N-Heterocyclic Carbene Catalyzed [2+3] Annulation Reaction for the Synthesis of Trifluoroethyl 3,2'-Spirooxindole γ-Lactam

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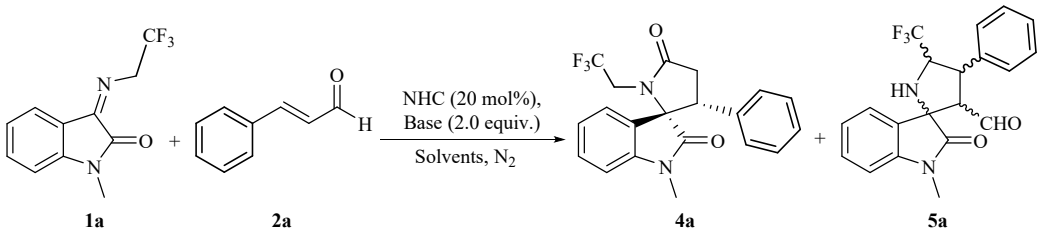
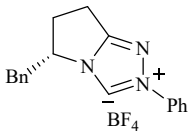
1. General Information

All the starting materials were obtained from commercial sources (Shanghai Macklin Biochemical Co., Ltd and Chengdu Pukang Biological Technology Co., Ltd) and used without further purification unless otherwise stated. All solvents were dried over activated molecular sieves of appropriate sizes and all reactions were carried out under an argon atmosphere (N_2). The progress of the reactions was monitored by thin-layer chromatography (TLC) or liquid chromatography-mass spectrometry (LC-MS), and flash column chromatography was performed using silica gel (200 - 300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-600 MHz or Bruker-700 MHz spectrometer. Chemical shifts (δ) are given in parts per million (ppm), and the residual solvent peaks were used as an internal reference ($CDCl_3$: δ 7.26 ppm ^{1}H; δ 77.2 ppm ^{13}C; d_6-DMSO: δ 2.50 ppm ^{1}H; δ 39.5 ppm ^{13}C). Enantiomeric excess (ee) values were determined by High Performance Liquid Chromatography (HPLC) analysis using chiral column (CHIRALPAK IB N-5) described below in detail. Specific rotation was measured on a Rudolph Research Analytical at 20 °C using a quartz glass cell (100 mm path length). Accurate mass measurements were performed on the electrospray ionization (ESI) apparatus using Agilent 1260-Bruker tims TOF mass.

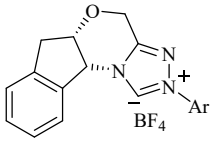
2. Supplementary Discussion

Table S1. Optimization of conditions[a]

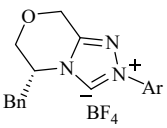




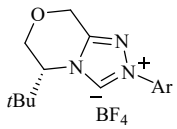
3a



3b: Ar = Mes
3c: Ar = C_6F_5



3d: Ar = Mes
3e: Ar = C_6F_5



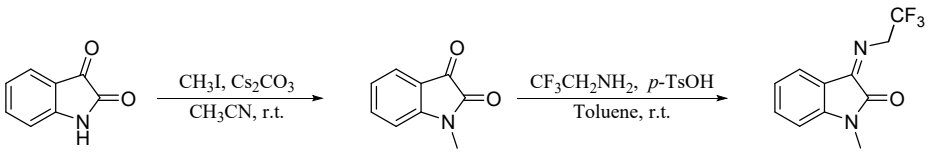
3f: Ar = Mes
3g: Ar = C_6F_5

Entry	NHC	Base	Solvent	Temp. (°C)	Yield (%)[b]		dr[c]	ee[d]
					4a	5a		
1	**3f**	Et_3N	DCE	20 °C	68	8	13:1	82
2	**3f**	Et_3N	CH_3CN	20 °C	49	10	10:1	62
3	**3f**	Et_3N	$CHCl_3$	20 °C	62	21	>20:1	88
4	**3f**	DMAP	DCM	20 °C	34	34	--	38
5	**3f**	*t*BuOK	DCM	20 °C	38	44	--	36
6	**3f**	DBU	DCM	20 °C	46	33	--	52
7	**3f**	K_2CO_3	DCM	20 °C	68	22	>20:1	84

[a]Reactions were performed with **1a** (0.10 mmol), **2a** (0.15 mmol), **3f** (20 mol%) and Base (2.0 equiv.) in solvent (1.0 mL) at 20 °C for 24 h under N_2. [b]Isolated yields. [c]dr values were determined by ^1H NMR analysis of the crude product. [d]ee values were determined by HPLC using a chiral column.

3. Synthesis and Characterization of *N*-2,2,2-Trifluoroethylisatinone Imines

General Procedure A:

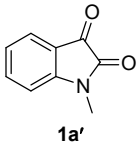


isatin **1a'** **1a**

Step 1: A mixture of isatin (1.0 g, 6.80 mmol), cesium carbonate (2.4 g, 7.51 mmol), and dry CH_3CN (40.0 ml) was stirred at room temperature for half an hour. The iodomethane (0.9 mL, 1.0 equiv.) was added to the reaction mixture and monitored by TLC until isatin was consumed. The reaction was quenched by pouring the emulsion into 30.0 mL water and extracted with ethyl acetate (60.0 mL × 3). The organic layer was separated, washed with brine, then the combined organic layers were dried over Na_2SO_4, and concentrated under reduced pressure to afford the product **1a'** (1.1 g, 97% yield) as a red solid. The **1a'** was used for the next step without further purification.

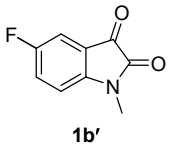
Step 2: The crude **1a'** (0.5 g, 3.12 mmol) was dissolved in toluene (15.0 mL), then the 2,2,2-Trifluoroethylamine (0.5 g, 4.70 mmol) and *p*-toluenesulfonic acid hydrate (0.1 g, 0.31 mmol) were added to the reaction mixture. The reaction was monitored by TLC until the reaction was finished. The resulting solution was filtered and concentrated in vacuo, followed by the addition of a saturated aqueous solution of sodium bicarbonate (10.0 mL), then the aqueous layer was extracted with ethyl acetate (20.0 mL × 3). The combined organic phases were dried over Na_2SO_4 and evaporated on a rotary evaporator to give the crude product, which was purified by flash chromatography on silica gel (petroleum ether : ethyl acetate = 4 : 1) to afford desired product **1a** (0.7 g, 91% yield) as a yellow solid.

Compounds **1b-1f** were synthesized according to the above procedure.



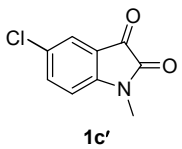
1a′

1-methylindoline-2,3-dione (**1a'**) was synthesized according to general procedure A (step 1) as a red solid in 98% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.65 – 7.58 (m, 2H), 7.14 (td, *J* = 7.6, 0.8 Hz, 1H), 6.90 (d, *J* = 8.1 Hz, 1H), 3.26 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 183.36, 158.25, 151.48, 138.39, 125.33, 123.85, 117.48, 109.91, 26.24.



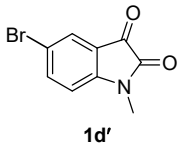
1b′

5-fluoro-1-methylindoline-2,3-dione (1b') was synthesized according to general procedure A (step 1) as a red solid in 97% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.38 – 7.29 (m, 2H), 6.89 (dd, *J* = 8.5, 3.6 Hz, 1H), 3.26 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 182.52 (d, *J* = 2.3 Hz), 159.95, 158.02 (d, *J* = 89.8 Hz), 147.25 (d, *J* = 2.2 Hz), 124.43 (d, *J* = 24.2 Hz), 117.74 (d, *J* = 7.0 Hz), 112.14 (d, *J* = 24.3 Hz), 110.83 (d, *J* = 7.2 Hz), 26.10.



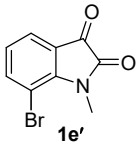
1c′

5-chloro-1-methylindoline-2,3-dione (1c') was synthesized according to general procedure A (step 1) as a red solid in 99% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.70 – 7.41 (m, 2H), 6.87 (dd, *J* = 8.3, 0.6 Hz, 1H), 3.26 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 182.34, 157.69, 149.71, 137.77, 129.70, 125.25, 118.25, 111.23, 26.40.



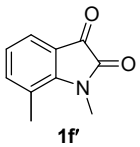
1d′

5-bromo-1-methylindoline-2,3-dione (1d') was synthesized according to general procedure A (step 1) as a red solid in 99% yield. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.73 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.70 (d, *J* = 1.9 Hz, 1H), 6.83 (d, *J* = 8.3 Hz, 1H), 3.26 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 182.18, 157.50, 150.14, 140.63, 128.07, 118.57, 116.67, 111.66, 26.37.



1e′

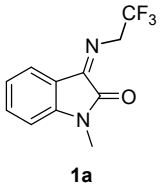
7-bromo-1-methylindoline-2,3-dione (1e') was synthesized according to general procedure A (step 1) as a red solid in 95% yield. **^{1}H NMR (600 MHz, CDCl3) δ** 7.71 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.57 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.00 (dd, *J* = 8.1, 7.2 Hz, 1H), 3.65 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 182.45, 158.57, 148.25, 143.78, 125.12, 124.48, 120.40, 104.32, 29.73.



1f′

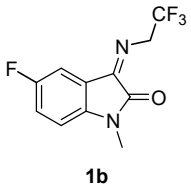
1,7-dimethylindoline-2,3-dione (1f') was synthesized according to general procedure A (step 1) as a red solid in 94% yield. **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.45 (d, *J* = 7.3 Hz,

1H), 7.33 (dt, *J* = 7.7, 0.7 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 3.52 (s, 3H), 2.57 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 183.79, 159.24, 148.99, 142.27, 123.89, 123.40, 121.92, 118.50, 29.73, 18.85.



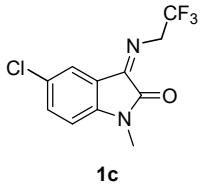
1a

1-methyl-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1a) was synthesized according to general procedure A (step 2) as a yellow solid in 91% yield. **^{1}H NMR (700 MHz, $CDCl_3$) δ** 7.70 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.46 (td, *J* = 7.7, 1.3 Hz, 1H), 7.11 (td, *J* = 7.5, 0.9 Hz, 1H), 6.83 (d, *J* = 7.7 Hz, 1H), 4.83 (q, *J* = 9.7 Hz, 2H), 3.22 (s, 3H). **^{13}C NMR (176 MHz, $CDCl_3$) δ** 158.64, 155.74, 146.26, 133.79, 125.03 (q, *J* = 276.0 Hz), 123.47, 122.98, 120.55, 108.76, 53.51 (q, *J* = 32.3 Hz), 25.82.



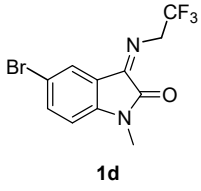
1b

5-fluoro-1-methyl-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1b) was synthesized according to general procedure A (step 2) as a yellow solid in 78% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.44 (dd, *J* = 7.3, 2.7 Hz, 1H), 7.18 (td, *J* = 8.7, 2.7 Hz, 1H), 6.79 (dd, *J* = 8.5, 3.8 Hz, 1H), 4.83 (q, *J* = 9.7 Hz, 2H), 3.23 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 160.37, 158.61 (d, *J* = 44.1 Hz), 155.31 (d, *J* = 3.1 Hz), 142.25 (d, *J* = 2.2 Hz), 124.86 (q, *J* = 276.3 Hz), 121.66 (d, *J* = 8.3 Hz), 120.04 (d, *J* = 24.2 Hz), 110.65 (d, *J* = 25.3 Hz), 109.60 (d, *J* = 7.8 Hz), 53.63 (q, *J* = 32.4 Hz), 25.98.



1c

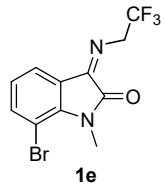
5-chloro-1-methyl-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1c) was synthesized according to general procedure A (step 2) as a yellow solid in 87% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.68 (d, *J* = 2.1 Hz, 1H), 7.43 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.78 (d, *J* = 8.3 Hz, 1H), 4.82 (q, *J* = 9.6 Hz, 2H), 3.22 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 158.17, 154.88, 144.59, 133.34, 129.23, 124.84 (q, *J* = 276.1 Hz), 123.20, 121.69, 109.91, 53.67 (q, *J* = 32.6 Hz), 25.98.



1d

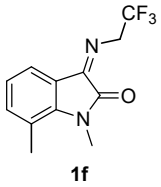
5-bromo-1-methyl-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1d) was synthesized according to general procedure A (step 2) as a yellow solid in 89% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.83 (d, *J* = 2.0 Hz, 1H), 7.58 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 1H), 4.82 (q, *J* = 9.6 Hz, 2H), 3.22 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 158.03, 154.74, 145.06, 136.22, 126.00, 124.84 (q, *J* = 276.3 Hz),122.01, 116.36,

110.35, 53.68 (q, J = 32.7 Hz), 25.97.



1e

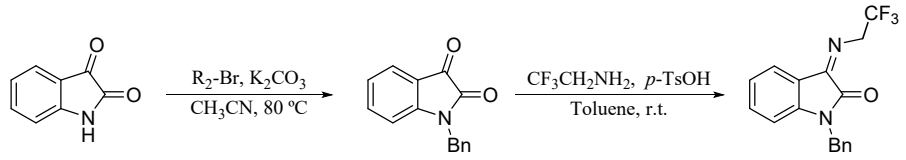
7-bromo-1-methyl-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1e) was synthesized according to general procedure A (step 2) as a yellow solid in 82% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.66 (dd, J = 7.3, 1.2 Hz, 1H), 7.55 (dd, J = 8.1, 1.2 Hz, 1H), 6.96 (dd, J = 8.1, 7.4 Hz, 1H), 4.81 (q, J = 9.7 Hz, 2H), 3.60 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 158.76, 154.64, 143.28, 139.16, 124.89 (q, J = 276.2 Hz), 124.61, 123.49, 122.04, 103.05, 53.86 (q, J = 32.5 Hz), 29.21.



1f

1,7-dimethyl-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1f) was synthesized according to general procedure A (step 2) as a yellow solid in 75% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.56 (d, J = 7.4 Hz, 1H), 7.18 (d, J = 7.7 Hz, 1H), 6.98 (t, J = 7.6 Hz, 1H), 4.81 (q, J = 9.8 Hz, 2H), 3.48 (s, 3H), 2.54 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 159.30, 155.76, 143.91, 137.57, 125.08 (q, J = 276.3 Hz), 123.40, 121.33, 120.96, 120.51, 53.60 (q, J = 32.2 Hz), 29.13, 18.77.

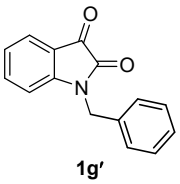
General Procedure B:



isatin 1g' 1g

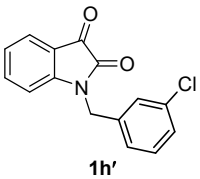
Step 1: To a solution of isatin (1.0 g, 6.80 mmol) and K_2CO_3 (2.8 g, 20.41 mmol) in CH_3CN (40.0 mL) was added benzyl bromide (1.2 g, 6.80 mmol) at room temperature. Then the mixture was stirred at 80 °C in an oil bath and monitored by TLC until isatin was consumed. The filtrate was concentrated under vacuum to give the residue, which was purified via silica gel column chromatography (petroleum ether : ethyl acetate = 4 : 1) to afford product **1g'** (1.6 g, 98% yield) as a red solid. The product **1g** was synthesized according to the above general procedure A Step 2.

Compounds **1h-1k** were synthesized according to the above procedure.



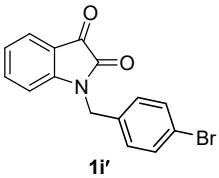
1g′

1-benzylindoline-2,3-dione (1g') was synthesized according to general procedure B (step 1) as a red solid in 99% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.61 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.48 (td, *J* = 7.8, 1.4 Hz, 1H), 7.38 – 7.27 (m, 5H), 7.09 (td, *J* = 7.5, 0.8 Hz, 1H), 6.78 (d, *J* = 7.9 Hz, 1H), 4.93 (s, 2H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 183.25, 158.27, 150.72, 138.33, 134.50, 129.05, 128.16, 127.43, 125.41, 123.87, 117.67, 111.01, 44.04.



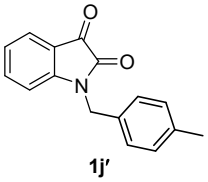
1h′

1-(3-chlorobenzyl)indoline-2,3-dione (1h') was synthesized according to general procedure B (step 1) as a red solid in 99% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.63 (ddd, *J* = 7.5, 1.3, 0.6 Hz, 1H), 7.52 (td, *J* = 7.8, 1.4 Hz, 1H), 7.33 (dt, *J* = 2.4, 1.2 Hz, 1H), 7.31 – 7.27 (m, 2H), 7.24 – 7.21 (m, 1H), 7.12 (td, *J* = 7.5, 0.8 Hz, 1H), 6.77 (d, *J* = 7.9 Hz, 1H), 4.91 (s, 2H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 182.90, 158.24, 150.36, 138.45, 136.59, 134.99, 130.39, 128.47, 127.48, 125.59, 125.53, 124.11, 117.69, 110.80, 43.49.



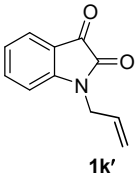
1i′

1-(4-bromobenzyl)indoline-2,3-dione (1i') was synthesized according to general procedure B (step 1) as a red solid in 96% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.62 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.53 – 7.47 (m, 3H), 7.25 – 7.20 (m, 2H), 7.11 (td, *J* = 7.6, 0.8 Hz, 1H), 6.75 (d, *J* = 8.0 Hz, 1H), 4.88 (s, 2H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 182.95, 158.23, 150.36, 138.38, 133.56, 132.22, 129.13, 125.57, 124.08, 122.19, 117.69, 110.81, 43.47.



1j′

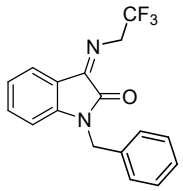
1-(4-methylbenzyl)indoline-2,3-dione (1j') was synthesized according to general procedure B (step 1) as a red solid in 98% yield. **^{1}H NMR (600 MHz, CDCl3) δ** 7.60 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.47 (td, *J* = 7.8, 1.4 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.08 (td, *J* = 7.6, 0.9 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 4.89 (s, 2H), 2.32 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 183.36, 158.25, 150.79, 138.29, 137.98, 131.44, 129.70, 127.46, 125.37, 123.80, 117.67, 111.05, 43.82, 21.12.



1k′

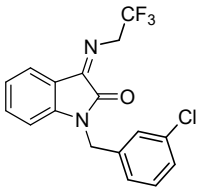
1-allylindoline-2,3-dione (1k') was synthesized according to general procedure B (step 1) as a red solid in 90% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.60 (ddd, *J* = 7.4, 1.4, 0.6 Hz, 1H), 7.56 (td, *J* = 7.8, 1.4 Hz, 1H), 7.11 (td, *J* = 7.5, 0.8 Hz, 1H), 6.89 (d, *J* = 7.9 Hz,

1H), 5.84 (ddt, *J* = 17.2, 10.5, 5.4 Hz, 1H), 5.36 – 5.24 (m, 2H), 4.36 (dt, *J* = 5.4, 1.7 Hz, 2H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 183.26, 157.92, 150.83, 138.35, 130.34, 125.39, 123.82, 118.66, 117.57, 110.92, 42.51.



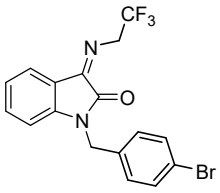
1g

1-benzyl-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1g) was synthesized according to general procedure B (step 2) as a yellow solid in 82% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.73 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.38 – 7.28 (m, 6H), 7.09 (td, *J* = 7.6, 0.9 Hz, 1H), 6.74 (d, *J* = 8.1 Hz, 1H), 4.97 – 4.75 (m, 4H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 158.61, 155.58, 145.49, 134.93, 133.72, 128.99, 128.03, 127.35,125.02 (q, *J* = 276.3 Hz), 123.50, 123.12, 120.72, 109.76, 53.64 (q, *J* = 32.5 Hz), 43.63.



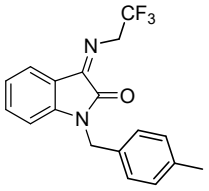
1h

1-(3-chlorobenzyl)-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1h) was synthesized according to general procedure B (step 2) as a yellow solid in 76% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.74 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.38 (td, *J* = 7.8, 1.3 Hz, 1H), 7.31 – 7.26 (m, 3H), 7.19 (td, *J* = 4.6, 1.5 Hz, 1H), 7.11 (td, *J* = 7.6, 0.9 Hz, 1H), 6.72 (d, *J* = 7.9 Hz, 1H), 4.91 – 4.83 (m, 4H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 158.53, 155.33, 145.16, 137.00, 134.93, 133.82, 130.30, 128.34, 127.43, 125.47,124.99 (q, *J* = 276.3 Hz), 123.73, 123.28, 120.72, 109.57, 53.70 (q, *J* = 32.5 Hz), 43.09.



1i

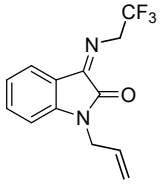
1-(4-bromobenzyl)-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1i) was synthesized according to general procedure B (step 2) as a yellow solid in 80% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.73 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.36 (td, *J* = 7.8, 1.3 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.11 (td, *J* = 7.6, 0.9 Hz, 1H), 6.70 (d, *J* = 7.9 Hz, 1H), 4.90 – 4.83 (m, 4H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 158.53, 155.37, 145.15, 133.97, 133.77, 132.14, 129.05, 124.98 (q, *J* = 276.3 Hz), 123.70, 123.27, 122.04, 120.72, 109.58, 53.68 (q, *J* = 32.3 Hz), 43.05.



1j

1-(4-methylbenzyl)-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1j) was synthesized according to general procedure B (step 2) as a yellow solid in 78% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.72 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.35 (td, *J* = 7.8, 1.3

Hz, 1H), 7.22 – 7.19 (m, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 7.08 (td, *J* = 7.6, 0.9 Hz, 1H), 6.78 – 6.74 (m, 1H), 4.91 – 4.85 (m, 4H), 2.32 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 157.28, 154.34, 144.23, 136.50, 132.37, 130.57, 128.32, 126.05, 123.71 (q, *J* = 276.3 Hz), 122.11, 121.76, 119.39, 108.46, 52.30 (q, *J* = 32.3 Hz), 42.08, 19.80.

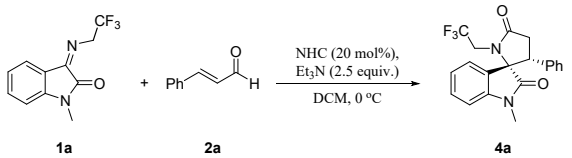


1k

1-allyl-3-((2,2,2-trifluoroethyl)imino)indolin-2-one (1k) was synthesized according to general procedure B (step 2) as a yellow solid in 75% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.72 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.43 (td, *J* = 7.8, 1.3 Hz, 1H), 7.11 (td, *J* = 7.6, 0.9 Hz, 1H), 6.84 (d, *J* = 7.9 Hz, 1H), 5.84 (ddt, *J* = 17.2, 10.6, 5.3 Hz, 1H), 5.34 – 5.25 (m, 2H), 4.84 (q, *J* = 9.7 Hz, 2H), 4.34 (dt, *J* = 5.3, 1.7 Hz, 2H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 158.27, 155.60, 145.55, 133.71, 130.63, 125.02 (q, *J* = 276.3 Hz), 123.43, 123.09, 120.63, 118.28, 109.65, 53.57 (q, *J* = 32.3 Hz), 42.11.

4. Synthesis and Characterization of Products (3*S*, 3'*R*)-4 and 5a.

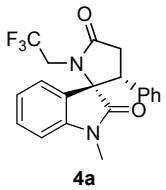
General Procedure C :



1a 2a 4a

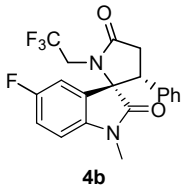
To a flame-dried Schlenk tube was added the co-incubation activation of NHC (16.0 mg, 0.20 mmol) and base (41.7 mg, 2.0 equiv.) in dry DCM for 0.5 h, then the vial was sealed under N_2, followed by the addition of **1a** (50.0 mg, 0.10 mmol) and **2a** (40.9 mg, 0.15 mmol), the reaction at 0 ℃ for 24 h. After the solvent was completely removed, the resulting residue was extracted with ethyl acetate (10.0 mL × 3), and then combined organic layers were dried over Na_2SO_4, filtered, and concentrated in vacuo. The crude residue was purified via silica gel column chromatography (petroleum ether : ethyl acetate = 4 : 1) to make product **4a** (80% yield, 98% ee) a white solid. Enantiomeric excess (ee %) values were determined by HPLC analysis using the chiral column described below.

Compounds **4b-4ae** were synthesized according to the above procedure.



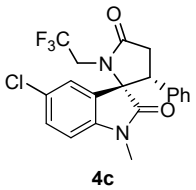
4a

(3*S*, 3'*R*)-1-methyl-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4a) was synthesized according to general procedure C as a white solid in 80% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.42 – 7.37 (m, 2H), 7.25 – 7.21 (m, 1H), 7.19 – 7.16 (m, 1H), 7.12 (t, *J* = 7.5 Hz, 2H), 6.85 (d, *J* = 7.4 Hz, 2H), 6.68 – 6.64 (m, 1H), 3.95 (dq, *J* = 15.3, 9.5 Hz, 1H), 3.81 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.61 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.53 (dt, *J* = 17.4, 8.7 Hz, 1H), 2.79 – 2.73 (m, 1H), 2.73 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.92, 173.11, 143.71, 134.02, 132.67, 128.63, 128.47, 128.04, 127.47, 126.39, 123.39 (d, *J* = 280.4 Hz), 115.94, 110.40, 73.70, 52.02, 42.64 (q, *J* = 35.6 Hz), 32.99, 25.96. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{17}F_3N_2O_2Na$: 397.1140, found: 397.1133. $[\alpha]^{20}_D$ = +67 (c = 0.1, $CHCl_3$). 98% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.643 min, t_R (major) = 9.690 min.



4b

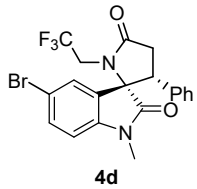
(3*S*, 3'*R*)-5-fluoro-1-methyl-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4b) was synthesized according to general procedure C as a light yellow solid in 81% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.25 – 7.07 (m, 5H), 6.91 – 6.83 (m, 2H), 6.60 (dd, *J* = 8.5, 4.0 Hz, 1H), 3.90 (dq, *J* = 15.4, 9.4 Hz, 1H), 3.77 (dd, *J* = 13.1, 7.8 Hz, 1H), 3.65 – 3.54 (m, 2H), 2.76 (ddd, *J* = 16.4, 7.9, 0.7 Hz, 1H), 2.72 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.89, 173.21, 159.36 (d, *J* = 243.2 Hz), 140.41 (d, *J* = 2.2 Hz), 132.56, 128.39, 128.24, 127.85, 125.73 (d, *J* = 7.7 Hz), 123.23 (q, *J* = 280.3 Hz), 117.39 (d, *J* = 23.3 Hz), 112.30 (d, *J* = 25.1 Hz), 109.49 (d, *J* = 7.9 Hz), 73.89, 51.74, 42.60 (q, *J* = 35.6 Hz), 32.87, 25.81. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{16}F_4N_2O_2Na$: 415.1046, found: 415.1040. $[\alpha]^{20}_D$ = +78 (c = 0.3, $CHCl_3$). 99% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.013 min, t_R (major) = 9.128 min.



4c

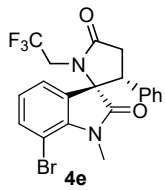
(3*S*, 3'*R*)-5-chloro-1-methyl-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4c) was synthesized according to general procedure C as a light yellow solid in 67% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.40 – 7.34 (m, 2H), 7.24 – 7.18 (m, 1H), 7.18 – 7.12 (m, 2H), 6.90 – 6.85 (m, 2H), 6.59 (d, *J* = 8.2

Hz, 1H), 3.99 (dq, *J* = 15.4, 9.5 Hz, 1H), 3.78 (dd, *J* = 13.1, 7.8 Hz, 1H), 3.62 – 3.48 (m, 2H), 2.75 (ddd, *J* = 16.4, 7.9, 0.8 Hz, 1H), 2.70 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.76, 173.03, 143.01, 132.48, 130.92, 128.69, 128.42, 128.26, 127.84, 125.85, 124.53, 123.19 (q, *J* = 280.3 Hz), 109.75, 73.59, 51.81, 42.46 (q, *J* = 35.7 Hz), 32.80, 25.78. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{16}ClF_3N_2O_2Na$: 431.0750, found: 431.0744. $[\alpha]^{20}_D$ = +52 (c = 0.1, $CHCl_3$). 92% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 6.757 min, t_R (major) = 8.492 min.



4d

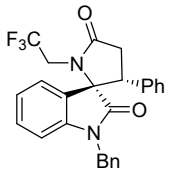
(3*S*, 3'*R*)-5-bromo-1-methyl-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4d) was synthesized according to general procedure C as a white solid in 75% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.55 – 7.50 (m, 2H), 7.24 – 7.18 (m, 1H), 7.18 – 7.11 (m, 2H), 6.88 (dd, *J* = 8.2, 1.3 Hz, 2H), 6.55 (d, *J* = 8.8 Hz, 1H), 4.01 (dq, *J* = 15.3, 9.5 Hz, 1H), 3.78 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.58 (dd, *J* = 16.4, 13.2 Hz, 1H), 3.52 (dt, *J* = 15.2, 8.7 Hz, 1H), 2.75 (dd, *J* = 16.3, 7.9 Hz, 1H), 2.70 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.72, 172.91, 143.51, 133.82, 132.47, 128.43, 128.26, 127.84, 127.26, 126.19, 123.19 (q, *J* = 280.3 Hz), 115.74, 110.20, 73.50, 51.82, 42.44 (q, *J* = 35.5 Hz), 32.79, 25.75. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{16}BrF_3N_2O_2Na$: 475.0245, found: 475.0239. $[\alpha]^{20}_D$ = +79 (c = 0.1, $CHCl_3$). 92% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.352 min, t_R (major) = 9.667 min.



4e

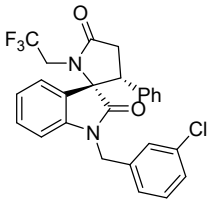
(3*S*, 3'*R*)-7-bromo-1-methyl-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4e) was synthesized according to general procedure C as a light yellow solid in 68% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.51 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.32 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.18 (t, *J* = 7.6 Hz, 2H), 7.09 (dd, *J* = 8.2, 7.3 Hz, 1H), 6.83 (dd, *J* = 7.3, 1.7 Hz, 2H), 3.94 (dq, *J* = 15.3, 9.4 Hz, 1H), 3.74 (dd, *J* = 13.1, 7.8 Hz, 1H), 3.62 – 3.47 (m, 2H), 3.07 (s, 3H), 2.76 (dd, *J* = 16.4, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.90, 173.93, 141.86, 136.46, 132.41, 128.54, 128.28, 127.73, 127.37, 124.31, 123.22, 123.21 (q, *J* = 280.9 Hz), 103.08, 73.28, 52.24, 42.45 (q, *J* = 35.8 Hz), 32.78, 29.25. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{16}BrF_3N_2O_2Na$: 475.0245, found: 475.0239. $[\alpha]^{20}_D$ = +55 (c = 0.2, $CHCl_3$). 94% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine

= 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.383 min, t_R (major) = 9.610 min.



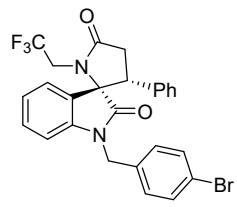
4f

(3*S*, 3'*R*)-1-benzyl-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4f) was synthesized according to general procedure C as a white solid in 72% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.41 (dd, *J* = 7.2 Hz, 1H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.23 – 7.12 (m, 4H), 7.08 (t, *J* = 7.6 Hz, 2H), 6.96 (d, *J* = 7.2 Hz, 2H), 6.45 (d, *J* = 7.8 Hz, 1H), 6.38 (d, *J* = 7.6 Hz, 2H), 4.95 (d, *J* = 16.0 Hz, 1H), 4.17 (d, *J* = 16.0 Hz, 1H), 4.05 (dq, *J* = 15.3, 9.6 Hz, 1H), 3.92 (dd, *J* = 13.3, 7.8 Hz, 1H), 3.71 (dd, *J* = 16.3, 13.3 Hz, 1H), 3.52 – 3.42 (m, 1H), 2.79 (dd, *J* = 16.3, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.93, 173.68, 143.99, 134.49, 133.07, 130.98, 128.64, 128.62, 128.42, 128.34, 127.28, 126.38, 124.26, 123.84, 123.30, 123.27 (q, *J* = 280.5 Hz), 110.20, 73.22, 51.39, 43.81, 42.24 (q, *J* = 35.7 Hz), 33.19. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{26}H_{21}F_3N_2O_2Na$: 473.1453, found: 473.1449. $[\alpha]^{20}_D$ = +82 (c = 0.2, $CHCl_3$). 98% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 6.792 min, t_R (major) = 8.888 min.



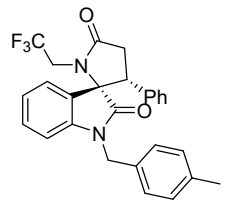
4g

(3*S*, 3'*R*)-1-(3-chlorobenzyl)-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4g) was synthesized according to general procedure C as a white solid in 68% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.42 (d, *J* = 7.4 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.19 – 7.11 (m, 3H), 6.98 (t, *J* = 7.8 Hz, 1H), 6.93 (d, *J* = 7.7 Hz, 2H), 6.79 (d, *J* = 2.0 Hz, 1H), 6.47 (d, *J* = 7.8 Hz, 1H), 6.06 (d, *J* = 7.7 Hz, 1H), 4.87 (d, *J* = 16.1 Hz, 1H), 4.16 – 4.05 (m, 2H), 3.91 (dd, *J* = 13.3, 7.8 Hz, 1H), 3.69 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.43 (dq, *J* = 16.8, 8.6 Hz, 1H), 2.78 (dd, *J* = 16.3, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.81, 173.80, 143.77, 136.71, 134.42, 132.83, 131.06, 130.05, 128.64, 128.54, 128.20, 127.76, 126.81, 124.58, 124.32, 123.83, 123.52, 123.23 (q, *J* = 280.9 Hz), 109.98, 73.10, 51.47, 43.42, 42.14 (q, *J* = 36.2 Hz), 33.12. **HRMS** (ESI) calculated [M+Na]+ for $C_{26}H_{20}ClF_3N_2O_2Na$: 507.1063, found: 507.1057. $[\alpha]^{20}_D$ = +74 (c = 0.1, $CHCl_3$). 99% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.818 min, t_R (major) = 10.700 min.



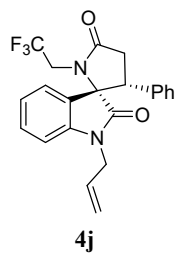
4h

(3*S*, 3'*R*)-1-(4-bromobenzyl)-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro-[indoline-3,2'-pyrrolidine]-2,5'-dione (4h) was synthesized according to general procedure C as a white solid in 72% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.42 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.35 – 7.30 (m, 1H), 7.29 – 7.26 (m, 2H), 7.22 (td, *J* = 7.5, 1.1 Hz, 1H), 7.20 – 7.17 (m, 4H), 6.99 – 6.91 (m, 2H), 6.45 – 6.37 (m, 1H), 6.22 (d, *J* = 8.4 Hz, 2H), 4.93 (d, *J* = 16.1 Hz, 1H), 4.15 – 4.05 (m, 2H), 3.92 (dd, *J* = 13.3, 7.8 Hz, 1H), 3.70 (dd, *J* = 16.3, 13.3 Hz, 1H), 3.43 (dq, *J* = 15.3, 8.6 Hz, 1H), 2.79 (dd, *J* = 16.3, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.79, 173.67, 143.67, 133.57, 133.04, 131.76, 131.04, 128.65, 128.43, 128.35, 128.12, 124.34, 123.80, 123.50, 123.24 (q, *J* = 280.9 Hz), 121.22, 110.01, 73.09, 51.43, 43.22, 42.15 (q, *J* = 35.1 Hz), 33.11. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{26}H_{20}BrF_3N_2O_2Na$: 551.0558, found: 551.0553. $[\alpha]^{20}_D$ = +66 (c = 0.3, $CHCl_3$). 97% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 10.632 min, t_R (major) = 12.948 min.



4i

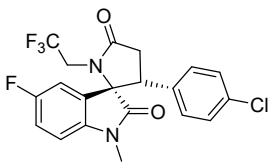
(3*S*, 3'*R*)-1-(4-methylbenzyl)-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4i) was synthesized according to general procedure C as a white solid in 65% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.40 (dd, *J* = 7.3 Hz, 1H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.24 (td, *J* = 7.7, 1.3 Hz, 1H), 7.19 (t, *J* = 7.7 Hz, 3H), 6.96 (d, *J* = 7.2 Hz, 2H), 6.89 (d, *J* = 7.8 Hz, 2H), 6.45 (d, *J* = 7.5 Hz, 1H), 6.28 (d, *J* = 7.8 Hz, 2H), 4.89 (d, *J* = 15.8 Hz, 1H), 4.14 (d, *J* = 15.8 Hz, 1H), 4.03 (dq, *J* = 15.4, 9.6 Hz, 1H), 3.91 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.71 (dd, *J* = 16.3, 13.3 Hz, 1H), 3.48 (dq, *J* = 15.3, 8.7 Hz, 1H), 2.79 (dd, *J* = 16.3, 7.8 Hz, 1H), 2.27 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.96, 173.63, 144.04, 136.96, 133.09, 131.42, 130.95, 129.30, 128.59, 128.40, 128.29, 126.38, 124.21, 123.84, 123.26 (q, *J* = 280.9 Hz), 123.22, 110.25, 73.24, 51.36, 43.60, 42.26 (q, *J* = 36.0 Hz), 33.21, 21.06. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{27}H_{23}F_3N_2O_2Na$: 487.1609, found: 487.1603. $[\alpha]^{20}_D$ = +53 (c = 0.1, $CHCl_3$). 87% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.547 min, t_R (major) = 10.188 min.



4j

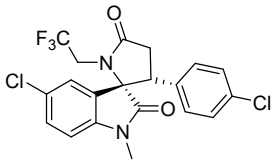
(3*S*, 3'*R*)-1-allyl-3'-phenyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-

2,5'-dione (4j) was synthesized according to general procedure C as a white solid in 71% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.40 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.36 (td, *J* = 7.8, 1.3 Hz, 1H), 7.26 – 7.17 (m, 2H), 7.14 (dd, *J* = 8.4, 6.9 Hz, 2H), 6.87 (dd, *J* = 7.3, 1.7 Hz, 2H), 6.65 (d, *J* = 7.8 Hz, 1H), 5.07 (dddd, *J* = 17.2, 10.4, 5.8, 4.7 Hz, 1H), 4.84 (dd, *J* = 10.4, 1.4 Hz, 1H), 4.46 (dd, *J* = 17.2, 1.3 Hz, 1H), 4.20 – 4.08 (m, 1H), 4.00 (dq, *J* = 15.3, 9.5 Hz, 1H), 3.84 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.73 – 3.60 (m, 2H), 3.52 (dq, *J* = 15.3, 8.7 Hz, 1H), 2.75 (dd, *J* = 16.3, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 176.03, 173.11, 143.86, 132.92, 130.83, 130.36, 128.35, 128.24, 128.14, 124.22, 123.87, 123.26 (q, *J* = 280.9 Hz), 123.18, 117.27, 109.81, 73.46, 51.73, 42.34 (q, *J* = 35.7 Hz), 42.12, 32.97. **^{19}F NMR (565 MHz, CDCl3) δ** -69.18 (t, *J* = 9.3 Hz). **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{22}H_{19}F_3N_2O_2Na$: 423.1296, found: 423.1290. $[\alpha]^{20}_D$ = +42 (c = 0.2, $CHCl_3$). 93% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.042 min, t_R (major) = 8.073 min.



4k

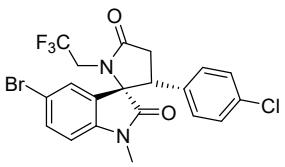
(3*S*, 3'*R*)-3'-(4-chlorophenyl)-5-fluoro-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4k) was synthesized according to general procedure C as a white solid in 70% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.19 – 7.09 (m, 4H), 6.86 – 6.80 (m, 2H), 6.65 (dd, *J* = 8.5, 4.0 Hz, 1H), 3.91 (dq, *J* = 15.4, 9.4 Hz, 1H), 3.74 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.62 – 3.48 (m, 2H), 2.78 (s, 4H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.44, 173.11, 159.40 (d, *J* = 243.8 Hz), 140.35 (d, *J* = 2.2 Hz), 134.34, 131.19, 129.27, 128.47, 125.40 (d, *J* = 7.4 Hz), 123.17 (q, *J* = 280.2 Hz), 117.62 (d, *J* = 23.6 Hz), 112.28 (d, *J* = 24.9 Hz), 109.73 (d, *J* = 8.0 Hz), 73.55, 51.03, 42.55 (q, *J* = 35.6 Hz), 32.98, 25.96. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{15}ClF_4N_2O2Na$: 449.0656, found: 449.0649. $[\alpha]^{20}_D$ = +72 (c = 0.2, $CHCl_3$). 98% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.973 min, t_R (major) = 11.593 min.



4l

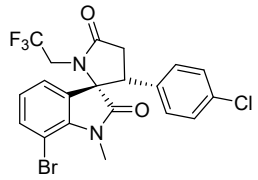
(3*S*, 3'*R*)-5-chloro-3'-(4-chlorophenyl)-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4l) was synthesized according to general procedure C as a white solid in 73% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.41 – 7.36 (m, 2H), 7.14 (d, *J* = 8.5 Hz, 2H), 6.83

(d, *J* = 8.5 Hz, 2H), 6.64 (d, *J* = 8.2 Hz, 1H), 4.01 (dq, *J* = 15.3, 9.5 Hz, 1H), 3.75 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.57 – 3.45 (m, 2H), 2.77 (s, 3H), 2.77 – 2.72 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.30, 172.93, 142.95, 134.38, 131.13, 131.12, 129.26, 128.87, 128.49, 125.51, 124.51, 123.14 (q, *J* = 280.9 Hz), 109.96, 73.26, 51.09, 42.41 (q, *J* = 35.7 Hz), 32.92, 25.93. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{15}C_{l2}F_3N_2O_2Na$: 465.0360, found: 465.0355. $[\alpha]^{20}_D$ = +70 (c = 0.1, $CHCl_3$). 99% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 8.172 min, t_R (major) = 10.593 min.



4m

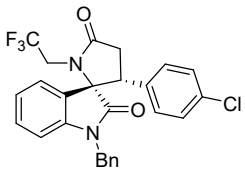
(3*S*, 3'*R*)-5-bromo-3'-(4-chlorophenyl)-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4m) was synthesized according to general procedure C as a white solid in 82% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.54 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.17 – 7.11 (m, 2H), 6.85 – 6.80 (m, 2H), 6.59 (d, *J* = 8.3 Hz, 1H), 4.02 (dq, *J* = 15.4, 9.5 Hz, 1H), 3.75 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.58 – 3.43 (m, 2H), 2.80 – 2.71 (m, 4H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.26, 172.81, 143.45, 134.39, 134.03, 131.11, 129.26, 128.50, 127.24, 125.86, 123.14 (q, *J* = 280.9 Hz), 115.91, 110.41, 73.18, 51.11, 42.39 (q, *J* = 35.7 Hz), 32.90, 25.90. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{15}BrClF_3N_2O_2Na$: 508.9855, found: 508.9849. $[\alpha]^{20}_D$ = +56 (c = 0.2, $CHCl_3$). 90% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.722 min, t_R (major) = 11.015 min.



4n

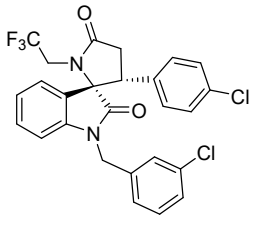
(3*S*, 3'*R*)-7-bromo-3'-(4-chlorophenyl)-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4n) was synthesized according to general procedure C as a white solid in 72% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.53 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.31 (dd, *J* = 7.3, 1.2 Hz, 1H), 7.19 – 7.14 (m, 2H), 7.09 (dd, *J* = 8.2, 7.3 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 2H), 3.95 (dq, *J* = 15.4, 9.4 Hz, 1H), 3.72 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.56 – 3.45 (m, 2H), 3.15 (s, 3H), 2.75 (dd, *J* = 16.4, 7.9 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.43, 173.84, 141.84, 136.71, 134.45, 131.08, 129.17, 128.53, 127.02, 124.46, 123.20, 123.16 (q, *J* = 279.4 Hz), 103.28, 72.88, 51.44, 42.39 (q, *J* = 35.6 Hz), 32.96, 29.39. **^{19}F NMR (565 MHz, $CDCl_3$) δ** -69.15 (t, *J* = 9.0 Hz). **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{15}BrClF_3N_2O2Na$: 508.9855, found: 508.9847. $[\alpha]^{20}_D$ = +63 (c = 0.3, $CHCl_3$). 95% ee as

determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 8.315 min, t_R (major) = 11.838 min.



4o

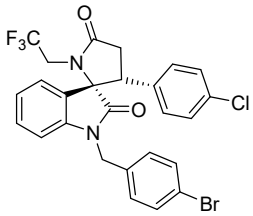
(3*S*, 3'*R*)-1-benzyl-3'-(4-chlorophenyl)-1'-(2,2,2-trifluoroethyl)spiro-[indoline-3,2'-pyrrolidine]-2,5'-dione (4o) was synthesized according to general procedure C as a white solid in 73% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.40 (dd, *J* = 6.8 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.23 – 7.17 (m, 4H), 7.16 – 7.12 (m, 2H), 6.90 – 6.85 (m, 2H), 6.52 (d, *J* = 7.8 Hz, 1H), 6.48 – 6.41 (m, 2H), 5.01 (d, *J* = 15.9 Hz, 1H), 4.16 (d, *J* = 15.9 Hz, 1H), 4.05 (dq, *J* = 15.4, 9.6 Hz, 1H), 3.88 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.65 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.45 (dq, *J* = 15.3, 8.6 Hz, 1H), 2.78 (dd, *J* = 16.2, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.49, 173.51, 144.00, 134.39, 134.37, 131.66, 131.18, 129.76, 128.80, 128.69, 127.56, 126.41, 124.23, 123.53, 123.44, 123.22 (q, *J* = 280.9 Hz), 110.26, 72.94, 50.68, 43.93, 42.23 (q, *J* = 36.2 Hz), 33.18. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{26}H_{20}ClF_3N_2O_2Na$:507.1063, found: 507.1051. $[\alpha]^{20}_D$ = +88 (c = 0.1, $CHCl_3$). 98% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 9.132 min, t_R (major) = 11.498 min.



4p

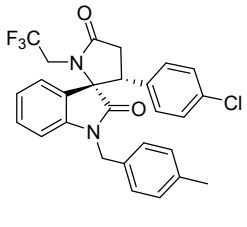
(3*S*, 3'*R*)-1-(3-chlorobenzyl)-3'-(4-chlorophenyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4p) was synthesized according to general procedure C as a white solid in 75% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.40 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.32 (td, *J* = 7.8, 1.3 Hz, 1H), 7.24 (td, *J* = 7.6, 1.0 Hz, 1H), 7.21 – 7.18 (m, 1H), 7.15 – 7.10 (m, 2H), 7.08 (t, *J* = 7.8 Hz, 1H), 6.98 (t, *J* = 2.0 Hz, 1H), 6.88 – 6.81 (m, 2H), 6.54 (dt, *J* = 7.9, 0.7 Hz, 1H), 6.01 (ddd, *J* = 7.7, 1.8, 0.9 Hz, 1H), 4.93 – 4.88 (m, 1H), 4.15 (d, *J* = 16.0 Hz, 1H), 4.09 (dq, *J* = 15.4, 9.6 Hz, 1H), 3.87 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.63 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.42 (dq, *J* = 15.3, 8.6 Hz, 1H), 2.77 (ddd, *J* = 16.3, 7.8, 0.7 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.39, 173.58, 143.70, 136.54, 134.46, 134.42, 131.52, 131.28, 130.10, 129.63, 128.77, 127.96, 127.13, 124.35, 124.33, 123.67, 123.54, 123.20 (q, *J* = 280.9 Hz), 110.05, 72.83, 50.75, 43.43, 42.15 (q, *J* = 36.2 Hz), 33.18. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{26}H_{19}Cl_2F_3N_2O_2Na$: 541.0673, found: 541.0668. $[\alpha]^{20}_D$ = +60 (c = 0.1, $CHCl_3$). 94% ee as determined by HPLC (CHIRALPAK IB N-5 Column,

hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 10.147 min, t_R (major) = 12.530 min.



4q

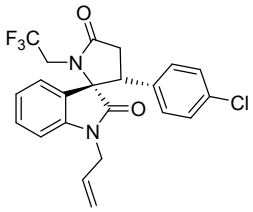
(3*S*, 3'*R*)-1-(4-bromobenzyl)-3'-(4-chlorophenyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4q) was synthesized according to general procedure C as a white solid in 68% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.40 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.23 (td, *J* = 7.6, 1.0 Hz, 1H), 7.18 – 7.12 (m, 2H), 6.89 – 6.83 (m, 2H), 6.48 (d, *J* = 7.8 Hz, 1H), 6.32 (d, *J* = 8.3 Hz, 2H), 4.94 (d, *J* = 16.0 Hz, 1H), 4.10 (dd, *J* = 15.7, 10.6 Hz, 2H), 3.87 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.64 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.41 (dt, *J* = 15.3, 8.5 Hz, 1H), 2.78 (dd, *J* = 16.2, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.39, 173.52, 143.69, 134.50, 133.44, 131.86, 131.61, 131.25, 129.74, 128.79, 128.16, 124.32, 123.65, 123.48, 123.20 (q, *J* = 279.4 Hz), 121.55, 110.06, 72.86, 50.77, 43.35, 42.15 (q, *J* = 35.6 Hz), 33.06. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{26}H_{19}BrClF_3N_2O_2Na$: 585.0168, found: 585.0162. $[\alpha]^{20}_D$ = +59 (c = 0.1, $CHCl_3$). 94% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1, 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 11.280 min, t_R (major) = 13.492 min.



4r

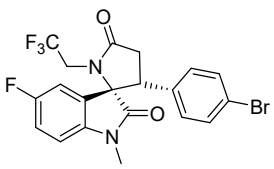
(3*S*, 3'*R*)-3'-(4-chlorophenyl)-1-(4-methylbenzyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4r) was synthesized according to general procedure C as a white solid in 73% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.39 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.19 (td, *J* = 7.6, 1.0 Hz, 1H), 7.15 – 7.08 (m, 2H), 6.99 (d, *J* = 7.8 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.54 (d, *J* = 7.8 Hz, 1H), 6.37 (d, *J* = 7.9 Hz, 2H), 4.94 (d, *J* = 15.8 Hz, 1H), 4.13 (d, *J* = 15.7 Hz, 1H), 4.02 (dq, *J* = 15.4, 9.5 Hz, 1H), 3.87 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.64 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.46 (dq, *J* = 15.3, 8.6 Hz, 1H), 2.77 (dd, *J* = 16.3, 7.8 Hz, 1H), 2.29 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.54, 173.45, 144.06, 137.28, 134.40, 131.65, 131.33, 131.17, 129.72, 129.37, 128.75, 126.46, 124.21, 123.54, 123.36, 123.22 (q, *J* = 280.9 Hz), 110.25, 72.94, 50.65, 43.69, 42.25 (q, *J* = 35.7 Hz), 33.18, 21.10. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{27}H_{22}ClF_3N_2O_2Na$:521.1220, found: 521.1215. $[\alpha]^{20}_D$ = +90 (c = 0.5, $CHCl_3$). 93% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min,

wavelength = 254 nm), t_R (minor) = 9.320 min, t_R (major) = 11.143 min.



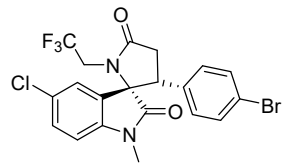
4s

(3*S*, 3'*R*)-1-allyl-3'-(4-chlorophenyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4s) was synthesized according to general procedure C as a white solid in 60% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.41 – 7.29 (m, 2H), 7.23 (td, *J* = 7.6, 1.0 Hz, 1H), 7.15 – 7.08 (m, 2H), 6.80 (d, *J* = 8.5 Hz, 2H), 6.68 (d, *J* = 7.8 Hz, 1H), 5.17 (ddt, *J* = 17.2, 10.5, 5.3 Hz, 1H), 4.93 (dq, *J* = 10.3, 1.4 Hz, 1H), 4.50 (dq, *J* = 17.1, 1.6 Hz, 1H), 4.17 (ddt, *J* = 16.4, 5.0, 1.8 Hz, 1H), 4.00 (dq, *J* = 15.3, 9.5 Hz, 1H), 3.80 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.73 (ddt, *J* = 16.4, 5.6, 1.6 Hz, 1H), 3.57 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.50 (dq, *J* = 15.3, 8.7 Hz, 1H), 2.75 (dd, *J* = 16.3, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.61, 172.97, 143.79, 134.33, 131.46, 131.04, 130.14, 129.49, 128.50, 124.20, 123.56, 123.34, 123.22 (q, *J* = 280.9 Hz), 117.39, 109.90, 73.24, 51.12, 42.34 (d, *J* = 35.6 Hz), 42.13, 32.94. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{22}H_{18}ClF_3N_2O_2Na$: 457.0907, found: 457.0900. $[\alpha]^{20}_D$ = +72 (c = 0.4, $CHCl_3$). 90% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.958 min, t_R (major) = 10.122 min.



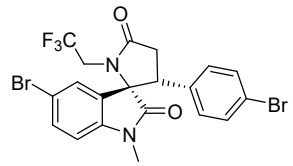
4t

(3*S*, 3'*R*)-3'-(4-bromophenyl)-5-fluoro-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4t) was synthesized according to general procedure C as a white solid in 69% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.30 – 7.27 (m, 2H), 7.17 – 7.09 (m, 2H), 6.79 – 6.74 (m, 2H), 6.65 (dd, *J* = 8.5, 4.0 Hz, 1H), 3.91 (dq, *J* = 15.4, 9.4 Hz, 1H), 3.73 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.61 – 3.48 (m, 2H), 2.79 (s, 3H), 2.78 – 2.74 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.40, 173.09, 159.40 (d, *J* = 244.0 Hz), 140.34 (d, *J* = 2.2 Hz), 131.72, 131.43, 129.59, 125.37 (d, *J* = 7.4 Hz), 123.16 (q, *J* = 280.4 Hz), 122.51, 117.63 (d, *J* = 23.6 Hz), 112.27 (d, *J* = 24.9 Hz), 109.76 (d, *J* = 7.9 Hz), 73.47, 51.08, 42.54 (q, *J* = 35.8 Hz), 32.93, 25.98. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{15}BrF_4N_2O_2Na$: 493.0151, found: 493.0146. $[\alpha]^{20}_D$ = +83 (c = 0.5, $CHCl_3$). 97% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.967 min, t_R (major) = 11.772 min.



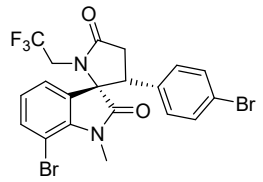
4u

(3*S*, 3'*R*)-3'-(4-bromophenyl)-5-chloro-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4u) was synthesized according to general procedure C as a white solid in 78% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.42 – 7.36 (m, 2H), 7.31 – 7.28 (m, 2H), 6.77 (d, *J* = 8.5 Hz, 2H), 6.64 (d, *J* = 8.2 Hz, 1H), 4.01 (dq, *J* = 15.4, 9.5 Hz, 1H), 3.74 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.57 – 3.43 (m, 2H), 2.78 (s, 3H), 2.75 (dd, *J* = 16.6, 8.2 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.27, 172.92, 142.95, 131.65, 131.45, 131.15, 129.59, 128.88, 125.49, 124.51, 123.14 (q, *J* = 280.3 Hz), 122.55, 109.99, 73.18, 51.13, 42.40 (q, *J* = 35.7 Hz), 32.87, 25.95. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{15}BrClF_3N_2O_2Na$: 508.9855, found: 508.9849. $[\alpha]^{20}_D$ = +80 (c = 0.4, $CHCl_3$). 95% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.658 min, t_R (major) = 10.988 min.



4v

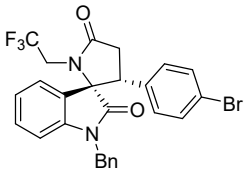
(3*S*, 3'*R*)-5-bromo-3'-(4-bromophenyl)-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4v) was synthesized according to general procedure C as a white solid in 79% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.54 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.31 – 7.28 (m, 2H), 6.80 – 6.74 (m, 2H), 6.60 (d, *J* = 8.3 Hz, 1H), 4.02 (dq, *J* = 15.4, 9.5 Hz, 1H), 3.74 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.58 – 3.43 (m, 2H), 2.79 – 2.72 (m, 4H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.25, 172.80, 143.44, 134.04, 131.63, 131.46, 129.58, 127.24, 125.83, 123.13 (q, *J* = 280.9 Hz), 122.56, 115.93, 110.44, 73.10, 51.15, 42.39 (q, *J* = 35.6 Hz), 32.85, 25.92. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{15}Br_2F_3N_2O_2Na$: 552.9350, found: 552.9342. $[\alpha]^{20}_D$ = +58 (c = 0.4, $CHCl_3$) 90% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 8.782 min, t_R (major) = 12.662 min.



4w

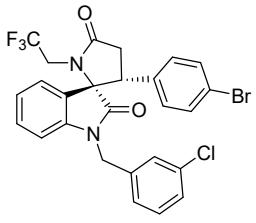
(3*S*, 3'*R*)-7-bromo-3'-(4-bromophenyl)-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4w) was synthesized according to general procedure C as a white solid in 68% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.53 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.34 – 7.28 (m, 3H), 7.09 (dd, *J* = 8.2, 7.3 Hz, 1H), 6.73 (d, *J* = 8.5 Hz, 2H), 3.94 (dq, *J* = 15.4, 9.4 Hz, 1H), 3.70 (dd, *J* = 13.1, 7.9 Hz, 1H), 3.56 – 3.44 (m, 2H), 3.15 (s, 3H), 2.75 (dd, *J* = 16.3, 7.9 Hz, 1H). **^{13}C NMR (151**

MHz, $CDCl_3$) δ 175.41, 173.83, 141.84, 136.72, 131.62, 131.50, 129.50, 127.00, 124.47, 123.21, 123.15 (q, *J* = 280.9 Hz), 122.63, 103.31, 72.79, 51.48, 42.39 (q, *J* = 35.5 Hz), 32.92, 29.41. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{20}H_{15}Br_2F_3N_2O_2Na$: 552.9350, found: 552.9345. $[\alpha]^{20}_D$ = +61 (c = 0.3, $CHCl_3$) 99% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (major) = 8.377 min, t_R (minor) = 12.160 min.



4x

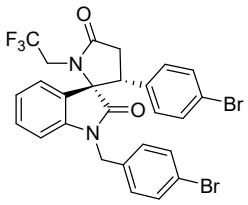
(3*S*, 3'*R*)-1-benzyl-3'-(4-bromophenyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4x) was synthesized according to general procedure C as a white solid in 70% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.40 (dd, *J* = 7.3 Hz, 1H), 7.31 – 7.27 (m, 3H), 7.24 – 7.15 (m, 4H), 6.82 (d, *J* = 8.5 Hz, 2H), 6.52 (d, *J* = 7.9 Hz, 1H), 6.48 – 6.43 (m, 2H), 5.02 (d, *J* = 16.0 Hz, 1H), 4.16 (d, *J* = 15.9 Hz, 1H), 4.05 (dq, *J* = 15.4, 9.6 Hz, 1H), 3.86 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.64 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.45 (dq, *J* = 15.3, 8.6 Hz, 1H), 2.78 (dd, *J* = 16.2, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.47, 173.52, 144.00, 134.36, 132.20, 131.75, 131.19, 130.09, 128.78, 127.57, 126.41, 124.23, 123.51, 123.44, 123.22 (q, *J* = 279.4 Hz), 122.57, 110.29, 72.85, 50.73, 43.96, 42.22 (q, *J* = 36.2 Hz), 33.15. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{26}H_{20}BrF_3N_2O_2Na$: 551.0558, found: 551.0551. $[\alpha]^{20}_D$ = +55 (c = 0.5, $CHCl_3$). 85% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 10.115 min, t_R (major) = 13.047 min.



4y

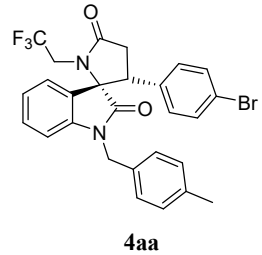
(3*S*, 3'*R*)-3'-(4-bromophenyl)-1-(3-chlorobenzyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4y) was synthesized according to general procedure C as a white solid in 66% yield. **^{1}H NMR (700 MHz, $CDCl_3$) δ** 7.40 (dd, *J* = 7.4, 1.2 Hz, 1H), 7.32 (td, *J* = 7.8, 1.3 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.25 – 7.19 (m, 2H), 7.11 (t, *J* = 7.9 Hz, 1H), 7.01 (t, *J* = 1.9 Hz, 1H), 6.82 – 6.77 (m, 2H), 6.54 (d, *J* = 7.9 Hz, 1H), 6.03 – 5.99 (m, 1H), 4.91 (d, *J* = 16.0 Hz, 1H), 4.16 (d, *J* = 16.0 Hz, 1H), 4.08 (dq, *J* = 15.4, 9.6 Hz, 1H), 3.85 (dd, *J* = 13.2, 7.8 Hz, 1H), 3.62 (dd, *J* = 16.3, 13.2 Hz, 1H), 3.46 – 3.38 (m, 1H), 2.77 (dd, *J* = 16.3, 7.8 Hz, 1H). **^{13}C NMR (176 MHz, $CDCl_3$) δ** 175.34, 173.59, 143.73, 136.55, 134.47, 132.10, 131.73, 131.30, 130.24, 129.97,

127.97, 127.19, 124.35, 124.33, 123.69, 123.56, 123.22 (q, J = 279.8 Hz), 122.64, 110.07, 72.76, 50.82, 43.47, 42.17 (q, J = 35.6 Hz), 33.16. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{26}H_{19}BrClF_3N_2O_2Na$: 585.0168, found: 585.0158. $[\alpha]^{20}_D$ = +81 (c = 0.5, $CHCl_3$). 96% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 11.190 min, t_R (major) = 14.158 min.



4z

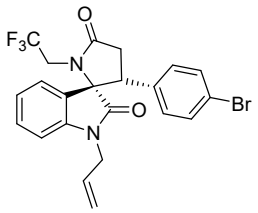
(3*S*, 3'*R*)-3'-(4-bromophenyl)-1-(4-methylbenzyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4z) was synthesized according to general procedure C as a white solid in 75% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.39 (dd, J = 7.3, 1.3 Hz, 1H), 7.31 – 7.26 (m, 3H), 7.20 (td, J = 7.6, 1.0 Hz, 1H), 7.02 (d, J = 7.9 Hz, 2H), 6.81 (d, J = 8.5 Hz, 2H), 6.54 (d, J = 7.7 Hz, 1H), 6.37 (d, J = 7.8 Hz, 2H), 4.96 (d, J = 15.8 Hz, 1H), 4.13 (d, J = 15.7 Hz, 1H), 4.02 (dq, J = 15.3, 9.5 Hz, 1H), 3.86 (dd, J = 13.2, 7.8 Hz, 1H), 3.64 (dd, J = 16.3, 13.3 Hz, 1H), 3.46 (dq, J = 15.3, 8.6 Hz, 1H), 2.77 (dd, J = 16.2, 7.8 Hz, 1H), 2.30 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.51, 173.46, 144.06, 137.27, 132.19, 131.71, 131.31, 131.18, 130.06, 129.45, 126.44, 124.21, 123.51, 123.37, 123.22 (q, J = 280.5 Hz), 122.60, 110.28, 72.85, 50.70, 43.71, 42.24 (q, J = 35.6 Hz), 33.16, 21.11. **HRM**S (ESI) calculated $[M+Na]^+$ for $C_{27}H_{22}BrF_3N_2O_2Na$:565.0714, found: 565.0709. $[\alpha]^{20}_D$ = +77 (c = 0.4, $CHCl_3$). 93% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1, 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 11.818 min, t_R (major) = 14.485 min.



4aa

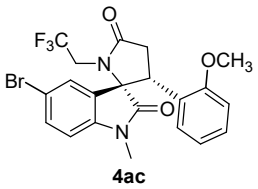
(3*S*, 3'*R*)-1-(4-bromobenzyl)-3'-(4-bromophenyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4aa) was synthesized according to general procedure C as a white solid in 67% yield. **^{1}H NMR (700 MHz, $CDCl_3$) δ** 7.40 (dd, J = 7.4, 1.3 Hz, 1H), 7.37 – 7.33 (m, 2H), 7.32 – 7.28 (m, 3H), 7.23 (td, J = 7.5, 1.0 Hz, 1H), 6.80 (d, J = 8.4 Hz, 2H), 6.48 (d, J = 7.8 Hz, 1H), 6.32 (d, J = 8.2 Hz, 2H), 4.95 (d, J = 16.1 Hz, 1H), 4.13 – 4.04 (m, 2H), 3.86 (dd, J = 13.2, 7.8 Hz, 1H), 3.63 (dd, J = 16.3, 13.2 Hz, 1H), 3.42 (dq, J = 16.7, 8.6 Hz, 1H), 2.77 (dd, J = 16.3, 7.8 Hz, 1H). **^{13}C NMR (176 MHz, $CDCl_3$) δ** 175.35, 173.54, 143.73, 133.45, 132.18, 131.96, 131.77, 131.26, 130.08, 128.15, 124.34, 123.66, 123.50, 123.21 (d, J = 281.3 Hz), 122.68, 121.57,

110.09, 72.80, 50.83, 43.39, 42.18 (q, J = 35.8 Hz), 33.05. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{26}H_{19}Br_2F_3N_2O_2Na$: 628.9663, found: 628.9652. $[\alpha]^{20}_D$ = +63 (c = 0.3, $CHCl_3$) 94% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), tR (minor) = 10.040 min, tR (major) = 12.255 min.



4ab

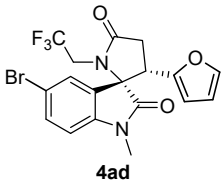
(3*S*, 3'*R*)-1-allyl-3'-(4-bromophenyl)-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4ab) was synthesized according to general procedure C as a white solid in 65% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** 7.38 (ddd, J = 9.1, 7.6, 1.3 Hz, 2H), 7.29 – 7.25 (m, 2H), 7.23 (td, J = 7.5, 0.9 Hz, 1H), 6.74 (d, J = 8.5 Hz, 2H), 6.68 (dd, J = 7.7, 1.1 Hz, 1H), 5.16 (ddt, J = 17.2, 10.4, 5.3 Hz, 1H), 4.94 (dd, J = 10.4, 1.4 Hz, 1H), 4.49 (dd, J = 17.2, 1.3 Hz, 1H), 4.18 (ddt, J = 16.5, 5.0, 1.8 Hz, 1H), 4.00 (dq, J = 15.3, 9.5 Hz, 1H), 3.78 (dd, J = 13.2, 7.8 Hz, 1H), 3.73 (ddt, J = 16.4, 5.6, 1.6 Hz, 1H), 3.57 (dd, J = 16.3, 13.2 Hz, 1H), 3.50 (dq, J = 15.2, 8.7 Hz, 1H), 2.75 (dd, J = 16.3, 7.8 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.58, 172.94, 143.78, 131.97, 131.46, 131.05, 130.11, 129.81, 124.20, 123.52, 123.35, 123.20 (q, J = 279.4 Hz), 122.46, 117.40, 109.90, 73.17, 51.18, 42.33 (q, J = 35.7 Hz), 42.12, 32.86. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{22}H_{18}BrF_3N_2O_2Na$: 501.0402, found: 501.0399. $[\alpha]^{20}_D$ = +45 (c = 0.5, $CHCl_3$). 96% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 8.270 min, t_R (major) = 11.155 min.



4ac

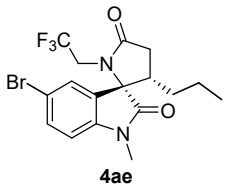
(3S, 3'R)-5-bromo-3'-(2-methoxyphenyl)-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4ac) was synthesized according to general procedure C as a white solid in 68% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** = 7.54 (d, J = 1.9, 1H), 7.43 (dd, J = 2.0, 8.3, 1H), 7.38 (dd, J = 1.6, 7.7, 1H), 7.15 (ddd, J = 1.7, 7.5, 8.4, 1H), 6.89 (td, J = 1.1, 7.6, 1H), 6.58 (dd, J = 1.1, 8.3, 1H), 6.50 (d, J = 8.3, 1H), 4.53 (dd, J = 8.1, 13.3, 1H), 3.99 (dq, J = 9.5, 15.4, 1H), 3.60 – 3.52 (m, 1H), 3.52 – 3.44 (m, 1H), 3.31 (s, 3H), 2.75 (s, 3H), 2.67 (dd, J = 8.1, 16.4, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 176.1, 173.4, 157.5, 143.2, 132.9, 129.1, 128.6, 128.4, 126.6, 121.1, 120.3, 115.2, 109.8, 109.6, 73.2, 54.1, 42.5, 33.0, 25.8. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{21}H_{18}BrF_3N_2O_3Na$: 505.0353, found: 505.0381. $[\alpha]^{20}_D$ = +57 (c = 0.3, $CHCl_3$). 94% ee as determined

by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 6.838 min, t_R (major) = 7.855 min.



4ad

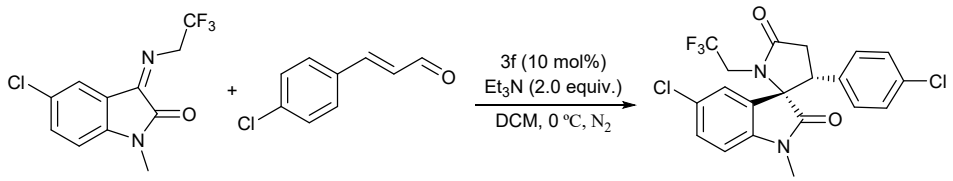
(3*S*, 3'*S*)-5-bromo-3'-(furan-2-yl)-1-methyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4ae) was synthesized according to general procedure C as a white solid in 71% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** = 7.36 (dd, *J* = 2.0, 8.3, 1H), 7.15 (dd, *J* = 0.8, 1.9, 1H), 6.63 (d, *J* = 8.3, 1H), 6.47 (d, *J* = 1.9, 1H), 6.17 (dd, *J* = 1.9, 3.3, 1H), 5.97 (dt, *J* = 0.8, 3.3, 1H), 3.95 (dq, *J* = 9.4, 15.5, 1H), 3.85 (dd, *J* = 5.3, 8.9, 1H), 3.44 – 3.33 (m, 1H), 3.33 – 3.24 (m, 1H), 3.15 (s, 3H), 2.86 – 2.78 (m, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 175.1, 174.2, 151.0, 142.3, 133.4, 128.4, 124.9, 115.5, 110.5, 110.1, 108.5, 70.1, 41.9, 33.2, 29.3, 26.6. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{18}H_{14}BrF_3N_2O_3Na$: 465.0040, found: 465.0051. $[\alpha]^{20}_D$ = +69 (c = 0.3, $CHCl_3$). 99% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 6.010 min, t_R (major) = 9.080 min.



4ae

(3*S*, 3'*S*)-5-bromo-1-methyl-3'-propyl-1'-(2,2,2-trifluoroethyl)spiro[indoline-3,2'-pyrrolidine]-2,5'-dione (4af) was synthesized according to general procedure C as a white solid in 74% yield. **^{1}H NMR (600 MHz, $CDCl_3$) δ** = 7.56 (dd, *J* = 1.9, 8.3, 1H), 7.34 (d, *J* = 1.9, 1H), 6.79 (d, *J* = 8.3, 1H), 4.01 – 3.79 (m, 1H), 3.42 – 3.31 (m, 1H), 3.19 (s, 3H), 2.75 (dd, *J* = 12.3, 16.4, 1H), 2.60 (dd, *J* = 8.0, 16.4, 1H), 2.56 – 2.46 (m, 1H), 1.38 – 1.26 (m, 1H), 1.14 – 1.00 (m, 2H), 0.80 (t, *J* = 7.2, 3H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 176.1, 173.9, 143.7, 133.7, 127.5, 126.9, 116.0, 109.7, 71.6, 46.0, 42.1 (q, *J* = 35.97), 34.3, 30.4, 26.3, 21.0, 13.9. **HRMS** (ESI) calculated $[M+Na]^+$ for $C_{17}H_{18}BrF_3N_2O_2Na$: 441.0404, found: 441.0402. $[\alpha]^{20}_D$ = +48 (c = 0.2, $CHCl_3$). 98% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 7.422 min, t_R (major) = 10.073 min.

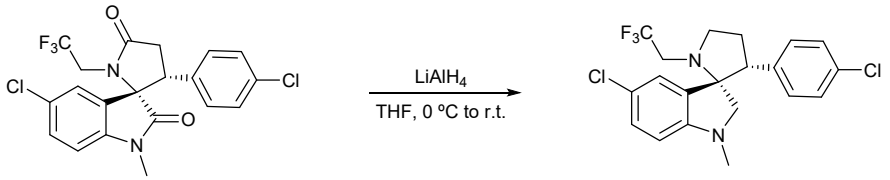
5. Gram-Scale Experiment.



1k,1.0 g **2c** **(3*S*, 3'*R*)-4l**, 73% yield and 94% ee

To a flame-dried Schlenk tube was added the co-incubation activation of 3f (0.2 g, 0.4 mmol) and Et_3N (2.0 equiv.) in dry DCM (20.0 mL) for 0.5 h, then the vial was sealed under N_2, followed by the addition of **1k** (1.0 g, 4.00 mmol) and **2c** (0.7 g, 5.00 mmol), the reaction at 0 ℃ for 48 h. Then the solvent was completely removed, the resulting residue was extracted with ethyl acetate (50.0 mL × 3), and then combined organic layers were dried over Na_2SO_4, filtered and concentrated in vacuo. The crude residue was purified via silica gel column chromatography (petroleum ether : ethyl acetate = 4 : 1) to afford the product (3*S*, 3'*R*)-**4l** (73% yield, 94% ee) as a white solid.

6. Synthetic Transformations of (3*S*, 3'*R*)-4l into (3S, 3'R)-6l.



(3*S*, 3'*R*)-4l **(3*S*, 3'*R*)-6l,** 81% yield and 94% ee

To a solution of (3*S*, 3'*R*)-**4l** (50.0 mg, 0.11 mmol) in THF (5.0 mL) was added $LiAlH_4$ (12.9 mg, 0.34 mmol) at 0 ℃. Then the mixture was stirred at room temperature and monitored by TLC until (3*S*, 3'*R*)-**4l** was consumed. The filtrate was concentrated under vacuum to give the residue, which was purified via silica gel column chromatography (petroleum ether : ethyl acetate = 3 : 1) to afford (3*S*, 3'*R*)-**6l** (85% yield, 94% ee) as a white solid. **^{1}H NMR (600 MHz, $CDCl_3$) δ** = 7.46 (d, *J* = 2.1, 1H), 7.35 – 7.27 (m, 2H), 7.16 – 7.00 (m, 2H), 6.82 (d, *J* = 8.5, 2H), 6.55 (d, *J* = 8.3, 1H), 4.72 (d, *J* = 12.6, 1H), 3.86 (dq, *J* = 8.9, 15.1, 1H), 3.64 – 3.47 (m, 1H), 2.93 (ddd, *J* = 6.6, 9.7, 14.6, 1H), 2.78 (s, 3H), 2.55 – 2.47 (m, 1H), 2.42 (dd, *J* = 9.8, 15.0, 1H). **^{13}C NMR (151 MHz, $CDCl_3$) δ** 142.3, 133.7, 133.0,

130.0, 129.4, 129.2, 128.8, 128.2, 124.8, 109.5, 85.2, 55.1, 44.1, 43.8 (q, J = 33.3 Hz), 38.7, 29.7, 26.0. 94% ee as determined by HPLC (CHIRALPAK IB N-5 Column, hexane/ethanol/diethylamine = 80/20/0.1; 1.0 ml/min, wavelength = 254 nm), t_R (minor) = 5.268 min, t_R (major) = 6.633 min.

7. Crystal Data for (3*S*, 3'*R*)-4aa

The absolute configuration of the product (3*S*, 3'*R*)-**4aa** by X-ray crystallographic analysis of a crystal. The X-ray crystallographic coordinates for the structure of (3*S*, 3'*R*)-**4aa** are available free of charge from the Cambridge Crystallographic Data Centre under deposition number CCDC 2106628.

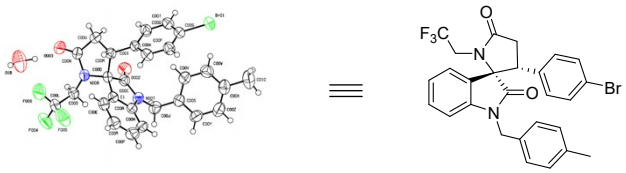


Figure. S1. X-ray structure of **(3*S*, 3'*R*)-4aa**.

Table S2. Sample and crystal data for 4aa.

Identification code	4aa
Empirical formula	$C_{27}H_{22}BrF_3N_2O_2$
Formula weight	542.08
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	monoclinic
Space group	P21
Unit cell dimensions	a = 11.3667(3) Å α = 90°
	b = 7.8133(2) Å β = 105.3130(10)°
	c = 14.3984(4) Å γ = 90°
Volume	1233.34(6) Å3
Z	2
Density (calculated)	1.512 g/cm3
Absorption coefficient	2.756 mm-1
F (000)	572

Crystal size	?×?×?
Theta range for data collection	3.18 to 68.26°
Index ranges	-13<=h<=13, -9<=k<=9, -17<=l<=17
Reflections collected	21753
Independent reflections	4471 [R(int) = 0.0373]
Coverage of independent reflections	99.8 %
Absorption correction	Multi-Scan
Refinement method	Full-matrix least-squares on F2
Data/restraints/parameters	4471 / 1 / 334
Goodness-of-fit on F2	1.050
Final R indices [I>2sigma(I)]	R1=0.0320, wR2=0.0891
Final R indices [all data]	R1=0.0342, wR2=0.0915
Largest diff. peak and hole	0.251 and -0.415 eÅ-3
Absolute structure parameter	0.020 (7)

8. Computational Details

All the density function theory (DFT) calculations were performed at B3LYP/6-31g* level [1-2] as implemented in Gaussian 16 software packages [3]. For each step, geometry optimization and transition state optimization ware employed. Frequency analysis was also conducted at the same level of theory to verify the nature of stationary points and the imaginary frequency of transition state. For more accurate energies, the Gibbs free energy was obtained by Shermo program [4] with thermal correction under 298.15 K and 1 atm. All the steps above were calculated in chloroform solvent environment based on IEFPCM model [5]

9. References

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[3] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016..

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[5] E. Cancès, B. Mennucci, and J. Tomasi. “A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anistropic dielectrics”. In: J. Chem. Phys. 107 (1997), pages 3032–41.

Cartesian coordinates of the structures

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H	-3.70645100	1.52451500	0.20412100
O	-2.18597400	2.81426700	0.56395500
N	-0.44531400	0.78161600	-0.16596000
C	0.57948200	-0.09913800	-0.37849500
N	1.29541600	1.70487000	0.84193900
N	1.62017500	0.49935800	0.22519800
C	2.98210000	0.04042400	0.31134100
C	3.84619700	0.27680900	-0.76779300
C	3.40005800	-0.60389600	1.48753200
C	5.16867900	-0.16361400	-0.64805200
C	4.73188200	-1.02354100	1.55505800
C	5.63074700	-0.81108800	0.50261700
H	5.85318600	0.00624400	-1.47593500
H	5.07360700	-1.53282900	2.45329800
C	3.37204100	0.96826400	-2.02341800
H	2.65202300	0.34898100	-2.57174000
H	2.87470300	1.91800900	-1.79650600
H	4.21337000	1.17530500	-2.69046200
C	2.43989500	-0.85939900	2.62430700
H	2.07113800	0.08133300	3.05011700
H	1.56674800	-1.42580800	2.27639100
H	2.93134100	-1.42336100	3.42232700
C	7.07174600	-1.24967500	0.61951100
H	7.67332300	-0.48964600	1.13536000
H	7.16164400	-2.17755500	1.19407500
H	7.52270900	-1.41024500	-0.36482500
C	-1.86170900	0.66263000	-0.57799500
H	-2.13418200	-0.38932400	-0.44702400
C	-2.10149500	1.05094700	-2.08113300
C	-1.42474900	0.01105800	-2.99752000

H	-0.34565700	-0.05189400	-2.82305200
H	-1.85062200	-0.98901200	-2.85715800
H	-1.57546400	0.29190100	-4.04607800
C	-3.61948300	1.01378600	-2.36227500
H	-4.07119300	0.07322300	-2.02305900
H	-4.15186900	1.84280400	-1.88486200
H	-3.79419100	1.09351700	-3.44073000
C	-1.55178700	2.44876900	-2.42893100
H	-2.01516800	3.23078300	-1.82310600
H	-0.46619900	2.50225800	-2.28597600
H	-1.75193500	2.66594300	-3.48450300
C	0.14609900	-1.99099200	-0.37431500
H	-0.62574900	-1.91203600	-1.15850100
C	1.39188400	-2.66062700	-0.89385900
H	2.29758600	-2.48825500	-0.31860900
C	1.46444000	-3.48317500	-1.95570600
H	2.45070100	-3.86768000	-2.21928400
C	0.37378700	-3.95271800	-2.83587700
C	-0.91149600	-4.26441600	-2.35232600
C	0.63403900	-4.15968100	-4.20310000
C	-1.90643600	-4.72756200	-3.21365700
H	-1.11875100	-4.16998500	-1.29067200
C	-0.36111200	-4.61948400	-5.06492700
H	1.62768600	-3.94742700	-4.59110200
C	-1.63872900	-4.90102400	-4.57423700
H	-2.89007800	-4.96635900	-2.81763500
H	-0.13777100	-4.76308700	-6.11889500
H	-2.41401900	-5.26566700	-5.24258100
O	-0.21975300	-2.18798100	0.82762300

M1

%chk=M1.chk

opt=(maxstep=5,notrust,gdiis,cartesian) freq b3lyp/6-31g(d)

scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	-0.01129800	1.42961600	0.41756000
C	-0.94411800	2.44768600	1.01673800
C	-2.65028300	0.91499400	0.37197700
H	-0.88135700	2.35471500	2.11101200
H	-0.64076700	3.46282200	0.74556000
H	-2.46090900	0.32382400	1.27968900
H	-3.72258300	0.91557800	0.18172900
O	-2.28036000	2.27811000	0.57374700
N	-0.45442300	0.43543600	-0.42165100
C	0.57391600	-0.44731800	-0.59238300
N	1.24503900	1.27223600	0.72582800
N	1.60673600	0.10478700	0.06801000
C	2.96546600	-0.35414800	0.21928900
C	3.93385100	0.11819400	-0.67994300
C	3.27025400	-1.21255000	1.28733900
C	5.25011800	-0.31462200	-0.49556900
C	4.60258800	-1.61603800	1.42253600
C	5.60367100	-1.17889500	0.54752600
H	6.01639800	0.03183900	-1.18497500
H	4.86200200	-2.29095400	2.23485100
C	3.57071700	1.04541500	-1.81472300
H	2.88907300	0.56231300	-2.52571600

H	3.06973200	1.94898900	-1.44945400
H	4.46509300	1.35080100	-2.36420900
C	2.20076200	-1.69174900	2.23719600
H	1.80443100	-0.85826600	2.83151300
H	1.35769100	-2.13127000	1.68488000
H	2.60792100	-2.43410500	2.92974800
C	7.03903500	-1.60844600	0.74027300
H	7.56825500	-0.91766400	1.40987700
H	7.10129000	-2.60574900	1.18739200
H	7.58356900	-1.62234900	-0.20926000
C	-1.88003900	0.28653900	-0.80378200
H	-2.07384100	-0.79045800	-0.78516600
C	-2.21647700	0.85638800	-2.22901400
C	-1.50141600	0.03132900	-3.31838400
H	-0.41119600	0.07277900	-3.22022700
H	-1.80954100	-1.01973100	-3.30298200
H	-1.75383300	0.43713200	-4.30454100
C	-3.73825000	0.71647400	-2.45386000
H	-4.08487000	-0.30374800	-2.24808400
H	-4.31635000	1.40820200	-1.83295400
H	-3.97616200	0.94209700	-3.49892400
C	-1.80711300	2.33375700	-2.40072900
H	-2.32783200	2.98828900	-1.69929200
H	-0.72774400	2.47114400	-2.26392500
H	-2.04774800	2.65883600	-3.41937100
C	0.32421500	-1.90504400	-1.03463400
H	-0.38493600	-1.82826600	-1.88245200
C	1.54503200	-2.62398300	-1.59451300
H	2.53060500	-2.30379200	-1.27077200
C	1.48961600	-3.67589500	-2.43318800

H	2.44047400	-4.09295900	-2.76777400
C	0.30414000	-4.35075400	-2.99236200
C	-0.94291100	-4.38686200	-2.33397700
C	0.42591800	-5.02322700	-4.22410400
C	-2.02887900	-5.04383500	-2.91448600
H	-1.03470200	-3.92574200	-1.35177800
C	-0.66183600	-5.67647400	-4.80088700
H	1.38641300	-5.02233600	-4.73518400
C	-1.89827100	-5.68534800	-4.14919200
H	-2.98189300	-5.06601800	-2.39121000
H	-0.54421900	-6.18211100	-5.75599500
H	-2.74713600	-6.19893100	-4.59301600
O	-0.22338300	-2.42637500	0.09261800

TS2

%chk=TS2Et3.chk

# opt=(maxstep=5,notrust,gdiis,cartesian) freq b3lyp/6-31g(d)
scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	0.15177100	1.63577600	0.73327400
C	-0.66897900	2.70313600	1.40748500
C	-2.57000900	1.47188300	0.74536100
H	-0.68715700	2.48625600	2.48843900
H	-0.21267800	3.68560400	1.26689600
H	-2.53217600	0.92300700	1.69945200
H	-3.61616600	1.63470500	0.48809100
O	-1.99332100	2.76771300	0.90631100

N	-0.44734100	0.55715100	0.11583200
C	0.56563200	-0.38563400	-0.14287800
N	1.43852200	1.53321400	0.80835400
N	1.73007300	0.30203400	0.21022900
C	3.10978600	-0.02610900	0.03528400
C	3.67934600	0.01975700	-1.25091600
C	3.88380000	-0.33203600	1.17118400
C	5.04043500	-0.27448000	-1.37994500
C	5.24295500	-0.60375000	0.99021500
C	5.84111800	-0.58216300	-0.27501700
H	5.48760100	-0.25039400	-2.37143500
H	5.84793900	-0.84789100	1.86092700
C	2.85077600	0.36101800	-2.46379400
H	2.13345800	-0.43702900	-2.69246900
H	2.27196600	1.27827400	-2.30714600
H	3.48799300	0.50329700	-3.34124900
C	3.26468100	-0.38347900	2.54681300
H	2.91109900	0.60451200	2.86155100
H	2.39530100	-1.05155400	2.56690500
H	3.98837300	-0.74220800	3.28435700
C	7.31788000	-0.85678400	-0.43867100
H	7.90502700	0.06597300	-0.33905900
H	7.68159500	-1.55529000	0.32225800
H	7.54016100	-1.27806700	-1.42449400
C	-1.85743700	0.64505900	-0.33757800
H	-2.25950800	-0.36725500	-0.30783700
C	-2.02964200	1.17532200	-1.81190000
C	-1.43832500	0.15850800	-2.80998300
H	-0.36076800	0.03116000	-2.67210900
H	-1.90438100	-0.82508700	-2.70580900

H	-1.60319800	0.51495300	-3.83381100
C	-3.54165500	1.29688700	-2.10763900
H	-4.07850900	0.37448600	-1.85200700
H	-4.00865100	2.12672400	-1.56694900
H	-3.69360400	1.48053600	-3.17718100
C	-1.35749000	2.54151500	-2.05572700
H	-1.77407300	3.32386800	-1.41768900
H	-0.27624300	2.49654000	-1.88044500
H	-1.50341200	2.83586000	-3.10202400
C	0.38647600	-1.70929100	-0.52714300
C	1.46751800	-2.63911600	-0.66068900
H	2.39489700	-2.28522200	-0.21927100
C	1.55889700	-3.91361200	-1.16071300
H	2.51511900	-4.39563400	-0.95635600
C	0.66743100	-4.76149300	-1.95081100
C	-0.44349100	-4.30632600	-2.69823300
C	0.98171200	-6.13868800	-2.04702000
C	-1.20206900	-5.18674000	-3.46926200
H	-0.70964800	-3.25834900	-2.66056900
C	0.22279000	-7.01533100	-2.81771900
H	1.84154700	-6.51816700	-1.49814000
C	-0.88175000	-6.54602900	-3.53573000
H	-2.04904500	-4.80278800	-4.03399600
H	0.49529000	-8.06741100	-2.86070200
H	-1.47512600	-7.22485600	-4.14263200
O	-0.93009300	-2.11411400	-0.73426200
H	-1.18772300	-2.75209400	-0.00343600
N	-1.86629100	-3.68023900	1.40003000
C	-1.34770300	-2.87559800	2.52426900
H	-0.25731200	-2.98703100	2.51941700

H	-1.55325500	-1.82639400	2.27273000
C	-3.32352400	-3.55126800	1.22284900
H	-3.88304000	-4.05724800	2.02551300
H	-3.55537700	-2.48253700	1.31257200
C	-1.33941200	-5.05729000	1.29695300
H	-1.44392300	-5.36600800	0.25161700
H	-0.26199700	-4.99372500	1.48304000
C	-1.95633500	-6.14514000	2.19029000
H	-1.49361300	-7.10892500	1.94721600
H	-1.79575500	-5.95895500	3.25572000
H	-3.03405700	-6.24980700	2.02358600
C	-1.88256500	-3.14609500	3.93981000
H	-1.59235200	-4.13176400	4.31406900
H	-1.47095400	-2.39717600	4.62690400
H	-2.97413200	-3.07016900	3.98619700
C	-3.81773800	-4.05635900	-0.13405500
H	-3.70832000	-5.14089300	-0.23637800
H	-4.88191900	-3.82133700	-0.24617400
H	-3.27055000	-3.58093300	-0.95458700

TS2-direct

%mem=128GB

%nprocshared=32

%chk=TS2.chk

opt=(calcfc,ts,noeigen,maxstep=5,notrust,gdiis,cartesian) freq

b3lyp/6-31g(d) scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	-0.27101500	1.03637100	0.62018600
C	-1.22000000	1.76440100	1.53882800
C	-2.94231400	0.74254700	0.26434800
H	-1.25395600	1.20600100	2.48735000
H	-0.85174300	2.77086900	1.75364500
H	-2.88010200	-0.15670200	0.89546100
H	-3.98885900	0.90892200	0.01248800
O	-2.52198600	1.89435500	0.99728000
N	-0.70856600	0.35008000	-0.48937500
C	0.35038600	-0.41932500	-0.94179100
N	0.98619300	0.82336800	0.86936300
N	1.38113500	-0.07974400	-0.10763500
C	2.73980200	-0.54797000	-0.06273100
C	3.72768900	0.19978400	-0.72353700
C	3.04186000	-1.68866300	0.69697600
C	5.04995800	-0.24332900	-0.62975200
C	4.38000200	-2.08956200	0.75884200
C	5.39518500	-1.38742000	0.09964200
H	5.82893900	0.32278300	-1.13520600
H	4.63427100	-2.97211700	1.34122100
C	3.37705000	1.44298000	-1.50572500
H	2.67908200	1.22266800	-2.32273900
H	2.89717900	2.19359900	-0.86716900
H	4.27399500	1.89048700	-1.94223500
C	1.96478200	-2.46644300	1.41199200
H	1.33853600	-1.81237700	2.02838600
H	1.30541000	-2.97393700	0.69735100
H	2.40525100	-3.22863000	2.06052800
C	6.82792700	-1.86225000	0.15878800
H	7.02853100	-2.41450600	1.08239300

H	7.05275800	-2.53532900	-0.67906700
H	7.53012100	-1.02436200	0.09929400
C	-2.09667200	0.53413200	-1.00049300
H	-2.36237600	-0.41781500	-1.46129600
C	-2.22420500	1.66206000	-2.09314500
C	-1.50967300	1.22651600	-3.38991300
H	-0.42722800	1.13276600	-3.24646400
H	-1.89612000	0.27183800	-3.75984900
H	-1.66640100	1.98304400	-4.16710700
C	-3.72391800	1.83756600	-2.42123200
H	-4.20318000	0.87708100	-2.64756200
H	-4.27519200	2.31359700	-1.60399900
H	-3.83343600	2.47783200	-3.30337400
C	-1.63916400	3.02139500	-1.65924500
H	-2.14937700	3.42712000	-0.78356700
H	-0.56847100	2.94854200	-1.43379500
H	-1.74556800	3.73846800	-2.48179200
C	0.30867400	-1.37128000	-2.01649500
H	-0.25789800	-0.94823700	-2.97638500
C	1.48886000	-2.18597500	-2.33327200
H	2.41323100	-1.61621900	-2.39823500
C	1.60002900	-3.49542800	-2.67582700
H	2.59074400	-3.78761400	-3.02551400
C	0.65947400	-4.61920700	-2.63283800
C	-0.54953700	-4.62766100	-1.90398800
C	1.01968300	-5.80536500	-3.30963600
C	-1.36080100	-5.76215600	-1.88142500
H	-0.86119200	-3.72761600	-1.38841700
C	0.20932700	-6.93796500	-3.28292000
H	1.95361700	-5.82909200	-3.86775500

C	-0.99118600	-6.92278500	-2.56683700
H	-2.28918100	-5.74160700	-1.31497200
H	0.51522300	-7.83312800	-3.81904100
H	-1.62485700	-7.80541600	-2.53676100
O	-1.02206400	-1.84658600	-2.39314400

M2

%chk=M2.chk

opt=(maxstep=5,notrust,gdiis,cartesian) freq b3lyp/6-31g(d)

scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	-0.14987900	1.35060600	0.56134400
C	-1.01935200	2.29387700	1.34933700
C	-2.86044000	1.22308700	0.34124800
H	-1.12656900	1.89004600	2.36934900
H	-0.55058800	3.27778100	1.42120200
H	-2.87950600	0.51461900	1.18353400
H	-3.88882100	1.43392700	0.05088600
O	-2.29793700	2.46621800	0.76116700
N	-0.69826200	0.42131900	-0.29980700
C	0.33551600	-0.44208500	-0.68693900
N	1.12679400	1.20774100	0.71781300
N	1.45704300	0.10488800	-0.07570100
C	2.77881000	-0.43042500	0.05196200
C	3.81497200	0.14866700	-0.70088000

C	3.01869700	-1.47608100	0.96050000
C	5.10669900	-0.36384100	-0.54649700
C	4.32589200	-1.96023400	1.07189400
C	5.38212700	-1.41914700	0.33061400
H	5.91646000	0.07070000	-1.12859800
H	4.52382400	-2.77614900	1.76366500
C	3.54234100	1.29122100	-1.64971300
H	2.79018900	1.02031500	-2.40028300
H	3.15673900	2.16737700	-1.11591200
H	4.45540800	1.58556300	-2.17487000
C	1.90446100	-2.06081000	1.79298400
H	1.37654300	-1.28030800	2.35298400
H	1.16137200	-2.56584800	1.16447000
H	2.29651500	-2.78858300	2.50898600
C	6.79090800	-1.93937900	0.49719700
H	7.32141200	-1.39410400	1.28913800
H	6.79634500	-2.99887900	0.77300100
H	7.37232800	-1.82150900	-0.42306100
C	-2.07546700	0.59618200	-0.82349500
H	-2.47850200	-0.40275200	-0.99436700
C	-2.14763100	1.38335400	-2.18810700
C	-1.58695100	0.51304100	-3.33274700
H	-0.53267100	0.26421900	-3.18141700
H	-2.14857400	-0.42131400	-3.43695800
H	-1.66810700	1.05931800	-4.27970600
C	-3.63099100	1.67454200	-2.50812700
H	-4.24770800	0.77040300	-2.42737800
H	-4.05617600	2.44032800	-1.85132000
H	-3.71917300	2.04231200	-3.53649000
C	-1.36687600	2.71265400	-2.16278800

H	-1.74226700	3.39076200	-1.39312800
H	-0.29717900	2.54995700	-1.98768000
H	-1.46377000	3.20983600	-3.13528300
C	0.22360600	-1.61957900	-1.41513600
C	1.31409000	-2.28673600	-2.04877100
H	2.22662100	-1.69810800	-2.08689900
C	1.37927700	-3.48065800	-2.72232200
H	2.29882300	-3.62782600	-3.28771000
C	0.45734700	-4.61489700	-2.81915000
C	-0.49893100	-4.95955800	-1.83544100
C	0.57849800	-5.48596100	-3.92765700
C	-1.30863500	-6.08570000	-1.98011300
H	-0.59944600	-4.34222100	-0.95100900
C	-0.22890700	-6.61131100	-4.06813900
H	1.32089900	-5.26076800	-4.69068000
C	-1.18692100	-6.91802300	-3.09627100
H	-2.03301000	-6.32255500	-1.20404000
H	-0.11053400	-7.25227300	-4.93866600
H	-1.81821100	-7.79625100	-3.20142200
O	-1.08434400	-2.09072300	-1.57721500
H	-1.16136000	-2.42799300	-2.48587800

R3

%mem=128GB

%nprocshared=32

%chk=R3.chk

opt=(maxstep=5,notrust,gdiis,cartesian) freq b3lyp/6-31g(d)

scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	3.28923200	-4.54020800	-7.55000200
C	2.22108700	-4.55804900	-8.46810900
C	2.99057200	-2.39722400	-8.55764200
C	3.83873000	-3.18261800	-7.54721000
N	2.06107100	-3.28491300	-9.05062500
O	3.10966200	-1.21909400	-8.86835400
N	4.81630500	-2.76609300	-6.84176300
C	5.25511800	-1.38548000	-6.94030000
C	6.39690700	-1.15747500	-5.96901300
F	6.82531400	0.12396800	-6.04482900
F	6.02936600	-1.38629200	-4.69017300
F	7.45487500	-1.95419100	-6.23053200
C	1.05740300	-2.93930600	-10.04079600
C	1.48482300	-5.71172600	-8.70287900
C	1.84566100	-6.86391700	-7.98815800
C	2.90427500	-6.85989300	-7.07315300
C	3.63685900	-5.68925400	-6.84777300
H	5.61111700	-1.13555200	-7.94606900
H	4.45731500	-0.67426800	-6.70025300
H	1.17835500	-3.54968100	-10.94176400
H	0.05024500	-3.08944300	-9.63809800
H	1.19308200	-1.88744600	-10.29474000
H	0.66175400	-5.73007900	-9.40939900
H	1.28533200	-7.77977200	-8.15328800
H	3.15734700	-7.76892900	-6.53650500
H	4.46134200	-5.66782500	-6.14153100

TS3A

%chk=TS3A.chk

opt=(calcall,ts,noeigen,maxstep=3,notrust,gdiis,cartesian) freq

b3lyp/6-31g(d) scrf=(solvent=dichloromethane)

Title Card Required

0 1

C	-4.14307800	-0.89703700	1.19176300
C	-5.01324400	-1.83579800	1.98384900
C	-3.30269100	-3.43670200	1.66385300
O	-4.70580800	-3.19262000	1.72635000
N	-2.96028900	-1.30756600	0.62016900
C	-2.32496800	-0.17907300	0.17183300
N	-4.31388700	0.39070600	1.07663800
N	-3.18160700	0.83334700	0.43100000
C	-3.01134900	2.25535800	0.24619300
C	-3.44023700	2.84020100	-0.95562600
C	-2.50653600	3.00185100	1.32102500
C	-3.32248900	4.22750400	-1.06905700
C	-2.41296300	4.38773100	1.15251500
C	-2.81437000	5.01760500	-0.03032300
C	-4.00709300	2.01442800	-2.08352400
C	-2.09957500	2.35087300	2.62139400
C	-2.73337700	6.51866600	-0.17694500
C	-2.65971900	-2.76209800	0.43860400
C	-3.09481000	-3.31361000	-0.97000200
C	-2.86516100	-4.84217500	-0.96334000
C	-4.56892500	-3.02229500	-1.31408500
C	-2.20407100	-2.70979900	-2.07637500
C	-1.00835500	-0.09152000	-0.43098100

C	0.03177700	-0.84424700	0.01520500
C	1.33436000	-1.03305100	-0.64272400
O	-0.95175600	0.75245300	-1.51979600
C	2.14363000	1.42597700	-0.39304000
C	2.85290000	1.82445800	-1.54007000
C	3.74385900	-0.22504100	-0.99062800
C	2.59540400	0.03710200	0.03365200
N	3.75691900	0.82094000	-1.90429100
O	4.50059500	-1.18604600	-1.05768000
N	2.76075500	-0.14494900	1.39502200
C	4.03964400	-0.57468700	1.88454800
C	4.98708000	0.58477400	2.17973200
F	6.18757900	0.14868300	2.65900500
F	5.26255200	1.32510100	1.07228600
F	4.49932100	1.44756100	3.10456700
C	4.70021300	0.91418800	-3.00032900
C	2.65851600	3.06622100	-2.13896800
C	1.73009200	3.93631900	-1.54906500
C	1.04261000	3.57426300	-0.38842600
C	1.26002900	2.31624400	0.20245100
C	2.56167500	-5.16870600	-0.31174700
C	2.40246900	-4.57708100	-1.56859000
C	2.01116300	-3.24196600	-1.67127600
C	1.76620000	-2.46998900	-0.52397500
C	1.92283000	-3.07679300	0.73445600
C	2.32626200	-4.41015500	0.83715100
H	-4.87132600	-1.60224900	3.05081900
H	-6.06561600	-1.67938300	1.73746700
H	-2.80848900	-3.07597000	2.57805200
H	-3.17837900	-4.51704000	1.61403200

H	-3.64394800	4.70364400	-1.99229900
H	-2.02344700	4.98730500	1.97154400
H	-3.23305000	1.37663400	-2.52393700
H	-4.81747800	1.36259700	-1.73755600
H	-4.40584400	2.66065500	-2.86995500
H	-2.95664600	1.87471300	3.11196100
H	-1.34050900	1.57461900	2.47075800
H	-1.68665300	3.09283500	3.30934500
H	-3.71920100	6.97944000	-0.03284400
H	-2.05350900	6.95716600	0.55959300
H	-2.38766600	6.80332500	-1.17644400
H	-1.58005300	-2.88568100	0.52722000
H	-1.85170100	-5.09960600	-0.63224300
H	-3.58268200	-5.36788400	-0.32566100
H	-2.98821800	-5.23008100	-1.97985200
H	-5.25490400	-3.47066600	-0.59262800
H	-4.77154500	-1.94585100	-1.36359000
H	-4.79318800	-3.43534200	-2.30388300
H	-2.33707200	-1.62852600	-2.17942100
H	-1.14181100	-2.90772200	-1.89805700
H	-2.47395000	-3.16062100	-3.03786600
H	1.25806300	-0.74177400	-1.69555200
H	-0.15313300	1.30676000	-1.42626000
H	3.92273000	-1.08736400	2.85313500
H	4.61071600	-1.25248600	1.23352300
H	4.17636300	1.02003000	-3.95691300
H	5.37263600	1.77027800	-2.86871200
H	5.28491700	-0.00658600	-3.00632800
H	-0.12626700	-1.38299500	0.94384100
H	3.21230600	3.36095000	-3.02516000

H	1.55622100	4.91032100	-1.99838400
H	0.34012700	4.26671100	0.06493100
H	0.76446200	2.04053400	1.12780600
H	2.86311600	-6.20980900	-0.23021800
H	2.58341500	-5.15610000	-2.47088400
H	1.89690600	-2.78808500	-2.65331300
H	1.76350400	-2.47885500	1.62609300
H	2.45202100	-4.85925000	1.81960700

TS3B

%chk=TS3B.chk

opt=(calcfc,ts,noeigen,maxstep=3,notrust,gdiis,cartesian) freq

b3lyp/6-31g(d) scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	3.43257200	2.24968600	-2.45368400
C	4.57479700	3.22930600	-2.48012400
C	5.89418900	1.41222400	-3.21615500
O	5.82639300	2.57680400	-2.39477700
N	3.62557600	0.89946600	-2.64419100
C	2.39091300	0.34058800	-2.74332300
N	2.16119500	2.54844700	-2.39277500
N	1.52178000	1.34921700	-2.57383700
C	0.07792300	1.28847700	-2.61052200
C	-0.60550800	1.10389700	-1.39645500
C	-0.57459100	1.45585200	-3.84055300
C	-1.99971900	1.07436400	-1.44568700
C	-1.97437900	1.41645300	-3.82646700

C	-2.70151900	1.22137000	-2.64960500
C	0.12959200	0.94090500	-0.08859200
C	0.16275900	1.65773100	-5.14293400
C	-4.21003800	1.15573900	-2.67209400
C	4.98896700	0.28706500	-2.68021600
C	5.41868700	-0.35178000	-1.30927800
C	6.88885400	-0.80890800	-1.44615200
C	5.29574500	0.61980900	-0.11858700
C	4.56121600	-1.59876000	-1.01617700
C	2.01387000	-1.03876000	3.07570600
C	2.15815800	-1.57447600	-4.30447100
C	1.58405000	-2.89440900	-4.61313800
O	1.37123000	-1.65974200	-2.03629200
C	2.63741800	-3.78243200	-7.59872400
C	1.45500900	-4.54403500	-7.78496400
C	0.70378600	-2.43593800	-7.28003200
C	2.21552300	-2.39529900	-7.34616700
N	0.33114700	-3.73741800	-7.60900800
O	-0.08577500	-1.51268400	-7.08994200
N	2.79402200	-1.23062100	-7.41772700
C	4.18295600	-1.14593000	-7.81758400
C	5.13164500	-0.89794400	-6.66104200
F	6.39581100	-0.70703100	-7.09833600
F	4.78471500	0.20957100	-5.95412000
F	5.16717000	-1.92591800	-5.77710200
C	-1.04297900	-4.18645200	-7.67567500
C	1.48998700	-5.89950600	-8.09182200
C	2.74279300	-6.51821900	-8.19535800
C	3.91977500	-5.79944600	-7.96930600
C	3.87294600	-4.43459600	-7.66100400

C	3.21612600	-6.69996200	-3.47446300
C	1.88193800	-6.57301600	-3.88618200
C	1.35908800	-5.33842800	-4.24753200
C	2.14588100	-4.14775300	-4.21696400
C	3.50593800	-4.31027000	-3.81724500
C	4.01652600	-5.55063800	-3.45031200
H	4.49862500	3.81043400	-3.41217300
H	4.50231400	3.92219400	-1.63865900
H	5.60658100	1.65201100	-4.24732300
H	6.93521500	1.09417700	-3.21818000
H	-2.55183400	0.93644400	-0.51921400
H	-2.50535100	1.54724500	-4.76616800
H	0.71880300	0.01689500	-0.08538100
H	0.81725600	1.77405800	0.09668400
H	-0.57669900	0.89488000	0.74440700
H	1.10766200	2.19116900	-5.00639200
H	0.38004300	0.69898600	-5.63058100
H	-0.45253500	2.24017900	-5.83515400
H	-4.64367600	1.62666400	-1.78362500
H	-4.61908500	1.64973500	-3.55865000
H	-4.55473500	0.11360300	-2.68752600
H	4.95135400	-0.50253400	-3.43395700
H	7.04304900	-1.41966200	-2.34409300
H	7.58687900	0.03352700	-1.47684000
H	7.15774800	-1.42239100	-0.58007800
H	5.92057900	1.50623000	-0.24503300
H	4.25995600	0.94496500	0.03609600
H	5.60932600	0.10533300	0.79662800
H	3.50707600	-1.35942300	-0.85377000
H	4.61746500	-2.33478200	-1.82522000

H	4.92702600	-2.07941400	-0.10202600
H	0.52712700	-2.89274400	-4.86968700
H	1.05374200	-2.50861900	-2.41962500
H	4.56284600	-2.01836700	-8.36329100
H	4.30174300	-0.27493900	-8.47531500
H	-1.27055500	-4.60419100	-8.66304300
H	-1.25051300	-4.94784300	-6.91426700
H	-1.67809100	-3.31721100	-7.49862900
H	2.59996800	-0.95512300	-5.09460600
H	0.57602500	-6.46633600	-8.23978500
H	2.79372700	-7.57641400	-8.43701000
H	4.88059400	-6.30328700	-8.02191200
H	4.79444100	-3.90856600	-7.44108100
H	3.62076400	-7.66671000	-3.18772500
H	1.24017600	-7.45179800	-3.91873700
H	0.31530700	-5.26351600	-4.54709100
H	4.15892500	-3.44216500	-3.82353700
H	5.06020000	-5.62553300	-3.14944200

TS3C

%chk=TS3C.chk

opt=(calcfc,ts,noeigen,maxstep=5,notrust,gdiis,cartesian) freq

b3lyp/6-31g(d) scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	3.05102100	2.32094600	-2.49162400
C	4.09543900	3.40371700	-2.53863600

C	5.51027300	1.77267600	-3.49915000
O	5.40558200	2.87309400	-2.59813100
N	3.33673800	1.01764200	-2.83301700
C	2.14509500	0.35437400	-2.88205900
N	1.77632900	2.49346900	-2.27354600
N	1.21840500	1.25829000	-2.51198700
C	-0.21849600	1.11598900	-2.47030100
C	-0.82639200	0.78544900	-1.24905500
C	-0.94285900	1.36911900	-3.64362900
C	-2.21897200	0.68919600	-1.23341400
C	-2.33624100	1.25336200	-3.56941400
C	-2.99029700	0.91572600	-2.38105800
C	-0.01336800	0.53236700	-0.00381500
C	-0.26586200	1.76124000	-4.93539000
C	-4.49680600	0.82351800	-2.32244100
C	4.74512700	0.53990900	-2.98413800
C	5.31090700	-0.13985400	-1.68307500
C	6.80675500	-0.44328400	-1.92627600
C	5.16854700	0.73841800	-0.42396600
C	4.59447000	-1.48292900	-1.42779900
C	1.89930700	-1.02936100	-3.27004700
C	2.48714900	-1.54982700	-4.37124100
C	2.34044600	-2.87145900	-4.99694700
O	1.02557900	-1.65138400	-2.40753400
C	2.70239200	-3.88109800	-7.45901700
C	1.55089000	-3.87877400	-8.27073300
C	1.56319300	-1.79066600	-7.31717000
C	2.80965900	-2.51921400	-6.79197800
N	0.89591100	-2.64269700	-8.17445100
O	1.19101300	-0.65214600	-7.04943700

N	3.90113300	-1.69020600	-6.83760600
C	5.21123700	-2.27864000	-6.78760300
C	5.91413400	-2.27059100	-8.14087500
F	7.17463500	-2.78305300	-8.04305000
F	5.27251600	-2.99958800	-9.08246500
F	6.04676000	-1.01861600	-8.64135500
C	-0.33376500	-2.29973100	-8.85841100
C	1.16108700	-4.97975000	-9.02650800
C	1.95402300	-6.13303300	-8.95908100
C	3.08789000	-6.16928900	-8.14759800
C	3.45950800	-5.04638000	-7.39074600
C	-1.24705500	-5.21331100	-4.40728600
C	0.01549600	-5.81559600	-4.36669900
C	1.16820500	-5.05394600	-4.54046500
C	1.10406100	-3.66198400	-4.76437800
C	-0.18123300	-3.07317300	-4.81560700
C	-1.33651200	-3.83903000	-4.63431800
H	3.88940800	4.03013600	-3.42053500
H	4.03138700	4.03453400	-1.64929400
H	5.12614800	2.05031600	-4.49140300
H	6.57162100	1.55088600	-3.59582500
H	-2.71372000	0.43116700	-0.29996400
H	-2.92190100	1.44179600	-4.46579800
H	0.60835100	-0.36222900	-0.12231300
H	0.65401700	1.37234700	0.22038100
H	-0.66759300	0.38051600	0.85874300
H	0.41984400	2.60299300	-4.78527900
H	0.31263300	0.93659700	-5.36834100
H	-1.01116300	2.06495700	-5.67560400
H	-4.92383600	1.69533600	-1.81029600

H	-4.93439000	0.78078600	-3.32423300
H	-4.82032400	-0.06473700	-1.76867500
H	4.74724100	-0.20207700	-3.78412800
H	6.96439300	-0.98332300	-2.86803400
H	7.41838200	0.46412100	-1.94168700
H	7.18376100	-1.07601900	-1.11609400
H	5.69793300	1.68800100	-0.52527800
H	4.11824500	0.95009100	-0.19086800
H	5.58554500	0.20230000	0.43590200
H	3.53284100	-1.35762200	-1.19583500
H	4.67577800	-2.15752000	-2.28693900
H	5.05747900	-1.97710300	-0.56642100
H	3.23291500	-3.47773400	-4.80584100
H	0.58788100	-2.38274800	-2.88725300
H	5.88032600	-1.68844100	-6.13828300
H	5.28474200	-3.31566100	-6.42305100
H	-0.21021800	-2.37523500	-9.94467100
H	-1.15159200	-2.96067600	-8.54840200
H	-0.57892200	-1.27055100	-8.59277200
H	3.16823900	-0.91409100	-4.94435800
H	0.26933900	-4.95250900	-9.64525900
H	1.67362700	-7.00725600	-9.54058200
H	3.68798300	-7.07349800	-8.09395000
H	4.33310000	-5.11093600	-6.75004100
H	- 2.14527300	-5.80780700	-4.26565500
H	0.10130500	-6.88523200	-4.19168600
H	2.14167500	-5.53607300	-4.50287900
H	-0.27111700	-2.01153100	-5.03183700
H	-2.30913700	-3.35516900	-4.67714000

TS3D

%chk=TS3D.chk

opt=(calcfc,ts,noeigen,maxstep=5,notrust,gdiis,cartesian) freq

b3lyp/6-31g(d) scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	4.55537900	-4.00366000	-0.21737900
C	3.70544900	-4.54862600	0.89887600
C	1.86023400	-3.70637200	-0.30394400
O	2.45448600	-3.89468500	0.97862700
N	4.01906800	-3.26591700	-1.25071300
C	5.01369600	-3.10428100	-2.17352200
N	5.81872000	-4.26147900	-0.41223900
N	6.10156900	-3.68988200	-1.63153400
C	7.41602500	-3.87741100	-2.20081600
C	8.42579000	-2.95755700	-1.88254000
C	7.63558100	-5.00515800	-3.00445200
C	9.69500600	-3.19054400	-2.41792800
C	8.92375100	-5.18606200	-3.51815000
C	9.96412200	-4.29425400	-3.23640500
C	8.15595600	-1.75501900	-1.01300200
C	6.53582700	-5.99661400	-3.29997300
C	11.35427500	-4.53147200	-3.77711100
C	2.64161200	-2.68685500	-1.15274400
C	2.63504600	-1.19963600	-0.63875700
C	1.16156100	-0.78747200	-0.41946600
C	3.41791100	-1.00407500	0.67495200
C	3.23107000	-0.26109100	-1.70958600

C	4.94799200	-2.46116300	-3.47768000
C	3.89269300	-2.65574100	-4.30931000
C	3.62287300	-2.13178000	-5.65386300
O	6.05862400	-1.68346100	-3.70351900
C	3.39169600	-4.32627000	-7.30676500
C	3.21005700	-4.02129100	-8.67000400
C	1.91495900	-2.47595900	-7.57349500
C	2.53836900	-3.37803100	-6.48549700
N	2.33556300	-2.93420900	-8.80694900
O	1.17619500	-1.51288600	-7.40594800
N	1.56289600	-3.82154500	-5.61985800
C	1.74993000	-5.11779100	-5.04296900
C	0.62874900	-5.39513400	-4.06227000
F	0.78722500	-6.60787200	-3.46655100
F	0.58363100	-4.48069100	-3.05111400
F	-0.59411900	-5.39680600	-4.63196000
C	1.94017100	-2.33848000	-10.06703400
C	3.83842500	-4.73396600	-9.68599000
C	4.67843900	-5.79431800	-9.31772500
C	4.87544400	-6.11610200	-7.97479700
C	4.23096200	-5.38095800	-6.96595100
C	6.77094200	-0.57213700	-8.17624000
C	5.55205700	0.10316800	-8.04647400
C	4.55137600	-0.39818500	-7.21758800
C	4.73100600	-1.59361100	-6.48967500
C	5.95940000	-2.27353800	-6.65120000
C	6.96646100	-1.76317900	-7.47606100
H	3.56906700	-5.62710900	0.72128600
H	4.21231900	-4.42194200	1.85800100
H	1.80142900	-4.65955500	-0.84600200

H	0.84481400	-3.35541900	-0.12933000
H	10.49344300	-2.48851700	-2.18991100
H	9.11692500	-6.05052000	-4.14864400
H	7.46173700	-1.06712700	-1.50890100
H	7.70979500	-2.04142400	-0.05386500
H	9.08279200	-1.21329400	-0.80690200
H	6.13178200	-6.43227000	-2.37867500
H	5.69976900	-5.52680400	-3.83130900
H	6.91154300	-6.81283700	-3.92215200
H	11.96565900	-5.08744200	-3.05428700
H	11.32960000	-5.11606000	-4.70200000
H	11.87037900	-3.58749500	-3.97992000
H	2.20561700	-2.70464600	-2.15190000
H	0.54339400	-1.00392600	-1.29901500
H	0.71592800	-1.28433300	0.44787600
H	1.11153100	0.29116200	-0.23796300
H	3.01117400	-1.60926900	1.48779200
H	4.48037600	-1.24882500	0.55774100
H	3.36354200	0.04957200	0.97088100
H	4.29460900	-0.44532500	-1.88784000
H	2.70543300	-0.34969900	-2.66645900
H	3.13602700	0.77592300	-1.36885700
H	2.81020700	-1.40179100	-5.57426000
H	6.14327500	-1.52454500	-4.66509800
H	1.73217400	-5.96381400	-5.75969000
H	2.68102400	-5.27160300	-4.45345000
H	2.81283700	-1.95582500	-10.60875400
H	1.42250200	-3.06826600	-10.69990900
H	1.26487800	-1.51260100	-9.83951800
H	3.06007200	-3.24464800	-3.93185000

H	3.68681800	-4.48147700	-10.73098400
H	5.18046900	-6.36812200	-10.09216500
H	5.53088700	-6.93944200	-7.70462300
H	4.40078300	-5.63847500	-5.92499500
H	7.55333200	-0.17651600	-8.81780600
H	5.38450900	1.03052600	-8.58859900
H	3.60866700	0.13476800	-7.12540900
H	6.11216200	-3.22676500	-6.15182000
H	7.90186400	-2.30783100	-7.57602900

M3

%mem=128GB

%nprocshared=32

%chk=C:\Users\win\Desktop\szu\coord\M3C.chk

opt=(maxstep=5,notrust,gdiis,cartesian) freq b3lyp/6-31g(d)

scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	2.94320400	2.29195200	-2.53380200
C	3.99258500	3.36363100	-2.66447700
C	5.18896300	1.80654600	-3.97909400
O	5.26134800	2.82084700	-2.97439500
N	3.14149500	1.02385000	-3.02803600
C	1.95684300	0.37032600	-2.90474400
N	1.72827100	2.44509900	-2.07382000
N	1.12210400	1.23362000	-2.30419100
C	-0.27436500	1.05029400	-1.98429000
C	-0.61571300	0.60941300	-0.69677300

C	-1.22609500	1.35552400	-2.96793900
C	-1.97572200	0.46823900	-0.41063900
C	-2.57241800	1.19250700	-2.62655200
C	-2.96659800	0.75408800	-1.35798000
C	0.43586600	0.28290300	0.33470600
C	-0.82584600	1.83919900	-4.34101000
C	-4.42886500	0.61742000	-1.00607100
C	4.49563800	0.54023400	-3.45479100
C	5.23811200	-0.24282200	-2.30376800
C	6.73404400	-0.35324600	-2.67539000
C	5.12127100	0.43946600	-0.92615100
C	4.66879000	-1.67572800	-2.20965800
C	1.66418600	-0.97567600	-3.38069600
C	2.01360100	-1.34850800	-4.62407400
C	1.91357300	-2.76345600	-5.13226600
O	1.09372600	-1.77890000	-2.41797200
C	2.82367200	-4.30374000	-6.96553400
C	2.25680800	-4.31720300	-8.24810900
C	2.14617900	-2.11186400	-7.60160900
C	2.82840400	-2.87707600	-6.40491000
N	1.85150900	-3.01620500	-8.60223800
O	1.93249400	-0.90332500	-7.68503100
N	4.09718100	-2.34890900	-6.00260300
C	4.99938900	-2.20621300	-7.10398200
C	6.29349800	-1.55920700	-6.66296800
F	7.16813000	-1.44262100	-7.69855300
F	6.11996500	-0.29651100	-6.17735000
F	6.94145400	-2.25240600	-5.69328500
C	1.27070400	-2.65059900	-9.87832400
C	2.16331700	-5.47986900	-9.00697900

C	2.66723800	-6.66331700	-8.44599500
C	3.25179000	-6.66627200	-7.17752700
C	3.33787500	-5.47684600	-6.43536300
C	-2.16632000	-4.23770200	-5.42548100
C	-1.18447900	-4.99376800	-4.78443200
C	0.12468200	-4.51196100	-4.69744800
C	0.47781100	-3.26913200	-5.24682900
C	-0.52465400	-2.51518500	-5.88196000
C	-1.83054900	-2.99665100	-5.97442500
H	3.66435100	4.06261600	-3.44987900
H	4.08546400	3.92055200	-1.72939900
H	4.64979000	2.18137500	-4.86137300
H	6.21073300	1.58450400	-4.27783100
H	-2.26706600	0.12461100	0.57893800
H	-3.33003000	1.41867000	-3.37269700
H	1.01946600	-0.59374500	0.03047200
H	1.13636900	1.11359100	0.47612400
H	-0.02764900	0.06274300	1.29984600
H	-0.18462200	2.72613700	-4.28427100
H	-0.27209300	1.07035600	-4.89312500
H	-1.71027400	2.09890400	-4.92815000
H	-4.78933800	1.51097900	-0.47996500
H	-5.04578600	0.49234500	-1.90111200
H	-4.60207100	-0.23865200	-0.34570200
H	4.35449600	-0.14204300	-4.29861400
H	6.87599200	-0.77261400	-3.67536800
H	7.24336300	0.61457200	-2.62283900
H	7.22887900	-1.02060500	-1.96149200
H	5.53298400	1.45210700	-0.93634900
H	4.08431900	0.48625500	-0.57264000

H	5.68166300	-0.14613700	-0.18856300
H	3.63923800	-1.69270800	-1.83843600
H	4.68777800	-2.17457200	-3.18525800
H	5.27318400	-2.25885800	-1.50495600
H	2.42827800	-3.39996300	-4.39832700
H	0.60960300	-2.49699100	-2.86501300
H	5.32026200	-3.15503200	-7.59715700
H	4.64907200	-1.56126600	-7.94432800
H	1.94474200	-2.90794800	-10.70380800
H	0.31366100	-3.16189300	-10.03278700
H	1.10784700	-1.57183200	-9.86661200
H	2.41104800	-0.61210400	-5.30780000
H	1.72073700	-5.47923600	-9.99870200
H	2.60700400	-7.58695800	-9.01576700
H	3.64662800	-7.59157400	-6.76633400
H	3.81358800	-5.46683900	-5.45710500
H	-3.18529000	-4.60880200	-5.49447900
H	-1.43297900	-5.95908600	-4.35146400
H	0.88653800	-5.11141300	-4.20490200
H	-0.27454100	-1.54939000	-6.31082700
H	-2.58942900	-2.39930200	-6.47314200

TS4

%mem=128GB

%nprocshared=32

%chk=TS4.chk

opt=(calcfc,ts,noeigen,maxstep=5,notrust,gdiis,cartesian) freq

b3lyp/6-31g(d) scrf=(solvent=dichloromethane) nosymm int=superfine

Title Card Required

0 1

C	1.92924800	1.99816800	-3.10302200
C	2.05552600	3.32259900	-3.80745400
C	3.95263800	2.39134000	-4.87387900
O	3.37381300	3.54982400	-4.27257300
N	2.87884900	1.01194900	-3.24681700
C	2.38421200	-0.10981500	-2.65258300
N	0.89945100	1.57707200	-2.42126000
N	1.19725900	0.26287600	-2.13261300
C	0.26263000	-0.53034000	-1.37100500
C	0.50044200	-0.72172300	-0.00090300
C	-0.87830600	-1.02517000	-2.02212800
C	-0.44400100	-1.46349600	0.71525200
C	-1.78805700	-1.75925700	-1.25637200
C	-1.58627700	-1.99575600	0.10806600
C	1.72280000	-0.16236400	0.68240100
C	-1.12749300	-0.77497600	-3.48876100
C	-2.57036600	-2.82170300	0.90201000
C	4.22023800	1.28809000	-3.83656500
C	5.30509900	1.61284100	-2.73983000
C	6.54819400	2.20024700	-3.44453800
C	4.81178900	2.61528800	-1.67712000
C	5.73481700	0.30873500	-2.03501900
C	2.94666500	-1.45682600	-2.69550300
C	3.13247100	-2.29957400	-3.72869800
C	2.84735500	-2.13652500	-5.19741000
O	3.28091400	-2.05642200	-1.51907700
C	3.88116800	-2.22206200	-7.54585400
C	3.73993200	-3.40248600	-8.29206600
C	4.20958900	-4.13298100	-6.16499900

C	4.09251600	-2.57767100	-6.08905900
N	3.91588100	-4.51911400	-7.45828800
O	4.54235400	-4.88972000	-5.26370900
N	5.27818900	-1.94614700	-5.50603500
C	6.54531600	-2.32896700	-6.11775500
C	7.64918700	-1.38629100	-5.68886600
F	8.83097800	-1.75610100	-6.22856700
F	7.41610500	-0.10924200	-6.06944000
F	7.80860500	-1.37595300	-4.34222300
C	3.91992200	-5.89812700	-7.90729900
C	3.49222300	-3.38113800	-9.66081100
C	3.40057000	-2.12852800	-10.28448800
C	3.55726300	-0.94517400	-9.55958500
C	3.79860900	-0.99010300	-8.17731500
C	-0.80786000	-4.16308600	-6.41474200
C	-0.47725900	-2.91769200	-6.95145900
C	0.69830000	-2.27403700	-6.55577600
C	1.56404200	-2.85850300	-5.61966900
C	1.21534700	-4.10730900	-5.08150300
C	0.04415400	-4.75443000	-5.47782600
H	3.48981500	-2.94618900	-2.40682500
H	5.27790600	-2.18874300	-4.51304500
H	1.34220000	3.32946600	-4.64656900
H	1.79588700	4.14178300	-3.13325100
H	3.29097100	2.00079900	-5.66172200
H	4.88135400	2.71557000	-5.33984400
H	-0.28111700	-1.62432500	1.77824600
H	-2.67764800	-2.15425000	-1.74105800
H	2.61983500	-0.67773800	0.32052100
H	1.84427600	0.90898600	0.48283700

H	1.65324000	-0.29830600	1.76515400
H	-2.05740500	-1.25376200	-3.80644400
H	-1.20512700	0.29687700	-3.70387100
H	-0.31772700	-1.17646100	-4.10774300
H	-2.57126800	-2.53676300	1.95892100
H	-3.58864600	-2.71300500	0.51475500
H	-2.31495900	-3.88830000	0.85159600
H	4.52792200	0.38439000	-4.37184900
H	6.88190100	1.56767100	-4.27420000
H	6.37004700	3.21182100	-3.82400200
H	7.37216800	2.26202800	-2.72540800
H	4.50806400	3.56602700	-2.12190900
H	3.97334600	2.21721900	-1.09397500
H	5.62497200	2.81551000	-0.97042200
H	4.90895200	-0.21481800	-1.54524800
H	6.19941700	-0.38576700	-2.74177100
H	6.47921300	0.54529900	-1.26560500
H	2.71643600	-1.07481100	-5.46154700
H	6.87436900	-3.35052500	-5.87686900
H	6.46597900	-2.24765600	-7.20548200
H	2.93779900	-6.17937500	-8.30209800
H	4.67494200	-6.05133300	-8.68661300
H	4.15711500	-6.52298900	-7.04544100
H	3.37952300	-4.29698100	-10.23208200
H	3.21043300	-2.08401900	-11.35332100
H	3.49437200	0.01319600	-10.06658400
H	3.92878800	-0.07248600	-7.60978800
H	-1.72242500	-4.66574400	-6.71847400
H	-1.13340500	-2.44320100	-7.67682700
H	0.94816400	-1.30559800	-6.98186100

H	1.86771400	-4.56121800	-4.34324800
H	-0.20672700	-5.72113400	-5.04834600

M4

%mem=30GB

%nprocshared=22

%chk=M4.chk

opt=(maxstep=5,notrust,gdiis,cartesian) freq b3lyp/6-31g(d)

scrf=(solvent=dichloromethane) nosymm

Title Card Required

0 1

C	2.23609500	1.90024100	-3.17217800
C	2.52478000	3.23007100	-3.81669400
C	4.43224200	2.19750800	-4.72526100
O	3.89475900	3.37815200	-4.12658300
N	3.09760000	0.83190800	-3.27169600
C	2.46357700	-0.22804200	-2.70456100
N	1.13166700	1.57142700	-2.55482700
N	1.28746400	0.24555200	-2.24970800
C	0.22355800	-0.41889400	-1.52235200
C	0.35460700	-0.57613200	-0.13260900
C	-0.93479200	-0.78243000	-2.22588500
C	-0.70994900	-1.17740300	0.54346000
C	-1.96556000	-1.38157500	-1.49548500
C	-1.87191700	-1.59296700	-0.11642400
C	1.57430700	-0.10928100	0.62133000
C	-1.08718200	-0.53429000	-3.70573400

C	-3.01285700	-2.21739700	0.65069100
C	4.51743700	1.03341900	-3.72988200
C	5.49272900	1.23460800	-2.50314100
C	6.79367800	1.90615500	-2.99792500
C	4.89510600	2.11657400	-1.38778900
C	5.86226100	-0.14200900	-1.91276400
C	2.88280100	-1.68731700	-2.61080500
C	3.56547700	-2.32788900	-3.76360400
C	2.88993600	-2.22727100	-5.15195700
O	2.62450500	-2.25751200	-1.55613300
C	3.49752700	-2.12485500	-7.64659700
C	3.62663300	-3.30367900	-8.39603000
C	4.49243800	-3.84849600	-6.33548300
C	4.04724400	-2.34411600	-6.23416200
N	4.19783800	-4.31406300	-7.60192900
O	5.03544700	-4.51759000	-5.46203600
N	5.08223000	-1.43529100	-5.84389400
C	6.28891200	-1.61213000	-6.59531800
C	7.36361300	-0.66062700	-6.12308100
F	8.49613300	-0.78695400	-6.86081700
F	6.99131400	0.64501600	-6.21280300
F	7.72480700	-0.86699800	-4.82944000
C	4.50627200	-5.65311200	-8.06214100
C	3.24627600	-3.37721800	-9.73287200
C	2.72994400	-2.21634300	-10.32727700
C	2.61679600	-1.02719600	-9.60350100
C	3.01185900	-0.97879800	-8.25673500
C	-0.47955600	-4.88448100	-5.87328600
C	-0.46776700	-3.58710200	-6.38778300
C	0.61718900	-2.74466100	-6.13694000

C	1.71449700	-3.17148500	-5.37116300
C	1.68806000	-4.48143500	-4.86578800
C	0.60461400	-5.32705400	-5.11281100
H	3.75946300	-3.36124500	-3.47492400
H	4.56016000	-1.86155100	-3.97167700
H	1.90718600	3.30257400	-4.72616900
H	2.23921200	4.04268500	-3.14511300
H	3.82052700	1.89277100	-5.58672500
H	5.42492400	2.44839600	-5.09126300
H	-0.62786500	-1.31879100	1.61826500
H	-2.86685200	-1.68463500	-2.02231200
H	2.45530100	-0.69141800	0.33313900
H	1.78738400	0.94853600	0.42691100
H	1.42509200	-0.22626100	1.69783500
H	-0.97387000	0.52866300	-3.94579800
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H	6.62625600	2.94725700	-3.29196600
H	7.52273800	1.91005600	-2.18038300
H	4.62041800	3.10795700	-1.75784900
H	4.01718900	1.65986300	-0.91763900
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H	-1.32321700	-5.54295300	-6.06198500
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O	-2.80326000	-4.66853300	-4.19157100

N	-0.58838300	-4.13278600	-5.84084800
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C	0.66305900	-0.97357800	-8.47302600
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C	2.10710900	0.99960100	-8.41620500
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O	-2.76661800	-4.75571900	-4.17905800
N	-0.58656900	-4.12319500	-5.82604200
C	0.45850100	-3.55477600	-6.50417400
N	-0.92731500	-1.94303900	-5.66728400
N	0.19267100	-2.23526600	-6.42745200
C	0.83481600	-1.13608400	-7.11006600
C	0.60127200	-0.97786600	-8.48488800
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C	-0.26643300	-1.92836400	-9.27726700
C	1.79904700	-0.36747200	-4.88560600
C	2.58902600	2.23038200	-9.14239400
C	-1.02761100	-5.53881600	-5.72854700
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N	3.29538200	-8.60970300	-6.53617000
O	1.31193500	-7.59175500	-7.17373300
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C	2.27141100	-5.39979300	-4.57293700
C	3.01777800	-4.44910900	-3.64658400
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C	6.91334200	-6.89418400	-5.38812600
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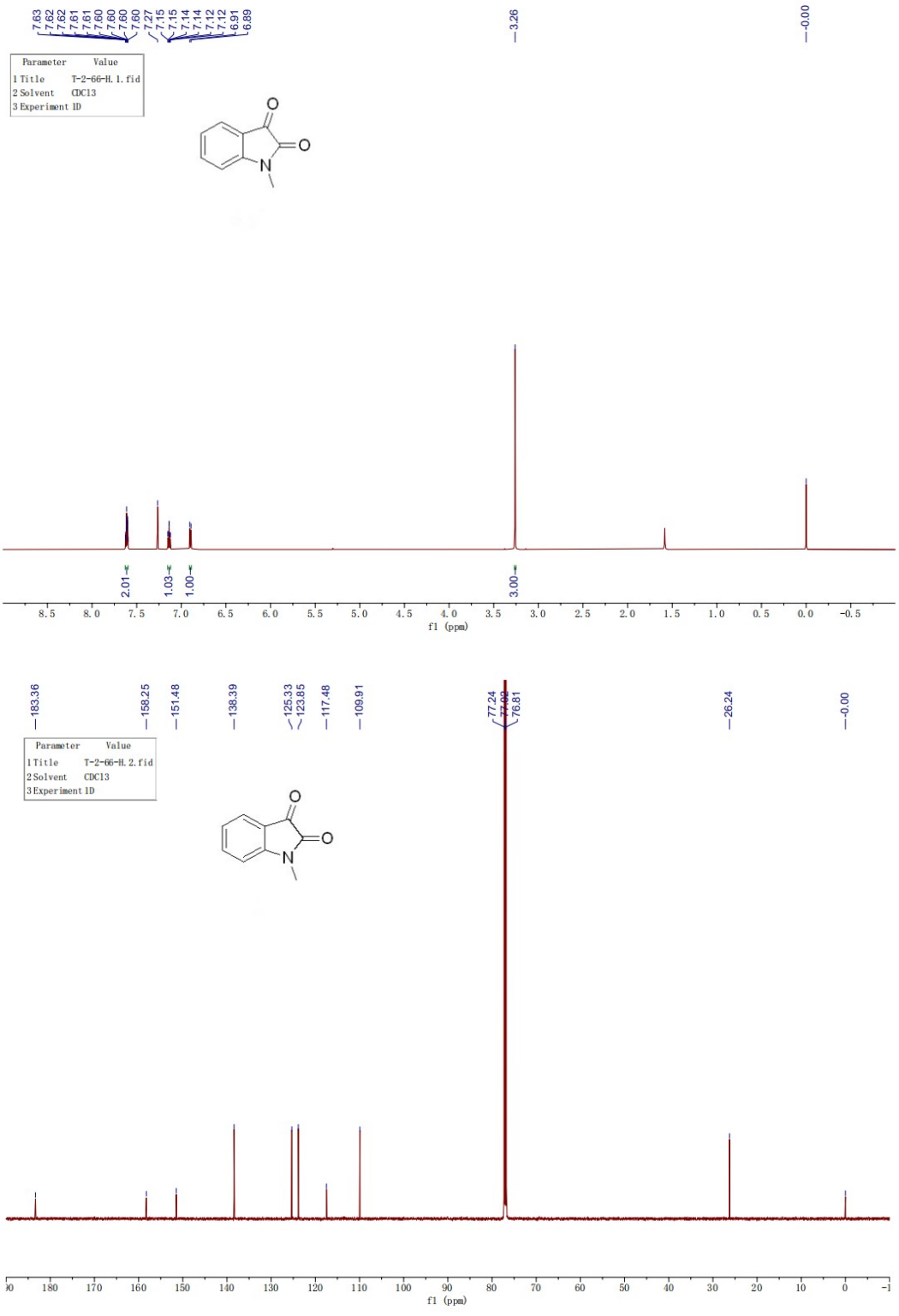

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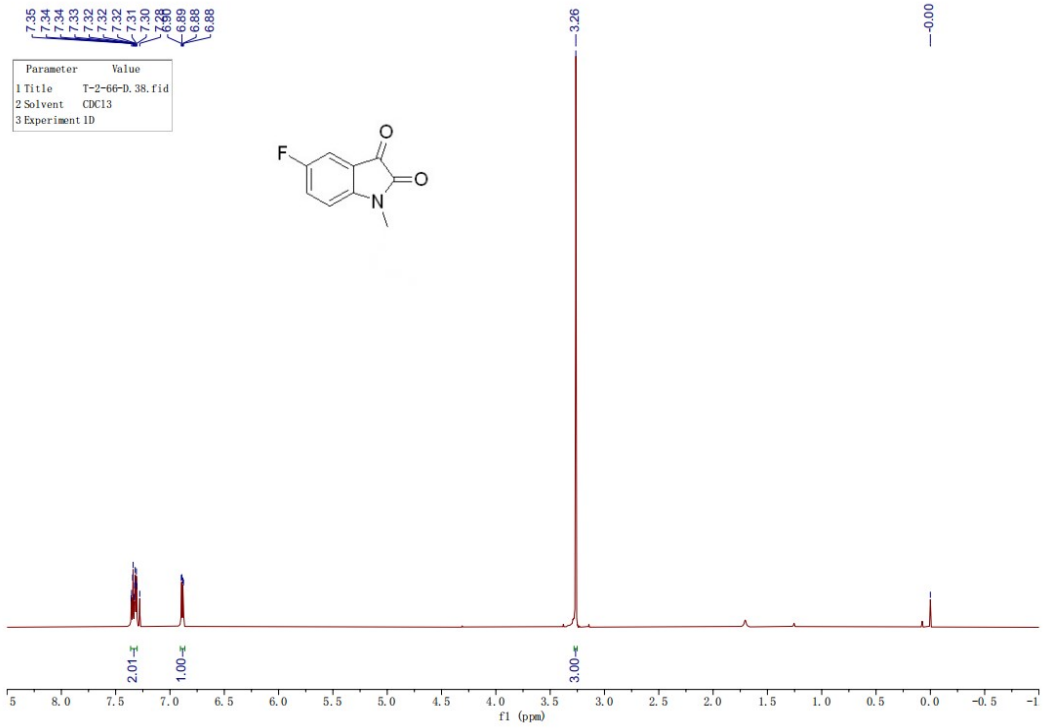

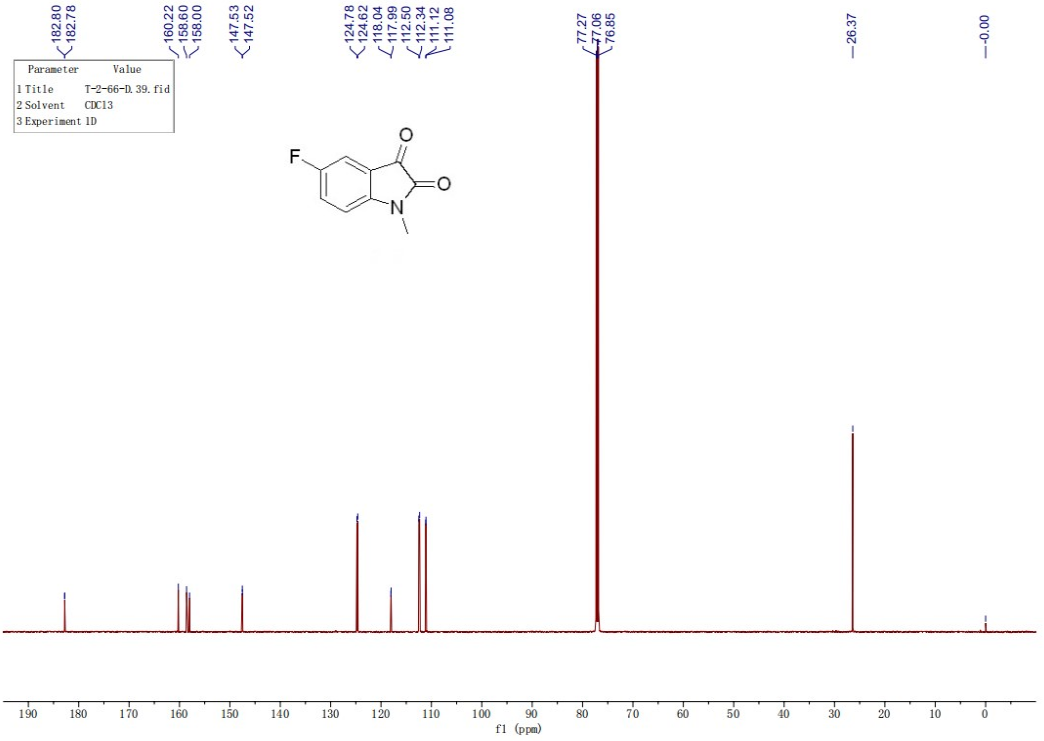

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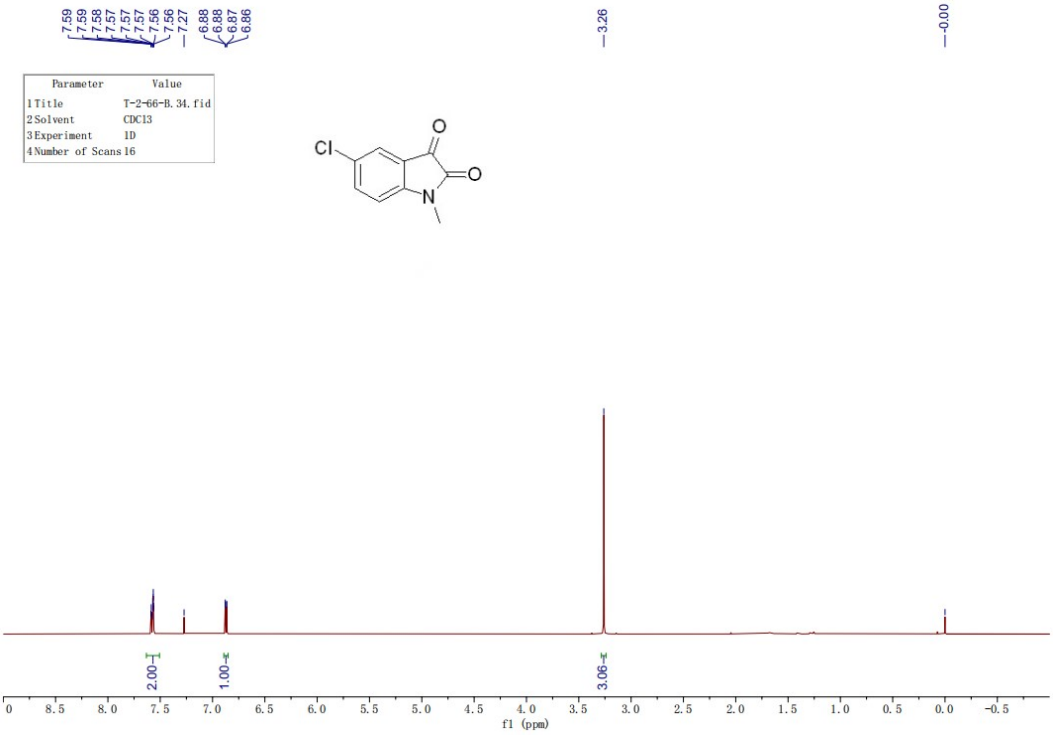

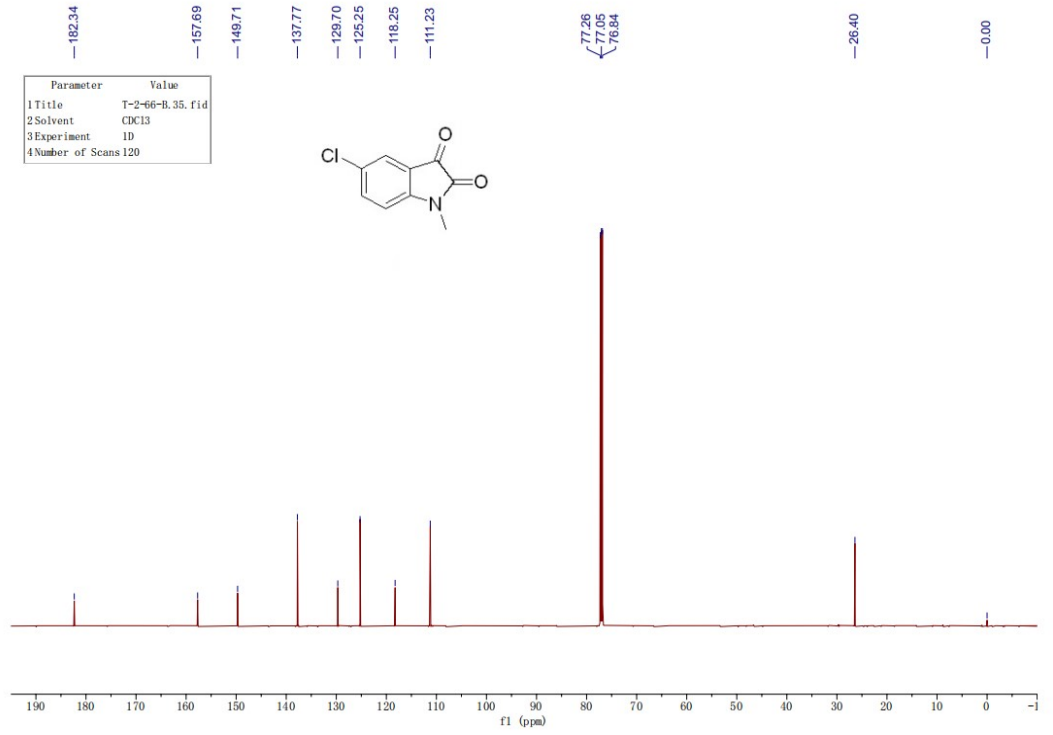

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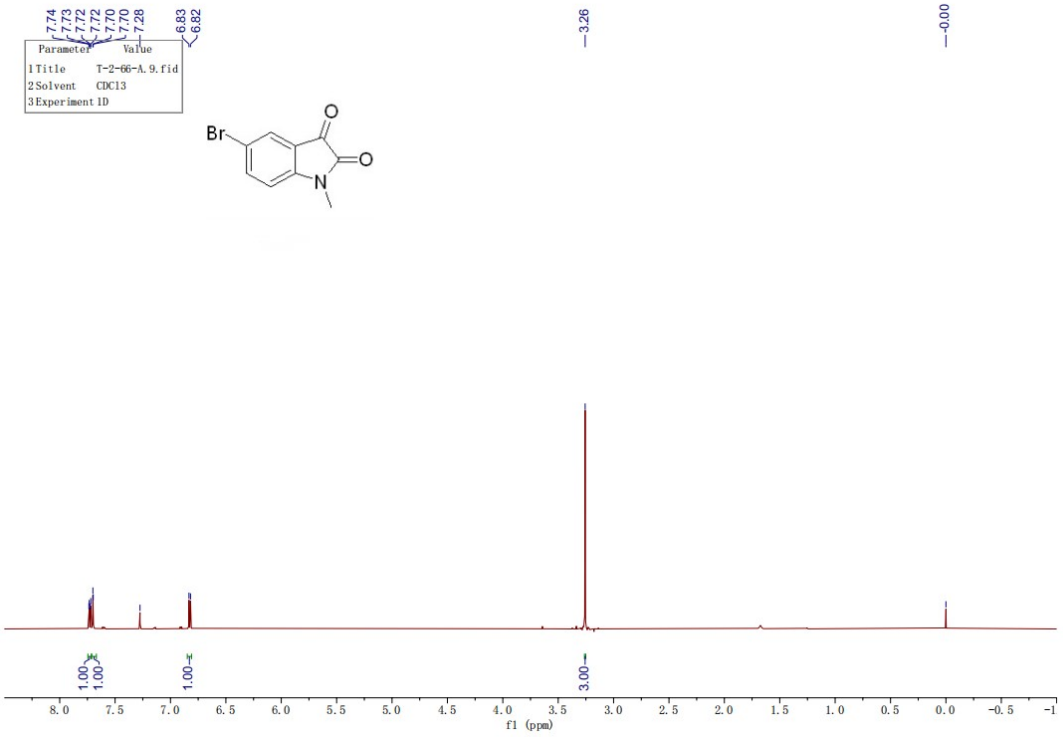

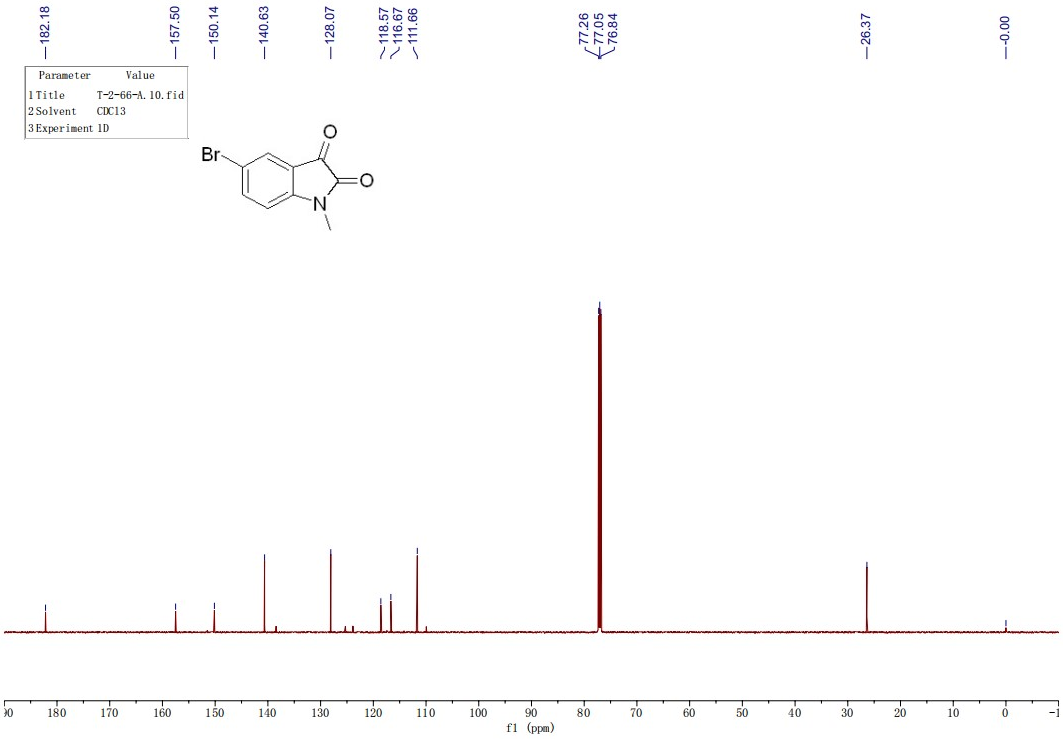

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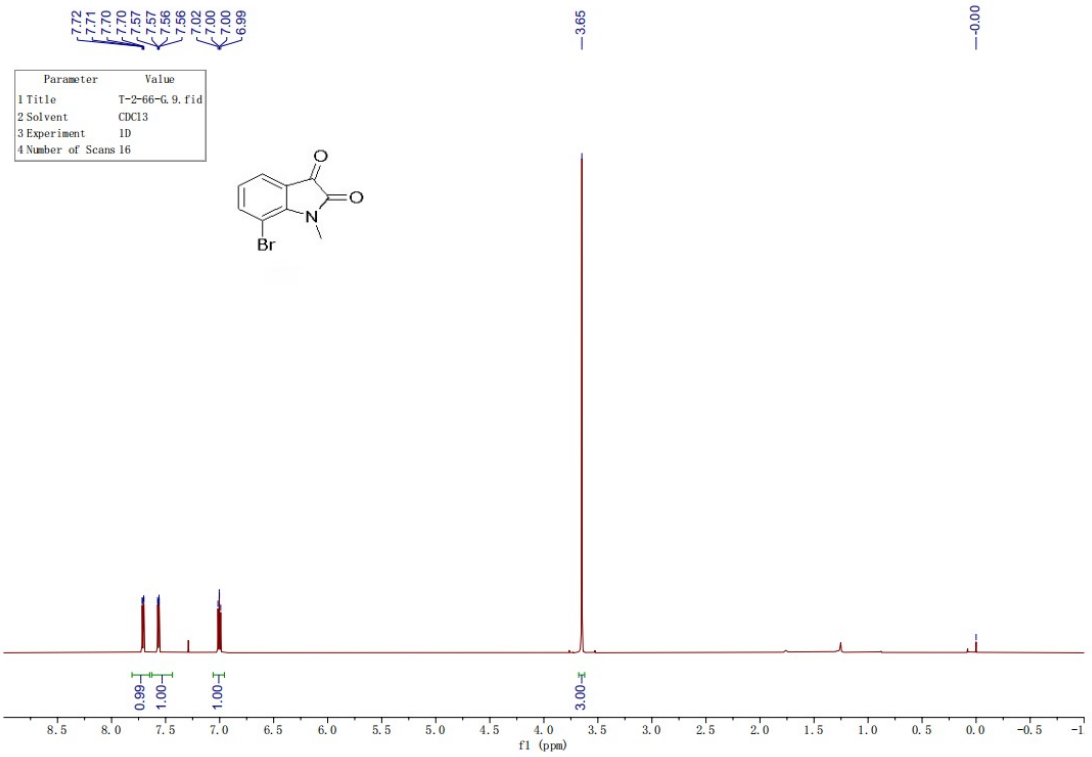

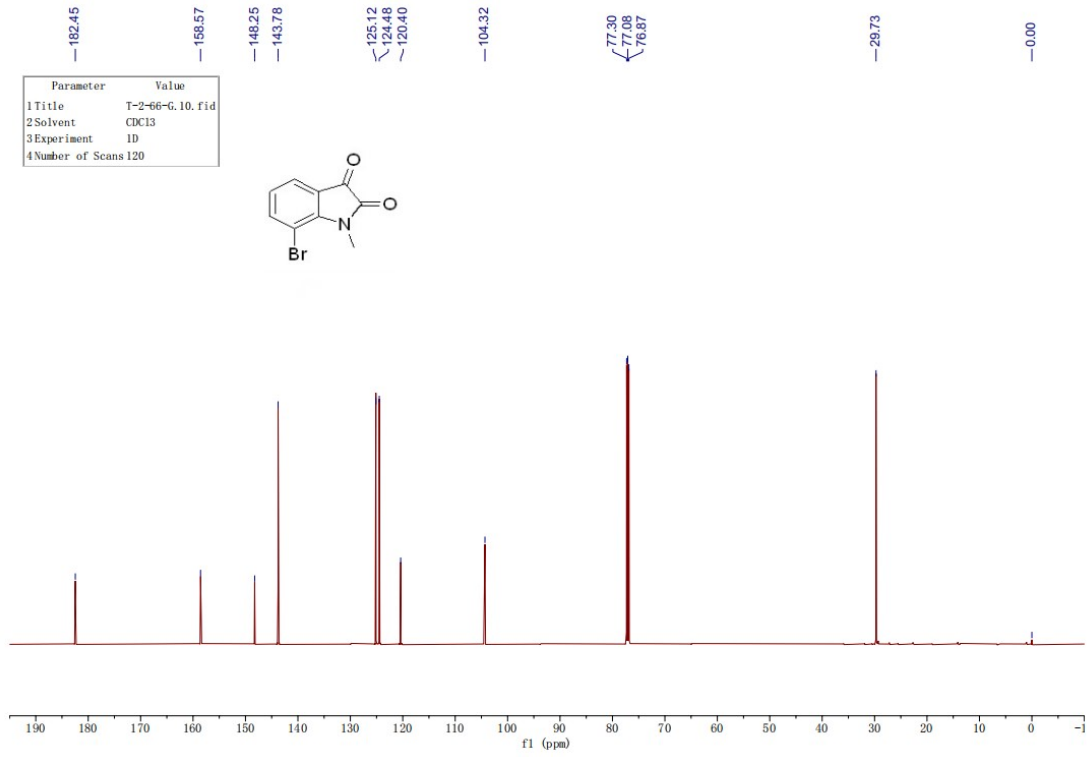

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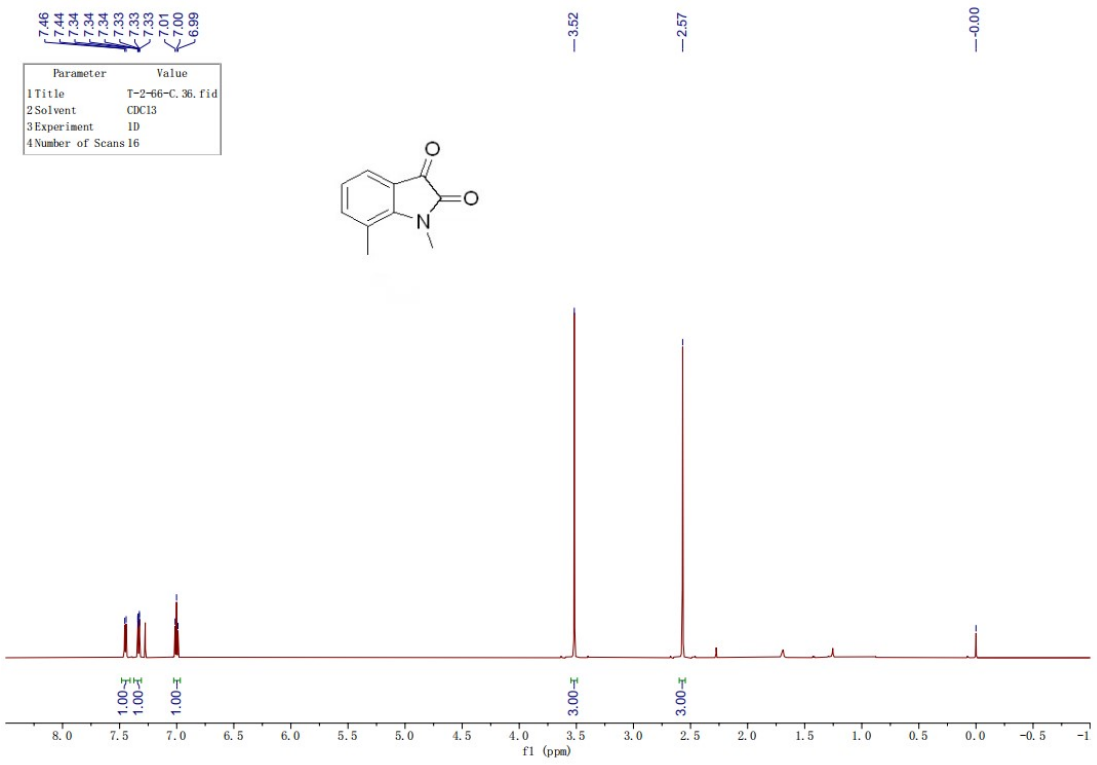
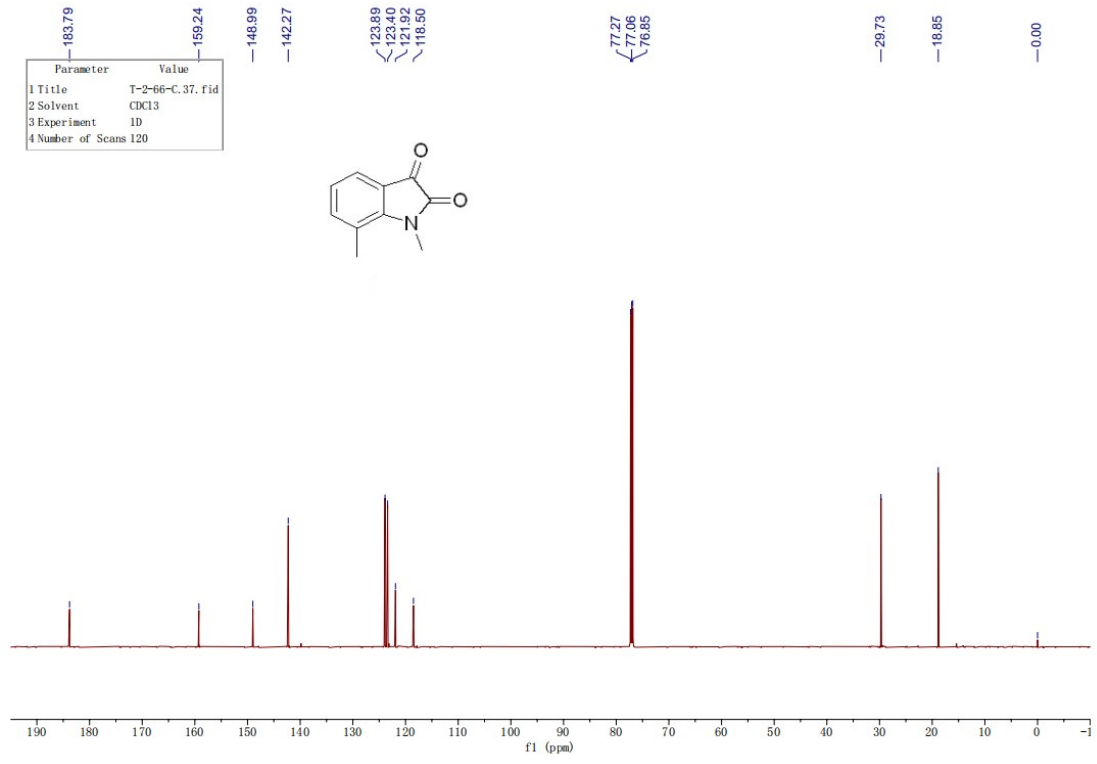
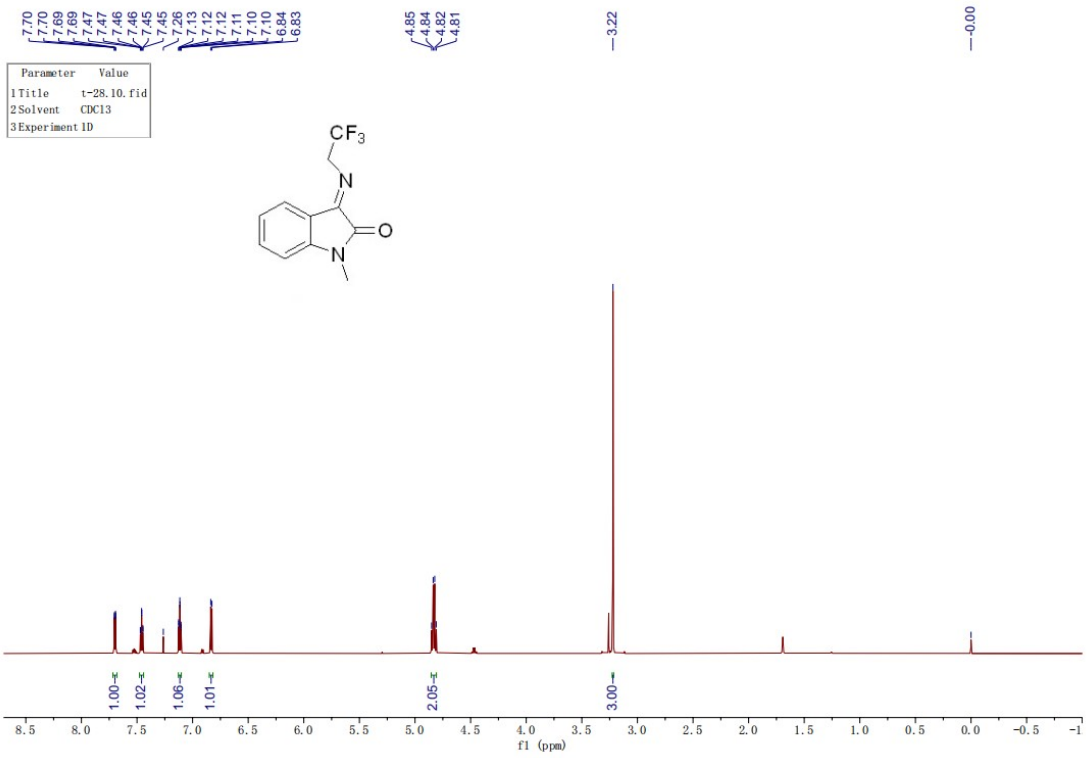
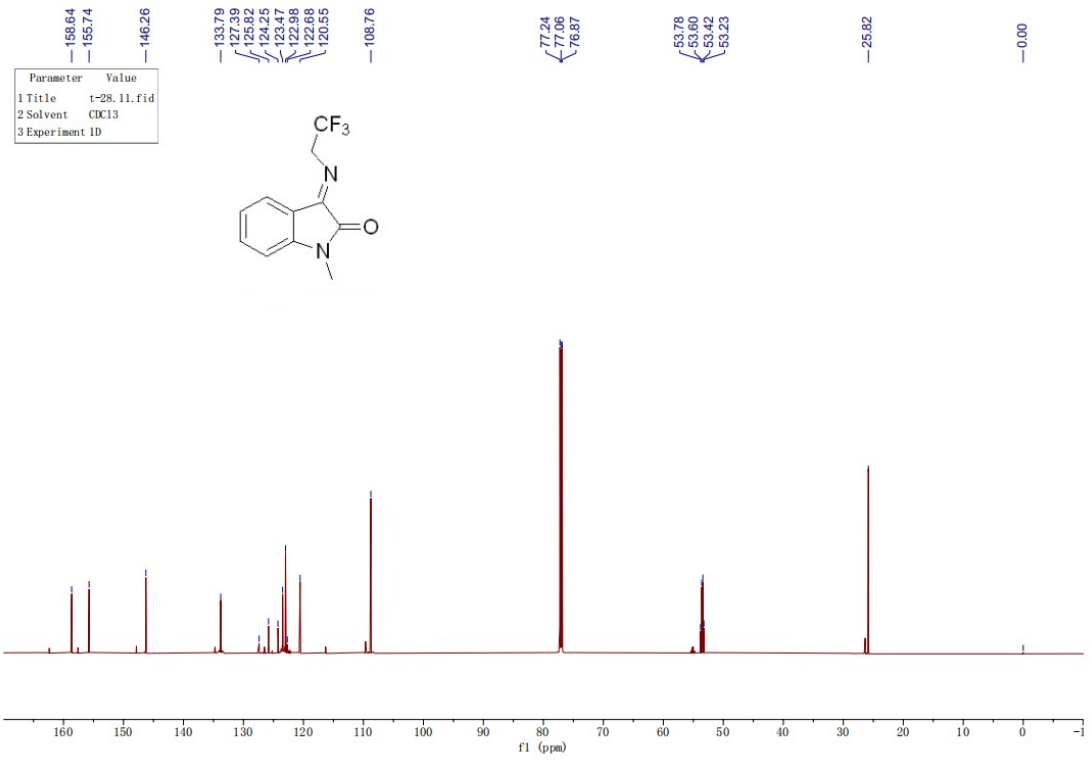


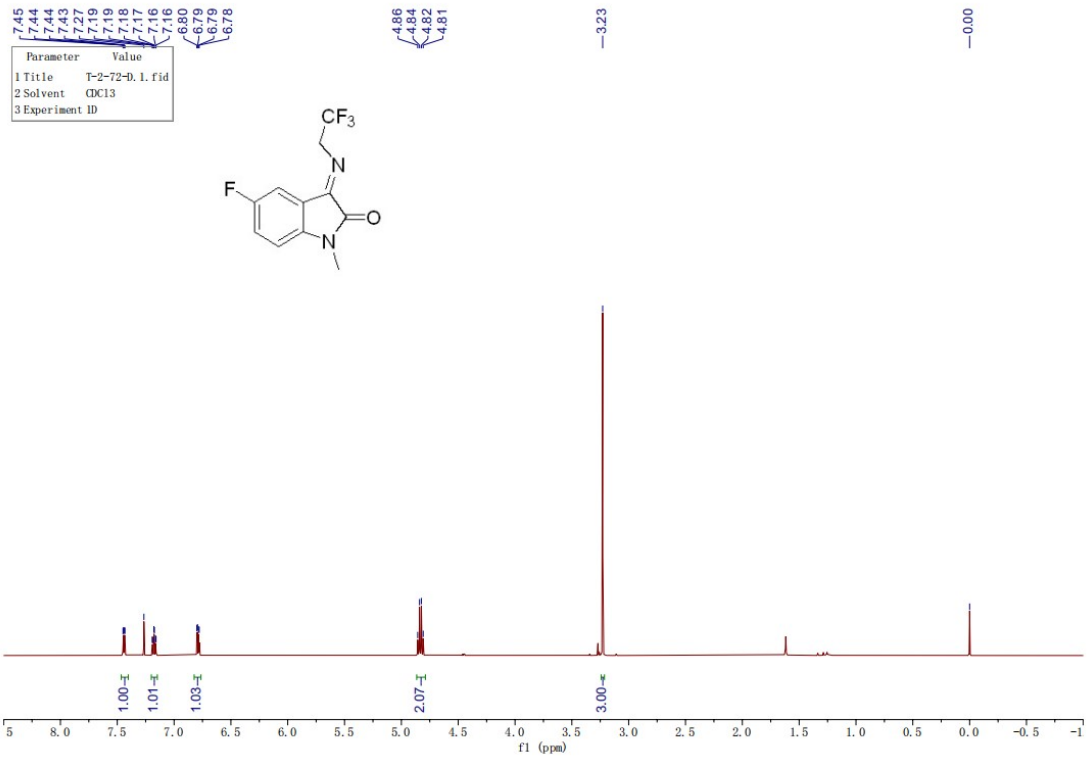


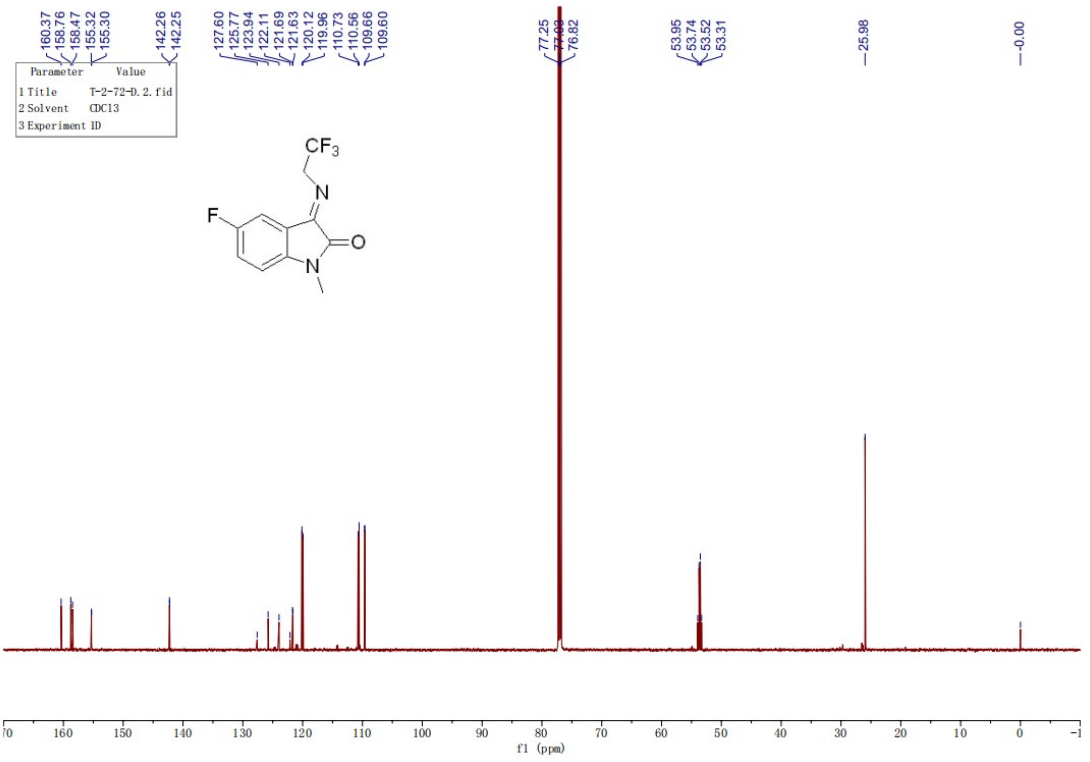
^{1}H-NMR and ^{13}C-NMR of **1f'**



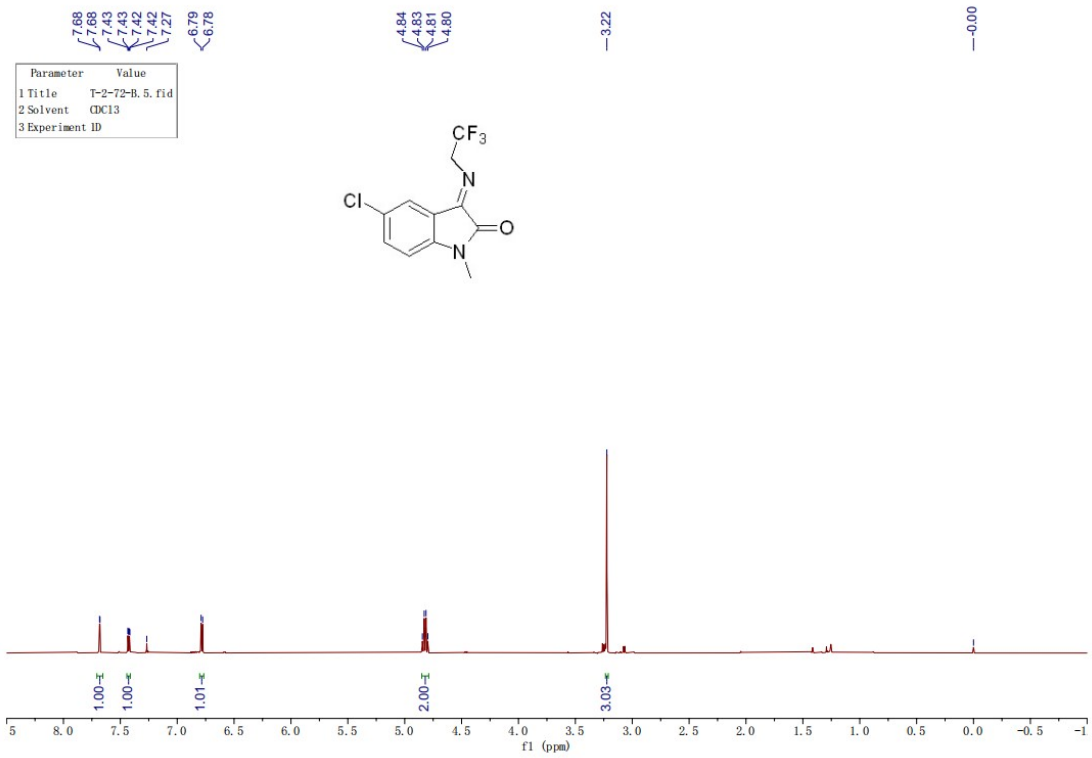


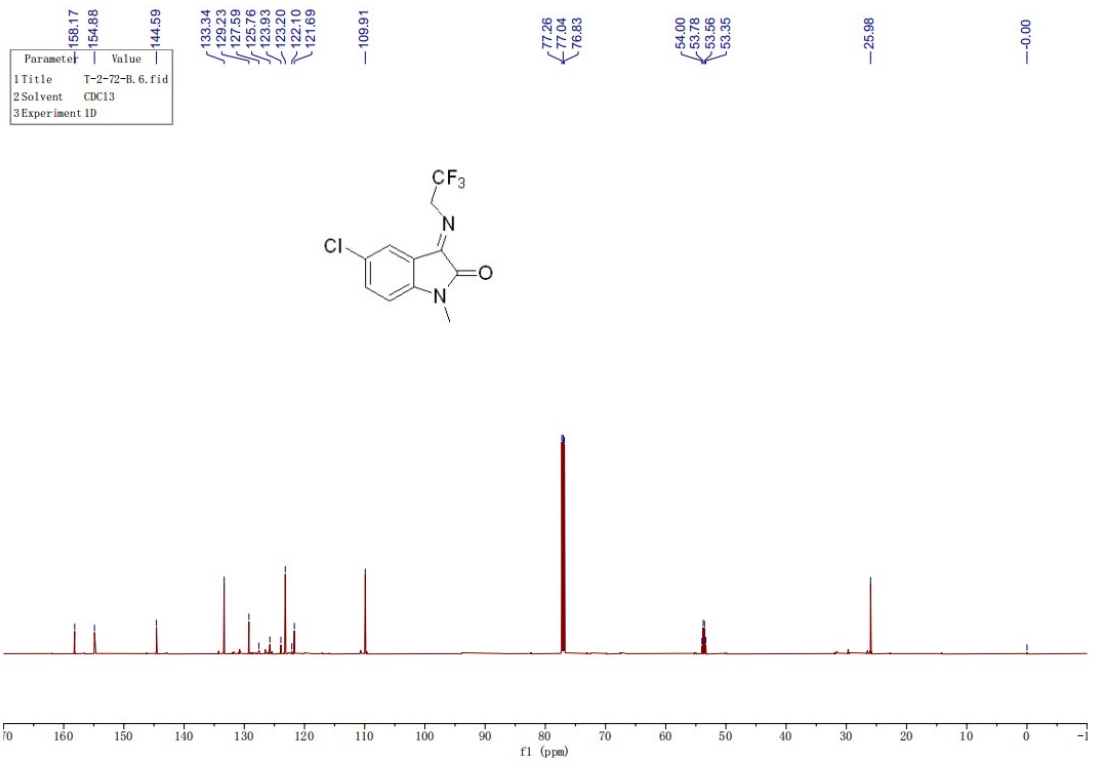
^{1}H-NMR and ^{13}C-NMR of **1a**



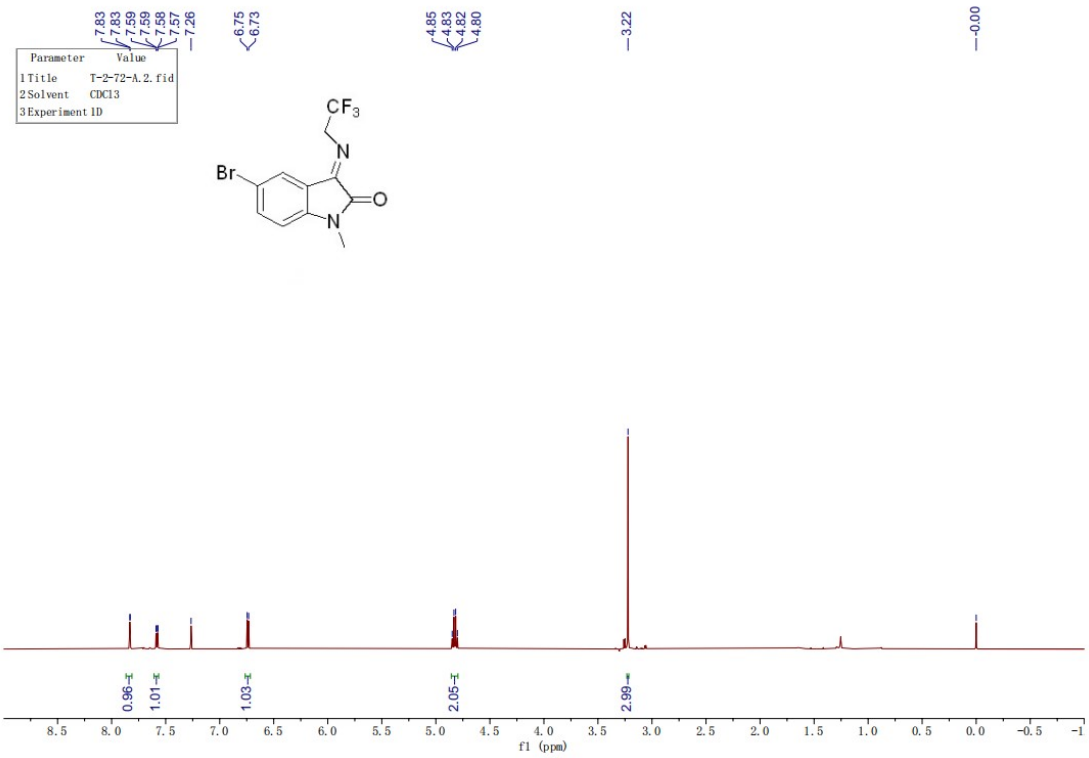


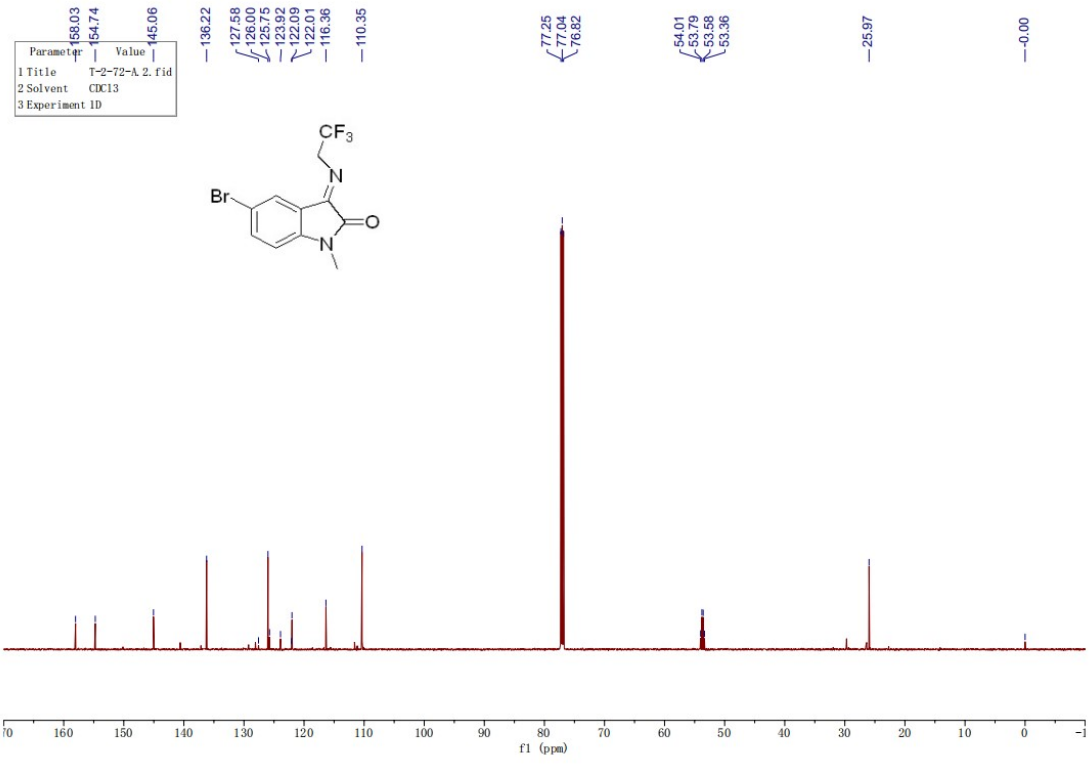
^{1}H-NMR and ^{13}C-NMR of **1b**





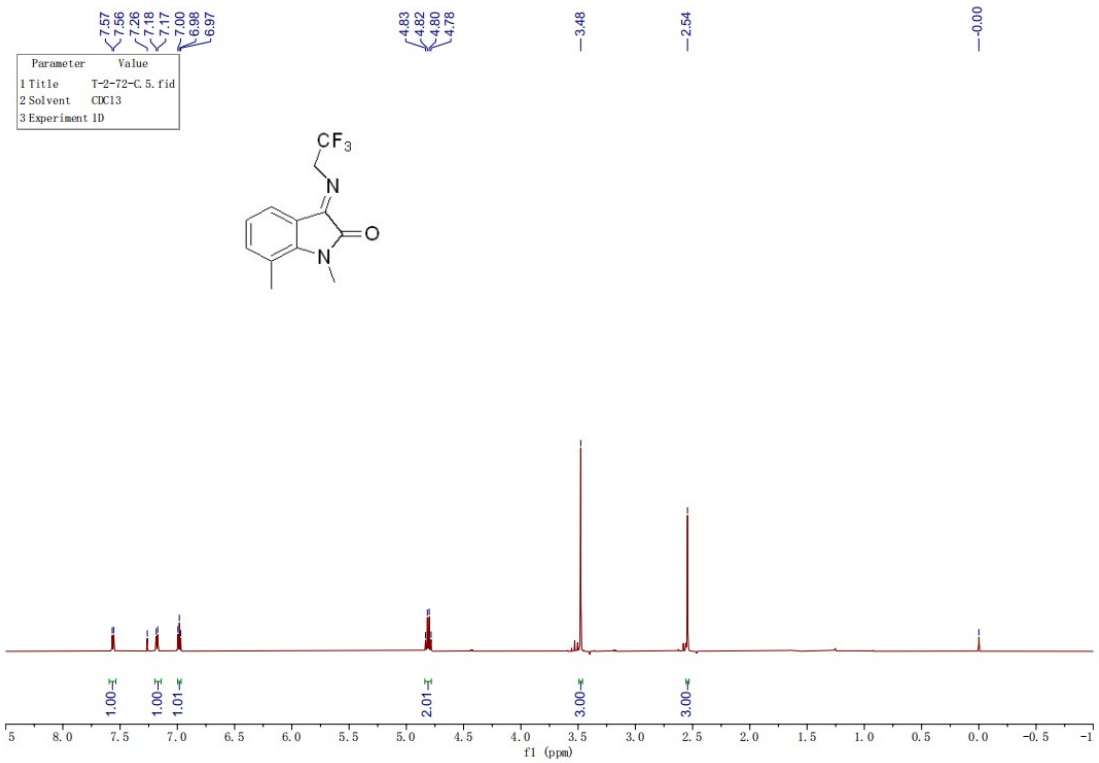
^{1}H-NMR and ^{13}C-NMR of **1c**

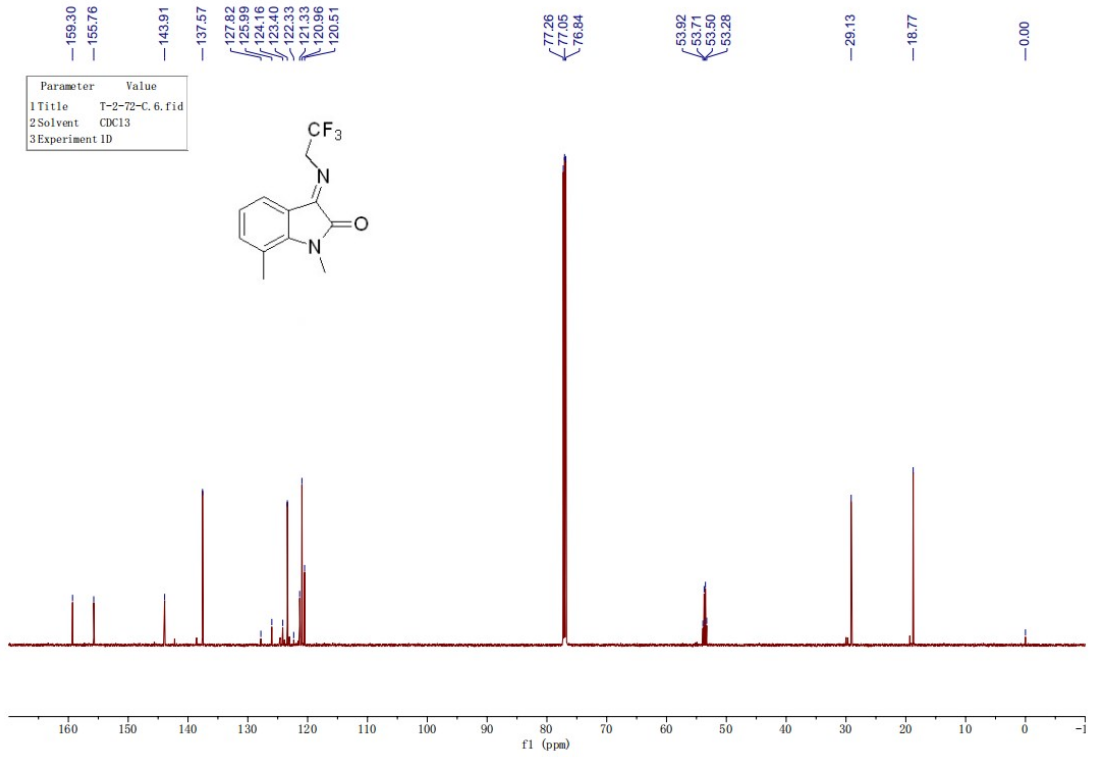




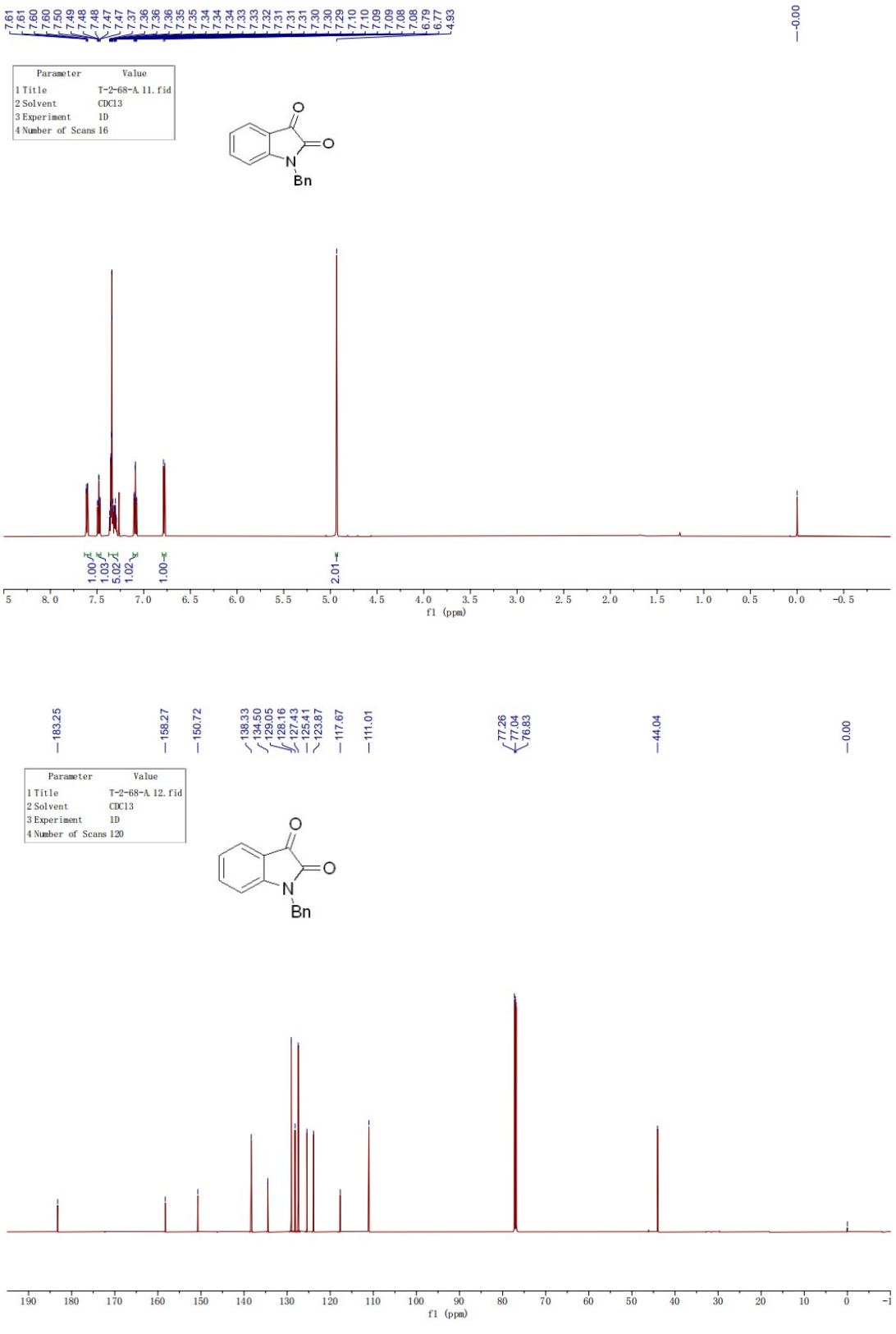
^{1}H-NMR and ^{13}C-NMR of **1d**

^{1}H-NMR and ^{13}C-NMR of **1e**

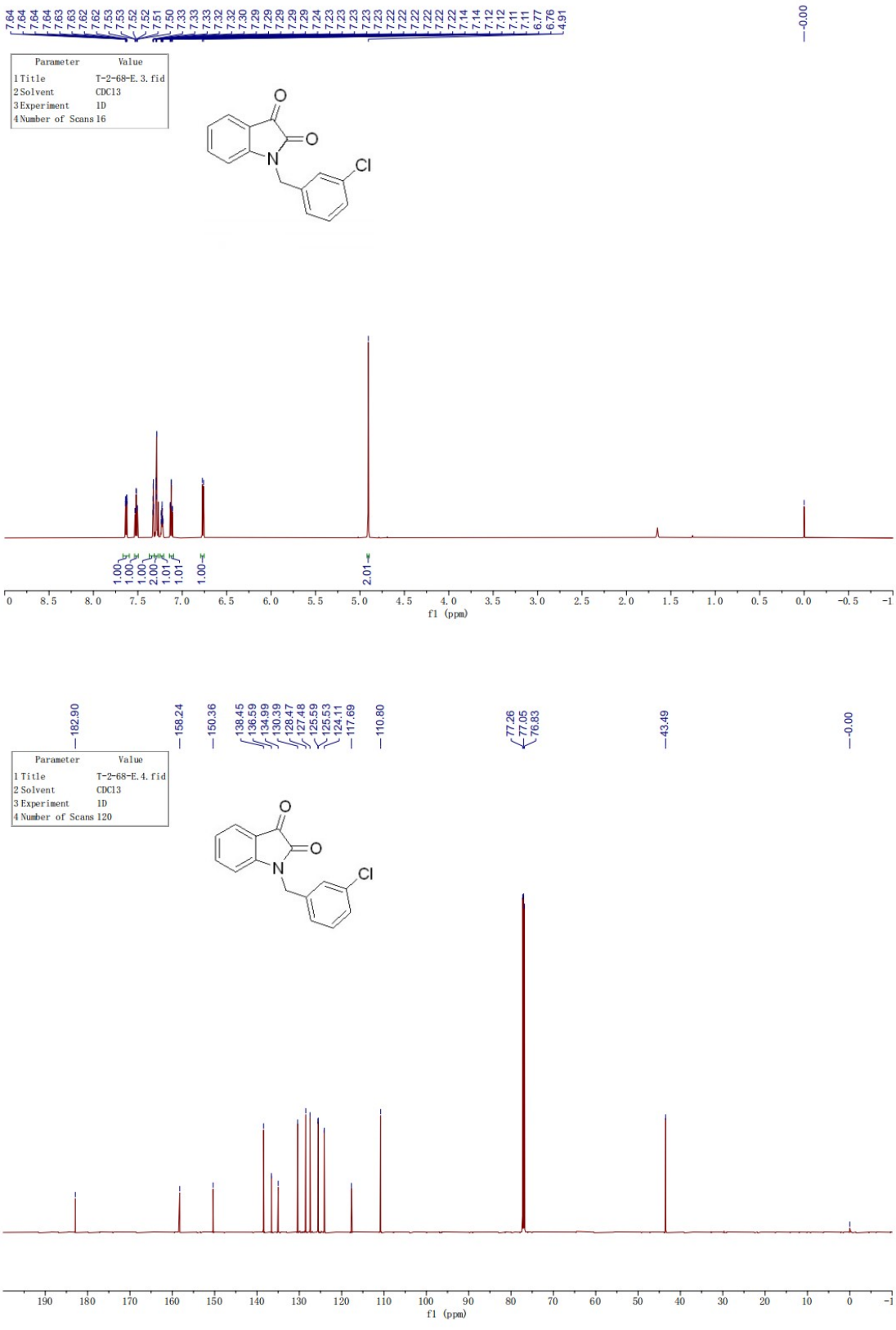




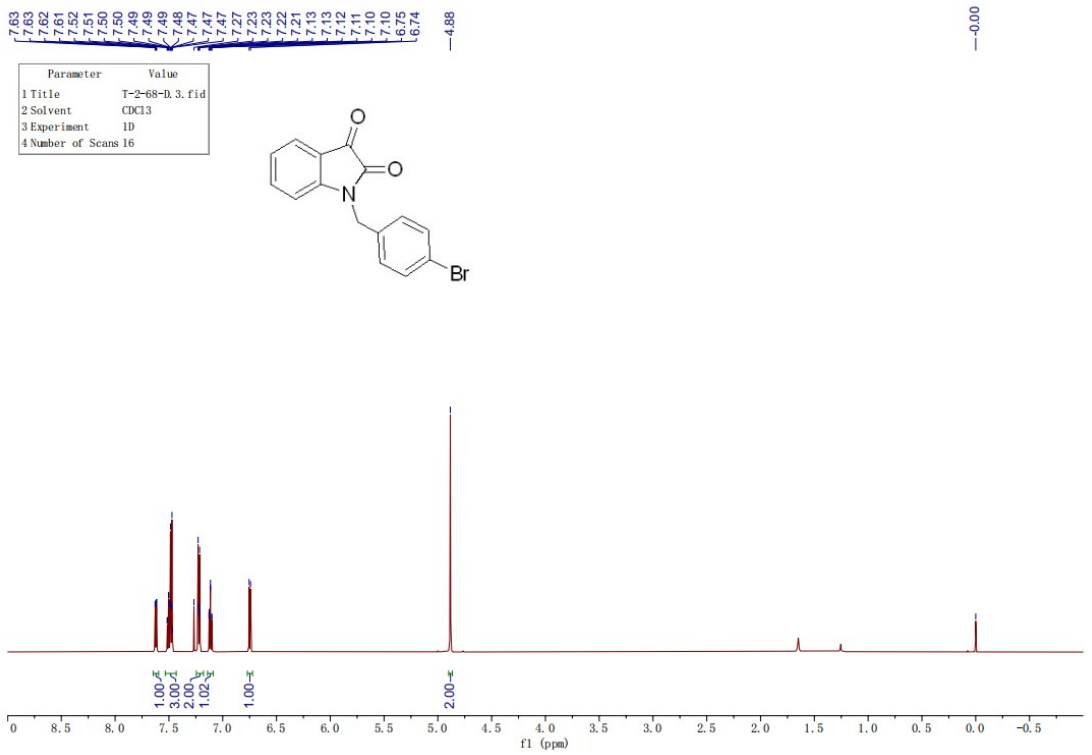
^{1}H-NMR and ^{13}C-NMR of **1f**

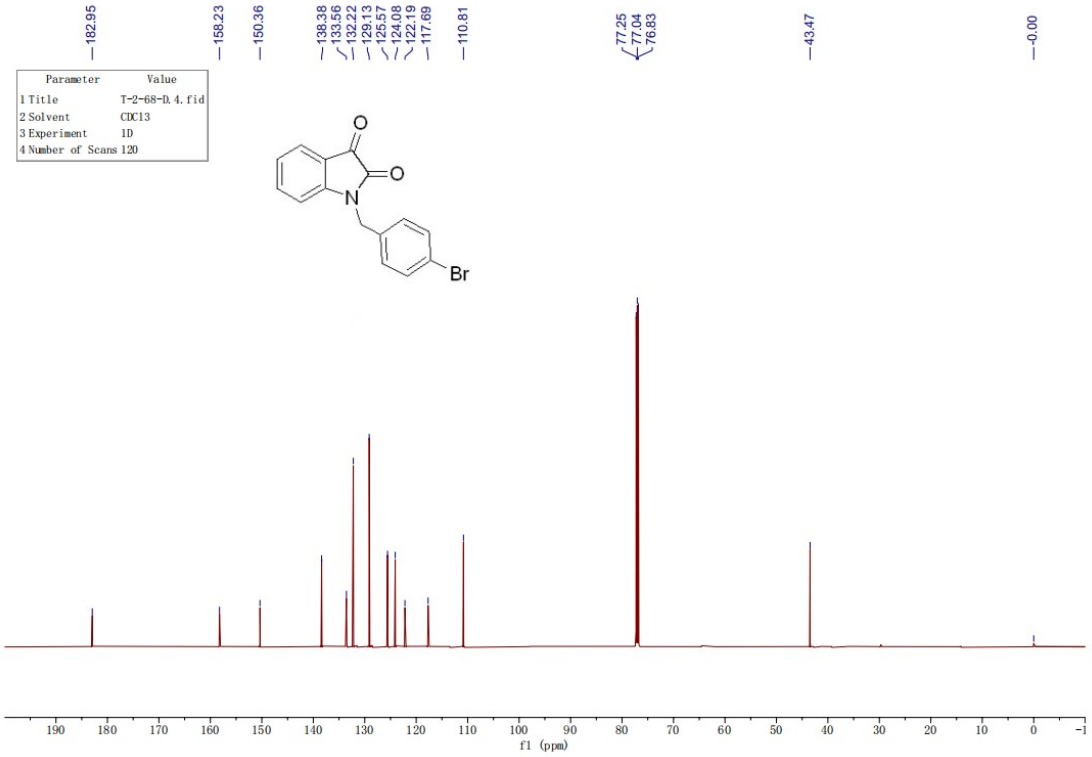


^{1}H-NMR and ^{13}C-NMR of **1g'**

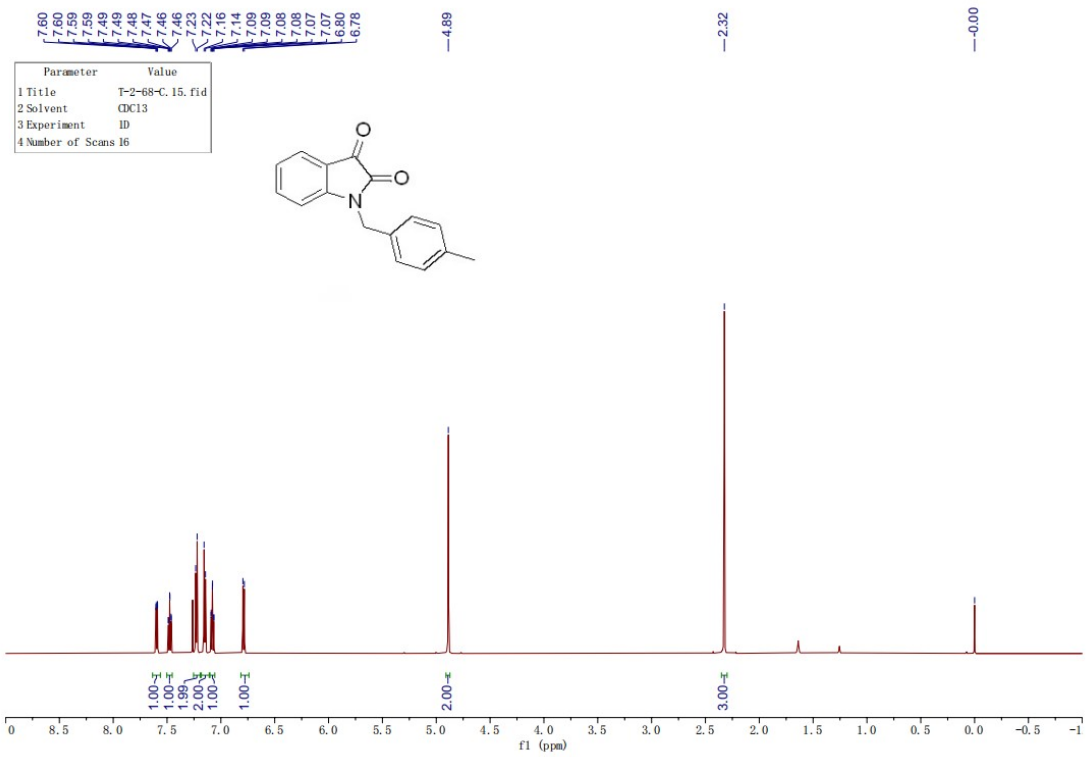


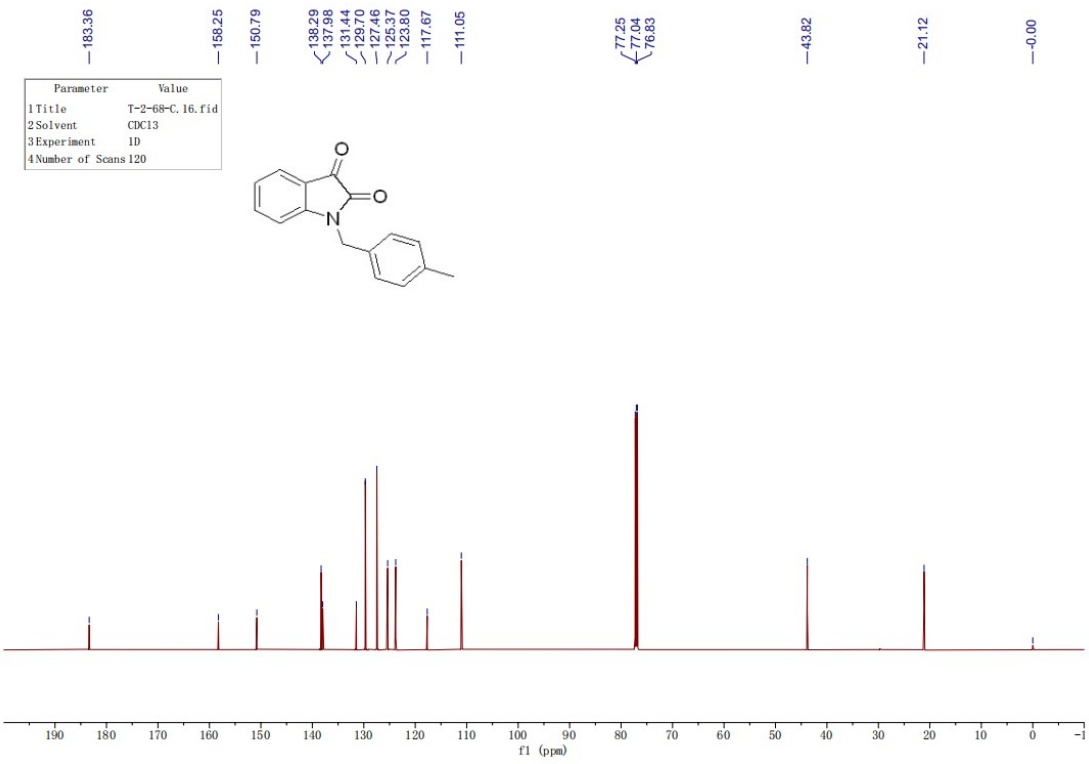
^{1}H-NMR and ^{13}C-NMR of **1h'**



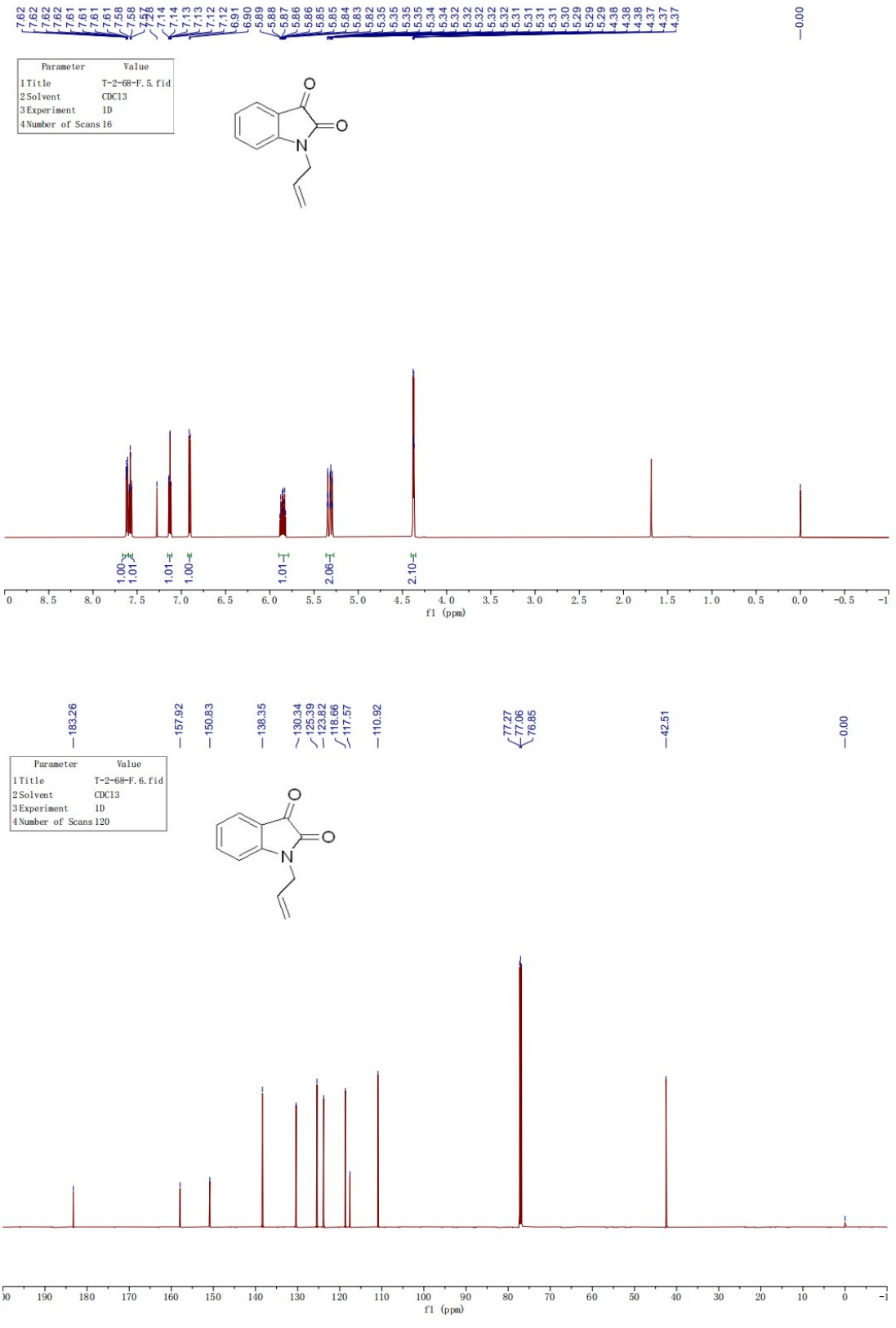


^{1}H-NMR and ^{13}C-NMR of **1i'**



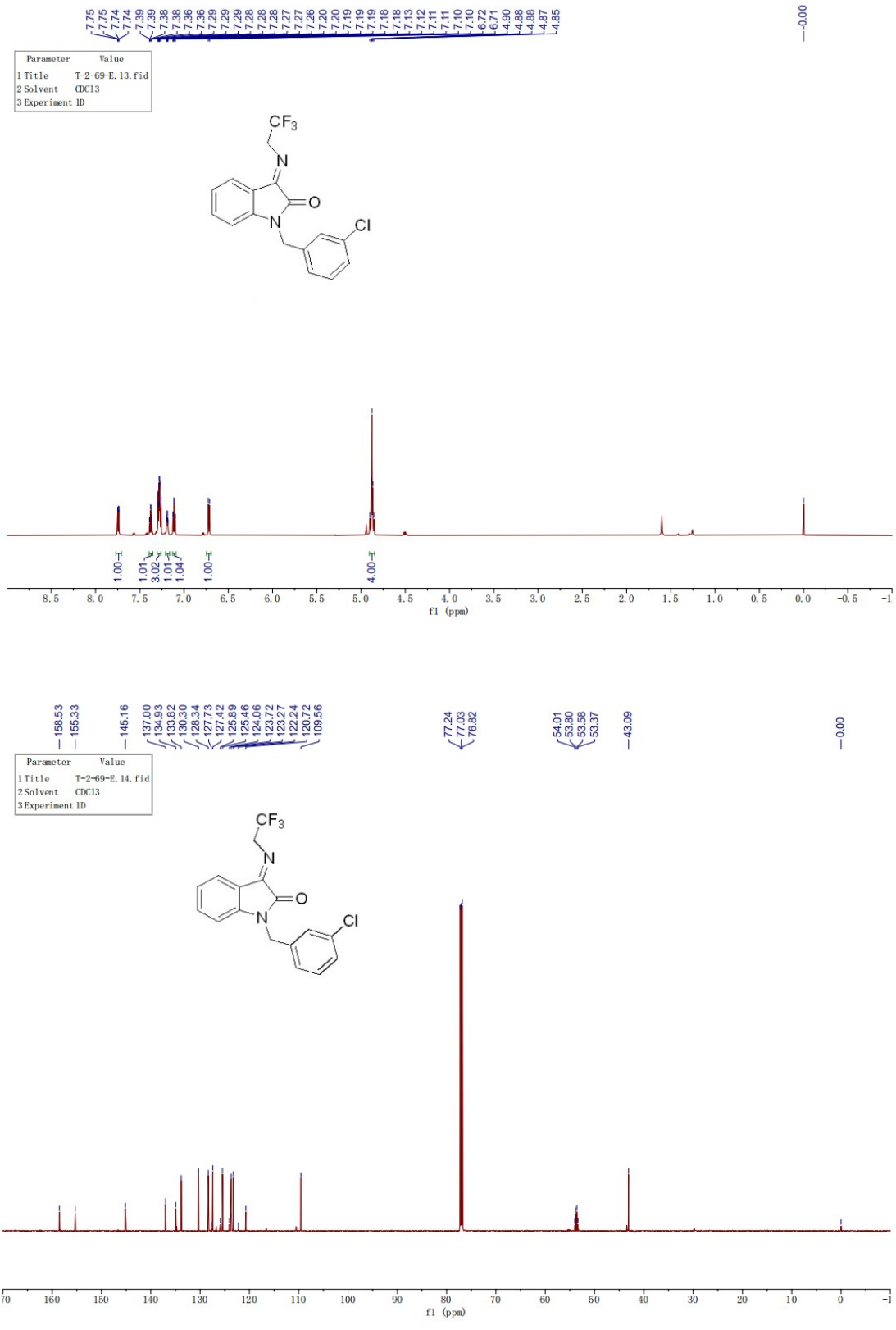


^{1}H-NMR and ^{13}C-NMR of **1j'**



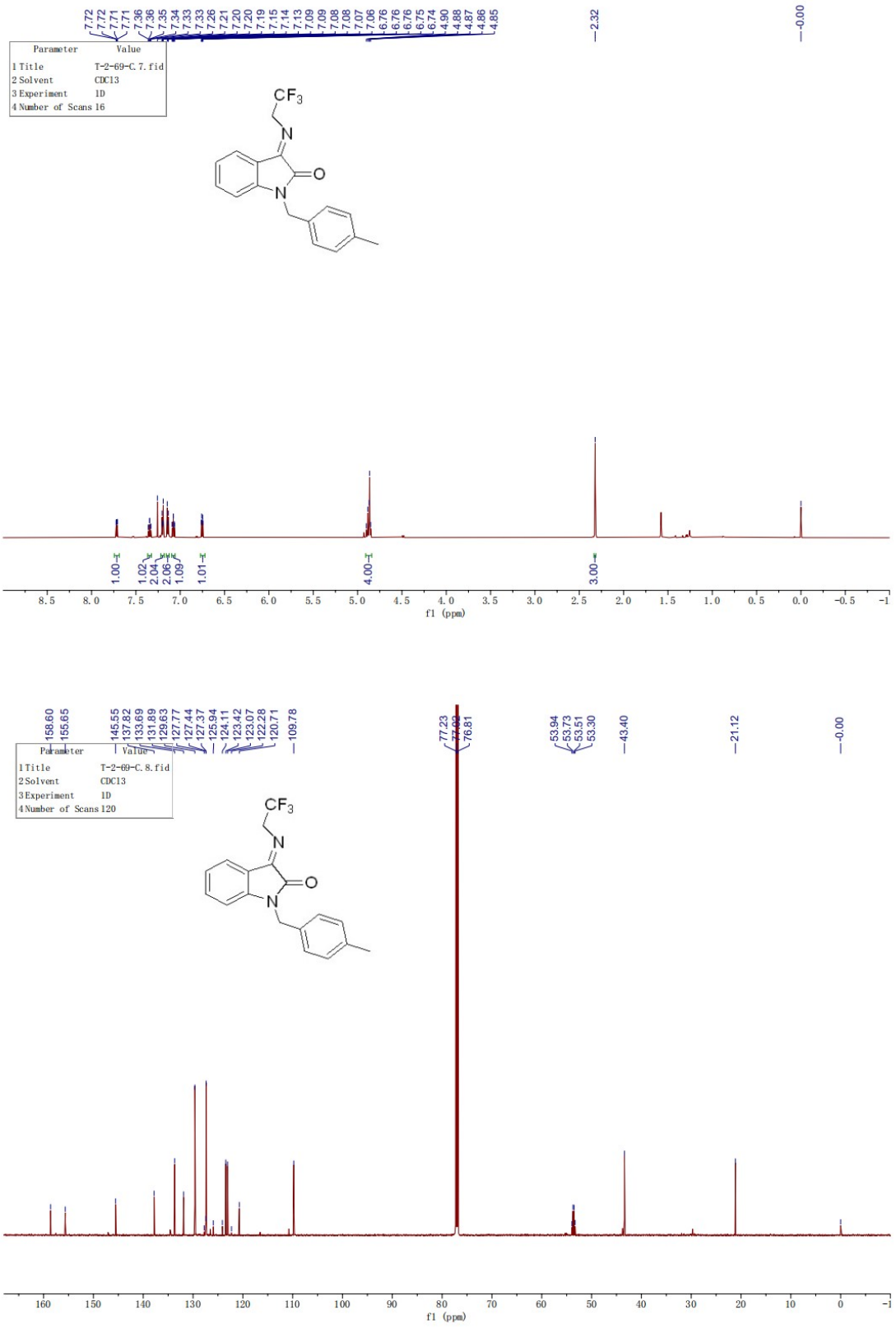
^{1}H-NMR and ^{13}C-NMR of **1k'**

^{1}H-NMR and ^{13}C-NMR of **1g**

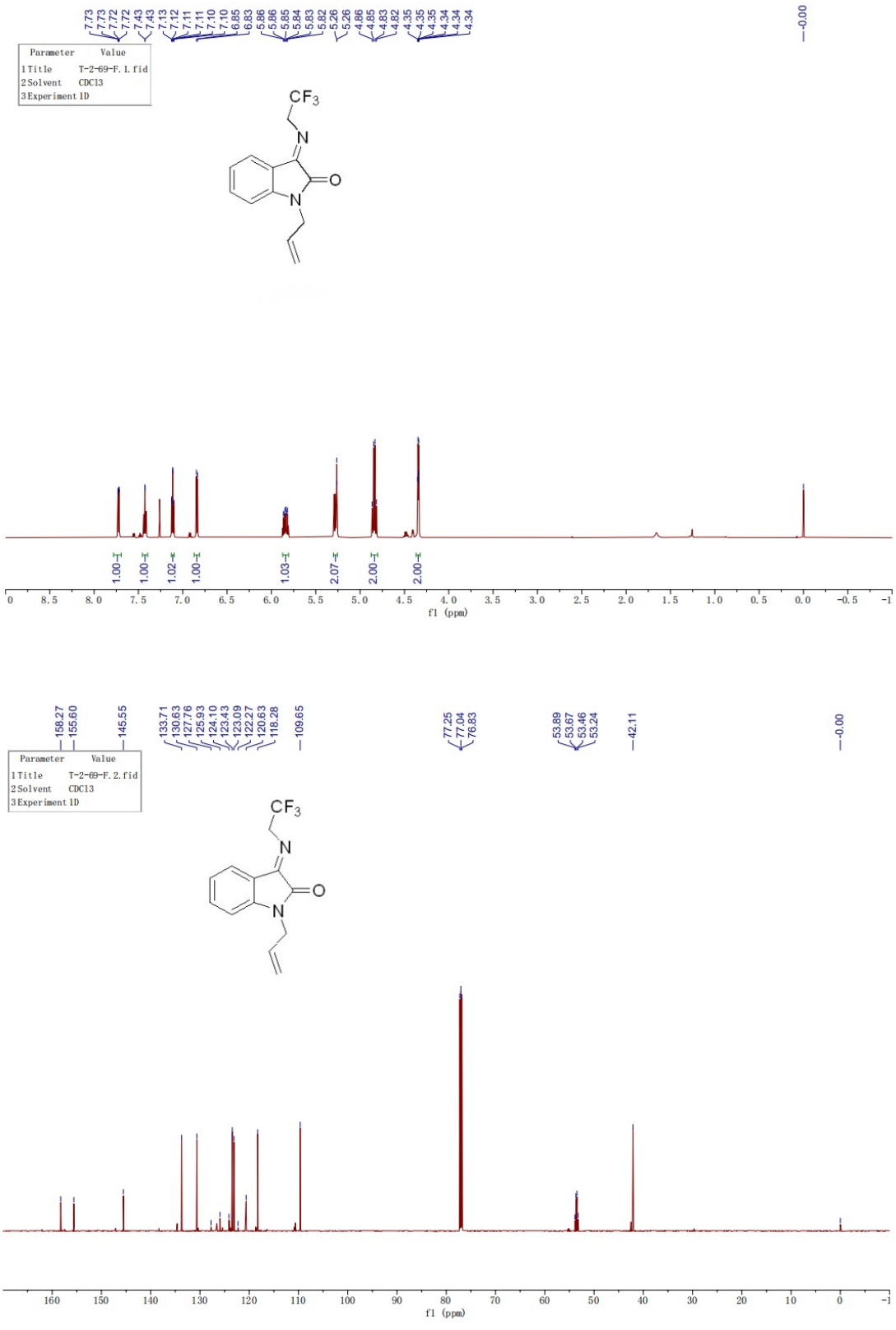


^{1}H-NMR and ^{13}C-NMR of **1h**

^{1}H-NMR and ^{13}C-NMR of **1i**



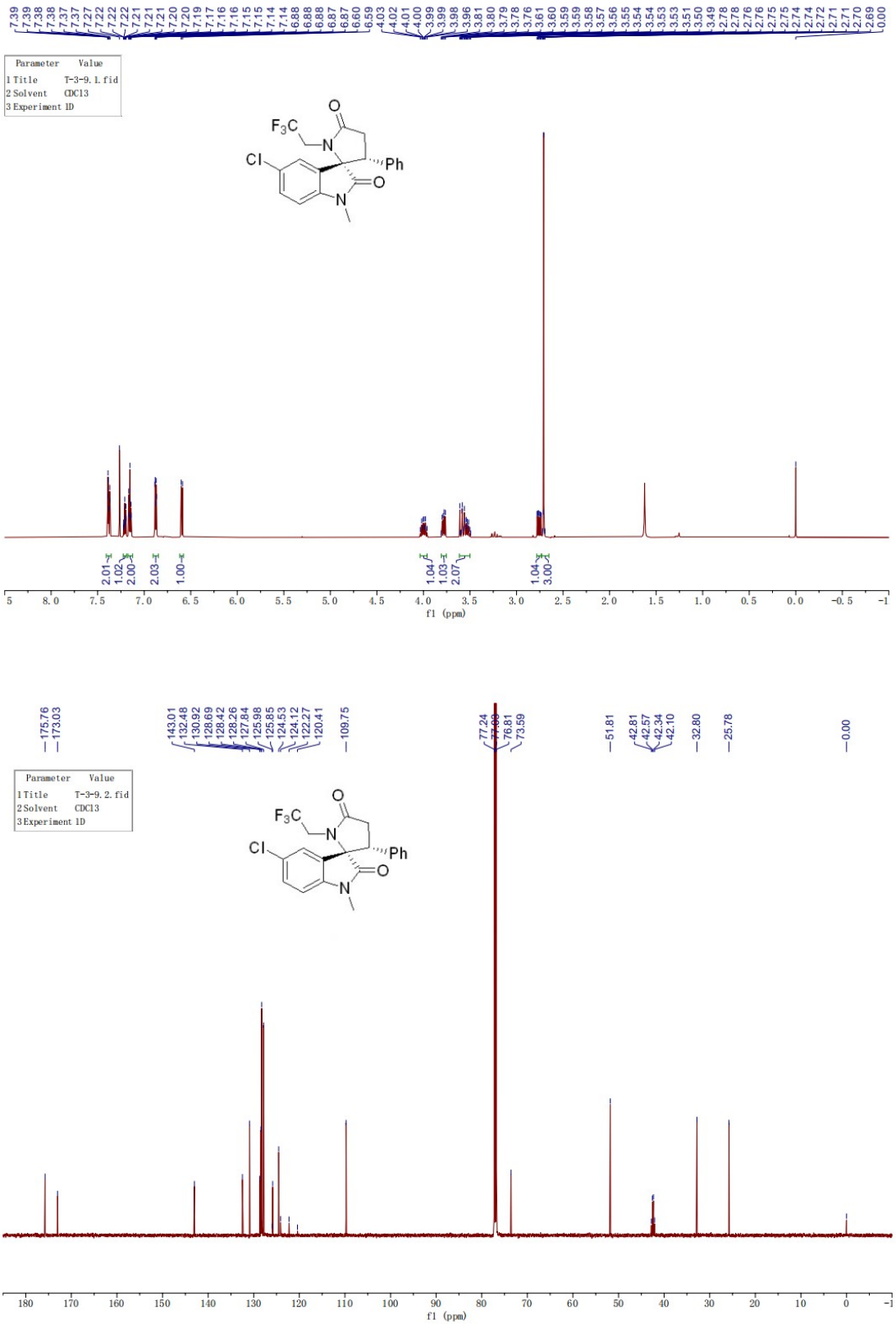
^{1}H-NMR and ^{13}C-NMR of **1j**



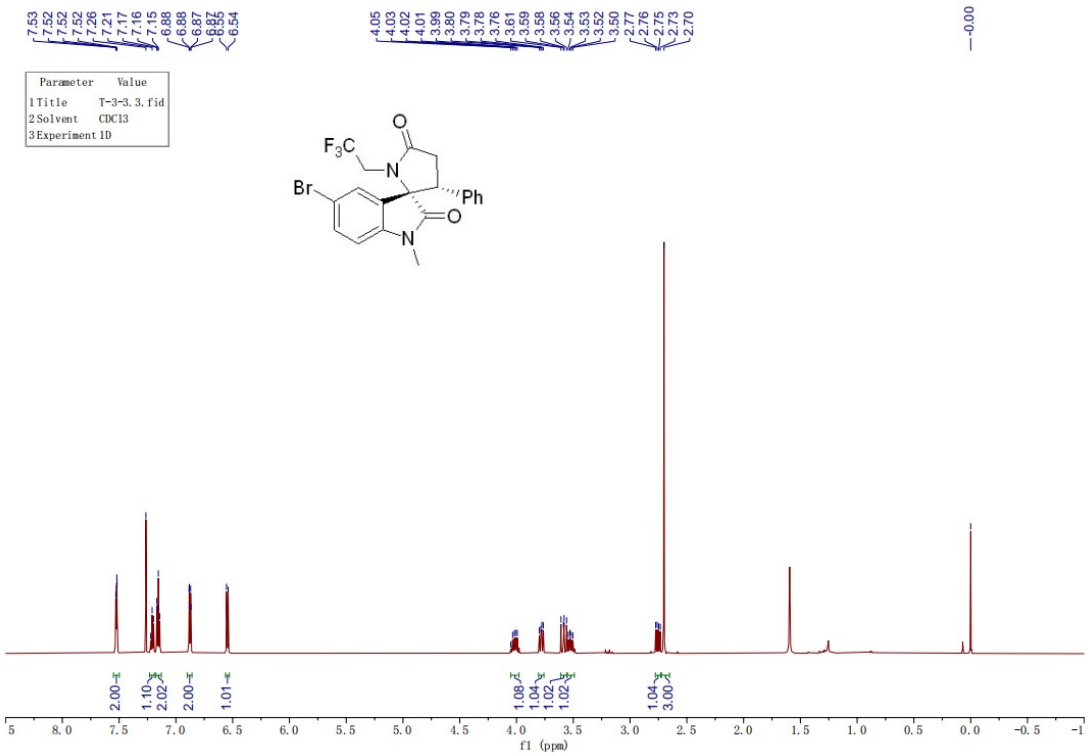
^{1}H-NMR and ^{13}C-NMR of **1k**

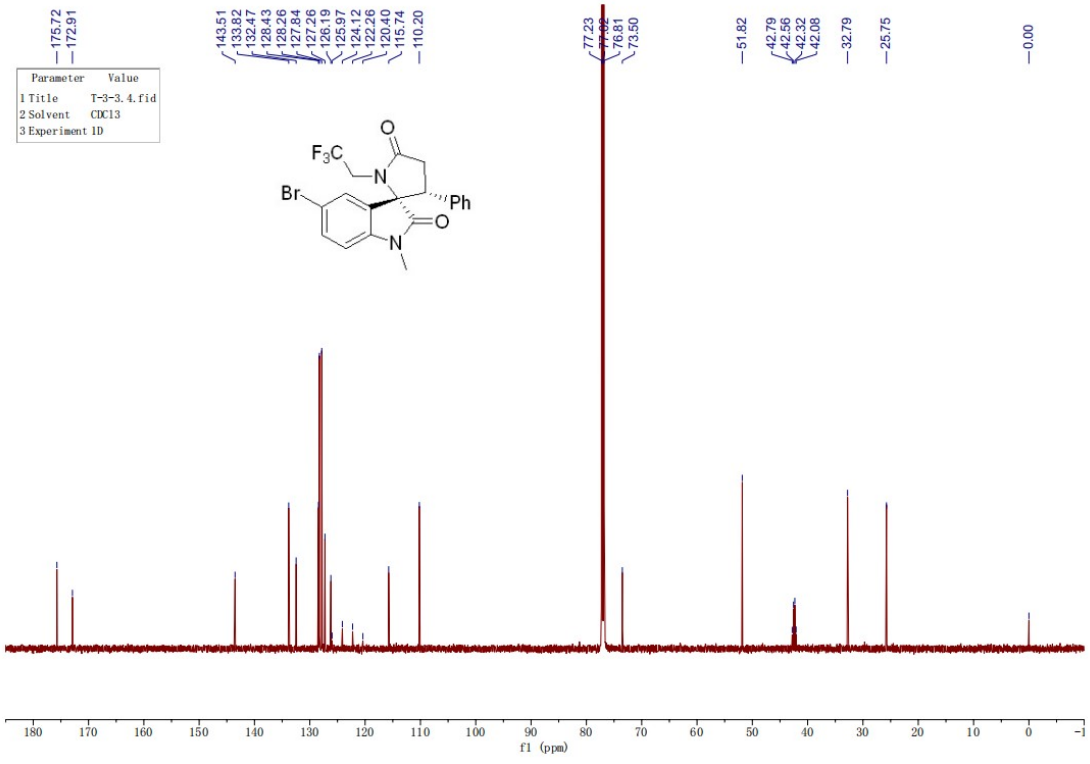
^{1}H-NMR and ^{13}C-NMR of **4a**

^{1}H-NMR and ^{13}C-NMR of **4b**

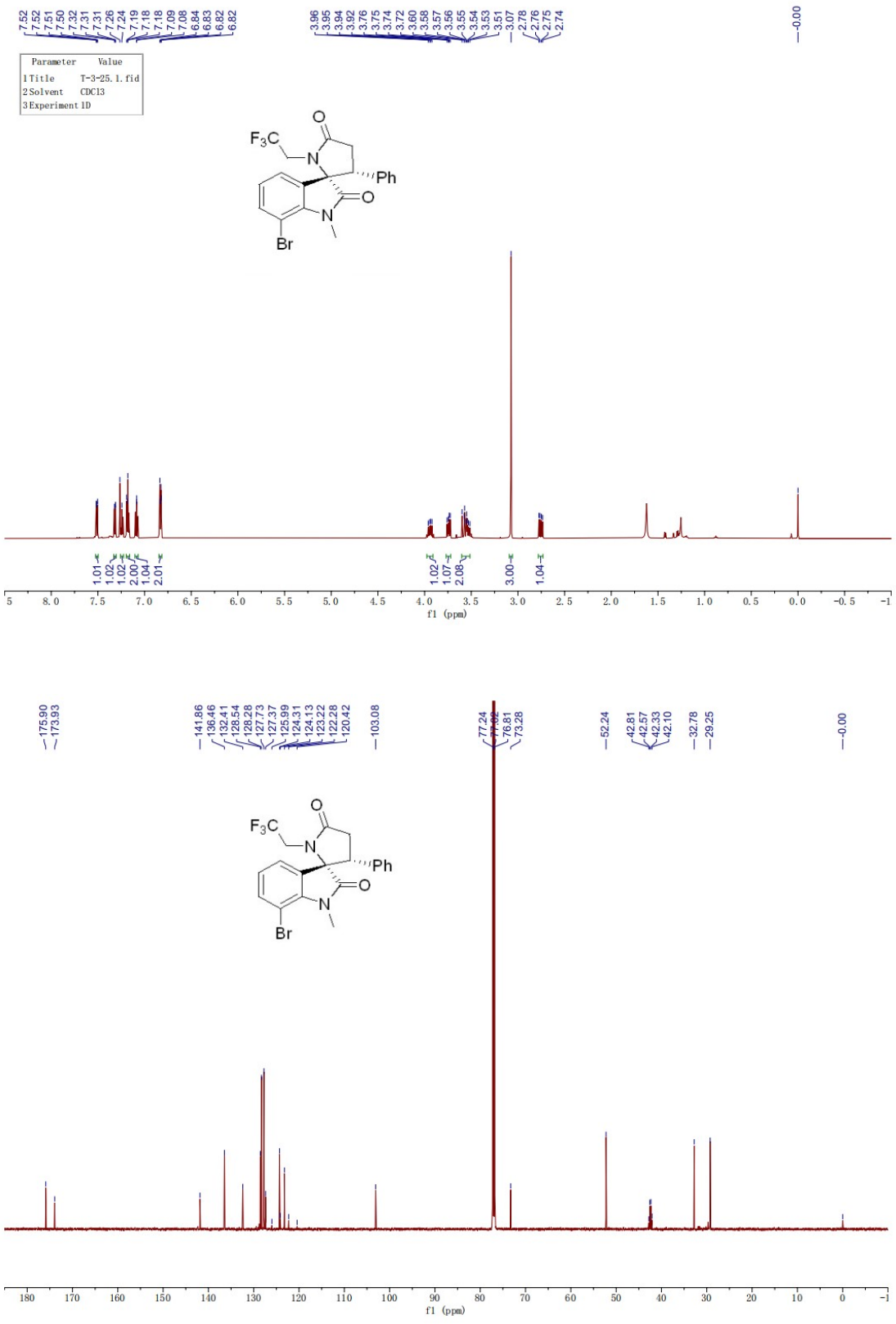


^{1}H-NMR and ^{13}C-NMR of **4c**

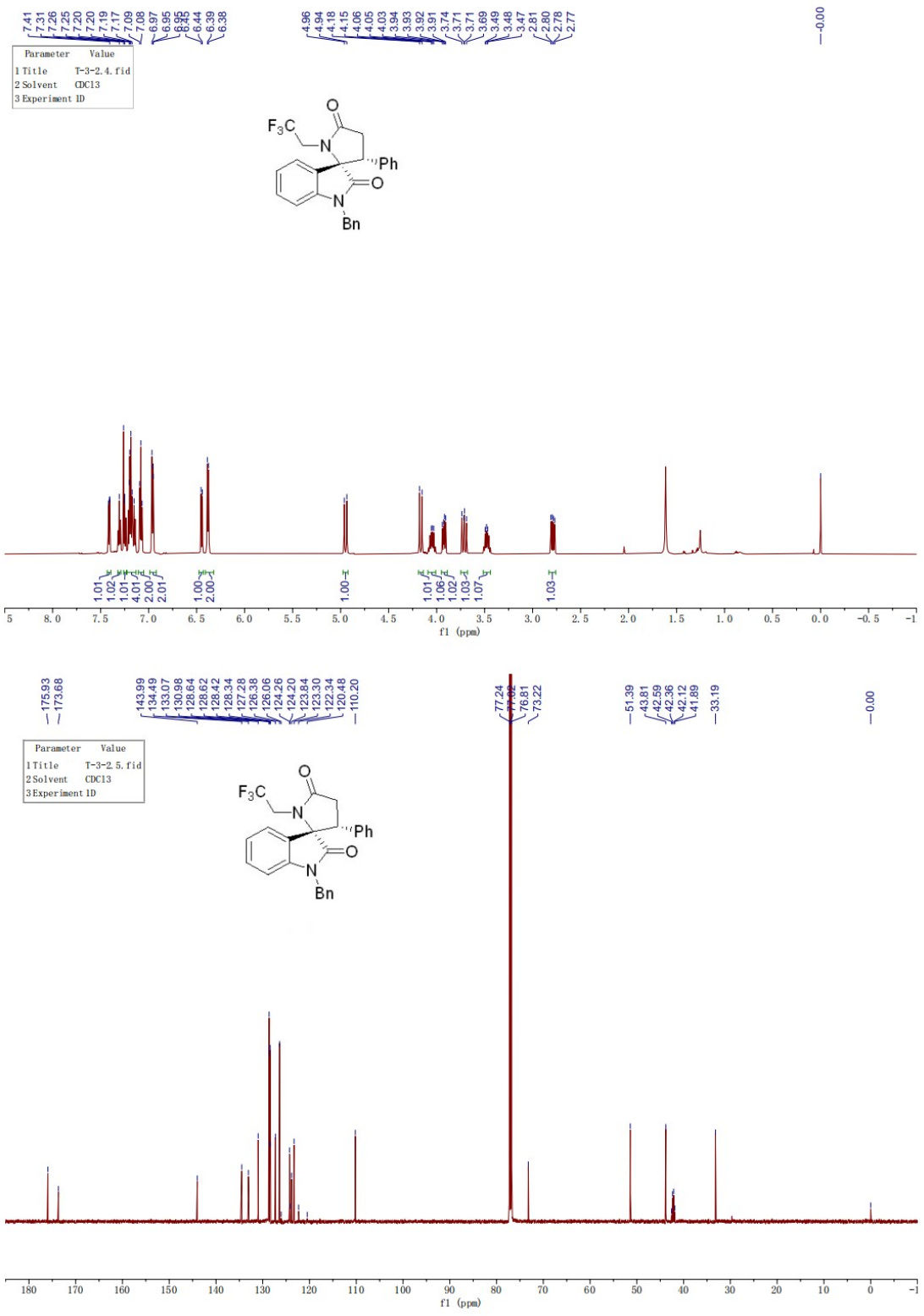




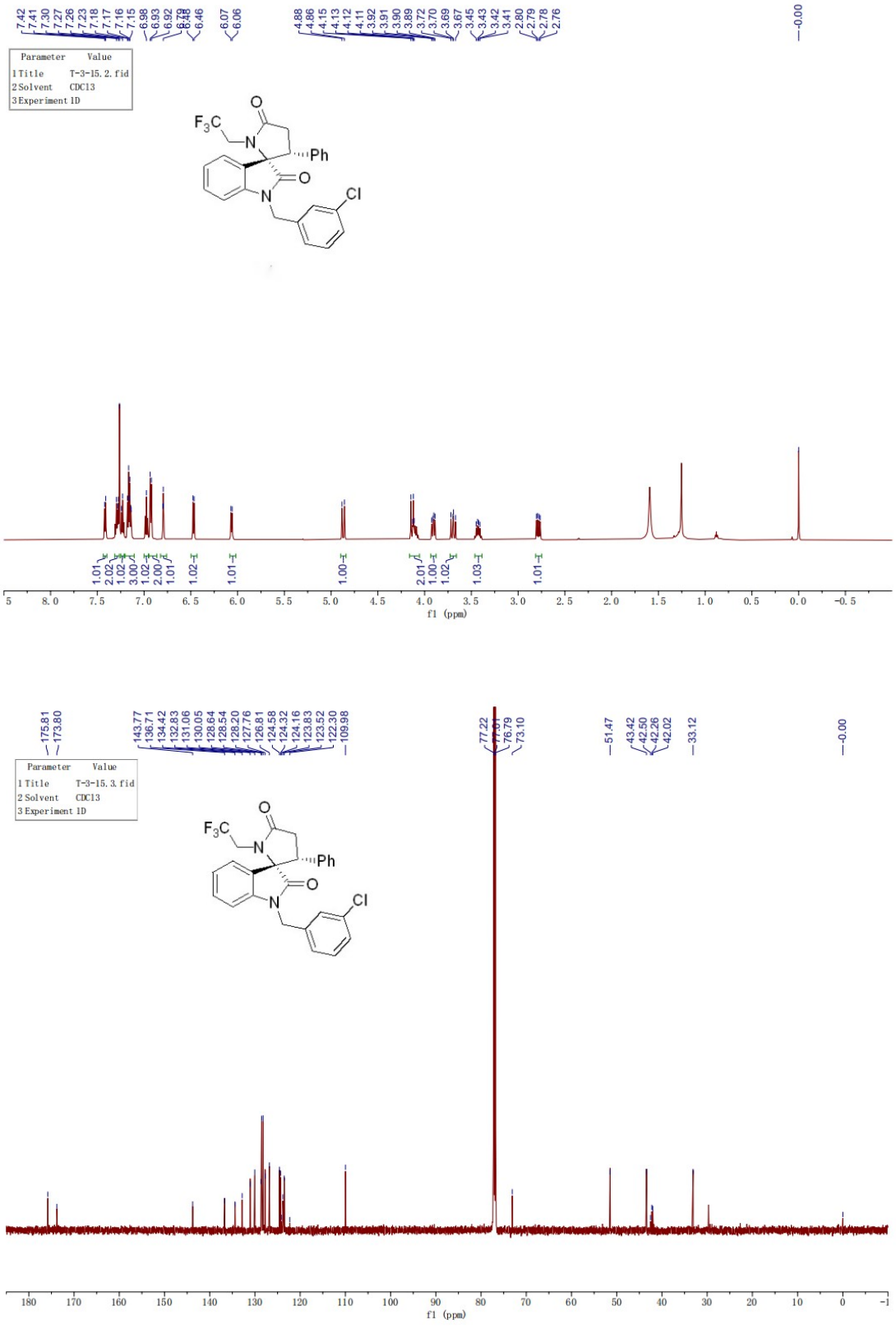
^{1}H-NMR and ^{13}C-NMR of **4d**



^{1}H-NMR and ^{13}C-NMR of **4e**

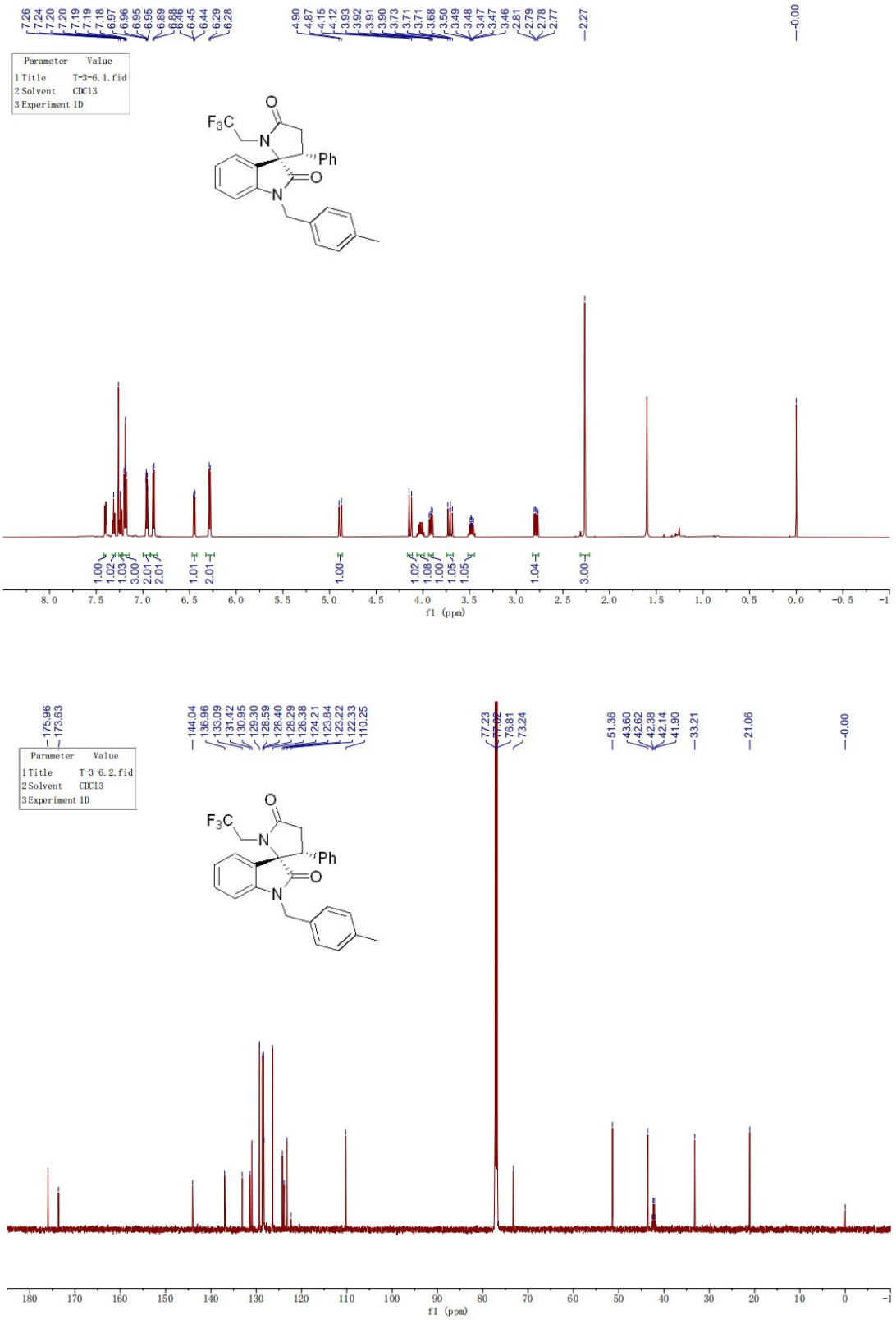


^{1}H-NMR and ^{13}C-NMR of **4f**

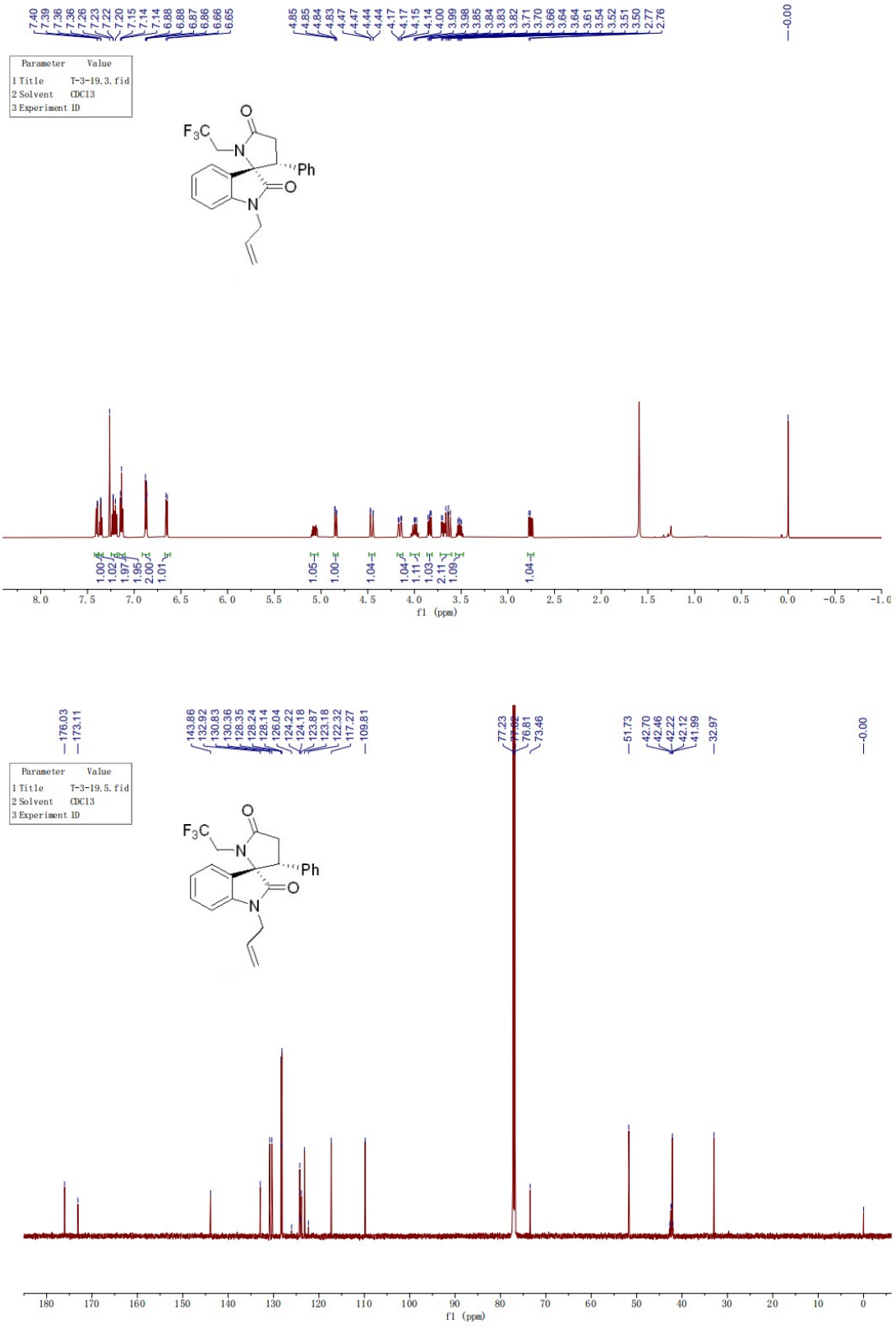


^{1}H-NMR and ^{13}C-NMR of **4g**

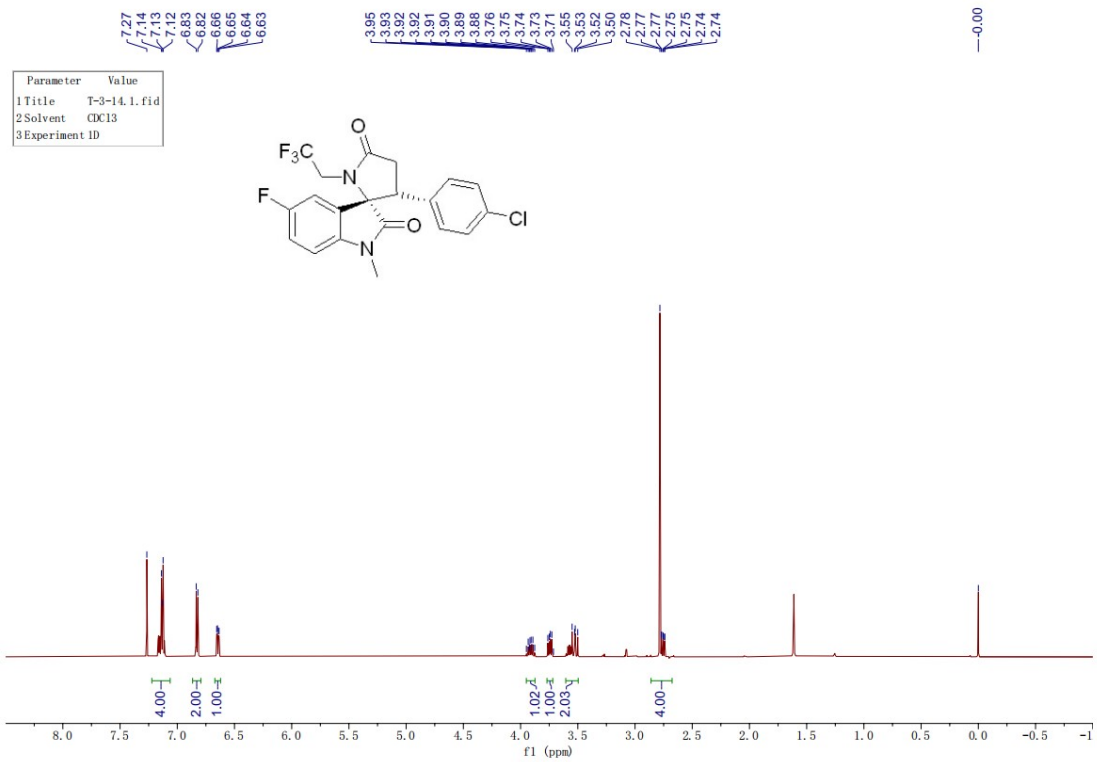
^{1}H-NMR and ^{13}C-NMR of **4h**

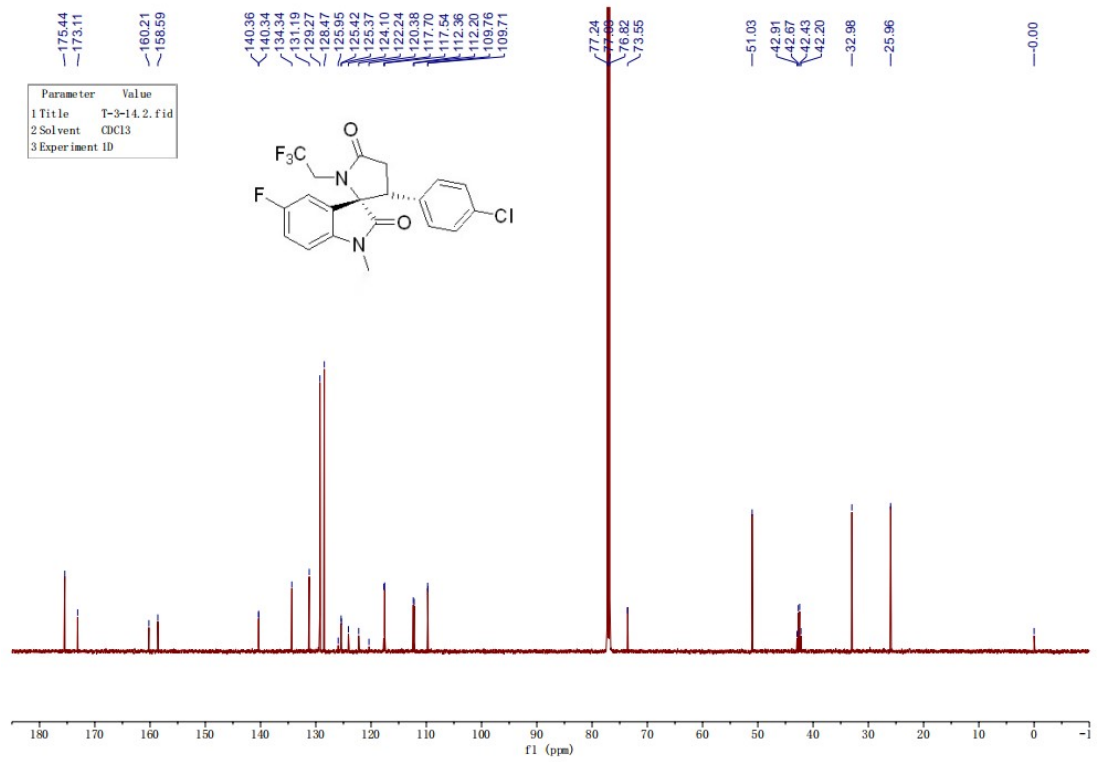


^{1}H-NMR and ^{13}C-NMR of **4i**

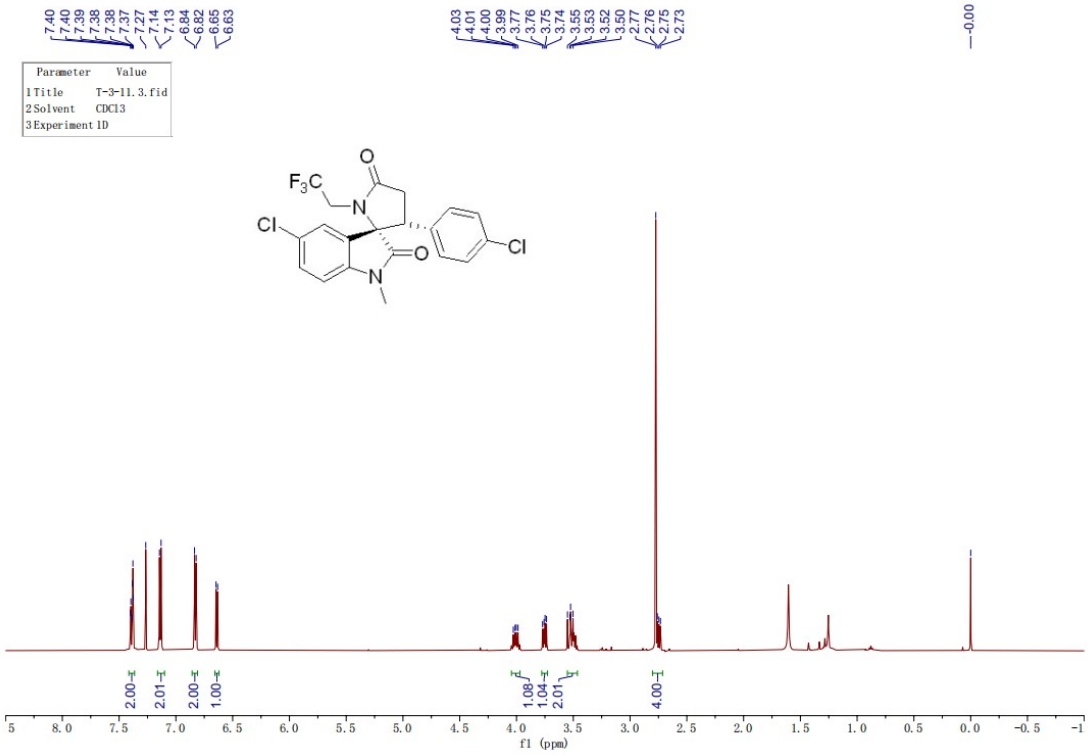


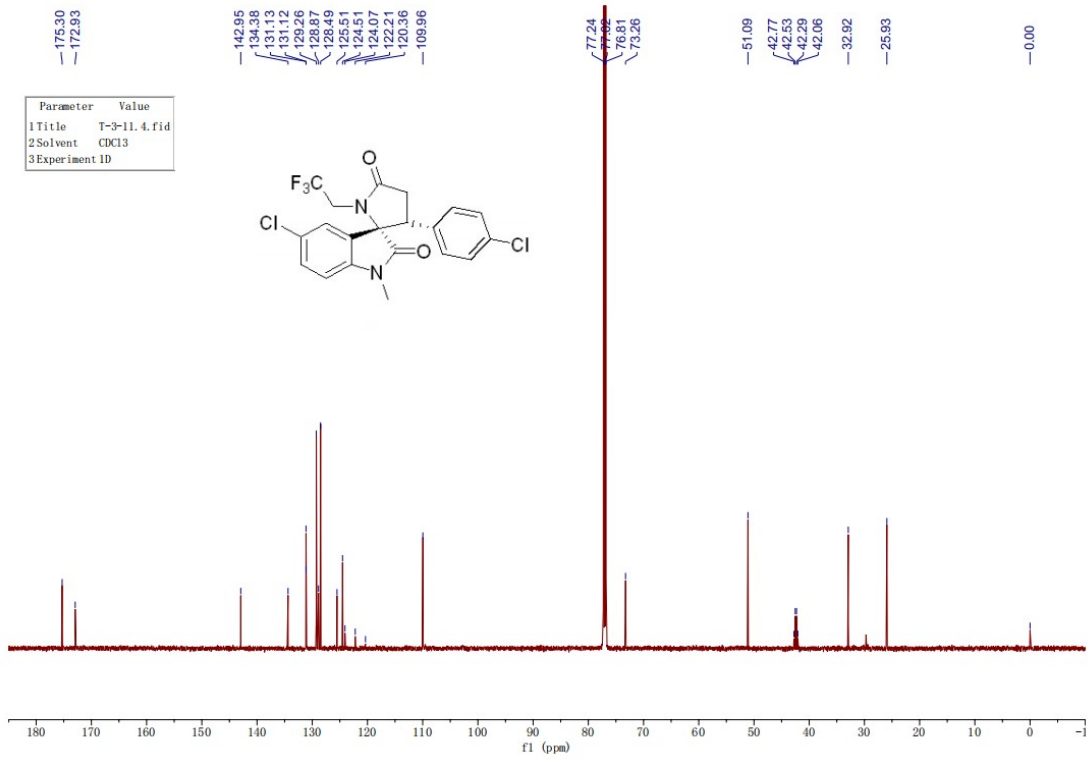
^{1}H-NMR and ^{13}C-NMR of **4j**



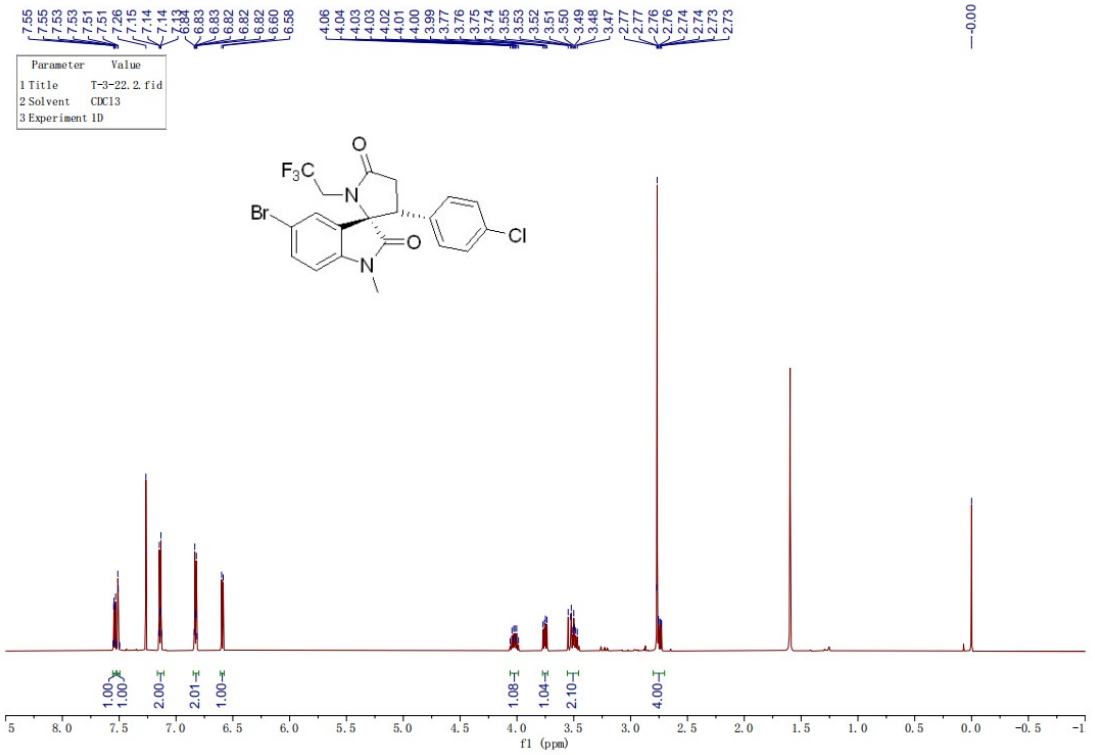


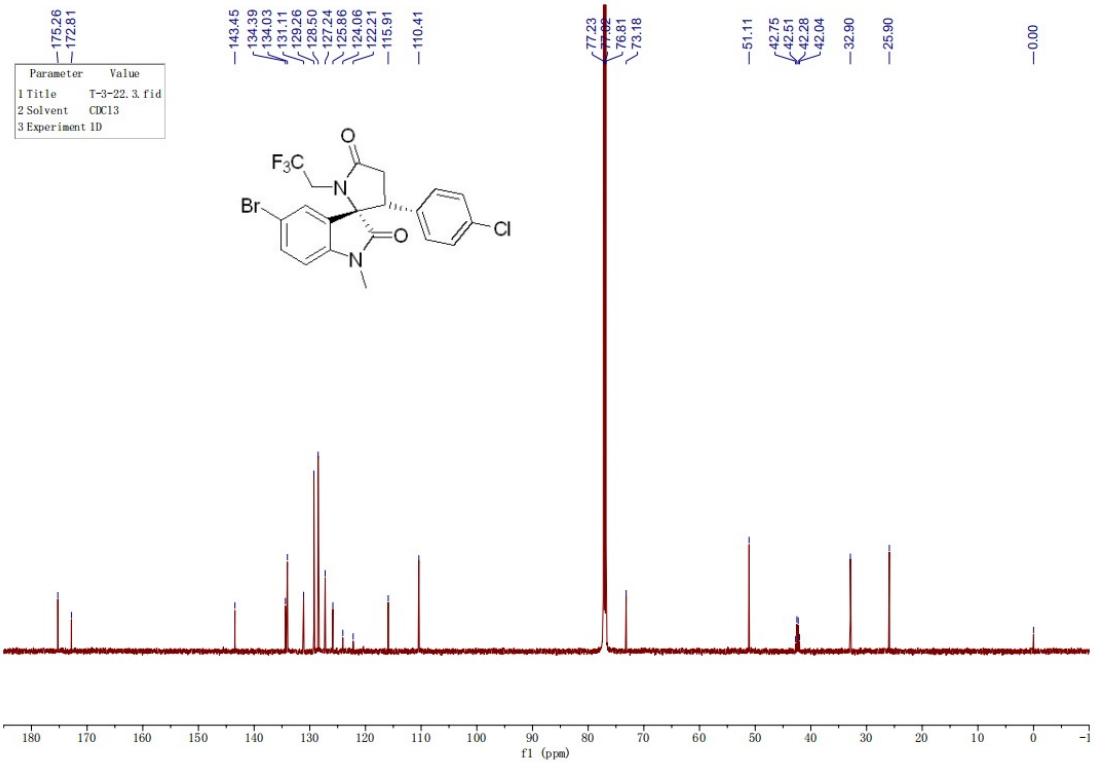
^{1}H-NMR and ^{13}C-NMR of **4k**



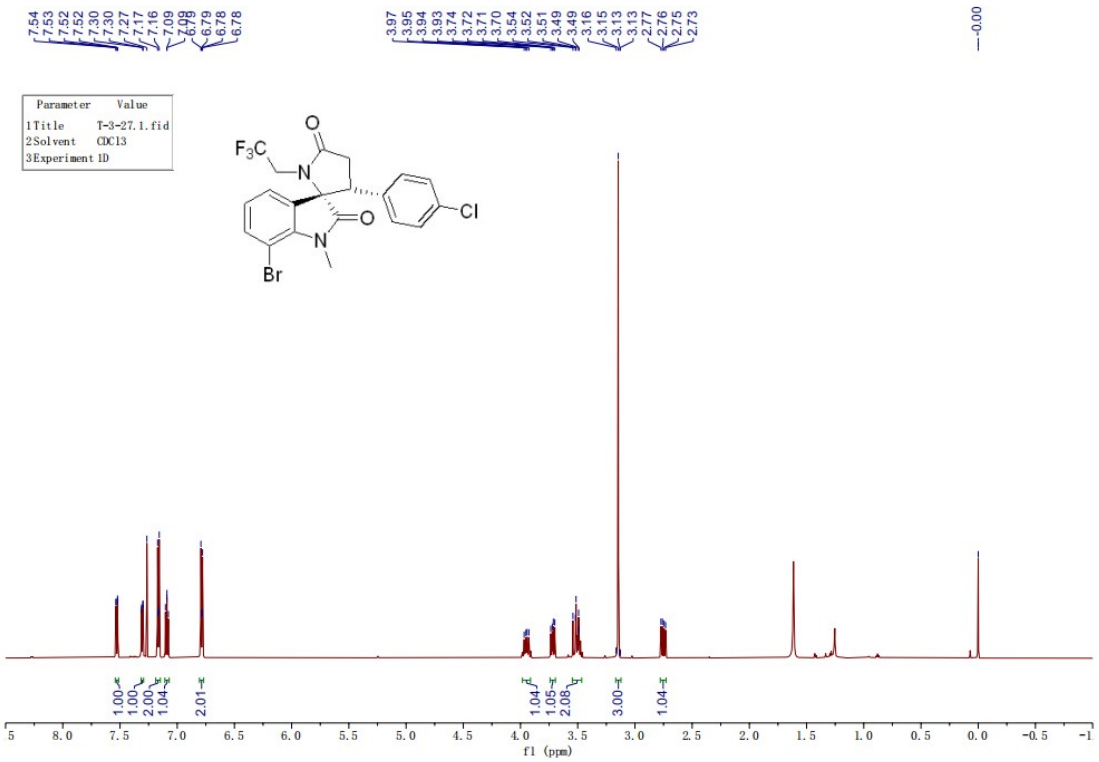


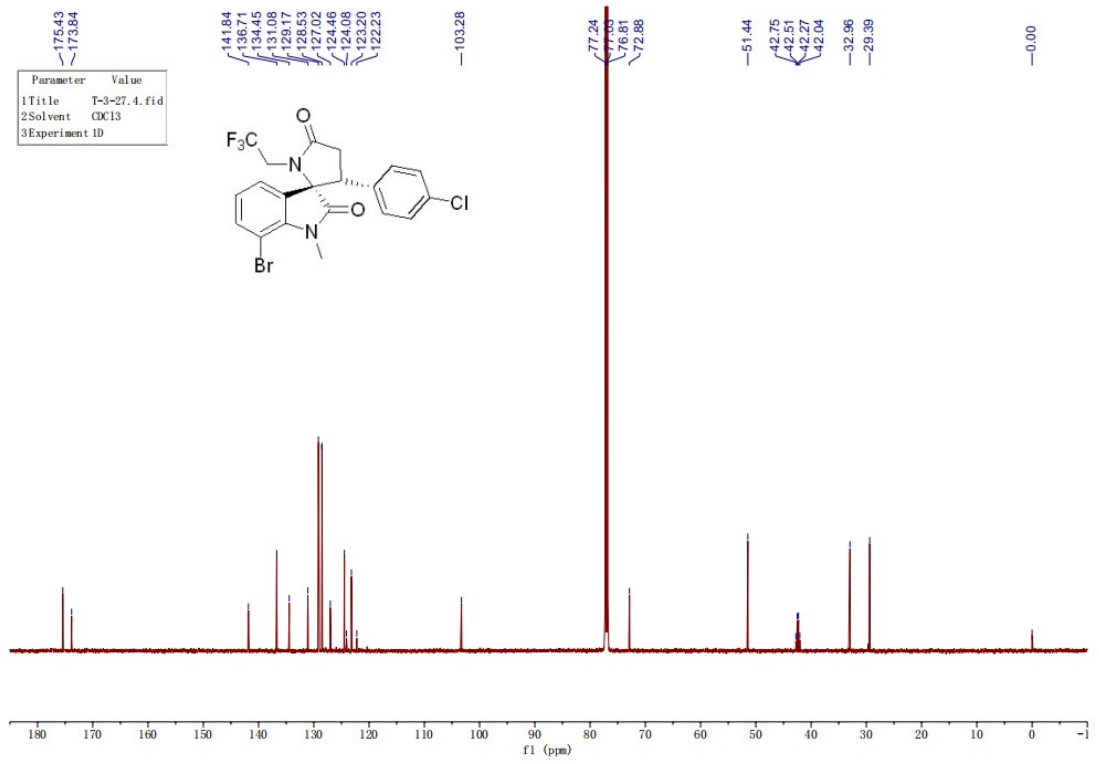
^{1}H-NMR and ^{13}C-NMR of **4l**



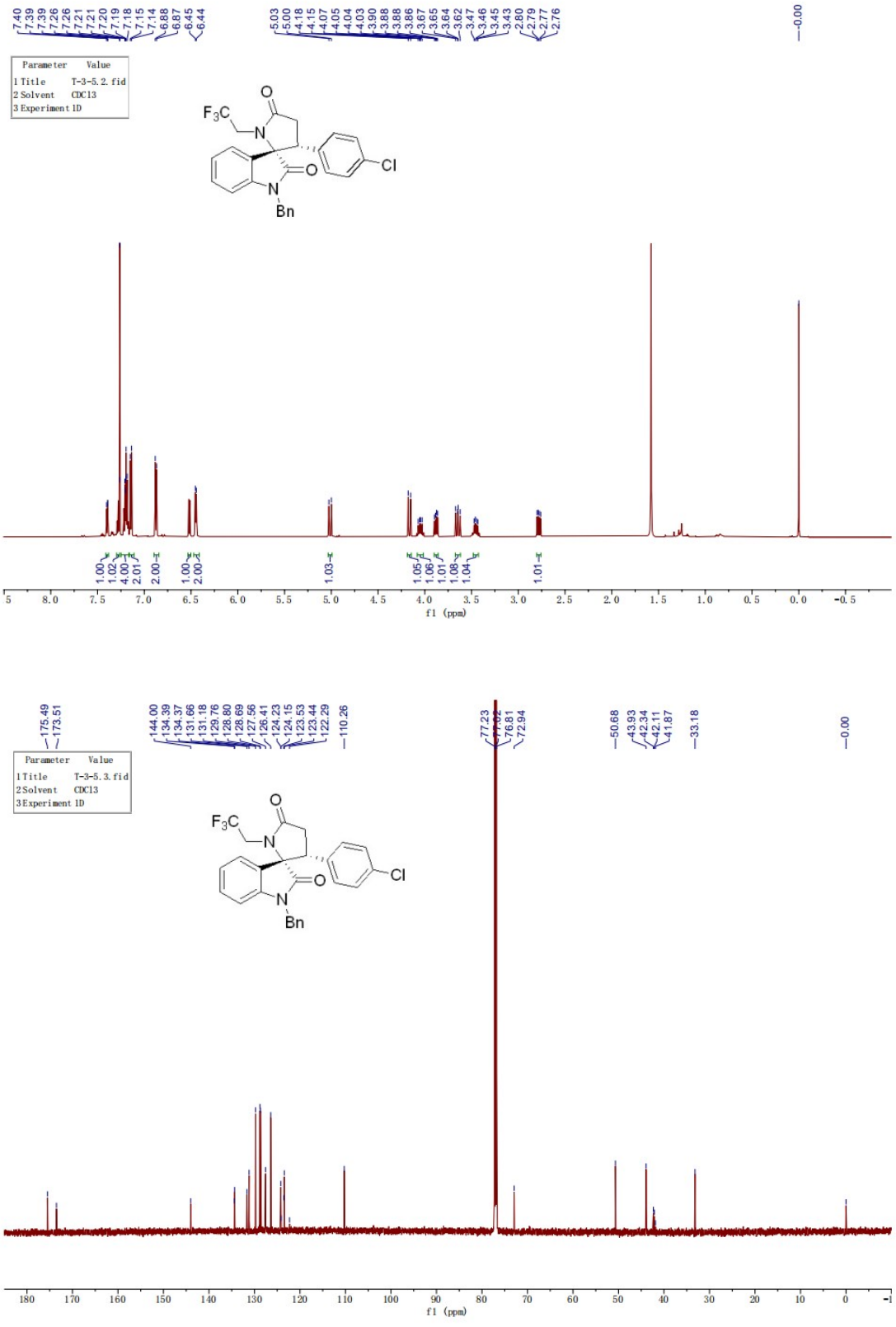


^{1}H-NMR and ^{13}C-NMR of **4m**

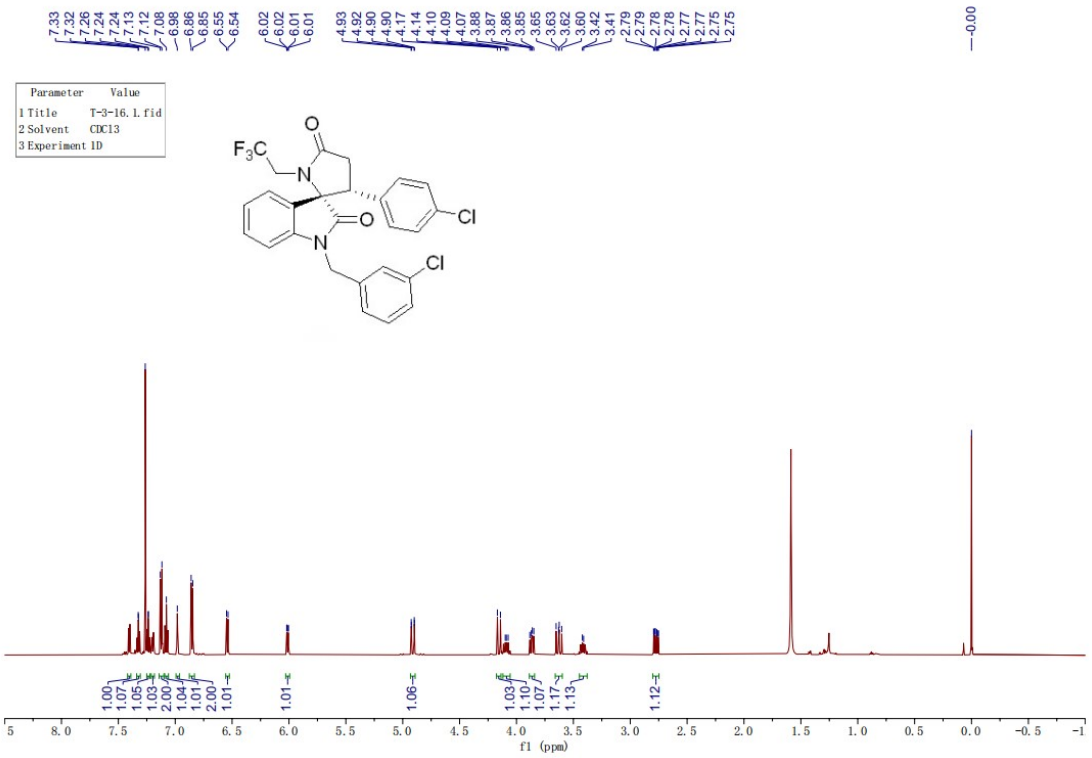


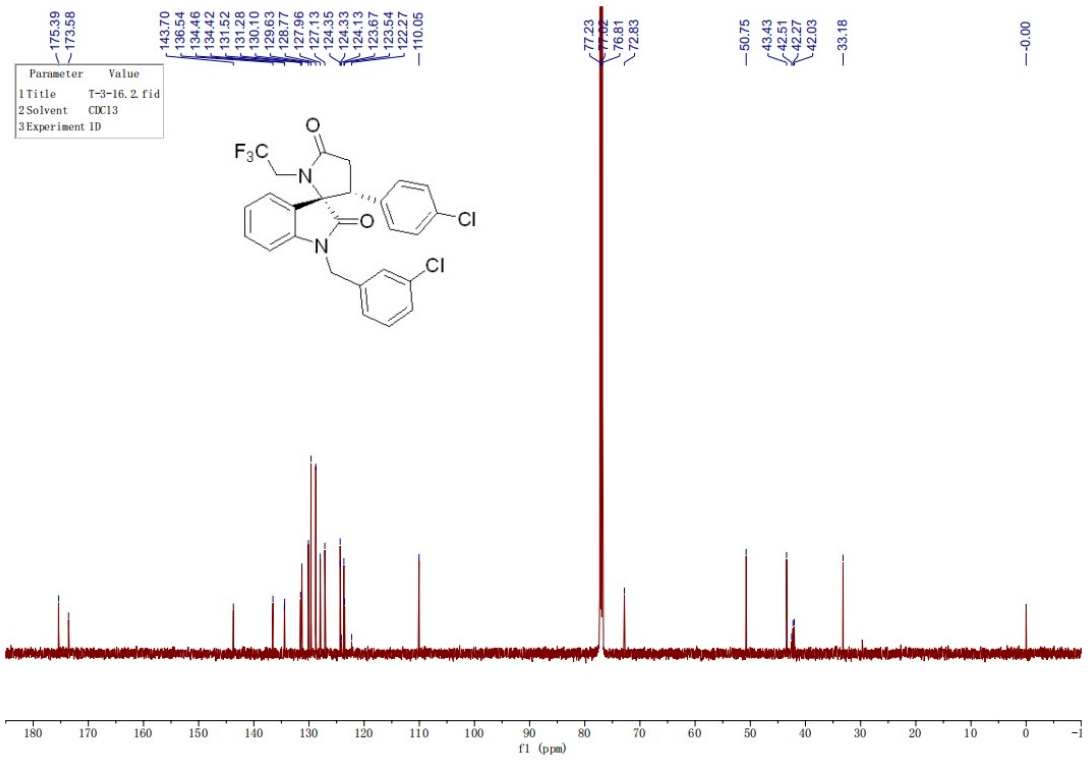


^{1}H-NMR and ^{13}C-NMR of **4n**



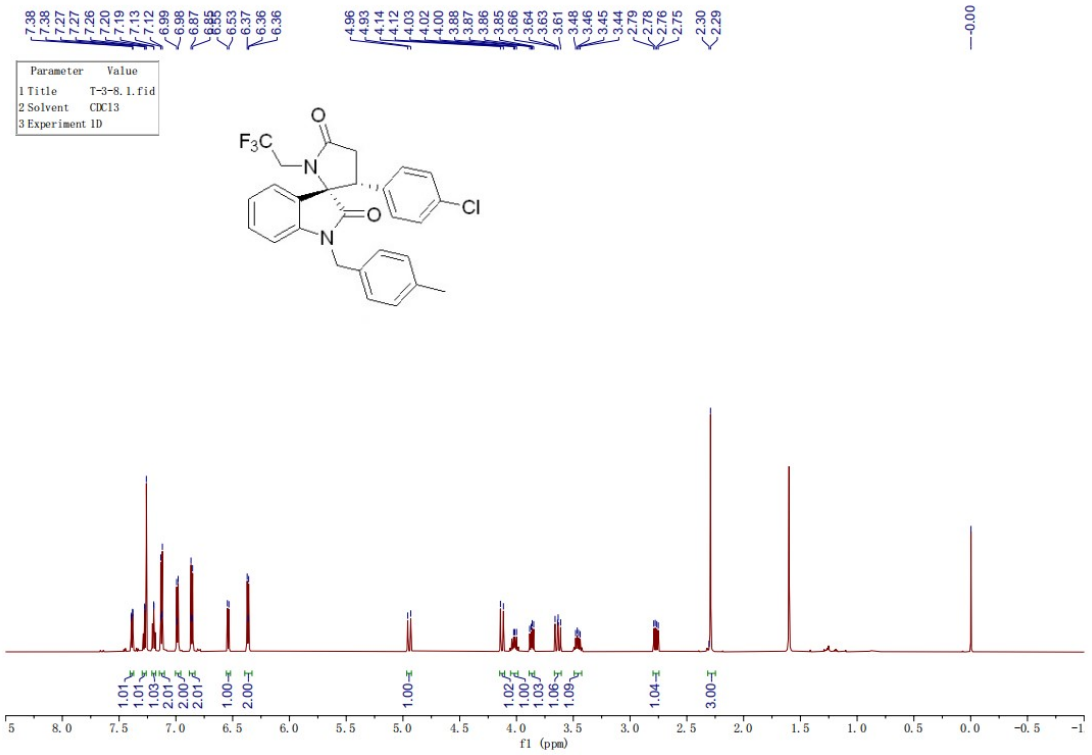
^{1}H-NMR and ^{13}C-NMR of **4o**

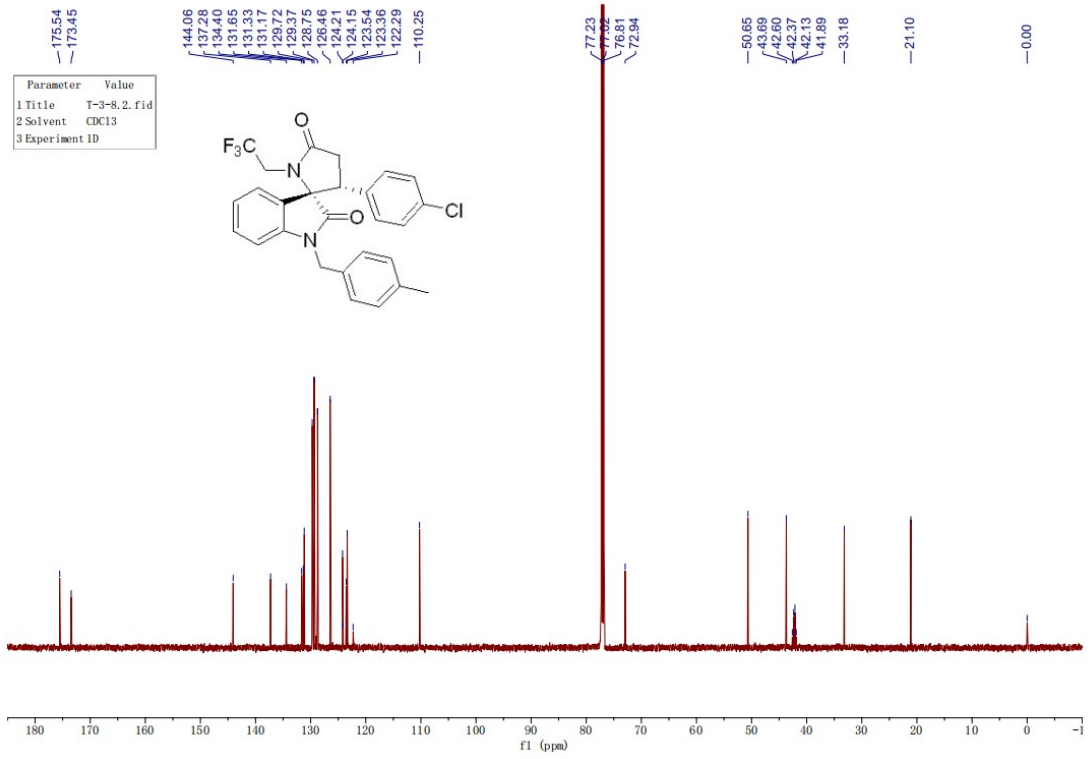




^{1}H-NMR and ^{13}C-NMR of **4p**

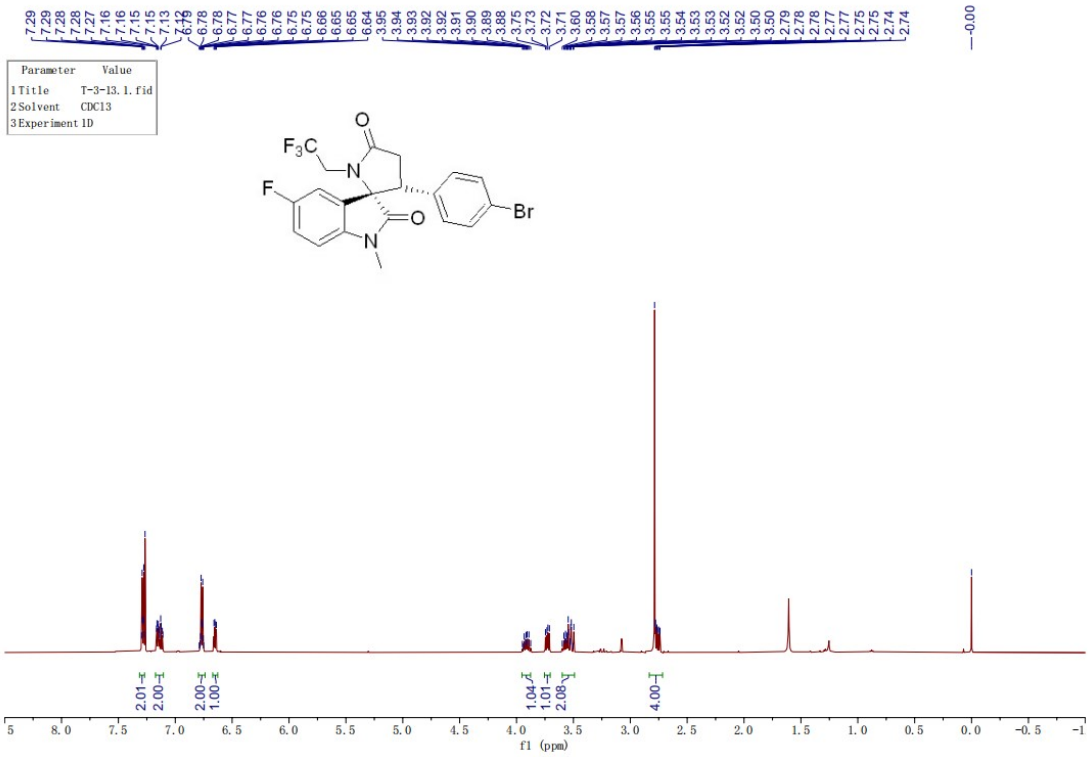
^{1}H-NMR and ^{13}C-NMR of **4q**

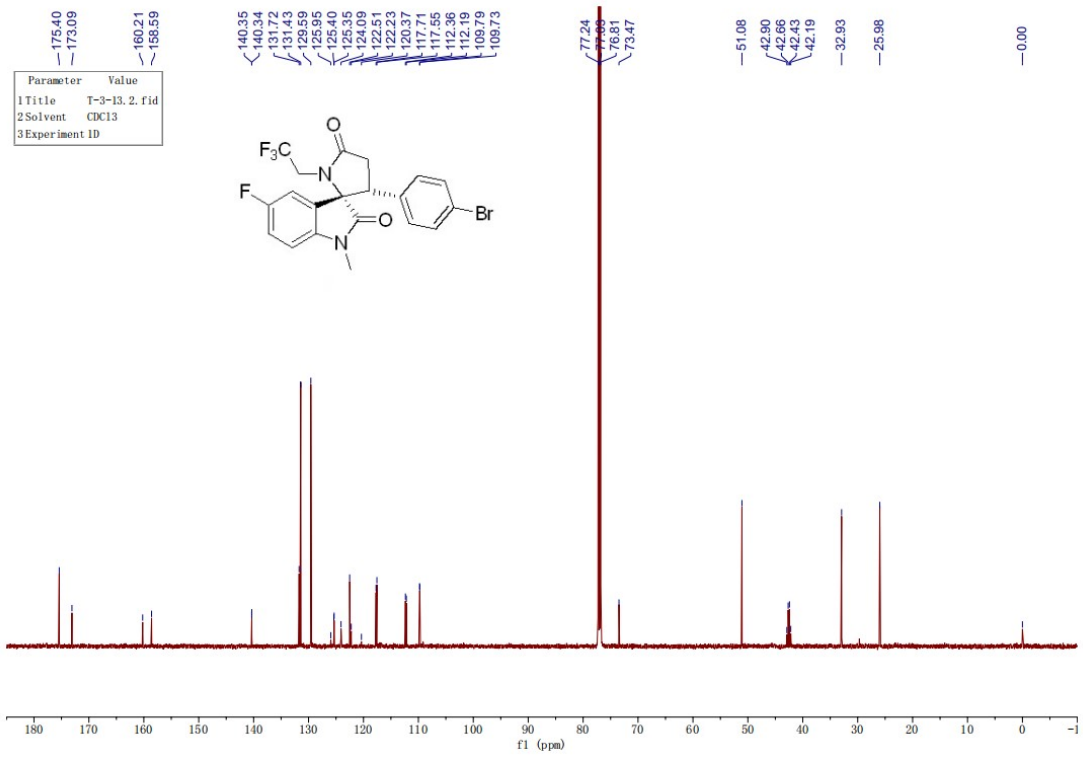




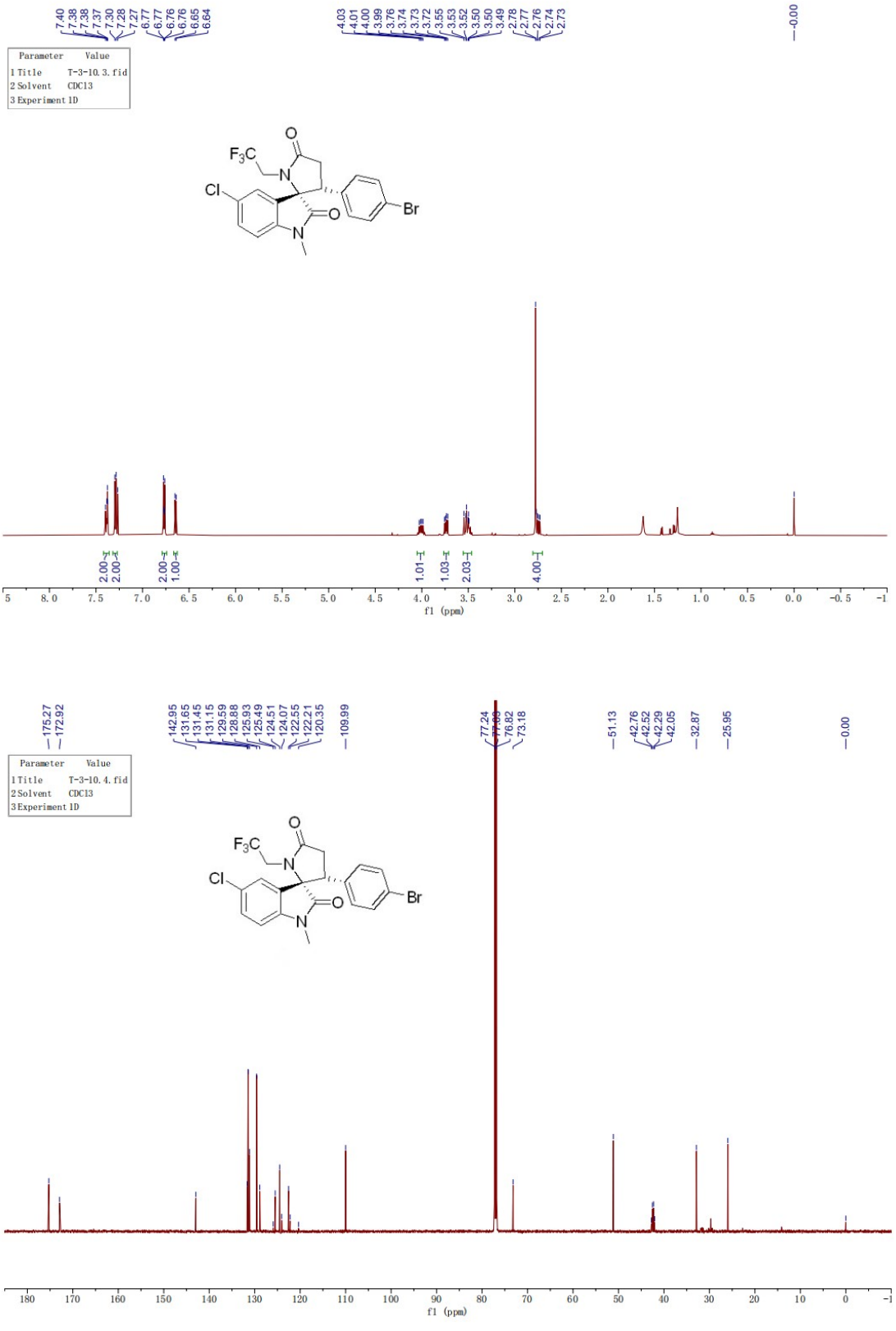
^{1}H-NMR and ^{13}C-NMR of **4r**

^{1}H-NMR and ^{13}C-NMR of **4s**





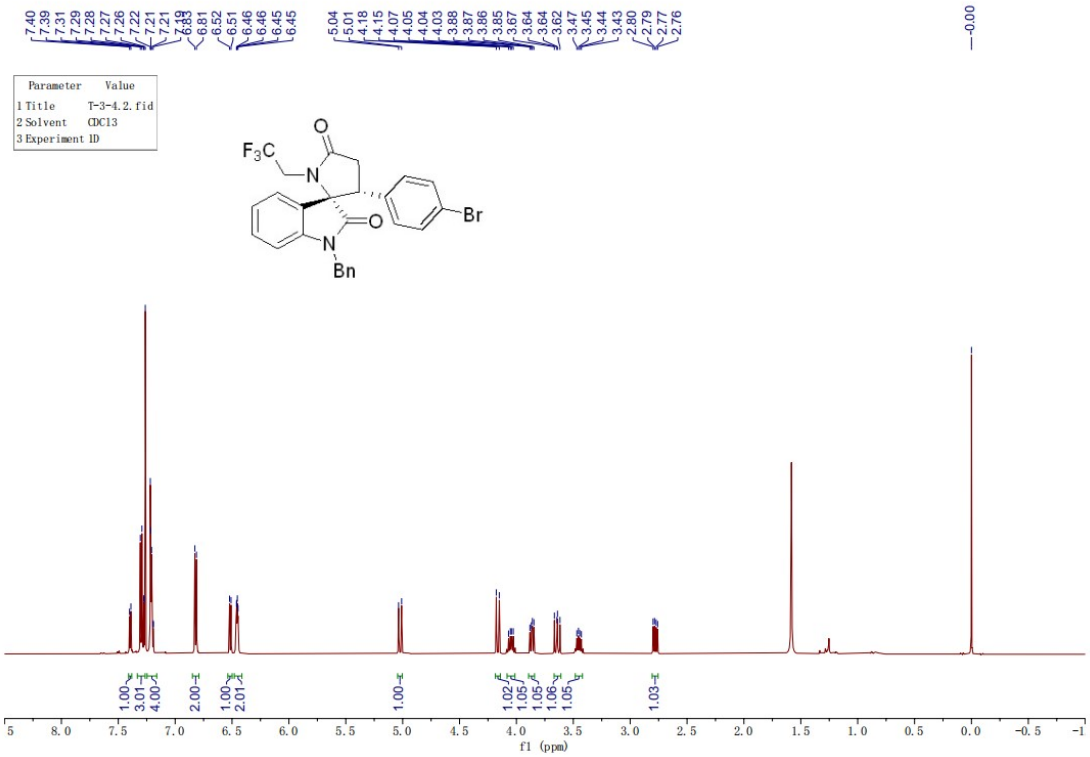
^{1}H-NMR and ^{13}C-NMR of **4t**

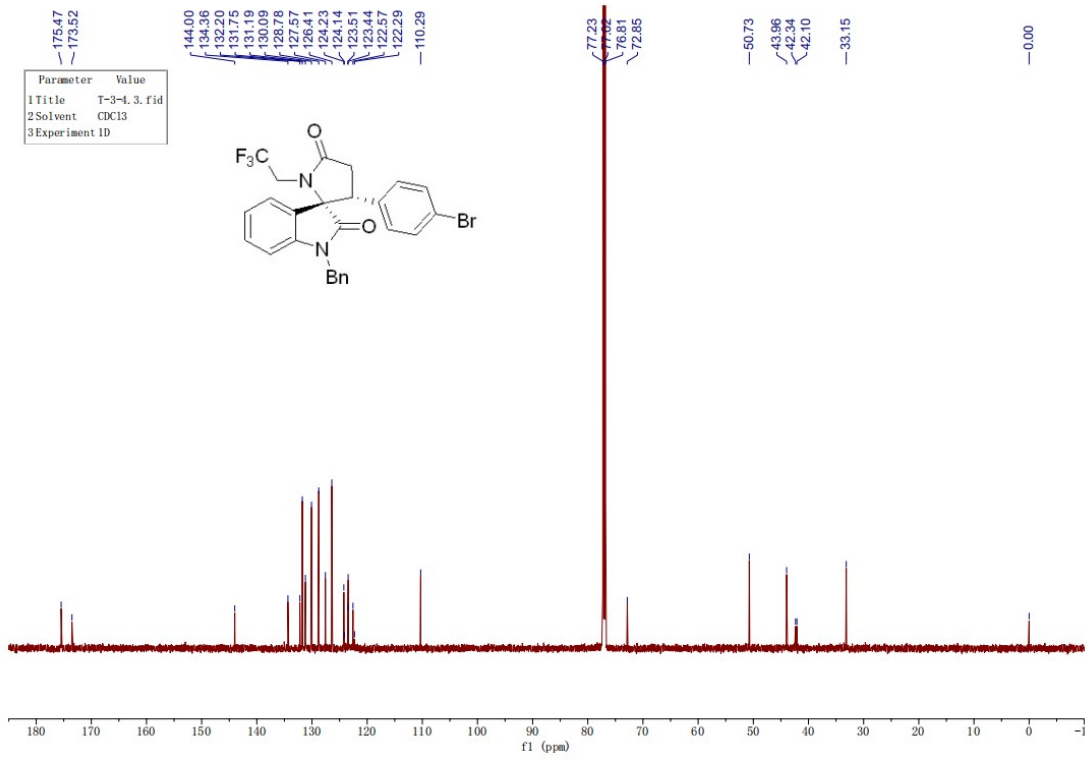


^{1}H-NMR and ^{13}C-NMR of **4u**

^{1}H-NMR and ^{13}C-NMR of **4v**

^{1}H-NMR and ^{13}C-NMR of **4w**

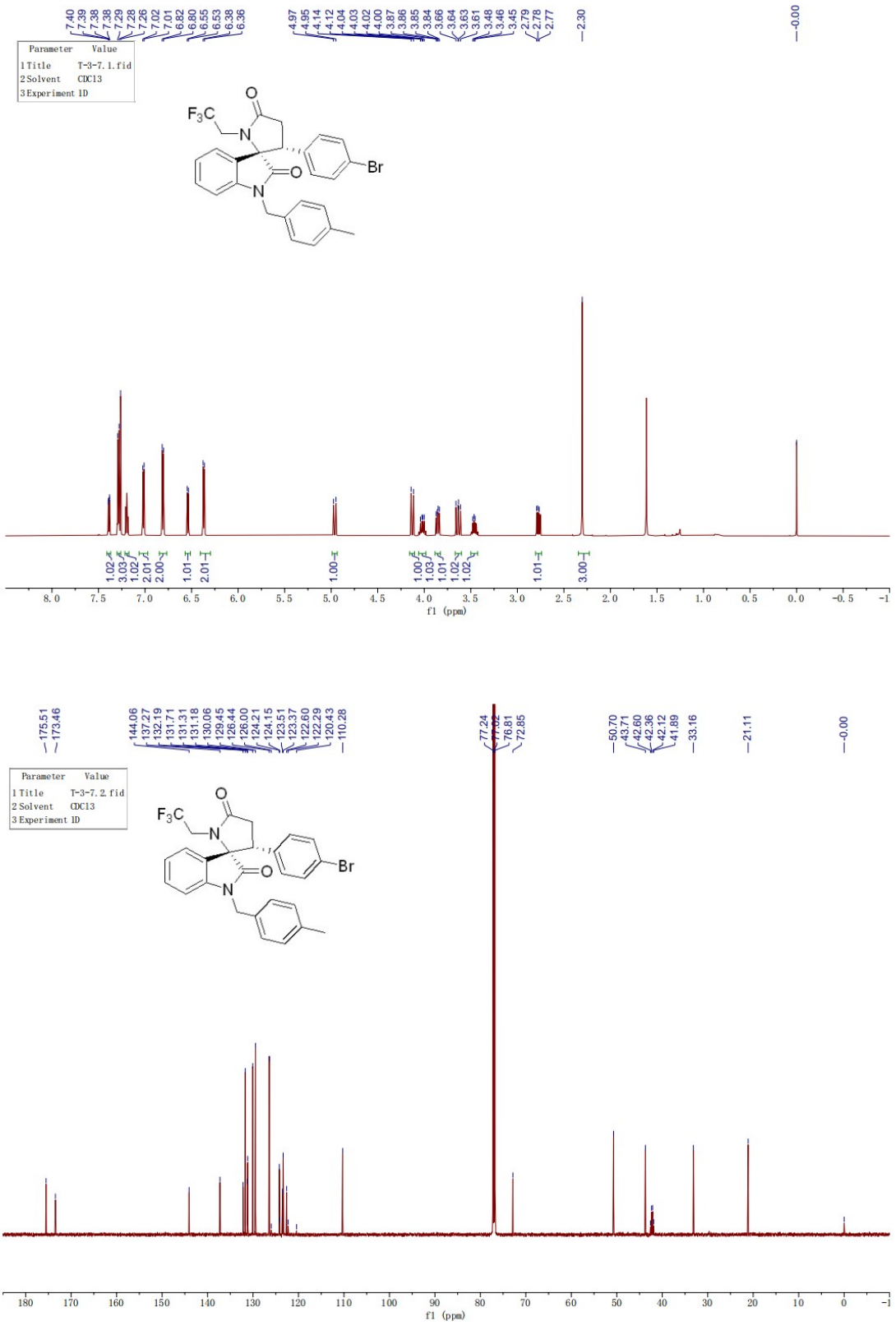




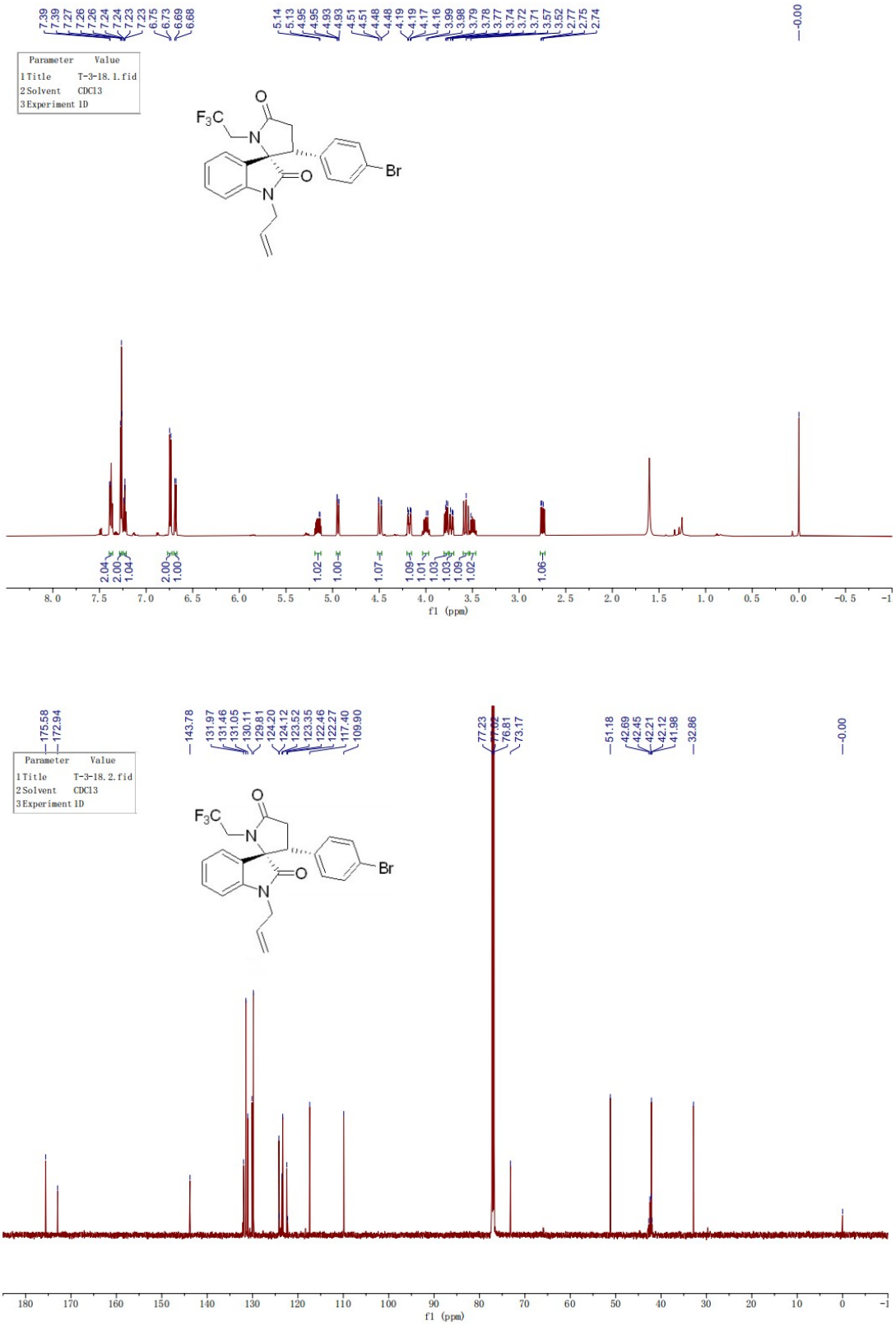
^{1}H-NMR and ^{13}C-NMR of **4x**

^{1}H-NMR and ^{13}C-NMR of **4y**

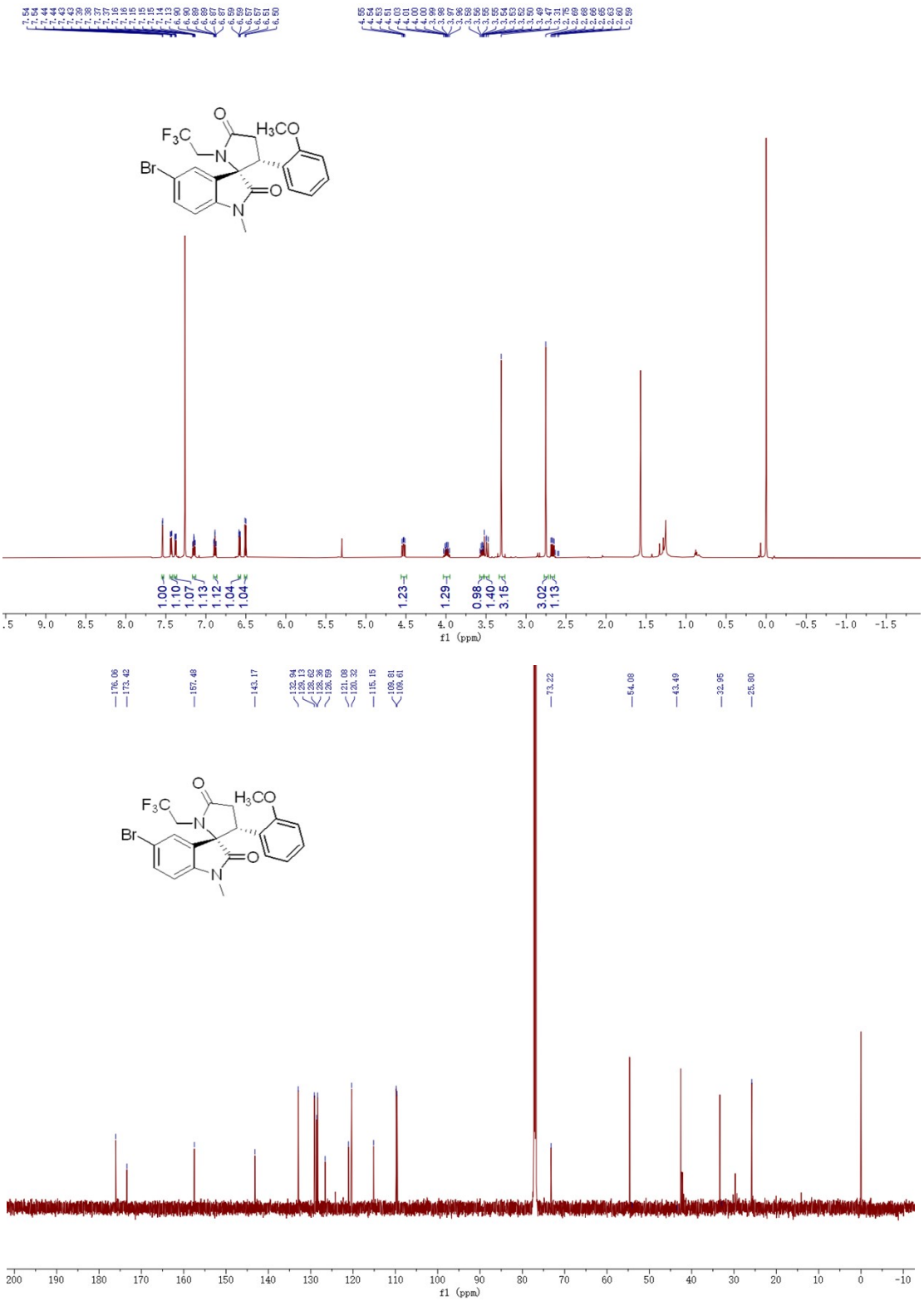
^{1}H-NMR and ^{13}C-NMR of **4z**



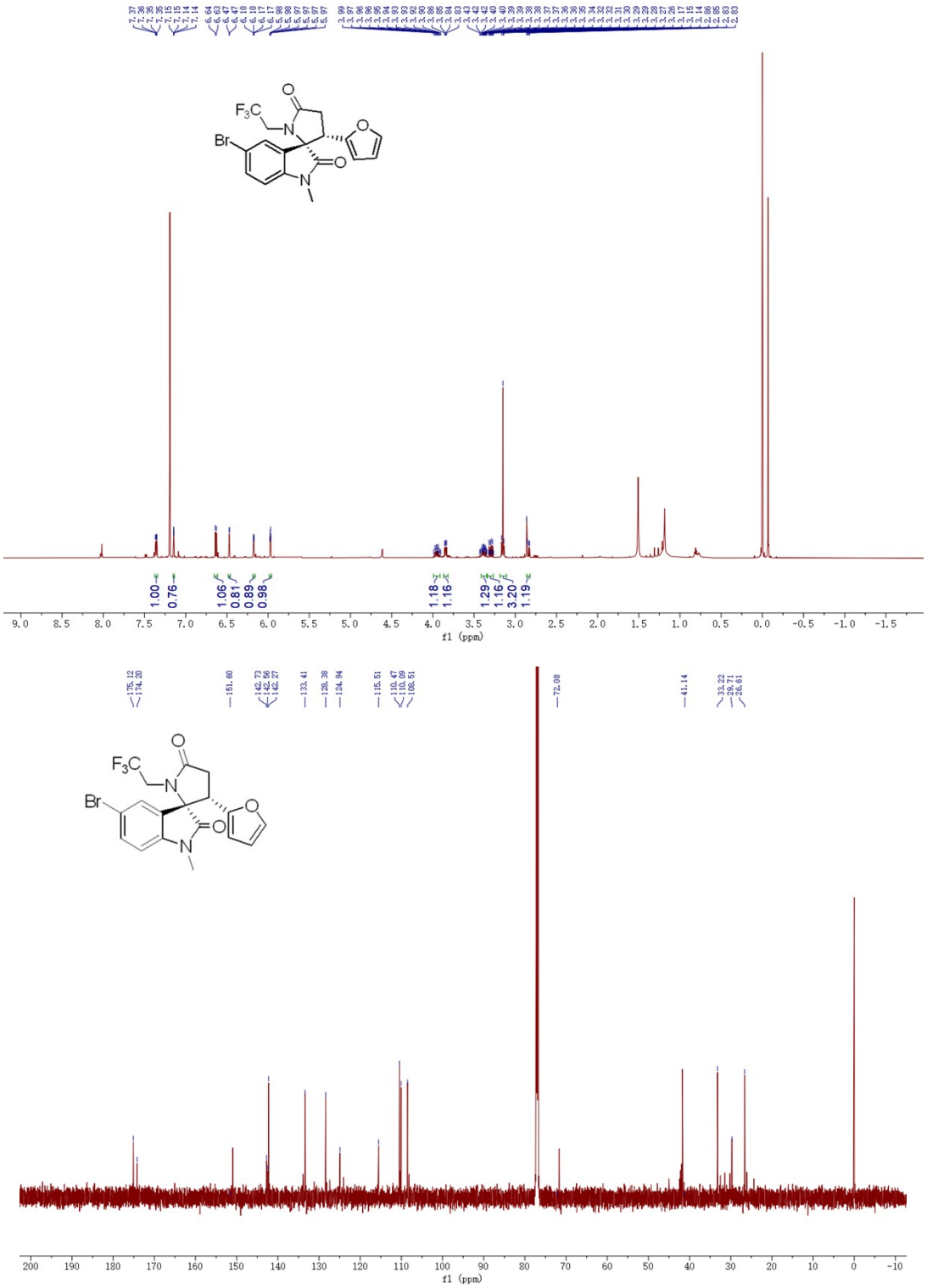
^{1}H-NMR and ^{13}C-NMR of **4aa**



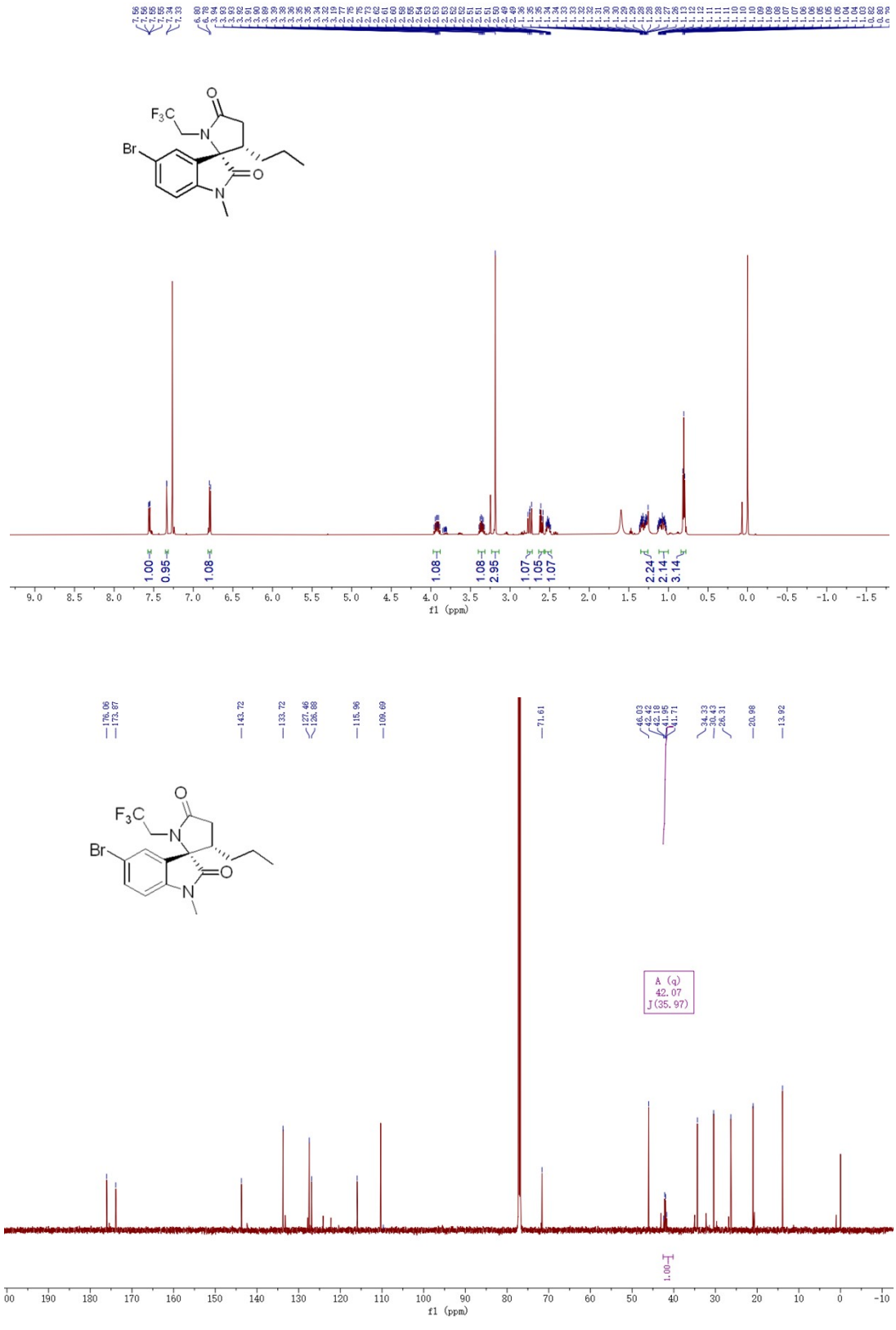
^{1}H-NMR and ^{13}C-NMR of **4ab**



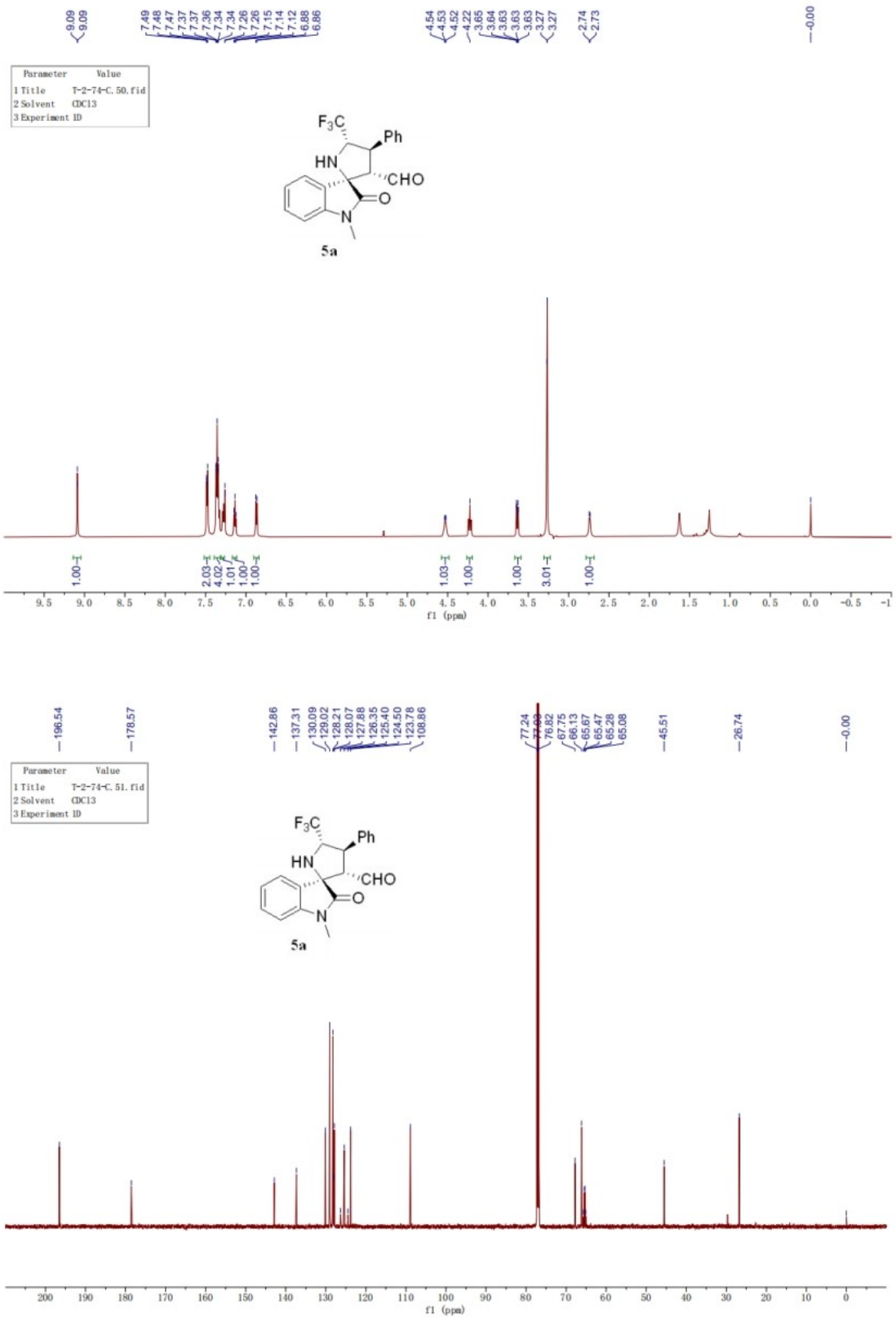
^{1}H-NMR and ^{13}C-NMR of **4ac**



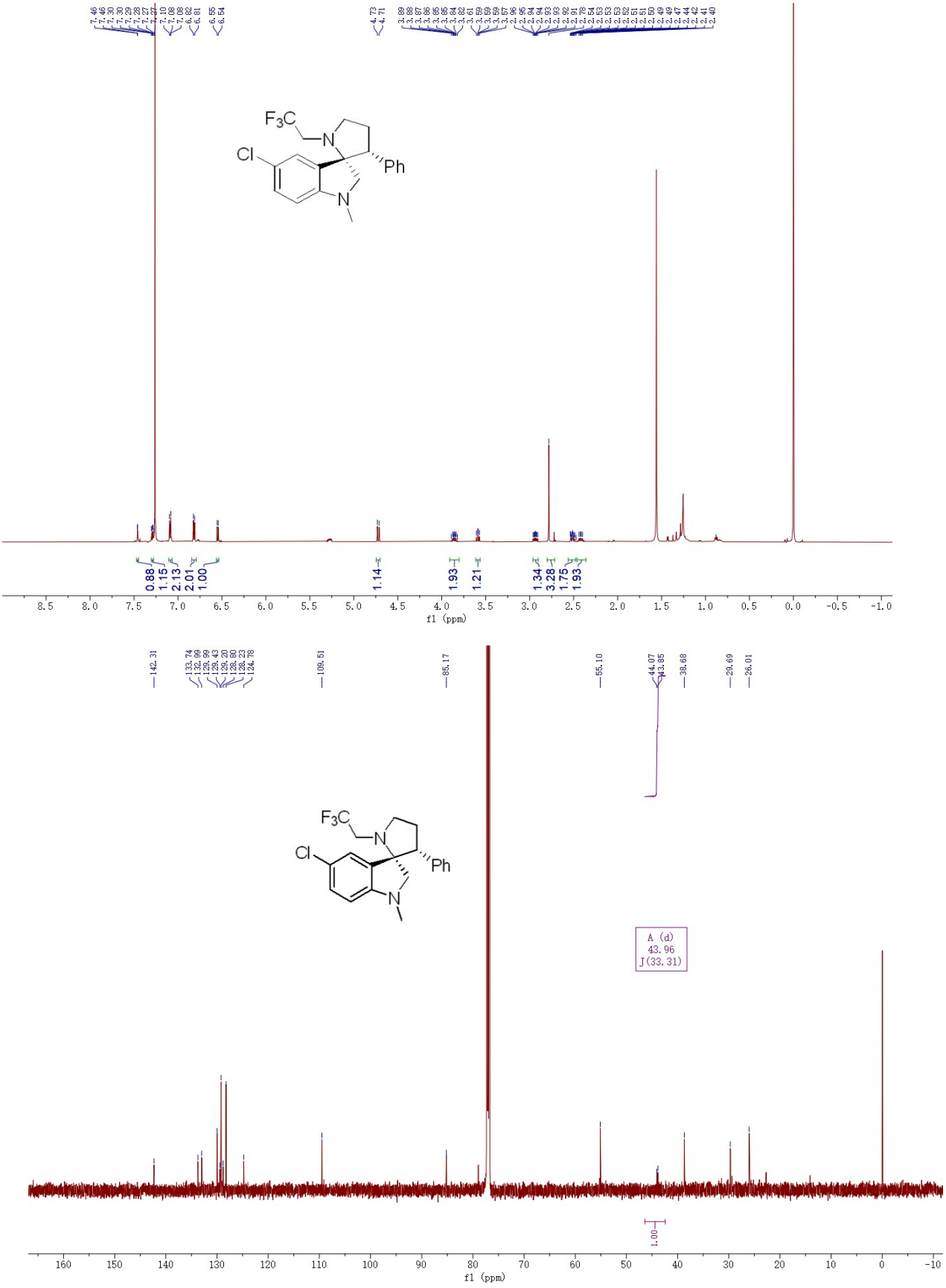
^{1}H-NMR and ^{13}C-NMR of **4ad**



^{1}H-NMR and ^{13}C-NMR of **4ae**

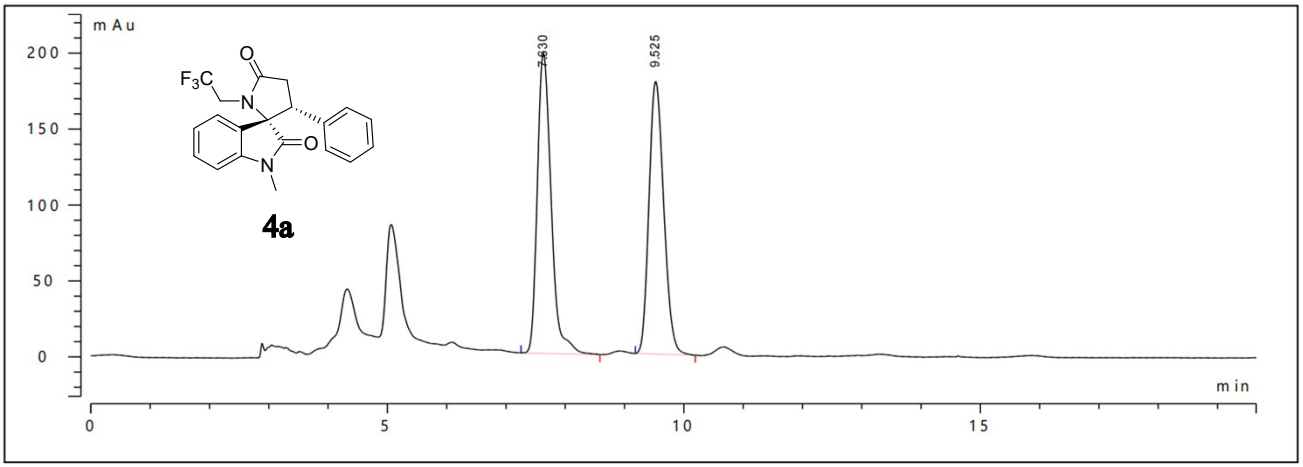


1H-NMR and 13C-NMR of 5a

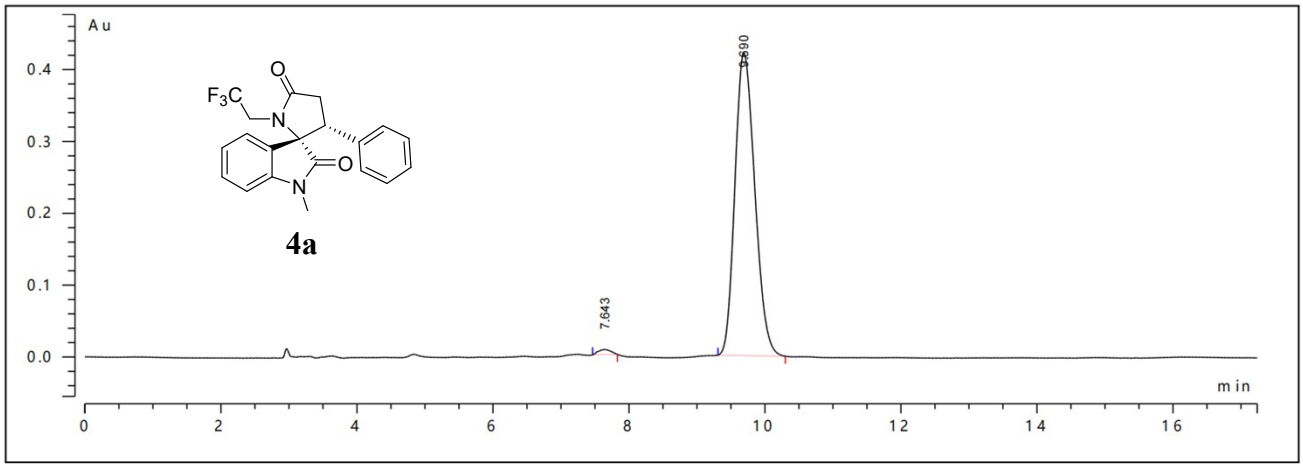


^{1}H-NMR and ^{13}C-NMR of **6l**

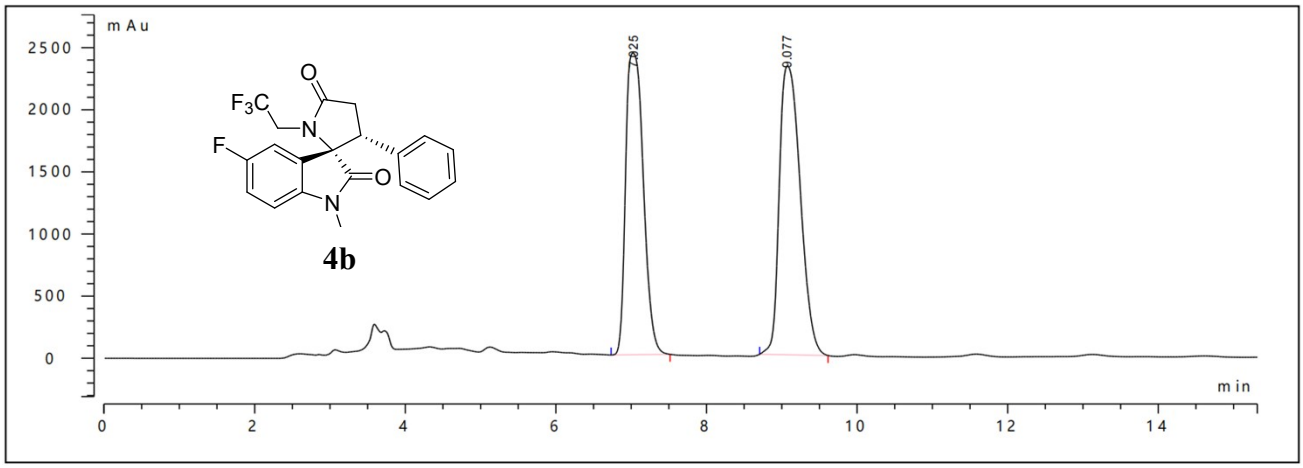
13 HPLC Traces



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.630	3206.265	0.399	198.114	50.746
2	N.A.	9.525	3112.031	0.446	179.900	49.254
3						

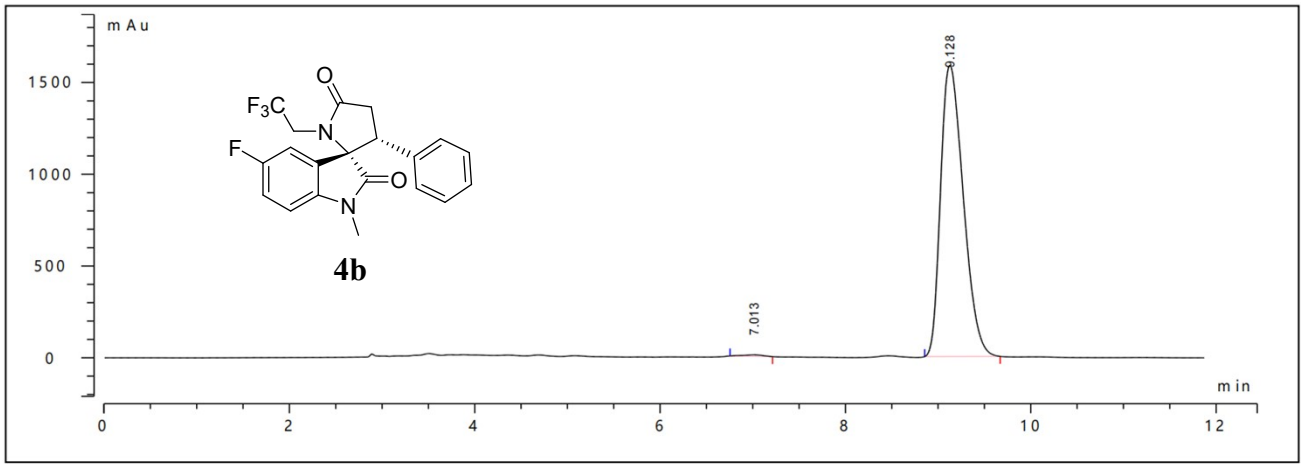


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area% (%) (NA)
1	N.A.	7.643	92.404	0.336	7.152	1.068
2	N.A.	9.690	8562.663	0.523	421.628	98.932
3			8655.067			



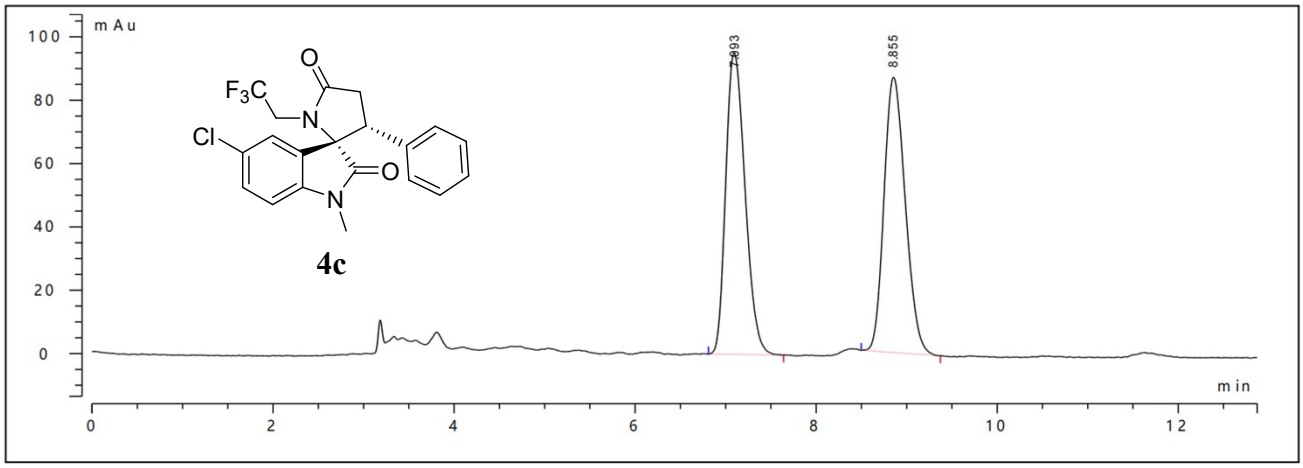
4b

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.025	39684.861	0.378	2429.398	46.898
2	N.A.	9.077	44935.472	0.468	2326.596	53.102
3						



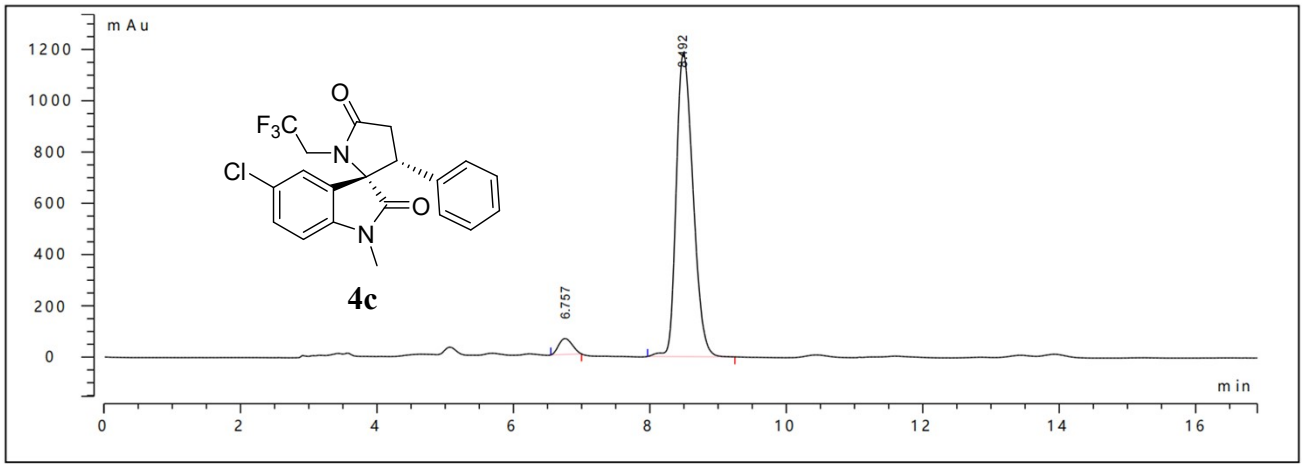
4b

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.013	119.022	0.440	8.242	0.438
2	N.A.	9.128	27033.292	0.433	1587.713	99.562
3						



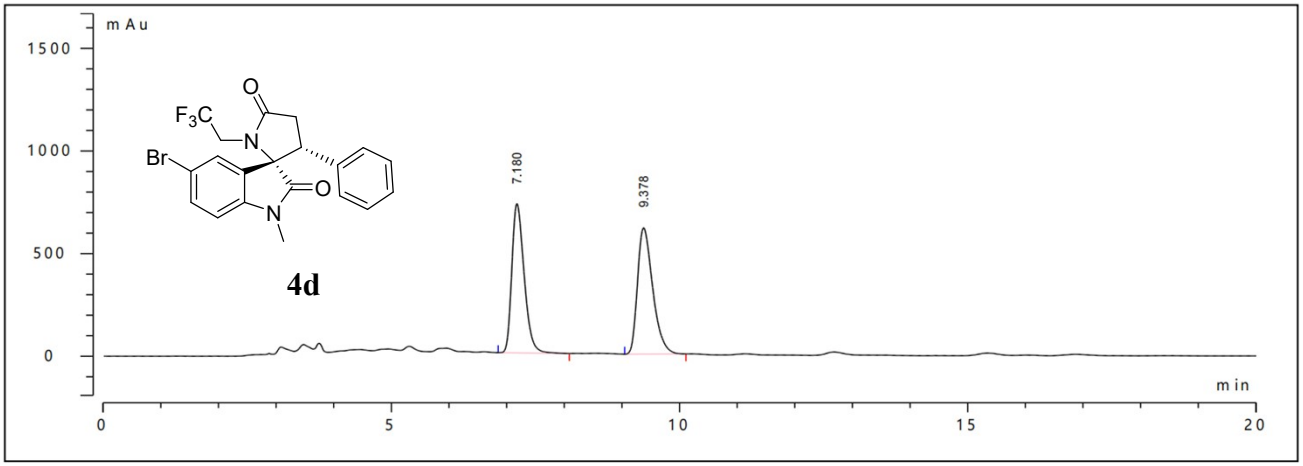
4c

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.093	1412.476	0.378	95.273	49.839
2	N.A.	8.855	1421.616	0.421	86.938	50.161
3						

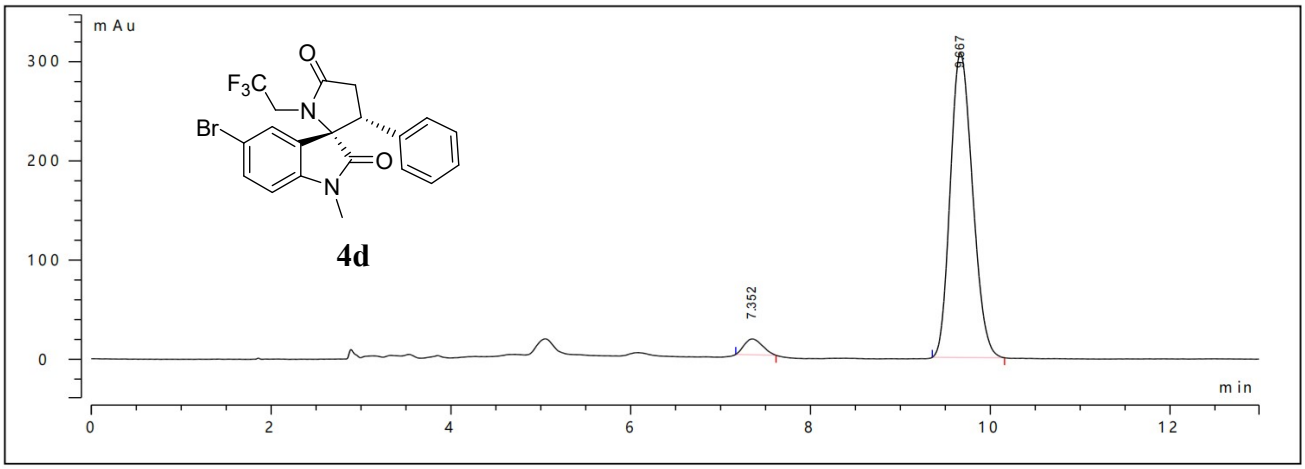


4c

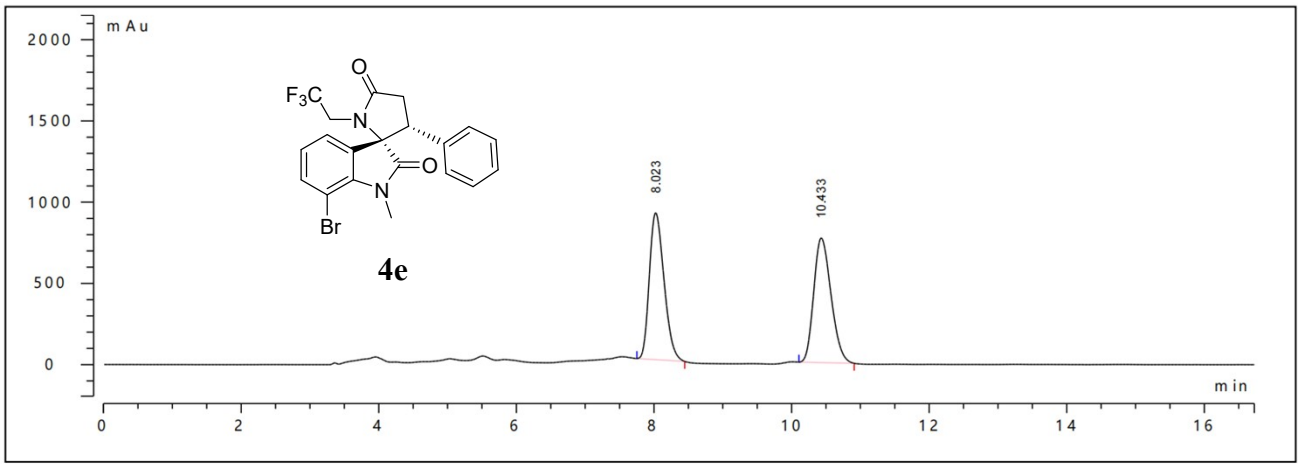
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	6.757	859.181	0.366	62.371	4.068
2	N.A.	8.492	20262.061	0.438	1185.897	95.932
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.180	10806.275	0.378	727.706	48.874
2	N.A.	9.378	11304.258	0.460	616.052	51.126
3						

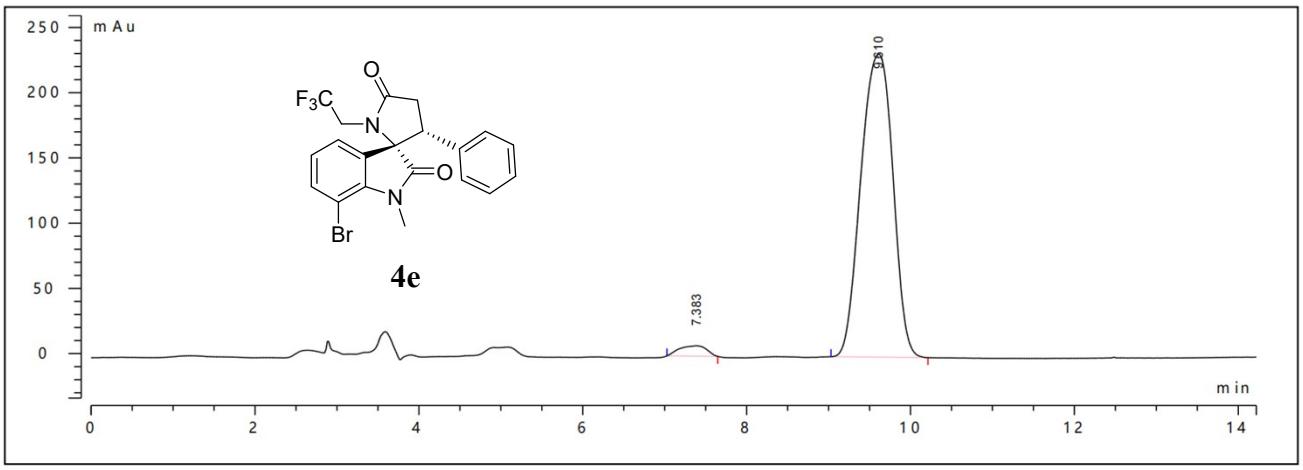


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.352	224.114	0.374	15.961	4.070
2	N.A.	9.667	5282.201	0.447	306.916	95.930
3						



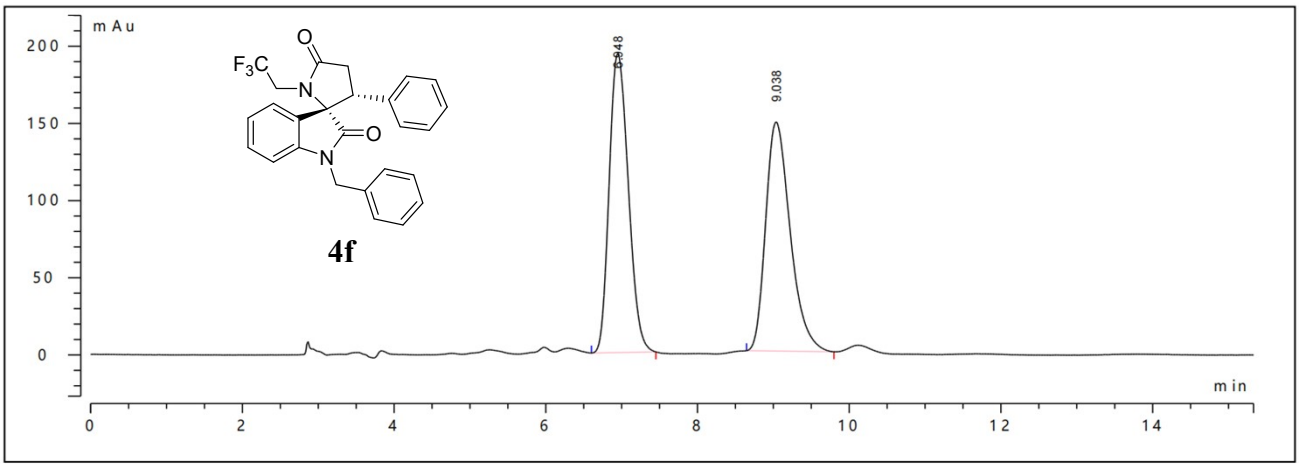
4e

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.023	13396.951	0.389	906.126	49.986
2	N.A.	10.433	13404.641	0.445	767.942	50.014
3						



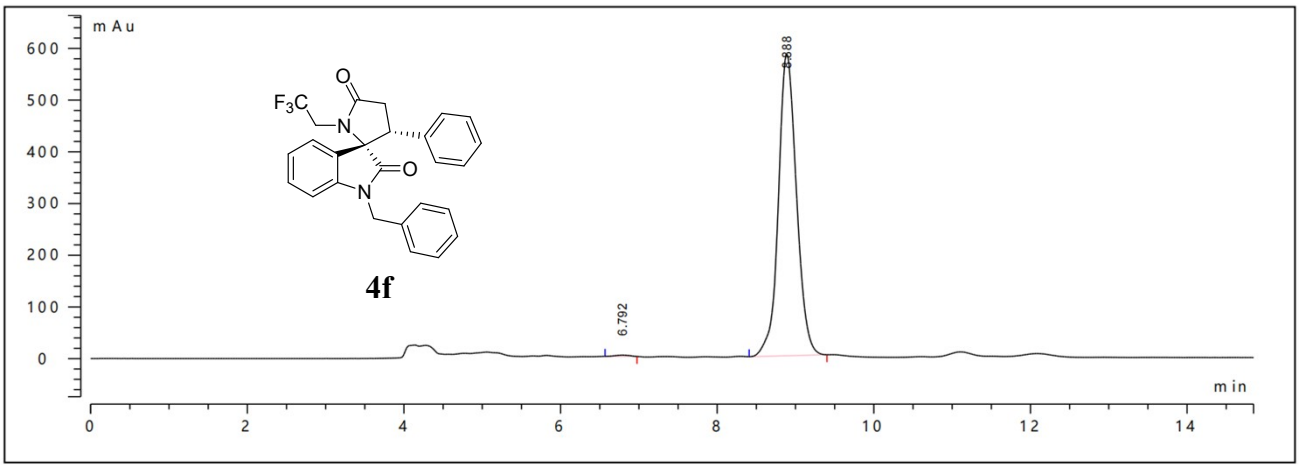
4e

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.383	184.686	0.571	7.912	2.842
2	N.A.	9.610	6313.642	0.682	232.456	97.158
3						



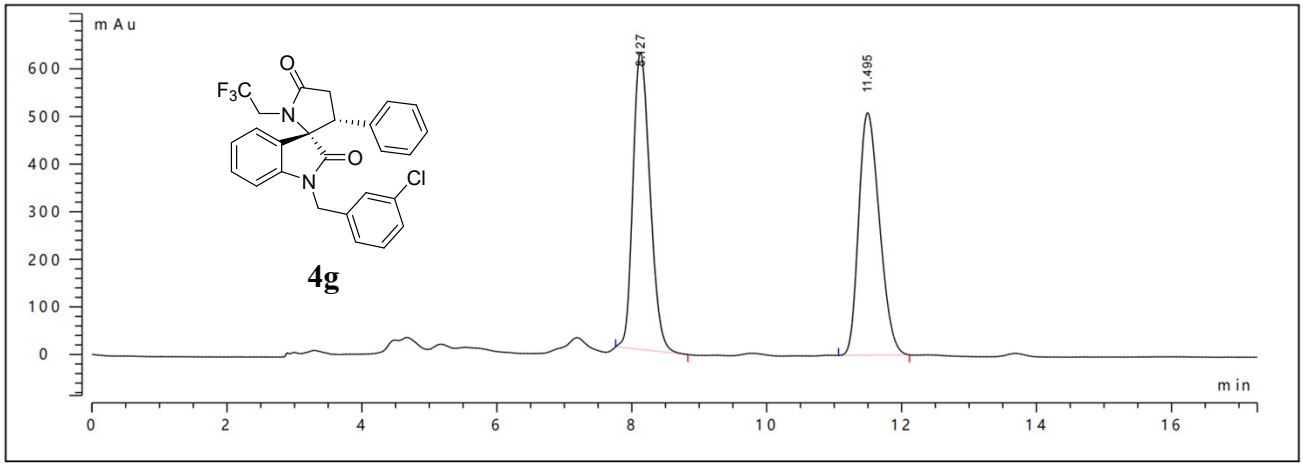
4f

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	6.948	3402.420	0.450	193.879	50.461
2	N.A.	9.038	3340.251	0.567	148.547	49.539
3						

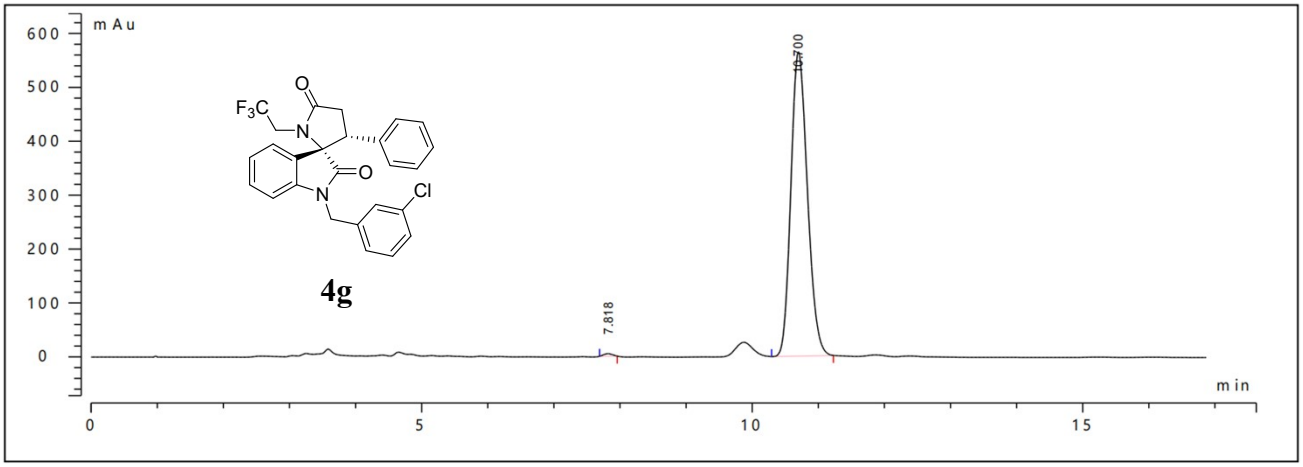


4f

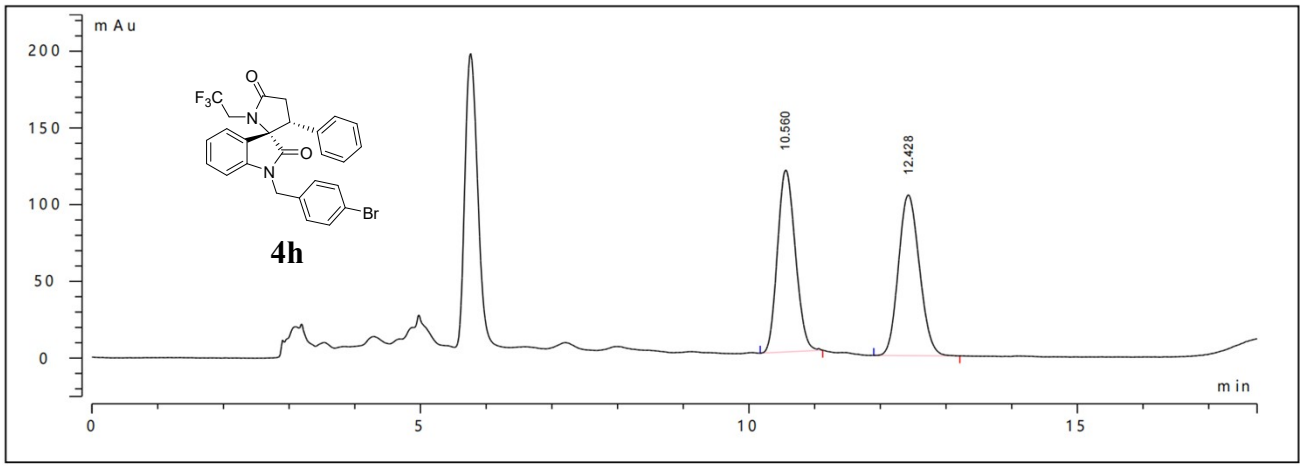
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	6.792	30.591	0.318	2.459	0.325
2	N.A.	8.888	9372.040	0.396	584.444	99.675
3						



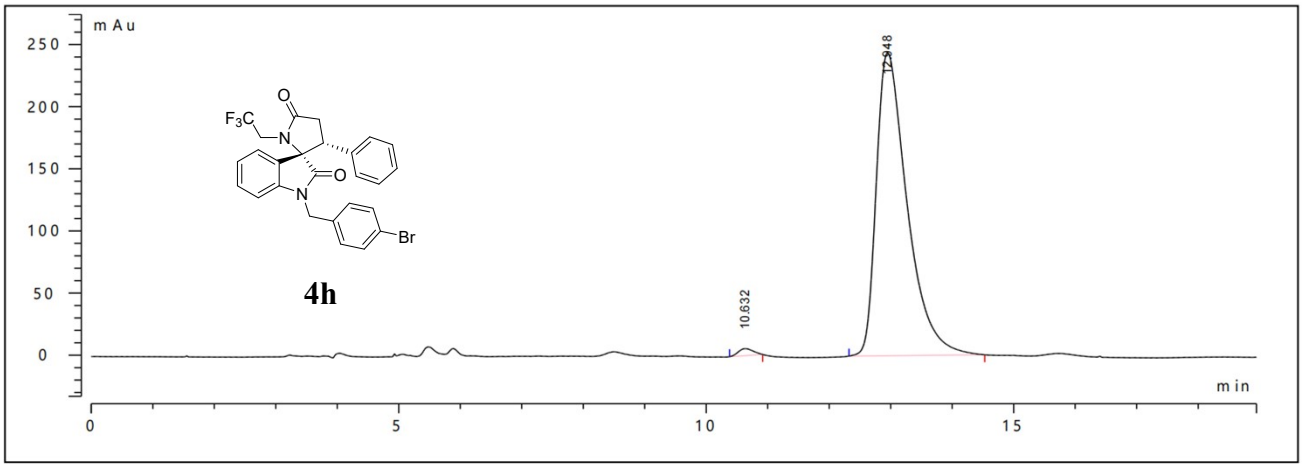
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.127	10966.262	0.454	625.183	50.132
2	N.A.	11.495	10908.597	0.559	509.815	49.868
3						



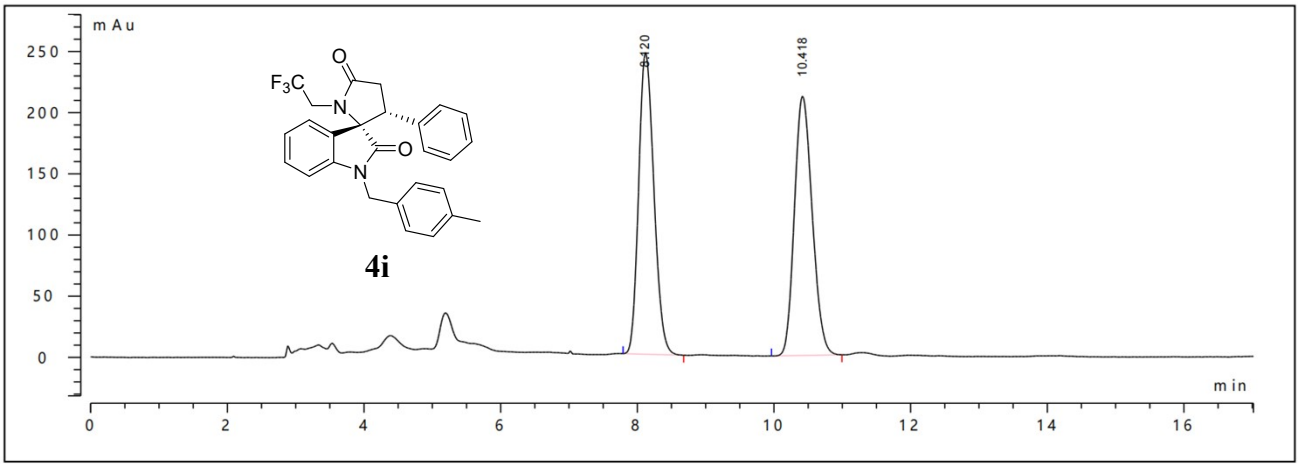
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.818	42.012	0.249	4.553	0.426
2	N.A.	10.700	9816.552	0.448	564.592	99.574
3						



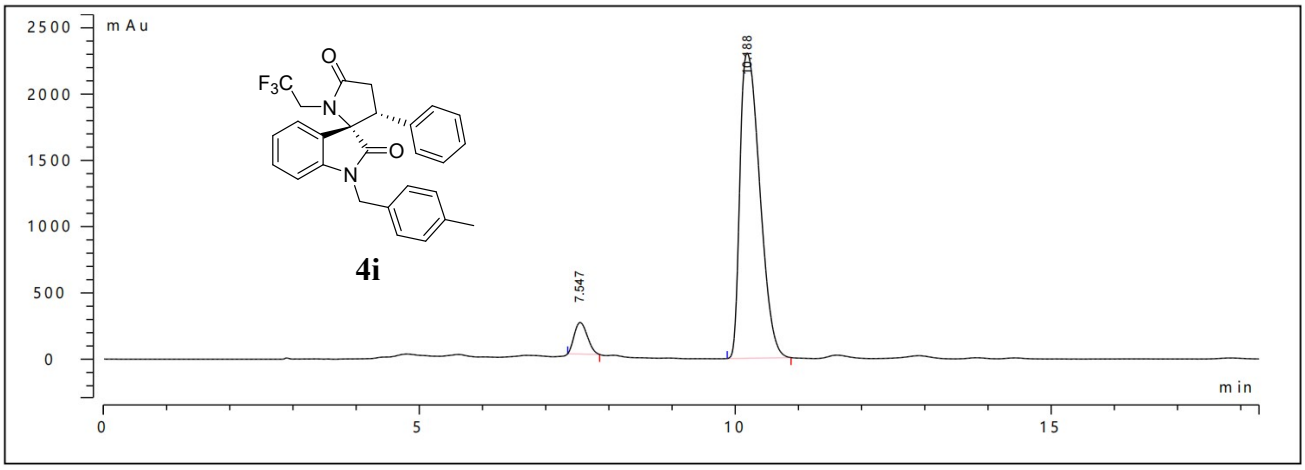
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	10.560	2244.540	0.493	118.725	49.069
2	N.A.	12.428	2329.708	0.579	104.801	50.931
3						



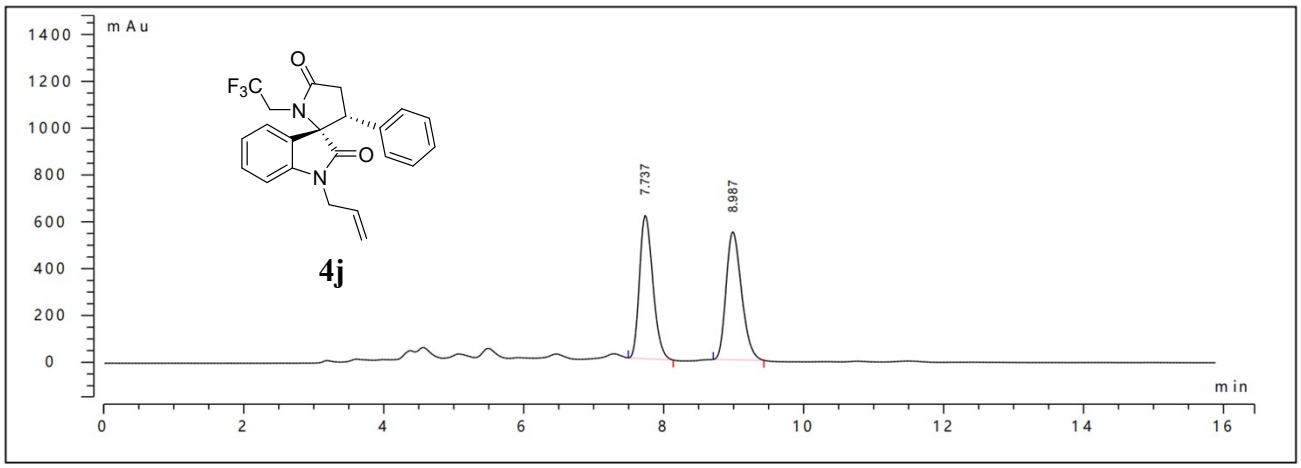
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area% (%) (NA)
1	N.A.	10.632	93.491	0.437	5.631	1.088
2	N.A.	12.948	8498.850	0.850	243.844	98.912
3			8592.341			



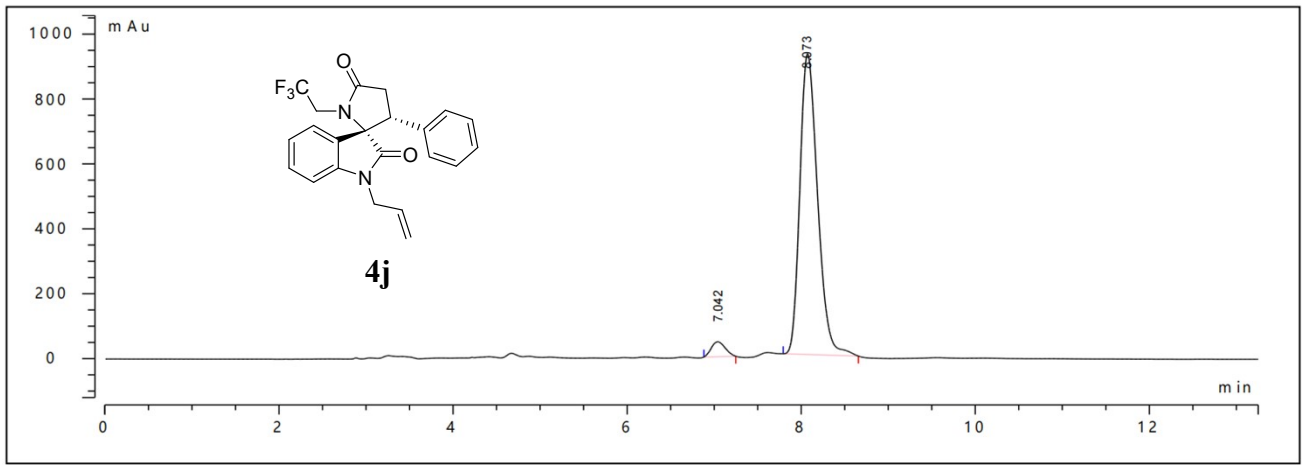
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.120	3825.186	0.396	246.588	49.927
2	N.A.	10.418	3836.344	0.470	211.825	50.073
3						



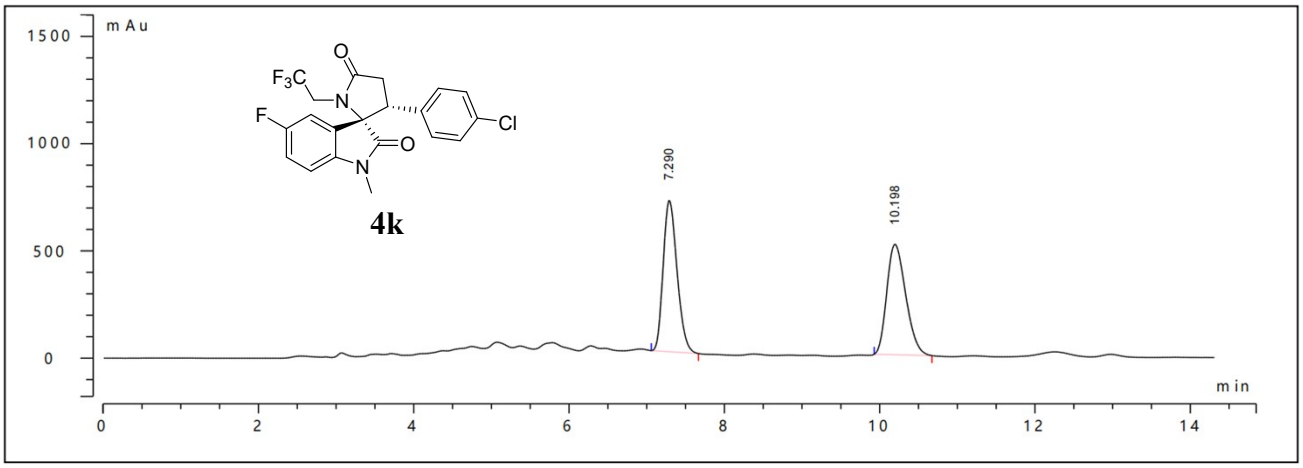
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.547	3433.490	0.375	239.220	6.408
2	N.A.	10.188	50144.472	0.547	2303.094	93.592
3						



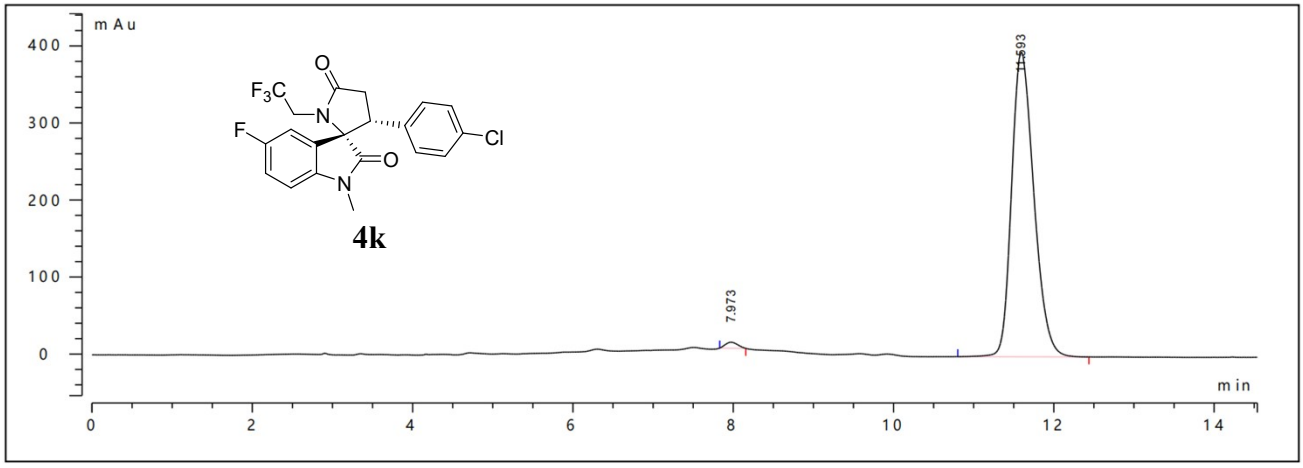
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.737	8135.275	0.342	613.089	49.210
2	N.A.	8.987	8396.604	0.394	546.845	50.790
3						



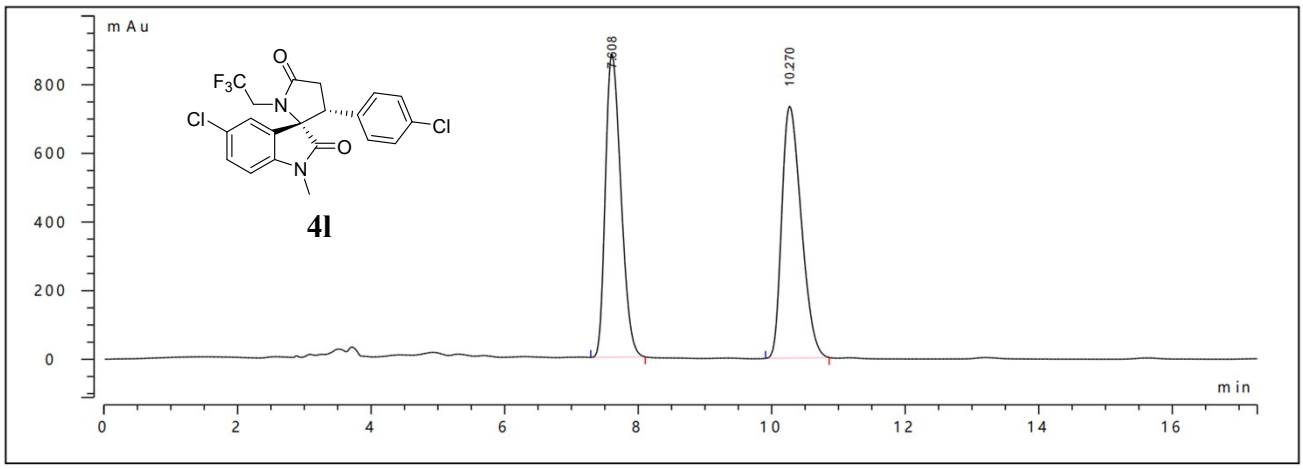
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.042	507.558	0.291	45.978	3.726
2	N.A.	8.073	13115.811	0.353	926.975	96.274
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.290	8777.816	0.317	707.764	50.183
2	N.A.	10.198	8713.906	0.434	516.246	49.817
3						

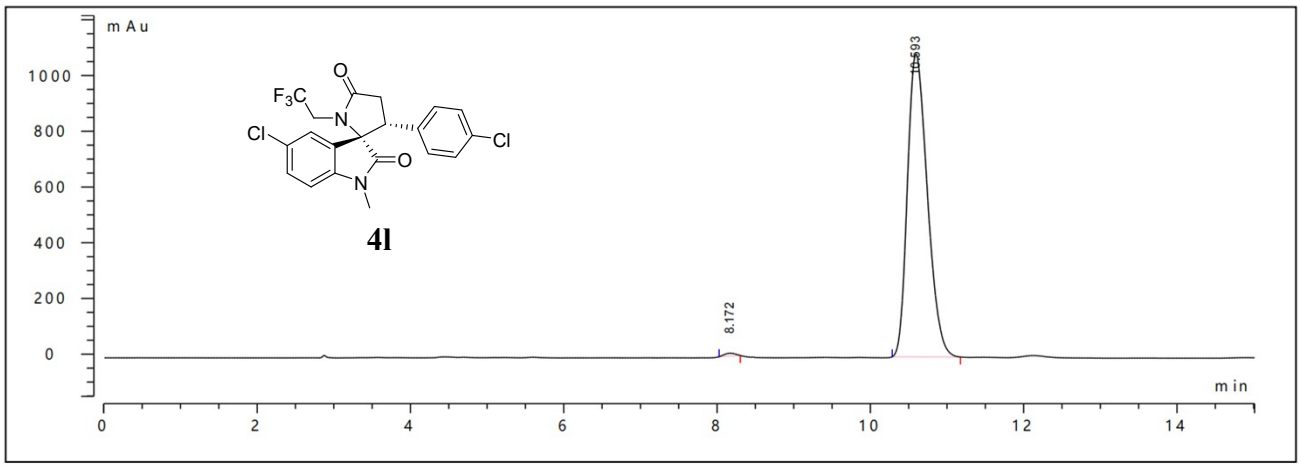


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.973	82.266	0.288	7.725	1.067
2	N.A.	11.593	7626.531	0.493	395.929	98.933
3						



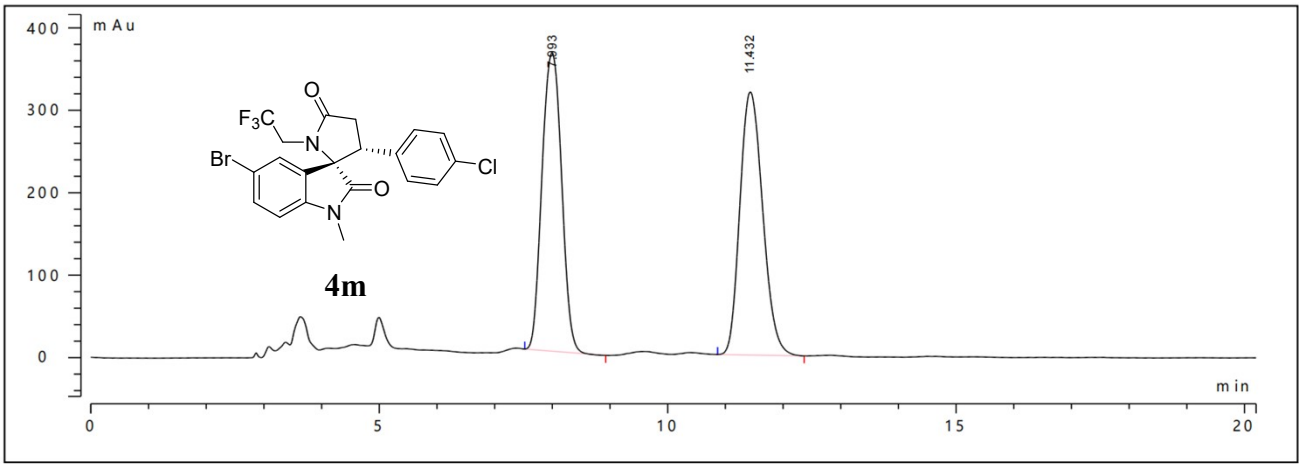
4l

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.608	14300.216	0.420	884.070	49.024
2	N.A.	10.270	14869.881	0.526	734.426	50.976
3						

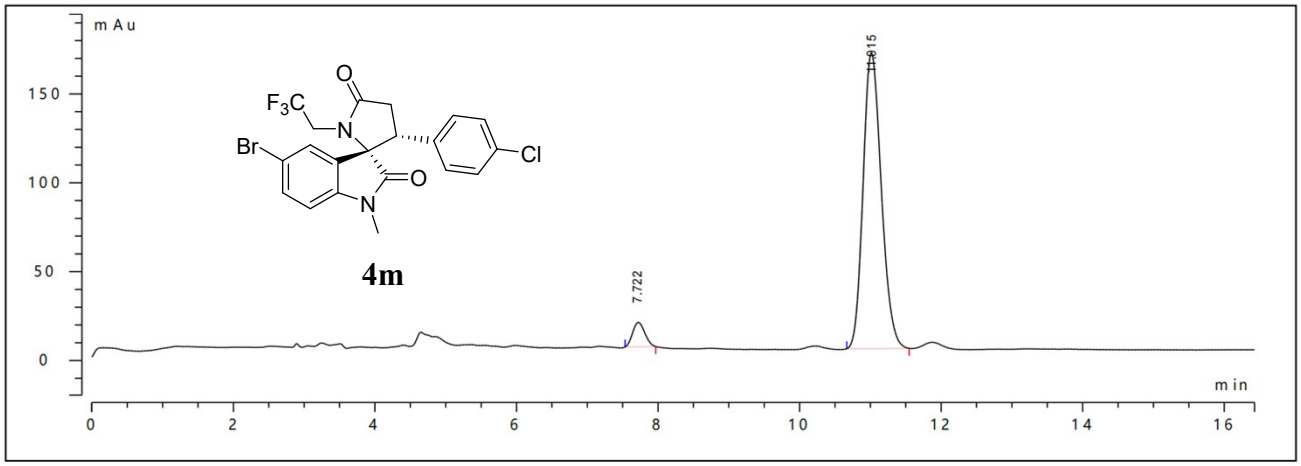


4l

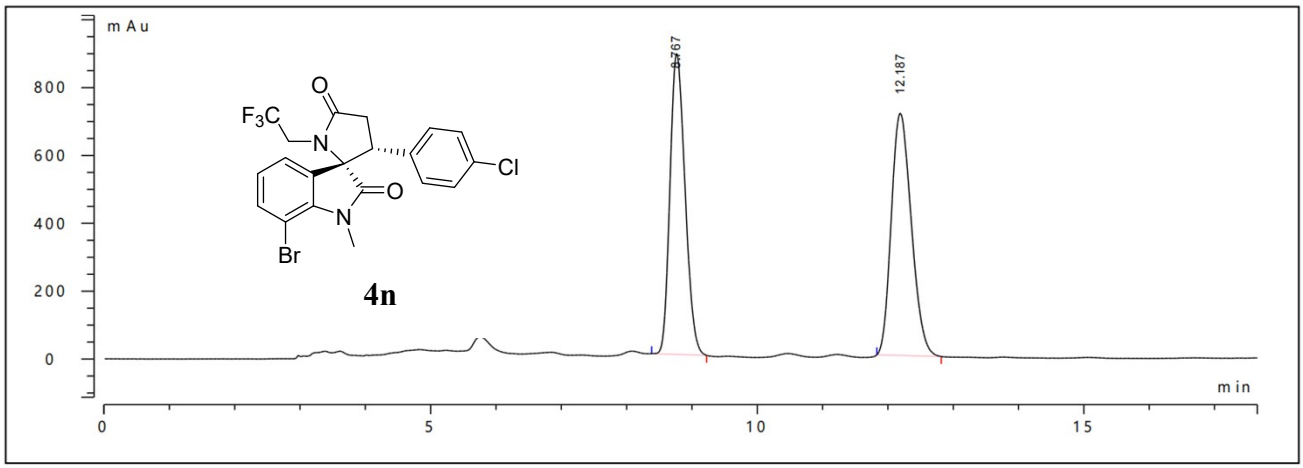
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.172	101.789	0.269	10.361	0.516
2	N.A.	10.593	19611.278	0.466	1088.176	99.484
3						



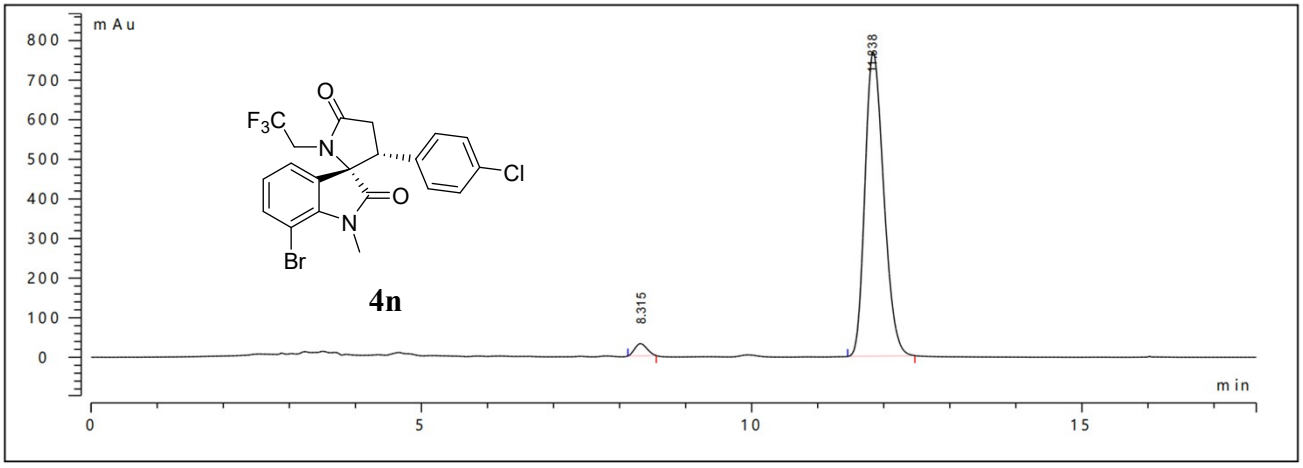
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.993	8551.684	0.601	362.109	49.331
2	N.A.	11.432	8783.538	0.698	319.302	50.669
3						



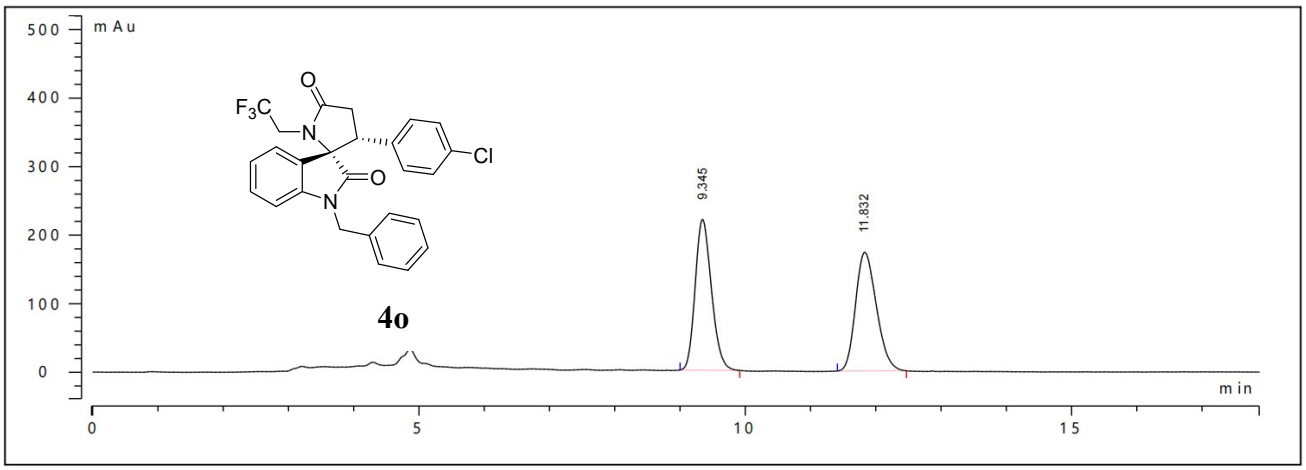
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.722	163.155	0.313	13.816	5.194
2	N.A.	11.015	2978.261	0.453	166.736	94.806
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.767	14239.053	0.417	886.892	48.337
2	N.A.	12.187	15219.106	0.552	714.366	51.663
3						

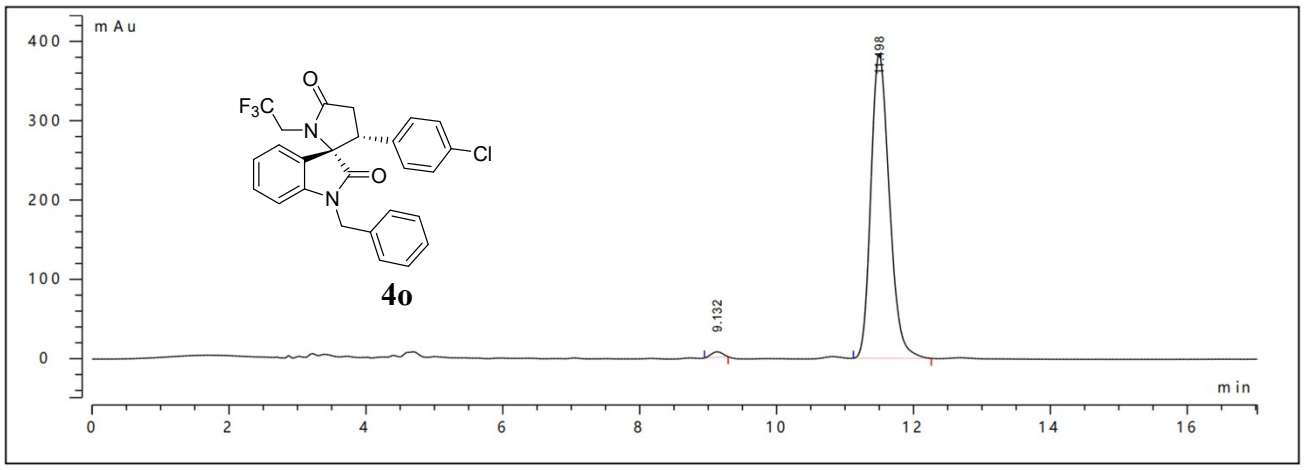


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.315	394.187	0.343	30.759	2.534
2	N.A.	11.838	15164.131	0.506	768.653	97.466
3						



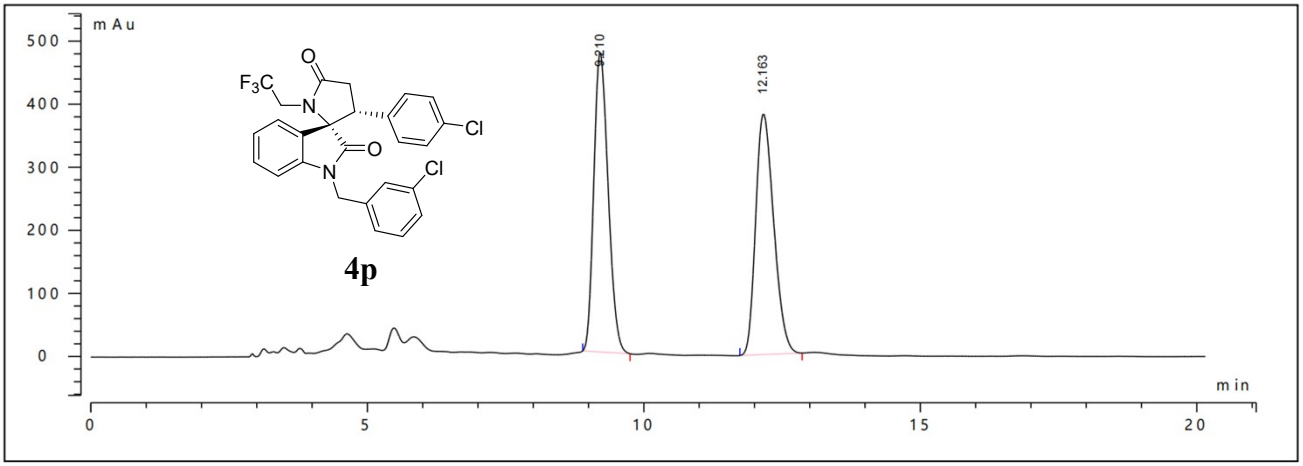
4o

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	9.345	3818.343	0.448	220.342	49.891
2	N.A.	11.832	3835.102	0.567	173.229	50.109
3						



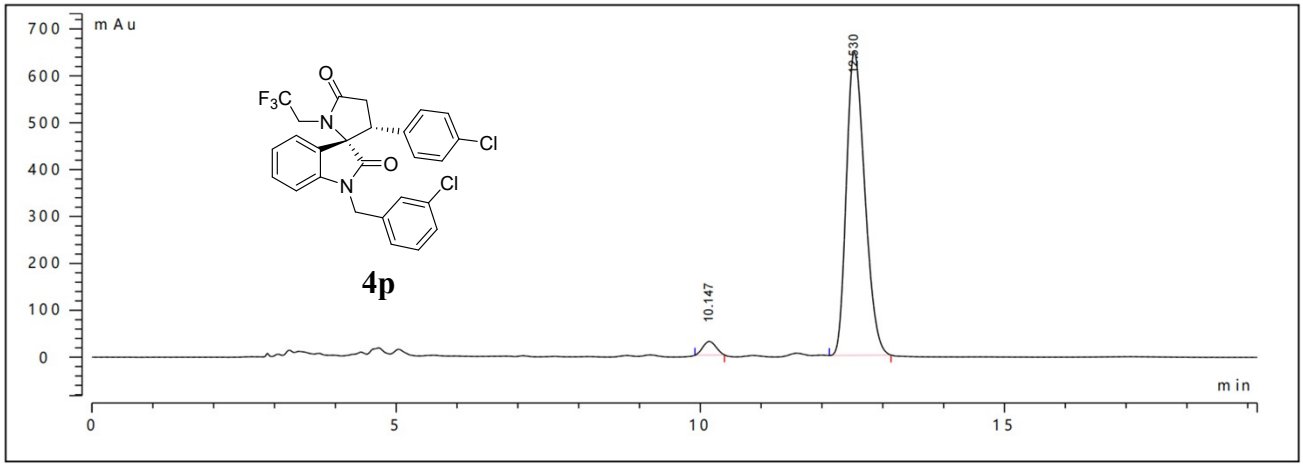
4o

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	9.132	78.938	0.311	6.895	1.085
2	N.A.	11.498	7199.555	0.477	383.849	98.915
3						



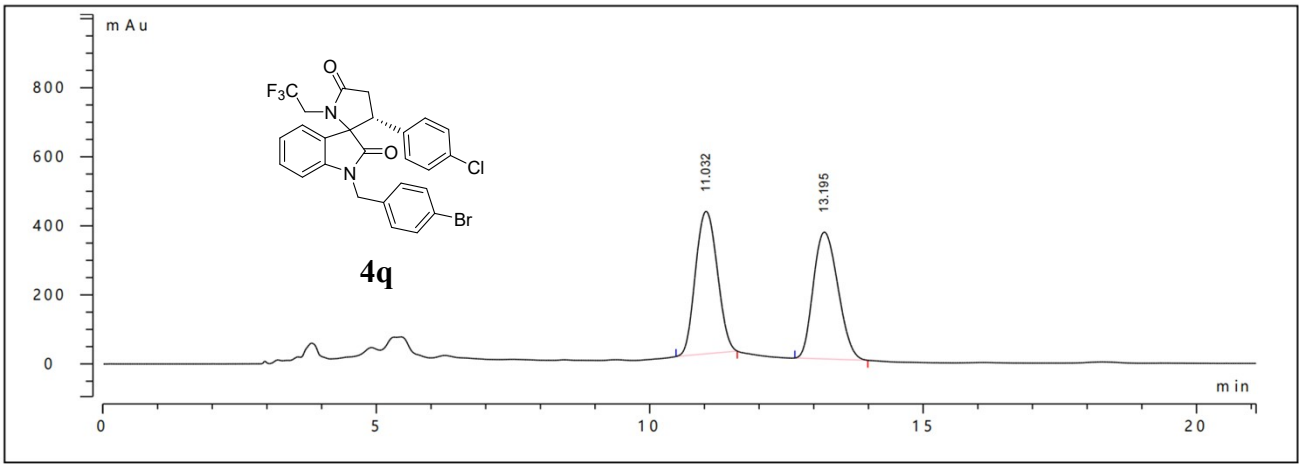
4p

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	9.210	8561.680	0.464	476.042	49.671
2	N.A.	12.163	8674.970	0.575	382.202	50.329
3						

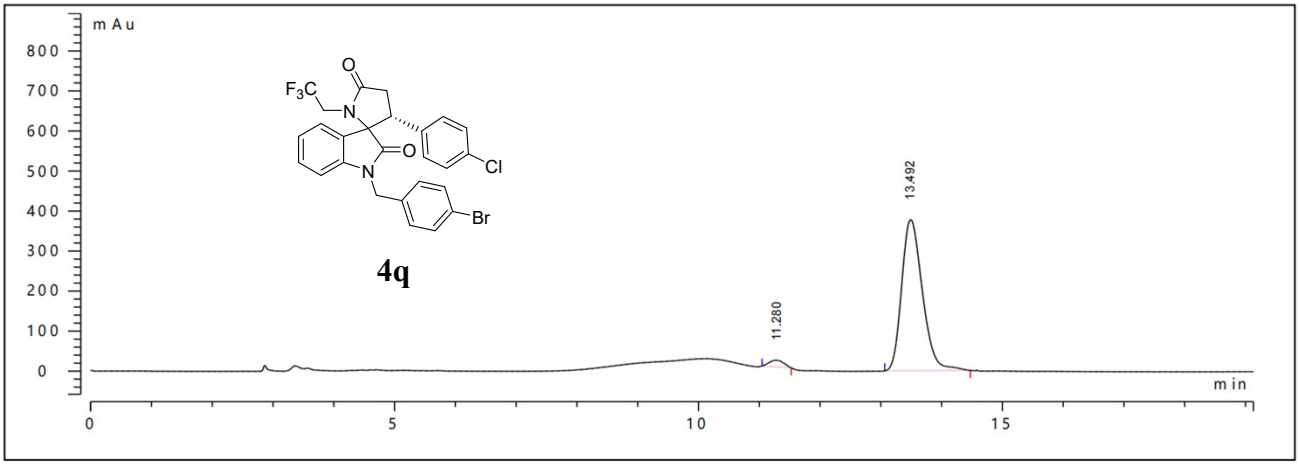


4p

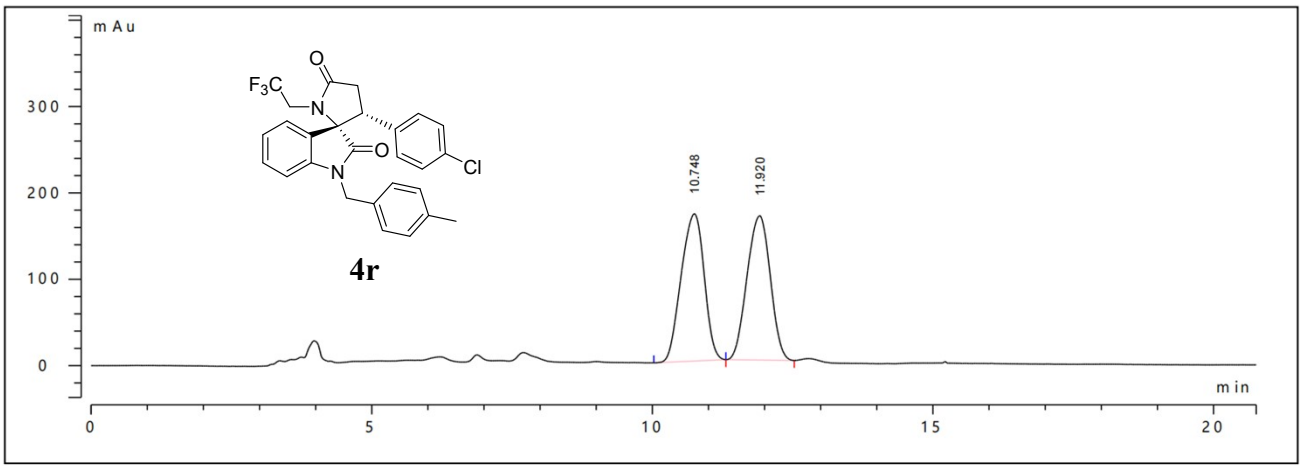
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	10.147	434.420	0.406	29.148	3.094
2	N.A.	12.530	13607.859	0.546	647.423	96.906
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	11.032	11464.294	0.713	413.116	49.876
2	N.A.	13.195	11521.472	0.802	367.625	50.124
3						

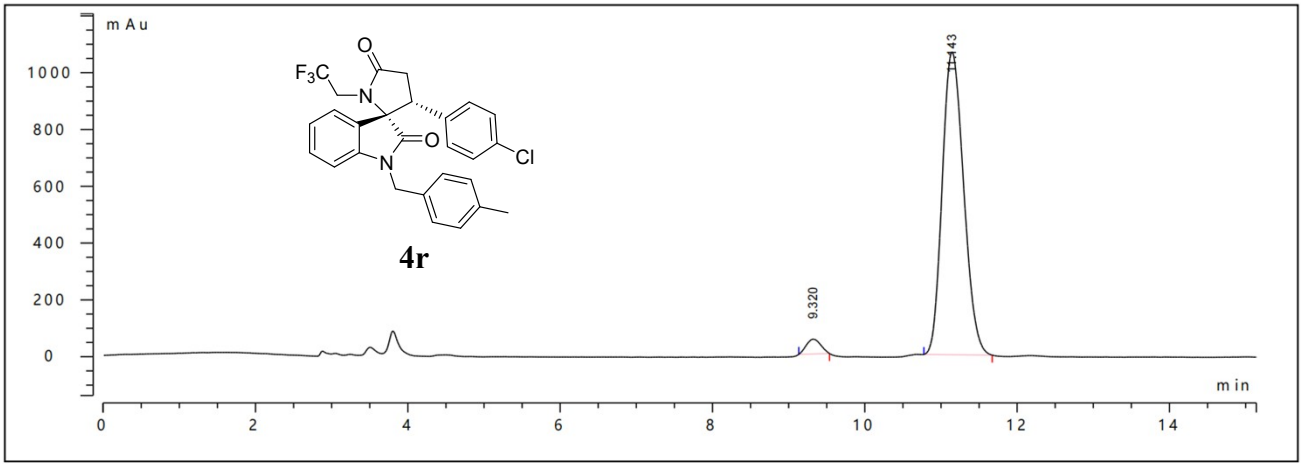


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	11.280	277.613	0.411	16.684	3.012
2	N.A.	13.492	8939.541	0.593	377.788	96.988
3						



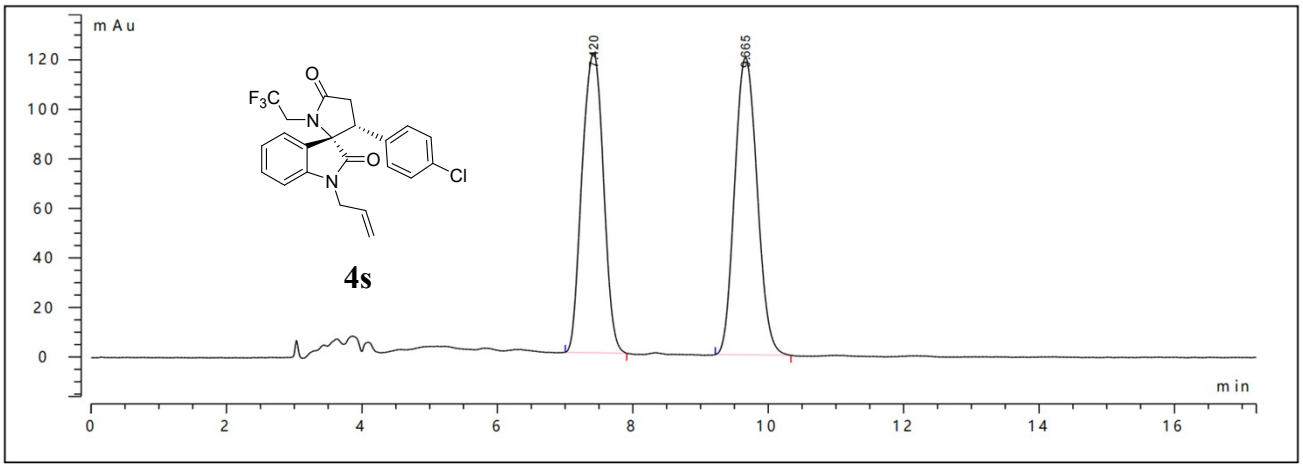
4r

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	10.748	4858.716	0.742	170.717	50.193
2	N.A.	11.920	4821.338	0.749	167.276	49.807
3						

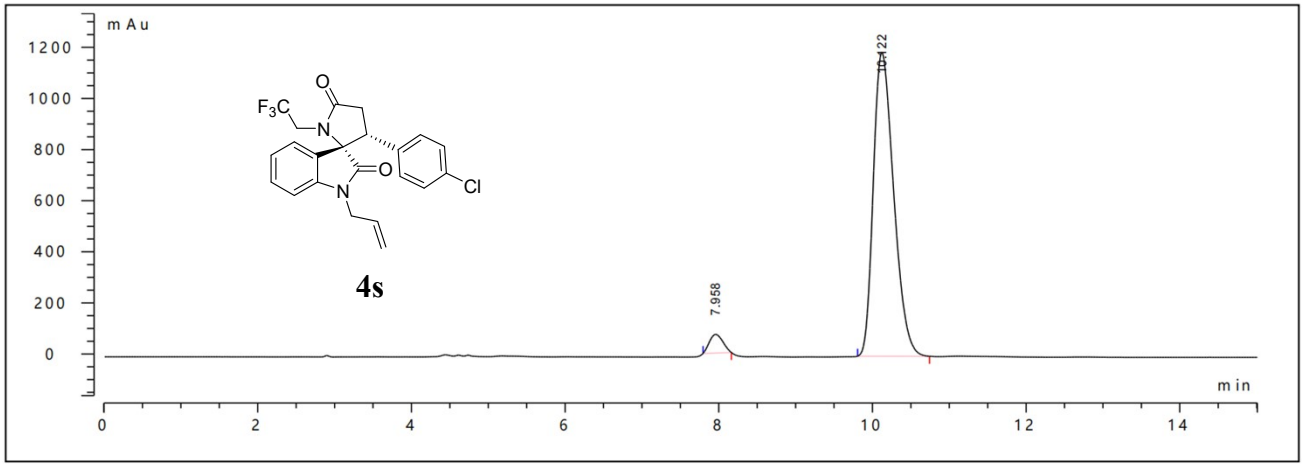


4r

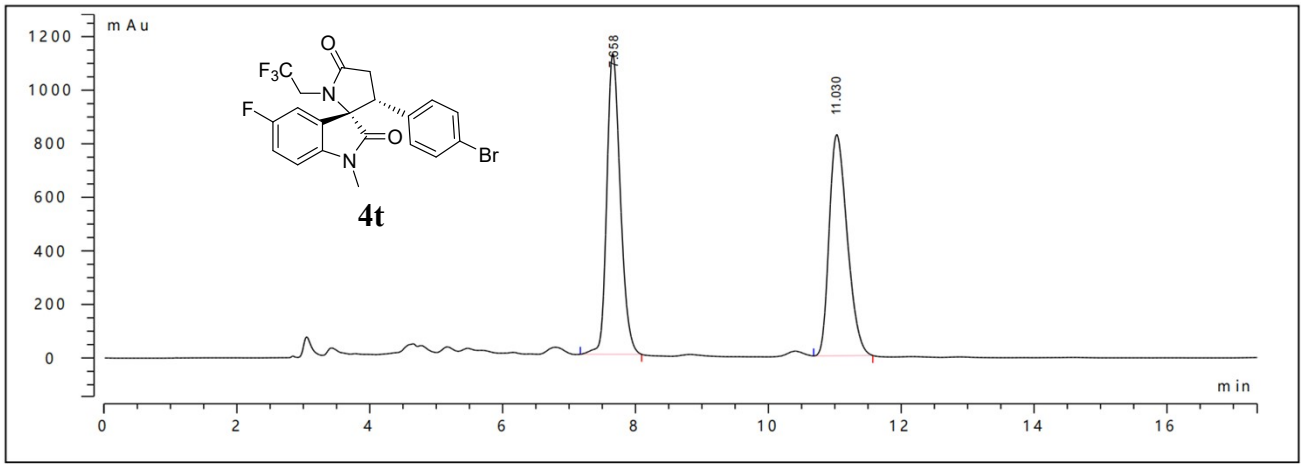
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	9.320	686.225	0.356	52.288	3.188
2	N.A.	11.143	20837.244	0.500	1066.637	96.812
3						



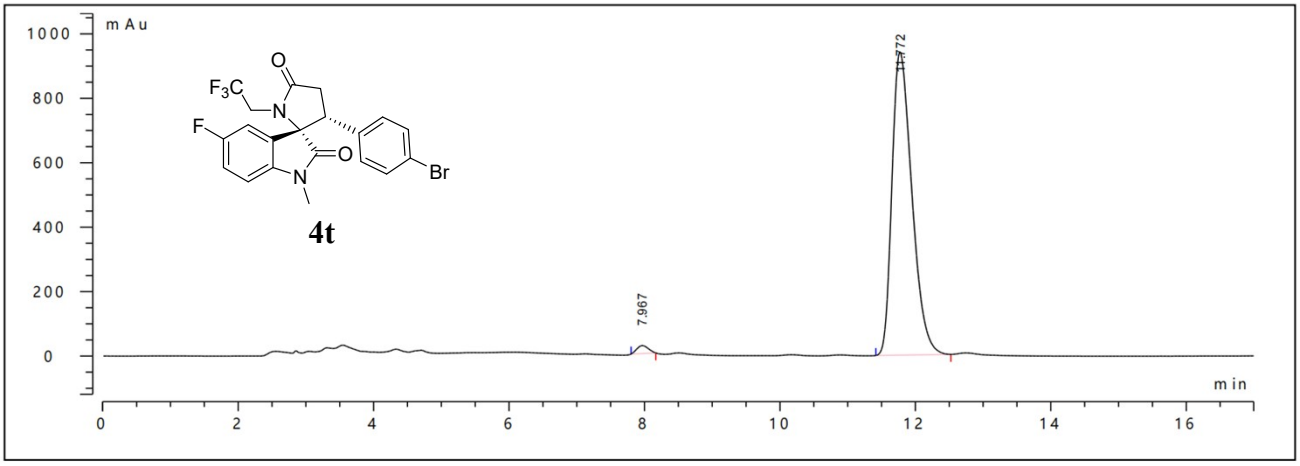
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.420	2661.498	0.564	121.099	48.928
2	N.A.	9.665	2778.120	0.599	120.133	51.072
3						



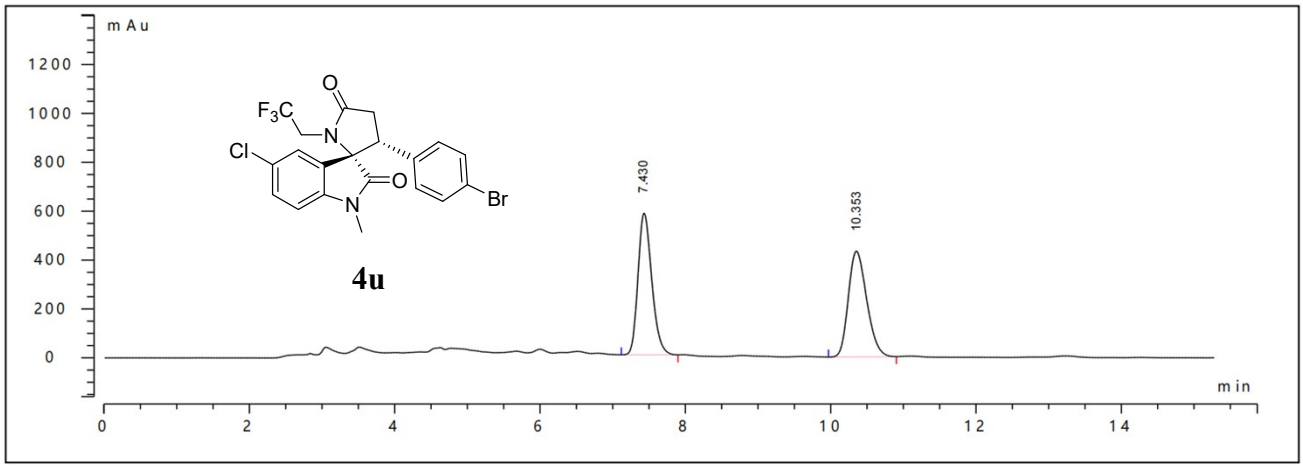
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.958	884.792	0.325	73.280	3.887
2	N.A.	10.122	21877.929	0.469	1191.146	96.113
3						



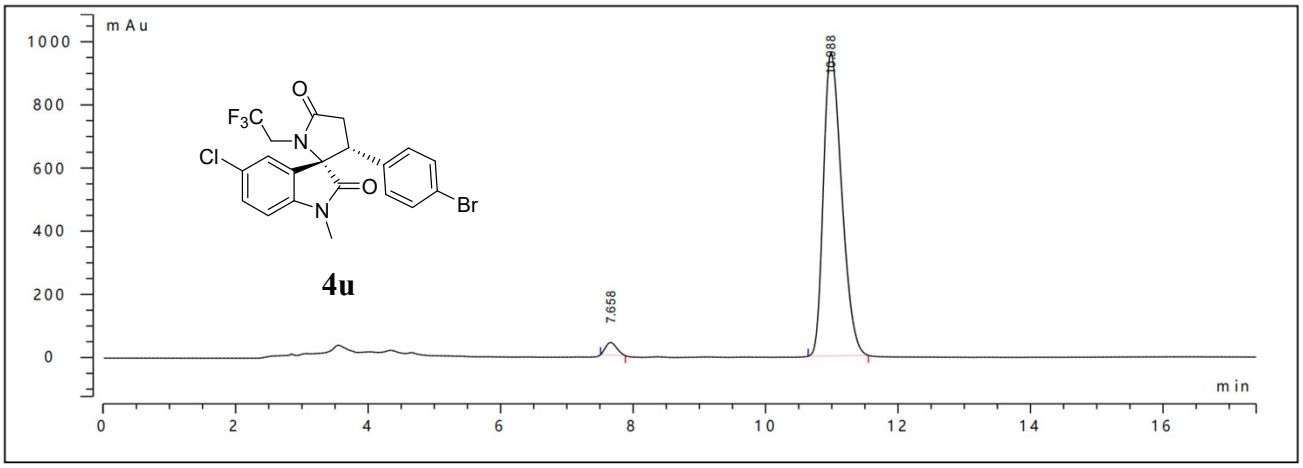
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.658	15905.023	0.354	1126.434	50.511
2	N.A.	11.030	15583.243	0.485	826.622	49.489
3						



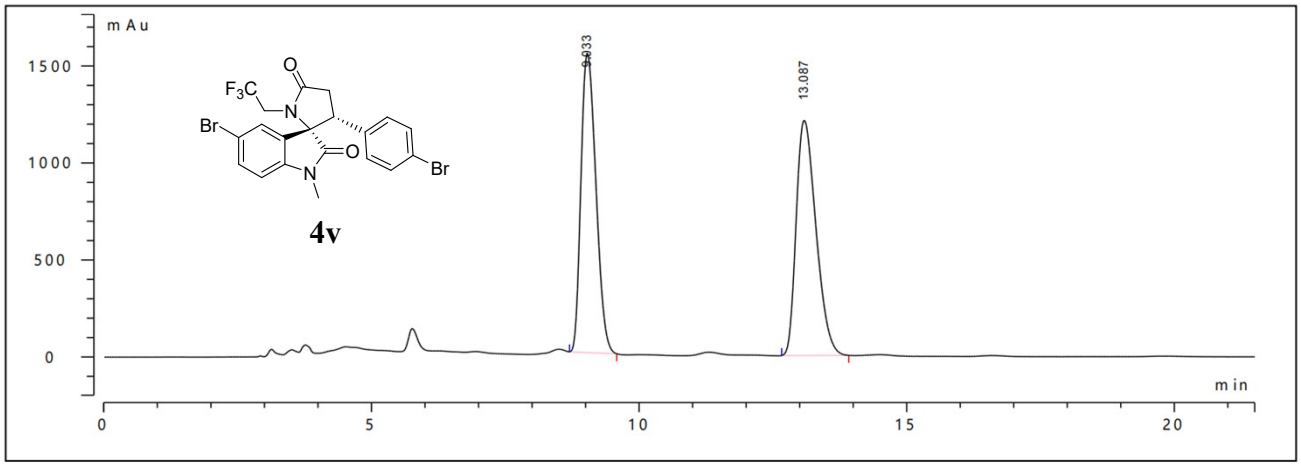
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.967	290.342	0.311	24.871	1.489
2	N.A.	11.772	19214.208	0.522	941.965	98.511
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.430	7646.266	0.336	581.030	50.174
2	N.A.	10.353	7593.246	0.447	433.425	49.826
3						

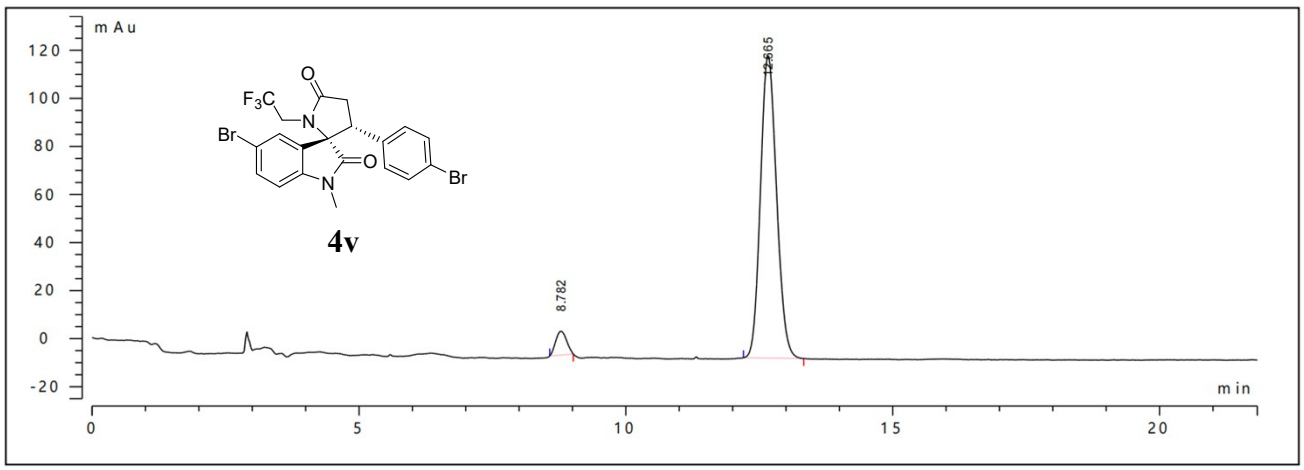


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.658	461.811	0.318	39.651	2.449
2	N.A.	10.988	18391.791	0.495	959.785	97.551
3						



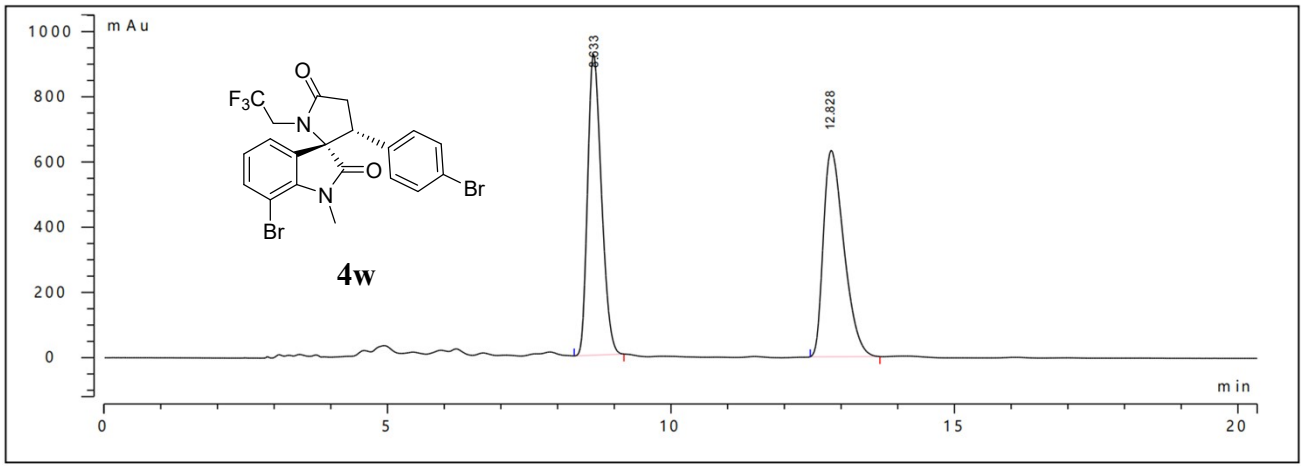
4v

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	9.033	29962.646	0.497	1546.765	49.055
2	N.A.	13.087	31117.615	0.659	1213.644	50.945
3						

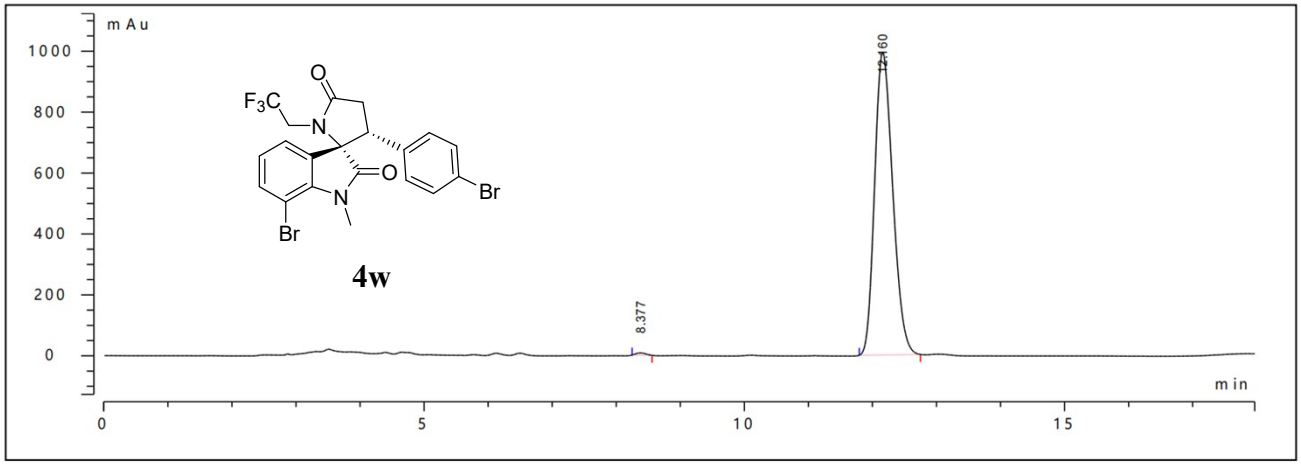


4v

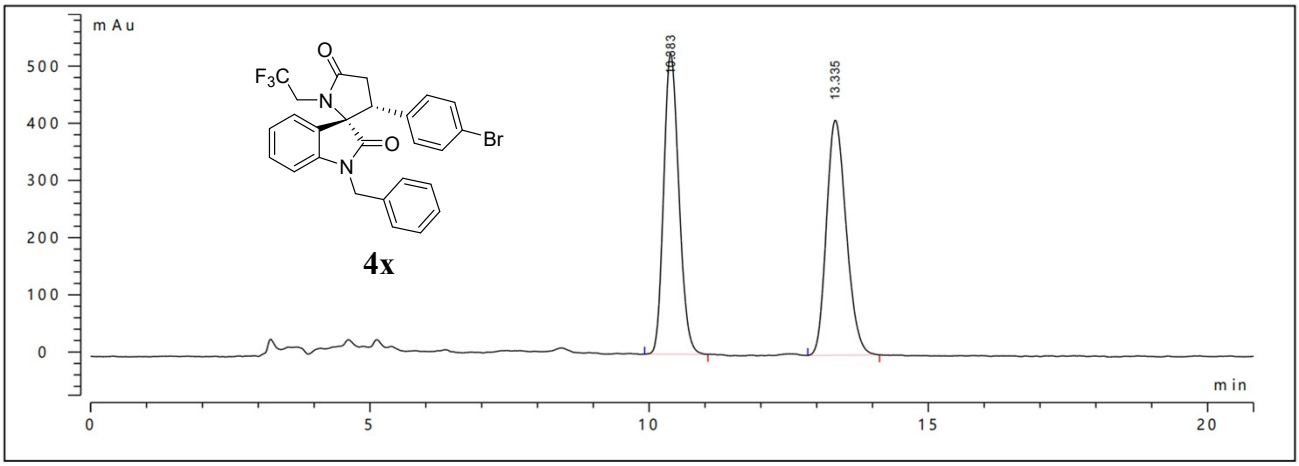
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.782	140.148	0.373	9.980	5.040
2	N.A.	12.665	2640.473	0.547	126.249	94.960
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.633	15599.201	0.437	927.038	49.384
2	N.A.	12.828	15988.563	0.640	633.616	50.616
3						

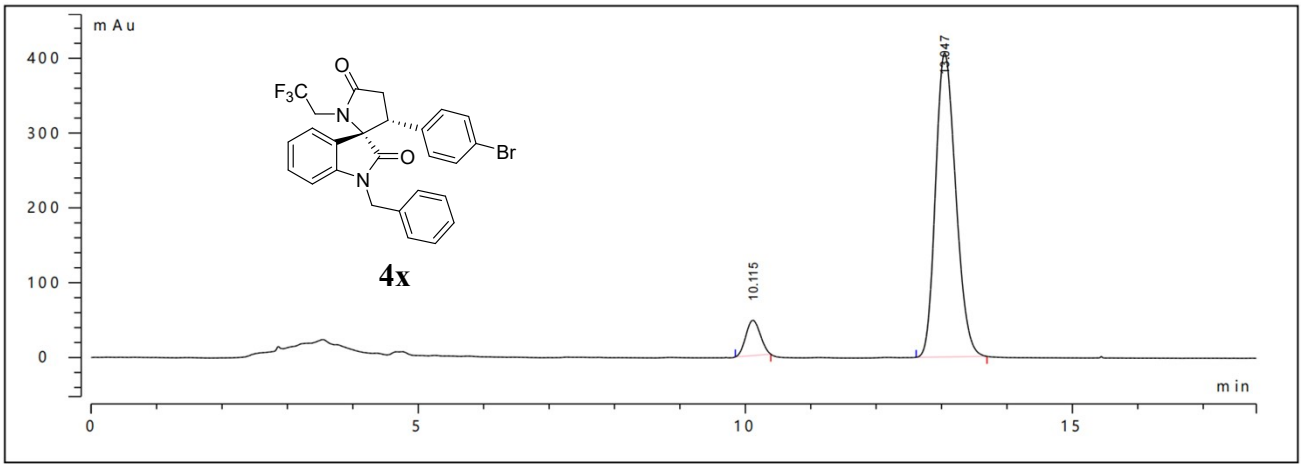


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.377	76.874	0.279	7.416	0.392
2	N.A.	12.160	19520.742	0.506	995.751	99.608
3						



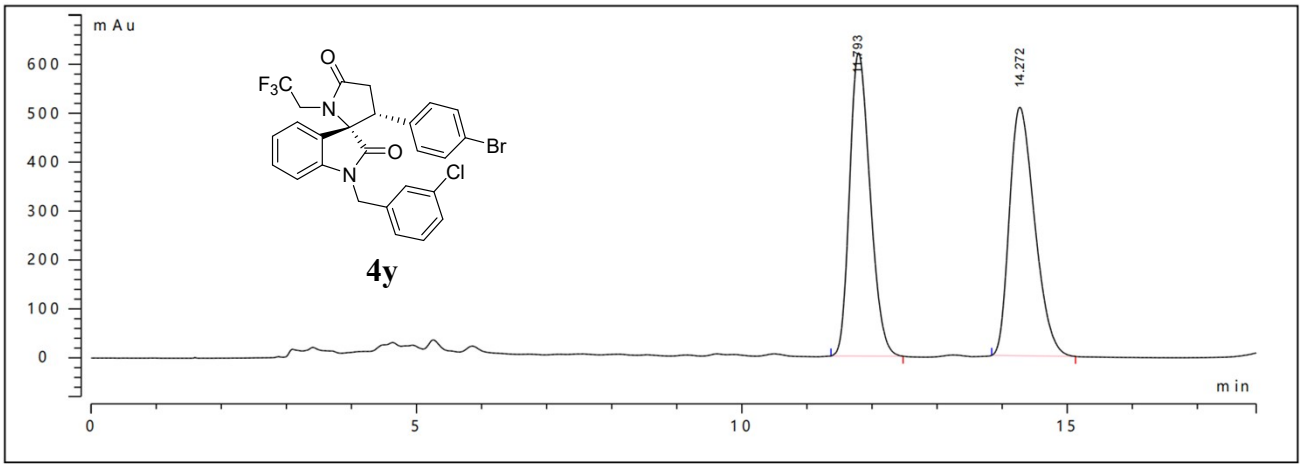
4x

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	10.383	9971.874	0.478	527.606	49.586
2	N.A.	13.335	10138.334	0.625	411.585	50.414
3						

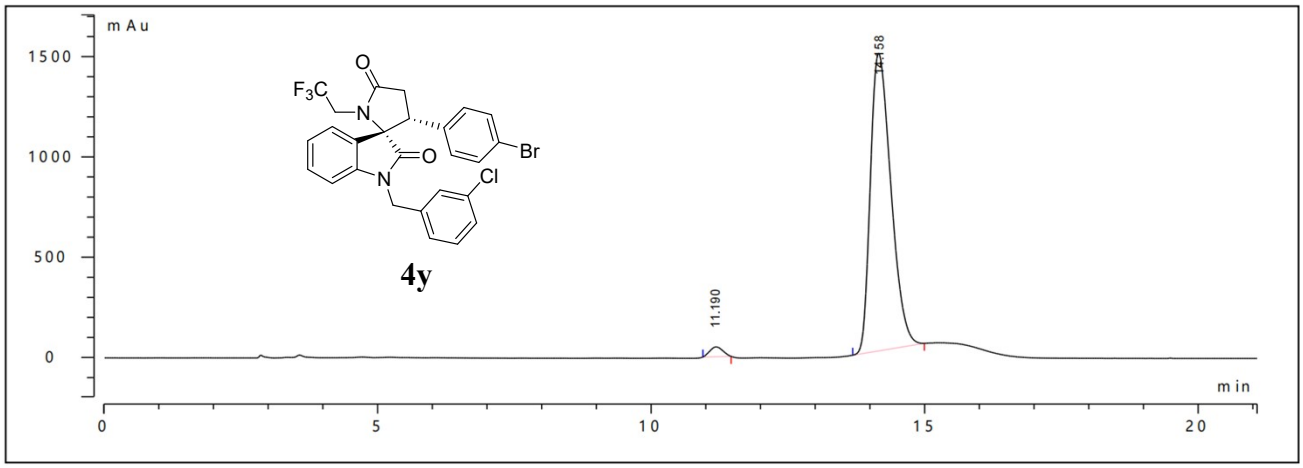


4x

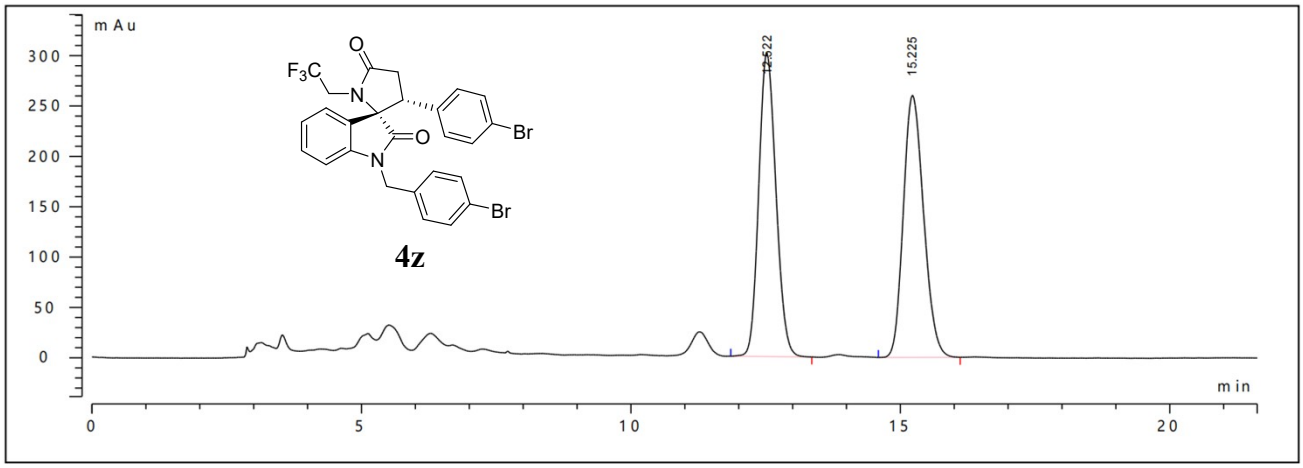
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	10.115	723.365	0.408	47.345	7.653
2	N.A.	13.047	8728.382	0.554	406.703	92.347
3						



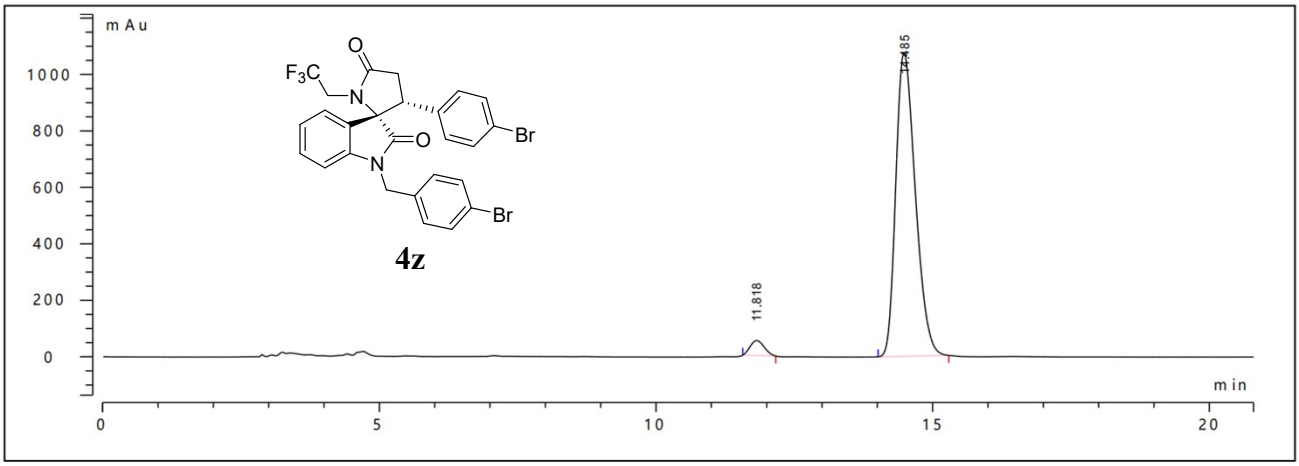
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	11.793	13537.944	0.562	620.068	49.661
2	N.A.	14.272	13722.621	0.690	508.170	50.339
3						



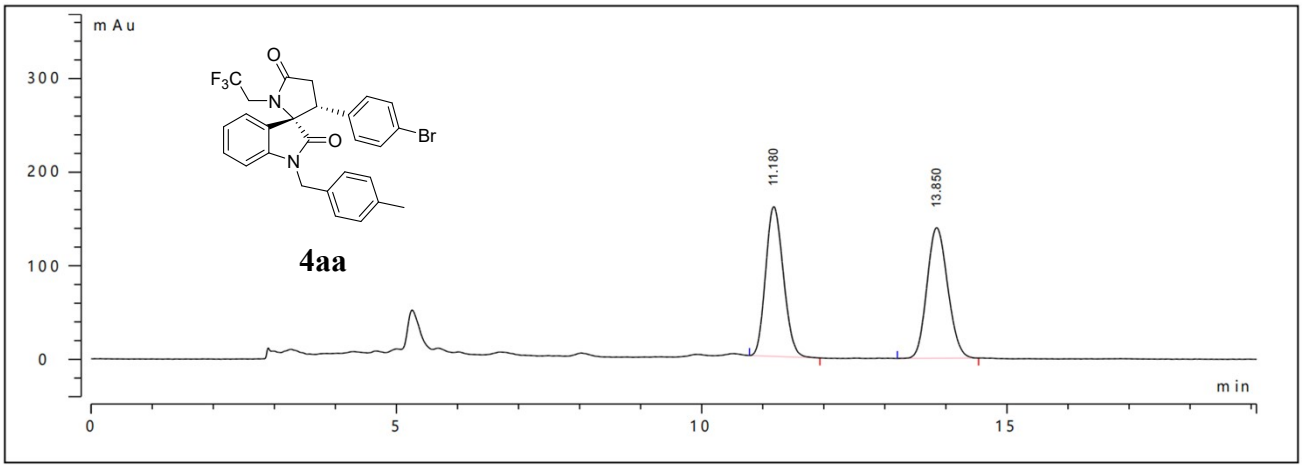
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	11.190	807.988	0.445	48.916	2.045
2	N.A.	14.158	38695.823	0.665	1485.688	97.955
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	12.522	6690.542	0.570	301.694	49.519
2	N.A.	15.225	6820.460	0.670	260.433	50.481
3						

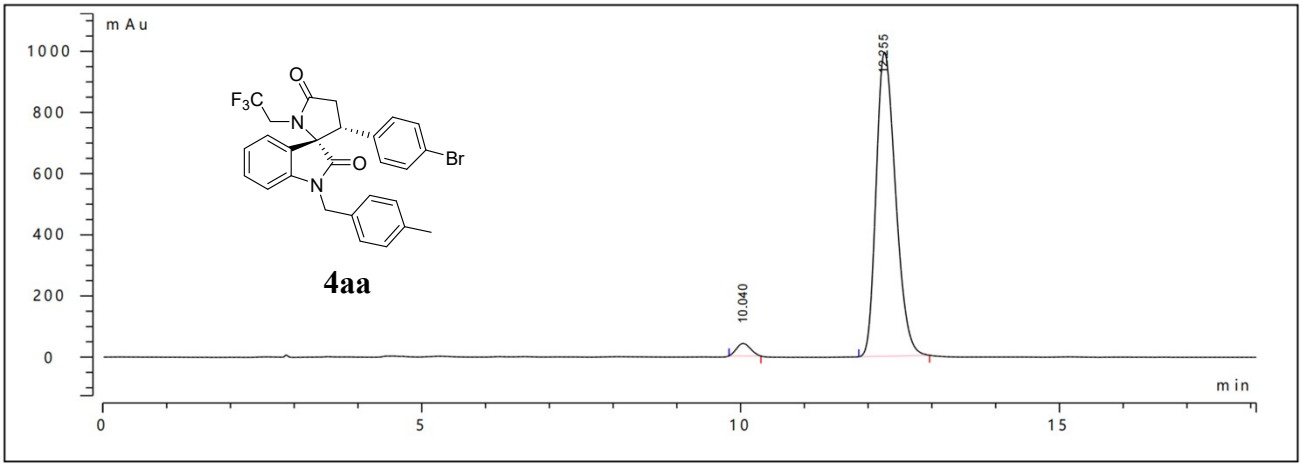


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	11.818	934.807	0.466	53.287	3.415
2	N.A.	14.485	26439.765	0.625	1076.750	96.585
3						



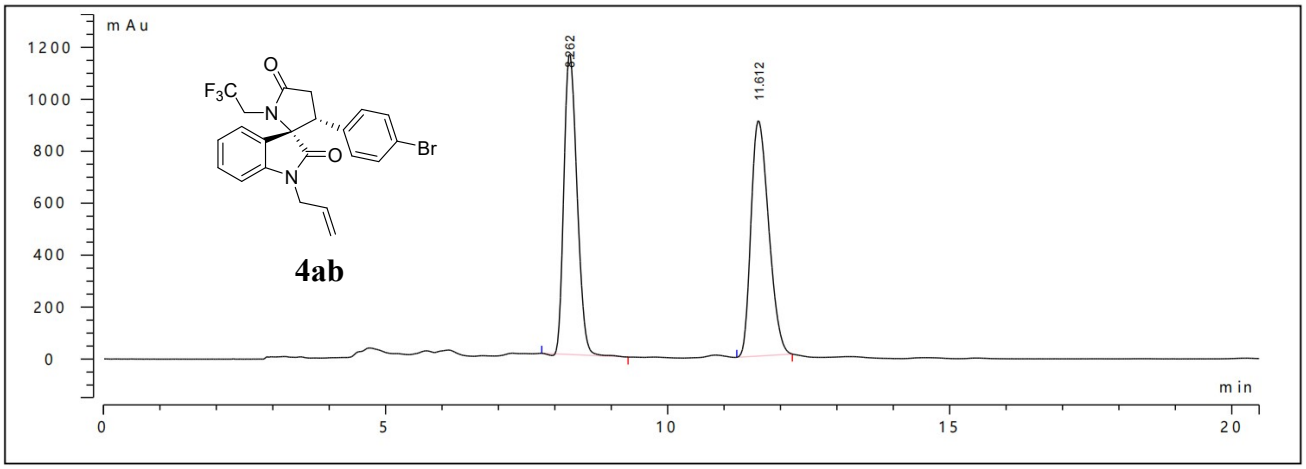
4aa

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	11.180	3237.939	0.519	160.141	49.506
2	N.A.	13.850	3302.535	0.610	139.753	50.494
3						

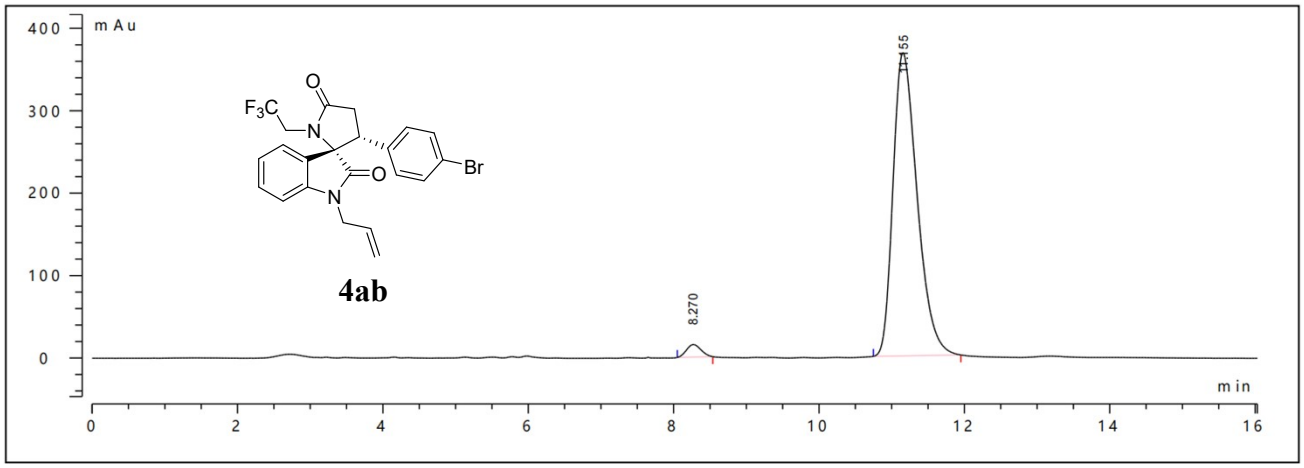


4aa

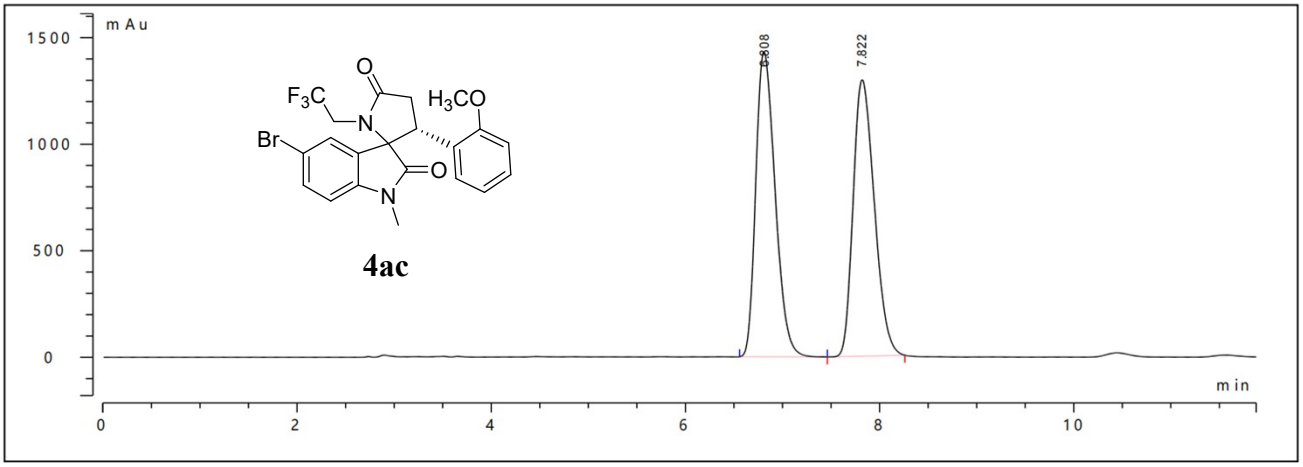
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	10.040	616.935	0.407	40.874	2.847
2	N.A.	12.255	21050.243	0.539	995.480	97.153
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	8.262	18678.041	0.417	1161.261	48.590
2	N.A.	11.612	19761.943	0.562	907.565	51.410
3						

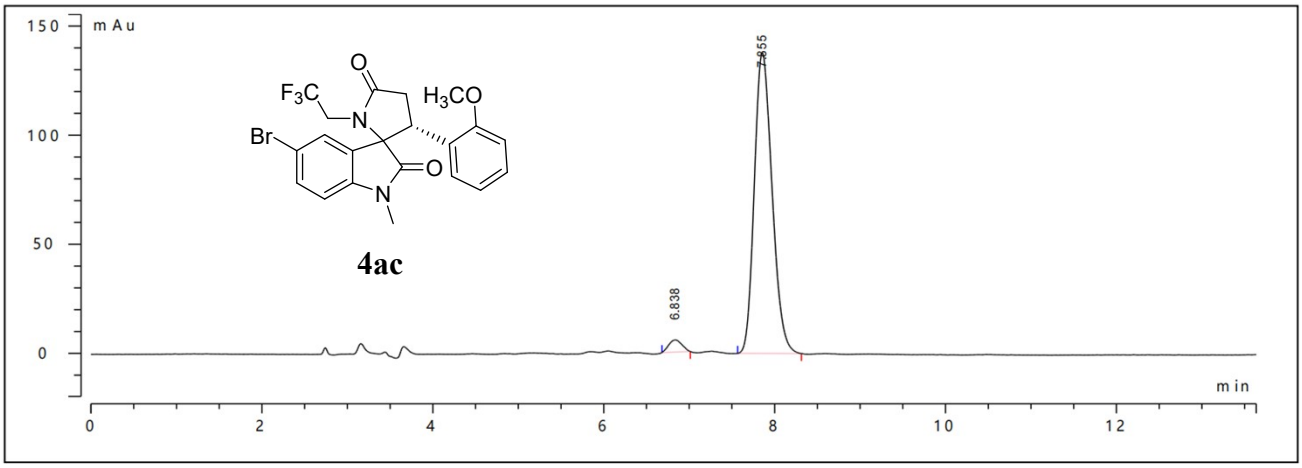


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area% (%) (NA)
1	N.A.	8.270	210.352	0.368	15.246	2.422
2	N.A.	11.155	8473.700	0.589	367.812	97.578
3			8684.052			



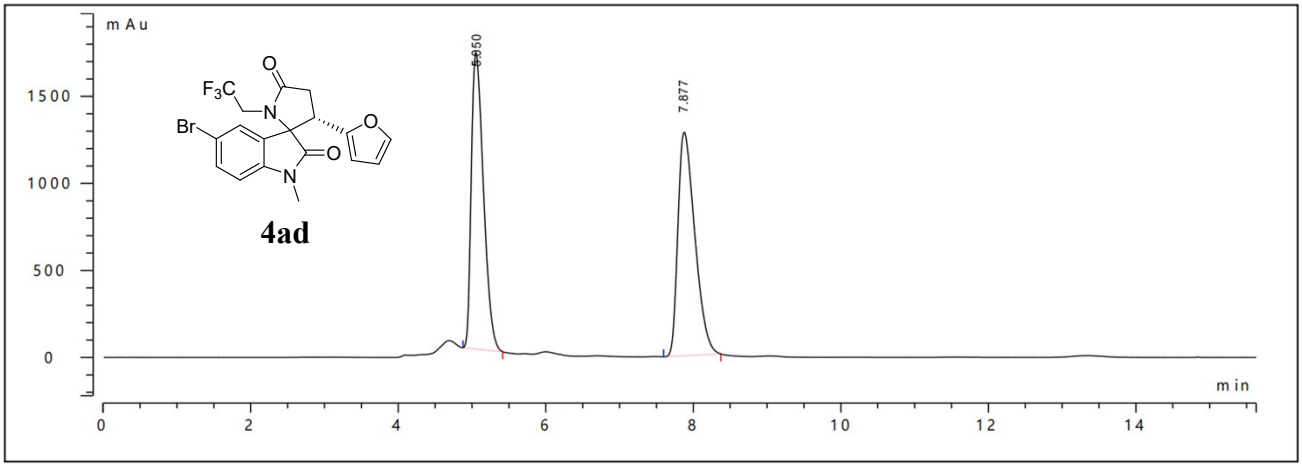
4ac

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	6.808	19805.057	0.353	1430.846	50.199
2	N.A.	7.822	19647.944	0.394	1296.626	49.801
3						

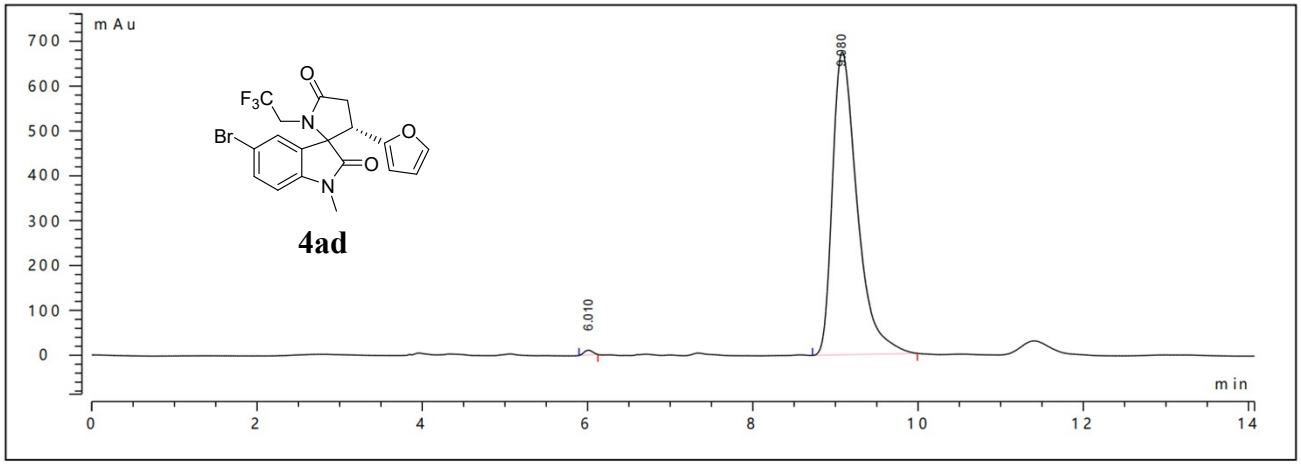


4ac

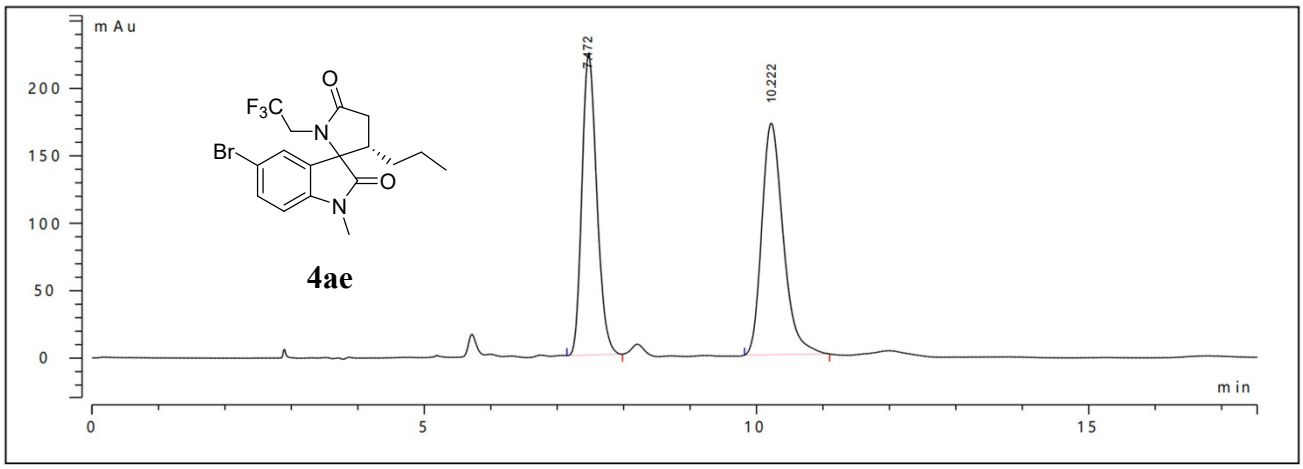
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	6.838	59.587	0.291	5.568	2.904
2	N.A.	7.855	1992.422	0.368	137.853	97.096
3						



No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	5.050	19518.295	0.292	1707.437	48.813
2	N.A.	7.877	20467.161	0.417	1287.445	51.187
3						

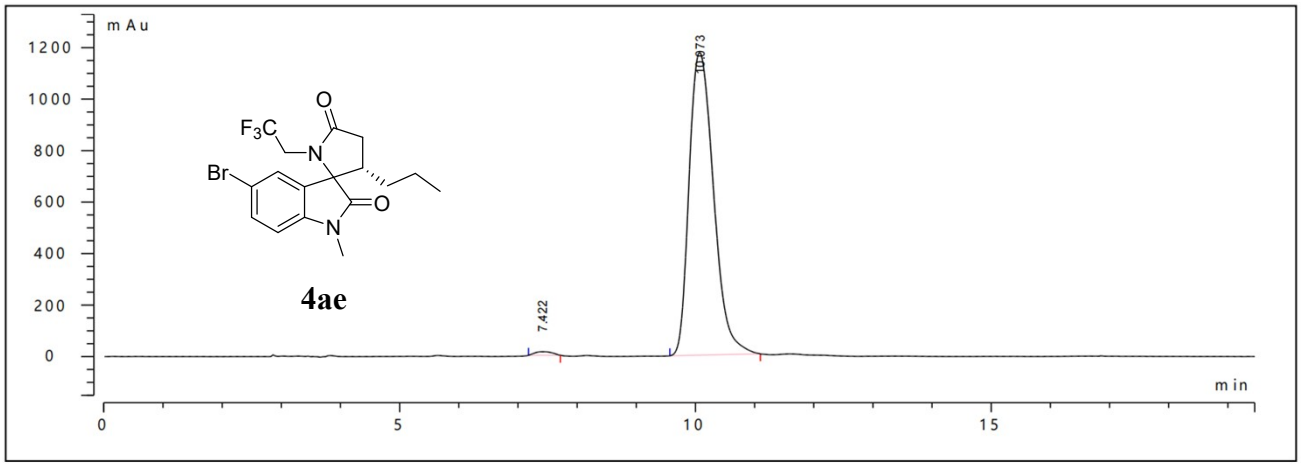


No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area% (%) (NA)
1	N.A.	6.010	76.105	0.194	10.663	0.539
2	N.A.	9.080	14038.921	0.506	675.999	99.461
3			14115.026			



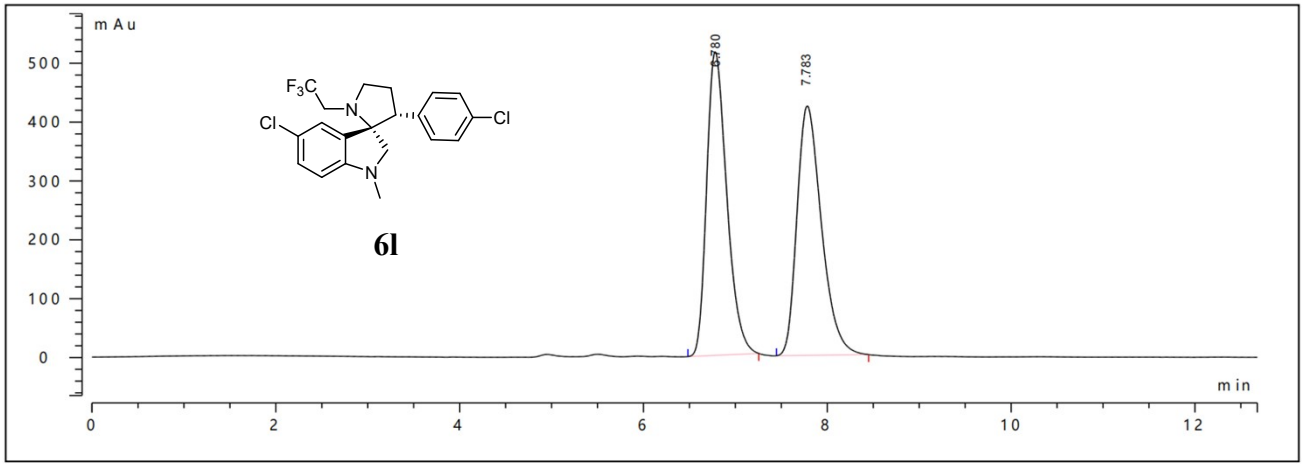
4ae

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.472	3474.530	0.397	223.367	47.471
2	N.A.	10.222	3844.690	0.558	171.924	52.529
3						



4ae

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	7.422	279.486	0.515	13.535	0.822
2	N.A.	10.073	33741.667	0.711	1175.528	99.178
3						



6l

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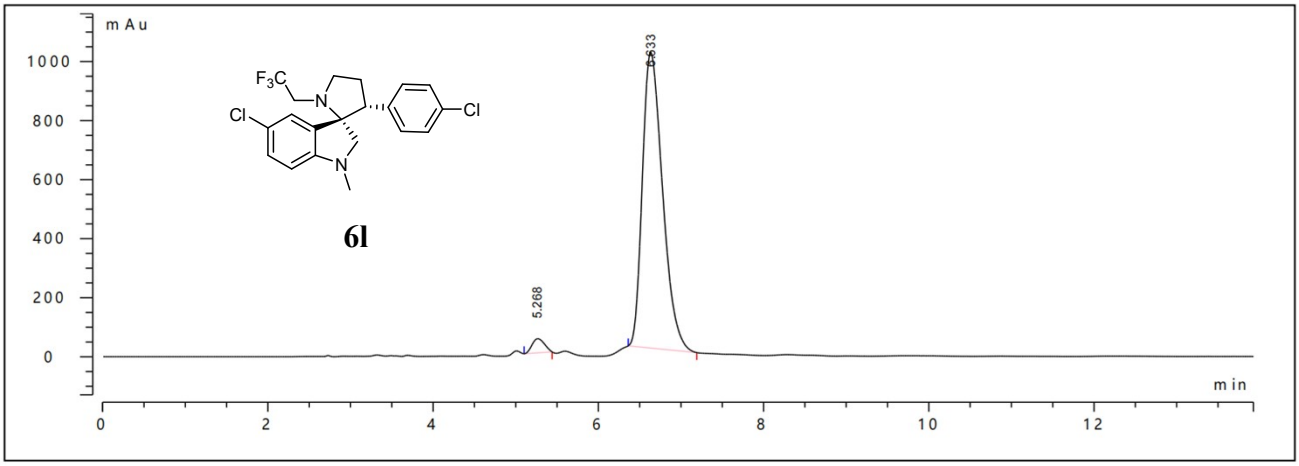
No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area% (%) (NA)
1	N.A.	6.780	7847.123	0.390	515.757	49.991
2	N.A.	7.783	7849.831	0.468	423.969	50.009
3	总计		15696.954			



6l

No	Name (NA)	Ret. time (min)	Area (mAu*s)	Plate number (min)	Tailing (mAu)	Area (%)(NA)
1	N.A.	5.268	496.205	0.282	48.155	2.833
2	N.A.	6.633	17020.935	0.430	1003.584	97.167
3						