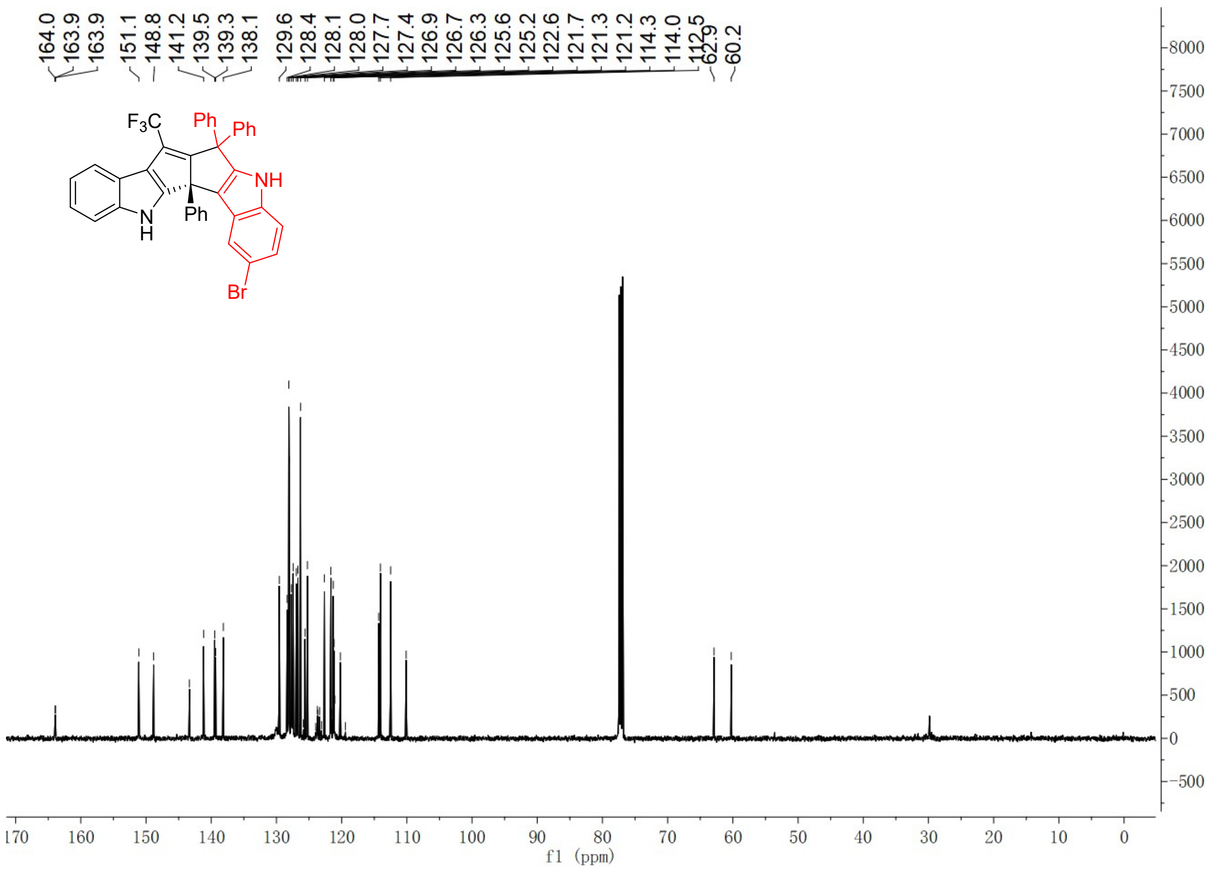


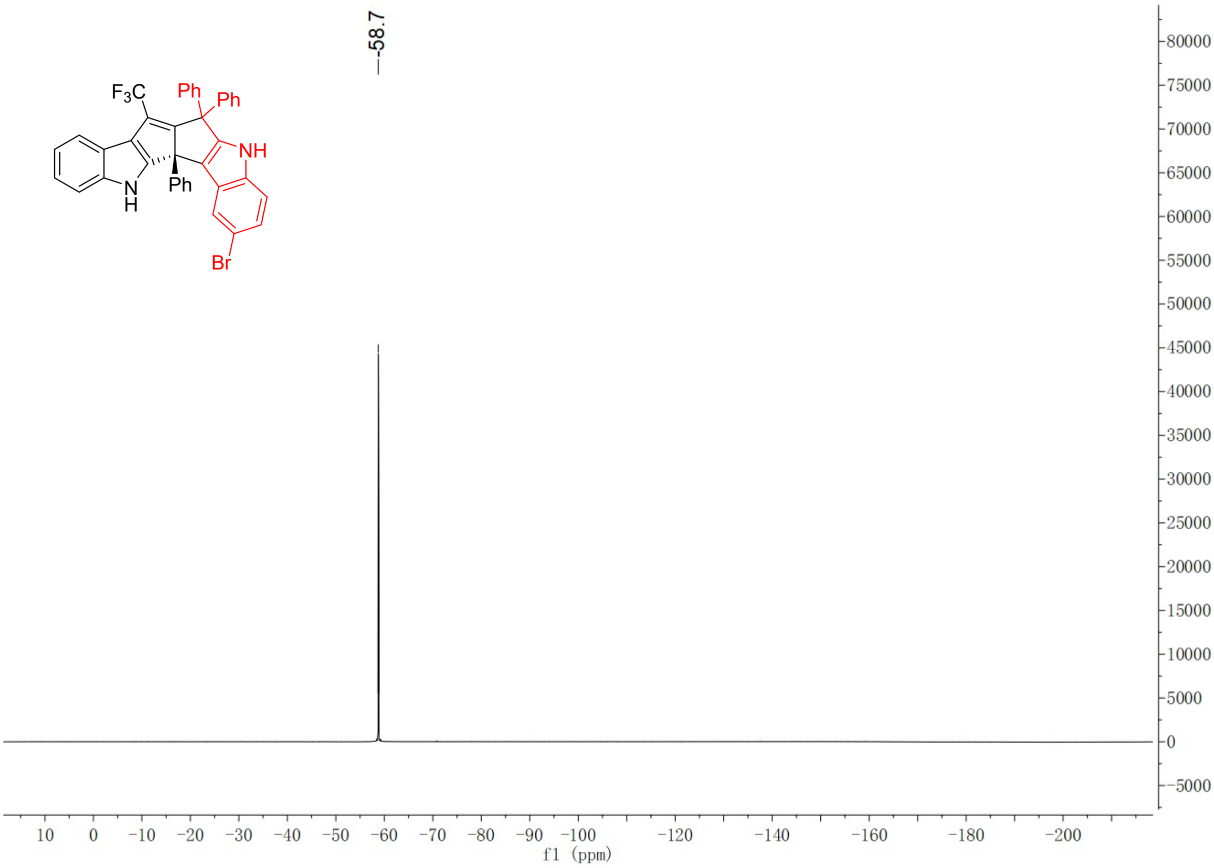
^{1}H NMR of compound 3s (in $CDCl_3$)



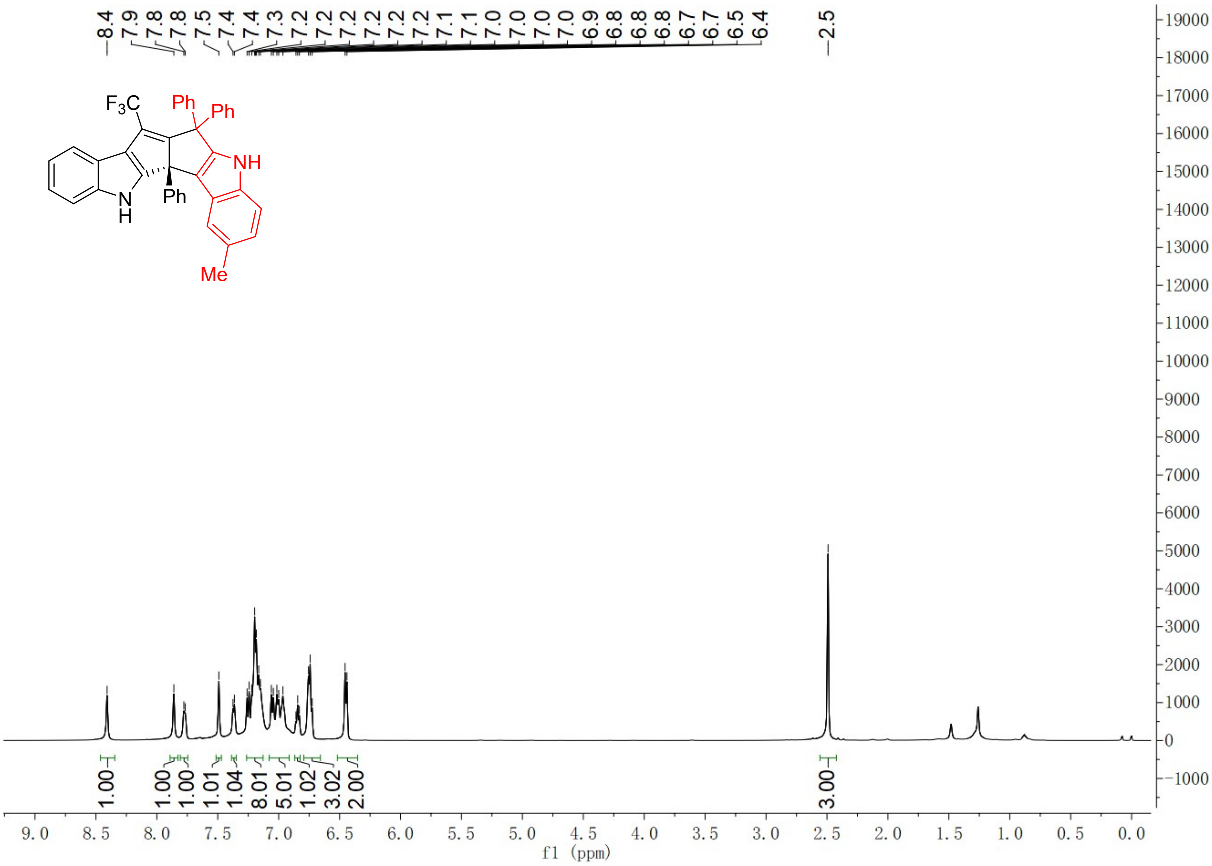
^{13}C NMR of compound 3s (in $CDCl_3$)



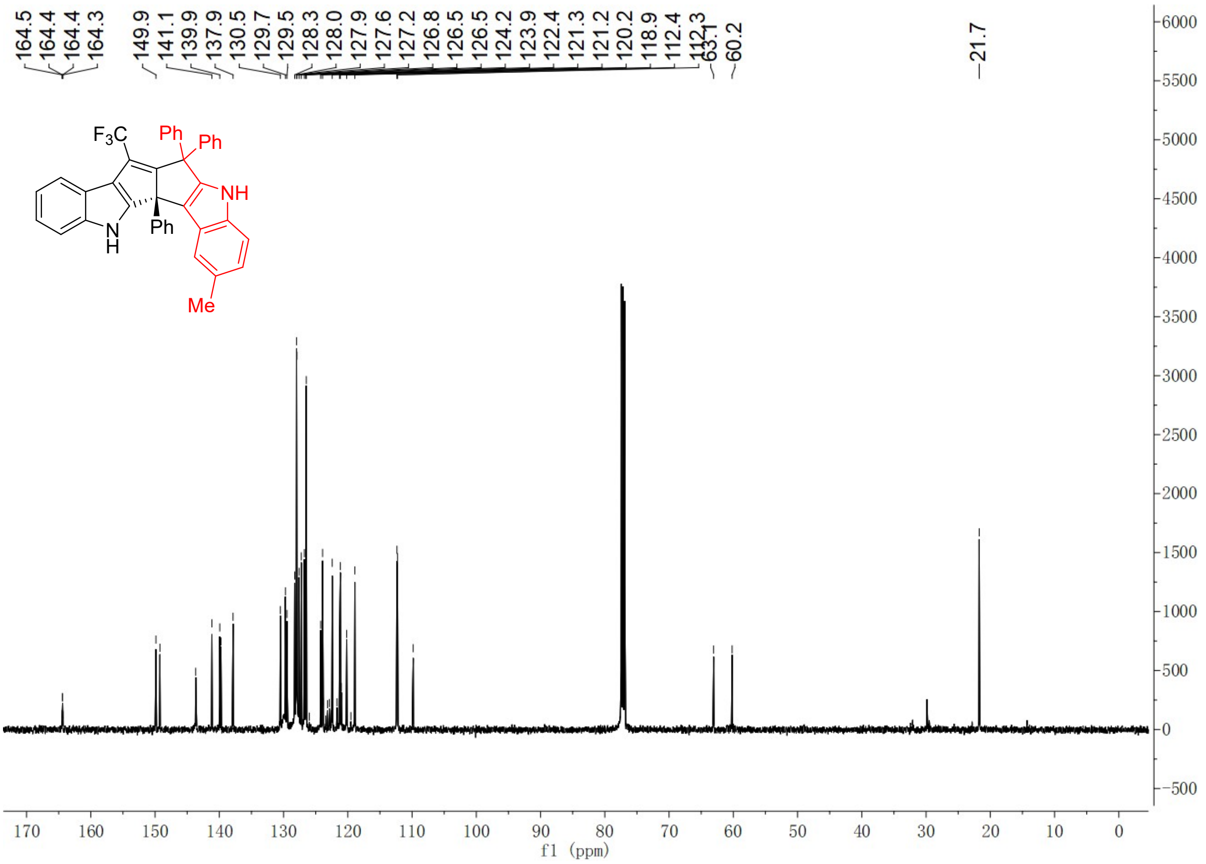
^{19}F NMR of compound 3s (in $CDCl_3$)



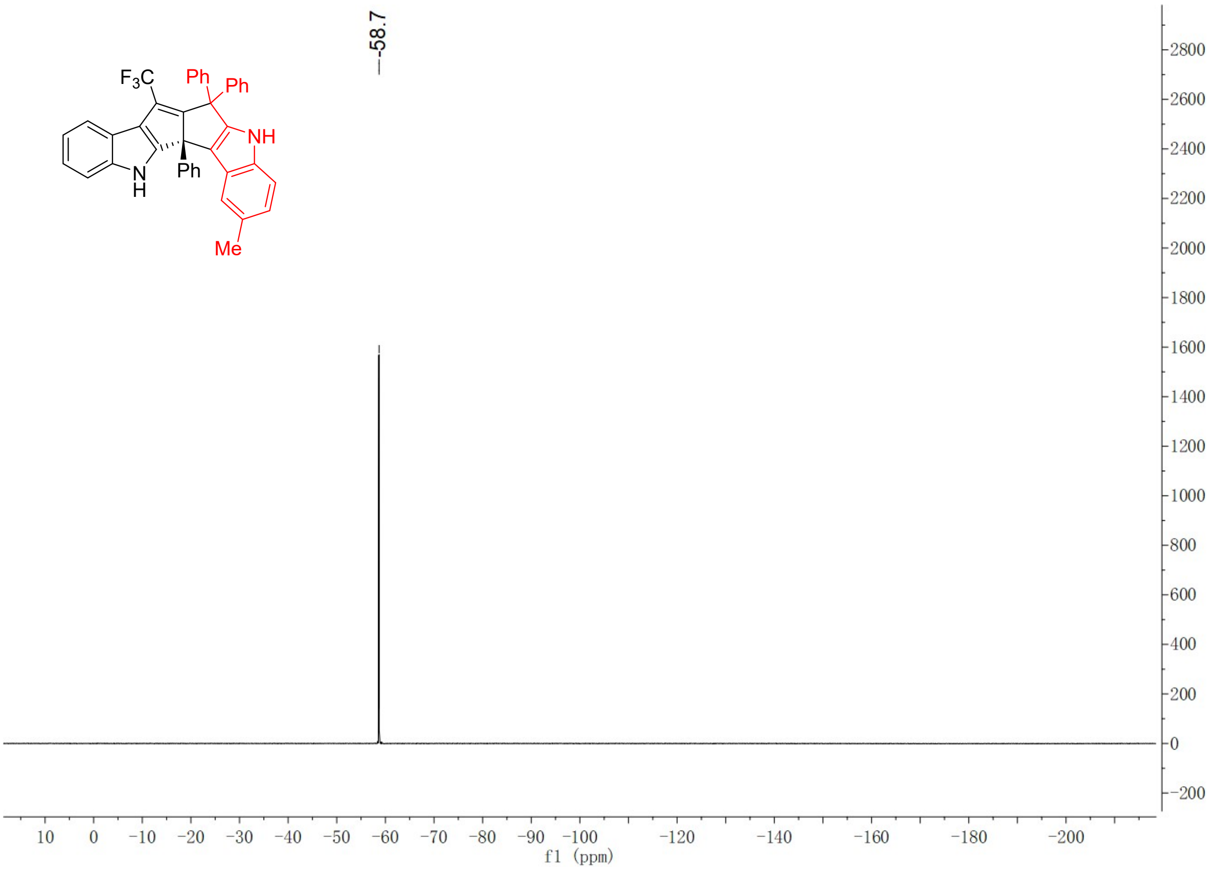
^{1}H NMR of compound 3t (in $CDCl_3$)



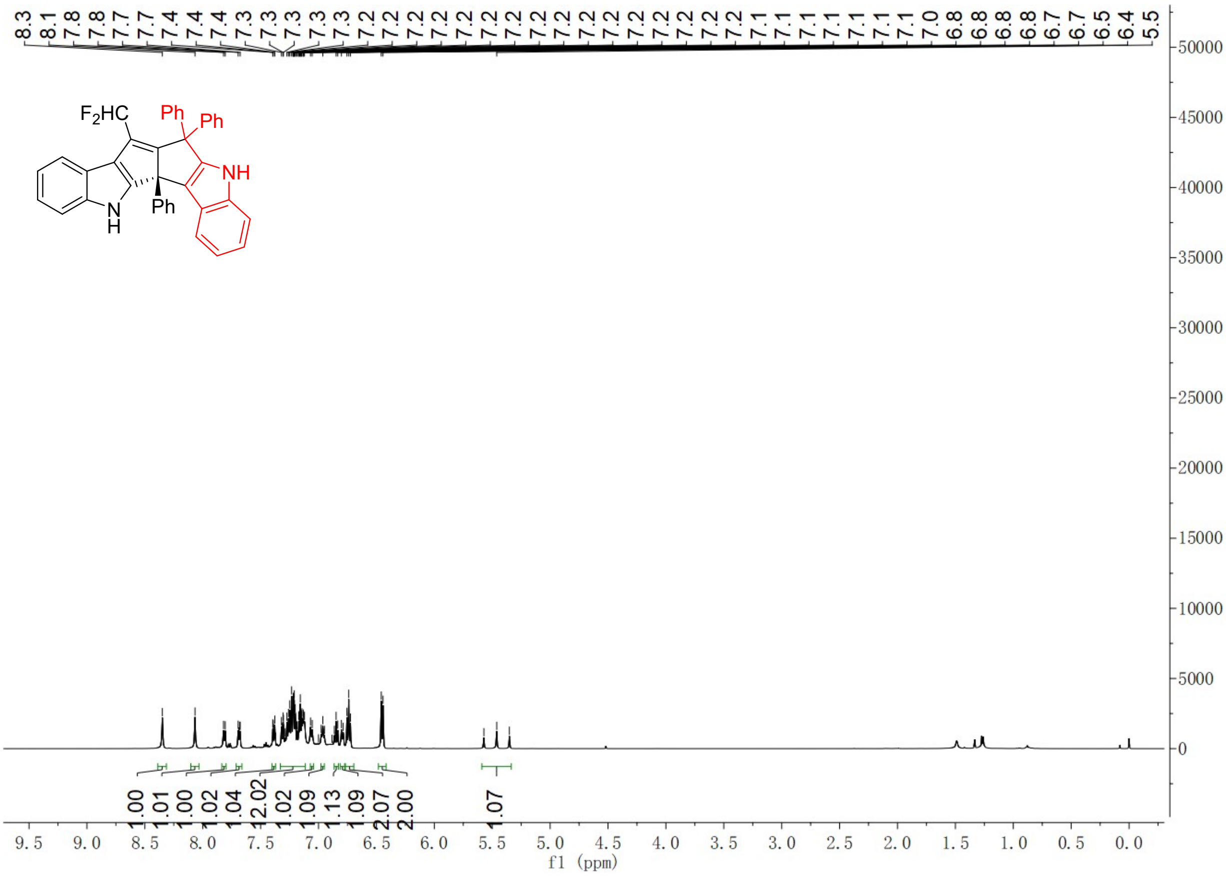
^{13}C NMR of compound 3t (in $CDCl_3$)



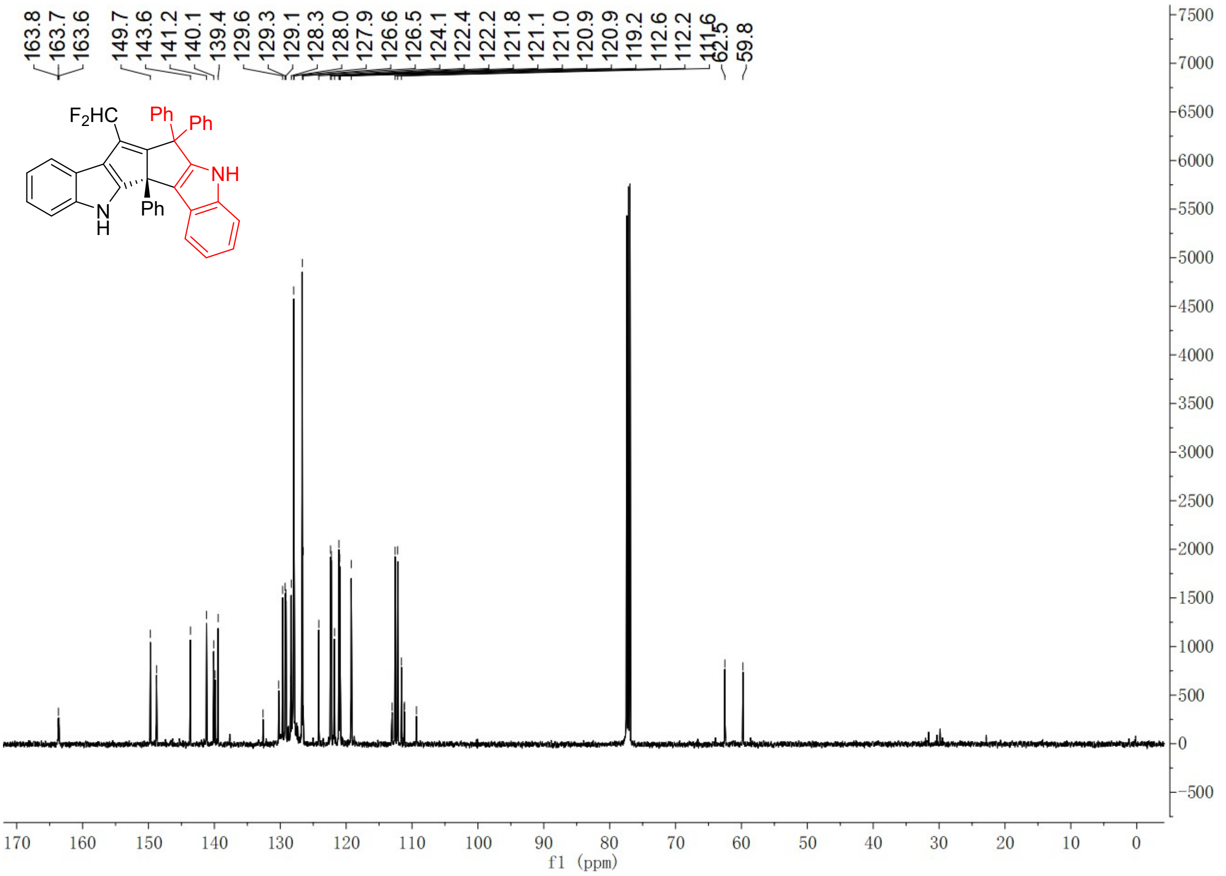
^{19}F NMR of compound 3t (in $CDCl_3$)



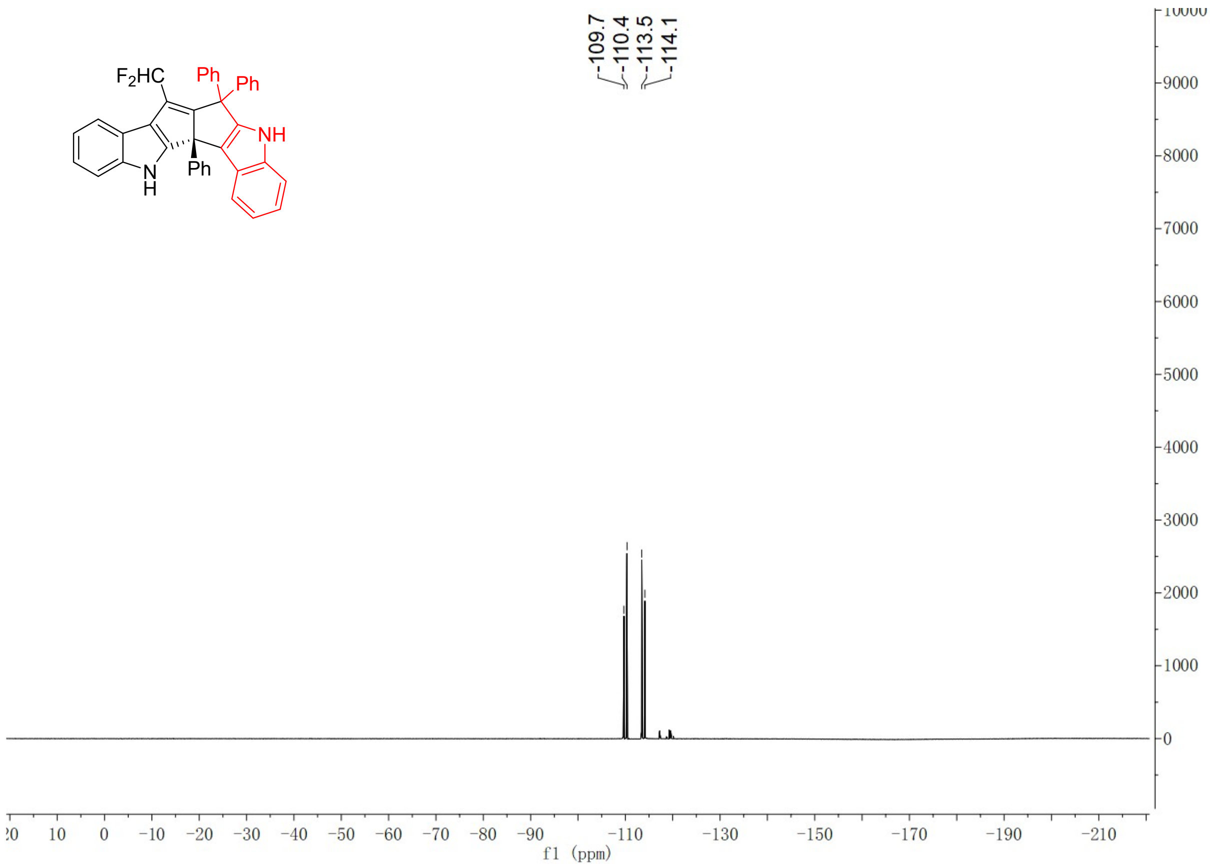
^{1}H NMR of compound 3u (in $CDCl_3$)



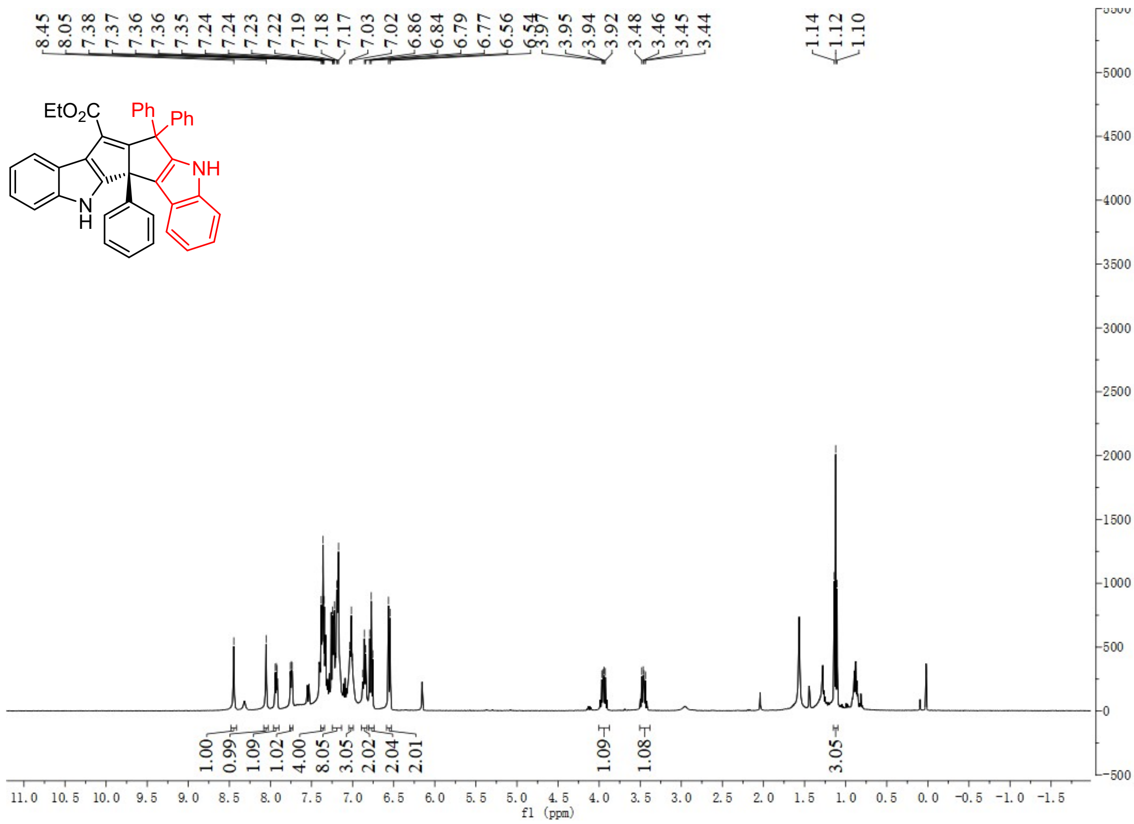
^{13}C NMR of compound 3u (in $CDCl_3$)



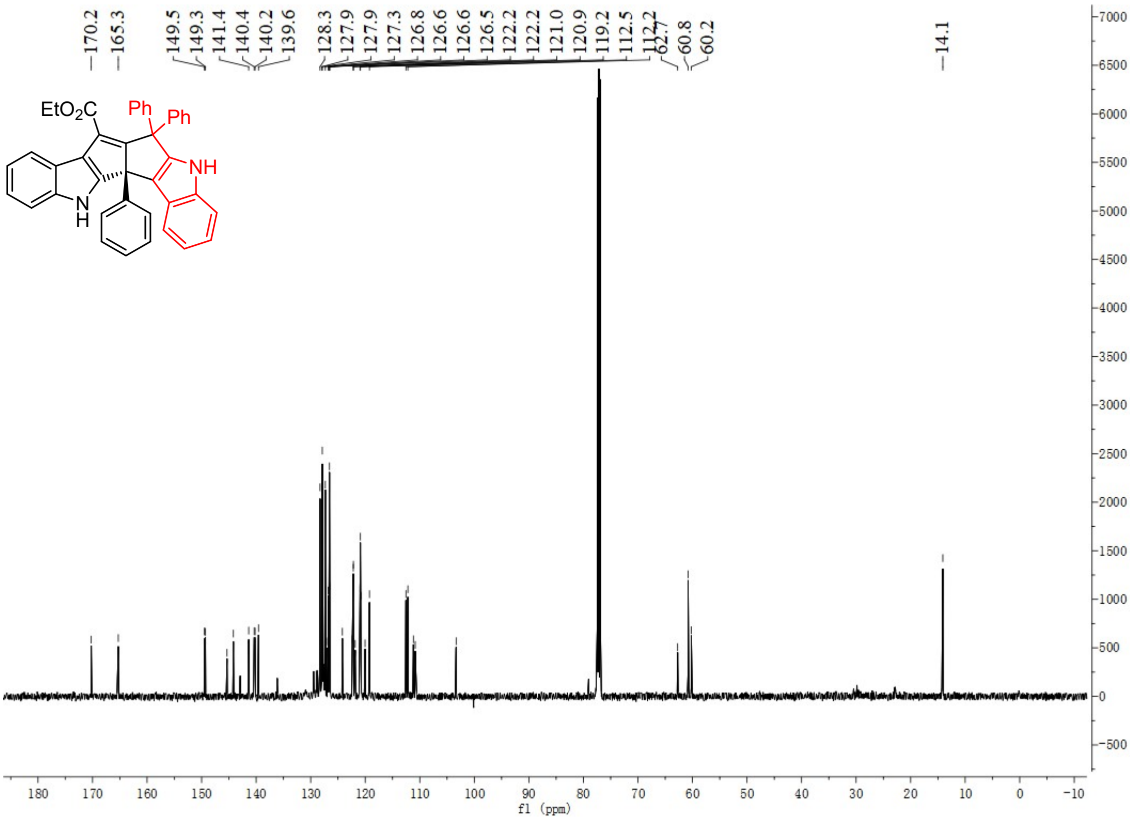
^{19}F NMR of compound 3u (in $CDCl_3$)



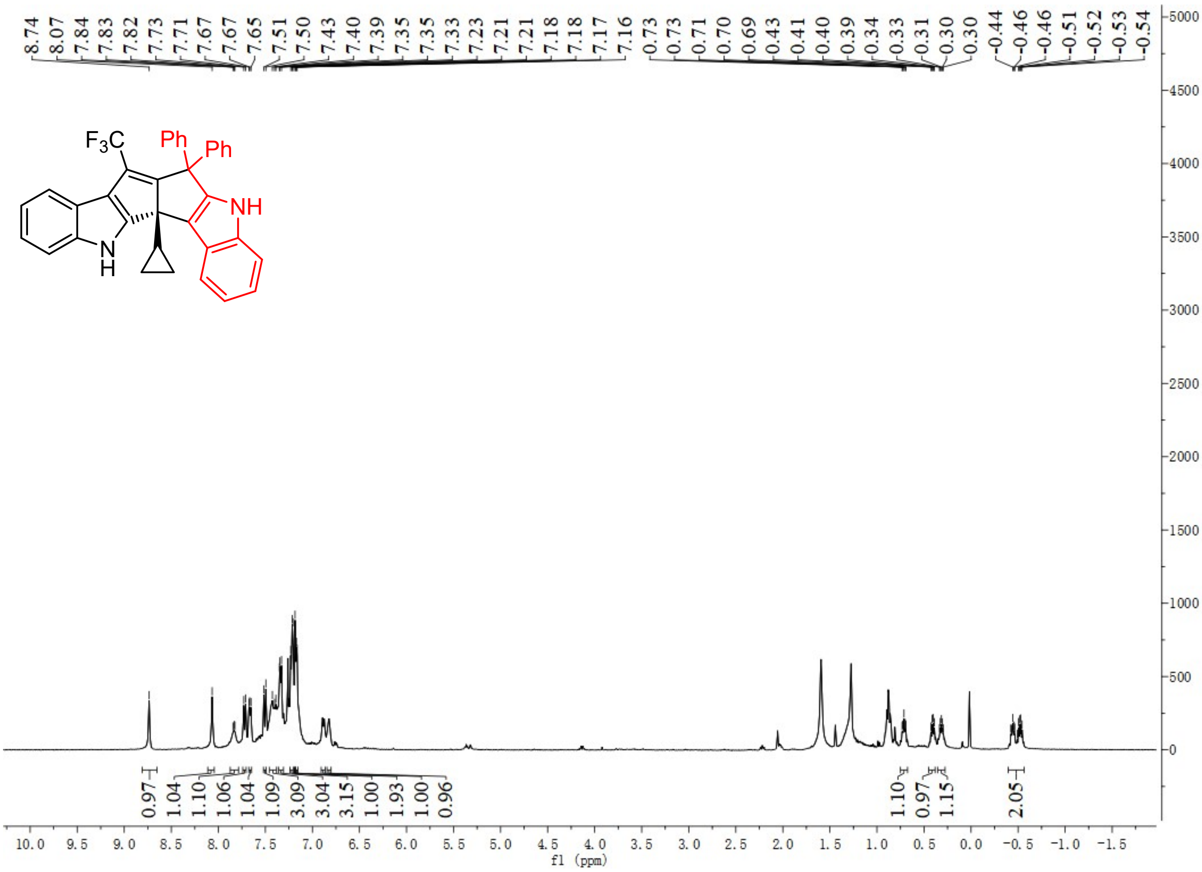
^{1}H NMR of compound 3v (in $CDCl_3$)



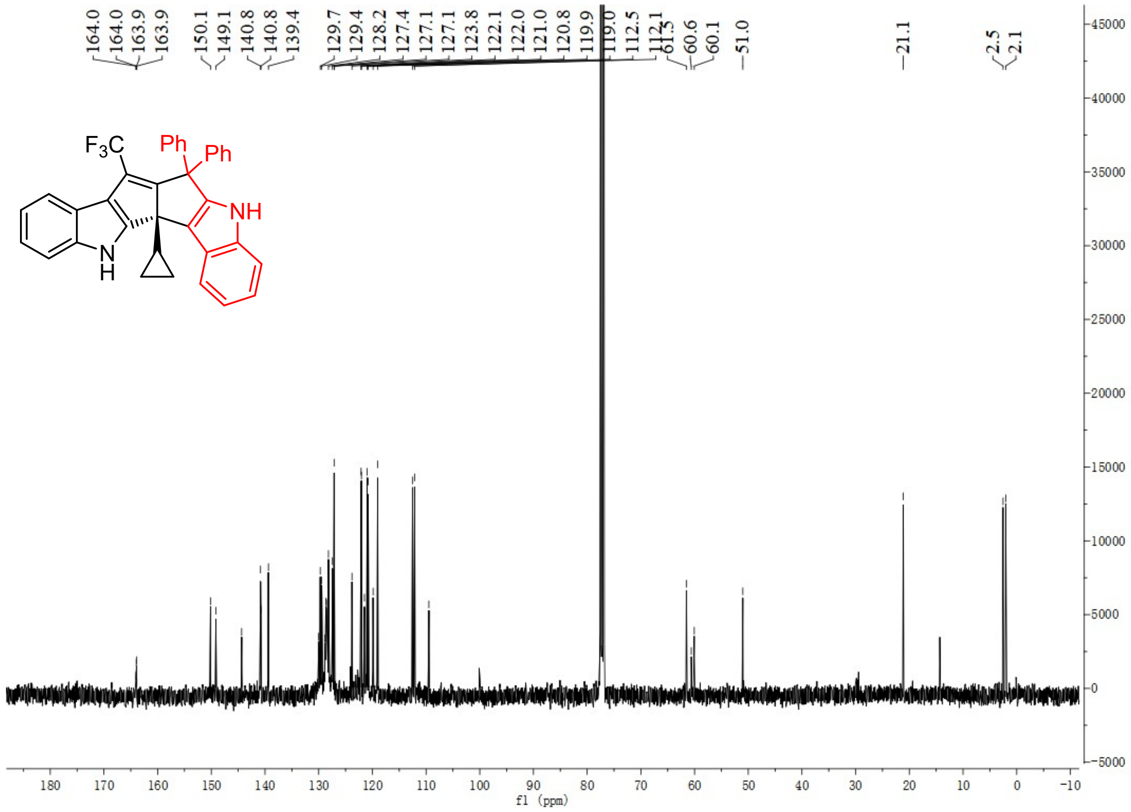
^{13}C NMR of compound 3v (in $CDCl_3$)



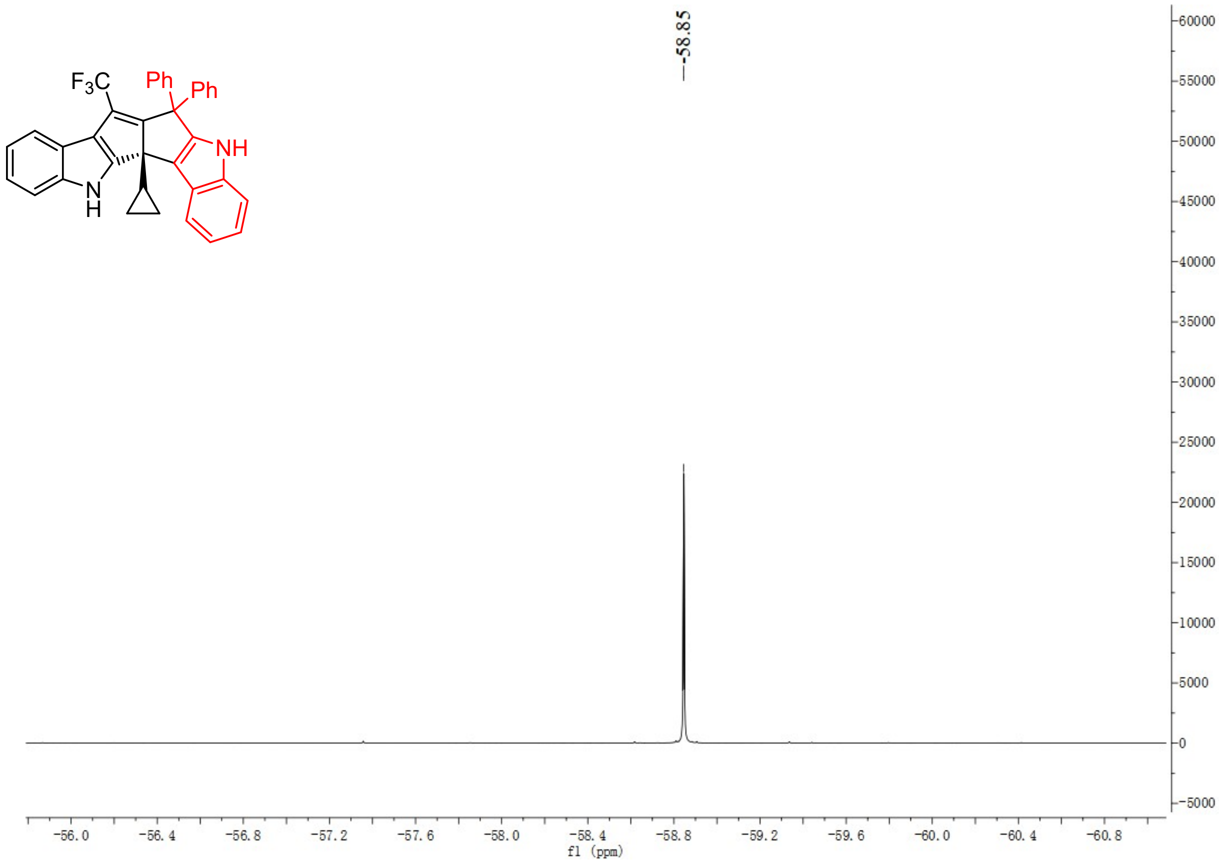
^{1}H NMR of compound 3w (in $CDCl_3$)



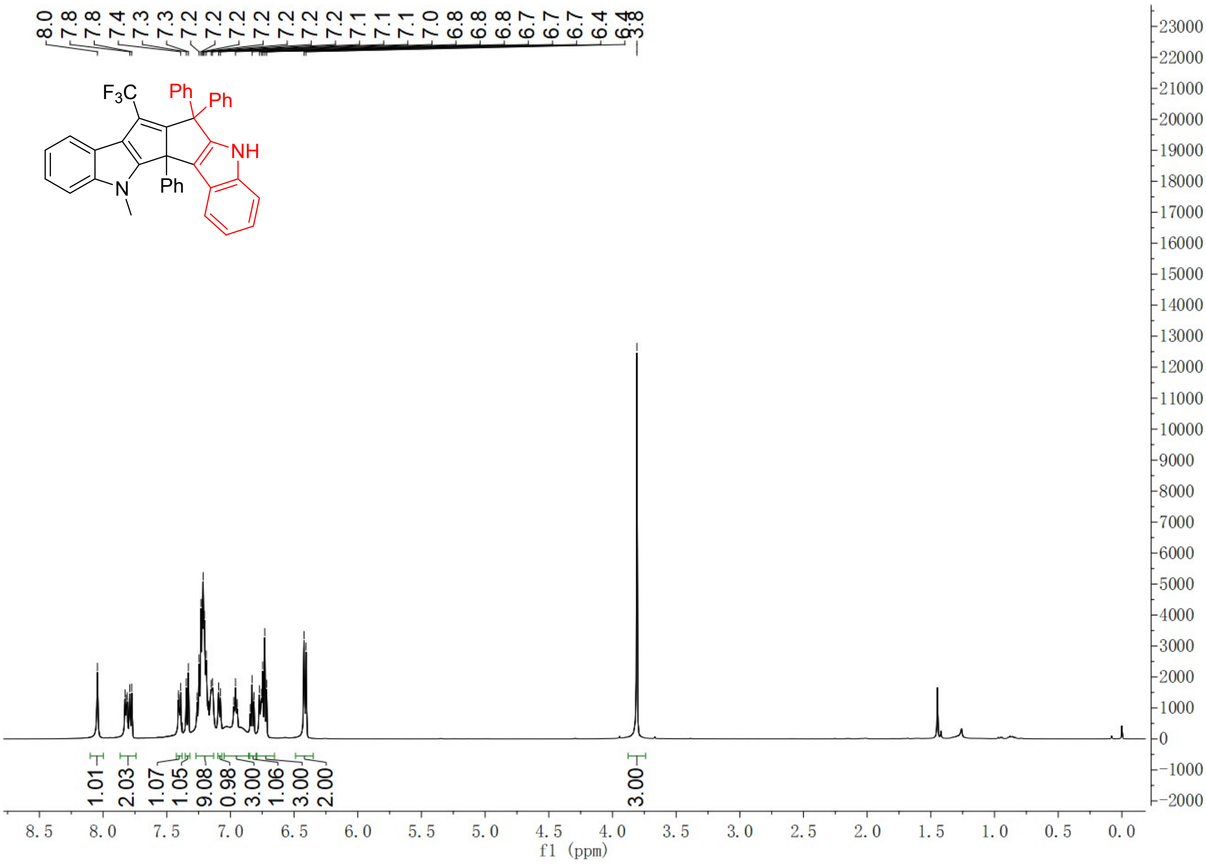
^{13}C NMR of compound 3w (in $CDCl_3$)



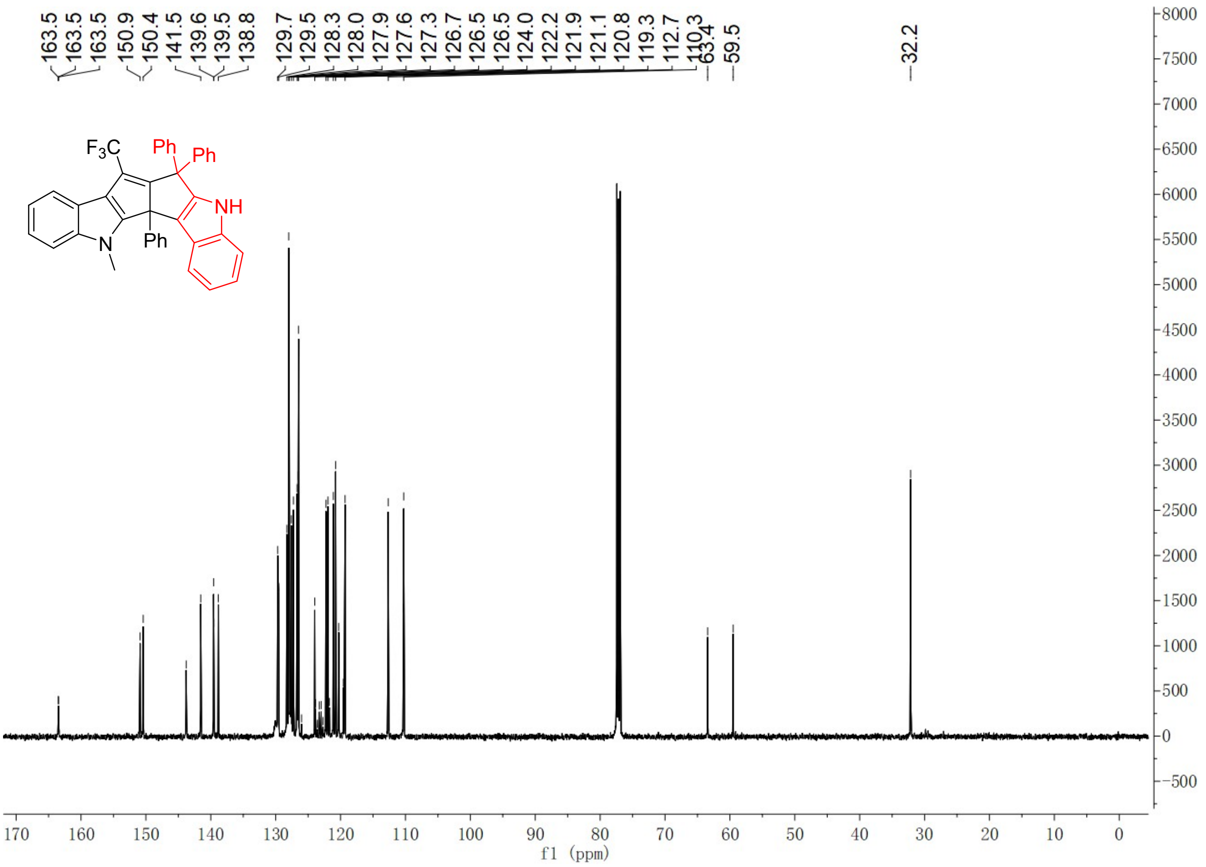
^{19}F NMR of compound 3w (in $CDCl_3$)



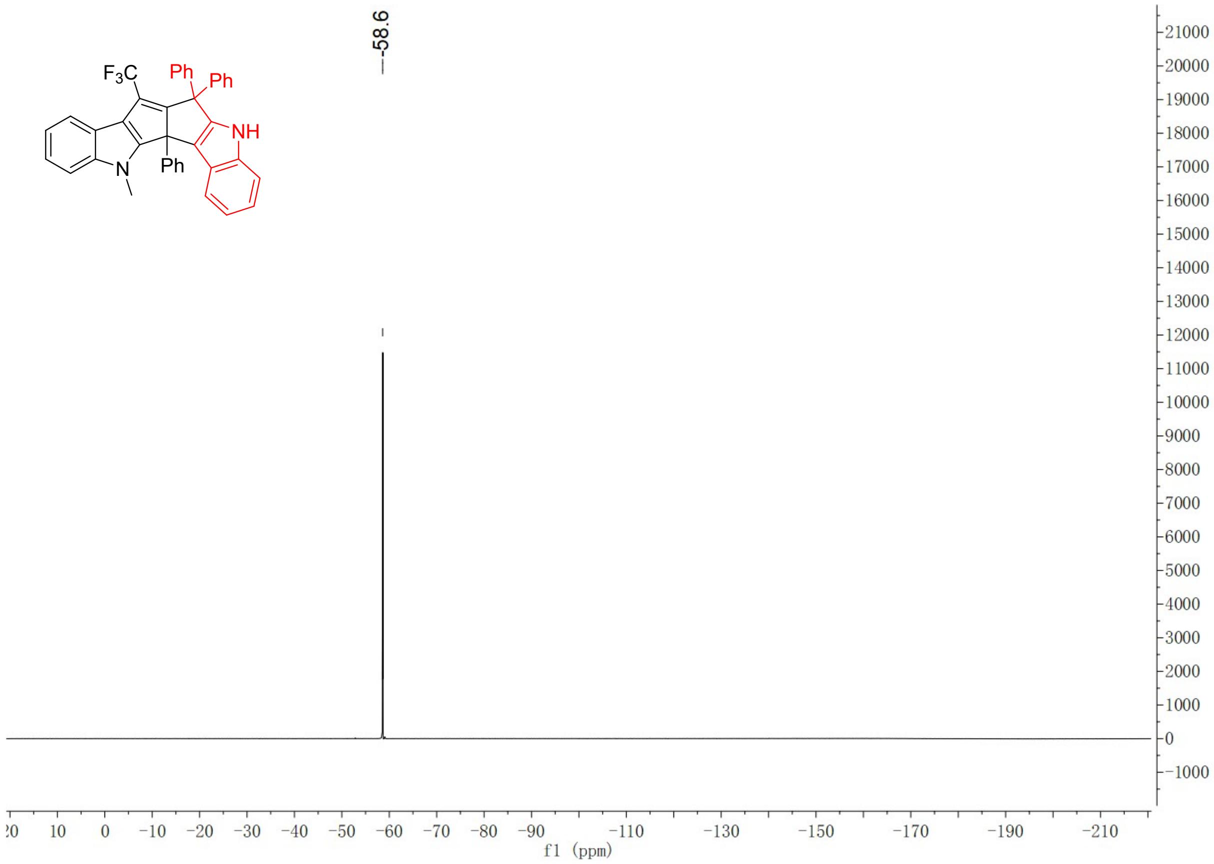
^{1}H NMR of compound 5 (in $CDCl_3$)



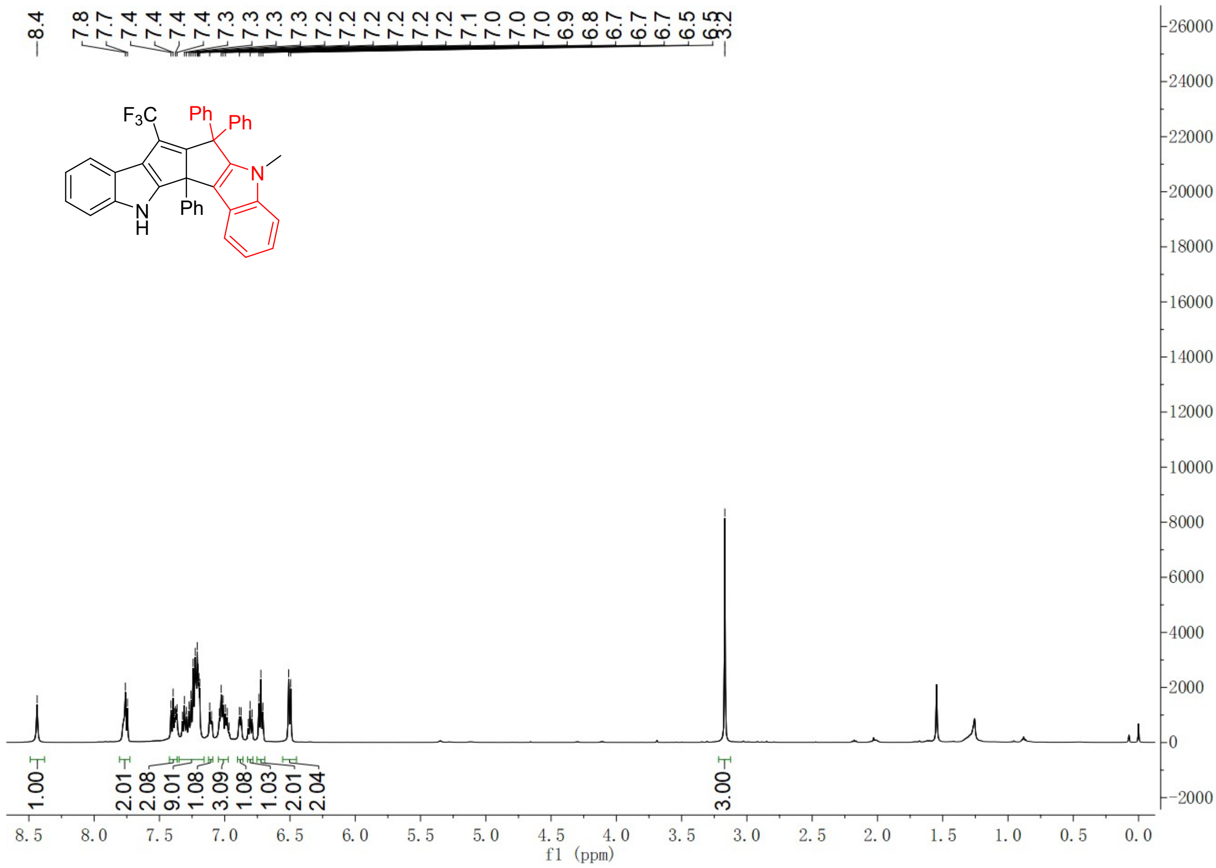
^{13}C NMR of compound 5 (in $CDCl_3$)



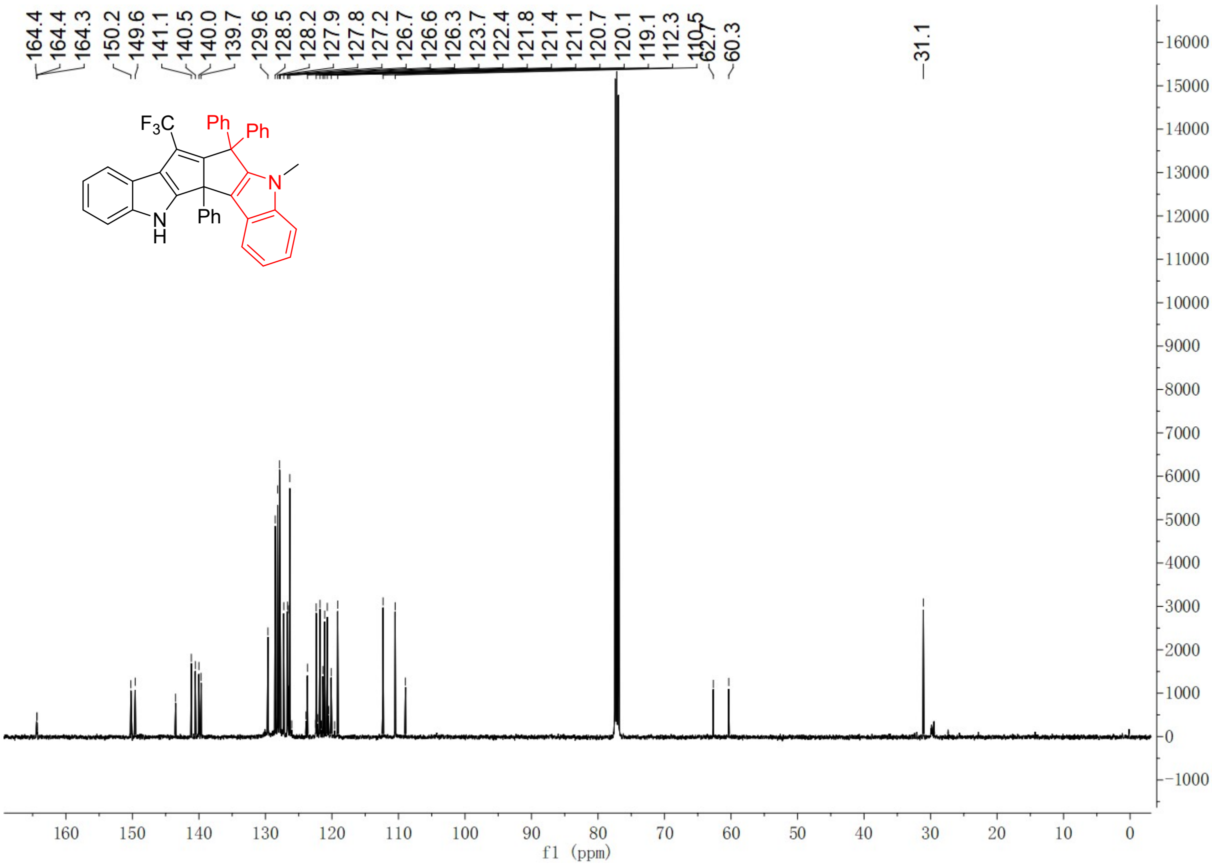
^{19}F NMR of compound 5 (in $CDCl_3$)



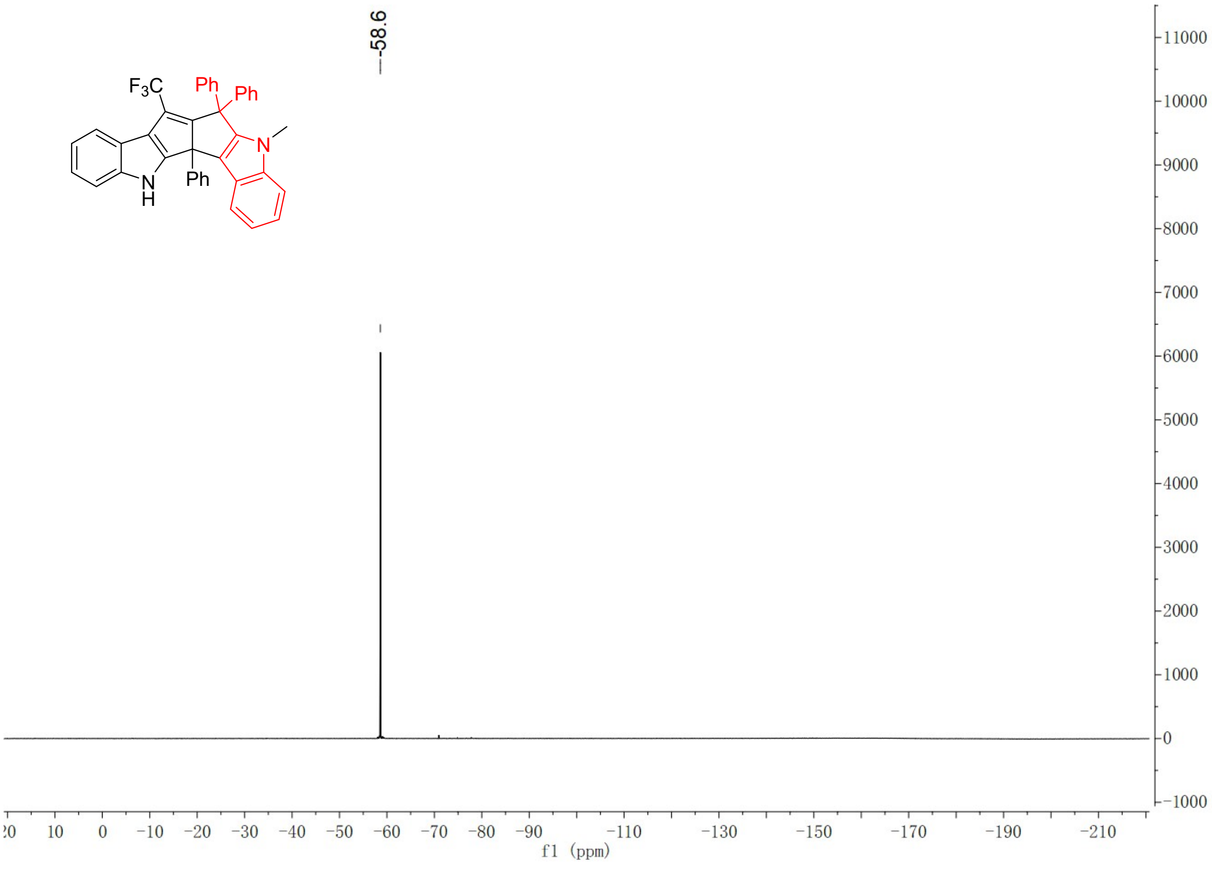
^{1}H NMR of compound 7 (in $CDCl_3$)



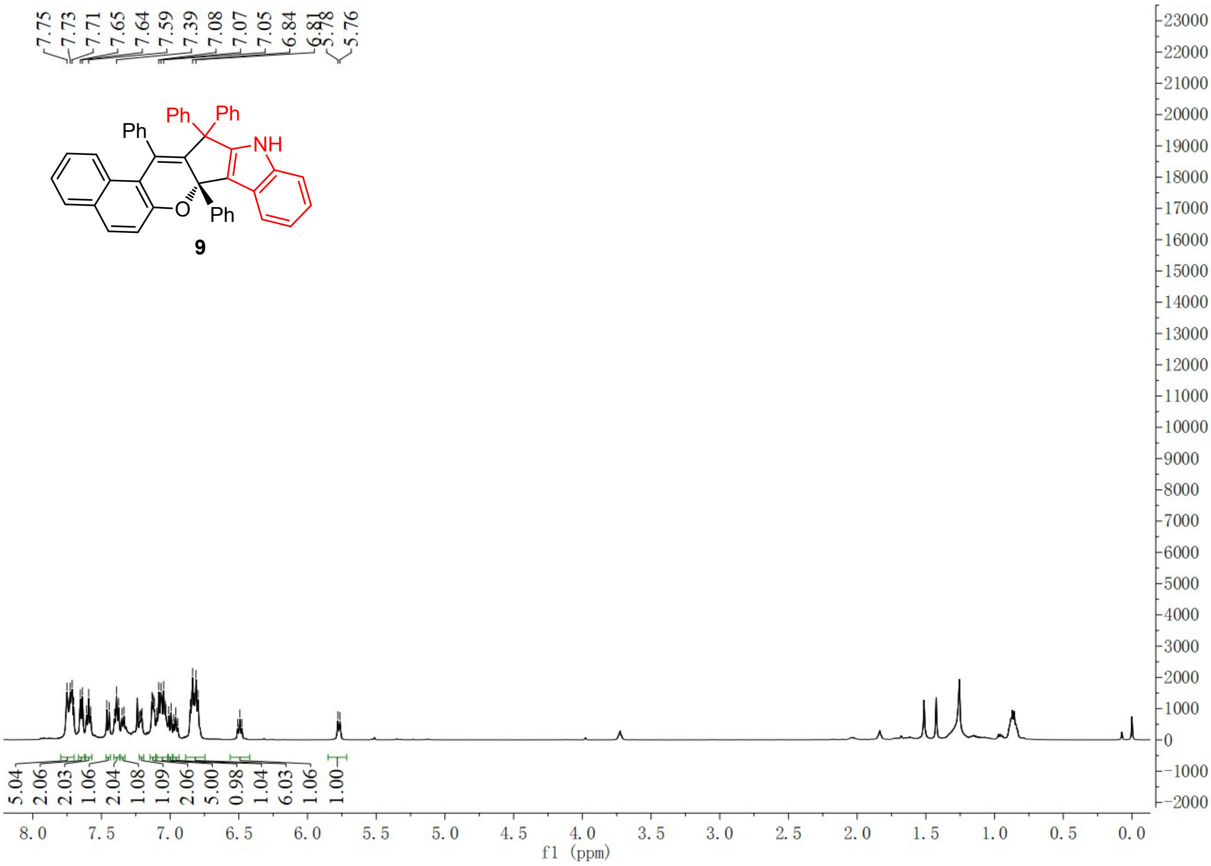
^{13}C NMR of compound 7 (in $CDCl_3$)



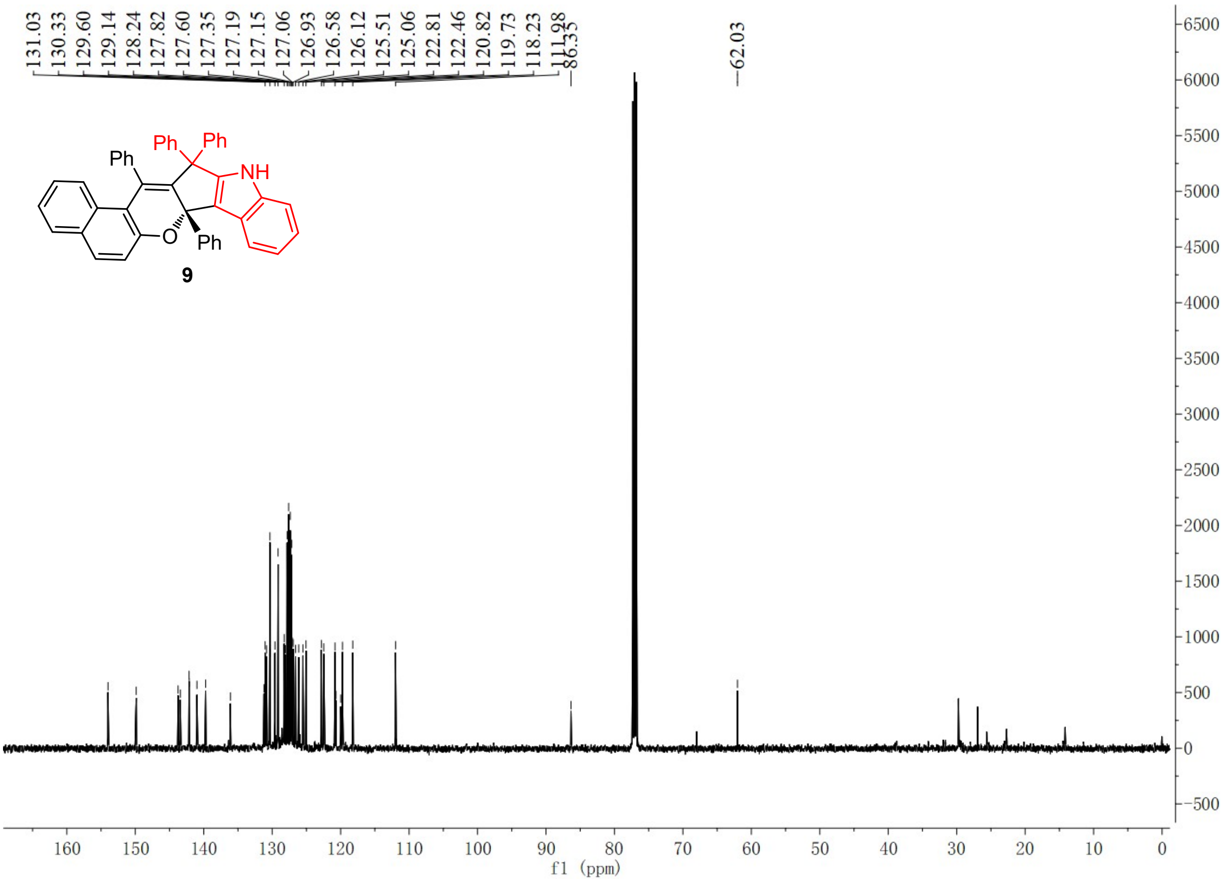
^{19}F NMR of compound 7 (in $CDCl_3$)



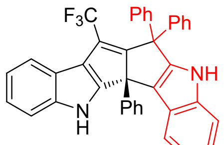
^{1}H NMR of compound 9 (in $CDCl_3$)



^{13}C NMR of compound 9 (in $CDCl_3$)

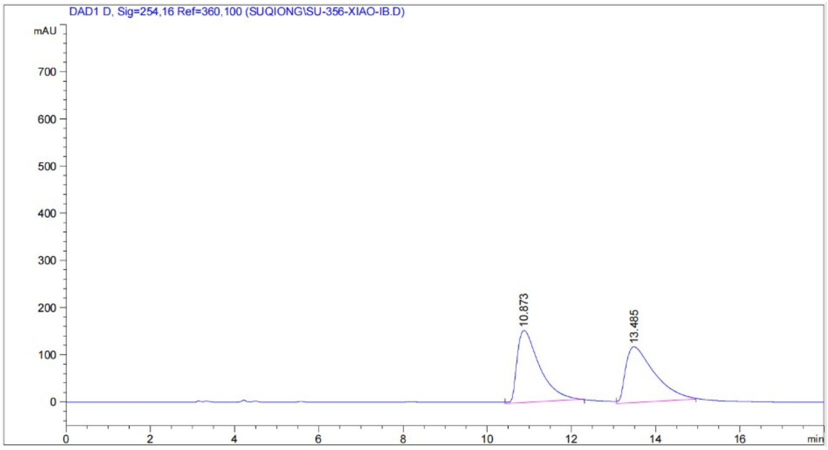


8. Copies of HPLC Spectra



3a

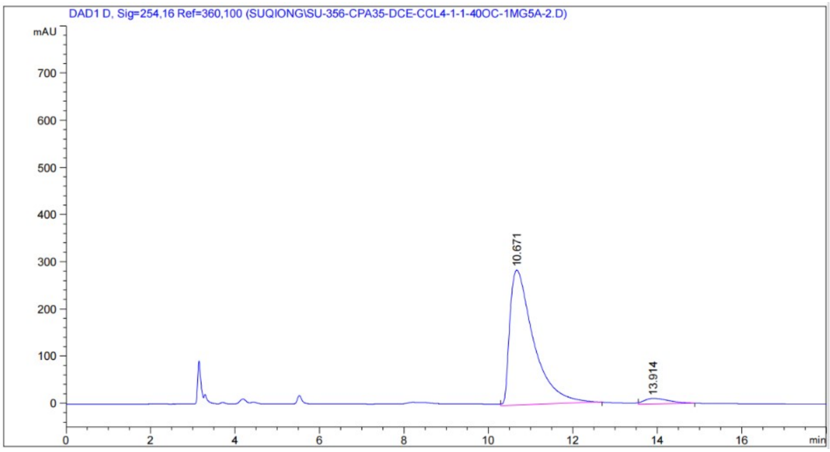
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

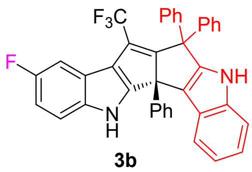
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.873	MM R	0.6183	5676.04590	153.00360	50.1581
2	13.485	MM R	0.7938	5640.25635	118.41669	49.8419

HPLC spectrum of the enantioenriched compound



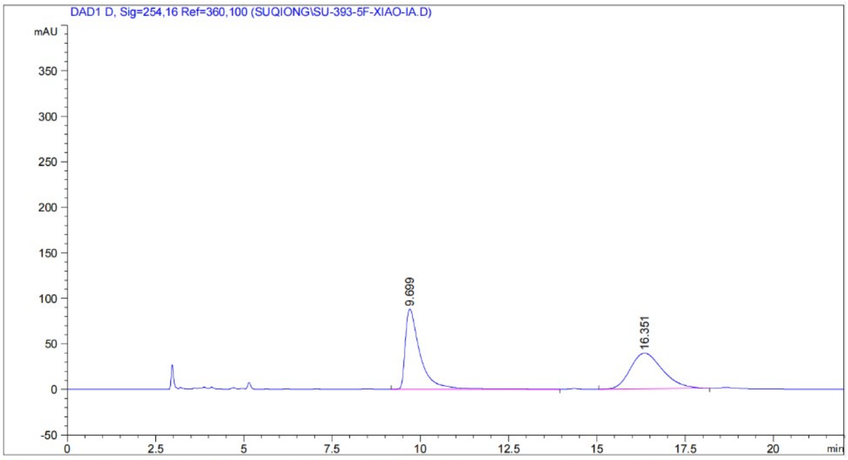
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.671	MM R	0.6506	1.11519e4	285.66281	95.9091
2	13.914	MM R	0.6713	475.66718	11.80954	4.0909



3b

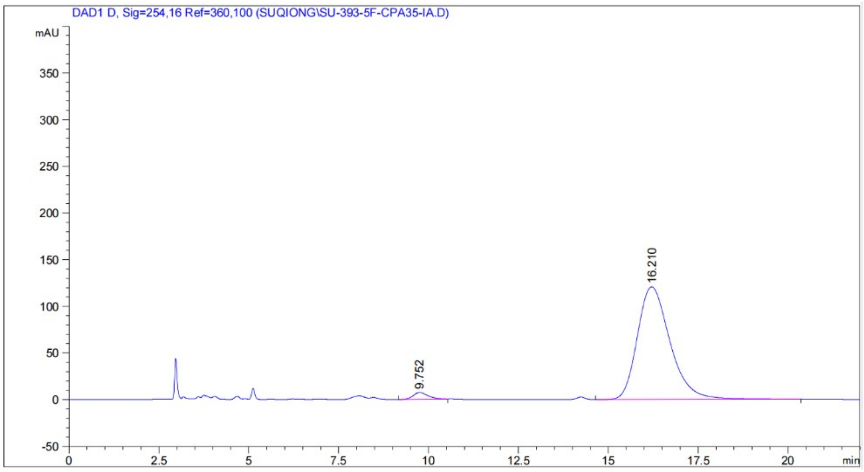
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

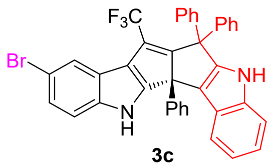
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.699	BB	0.4299	2578.75049	87.99345	50.9629
2	16.351	BB	0.9472	2481.29932	39.05825	49.0371

HPLC spectrum of the enantioenriched compound



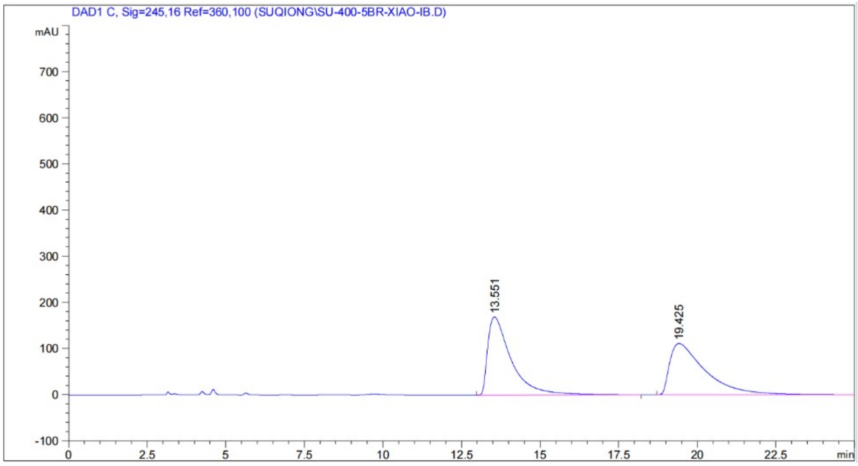
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.752	BB	0.4152	208.94456	7.36093	2.6588
2	16.210	BB	0.9683	7649.60889	120.55412	97.3412



3c

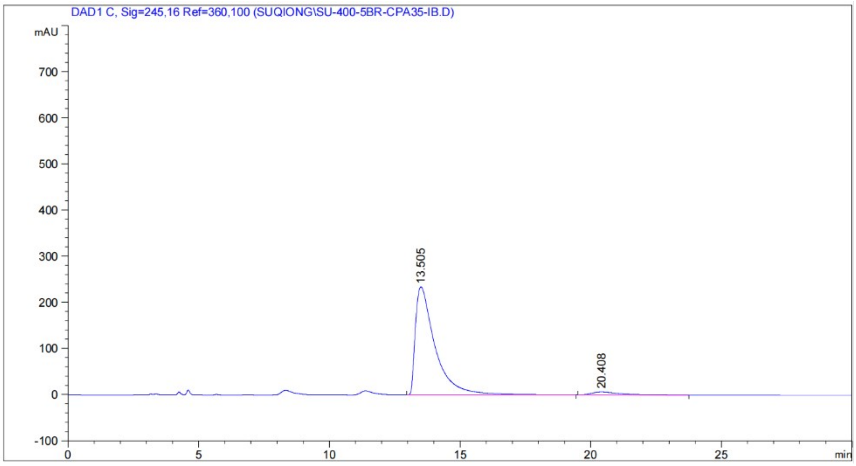
HPLC spectrum of the racemate



信号 1: DAD1 C, Sig=245,16 Ref=360,100

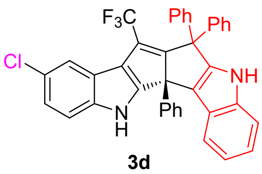
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.551	BB	0.7642	8816.94629	169.13531	50.0694
2	19.425	BB	1.1310	8792.49219	111.13631	49.9306

HPLC spectrum of the enantioenriched compound



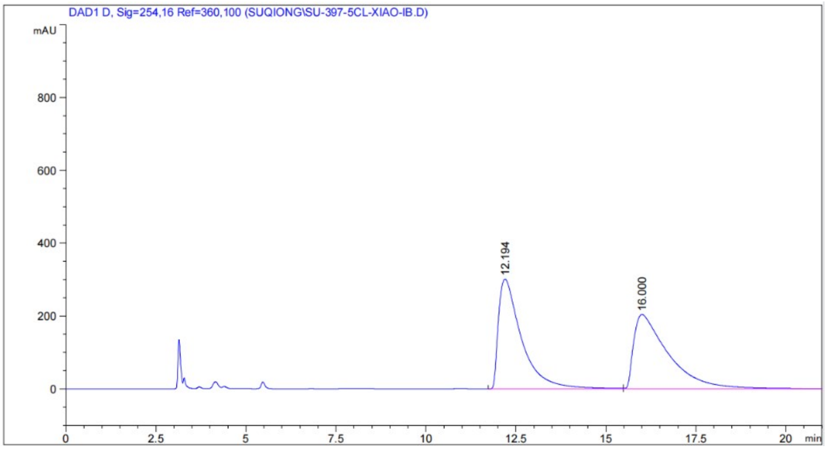
信号 1: DAD1 C, Sig=245,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	13.505	BB	0.7773	1.23031e4	234.02071	96.5608
2	20.408	BB	0.8389	438.20074	6.15302	3.4392



3d

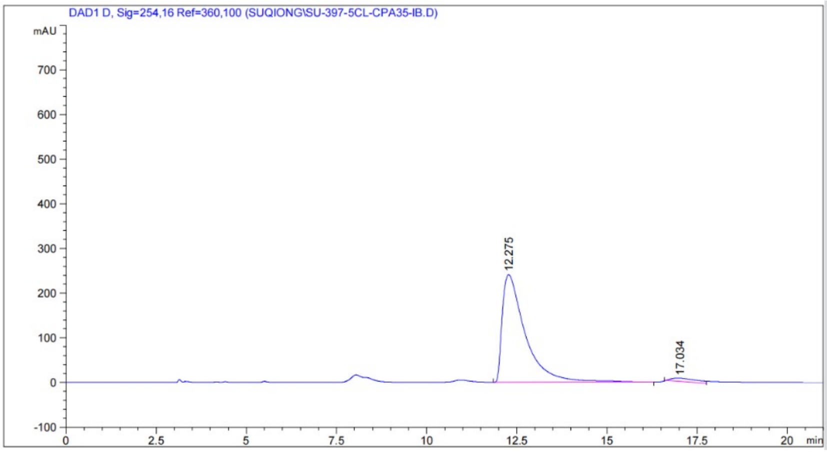
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

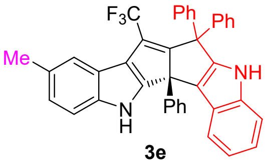
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.194	BV	0.6588	1.35088e4	301.46106	49.6878
2	16.000	VBA	0.9538	1.36785e4	204.12175	50.3122

HPLC spectrum of the enantioenriched compound



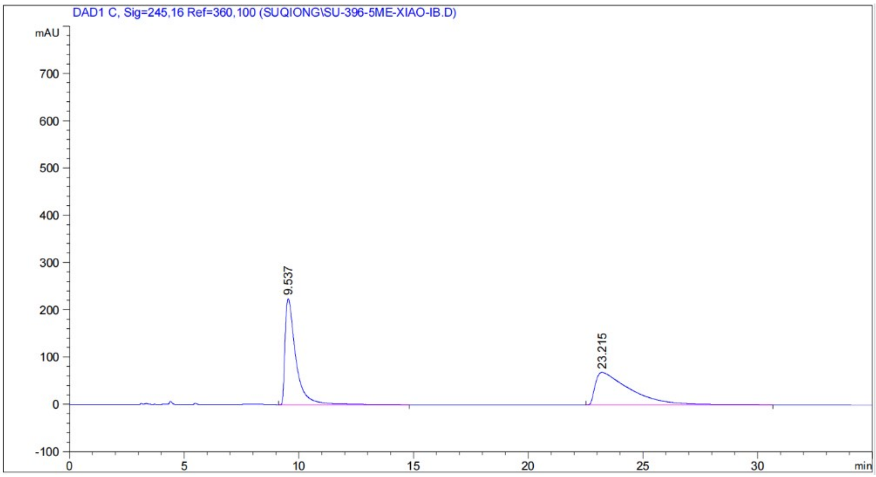
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.275	BB	0.6539	1.06919e4	240.84969	96.5297
2	17.034	MM R	0.8472	384.38080	7.56154	3.4703



3e

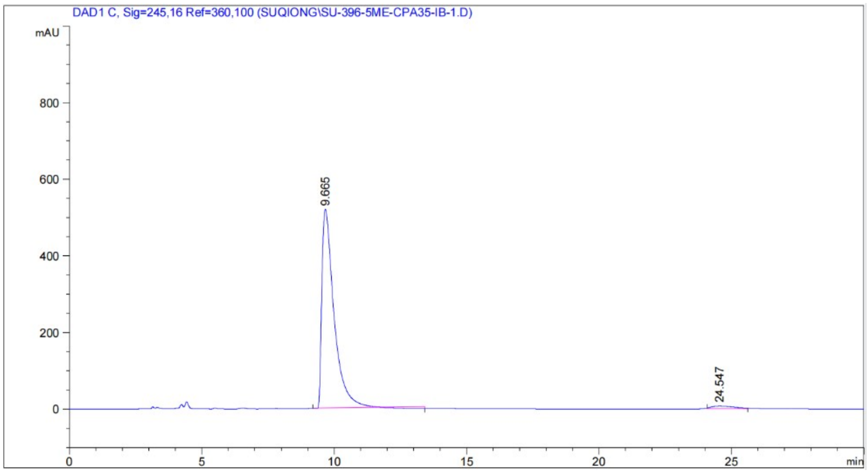
HPLC spectrum of the racemate



信号 1: DAD1 C, Sig=245,16 Ref=360,100

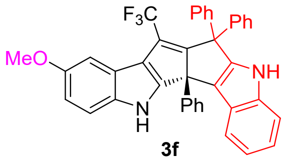
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.537	BB	0.4870	7364.49023	224.31772	50.5871
2	23.215	BB	1.4082	7193.55176	68.55206	49.4129

HPLC spectrum of the enantioenriched compound



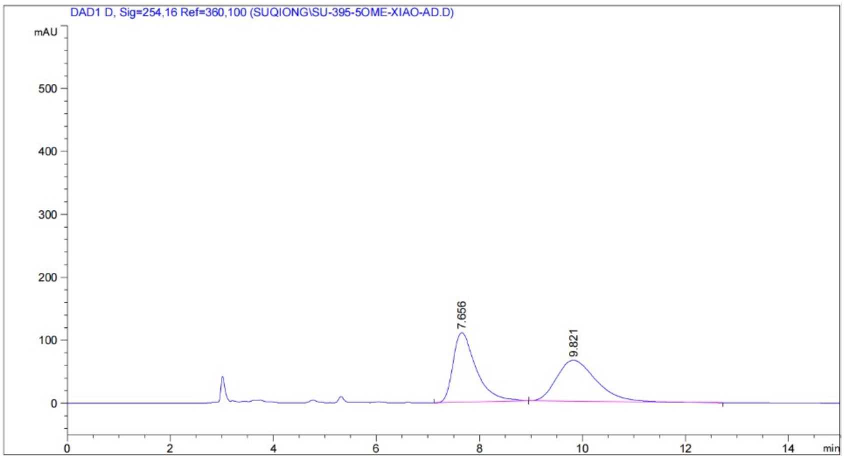
信号 1: DAD1 C, Sig=245,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.665	MM R	0.5326	1.65877e4	519.10730	97.4115
2	24.547	MM R	1.0129	440.78732	7.25292	2.5885



3f

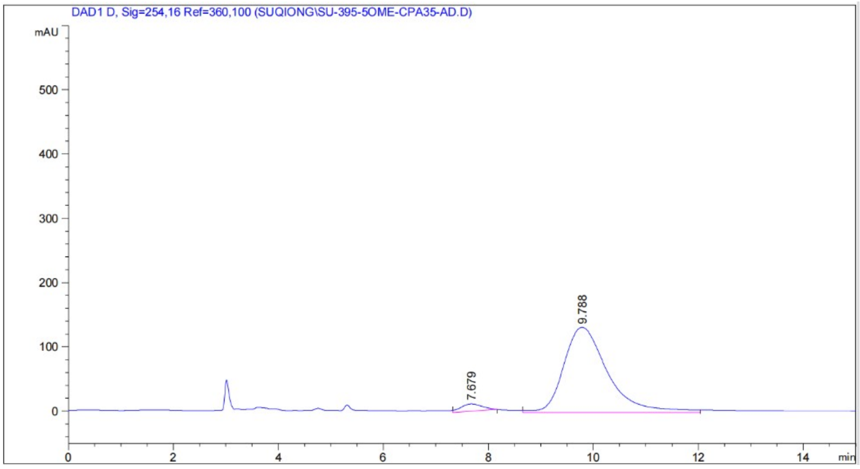
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

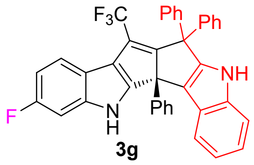
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.656	BB	0.4672	3438.89990	110.46636	49.7690
2	9.821	BB	0.8057	3470.82764	65.13085	50.2310

HPLC spectrum of the enantioenriched compound



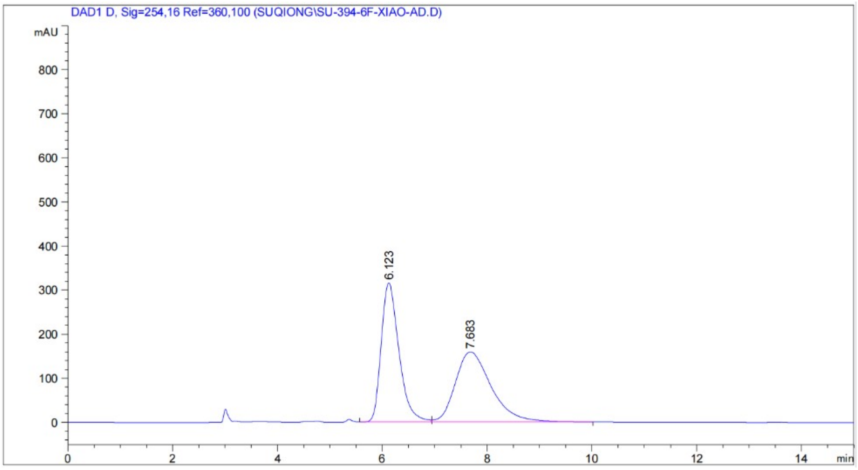
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.679	MM R	0.4712	313.37573	11.08512	3.9032
2	9.788	MM R	0.9716	7715.27539	132.34190	96.0968



3g

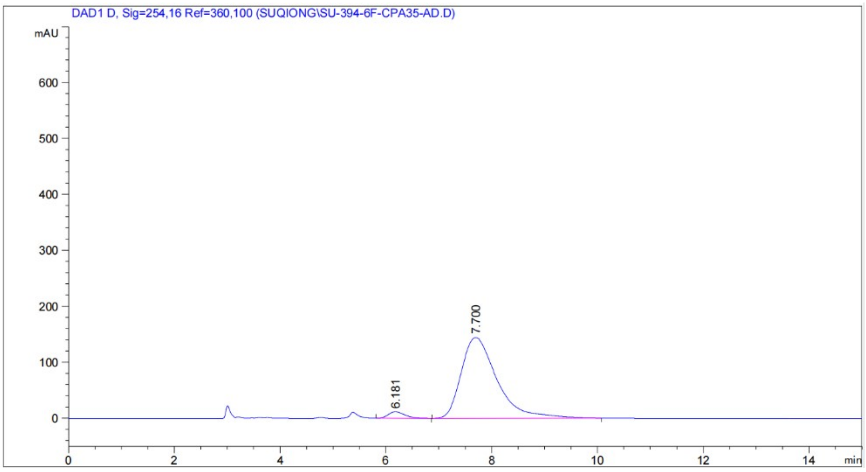
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

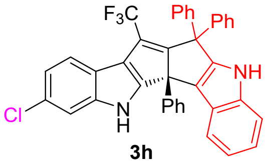
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.123	BV	0.3605	7418.00732	315.23819	49.4887
2	7.683	VB	0.7277	7571.29688	158.95178	50.5113

HPLC spectrum of the enantioenriched compound



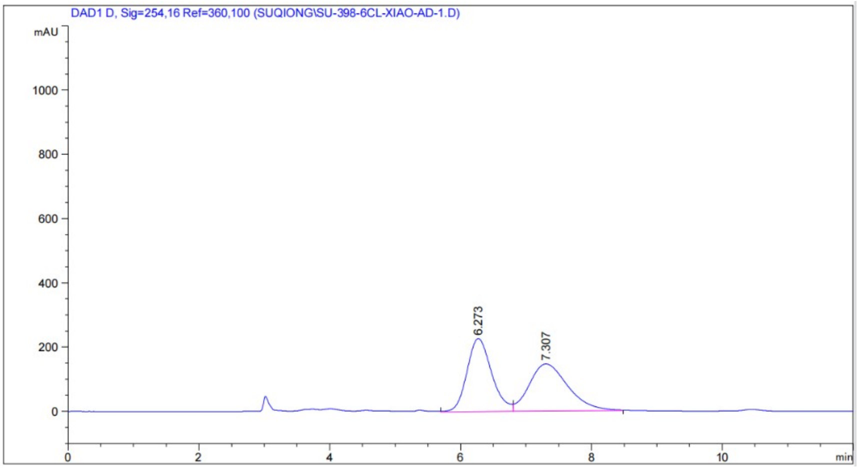
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.181	BB	0.3337	252.38934	11.69851	3.5933
2	7.700	BB	0.7147	6771.57178	144.50438	96.4067



3h

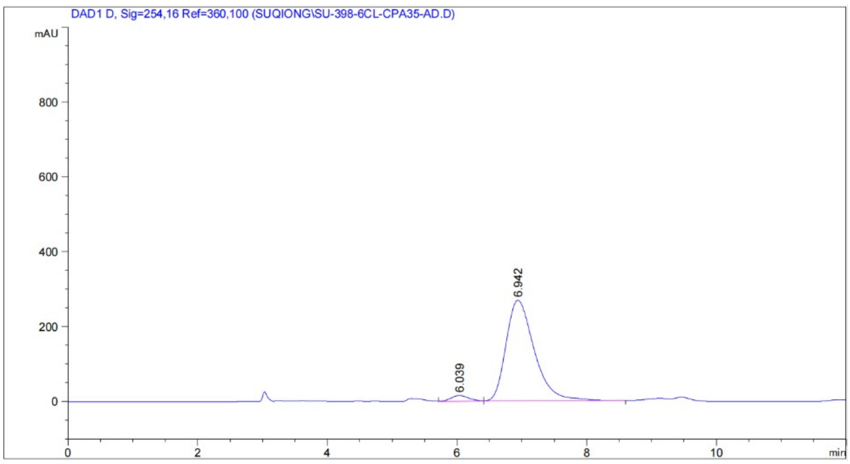
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

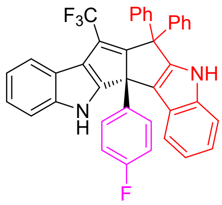
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.273	MF R	0.4377	5978.38623	227.63902	49.7327
2	7.307	FM R	0.6854	6042.65430	146.93446	50.2673

HPLC spectrum of the enantioenriched compound



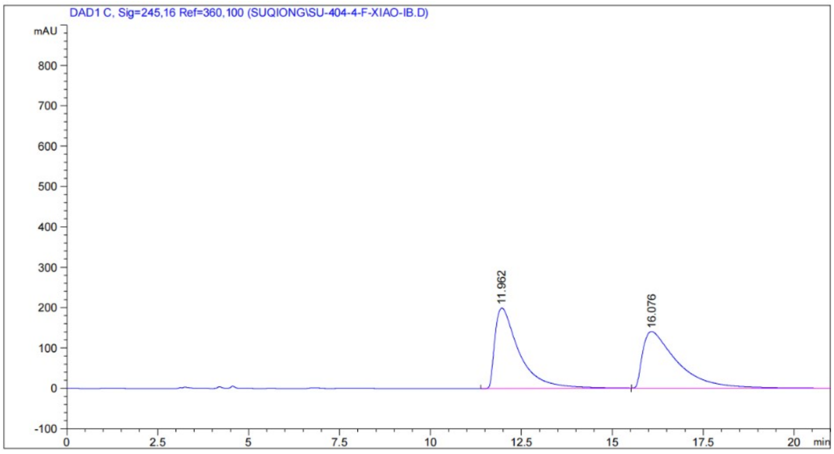
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.039	VV	0.2972	289.76547	15.14319	3.4242
2	6.942	VB	0.4664	8172.57666	269.05099	96.5758



3i

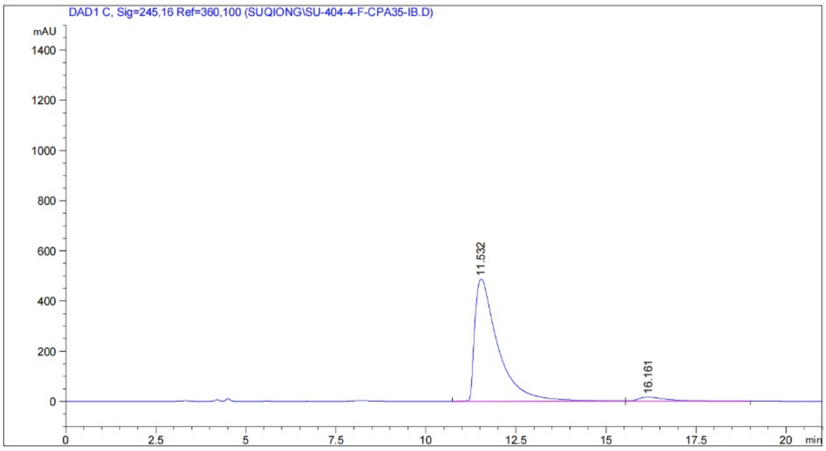
HPLC spectrum of the racemate



信号 1: DAD1 C, Sig=245,16 Ref=360,100

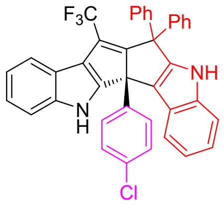
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.962	BB	0.6852	9226.88867	198.88986	49.8352
2	16.076	BBA	0.9485	9287.90527	140.26390	50.1648

HPLC spectrum of the enantioenriched compound



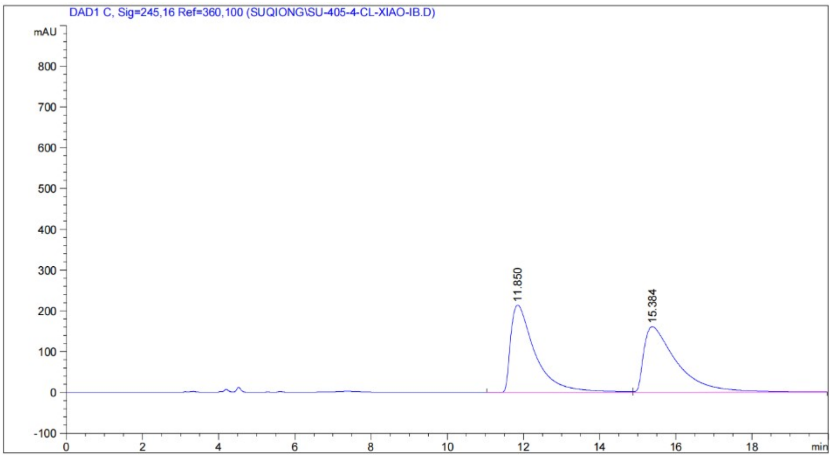
信号 1: DAD1 C, Sig=245,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.532	BB	0.6528	2.17626e4	487.47021	96.3237
2	16.161	BB	0.7742	830.58527	15.47383	3.6763



3j

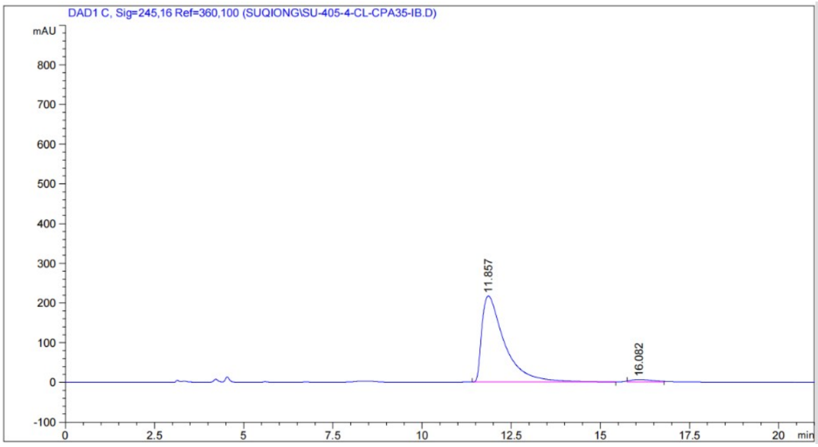
HPLC spectrum of the racemate



信号 1: DAD1 C, Sig=245,16 Ref=360,100

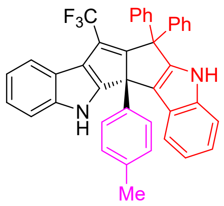
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.850	BV	0.6580	9532.00586	213.86977	49.7827
2	15.384	VBA	0.8719	9615.21875	160.73650	50.2173

HPLC spectrum of the enantioenriched compound



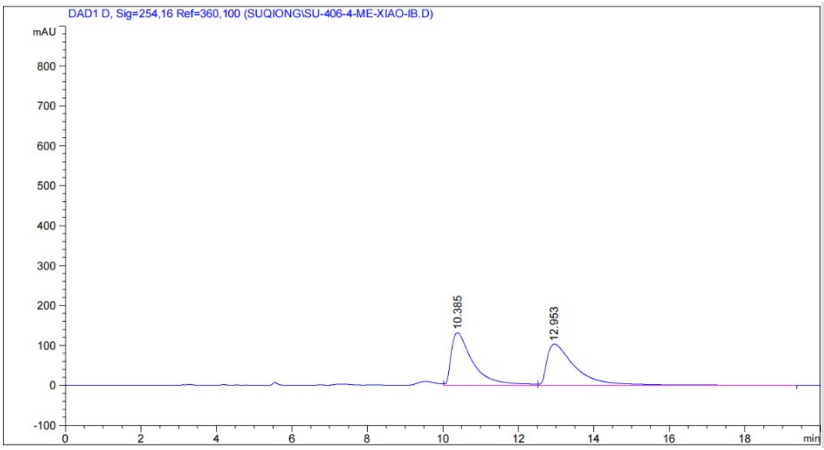
信号 1: DAD1 C, Sig=245,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.857	BB	0.6516	9568.56543	216.49388	97.1472
2	16.082	MM R	0.7123	280.98480	6.57450	2.8528



3k

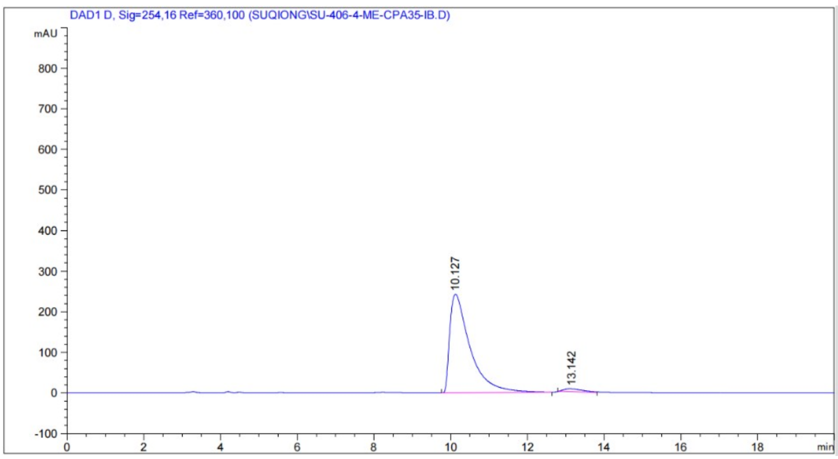
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

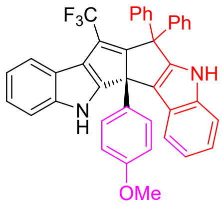
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.385	VV	0.5779	5197.17871	131.27740	49.3217
2	12.953	VB	0.7632	5340.13135	102.94147	50.6783

HPLC spectrum of the enantioenriched compound



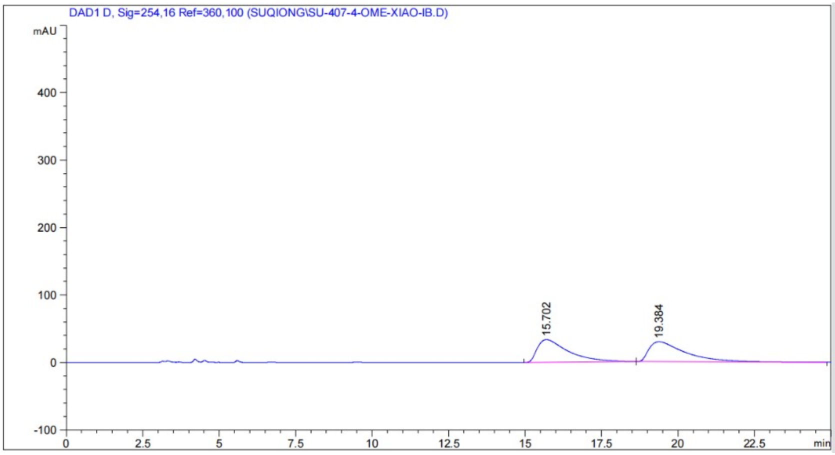
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.127	BB	0.5445	8956.59570	242.74779	97.2916
2	13.142	MM R	0.6020	249.33090	6.90240	2.7084



3l

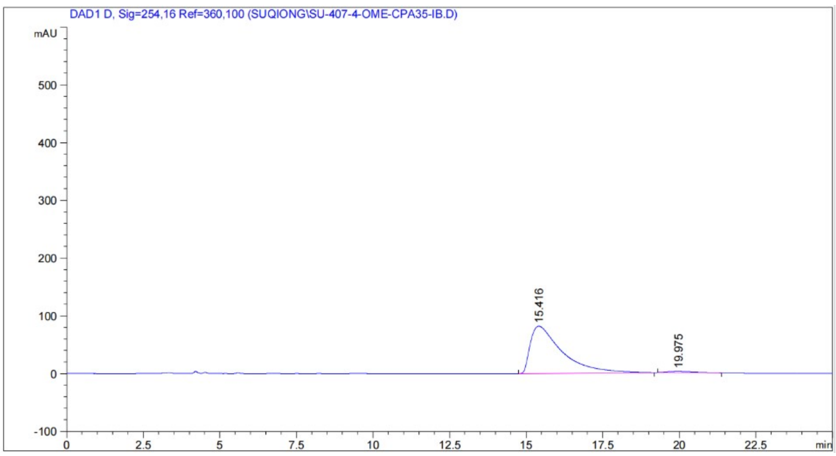
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

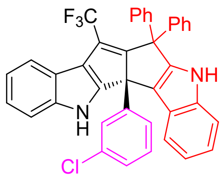
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.702	BB	1.0130	2407.94287	33.80563	49.3171
2	19.384	BB	1.1601	2474.62500	29.57738	50.6829

HPLC spectrum of the enantioenriched compound



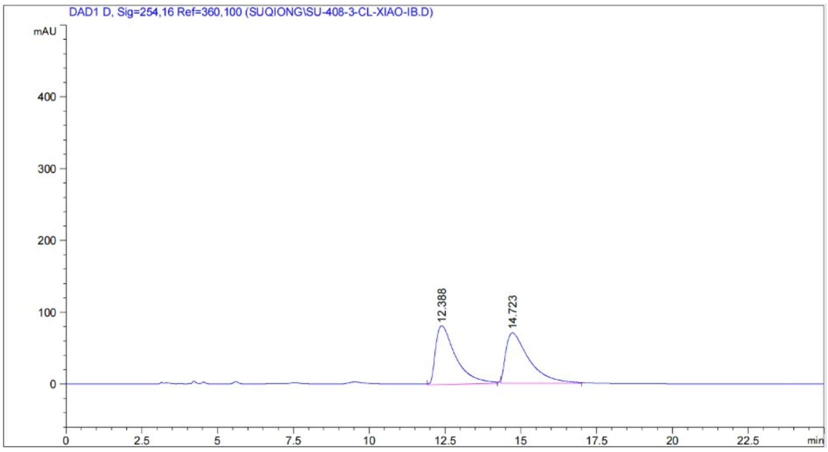
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	15.416	BB	1.0328	5923.20605	81.98966	98.1514
2	19.975	MM R	0.9678	111.55567	1.92107	1.8486



3m

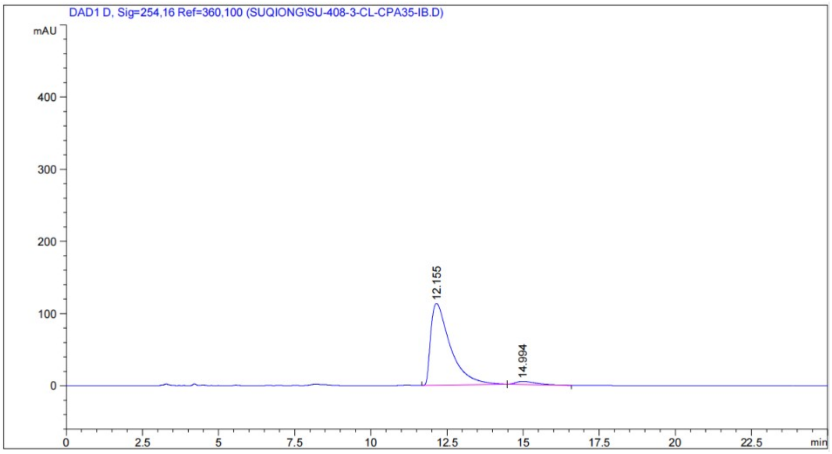
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

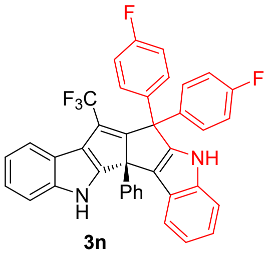
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.388	MM R	0.7751	3809.15112	81.91010	50.2003
2	14.723	MM R	0.8954	3778.75781	70.33413	49.7997

HPLC spectrum of the enantioenriched compound



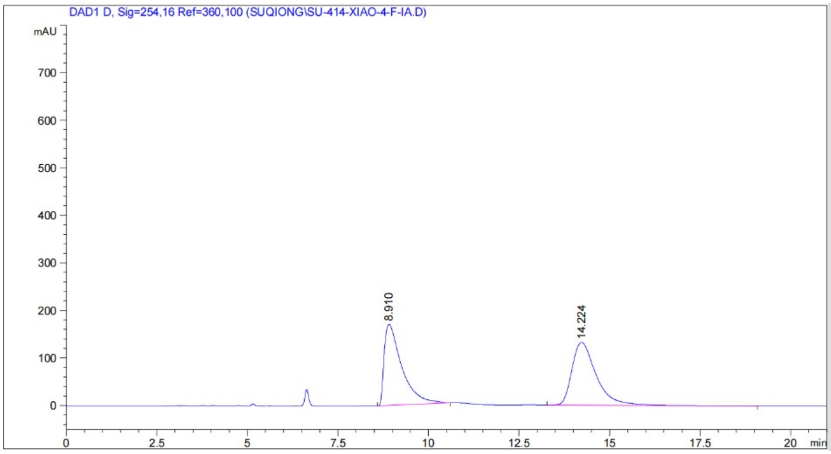
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.155	BB	0.6609	5099.30957	113.34273	96.4014
2	14.994	BB	0.6004	190.35158	4.31718	3.5986



3n

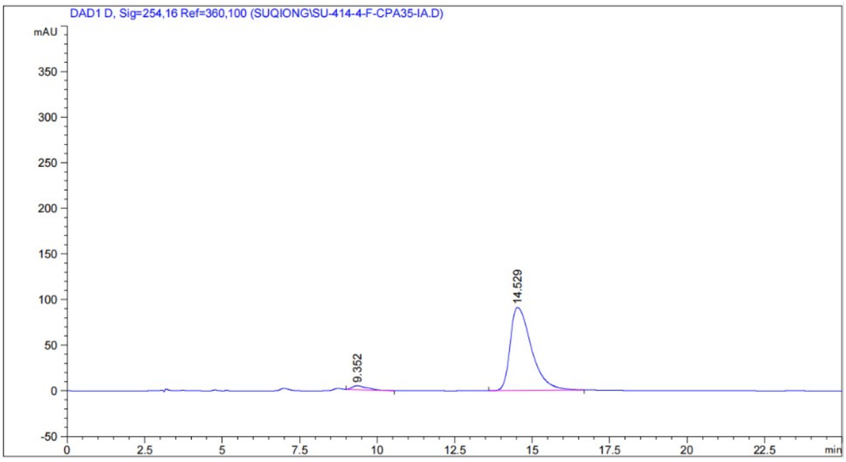
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

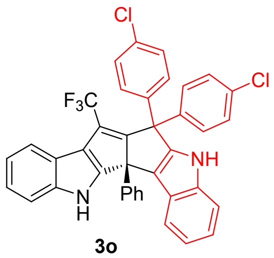
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.910	BB	0.4945	5766.10645	170.51221	48.1247
2	14.224	BB	0.7034	6215.49756	132.47508	51.8753

HPLC spectrum of the enantioenriched compound



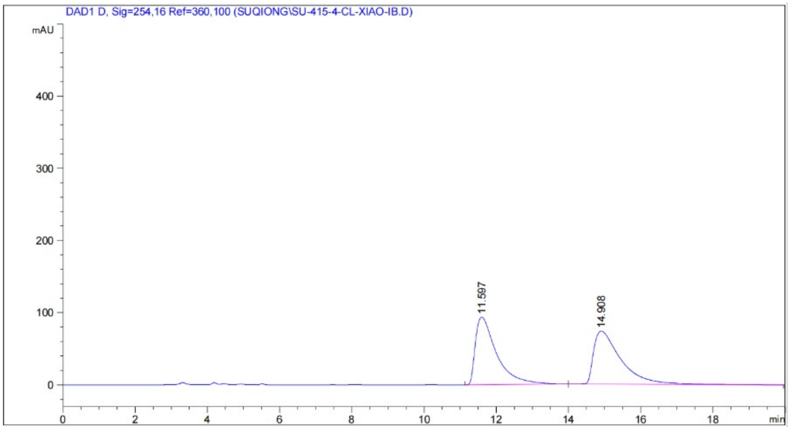
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.352	BB	0.4712	136.64609	4.22660	3.0568
2	14.529	BB	0.7285	4333.53760	90.84709	96.9432



3o

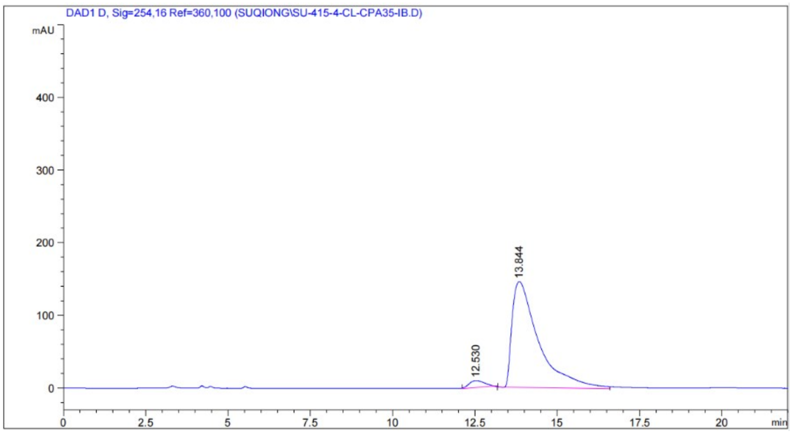
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

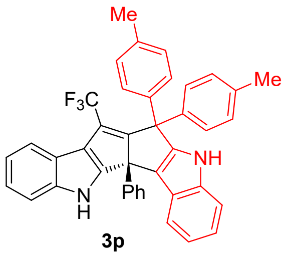
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.597	BB	0.6091	3829.26611	93.64758	49.5590
2	14.908	BBA	0.7703	3897.41772	73.53433	50.4410

HPLC spectrum of the enantioenriched compound



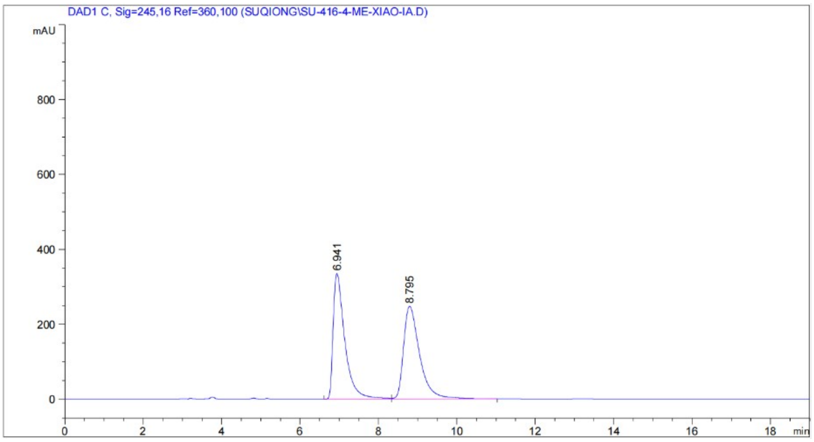
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.530	MM R	0.5223	295.15820	9.41770	3.4834
2	13.844	MM R	0.9356	8178.06934	145.68179	96.5166



3p

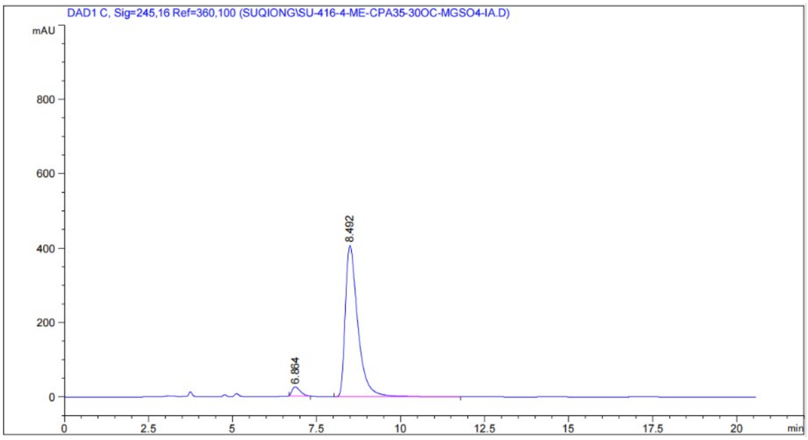
HPLC spectrum of the racemate



信号 1: DAD1 C, Sig=245,16 Ref=360,100

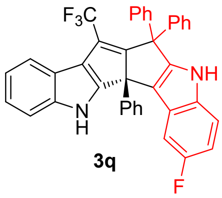
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.941	BV	0.3070	6914.88867	334.71680	49.5424
2	8.795	VB	0.4299	7042.62256	247.59163	50.4576

HPLC spectrum of the enantioenriched compound



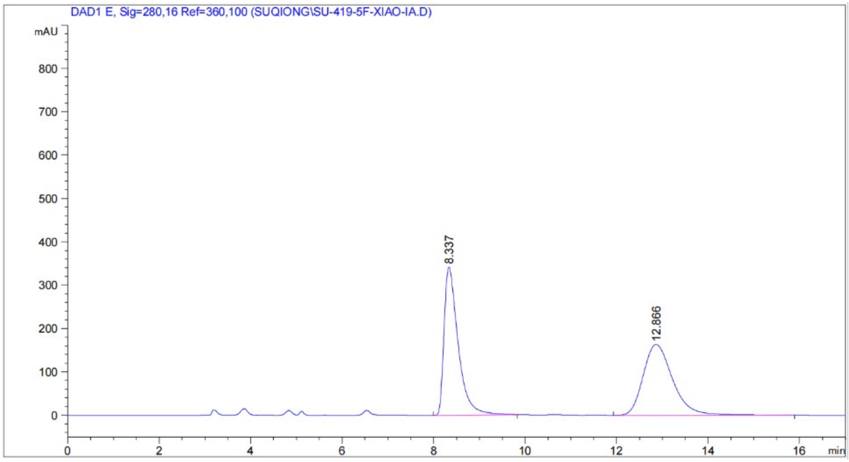
信号 1: DAD1 C, Sig=245,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.864	MM R	0.2794	405.80634	24.20663	3.6757
2	8.492	BB	0.3950	1.06344e4	406.79831	96.3243



3q

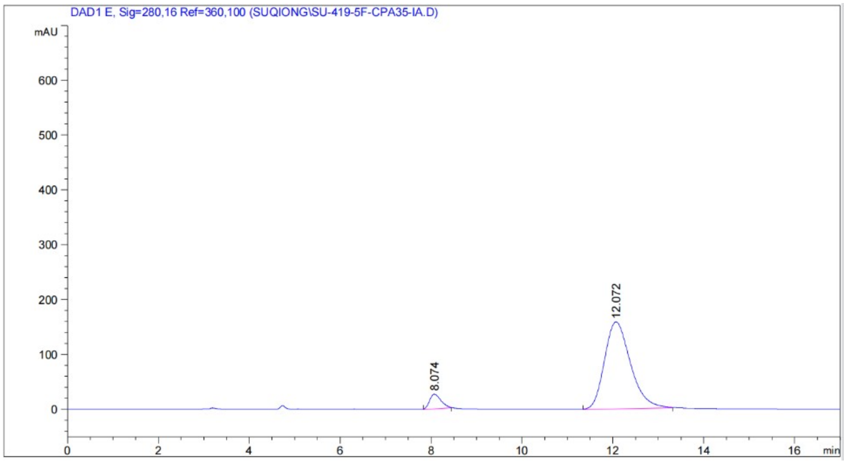
HPLC spectrum of the racemate



信号 1: DAD1 E, Sig=280,16 Ref=360,100

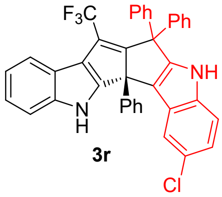
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.337	BB	0.3231	7287.90332	341.34735	49.8853
2	12.866	BB	0.6895	7321.41602	163.17613	50.1147

HPLC spectrum of the enantioenriched compound



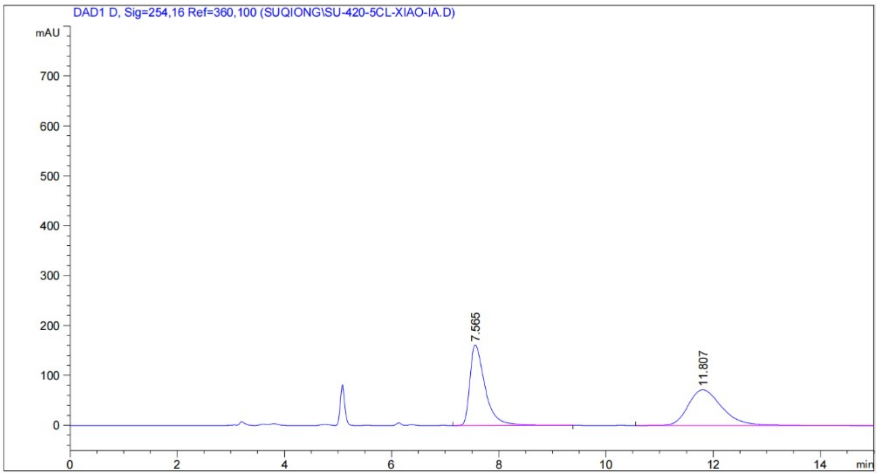
信号 1: DAD1 E, Sig=280,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	8.074	MM R	0.2925	472.14484	26.89991	6.9333
2	12.072	MM R	0.6653	6337.67920	158.76044	93.0667



3r

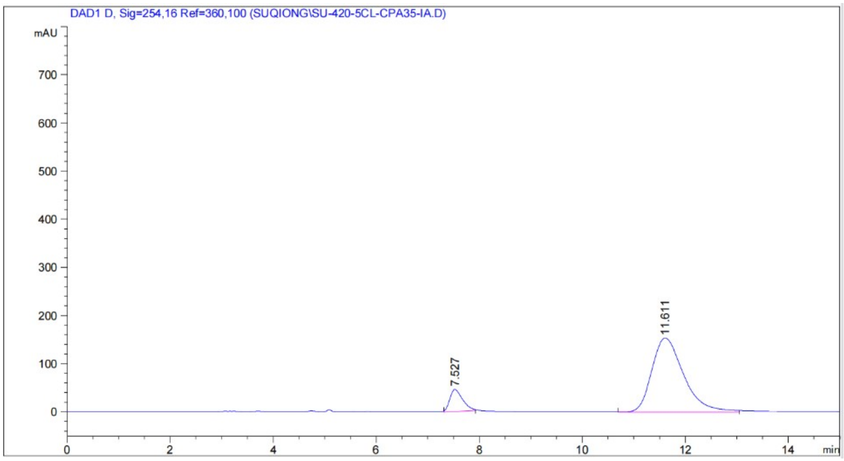
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

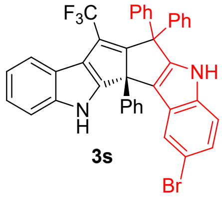
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.565	BB	0.2966	3190.10913	161.38489	49.7325
2	11.807	BB	0.6861	3224.43115	71.77167	50.2675

HPLC spectrum of the enantioenriched compound



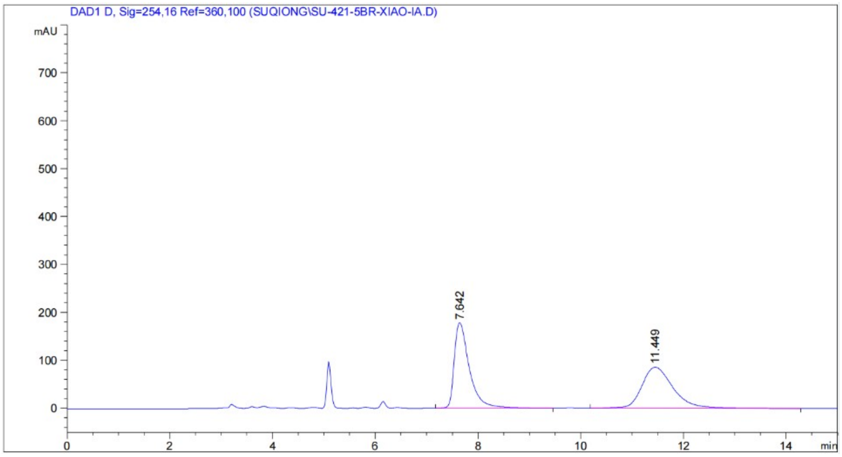
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.527	MM R	0.2900	803.18469	46.15590	10.7743
2	11.611	MM R	0.7215	6651.47412	153.64421	89.2257



3s

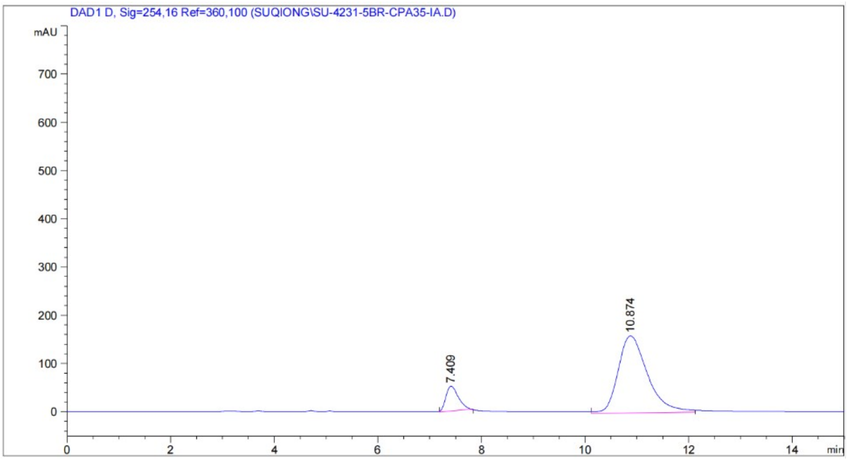
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

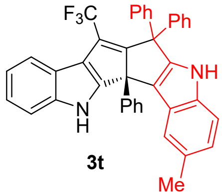
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.642	BB	0.3054	3660.49805	178.38788	50.1868
2	11.449	BB	0.6504	3633.25439	85.74265	49.8132

HPLC spectrum of the enantioenriched compound



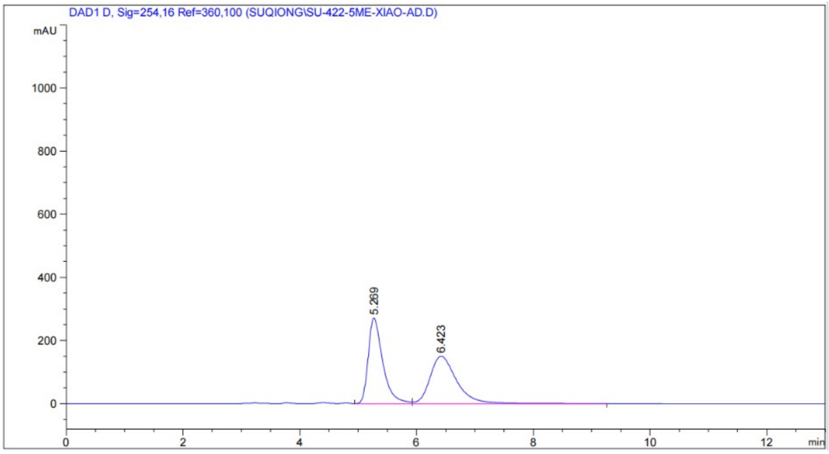
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.409	MM R	0.2758	852.04376	51.48931	11.8579
2	10.874	MM R	0.6606	6333.42871	159.77948	88.1421



3t

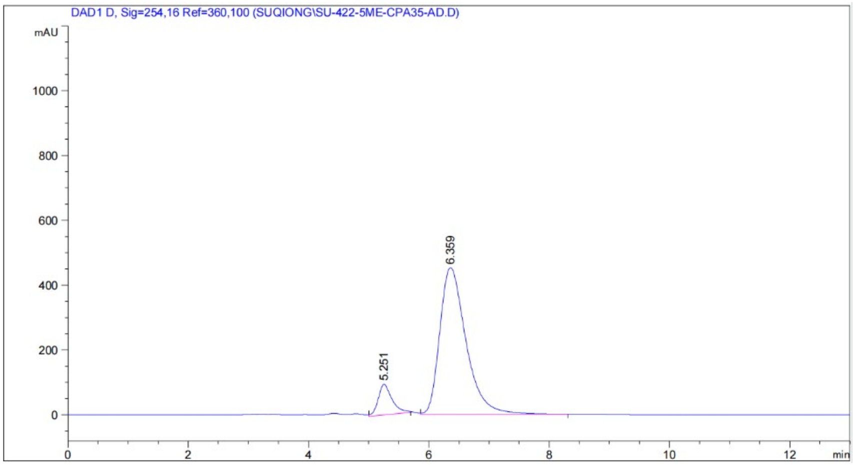
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

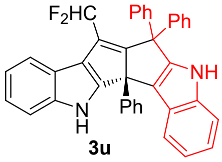
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.269	BV	0.2580	4690.27490	270.89209	49.6087
2	6.423	VB	0.4830	4764.27002	149.83893	50.3913

HPLC spectrum of the enantioenriched compound



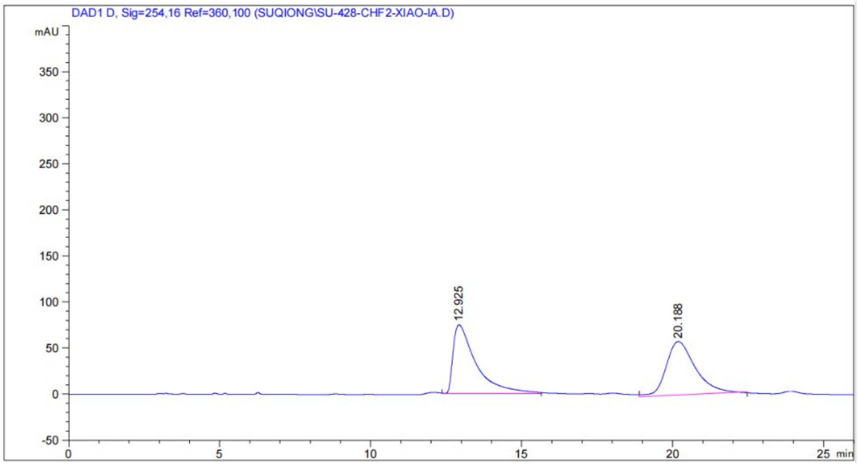
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.251	MM R	0.2626	1501.28455	95.28012	9.8098
2	6.359	VB	0.4651	1.38026e4	453.45667	90.1902



3u

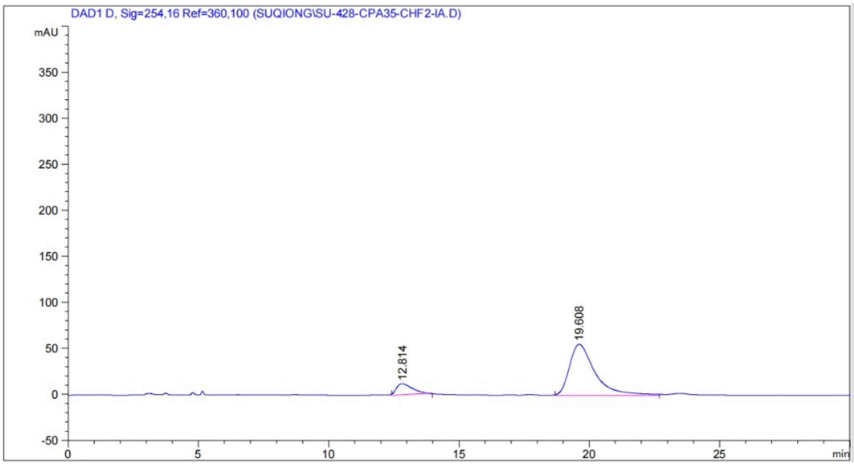
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

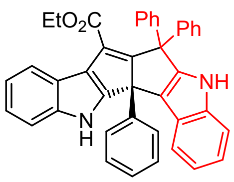
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.925	MM R	0.8833	3953.15259	74.58946	50.4189
2	20.188	MM R	1.1170	3887.46729	58.00404	49.5811

HPLC spectrum of the enantioenriched compound



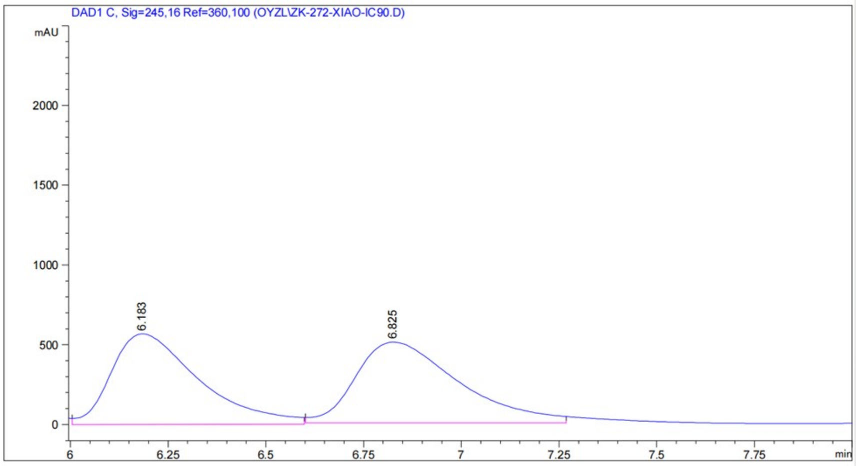
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.814	MM R	0.7029	503.55838	11.94076	11.8567
2	19.608	MM R	1.1273	3743.47485	55.34687	88.1433



3v

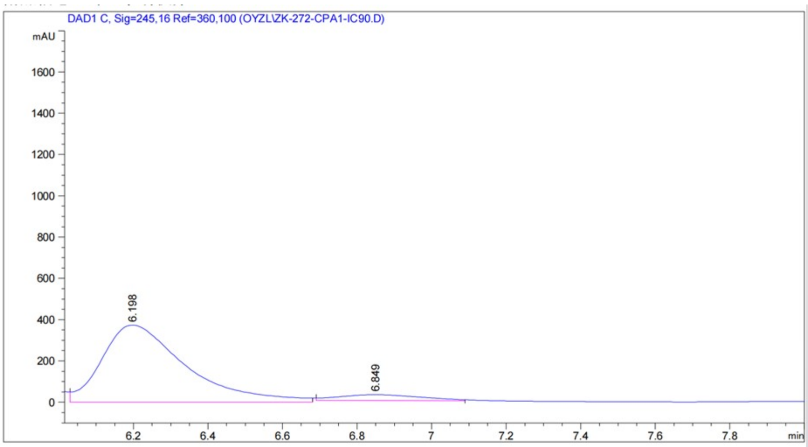
HPLC spectrum of the racemate



信号 1: DAD1 C, Sig=245,16 Ref=360,100

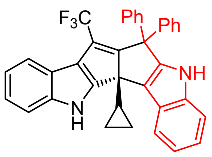
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.183	VV	0.2336	8826.76270	566.92938	48.8329
2	6.825	MM R	0.3052	9248.69238	505.00375	51.1671

HPLC spectrum of the enantioenriched compound



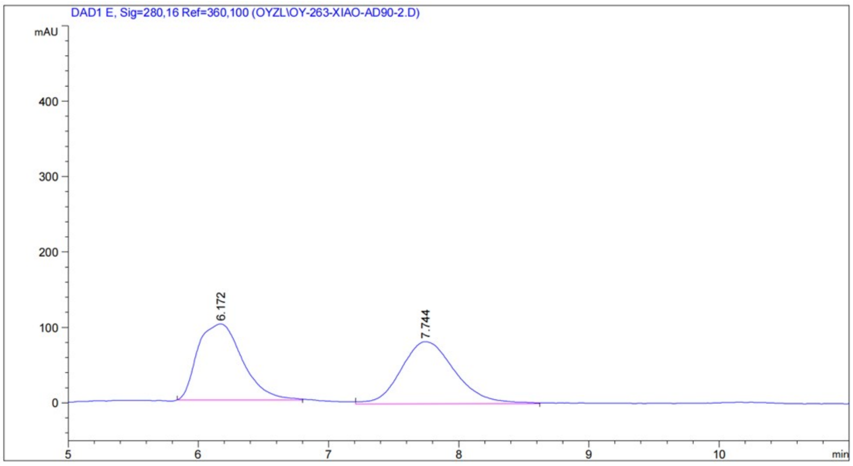
信号 1: DAD1 C, Sig=245,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.198	VV	0.2313	5810.36182	373.91232	93.0082
2	6.849	MM R	0.2564	436.78491	28.39303	6.9918



3w

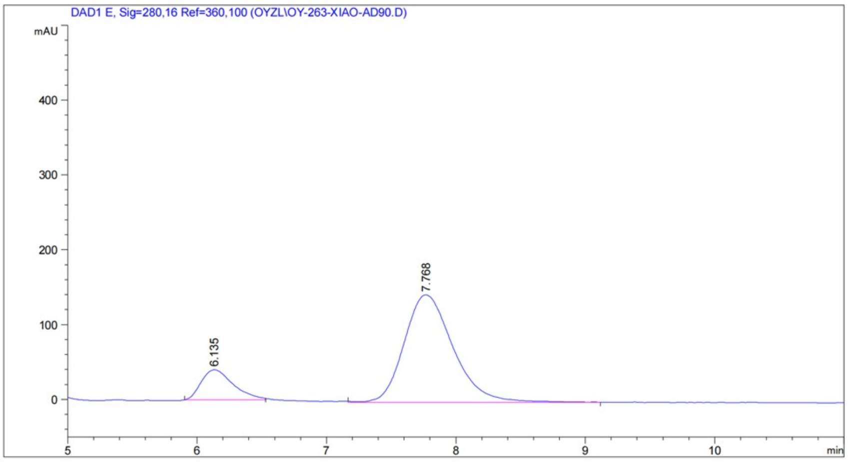
HPLC spectrum of the racemate



信号 1: DAD1 E, Sig=280,16 Ref=360,100

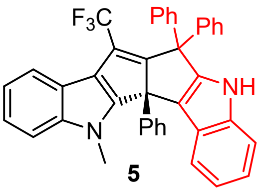
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.172	MM R	0.3981	2412.56885	101.00908	50.5102
2	7.744	MM R	0.4794	2363.83374	82.17830	49.4898

HPLC spectrum of the enantioenriched compound



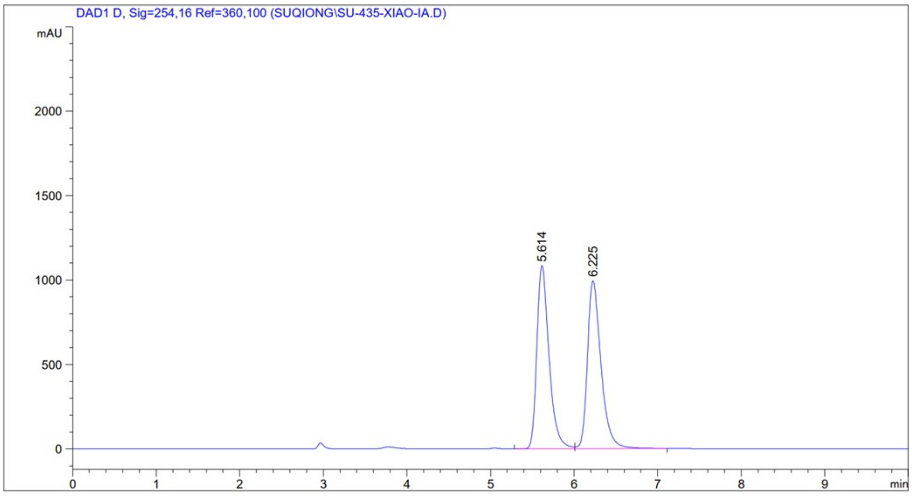
信号 1: DAD1 E, Sig=280,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	6.135	MM R	0.2849	683.05865	39.96221	15.2682
2	7.768	MM R	0.4393	3790.68433	143.81737	84.7318



5

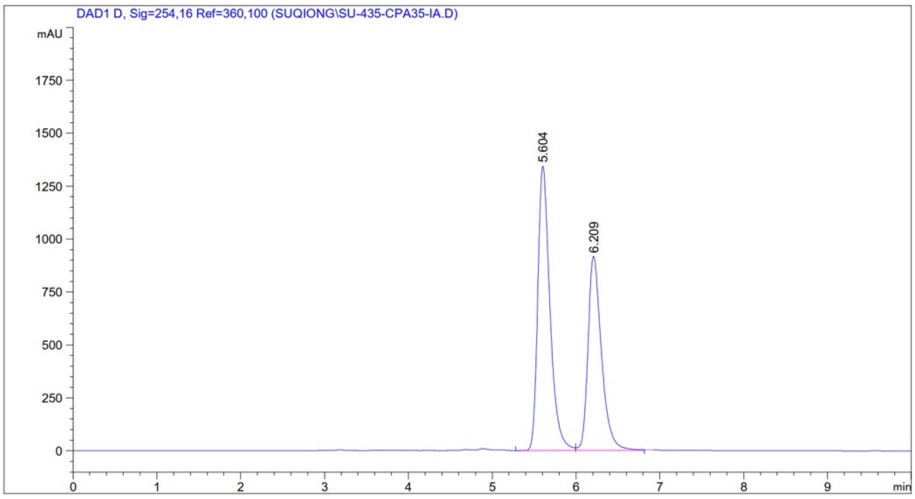
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

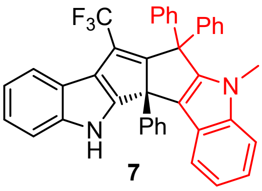
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.614	BV	0.1543	1.09990e4	1084.57617	49.4625
2	6.225	VB	0.1698	1.12380e4	994.77118	50.5375

HPLC spectrum of the enantioenriched compound



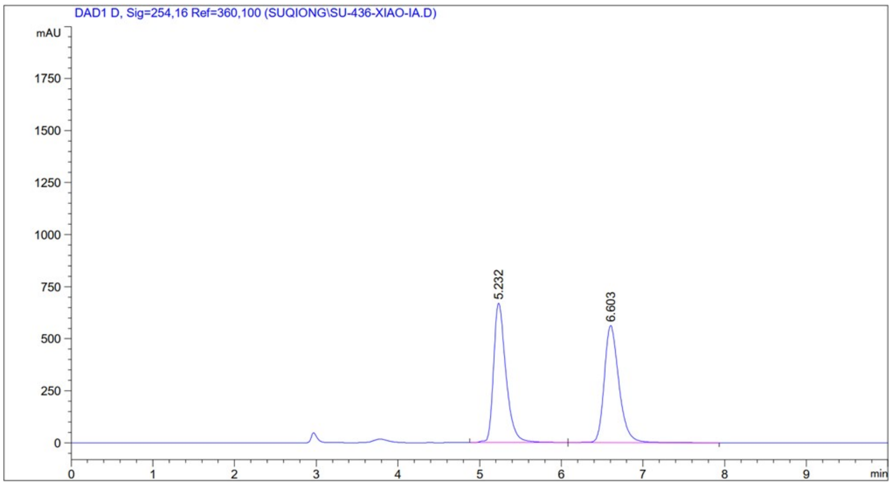
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.604	BV	0.1535	1.35301e4	1343.29504	56.8611
2	6.209	VV	0.1706	1.02649e4	916.80322	43.1389



7

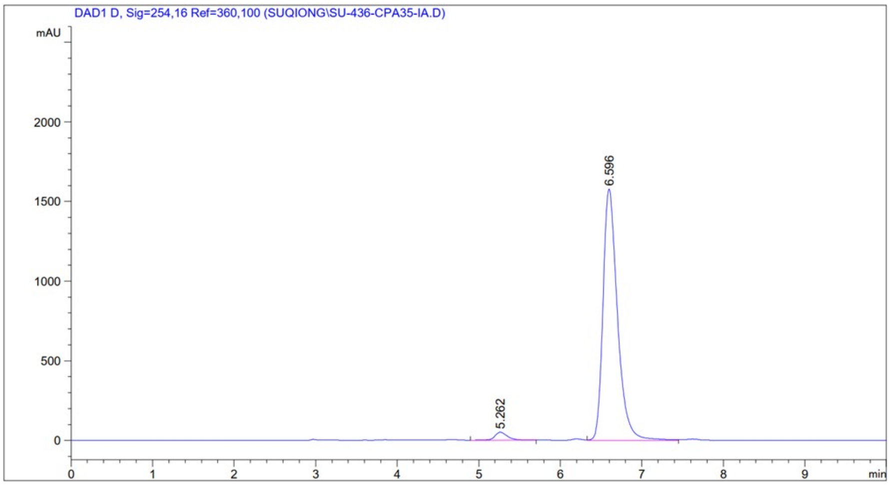
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

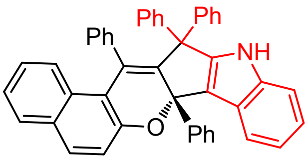
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.232	VB	0.1612	7081.91406	670.38788	50.1964
2	6.603	BB	0.1899	7026.48779	562.03778	49.8036

HPLC spectrum of the enantioenriched compound



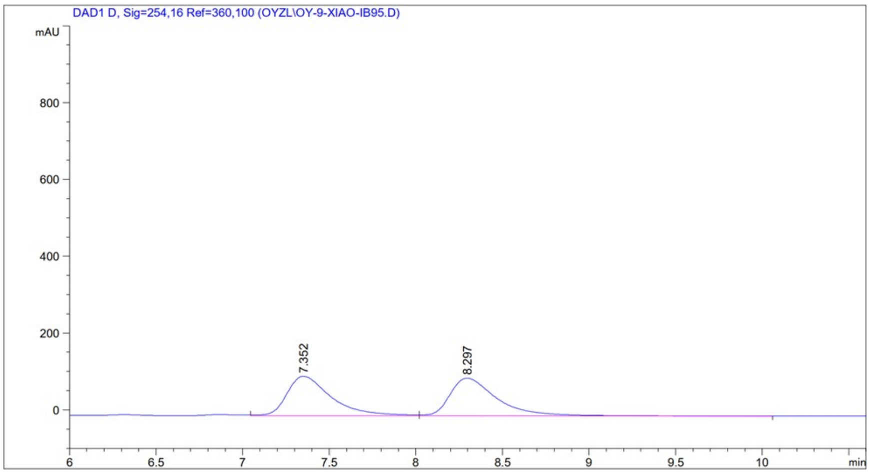
信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	5.262	BB	0.1587	522.68707	49.71313	2.6219
2	6.596	VV	0.1875	1.94128e4	1578.03247	97.3781



9

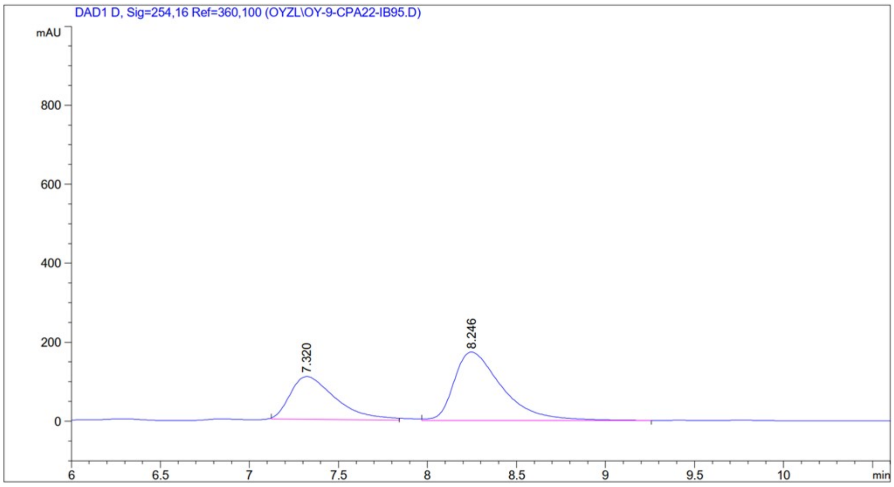
HPLC spectrum of the racemate



信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.352	VV	0.2662	1835.54102	102.84097	49.7955
2	8.297	VB	0.2821	1850.61877	98.11518	50.2045

HPLC spectrum of the enantioenriched compound



信号 1: DAD1 D, Sig=254,16 Ref=360,100

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.320	MM R	0.2942	1915.77283	108.51183	37.2603
2	8.246	VB	0.2815	3225.82251	173.03253	62.7397

9. Plausible reaction mechanism

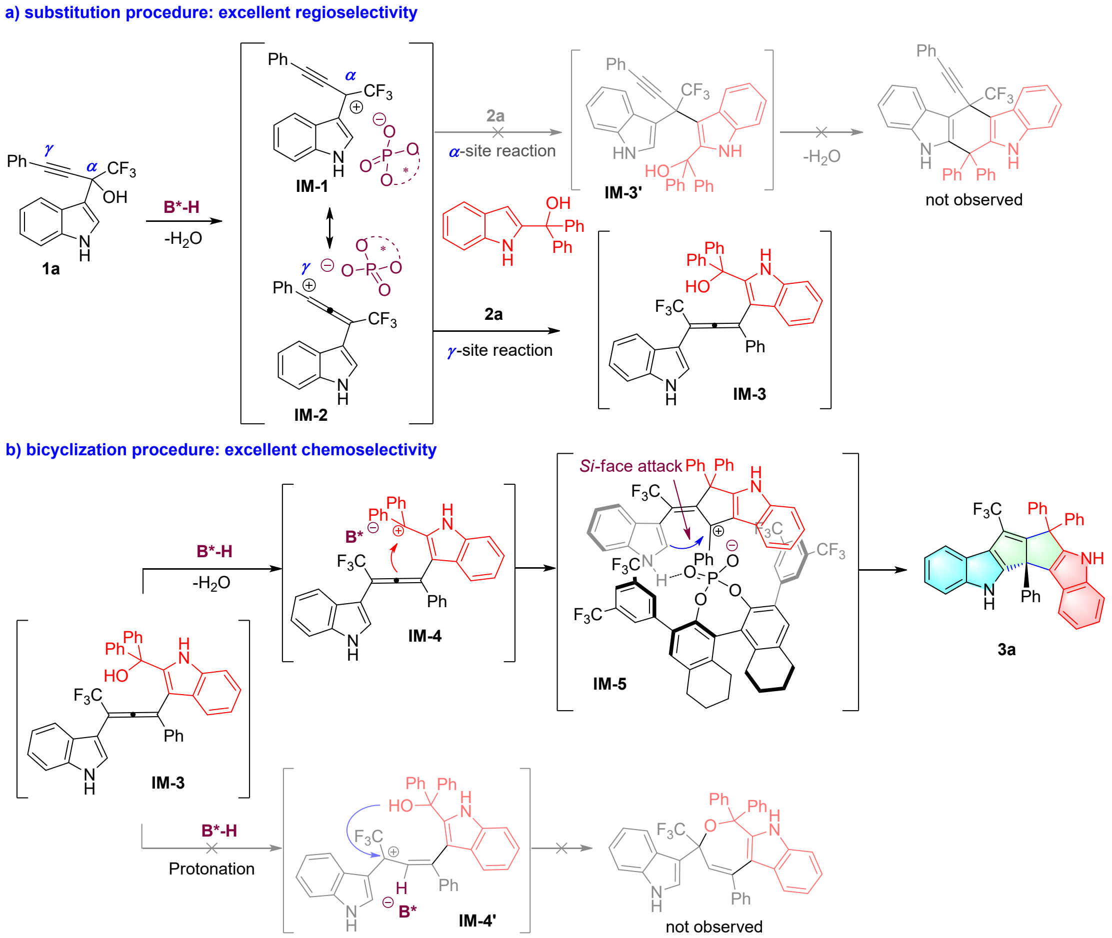


Fig. S1 Plausible reaction mechanism.

As shown in **Fig. S1a**, the excellent regioselectivity results from the nucleophilic substitution procedure of **1a** and **2a**. The dehydration of **1a** to form carbonium ion might occur at either α- or γ-position due to the influence of spatial steric hindrance and electronegativity. 2-indolylmethanol **2a**, as a sterically hindered nucleophilic reagent, tends to attack the less hindered γ-position of **1a**, resulting in the formation of allene intermediate **IM-3**.

As shown in **Fig. S1b**, the excellent chemoselectivity arises from further cyclization process of allene intermediate **IM-3**. We hypothesize that the preferential formation of intermediate **IM-4** is due to intramolecular dehydration occurring at a faster rate than its intermolecular protonation. **IM-4** then undergoes the first intramolecular cyclization to give intermediate **IM-5**. Subsequently, **IM-5** performs the second cyclization to give the desired product **3a** in the presence of catalyst (*R*)-**C1**. During the cyclization of intermediate **IM-5**, the activated C2 position of indole group attacks the indolyl benzylic cation (*Si*-face). Chiral phosphoric acid catalyst (*R*)-**C1** exerts efficient chiral induction through ion-pair and hydrogen-bonding with the corresponding carbocation and the N−H moiety in indole simultaneously, to deliver the desired cyclization product **3a** with excellent enantioselectivity.

10. Results of DFT Calculations

a. Computational Details

All reaction mechanisms were calculated with Gaussian 16 package (G16 A.03)[1]. Geometry optimization and frequency calculations were performed at the B3LYP-D3(BJ)/6-31G(d,p) level with PCM implicit solvent model (dichloromethane, ε=8.93)[2-4]. Berny algorithm was used to search transition-state structures. Transition-state structures were verified with IRC calculations. In all single point calculations, M06-2X-D3/6-311+G(d,p) level was used for all structure with SMD implicit solvent model (dichloromethane, ε=8.93) and Gibbs free energy correction was applied[5-6].

b. Computational Results

As shown in **Fig. S2**, both γ-site and α-site reactions of **IM-2** have favorable energy barrier (13.3 and 11.6 kcal/mol). However, the *γ*-site reaction is more exothermic (-12.7 kcal/mol) than *α*-site reaction (-2.1 kcal/mol), which means **IM-3** intermediate was thermodynamically favorable compared with **IM-3'** intermediate. Therefore, according to thermodynamic stability of products **IM-3** and **IM-3'**, *γ*-site reaction pathway could be more advantageous than *α*-site reaction pathway.

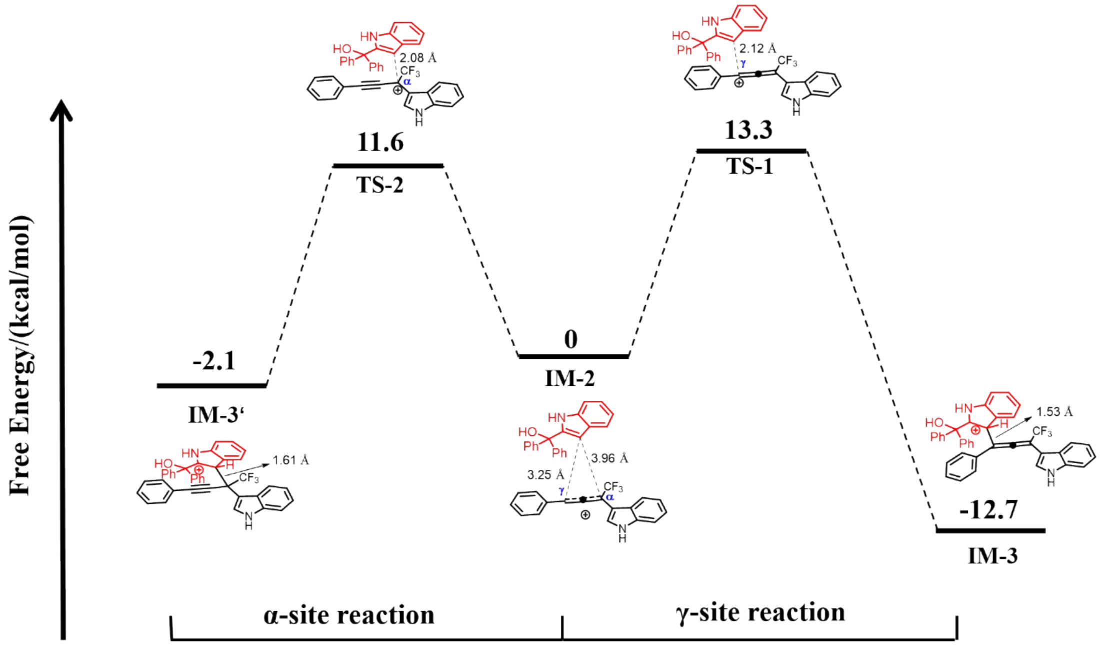


Fig. S2. Reaction energy profile of *α*-stie reaction and *γ*-site reaction for **IM-2** intermediate.

Regarding the chemoselectivity of **IM-3** (**Fig. S3**), the energy barrier of protonation reaction is 16.1 kcal/mol, which is slightly higher than the dehydration reaction (13.3 kcal/mol) with similar endothermicity (5.0 and 5.5 kcal/mol). In terms of reaction energy barrier, the dehydration reaction is more slightly advantageous. Also, the reactant energy of the protonation reaction is approximately 5.8 kcal/mol higher than that of the dehydration reaction. Therefore, both the transition state and the product energies are overall higher than those of the dehydration reaction. Furthermore, based on the distinction in the final products, the conformations of **IM-3** dehydration reaction (**IM-3** conformation **1**) and protonation reaction (**IM-3** conformation **2**) are likely different.

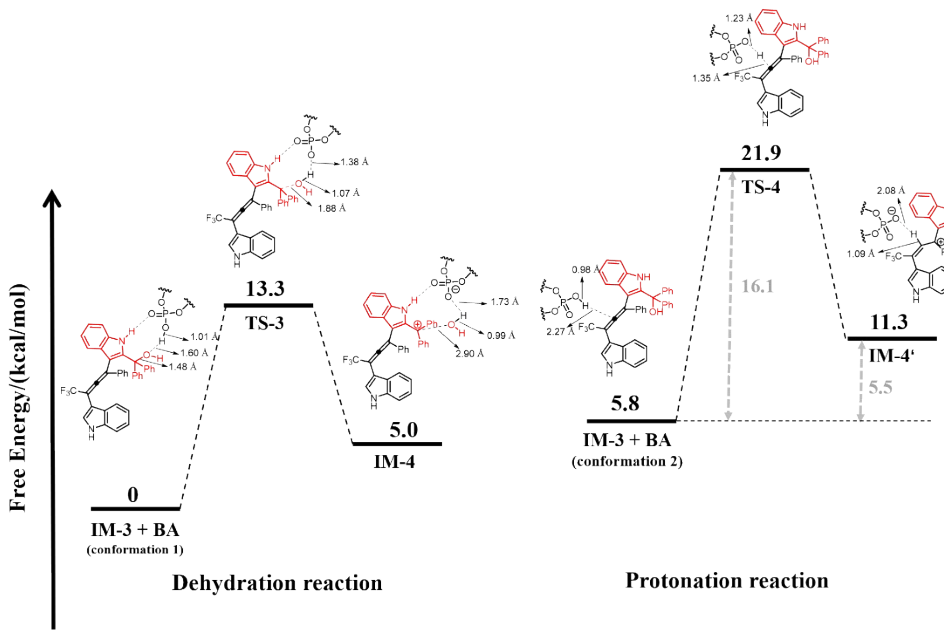


Fig. S3. Reaction energy profile of dehydration and protonation energy for **IM-3** intermediate.

As can be seen in **Fig. S4,** in **IM-3** conformation **1**, the hydroxyl group needs to be on the same side as the amino group of indole, which is beneficial for the binding to CPA, leading to subsequent dehydration reaction. In **IM-3** conformation **2**, the hydroxyl needs to attack allene carbon, leading to the hydroxyl group and the indole amino group not being on the same side. Energy calculations for both conformations reveal that the energy of **IM-3** conformation **2** is approximately 5.0 kcal/mol higher than that of **IM-3** conformation **1**. Therefore, **IM-3** conformation **1** is more advantageous. In conclusion, through the comparison of reaction energy profiles and conformation analysis, **IM-3** is more conducive to undergoing dehydration reaction to yield **IM-5**.

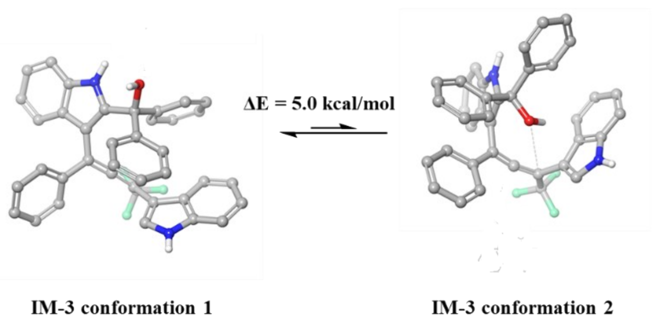


Fig. S4. Two conformations of **IM-3** intermediate. **IM-3** conformations **1** and **2** are separately pre-reaction conformations of dehydration and protonation reaction. The energy of conformation **2** is about 5.0 kcal/mol higher than conformation **1**.

c. References

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d. The cartesian coordinates of optimized structures

γ-site and α-site reaction

IM-2

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C	0.51791800	1.99918200	-0.72544000
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TS-1

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H	2.82802700	4.58573300	-2.86699200
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H	-7.68290000	-1.64245700	-0.77794100
O	2.66497900	-1.80210200	1.55319600
H	2.36133400	-1.08555100	2.13484400
H	0.35090900	0.25804100	-1.39533300

IM-3

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H	4.72163100	1.80031300	2.39836300
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H	-4.20682600	-0.05143600	-0.93990700
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C	4.01405800	0.58686700	-0.51639100
C	3.52781900	0.21139800	1.66690400
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C	3.28185100	-0.25924100	0.39519300
C	-0.80300400	1.88046300	0.38501200
C	-1.79332000	-2.18408300	-1.33021900
C	-1.33366000	-3.42508100	-1.74125900
H	-0.29322700	-3.70189500	-1.61482700
C	-1.08430700	-1.00210300	-0.70721000
C	-1.98367000	-2.31782200	1.96145600
H	-2.43581300	-2.78698300	1.09535900
C	-0.19511500	-1.30722800	0.49513600
C	0.97181400	2.87531700	1.69513100
H	1.35798800	3.18904400	2.65948400
C	-3.17781200	2.29965900	-0.31006000
C	4.12464000	0.66038200	-1.91475200
H	3.61710100	-0.06316000	-2.54231100
C	-0.29425300	2.29156600	1.61833700
H	-0.88714400	2.17173600	2.51693700
C	-0.23419700	-0.97346500	2.96342700
H	0.65088100	-0.35754800	2.84748400
C	-3.29521100	2.45412900	-1.69655400
H	-2.74457300	1.81106400	-2.37580500
C	1.10020000	-1.35248900	0.30423300
C	-2.22071400	-0.03378400	-0.47125200
C	-0.04039000	2.07823600	-0.77268300
H	-0.43376900	1.80162300	-1.74563500
C	-2.21044900	1.28247100	0.30079800
C	-4.12899400	3.43944400	-2.22539200
H	-4.21423200	3.54724000	-3.30157200
C	-3.14299000	-1.85330000	-1.48486300
C	-0.81631700	-1.15207500	4.21793900
H	-0.36631200	-0.68866600	5.08961000

C	-1.98096100	-1.91104800	4.34768200
H	-2.43812100	-2.04373300	5.32245900
C	5.46935300	2.56887500	-0.27640900
H	5.97715200	3.29594800	0.34904400
C	1.22565800	2.65203200	-0.69276900
H	1.81990700	2.77816000	-1.59096500
C	-2.56047100	-2.49222000	3.21793900
H	-3.46460300	-3.08414000	3.31353500
C	-3.89844600	3.14295600	0.54099700
H	-3.80495700	3.02322100	1.61297900
C	1.73303600	3.05690000	0.54318000
H	2.71891800	3.50187000	0.60113200
C	-4.84872400	4.27789600	-1.37428200
H	-5.49818000	5.04354200	-1.78575300
C	4.89315300	1.67368900	-2.47292100
H	4.98606200	1.74305900	-3.55211400
C	-3.60990500	-3.95166500	-2.45986500
H	-4.30195700	-4.65956800	-2.90160400
C	-4.08375200	-2.70306600	-2.04667700
H	-5.12485500	-2.42192800	-2.15389300
C	-4.73068400	4.12629300	0.00836900
H	-5.28815600	4.77441500	0.67677300
C	-2.26253500	-4.30626600	-2.30851500
H	-1.93346400	-5.28673600	-2.63455800
C	5.55983700	2.61686500	-1.66268900
H	6.15421300	3.39528200	-2.13017700
O	-2.72913100	0.92496100	1.57910200
H	-2.06016500	0.40275500	2.05381900
H	-0.44724800	-0.52872300	-1.46686200

TS-2

F	1.48439500	-2.34094600	-2.42762600
F	-0.10011400	-1.46994100	-3.61343100
F	-0.59008400	-2.81901800	-1.98830000
N	-2.05633600	2.18694700	-2.15930800
H	-2.22938200	3.17166900	-2.29447800
N	1.47021100	-0.59008100	1.83770500
H	1.82916900	0.00353700	2.57945100
C	0.24913900	-1.82501100	-2.36388400
C	-2.36631700	-0.04403100	-1.90999300
C	-0.84590400	1.65448800	-1.87471400
H	0.03887900	2.26616000	-1.82170400
C	0.18044900	-0.58432800	-1.43572400
C	3.78557200	1.10873800	-0.71720900

C	-3.02329800	1.19154000	-2.16571800
C	-0.96259500	0.27846700	-1.70402000
C	-0.79642400	1.88737000	1.34861500
C	1.12566700	-2.40612700	0.54057500
C	1.43430400	-3.67003600	0.03681500
H	0.72281900	-4.22024300	-0.56429800
C	-0.03766400	-1.49791900	0.41996900
C	4.88655200	0.27129000	-0.45012100
H	4.76505300	-0.80367800	-0.51876900
C	2.52626600	0.53942600	-1.04159400
C	0.35516500	3.82387200	0.44243000
H	1.28079600	4.31651700	0.16336200
C	-1.99265800	-0.14502500	2.44643000
C	-3.14606000	-1.21254400	-1.85764600
H	-2.69605200	-2.17784000	-1.67353600
C	0.38985300	2.53594400	0.96886300
H	1.34475700	2.04026000	1.09486700
C	3.93234300	2.50664400	-0.62916700
H	3.08319900	3.14439100	-0.84770100
C	-2.95176300	-0.38811600	1.45671700
H	-2.79363500	-0.03487400	0.44786400
C	1.44431900	0.05292500	-1.30477200
C	0.22127900	-0.46254600	1.41205400
C	-2.01262800	2.56016200	1.20634500
H	-2.93593300	2.09248300	1.52117700
C	-0.67118900	0.55936400	2.11250700
C	-4.12260700	-1.07935000	1.76002400
H	-4.85158300	-1.25552400	0.97611800
C	2.08029600	-1.75460800	1.34479400
C	5.16098100	3.05361600	-0.27455900
H	5.27199800	4.13081500	-0.20916200
C	6.24865000	2.21862400	-0.00407100
H	7.20509500	2.64944900	0.27339600
C	-4.40097100	1.29711800	-2.35069200
H	-4.87027900	2.25776700	-2.53434100
C	-2.04600500	3.84909000	0.66956100
H	-2.99884700	4.35768000	0.56561700
C	6.10908200	0.83075700	-0.09302500
H	6.95572400	0.18476800	0.11436000
C	-2.21600700	-0.61416100	3.74367300
H	-1.46833800	-0.44103100	4.50723400
C	-0.86640300	4.48410900	0.28474100
H	-0.89436800	5.48864400	-0.12450200
C	-4.34750400	-1.53769400	3.05966500

H	-5.25919400	-2.07574900	3.29867800
C	-4.52130700	-1.11432200	-2.04259600
H	-5.12593000	-2.01427800	-2.00124300
C	3.63547400	-3.51778100	1.08678200
H	4.60390700	-3.96572200	1.28017200
C	3.33985400	-2.26386900	1.62524900
H	4.04795100	-1.72197300	2.24076200
C	-3.39176100	-1.30259600	4.04800100
H	-3.55577900	-1.65874900	5.06003600
C	2.68889600	-4.21390200	0.32165400
H	2.93515400	-5.19967800	-0.05771600
C	-5.14478500	0.12369700	-2.28333300
H	-6.22015200	0.16445700	-2.41953000
O	0.06215400	0.84915200	3.31583900
H	-0.26114700	1.69590900	3.65447200
H	-1.04774300	-1.85697500	0.28237000

IM-3'

F	1.24940900	-2.08248500	-2.79856400
F	0.11246200	-0.51538200	-3.74928500
F	-0.92683100	-2.15630700	-2.76990900
N	-1.76014900	2.65925300	-1.84951200
H	-1.80961400	3.66613600	-1.85982600
N	1.18486900	-1.46085600	1.71651000
H	1.58923600	-1.18477600	2.61091700
C	0.14257400	-1.32827000	-2.68339800
C	-2.34485600	0.47585900	-1.74499900
C	-0.61652700	1.94293600	-1.63051600
H	0.33715800	2.43364000	-1.52901900
C	0.11074300	-0.49147200	-1.36405500
C	3.83685200	0.97086500	-0.52378800
C	-2.84244100	1.80336200	-1.89984000
C	-0.91574600	0.60229000	-1.54210000
C	-0.31937900	1.73729700	1.58605200
C	0.56977800	-2.72759700	-0.05329700
C	0.54206500	-3.89175100	-0.81010900
H	-0.16075000	-4.01989500	-1.62146100
C	-0.23457200	-1.43215300	-0.09876200
C	4.74094000	0.15552900	0.18193600
H	4.46967800	-0.87141600	0.40253000
C	2.56267600	0.45838500	-0.90319700
C	1.14800200	3.56183700	0.94849600
H	2.14818100	3.92599000	0.73911000
C	-1.81834700	-0.22726100	2.45025800

C	-3.26707300	-0.58872000	-1.77781700
H	-2.93869000	-1.61632900	-1.68917000
C	0.96572300	2.23368300	1.31848000
H	1.82602100	1.58320000	1.41312300
C	4.18225100	2.30380800	-0.81476600
H	3.48222700	2.92758900	-1.35959100
C	-2.86278900	-0.14622900	1.52270400
H	-2.70818600	0.33301200	0.56770000
C	1.45513300	0.04978400	-1.16751500
C	0.19896100	-0.77150400	1.21640400
C	-1.41220700	2.60344500	1.52514200
H	-2.40643500	2.25323700	1.76694900
C	-0.41073800	0.30658100	2.12285900
C	-4.11540600	-0.67811400	1.82050200
H	-4.90900800	-0.60267500	1.08499100
C	1.47444000	-2.64696000	1.00836500
C	5.41246400	2.80815600	-0.40297900
H	5.67490000	3.83634000	-0.62937100
C	6.30638400	1.99461500	0.29784300
H	7.26448000	2.39184900	0.61677800
C	-4.20209500	2.08744000	-2.05104700
H	-4.55095700	3.10926300	-2.15772800
C	-1.22718100	3.93708500	1.15431900
H	-2.08551200	4.59909800	1.10632700
C	5.96888400	0.67022800	0.58762300
H	6.66394300	0.03814200	1.13050100
C	-2.03815600	-0.86777100	3.67470400
H	-1.22802400	-0.94662700	4.38788600
C	0.04676800	4.41772400	0.85627300
H	0.18526700	5.45487000	0.56873800
C	-4.33624400	-1.30302000	3.04898800
H	-5.31113900	-1.71853300	3.28259600
C	-4.61944500	-0.30846600	-1.92553700
H	-5.33193200	-1.12674500	-1.94553000
C	2.37716300	-4.77784500	0.54014200
H	3.07295900	-5.58257800	0.74878400
C	2.39575400	-3.62878000	1.33500500
H	3.07414800	-3.51865900	2.17282900
C	-3.29482200	-1.39512400	3.97294600
H	-3.45567200	-1.88313400	4.92876100
C	1.45327700	-4.90990000	-0.50140500
H	1.43619700	-5.82429400	-1.08411600
C	-5.08523600	1.01512500	-2.05668000
H	-6.14853100	1.19914900	-2.16935200

O	0.41486900	0.24429800	3.29479500
H	0.35906800	1.10035600	3.74138900
H	-1.31179100	-1.60241000	-0.09568200

Dehydration and protonation reaction

IM-3

F	5.43377100	-2.19958600	-2.10410100
F	6.97235000	-0.66842900	-2.02218200
F	5.42715700	-0.56886900	-3.54549500
N	5.99728600	3.44568600	-1.32353700
H	6.72049800	4.14752600	-1.30588700
N	-0.47952600	-1.94873500	-0.21681400
H	-1.48290900	-1.76243000	-0.15957000
C	5.64690500	-0.87434500	-2.24672100
C	3.98291400	2.43210700	-1.39861000
C	6.22000000	2.08780600	-1.31932700
H	7.22283800	1.69295400	-1.28429400
C	4.80045900	-0.03686500	-1.32045500
C	3.68487500	-1.73820600	1.59893900
C	4.63996300	3.69364000	-1.37038000
C	5.01201700	1.42135900	-1.35555200
C	1.24706600	0.44835900	2.15118200
C	1.48360600	-2.70102100	-1.02586800
C	2.30367900	-3.53206700	-1.80771300
H	3.38092100	-3.41340100	-1.78662600
C	1.74964100	-1.63281300	-0.09182500
C	4.84866000	-1.17570200	2.14144800
H	5.32877500	-0.35039800	1.62676400
C	3.13038600	-1.25215200	0.30278100
C	2.52396500	0.25756600	4.20534600
H	2.71479700	-0.25572100	5.14133500
C	-0.52785500	1.10862500	0.44949100
C	2.58285300	2.39269200	-1.49291700
H	2.06214900	1.44158600	-1.53246600
C	1.50608300	-0.19546800	3.36795000
H	0.93142500	-1.06877300	3.65598500
C	3.05734400	-2.78887600	2.28184000
H	2.15655800	-3.22758200	1.86795600
C	-0.73625400	1.03400500	-0.93056200
H	-0.39394600	0.17139200	-1.48720100
C	3.92271300	-0.63135300	-0.54394500
C	0.51716600	-1.19499800	0.37484200
C	2.05013200	1.52639000	1.76950900
H	1.86802800	2.03111000	0.83084700

C	0.10694100	-0.03625800	1.25642100
C	-1.39210300	2.06632300	-1.60597000
H	-1.55256300	1.98636900	-2.67598500
C	0.07421800	-2.86475400	-1.07826700
C	3.57964100	-3.26238200	3.48406400
H	3.08198000	-4.07704600	4.00140500
C	4.73478000	-2.69253700	4.02134300
H	5.13865400	-3.05746300	4.96066700
C	3.93581200	4.90188200	-1.39988500
H	4.45325100	5.85562700	-1.37134400
C	3.08691000	1.96018600	2.59290900
H	3.70666200	2.79211300	2.27343300
C	5.36839800	-1.64881800	3.34219200
H	6.26324500	-1.19417900	3.75631600
C	-0.97309600	2.24606500	1.13901500
H	-0.80986200	2.32544400	2.20874600
C	3.31888200	1.33532400	3.81888000
H	4.12254100	1.67766300	4.46307700
C	-1.82938300	3.19311800	-0.91314600
H	-2.33347200	3.99726900	-1.43956800
C	1.87944900	3.59044900	-1.52476800
H	0.79794700	3.57082400	-1.58604200
C	0.29592100	-4.62502400	-2.66606000
H	-0.14138900	-5.37537900	-3.31758300
C	-0.53708400	-3.82122800	-1.89757200
H	-1.61713500	-3.92077800	-1.92904300
C	-1.61019100	3.28322800	0.46458600
H	-1.93826400	4.16038300	1.01359000
C	1.70097900	-4.48346100	-2.62020900
H	2.31781900	-5.12992500	-3.23698700
C	2.54928400	4.83087100	-1.47116500
H	1.97020800	5.74886800	-1.49255700
O	-0.96511600	-0.56760900	2.12776900
H	-0.85347300	-0.16076200	3.00100300
P	-4.08531100	-0.58598600	0.32968800
O	-3.47572000	-0.04385900	1.67402200
O	-3.21895200	-1.46102300	-0.50141000
O	-5.46071800	-1.24234300	0.87319700
O	-4.60235900	0.67409900	-0.53858000
C	-6.51886900	-1.46628000	-0.01842300
C	-7.28423500	-0.38036600	-0.46982500
C	-6.81895200	-2.78000400	-0.35784200
C	-8.38911800	-0.66976100	-1.28659700
C	-7.92186600	-3.03835000	-1.17062100

C	-8.70766900	-1.98049900	-1.63313700
H	-8.98831300	0.15235500	-1.66349900
H	-8.16292900	-4.06078700	-1.44127800
H	-9.56338400	-2.17549200	-2.27081100
C	-5.64368400	1.49234000	-0.08073500
C	-6.96165300	1.01065100	-0.08421200
C	-5.32954000	2.79501500	0.28608700
C	-7.97413300	1.91013200	0.28751100
C	-6.35470500	3.66607300	0.65155400
C	-7.67894700	3.22256100	0.64809800
H	-9.00043100	1.55907200	0.30940400
H	-6.11770800	4.68514100	0.93870400
H	-8.48040900	3.89451100	0.93637500
H	-6.19353700	-3.57816100	0.02531800
H	-4.29210300	3.10395800	0.26953200
H	-2.49154500	-0.23597900	1.78136300

TS-3

F	4.77292000	-1.25041100	-2.97822400
F	6.21888900	0.36275800	-2.75728200
F	4.26787000	0.76910600	-3.62288000
N	5.16959400	3.67318000	0.14283900
H	5.75366400	4.30159900	0.67159700
N	-0.40194400	-1.87739500	-0.37636800
H	-1.40205000	-1.60828600	-0.34900000
C	4.90355200	0.05307200	-2.66246700
C	3.48472500	2.83627600	-1.10513600
C	5.45465100	2.34843400	-0.10341300
H	6.35149200	1.89129700	0.28674700
C	4.35607600	0.38413000	-1.29795500
C	4.05418900	-2.28876800	1.14429400
C	3.96394600	4.00304700	-0.44684000
C	4.44940000	1.79540600	-0.86184200
C	1.53872500	0.52062400	1.79489700
C	1.47922200	-3.01567100	-0.88648800
C	2.21677300	-4.05433100	-1.48741700
H	3.29866600	-4.07649000	-1.40609900
C	1.84692600	-1.86696900	-0.11225200
C	5.38610900	-1.94755200	1.42852000
H	5.84803700	-1.12107300	0.89818200
C	3.26509800	-1.50938300	0.15467100
C	3.12269000	0.00955900	3.56026100
H	3.52430900	-0.69367200	4.28178700
C	-0.38744000	1.11430200	0.22376600

C	2.25119600	2.88002500	-1.77306900
H	1.87016400	1.99738200	-2.27508700
C	2.06084900	-0.37035100	2.74906400
H	1.63103000	-1.35973500	2.84364100
C	3.46501000	-3.35104700	1.84334100
H	2.43723600	-3.62392400	1.63380400
C	-0.67911500	1.03132200	-1.14567400
H	-0.30927200	0.19805300	-1.72814000
C	3.80815700	-0.55944000	-0.57360200
C	0.65975700	-1.18777700	0.18271800
C	2.09327600	1.80303800	1.67820900
H	1.71883500	2.49071500	0.93312500
C	0.43318200	0.06908300	0.90135100
C	-1.43419100	2.02312400	-1.76780700
H	-1.65560700	1.94101700	-2.82630600
C	0.06255300	-2.99250500	-1.01635500
C	4.18829700	-4.05103900	2.80908200
H	3.71522800	-4.86935900	3.34288600
C	5.50885900	-3.70136500	3.08961600
H	6.07023700	-4.24350400	3.84390100
C	3.23909900	5.19892200	-0.43468900
H	3.61381600	6.07975000	0.07708500
C	3.16264500	2.17632400	2.48944400
H	3.59821000	3.16155300	2.37068400
C	6.10540000	-2.64630400	2.39142200
H	7.13259200	-2.36579600	2.60312000
C	-0.86182900	2.21914300	0.95239300
H	-0.65577400	2.29160500	2.01397500
C	3.68025500	1.28380400	3.42766200
H	4.51668800	1.57781300	4.05382400
C	-1.89595800	3.11496200	-1.03609800
H	-2.48413500	3.88670700	-1.52187900
C	1.52767100	4.06510100	-1.75984500
H	0.56521100	4.10897200	-2.25630900
C	0.11466500	-5.00370000	-2.28674400
H	-0.38971700	-5.79121200	-2.83794800
C	-0.63638500	-3.98925200	-1.71333500
H	-1.71700800	-3.95325600	-1.79864300
C	-1.60036200	3.21434400	0.32645200
H	-1.95361100	4.06344000	0.90225400
C	1.52731400	-5.03716900	-2.17744300
H	2.07319200	-5.84930200	-2.64679800
C	2.01611400	5.21095400	-1.09689300
H	1.42413700	6.12077700	-1.10238500

O	-0.76857200	-0.55967800	2.20145500
H	-0.56505200	-0.04937300	3.00114400
P	-3.81104400	-0.54042300	0.43899800
O	-3.11732300	-0.05956800	1.70140200
O	-3.04963200	-1.33923400	-0.57697700
O	-5.14586200	-1.32969200	0.98364200
O	-4.49527500	0.71846500	-0.35874600
C	-6.21129300	-1.57351100	0.12554000
C	-7.07789600	-0.52355600	-0.22413300
C	-6.43814800	-2.88058700	-0.29575900
C	-8.19720600	-0.84020500	-1.01020100
C	-7.55635700	-3.16830000	-1.07700100
C	-8.43870500	-2.14552400	-1.43229600
H	-8.87091300	-0.04174800	-1.30398400
H	-7.73538300	-4.18642500	-1.40701200
H	-9.30779400	-2.36230700	-2.04470900
C	-5.54894900	1.42918000	0.20214600
C	-6.83404900	0.86067500	0.23700800
C	-5.31276600	2.73017200	0.63647600
C	-7.88481600	1.66060600	0.71378100
C	-6.37335100	3.50292000	1.10676700
C	-7.66285700	2.96749800	1.14181700
H	-8.88221900	1.23582400	0.76304400
H	-6.19159500	4.51781500	1.44553600
H	-8.49182000	3.56206000	1.51156200
H	-5.73948400	-3.65373600	0.00374700
H	-4.30183100	3.11535900	0.58911400
H	-1.78940300	-0.34255500	1.94686800

IM-4

F	-4.60619600	1.21389700	-3.18742300
F	-6.02017200	-0.43774500	-3.06936600
F	-3.98219900	-0.80222800	-3.72925900
N	-5.13574000	-3.60634700	0.10973900
H	-5.70507200	-4.20777800	0.68399800
N	0.32625100	1.60103300	-0.37638100
H	1.31750800	1.26452200	-0.30848900
C	-4.73161600	-0.08537900	-2.85526600
C	-3.46486200	-2.82136500	-1.18956700
C	-5.41205900	-2.28645400	-0.16498200
H	-6.29519000	-1.80815200	0.23089000
C	-4.31321100	-0.36857400	-1.43424400
C	-4.22569300	2.37611000	0.96428600
C	-3.94160700	-3.96276800	-0.48648300

C	-4.41902000	-1.76619200	-0.96202700
C	-1.74984000	-0.77559700	1.60019000
C	-1.39417900	3.06375400	-0.58170800
C	-1.97374200	4.30074700	-0.96090800
H	-3.04140700	4.45946000	-0.86035600
C	-1.91743600	1.86130300	-0.05490800
C	-5.62305700	2.24281100	0.92427500
H	-6.07253600	1.56352000	0.20696800
C	-3.36348200	1.56150900	0.07050000
C	-3.23978500	-0.25599900	3.44638500
H	-3.63532400	0.46004000	4.15863500
C	0.27097200	-1.26703900	0.18435400
C	-2.22980600	-2.88664200	-1.85239100
H	-1.85463200	-2.02432000	-2.39221400
C	-2.27350100	0.14292000	2.53544600
H	-1.86820600	1.14444600	2.56494900
C	-3.65659900	3.26349000	1.88909400
H	-2.57999600	3.38254800	1.92942200
C	0.74252100	-1.24203600	-1.14635300
H	0.33969900	-0.51641000	-1.84169300
C	-3.84637700	0.59926100	-0.68694100
C	-0.81574900	0.96243400	0.08977800
C	-2.18373600	-2.11767400	1.64309400
H	-1.79398000	-2.82887500	0.92815900
C	-0.76565400	-0.34386900	0.62073800
C	1.67831800	-2.17014900	-1.57823700
H	2.02370400	-2.14886700	-2.60575900
C	0.01736200	2.86730400	-0.74308900
C	-4.46585100	3.99483600	2.75804600
H	-4.00829100	4.67554800	3.46881000
C	-5.85238000	3.85122400	2.71592100
H	-6.48165500	4.42013200	3.39278600
C	-3.20994500	-5.15253000	-0.42212400
H	-3.58005500	-6.01280800	0.12643900
C	-3.14969600	-2.51085600	2.56099700
H	-3.49377200	-3.53859500	2.56663700
C	-6.42745100	2.97187700	1.79313300
H	-7.50596900	2.85724900	1.74952600
C	0.79068100	-2.23340100	1.07143400
H	0.47373400	-2.22626600	2.10644500
C	-3.68770900	-1.58157700	3.45451500
H	-4.44441400	-1.89199800	4.16809600
C	2.17162300	-3.12980800	-0.69120600
H	2.90895700	-3.84994700	-1.03023300

C	-1.49504200	-4.06284500	-1.78044700
H	-0.52551200	-4.11840400	-2.26341100
C	0.26288400	5.08306800	-1.56238000
H	0.87617700	5.89422500	-1.94160000
C	0.86105800	3.88690600	-1.22162900
H	1.92720900	3.71750200	-1.31752800
C	1.72982100	-3.15609400	0.63433000
H	2.12862400	-3.88832600	1.32818300
C	-1.14352600	5.28947400	-1.43856700
H	-1.55771800	6.24950900	-1.72749800
C	-1.98022200	-5.18276900	-1.07236900
H	-1.38072800	-6.08664600	-1.03224800
O	0.77270100	0.77898100	2.81003800
H	0.58523300	0.10601400	3.47526600
P	3.77505900	0.45110700	0.57186200
O	3.22142700	0.03561900	1.90277100
O	2.91334500	1.10717500	-0.47709000
O	5.09210900	1.39799000	0.90665000
O	4.51668700	-0.80725200	-0.20145500
C	6.03522400	1.65418300	-0.07325800
C	6.96305400	0.65786300	-0.42806100
C	6.09488800	2.93179000	-0.62510400
C	7.96483800	0.99817300	-1.35066500
C	7.09832100	3.24443100	-1.54092000
C	8.03723000	2.27539100	-1.90230500
H	8.68120700	0.23831100	-1.64653200
H	7.14507700	4.24007800	-1.97039900
H	8.81780700	2.51082800	-2.61844500
C	5.67239500	-1.37002800	0.30946600
C	6.89844800	-0.69479600	0.16751900
C	5.60481800	-2.64184600	0.87381600
C	8.06040400	-1.35510000	0.59686400
C	6.77306000	-3.27550800	1.29452900
C	8.00444800	-2.63195800	1.15144400
H	9.01376100	-0.84401200	0.50764900
H	6.72043600	-4.26662400	1.73381600
H	8.91694000	-3.11781800	1.48140400
H	5.35773400	3.66509300	-0.31733600
H	4.63526200	-3.11604000	0.96647700
H	1.66568200	0.53599600	2.47078800

IM-3’

F	1.49212000	-3.15530400	0.95052700
F	1.42279100	-4.29496900	-0.90714100

F	0.08354700	-4.79651600	0.72469700
N	-2.41800500	-4.43978200	-3.08953500
H	-2.54796900	-5.01596500	-3.90650000
N	-3.26465800	0.92025800	2.38229400
H	-4.15560200	1.35456200	2.57346700
C	0.65574200	-3.76077400	0.07076400
C	-2.80550200	-3.08424500	-1.32911400
C	-1.20877800	-4.21146200	-2.47364600
H	-0.29973100	-4.64946200	-2.85545600
C	-0.37923100	-2.82025800	-0.48332600
C	0.00822400	0.76904100	-0.76960800
C	-3.41747700	-3.76283600	-2.41836700
C	-1.39533800	-3.37793700	-1.39058300
C	-4.79712500	1.85444000	0.14235700
C	-1.45414200	-0.41219600	2.54219400
C	-0.56291500	-1.27331600	3.20549400
H	0.27175500	-1.72444600	2.68060800
C	-1.53852800	0.10267200	1.19533900
C	0.22317900	0.53853600	-2.13407400
H	-0.10188100	-0.39944600	-2.57090700
C	-0.64132100	-0.26907600	0.07810500
C	-7.09528600	1.27966900	-0.38629600
H	-7.79844800	0.68847100	-0.96496800
C	-2.60859200	2.98551800	-0.29411500
C	-3.60789800	-2.35322900	-0.43566100
H	-3.16818300	-1.87807600	0.43534500
C	-5.72468600	1.10650600	-0.58753000
H	-5.37956800	0.39679700	-1.32747300
C	0.43020600	1.97540600	-0.20035500
H	0.27096000	2.14776200	0.85724600
C	-2.10218200	3.73784400	0.76934600
H	-2.12395700	3.33495400	1.77663900
C	-0.40793200	-1.55290600	-0.13721100
C	-2.67476100	0.90027000	1.13462500
C	-5.27228800	2.80747200	1.05529000
H	-4.57355100	3.44323000	1.58886900
C	-3.28089700	1.62785000	-0.05938000
C	-1.53894800	4.99360800	0.54195200
H	-1.14380800	5.56395200	1.37693300
C	-2.55207000	0.13158600	3.26198500
C	1.04485700	2.94607200	-0.98643800
H	1.35730200	3.88199300	-0.53669900
C	1.23744300	2.72188600	-2.34937500
H	1.70139400	3.48577900	-2.96587500

C	-4.79418800	-3.69596600	-2.65522100
H	-5.24585500	-4.21413800	-3.49498100
C	-6.64154300	2.97485900	1.26332100
H	-6.98801500	3.71586600	1.97692200
C	0.82955300	1.51340100	-2.92098600
H	0.97763200	1.33448300	-3.98147200
C	-2.54862100	3.50616400	-1.58923000
H	-2.93513700	2.91997500	-2.41397000
C	-7.55998100	2.20656800	0.54614700
H	-8.62560000	2.33930200	0.70348600
C	-1.46861000	5.50454000	-0.75385900
H	-1.02109000	6.47699700	-0.93430200
C	-4.97919100	-2.29405600	-0.66439200
H	-5.61221900	-1.74139300	0.02140400
C	-1.87939900	-1.00439900	5.24285700
H	-2.02429300	-1.25040900	6.28996500
C	-2.77865700	-0.15291300	4.61187100
H	-3.62431800	0.27249700	5.14229500
C	-1.97314600	4.75461000	-1.81799300
H	-1.91723200	5.14186000	-2.83081400
C	-0.78402200	-1.55788600	4.54661200
H	-0.10487300	-2.22307400	5.07039400
C	-5.56285000	-2.94725200	-1.77033400
H	-6.63453700	-2.87574900	-1.92557300
O	-3.04253900	0.84632300	-1.22756600
H	-3.29296200	-0.07272300	-1.03844000
P	3.32478100	-0.65060200	-0.25094800
O	2.39039500	-0.46011300	1.02616900
O	2.78696900	-1.42775000	-1.38409200
O	3.74979200	0.88826300	-0.51664100
O	4.69426700	-1.30261500	0.31666100
C	4.91602600	1.16400000	-1.23759400
C	6.16237500	1.00559100	-0.61257100
C	4.78732000	1.66544800	-2.52729000
C	7.29953600	1.38677700	-1.34276500
C	5.93363900	2.03537700	-3.22935100
C	7.18983800	1.89726400	-2.63415600
H	8.27741800	1.26003800	-0.89021800
H	5.84446600	2.42775000	-4.23692800
H	8.08494300	2.17838400	-3.17899600
C	5.51867400	-0.61215300	1.21153800
C	6.27542300	0.48390200	0.76731400
C	5.61926400	-1.10587000	2.50716900
C	7.16000300	1.06805800	1.68855100

C	6.50494500	-0.50590900	3.40083900
C	7.27830800	0.58119100	2.98791200
H	7.74403600	1.92733200	1.37608100
H	6.58805200	-0.88629100	4.41341700
H	7.96562500	1.05594900	3.68014400
H	3.79456400	1.76758000	-2.94881600
H	5.01111800	-1.95696100	2.79160400
H	1.48859200	-0.79236000	0.84890700

TS-4

F	1.67369600	-3.76568400	-0.42335000
F	1.04294400	-3.90242000	-2.50353500
F	-0.10159200	-4.90237400	-0.95121200
N	-2.95740700	-2.55913700	-3.60371400
H	-3.29389700	-2.58229400	-4.55362000
N	-3.08711600	0.32297500	2.43106800
H	-4.00852100	0.66138800	2.67695100
C	0.59378900	-3.77009000	-1.22774100
C	-2.87418900	-2.45216500	-1.35071200
C	-1.63299300	-2.63283100	-3.23456400
H	-0.85461600	-2.72509700	-3.97623900
C	-0.27707000	-2.55324300	-1.07345300
C	0.02596900	0.85968700	-0.74804300
C	-3.74618400	-2.45104300	-2.47822400
C	-1.52683400	-2.55922600	-1.86195900
C	-4.68306400	1.62110700	0.50451300
C	-1.26337000	-0.99903500	2.33819600
C	-0.36645700	-1.96562100	2.81735400
H	0.50364200	-2.25258800	2.23869700
C	-1.30946300	-0.16007000	1.14934300
C	0.23241900	0.76372500	-2.13577700
H	-0.01291800	-0.15967900	-2.64619700
C	-0.45987500	-0.29453000	0.00631800
C	-6.98450800	1.07335300	-0.02617900
H	-7.69638200	0.56573700	-0.66959000
C	-2.58170500	2.89704100	0.09819000
C	-3.43129300	-2.40382700	-0.05858200
H	-2.78939900	-2.43610000	0.81349800
C	-5.62064800	0.98098300	-0.30809200
H	-5.29172800	0.41509700	-1.16843200
C	0.36803100	2.04256600	-0.07248600
H	0.25296400	2.09058800	1.00245200
C	-2.08583800	3.55703300	1.22602300
H	-2.04210600	3.04405000	2.18173300

C	0.10621100	-1.54275700	-0.29002600
C	-2.47331400	0.63332900	1.25841700
C	-5.13924100	2.38442000	1.59014100
H	-4.43521500	2.93801300	2.20247400
C	-3.17281100	1.48921400	0.19666100
C	-1.61069400	4.86438500	1.12620700
H	-1.22056800	5.36280600	2.00794100
C	-2.38042900	-0.64545700	3.13071600
C	0.88437600	3.12378000	-0.77714400
H	1.15084300	4.03255300	-0.25072400
C	1.03250200	3.04169600	-2.16183400
H	1.41273800	3.89453000	-2.71562400
C	-5.13779500	-2.37987000	-2.34372800
H	-5.78589200	-2.37942200	-3.21415200
C	-6.50160200	2.46819600	1.87750300
H	-6.83455000	3.06025000	2.72401300
C	0.70706700	1.86128200	-2.84071300
H	0.83582800	1.79933000	-3.91604700
C	-2.60359500	3.55936700	-1.13119100
H	-2.98269100	3.04406100	-2.00477900
C	-7.43066600	1.80822400	1.07124100
H	-8.49122800	1.87669600	1.29103200
C	-1.62287600	5.52009400	-0.10510500
H	-1.24534900	6.53444000	-0.18684600
C	-4.81196600	-2.33316800	0.07564600
H	-5.25029800	-2.28591000	1.06697400
C	-1.74909300	-2.19074600	4.81843200
H	-1.91866800	-2.67184900	5.77595300
C	-2.64418000	-1.22405700	4.37241800
H	-3.50726900	-0.93064200	4.96014200
C	-2.11851700	4.86188800	-1.23225000
H	-2.12583000	5.36328000	-2.19505900
C	-0.62388000	-2.55223500	4.05161700
H	0.05573700	-3.30730000	4.43266300
C	-5.65579900	-2.32029300	-1.05523000
H	-6.72990600	-2.25660500	-0.91595100
O	-2.97238800	0.86102700	-1.06470800
H	-3.19008000	-0.08155800	-0.97567500
P	3.46767300	-0.79389000	-0.52372700
O	2.50326100	-1.21348500	0.60877400
O	3.15312400	-1.12492200	-1.93525700
O	3.68465200	0.80962200	-0.23372600
O	4.95251100	-1.38399500	-0.14830900
C	4.80551800	1.46025100	-0.73202900

C	6.05098200	1.27116700	-0.10857300
C	4.64267100	2.35169500	-1.78832600
C	7.13439000	2.02978800	-0.57947800
C	5.73515700	3.09158300	-2.23815400
C	6.98247300	2.93235100	-1.62976400
H	8.10828700	1.88874200	-0.12185300
H	5.61184100	3.78783700	-3.06149100
H	7.83751200	3.50177300	-1.97925500
C	5.62417200	-0.95343400	0.98948000
C	6.21032500	0.32403300	1.01666100
C	5.77016500	-1.84782000	2.04587900
C	6.96720500	0.66602900	2.14872200
C	6.52524600	-1.48276800	3.15930600
C	7.12777800	-0.22364600	3.20838800
H	7.41617300	1.65289600	2.19631300
H	6.64076600	-2.17892500	3.98367500
H	7.71300100	0.06855700	4.07415300
H	3.65899600	2.45606800	-2.22928200
H	5.29730400	-2.82065900	1.97291000
H	1.36435800	-1.46226500	0.20425000

IM-4'

F	0.25337800	-4.32736200	-1.84337700
F	-1.52565000	-4.18838400	-3.08779800
F	-1.70866500	-4.71990500	-0.98642600
N	-4.39847500	-0.86605300	-2.30104900
H	-5.00363700	-0.38460600	-2.94886400
N	-2.57941700	0.59925100	1.91794400
H	-3.36350800	1.13952400	2.26433200
C	-1.03134300	-3.92812100	-1.85676600
C	-3.69307500	-2.21829300	-0.63003900
C	-3.07037100	-1.15757600	-2.53688200
H	-2.56945400	-0.79412700	-3.42210600
C	-1.20856500	-2.47950300	-1.47828400
C	0.47964400	0.68387200	-1.34697000
C	-4.80831100	-1.49842800	-1.14052600
C	-2.59117400	-1.97141700	-1.53073700
C	-3.83850000	2.48590900	0.33634700
C	-1.20208400	-1.14356000	1.55517900
C	-0.57016200	-2.35026400	1.87862200
H	0.22533500	-2.73642500	1.25699200
C	-1.03085400	-0.16365400	0.48106900
C	0.72673300	0.60673200	-2.73433500
H	0.35112200	-0.23981900	-3.29800400

C	-0.23517600	-0.36817100	-0.66883400
C	-6.22212700	2.31648600	-0.07692500
H	-7.03787500	1.96502300	-0.70071100
C	-1.49360300	3.34547000	0.15741400
C	-3.82974600	-2.93001400	0.57387400
H	-2.99156900	-3.47953400	0.98319700
C	-4.90581700	2.04260000	-0.44789600
H	-4.71098800	1.49197900	-1.35743000
C	1.00430400	1.76391000	-0.61124900
H	0.91340600	1.75360800	0.46453200
C	-0.79837300	3.56110100	1.34966000
H	-0.83920800	2.82632400	2.14745400
C	-0.12562600	-1.73707900	-1.19006100
C	-1.92456800	0.91256600	0.78109800
C	-4.11329400	3.22990900	1.49317600
H	-3.29944800	3.62064000	2.09439500
C	-2.38460800	2.11875600	-0.04913600
C	-0.01788400	4.70660100	1.51240100
H	0.52811100	4.85629700	2.43817600
C	-2.16637900	-0.62271900	2.43926600
C	1.70231400	2.77604100	-1.25383500
H	2.10332100	3.60158600	-0.67792000
C	1.88869000	2.72041900	-2.63531800
H	2.43069300	3.51400400	-3.13987000
C	-6.04011900	-1.46235500	-0.47997400
H	-6.87524200	-0.89582200	-0.87764700
C	-5.43077400	3.49580900	1.86930500
H	-5.62415100	4.07206000	2.76836800
C	1.40803200	1.63028900	-3.37474700
H	1.57294200	1.58503200	-4.44587700
C	-1.42090900	4.29684400	-0.86350100
H	-1.96052100	4.12715500	-1.78715200
C	-6.49074500	3.03683500	1.08674200
H	-7.51520200	3.24688500	1.37636600
C	0.06821700	5.64592400	0.48478900
H	0.68069900	6.53348200	0.60724500
C	-5.05213700	-2.89963900	1.22900300
H	-5.16872300	-3.43765300	2.16409000
C	-1.97588100	-2.49923600	3.87246200
H	-2.26794800	-3.05054500	4.75995200
C	-2.57981000	-1.27587500	3.59754900
H	-3.33023800	-0.84793200	4.25253300
C	-0.63811500	5.43777900	-0.70214300
H	-0.57637200	6.16429900	-1.50627700

C	-0.97567100	-3.01971600	3.02984200
H	-0.50542800	-3.96297800	3.28743200
C	-6.14462100	-2.17301600	0.70939900
H	-7.08521000	-2.16597800	1.25086800
O	-2.30069900	1.77716400	-1.42648200
H	-2.66778200	0.88855900	-1.55384600
P	3.12784700	-1.18336600	-0.09089300
O	1.99024800	-0.98263700	0.86771400
O	2.95850600	-1.93771700	-1.37636300
O	3.75383400	0.33579700	-0.35740700
O	4.43967300	-1.87747600	0.67146900
C	5.00632500	0.48826700	-0.91139200
C	6.14708300	0.29481800	-0.11027600
C	5.11248500	0.91775700	-2.23302800
C	7.40071500	0.56758600	-0.67958500
C	6.36932900	1.18001400	-2.77625600
C	7.51593800	1.00818100	-1.99659400
H	8.29206700	0.41097200	-0.08009400
H	6.45263900	1.51519200	-3.80544400
H	8.49718600	1.20562000	-2.41616800
C	5.13680500	-1.19591100	1.64784400
C	6.02030600	-0.15796900	1.29232500
C	5.01726100	-1.61883800	2.97098700
C	6.78851900	0.42537800	2.31228900
C	5.78937700	-1.02174300	3.96604500
C	6.68091200	0.00135100	3.63496900
H	7.46431200	1.23548700	2.05635500
H	5.69388800	-1.35426700	4.99492500
H	7.28219000	0.47396600	4.40498600
H	4.20293800	1.04937500	-2.80725300
H	4.32355400	-2.42143500	3.19610800
H	0.88615600	-2.11266700	-1.34975800

IM-3 conformation 1

F	0.11238800	0.19465700	-3.31429200
F	-0.84422500	2.14748500	-3.38983000
F	-2.05432600	0.35075600	-3.22009200
N	-3.32834400	2.74822500	0.76323900
H	-3.61099300	3.49604100	1.37659800
N	2.53298600	-2.62128600	0.84001500
H	2.34295900	-3.48108800	1.33278900
C	-0.90307400	0.92396400	-2.80051900
C	-3.32620400	0.83875100	-0.44724900
C	-2.08475600	2.62260600	0.19420700

H	-1.31347000	3.35923400	0.36192000
C	-0.83258000	1.03517300	-1.29607700
C	2.34359900	2.03227700	-0.07036200
C	-4.11083300	1.66818600	0.40280200
C	-2.03459500	1.47541400	-0.56714600
C	-0.38327600	-0.69983500	2.06131700
C	3.52661700	-0.89822700	-0.21258600
C	4.58281800	-0.26334500	-0.88961700
H	4.46456400	0.74364100	-1.27269500
C	2.17104600	-0.51501300	0.13520500
C	2.15003800	3.12209000	-0.93303600
H	1.44669800	3.02954300	-1.75483700
C	1.55683100	0.77348700	-0.23851900
C	-0.07033800	1.15259400	3.60578300
H	0.59865900	1.79242700	4.17297600
C	-0.67459100	-2.51142000	0.24624500
C	-3.87103800	-0.37170900	-0.90566500
H	-3.28603300	-1.03287100	-1.53161900
C	0.45628800	0.12869400	2.82155100
H	1.52981000	-0.01962600	2.78714900
C	3.25972800	2.15439400	0.98358700
H	3.41975300	1.31321400	1.64859000
C	-0.44669100	-2.28178900	-1.11354200
H	0.39479500	-1.68011700	-1.42812300
C	0.34060300	0.86862500	-0.73281400
C	1.60558800	-1.60633300	0.77886000
C	-1.76337400	-0.48650100	2.11709000
H	-2.43241300	-1.09542000	1.52468800
C	0.22483100	-1.90854800	1.33459900
C	-1.29192000	-2.82794900	-2.08025600
H	-1.10154700	-2.62306100	-3.12882200
C	3.71588500	-2.22724000	0.25708300
C	3.96355700	3.34270700	1.17384500
H	4.66843100	3.42337900	1.99565900
C	3.76452600	4.42331400	0.31309100
H	4.31662000	5.34648000	0.45880000
C	-5.41387600	1.33120700	0.78214700
H	-5.99515400	1.97918600	1.43067800
C	-2.29285900	0.52397800	2.91985700
H	-3.36655900	0.67248600	2.94287800
C	2.85470200	4.30798100	-0.74130400
H	2.69957100	5.14088500	-1.42018500
C	-1.75352500	-3.32419300	0.61964800
H	-1.91841700	-3.53216300	1.66985100

C	-1.45104500	1.35086800	3.66112600
H	-1.86513300	2.14566300	4.27404000
C	-2.37359300	-3.62206300	-1.69996400
H	-3.03217100	-4.04710500	-2.45107600
C	-5.16123000	-0.71487900	-0.52210900
H	-5.58614700	-1.65400300	-0.86313200
C	5.95075400	-2.25874600	-0.56635000
H	6.89999000	-2.76455100	-0.71279600
C	4.92115800	-2.91758100	0.09548400
H	5.04178700	-3.93020100	0.46696900
C	-2.59927500	-3.87054800	-0.34453700
H	-3.43258500	-4.49424800	-0.03593200
C	5.78043200	-0.94750500	-1.05737400
H	6.60233400	-0.46564900	-1.57784600
C	-5.92780500	0.12894500	0.30846100
H	-6.93404000	-0.16702400	0.58837200
O	0.37770100	-2.96836100	2.31748000
H	0.65491100	-2.54379600	3.14263300

IM-3 conformation 2

F	3.10557000	-3.52143200	-0.53976500
F	4.21606100	-3.04540000	1.27439600
F	4.37242200	-1.74942700	-0.45973100
N	2.64618100	1.01394600	3.25787300
H	2.56730000	1.39895600	4.18620700
N	-0.90597900	0.96997600	-2.31320400
H	-1.14414600	1.93389000	-2.49083000
C	3.50185100	-2.50719500	0.25695600
C	2.95782500	0.81120200	1.03270200
C	2.43129600	-0.30721900	2.93009300
H	2.14506500	-1.02605200	3.68304100
C	2.34908900	-1.68847900	0.75717200
C	-1.26141800	-2.50494800	0.64552300
C	2.96572900	1.72883200	2.12058400
C	2.61800700	-0.48333300	1.57832500
C	-1.24382100	2.67453300	-0.02045200
C	-0.04682900	-1.10331700	-2.53609800
C	0.52276100	-2.17895500	-3.23623600
H	0.82451700	-3.07573900	-2.70383800
C	-0.36585200	-0.87812000	-1.15128300
C	-1.10855800	-3.06760900	1.92225100
H	-0.14581600	-3.00136000	2.42027300
C	-0.13535700	-1.81418400	-0.01866300
C	0.19419200	4.58647600	-0.44791100

H	1.18162100	4.97851600	-0.66915200
C	-2.77840900	0.70396800	0.51170900
C	3.24626500	1.27288400	-0.26337500
H	3.24390800	0.58233700	-1.09980200
C	0.01815200	3.21202700	-0.31623400
H	0.87364300	2.55698600	-0.44643200
C	-2.50895300	-2.58138200	0.01305500
H	-2.63497300	-2.13432200	-0.96585400
C	-3.73971700	0.61822900	-0.50179800
H	-3.46811600	0.85992200	-1.52422700
C	1.12130500	-1.91217600	0.35459800
C	-0.86109200	0.40889500	-1.04882400
C	-2.32617100	3.54389400	0.13657700
H	-3.30740200	3.14722600	0.36738900
C	-1.35151800	1.15179500	0.18371200
C	-5.03993900	0.20962900	-0.21137900
H	-5.77355900	0.14348900	-1.00901700
C	-0.40290900	0.07980300	-3.24163800
C	-3.58358600	-3.20327400	0.64460000
H	-4.54767600	-3.24089900	0.14831300
C	-3.42589600	-3.75813900	1.91481700
H	-4.26535900	-4.23623900	2.41003500
C	3.25495600	3.08590900	1.94204000
H	3.25475800	3.77588900	2.77933600
C	-2.15124100	4.92392200	0.00133300
H	-3.00246500	5.58596500	0.12743200
C	-2.18287200	-3.68861300	2.55148600
H	-2.05457900	-4.11317700	3.54256900
C	-3.13887000	0.38019500	1.82103600
H	-2.39262300	0.43393000	2.60260000
C	-0.89326500	5.44955900	-0.28981600
H	-0.75945600	6.52191600	-0.39327900
C	-5.39352000	-0.12288900	1.09779900
H	-6.40335300	-0.45087400	1.32422600
C	3.53759500	2.61956200	-0.44056800
H	3.76282500	2.99408600	-1.43403800
C	0.34371700	-0.87679000	-5.29141700
H	0.50551500	-0.81192500	-6.36282800
C	-0.21395600	0.20696500	-4.62093300
H	-0.48846300	1.11667600	-5.14538900
C	-4.43887100	-0.03584400	2.11046300
H	-4.70180800	-0.30010900	3.13018700
C	0.71062900	-2.05559800	-4.60697300
H	1.15132500	-2.87599900	-5.16484900

C	3.54136600	3.51483500	0.65110400
H	3.77131800	4.56144700	0.47905500
O	-0.54257100	0.78249700	1.30728200
H	0.38797400	0.88406400	1.05781500