

Supporting Information

Enantioselective Photoredox- and Cu-Catalyzed Alkoxyacylation of Styrenes to Synthesize β -Chiral Cyanide Ethers

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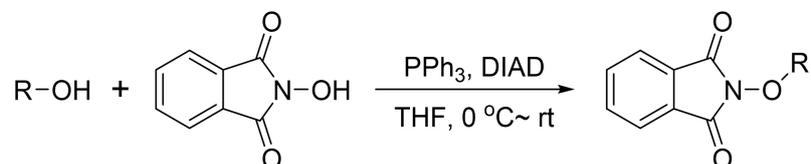
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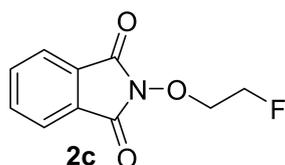
1 General considerations.

All commercially available compounds were purchased from Aldrich, Alfa Aesar or Adamas. NMR spectra were recorded on Bruker 600 (600 MHz for ^1H , 564 MHz for ^{19}F , 150 MHz for ^{13}C) spectrometer. The chemical shifts (δ) are given in parts per million relative to CDCl_3 (7.26 ppm for ^1H) or TMS (0 ppm for ^1H) and CDCl_3 (77.0 ppm for ^{13}C). High performance liquid chromatography was performed on Waters 2487-600E, Waters ACQUITY UPC2, and Ultimate 3000 Series HPLC, using AD-H, IG, IC-3 and AY-3 chiral column eluted with a mixture of hexane and isopropyl alcohol. Optical rotation was measured on a Rudolph-Autopol I. Flash column chromatography was performed on silica gel (particle size 200-300 mesh, purchased from Canada) and eluted with EA/PE. Solvent was purified according to the procedure from the book named —Purification of Laboratory Chemicals.

2 General procedure for the synthesis of substrates

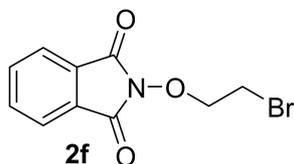


General procedure: To a stirred solution of primary or secondary alcohol (5 mmol, 1.0 equiv), N-hydroxyphthalimide (6 mmol, 1.2 equiv) and triphenylphosphine (6 mmol, 1.2 equiv.) in 20 mL THF was added diisopropyl azodicarboxylate (6 mmol, 1.2 equiv) dropwise at 0 °C. Then the reaction was allowed to room temperature. After stirring for 8 h, the solvent was removed under reduced pressure. The resulting residue was purified by column chromatography (petroleum ether/ethyl acetate = 5:1).^{ref 1}

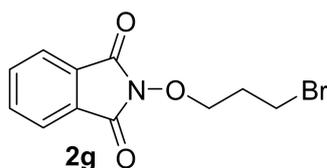


Prepared according to General procedure afforded **2c** as white solid in 60% yield.^{ref 2}

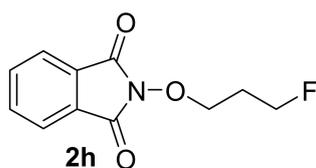
^1H NMR (600 MHz, CDCl_3) δ 7.90 – 7.80 (m, 2H), 7.79 – 7.70 (m, 2H), 4.78 (dt, J = 47.4 Hz, 3.6 Hz, 2H), 4.49 (dt, J = 28.2 Hz, 3.6 Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3) δ 163.3, 134.6, 128.8, 123.6, 81.9 (d, J = 170.1 Hz), 76.6; ^{19}F NMR (564 MHz, CDCl_3) δ -223.7 (m).



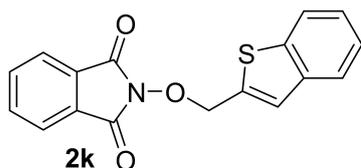
Prepared according to General procedure afforded **2f** as white solid in 82% yield.^{ref 3}
 ^1H NMR (600 MHz, CDCl_3) δ 7.87 – 7.84 (m, 2H), 7.78 – 7.75 (m, 2H), 4.48 (t, J = 7.2 Hz, 2H), 3.64 (t, J = 7.2 Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3) δ 163.4, 134.7, 128.7, 123.7, 26.6.



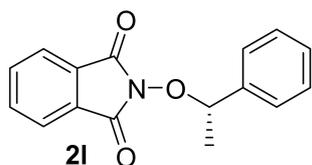
Prepared according to General procedure afforded **2g** as white solid in 66% yield.^{ref 3}
 ^1H NMR (600 MHz, CDCl_3) δ 7.85 – 7.83 (m, 2H), 7.77 – 7.75 (m, 2H), 4.36 (t, J = 6.0 Hz, 2H), 3.70 (t, J = 6.0 Hz, 2H), 2.32 – 2.28 (m, 2H); ^{13}C NMR (150 MHz, CDCl_3) δ 163.5, 134.5, 128.8, 123.5, 76.0, 31.4, 29.2.



Prepared according to General procedure afforded **2h** as white solid in 65% yield. ^1H NMR (600 MHz, CDCl_3) δ 7.90 – 7.82 (m, 2H), 7.80 – 7.71 (m, 2H), 4.76 (dt, J = 46.8 Hz, 6.0 Hz, 2H), 4.35 (t, J = 6.0 Hz, 2H), 2.20 – 2.12 (m, 2H); ^{13}C NMR (150 MHz, CDCl_3) δ 163.5, 134.5, 128.8, 123.5, 80.8 (d, J = 654.6 Hz), 74.3 (d, J = 17.4 Hz), 29.5 (d, J = 82.8 Hz); ^{19}F NMR (564 MHz, CDCl_3) δ -221.3 (m). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{11}\text{H}_{10}\text{FNO}_3$ 224.0717, found: 224.0717.



Prepared according to General procedure afforded **2k** as white solid in 83% yield.^{ref 4}
¹H NMR (600 MHz, CDCl₃) δ 7.83 – 7.80 (m, 3H), 7.75 – 7.72 (m, 3H), 7.42 (s, 1H), 7.35 – 7.33 (m, 2H), 5.48 (m, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 163.4, 141.2, 139.0, 136.3, 134.5, 128.8, 126.7, 125.0, 124.4, 124.0, 123.6, 122.5, 74.0.



Prepared according to General procedure afforded **2l** as white solid in 66% yield.^{ref 5}
¹H NMR (600 MHz, CDCl₃) δ 7.75 – 7.35 (m, 2H), 7.70 – 7.67 (m, 2H), 7.51 (d, *J* = 7.2 Hz, 2H), 7.35 – 7.29 (m, 3H), 5.51 (q, *J* = 6.6 Hz, 1H), 1.72 (d, *J* = 6.6 Hz, 3H);
¹³C NMR (150 MHz, CDCl₃) δ 163.8, 138.9, 134.2, 128.9, 128.8, 128.3, 127.6, 123.3, 85.1, 20.4.

Reference:

- Zhi, R.; Fangyang, M.; Guangbin, D. *J. Am. Chem. Soc.* **2012**, *134*, 16991–16994.
- Sarró, P.; Gallego-Gamo, A.; Molins, E.; Pleixats, R.; Gimbert-Surinach, C.; Vallribera, A.; Granados, A. *Org. Lett.* **2025**, *27*, 11372–11377.
- Musolino, M.; Fleming, I. N.; Schweiger, L. F.; O'Hagan, D.; Dall'Angelo, S.; Zanda, M. *Eur. J. Org. Chem.* **2021**, *9*, 1429–1439.
- Grottelli, S.; Annunziato, G.; Pampalone, G.; Pieroni, M.; Dindo, M.; Ferlenghi, F.; Costantino, G.; Cellini, B. *J. Med. Chem.* **2022**, *65*, 9718–9734.
- Li, F.; Liu, X.-M.; Pan, J.-B.; Dai, L.; Yang, Y.; Xiao, L.-J.; Fan, C.; Zhou, Q.-L. *J. Am. Chem. Soc.* **2025**, *147*, 19093–19100.

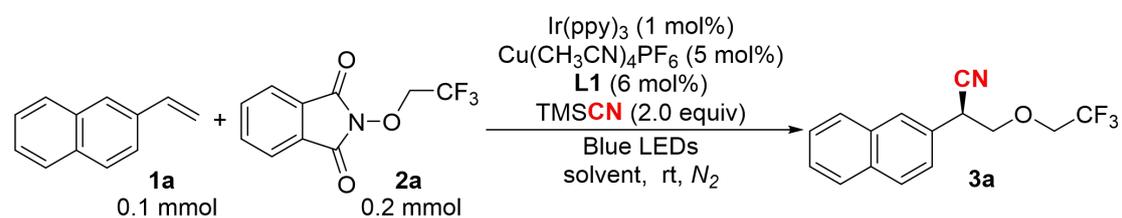
3 Optimization of the reaction conditions

3.1 Optimization of solvent

These reactions were performed according to the general procedure on a 0.1

mmol scale and the results were listed in Table S1

Table S1. Optimization of solvents^a



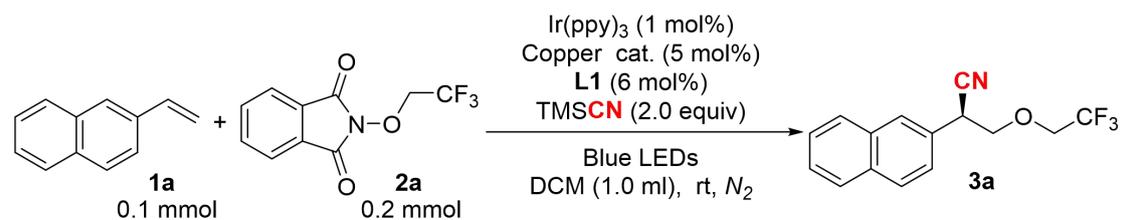
Entry	Solvents	Yield of 3a ^b (ee) ^c
1	CH_3CN	62% (85% ee)
2	DCM	58% (90% ee)
3	DCE	58% (89% ee)
4	PhCl	<10% (86% ee)
5	CHCl_3	46% (85% ee)
6	MTBE	<10%(90% ee)

[a] All reactions were run on 0.1 mmol scale in solvent (1 mL) at room temperature under nitrogen atmosphere. [b] Isolated yield of **3a** based on **1a**. [c] Enantiomeric excess (ee) values determined by HPLC on a chiral stationary phase.

3.2 Optimization of copper catalyst

These reactions were performed according to the general procedure on a 0.1 mmol scale and the results were listed in Table S2.

Table S2. Optimization of copper catalyst^a



Entry	Copper cat.	Yield of 2a ^b (ee) ^c
1	$\text{Cu}(\text{CH}_3\text{CN})_4\text{PF}_6$	66% (90% ee)
2	$\text{Cu}(\text{CH}_3\text{CN})_4\text{BF}_6$	46% (88% ee)
3	CuBr_2	50% (78% ee)
4	CuCl_2	46% (81% ee)
5	CuBr	63% (81% ee)
6	CuCl	50% (84% ee)
7	CuOAc	48% (79% ee)
8	CuCN	48% (80% ee)

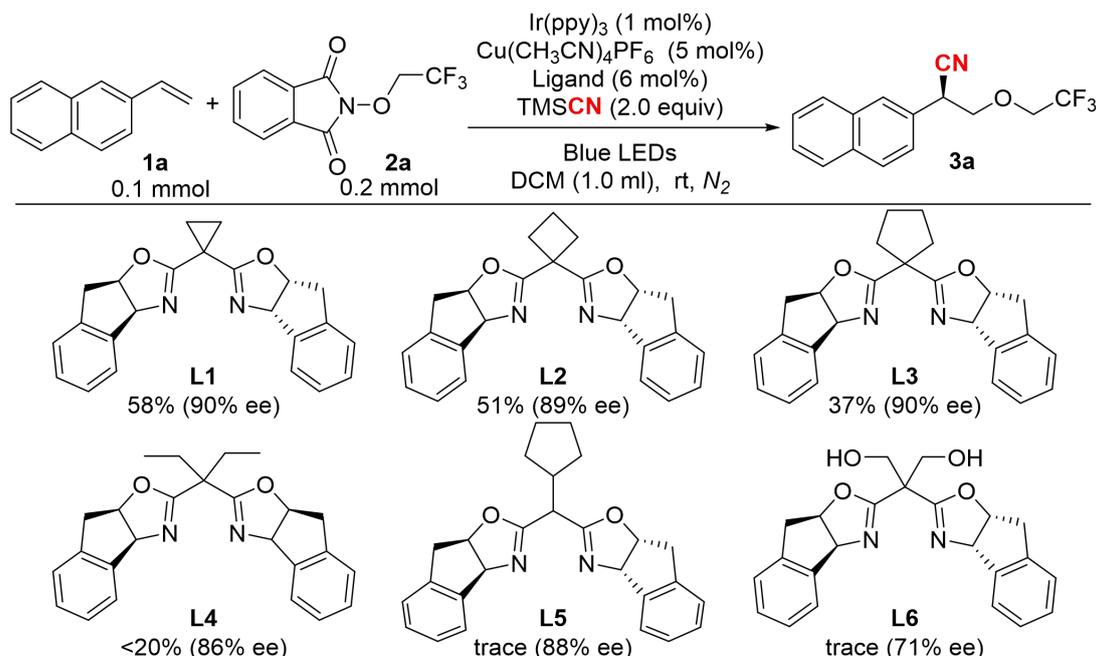
[a] All reactions were run on 0.1 mmol scale in DCM (1 mL) at room temperature under nitrogen atmosphere. [b] Isolated yield of **3a** based on **1a**. [c] Enantiomeric

excess (ee) values determined by HPLC on a chiral stationary phase.

3.3 Optimization of ligands

These reactions were performed according to the general procedure on a 0.1 mmol scale and the results were listed in Table S3

Table S3. Optimization of ligands^a



[a] All reactions were run on 0.1 mmol scale in DCM (1 mL) at room temperature under nitrogen atmosphere. [b] Isolated yield of **3a** based on **1a**. [c] Enantiomeric excess (ee) values determined by HPLC on a chiral stationary phase.

[b]

3.4 Optimization of solvent dosage

These reactions were performed according to the general procedure on a 0.1 mmol scale and the results were listed in Table S4

Table S4. Optimization of solvent dosage^a



Entry	Solvents dosage	Yield of 3a ^b (ee) ^c
1	0.5 mL	62% (90% ee)
2	1 mL	58% (90% ee)

3	2 mL	58% (90% ee)
4	3 mL	46% (90% ee)

[a] All reactions were run on 0.1 mmol scale in DCM at room temperature under nitrogen atmosphere. [b] Isolated yield of **3a** based on **1a**. [c] Enantiomeric excess (ee) values determined by HPLC on a chiral stationary phase.

3.5 Optimization of TMSCN dosage

These reactions were performed according to the general procedure on a 0.1 mmol scale and the results were listed in Table S5.

Table S5. Optimization of TMSCN dosage^a



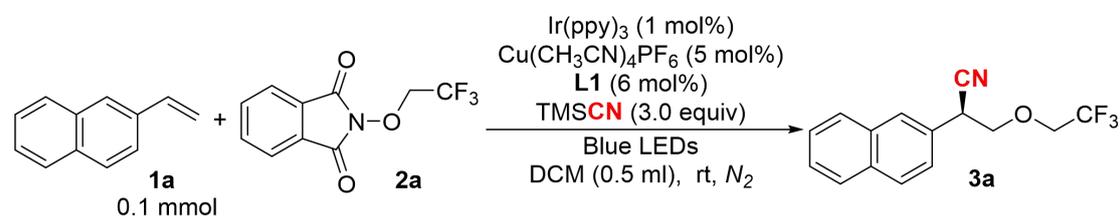
Entry	TMSCN dosage	Yield of 3a ^b (ee) ^c
1	2 equiv	62% (90% ee)
2	3 equiv	65% (90% ee)

[a] All reactions were run on 0.1 mmol scale in DCM (0.5 mL) at room temperature under nitrogen atmosphere. [b] Isolated yield of **3a** based on **1a**. [c] Enantiomeric excess (ee) values determined by HPLC on a chiral stationary phase.

3.6 Optimization of 2a dosage

These reactions were performed according to the general procedure on a 0.1 mmol scale and the results were listed in Table S6.

Table S6. Optimization of oxidant dosage^a



Entry	2a dosage	Yield of 2a ^b (ee) ^c
1	1.5 equiv	51% (90% ee)
2	2.0 equiv	65% (90% ee)
3	2.5 equiv	66% (90% ee)
4	3.0 equiv	48% (90% ee)

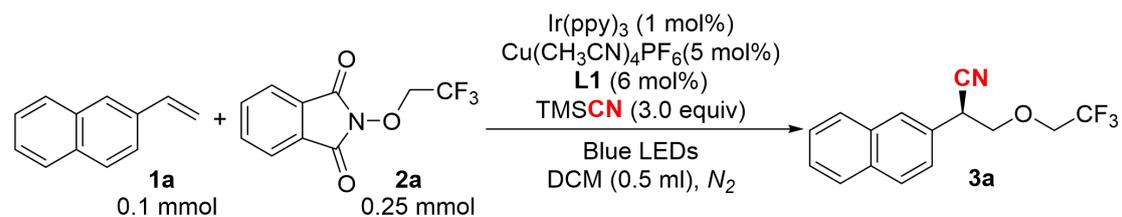
[a] All reactions were run on 0.1 mmol scale in DCM (0.5 mL) at room temperature

under nitrogen atmosphere. [b] Isolated yield of **3a** based on **1a**. [c] Enantiomeric excess (ee) values determined by HPLC on a chiral stationary phase.

3.7 Optimization of reaction temperature.

These reactions were performed according to the general procedure on a 0.1 mmol scale and the results were listed in Table S7.

Table S7. Optimization of reaction temperature ^a



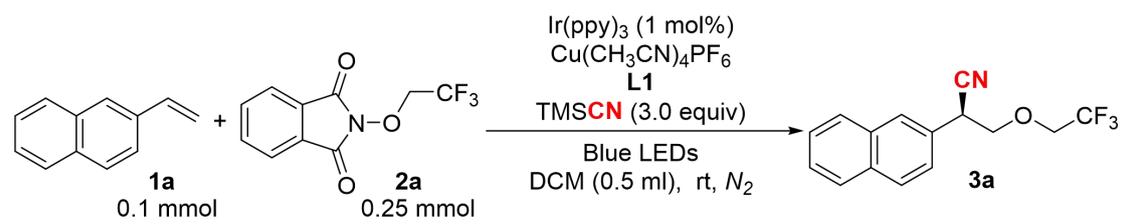
Entry	Temperature	Yield of 2a ^b (ee) ^c
1	0 °C	63% (85% ee)
2	rt	66% (90% ee)
3	40 °C	65% (90% ee)

[a] All reactions were run on 0.1 mmol scale in DCM (0.5 mL) under nitrogen atmosphere. [b] Isolated yield of **3a** based on **1a**. [c] Enantiomeric excess (ee) values determined by HPLC on a chiral stationary phase.

3.8 Optimization of copper catalyst dosage

These reactions were performed according to the general procedure on a 0.1 mmol scale and the results were listed in Table S8.

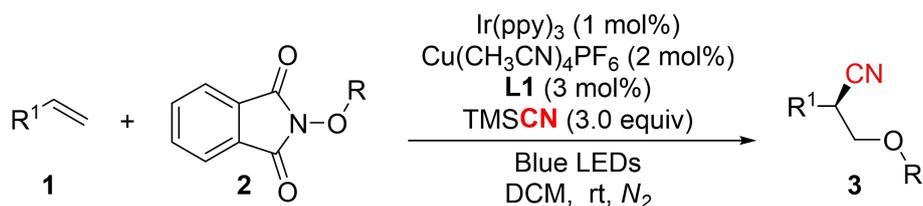
Table S8. Optimization of copper catalyst dosage ^a



Entry	Copper cat. dosage	Ligand dosage	Yield of 2a ^b (ee) ^c
1	1 mol%	2 mol%	56% (85% ee)
2	2 mol%	3 mol%	68% (90% ee)
3	3 mol%	4 mol%	65% (90% ee)

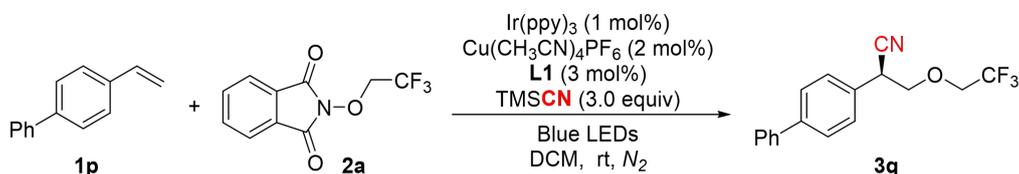
[a] All reactions were run on 0.1 mmol scale in DCM (0.5 mL) at room temperature under nitrogen atmosphere. [b] Isolated yield of **3a** based on **1a**. [c] Enantiomeric excess (ee) values determined by HPLC on a chiral stationary phase.

4 General experimental procedures for the asymmetric alkoxyacylation of styrenes



In a dried sealed tube, **L1** (0.006 mmol, 3 mol%), Ir(ppy)₃ (0.002 mmol, 1 mol%) and Cu(CH₃CN)₄PF₆ (0.004 mmol, 2 mol%) were dissolved in DCM (1.0 mL) under the atmosphere of nitrogen. The solution was stirred at room temperature for 5 min, then alkene **1** (0.2 mmol, 1 equiv), **2** (0.5 mmol, 2 equiv), TMS-CN (0.6 mmol, 3 equiv) were added sequentially. The mixture was stirred for 12 h at room temperature with 2 × 3 W blue LEDs. After the reaction was completed, the product was purified by flash column chromatography on silica gel with gradient of petroleum ether/ethyl acetate.

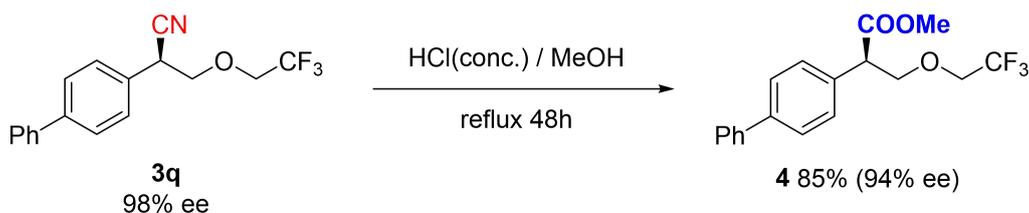
5 Scale-up reaction



To a 100 mL sealed tube, **L1** (42 mg, 0.12 mmol, 3 mol%), Ir(ppy)₃ (26 mg, 0.04 mmol, 1 mol%) and Cu(CH₃CN)₄PF₆ (28 mg, 0.08 mmol, 2 mol%) were dissolved in DCM (20 mL) under the atmosphere of nitrogen. The solution was stirred at room temperature for 5 min, then substrate **1p** (0.72g, 4 mmol, 1.0 equiv), **2a** (2.46 g, 10 mmol, 2.5 equiv), TMS-CN (1.56 mL, 12 mmol, 3 equiv) were added sequentially. The mixture was stirred for 12 h at room temperature with 2 × 10 W blue LEDs. After the reaction was completed, the product was purified by flash column chromatography on silica gel with gradient of petroleum ether/ethyl acetate to afford product **3p** (1.16 g) in 95% yield with 98% ee.

6 Further transformations of products

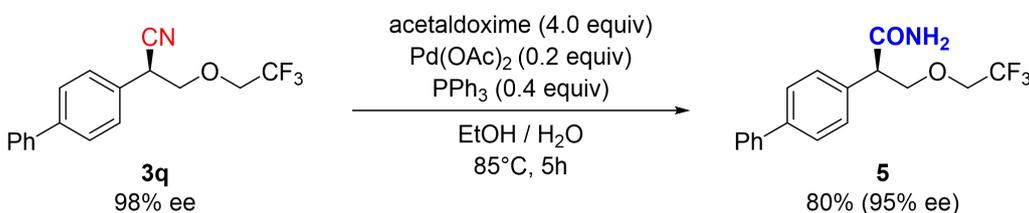
6.1 Esterification of the cyano group



Under a nitrogen atmosphere, a Schlenk tube equipped with a stir bar was charged with **3q** (30.5 mg, 0.1 mmol), 37% HCl (2.0 mL), MeOH (2.0 mL). The reaction mixture was stirred at 80 °C in oil bath for 48 h until the complete consumption of the starting material (monitored by TLC). After cooling to room temperature, the mixture was extracted with ethyl acetate three times. The combined organic layer was dried over anhydrous Na₂SO₄ and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (10:1) to afford product **4** (28.7 mg) in 85% yield with 94% ee.

4 (28.7 mg, 85% yield, 94% ee) as white solid. ¹H NMR (600 MHz, CDCl₃) δ 7.57 (d, *J* = 8.4 Hz, 4H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.37 – 7.34 (m, 3H), 4.20 (t, *J* = 9.6 Hz, 1H), 3.98 – 3.94 (m, 1H), 3.92 – 3.84 (m, 3H), 3.73 (s, 3H). ¹³C NMR (150 MHz, CDCl₃) δ 172.3, 140.9, 140.4, 133.8, 128.8, 128.4, 127.6, 127.4, 127.0, 123.8 (q, *J* = 278.4 Hz), 74.0, 68.8 (q, *J* = 34.7 Hz), 52.3, 51.6. ¹⁹F NMR (564 MHz, CDCl₃) δ -74.1 (t, *J* = 7.9 Hz). HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₈H₁₇F₃NaO₃ 361.1022, found: 361.1025. [α]_D^{23.1} +33.5890 (c 0.7, CHCl₃). HPLC (IG, 0.46*25 cm, 5 μm, hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 10.340 min (major) and 11.639 min (minor).

6.2 Amidation of the cyano group



Under a nitrogen atmosphere, a mixture of **3q** (30.5 mg, 0.10 mmol, 1.0 equiv), acetaldoxime (24 μL, 0.40 mmol, 4.0 equiv), Pd(OAc)₂ (5 mg, 0.02mmol, 0.2 equiv), and PPh₃ (11 mg, 0.04 mmol, 0.4 equiv) in aqueous EtOH (EtOH/H₂O=4/1, 1.5 mL) was heated to 85 °C in a 10 mL Schlenk tube for 5 h. The reaction mixture was

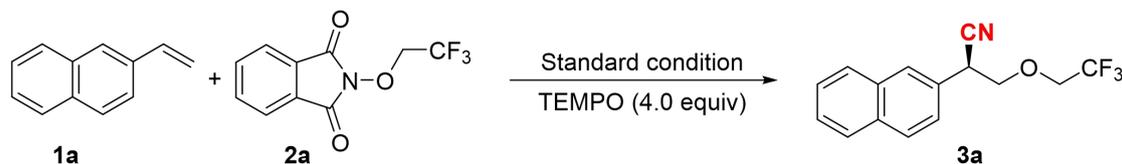
filtered through a Celite pad and washed with EtOH/CH₂Cl₂. The combined organic layers were concentrated under vacuum. The product was purified by column chromatography on silica gel(ethyl acetate/petroleum ether) to afford product **5** (25.8 mg) in 80% yield with 95% ee.

5 (25.8 mg, 80% yield, 95% ee) as white solid. ¹H NMR (600 MHz, CDCl₃) δ 7.58 – 7.56 (m, 4H), 7.45 – 7.40 (m, 4H), 7.35 (t, *J* = 7.2 Hz, 1H), 5.54 (d, *J* = 126 Hz, 2H), 4.24 (dd, *J* = 8.4 Hz, 9.6 Hz, 1H), 3.99 – 3.95 (m, 1H), 3.94 – 3.85 (m, 2H), 3.79 (dd, *J* = 5.4 Hz, 7.8 Hz, 1H). ¹³C NMR (150 MHz, CDCl₃) δ 173.2, 140.9, 140.4, 135.0, 128.8, 128.6, 127.7, 127.5, 127.0, 123.8 (q, *J* = 278.4 Hz), 73.8, 68.9 (q, *J* = 33.6 Hz), 52.5. ¹⁹F NMR (564 MHz, CDCl₃) δ -74.1 (t, *J* = 7.9 Hz). HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₇H₁₇F₃NO₂ 324.1206, found: 324.1205.

[α]_D^{23.1} +33.2778 (c 0.4, CHCl₃). HPLC (AD-H, 0.46*25 cm, 5 μm, hexane/isopropanol = 85/15, flow 0.7 mL/min, detection at 254 nm), retention time = 13.713 min (major) and 21.741 min (minor).

7 Mechanistic study

7.1 Using TEMPO as a radical scavenger



In a dried sealed tube, **L1** (0.003 mmol, 3 mol%), Ir(ppy)₃ (0.7 mg, 0.001 mmol, 1 mol%) and Cu(CH₃CN)₄PF₆ (0.002 mmol, 2 mol%) were dissolved in DCM (0.5 mL) under the atmosphere of nitrogen. The solution was stirred at room temperature for 5 min, and then substrate **1a** (0.1 mmol, 1.0 equiv), **2a** (0.25 mmol, 2.5 equiv), TMSCN (39 μL, 0.3 mmol, 3.0 equiv) and TEMPO (62.6 mg, 0.4 mmol, 4.0 equiv) were added sequentially. The mixture was stirred for 12 h at room temperature with 2 × 3 W blue LEDs. For the reaction workup, solvent was evaporated under reduced pressure, the product **3a** was not obtained in the reaction.

7.2 Radical Clock Experiment

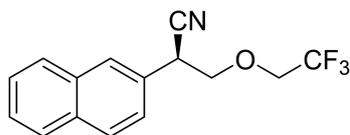


In a dried sealed tube, **L1** (0.003 mmol, 3 mol%), Ir(ppy)₃ (0.7 mg, 0.001 mmol, 1 mol%) and Cu(CH₃CN)₄PF₆ (0.002 mmol, 2 mol%) were dissolved in DCM (0.5 mL) under the atmosphere of nitrogen. The solution was stirred at room temperature for 5 min, and then substrate **6** (0.1 mmol, 1.0 equiv), **2a** (0.25 mmol, 2.5 equiv), TMSCN (39 μL, 0.3 mmol, 3.0 equiv) were added sequentially. The mixture was stirred for 12 h at room temperature with 2 × 3 W blue LEDs. After the reaction was completed, the product was purified by flash column chromatography on silica gel with gradient of petroleum ether/ethyl acetate afford the product **7** (12.3 mg, 38% yield, 77% ee).

7 (12.3 mg, 38 % yield, 77% ee) as white solid. ¹H NMR (600 MHz, CDCl₃) δ 7.42 – 7.29 (m, 9H), 7.22 – 7.00 (m, 1H), 6.01 – 5.77 (m, 1H), 4.44 – 4.26 (m, 2H), 3.98 – 3.66 (m, 3H), 2.91 – 2.61 (m, 2H). ¹³C NMR (150 MHz, CDCl₃) δ 140.9, 140.2, 139.5, 137.0, 134.8, 129.2, 129.1, 128.5, 128.4, 128.2, 128.0, 127.8, 127.7, 127.4, 127.3, 126.3, 124.6, 124.0 (q, *J* = 278.4 Hz), 120.3, 120.2, 76.3, 68.8, 67.0 (q, *J* = 33.6 Hz), 37.5, 37.2, 34.6 (q, *J* = 3.3 Hz). ¹⁹F NMR (564 MHz, CDCl₃) δ -73.6 (t, *J* = 10.2 Hz), -73.8 (t, *J* = 7.9 Hz). HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₀H₁₉F₃NO 346.1413, found: 346.1412.

[α]_D^{23.1} -252.3322 (c 0.3, CHCl₃). HPLC (AD-H, 0.46*25 cm, 5 μm, hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 14.932 min (major) and 16.578 min (minor).

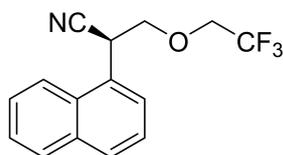
8 Analytical data for new compounds



(S)-2-(naphthalen-2-yl)-3-(2,2,2-trifluoroethoxy)propanenitrile (3a): (37.8 mg, 68%, 90% ee). ¹H NMR (600 MHz, CDCl₃) δ 7.89 – 7.85 (m, 4H), 7.55 – 7.52 (m,

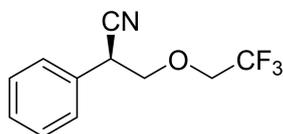
2H), 7.44 (d, $J = 8.4$ Hz, 1H), 4.25 (t, $J = 6.6$ Hz, 1H), 4.01 (d, $J = 6.6$ Hz, 2H), 3.99 – 3.86 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 133.2, 133.0, 129.2, 128.9, 127.9, 127.7, 127.2, 126.9, 126.8, 124.8, 123.5 (q, $J = 278.4$ Hz), 118.7, 74.2, 68.9 (q, $J = 34.7$ Hz), 38.7. ^{19}F NMR (564 MHz, CDCl_3) δ -73.9 (t, $J = 10.1$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{F}_3\text{NNaO}$ 302.0763, found: 302.0764.

$[\alpha]_{\text{D}}^{23.1}$ -25.9576 (c 1.7, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 13.897 min (major) and 17.071 min (minor).



(S)-2-(naphthalen-1-yl)-3-(2,2,2-trifluoroethoxy)propanenitrile (3b): (33.5 mg, 60%, 97% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.93 – 7.88 (m, 3H), 7.75 (d, $J = 7.2$ Hz, 1H), 7.62 (t, $J = 7.8$ Hz, 1H), 7.56 (t, $J = 7.8$ Hz, 1H), 7.51 (t, $J = 7.2$ Hz, 1H), 4.86 (dd, $J = 9.0$ Hz, 4.8 Hz, 1H), 4.12 (dd, $J = 10.2$ Hz, 4.8 Hz, 1H), 4.02 – 3.96 (m, 2H), 3.90 – 3.84 (m, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 133.9, 130.0, 129.7, 129.4, 127.3, 127.0, 126.5, 126.3, 125.4, 123.5 (q, $J = 278.6$ Hz), 121.5, 119.3, 73.4, 69.0 (q, $J = 33.6$ Hz), 35.6. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, $J = 8.5$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{13}\text{F}_3\text{NO}$ 280.0944, found: 280.0940.

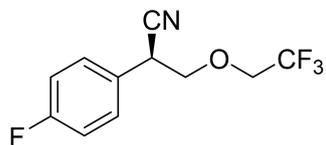
$[\alpha]_{\text{D}}^{23.1}$ -158.9467 (c 0.5, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 12.118 min (major) and 15.820 min (minor).



(S)-2-phenyl-3-(2,2,2-trifluoroethoxy)propanenitrile (3c): (44.8mg, 98%, 84% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.42 – 7.36 (m, 5H), 4.07 (t, $J = 6.6$ Hz, 1H), 3.95 – 3.84 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 131.6, 129.2, 128.8, 127.7, 123.5 (q, $J = 278.4$ Hz), 118.7, 74.2, 68.9 (q, $J = 34.7$ Hz), 38.5. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, $J = 10.2$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{11}\text{H}_{11}\text{F}_3\text{NO}$ 230.0787,

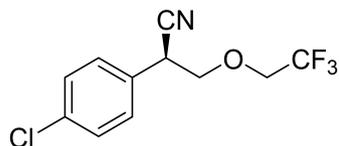
found: 230.0787.

$[\alpha]_D^{23.1}$ -75.1811 (c 1.2, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 8.524 min (major) and 13.778 min (minor).



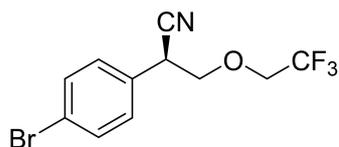
(S)-2-(4-fluorophenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile (3d): (44.5 mg, 90%, 85% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.38 – 7.32 (m, 2H), 7.10 (t, J = 8.4 Hz, 2H), 4.06 (t, J = 6.6 Hz, 1H), 3.96 – 3.83 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 163.6 (d, J = 247.1 Hz), 129.6 (d, J = 7.7 Hz), 127.5 (d, J = 3.3 Hz), 123.5 (q, J = 277.4 Hz), 118.4, 116.3 (d, J = 21.8 Hz), 74.0, 68.9 (q, J = 34.7 Hz), 37.8. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, J = 8.5 Hz), -112.5 (m). HRMS (ESI) m/z : (ESI) $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{11}\text{H}_9\text{F}_4\text{NNaO}$ 270.0512, measured: 270.0515.

$[\alpha]_D^{23.1}$ -102.4095 (c 0.5, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 9.662 min (major) and 12.078 min (minor).

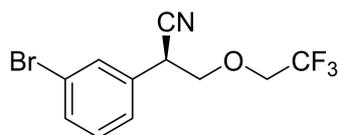


(S)-2-(4-chlorophenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile (3e): (37.9 mg, 72%, 90% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.39 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.4 Hz, 2H), 4.05 (t, J = 6.6 Hz, 1H), 3.95 – 3.83 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 135.0, 130.3, 129.4, 129.2, 123.5 (q, J = 278.4 Hz), 118.2, 73.8, 68.9 (q, J = 34.8 Hz), 37.9. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, J = 10.2 Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{11}\text{H}_{10}\text{ClF}_3\text{NO}$ 264.0398, found: 264.0396.

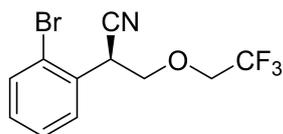
$[\alpha]_D^{23.1}$ -20.0928 (c 0.7, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 8.719 min (major) and 11.306 min (minor).



(S)-2-(4-bromophenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile (3f): (50.4 mg, 82%, 86% ee). ¹H NMR (600 MHz, CDCl₃) δ 7.55 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 4.04 (t, *J* = 6.6 Hz, 1H), 3.95 – 3.83 (m, 4H). ¹³C NMR (150 MHz, CDCl₃) δ 132.4, 130.7, 129.4, 123.5 (q, *J* = 277.4 Hz), 123.0, 118.1, 73.8, 68.9 (q, *J* = 33.6 Hz), 38.0. ¹⁹F NMR (564 MHz, CDCl₃) δ -73.9 (t, *J* = 7.9 Hz). HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₁H₉F₃BrNaNO 329.9712, found: 329.9713. [α]_D^{23.1} -16.0986 (c 0.7, CHCl₃). HPLC (AY-3, 0.46*15 cm, 3 μm, hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 9.565 min (major) and 12.950 min (minor).



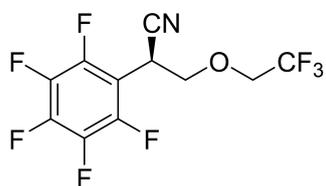
(S)-2-(3-bromophenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile(3g): (44.4 mg, 73%, 84% ee). ¹H NMR (600 MHz, CDCl₃) δ 7.53 (s, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 1H), 4.04 (t, *J* = 6.6 Hz, 1H), 3.96 – 3.84 (m, 4H). ¹³C NMR (150 MHz, CDCl₃) δ 133.8, 132.0, 130.8, 130.7, 126.4, 123.5 (q, *J* = 278.4), 123.1, 118.0, 73.8, 68.9 (q, *J* = 34.7), 38.0. ¹⁹F NMR (564 MHz, CDCl₃) δ -73.9 (t, *J* = 10.2 Hz). HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₁H₉F₃BrNaNO 329.9712, found: 329.9713. [α]_D^{23.1} -22.4946 (c 0.9, CHCl₃). HPLC (AY-3, 0.46*15 cm, 3 μm, hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 9.662 min (major) and 12.078 min (minor).



(S)-2-(2-bromophenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile (3h): (38.7 mg, 63%, 95% ee). ¹H NMR (600 MHz, CDCl₃) δ 7.64 (dd, *J* = 15.0 Hz, 7.8 Hz, 2H), 7.40

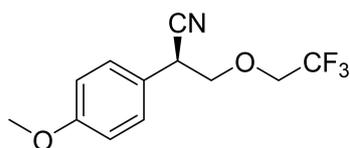
(t, $J = 7.8$ Hz, 1H), 7.26 – 7.24 (m, 1H), 4.59 (dd, $J = 4.8$ Hz, 7.8 Hz, 1H), 4.01 (dd, $J = 4.8$ Hz, 9.6 Hz, 1H), 3.96 – 3.89 (m, 2H), 3.85 (t, $J = 9.0$ Hz, 1H). ^{13}C NMR (150 MHz, CDCl_3) δ 133.4, 131.0, 130.5, 129.9, 128.3, 123.5 (q, $J = 278.4$ Hz), 123.1, 118.4, 72.3, 69.3 (q, $J = 33.6$ Hz), 38.4. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, $J = 10.2$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{11}\text{H}_9\text{F}_3\text{BrNaNO}$ 329.9712, found: 329.9713.

$[\alpha]_{\text{D}}^{23.1}$ -55.4269 (c 1.0, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 7.800 min (major) and 9.472 min (minor).



(S)-2-(perfluorophenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile(3i): (28.7 mg, 45%, 61% ee). ^1H NMR (600 MHz, CDCl_3) δ 4.44 (t, $J = 6.6$ Hz, 1H), 4.13 (dd, $J = 9.0$ Hz, 7.2 Hz, 1H), 4.01 – 3.87 (m, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 146.0 – 144.2 (dm), 142.8 – 140.9 (dm), 138.8 – 136.9 (dm), 123.3 (q, $J = 278.6$ Hz), 115.0, 106.2 (td, $J = 15.1$ Hz, 4.3 Hz), 70.6, 68.8 (q, $J = 34.7$ Hz), 26.9. ^{19}F NMR (564 MHz, CDCl_3) δ -74.1 (t, $J = 8.5$ Hz), -140.5 (dd, $J = 20.3$, 6.2 Hz), -150.7 (t, $J = 19.7$ Hz), -159.5 (m). HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{11}\text{H}_6\text{F}_8\text{NNaO}$ 320.0316, found: 320.0318.

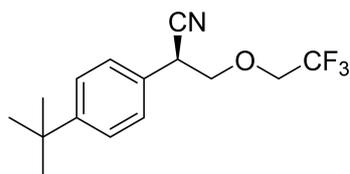
$[\alpha]_{\text{D}}^{23.1}$ -102.7809 (c 0.4, CHCl_3). HPLC (IG, 0.46*25 cm, 5 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 8.566 min (minor) and 9.118 min (major).



(S)-2-(4-methoxyphenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile(3j): (38.7 mg, 75%, 75% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.28 (d, $J = 8.4$ Hz, 2H), 6.92 (d, $J = 9.0$ Hz, 2H), 4.02 (t, $J = 7.2$ Hz, 1H), 3.95 – 3.83 (m, 4H), 3.82 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 159.8, 128.9, 123.6 (q, $J = 278.4$ Hz), 123.5, 118.9, 114.6, 74.3,

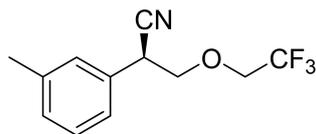
68.9 (q, $J = 34.7$ Hz), 55.3, 37.8. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, $J = 8.5$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{13}\text{F}_3\text{NO}_2$ 260.0893, found: 260.0894.

$[\alpha]_{\text{D}}^{23.1}$ -131.6344 (c 0.6, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 16.902 min (major) and 20.883 min (minor).



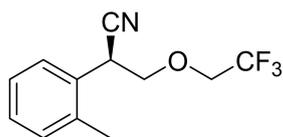
(S)-2-(4-(tert-butyl)phenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile(3k): (16.2 mg, 61%, 78% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.42 (d, $J = 8.4$ Hz, 2H), 7.30 (d, $J = 8.4$ Hz, 2H), 4.05 (dd, $J = 8.4$ Hz, 6.0 Hz, 1H), 3.97 – 3.85 (m, 4H), 1.32 (s, 9H). ^{13}C NMR (150 MHz, CDCl_3) δ 151.9, 128.4, 127.4, 126.2, 123.6 (q, $J = 278.4$ Hz), 118.9, 74.3, 68.9 (q, $J = 34.7$ Hz), 38.1, 34.6, 31.1. ^{19}F NMR (564 MHz, CDCl_3) δ -73.9 (t, $J = 7.9$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{19}\text{F}_3\text{NO}$ 286.1413, found: 286.1414.

$[\alpha]_{\text{D}}^{23.1}$ -19.5035 (c 1.7, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 6.594 min (minor) and 6.872 min (major).



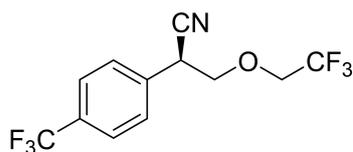
(S)-2-(m-tolyl)-3-(2,2,2-trifluoroethoxy)propanenitrile(3l): (24.8 mg, 51%, 84% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.29 (t, $J = 8.4$ Hz, 1H), 7.18 – 7.15 (m, 3H), 4.04 (t, $J = 7.2$ Hz, 1H), 3.96 – 3.84 (m, 4H), 2.38 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 139.1, 131.4, 129.5, 129.1, 128.4, 124.7, 123.5 (q, $J = 278.6$ Hz), 118.8, 74.3, 68.9 (q, $J = 33.6$ Hz), 38.5, 21.3. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, $J = 9.6$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{13}\text{F}_3\text{NO}$ 244.0944, found: 244.0943.

$[\alpha]_{\text{D}}^{23.1}$ -19.7000 (c 0.4, CHCl_3). HPLC (IG, 0.46*25 cm, 5 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 10.816 min (minor) and 11.532 min (major).



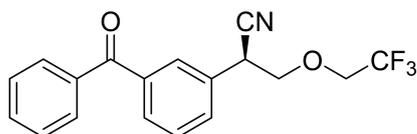
(S)-2-(o-tolyl)-3-(2,2,2-trifluoroethoxy)propanenitrile(3m): (29.2 mg, 60%, 95% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.47 – 7.44 (m, 1H), 7.28 – 7.25 (m, 2H), 7.22 – 7.19 (m, 1H), 4.27 (dd, $J = 5.4$ Hz, 8.4 Hz, 1H), 3.99 – 3.82 (m, 4H), 2.36 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 135.5, 131.1, 129.8, 128.8, 127.9, 127.0, 123.5 (q, $J = 278.6$ Hz), 119.2, 73.2, 68.9 (q, $J = 34.7$ Hz), 35.4, 19.0. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, $J = 7.9$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{12}\text{H}_{12}\text{F}_3\text{NNaO}$ 266.0763, found: 266.0762.

$[\alpha]_{\text{D}}^{23.1}$ -47.3244 (c 0.9, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 16.902 min (major) and 20.883 min (minor).



(S)-3-(2,2,2-trifluoroethoxy)-2-(4-(trifluoromethyl)phenyl)propanenitrile(3n): (36.8 mg, 62%, 78% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.69 (d, $J = 7.8$ Hz, 2H), 7.53 (d, $J = 8.4$ Hz, 2H), 4.14 (t, $J = 6.0$ Hz, 1H), 3.96 – 3.86 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 135.7, 131.2 (q, $J = 32.6$ Hz), 128.3, 126.2 (q, $J = 3.3$ Hz), 123.6 (q, $J = 270.9$ Hz), 123.4 (q, $J = 278.4$ Hz), 117.8, 73.6, 68.9 (q, $J = 34.7$ Hz), 38.3. ^{19}F NMR (564 MHz, CDCl_3) δ -62.8 (s), -73.9 (t, $J = 7.9$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{12}\text{H}_9\text{F}_6\text{NNaO}$ 320.0481, found: 320.0485.

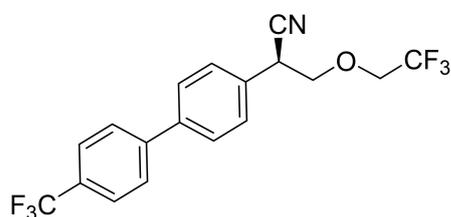
$[\alpha]_{\text{D}}^{23.1}$ -15.4375 (c 0.6, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 7.104 min (major) and 8.013 min (minor).



(S)-2-(3-benzoylphenyl)-3-(2,2,2-trifluoroethoxy)propanenitrile(3o): (51.3 mg, 77%, 78% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.79 (dd, $J = 8.4$ Hz, 1.2 Hz, 4H), 7.65

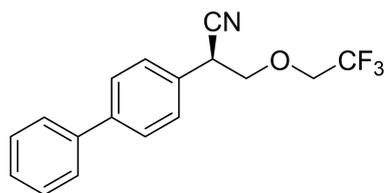
- 7.60 (m, 2H), 7.55 (t, $J = 7.2$ Hz, 1H), 7.50 (t, $J = 7.2$ Hz, 2H), 4.16 (t, $J = 6.6$ Hz, 1H), 3.97 (d, $J = 6.0$ Hz, 2H), 3.95 – 3.85 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 195.8, 138.5, 137.0, 132.9, 132.3, 131.6, 130.5, 130.0, 129.3, 129.2, 128.5, 123.5 (q, $J = 21.6$ Hz), 118.2, 73.8, 68.9 (q, $J = 34.7$ Hz), 38.3. ^{19}F NMR (564 MHz, CDCl_3) δ -73.9 (t, $J = 7.9$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{15}\text{F}_3\text{NO}_2$ 334.1049, found: 334.1048.

$[\alpha]_{\text{D}}^{23.1}$ -28.9984 (c 1.3, CHCl_3). HPLC (AD-H, 0.46*25 cm, 5 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 16.902 min (major) and 20.883 min (minor).



(S)-3-(2,2,2-trifluoroethoxy)-2-(4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)propane nitrile(3p): (64.0 mg, 86%, 87% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.72 (d, $J = 7.8$ Hz, 2H), 7.68 (d, $J = 8.4$ Hz, 2H), 7.64 (d, $J = 7.8$ Hz, 2H), 7.49 (d, $J = 7.8$ Hz, 2H), 4.14 (t, 6.6Hz, 1H), 4.00 – 3.86 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 143.5, 140.3, 131.6, 129.8 (q, $J = 32.6$ Hz), 128.4, 128.0, 127.4, 125.8 (q, $J = 3.2$ Hz), 124.1 (q, $J = 270.8$ Hz), 123.5 (q, $J = 278.4$ Hz), 118.4, 74.0, 68.9 (q, $J = 34.7$ Hz), 38.2. ^{19}F NMR (564 MHz, CDCl_3) δ -62.4 (s), -73.9 (t, $J = 7.9$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{14}\text{F}_6\text{NO}$ 374.0974, found: 374.0975.

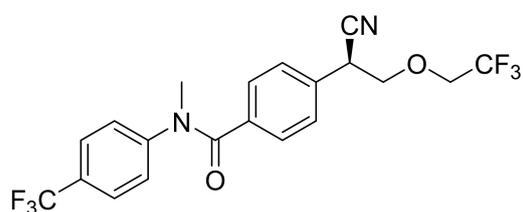
$[\alpha]_{\text{D}}^{23.1}$ -14.5505 (c 0.9, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 11.520 min (major) and 13.283 min (minor).



(S)-2-([1,1'-biphenyl]-4-yl)-3-(2,2,2-trifluoroethoxy)propanenitrile(3q): (27.4 mg, 90%, 98% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.63 (d, $J = 8.4$ Hz, 2H), 7.58 (d, $J =$

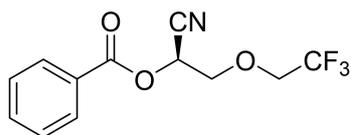
7.2 Hz, 2H), 7.47 – 7.44 (m, 4H), 7.38 (t, $J = 7.2$ Hz, 1H), 4.13 (t, $J = 6.6$ Hz, 1H), 4.00 – 3.86 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3) δ 141.8, 140.0, 130.5, 128.9, 128.2, 127.9, 127.7, 127.1, 123.5 (q, $J = 278.6$ Hz), 118.6, 74.2, 68.9 (q, $J = 34.7$ Hz), 38.2. ^{19}F NMR (564 MHz, CDCl_3) δ -73.9 (t, $J = 7.9$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{15}\text{F}_3\text{NO}$ 306.1100, found: 306.1104.

$[\alpha]_{\text{D}}^{23.1}$ -19.6499 (c 0.9, CHCl_3). HPLC (AD-H, 0.46*25 cm, 5 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 16.902 min (major) and 20.883 min (minor).



(S)-4-(1-cyano-2-(2,2,2-trifluoroethoxy)ethyl)-N-methyl-N-(4-(trifluoromethyl)phenyl)benzamide (3r): (66.3 mg, 77%, 62% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.51 (d, $J = 8.4$ Hz, 2H), 7.34 (d, $J = 7.2$ Hz, 2H), 7.24 (d, $J = 7.8$ Hz, 2H), 7.15 (d, $J = 8.4$ Hz, 2H), 4.00 (t, $J = 6.0$ Hz, 1H), 3.87 – 3.75 (m, 4H), 3.51 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 169.5, 147.6, 135.9, 133.7, 129.4, 128.6 (q, $J = 32.6$ Hz), 127.6, 126.8, 126.4 (q, $J = 3.3$ Hz), 123.5 (q, $J = 270.9$ Hz), 123.4 (q, $J = 278.6$ Hz), 118.0, 73.6, 68.8 (q, $J = 34.7$ Hz), 38.2, 38.1. ^{19}F NMR (564 MHz, CDCl_3) δ -62.5 (s), -74.0 (t, $J = 7.9$ Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{20}\text{H}_{17}\text{F}_6\text{N}_2\text{O}_2$ 431.1189, found: 431.1187.

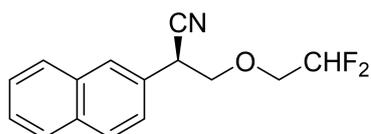
$[\alpha]_{\text{D}}^{23.1}$ 334.1000 (c 0.5, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 12.118 min (major) and 15.820 min (minor).



(S)-1-cyano-2-(2,2,2-trifluoroethoxy)ethyl benzoate(3s): (18.6 mg, 34%, 0% ee). ^1H NMR (600 MHz, CDCl_3) δ 8.07 (dd, $J = 1.2$ Hz, 8.4 Hz, 2H), 7.66 – 7.63 (m, 1H), 7.49 (t, $J = 7.8$ Hz, 2H), 5.76 (t, $J = 5.4$ Hz, 1H), 4.14 – 4.11 (m, 2H), 4.04 – 3.97 (m,

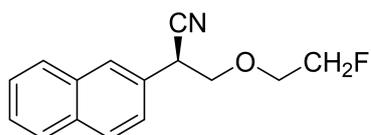
2H). ^{13}C NMR (150 MHz, CDCl_3) δ 164.4, 134.3, 130.0, 128.7, 127.6, 123.4 (q, J = 278.4 Hz), 114.6, 70.8, 69.1 (q, J = 34.8 Hz), 60.4. ^{19}F NMR (564 MHz, CDCl_3) δ -74.0 (t, J = 8.5 Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{11}\text{F}_3\text{NO}_3$ 274.0686, measured: 274.0686.

$[\alpha]_{\text{D}}^{23.1}$ 5.0897 (c 1.5, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 12.678 min (minor) and 15.593 min (major).



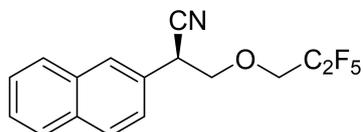
(S)-3-(2,2-difluoroethoxy)-2-(naphthalen-2-yl)propanenitrile(3t): (36.5 mg, 70%, 89% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.89 – 7.85 (m, 4H), 7.55 – 7.52 (m, 2H), 7.43 (dd, J = 1.8 Hz, 8.4 Hz, 1H), 5.97 – 5.78 (m, 1H), 4.23 (t, J = 6.6 Hz, 1H), 3.97 – 3.93 (m, 2H), 3.82 – 3.69 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 133.2, 133.0, 129.1, 127.9, 127.7, 127.1, 126.8, 126.8, 124.9, 119.0, 114.1 (t, J = 240.5 Hz), 73.8, 70.7 (t, J = 27.0 Hz), 38.7. ^{19}F NMR (564 MHz, CDCl_3) δ -124.9 (dq, J = 55.8 Hz, 14.1 Hz). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{14}\text{F}_2\text{NO}$ 262.1038, found: 262.1041.

$[\alpha]_{\text{D}}^{23.1}$ -31.8977 (c 0.4, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 21.886 min (major) and 26.827 min (minor).



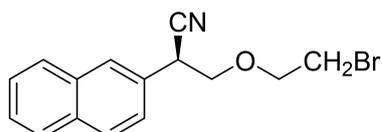
(S)-3-(2-fluoroethoxy)-2-(naphthalen-2-yl)propanenitrile(3u): (23.3 mg, 48%, 85% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.88 – 7.84 (m, 4H), 7.54 – 7.51 (m, 2H), 7.45 (d, J = 8.4 Hz, 1H), 4.64 – 4.51 (m, 2H), 4.24 (t, J = 6.6 Hz, 1H), 3.95 – 3.90 (m, 2H), 3.85 – 3.73 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 133.2, 132.9, 129.6, 129.0, 127.8, 127.7, 127.1, 126.8, 126.7, 125.0, 119.3, 83.6, 82.5, 73.4, 70.8 (d, J = 19.5 Hz), 38.8. ^{19}F NMR (564 MHz, CDCl_3) δ -222.3 – -222.7 (m). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{15}\text{FNO}$ 244.1132, found: 244.1132.

$[\alpha]_D^{23.1}$ -32.4432 (c 0.4, CHCl₃). HPLC (AY-3, 0.46*15 cm, 3 μm, hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 46.137 min (minor) and 48.043 min (major).



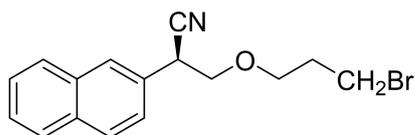
(S)-2-(naphthalen-2-yl)-3-(2,2,3,3,3-pentafluoropropoxy)propanenitrile(3v): (39.5 mg, 60%, 89% ee). ¹H NMR (600 MHz, CDCl₃) δ 7.89 – 7.85 (m, 4H), 7.56 – 7.52 (m, 2H), 7.43 (dd, *J* = 8.4 Hz, 1.8 Hz, 1H), 4.24 (t, *J* = 6.6 Hz, 1H), 4.06 – 3.92 (m, 4H). ¹³C NMR (150 MHz, CDCl₃) δ 133.2, 133.0, 129.2, 128.8, 127.8, 127.7, 127.2, 126.9, 126.8, 124.8, 118.6, 118.4 (qt, *J* = 284.8 Hz, 34.6 Hz), 112.7 (qt, *J* = 254.5 Hz, 36.9 Hz), 74.4, 68.1 (t, *J* = 26.1 Hz), 38.6. ¹⁹F NMR (564 MHz, CDCl₃) δ -83.5 (s), 123.1 (q, *J* = 11.8 Hz). HRMS (ESI) *m/z*: [M+Na]⁺ calcd for C₁₆H₁₂F₅NNaO 352.0731, found: 352.0735.

$[\alpha]_D^{23.1}$ -17.4609 (c 0.2, CHCl₃). HPLC (AY-3, 0.46*15 cm, 3 μm, hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 8.382 min (major) and 9.122 min (minor).



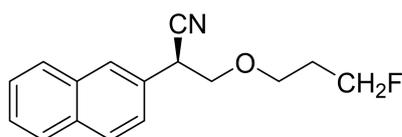
(S)-3-(2-bromoethoxy)-2-(naphthalen-2-yl)propanenitrile(3x): (31.5 mg, 52%, 87% ee). ¹H NMR (600 MHz, CDCl₃) δ 7.89 – 7.84 (m, 4H), 7.54 – 7.51 (m, 2H), 7.45 (dd, *J* = 1.8 Hz, 8.4 Hz, 1H), 4.23 (dd, *J* = 6.6 Hz, 7.8 Hz 1H), 3.94 – 3.80 (m, 4H), 3.46 (t, *J* = 6.0 Hz, 2H). ¹³C NMR (150 MHz, CDCl₃) δ 133.2, 132.9, 129.5, 129.0, 127.8, 127.7, 127.1, 126.8, 126.7, 125.0, 119.2, 73.0, 71.5, 38.7, 29.7. HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₁₅H₁₅BrNO 304.0332, found: 304.0332.

$[\alpha]_D^{23.1}$ -50.2299 (c 0.8, CHCl₃). HPLC (AD-H, 0.46*25 cm, 5 μm, hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 23.691 min (minor) and 24.882 min (major).



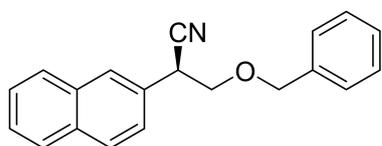
(S)-3-(3-bromopropoxy)-2-(naphthalen-2-yl)propanenitrile(3y): (28.5 mg, 45%, 82% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.88 – 7.84 (m, 4H), 7.53 – 7.51 (m, 2H), 7.44 (dd, $J = 1.8$ Hz, 6.0 Hz, 1H), 4.22 (dd, $J = 6.6$ Hz, 7.8 Hz, 1H), 3.87 – 3.81 (m, 2H), 3.66 (t, $J = 6.0$ Hz, 2H), 3.51 – 3.48 (m, 2H), 2.13 – 2.09 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 133.2, 132.9, 129.7, 129.0, 127.8, 127.7, 127.0, 126.8, 126.6, 125.0, 119.3, 72.8, 68.8, 38.7, 32.5, 30.2. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{17}\text{BrNO}$ 318.0488, found: 318.0486.

$[\alpha]_{\text{D}}^{23.1}$ -167.7471 (c 0.3, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 20.430 min (major) and 24.434 min (minor).



(S)-3-(3-fluoropropoxy)-2-(naphthalen-2-yl)propanenitrile(3z): (23.7 mg, 46%, 83% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.88 – 7.84 (m, 4H), 7.54 – 7.51 (m, 2H), 7.44 (d, $J = 8.4$ Hz, 1H), 4.58 (dt, $J = 46.8$ Hz, 6.0 Hz, 2H), 4.22 (t, $J = 6.6$ Hz, 1H), 3.86 – 3.80 (m, 2H), 3.65 (t, $J = 6.0$ Hz, 2H), 2.01 – 1.93 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 133.2, 132.9, 129.7, 129.0, 127.8 (d, $J = 21.6$ Hz), 127.0, 126.7, 126.6, 125.0, 119.4, 81.3, 80.2, 72.8, 67.1 (d, $J = 5.6$ Hz), 38.7, 30.6 (d, $J = 19.5$ Hz). ^{19}F NMR (564 MHz, CDCl_3) δ -222.1 – -222.5 (m). HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{17}\text{FNO}$ 258.1289, found: 258.1289.

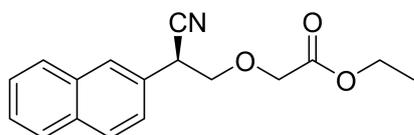
$[\alpha]_{\text{D}}^{23.1}$ -544.7114 (c 0.1, CHCl_3). HPLC (AD-H, 0.46*25 cm, 5 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 18.021 min (minor) and 19.045 min (major).



(S)-3-(benzyloxy)-2-(naphthalen-2-yl)propanenitrile(3aa): (34.4 mg, 60%, 81% ee).

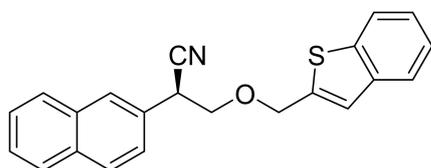
^1H NMR (600 MHz, CDCl_3) δ 7.86 – 7.83 (m, 4H), 7.53 – 7.50 (m, 2H), 7.42 (d, J = 8.4 Hz, 1H), 7.34 – 7.28 (m, 5H), 4.63 (q, J = 12.0 Hz, 2H), 4.22 (t, J = 6.6 Hz, 1H), 3.88 – 3.80 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 137.1, 133.2, 132.9, 129.8, 128.9, 128.5, 127.9, 127.8, 127.7, 127.1, 126.7, 126.6, 125.1, 119.4, 73.5, 71.8, 38.7, 29.6. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{20}\text{H}_{18}\text{NO}$ 288.1383, found: 288.1379.

$[\alpha]_{\text{D}}^{23.1}$ -81.4635 (c 0.017, CHCl_3). HPLC (AY-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 25.994 min (major) and 28.079 min (minor).



ethyl (*S*)-2-(2-cyano-2-(naphthalen-2-yl)ethoxy)acetate(3ab): (44.1 mg, 78%, 84% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.90 – 7.84 (m, 4H), 7.53 – 7.51 (m, 2H), 7.46 (dd, J = 1.8 Hz, 8.4 Hz, 1H), 4.32 (dd, J = 8.4 Hz, 6.0 Hz, 1H), 4.22 – 4.19 (m, 3H), 4.13 (d, J = 16.8 Hz, 1H), 4.00 – 3.95 (m, 2H), 1.27 (t, J = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 169.8, 133.2, 133.0, 129.4, 129.0, 127.9, 127.7, 127.1, 126.7, 126.7, 125.0, 119.2, 73.3, 68.7, 61.0, 38.0, 14.1. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{18}\text{NO}_3$ 284.1281, found: 284.1281.

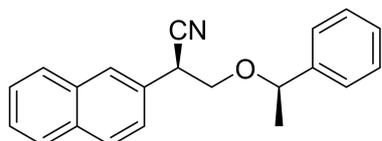
$[\alpha]_{\text{D}}^{23.1}$ -114.9895 (c 0.4, CHCl_3). HPLC (IC-3, 0.46*15 cm, 3 μm , hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 64.769 min (minor) and 74.043 min (major).



(*S*)-3-(benzo[b]thiophen-2-ylmethoxy)-2-(naphthalen-2-yl)propanenitrile(3ac): (20.9 mg, 59%, 84% ee). ^1H NMR (600 MHz, CDCl_3) δ 7.86 – 7.82 (m, 4H), 7.80 (d, J = 7.8 Hz, 1H), 7.70 (dd, J = 1.8 Hz, 6.6 Hz, 1H), 7.53 – 7.51 (m, 2H), 7.42 (dd, J = 1.8 Hz, 8.4 Hz, 1H), 7.33 – 7.31 (m, 2H), 7.18 (s, 1H), 4.89 (q, J = 13.2 Hz, 2H), 4.23 (t, J = 7.2 Hz, 1H), 3.93 – 3.87 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3) δ 140.7, 140.2, 139.2, 133.2, 132.9, 129.6, 129.0, 127.8, 127.7, 127.1, 126.7, 126.6, 125.0, 124.4,

124.3, 123.5, 123.1, 122.4, 119.2, 71.5, 68.6, 38.7. HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{22}H_{18}NOS$ 344.1104, found: 344.1104.

$[\alpha]_D^{23.1}$ 736.0058 (c 0.2, $CHCl_3$). HPLC (IC-3, 0.46*15 cm, 3 μ m, hexane/isopropanol = 9/1, flow 0.7 mL/min, detection at 254 nm), retention time = 26.664 min (minor) and 28.533 min (major).



(S)-2-(naphthalen-2-yl)-3-((R)-1-phenylethoxy)propanenitrile(3ad): (21.1 mg, 35%, 90% ee). 1H NMR (600 MHz, $CDCl_3$) δ 7.84 – 7.81 (m, 5H), 7.52 – 7.49 (m, 2H), 7.39 (dd, J = 8.4 Hz, 1.8 Hz, 1H), 7.32 – 7.26 (m, 4H), 4.46 (q, J = 6.6 Hz, 1H), 4.22 (dd, J = 7.8 Hz, 6 Hz, 1H), 3.72 – 3.63 (m, 2H), 1.46 (d, J = 6.6 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 142.5, 133.1, 132.9, 129.9, 128.8, 128.5, 127.8, 127.7, 127.6, 127.0, 126.6, 126.5, 126.1, 125.1, 119.5, 78.8, 70.3, 38.8, 23.9. HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{21}H_{20}NO$ 302.1539, found: 302.1539.

$[\alpha]_D^{23.1}$ -248.6213 (c 0.3, $CHCl_3$). HPLC (AY-3, 0.46*15 cm, 3 μ m, hexane/isopropanol = 95/5, flow 0.7 mL/min, detection at 254 nm), retention time = 13.719 min (minor) and 14.396 min (major).

9 X-Ray Data (3q)

The crystal of **3q** (CCDC 2521832) suitable for crystallographic analysis was grown from dichloromethane by slow crystallization in 2 mL flat bottom bottle. Single crystal X-ray diffraction data were recorded on a Rigaku XtaLAB Synergy-R Diffraction equipped with a digital camera diffractometer comprising a microfocus rotating anode X-ray source (Cu $K\alpha$, λ =1.54178 Å) and an HPC detector [HyPix-6000C] radiation for the crystal structures. The diffraction data were processed during data collection using CrysAlisPro. The structures were solved and refined during data collection with AutoChem. Final structure refinements were performed using SHELXL implemented in Olex2.

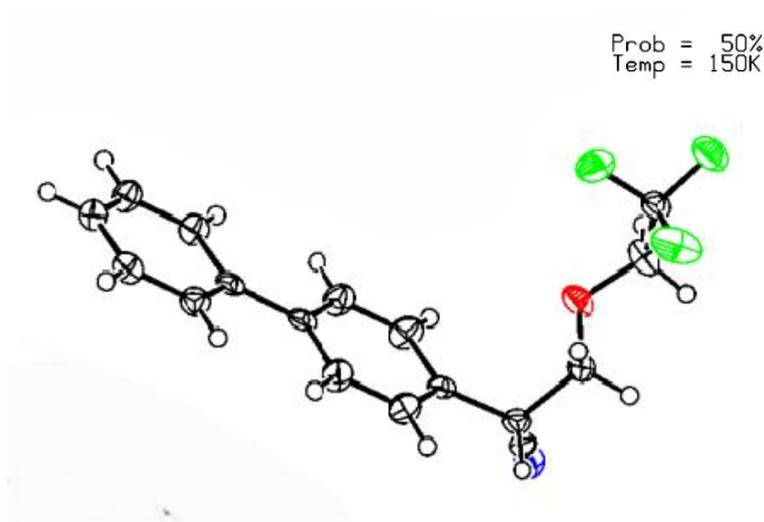


Table 1 Crystal data and structure refinement for ZGY.

Identification code	ZGY
Empirical formula	C ₁₇ H ₁₄ F ₃ NO
Formula weight	305.29
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	P2 ₁
a/Å	5.54510(10)
b/Å	23.8249(8)
c/Å	32.5396(16)
α/°	90
β/°	90.416(2)
γ/°	90
Volume/Å ³	4298.7(3)
Z	12
ρ _{calc} /cm ³	1.415
μ/mm ⁻¹	0.979
F(000)	1896.0
Crystal size/mm ³	0.13 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	4.596 to 144.186
Index ranges	-5 ≤ h ≤ 6, -23 ≤ k ≤ 29, -40 ≤ l ≤ 38
Reflections collected	28270
Independent reflections	13016 [R _{int} = 0.0292, R _{sigma} = 0.0339]
Data/restraints/parameters	13016/1/1189
Goodness-of-fit on F ²	1.027
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0494, wR ₂ = 0.1367
Final R indexes [all data]	R ₁ = 0.0520, wR ₂ = 0.1385

Largest diff. peak/hole / e Å ⁻³	0.26/-0.26
Flack parameter	0.14(6)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for ZGY. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U(\text{eq})$
F001	3221(5)	7636.5(11)	4854.6(9)	45.3(6)
F002	7923(5)	9111.6(11)	158.5(9)	43.6(6)
F003	7071(6)	12223.3(12)	791.7(8)	48.1(7)
F004	7783(6)	12419.3(11)	158.7(9)	48.4(7)
F005	2267(5)	10951.1(11)	4862.1(9)	46.6(7)
F006	-646(5)	4781.7(13)	4670.5(10)	53.5(8)
F007	6910(5)	5763.7(11)	114.6(9)	47.8(7)
F008	8225(6)	8889.9(12)	797.2(9)	52.8(7)
F009	2427(5)	4306.0(11)	4862.1(9)	47.7(7)
O00A	2260(5)	5600.0(12)	4333.6(8)	29.3(6)
O00B	7431(5)	11104.9(11)	652.1(8)	28.5(6)
F00C	10228(5)	8441.3(12)	348.4(11)	56.2(9)
F00D	4624(5)	11948.5(12)	322.2(10)	50.3(7)
F00E	1779(6)	4465.1(12)	4221.1(8)	53.2(8)
F00F	3172(6)	7833.1(12)	4212.1(9)	56.3(8)
F00G	6445(7)	5613.3(12)	757.9(9)	58.9(8)
O00H	5903(5)	7893.1(12)	693.9(9)	32.6(6)
O00I	6767(5)	4479.3(12)	657.1(9)	33.3(6)
F00J	2704(7)	11123.7(13)	4216.6(9)	56.4(8)
F00K	4800(4)	11577.3(12)	4658.3(10)	50.9(7)
F00L	3857(5)	5300.6(14)	322.3(12)	61.6(9)
O00M	702(5)	12168.9(13)	4283.8(9)	38.3(7)
F00N	5617(5)	8262.7(12)	4614.5(12)	58.6(9)
O00O	1321(5)	8880.7(14)	4336.2(9)	37.8(7)
N00P	-1452(7)	6844.3(17)	4313.8(11)	37.5(8)
N00Q	3633(6)	9855.0(16)	692.2(11)	32.5(8)
N00R	2360(6)	6656.0(16)	703.7(11)	33.0(8)
N00S	-2065(7)	10143.5(18)	4308.2(11)	37.5(8)
N00T	-2674(7)	13424.3(17)	4279.3(11)	36.4(8)
C1	7252(6)	10771.0(15)	2250.7(11)	21.5(7)
C4	1838(6)	12625.7(15)	2740.4(11)	20.5(7)
C6	6719(6)	7125.6(15)	1405.1(11)	20.7(7)
N00X	2960(7)	3263.3(17)	694.8(11)	35.9(8)
C8	2240(6)	9119.8(15)	2329.1(11)	21.3(7)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	$U(\text{eq})$
C10	7551(6)	10415.9(15)	1423.8(11)	22.3(7)
C12	6896(6)	4290.2(15)	2697.2(11)	22.3(7)
C14	7011(6)	7439.9(15)	2245.2(11)	21.3(7)
C16	7183(6)	7613.6(15)	2683.7(11)	22.1(7)
C18	2185(6)	9295.6(16)	2768.3(11)	22.3(7)
C20	8112(7)	8680.1(17)	421.5(12)	27.6(8)
C22	7114(7)	10957.9(16)	2686.6(12)	23.8(8)
C24	2082(6)	5962.5(15)	2735.2(11)	20.6(7)
C26	8842(7)	3609.6(17)	1697.1(13)	30.3(9)
C28	2390(6)	6309.0(16)	3568.4(11)	21.9(7)
C30	6932(6)	4112.0(15)	2259.2(11)	22.1(7)
C32	1985(6)	12452.8(15)	2302.3(11)	21.3(7)
C34	1610(6)	12942.9(16)	3579.7(11)	23.7(7)
C36	1915(6)	5781.4(16)	2299.3(11)	22.4(7)
C38	8618(7)	6948.3(18)	1651.9(12)	30.2(9)
C40	7048(7)	3772.0(16)	1426.0(11)	23.5(7)
C42	6661(7)	6971.1(16)	953.8(12)	25.6(8)
C44	4788(8)	3406.6(17)	821.0(12)	28.0(8)
C46	5439(7)	10016.3(16)	817.9(12)	26.9(8)
C48	3382(8)	8056.3(18)	4585.5(13)	32.3(9)
C50	1595(7)	13092.9(17)	4033.6(12)	27.9(8)
C52	2074(7)	9622.3(16)	3603.6(12)	24.3(8)
C54	4231(7)	6796.2(16)	815.8(12)	25.6(8)
C56	7792(6)	10207.0(16)	981.3(12)	24.7(8)
C58	4197(7)	9265.4(17)	2074.4(12)	28.7(8)
C60	451(7)	8641.6(17)	1741.2(13)	30.0(9)
C62	-193(7)	12614.2(18)	3399.8(13)	29.5(8)
C64	5191(7)	4102.9(18)	1571.6(12)	30.3(9)
C66	3153(8)	5216.2(18)	4625.1(12)	29.9(8)
C68	2136(7)	9787.7(17)	4057.2(12)	28.0(8)
C70	9319(7)	7622.2(18)	3336.7(13)	30.1(9)
C72	9156(7)	7461.9(17)	2929.5(12)	28.3(8)
C74	487(7)	5978.7(18)	3429.5(13)	30.3(9)
C76	2663(7)	6502.2(16)	4009.5(12)	26.3(8)
C78	-77(7)	12460.4(18)	2990.4(12)	28.4(8)
C80	3987(7)	6291.2(18)	2879.3(12)	29.3(8)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	$U(\text{eq})$
C82	391(7)	8801.5(17)	2150.4(12)	27.2(8)
C84	1660(8)	4695.3(18)	4594.1(13)	31.0(9)
C86	5123(7)	4271.2(18)	1979.1(12)	28.6(8)
C88	-806(7)	13282.1(17)	4166.4(12)	26.9(8)
C90	5553(7)	8096.4(18)	3277.3(13)	31.5(9)
C92	4247(7)	9103.8(19)	1667.4(13)	31.4(9)
C94	3613(7)	12961.6(18)	2925.9(12)	30.0(8)
C96	328(7)	6691.9(17)	4181.9(11)	26.3(8)
C98	-113(8)	5296(2)	1738.9(13)	36.8(10)
C100	4937(7)	7455.5(18)	1585.0(13)	30.3(9)
C102	5680(7)	10754.9(18)	1553.7(12)	29.6(8)
C51	3508(7)	13114.9(17)	3333.2(13)	29.0(8)
C13	3928(7)	9800.8(18)	3348.1(13)	31.8(9)
C53	293(8)	9285(2)	3439.9(13)	34.8(9)
C27	8378(7)	11490.8(17)	368.5(12)	28.8(8)
C55	4142(7)	6463.3(17)	3284.8(12)	28.0(8)
C7	333(7)	5810.5(18)	3027.0(12)	28.7(8)
C57	7566(7)	7437.9(17)	672.8(12)	26.5(8)
C29	5037(7)	11444.3(18)	3239.0(13)	31.7(9)
C59	8769(7)	7103.7(18)	2061.5(12)	30.1(9)
C15	5398(6)	7938.9(18)	2870.3(12)	27.2(8)
C61	7178(7)	3579.4(16)	980.4(12)	26.0(8)
C31	8781(7)	3777.9(18)	2103.1(12)	29.7(8)
C63	9290(7)	10258.5(18)	1707.8(13)	31.3(9)
C2	6867(8)	11302.5(18)	3513.1(12)	32.0(9)
C65	3814(7)	6071.5(17)	4298.6(12)	27.7(8)
C33	9148(7)	10435.2(18)	2112.7(12)	30.4(9)
C67	5532(7)	10930.0(19)	1957.2(12)	31.4(9)
C17	8913(8)	10822.8(19)	2972.2(13)	33.7(9)
C69	6941(8)	12018.8(18)	411.6(13)	32.6(9)
C35	5165(7)	11271.3(18)	2830.8(12)	29.4(8)
C71	1667(7)	5448.4(17)	1467.8(12)	29.5(8)
C9	7524(7)	7940.0(18)	3515.8(12)	29.1(8)
C73	3925(7)	12608.9(18)	2055.2(13)	31.7(9)
C37	3690(7)	5928(2)	2017.5(13)	34.7(10)
C75	8943(7)	10627.2(16)	689.3(12)	26.9(8)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U_{eq}
C19	2273(7)	12125.1(18)	1470.3(12)	29.9(8)
C77	3951(7)	9639.7(18)	2941.2(13)	31.8(9)
C39	335(7)	9124.4(19)	3031.6(12)	31.9(9)
C79	2405(7)	8793.1(18)	1496.8(12)	29.9(9)
C5	6039(8)	8280(2)	371.3(13)	34.3(9)
C81	6159(8)	5381.7(19)	387.6(13)	35.6(10)
C41	2612(8)	11363.9(19)	4588.0(13)	33.8(9)
C83	336(8)	11960(2)	1709.1(13)	35.1(9)
C21	5100(7)	7610.4(18)	1992.4(13)	31.0(9)
C85	4067(8)	12448.2(19)	1649.6(14)	34.9(9)
C43	3057(7)	9320.1(19)	4341.0(12)	31.9(9)
C87	19(7)	5462.7(19)	2147.4(12)	33.7(9)
C11	6883(8)	4624.8(18)	3524.9(12)	32.0(9)
C89	8792(8)	10992(2)	3376.5(13)	36.9(10)
C45	5059(8)	4616(2)	2855.2(13)	36.6(10)
C91	-235(8)	9988.7(18)	4197.8(12)	30.2(9)
C23	8316(7)	4009.1(17)	690.4(12)	30.5(9)
C93	2429(7)	12613.2(19)	4313.8(13)	32.4(9)
C47	193(7)	12123.3(19)	2117.6(12)	30.7(9)
C95	1510(8)	8486(2)	4659.8(14)	39.2(11)
C3	8733(8)	4306(2)	3374.3(14)	40.0(11)
C97	5038(8)	4778(2)	3268.2(14)	40.3(11)
C49	8749(8)	4138(2)	2966.8(13)	37.8(10)
C99	7635(8)	4855.0(18)	353.2(12)	32.0(9)
C25	663(8)	11788(2)	4614.5(14)	38.6(10)
C101	3581(8)	5766(2)	1612.9(13)	38.2(10)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+...]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F001	53.2(16)	30.6(15)	52.2(15)	14.2(12)	0.7(12)	3.3(12)
F002	46.9(15)	30.3(14)	53.9(16)	11.4(12)	15.8(12)	-0.4(11)
F003	77(2)	31.4(15)	35.5(13)	-6.4(11)	6.9(13)	9.1(13)
F004	68.5(18)	26.4(14)	50.6(16)	15.7(12)	13.4(13)	1.3(13)
F005	56.2(16)	33.8(15)	49.6(15)	18.3(12)	-5.9(12)	-4.0(12)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
F006	31.9(13)	44.0(17)	85(2)	14.2(15)	12.5(13)	-4.7(12)
F007	64.4(17)	29.7(15)	49.7(15)	17.1(12)	22.7(13)	6.0(13)
F008	82(2)	32.8(15)	43.4(15)	-10.8(12)	-9.3(14)	0.6(14)
F009	65.1(18)	30.4(15)	47.4(15)	16.1(12)	-5.6(13)	-0.9(12)
O00A	32.3(14)	23.8(15)	31.8(14)	6.5(11)	-2.0(11)	-8.6(11)
O00B	32.8(14)	19.6(14)	33.3(14)	5.1(11)	12.4(11)	5.0(11)
F00C	27.0(13)	36.3(16)	106(3)	10.9(15)	26.1(14)	3.0(11)
F00D	35.7(14)	38.5(16)	77(2)	7.5(14)	-0.5(12)	7.7(12)
F00E	92(2)	30.7(15)	36.2(14)	-6.3(12)	-3.0(14)	-9.2(15)
F00F	95(2)	32.6(16)	41.1(15)	-9.2(12)	11.6(15)	-7.2(15)
F00G	105(3)	32.8(16)	38.9(15)	-9.0(12)	14.9(15)	8.0(16)
O00H	29.8(14)	26.8(15)	41.4(16)	11.9(12)	12.6(11)	4.8(12)
O00I	41.1(16)	25.4(15)	33.7(15)	7.5(12)	14.3(12)	8.7(12)
F00J	88(2)	39.5(17)	41.7(15)	-12.4(13)	7.4(14)	0.0(15)
F00K	28.6(13)	42.7(16)	81(2)	11.1(15)	-5.5(12)	-1.7(11)
F00L	34.4(15)	48.3(18)	102(3)	19.3(17)	6.2(14)	9.5(13)
O00M	40.3(16)	34.1(17)	40.2(16)	14.4(13)	-3.3(13)	-4.1(13)
F00N	24.4(13)	39.1(17)	112(3)	6.1(17)	-0.1(14)	-1.1(11)
O00O	35.4(15)	40.3(18)	37.5(16)	13.6(14)	0.1(12)	-1.5(13)
N00P	38(2)	38(2)	36.6(19)	-1.9(16)	8.2(15)	-1.5(16)
N00Q	35.1(19)	32(2)	30.4(17)	-3.1(15)	3.3(14)	1.7(15)
N00R	27.6(17)	36(2)	35.8(18)	-3.0(15)	6.3(13)	1.0(15)
N00S	34.5(19)	46(2)	31.7(18)	-1.7(17)	6.5(14)	7.2(17)
N00T	36(2)	43(2)	30.4(18)	-3.0(16)	6.3(14)	-1.3(16)
C1	22.0(17)	12.1(17)	30.3(18)	4.5(14)	3.0(13)	-3.6(13)
C4	16.9(16)	15.6(18)	29.2(18)	5.9(14)	4.4(13)	1.8(13)
C6	19.5(16)	12.8(17)	29.9(18)	0.4(14)	6.8(13)	-0.7(13)
N00X	37(2)	35(2)	35.5(19)	-2.1(16)	0.9(15)	4.5(16)
C8	25.2(17)	11.6(17)	27.2(18)	4.8(14)	5.0(14)	3.7(13)
C10	26.3(18)	11.1(17)	29.4(19)	-0.3(14)	6.3(14)	0.2(14)
C12	22.5(17)	14.3(18)	30.1(19)	2.6(15)	4.7(14)	-2.8(13)
C14	21.4(17)	12.2(17)	30.4(19)	3.6(14)	5.8(14)	-2.7(13)
C16	21.0(17)	14.1(18)	31.5(19)	4.9(15)	9.4(14)	-1.7(13)
C18	23.1(17)	15.7(18)	28.1(18)	6.4(14)	5.8(13)	3.3(14)
C20	27.5(19)	22(2)	34(2)	3.3(16)	8.5(15)	0.4(15)
C22	26.2(18)	15.4(19)	30.0(19)	4.7(15)	3.9(14)	-5.6(14)
C24	16.0(15)	17.2(18)	28.5(18)	4.3(14)	6.9(13)	2.5(13)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C26	32(2)	28(2)	31(2)	1.0(17)	4.1(15)	4.9(16)
C28	21.2(17)	16.2(18)	28.4(18)	2.8(15)	8.4(13)	0.1(14)
C30	21.8(17)	15.1(18)	29.5(19)	4.3(14)	5.8(13)	-2.1(13)
C32	22.7(17)	11.6(17)	29.6(19)	4.6(14)	4.6(14)	1.1(13)
C34	25.1(18)	16.6(18)	29.4(18)	2.6(15)	3.2(14)	-0.1(14)
C36	21.8(17)	15.5(18)	30.0(19)	4.4(15)	6.5(14)	4.6(13)
C38	26.0(19)	31(2)	34(2)	-1.4(17)	6.1(15)	8.5(16)
C40	29.5(18)	15.0(18)	26.2(18)	-0.2(14)	6.2(14)	-1.5(14)
C42	27.4(18)	18.6(19)	30.9(19)	0.5(15)	7.1(14)	4.4(15)
C44	39(2)	21(2)	24.6(18)	-0.2(15)	5.3(16)	6.8(16)
C46	35(2)	18.0(19)	27.5(19)	-0.3(15)	5.4(15)	3.9(16)
C48	37(2)	28(2)	32(2)	1.7(17)	4.6(16)	-2.0(17)
C50	29.7(19)	23(2)	31(2)	-0.3(16)	0.2(15)	-1.2(15)
C52	23.8(17)	18.2(19)	30.9(19)	2.8(15)	3.1(14)	4.0(14)
C54	32(2)	18.7(19)	26.4(18)	-2.1(15)	7.0(15)	3.8(15)
C56	25.3(18)	16.5(19)	32(2)	-1.0(15)	4.8(14)	3.4(14)
C58	26.6(19)	27(2)	33(2)	4.0(17)	6.9(15)	-3.8(16)
C60	29(2)	26(2)	35(2)	-1.5(17)	3.1(16)	-2.5(16)
C62	25.4(19)	28(2)	35(2)	-3.4(17)	7.6(15)	-7.0(16)
C64	28.7(19)	30(2)	32(2)	-1.8(17)	-2.3(15)	5.8(16)
C66	38(2)	28(2)	23.6(18)	4.2(16)	1.5(15)	-4.5(17)
C68	25.9(18)	26(2)	32(2)	-0.9(16)	4.4(15)	1.3(15)
C70	27.5(19)	28(2)	35(2)	4.7(17)	1.5(15)	0.2(16)
C72	27.3(19)	25(2)	33(2)	1.1(16)	2.7(15)	3.0(16)
C74	22.0(18)	34(2)	36(2)	-1.1(18)	11.8(15)	-6.8(16)
C76	29.2(19)	19(2)	31.2(19)	-1.6(15)	5.7(15)	-3.4(15)
C78	19.3(17)	33(2)	33(2)	-3.2(17)	7.4(14)	-7.6(16)
C80	27.9(19)	28(2)	32(2)	1.3(17)	9.9(15)	-8.6(16)
C82	24.1(18)	25(2)	32(2)	2.8(16)	5.8(14)	0.8(15)
C84	39(2)	24(2)	30(2)	5.4(16)	2.0(16)	-1.8(17)
C86	24.6(18)	30(2)	32(2)	-4.3(17)	1.9(15)	8.3(16)
C88	33(2)	24(2)	24.4(18)	0.5(15)	1.5(15)	-4.4(16)
C90	27.6(19)	33(2)	34(2)	-3.1(18)	9.1(15)	5.5(17)
C92	28(2)	33(2)	33(2)	7.6(17)	12.1(15)	4.5(17)
C94	27.8(19)	30(2)	32(2)	1.1(17)	6.8(15)	-9.0(16)
C96	34(2)	21(2)	24.7(18)	-1.8(15)	4.8(15)	-4.7(16)
C98	35(2)	40(3)	36(2)	-0.3(19)	4.0(17)	-14.4(19)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*^2U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C100	23.0(18)	33(2)	36(2)	-4.0(17)	0.1(15)	10.8(16)
C102	25.6(18)	33(2)	30(2)	-3.9(17)	-0.6(15)	9.1(17)
C51	24.7(18)	26(2)	36(2)	0.1(17)	3.5(15)	-9.1(16)
C13	28.4(19)	31(2)	36(2)	-0.6(18)	5.1(16)	-9.3(17)
C53	35(2)	38(3)	32(2)	-1.5(18)	9.8(16)	-7.6(18)
C27	36(2)	24(2)	26.5(19)	3.4(16)	11.0(15)	0.8(16)
C55	23.9(18)	26(2)	34(2)	0.2(16)	7.3(15)	-11.1(15)
C7	19.1(17)	33(2)	34(2)	-1.1(17)	10.3(14)	-11.6(16)
C57	25.9(18)	23(2)	30.8(19)	0.9(15)	8.7(14)	0.5(15)
C29	33(2)	31(2)	31(2)	-1.6(17)	9.0(16)	3.4(17)
C59	25.4(18)	33(2)	32(2)	-0.1(17)	3.7(15)	10.7(16)
C15	19.4(17)	29(2)	34(2)	0.1(17)	5.0(14)	3.9(15)
C61	28.8(19)	20(2)	30(2)	-0.4(15)	6.4(15)	2.2(15)
C31	28.1(19)	30(2)	30(2)	-0.6(17)	1.5(15)	6.6(16)
C63	29(2)	28(2)	37(2)	-0.9(17)	2.8(16)	11.5(17)
C2	42(2)	28(2)	25.9(19)	2.1(17)	6.6(16)	-9.6(18)
C65	28.7(19)	22(2)	33(2)	2.4(16)	0.3(15)	-8.6(15)
C33	29.4(19)	30(2)	32(2)	0.5(17)	-2.2(15)	7.0(17)
C67	25.9(19)	37(2)	32(2)	-3.8(18)	-0.5(15)	11.0(17)
C17	33(2)	36(2)	32(2)	1.2(18)	-0.8(16)	3.1(18)
C69	41(2)	26(2)	31(2)	5.7(17)	5.4(16)	0.5(18)
C35	28.6(19)	29(2)	31(2)	0.8(17)	2.5(15)	2.1(16)
C71	39(2)	25(2)	24.6(19)	-1.2(16)	3.6(15)	0.8(17)
C9	34(2)	27(2)	26.4(19)	-0.2(16)	4.2(15)	-0.6(17)
C73	30(2)	33(2)	32(2)	-0.2(18)	8.2(16)	-9.7(17)
C37	29(2)	41(3)	35(2)	-1.9(19)	11.3(16)	-11.0(18)
C75	29.2(19)	22(2)	29.4(19)	0.0(16)	8.6(15)	4.6(15)
C19	36(2)	27(2)	26.8(19)	0.4(16)	7.1(15)	3.0(17)
C77	26.1(19)	34(2)	36(2)	0.4(18)	8.5(15)	-7.3(17)
C39	28.4(19)	37(2)	30(2)	-4.1(18)	7.1(15)	-10.1(17)
C79	34(2)	28(2)	27.1(19)	-0.7(16)	6.2(15)	7.2(17)
C5	34(2)	34(2)	35(2)	12.5(18)	-1.4(17)	-4.0(18)
C81	50(3)	26(2)	30(2)	4.7(17)	12.9(18)	2.9(19)
C41	36(2)	35(2)	30(2)	3.3(18)	-1.4(16)	-3.9(18)
C83	38(2)	37(3)	31(2)	-3.6(18)	3.9(16)	-8.4(18)
C21	29(2)	33(2)	32(2)	-3.1(17)	2.8(15)	9.6(17)
C85	39(2)	31(2)	34(2)	3.2(18)	11.2(17)	-4.0(18)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C43	27.8(19)	36(2)	31(2)	0.6(17)	-1.1(15)	0.5(17)
C87	34(2)	37(2)	31(2)	-0.3(18)	9.4(16)	-8.6(18)
C11	42(2)	29(2)	25.6(19)	-0.6(17)	4.8(16)	-2.2(18)
C89	40(2)	39(3)	32(2)	4.6(19)	-0.6(17)	0.4(19)
C45	35(2)	43(3)	32(2)	-1.8(19)	-1.3(17)	12.1(19)
C91	37(2)	28(2)	25.4(19)	-1.3(16)	1.8(16)	2.7(17)
C23	35(2)	25(2)	31(2)	2.5(16)	10.4(16)	3.7(16)
C93	29(2)	34(2)	34(2)	4.4(18)	-1.8(16)	-0.9(17)
C47	25.9(19)	34(2)	32(2)	-0.8(18)	8.7(15)	-8.5(17)
C95	34(2)	51(3)	33(2)	15(2)	9.2(17)	10(2)
C3	37(2)	49(3)	35(2)	-2(2)	-5.8(17)	12(2)
C97	44(2)	46(3)	31(2)	-6(2)	7.7(18)	15(2)
C49	35(2)	44(3)	34(2)	-7(2)	-3.1(17)	13(2)
C99	39(2)	30(2)	28(2)	4.4(17)	10.3(16)	3.2(17)
C25	33(2)	43(3)	40(2)	14(2)	11.8(17)	4.0(19)
C101	38(2)	46(3)	31(2)	-0.3(19)	15.7(17)	-8(2)

Table 4 Bond Lengths for ZGY.

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA
F001	C48	1.333(5)	C28	C74	1.390(5)
F002	C20	1.341(5)	C28	C76	1.514(5)
F003	C69	1.331(5)	C28	C55	1.394(5)
F004	C69	1.346(5)	C30	C86	1.403(5)
F005	C41	1.342(5)	C30	C31	1.396(5)
F006	C84	1.321(5)	C32	C73	1.398(5)
F007	C81	1.340(5)	C32	C47	1.399(5)
F008	C20	1.322(5)	C34	C50	1.520(5)
F009	C84	1.340(5)	C34	C62	1.396(5)
O00A	C66	1.405(5)	C34	C51	1.390(5)
O00A	C65	1.421(4)	C36	C37	1.395(5)
O00B	C27	1.407(5)	C36	C87	1.385(6)
O00B	C75	1.418(5)	C38	C59	1.386(6)
F00C	C20	1.327(5)	C40	C64	1.383(5)
F00D	C69	1.326(5)	C40	C61	1.523(5)
F00E	C84	1.334(5)	C42	C54	1.477(5)
F00F	C48	1.330(5)	C42	C57	1.527(5)
F00G	C81	1.334(5)	C44	C61	1.478(6)

Table 4 Bond Lengths for ZGY.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O00H	C57	1.426(5)	C46	C56	1.477(5)
O00H	C5	1.400(5)	C48	C95	1.480(6)
O00I	C23	1.415(5)	C50	C88	1.474(6)
O00I	C99	1.421(5)	C50	C93	1.531(6)
F00J	C41	1.339(5)	C52	C68	1.528(5)
F00K	C41	1.334(5)	C52	C13	1.393(6)
F00L	C81	1.307(6)	C52	C53	1.377(6)
O00M	C93	1.430(5)	C56	C75	1.523(5)
O00M	C25	1.408(5)	C58	C92	1.380(6)
F00N	C48	1.336(5)	C60	C82	1.386(6)
O00O	C43	1.422(5)	C60	C79	1.396(6)
O00O	C95	1.414(5)	C62	C78	1.383(6)
N00P	C96	1.139(5)	C64	C86	1.386(6)
N00Q	C46	1.146(5)	C66	C84	1.495(6)
N00R	C54	1.147(5)	C68	C43	1.532(6)
N00S	C91	1.140(5)	C68	C91	1.475(6)
N00T	C88	1.153(6)	C70	C72	1.381(6)
C1	C22	1.489(5)	C70	C9	1.383(6)
C1	C33	1.398(5)	C74	C7	1.372(6)
C1	C67	1.397(5)	C76	C96	1.485(5)
C4	C32	1.486(5)	C76	C65	1.529(5)
C4	C78	1.399(5)	C80	C55	1.384(6)
C4	C94	1.402(5)	C90	C15	1.379(6)
C6	C38	1.386(5)	C90	C9	1.387(6)
C6	C42	1.514(5)	C92	C79	1.375(6)
C6	C100	1.395(5)	C94	C51	1.376(6)
N00X	C44	1.143(5)	C98	C71	1.377(6)
C8	C18	1.490(5)	C98	C87	1.388(6)
C8	C58	1.413(5)	C100	C21	1.378(6)
C8	C82	1.398(5)	C102	C67	1.380(6)
C10	C56	1.530(5)	C13	C77	1.379(6)
C10	C102	1.383(5)	C53	C39	1.383(6)
C10	C63	1.382(5)	C27	C69	1.496(6)
C12	C30	1.487(5)	C29	C2	1.388(6)
C12	C45	1.383(6)	C29	C35	1.393(6)
C12	C49	1.394(5)	C61	C23	1.532(6)
C14	C16	1.488(5)	C63	C33	1.386(6)
C14	C59	1.399(5)	C2	C89	1.375(7)

Table 4 Bond Lengths for ZGY.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C14	C21	1.397(5)	C17	C89	1.378(6)
C16	C72	1.398(5)	C71	C101	1.384(6)
C16	C15	1.399(5)	C73	C85	1.377(6)
C18	C77	1.393(5)	C37	C101	1.373(6)
C18	C39	1.402(5)	C19	C83	1.387(6)
C20	C5	1.501(6)	C19	C85	1.384(6)
C22	C17	1.396(5)	C81	C99	1.503(6)
C22	C35	1.398(6)	C41	C25	1.483(6)
C24	C36	1.485(5)	C83	C47	1.388(6)
C24	C80	1.394(5)	C11	C3	1.370(6)
C24	C7	1.409(5)	C11	C97	1.366(6)
C26	C40	1.380(5)	C45	C97	1.398(6)
C26	C31	1.381(6)	C3	C49	1.385(6)

Table 5 Bond Angles for ZGY.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C66	O00A	C65	111.0(3)	C91	C68	C43	110.1(3)
C27	O00B	C75	110.9(3)	C72	C70	C9	120.9(4)
C5	O00H	C57	115.3(3)	C70	C72	C16	121.5(4)
C23	O00I	C99	110.1(3)	C7	C74	C28	121.2(4)
C25	O00M	C93	116.0(3)	C28	C76	C65	114.7(3)
C95	O00O	C43	115.7(3)	C96	C76	C28	111.7(3)
C33	C1	C22	121.4(3)	C96	C76	C65	109.5(3)
C67	C1	C22	122.0(3)	C62	C78	C4	121.8(3)
C67	C1	C33	116.5(3)	C55	C80	C24	121.9(4)
C78	C4	C32	121.8(3)	C60	C82	C8	121.7(4)
C78	C4	C94	116.3(3)	F006	C84	F009	106.8(3)
C94	C4	C32	121.9(3)	F006	C84	F00E	106.8(4)
C38	C6	C42	119.9(3)	F006	C84	C66	113.2(4)
C38	C6	C100	117.8(3)	F009	C84	C66	111.0(3)
C100	C6	C42	122.3(3)	F00E	C84	F009	106.9(4)
C58	C8	C18	121.0(3)	F00E	C84	C66	111.8(3)
C82	C8	C18	122.1(3)	C64	C86	C30	121.3(4)
C82	C8	C58	116.9(4)	N00T	C88	C50	178.4(4)
C102	C10	C56	123.3(3)	C15	C90	C9	120.5(4)
C63	C10	C56	118.4(3)	C79	C92	C58	121.2(4)
C63	C10	C102	118.4(3)	C51	C94	C4	122.1(4)

Table 5 Bond Angles for ZGY.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C45	C12	C30	122.1(3)	N00P	C96	C76	179.1(5)
C45	C12	C49	117.0(4)	C71	C98	C87	120.3(4)
C49	C12	C30	120.9(3)	C21	C100	C6	120.8(3)
C59	C14	C16	121.9(3)	C67	C102	C10	121.1(3)
C21	C14	C16	121.8(3)	C94	C51	C34	121.0(3)
C21	C14	C59	116.3(4)	C77	C13	C52	120.0(4)
C72	C16	C14	121.4(3)	C52	C53	C39	121.1(4)
C72	C16	C15	116.6(3)	O00B	C27	C69	106.6(3)
C15	C16	C14	122.0(3)	C80	C55	C28	121.0(3)
C77	C18	C8	122.3(3)	C74	C7	C24	122.0(3)
C77	C18	C39	116.1(4)	O00H	C57	C42	108.0(3)
C39	C18	C8	121.7(3)	C2	C29	C35	119.9(4)
F002	C20	C5	111.1(3)	C38	C59	C14	121.8(3)
F008	C20	F002	107.7(3)	C90	C15	C16	121.9(3)
F008	C20	F00C	107.0(3)	C40	C61	C23	114.1(3)
F008	C20	C5	111.8(3)	C44	C61	C40	111.7(3)
F00C	C20	F002	106.2(3)	C44	C61	C23	110.0(3)
F00C	C20	C5	112.7(4)	C26	C31	C30	122.4(4)
C17	C22	C1	121.6(4)	C10	C63	C33	120.6(4)
C17	C22	C35	116.8(4)	C89	C2	C29	119.3(4)
C35	C22	C1	121.6(3)	O00A	C65	C76	109.2(3)
C80	C24	C36	121.8(3)	C63	C33	C1	121.8(3)
C80	C24	C7	116.2(3)	C102	C67	C1	121.6(4)
C7	C24	C36	122.0(3)	C89	C17	C22	121.9(4)
C40	C26	C31	120.5(4)	F003	C69	F004	107.0(4)
C74	C28	C76	123.4(3)	F003	C69	C27	111.7(3)
C74	C28	C55	117.7(3)	F004	C69	C27	110.6(3)
C55	C28	C76	118.8(3)	F00D	C69	F003	107.2(4)
C86	C30	C12	122.1(3)	F00D	C69	F004	107.2(3)
C31	C30	C12	121.7(3)	F00D	C69	C27	112.9(4)
C31	C30	C86	116.2(3)	C29	C35	C22	121.5(4)
C73	C32	C4	121.7(3)	C98	C71	C101	118.5(4)
C73	C32	C47	116.7(4)	C70	C9	C90	118.6(4)
C47	C32	C4	121.6(3)	C85	C73	C32	121.8(4)
C62	C34	C50	122.1(3)	C101	C37	C36	122.3(4)
C51	C34	C50	120.1(3)	O00B	C75	C56	109.3(3)
C51	C34	C62	117.8(4)	C85	C19	C83	118.6(4)
C37	C36	C24	121.0(3)	C13	C77	C18	122.7(4)

Table 5 Bond Angles for ZGY.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C87	C36	C24	122.8(3)	C53	C39	C18	121.6(4)
C87	C36	C37	116.1(4)	C92	C79	C60	119.1(4)
C59	C38	C6	121.1(3)	O00H	C5	C20	112.4(3)
C26	C40	C64	118.4(4)	F007	C81	C99	110.2(3)
C26	C40	C61	119.0(3)	F00G	C81	F007	106.4(4)
C64	C40	C61	122.6(3)	F00G	C81	C99	110.6(4)
C6	C42	C57	113.5(3)	F00L	C81	F007	107.5(4)
C54	C42	C6	112.1(3)	F00L	C81	F00G	108.5(4)
C54	C42	C57	109.1(3)	F00L	C81	C99	113.3(4)
N00X	C44	C61	178.6(5)	F005	C41	C25	110.7(4)
N00Q	C46	C56	178.3(4)	F00J	C41	F005	107.0(4)
F001	C48	F00N	107.2(3)	F00J	C41	C25	112.1(4)
F001	C48	C95	111.2(3)	F00K	C41	F005	107.4(3)
F00F	C48	F001	107.1(4)	F00K	C41	F00J	106.1(4)
F00F	C48	F00N	106.6(4)	F00K	C41	C25	113.1(4)
F00F	C48	C95	111.7(4)	C19	C83	C47	120.4(4)
F00N	C48	C95	112.6(4)	C100	C21	C14	122.2(4)
C34	C50	C93	113.5(3)	C73	C85	C19	120.8(4)
C88	C50	C34	111.6(3)	O00O	C43	C68	107.8(3)
C88	C50	C93	108.9(3)	C36	C87	C98	122.2(4)
C13	C52	C68	119.1(3)	C97	C11	C3	119.3(4)
C53	C52	C68	122.4(3)	C2	C89	C17	120.6(4)
C53	C52	C13	118.5(4)	C12	C45	C97	121.6(4)
N00R	C54	C42	178.9(4)	N00S	C91	C68	179.7(5)
C46	C56	C10	110.8(3)	O00I	C23	C61	108.9(3)
C46	C56	C75	110.5(3)	O00M	C93	C50	108.2(3)
C75	C56	C10	114.4(3)	C83	C47	C32	121.6(4)
C92	C58	C8	121.0(4)	O00O	C95	C48	112.7(4)
C82	C60	C79	120.0(4)	C11	C3	C49	120.9(4)
C78	C62	C34	121.0(4)	C11	C97	C45	120.2(4)
C40	C64	C86	121.2(3)	C3	C49	C12	121.1(4)
O00A	C66	C84	107.6(3)	O00I	C99	C81	106.7(3)
C52	C68	C43	113.6(3)	O00M	C25	C41	112.3(4)
C91	C68	C52	111.7(3)	C37	C101	C71	120.6(4)

Table 6 Torsion Angles for ZGY.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
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Table 6 Torsion Angles for ZGY.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
F001	C48	C95	O00O	-168.6(4)	C78	C4	C32	C73	-178.7(4)
F002	C20	C5	O00H	-167.5(3)	C78	C4	C32	C47	1.0(5)
F005	C41	C25	O00M	-168.8(4)	C78	C4	C94	C51	1.0(6)
F007	C81	C99	O00I	178.7(4)	C80	C24	C36	C37	0.9(5)
F008	C20	C5	O00H	-47.1(5)	C80	C24	C36	C87	-178.9(4)
O00A	C66	C84	F006	-60.5(4)	C80	C24	C7	C74	0.4(6)
O00A	C66	C84	F009	179.4(3)	C82	C8	C18	C77	-176.2(4)
O00A	C66	C84	F00E	60.2(5)	C82	C8	C18	C39	3.6(5)
O00B	C27	C69	F003	59.0(4)	C82	C8	C58	C92	0.7(6)
O00B	C27	C69	F004	178.0(3)	C82	C60	C79	C92	-0.4(6)
O00B	C27	C69	F00D	-61.9(4)	C86	C30	C31	C26	-0.2(6)
F00C	C20	C5	O00H	73.4(5)	C88	C50	C93	O00M	59.2(4)
F00F	C48	C95	O00O	-49.0(5)	C94	C4	C32	C73	1.1(5)
F00G	C81	C99	O00I	61.3(5)	C94	C4	C32	C47	-179.2(4)
F00J	C41	C25	O00M	-49.3(5)	C94	C4	C78	C62	-0.8(6)
F00K	C41	C25	O00M	70.6(5)	C96	C76	C65	O00A	61.1(4)
F00L	C81	C99	O00I	-60.8(5)	C98	C71	C101	C37	-0.4(7)
F00N	C48	C95	O00O	71.0(5)	C100	C6	C38	C59	-1.4(6)
C1	C22	C17	C89	-179.7(4)	C100	C6	C42	C54	-44.2(5)
C1	C22	C35	C29	179.8(4)	C100	C6	C42	C57	80.0(4)
C4	C32	C73	C85	179.9(4)	C102	C10	C56	C46	-43.4(5)
C4	C32	C47	C83	-179.7(4)	C102	C10	C56	C75	82.4(5)
C4	C94	C51	C34	-0.3(6)	C102	C10	C63	C33	0.3(6)
C6	C38	C59	C14	0.6(6)	C51	C34	C50	C88	136.6(4)
C6	C42	C57	O00H	-66.6(4)	C51	C34	C50	C93	-99.9(4)
C6	C100	C21	C14	-1.1(7)	C51	C34	C62	C78	0.7(6)
C8	C18	C77	C13	-179.4(4)	C13	C52	C68	C43	-100.3(4)
C8	C18	C39	C53	179.6(4)	C13	C52	C68	C91	134.5(4)
C8	C58	C92	C79	-0.4(6)	C13	C52	C53	C39	0.2(6)
C10	C56	C75	O00B	-64.3(4)	C53	C52	C68	C43	77.3(5)
C10	C102	C67	C1	-0.3(7)	C53	C52	C68	C91	-47.8(5)
C10	C63	C33	C1	0.7(6)	C53	C52	C13	C77	0.0(6)
C12	C30	C86	C64	179.7(4)	C27	O00B	C75	C56	-177.1(3)
C12	C30	C31	C26	-179.9(4)	C55	C28	C74	C7	-0.1(6)
C12	C45	C97	C11	1.4(8)	C55	C28	C76	C96	138.0(4)
C14	C16	C72	C70	-180.0(4)	C55	C28	C76	C65	-96.7(4)
C14	C16	C15	C90	179.6(4)	C7	C24	C36	C37	-178.8(4)
C16	C14	C59	C38	-179.2(4)	C7	C24	C36	C87	1.4(6)

Table 6 Torsion Angles for ZGY.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C16	C14	C21	C100	179.4(4)	C7	C24	C80	C55	-0.6(6)
C18	C8	C58	C92	-179.9(4)	C57	O00H	C5	C20	-78.3(5)
C18	C8	C82	C60	179.7(4)	C29	C2	C89	C17	0.1(7)
C22	C1	C33	C63	179.9(4)	C59	C14	C16	C72	2.0(5)
C22	C1	C67	C102	179.9(4)	C59	C14	C16	C15	-178.5(4)
C22	C17	C89	C2	0.1(7)	C59	C14	C21	C100	0.3(6)
C24	C36	C37	C101	180.0(4)	C15	C16	C72	C70	0.5(6)
C24	C36	C87	C98	-180.0(4)	C15	C90	C9	C70	-0.2(6)
C24	C80	C55	C28	0.5(6)	C61	C40	C64	C86	180.0(4)
C26	C40	C64	C86	0.2(6)	C31	C26	C40	C64	-0.4(6)
C26	C40	C61	C44	138.4(4)	C31	C26	C40	C61	179.9(4)
C26	C40	C61	C23	-96.1(4)	C31	C30	C86	C64	0.0(6)
C28	C74	C7	C24	0.0(7)	C63	C10	C56	C46	136.7(4)
C28	C76	C65	O00A	-65.3(4)	C63	C10	C56	C75	-97.6(4)
C30	C12	C45	C97	179.6(4)	C63	C10	C102	C67	-0.5(6)
C30	C12	C49	C3	179.5(4)	C2	C29	C35	C22	-0.4(6)
C32	C4	C78	C62	179.0(4)	C65	O00A	C66	C84	-170.8(3)
C32	C4	C94	C51	-178.8(4)	C33	C1	C22	C17	2.3(6)
C32	C73	C85	C19	0.3(7)	C33	C1	C22	C35	-176.9(4)
C34	C50	C93	O00M	-65.8(4)	C33	C1	C67	C102	1.2(6)
C34	C62	C78	C4	0.0(7)	C67	C1	C22	C17	-176.3(4)
C36	C24	C80	C55	179.6(4)	C67	C1	C22	C35	4.4(6)
C36	C24	C7	C74	-179.9(4)	C67	C1	C33	C63	-1.4(6)
C36	C37	C101	C71	0.3(7)	C17	C22	C35	C29	0.5(6)
C38	C6	C42	C54	137.3(4)	C35	C22	C17	C89	-0.4(6)
C38	C6	C42	C57	-98.6(4)	C35	C29	C2	C89	0.1(6)
C38	C6	C100	C21	1.6(6)	C71	C98	C87	C36	-0.3(7)
C40	C26	C31	C30	0.4(6)	C9	C70	C72	C16	0.0(6)
C40	C64	C86	C30	-0.1(6)	C9	C90	C15	C16	0.7(6)
C40	C61	C23	O00I	-67.5(4)	C73	C32	C47	C83	0.0(6)
C42	C6	C38	C59	177.2(4)	C37	C36	C87	C98	0.2(6)
C42	C6	C100	C21	-177.0(4)	C75	O00B	C27	C69	-169.3(3)
C44	C61	C23	O00I	58.9(4)	C19	C83	C47	C32	-0.6(7)
C46	C56	C75	O00B	61.6(4)	C77	C18	C39	C53	-0.6(6)
C50	C34	C62	C78	-176.8(4)	C39	C18	C77	C13	0.8(6)
C50	C34	C51	C94	177.0(4)	C79	C60	C82	C8	0.7(6)
C52	C68	C43	O00O	-67.5(4)	C5	O00H	C57	C42	-161.7(3)
C52	C13	C77	C18	-0.6(7)	C83	C19	C85	C73	-0.8(7)

Table 6 Torsion Angles for ZGY.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C52	C53	C39	C18	0.1(7)	C21	C14	C16	C72	-177.1(4)
C54	C42	C57	O00H	59.1(4)	C21	C14	C16	C15	2.4(5)
C56	C10	C102	C67	179.6(4)	C21	C14	C59	C38	-0.1(6)
C56	C10	C63	C33	-179.8(4)	C85	C19	C83	C47	1.0(7)
C58	C8	C18	C77	4.4(5)	C43	O00O	C95	C48	-80.9(5)
C58	C8	C18	C39	-175.9(4)	C87	C36	C37	C101	-0.2(6)
C58	C8	C82	C60	-0.8(6)	C87	C98	C71	C101	0.4(7)
C58	C92	C79	C60	0.2(6)	C11	C3	C49	C12	0.4(8)
C62	C34	C50	C88	-46.0(5)	C45	C12	C30	C86	0.9(6)
C62	C34	C50	C93	77.5(5)	C45	C12	C30	C31	-179.4(4)
C62	C34	C51	C94	-0.5(6)	C45	C12	C49	C3	0.2(7)
C64	C40	C61	C44	-41.4(5)	C91	C68	C43	O00O	58.5(4)
C64	C40	C61	C23	84.2(5)	C23	O00I	C99	C81	-170.4(3)
C66	O00A	C65	C76	-174.8(3)	C93	O00M	C25	C41	-79.9(5)
C68	C52	C13	C77	177.7(4)	C47	C32	C73	C85	0.1(6)
C68	C52	C53	C39	-177.4(4)	C95	O00O	C43	C68	-163.3(4)
C72	C16	C15	C90	-0.9(6)	C3	C11	C97	C45	-0.8(7)
C72	C70	C9	C90	-0.2(6)	C97	C11	C3	C49	-0.1(7)
C74	C28	C76	C96	-42.6(5)	C49	C12	C30	C86	-178.4(4)
C74	C28	C76	C65	82.6(5)	C49	C12	C30	C31	1.3(6)
C74	C28	C55	C80	-0.2(6)	C49	C12	C45	C97	-1.1(7)
C76	C28	C74	C7	-179.4(4)	C99	O00I	C23	C61	-173.1(3)
C76	C28	C55	C80	179.2(4)	C25	O00M	C93	C50	-158.2(4)

Table 7 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for ZGY.

Atom	x	y	z	U(eq)
H26	10127.97	3380.3	1603.8	36
H38	9837.26	6716.33	1538.26	36
H42	7758.12	6641.97	917.31	31
H50	2738.59	13412.91	4074.63	34
H56	8871.44	9870.86	989.92	30
H58	5497.51	9477.75	2185.22	34
H60	-838.23	8428.94	1626.8	36
H62	-1519.72	12494.33	3560.69	35
H64	3939.63	4216.9	1389.01	36
H66A	3042.51	5376.89	4904.86	36

Table 7 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for ZGY.

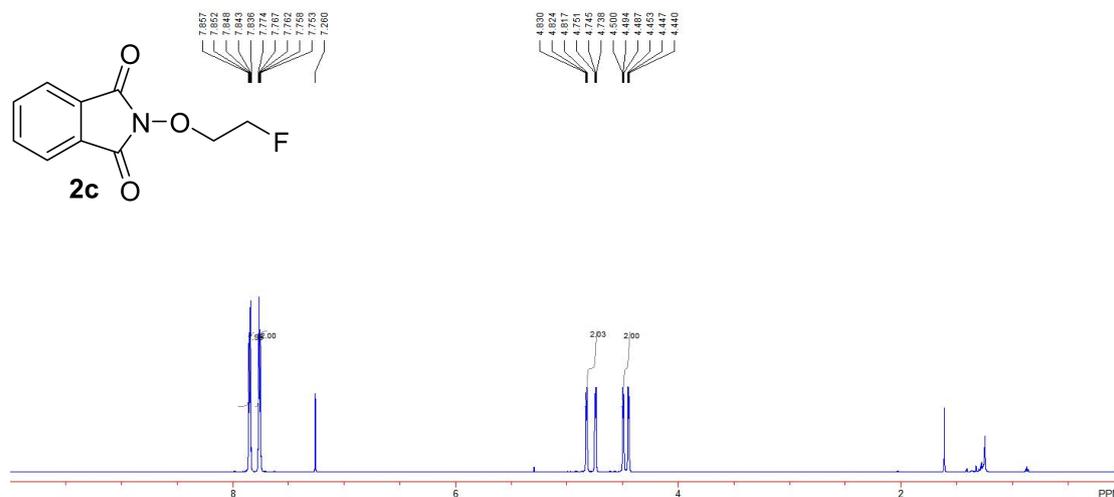
Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H66B	4865.22	5129.21	4568.81	36
H68	3286.27	10108.95	4084.55	34
H70	10682.44	7512.73	3495.85	36
H72	10413.86	7243.54	2813.77	34
H74	-730.18	5867.3	3616.67	36
H76	3753.31	6836.37	4006.76	32
H78	-1331.03	12236.65	2876.09	34
H80	5215.68	6400.41	2693.68	35
H82	-941.34	8692	2313.94	33
H86	3826.01	4498.75	2070.5	34
H90	4299.7	8313.75	3395.4	38
H92	5577.87	9209.05	1502.01	38
H94	4930.79	13087.49	2765.34	36
H98	-1437.26	5076.21	1646.04	44
H100	3593.08	7574.99	1424.66	36
H102	4476.04	10869.15	1362.04	36
H51	4752.26	13341.63	3447.59	35
H13	5176.18	10033.53	3454.31	38
H53	-985.98	9161.59	3610.13	42
H27A	8232.85	11342.03	85.29	35
H27B	10102.26	11563.4	428.86	35
H55	5461.62	6689.77	3371.21	34
H7	-992.13	5584.65	2942.37	34
H57A	9188.27	7562.92	763.04	32
H57B	7677.86	7299.49	386.74	32
H29	3699.03	11659.03	3329.6	38
H59	10102.11	6978.67	2222.08	36
H15	4039.72	8054.54	2712.02	33
H61	8230.12	3238.6	975.85	31
H31	10043.92	3662.19	2282.85	36
H63	10593.24	10027.1	1624.63	38
H2	6790.56	11418.74	3791.92	38
H65A	5393.99	5951.52	4189.18	33
H65B	4084.72	6241.61	4572.63	33
H33	10373.3	10325.14	2301.61	36
H67	4230.13	11164.16	2037.06	38
H17	10259.91	10608.16	2885.28	40

Table 7 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for ZGY.

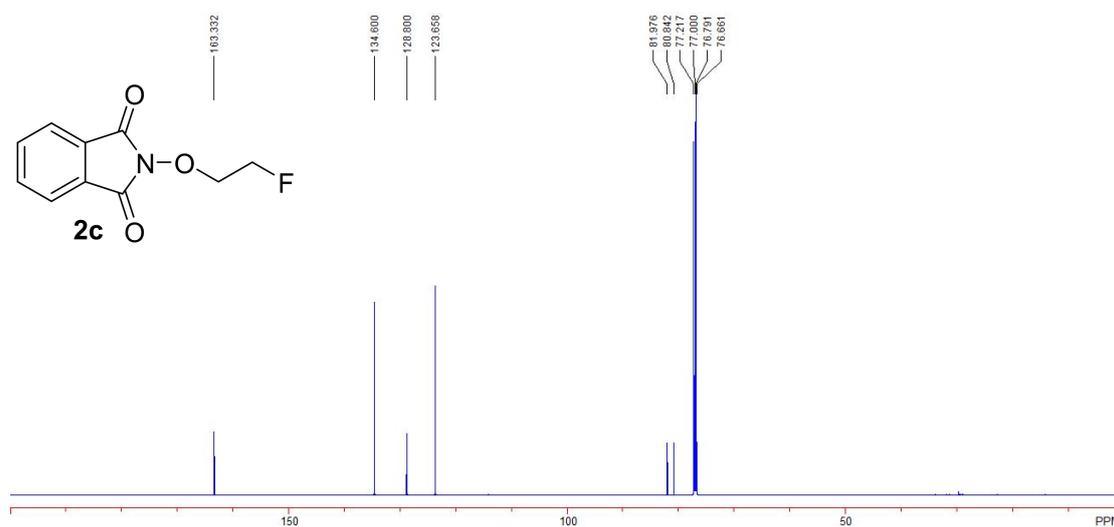
Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H35	3897.28	11368.58	2646.09	35
H71	1582.39	5337.76	1187.6	35
H9	7638.28	8048.74	3796.12	35
H73	5179.09	12832.02	2170.25	38
H37	5019.91	6147.81	2108.69	42
H75A	10545.25	10740.9	796.48	32
H75B	9166.41	10452.32	416.26	32
H19	2364.65	12018.89	1189.5	36
H77	5223.51	9768.82	2771.75	38
H39	-920.45	8892.2	2927.11	38
H79	2461.79	8682.87	1216.5	36
H5A	4515.5	8496.34	357.02	41
H5B	6215.39	8074.71	108.82	41
H83	-900.38	11732.74	1592.36	42
H21	3872.01	7840.72	2105.06	37
H85	5414.88	12560.52	1490.87	42
H43A	4630.47	9178.8	4243.32	38
H43B	3272.19	9465.12	4624.01	38
H87	-1233.27	5354.47	2328.68	40
H11	6883.61	4737.92	3804.9	38
H89	10049.4	10892.79	3562.65	44
H45	3782.05	4733.41	2678.94	44
H23A	9908.02	4127.73	799.4	37
H23B	8556.67	3839.01	416.17	37
H93A	4035.32	12477.74	4227.53	39
H93B	2552.9	12746	4601.43	39
H47	-1154.14	12008.84	2275.59	37
H95A	-66.38	8298.21	4695.08	47
H95B	1895.75	8687.29	4918.41	47
H3	10021.22	4198.79	3551.6	48
H97	3736.95	4995.52	3370.47	48
H49	10044.42	3914.72	2869.33	45
H99A	7447.01	4688.81	75.97	38
H99B	9363.07	4938.07	401.27	38
H25A	-915.98	11594.45	4618.14	46
H25B	838.09	11998.37	4875.49	46
H101	4831.38	5873.43	1430.83	46

10 NMR spectra of new compound

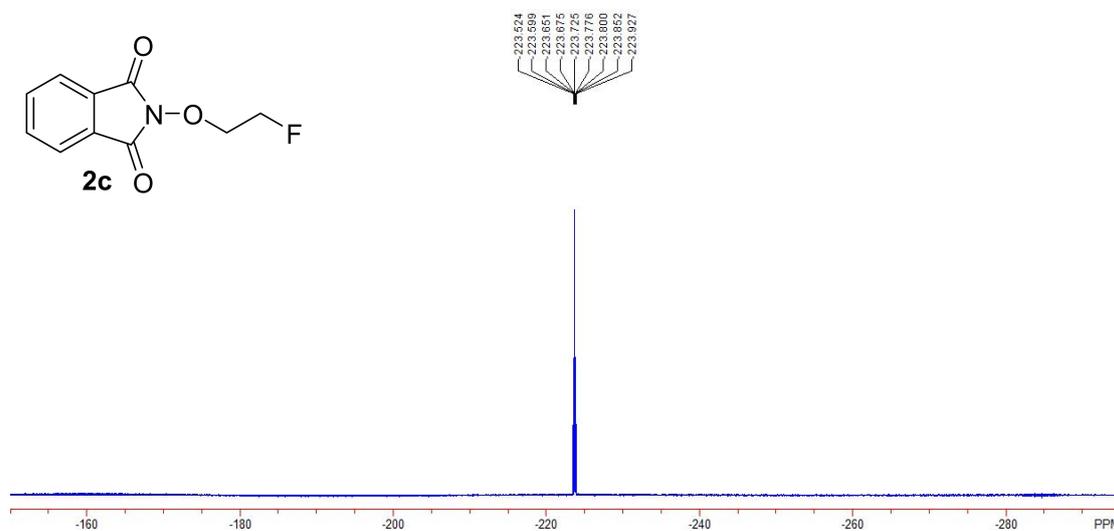
^1H NMR (600 MHz, CDCl_3) spectra of **2c**



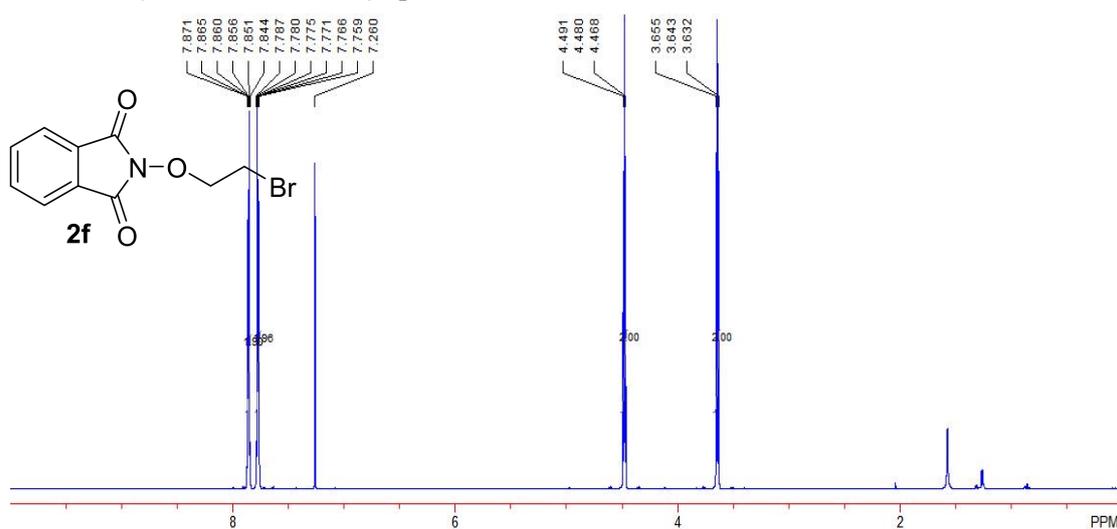
^{13}C NMR (150 MHz, CDCl_3) spectra of **2c**



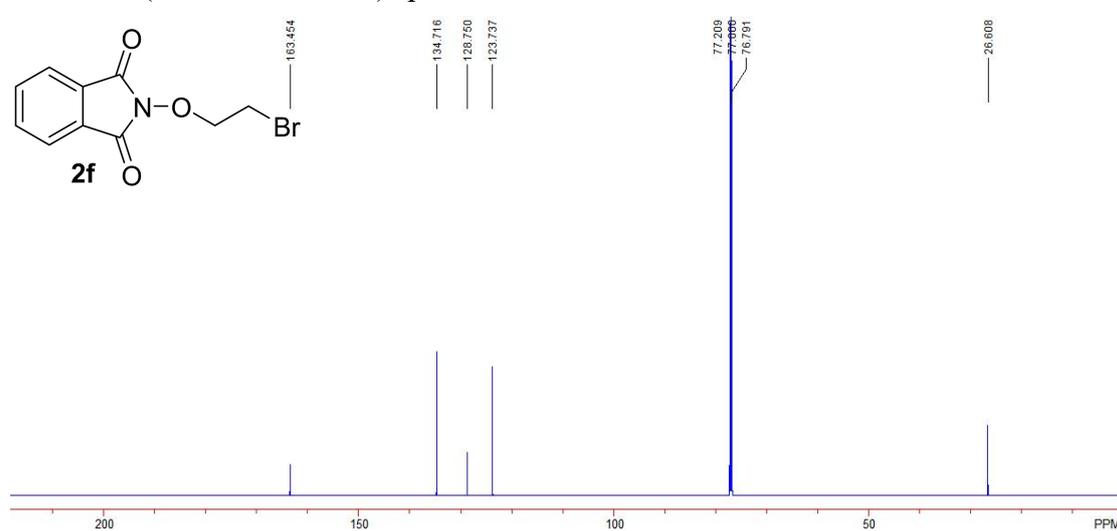
^{19}F NMR (564 MHz, CDCl_3) spectra of **2c**



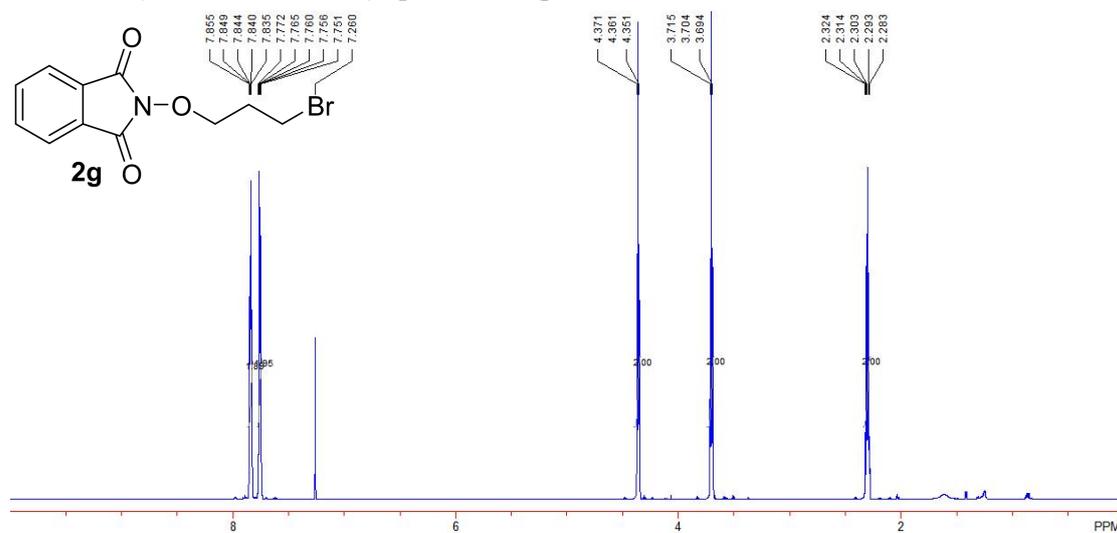
^1H NMR (600 MHz, CDCl_3) spectra of **2f**



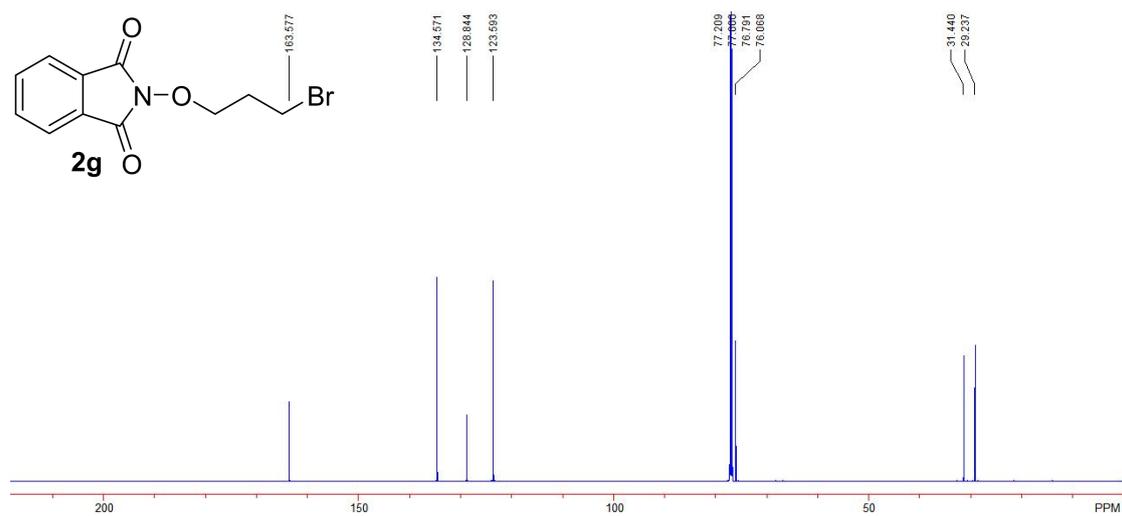
^{13}C NMR (150 MHz, CDCl_3) spectra of **2f**



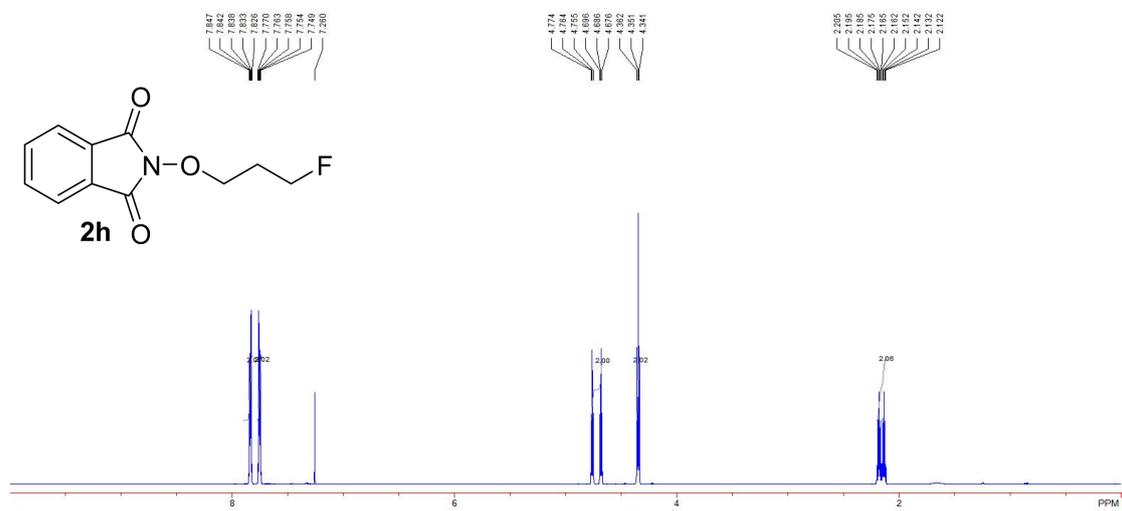
^1H NMR (600 MHz, CDCl_3) spectra of **2g**



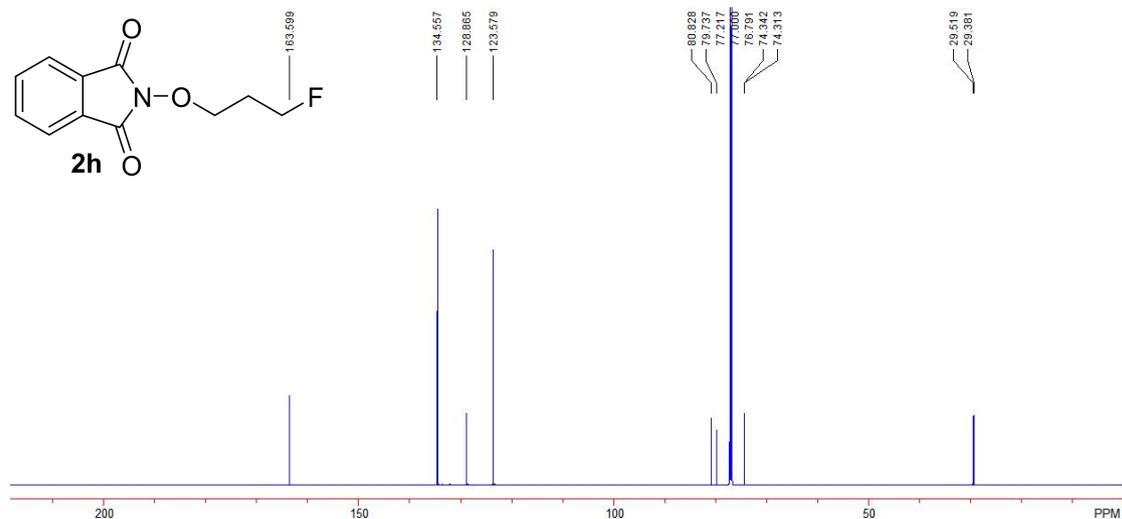
¹³C NMR (150 MHz, CDCl₃) spectra of **2g**



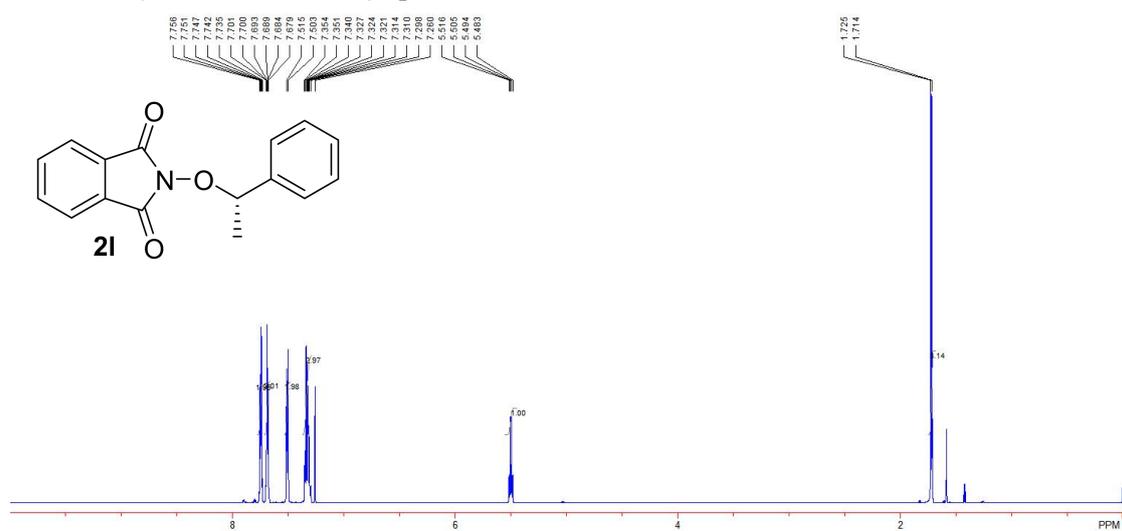
¹H NMR (600 MHz, CDCl₃) spectra of **2h**



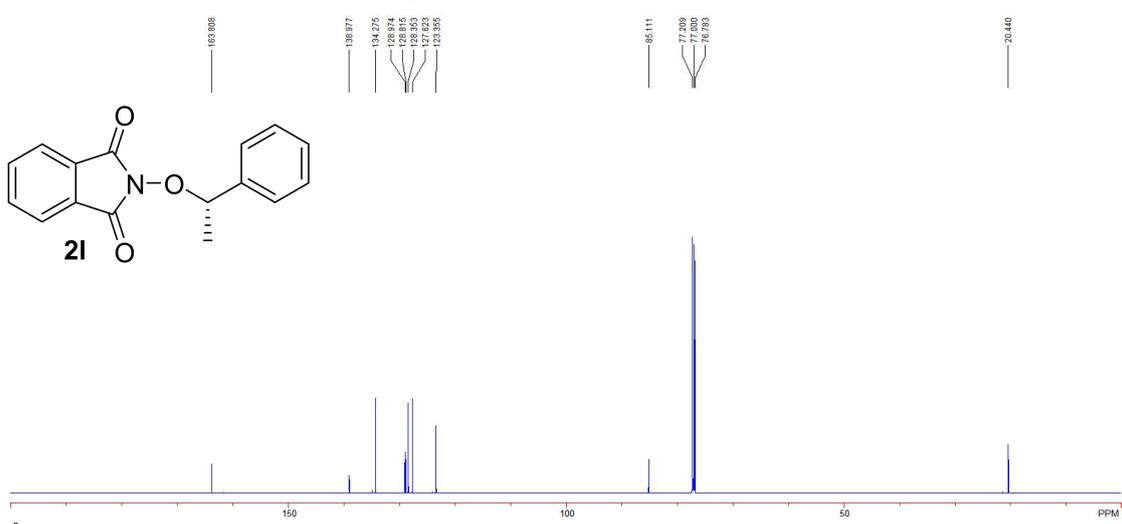
¹³C NMR (150 MHz, CDCl₃) spectra of **2h**



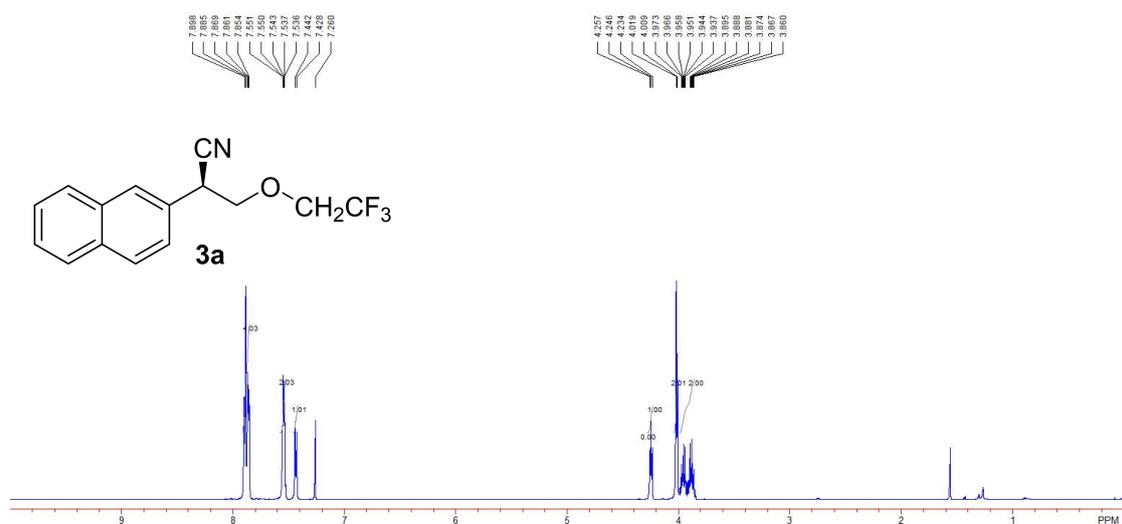
^1H NMR (600 MHz, CDCl_3) spectra of **21**



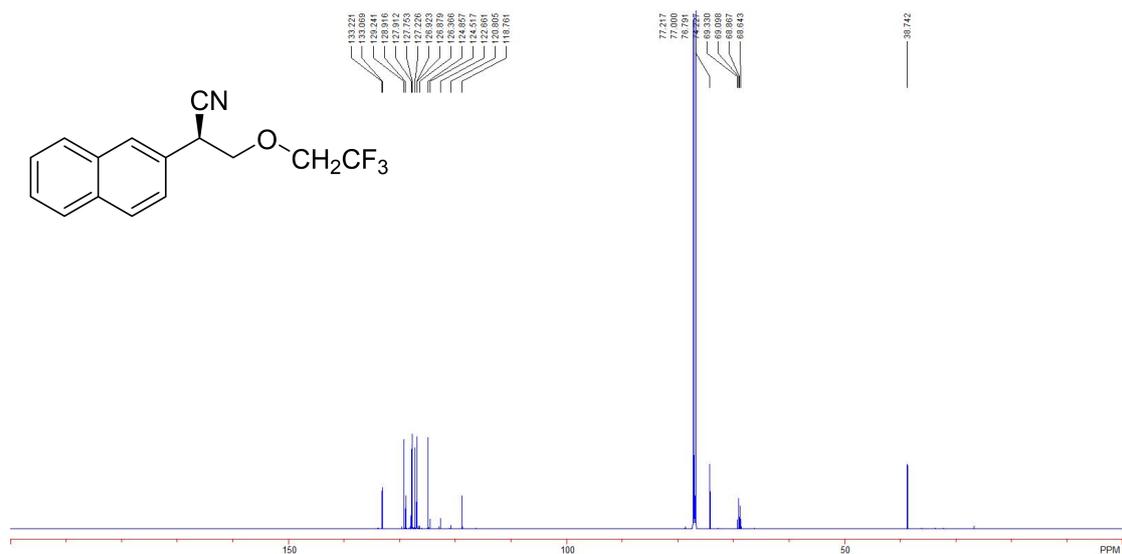
^{13}C NMR (150 MHz, CDCl_3) spectra of **21**



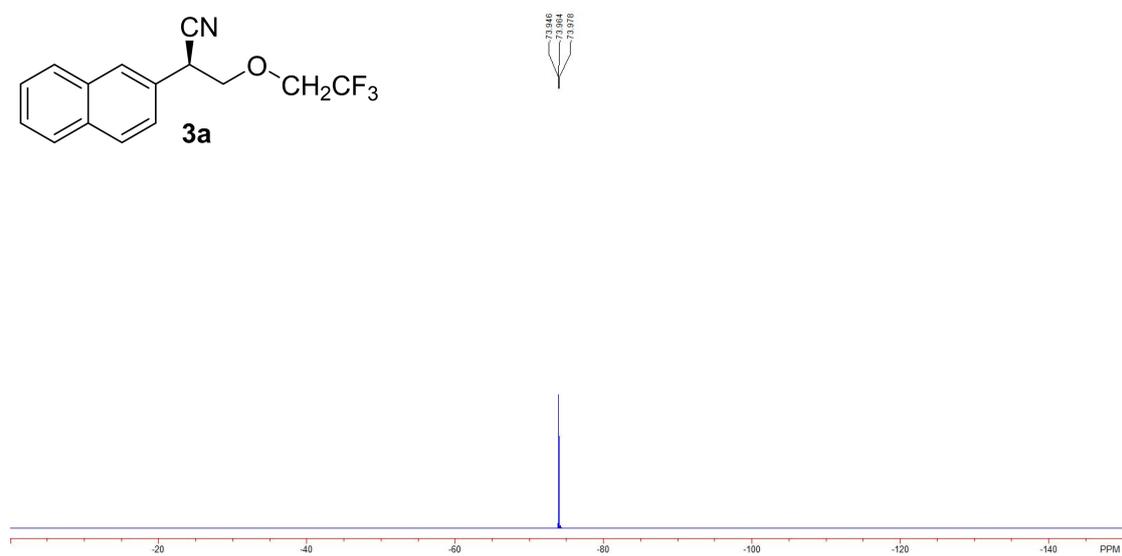
^1H NMR (600 MHz, CDCl_3) spectra of **3a**



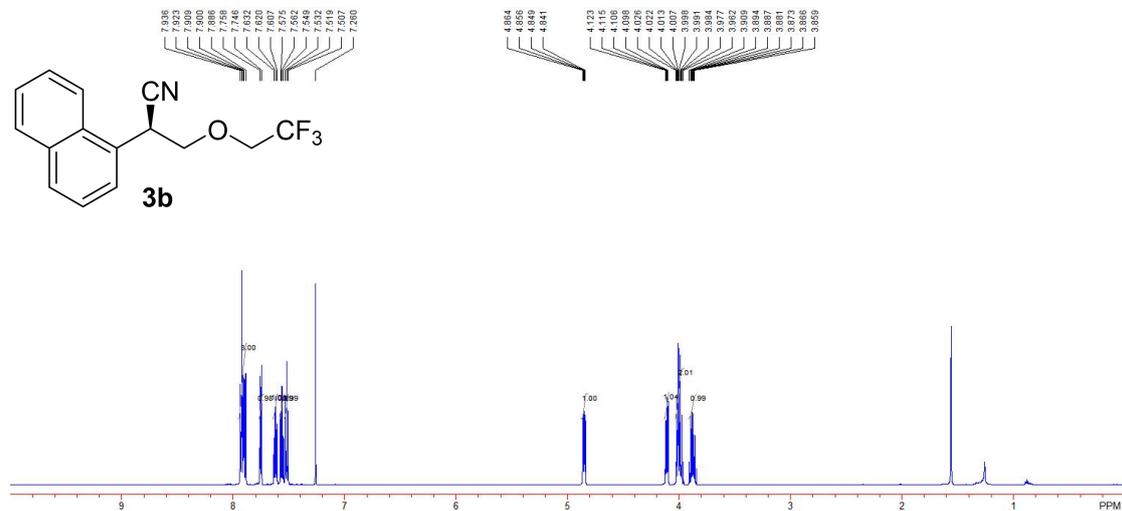
¹³C NMR (150 MHz, CDCl₃) spectra of **3a**



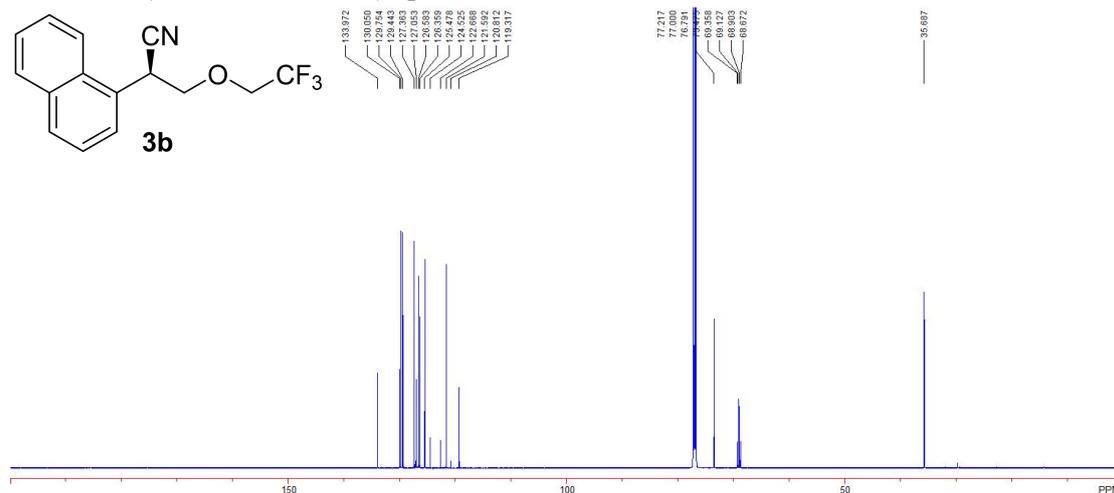
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3a**



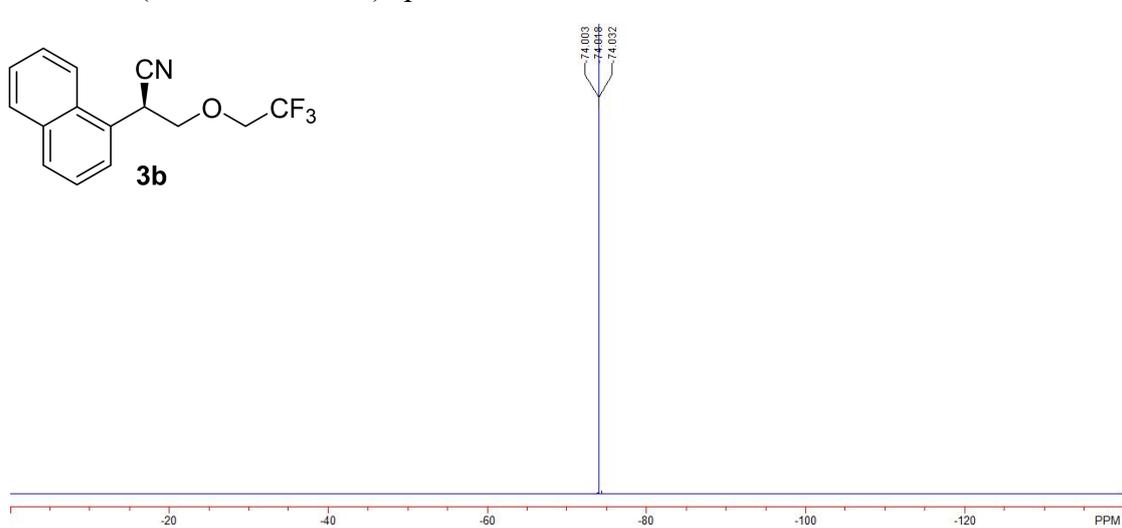
¹H NMR (600 MHz, CDCl₃) spectra of **3b**



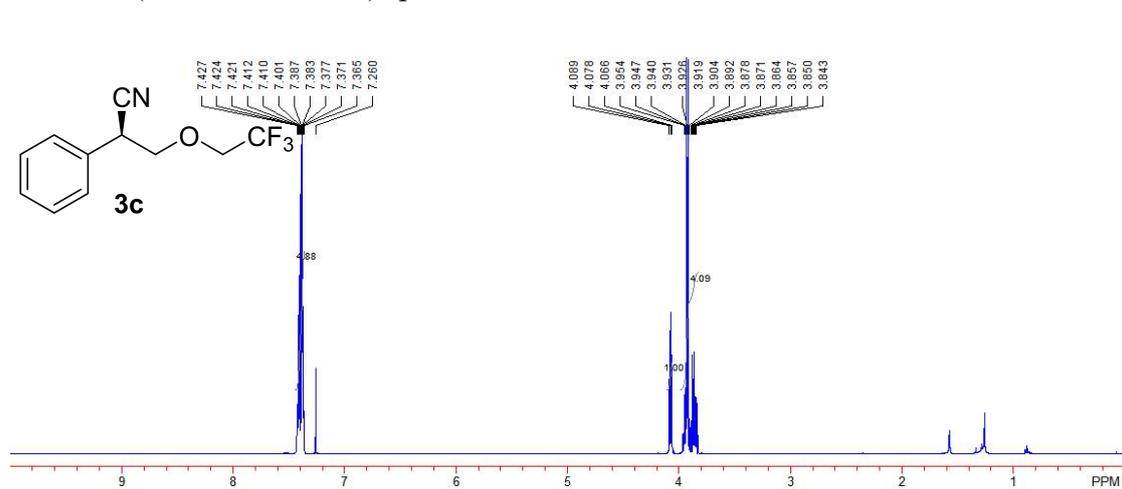
¹³C NMR (150 MHz, CDCl₃) spectra of **3b**



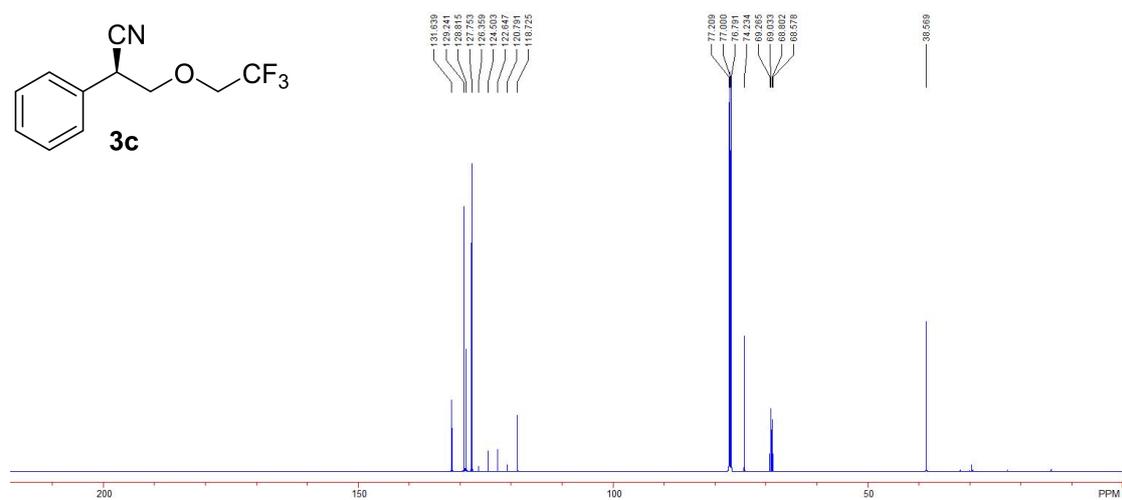
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3b**



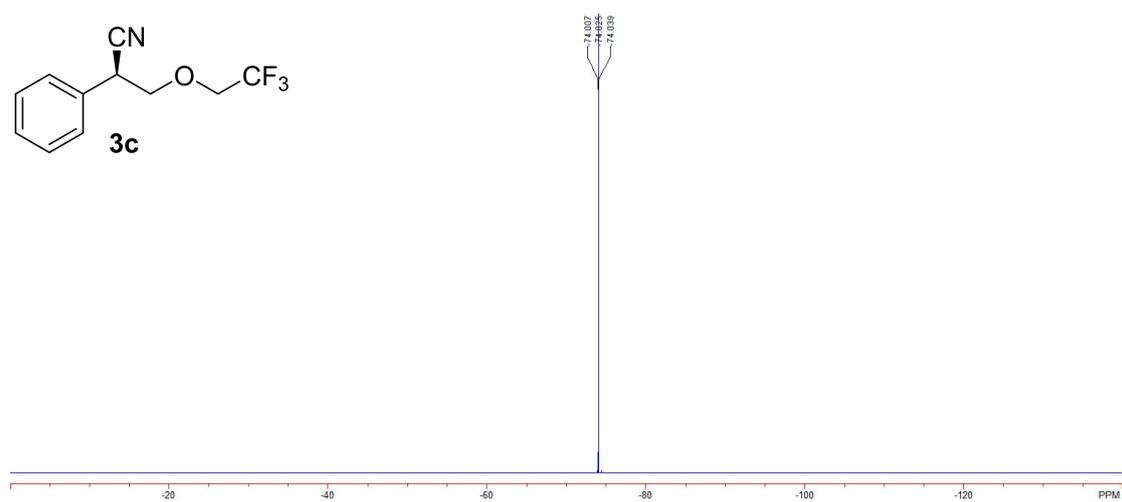
¹H NMR (600 MHz, CDCl₃) spectra of **3c**



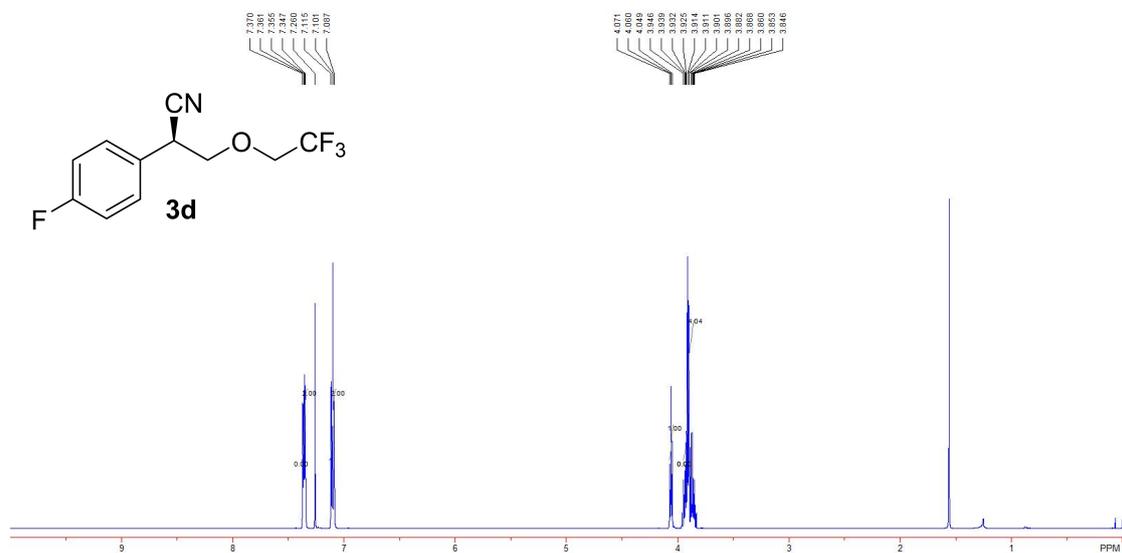
^{13}C NMR (150 MHz, CDCl_3) spectra of **3c**



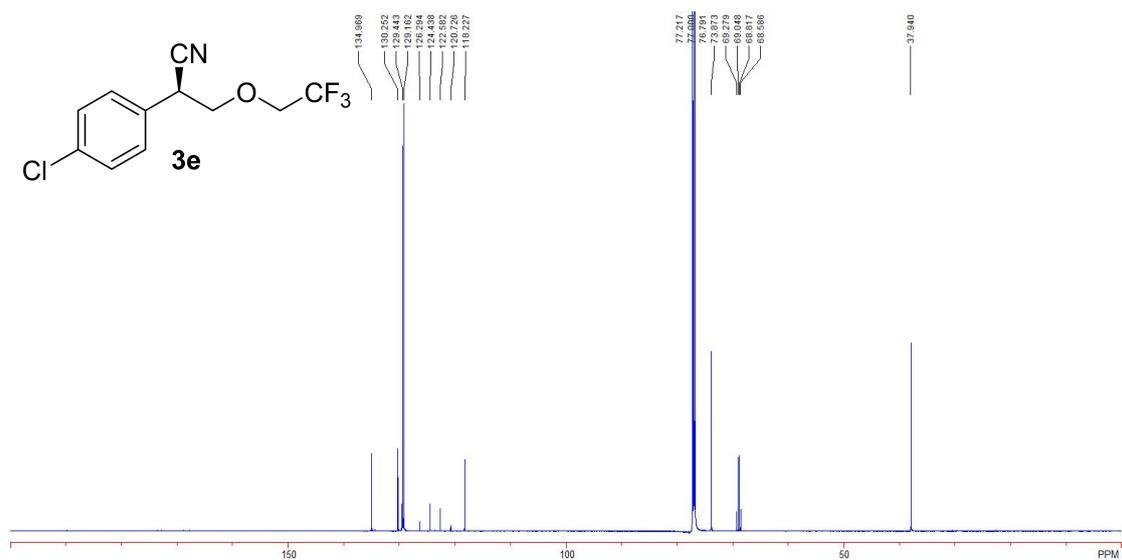
^{19}F NMR (564 MHz, CDCl_3) spectra of **3c**



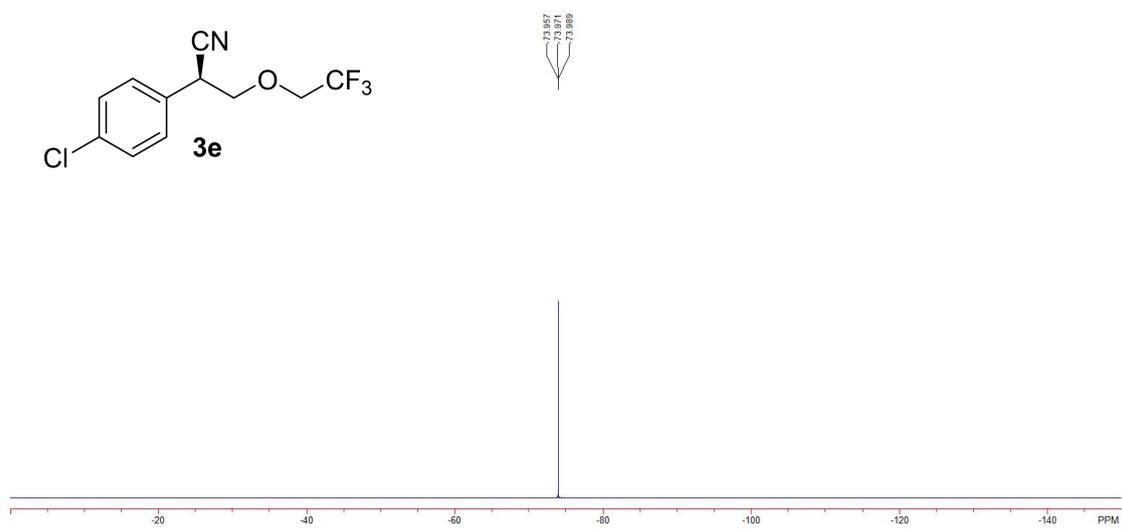
^1H NMR (600 MHz, CDCl_3) spectra of **3d**



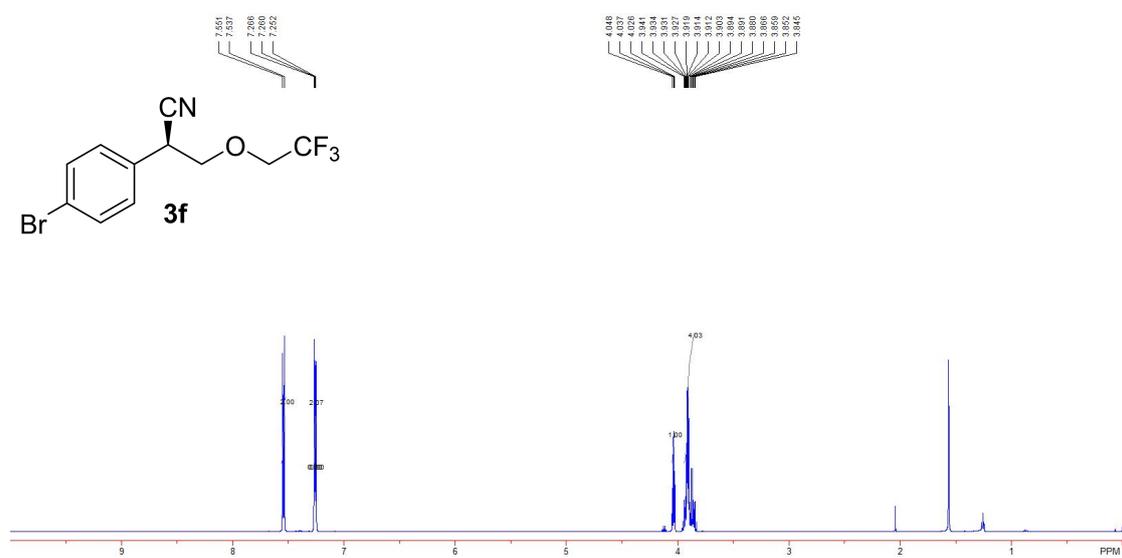
^{13}C NMR (150 MHz, CDCl_3) spectra of **3e**



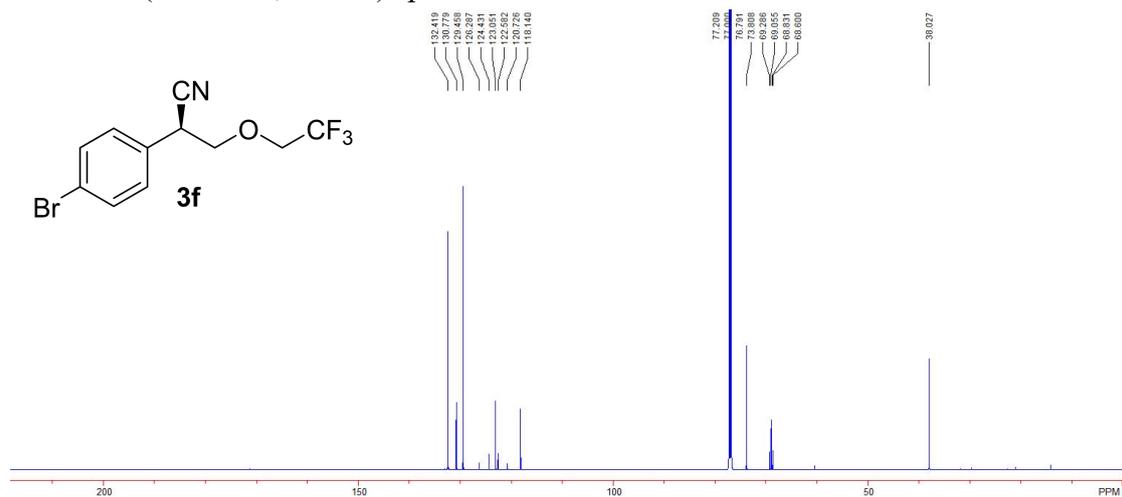
^{19}F NMR (564 MHz, CDCl_3) spectra of **3e**



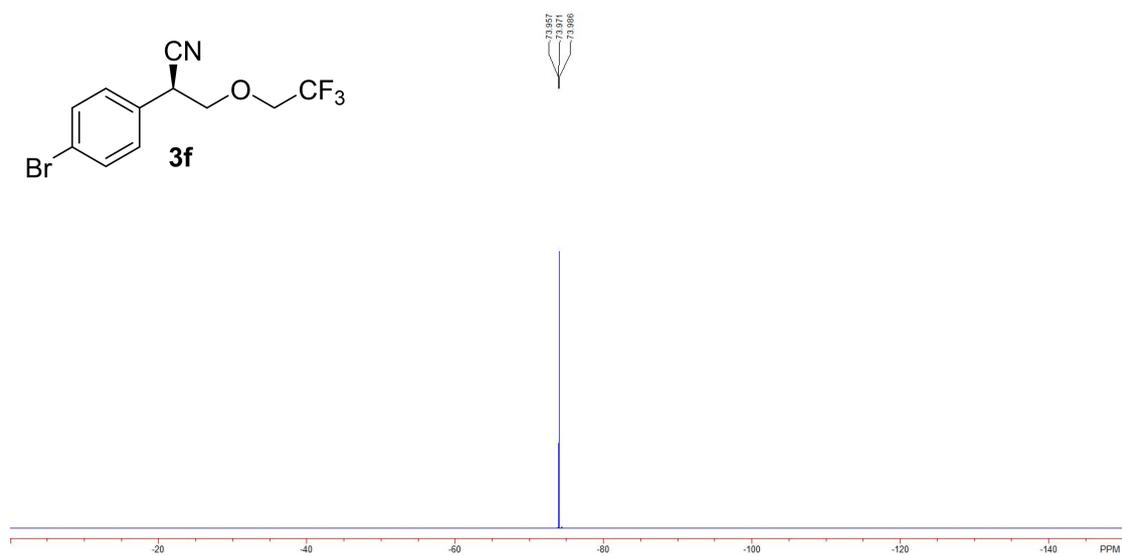
^1H NMR (600 MHz, CDCl_3) spectra of **3f**



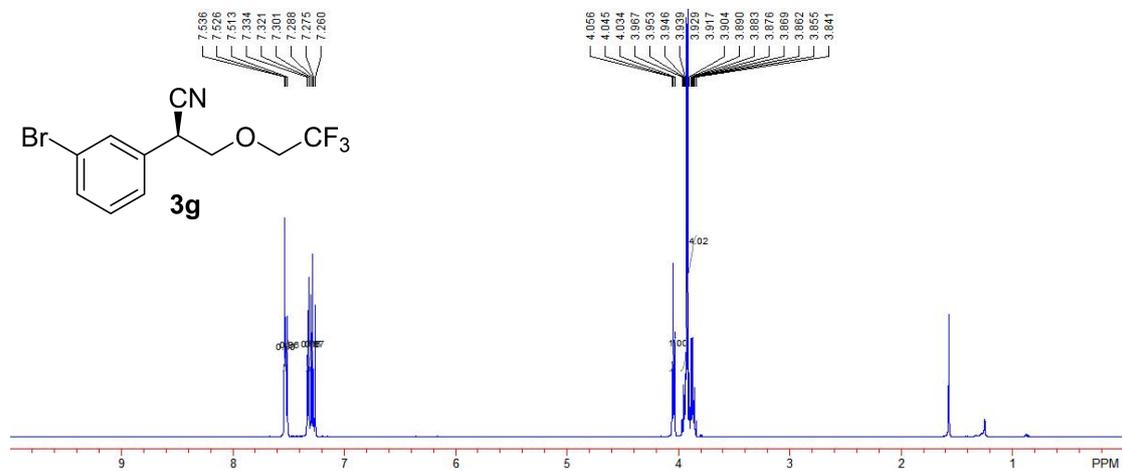
^{13}C NMR (150 MHz, CDCl_3) spectra of **3f**



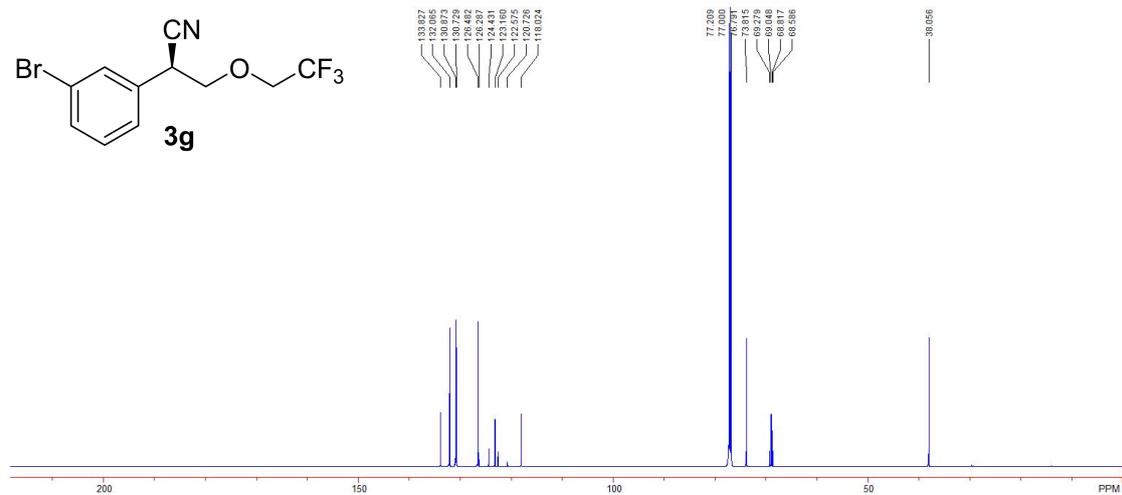
^{19}F NMR (564 MHz, CDCl_3) spectra of **3f**



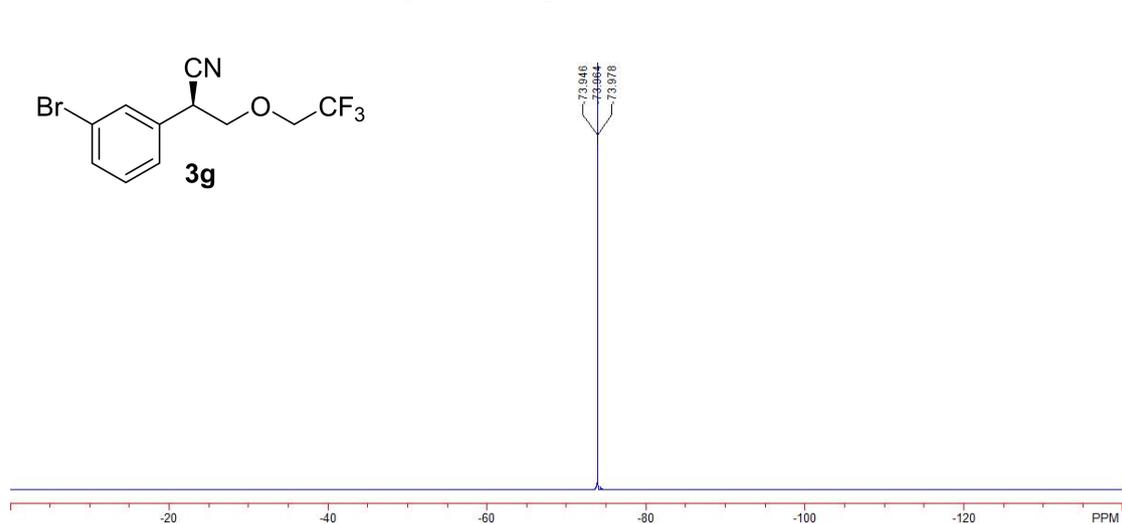
^1H NMR (600 MHz, CDCl_3) spectra of **3g**



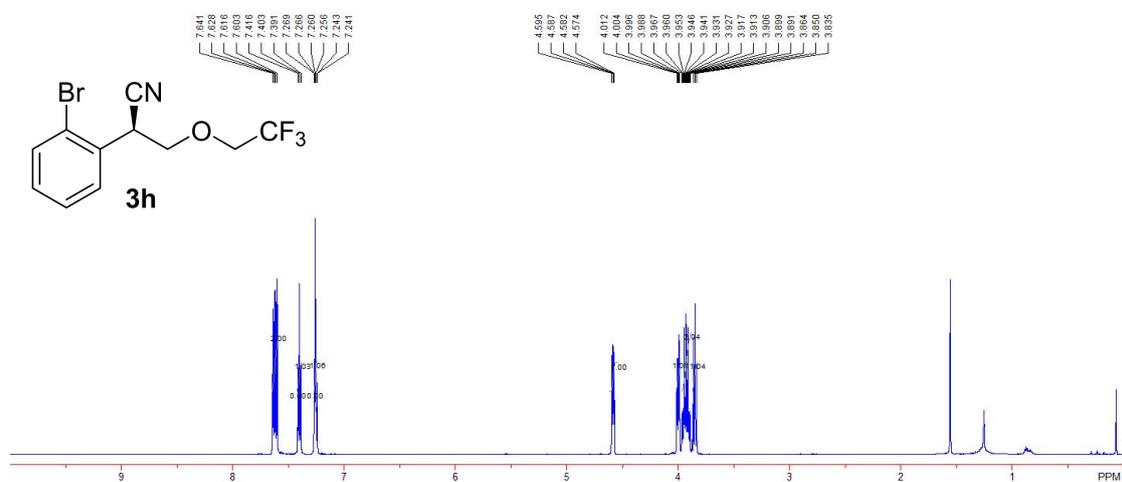
¹³C NMR (150 MHz, CDCl₃) spectra of **3g**



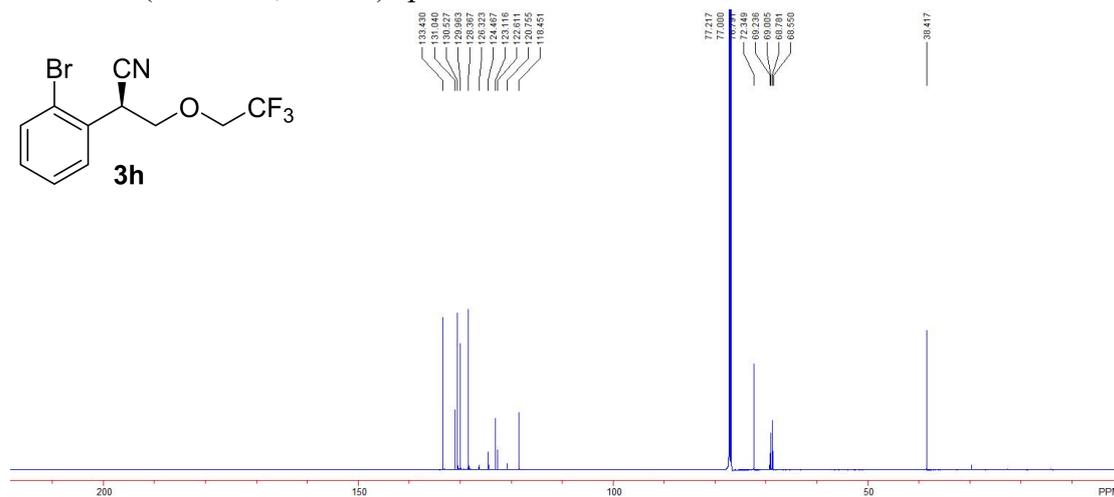
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3g**



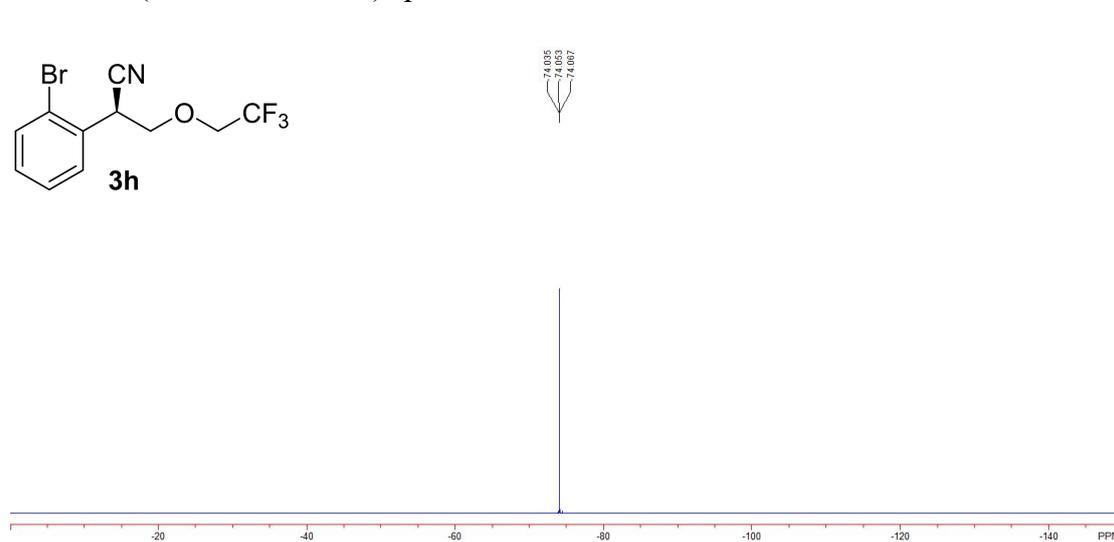
¹H NMR (600 MHz, CDCl₃) spectra of **3h**



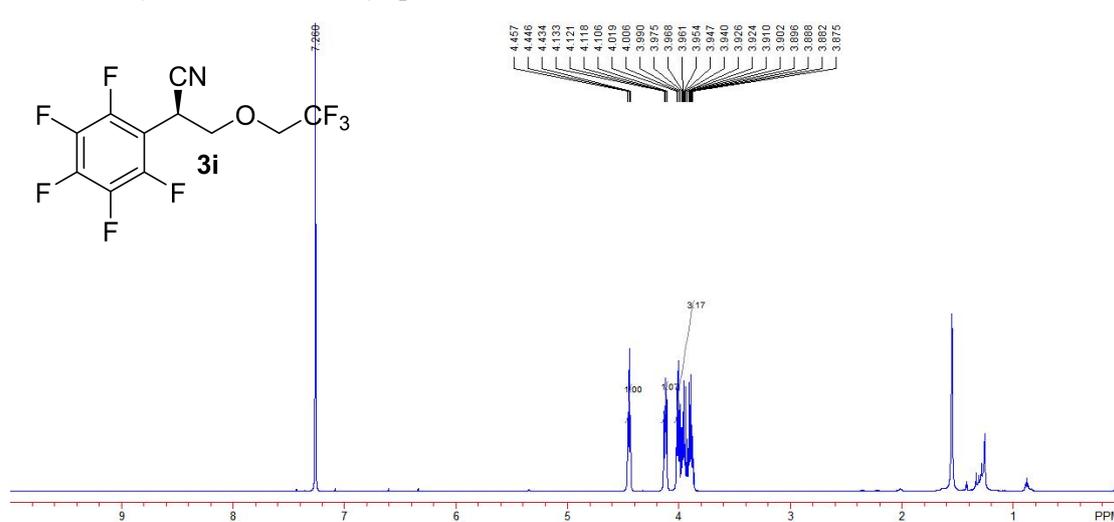
¹³C NMR (150 MHz, CDCl₃) spectra of **3h**



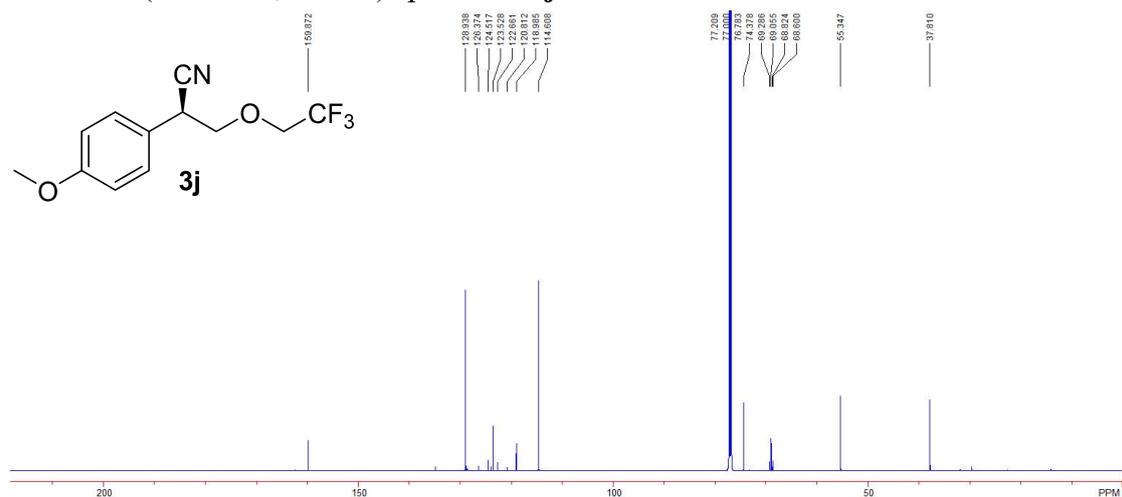
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3h**



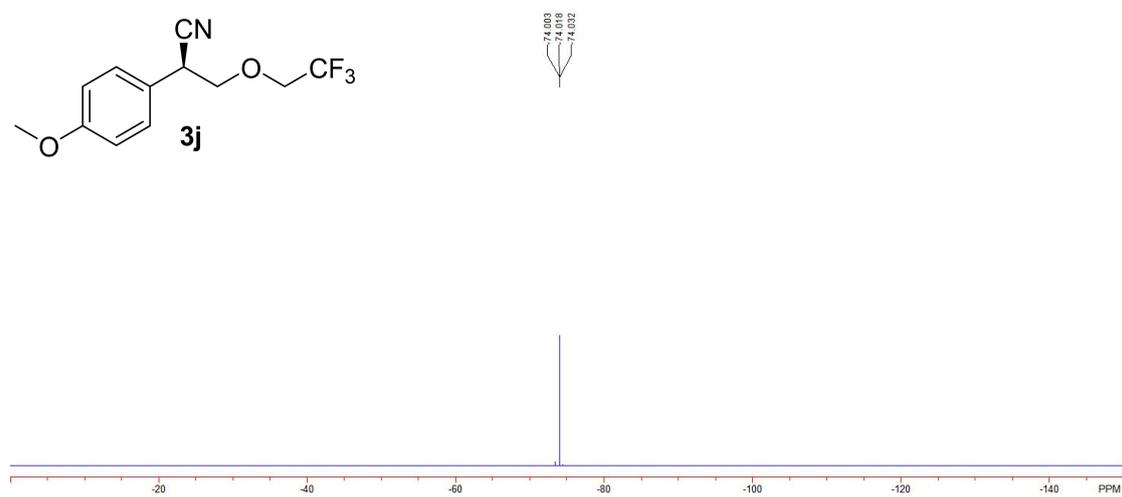
¹H NMR (600 MHz, CDCl₃) spectra of **3i**



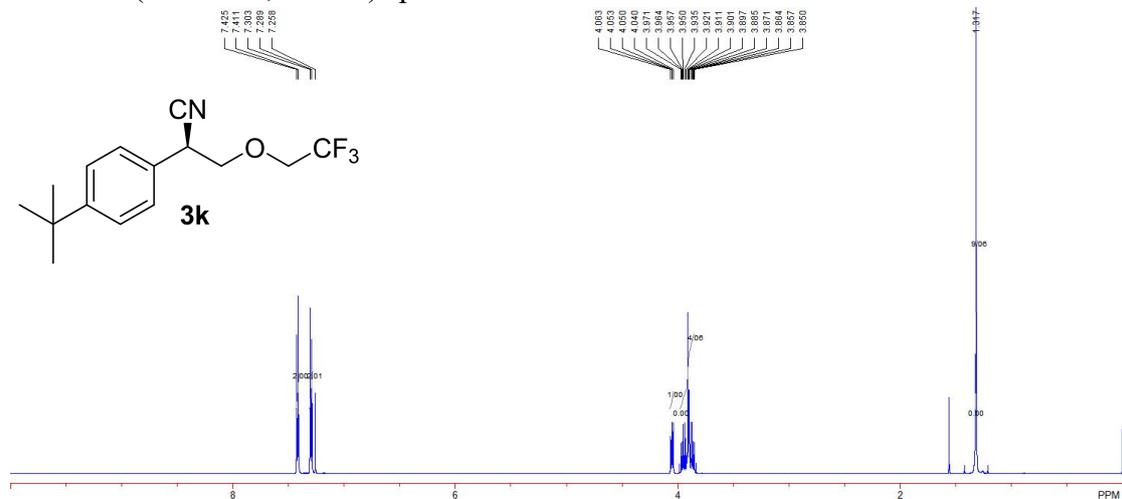
^{13}C NMR (150 MHz, CDCl_3) spectra of **3j**



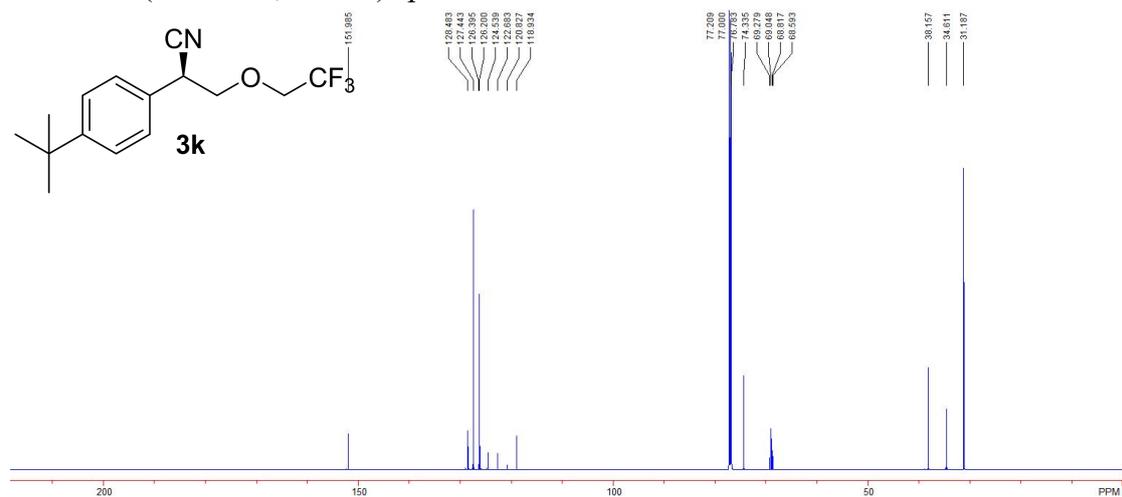
^{19}F NMR (564 MHz, CDCl_3) spectra of **3j**



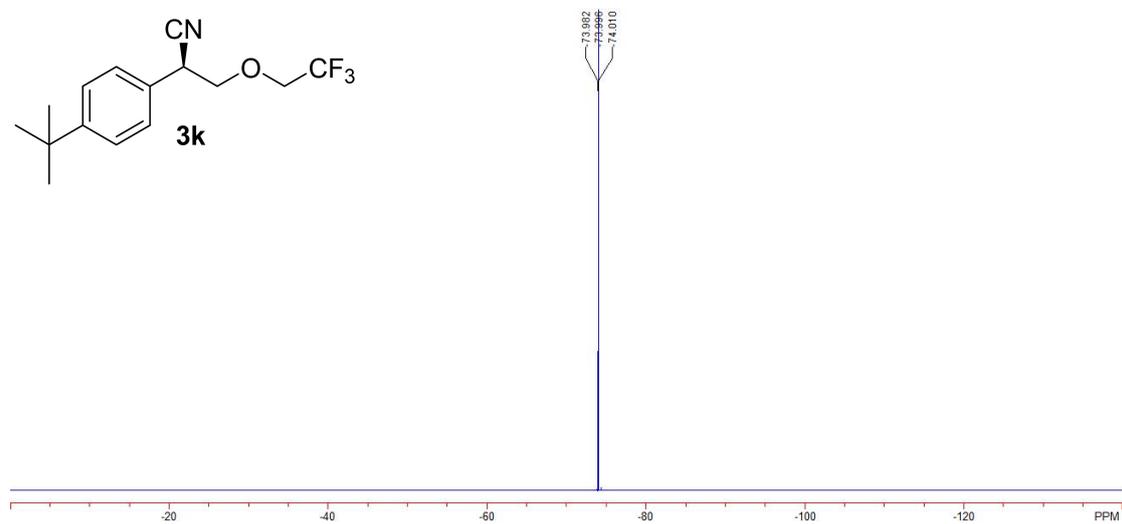
^1H NMR (600 MHz, CDCl_3) spectra of **3k**



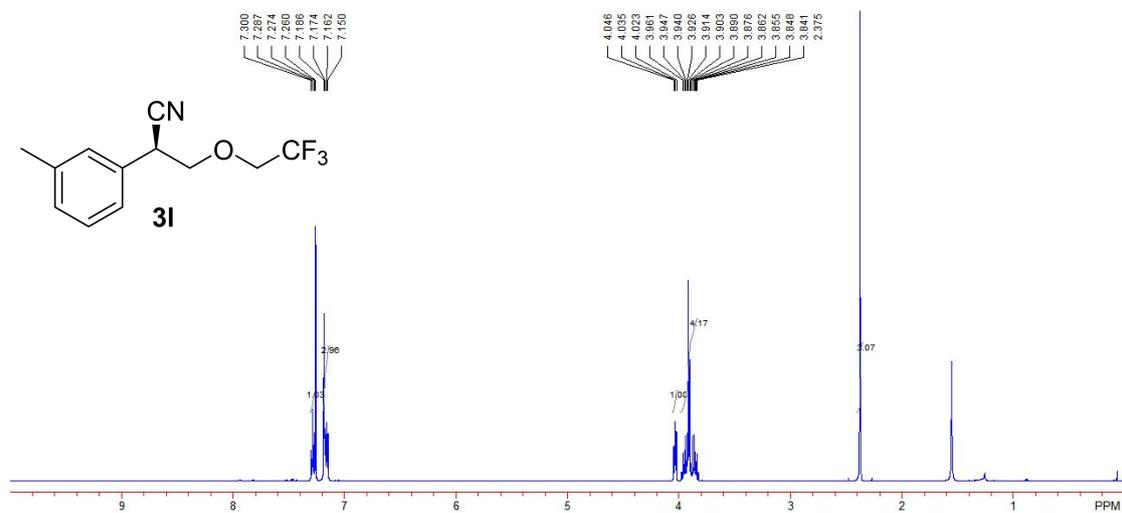
^{13}C NMR (150 MHz, CDCl_3) spectra of **3k**



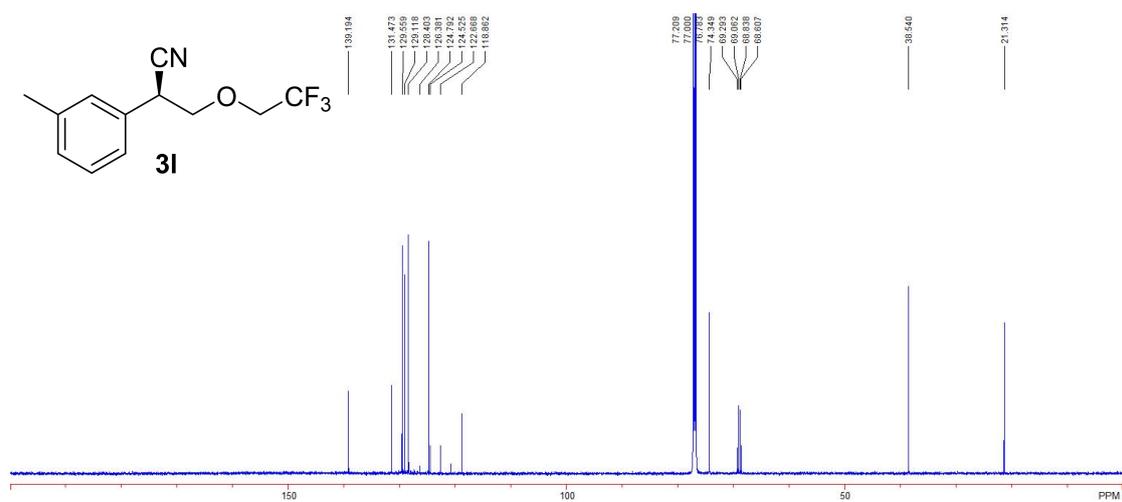
^{19}F NMR (564 MHz, CDCl_3) spectra of **3k**



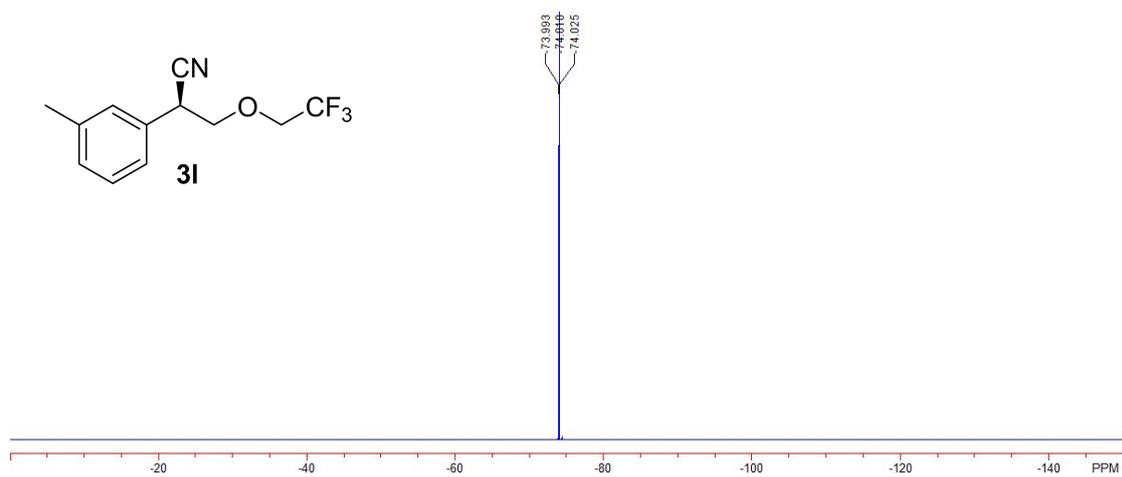
^1H NMR (600 MHz, CDCl_3) spectra of **3l**



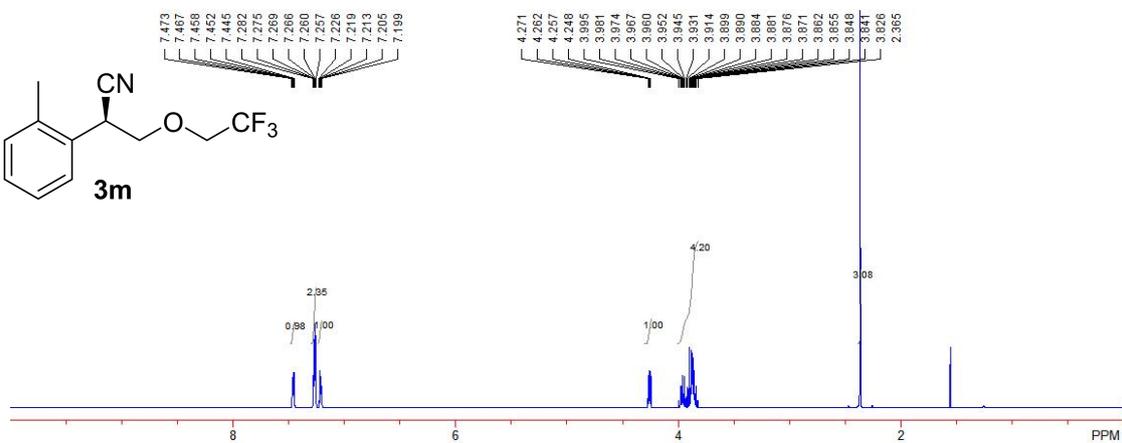
^{13}C NMR (150 MHz, CDCl_3) spectra of **3I**



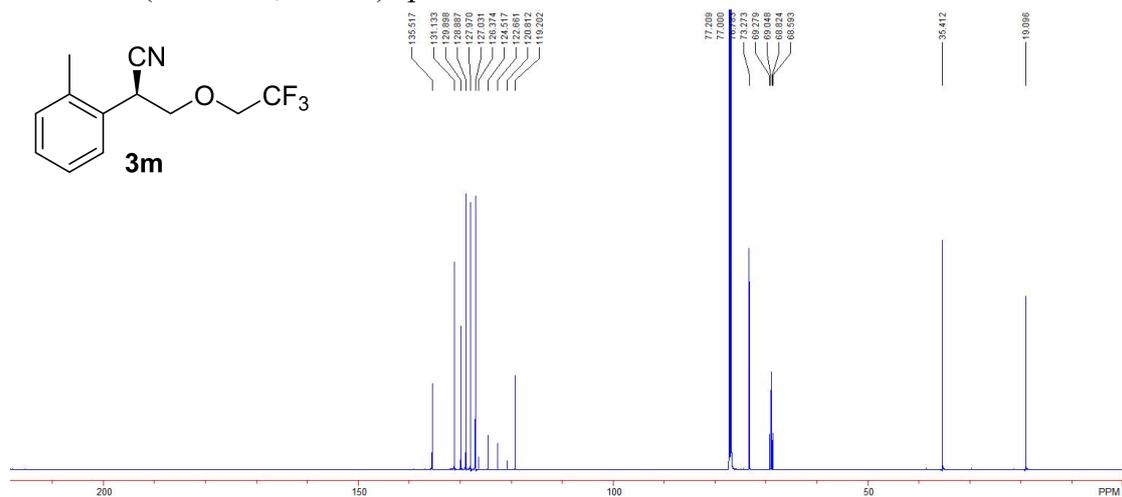
^{19}F NMR (564 MHz, CDCl_3) spectra of **3I**



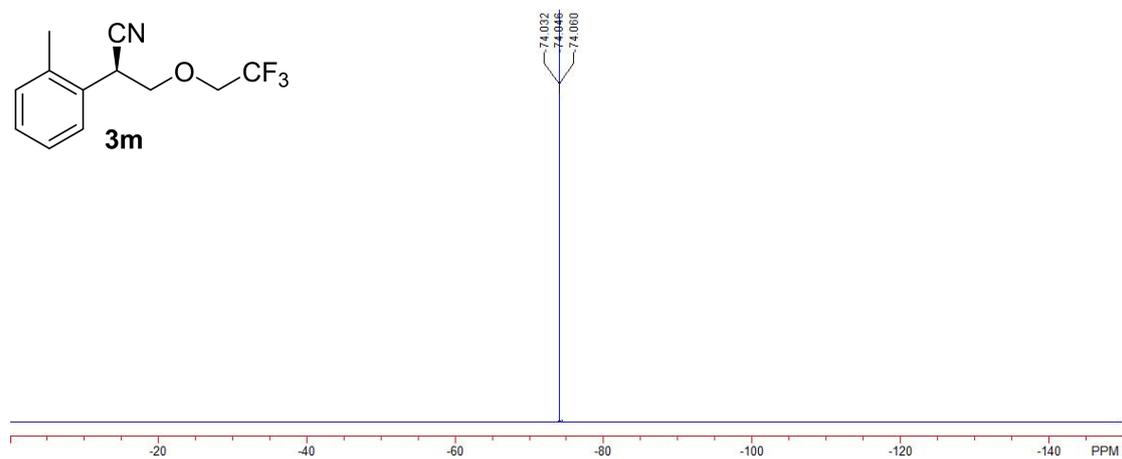
^1H NMR (600 MHz, CDCl_3) spectra of **3m**



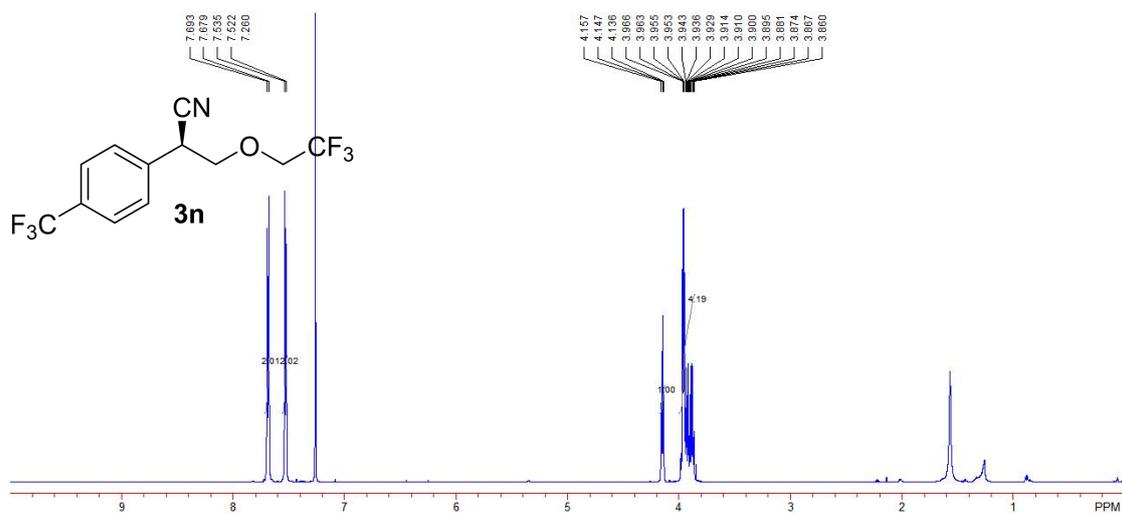
¹³C NMR (150 MHz, CDCl₃) spectra of **3m**



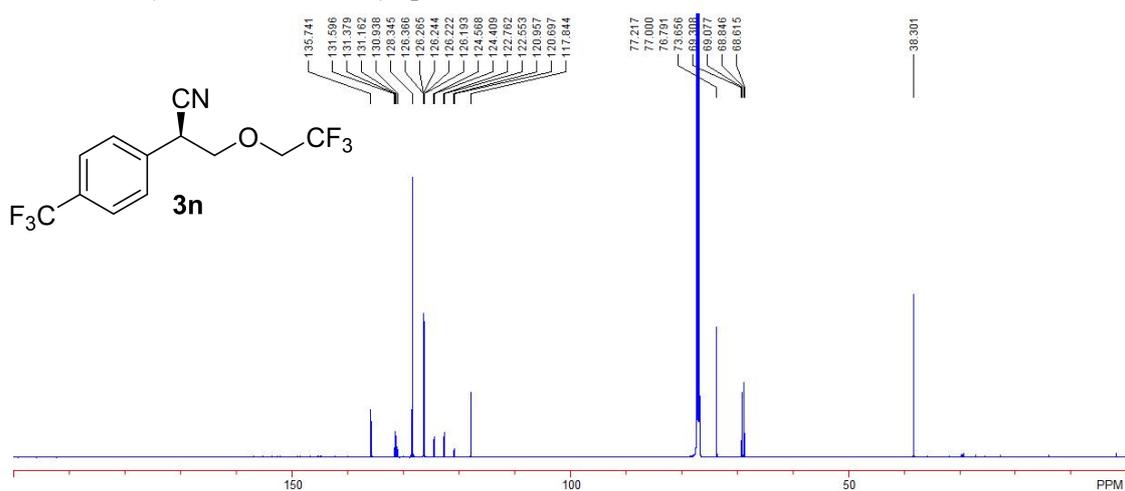
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3m**



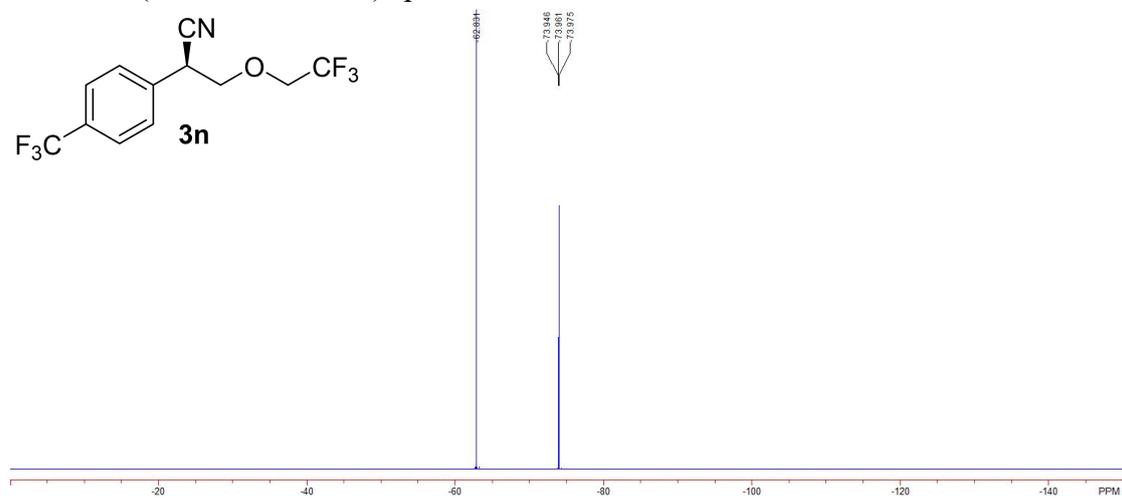
¹H NMR (600 MHz, CDCl₃) spectra of **3n**



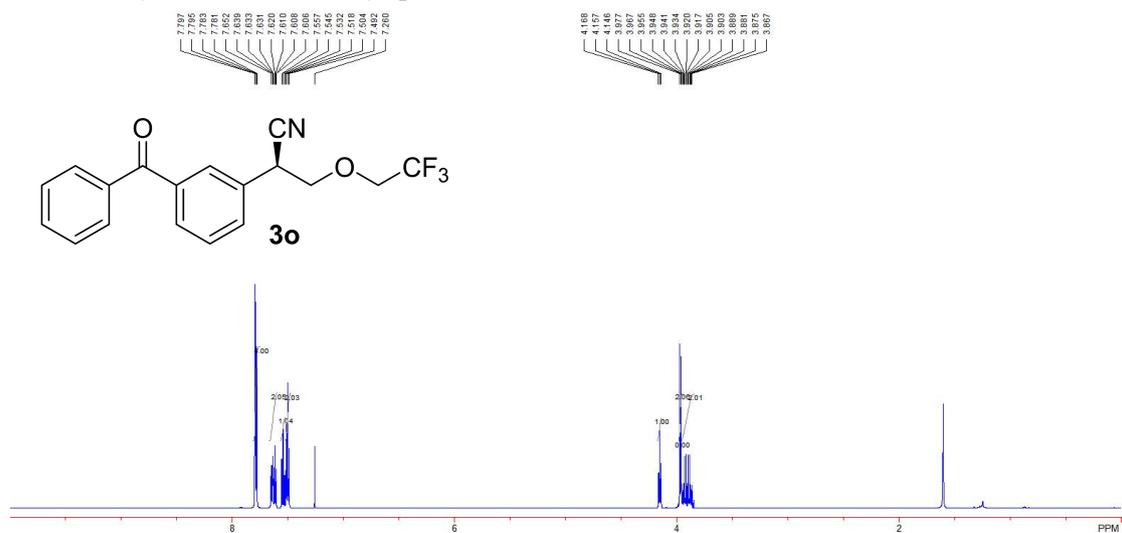
^{13}C NMR (150 MHz, CDCl_3) spectra of **3n**



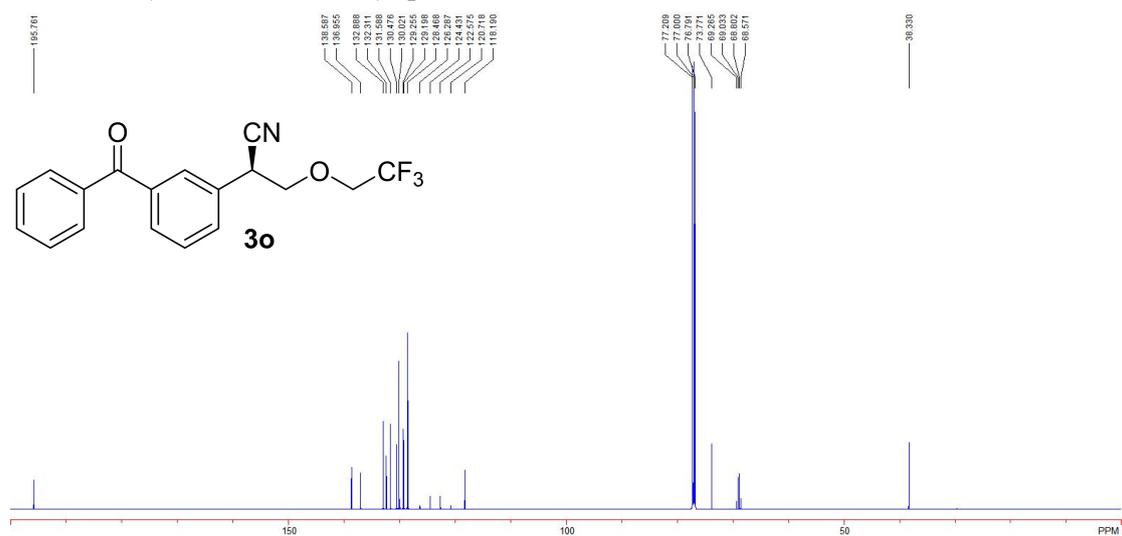
^{19}F NMR (564 MHz, CDCl_3) spectra of **3n**



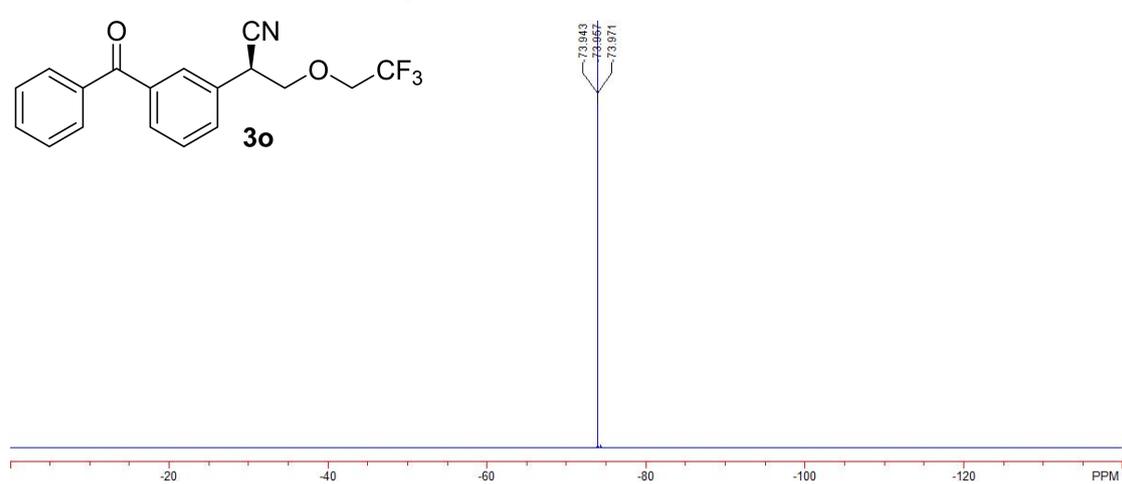
^1H NMR (600 MHz, CDCl_3) spectra of **3o**



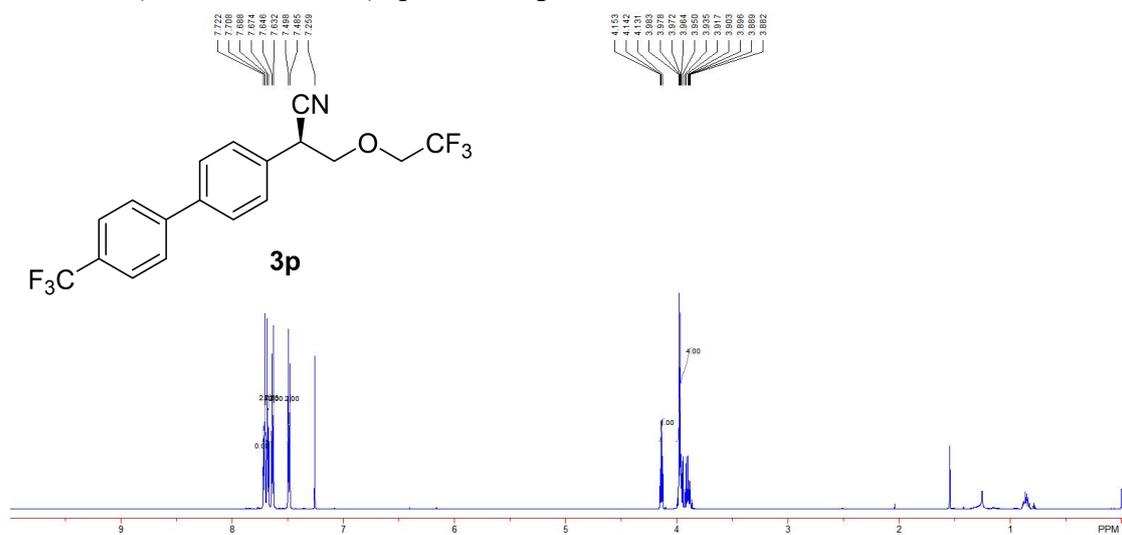
^{13}C NMR (150 MHz, CDCl_3) spectra of **3o**



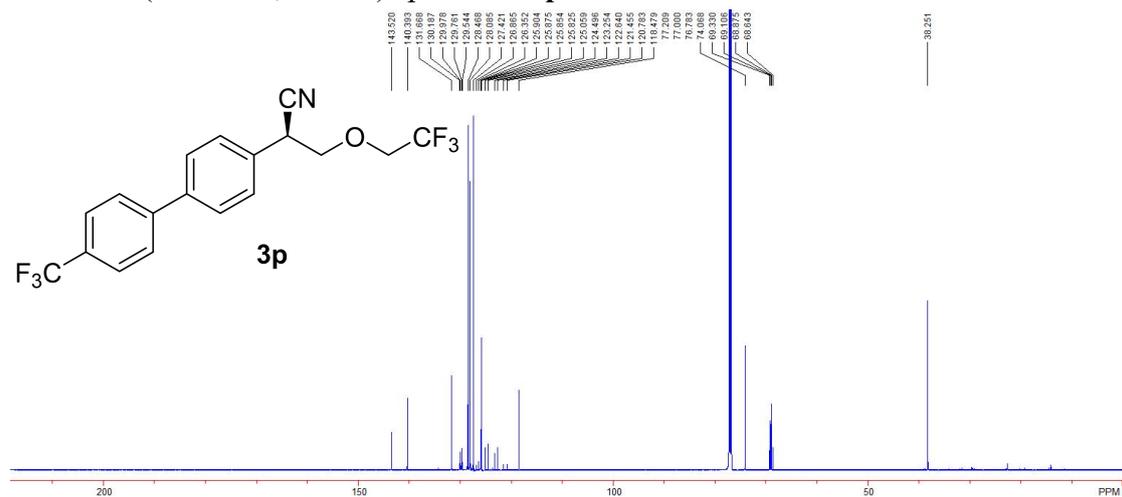
^{19}F NMR (564 MHz, CDCl_3) spectra of **3o**



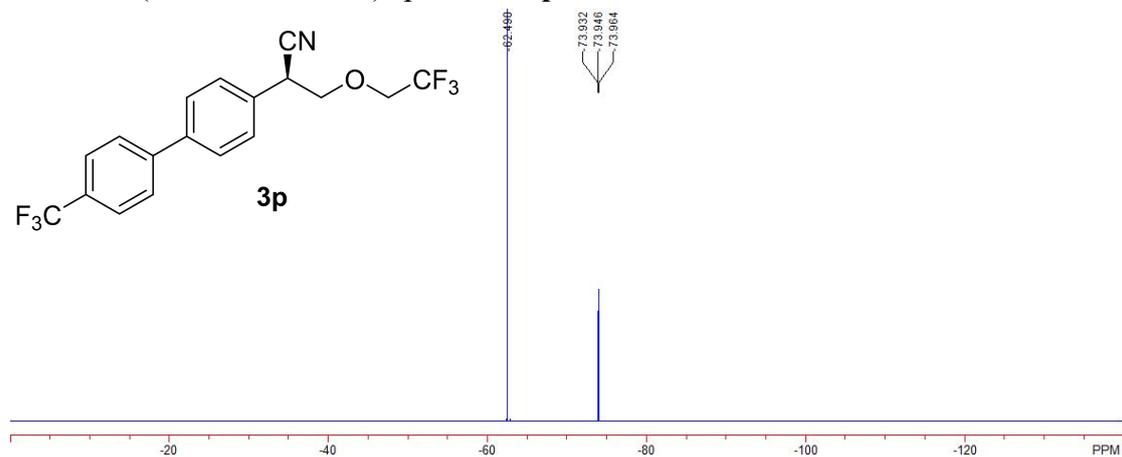
^1H NMR (600 MHz, CDCl_3) spectra of **3p**



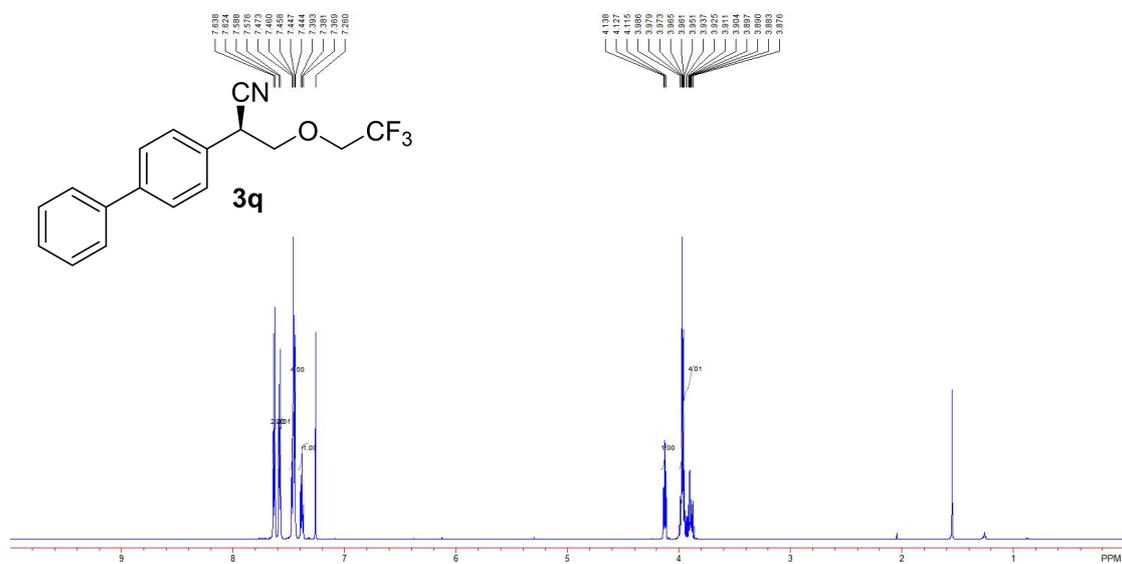
^{13}C NMR (150 MHz, CDCl_3) spectra of **3p**



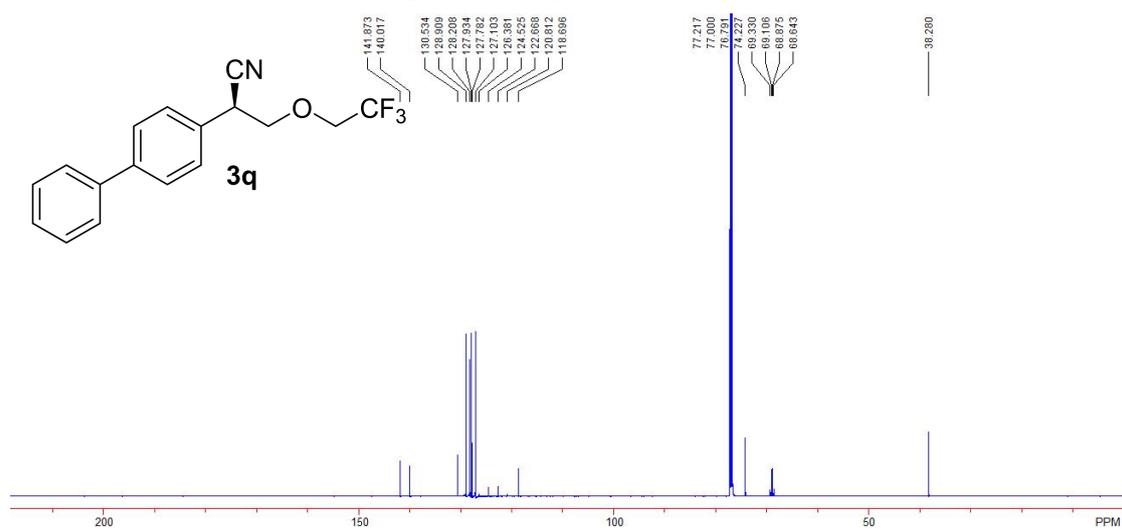
^{19}F NMR (564 MHz, CDCl_3) spectra of **3p**



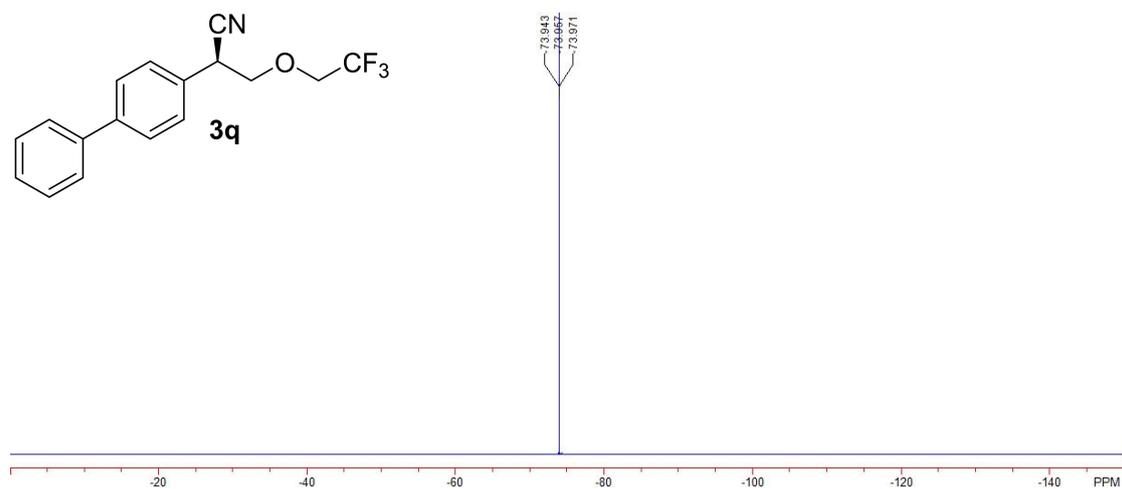
^1H NMR (600 MHz, CDCl_3) spectra of **3q**



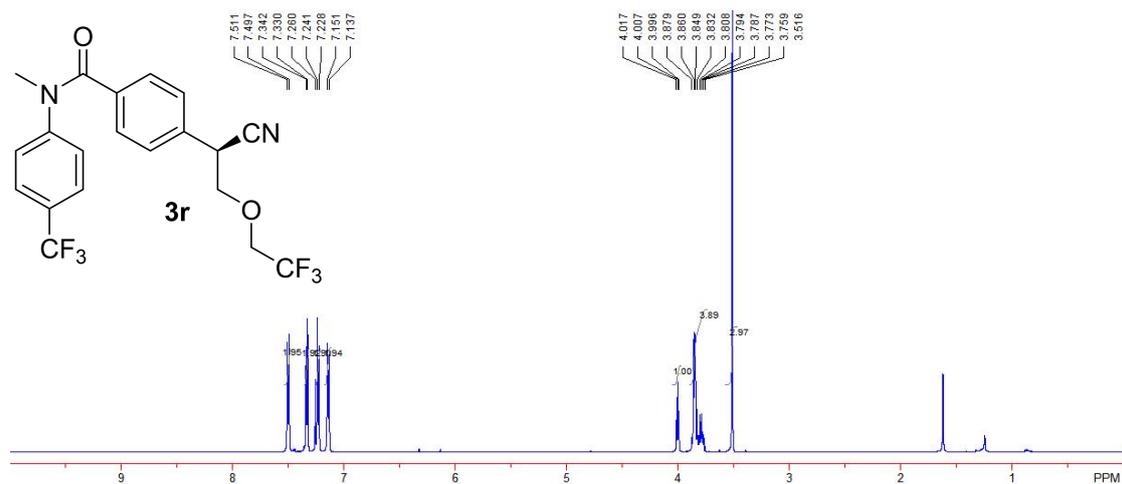
^{13}C NMR (150 MHz, CDCl_3) spectra of **3q**



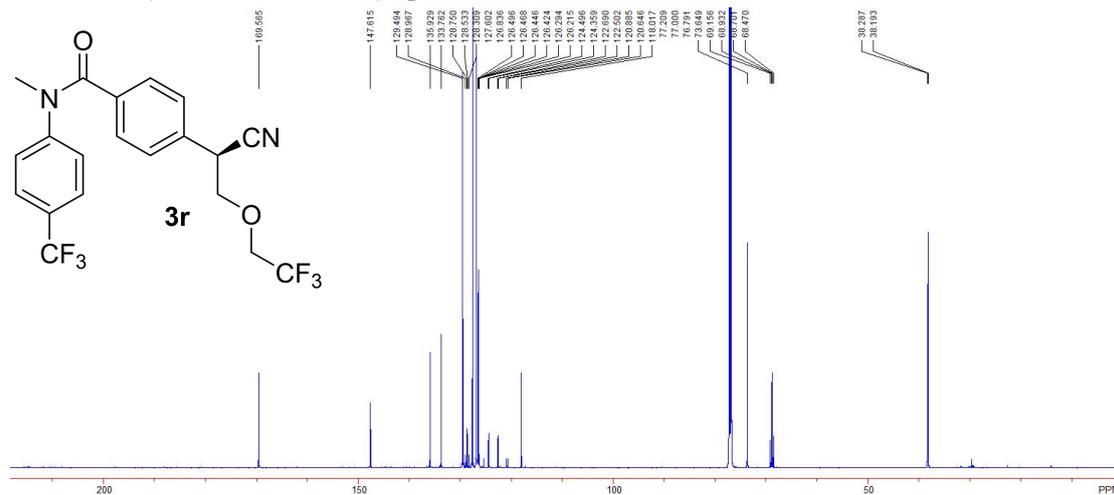
^{19}F NMR (564 MHz, CDCl_3) spectra of **3q**



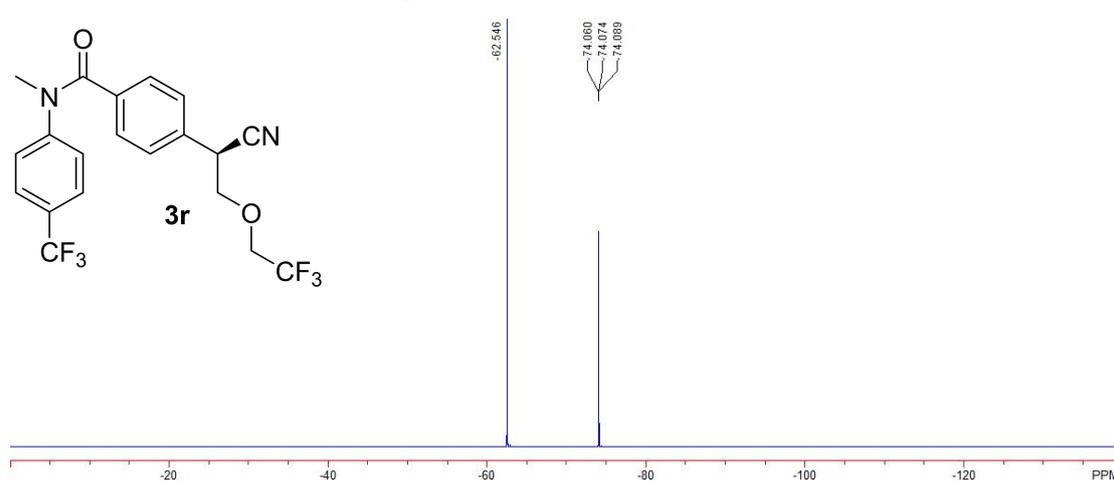
^1H NMR (600 MHz, CDCl_3) spectra of **3r**



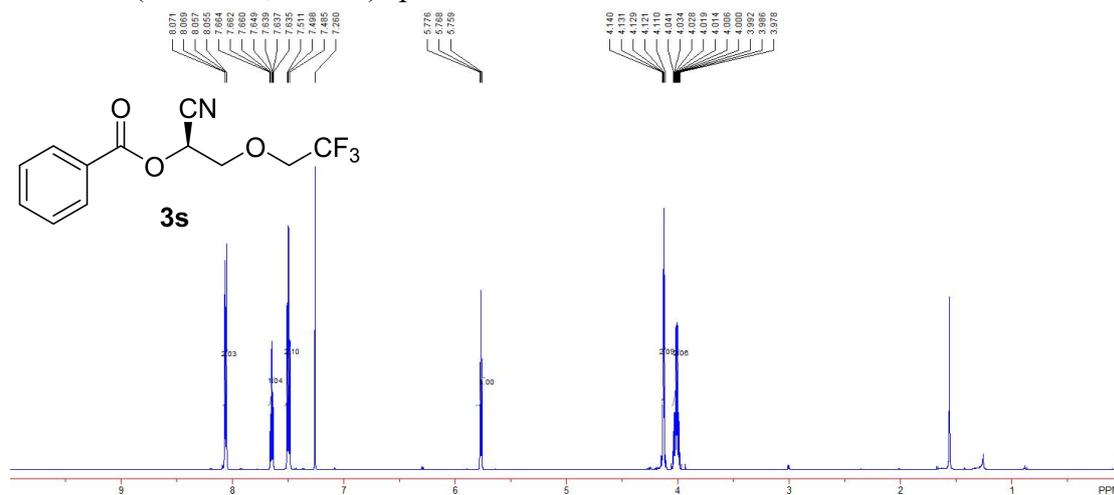
¹³C NMR (150 MHz, CDCl₃) spectra of **3r**



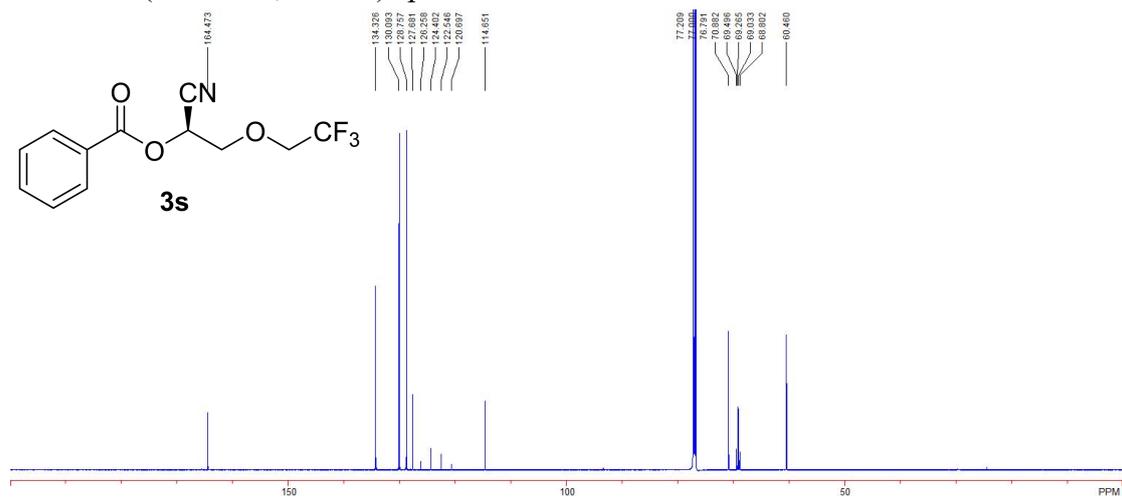
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3r**



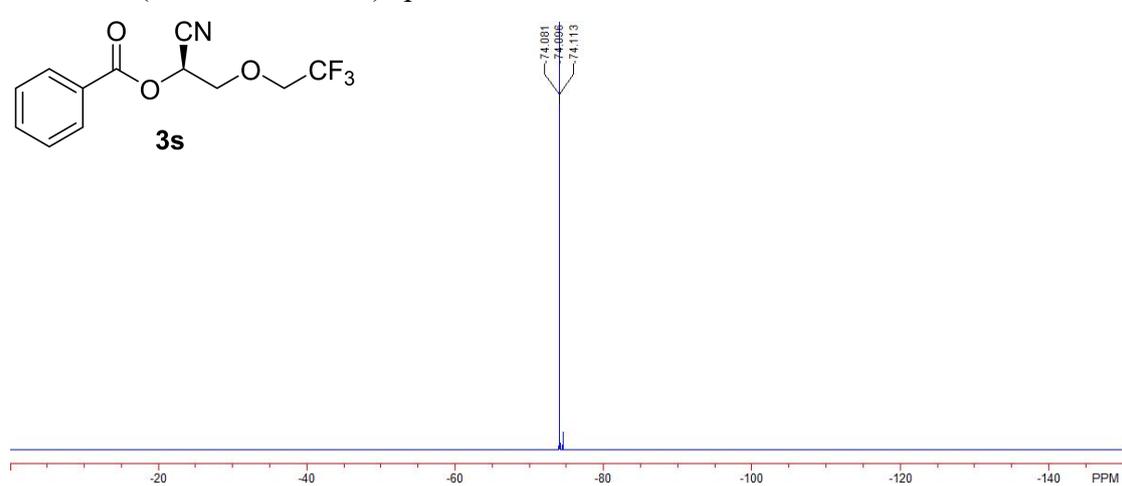
¹H NMR (600 MHz, CDCl₃) spectra of **3s**



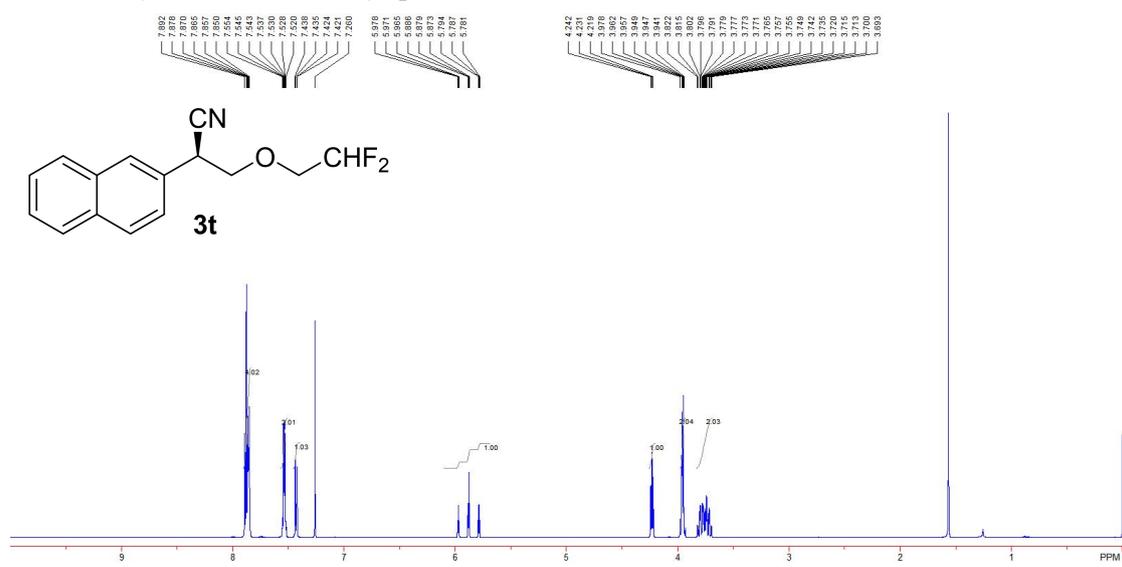
¹³C NMR (150 MHz, CDCl₃) spectra of **3s**



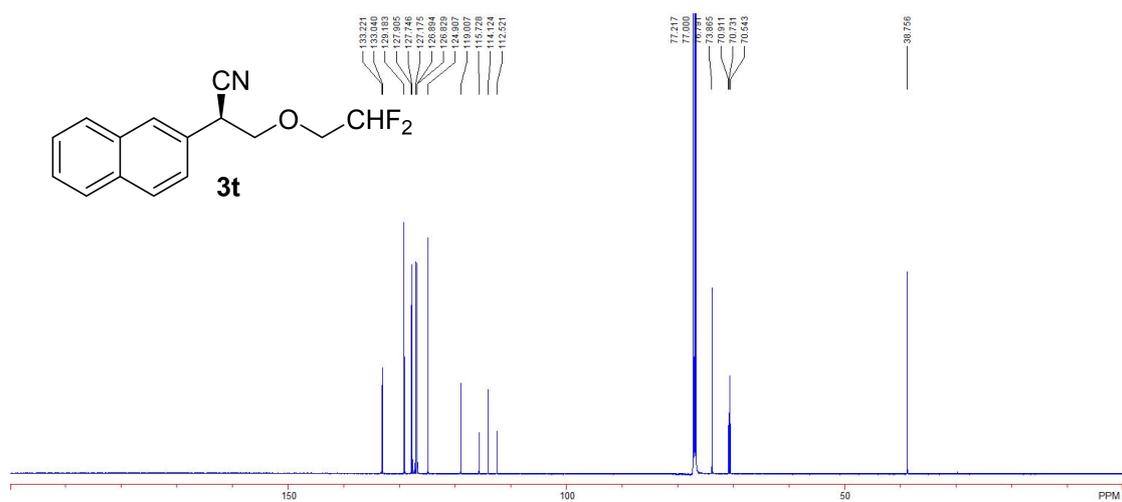
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3s**



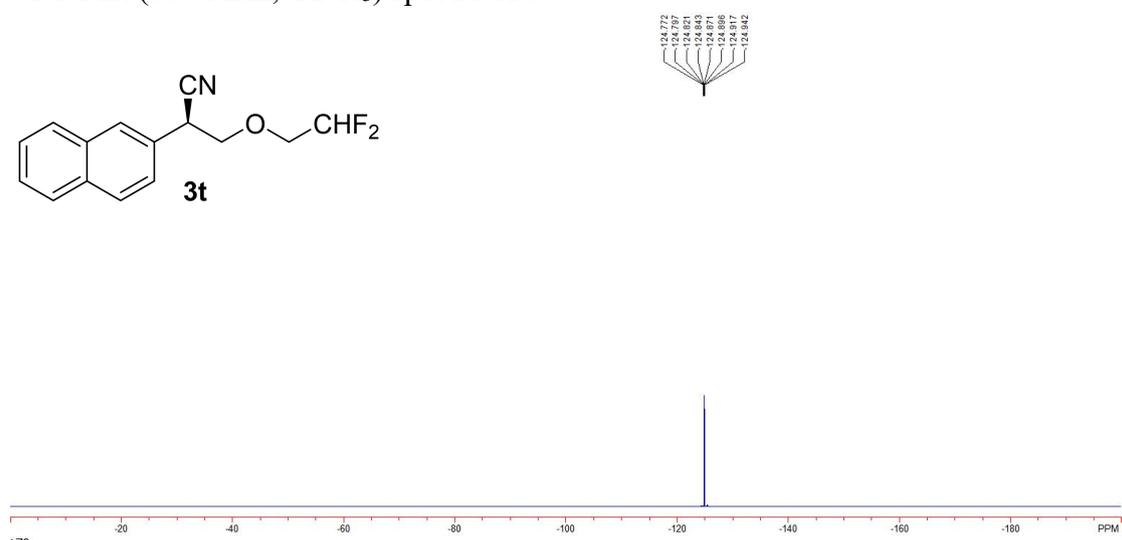
¹H NMR (600 MHz, CDCl₃) spectra of **3t**



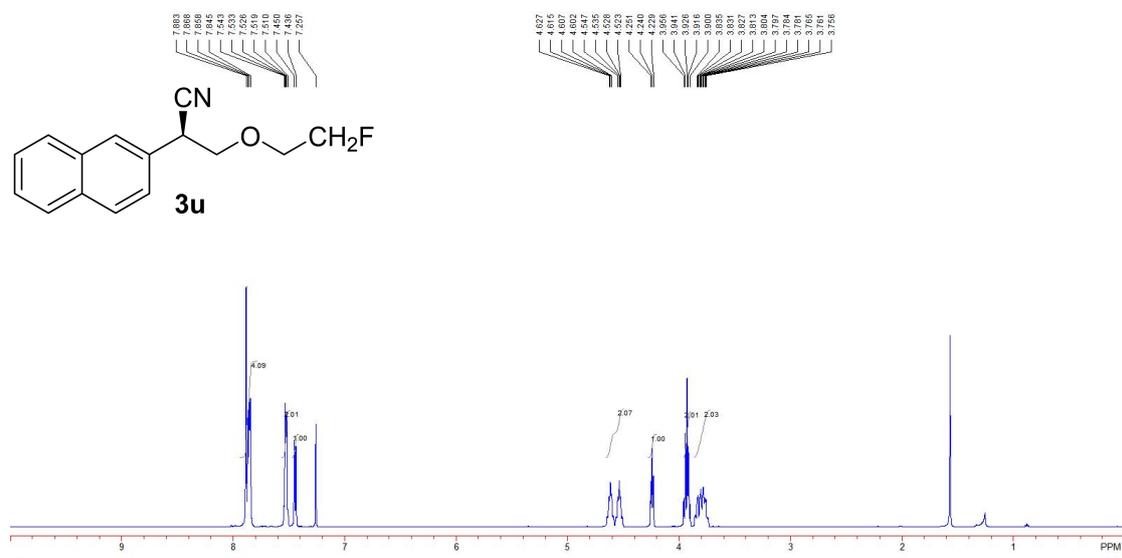
^{13}C NMR (150 MHz, CDCl_3) spectra of **3t**



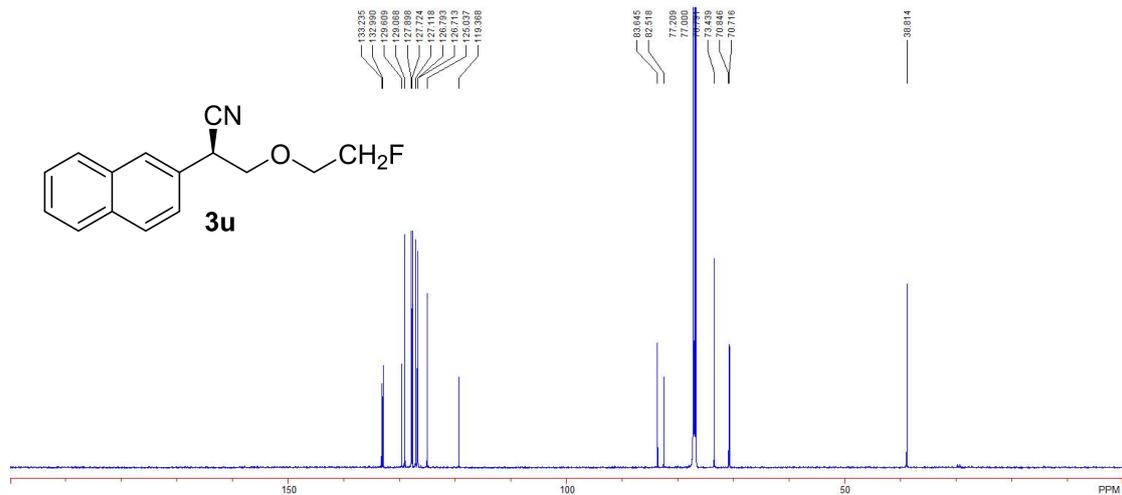
^{19}F NMR (564 MHz, CDCl_3) spectra of **3t**



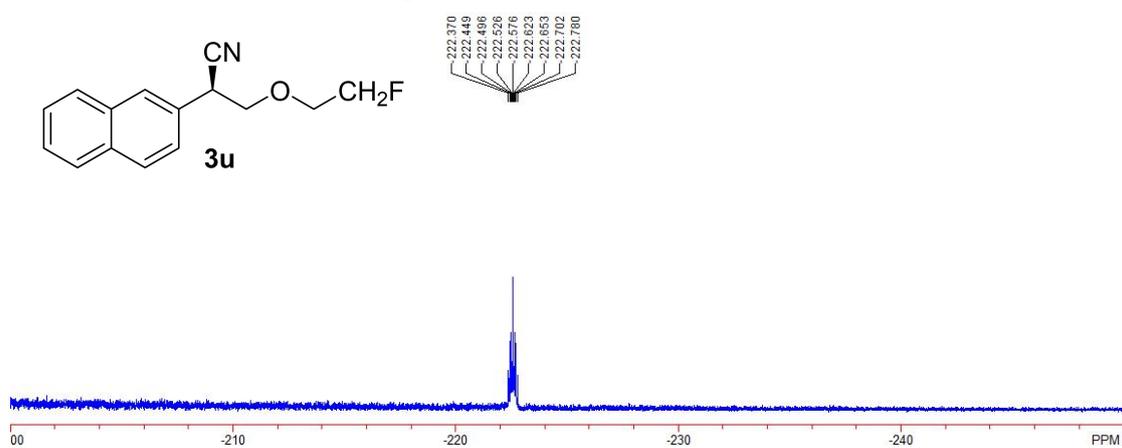
^1H NMR (600 MHz, CDCl_3) spectra of **3u**



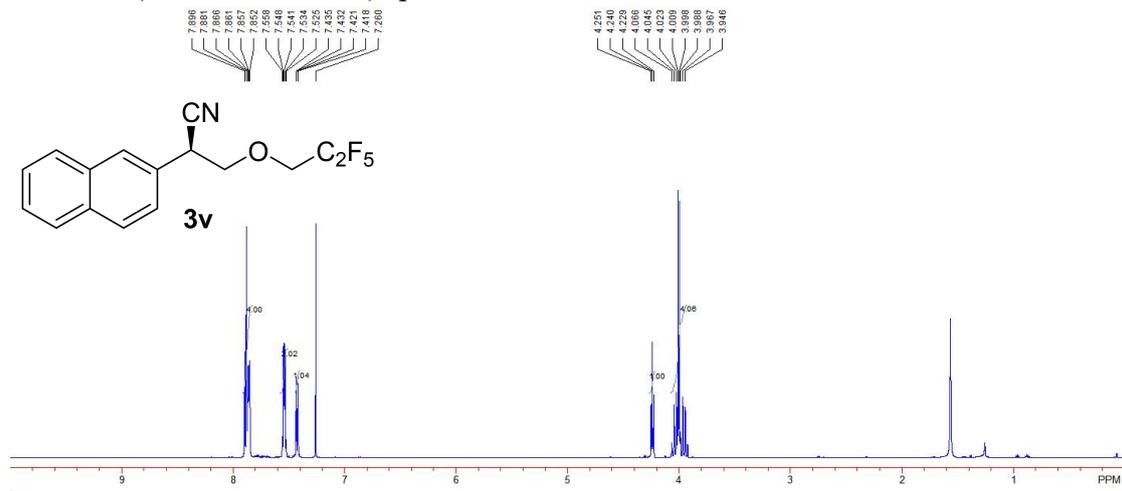
¹³C NMR (150 MHz, CDCl₃) spectra of **3u**



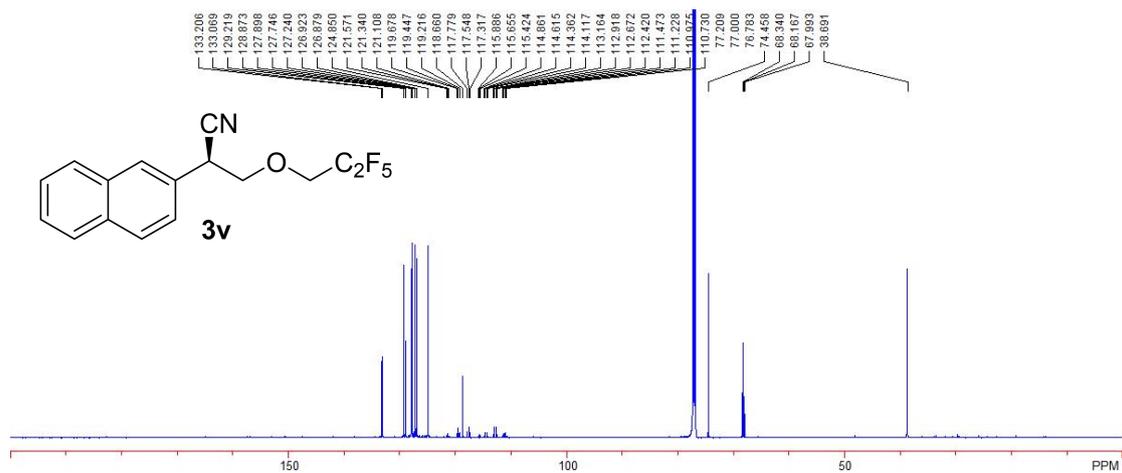
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3u**



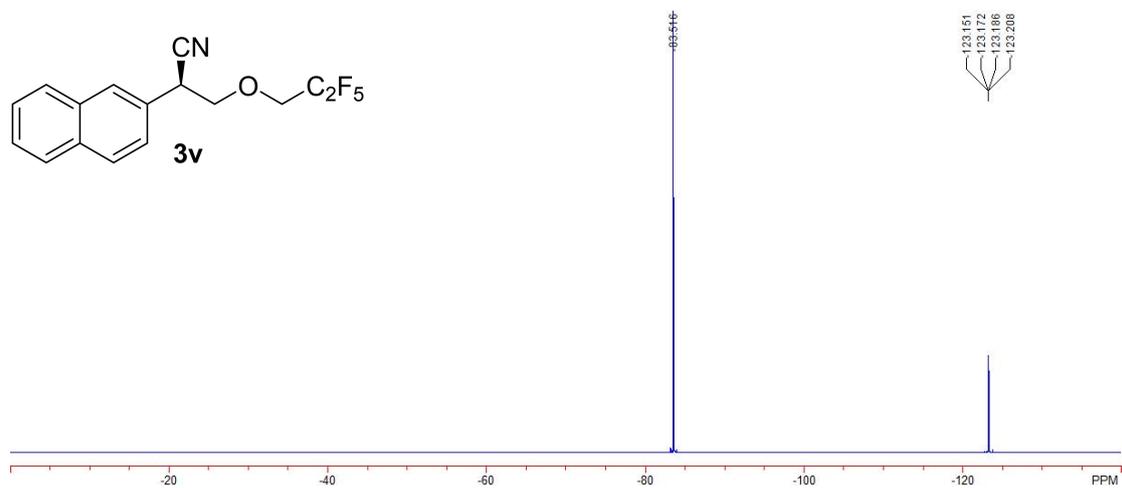
¹H NMR (600 MHz, CDCl₃) spectra of **3v**



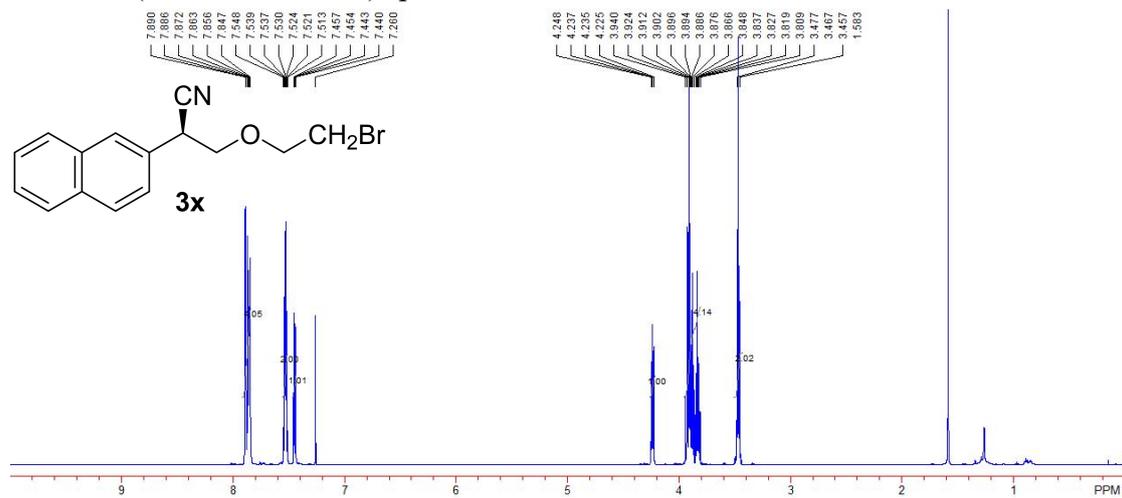
¹³C NMR (150 MHz, CDCl₃) spectra of **3v**



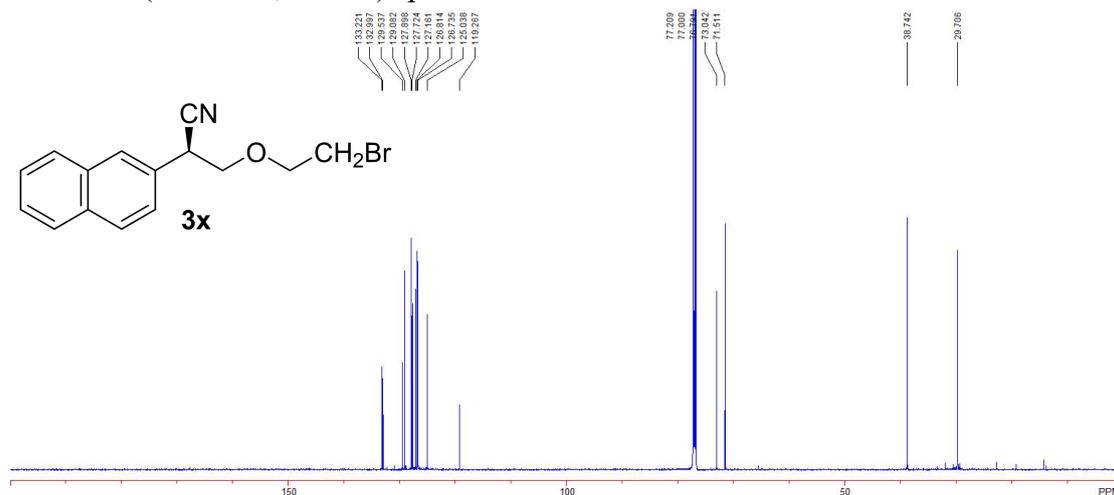
¹⁹F NMR (564 MHz, CDCl₃) spectra of **3v**



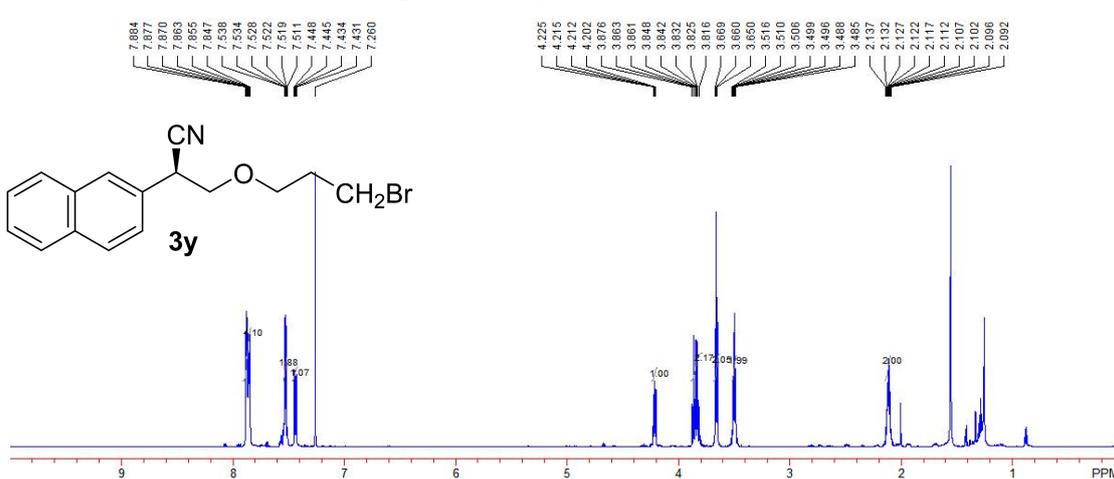
¹H NMR (600 MHz, CDCl₃) spectra of **3x**



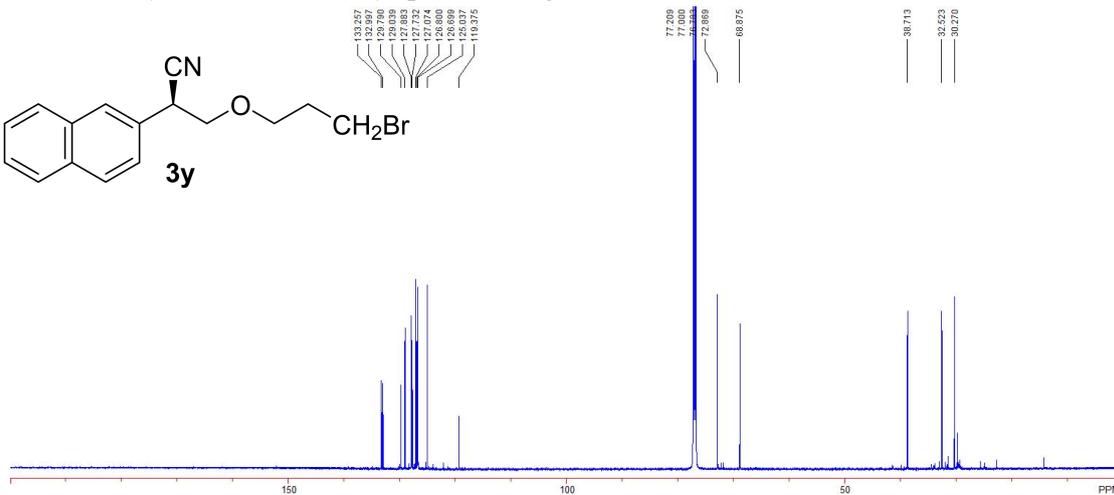
¹³C NMR (150 MHz, CDCl₃) spectra of **3x**



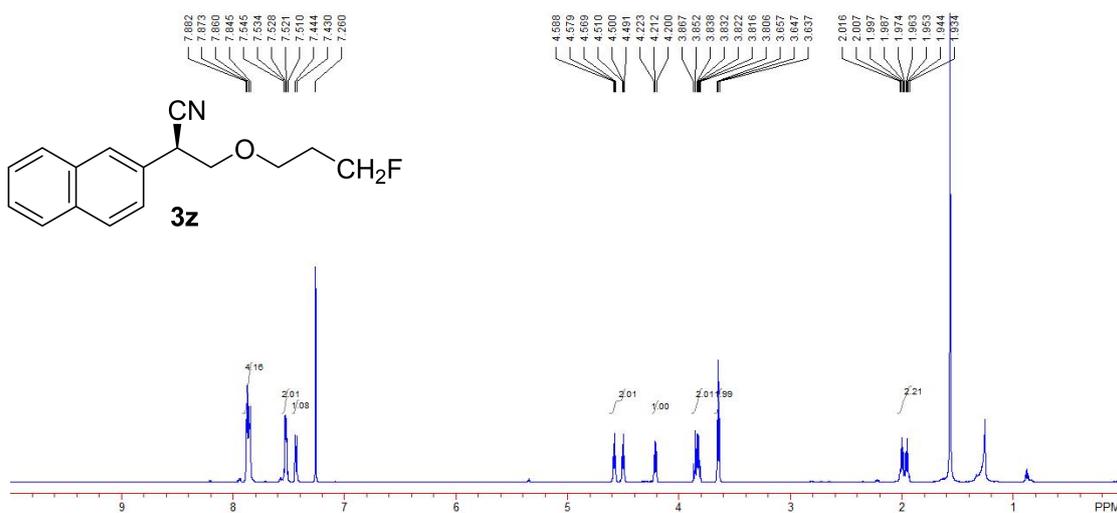
¹H NMR (600 MHz, CDCl₃) spectra of **3y**



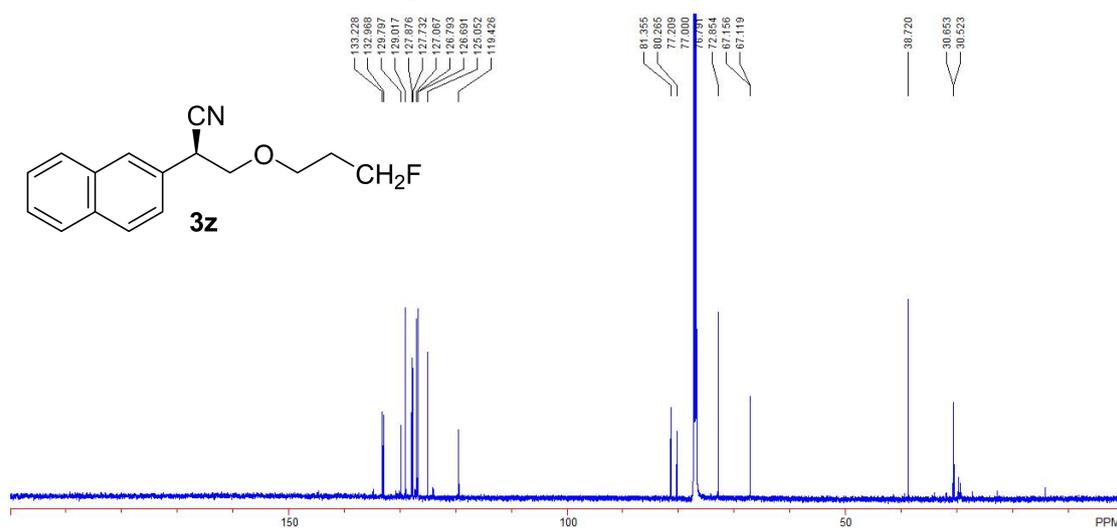
¹³C NMR (150 MHz, CDCl₃) spectra of **3y**



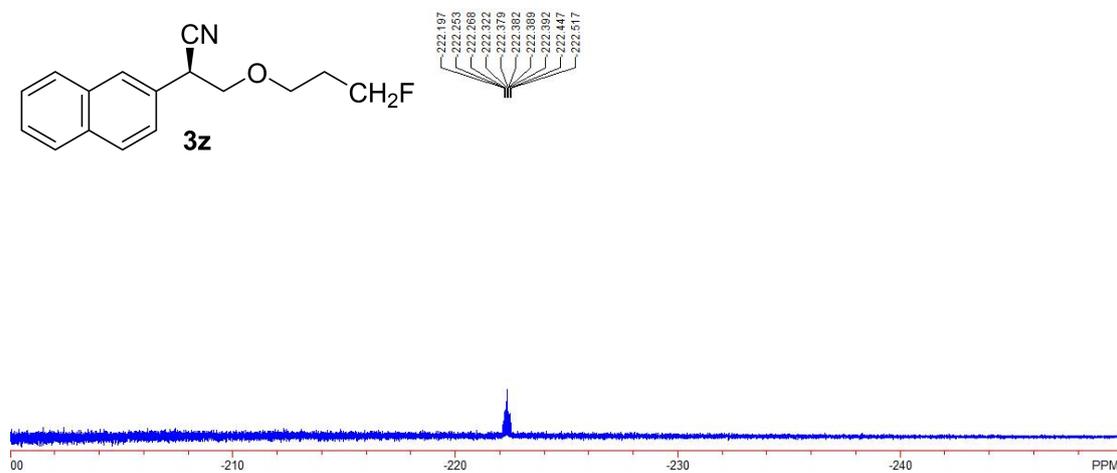
^1H NMR (600 MHz, CDCl_3) spectra of **3z**



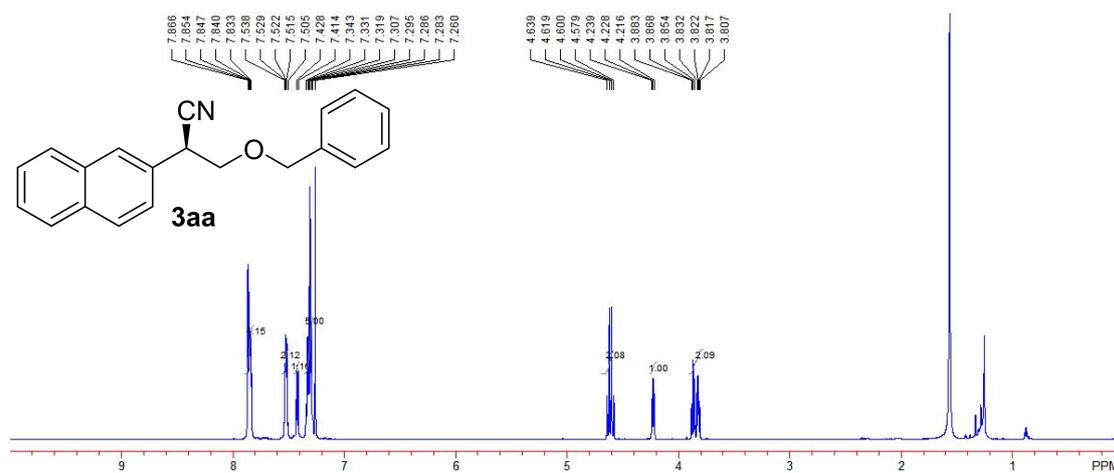
^{13}C NMR (150 MHz, CDCl_3) spectra of **3z**



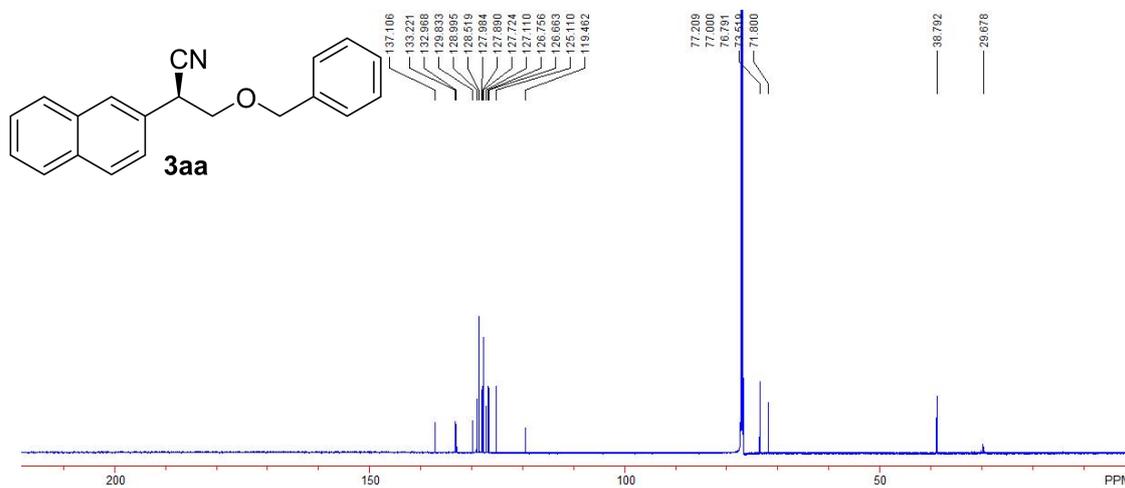
^{19}F NMR (564 MHz, CDCl_3) spectra of **3z**



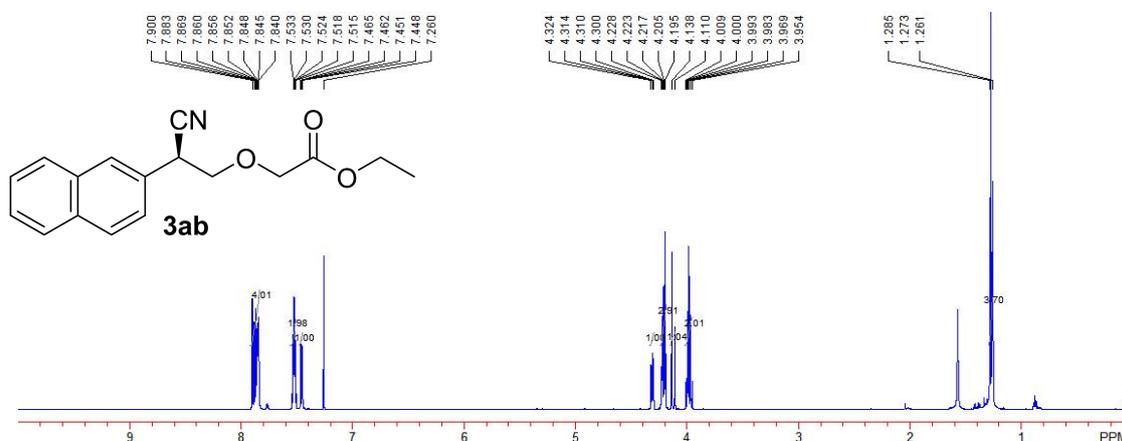
¹H NMR (600 MHz, CDCl₃) spectra of **3aa**



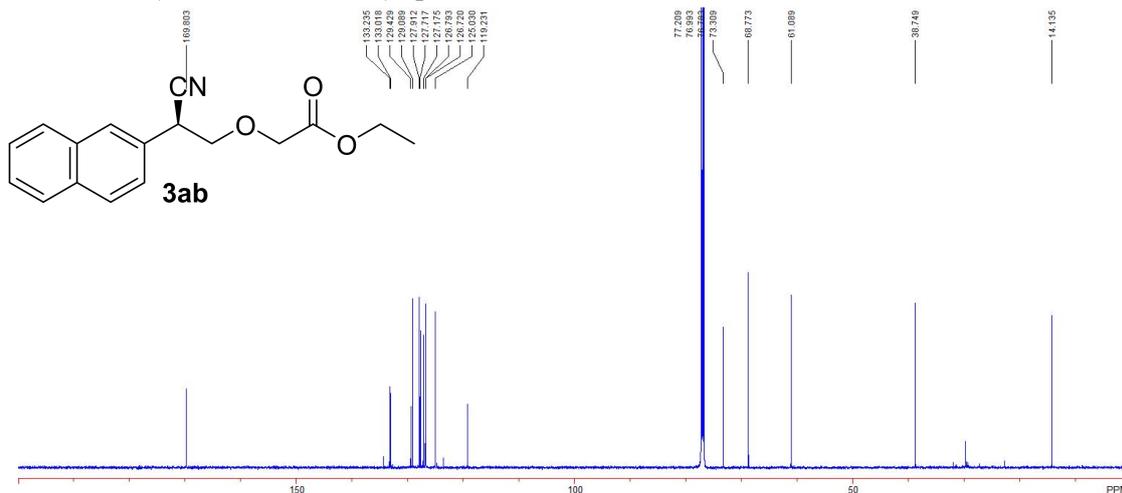
¹³C NMR (150 MHz, CDCl₃) spectra of **3aa**



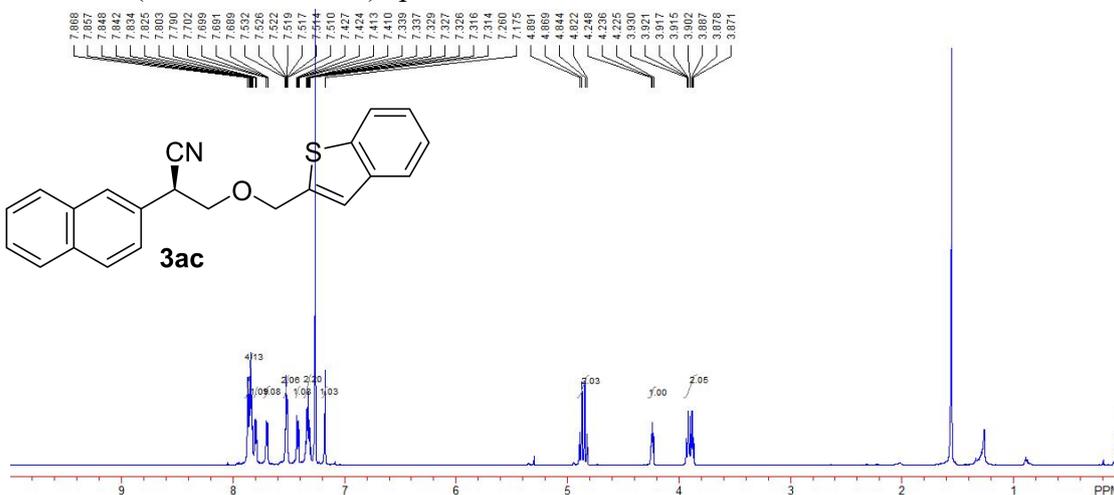
¹H NMR (600 MHz, CDCl₃) spectra of **3ab**



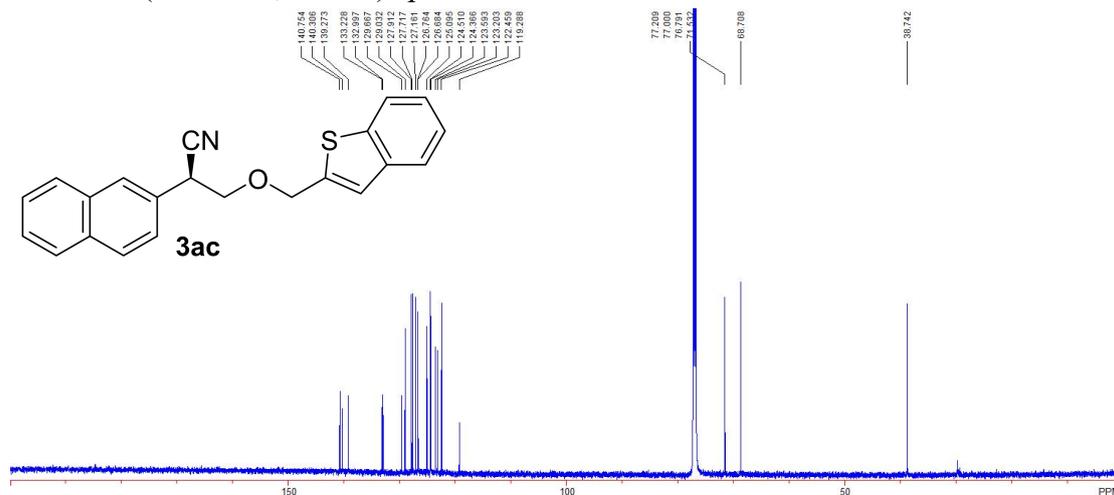
¹³C NMR (150 MHz, CDCl₃) spectra of **3ab**



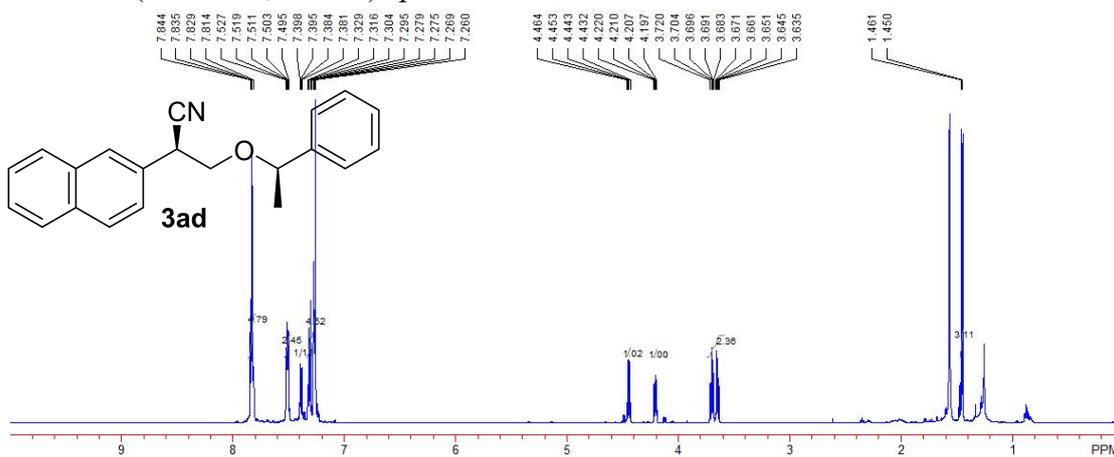
¹H NMR (600 MHz, CDCl₃) spectra of **3ac**



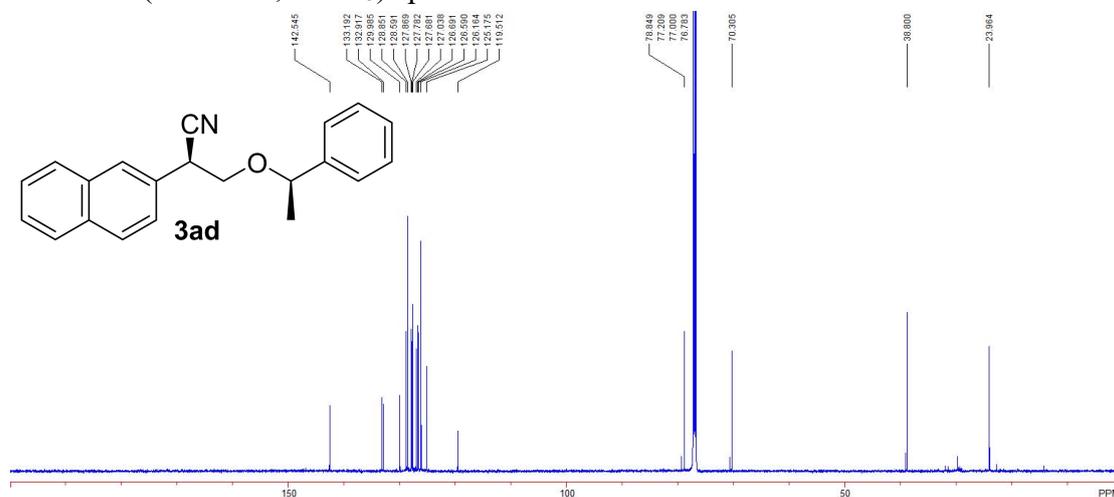
¹³C NMR (150 MHz, CDCl₃) spectra of **3ac**



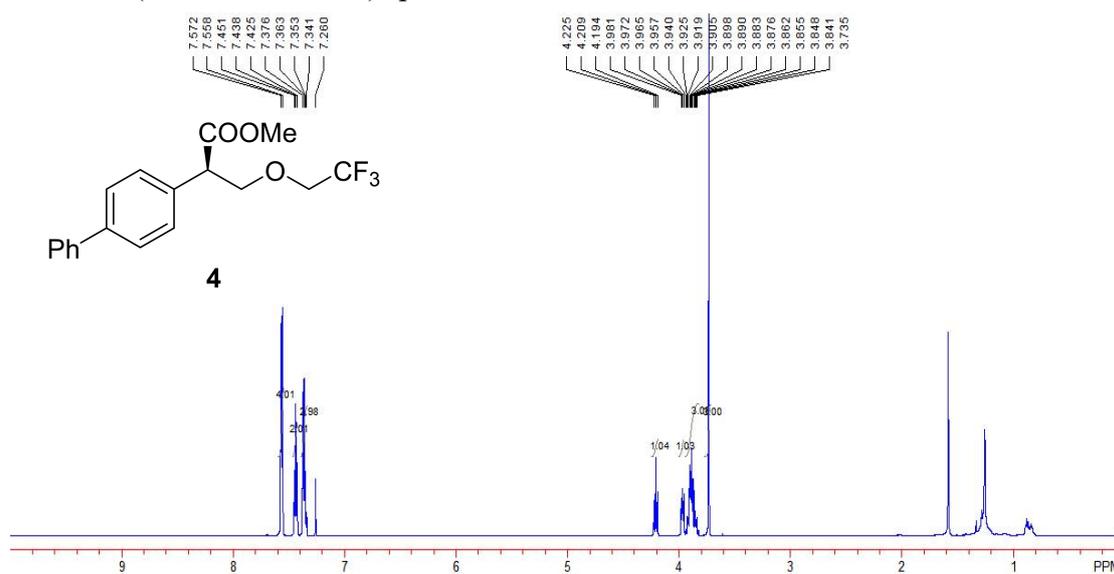
¹H NMR (600 MHz, CDCl₃) spectra of **3ad**



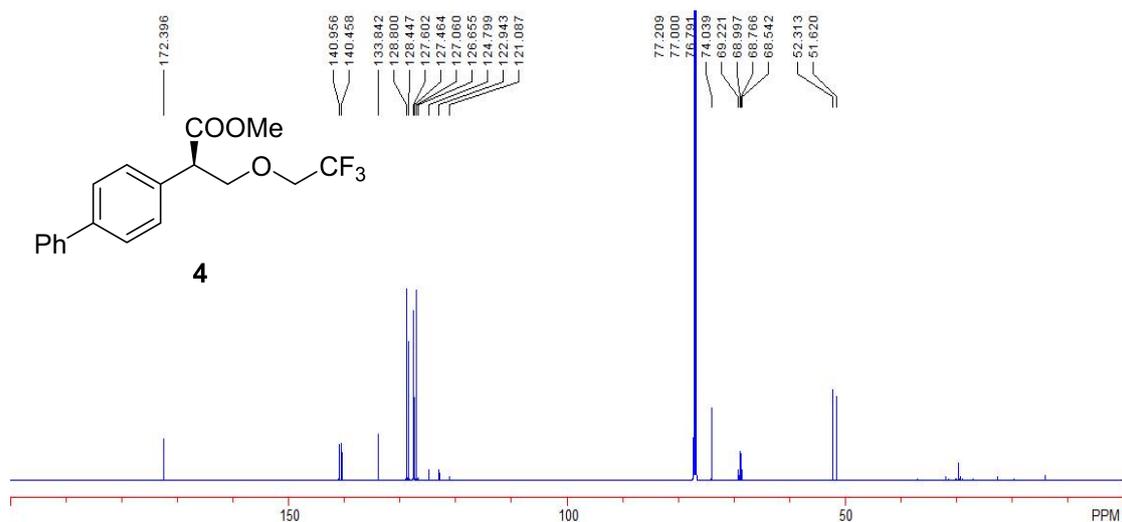
¹³C NMR (150 MHz, CDCl₃) spectra of **3ad**



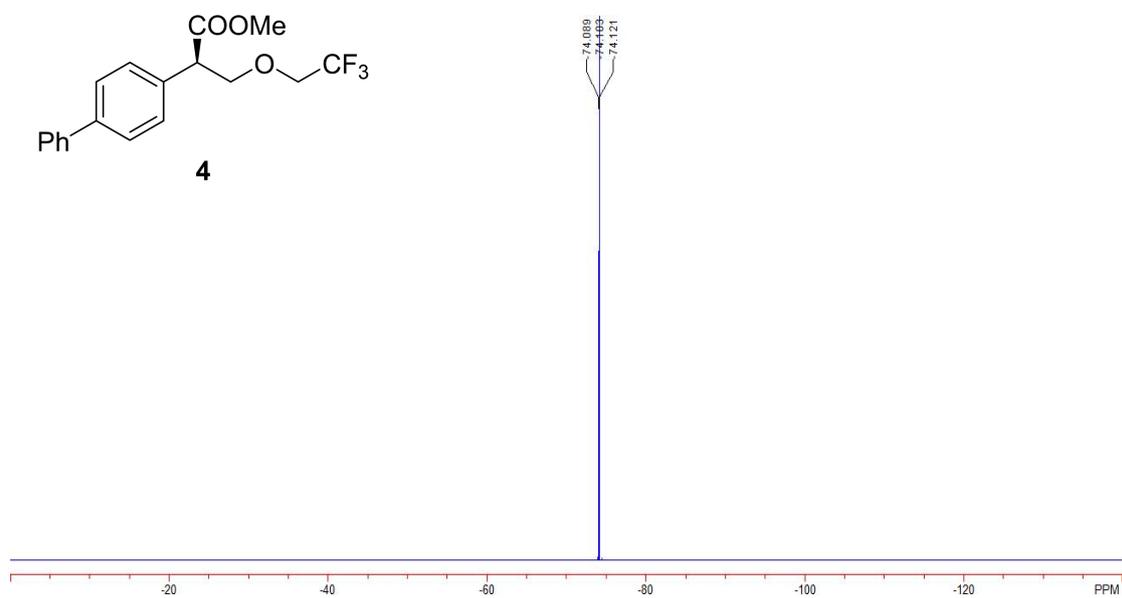
¹H NMR (600 MHz, CDCl₃) spectra of **4**



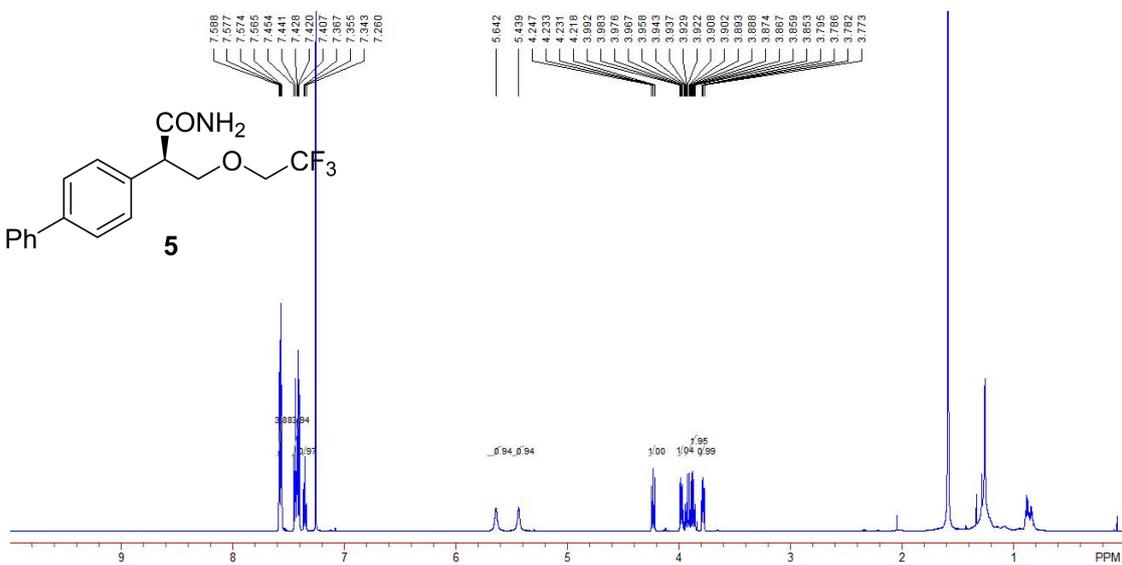
¹³C NMR (150 MHz, CDCl₃) spectra of **4**



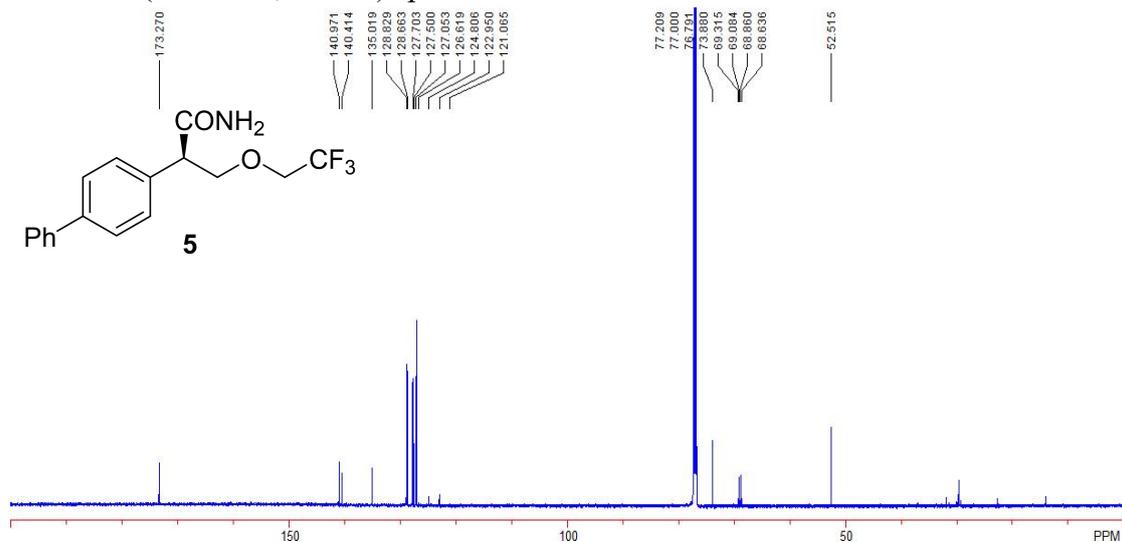
¹⁹F NMR (564 MHz, CDCl₃) spectra of **4**



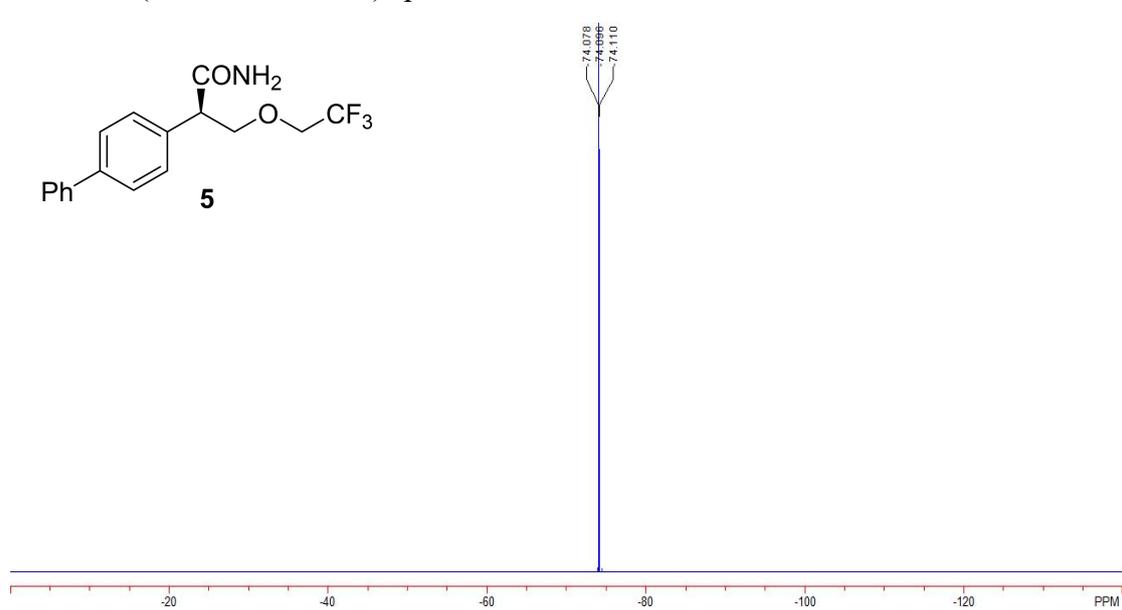
¹H NMR (600 MHz, CDCl₃) spectra of **5**



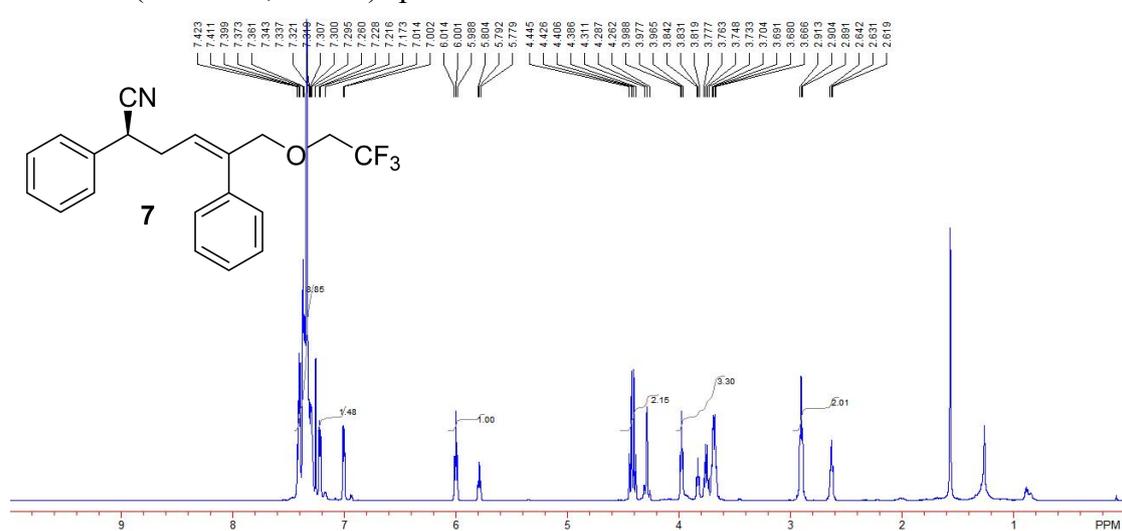
¹³C NMR (150 MHz, CDCl₃) spectra of **5**



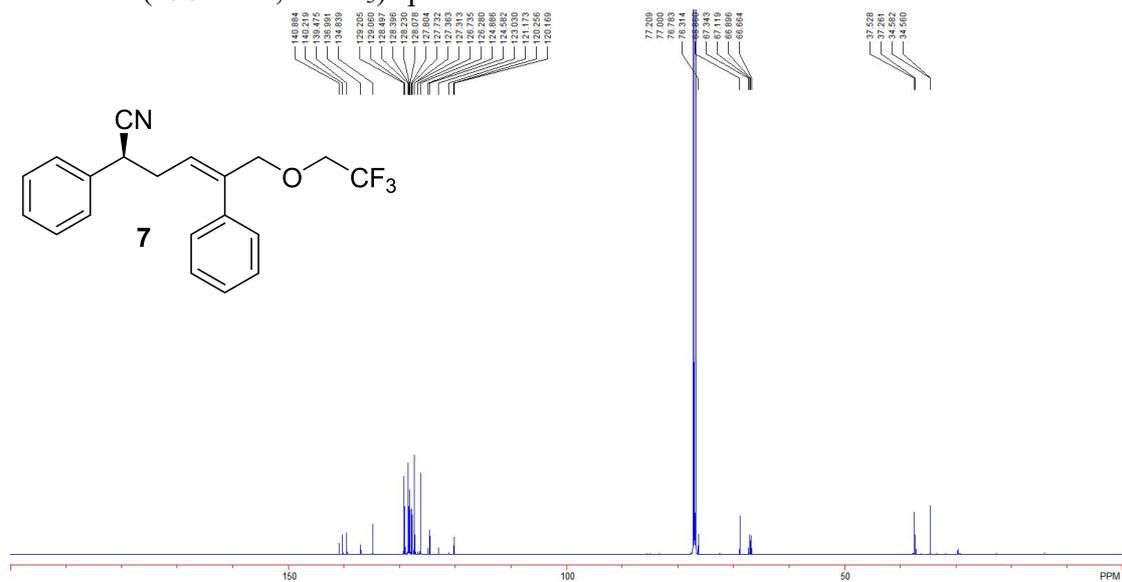
¹⁹F NMR (564 MHz, CDCl₃) spectra of **5**



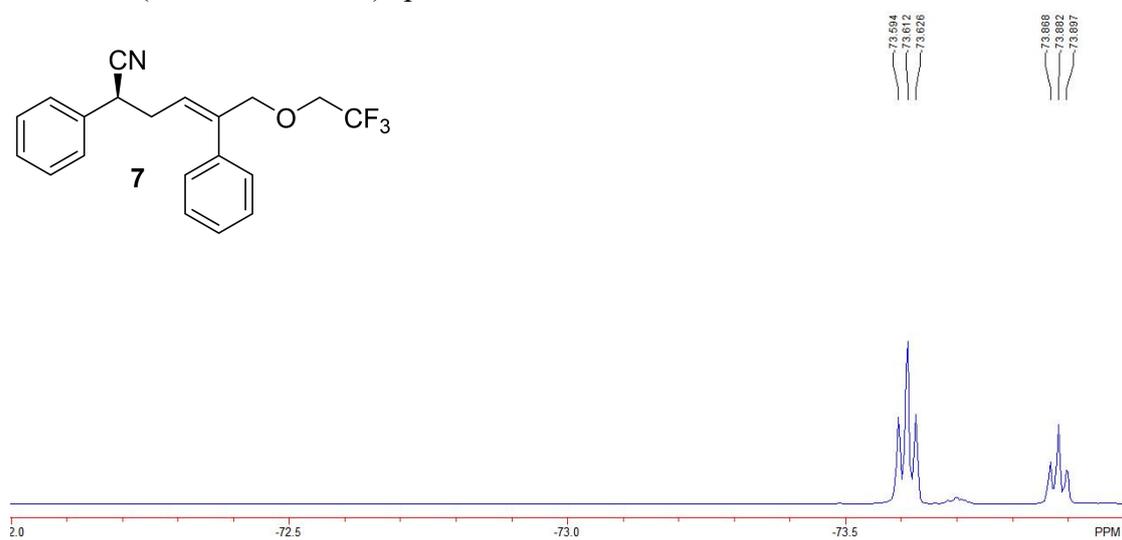
¹H NMR (600 MHz, CDCl₃) spectra of **7**



¹³C NMR (150 MHz, CDCl₃) spectra of **7**

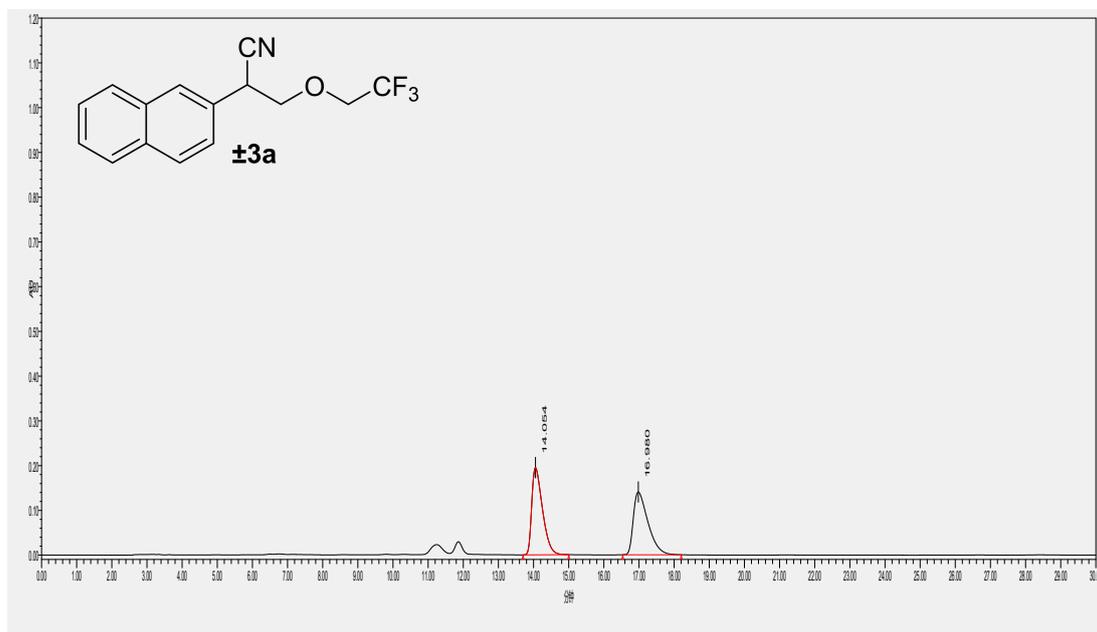


¹⁹F NMR (564 MHz, CDCl₃) spectra of **7**

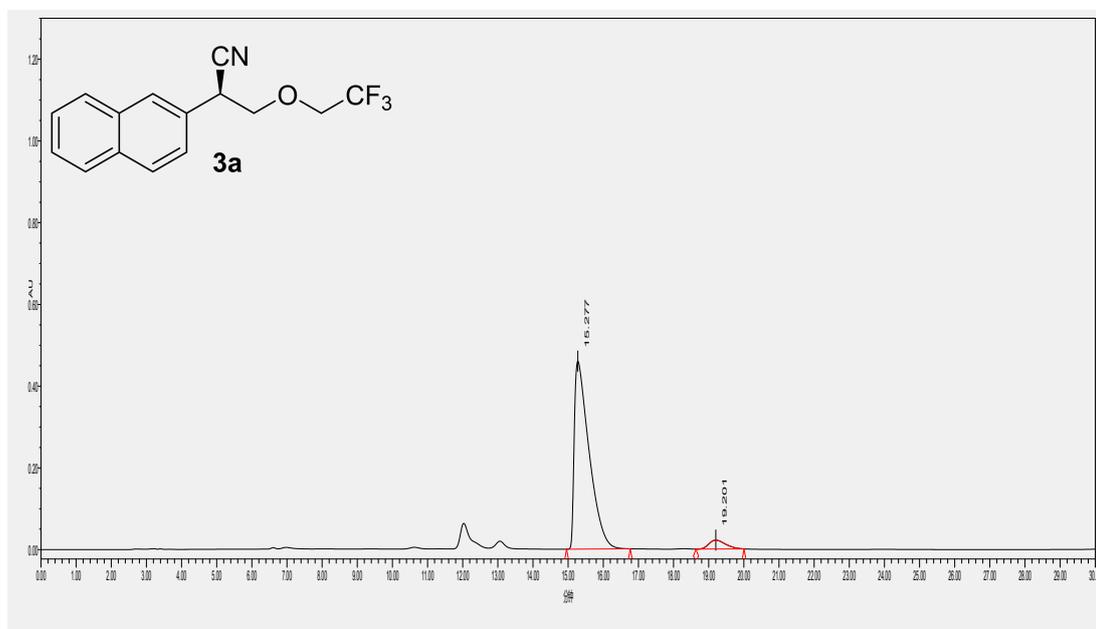


11 HPLC spectra of new compounds

HPLC spectra of 3a

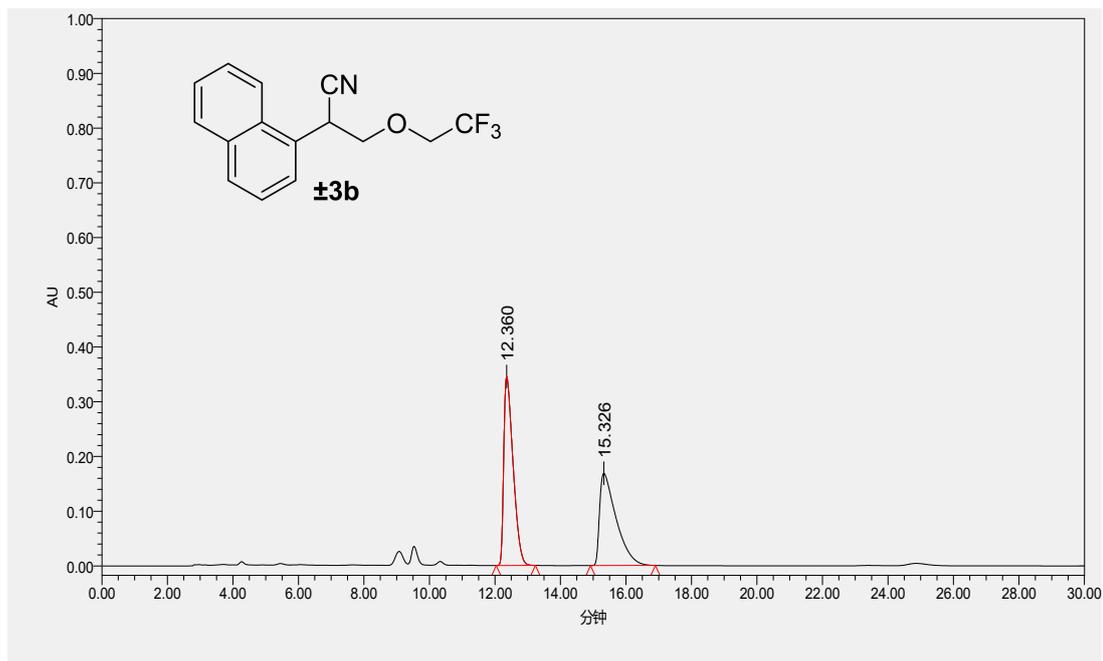


		RT(min)	Area	Area%	Height	Type
1		14.054	4126124	50.44	194817	BB
2		16.980	4053749	49.56	140275	BB

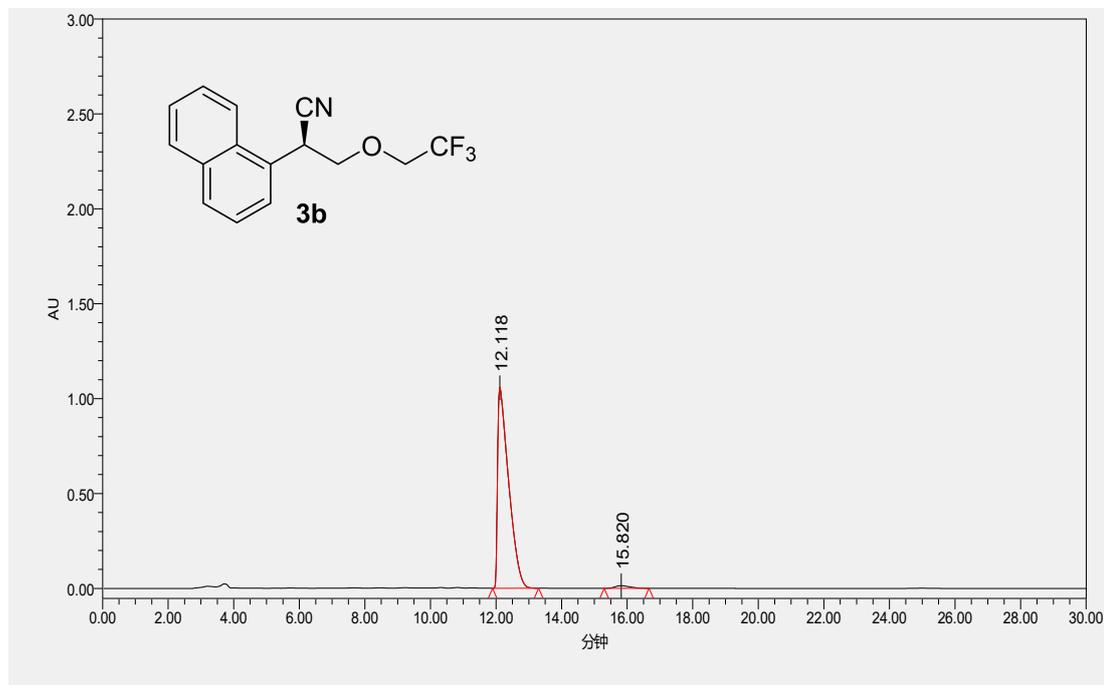


		RT(min)	Area	Area%	Height	Type
1		13.897	5668319	95.04	273011	Bb
2		17.071	295641	4.96	10336	bb

HPLC spectra of **3b**

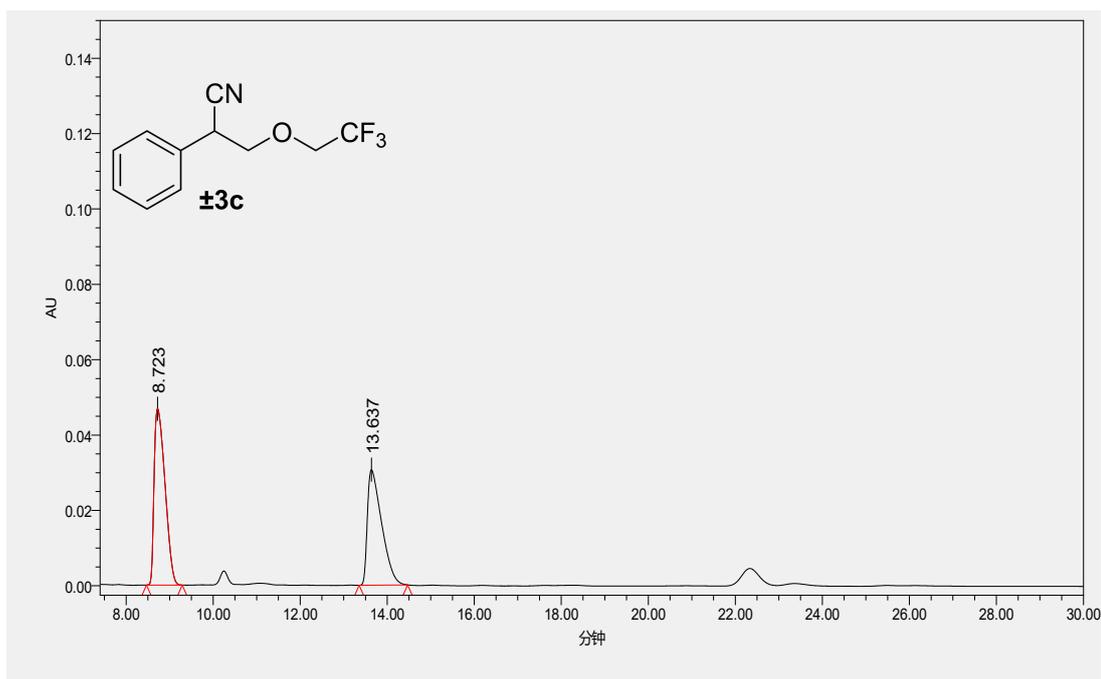


	RT(min)	Area	Area%	Height	Type
1	12.360	6811714	53.52	345074	BB
2	15.326	5914559	46.48	168644	BB

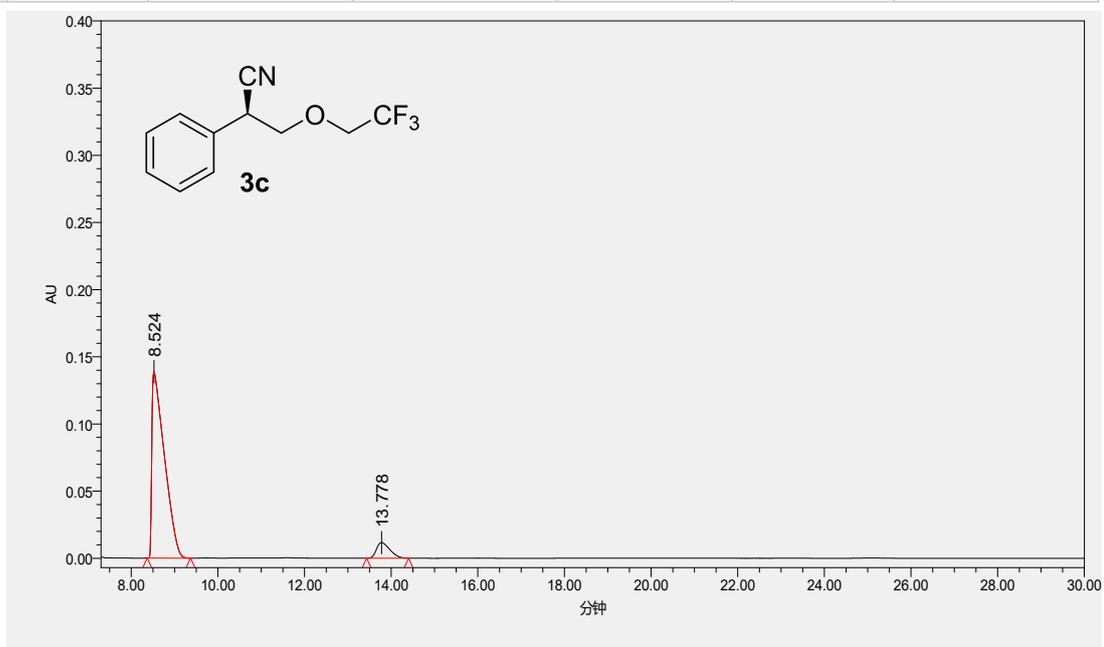


	RT(min)	Area	Area%	Height	Type
1	12.118	24781514	98.27	1056776	BB
2	15.820	436106	1.73	13805	BB

HPLC spectra of **3c**

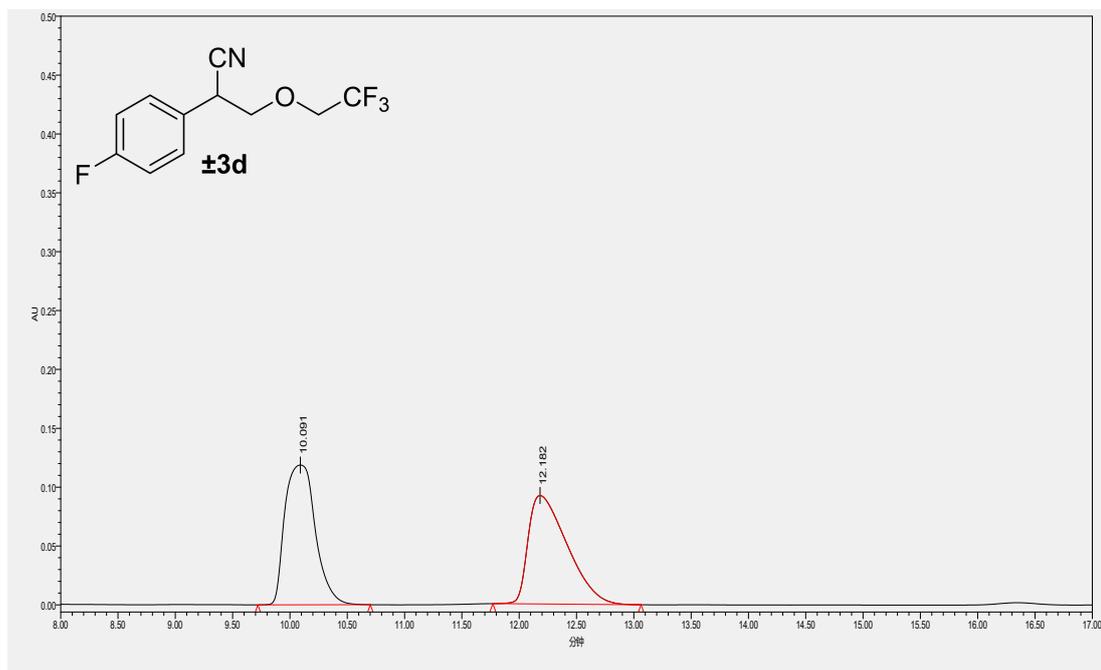


	RT(min)	Area	Area%	Height	Type
1	8.723	813497	53.81	46786	BB
2	13.637	698216	46.19	30667	BB

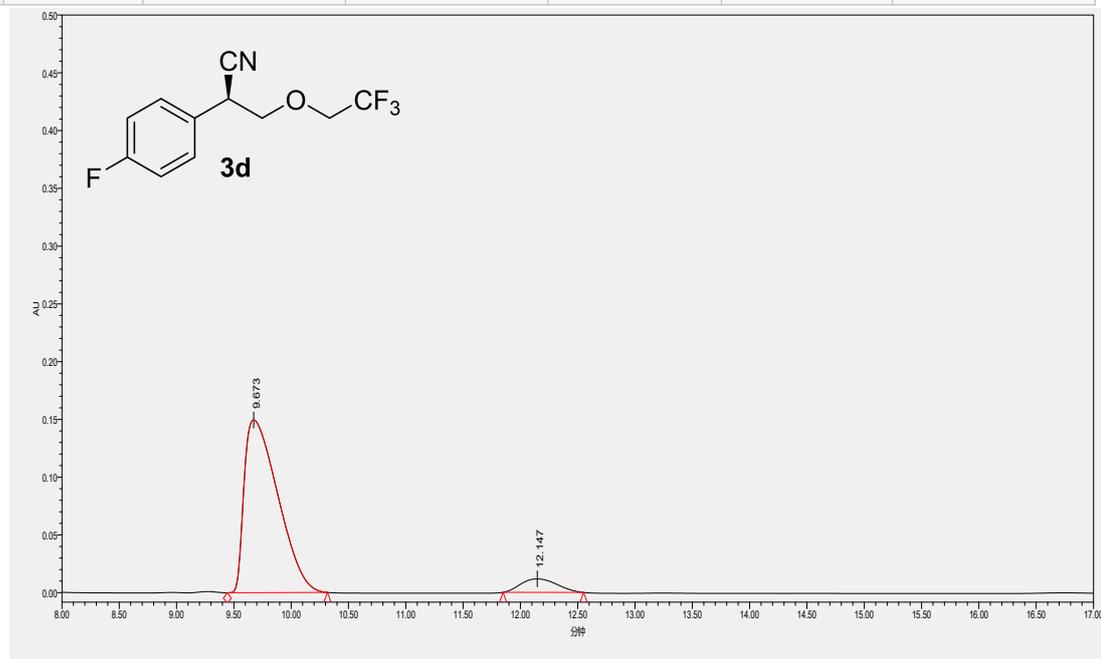


	RT(min)	Area	Area%	Height	Type
1	8.524	2793877	91.82	138807	BB
2	13.778	248920	8.18	11612	BB

HPLC spectra of 3d

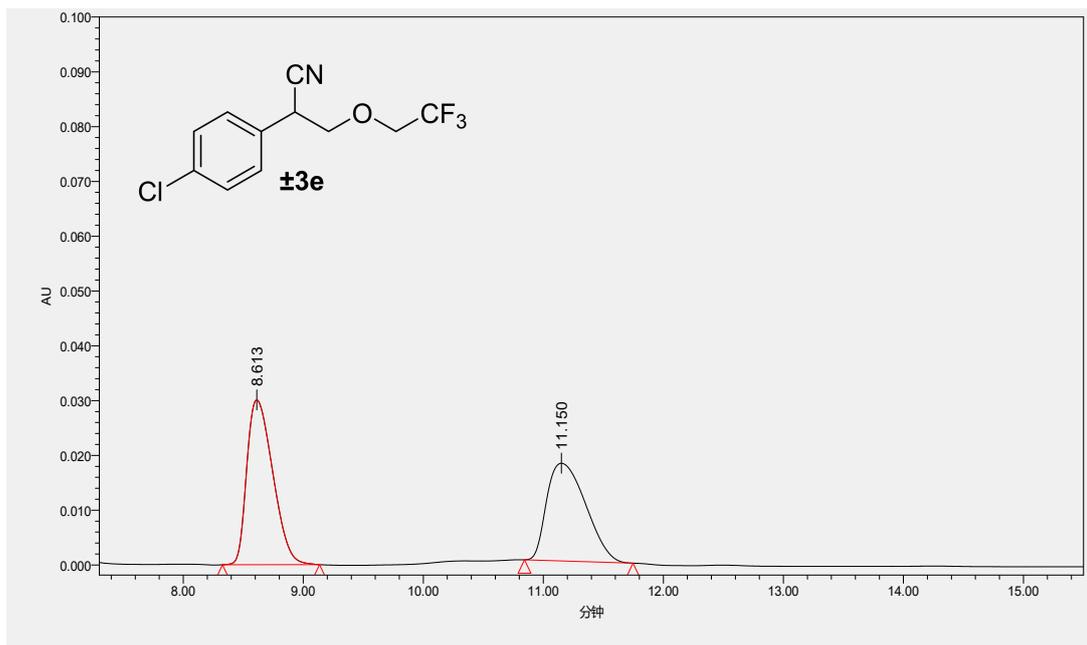


	RT(min)	Area	Area%	Height	Type
1	10.091	2197911	50.23	118705	BB
2	12.182	2177928	49.77	92158	BB

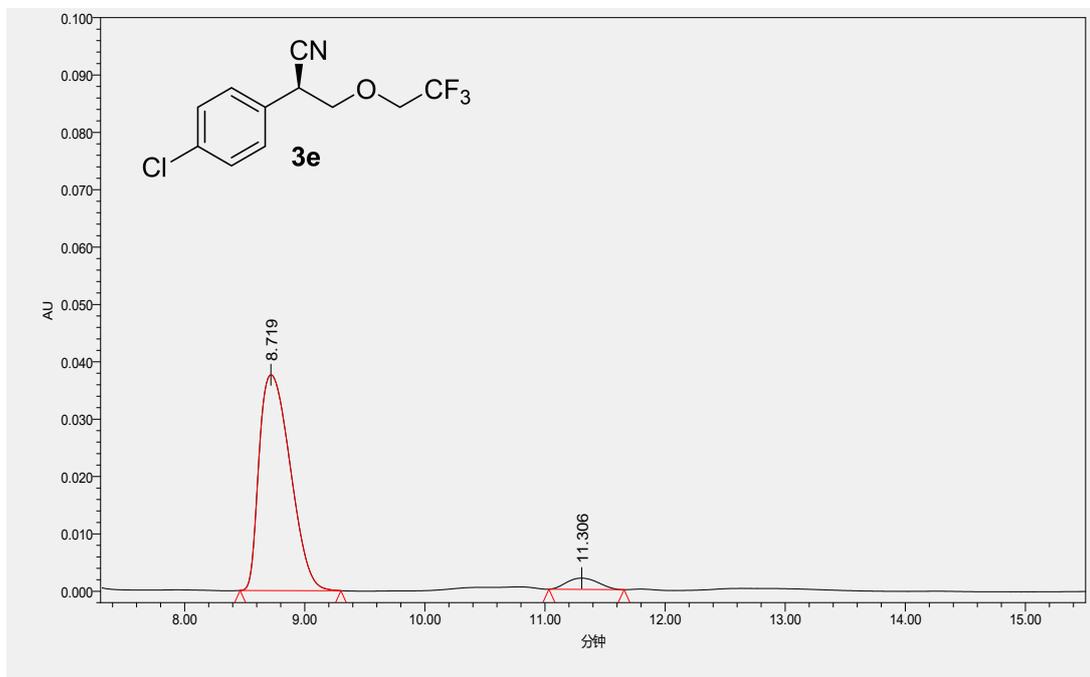


	RT(min)	Area	Area%	Height	Type
1	9.673	3060029	92.28	149518	Vb
2	12.147	255943	7.72	11671	bb

HPLC spectra of **3e**

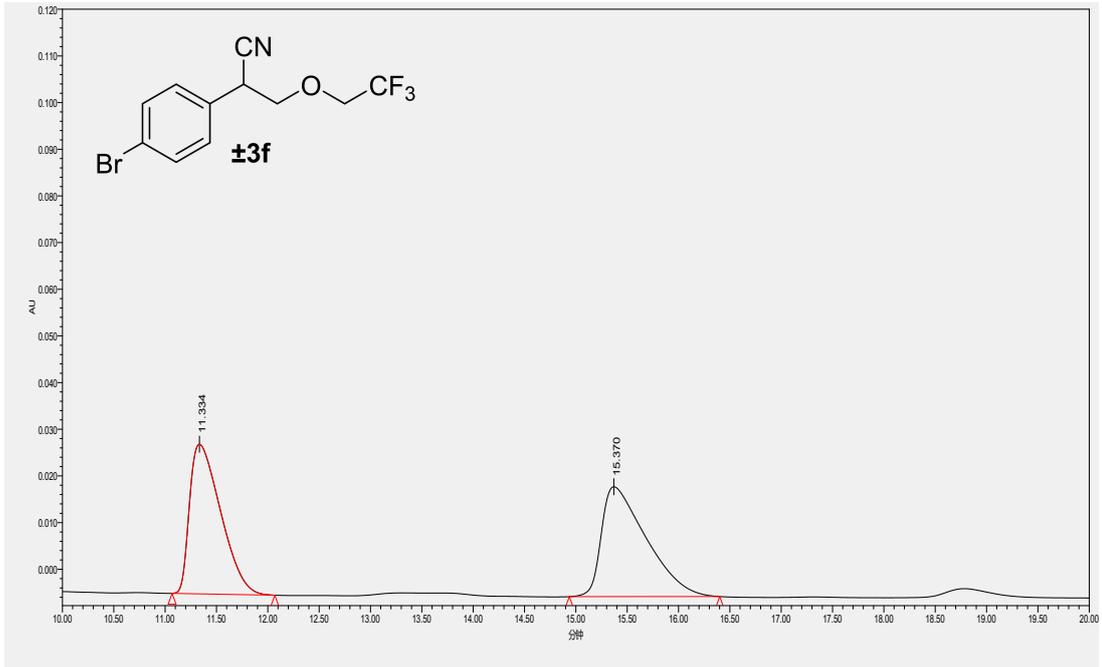


	RT(min)	Area	Area%	Height	Type
1	8.613	452475	52.92	30088	BB
2	11.150	402560	47.08	17830	BB

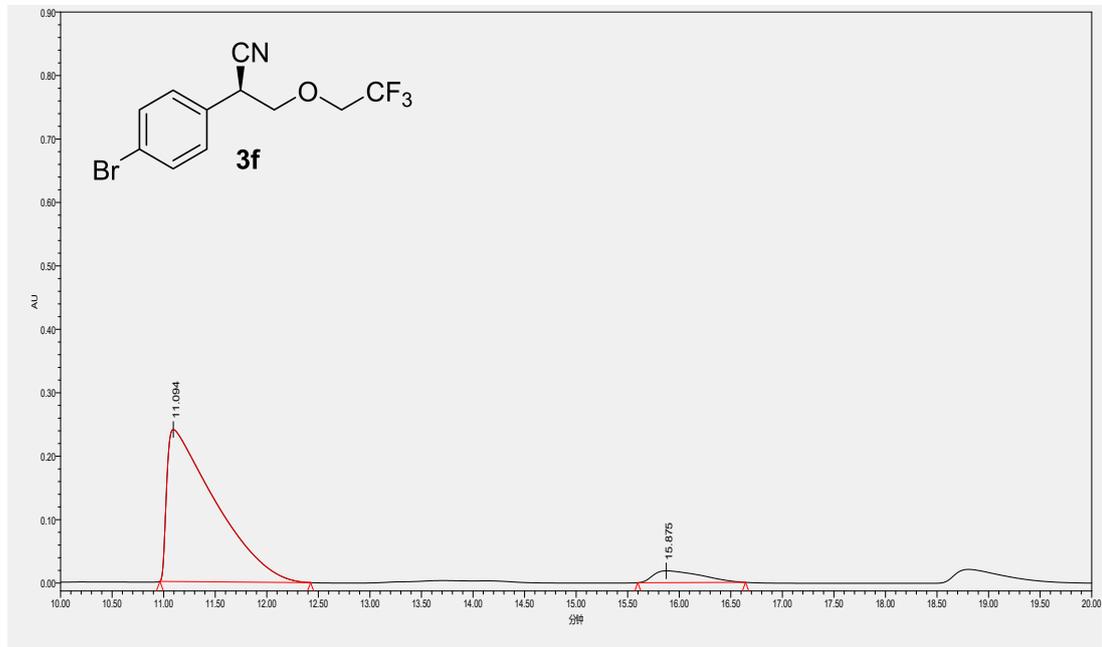


	RT(min)	Area	Area%	Height	Type
1	8.719	677845	94.93	37604	BB
2	11.306	36178	5.07	1967	BB

HPLC spectra of **3f**

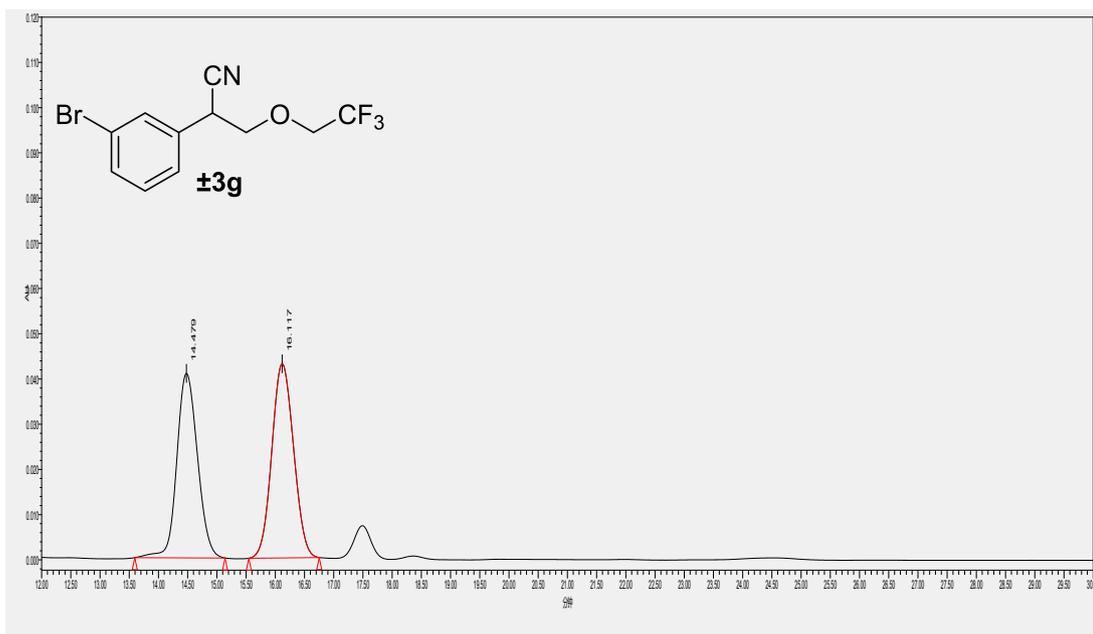


	RT(min)	Area	Area%	Height	Type
1	11.334	674695	48.62	32062	BB
2	15.370	713131	51.38	23543	BB

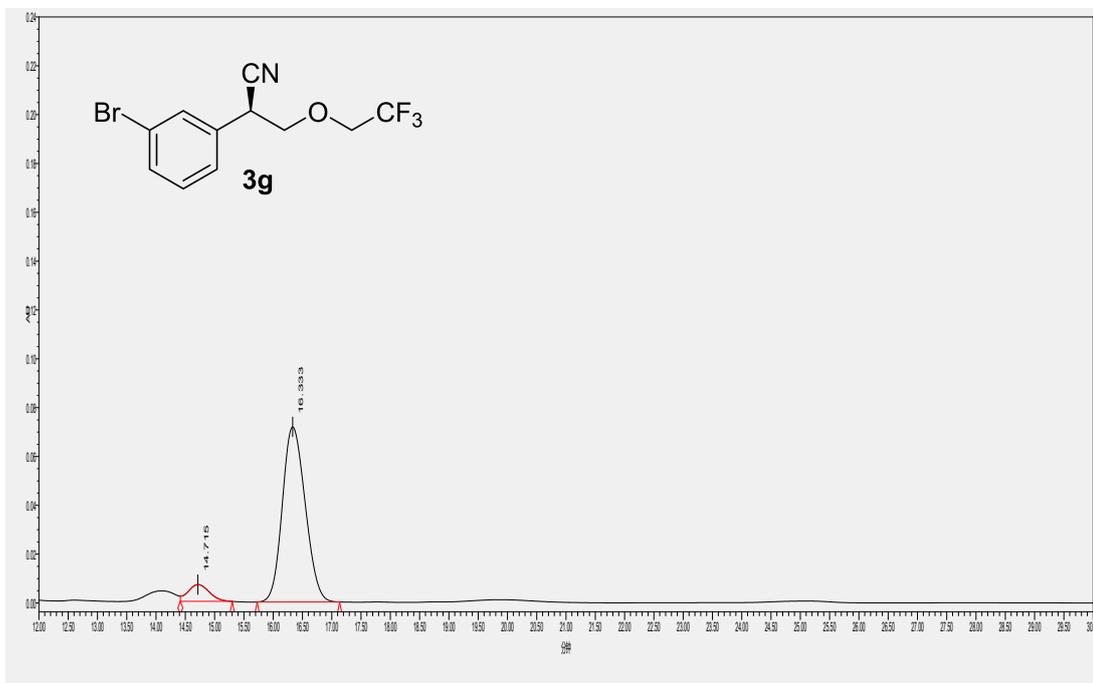


	RT(min)	Area	Area%	Height	Type
1	11.094	7851299	92.94	239578	bb
2	15.875	596470	7.06	18633	bb

HPLC spectra of **3g**

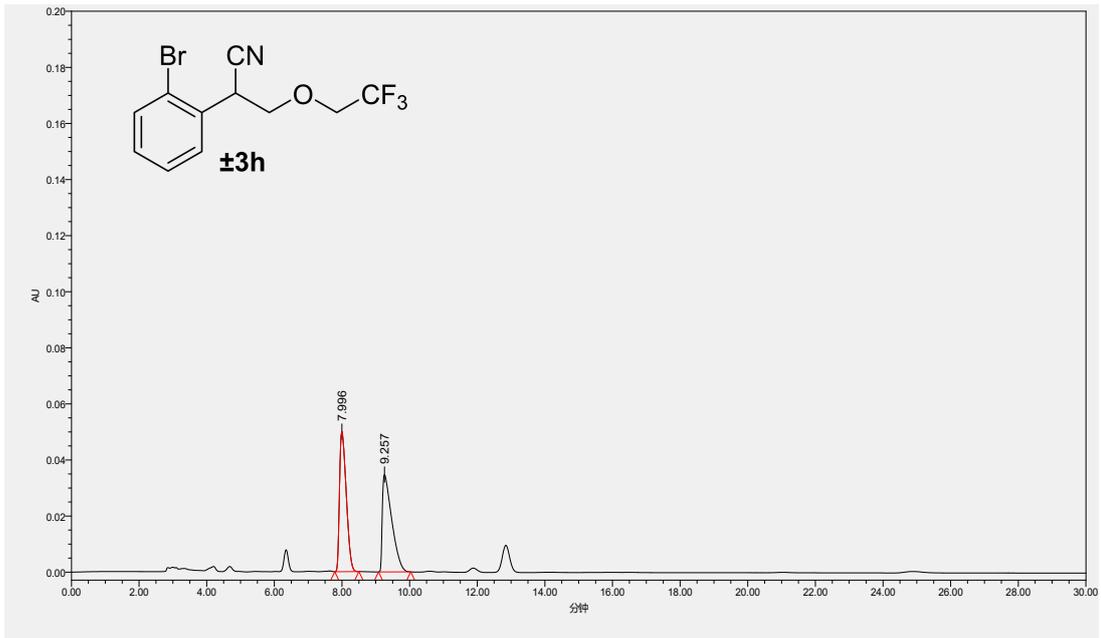


	RT(min)	Area	Area%	Height	Type
1	14.479	989266	47.46	40590	bb
2	16.117	1095081	52.54	42660	bV

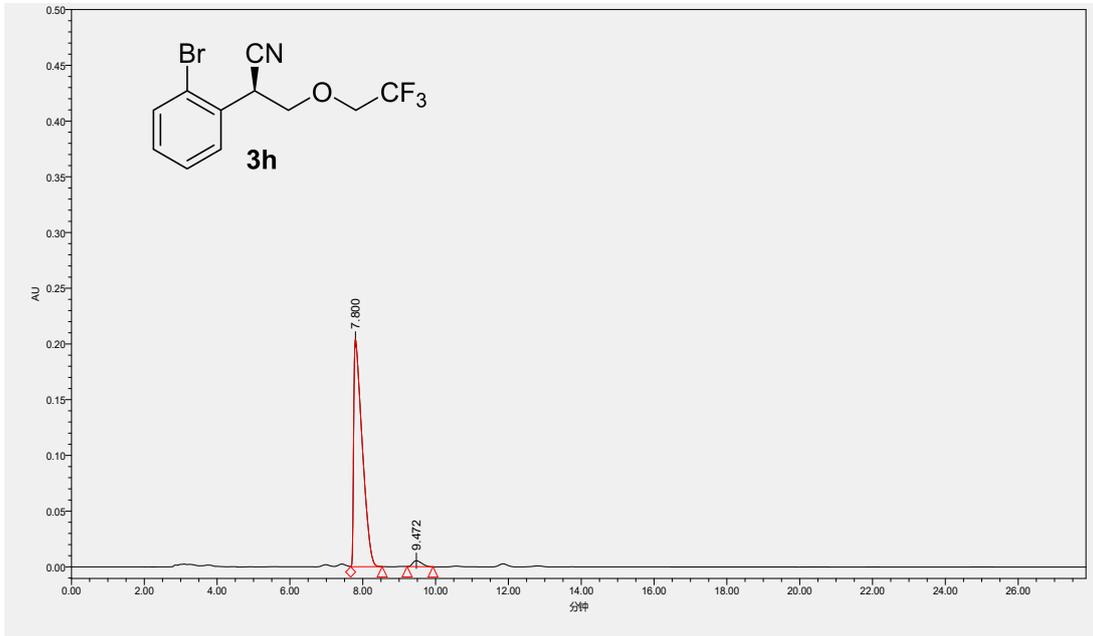


	RT(min)	Area	Area%	Height	Type
1	14.715	173343	8.16	6862	VB
2	16.333	1950526	91.84	71723	BB

HPLC spectra of **3h**

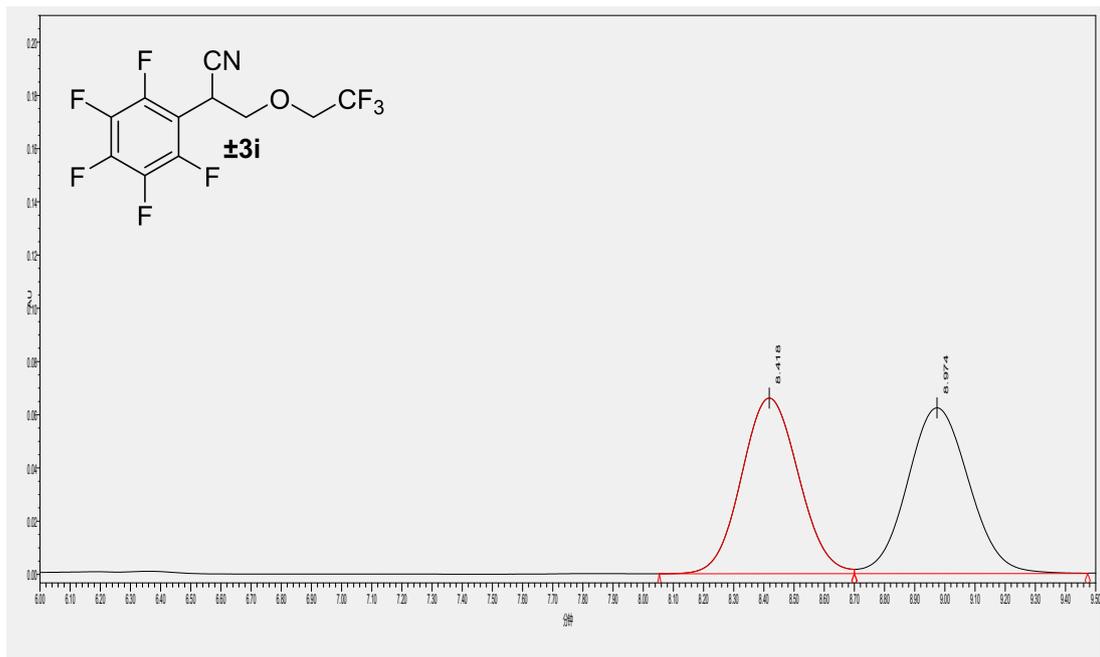


	RT(min)	Area	Area%	Height	Type
1	7.996	691935	50.61	49969	BB
2	9.257	675277	49.39	34719	BB

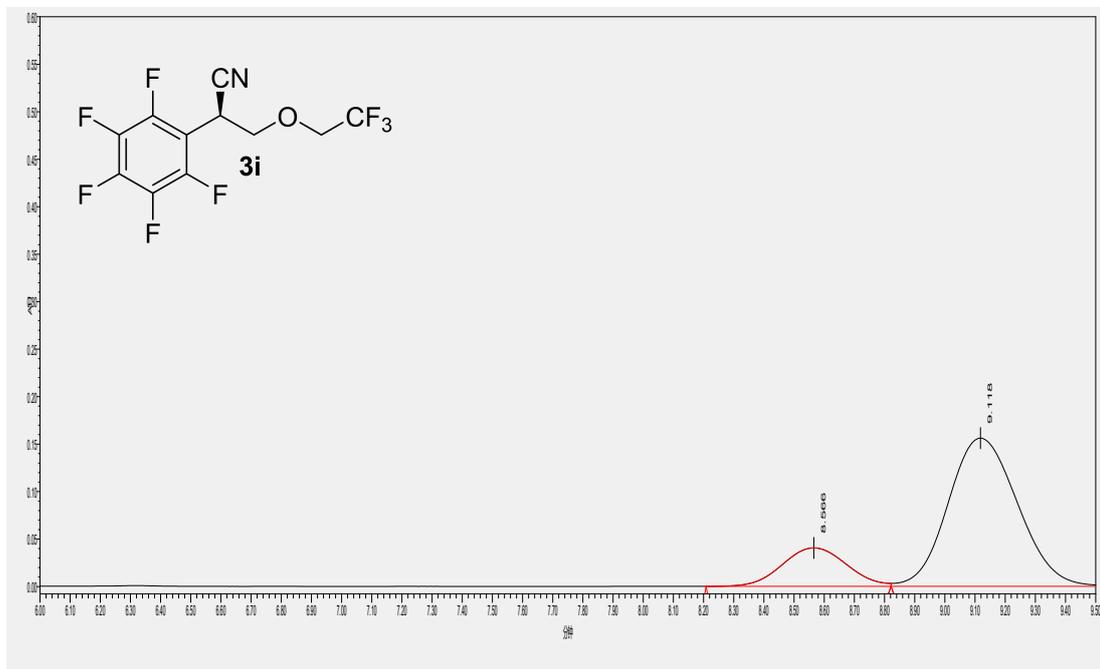


	RT(min)	Area	Area%	Height	Type
1	7.800	3315422	97.32	203951	VB
2	9.472	91235	2.68	5247	BB

HPLC spectra of **3i**

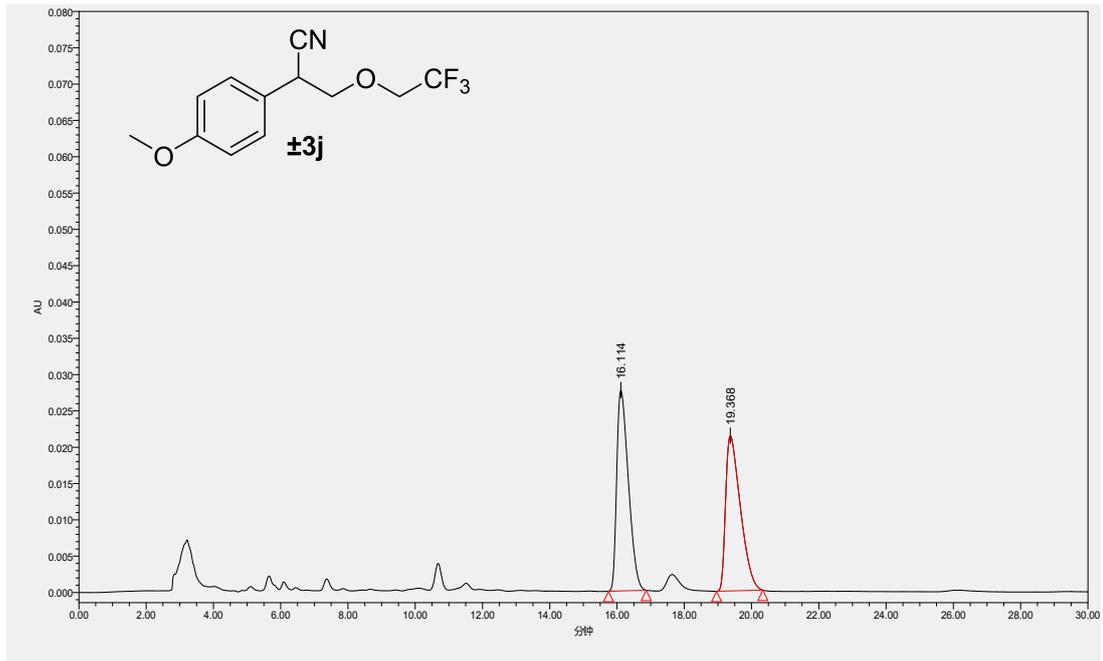


	RT(min)	Area	Area%	Height	Type
1	8.418	869489	49.55	66000	BV
2	8.974	885320	50.45	62308	VV

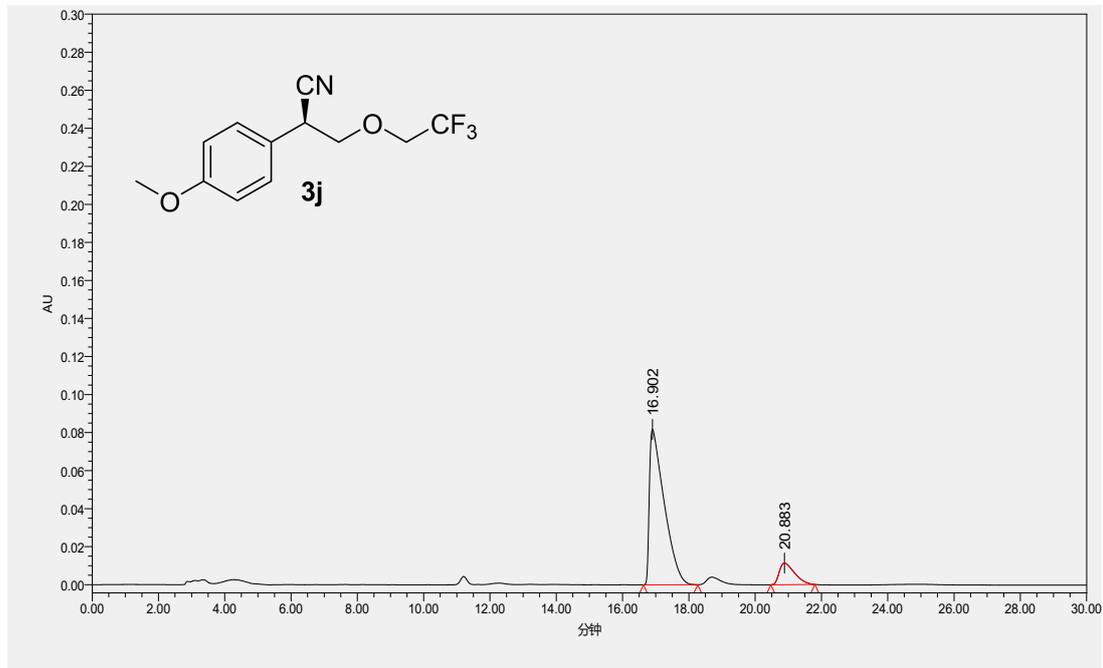


	RT(min)	Area	Area%	Height	Type
1	8.566	600175	19.35	40451	BV
2	9.118	2500820	80.65	156008	VV

HPLC spectra of **3j**

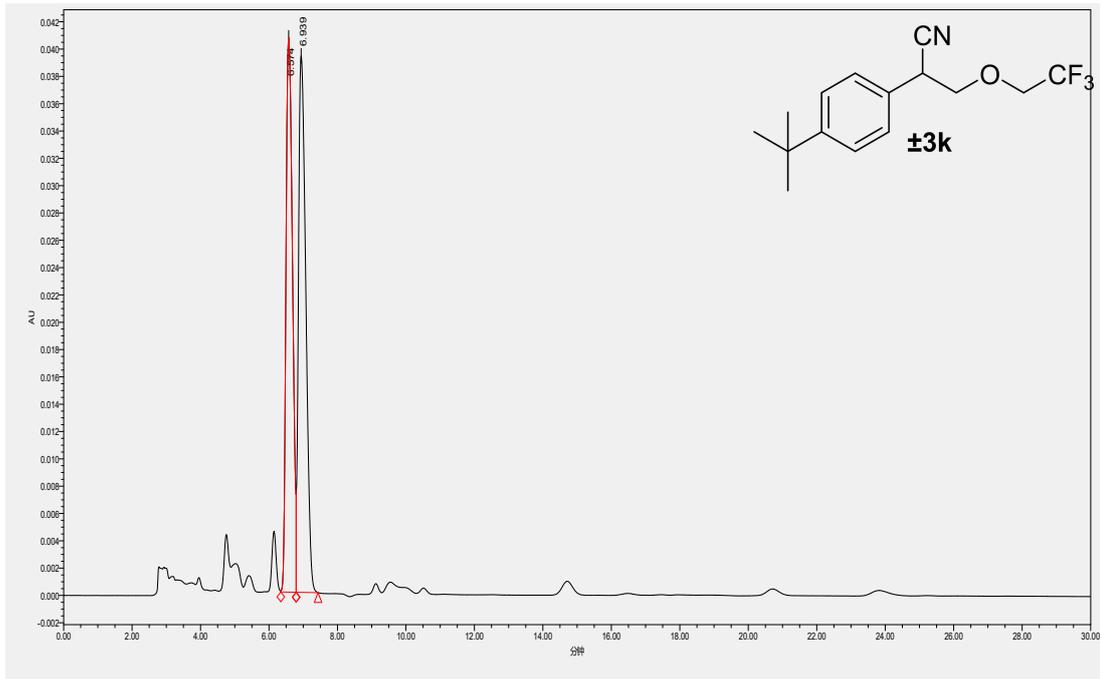


	RT(min)	Area	Area%	Height	Type
1	16.114	665755	50.59	27661	BB
2	19.368	650302	49.41	21385	BB

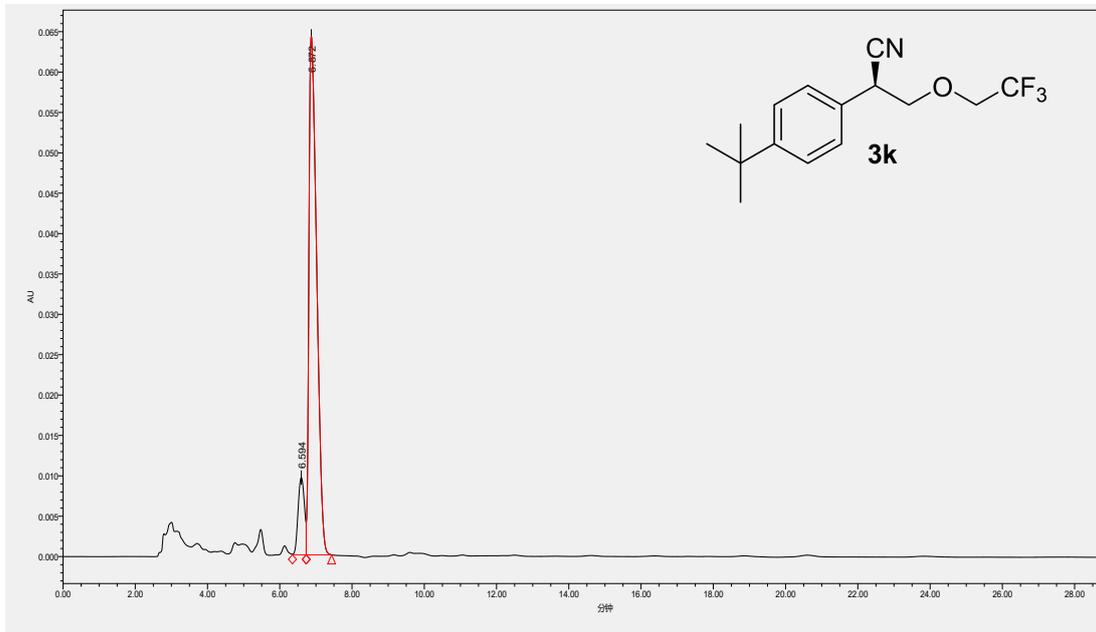


	RT(min)	Area	Area%	Height	Type
1	16.902	2536686	87.39	81691	BB
2	20.883	366040	12.61	11385	BB

HPLC spectra of 3k

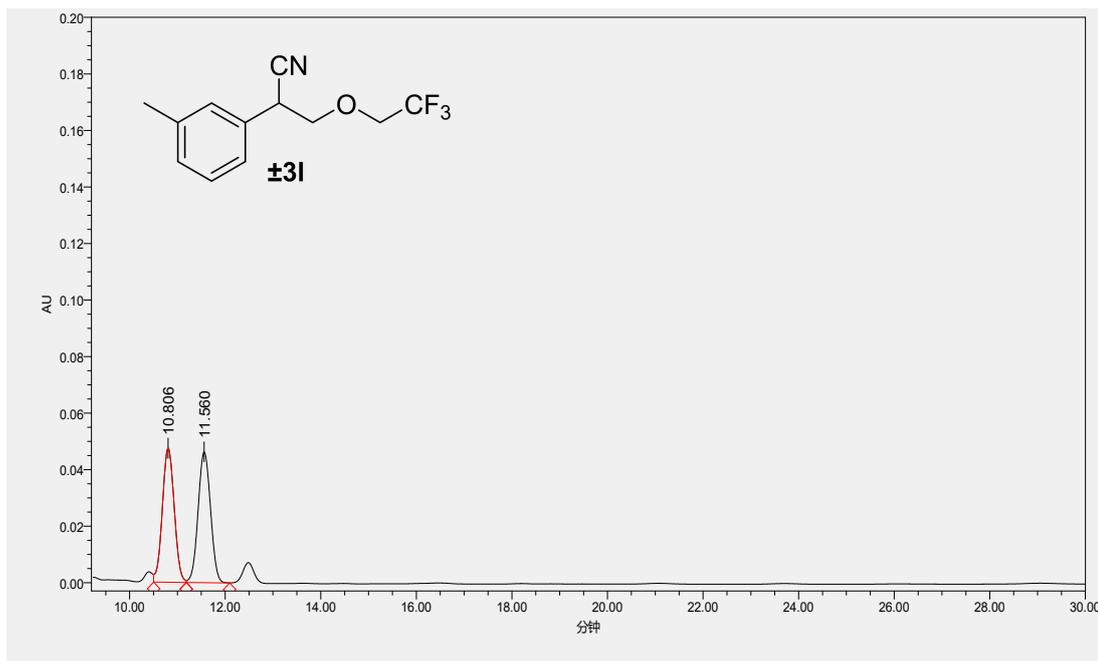


	RT(min)	Area	Area%	Height	Type
1	6.574	537617	47.89	40586	VV
2	6.939	584893	52.11	39283	VB

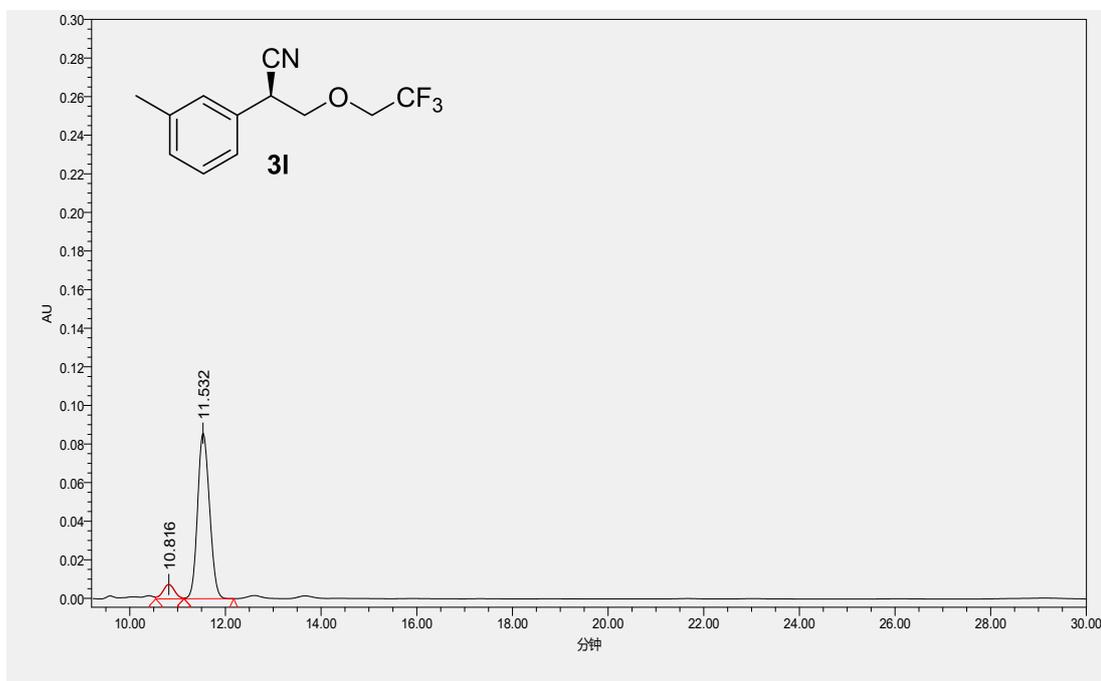


	RT(min)	Area	Area%	Height	Type
1	6.594	115682	10.82	9558	VV
2	6.872	953886	89.18	64214	VB

HPLC spectra of **3I**

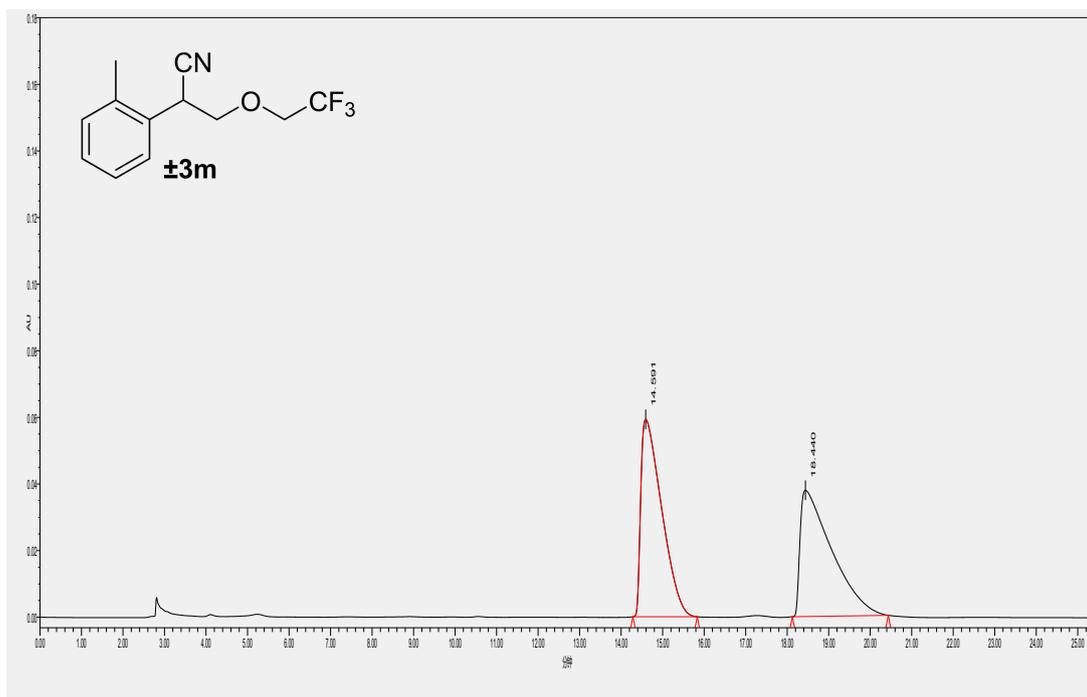


	RT(min)	Area	Area%	Height	Type
1	10.806	817549	49.37	47402	VV
2	11.560	838328	50.63	46256	VV

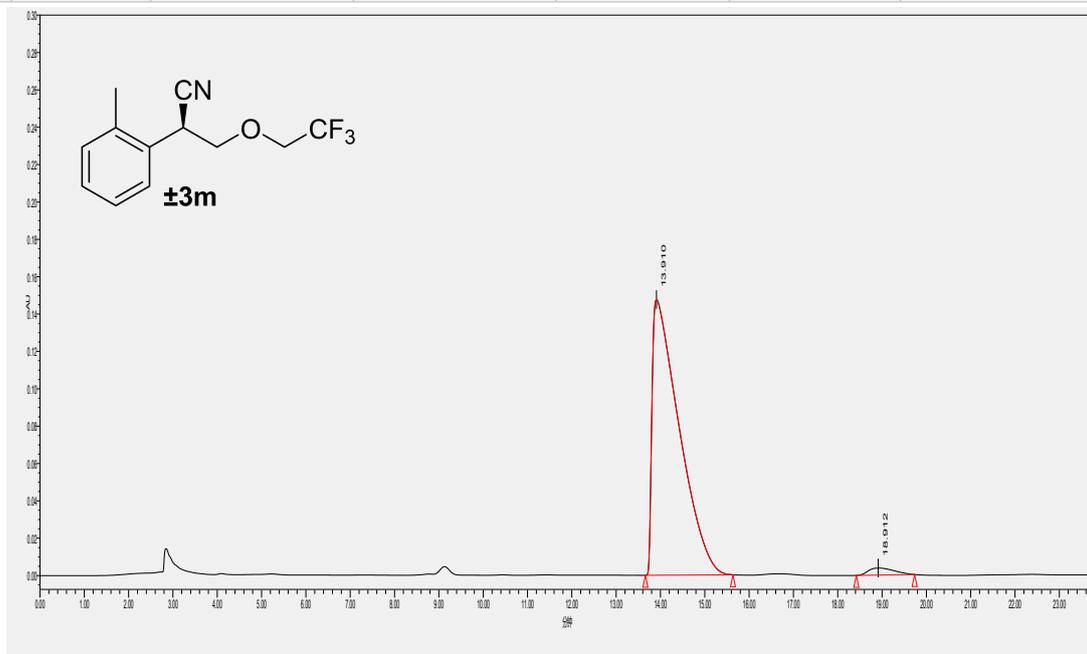


	RT(min)	Area	Area%	Height	Type
1	10.816	126089	7.79	7430	VV
2	11.532	1493171	92.21	85776	VB

HPLC spectra of **3m**

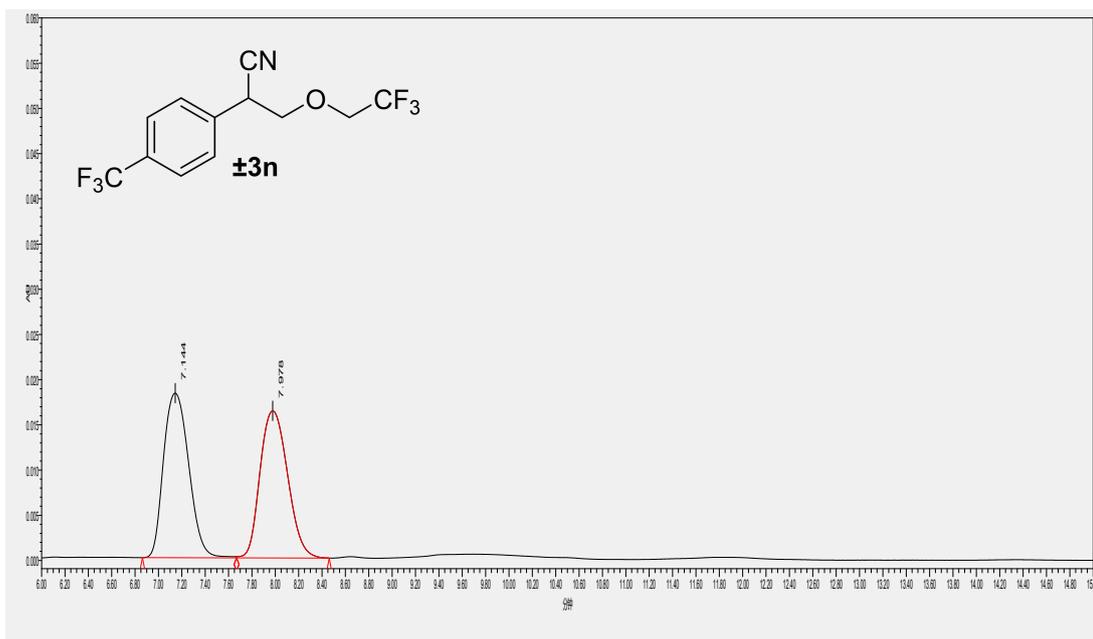


	RT(min)	Area	Area%	Height	Type
1	14.591	2065424	50.74	59294	BB
2	18.440	2005476	49.26	37895	BB

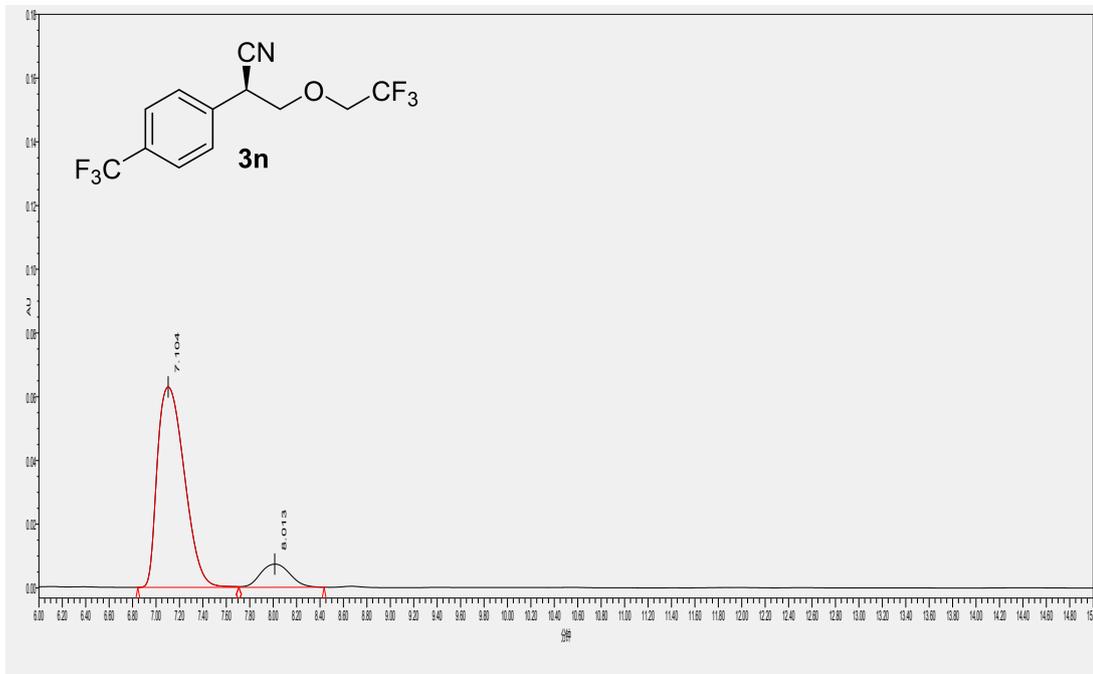


	RT(min)	Area	Area%	Height	Type
1	13.910	6256211	97.63	147599	BB
2	18.912	152043	2.37	3783	BB

HPLC spectra of **3n**

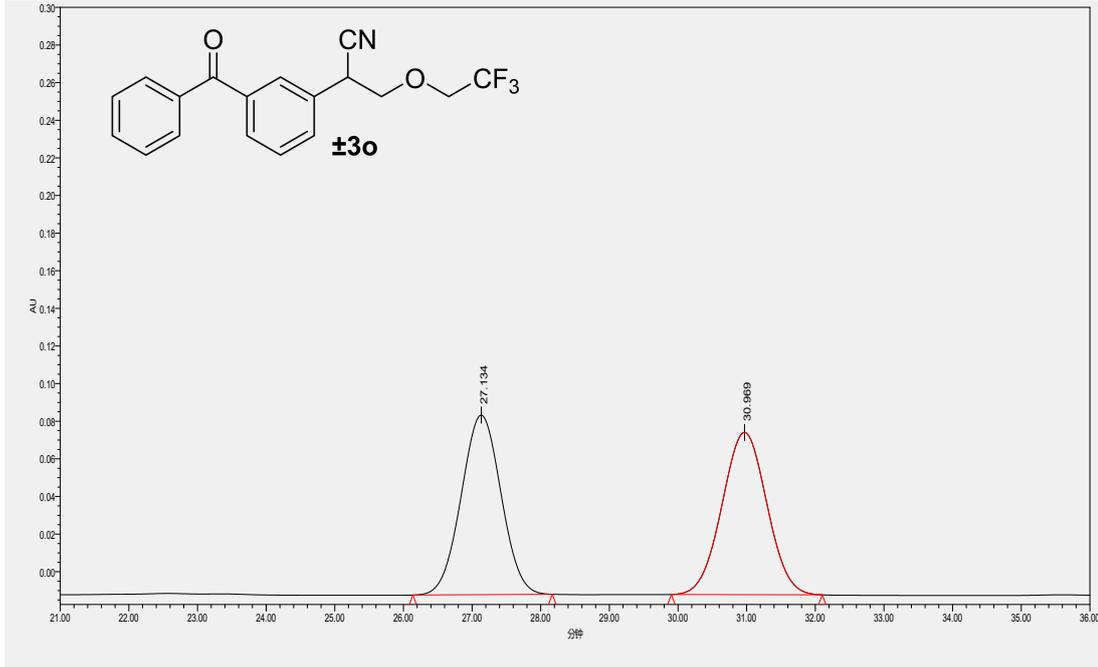


	RT(min)	Area	Area%	Height	Type
1	7.144	274183	50.67	18205	BV
2	7.978	266967	49.33	16276	VB

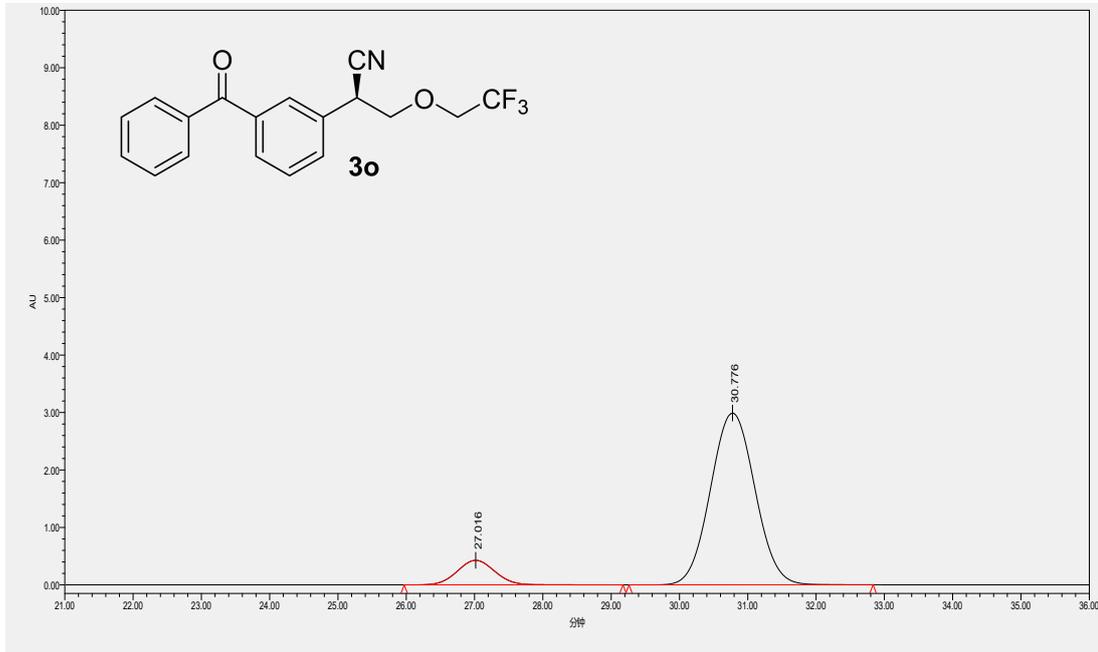


	RT(min)	Area	Area%	Height	Type
1	7.104	1011613	88.78	62894	BV
2	8.013	127825	11.22	7270	VB

HPLC spectra of **3o**

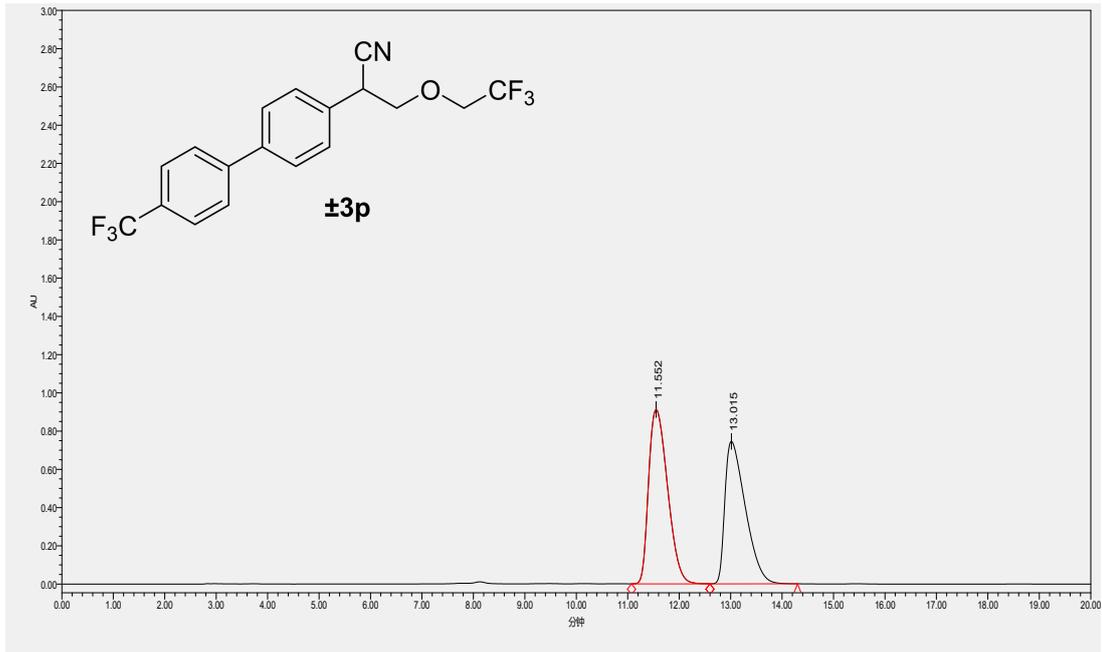


	RT(min)	Area	Area%	Height	Type
1	27.134	3856663	49.60	95451	BB
2	30.969	3918158	50.40	86242	BB

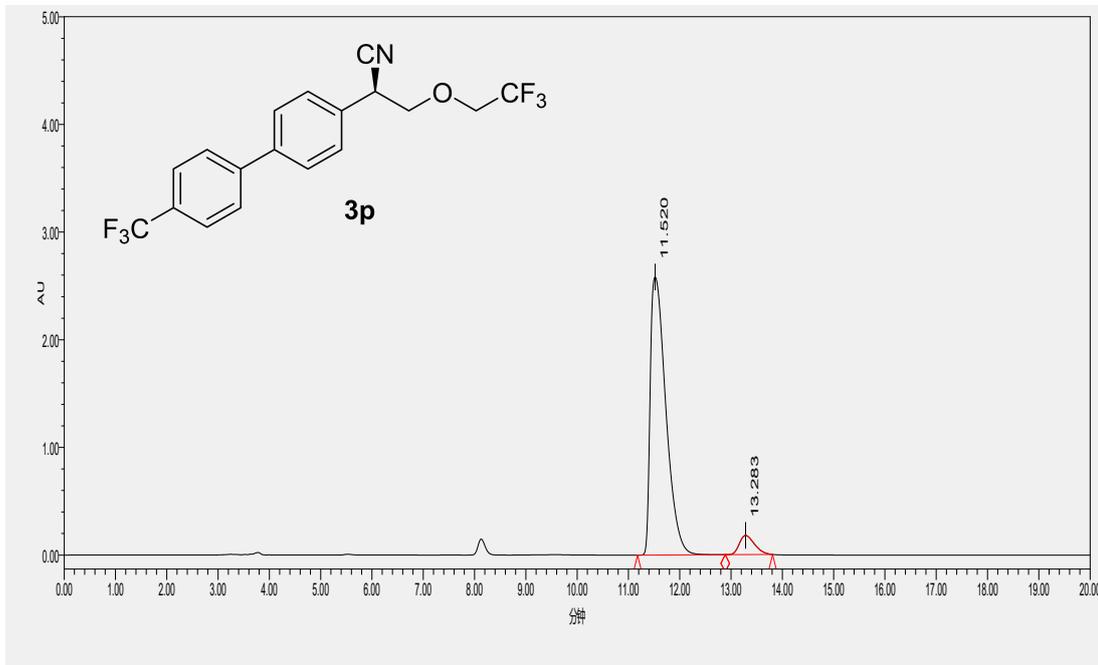


	RT(min)	Area	Area%	Height	Type
1	27.016	16438154	10.83	427491	BB
2	30.776	135402867	89.17	2990126	BB

HPLC spectra of 3p

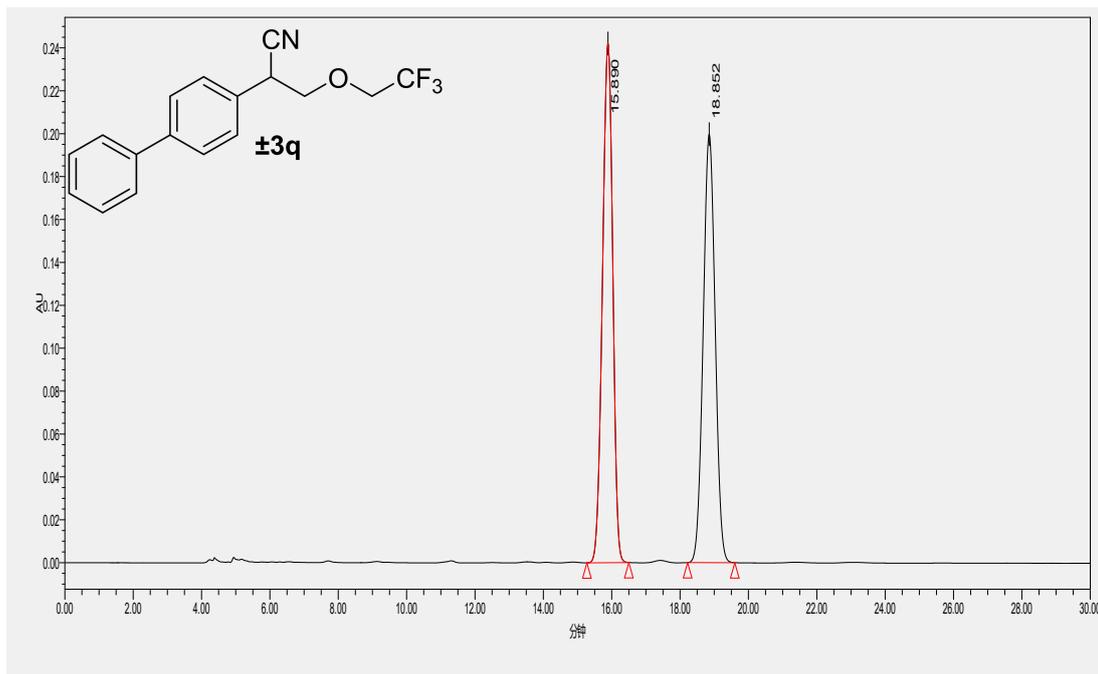


	RT(min)	Area	Area%	Height	Type
1	11.552	23332279	53.16	911677	VV
2	13.015	20556764	46.84	744976	VB

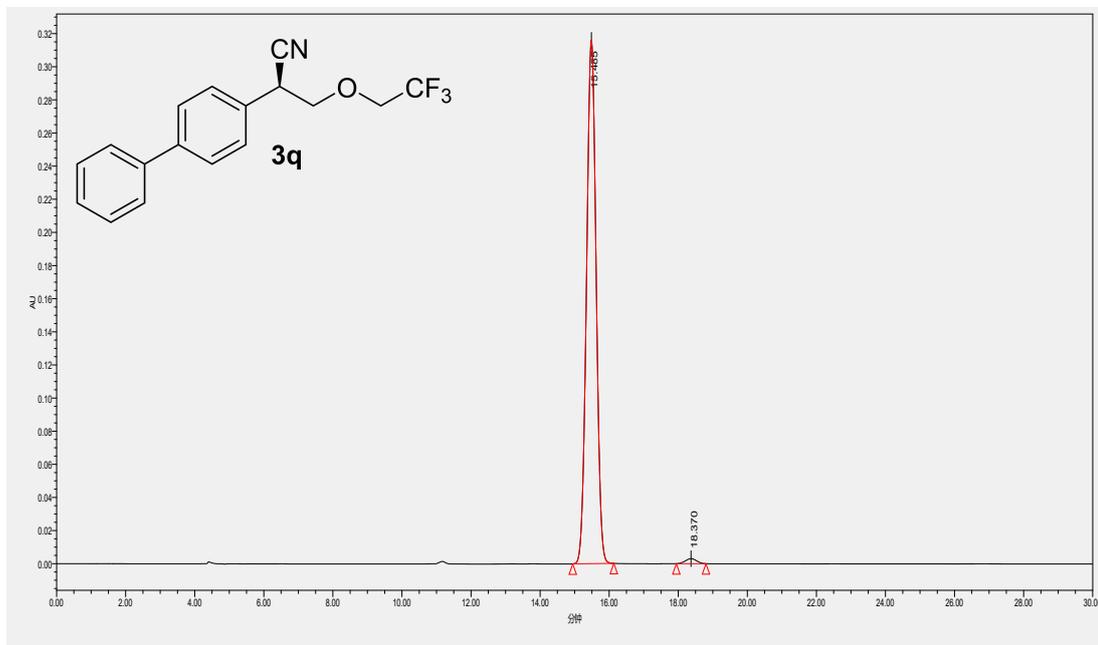


	RT(min)	Area	Area%	Height	Type
1	11.520	54676414	93.73	2582289	BV
2	13.283	3659349	6.27	178086	Vb

HPLC spectra of 3q

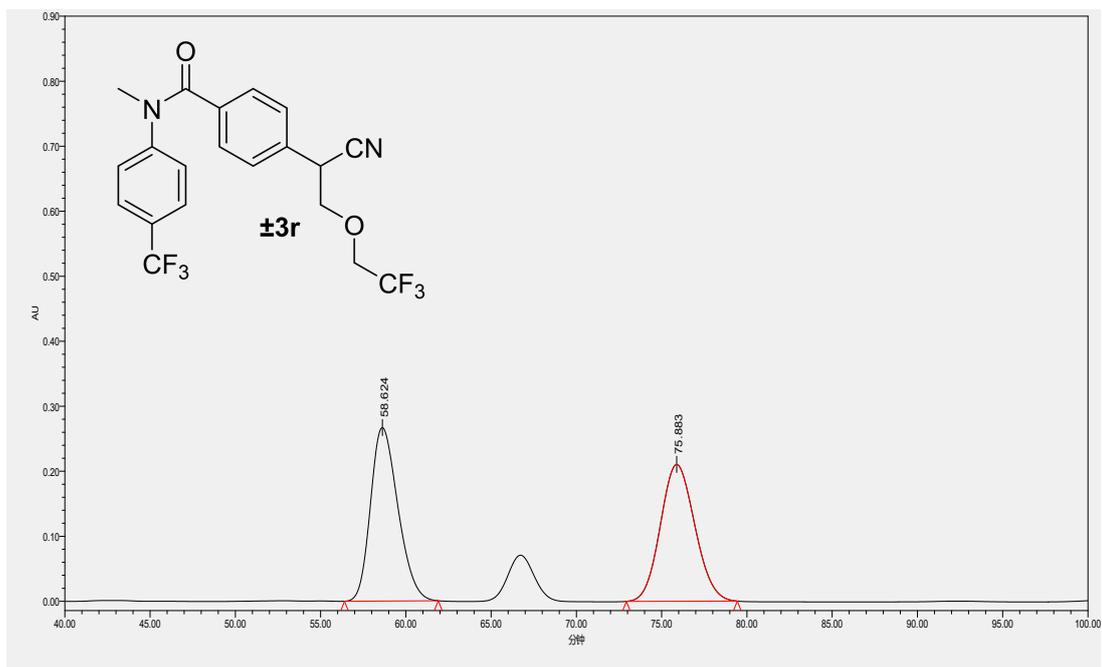


	RT(min)	Area	Area%	Height	Type
1	15.890	5057738	51.02	242093	BB
2	18.852	4854839	48.98	199768	BB

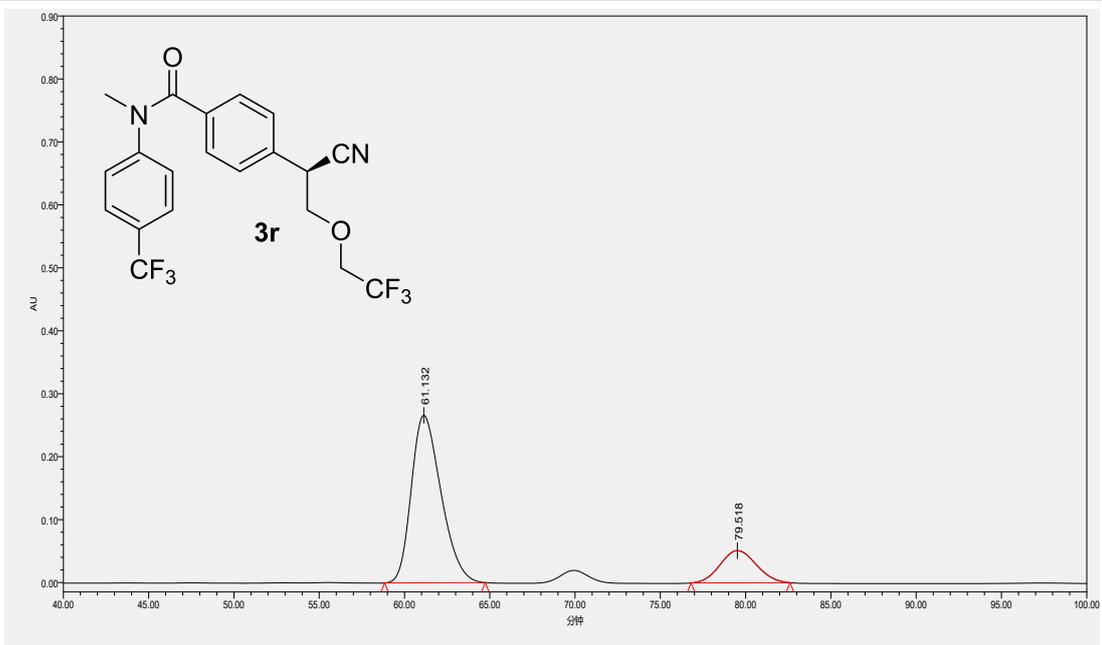


	RT(min)	Area	Area%	Height	Type
1	15.485	6088488	98.90	315958	BB
2	18.370	67776	1.10	2988	BB

HPLC spectra of **3r**

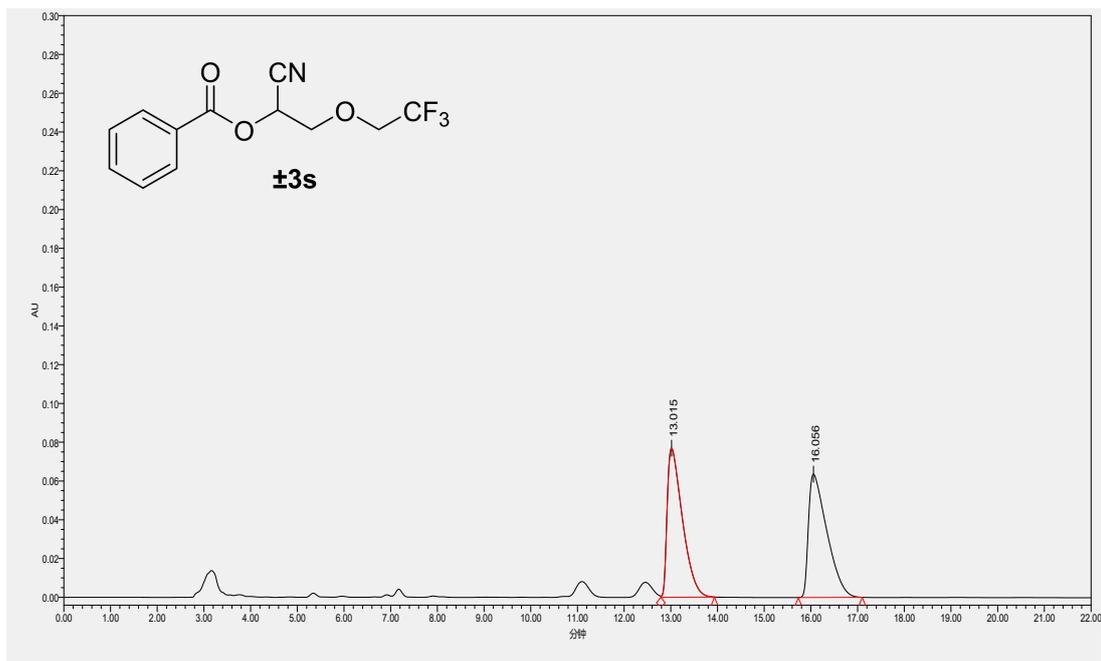


	RT(min)	Area	Area%	Height	Type
1	58.624	29870479	50.28	266854	BB
2	75.883	29539015	49.72	210472	BB

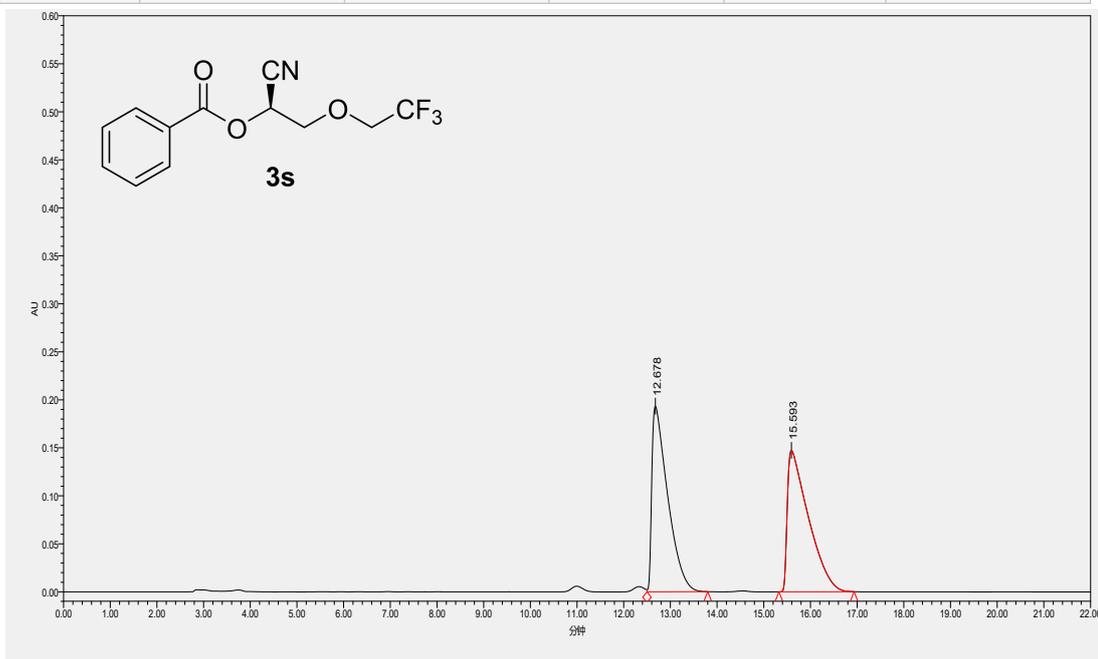


	RT(min)	Area	Area%	Height	Type
1	61.132	32263109	81.06	266055	BB
2	79.518	7539925	18.94	51109	BB

HPLC spectra of 3s

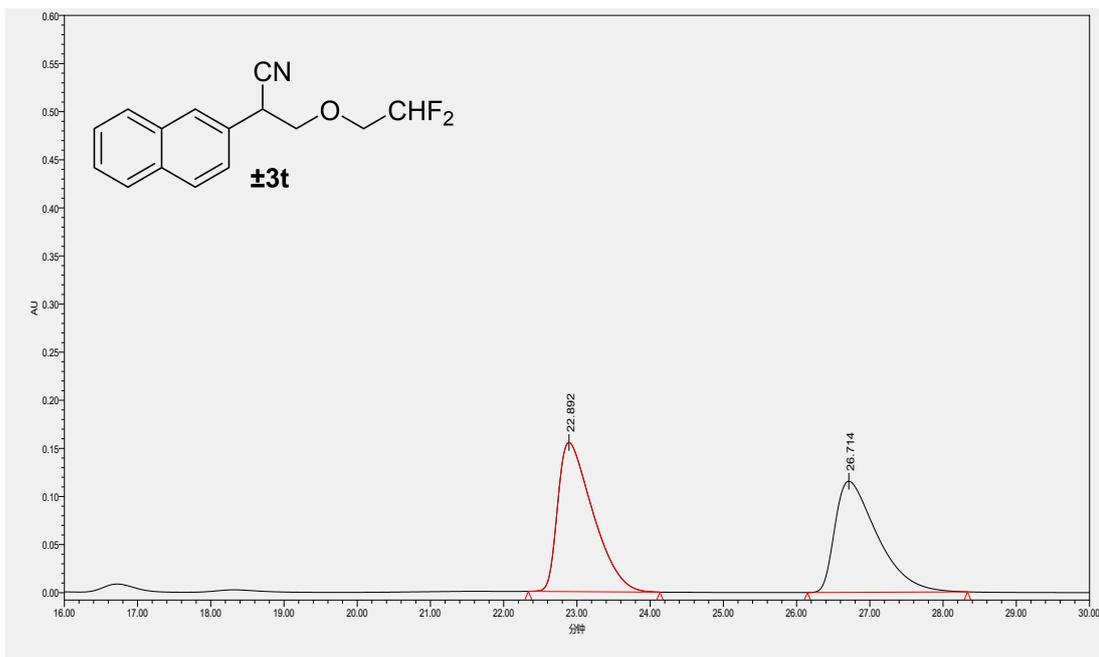


	RT(min)	Area	Area%	Height	Type
1	13.015	1740126	49.94	76894	VB
2	16.056	1744481	50.06	63598	BB

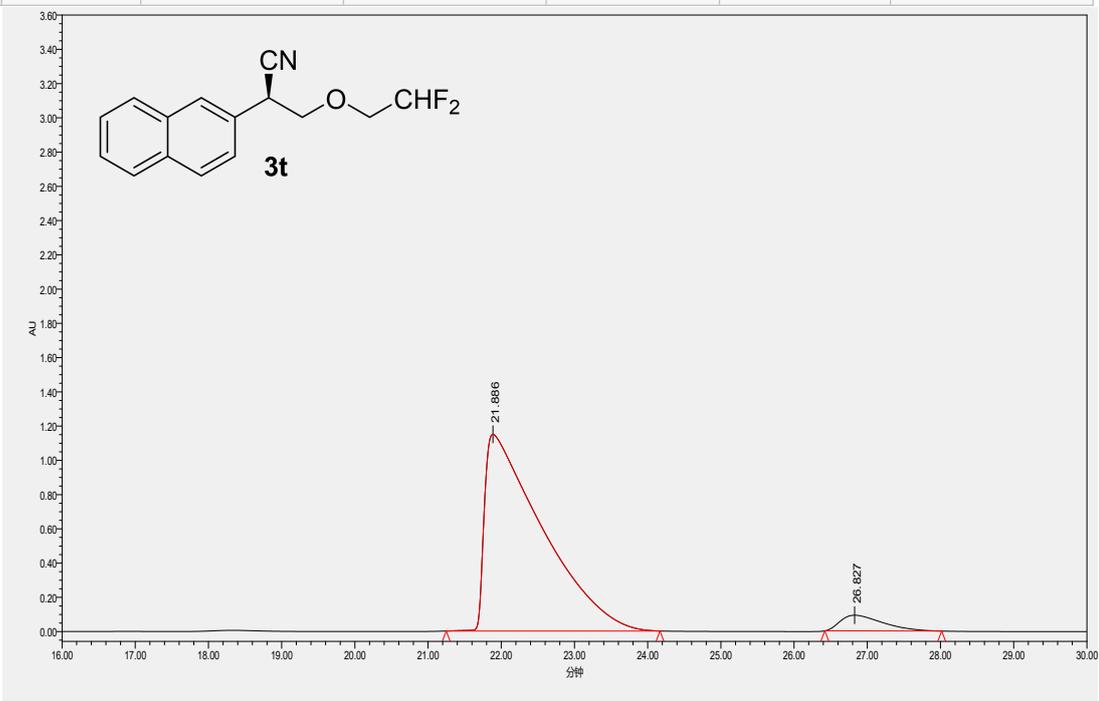


	RT(min)	Area	Area%	Height	Type
1	12.678	4571320	49.73	193418	VB
2	15.593	4620751	50.27	147391	BB

HPLC spectra of **3t**

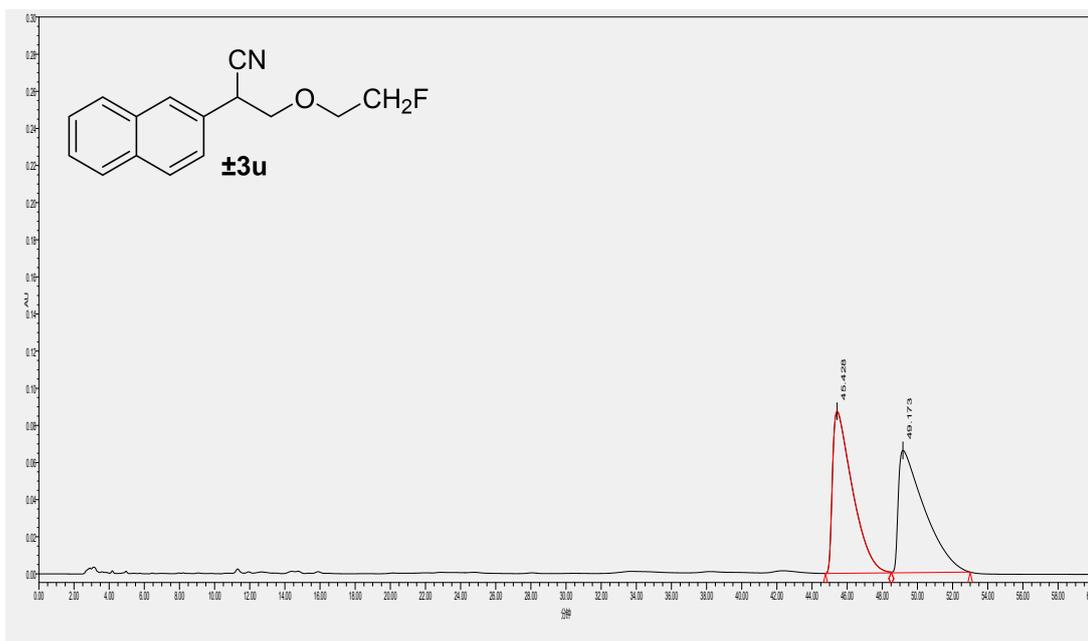


	RT(min)	Area	Area%	Height	Type
1	22.892	5167206	52.68	155009	BB
2	26.714	4641027	47.32	115480	BB

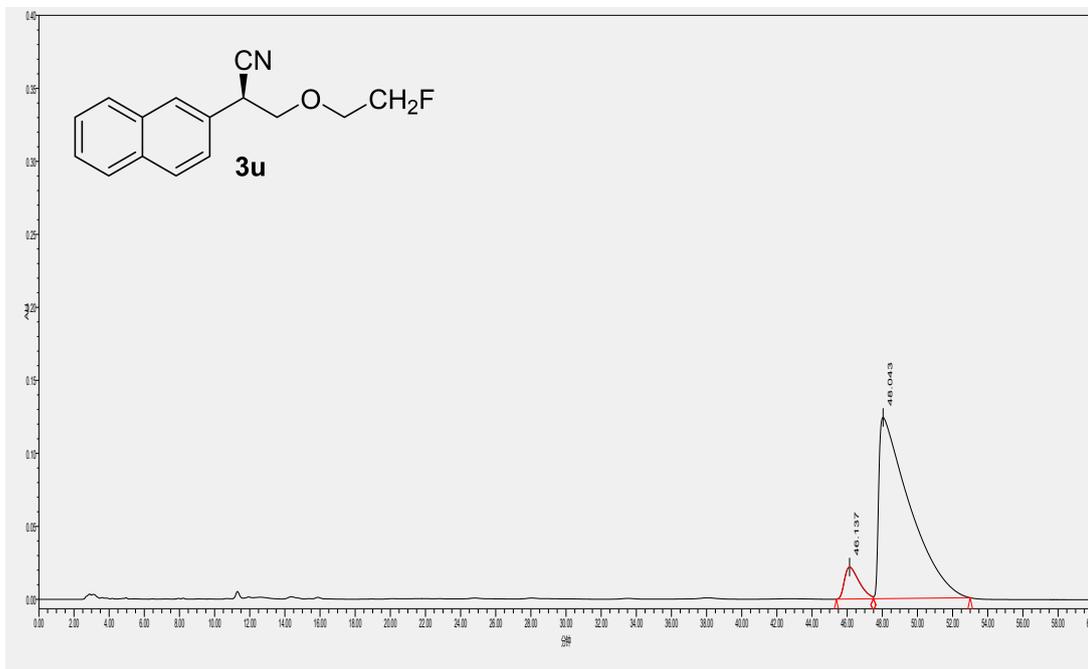


	RT(min)	Area	Area%	Height	Type
1	21.886	62933176	94.47	1148906	bb
2	26.827	3682957	5.53	91576	bb

HPLC spectra of **3u**

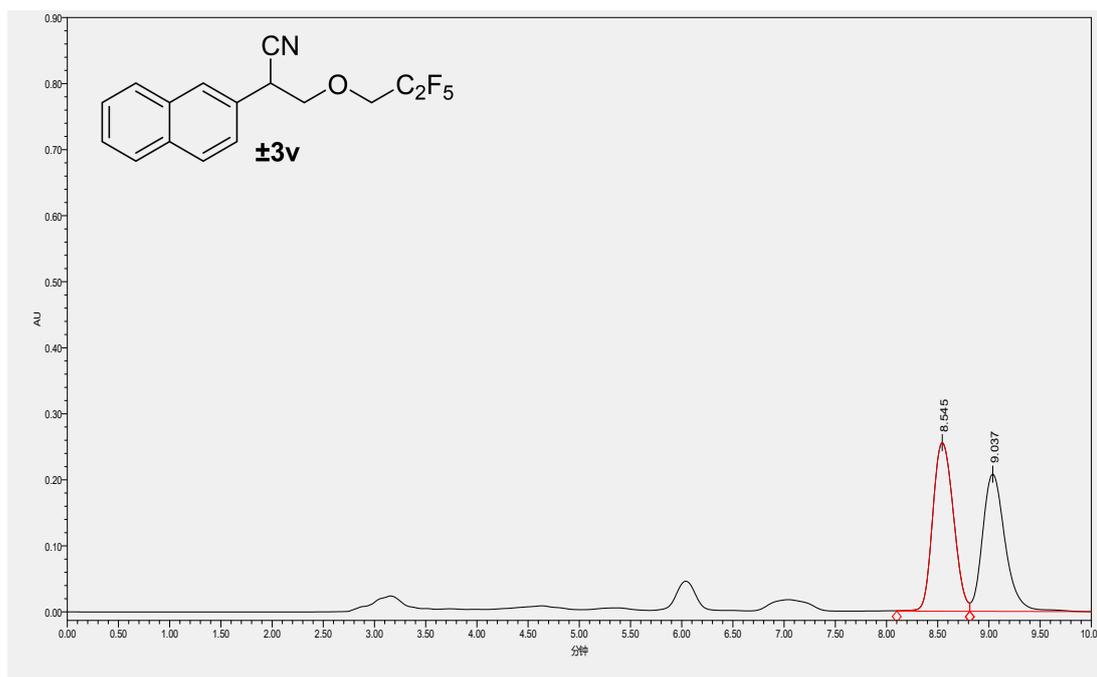


		RT(min)	Area	Area%	Height	Type
1		45.428	6875422	50.18	87298	BV
2		49.173	6826365	49.82	65908	VB

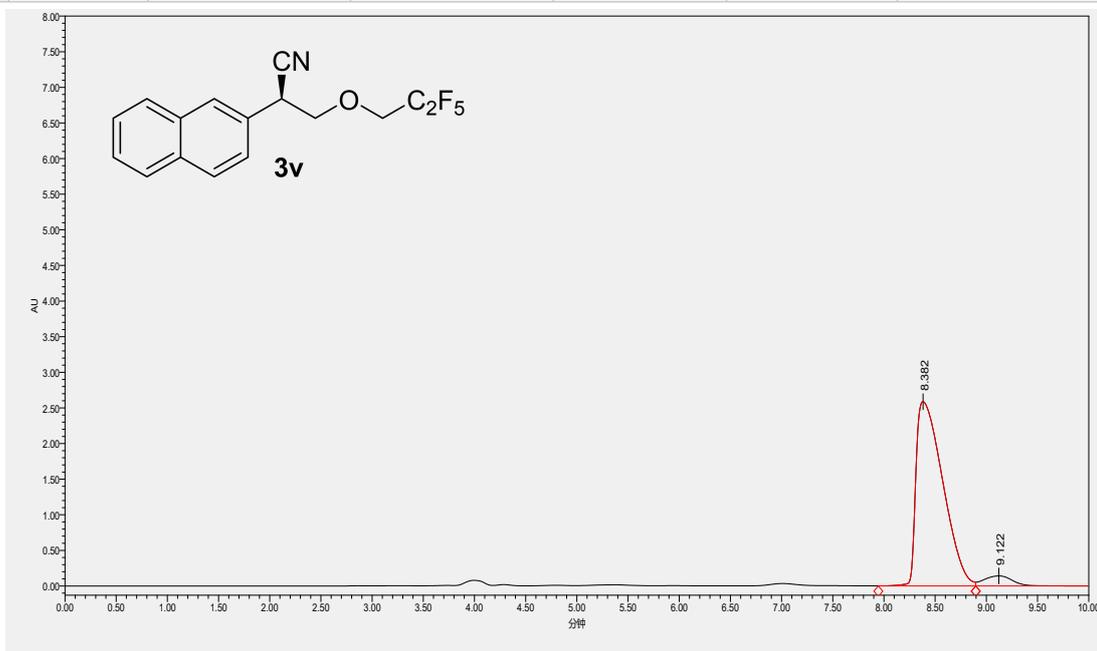


		RT(min)	Area	Area%	Height	Type
1		46.137	1268428	7.70	21907	BV
2		48.043	15197047	92.30	124148	VB

HPLC spectra of 3v

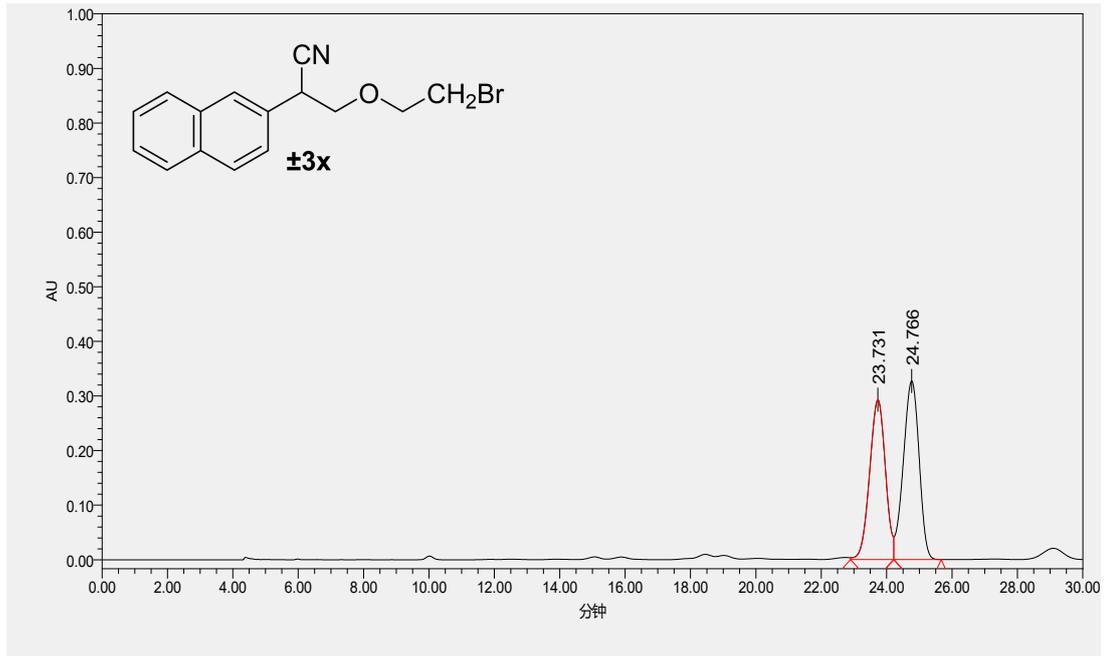


	RT(min)	Area	Area%	Height	Type
1	8.545	3582692	52.85	255200	VV
2	9.037	3196186	47.15	207876	VB

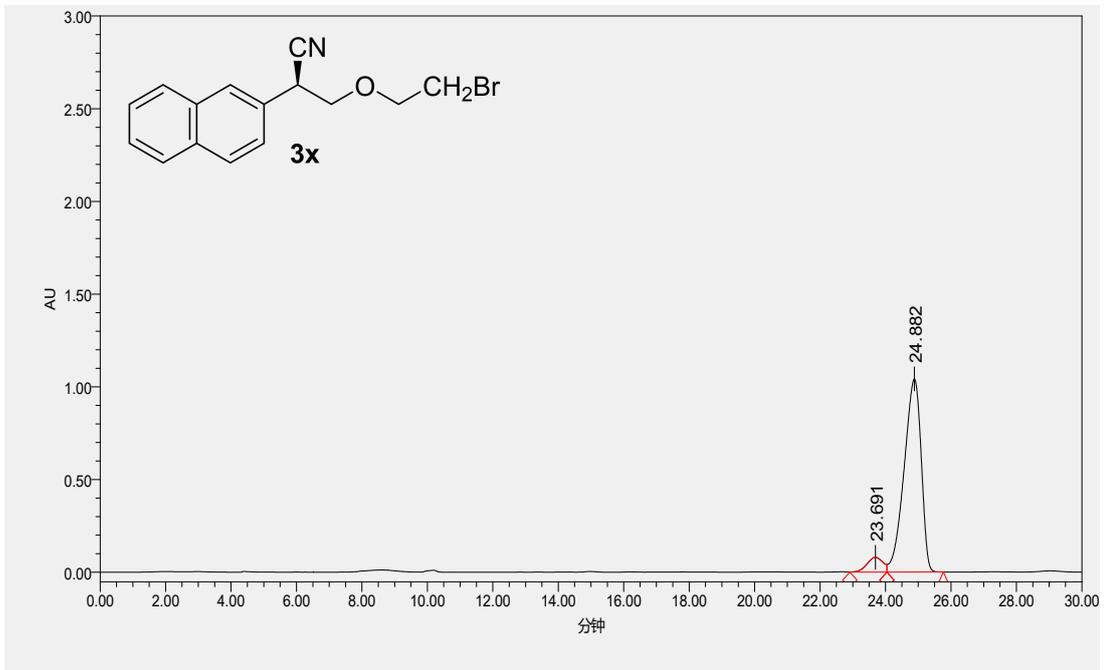


	RT(min)	Area	Area%	Height	Type
1	8.382	47077442	94.54	2586319	VV
2	9.122	2721475	5.46	140568	VB

HPLC spectra of **3x**

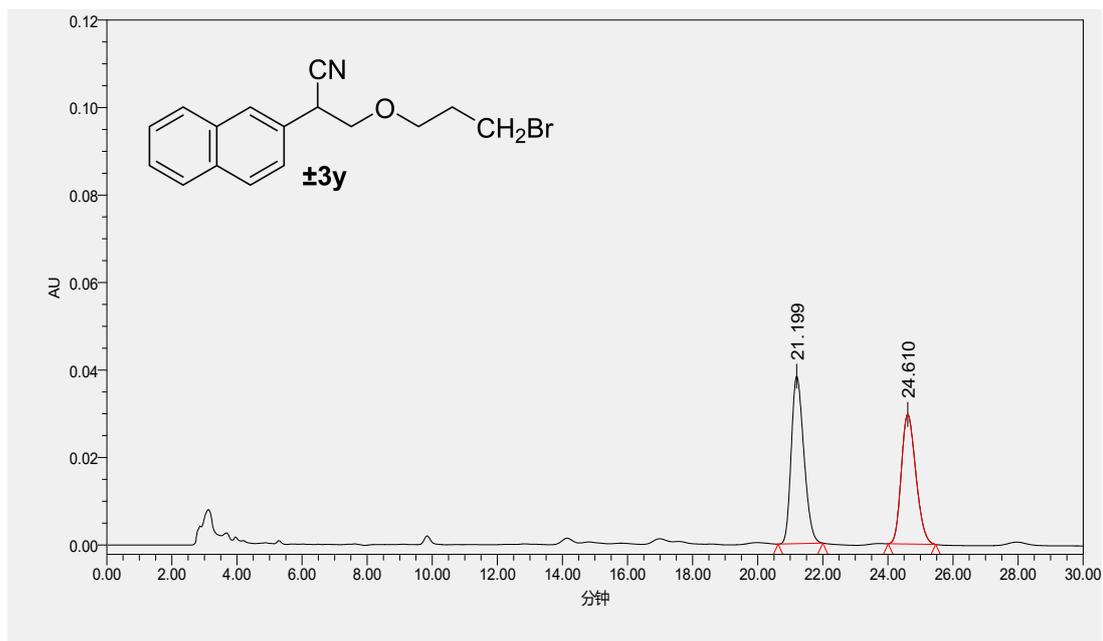


		RT(min)	Area	Area%	Height	Type
1		23.731	9811777	47.21	292747	VV
2		24.766	10971717	52.79	327205	VB

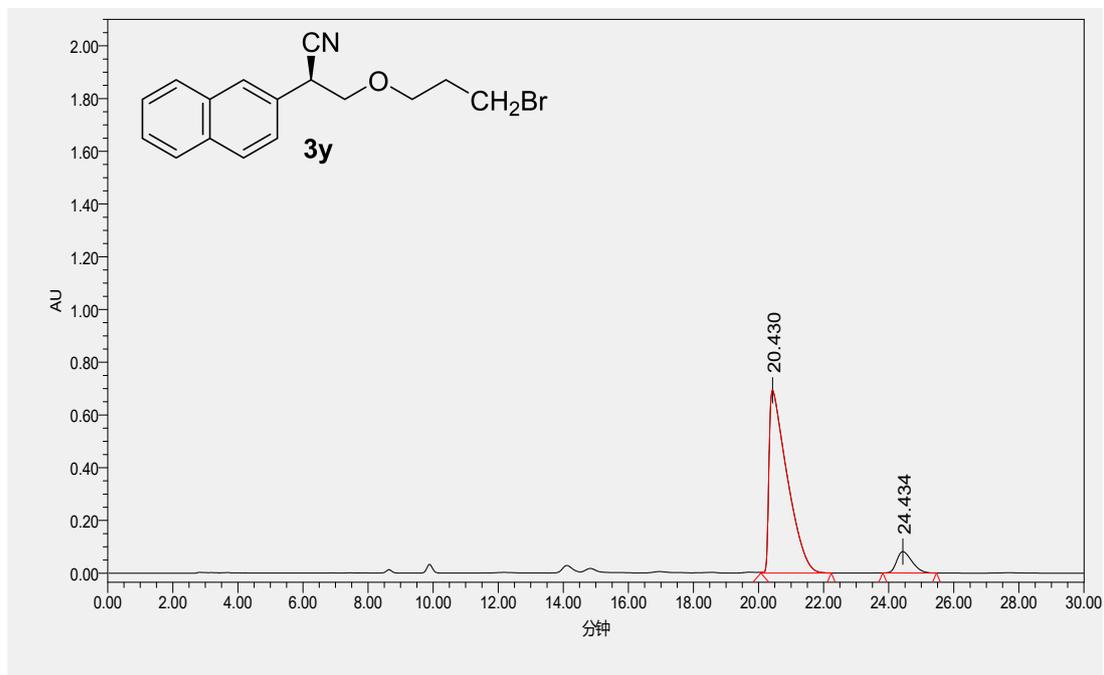


		RT(min)	Area	Area%	Height	Type
1		23.691	2678765	6.62	79447	VV
2		24.882	37789717	93.38	1041786	VB

HPLC spectra of **3y**

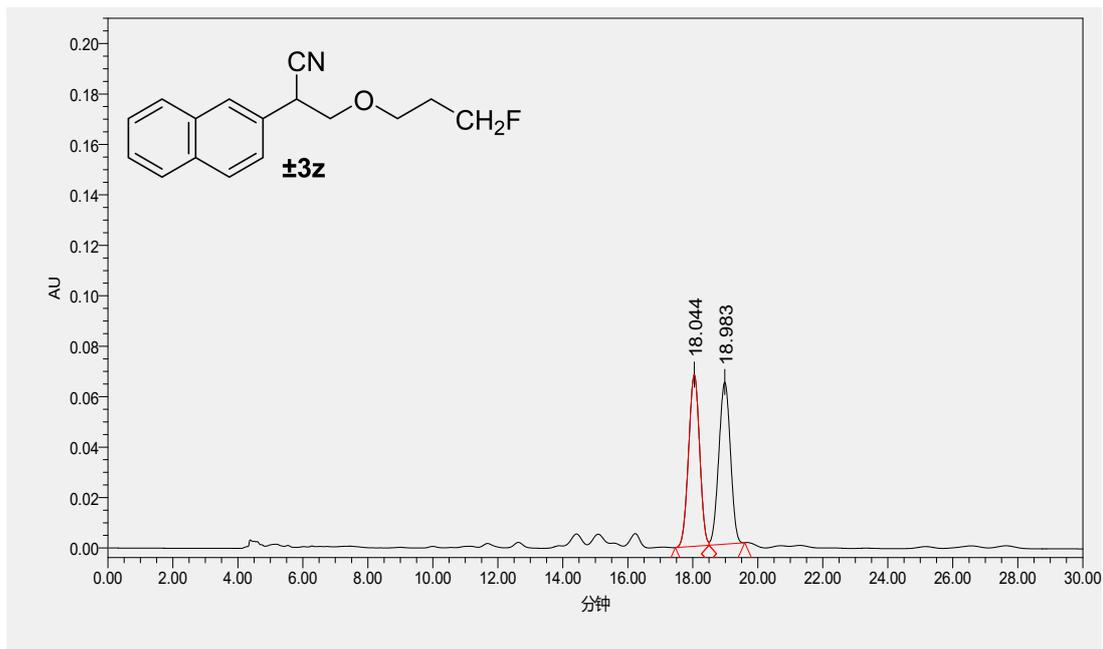


	RT(min)	Area	Area%	Height	Type
1	21.399	1017439	52.44	37892	bB
2	24.808	922893	47.56	29203	BB

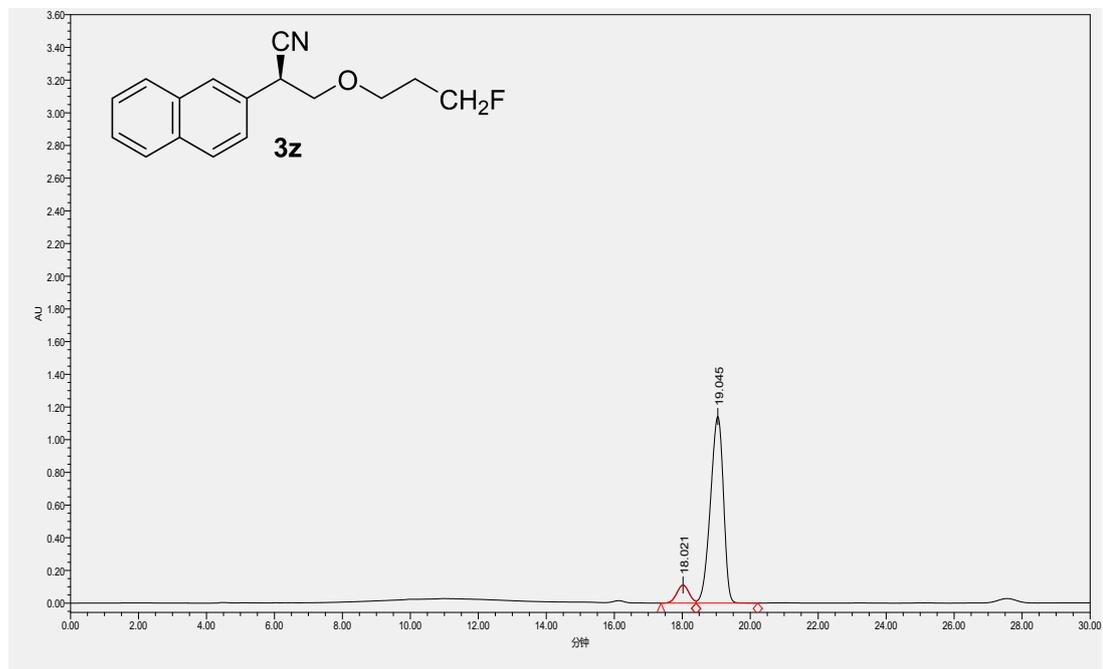


	RT(min)	Area	Area%	Height	Type
1	20.430	26938118	91.10	692957	VB
2	24.434	2632210	8.90	80897	BB

HPLC spectra of 3z

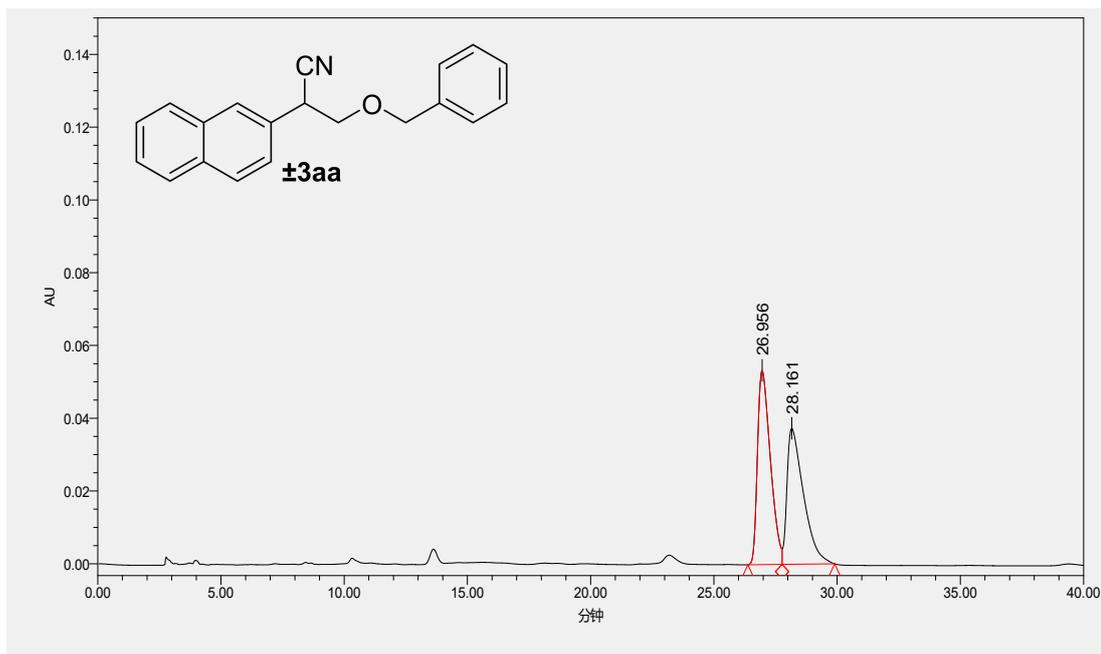


	RT(min)	Area	Area%	Height	Type
1	18.044	1608017	50.20	68058	BV
2	18.983	1594967	49.80	64242	VB

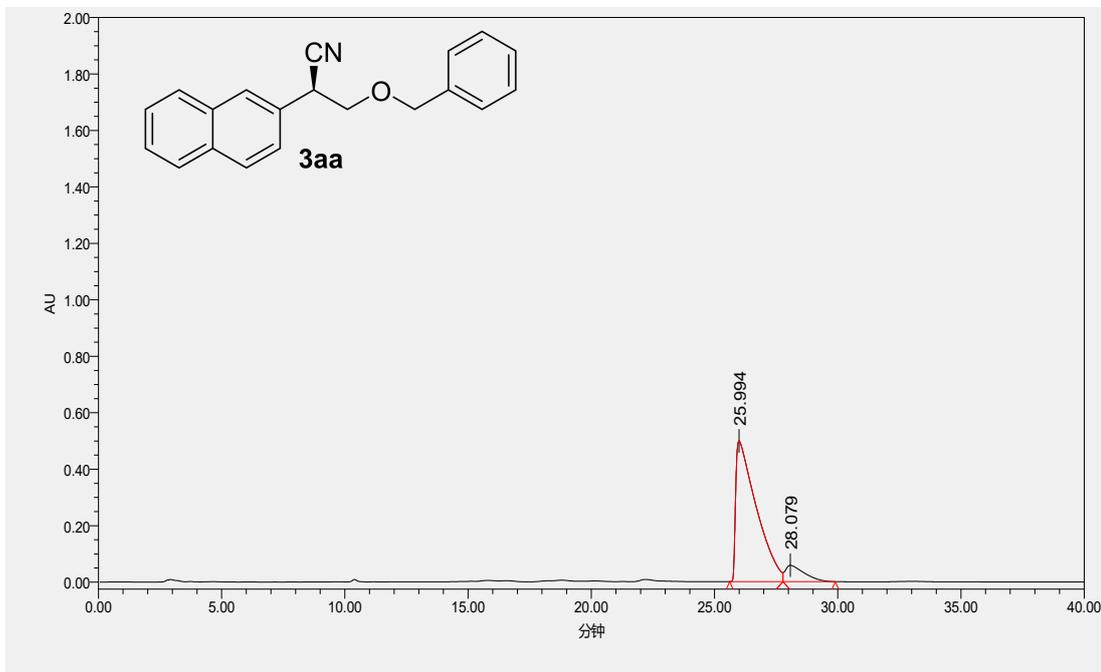


	RT(min)	Area	Area%	Height	Type
1	18.021	2761063	8.33	110144	BV
2	19.045	30376155	91.67	1141759	VV

HPLC spectra of 3aa

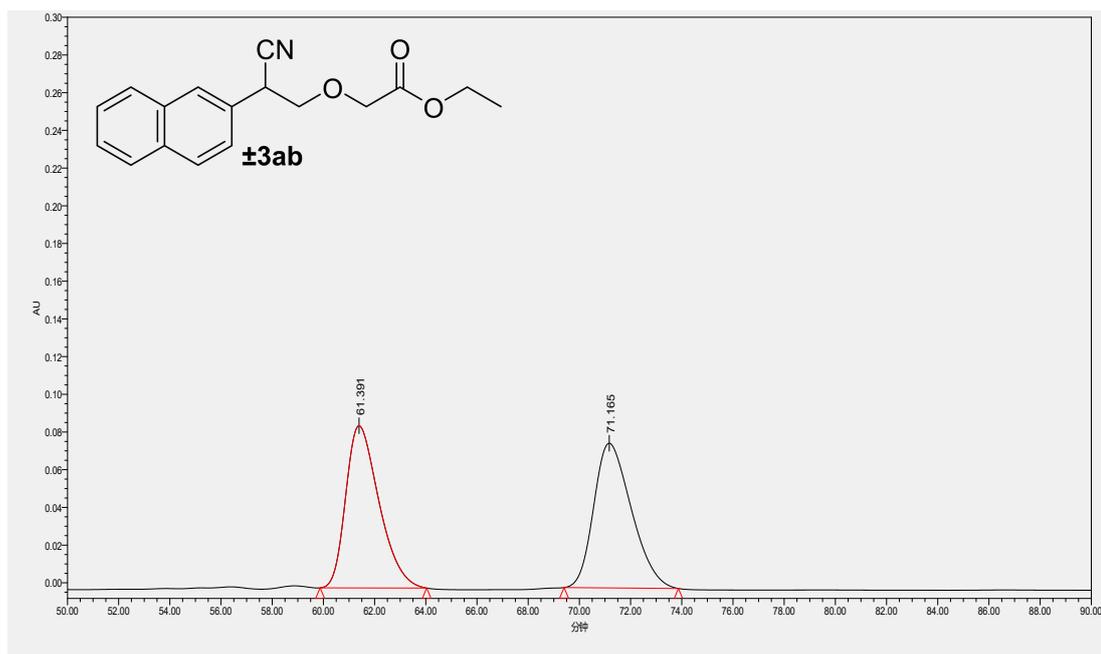


	RT(min)	Area	Area%	Height	Type
1	26.956	1936596	52.63	53360	BV
2	28.161	1743246	47.37	37385	VB

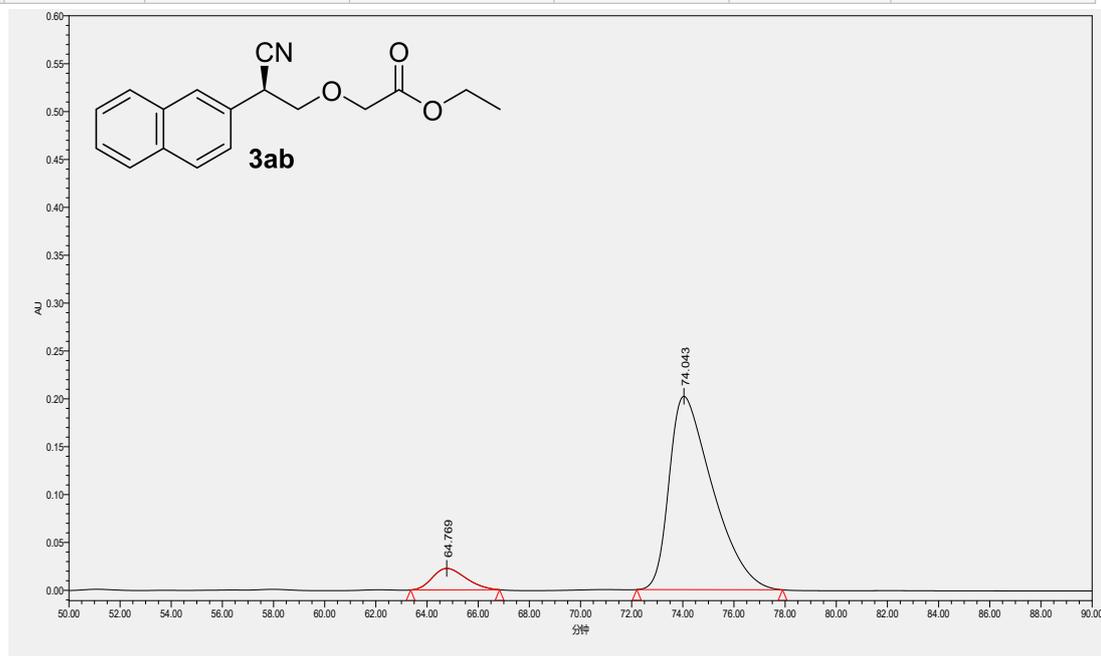


	RT(min)	Area	Area%	Height	Type
1	25.994	28970021	90.27	498789	BV
2	28.079	3121355	9.73	58045	VB

HPLC spectra of **3ab**

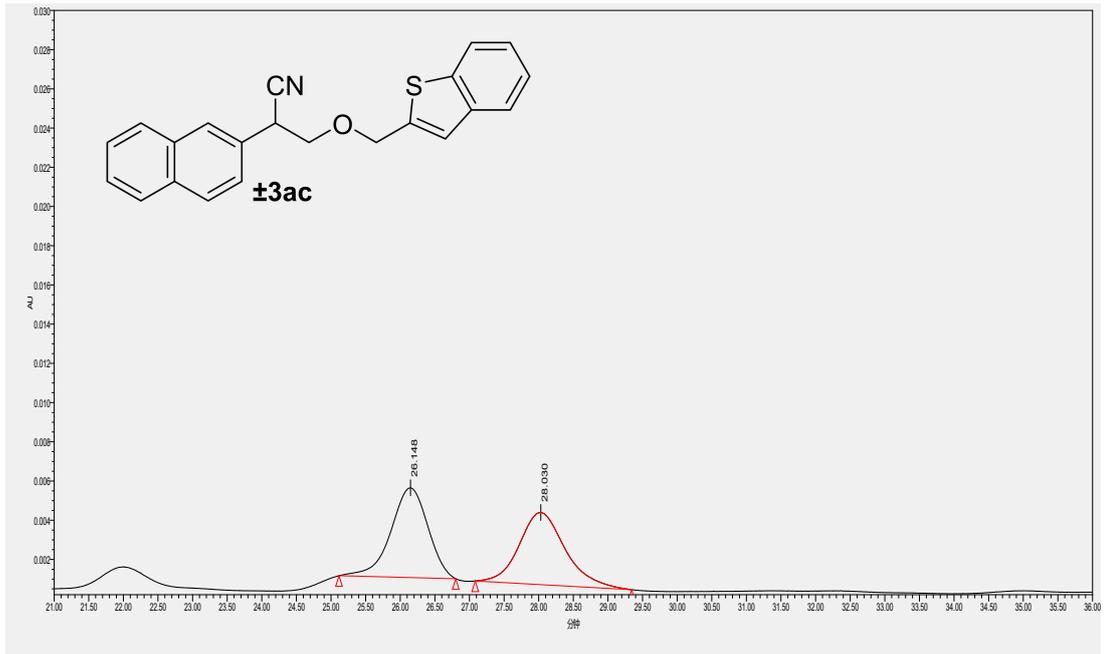


	RT(min)	Area	Area%	Height	Type
1	61.391	7778393	49.81	86062	BB
2	71.165	7837759	50.19	76762	BB

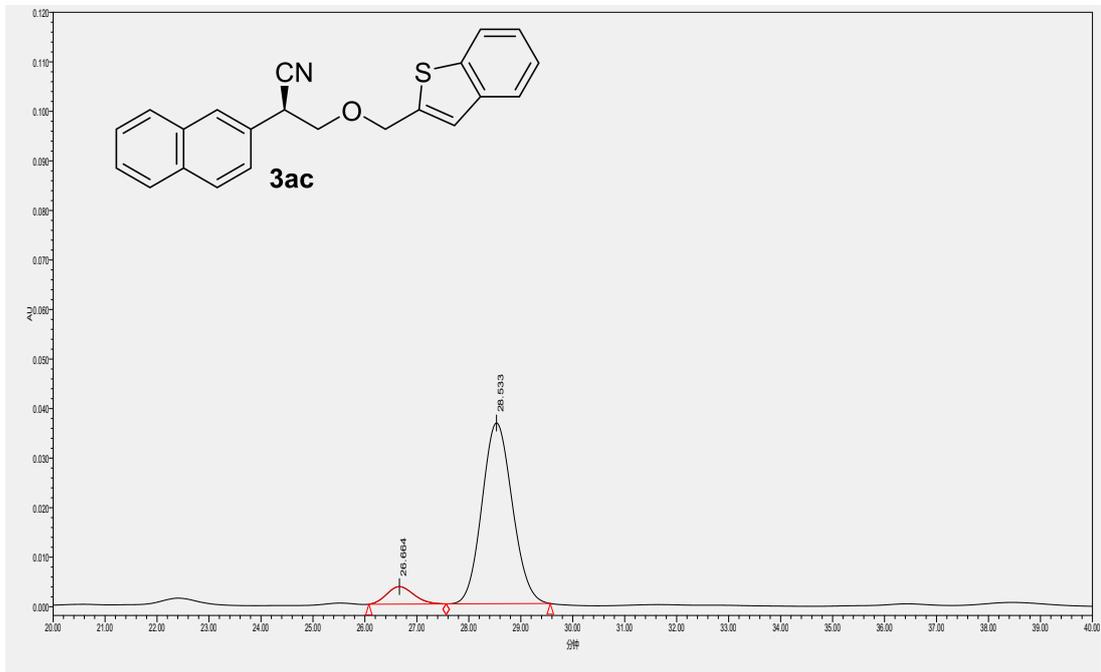


	RT(min)	Area	Area%	Height	Type
1	64.769	2033693	7.85	22417	BB
2	74.043	23863770	92.15	201973	BB

HPLC spectra of **3ac**

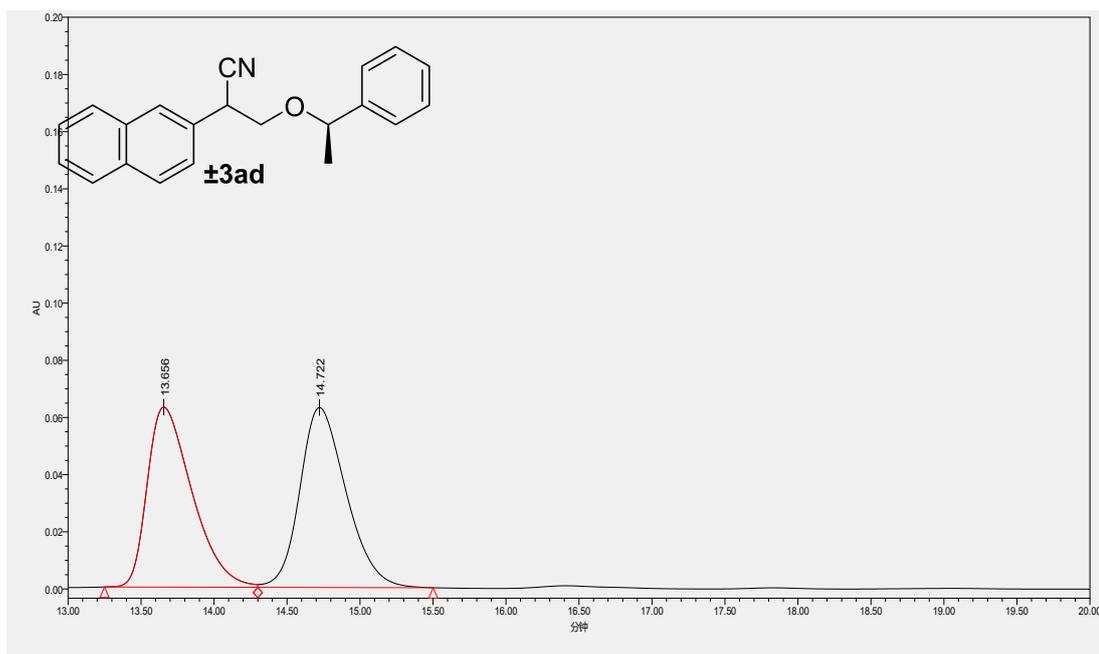


	RT(min)	Area	Area%	Height	Type
1	26.148	170121	50.03	4578	bB
2	28.030	169891	49.97	3680	bb

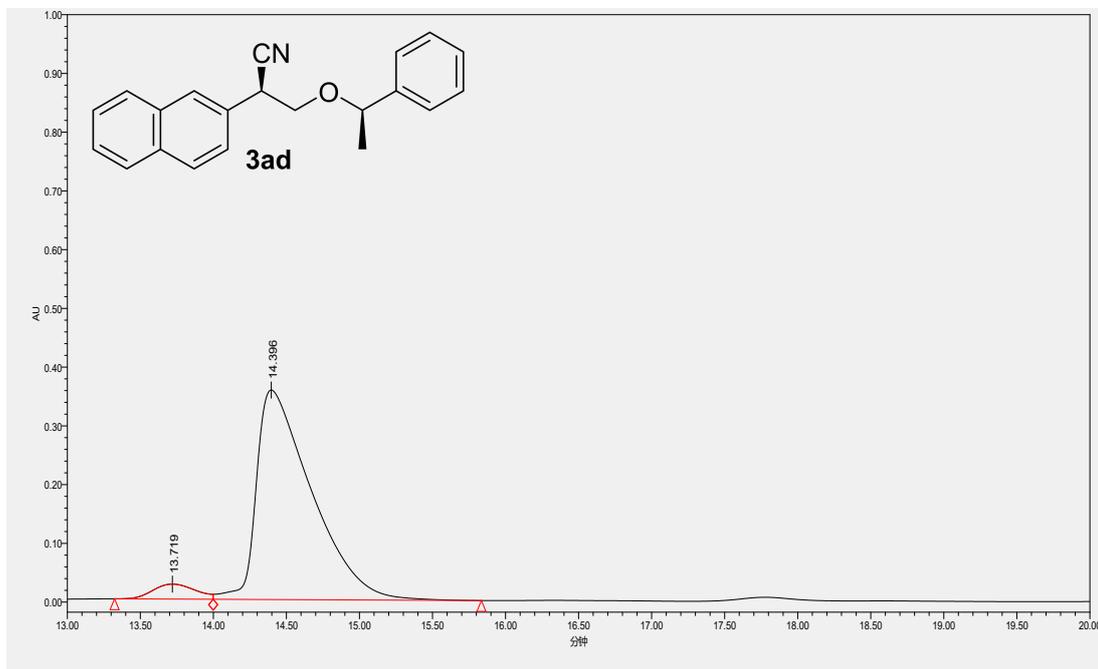


	RT(min)	Area	Area%	Height	Type
1	26.664	127626	7.91	3529	BV
2	28.533	1485303	92.09	36488	VB

HPLC spectra of 3ad

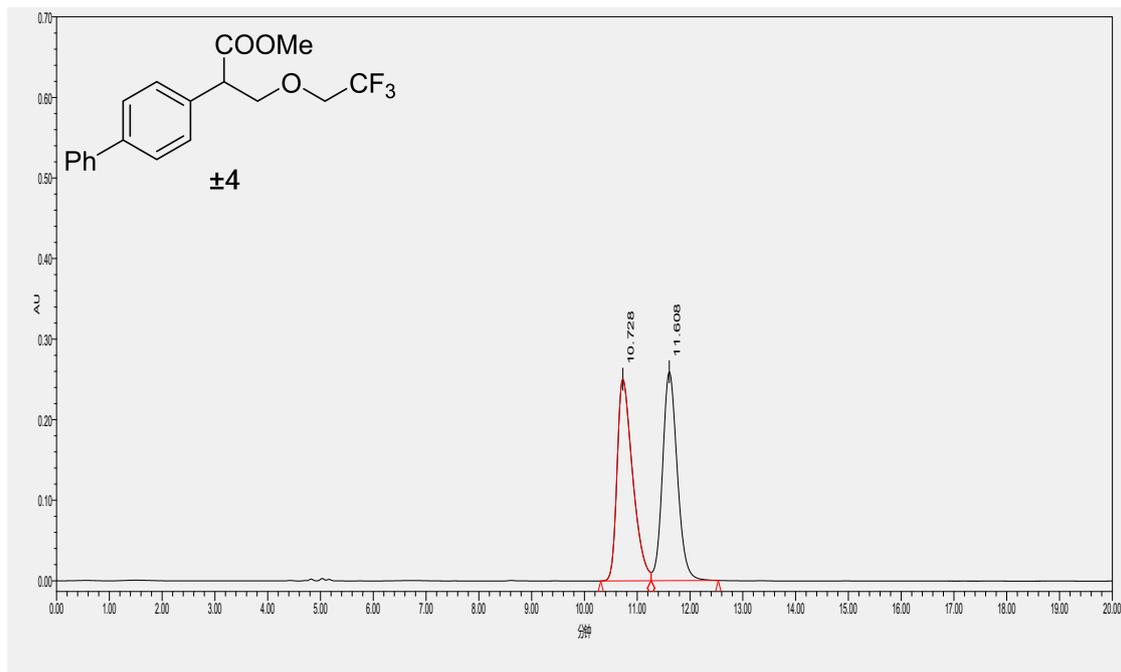


	RT(min)	Area	Area%	Height	Type
1	13.656	1345561	49.20	62970	BV
2	14.722	1389560	50.80	62955	VB

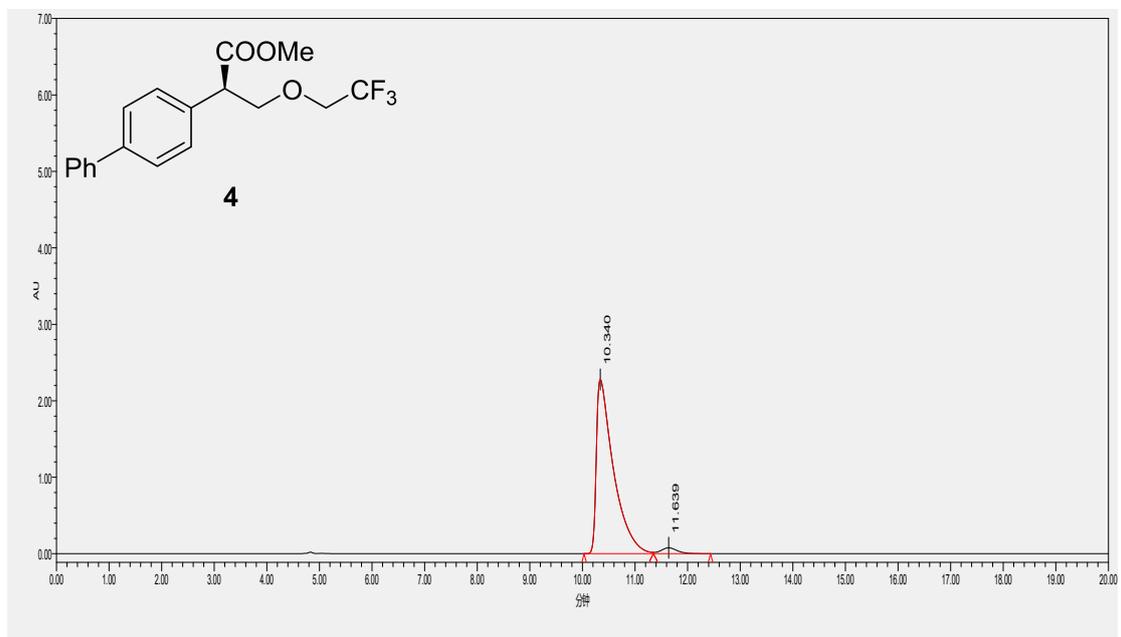


	RT(min)	Area	Area%	Height	Type
1	13.719	519503	5.25	25543	BV
2	14.396	9383385	94.75	356765	VB

HPLC spectra of 4

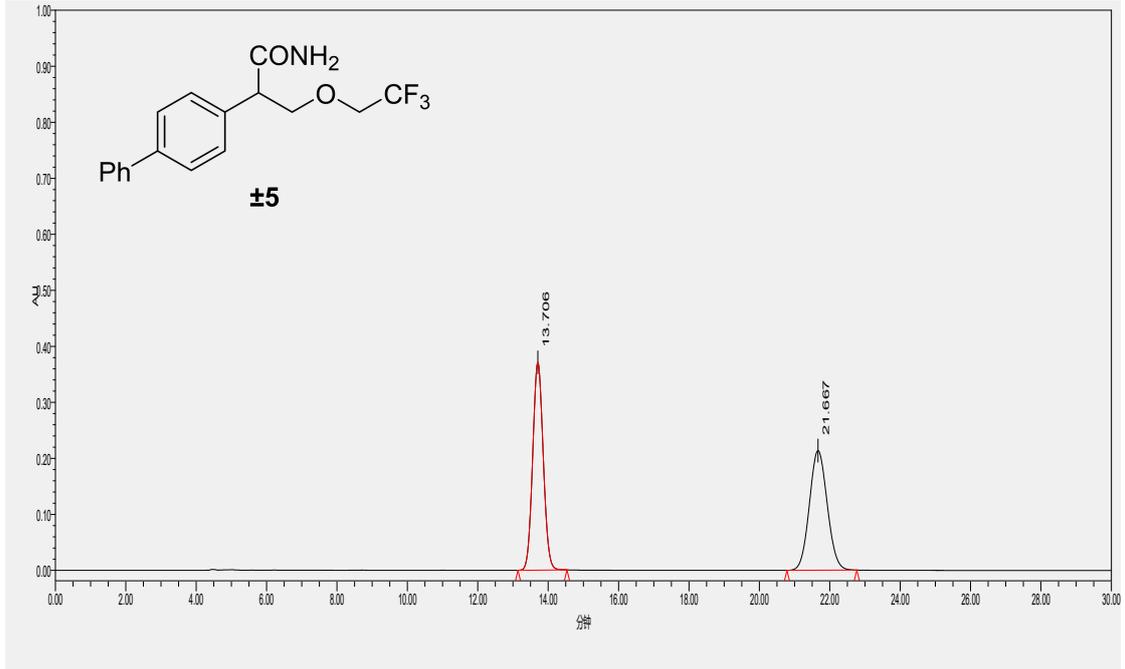


	RT(min)	Area	Area%	Height	Type
1	10.728	5127021	50.42	250414	BV
2	11.608	5041856	49.58	259229	VB

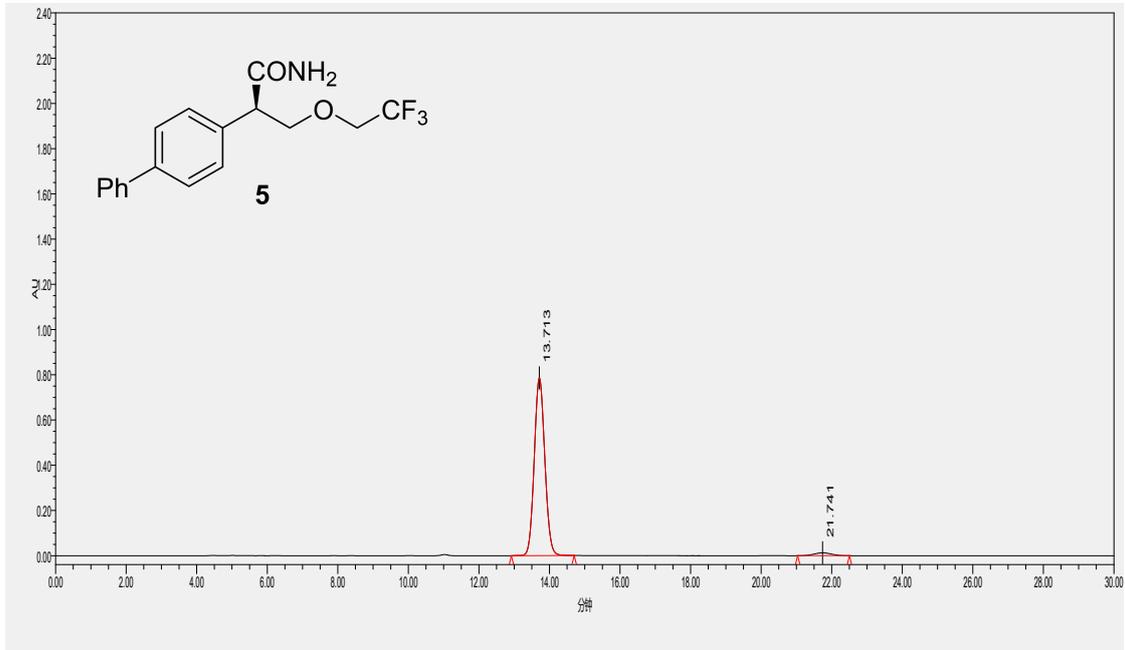


	RT(min)	Area	Area%	Height	Type
1	10.340	51578927	96.89	2278134	BV
2	11.639	1653564	3.11	76989	VB

HPLC spectra of 5

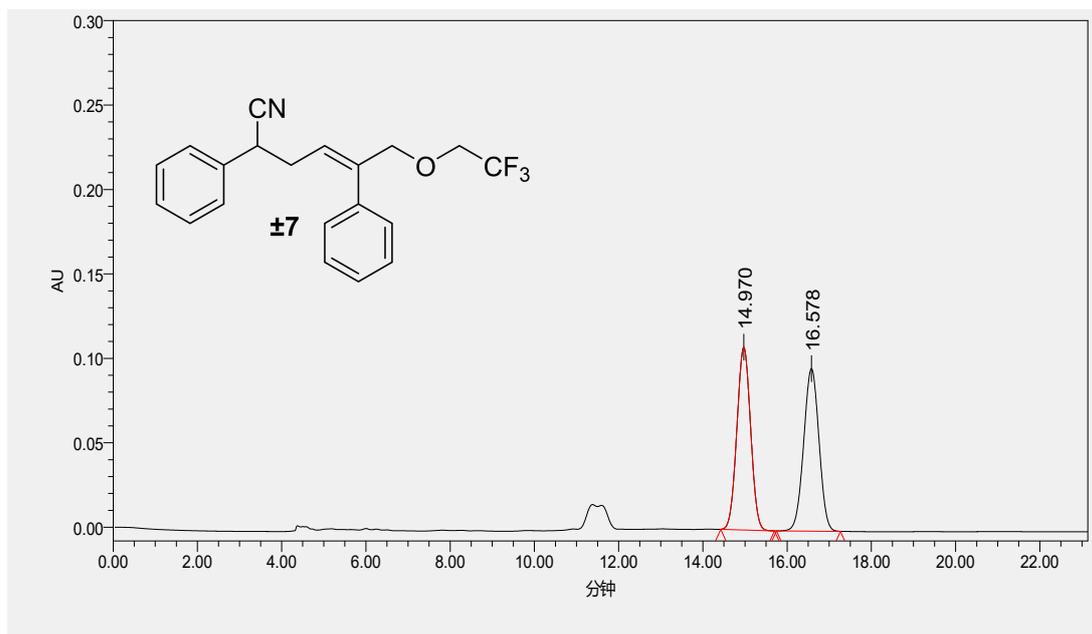


	RT(min)	Area	Area%	Height	Type
1	13.706	7733303	50.65	370888	BB
2	21.667	7536179	49.35	213573	BB

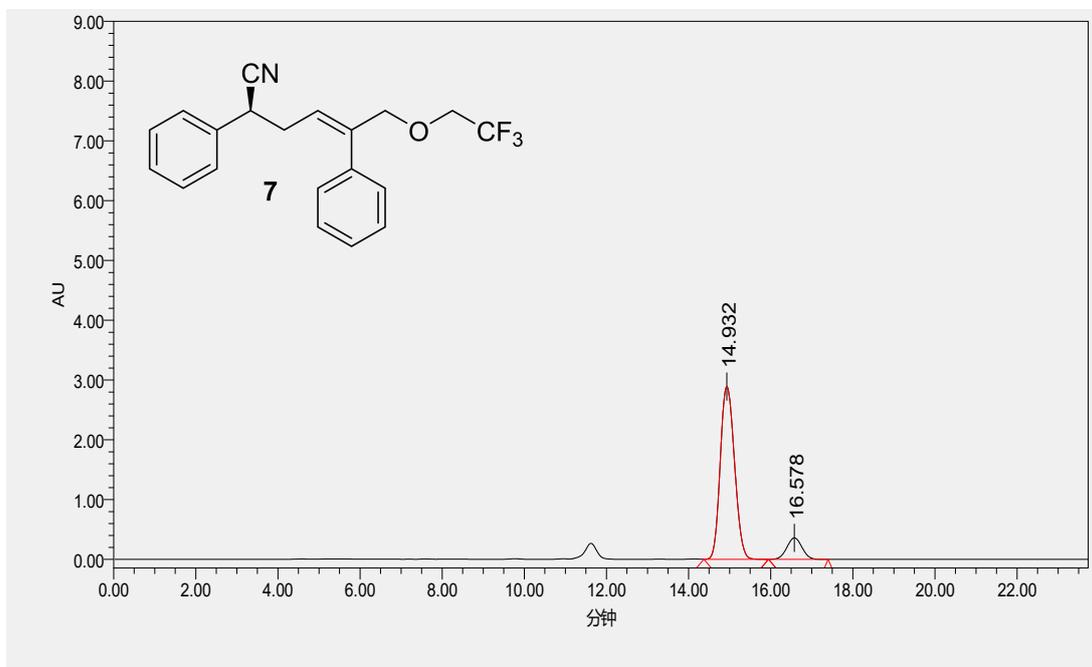


	RT(min)	Area	Area%	Height	Type
1	13.713	16365676	97.39	785990	BB
2	21.741	438883	2.61	12655	BB

HPLC spectra of 7



	RT(min)	Area	Area%	Height	Type
1	14.970	2451095	50.19	108271	BB
2	16.578	2432559	49.81	96248	BB



	RT(min)	Area	Area%	Height	Type
1	14.932	69860451	88.31	2891041	VV
2	16.578	9250541	11.69	359105	VB

