

**Diastereoselective Diastereoselective Formal 1,3-Dipolar
Cycloaddition of Trifluoroethyl Amine-derived Ketimines Enables
the Desymmetrization of Cyclopentenediones**

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Supporting Information

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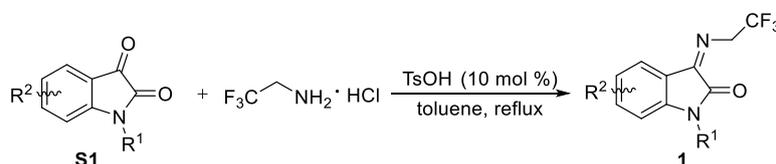
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1. General experimental information

Reagents were purchased from commercial sources and were used as received unless mentioned otherwise. Reactions were monitored by TLC. ^1H NMR and ^{13}C NMR spectra were recorded in CDCl_3 or $\text{DMSO-}d_6$. ^1H NMR chemical shifts are reported in ppm employed as the internal standard (CDCl_3 at 7.26 ppm, $\text{DMSO-}d_6$ at 2.50 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, br s = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR chemical shifts are reported in ppm with the solvent resonance as the internal standard (CDCl_3 at 77.16 ppm, $\text{DMSO-}d_6$ at 39.52 ppm). Melting points products were recorded on a Büchi Melting Point B-545. The HRMS were recorded by The HRMS were recorded by Agilent 6545 LC/Q-TOF mass spectrometer.

2. General experimental procedures for synthesis of compounds 1.

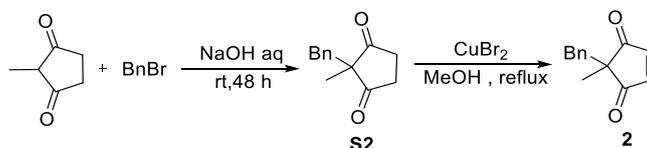
The *N*-2,2,2-trifluoroethylisatin ketimines **1** are known compounds, which were prepared according to literatures. Compounds **1a-1q** were synthesized with same method^[1].



In the dry reaction flask equipped with a water separator and a condenser was added the mixture of isatin **S1** (10.0 mmol), 2,2,2-trifluoroethylamine hydrochloride (15.0 mmol) and TsOH (1.0 mmol) in toluene (10.0 mL). Then, the mixture was refluxed to separate the water until complete disappearance of the isatin **S1**. Let cool slightly before evaporation of the toluene, and the crude residue was purified by flash chromatography on silica gel (petroleum ether / ethyl acetate = 15:1 to 8:1) to give the corresponding *N*-2,2,2-trifluoroethylisatin ketimines **1**.

3. General experimental procedures for synthesis of compound 2.

The 2-methyl-2-(phenylmethyl)-4-cyclopentene-1,3-dione **2** are known compounds, which were prepared according to literatures. Compounds **2a-2n** were synthesized with same method^[2].

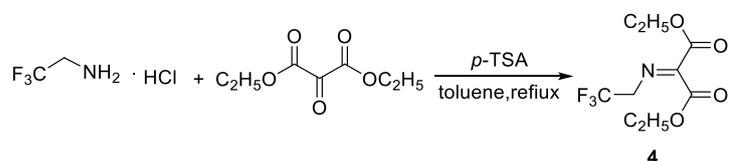


2-methylcyclopentane-1,3-dione (2.2 g, 20.0 mmol, 1.0 equiv) was stirred with 1.0 M aq. NaOH solution (1.0 equiv) at room temperature for 10 min. To this suspension benzyl bromide (6.8 g, 40.0 mmol, 2.0 equiv) was added at once and the resulting bi-phasic solution was stirred vigorously. After being stirred for 48 hours, the reaction mixture was diluted with EtOAc (50.0 mL). The aqueous phase was back-extracted with EtOAc twice (50.0 mL \times 2). The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. After an evaporation of the organic solvent, the crude residue was purified by chromatography (silica gel, hexane/ethyl acetate = 7:1). Compound **S2** (3.5 g, 87% yield) was obtained as a white solid according to the procedure mentioned above.

To a solution of 2,2-disubstituted cyclopentane-1,3-dione (1.6 g, 8.0 mmol, 1.0 equiv) in MeOH (50.0 mL) under argon atmosphere was added copper (II) bromide (3.9 g, 17.6 mmol, 2.2 equiv) and the resulting brown solution was refluxed for 1.0 hour. The reaction mixture was cooled to room temperature and then added in sequence: 10.0 mL of H₂O, 10.0 mL of HCl aq (1.0 M), and 50.0 mL of DCM. The aqueous phase was separated and extracted for 2 times with DCM. The collected organic phases were dried over MgSO₄, filtered and concentrated under reduced pressure. After an evaporation of the organic solvent, the crude residue was purified by chromatography (silica gel, hexane / ethyl acetate = 10:1). Compound **2** (1.5 g, 94% yield) was obtained as a yellow solid according to the procedure mentioned above.

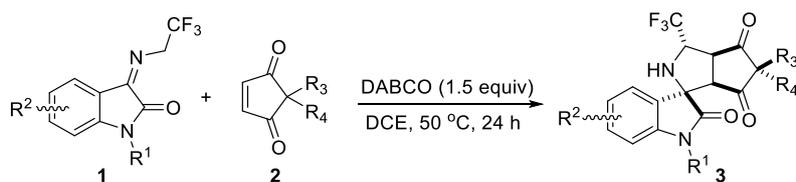
4. General experimental procedures for synthesis of compound **4**^[3].

The diethyl 2-((2,2,2-trifluoroethyl)imino)malonate **4** is known compound, which was prepared according to literatures.



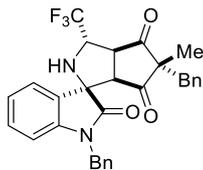
Diethyl ketomalonate (2.4 g, 14.0 mmol, 1.0 equiv); 2,2,2-trifluoroethyl-amine hydrochloride (3.8 g, 28.0 mmol, 2.0 equiv), and *p*-toluenesulfonic acid (0.2 g, 1.4 mmol, 0.1 equiv) were suspended in toluene (40.0 mL) in a two-neck flask with a water separator and a condenser. The mixture was then heated to separate the water until complete disappearance of the starting materials (about 30-60 minutes), after which it was cooled to room temperature, washed with a small quantity of saturated NaHCO₃ solution, extracted with ethyl acetate and washed with brine, and dried over anhydrous Na₂SO₄. After an evaporation of the organic solvent, the crude residue was purified by chromatography (silica gel, hexane / ethyl acetate = 5:1). Ketimine **4** (3.0 g, 84% yield) was obtained as a pale yellow liquid according to the procedure mentioned above.

5. General experimental procedures for synthesis of compounds **3**.



In a dry reaction tube equipped with a magnetic stirring bar, *N*-2,2,2-trifluoroethylisatin ketimines **1** (0.3 mmol), DABCO (33.6 mg, 0.3 mmol, 1.5 equiv), and **2** (40.2 mg, 0.2 mmol, 1.0 equiv), DCE (2.0 mL) were added in sequence. Then the mixture was stirred for 24 h at 50 °C. After completion, the reaction mixture was directly purified by flash chromatography on silica gel (petroleum ether / ethyl acetate, 15:1 - 10:1) to give the corresponding products **3**.

1',5-dibenzyl-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3aa)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

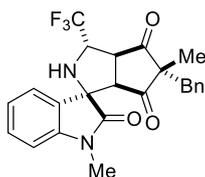
White solid; 99.5 mg, 96% yield; 85:15 *dr*, mp 194.4-195.3 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.38 (d, *J* = 7.3 Hz, 1H), 7.35 – 7.19 (m, 9H), 7.11 (m, 1H), 7.07 – 7.01 (m, 2H), 6.74 (d, *J* = 7.8 Hz, 1H), 4.85 (d, *J* = 15.9 Hz, 1H), 4.66 (d, *J* = 5.6 Hz, 1H), 4.59 (d, *J* = 15.9 Hz, 1H), 4.44 (m, 1H), 4.04 (d, *J* = 3.1 Hz, 2H), 3.01 (d, *J* = 13.3 Hz, 1H), 2.85 (d, *J* = 13.3 Hz, 1H), 0.95 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.8, 210.8, 178.0, 143.1, 135.5, 134.5, 130.2, 129.6, 128.6, 128.4, 128.08, 127.4, 127.2, 127.1, 125.6 (q, *J* = 276.8 Hz, 1C), 124.1, 123.1, 109.7, 70.9, 62.0, 58.7 (q, *J* = 30.4 Hz, 1C), 57.8, 51.3, 42.7, 41.4, 14.3.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₀H₂₆F₃N₂O₃, 519.1890, found: 519.1895.

5-benzyl-1',5-dimethyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ba)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

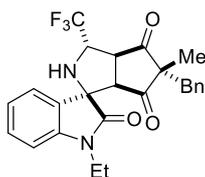
White solid; 81.4 mg, 92% yield; 83:17 *dr*, mp 239.0-239.7 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.42 – 7.31 (m, 2H), 7.30 – 7.19 (m, 3H), 7.14 (m, 1H), 7.02 (m, 3H), 4.50 (d, *J* = 5.6 Hz, 1H), 4.39 (m, 1H), 4.02 (dd, *J* = 12.0, 4.0 Hz, 1H), 3.97 (d, *J* = 12.0 Hz, 1H), 2.96 (s, 3H), 2.93 (s, 1H), 2.83 (d, *J* = 13.3 Hz, 1H), 0.92 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.7, 210.8, 177.8, 144.0, 134.4, 130.2, 129.7, 128.6, 128.0, 127.1, 125.6 (q, *J* = 276.8 Hz, 1C), 123.9, 123.0, 108.9, 70.94, 62.0, 58.7 (q, *J* = 30.4 Hz, 1C), 57.7, 51.1, 41.3, 25.7, 14.4.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₄H₂₂F₃N₃O₃, 443.1577, found: 443.1572.

5-benzyl-1'-ethyl-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ca)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

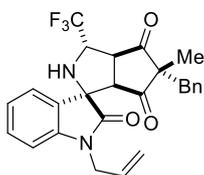
White solid; 83.8 mg, 92% yield; 90:10 *dr*, mp 158.1-158.8 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.29 – 7.16 (m, 5H), 7.03 (m, 1H), 6.94 – 6.85 (m, 2H), 6.75 (d, *J* = 7.8 Hz, 1H), 4.56 – 4.43 (m, 1H), 3.61 (m, 1H), 3.38 (m, 1H), 3.03 (d, *J* = 12.0 Hz, 1H), 2.84 (d, *J* = 12.9 Hz, 1H), 2.75 (d, *J* = 12.9 Hz, 1H), 2.61 (dd, *J* = 12.0, 4.5 Hz, 1H), 2.18 (s, 1H), 1.19 (s, 3H), 1.10 (t, *J* = 7.2 Hz, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.3, 210.8, 177.6, 142.9, 134.5, 130.2, 129.7, 128.8, 128.0, 127.1, 125.6 (q, *J* = 279.8 Hz, 1C), 124.1, 122.9, 109.0, 70.6, 61.8, 58.8 (q, *J* = 30.3 Hz, 1C), 58.0, 51.1, 41.3, 33.8, 14.3, 12.2.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₅H₂₄F₃N₂O₃, 457.1734, found: 457.1736.

1'-allyl-5-benzyl-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3da)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

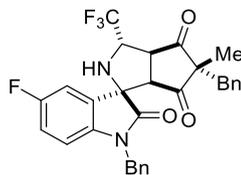
White solid; 90.1 mg, 96% yield, 83:17 *dr*, mp 149.0-149.7 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.36 (m, 2H), 7.28 (m, *J* = 3.7 Hz, 3H), 7.15 m, 1H), 7.03 (dd, *J* = 7.3, 2.3 Hz, 2H), 6.92 (d, *J* = 7.8 Hz, 1H), 5.70 (m, 1H), 5.22 (dd, *J* = 17.3, 1.7 Hz, 1H), 5.13 (dd, *J* = 10.4, 1.7 Hz, 1H), 4.58 (d, *J* = 5.6 Hz, 1H), 4.42 (m, 1H), 4.22 (m, 1H), 4.05 (dd, *J* = 9.9, 6.6 Hz, 1H), 4.01 (d, *J* = 3.8 Hz, 1H), 3.98 (d, *J* = 11.9 Hz, 1H), 2.95 (d, *J* = 13.3 Hz, 1H), 2.87 (d, *J* = 13.3 Hz, 1H), 0.92 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.6, 210.9, 177.7, 143.1, 134.5, 131.3, 130.3, 129.6, 128.6, 128.0, 127.1, 125.6 (q, *J* = 279.1 Hz, 1C), 124.1, 123.0, 116.9, 109.6, 70.8, 61.9, 58.7 (q, *J* = 30.6 Hz, 1C), 57.9, 51.1, 41.4, 41.3, 14.3.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₆H₂₄F₃N₂O₃, 469.1734, found: 469.1735.

1',5-dibenzyl-5'-fluoro-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ea)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

White solid; 84.7 mg, 79% yield; 84:16 *dr*, mp 209.0-209.7 °C;

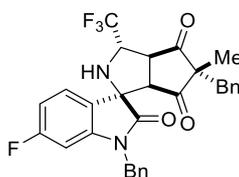
¹H NMR (400 MHz, DMSO-*d*₆) δ 7.32 (d, *J* = 3.3 Hz, 4H), 7.28 (m, 4H), 7.25 (d, *J* = 2.5 Hz, 1H), 7.13 (m, 1H), 7.09 – 6.99 (m, 2H), 6.76 (dd, *J* = 8.6, 4.1 Hz, 1H), 4.86 (d, *J* = 16.0 Hz, 1H), 4.76

(d, $J = 5.6$ Hz, 1H), 4.61 (d, $J = 16.0$ Hz, 1H), 4.52 – 4.36 (m, 1H), 4.13 (d, $J = 12.0$ Hz, 1H), 4.05 (dd, $J = 12.1, 4.4$ Hz, 1H), 3.01 (d, $J = 13.3$ Hz, 1H), 2.88 (d, $J = 13.3$ Hz, 1H), 0.97 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO- d_6) δ 213.2, 211.2, 178.4, 160.6, 158.2, 139.7 (d, $J = 1.8$ Hz, 1C), 135.7, 134.9, 130.9 (d, $J = 7.9$ Hz, 1C), 129.6 (d, $J = 217.1$ Hz, 1C), 128.9, 127.9, 127.7, 127.6, 126.0 (q, $J = 279.4$ Hz, 1C), 116.4 (d, $J = 23.3$ Hz, 1C), 112.6 (d, $J = 25.0$ Hz, 1C), 111.2 (d, $J = 8.0$ Hz, 1C), 71.5 (d, $J = 1.0$ Hz, 1C), 62.5, 59.3 (q, $J = 31.3$ Hz, 1C), 58.2, 51.6, 43.3, 41.9, 14.8.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{30}\text{H}_{25}\text{F}_4\text{N}_2\text{O}_3$, 537.1796, found: 537.1806.

1',5-dibenzyl-6'-fluoro-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3fa)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

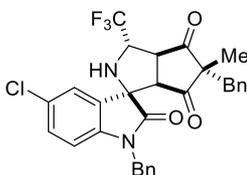
White solid; 87.9 mg, 82% yield; 87:13 *dr*, mp. 209.1-209.7 °C;

^1H NMR (400 MHz, DMSO- d_6) δ 7.32 (dd, $J = 8.3, 5.5$ Hz, 1H), 7.28 – 7.11 (m, 8H), 6.97 (dd, $J = 7.2, 2.3$ Hz, 2H), 6.84 (m, 1H), 6.64 (dd, $J = 9.4, 2.3$ Hz, 1H), 4.76 (d, $J = 15.9$ Hz, 1H), 4.59 (d, $J = 5.5$ Hz, 1H), 4.53 (d, $J = 15.9$ Hz, 1H), 4.34 (m, $J = 6.8, 6.3$ Hz, 1H), 3.97 (d, $J = 2.0$ Hz, 2H), 2.92 (d, $J = 13.3$ Hz, 1H), 2.77 (d, $J = 13.3$ Hz, 1H), 0.86 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO- d_6) δ 213.2, 211.2, 178.8, 164.8, 162.3, 145.3 (d, $J = 12.1$ Hz, 1C), 135.6, 134.9, 128.9, 128.1 (d, $J = 218.1$ Hz, 1C), 127.9, 127.8, 127.6, 126.3 (d, $J = 10.2$ Hz, 1C), 126.0 (q, $J = 279.8$ Hz, 1C), 124.8 (d, $J = 2.8$ Hz, 1C), 109.6 (d, $J = 22.5$ Hz, 1C), 98.8 (d, $J = 28.1$ Hz, 1C), 70.9, 62.5, 59.1 (q, $J = 31.0$ Hz, 1C), 58.2, 51.6, 43.3, 41.9, 14.7.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{30}\text{H}_{25}\text{F}_4\text{N}_2\text{O}_3$, 537.1796, found: 537.1800.

1',5-dibenzyl-5'-chloro-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ga)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

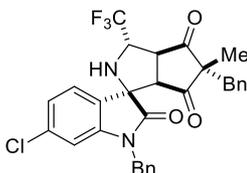
White solid; 100.5 mg, 91% yield; 85:15 *dr*, mp 249.3-250.0 °C;

^1H NMR (400 MHz, DMSO- d_6) δ 7.42 (d, $J = 2.2$ Hz, 1H), 7.38 – 7.21 (m, 9H), 7.09 – 7.02 (m, 2H), 6.77 (d, $J = 8.4$ Hz, 1H), 4.86 (d, $J = 16.0$ Hz, 1H), 4.76 (d, $J = 5.6$ Hz, 1H), 4.60 (d, $J = 16.0$ Hz, 1H), 4.44 (m, 1H), 4.19 (d, $J = 12.1$ Hz, 1H), 4.05 (dd, $J = 12.0, 4.5$ Hz, 1H), 2.99 (d, $J = 13.3$ Hz, 1H), 2.88 (d, $J = 13.3$ Hz, 1H), 0.95 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO- d_6) δ 212.7, 210.7, 177.7, 142.0, 135.1, 134.4, 130.6, 130.3, 129.5, 128.5, 128.1, 127.5, 127.3, 127.2, 127.2, 125.8 (q, J = 260.1 Hz, 1C), 124.5, 111.2, 70.8, 62.8, 58.7 (q, J = 30.6 Hz, 1C), 57.7, 51.1, 42.8, 41.5, 14.3.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{30}\text{H}_{25}^{35}\text{ClF}_3\text{N}_2\text{O}_3$, 553.1500, found: 553.1512; calcd for $\text{C}_{30}\text{H}_{24}^{37}\text{ClF}_3\text{N}_2\text{O}_3$, 555.1486, found: 555.1494.

1',5-dibenzyl-6'-chloro-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ha)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

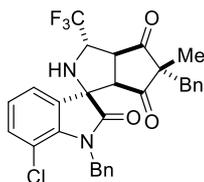
White solid; 68.5 mg, 82% yield; 88:12 *dr*, mp 253.8-254.4 °C;

^1H NMR (400 MHz, DMSO- d_6) δ 7.39 (d, J = 8.0 Hz, 1H), 7.37 – 7.21 (m, 8H), 7.17 (dd, J = 7.9, 1.9 Hz, 1H), 7.05 (dd, J = 7.2, 2.3 Hz, 2H), 6.88 (d, J = 1.9 Hz, 1H), 4.86 (d, J = 16.0 Hz, 1H), 4.70 (d, J = 5.5 Hz, 1H), 4.63 (d, J = 16.0 Hz, 1H), 4.47 – 4.37 (m, 1H), 4.06 (d, J = 1.9 Hz, 2H), 3.01 (d, J = 13.3 Hz, 1H), 2.85 (d, J = 13.3 Hz, 1H), 0.94 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO- d_6) δ 212.7, 210.6, 178.1, 144.6, 135.1, 134.4, 134.0, 130.2, 128.5, 128.1, 127.49, 127.47, 127.3, 127.2, 125.7, 125.6 (q, J = 271.2 Hz, 1C), 122.9, 110.0, 70.5, 62.1, 58.7 (q, J = 30.9 Hz, 1C), 57.8, 51.1, 42.8, 41.4, 14.2.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{30}\text{H}_{25}^{35}\text{ClF}_3\text{N}_2\text{O}_3$, 553.1500, found: 553.1511; calcd for $\text{C}_{30}\text{H}_{24}^{37}\text{ClF}_3\text{N}_2\text{O}_3$, 555.1486, found: 555.1493.

1',5-dibenzyl-7'-chloro-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ia)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

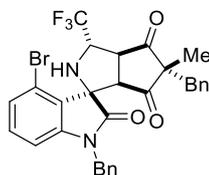
White solid; 68.5 mg, 62% yield; 86:14 *dr*, mp 190.7-191.6 °C;

^1H NMR (400 MHz, CDCl_3) 7.31 – 7.18 (m, 5H), 7.19 – 7.04 (m, 5H), 7.03 – 6.81 (m, 3H), 5.09 (d, J = 16.2 Hz, 1H), 5.01 (d, J = 16.2 Hz, 1H), 4.45 (m, 1H), 3.02 (d, J = 12.0 Hz, 1H), 2.85 (d, J = 12.9 Hz, 1H), 2.73 (d, J = 12.9 Hz, 1H), 2.56 (dd, J = 12.1, 4.5 Hz, 1H), 2.24 (s, 1H), 1.07 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 214.2, 211.7, 178.6, 139.1, 136.6, 134.6, 132.8, 130.9, 129.4, 128.9, 128.6, 128.0, 127.3, 126.5, 124.9 (q, J = 279.5 Hz, 1C), 124.8, 123.1, 116.0, 70.5, 63.0, 59.6, 59.5 (q, J = 32.0 Hz, 1C), 52.7, 46.2, 45.1, 17.7.

HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{30}H_{25}^{35}ClF_3N_2O_3$, 553.1500, found: 553.1511; calcd for $C_{30}H_{24}^{37}ClF_3N_2O_3$, 555.1486, found: 555.1492.

1',5-dibenzyl-4'-bromo-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ja)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

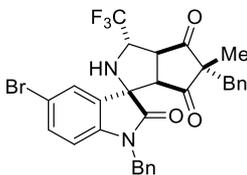
White solid; 81.2 mg, 68% yield; 91: 9 *dr*, mp 238.1-238.8 °C;

1H NMR (400 MHz, DMSO- d_6) δ 7.41 – 7.16 (m, 10H), 7.06 (dd, J = 7.1, 2.4 Hz, 2H), 6.78 (d, J = 7.6 Hz, 1H), 4.87 (d, J = 16.0 Hz, 1H), 4.68 – 4.54 (m, 2H), 4.41 (dd, J = 12.4, 6.6 Hz, 2H), 3.99 (dd, J = 12.3, 4.6 Hz, 1H), 3.07 (d, J = 13.2 Hz, 1H), 2.87 (d, J = 13.2 Hz, 1H), 0.98 (s, 3H).

$^{13}C\{^1H\}$ NMR (101 MHz, DMSO- d_6) δ 213.6, 211.0, 177.5, 145.4, 135.0, 134.5, 131.6, 130.2, 128.5, 128.1, 127.5, 127.2, 127.2, 125.9 (q, J = 256.4 Hz, 1C), 125.0, 119.0, 109.3, 72.2, 62.2, 58.5 (q, J = 30.9 Hz, 1C), 54.0, 51.1, 42.9, 41.6, 14.7.

HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{30}H_{25}^{79}BrF_3N_2O_3$, 597.0995, found: 597.1014; calcd for $C_{30}H_{24}^{81}BrF_3N_2O_3$, 599.0980, found: 599.0999.

1',5-dibenzyl-5'-bromo-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ka)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

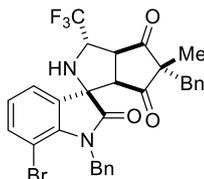
White solid; 116.8 mg, 98% yield; 85:15 *dr*, mp 204.3-205.2 °C;

1H NMR (400 MHz, DMSO- d_6) δ 7.42 – 7.30 (m, 6H), 7.28 (d, J = 6.7 Hz, 4H), 7.11 – 7.03 (m, 2H), 7.02 (s, 1H), 4.87 (d, J = 16.0 Hz, 1H), 4.72 (d, J = 5.6 Hz, 1H), 4.64 (d, J = 16.0 Hz, 1H), 4.44 (m, 1H), 4.08 (d, J = 1.9 Hz, 2H), 3.02 (d, J = 13.3 Hz, 1H), 2.87 (d, J = 13.3 Hz, 1H), 0.94 (s, 3H).

$^{13}C\{^1H\}$ NMR (101 MHz, DMSO- d_6) δ 212.7, 210.6, 178.0, 144.6, 135.1, 134.4, 130.2, 128.5, 128.1, 127.9, 127.5, 127.2, 127.2, 126.0, 125.8, 125.5 (q, J = 280.1 Hz, 1C), 122.3, 112.7, 70.5, 62.1, 58.7 (q, J = 31.2 Hz, 1C), 57.7, 51.1, 42.7, 41.3, 14.2.

HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{30}H_{25}^{79}BrF_3N_2O_3$, 597.0995, found: 597.0992; calcd for $C_{30}H_{24}^{81}BrF_3N_2O_3$, 599.0980, found: 599.0977.

1',5-dibenzyl-7'-bromo-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3la)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

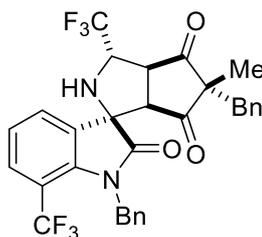
White solid; 75.1 mg, 63% yield; 85:15 *dr*, mp 151.5-152.3 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.46 (m, 2H), 7.34 – 7.25 (m, 5H), 7.25 – 7.21 (m, 1H), 7.21 – 7.16 (m, 2H), 7.11 (m, 1H), 7.08 – 7.00 (m, 2H), 5.06 (s, 2H), 4.75 (d, *J* = 5.5 Hz, 1H), 4.41 (dd, *J* = 9.8, 4.9 Hz, 1H), 4.08 (d, *J* = 2.8 Hz, 2H), 3.00 (d, *J* = 13.3 Hz, 1H), 2.86 (d, *J* = 13.3 Hz, 1H), 0.86 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.7, 210.5, 179.0, 140.5, 137.0, 135.2, 134.4, 132.2, 130.2, 28.2, 128.1, 127.2, 126.8, 125.9, 125.6 (q, *J* = 271.4 Hz, 1C), 125.1, 124.0, 101.7, 70.2, 62.0, 58.8 (q, *J* = 31.4 Hz, 1C), 58.1, 51.1, 44.2, 41.3, 14.1.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₀H₂₅⁷⁹BrF₃N₂O₃, 597.0995, found: 597.0996; calcd for C₃₀H₂₄⁸¹BrF₃N₂O₃, 599.0980, found: 599.0979.

1',5-dibenzyl-5-methyl-3,7'-bis(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ma)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

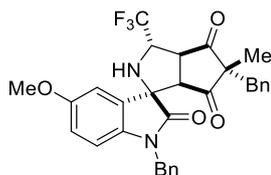
White solid; 80.9 mg, 69% yield; 83:17 *dr*, mp 248.2-248.8 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.77 (d, *J* = 7.4 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.40 (m, 1H), 7.26 (m, 5H), 7.19 (m, 1H), 7.12 (d, *J* = 7.6 Hz, 2H), 7.09 – 7.00 (m, 2H), 4.92 (d, *J* = 17.6 Hz, 1H), 4.82 (s, 1H), 4.78 (s, 1H), 4.41 (m, 1H), 4.17 (d, *J* = 12.0 Hz, 1H), 4.12 (dd, *J* = 12.0, 3.8 Hz, 1H), 2.99 (d, *J* = 13.3 Hz, 1H), 2.87 (d, *J* = 13.3 Hz, 1H), 0.81 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 213.2, 210.9, 180.3, 141.8, 136.3, 134.8, 132.2, 130.7, 129.5, 128.6, 128.5, 128.2, 127.6, 127.0, 126.4 (q, *J* = 273.7 Hz, 1C), 126.0 (q, *J* = 278.8 Hz), 125.7, 124.0, 112.0 (q, *J* = 33.3 Hz), 69.2, 62.5, 59.1 (q, *J* = 31.3 Hz, 1C), 58.4, 51.5, 46.3, 41.8, 14.5.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₁H₂₅F₆N₂O₃, 587.1764, found: 587.1772.

1',5-dibenzyl-5'-methoxy-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3na)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

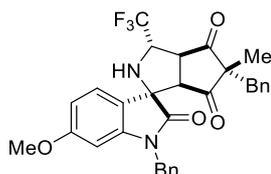
White solid; 105.3 mg, 96% yield; 80:20 *dr*, mp 188.5-189.4 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.38 – 7.20 (m, 8H), 7.13 – 7.02 (m, 2H), 6.99 (d, *J* = 2.5 Hz, 1H), 6.83 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.65 (d, *J* = 8.5 Hz, 1H), 4.84 (d, *J* = 15.9 Hz, 1H), 4.68 (d, *J* = 5.6 Hz, 1H), 4.58 (d, *J* = 15.9 Hz, 1H), 4.47 (m, *J* = 10.5, 5.2 Hz, 1H), 4.14 – 3.99 (m, 2H), 3.74 (s, 3H), 3.01 (d, *J* = 13.3 Hz, 1H), 2.87 (d, *J* = 13.3 Hz, 1H), 0.98 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.8, 210.8, 177.7, 156.0, 136.3, 135.5, 134.5, 130.3, 129.9, 128.4, 128.1, 127.3, 127.2, 127.2, 125.6 (q, *J* = 279.3 Hz, 1C), 114.1, 111.1 110.3, 71.3, 62.0, 58.8 (q, *J* = 30.9 Hz, 1C), 57.9, 55.6, 51.3, 42.8, 41.5, 14.4.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₁H₂₈F₃N₂O₄, 549.1996, found: 549.1998.

1',5-dibenzyl-6'-methoxy-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3oa)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

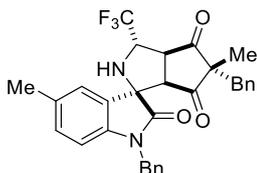
White solid; 88.8 mg, 81% yield; 85:15 *dr*, mp 205.1-205.9 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.27 – 7.11 (m, 9H), 7.04 – 6.93 (m, 2H), 6.58 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.28 (d, *J* = 2.3 Hz, 1H), 4.75 (d, *J* = 15.8 Hz, 1H), 4.57 – 4.43 (m, 2H), 4.33 (m, *J* = 9.7, 5.2 Hz, 1H), 3.98 – 3.78 (m, 2H), 3.62 (s, 3H), 2.93 (d, *J* = 13.4 Hz, 1H), 2.76 (d, *J* = 13.9 Hz, 1H), 0.86 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.8, 210.9, 178.5, 160.8, 144.4, 135.6, 134.5, 130.2, 128.4, 128.1, 127.4, 127.3, 127.2, 125.6 (q, *J* = 279.8 Hz, 1C), 125.0, 120.2, 106.9, 97.6, 70.7, 62.0, 58.5 (q, *J* = 31.0 Hz, 1C), 57.7, 55.4, 51.2, 42.7, 41.5, 14.4.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₁H₂₈F₃N₂O₄, 549.1996, found: 549.1998.

1',5-dibenzyl-5,5'-dimethyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3pa)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1

as the eluent);

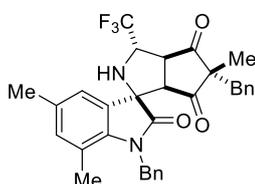
White solid; 101.1 mg, 95% yield; 89:11 *dr*, mp 231.8-232.4 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.50 – 7.22 (m, 8H), 7.20 (s, 1H), 7.13 – 6.94 (m, 3H), 6.62 (d, *J* = 7.9 Hz, 1H), 4.83 (d, *J* = 15.9 Hz, 1H), 4.64 (d, *J* = 5.6 Hz, 1H), 4.57 (d, *J* = 15.9 Hz, 1H), 4.44 (m, 1H), 3.99 (m, 2H), 3.01 (d, *J* = 13.3 Hz, 1H), 2.86 (d, *J* = 13.3 Hz, 1H), 2.30 (s, 3H), 0.96 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.8, 210.8, 177.9, 140.7, 135.5, 134.5, 132.3, 130.2, 129.7, 128.5, 128.4, 128.1, 127.3, 127.2, 127.1, 125.8 (q, *J* = 287.9 Hz, 1C), 124.8, 109.5, 71.0, 62.0, 58.7 (q, *J* = 30.7 Hz, 1C), 57.8, 51.3, 42.7, 41.6, 20.6, 14.4.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₁H₂₈F₃N₂O₃, 533.2047, found: 533.2048.

1',5-dibenzyl-5,5',7'-trimethyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3qa)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate = 15:1 as the eluent);

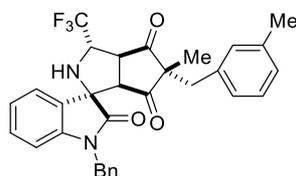
White solid; 87.4 mg, 80% yield; 83:17 *dr*, mp.190.7-191.6 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.32 – 7.19 (m, 5H), 7.16 (m, 1H), 7.08 – 6.99 (m, 2H), 6.93 (dd, *J* = 6.4, 2.9 Hz, 2H), 6.90 (d, *J* = 1.9 Hz, 1H), 6.72 (d, *J* = 1.9 Hz, 1H), 5.00 (d, *J* = 16.9 Hz, 1H), 4.73 (d, *J* = 16.9 Hz, 1H), 4.58 – 4.34 (m, 1H), 3.04 (d, *J* = 12.0 Hz, 1H), 2.86 (d, *J* = 12.9 Hz, 1H), 2.74 (d, *J* = 12.9 Hz, 1H), 2.56 (dd, *J* = 12.0, 4.6 Hz, 1H), 2.19 (s, 4H), 2.05 (s, 3H), 1.09 (s, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 214.8, 212.1, 179.0, 138.7, 136.9, 134.9, 134.8, 133.7, 129.5, 129.0, 129.0, 128.5, 128.0, 127.4, 125.7, 125.1 (q, *J* = 279.8Hz, 1C), 123.0, 120.4, 70.8, 63.1, 59.6 (q, *J* = 31.8Hz, 1C), 59.5, 52.9, 46.3, 45.2, 20.8, 18.4, 17.9.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₂H₃₀F₃N₂O₃, 547.2203, found: 547.2199.

1'-benzyl-5-methyl-5-(3-methylbenzyl)-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ab)



The product was purified by flash column chromatography (petroleum ether /ethyl acetate =15:1 as the eluent);

White solid; 102.1 mg, 96% yield; 84:16 *dr*, mp 190.6-191.4 °C;

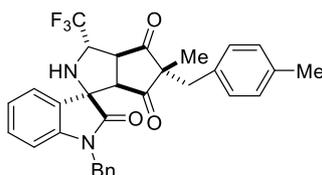
¹H NMR (400 MHz, CDCl₃) δ 7.38 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.31 (d, *J* = 4.3 Hz, 4H), 7.29 – 7.21 (m, 2H), 7.17 (m, 1H), 7.11 (m, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.86 (s, 1H), 6.82 (d, *J* = 7.6 Hz, 1H), 6.75 (d, *J* = 7.8 Hz, 1H), 4.85 (d, *J* = 16.0 Hz, 1H), 4.65 (d, *J* = 5.6 Hz, 1H), 4.59 (d, *J* =

16.0 Hz, 1H), 4.43 (q, $J = 6.9$ Hz, 1H), 3.97 (d, $J = 2.3$ Hz, 2H), 2.96 (d, $J = 13.3$ Hz, 1H), 2.80 (d, $J = 13.3$ Hz, 1H), 2.25 (s, 3H), 0.96 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 213.8, 211.8, 178.9, 144.1, 138.1, 136.4, 135.4, 131.8, 130.6, 129.6, 129.4, 129.0, 128.8, 128.3, 128.2, 128.2, 126.6 (q, $J = 279.8$ Hz, 1C), 125.1, 124.1, 110.7, 71.9, 63.0, 59.7 (q, $J = 30.6$ Hz, 1C), 58.8, 52.3, 43.7, 42.6, 21.9, 15.5.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{31}\text{H}_{28}\text{F}_3\text{N}_2\text{O}_3$, 533.2047, found: 533.2046.

1'-benzyl-5-methyl-5-(4-methylbenzyl)-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ac)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

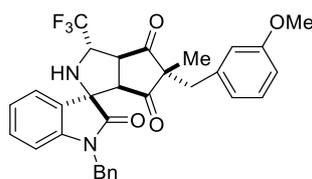
White solid; 100.0 mg, 94% yield; 82:18 *dr*, mp 131.2-132.0 °C;

^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 7.31 – 7.21 (m, 3H), 7.21 – 7.14 (m, 3H), 7.11 (m, 1H), 7.04 – 6.94 (m, 3H), 6.80 (d, $J = 7.8$ Hz, 2H), 6.55 (d, $J = 7.8$ Hz, 1H), 4.84 (d, $J = 15.7$ Hz, 1H), 4.54 – 4.46 (m, 1H), 4.43 (d, $J = 15.8$ Hz, 1H), 3.10 (d, $J = 12.0$ Hz, 1H), 2.83 (d, $J = 13.0$ Hz, 1H), 2.72 (d, $J = 13.0$ Hz, 1H), 2.64 (dd, $J = 12.0, 4.6$ Hz, 1H), 2.25 (s, 3H), 2.21 (s, 1H), 1.15 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, $\text{DMSO}-d_6$) δ 214.7, 212.2, 178.1, 143.0, 137.8, 134.9, 131.5, 130.3, 129.6, 129.4, 128.9, 128.1, 127.9, 127.3, 125.1 (q, $J = 276.7$ Hz, 1C), 123.9, 123.7, 110.0, 71.3, 63.2, 59.7 (q, $J = 31.5$ Hz, 1C), 59.2, 52.8, 45.9, 43.9, 21.2, 17.8.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{31}\text{H}_{28}\text{F}_3\text{N}_2\text{O}_3$, 533.2047, found: 533.2043.

1'-benzyl-5-(3-methoxybenzyl)-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ad)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

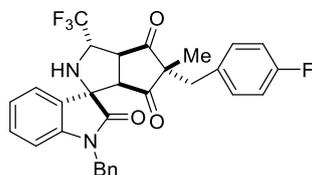
White solid; 103.1 mg, 94% yield; 85:15 *dr*, mp 182.6-183.4 °C;

^1H NMR (400 MHz, CDCl_3) δ 7.26 (dd, $J = 8.0, 6.5$ Hz, 2H), 7.23 – 7.17 (m, 2H), 7.17 – 7.14 (m, 2H), 7.11 (m, 2H), 6.98 (m, 1H), 6.79 – 6.69 (m, 1H), 6.55 (d, $J = 7.8$ Hz, 1H), 6.49 (m, 1H), 6.45 (t, $J = 2.1$ Hz, 1H), 4.84 (d, $J = 15.7$ Hz, 1H), 4.54 – 4.45 (m, 1H), 4.42 (d, $J = 15.7$ Hz, 1H), 3.65 (s, 3H), 3.11 (d, $J = 12.1$ Hz, 1H), 2.84 (d, $J = 12.8$ Hz, 1H), 2.72 (d, $J = 12.8$ Hz, 1H), 2.66 (dd, $J = 12.1, 4.5$ Hz, 1H), 2.19 (s, 1H), 1.17 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 214.5, 212.1, 178.1, 159.9, 143.0, 136.2, 134.9, 130.3, 130.1, 128.9, 128.0, 127.9, 127.3, 125.1 (q, $J = 276.8$ Hz, 1C), 124.3, 123.9, 121.7, 114.8, 113.8, 110.0, 71.3, 63.0, 59.6 (q, $J = 31.5$ Hz, 1C), 59.4, 55.4, 53.0, 46.4, 43.9, 18.0.

HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{31}H_{28}F_3N_2O_4$, 549.1996, found: 549.2004.

1'-benzyl-5-(4-fluorobenzyl)-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ae)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

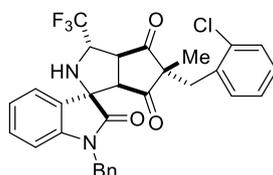
White solid; 102.9 mg, 96% yield; 88:12 *dr*, mp 172.9-173.7 °C;

1H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.22 (m, 3H), 7.22 – 7.07 (m, 4H), 7.04 – 6.96 (m, 1H), 6.95 – 6.81 (m, 4H), 6.56 (d, J = 7.8 Hz, 1H), 4.85 (d, J = 15.7 Hz, 1H), 4.52 (m, 1H), 4.44 (d, J = 15.7 Hz, 1H), 3.15 (d, J = 12.1 Hz, 1H), 2.87 – 2.81 (m, 1H), 2.81 – 2.76 (m, 1H), 2.74 (d, J = 13.2 Hz, 1H), 2.25 (s, 1H), 1.14 (s, 3H).

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 214.3, 211.8, 178.1, 162.4 (d, J = 248.3 Hz, 1C), 143.0, 134.8, 131.2 (d, J = 8.0 Hz, 1C), 130.4 (d, J = 3.0 Hz, 1C), 129.0, 127.9, 127.3, 125.0 (q, J = 279.4 Hz, 1C), 124.4, 124.0, 115.9 (d, J = 21.3 Hz, 1C), 110.1, 71.4, 62.9, 62.8, 59.8 (q, J = 31.9 Hz, 1C), 59.2, 52.7, 44.8, 43.9, 17.6.

HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{30}H_{25}F_4N_2O_3$, 537.1796, found: 537.1802.

1'-benzyl-5-(2-chlorobenzyl)-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione(3af)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

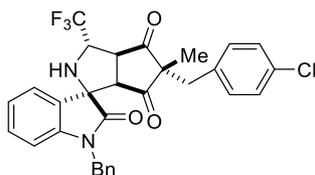
White solid; 83.9 mg, 76% yield; 71:29 *dr*, mp 174.8-175.6 °C;

1H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.22 (m, 3H), 7.16 (m, 4H), 7.05 – 6.96 (m, 1H), 6.90 (d, J = 2.4 Hz, 2H), 6.89 (s, 2H), 6.56 (d, J = 7.8 Hz, 1H), 4.85 (d, J = 15.7 Hz, 1H), 4.52 (m, 1H), 4.44 (d, J = 15.7 Hz, 1H), 3.15 (d, J = 12.1 Hz, 1H), 2.96 – 2.62 (m, 3H), 2.25 (s, 1H), 1.15 (s, 3H).

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 214.3, 211.9, 178.1, 163.7, 161.2, 143.1, 134.9, 131.3, 131.2, 130.4, 130.4, 129.07, 127.9, 127.3, 125.0 (q, J = 279.4 Hz, 1C), 124.4, 124.0, 116.0, 115.8, 110.1, 71.4, 62.9, 59.8 (q, J = 31.9 Hz, 1C), 59.2, 52.7, 44.8, 44.0, 17.6.

HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{30}H_{25}^{35}ClF_3N_2O_3$, 553.1500, found: 553.1500; calcd for $C_{30}H_{24}^{37}ClF_3N_2O_3$, 555.1486, found: 555.1485.

1'-benzyl-5-(4-chlorobenzyl)-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ag)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

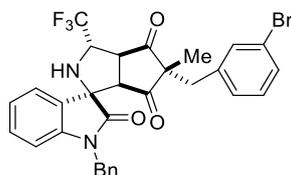
White solid; 103.8 mg, 94% yield; 86:14 *dr*, mp 198.1-198.8 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.26 (dd, *J* = 7.9, 6.5 Hz, 3H), 7.23 – 7.07 (m, 6H), 7.00 (m, 1H), 6.90 – 6.79 (m, 2H), 6.56 (d, *J* = 7.8 Hz, 1H), 4.84 (d, *J* = 15.7 Hz, 1H), 4.65 – 4.49 (m, 1H), 4.44 (d, *J* = 15.7 Hz, 1H), 3.20 (d, *J* = 12.1 Hz, 1H), 2.86 (dd, *J* = 12.1, 4.6 Hz, 1H), 2.83 – 2.64 (m, 2H), 2.27 (s, 1H), 1.14 (s, 3H).

¹³C{¹H}NMR (101 MHz, CDCl₃) δ 214.0, 211.6, 178.1, 143.0 134.8, 134.0, 133.0, 131.0, 130.4, 129.0 129.0, 127.9 127.9, 127.3, 125.0 (q, *J* = 276.7 Hz, 1C) 124.4, 124.0, 110.1, 71.4, 62.7, 59.8 (q, *J* = 31.0 Hz, 1C), 59.1, 52.6 44.7, 43.9, 17.5.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₀H₂₅³⁵Cl F₃N₂O₃, 553.1500, found: 553.1502; calcd for C₃₀H₂₄³⁷Cl F₃N₂O₃, 555.1486, found: 555.1486.

1'-benzyl-5-(3-bromobenzyl)-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ah)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

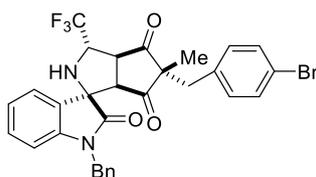
White solid; 100.1 mg, 84% yield; 84:16 *dr*, mp 175.0-175.6 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.32 (m, 1H), 7.31 – 7.23 (m, 3H), 7.23 – 7.11 (m, 4H), 7.11 – 7.04 (m, 2H), 7.01 (m, 1H), 6.84 (d, *J* = 7.9 Hz, 1H), 6.57 (d, *J* = 7.7 Hz, 1H), 4.85 (d, *J* = 15.7 Hz, 1H), 4.53 (m, 1H), 4.44 (d, *J* = 15.7 Hz, 1H), 3.21 (d, *J* = 12.0 Hz, 1H), 2.88 – 2.76 (m, 2H), 2.71 (d, *J* = 13.0 Hz, 1H), 2.43 – 2.01 (s, 1H), 1.15 (s, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 214.3, 211.9, 178.1, 163.7, 161.2, 143.1, 134.9, 131.3, 131.2, 130.4, 130.4, 129.0, 127.9, 127.3, 125.0 (q, *J* = 276.6 Hz, 1C), 124.4, 124.0, 116.0, 115.8, 110.1, 71.4, 62.9, 59.8 (q, *J* = 31.6 Hz, 1C), 59.2, 52.7, 44.8, 44.0, 17.6.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₀H₂₅⁷⁹BrF₃N₂O₃, 597.0995, found, 597.0995, calcd for C₃₀H₂₄⁸¹BrF₃N₂O₃, 599.0980, found: 599.0981.

1'-benzyl-5-(4-bromobenzyl)-5-methyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ai)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

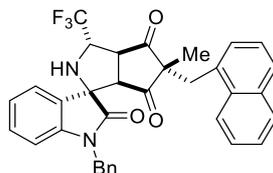
White solid; 112.1 mg, 94% yield; 85:15 *dr*, mp 176.1-176.9 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.47 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 7.3 Hz, 1H), 7.31 (d, *J* = 4.3 Hz, 4H), 7.26 (m, 2H), 7.12 (m, 1H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.75 (d, *J* = 7.8 Hz, 1H), 4.84 (d, *J* = 15.9 Hz, 1H), 4.68 (d, *J* = 5.5 Hz, 1H), 4.60 (d, *J* = 15.9 Hz, 1H), 4.45 (m, 1H), 4.29 (dd, *J* = 12.1, 4.4 Hz, 1H), 4.15 (d, *J* = 12.0 Hz, 1H), 3.08 – 2.78 (m, 2H), 0.92 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.4, 210.6, 178.0, 143.1, 135.5, 133.9, 132.6, 130.9, 129.6, 128.6, 128.4, 127.4, 127.2, 125.7 (q, *J* = 272.1 Hz, 1C), 124.2, 123.2, 120.5, 109.7, 71.0, 61.6, 58.7 (q, *J* = 30.5 Hz, 1C), 57.7, 51.0, 42.8, 39.9, 13.8.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₀H₂₅⁷⁹BrF₃N₂O₃, 597.0995, found, 597.0995, calcd for C₃₀H₂₄⁸¹BrF₃N₂O₃, 599.0980, found: 599.0978.

1'-benzyl-5-methyl-5-(naphthalen-1-ylmethyl)-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3aj)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

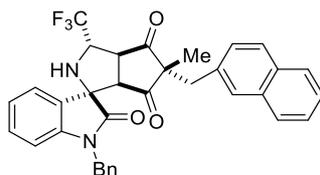
White solid; 111.3 mg, 98% yield; 89:11 *dr*, mp 190.2-191.1 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 8.07 – 8.00 (m, 1H), 7.97 – 7.89 (m, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.51 (dd, *J* = 6.5, 3.3 Hz, 2H), 7.45 (m, 1H), 7.37 – 7.20 (m, 8H), 7.10 (m, 1H), 6.75 (d, *J* = 7.7 Hz, 1H), 4.86 (d, *J* = 16.0 Hz, 1H), 4.65 (d, *J* = 5.5 Hz, 1H), 4.59 (d, *J* = 16.0 Hz, 1H), 4.44 (t, *J* = 7.0 Hz, 1H), 3.81 (s, 2H), 3.60 – 3.44 (m, 2H), 1.08 (s, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 213.2, 211.2, 178.6, 143.1, 135.4, 133.3, 132.0, 131.0, 129.6, 129.1, 128.6, 128.6, 128.4, 128.0, 127.4, 127.2, 126.0, 125.8, 125.5 (q, *J* = 276.6 Hz, 1C), 125.1, 124.0, 123.9, 123.2, 109.7, 71.0, 62.3, 58.7 (q, *J* = 30.6 Hz, 1C), 58.3, 51.7, 42.8, 37.8, 15.5.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₄H₂₈F₃N₂O₃, 569. 2047, found: 569.2072.

1'-benzyl-5-methyl-5-(naphthalen-2-ylmethyl)-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3ak)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

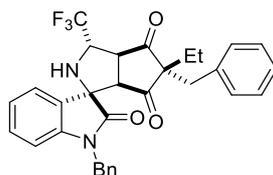
White solid; 112.6 mg, 99% yield; 86:14 *dr*, mp 138.2-138.9 °C

¹H NMR (400 MHz, CDCl₃) δ 7.78 – 7.69 (m, 1H), 7.66 (dd, *J* = 9.0, 5.4 Hz, 2H), 7.39 (dd, *J* = 6.3, 2.9 Hz, 3H), 7.25 (dd, *J* = 8.1, 6.5 Hz, 2H), 7.21 – 7.12 (m, 4H), 7.09 (m, 1H), 7.00 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.93 (m, 1H), 6.53 (d, *J* = 7.8 Hz, 1H), 4.84 (d, *J* = 15.7 Hz, 1H), 4.50 (m, *J* = 11.3, 5.6 Hz, 1H), 4.41 (d, *J* = 15.7 Hz, 1H), 3.08 (d, *J* = 12.0 Hz, 1H), 3.00 (d, *J* = 13.0 Hz, 1H), 2.92 (d, *J* = 13.0 Hz, 1H), 2.75 (dd, *J* = 12.1, 4.7 Hz, 1H), 2.12 (s, 1H), 1.21 (s, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 214.5, 212.1, 178.1, 143.0, 134.9, 133.3, 132.7, 132.1, 130.3, 128.9, 128.7, 128.5, 127.9, 127.8, 127.8, 127.4, 127.3, 126.7, 126.4, 125.0 (q, *J* = 276.7 Hz, 1C), 123.9, 123.6, 110.0, 71.3, 63.2, 59.7 (q, *J* = 29.1 Hz, 1C), 59.2, 52.8, 46.1, 43.9, 17.9.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₄H₂₈F₃N₂O₃, 569. 2047, found: 569.2049.

1',5-dibenzyl-5-ethyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3aI)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

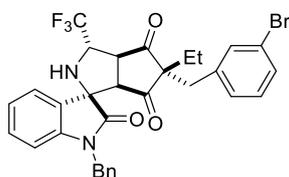
White solid; 73.4 mg, 69% yield; 88:12 *dr*, mp 171.2-171.8 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.34 (m, 5H), 7.30 – 7.20 (m, 5H), 7.11 (m, 1H), 7.08 – 6.98 (m, 2H), 6.73 (d, *J* = 7.8 Hz, 1H), 4.91 (d, *J* = 16.1 Hz, 1H), 4.64 (d, *J* = 5.2 Hz, 1H), 4.59 (d, *J* = 15.8 Hz, 1H), 4.47 (m, 1H), 4.01 (d, *J* = 12.4 Hz, 1H), 3.87 (dd, *J* = 12.5, 5.2 Hz, 1H), 3.09 (d, *J* = 13.5 Hz, 1H), 2.99 (d, *J* = 13.5 Hz, 1H), 1.54 (m, *J* = 7.5 Hz, 2H), 0.87 (t, *J* = 7.6 Hz, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 212.3, 210.5, 177.7, 143.2, 135.6, 134.5, 130.1, 129.6, 128.9, 128.4, 128.2, 127.3, 127.2, 127.2, 125.5 (q, *J* = 276.8 Hz, 1C), 124.1, 123.0, 109.6, 70.1, 66.2, 58.6 (q, *J* = 30.5 Hz, 1C), 57.8, 51.3, 42.8, 40.3, 22.1, 8.1.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₁H₂₈F₃N₂O₃, 533. 2047, found: 533.2048.

1'-benzyl-5-(3-bromobenzyl)-5-ethyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione (3am)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

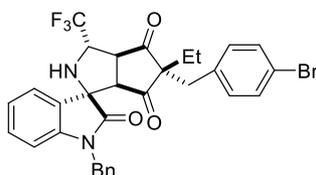
White solid; 102.5 mg, 84% yield; 72:28 *dr*, mp 166.5-167.4 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.46 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.37 – 7.28 (m, 5H), 7.25 (dd, *J* = 8.9, 7.2 Hz, 3H), 7.12 (m, 1H), 7.07 (d, *J* = 7.7 Hz, 1H), 6.73 (d, *J* = 7.8 Hz, 1H), 4.90 (d, *J* = 16.0 Hz, 1H), 4.65 (d, *J* = 5.3 Hz, 1H), 4.59 (d, *J* = 16.0 Hz, 1H), 4.54 – 4.40 (m, 1H), 4.30 – 4.01 (m, 2H), 3.10 (d, *J* = 13.6 Hz, 1H), 3.01 (d, *J* = 13.6 Hz, 1H), 1.49 (m, *J* = 9.8, 5.0 Hz, 2H), 0.84 (t, *J* = 7.5 Hz, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 213.8, 211.3, 178.0, 143.0, 136.9, 134.8, 132.6, 131.2, 130.5, 130.4, 129.0, 128.3, 127.9, 127.9, 127.3, 125.0 (q, *J* = 279.4 Hz, 1C), 124.4, 124.0, 122.9, 110.2, 77.5, 77.2, 76.8, 71.4, 62.6, 59.7 (q, *J* = 31.7 Hz, 1C), 59.1, 52.7, 44.8, 44.0, 17.5.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₁H₂₇⁷⁹BrF₃N₂O₃, 611.1152, found: 611.1149; calcd for C₃₁H₂₆⁸¹BrF₃N₂O₃, 613.1136, found: 613.1139.

1'-benzyl-5-(4-bromobenzyl)-5-ethyl-3-(trifluoromethyl)-2,3,3a,6a-tetrahydro-4H-spiro[cyclopenta[c]pyrrole-1,3'-indoline]-2',4,6(5H)-trione(3an)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =15:1 as the eluent);

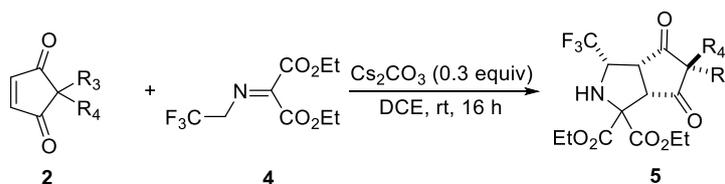
White solid; 107.3 mg, 88% yield; 84:16 *dr*, mp. 120.1-120.7 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.48 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 7.3 Hz, 1H), 7.39 – 7.28 (m, 4H), 7.25 (m, 2H), 7.11 (m, 1H), 7.02 (d, *J* = 8.1 Hz, 2H), 6.73 (d, *J* = 7.8 Hz, 1H), 4.90 (d, *J* = 16.0 Hz, 1H), 4.65 (d, *J* = 5.3 Hz, 1H), 4.58 (d, *J* = 16.0 Hz, 1H), 4.48 (m, 1H), 4.19 (d, *J* = 12.5 Hz, 1H), 4.14 (dd, *J* = 12.5, 4.7 Hz, 1H), 3.07 (d, *J* = 13.6 Hz, 1H), 3.00 (d, *J* = 13.6 Hz, 1H), 1.48 (dt, *J* = 11.7, 7.0 Hz, 2H), 0.83 (t, *J* = 7.5 Hz, 3H).

¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 211.8, 210.1, 177.7, 143.2, 135.6, 133.9, 132.4, 131.0, 129.6, 128.8, 128.4, 127.3, 127.1, 125.5 (q, *J* = 276.9 Hz, 1C) 124.2, 123.0, 120.6, 109.6, 70.0, 66.0, 58.6 (q, *J* = 30.8 Hz, 1C), 57.6, 51.0, 42.8, 38.9, 21.5, 8.1.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₃₁H₂₇⁷⁹BrF₃N₂O₃, 611. 1152, found: 611.1153; calcd for C₃₁H₂₆⁸¹BrF₃N₂O₃, 613.1136, found: 613.1138.

6. General experimental procedures for synthesis of compounds 5.

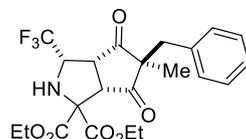


In a dry reaction tube equipped with a magnetic stirring bar, **2** (60.2 mg, 0.3 mmol, 3.0 equiv), and 2-((2,2,2-trifluoroethyl)imino) malonate **4** (0.1 mmol), Cs₂CO₃ (31.8 mg, 0.09 mmol), DCE (3.0 mL) were added in sequence, Then the mixture was stirred at room temperature for 24 h.

After completion, the reaction mixture was directly purified by flash chromatography on silica gel (petroleum ether / ethyl acetate = 15:1 - 10:1) to give the corresponding products **5**.

Diethyl

5-benzyl-5-methyl-4,6-dioxo-3-(trifluoromethyl)hexahydrocyclopenta[c]pyrrole-1,1(2H)-dicarboxylate(**5a**)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

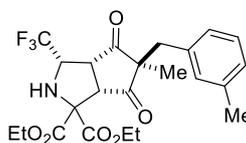
White solid; 77.8 mg, 57% yield; > 20:1 *dr*, mp 162.1-162.9 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.25 – 7.12 (m, 3H), 6.98 – 6.86 (m, 2H), 4.26 (q, 2H), 4.21 – 4.06 (m, 2H), 3.63 – 3.50 (m, 1H), 3.08 (d, *J* = 10.1 Hz, 1H), 2.99 (d, *J* = 12.9 Hz, 1H), 2.86 (t, *J* = 9.7 Hz, 1H), 2.83 – 2.76 (m, 2H), 1.26 (t, *J* = 7.2 Hz, 3H), 1.20 – 1.12 (m, 6H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 213.6, 212.9, 168.7, 166.2, 135.3, 129.6, 128.9, 127.5, 123.6 (q, *J* = 280.5 Hz, 1C), 74.7, 63.0, 62.4, 61.4 (q, *J* = 32.6 Hz, 1C), 60.7, 56.2, 49.8, 44.2, 19.5, 13.9, 13.8.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₂H₂₅F₃NO₆, 456.1628, found: 456.1635.

Diethyl 5-methyl-5-(3-methylbenzyl)-4,6-dioxo-3-(trifluoromethyl)hexahydrocyclopenta[c]pyrrole-1,1(2H)-dicarboxylate(**5b**)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

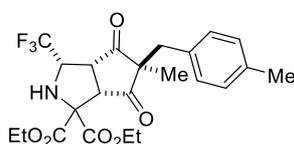
White solid; 70.4 mg, 50% yield; > 20:1 *dr*, mp 136.9-137.7 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.13 (m, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.86 – 6.72 (m, 2H), 4.38 – 4.27 (m, 2H), 4.27 – 4.05 (m, 2H), 3.71 – 3.52 (m, 1H), 3.12 (d, *J* = 10.1 Hz, 1H), 3.01 (d, *J* = 12.9 Hz, 1H), 2.94 (t, *J* = 9.9 Hz, 1H), 2.87 (d, *J* = 4.1 Hz, 1H), 2.82 (d, *J* = 12.9 Hz, 1H), 2.28 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H), 1.28 – 1.13 (m, 6H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 213.6, 212.9, 168.7, 166.3, 138.5, 135.2, 130.3, 128.7, 128.3, 126.5, 123.6 (q, *J* = 280.5 Hz, 1C), 74.6, 63.0, 62.4, 61.3 (q, *J* = 32.5 Hz, 1C), 60.7, 56.3, 49.8, 44.4, 21.3, 19.4, 13.9 (2C).

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₃H₂₇F₃NO₆, 470.1785, found: 470.1790.

Diethyl 5-methyl-5-(4-methylbenzyl)-4,6-dioxo-3-(trifluoromethyl)hexahydrocyclopenta[c]pyrrole-1,1(2H)-dicarboxylate(**5c**)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

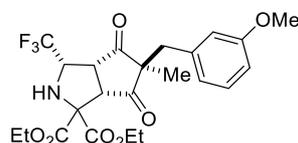
White solid; 59.1 mg, 42% yield; > 20:1 *dr*, mp 113.3-114.2 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.04 (d, *J* = 7.8 Hz, 2H), 6.96 – 6.74 (m, 2H), 4.33 (m, 2H), 4.28 – 4.09 (m, 2H), 3.63 (m, 1H), 3.20 (d, *J* = 10.2 Hz, 1H), 3.00 (d, *J* = 12.9 Hz, 1H), 2.93 (t, *J* = 9.8 Hz, 1H), 2.88 (s, 1H), 2.83 (d, *J* = 13.0 Hz, 1H), 2.29 (s, 3H), 1.33 (t, *J* = 7.2 Hz, 3H), 1.29 – 1.13 (m, 6H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 213.8, 213.0, 168.7, 166.3, 137.2, 132.2, 129.5, 129.4, 123.7 (q, *J* = 278.1 Hz, 1C), 74.8, 63.0, 62.4, 61.4 (q, *J* = 32.3 Hz, 1C), 60.7, 56.2, 49.8, 43.8, 21.1, 19.4, 13.9 (2C).

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₃H₂₇F₃NO₆, 470.1785, found: 470.1788.

Diethyl 5-(3-methoxybenzyl)-5-methyl-4,6-dioxo-3-(trifluoromethyl)hexahydrocyclopenta[c] pyrrole-1,1(2H)-dicarboxylate(5d)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

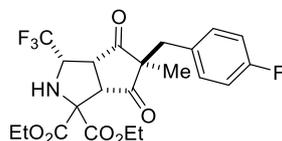
White solid; 78.6 mg, 54% yield; > 20:1 *dr*, mp 110.8-111.4 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.15 (m, 1H), 6.77 (dd, *J* = 8.2, 2.6 Hz, 1H), 6.57 (d, *J* = 7.5 Hz, 1H), 6.53 (m, 1H), 4.32 (m, 2H), 4.28 – 4.12 (m, 2H), 3.75 (d, *J* = 1.9 Hz, 3H), 3.63 (m, 1H), 3.19 (d, *J* = 10.2 Hz, 1H), 3.03 (d, *J* = 12.7 Hz, 1H), 2.97 (t, *J* = 9.9 Hz, 1H), 2.85 (d, *J* = 12.8 Hz, 2H), 1.32 (m, 3H), 1.27 – 1.18 (m, 6H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 213.8, 212.9, 168.8, 166.4, 159.8, 137.0, 129.9, 123.7 (q, *J* = 280.5 Hz, 1C), 121.9, 115.2, 113.3, 74.8, 63.1, 62.5, 61.5 (q, *J* = 32.6 Hz, 1C), 60.7, 56.4, 55.3, 50.0, 44.4, 19.7, 14.1, 14.0.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₃H₂₇F₃NO₇, 486.1734, found: 486.1714.

Diethyl 5-(4-fluorobenzyl)-5-methyl-4,6-dioxo-3-(trifluoromethyl)hexahydrocyclopenta [c] pyrrole-1,1(2H)-dicarboxylate(5e)



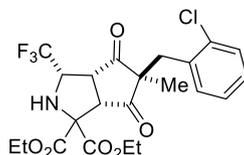
The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

White solid; 85.2 mg, 60% yield; > 20:1 *dr*, mp 152.6-153.4 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.05 – 6.82 (m, 4H), 4.32 (m, 2H), 4.28 – 4.11 (m, 2H), 3.68 – 3.59 (m, 1H), 3.25 (d, *J* = 10.1 Hz, 1H), 3.01 (d, *J* = 13.1 Hz, 1H), 2.96 (d, *J* = 9.8 Hz, 1H), 2.93 – 2.89 (m, 1H), 2.86 (d, *J* = 13.2 Hz, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 1.29 – 1.18 (m, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 213.7, 212.9, 168.8, 166.3, 162.2 (d, $J = 247.6$ Hz, 1C), 131.4 (d, $J = 8.0$ Hz, 1C), 131.3 (d, $J = 3.3$ Hz, 1C), 123.7 (q, $J = 280.4$ Hz, 1C), 115.7 (d, $J = 21.3$ Hz, 1C), 75.0, 63.2, 62.6, 61.6 (q, $J = 32.5$ Hz, 1C), 60.7, 60.7, 56.3, 49.8, 42.7, 19.8, 14.0.
HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{24}\text{F}_4\text{NO}_6$, 474.1534, found: 474.1534.

Diethyl 5-(2-chlorobenzyl)-5-methyl-4,6-dioxo-3-(trifluoromethyl)hexahydrocyclopenta[c]pyrrole-1,1(2H)-dicarboxylate(5f)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

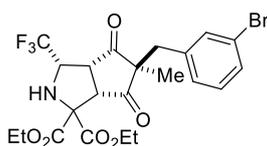
White solid; 64.6 mg, 44% yield; > 20:1 *dr*, mp 159.1-159.8°C;

^1H NMR (400 MHz, CDCl_3) δ 7.38 – 7.31 (m, 1H), 7.26 – 7.23 (m, 2H), 7.08 (dd, $J = 6.8, 2.5$ Hz, 1H), 4.42 – 4.28 (m, 2H), 4.27 – 4.10 (m, 2H), 3.77 (d, $J = 10.2$ Hz, 2H), 3.37 (t, $J = 10.1$ Hz, 1H), 3.10 (d, $J = 2.9$ Hz, 2H), 2.90 (d, $J = 4.2$ Hz, 1H), 1.31 (t, $J = 7.2$ Hz, 3H), 1.25 (t, $J = 7.1$ Hz, 3H), 1.20 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 211.0 (2C), 168.7, 166.3, 134.6, 132.7, 132.1, 130.0, 129.2, 127.0, 123.6 (q, $J = 280.5$ Hz, 1C), 74.0, 63.0, 62.3, 61.0 (q, $J = 32.4$ Hz, 1C), 59.3, 55.6, 49.9, 40.3, 17.8, 14.0, 13.9.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{24}^{35}\text{ClF}_3\text{NO}_6$, 490.1239, found: 490.1242; calcd for $\text{C}_{22}\text{H}_{23}^{37}\text{ClF}_3\text{NO}_6$, 492.1225, found: 492.1225.

Diethyl 5-(4-bromobenzyl)-5-methyl-4,6-dioxo-3-(trifluoromethyl)hexahydrocyclopenta[c]pyrrole-1,1(2H)-dicarboxylate(5g)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

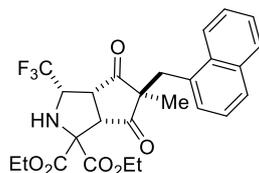
White solid; 84.8 mg, 53% yield; > 20:1 *dr*, mp 149.1-150.0 °C;

^1H NMR (400 MHz, CDCl_3) δ 7.36 (dd, $J = 8.0, 1.9$ Hz, 1H), 7.12 (dd, $J = 14.4, 6.6$ Hz, 2H), 6.92 (d, $J = 7.6$ Hz, 1H), 4.32 (m, 2H), 4.29 – 4.13 (m, 2H), 3.66 (m, 1H), 3.29 (d, $J = 10.1$ Hz, 1H), 3.08 – 2.96 (m, 2H), 2.92 (d, $J = 3.9$ Hz, 1H), 2.83 (d, $J = 13.1$ Hz, 1H), 1.33 (t, $J = 7.2$ Hz, 3H), 1.29 – 1.20 (m, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 213.1, 212.3, 168.7, 166.1, 137.8, 132.7, 130.7, 130.3, 128.4, 123.5 (q, $J = 280.3$ Hz, 1C), 122.7, 74.9, 63.1, 62.5, 61.5 (q, $J = 32.4$ Hz, 1C), 60.4, 56.1, 49.7, 42.7, 19.8, 14.0, 13.9.

HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{24}^{79}\text{BrF}_3\text{NO}_6$, 534.0734, found: 534.0732; calcd for $\text{C}_{22}\text{H}_{23}^{81}\text{BrF}_3\text{NO}_6$, 536.0716, found: 536.0717.

Diethyl 5-methyl-5-(naphthalen-1-ylmethyl)-4,6-dioxo-3-(trifluoromethyl) hexahydrocyclopenta[c]pyrrole-1,1(2H)-dicarboxylate(5h)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

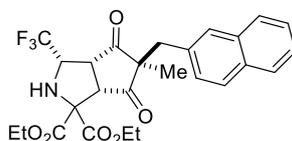
White solid; 89.4 mg, 59% yield; > 20:1 *dr*, mp 158.3-159.1 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.98 – 7.91 (m, 1H), 7.87 – 7.80 (m, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.49 (m, 2H), 7.37 (m, 1H), 7.18 (d, *J* = 7.0 Hz, 1H), 4.37 – 4.15 (m, 2H), 4.15 – 3.97 (m, 2H), 3.56 (m, 6.8 Hz, 1H), 3.48 (s, 2H), 2.88 – 2.72 (m, 2H), 2.64 (d, *J* = 10.4 Hz, 1H), 1.34 (s, 3H), 1.23 (t, *J* = 7.2 Hz, 3H), 1.13 (t, *J* = 7.1 Hz, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 213.2, 212.8, 168.5, 166.2, 133.9, 131.7, 131.6, 128.9, 128.7, 128.4, 126.5, 126.1, 125.3, 124.1, 123.7 (q, *J* = 280.4 Hz, 1C), 74.0, 62.9, 62.2, 61.0 (q, *J* = 32.4 Hz, 1C), 60.6, 56.5, 50.2, 41.0, 19.5, 13.9 (2C).

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₆H₂₇F₃NO₆, 506.1785, found: 506.1789.

Diethyl 5-methyl-5-(naphthalen-2-ylmethyl)-4,6-dioxo-3-(trifluoromethyl) hexahydrocyclopenta[c]pyrrole-1,1(2H)-dicarboxylate(5i)



The product was purified by flash column chromatography (petroleum ether / ethyl acetate =10:1 as the eluent);

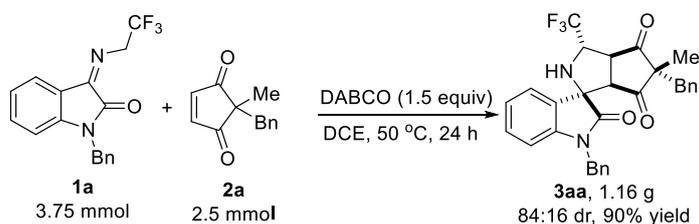
White solid; 75.8 mg, 50% yield; > 20:1 *dr*, mp 122.5-123.4 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.82 – 7.74 (m, 2H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.51 – 7.41 (m, 3H), 7.11 (dd, *J* = 8.4, 1.7 Hz, 1H), 4.33 (m, *J* = 7.1 Hz, 2H), 4.22 – 4.05 (m, 2H), 3.59 (m, 3.8 Hz, 1H), 3.21 (t, *J* = 11.8 Hz, 2H), 3.06 (d, *J* = 13.0 Hz, 1H), 2.95 – 2.83 (m, 2H), 1.39 – 1.27 (m, 6H), 1.15 (t, *J* = 7.1 Hz, 3H).

¹³C{¹H} NMR (101 MHz, CDCl₃) δ 213.8, 212.9, 168.8, 166.3, 133.4, 133.0, 132.5, 128.7, 128.5, 127.9, 127.7, 127.7, 126.5, 126.2, 123.7 (q, *J* = 280.4 Hz, 1C), 74.9, 63.1, 62.5, 61.6 (q, *J* = 32.6 Hz, 1C), 60.9, 56.3, 49.8, 44.0, 19.9, 14.0, 13.9.

HRMS (ESI) *m/z*: [M+H]⁺ calcd for C₂₆H₂₇F₃NO₆, 506.1785, found: 506.1790.

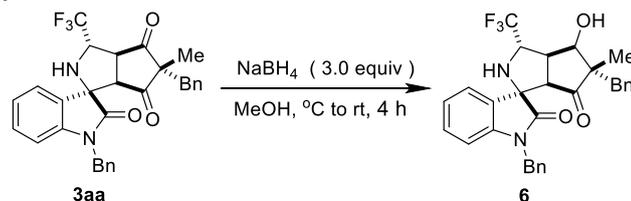
7. Scale-up experiment.



In a dry 100 mL round-bottom flask equipped with a magnetic stirring bar, *N*-2,2,2-trifluoroethylisatin ketimines **1a** (1.2 g, 3.75 mmol, 1.5 equiv), DABCO (0.4 g, 3.75 mmol, 1.5 equiv), and **2a** (0.5 g, 2.5 mmol, 1.0 equiv), DCE (25.0 mL) were added in sequence. Then the mixture was stirred for 24 h at 50 °C. After completion, the reaction mixture was directly purified by flash chromatography on silica gel (petroleum ether / ethyl acetate = 15:1) to give the corresponding product **3aa**.

8. Different transformations of products.

8.1. Procedure for the synthesis of 6.



Compound **3aa** (0.1 g, 0.2 mmol) was dissolved in MeOH (2.0 mL), and then NaBH₄ (22.7 mg, 3.0 equiv) was added slowly at 0 °C. The reaction mixture was then allowed to stir at room temperature for 4 h. The reaction system was monitored by TLC until **3aa** disappeared completely. After that, the reaction mixture was quenched by a drop of water and directly purified by column chromatography on silica gel (petroleum ether / ethyl acetate = 15:1) to provide compound **6** as a white solid (89.5 mg, 86% yield).

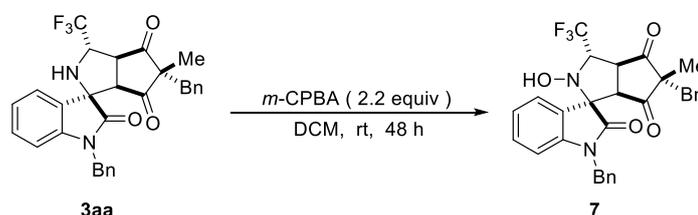
White solid; 89.5 mg, 86% yield; 83:17 *dr*, mp 188.2-188.9 °C;

¹H NMR (300 MHz, DMSO-*d*₆) δ 7.44 – 7.27 (m, 5H), 7.28 – 7.18 (m, 5H), 7.13 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.11 – 7.01 (m, 2H), 6.79 – 6.70 (m, 1H), 5.58 (s, 1H), 4.92 (d, *J* = 15.9 Hz, 1H), 4.70 (d, *J* = 16.0 Hz, 1H), 4.63 – 4.50 (m, 1H), 3.95 (d, *J* = 11.6 Hz, 2H), 3.68 (ddd, *J* = 11.1, 6.3, 3.8 Hz, 2H), 2.86 – 2.69 (m, 2H), 0.90 (s, 3H).

¹³C NMR{¹H} (75 MHz, CDCl₃) δ 218.1, 180.1, 141.7, 136.2, 135.2, 132.5, 130.3, 129.1, 128.5, 127.9, 127.4, 127.3, 126.7 (q, *J* = 277.5 Hz, 1C), 126.6, 123.88, 123.6, 110.0, 75.5, 70.8, 59.4, 59.3, 58.7 (q, *J* = 30.0 Hz, 1C), 44.2, 43.2, 41.2, 14.8.

HRMS (ESI) *m/z* [M+H]⁺ calcd for C₃₀H₂₈F₃N₂O₃, 521.2047, found: 521.2046.

8.2 Procedure for the synthesis of 7.



The solution of compound **3aa** (0.1 g, 0.20 mmol) in DCM (2.0 mL) was stirred at room temperature in a sealed tube. Subsequently, *m*-CPBA (76.1 mg, 0.44 mmol) was added to the above solution. The reaction mixture was then allowed to stir 48 h. The reaction mixture was quenched by the addition of NaHCO₃ aq (15 mL), and diluted with EtOAc (15 mL). The organic layer was separated, and the aqueous layer was extracted twice with EtOAc (2 × 15 mL). The combined organic layers were dried over Na₂SO₄. Subsequently, the organic phase was concentrated under reduced pressure. The crude product was purified by flash column

chromatography on silica gel (petroleum ether / ethyl acetate = 15:1) to afford the desired product **7** as a white solid (44.9 mg, 42% yield).

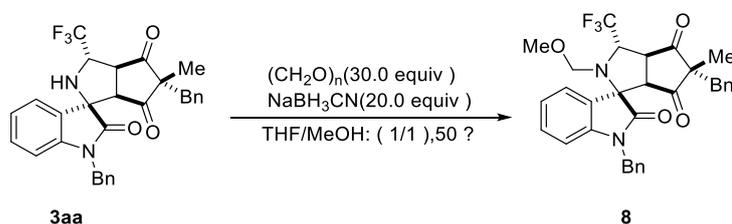
White solid; 44.9 mg, 42% yield; 86:14 *dr*, mp 135.8-136.6 °C;

¹H NMR (300 MHz, CDCl₃) δ 7.37 – 7.24 (m, 7H), 7.24 – 7.14 (m, 3H), 7.07 (m, *J* = 7.6, 1.0 Hz, 1H), 7.04 – 6.93 (m, 2H), 6.60 (d, *J* = 7.8 Hz, 1H), 5.07 (s, 1H), 4.76 (s, 2H), 4.60 (m, *J* = 6.2 Hz, 1H), 3.00 (d, *J* = 11.9 Hz, 1H), 2.93 (d, *J* = 12.9 Hz, 1H), 2.84 (d, *J* = 12.9 Hz, 1H), 2.46 (dd, *J* = 11.9, 6.0 Hz, 1H), 1.27 (s, 3H).

¹³C NMR{¹H} (75 MHz, CDCl₃) δ 214.2, 211.2, 174.7, 144.3, 134.9, 134.6, 130.8, 129.5, 129.1, 128.9, 128.2, 127.8, 127.2, 126.6, 125.8, 124.9 (q, *J* = 277.2 Hz, 1C), 124.2, 123.6, 110.1, 65.6 (q, *J* = 30.5 Hz, 1C), 62.3, 54.3, 48.2, 46.4, 43.8, 18.2.

HRMS (ESI) *m/z* [M+H]⁺ calcd for C₃₀H₂₆F₃N₂O₄, 535.1839, found: 535.1845.

8.3 Procedure for the synthesis of **8**.



Compound **3aa** (0.10 g, 0.20 mmol) and polyformaldehyde (0.5 g, 30.0 equiv) was dissolved in the mixture solvents of MeOH /THF (1:1, 4.0 mL). Then the NaBH₃CN (0.3 g, 20.0 equiv) was added into the mixture at room temperature for 30 minutes. The reaction mixture was then allowed to stir 72 h at 50 °C. After completion, the reaction mixture was quenched by addition of 1.0 M NaOH (10.0 mL). The aqueous layer was extracted with DCM (2×10.0 mL). The combined organic layers were dried over anhydrous Na₂SO₄. After filtration, the solution was concentrated under reduced pressure and the resulting crude mixture was purified by hexane beating twice to provide compound **8** as a white solid (100.1 mg, 89% yield).

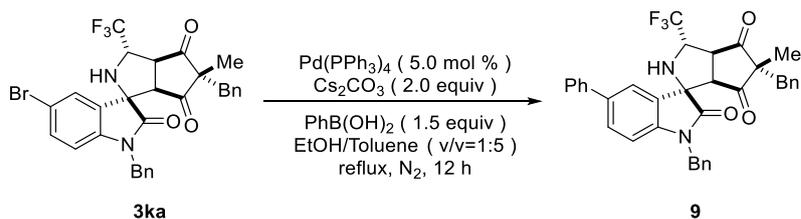
White solid; 100.1 mg, 89% yield; 86:14 *dr*, mp 192.3-193.1 °C;

¹H NMR (400 MHz, CDCl₃) δ 7.31 (m, 5H), 7.27 (d, *J* = 6.5 Hz, 3H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.08 (m, 1H), 7.04 – 6.96 (m, 2H), 6.65 (d, *J* = 7.8 Hz, 1H), 4.72 (s, 3H), 4.06 (d, *J* = 11.0 Hz, 1H), 3.73 (d, *J* = 11.0 Hz, 1H), 3.13 (d, *J* = 10.2 Hz, 1H), 2.99 (s, 3H), 2.96 (d, *J* = 12.7 Hz, 1H), 2.84 (d, *J* = 12.7 Hz, 1H), 2.60 (dd, *J* = 12.0, 4.0 Hz, 1H), 1.28 (s, 3H).

¹³C NMR{¹H} (101 MHz, CDCl₃) δ 214.5, 211.0, 177.5, 144.0, 135.3, 134.9, 130.6, 129.5, 129.0, 128.9, 128.1, 127.8, 127.4, 126.1, 125.7 (q, *J* = 304.0 Hz, 1C), 124.4, 123.6, 110.0, 79.2, 73.8, 63.3, 60.6 (q, *J* = 30.0 Hz, 1C), 58.5, 56.4, 52.1, 46.4, 43.9, 17.7.

HRMS (ESI) *m/z* [M+H]⁺ calcd for C₃₂H₃₀F₃N₂O₄, 563.2152, found: 563.2163.

8.4 Procedure for the synthesis of **9**.



To an oven-dried schlenk tube, **3ak** (119.2 mg, 0.20 mmol), PhB(OH)₂ (36.6 mg, 0.30mmol), Cs₂CO₃ (130.4 mg, 0.40 mmol) were added and then the mixture solvents of ethanol (0.4 mL) and toluene (2.0 mL) was added into reaction tube. The reaction mixture was stirred at 120 °C under N₂ atmosphere for 12 hours. The heat source is an oil bath. When the mixture was cooled to room temperature, the brine (10 mL) was added to quench the reaction. The aqueous layer was extracted with DCM (2×10.0 mL), and the combined organic layers were dried over anhydrous Na₂SO₄. After filtration, the organic phase was concentrated and purified by column chromatography on silica gel (petroleum ether / ethyl acetate = 15:1) to afford product **9** as a white solid (108.1 mg, 91% yield).

White solid; 108.1 mg, 91% yield; 86:14 dr, mp.140.0-140.7 °C;

¹H NMR (400 MHz, DMSO-*d*₆) δ 7.64 – 7.53 (m, 2H), 7.46 (m, 3H), 7.43 – 7.39 (m, 1H), 7.39 – 7.37 (m, 1H), 7.36 – 7.23 (m, 8H), 7.13 – 6.95 (m, 3H), 4.93 (d, *J* = 15.9 Hz, 1H), 4.73 (d, *J* = 15.9 Hz, 1H), 4.69 (d, *J* = 5.6 Hz, 1H), 4.52 – 4.38 (m, 1H), 4.06 (d, *J* = 3.9 Hz, 2H), 3.02 (d, *J* = 13.3 Hz, 1H), 2.87 (d, *J* = 13.3 Hz, 1H), 0.96 (s, 3H).

¹³C NMR{¹H} (101 MHz, DMSO-*d*₆) δ 212.8, 210.8, 178.2, 143.9, 142.0, 139.9, 135.6, 134.5, 130.2, 129.0, 128.4, 128.1, 127.8, 127.7, 127.3, 127.3, 127.2, 126.7, 125.6 (q, *J* = 276.4 Hz, 1C), 124.6, 121.7, 108.1, 70.8, 62.0, 58.7 (q, *J* = 31.0 Hz, 1C) 57.8, 51.3, 42.7, 41.5, 14.3.

HRMS (ESI) *m/z* [M+H]⁺ calcd for C₃₆H₃₀F₃N₂O₃, 595.2203 found: 595.2209

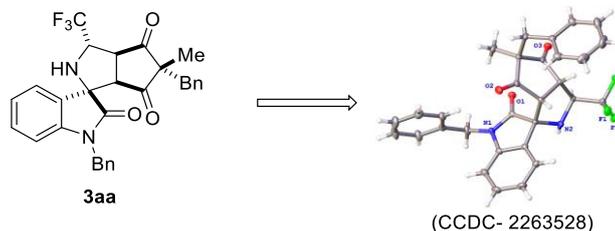
9. X-ray crystal structure of compounds **3aa**, **8** and **5a**.

Single crystal of compound **3aa** was prepared from the mixture solvent of MeOH/Dichloromethane (*V* : *V* = 6/1) at room temperature by slow evaporation of solvent. A suitable crystal was selected for structure determination on a Xcalibur, Eos, Gemini diffractometer. The crystal was kept at 293(2) K during data collection. Using Olex2^[1], the structure was solved with the ShelXS^[2] structure solution program using Direct Methods and refined with the ShelXL^[3] refinement package using Least Squares minimisation.

[1] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J, Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339-341.

[2]Sheldrick, G. M. *Acta Cryst.* **2008**, A64, 112-122.

[3]Sheldrick, G. M. *Acta Cryst.* **2015**, C71, 3-8.



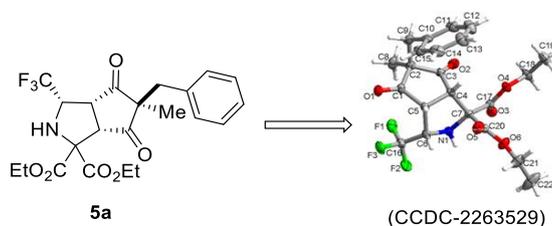
ORTEP of **3aa** (at 50% level)

Crystal data and structure refinement for **3aa**.

| Identification code | 3aa |
|---------------------|--|
| Empirical formula | C ₃₀ H ₂₅ F ₃ N ₂ O ₃ |
| Formula weight | 518.52 |
| Temperature/K | 179.99(10) |
| Crystal system | triclinic |
| Space group | P-1 |

| | |
|---|--|
| a/Å | 8.6814(4) |
| b/Å | 10.3082(6) |
| c/Å | 14.7740(8) |
| α /° | 88.935(5) |
| β /° | 81.813(4) |
| γ /° | 71.234(5) |
| Volume/Å ³ | 1238.55(12) |
| Z | 2 |
| ρ calcg/cm ³ | 1.390 |
| μ /mm ⁻¹ | 0.105 |
| F(000) | 540.0 |
| Crystal size/mm ³ | 0.15 × 0.13 × 0.11 |
| Radiation | Mo K α (λ = 0.71073) |
| 2 θ range for data collection/° | 4.174 to 49.998 |
| Index ranges | -8 ≤ h ≤ 10, -8 ≤ k ≤ 12, -17 ≤ l ≤ 17 |
| Reflections collected | 8048 |
| Independent reflections | 4362 [Rint = 0.0190, Rsigma = 0.0344] |
| Data/restraints/parameters | 4362/0/348 |
| Goodness-of-fit on F ² | 1.082 |
| Final R indexes [$I \geq 2\sigma(I)$] | R1 = 0.0424, wR2 = 0.0968 |
| Final R indexes [all data] | R1 = 0.0508, wR2 = 0.1027 |
| Largest diff. peak/hole / e Å ⁻³ | 0.18/-0.32 |

Single crystal of compound **5a** was prepared from the mixture solvent of Hexane/Ethyl acetate ($V : V = 8/1$) at room temperature by slow evaporation of solvent.



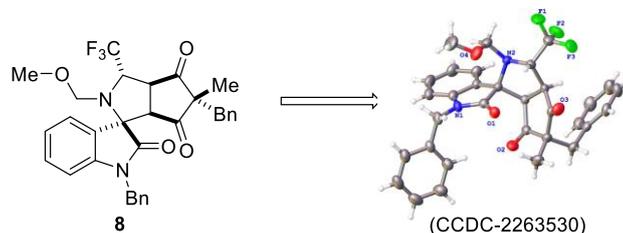
ORTEP of **5a** (at 50% level)

Crystal data and structure refinement for **5a**

| | |
|---------------------|--|
| Identification code | 5a |
| Empirical formula | C ₂₂ H ₂₄ F ₃ NO ₆ |
| Formula weight | 455.42 |
| Temperature/K | 293(2) |
| Crystal system | triclinic |
| Space group | P-1 |
| a/Å | 10.1328(11) |
| b/Å | 11.3561(14) |
| c/Å | 11.5752(17) |
| α /° | 67.509(13) |
| β /° | 64.451(13) |

| | |
|---|---|
| $\gamma/^\circ$ | 81.505(10) |
| Volume/ \AA^3 | 1110.1(3) |
| Z | 2 |
| $\rho_{\text{calc}}/\text{cm}^3$ | 1.363 |
| μ/mm^{-1} | 0.988 |
| F(000) | 476.0 |
| Crystal size/ mm^3 | $0.15 \times 0.11 \times 0.1$ |
| Radiation | $\text{CuK}\alpha$ ($\lambda = 1.54184$) |
| 2θ range for data collection/ $^\circ$ | 8.428 to 134.114 |
| Index ranges | $-9 \leq h \leq 12, -13 \leq k \leq 12, -13 \leq l \leq 13$ |
| Reflections collected | 7940 |
| Independent reflections | 3935 [Rint = 0.0248, Rsigma = 0.0330] |
| Data/restraints/parameters | 3935/0/296 |
| Goodness-of-fit on F2 | 1.049 |
| Final R indexes [$I \geq 2\sigma(I)$] | R1 = 0.0502, wR2 = 0.1356 |
| Final R indexes [all data] | R1 = 0.0612, wR2 = 0.1496 |
| Largest diff. peak/hole / $e \text{\AA}^{-3}$ | 0.27/-0.23 |

Single crystal of compound **8** was prepared from the mixture solvent of MeOH/Ethyl acetate ($V : V = 5/1$) at room temperature by slow evaporation of solvent.



ORTEP of **8** (at 50% level)

Crystal data and structure refinement for **8**.

| | |
|----------------------------------|--|
| Identification code | 8 |
| Empirical formula | $\text{C}_{32}\text{H}_{29}\text{F}_3\text{N}_2\text{O}_4$ |
| Formula weight | 562.57 |
| Temperature/K | 296.15 |
| Crystal system | triclinic |
| Space group | P-1 |
| a/ \AA | 10.034(10) |
| b/ \AA | 12.228(12) |
| c/ \AA | 12.997(13) |
| $\alpha/^\circ$ | 69.56(2) |
| $\beta/^\circ$ | 86.77(2) |
| $\gamma/^\circ$ | 87.29(2) |
| Volume/ \AA^3 | 1491(3) |
| Z | 2 |
| $\rho_{\text{calc}}/\text{cm}^3$ | 1.253 |

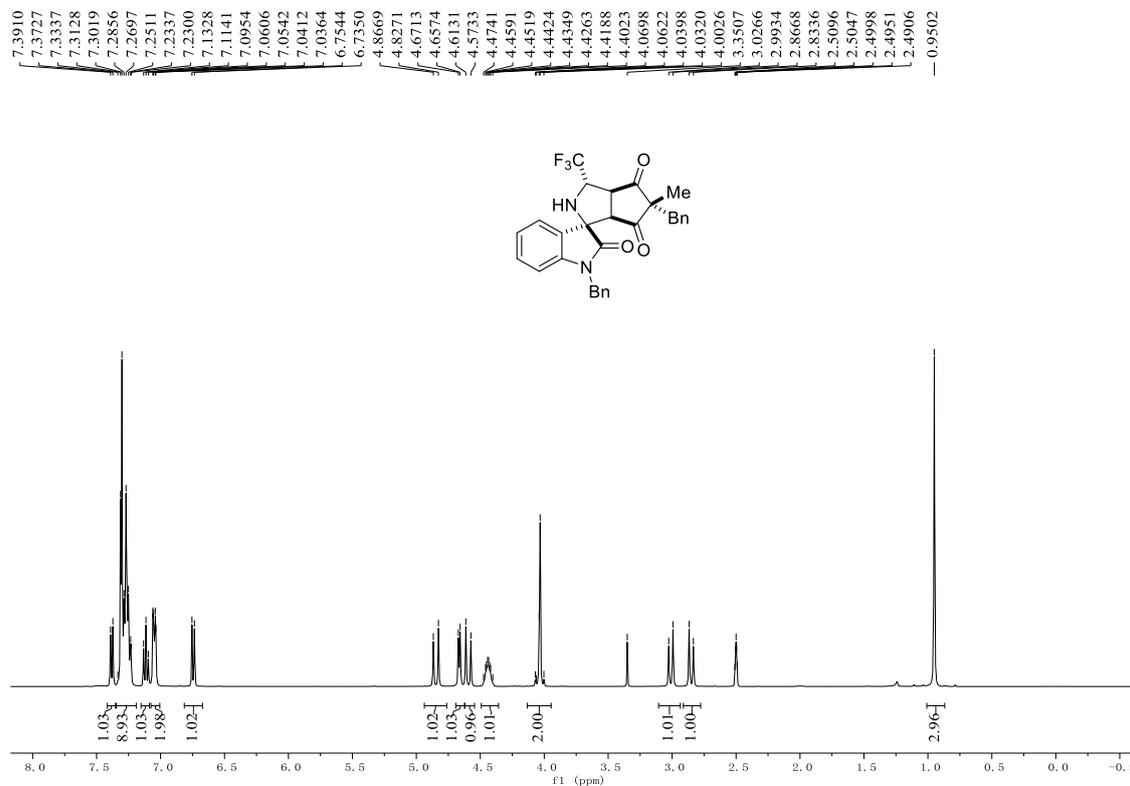
| | |
|--|--|
| μ/mm^{-1} | 0.095 |
| F(000) | 588.0 |
| Crystal size/mm ³ | 0.15 × 0.12 × 0.11 |
| Radiation | MoK α ($\lambda = 0.71073$) |
| 2 Θ range for data collection/ $^{\circ}$ | 5.158 to 50.416 |
| Index ranges | -11 \leq h \leq 11, -14 \leq k \leq 14, -15 \leq l \leq 15 |
| Reflections collected | 40902 |
| Independent reflections | 5302 [Rint = 0.0772, Rsigma = 0.0602] |
| Data/restraints/parameters | 5302/0/376 |
| Goodness-of-fit on F ² | 1.037 |
| Final R indexes [$I \geq 2\sigma(I)$] | R1 = 0.0622, wR2 = 0.1240 |
| Final R indexes [all data] | R1 = 0.1239, wR2 = 0.1531 |
| Largest diff. peak/hole / e \AA^{-3} | 0.18/-0.23 |

References:

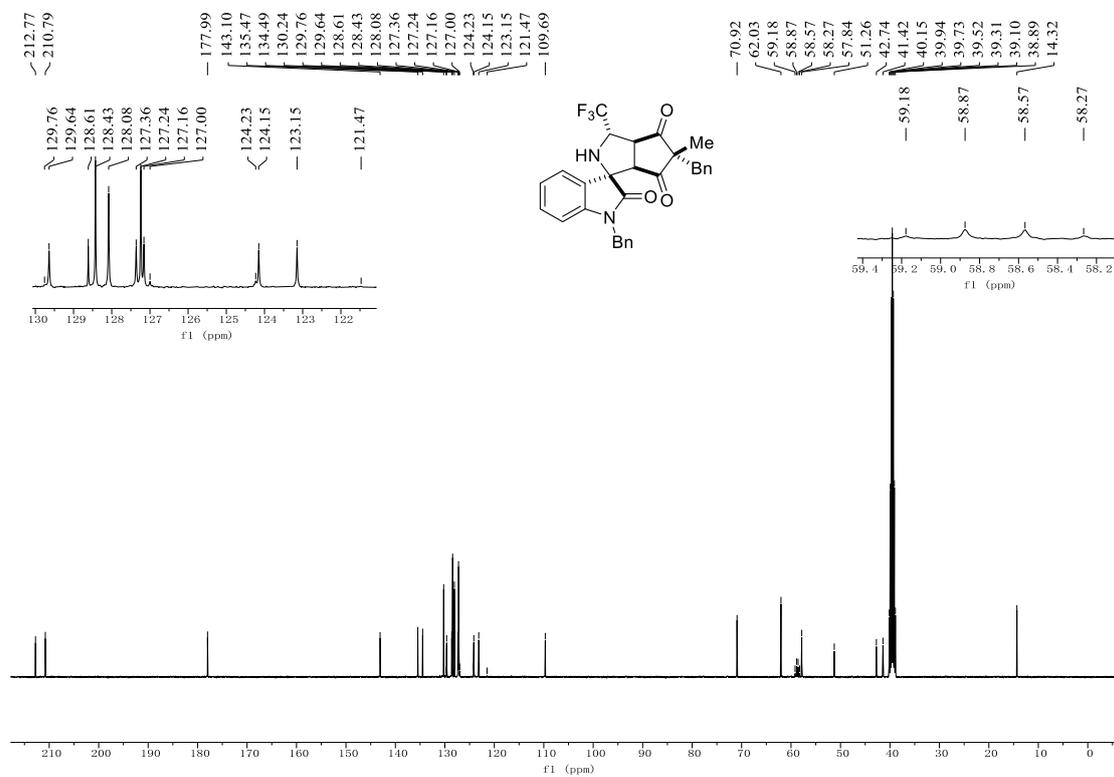
- [1] (a) Ma, M.; Zhu, Y.; Sun, Q.; Li, X.; Su, J.; Zhao, L.; Zhao, Y.; Qiu, S.; Yan, W.; Wang, K.; Wang, R. The asymmetric synthesis of CF₃-containing spiro[pyrrolidin-3,2'-oxindole] through the organocatalytic 1,3-dipolar cycloaddition reaction. *Chem. Commun.*, **2015**, 51, 8789. (b) Ryu, H.; Seo, J.; Ko H. M. Synthesis of Spiro[oxindole-3,2'-pyrrolidine] Derivatives from Benzynes and Azomethine Ylides through 1,3-Dipolar Cycloaddition Reactions. *J. Org. Chem.* **2018**, 83, 14102.
- [2] Das, T.; Saha, P.; Singh, V. K. Silver(I)-Ferrophox Catalyzed Enantioselective Desymmetrization of Cyclopentenedione: Synthesis of Highly Substituted Bicyclic Pyrrolidines *Org. Lett.*, **2015**, 17, 5088.
- [3] Zhi Y., Zhao, K., Liu, Q.; Wang, A.; Enders, D. Asymmetric synthesis of functionalized trifluoromethyl-substituted pyrrolidines: Via an organocatalytic domino Michael/Mannich [3+2] cycloaddition. *Chem. Commun.* **2016**, 52, 14011.

10. ^1H NMR, $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compounds 3, 5, 6, 7, 8, 9.

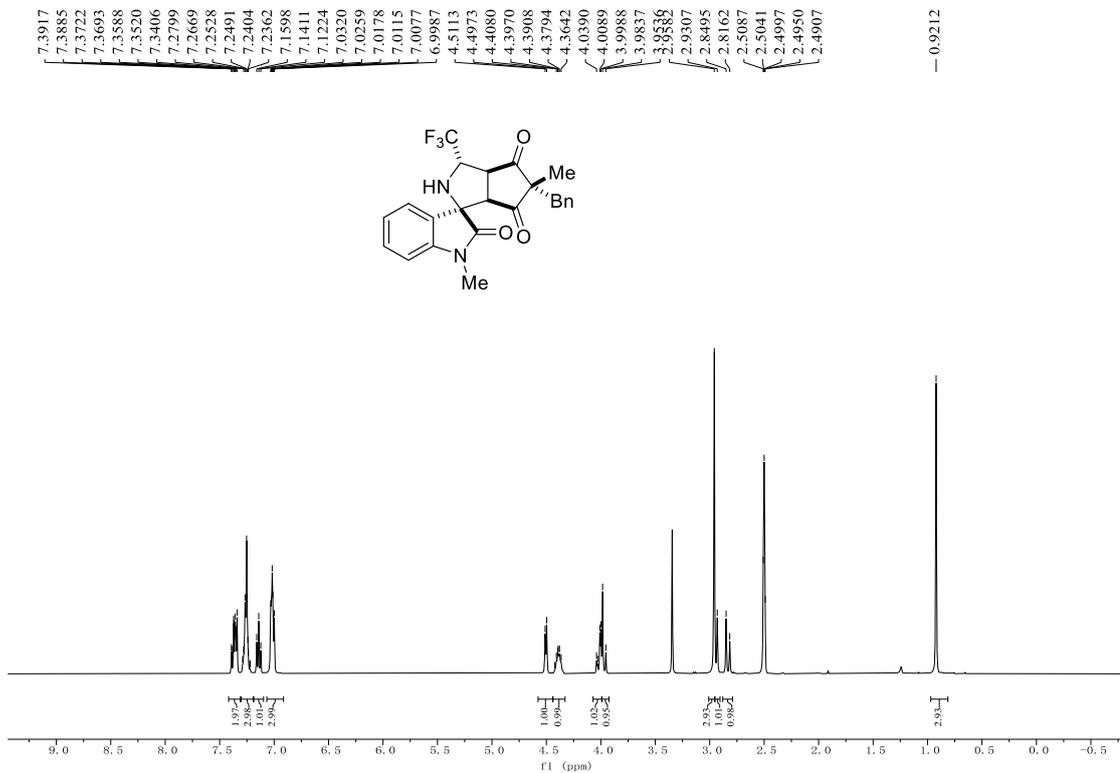
^1H NMR (400 MHz, $\text{DMSO-}d_6$) of 3aa



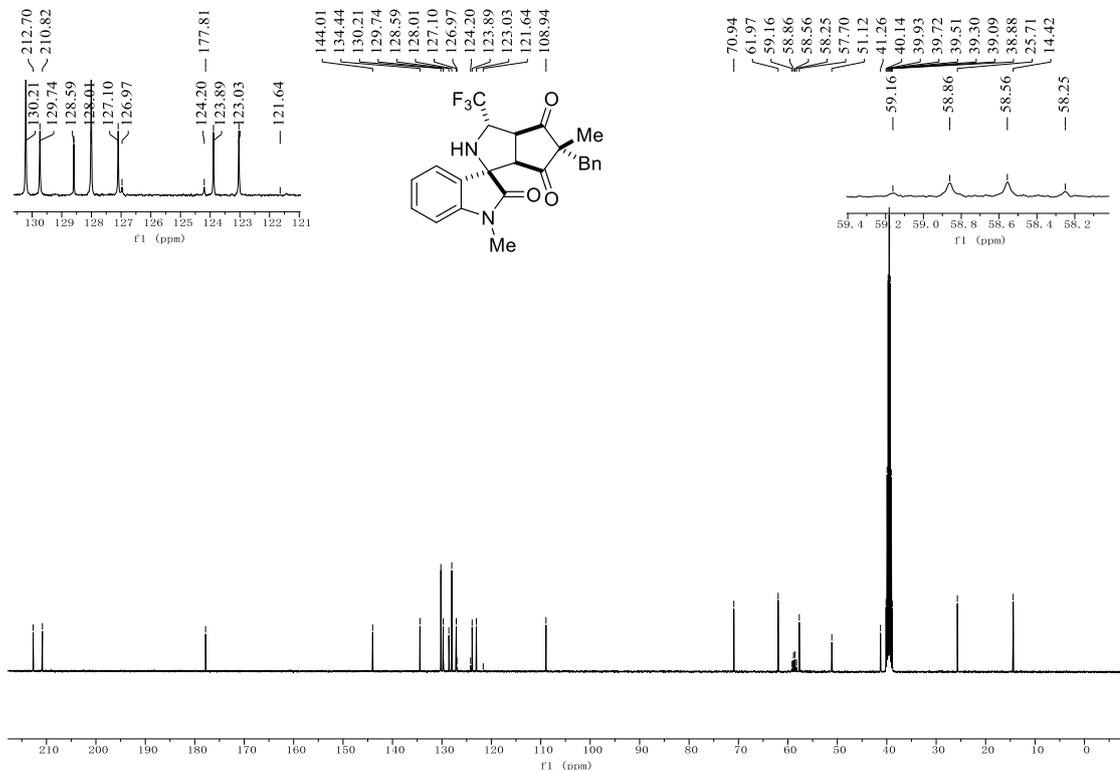
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, $\text{DMSO-}d_6$) of 3aa



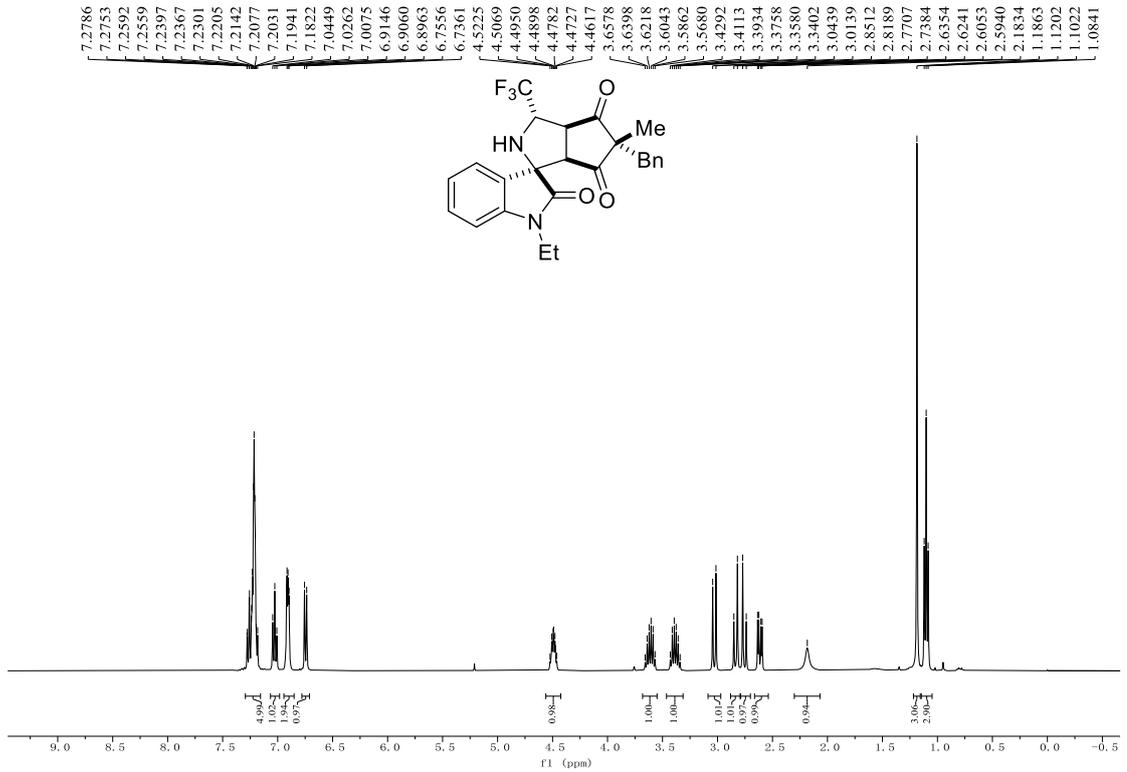
¹H NMR (400 MHz, DMSO-d₆) of **3ba**



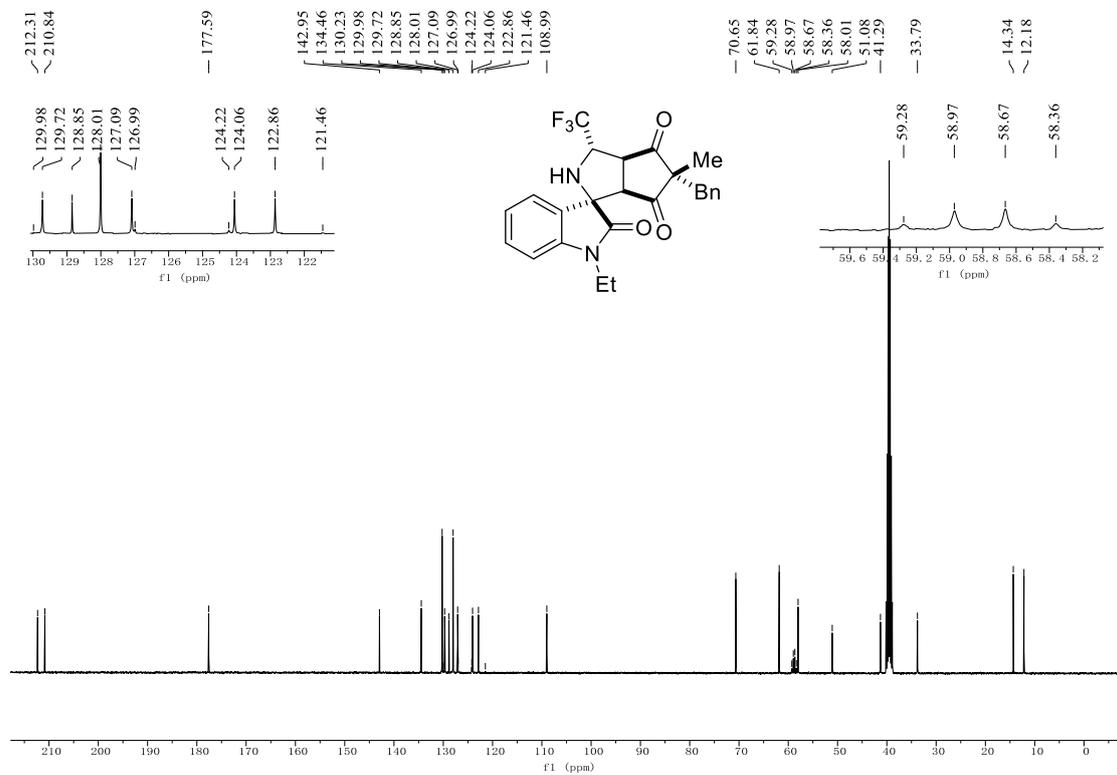
¹³C{¹H} NMR (101 MHz, DMSO-d₆) of **3ba**



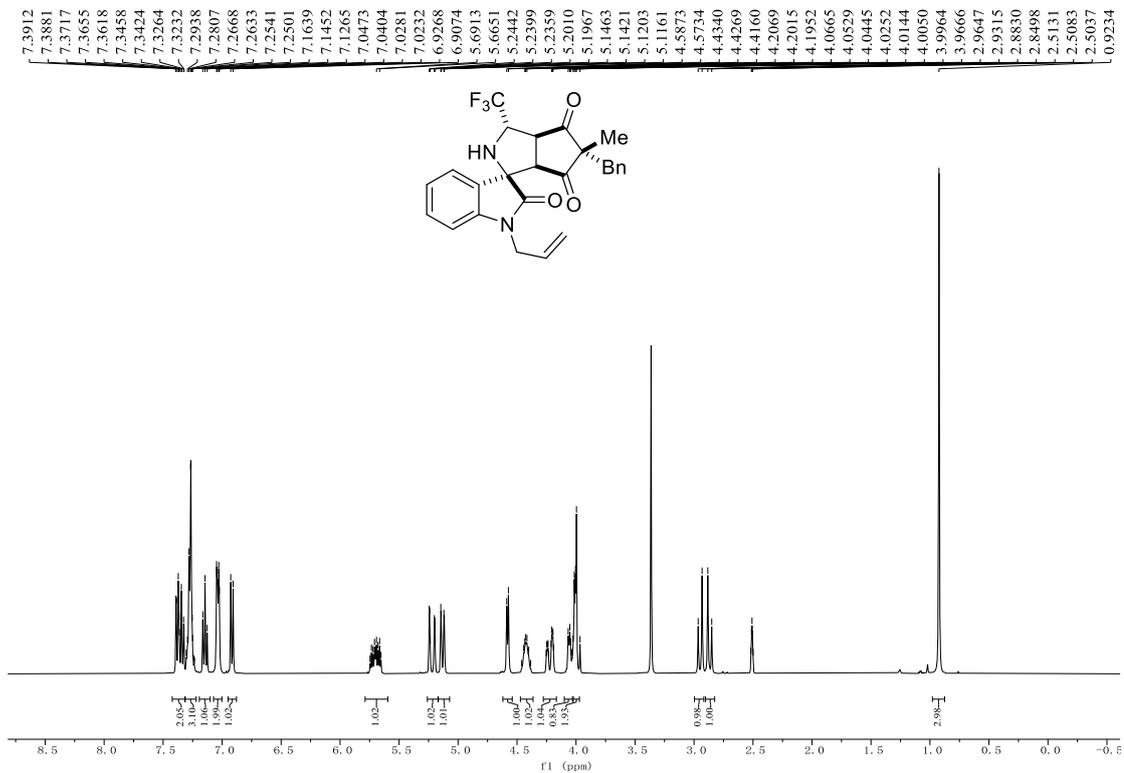
¹H NMR (400 MHz, CDCl₃) of **3ca**



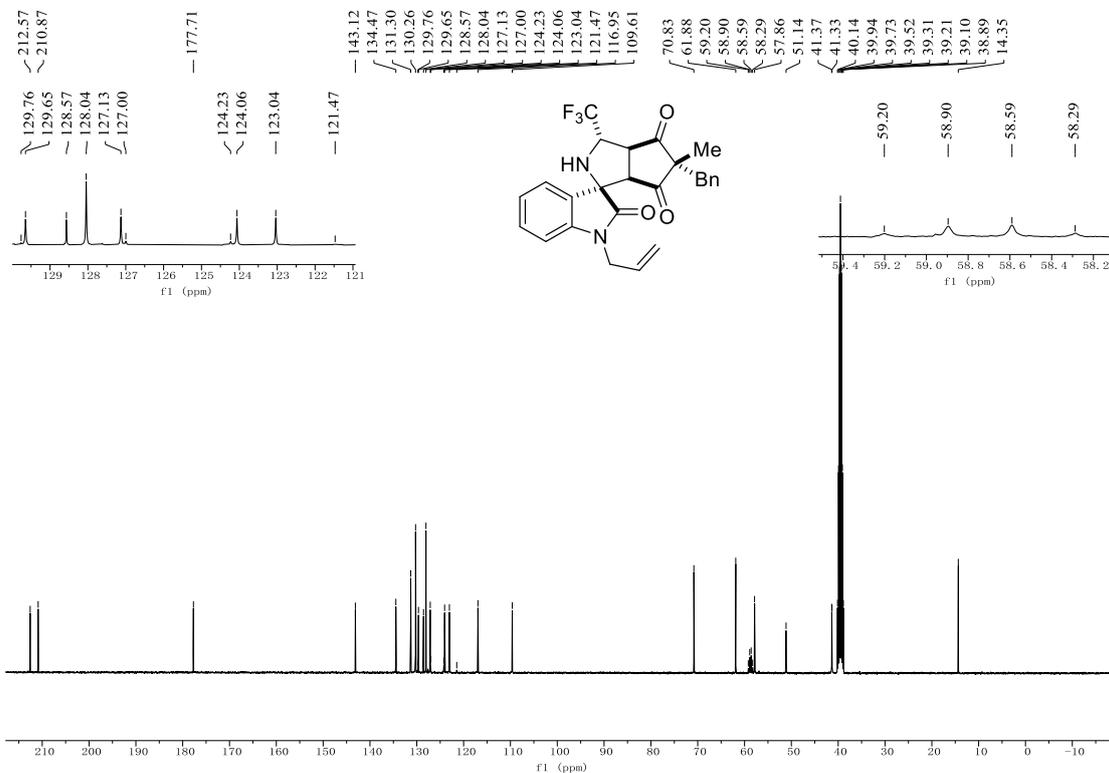
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **3ca**



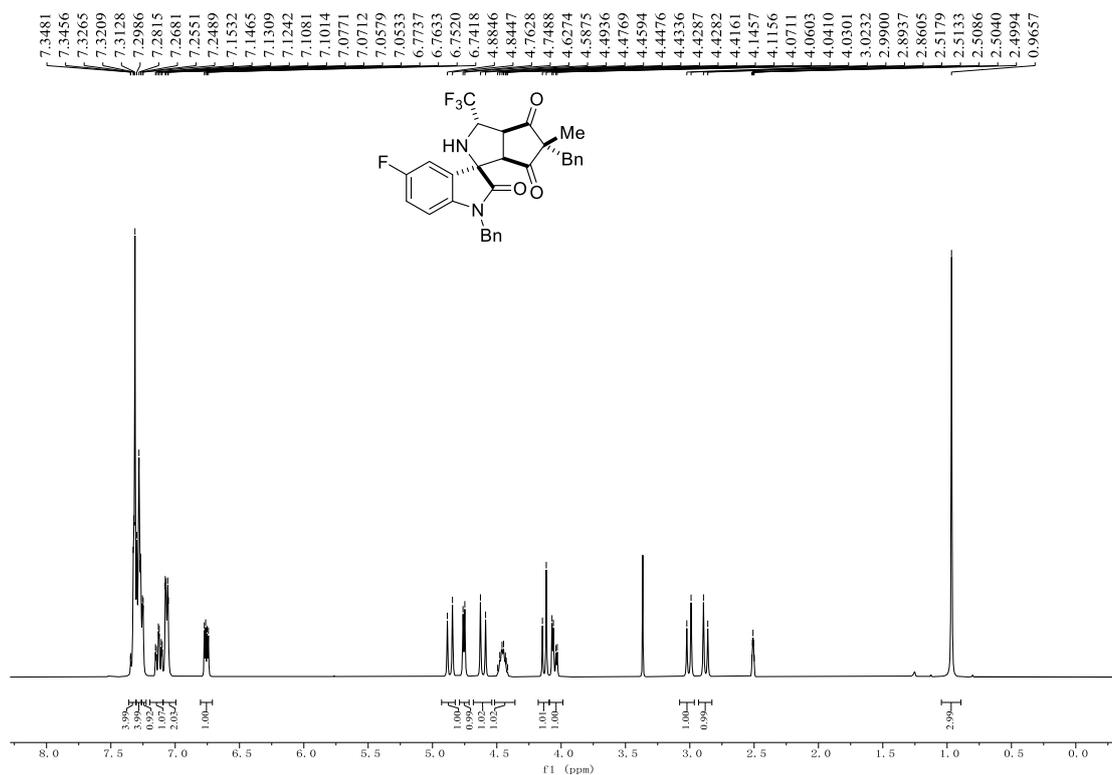
¹H NMR (400 MHz, DMSO-d₆) of 3da



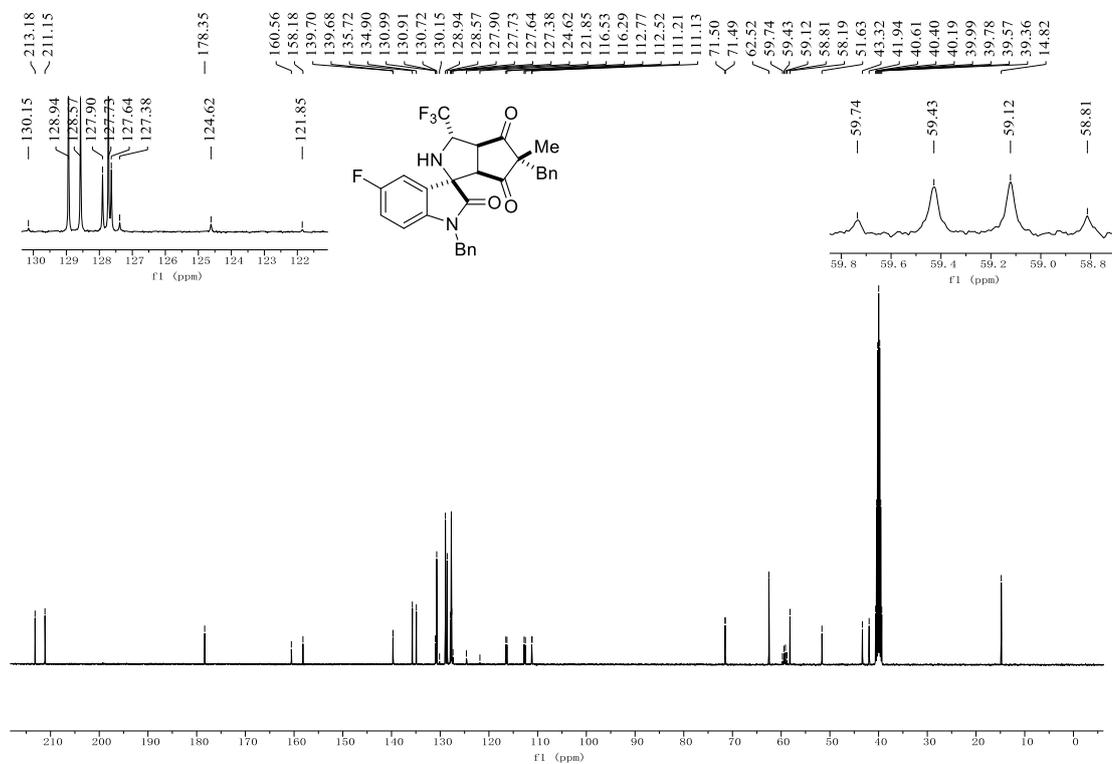
¹³C{¹H} NMR (101 MHz, DMSO-d₆) of 3da



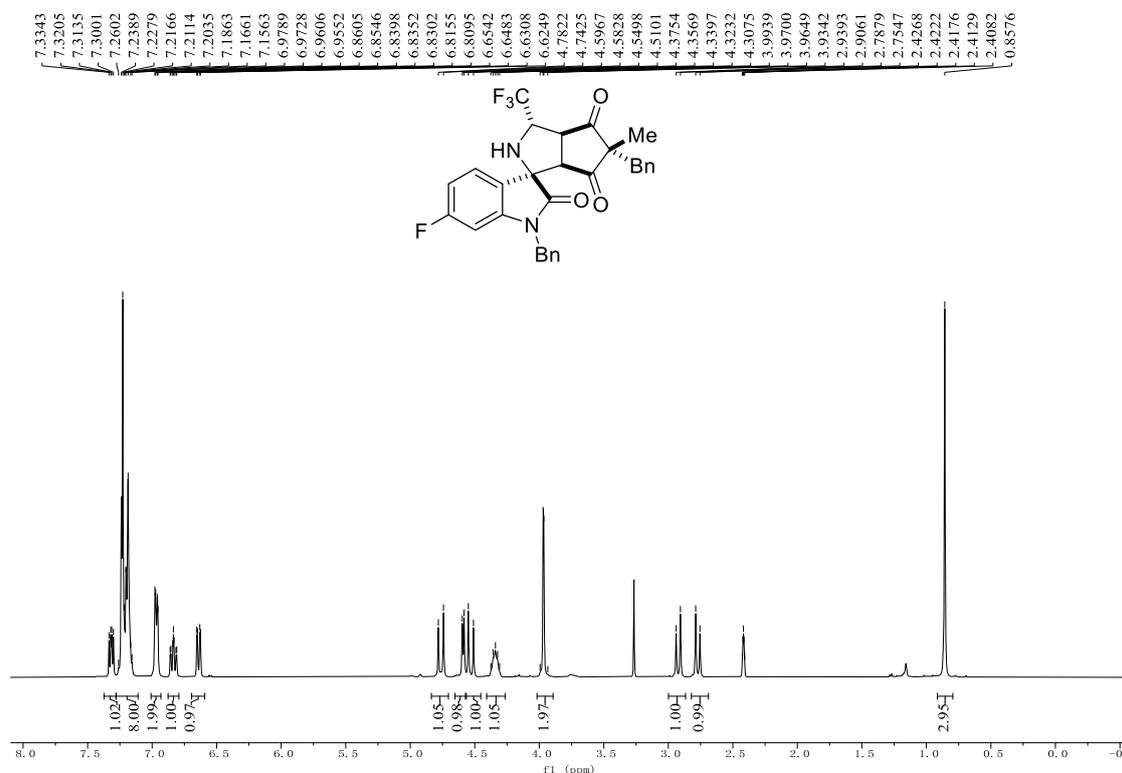
¹H NMR (400 MHz, DMSO-*d*₆) of 3ea



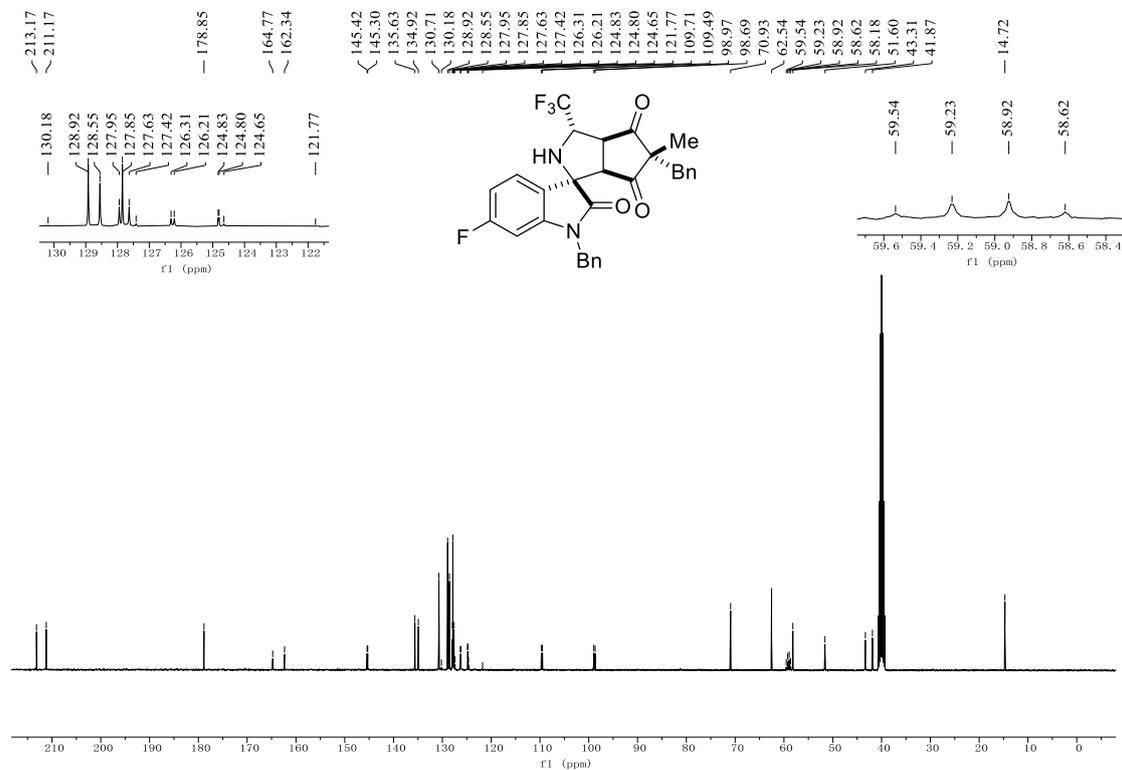
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of 3ea



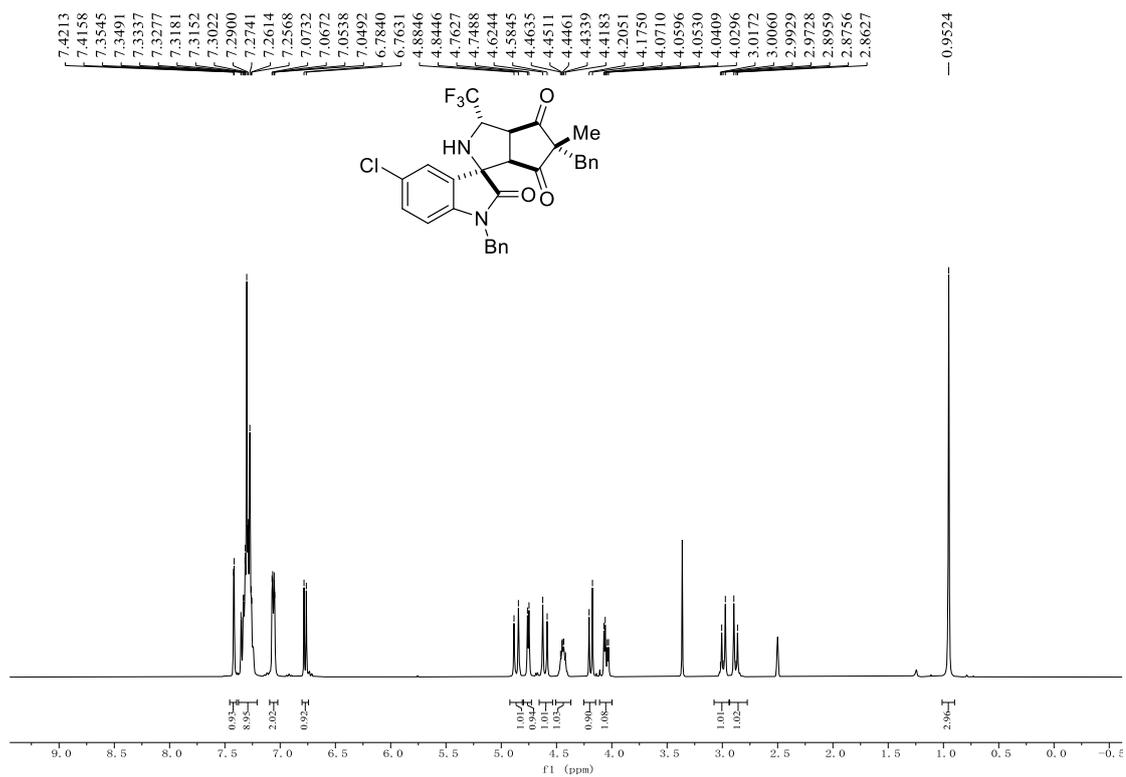
¹H NMR (400 MHz, DMSO-*d*₆) of **3fa**



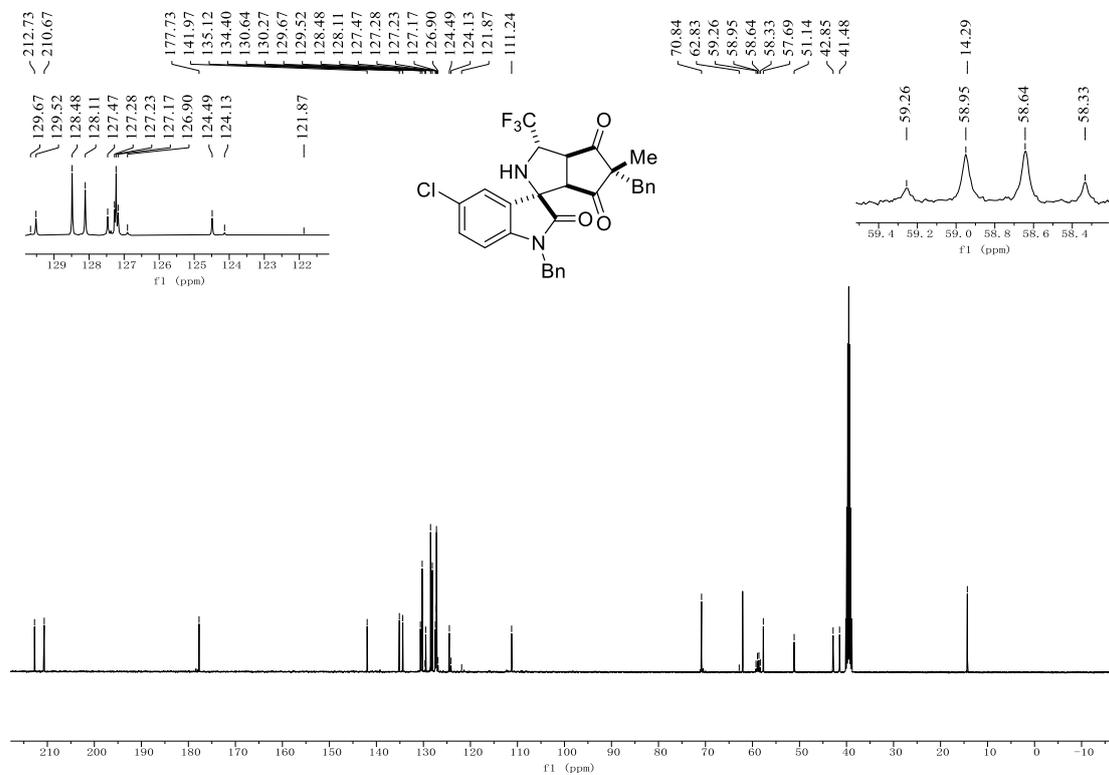
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **3fa**



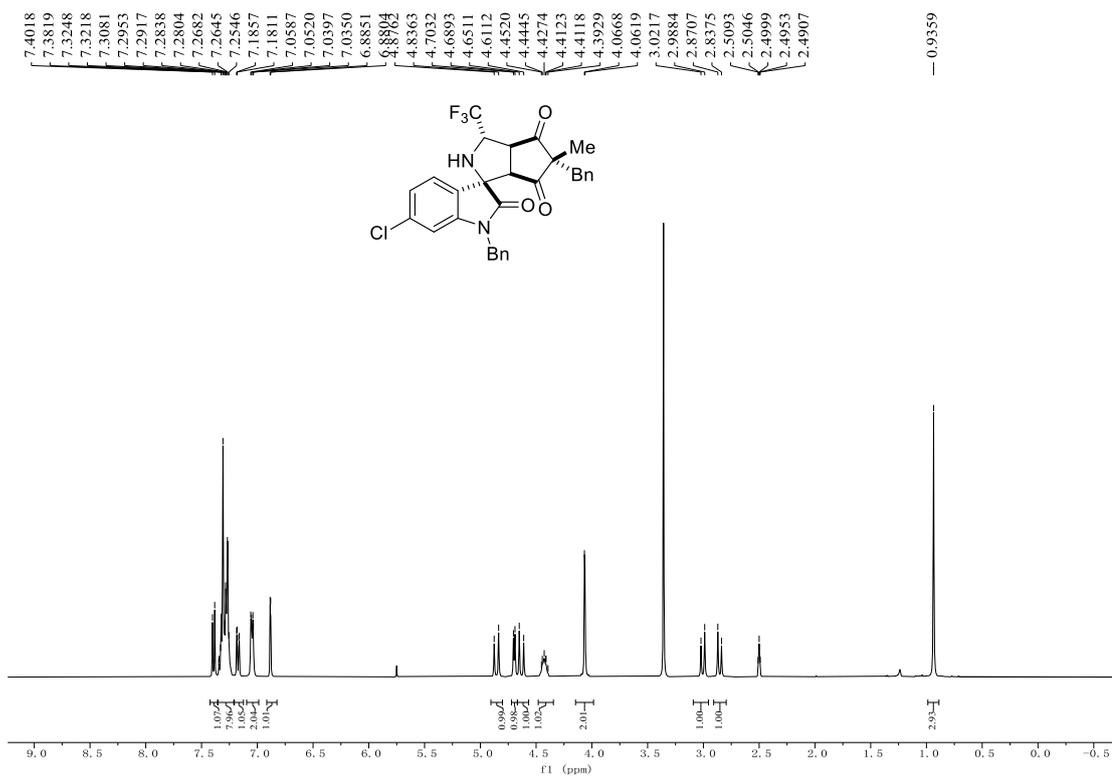
¹H NMR (400 MHz, DMSO-*d*₆) of **3ga**



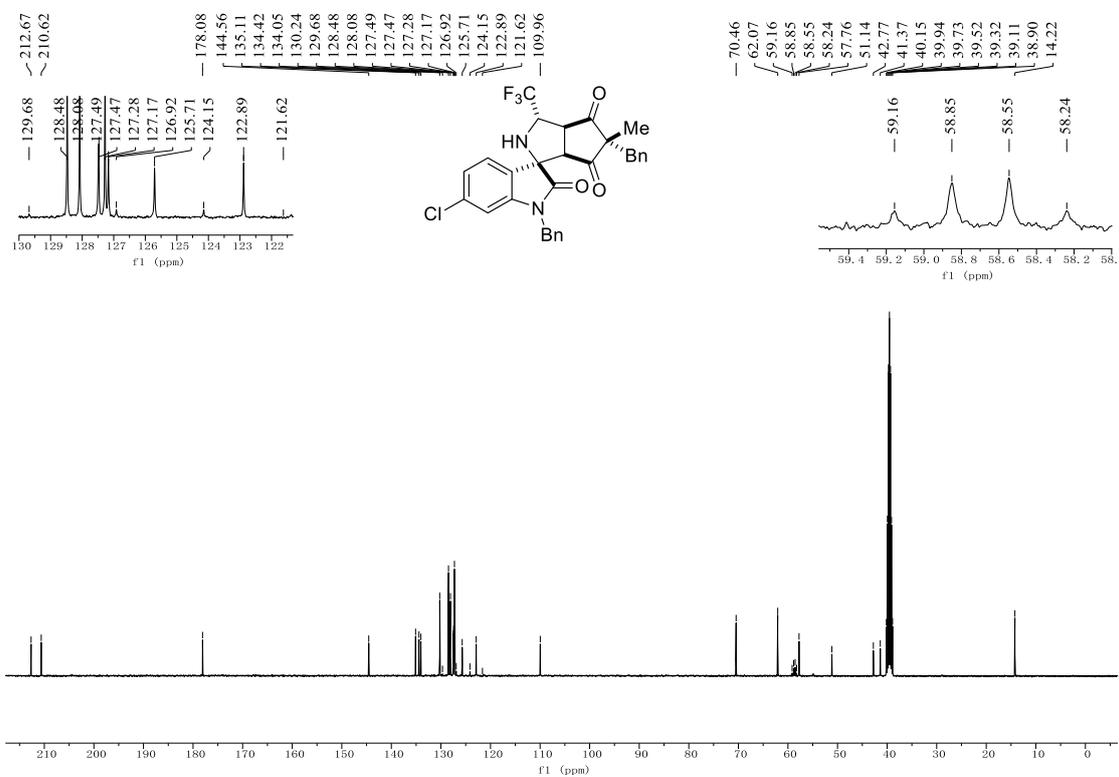
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **3ga**



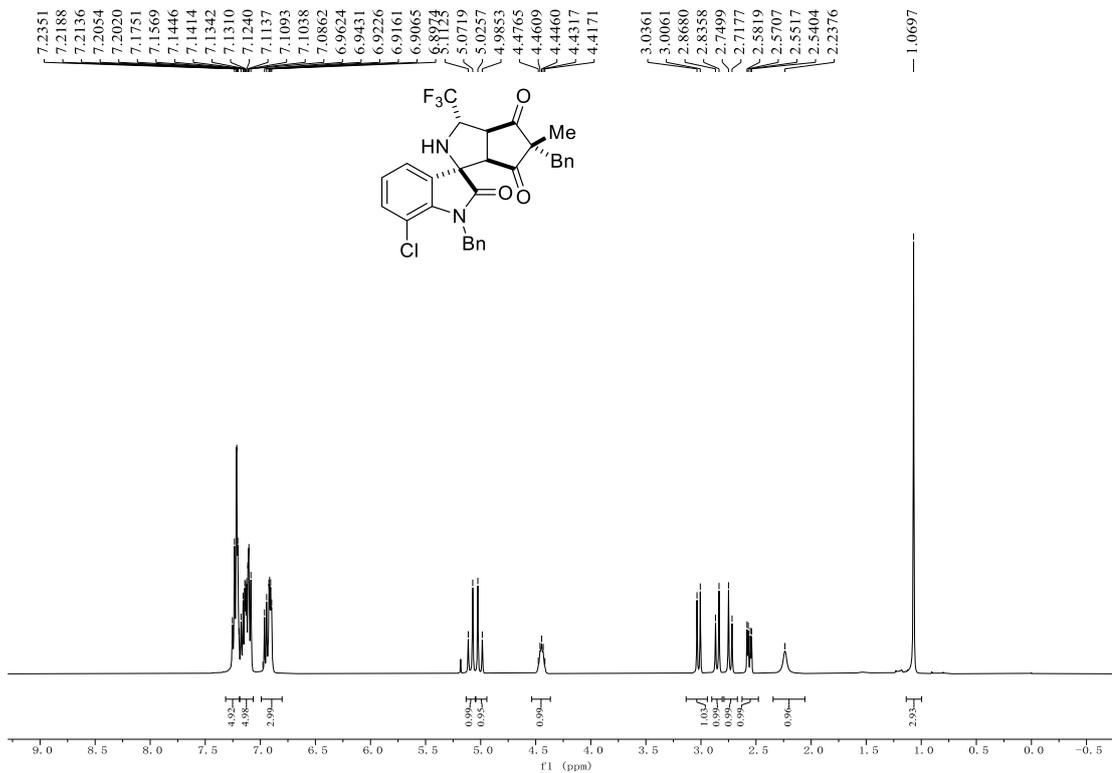
¹H NMR (400 MHz, DMSO-d₆) of **3ha**



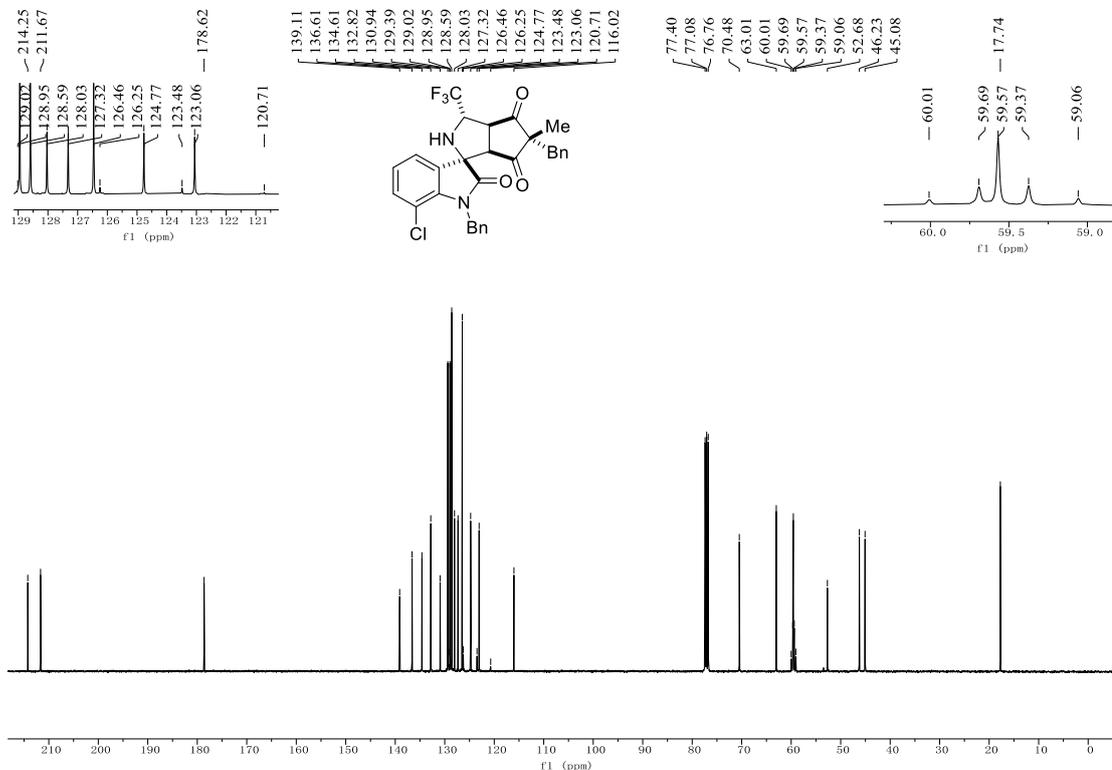
¹³C{¹H} NMR (101 MHz, DMSO-d₆) of **3ha**



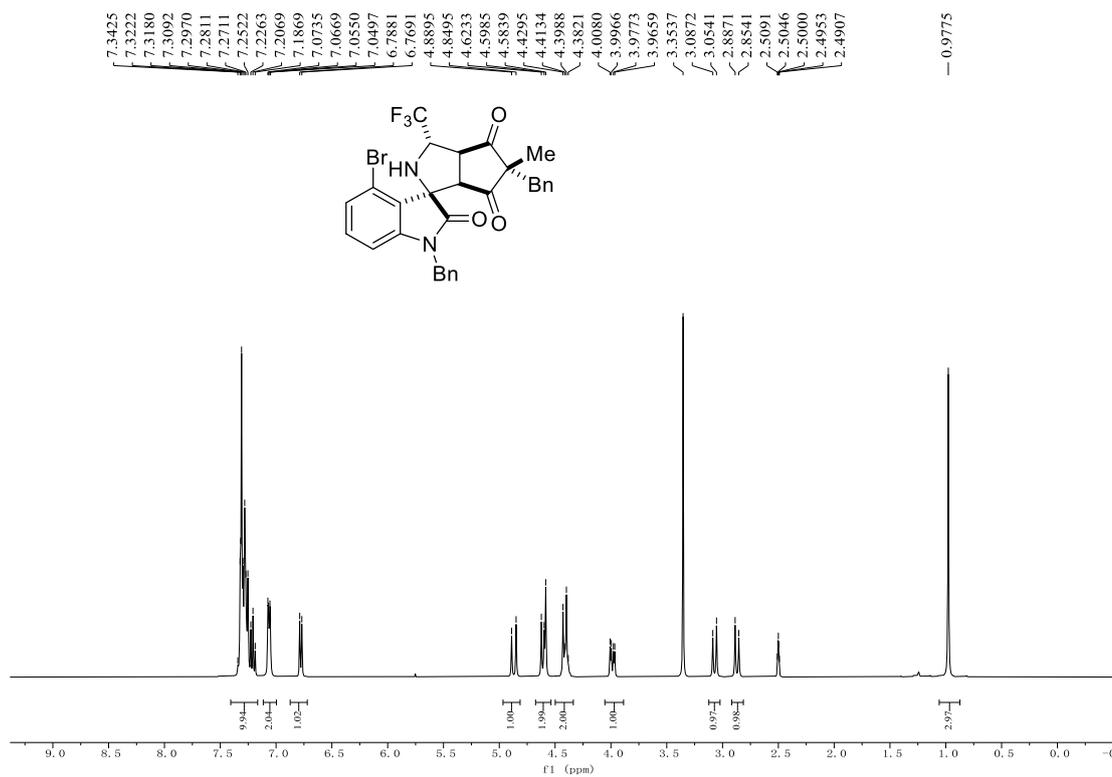
^1H NMR (400 MHz, CDCl_3) of **3ia**



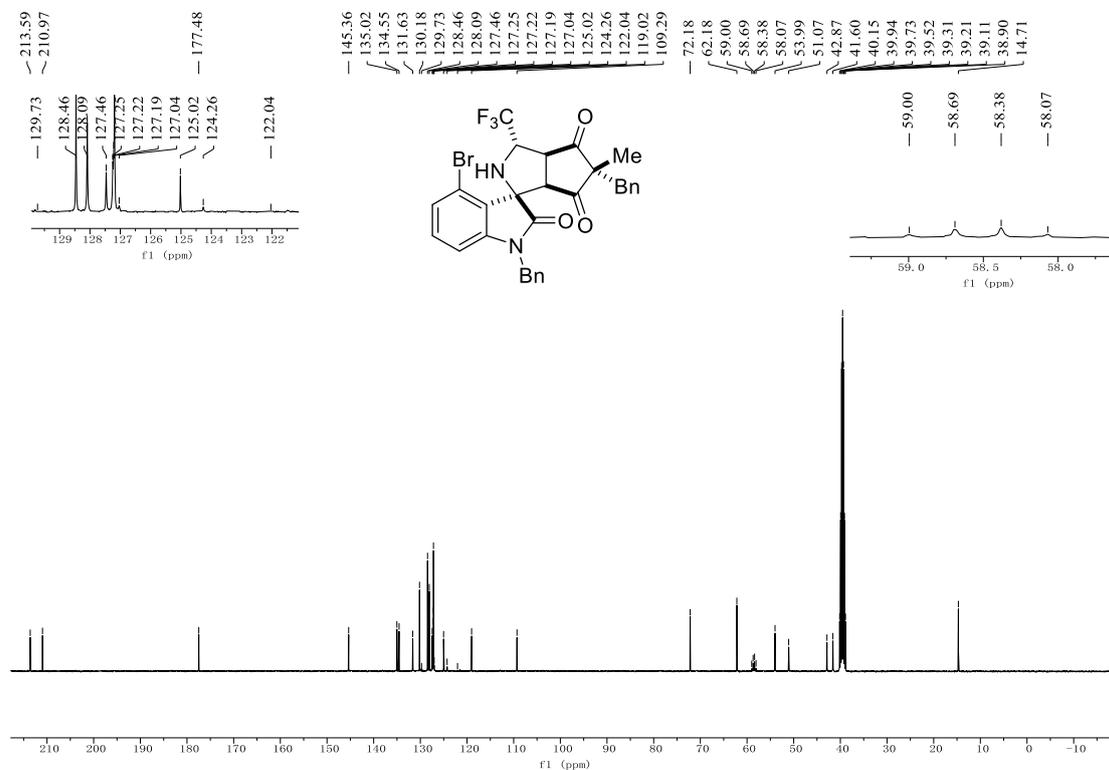
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of **3ia**



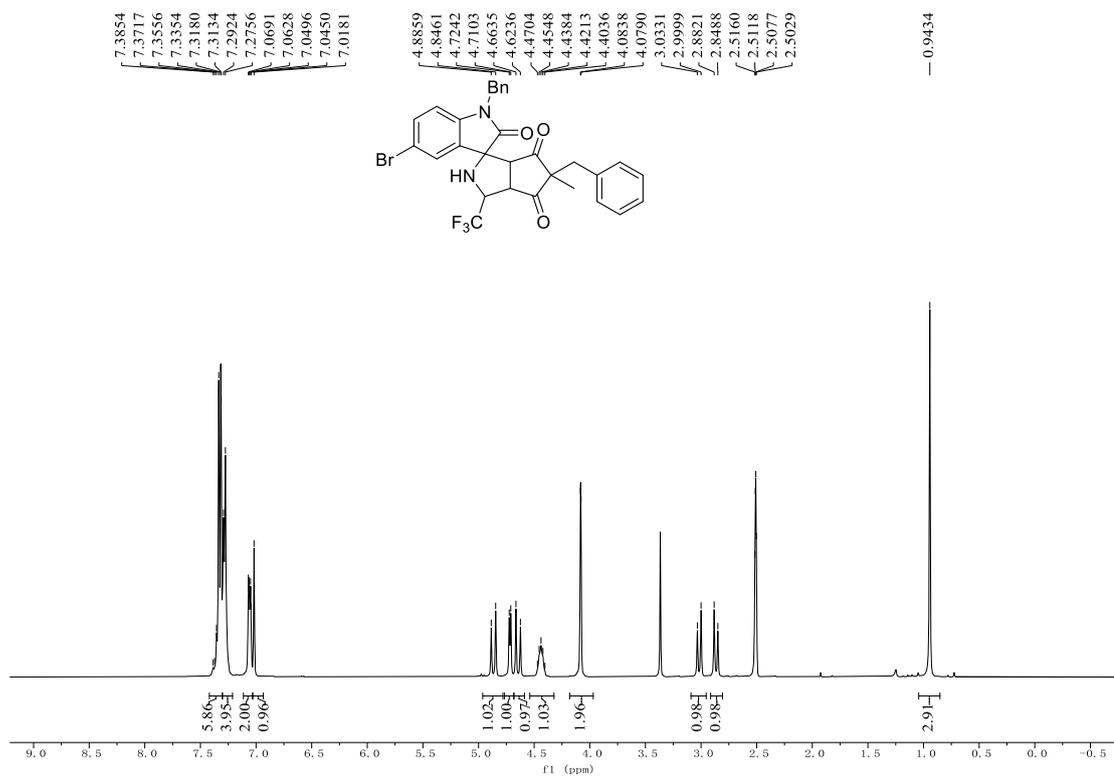
¹H NMR (400 MHz, DMSO-d₆) of **3ja**



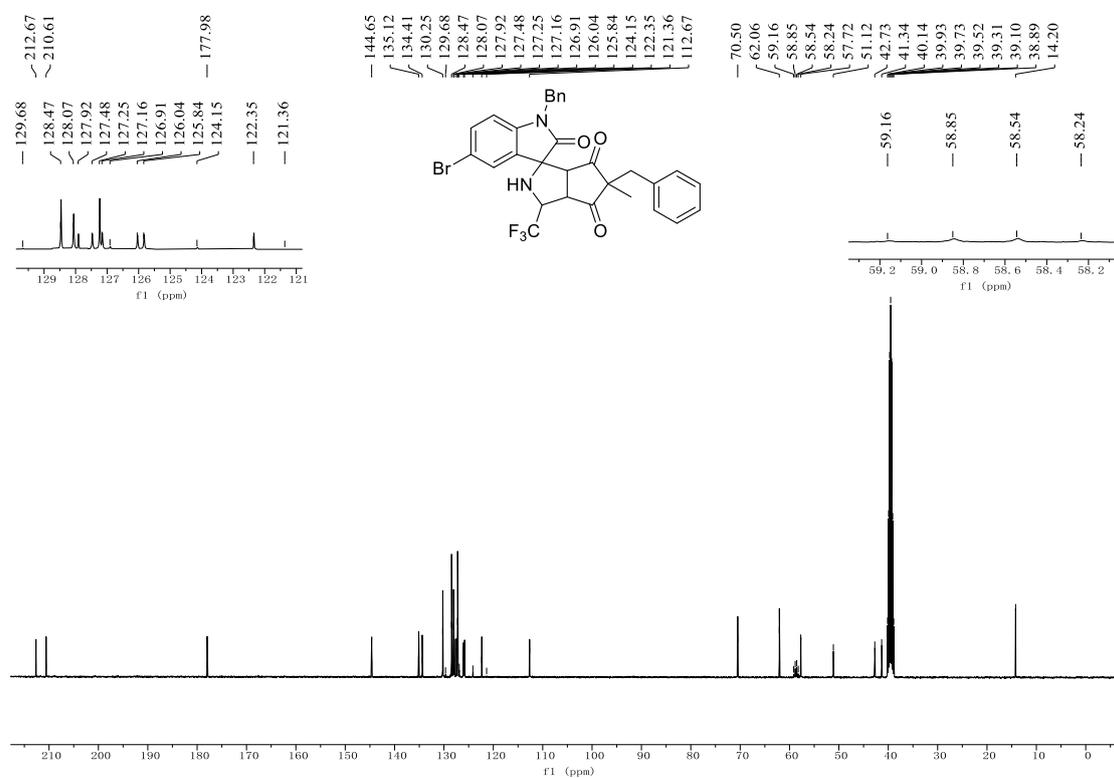
¹³C{¹H} NMR (101 MHz, DMSO-d₆) of **3ja**



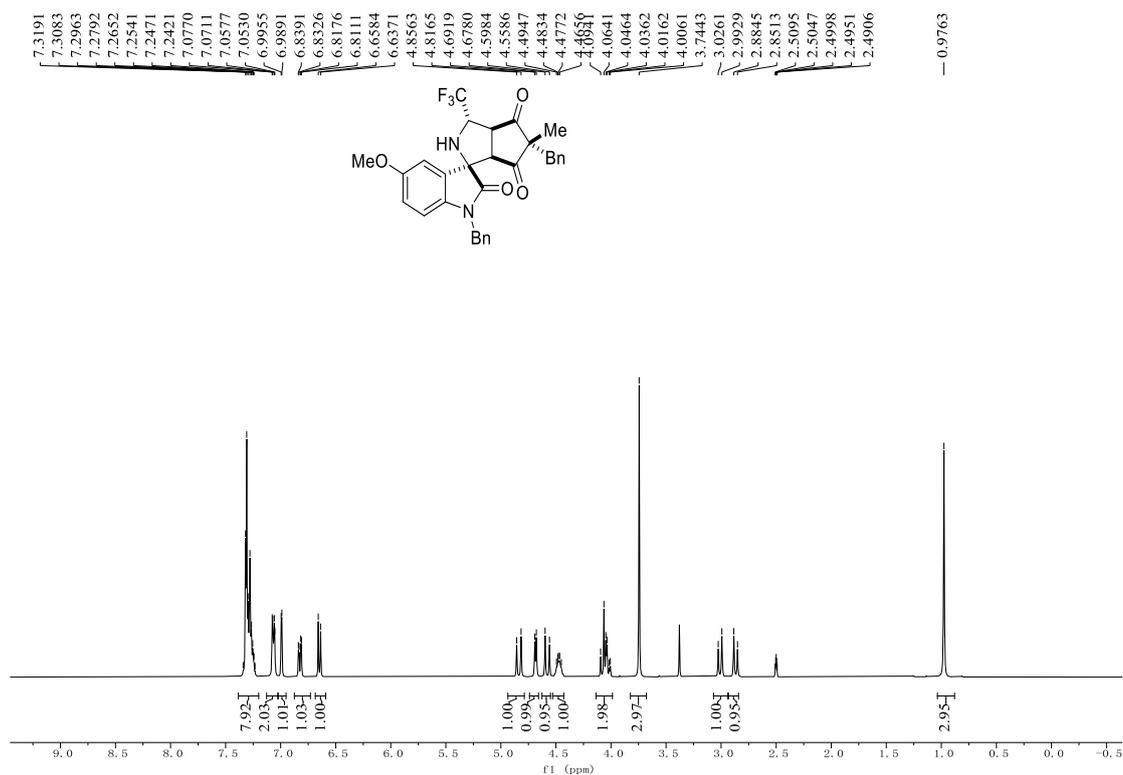
¹H NMR (400 MHz, DMSO-*d*₆) of **3ka**



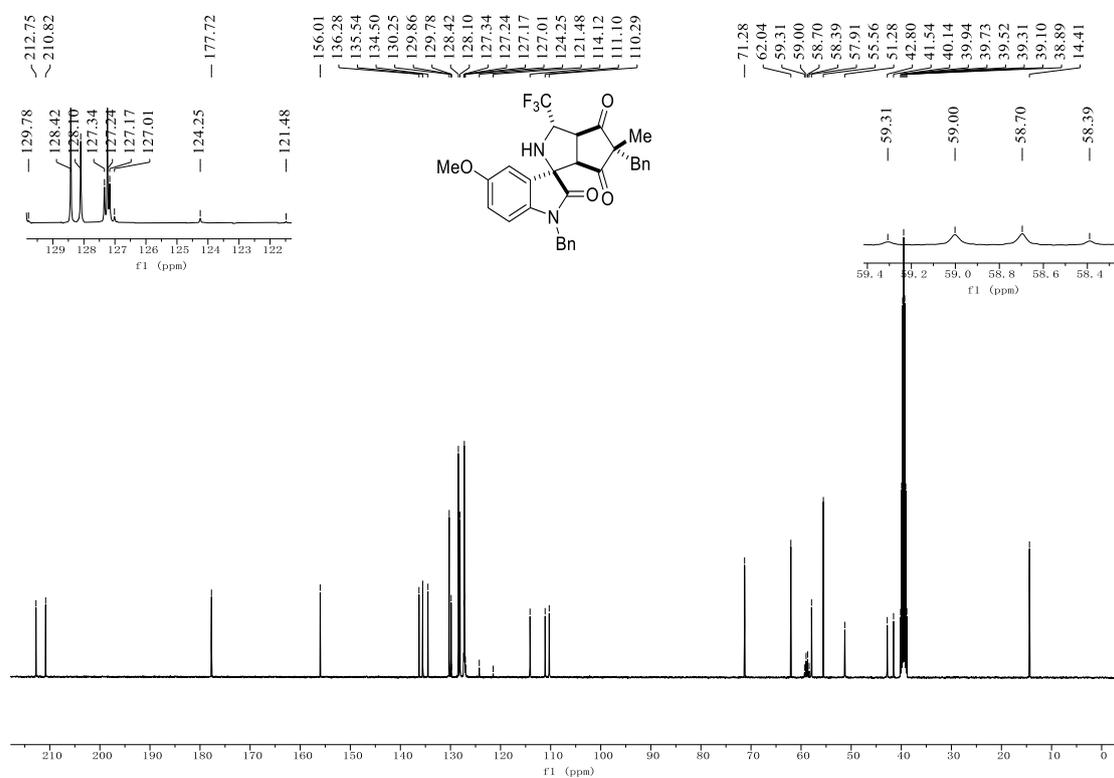
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **3ka**



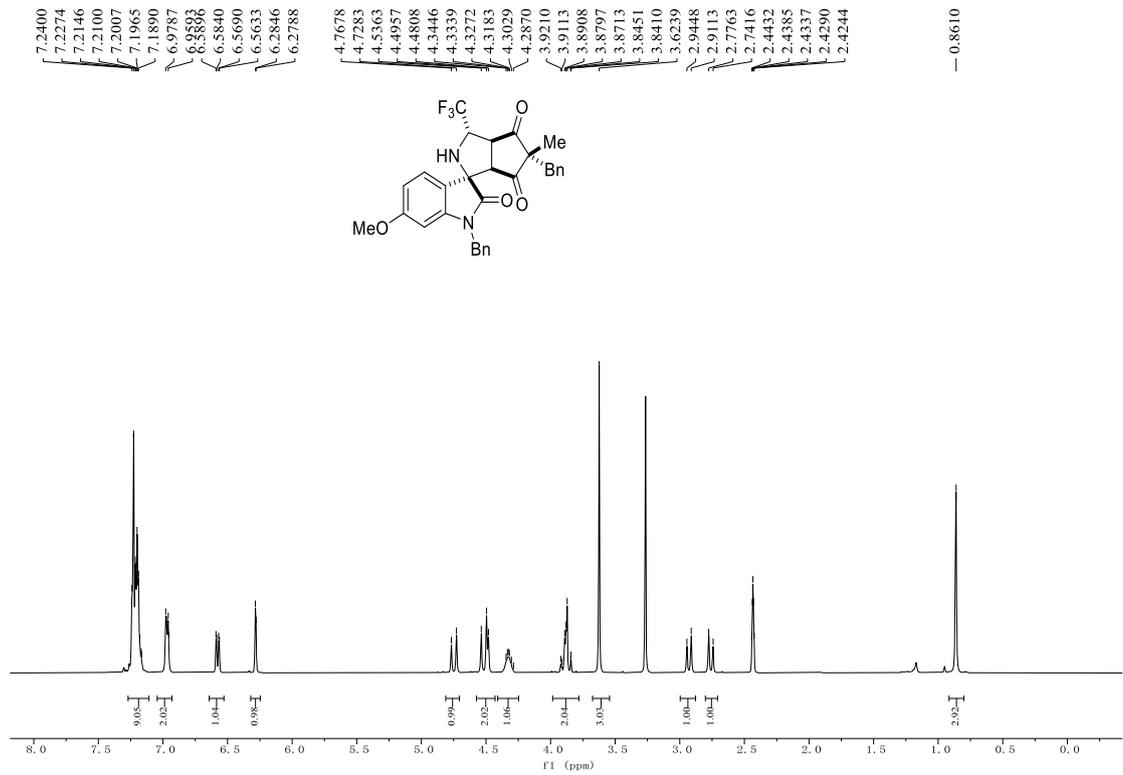
¹H NMR (400 MHz, DMSO-d₆) of **3na**



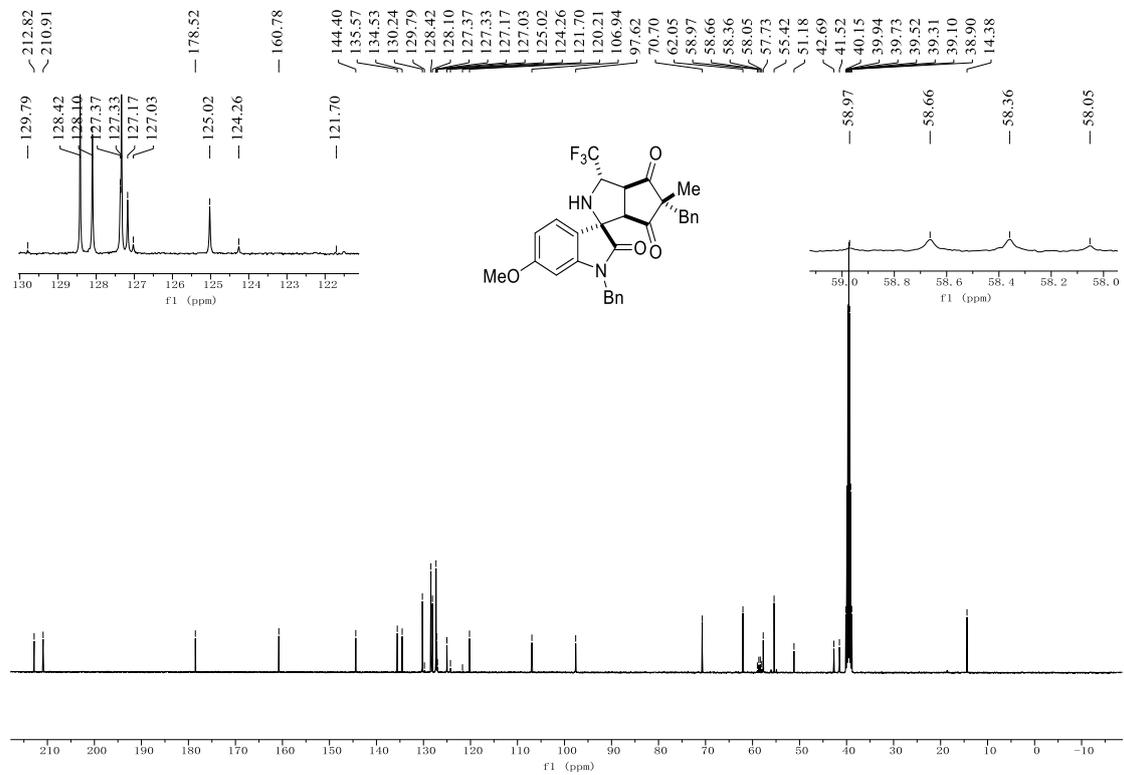
¹³C{¹H} NMR (101 MHz, DMSO-d₆) of **3na**



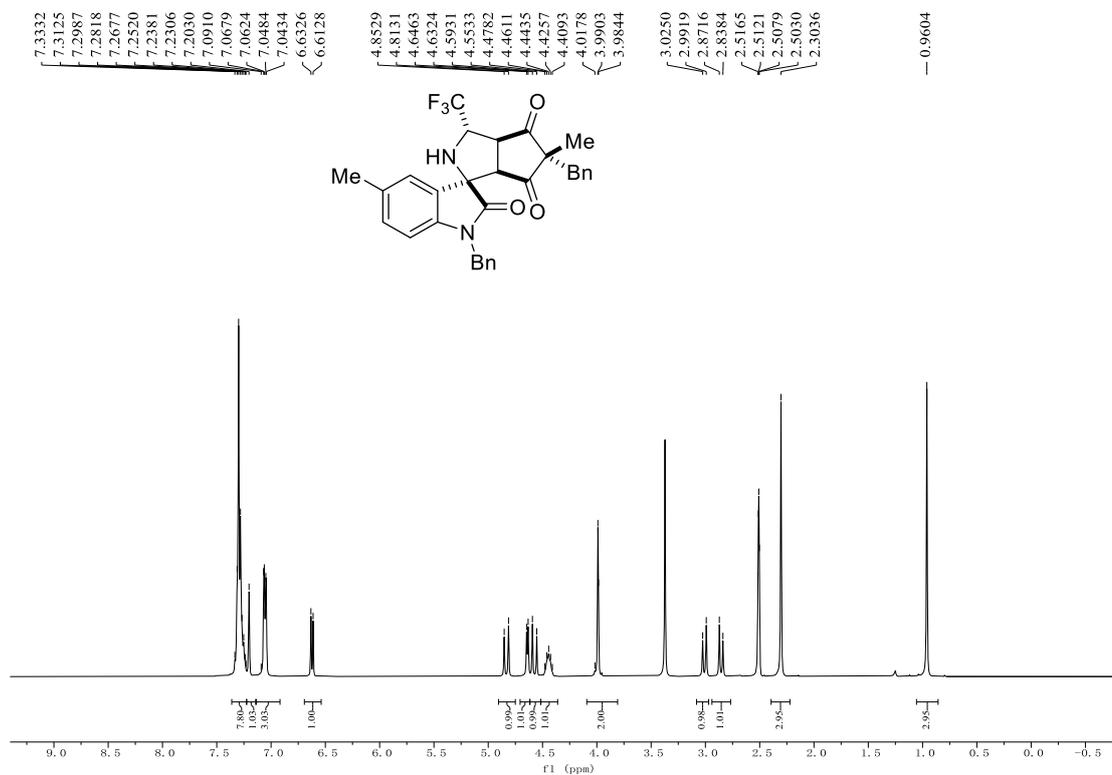
¹H NMR (400 MHz, DMSO-*d*₆) of **30a**



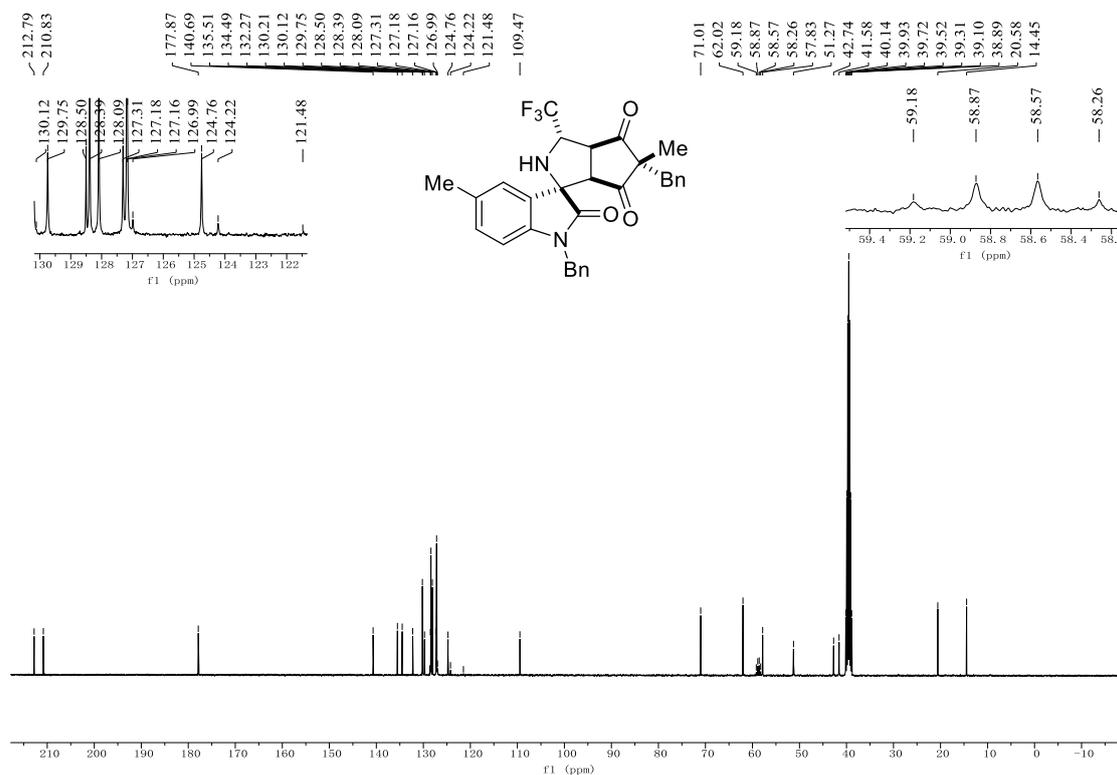
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **30a**



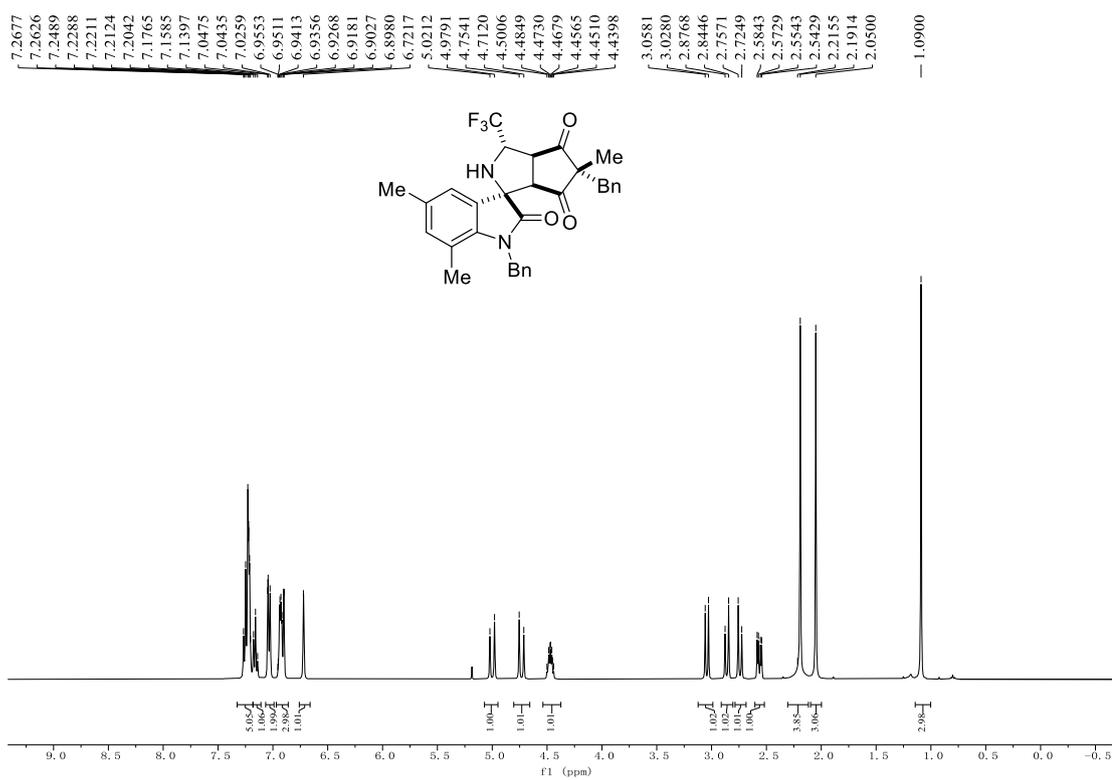
¹H NMR (400 MHz, DMSO-*d*₆) of **3pa**



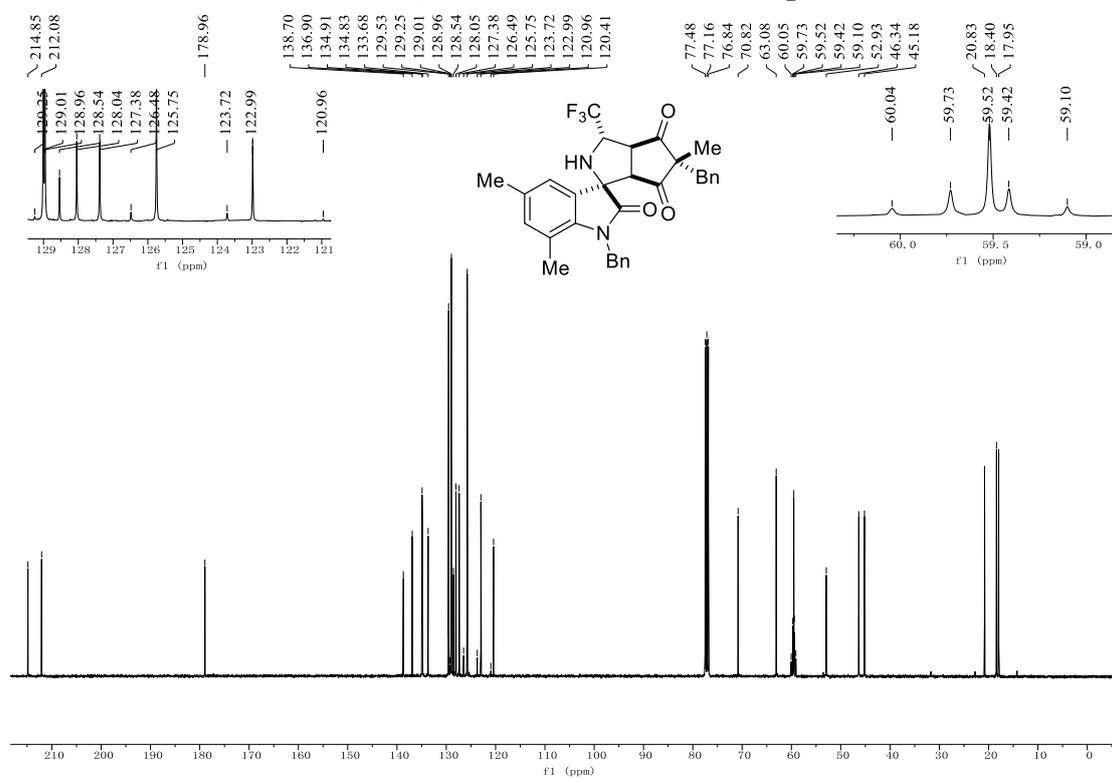
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **3pa**



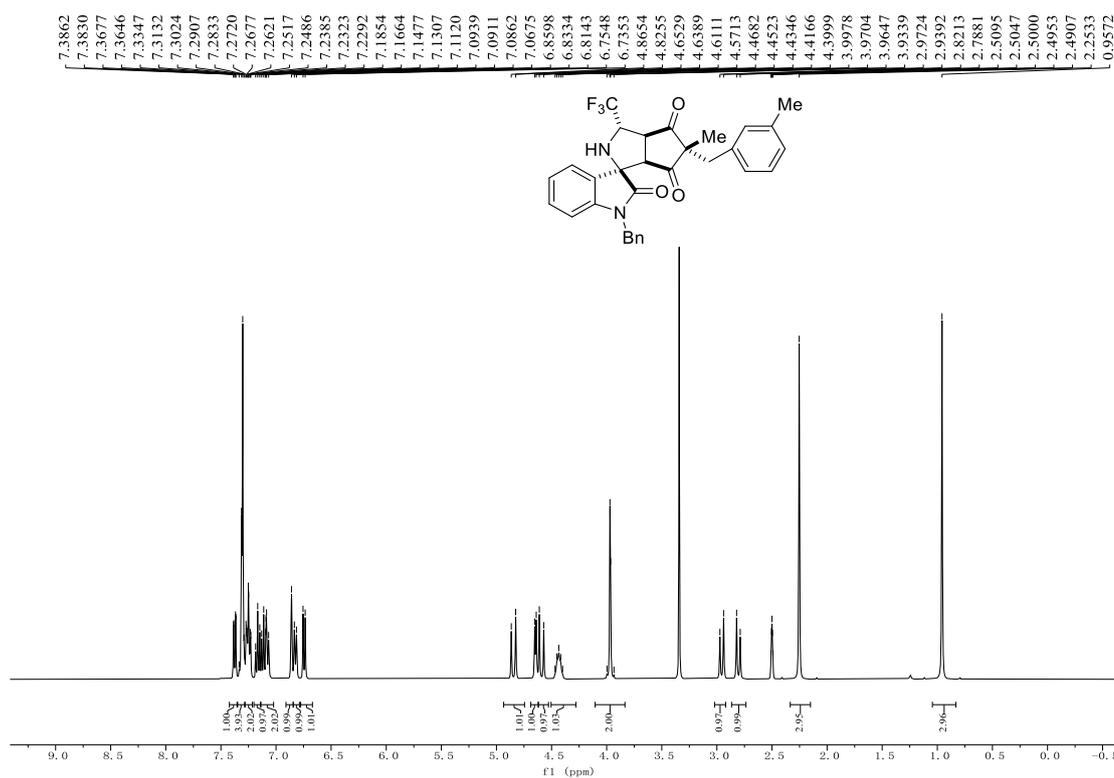
^1H NMR (400 MHz, CDCl_3) of **3qa**



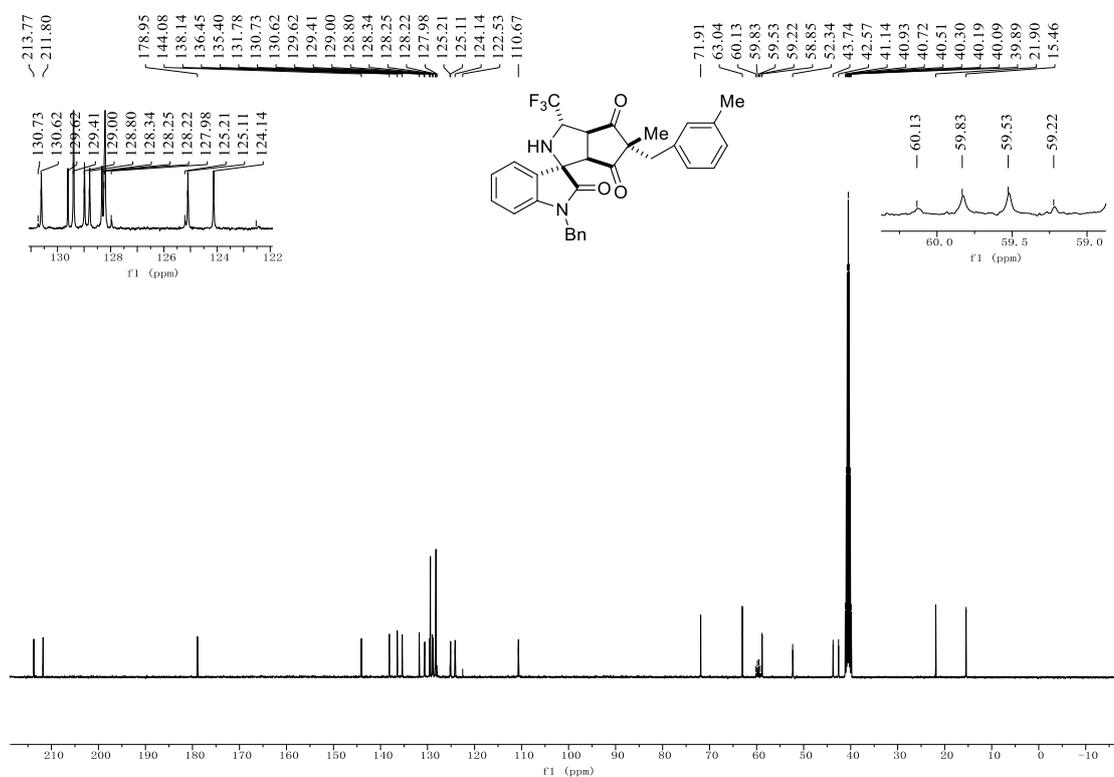
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of **3qa**



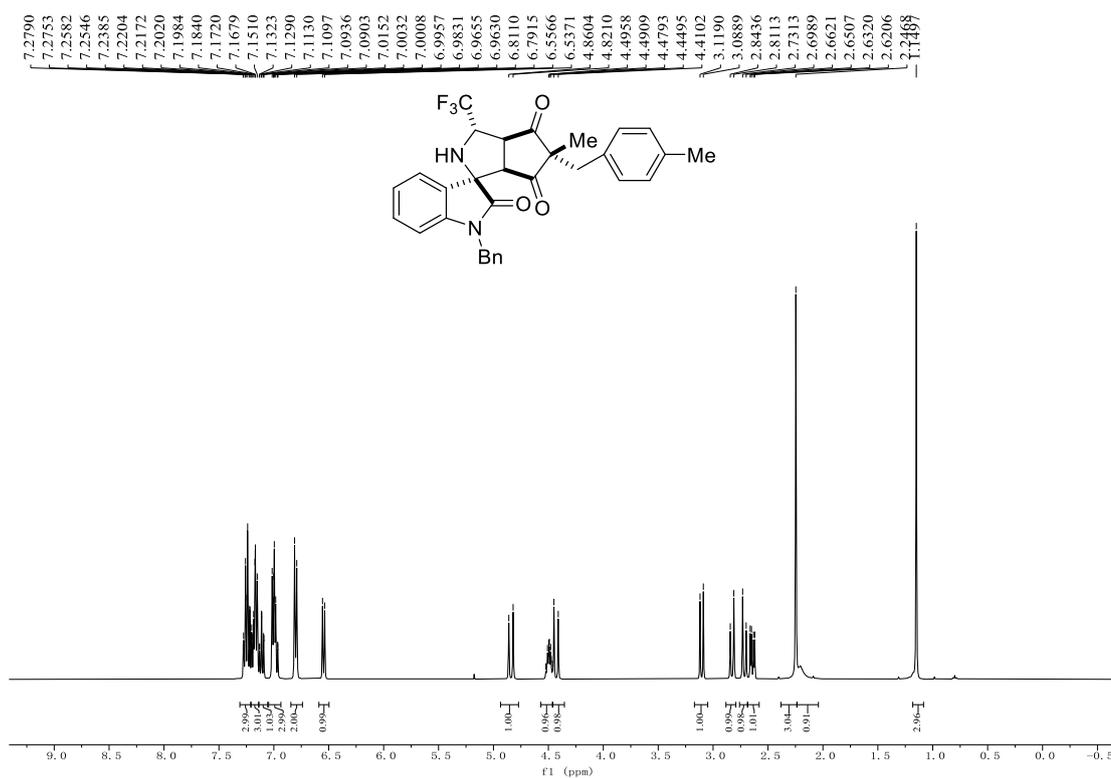
¹H NMR (400 MHz, DMSO-d₆) of **3ab**



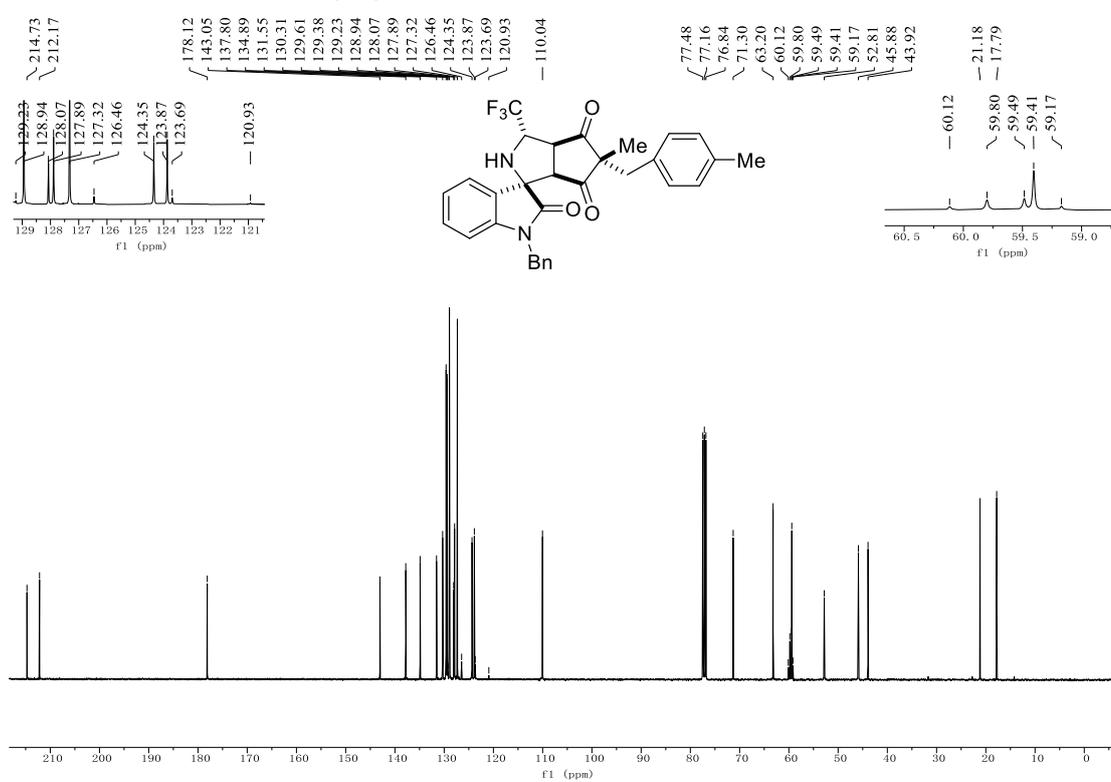
¹³C{¹H} NMR (101 MHz, DMSO-d₆) of **3ab**



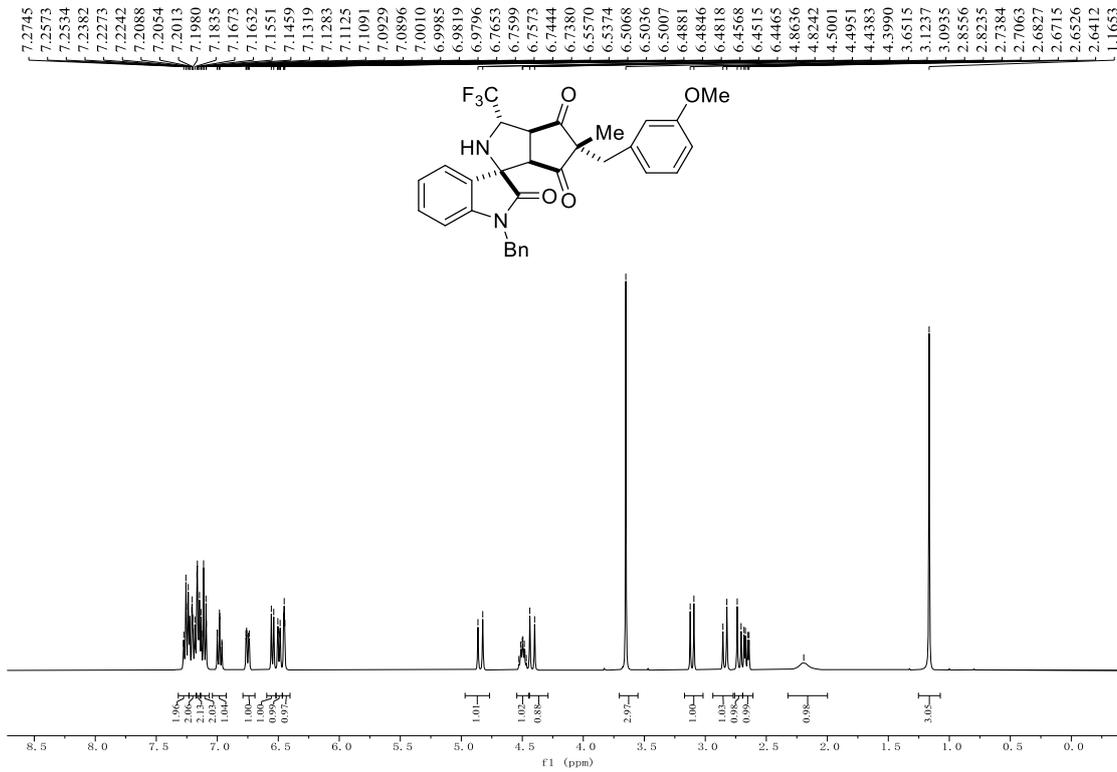
¹H NMR (400 MHz, CDCl₃) of **3ac**



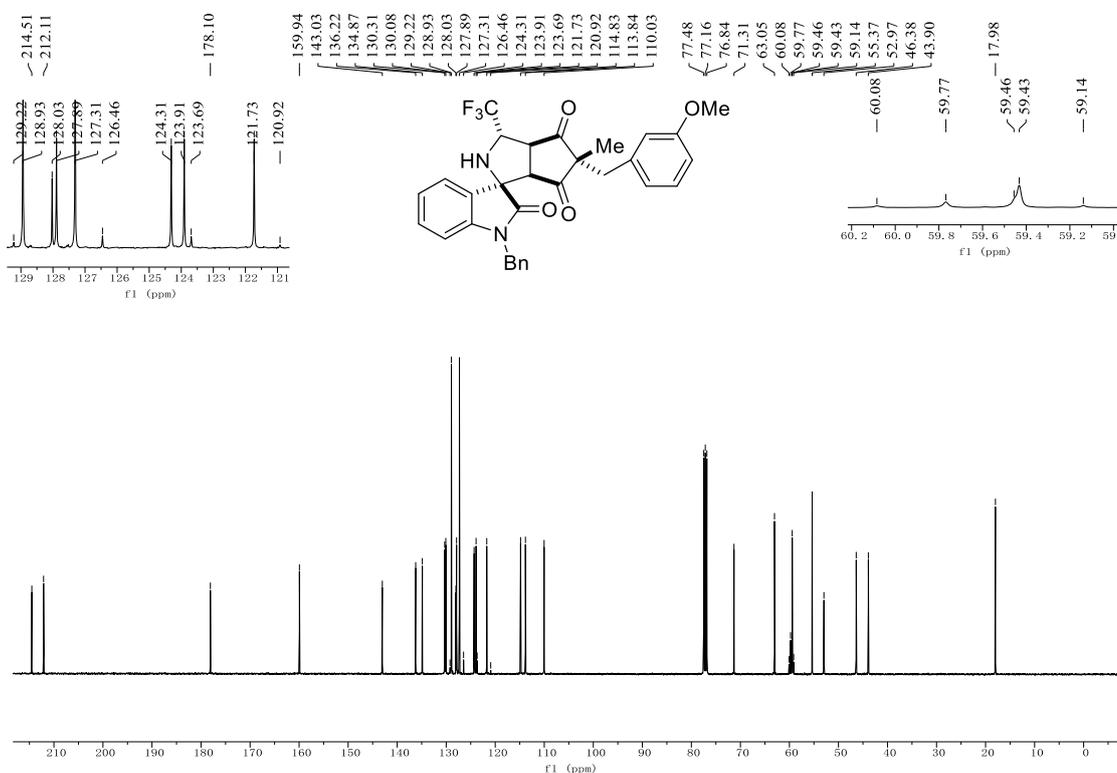
¹³C{¹H} NMR (101 MHz, CDCl₃) of **3ac**



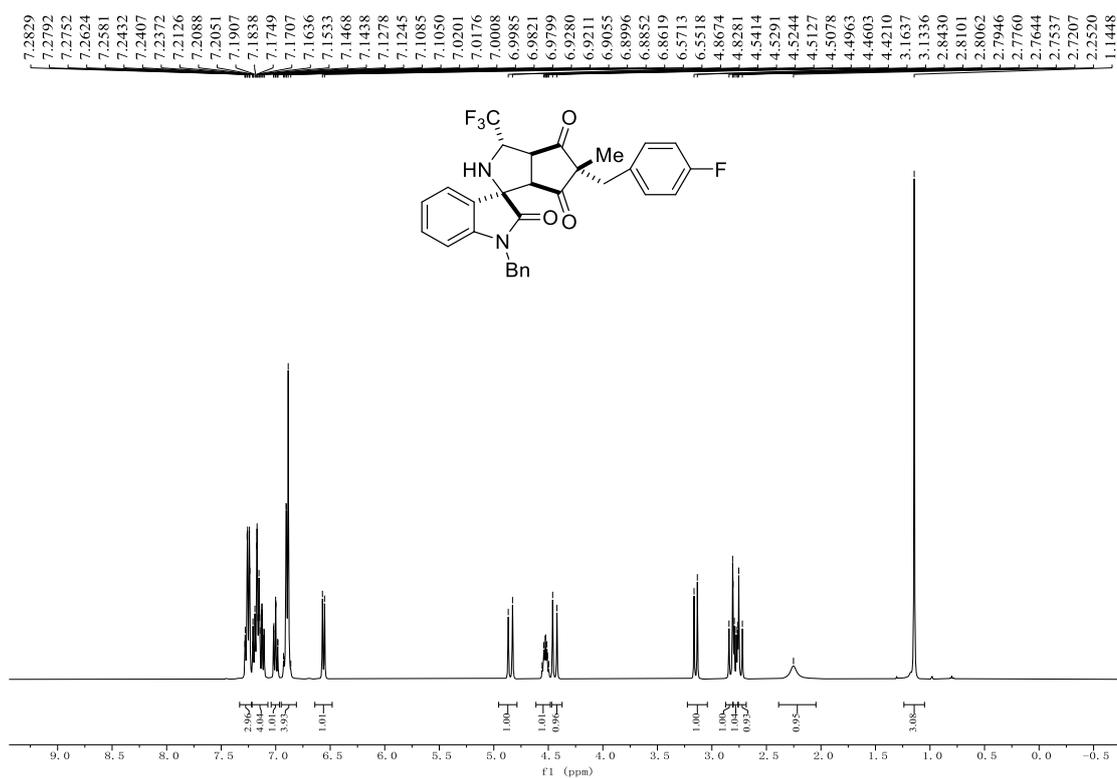
¹H NMR (400 MHz, CDCl₃) of **3ad**



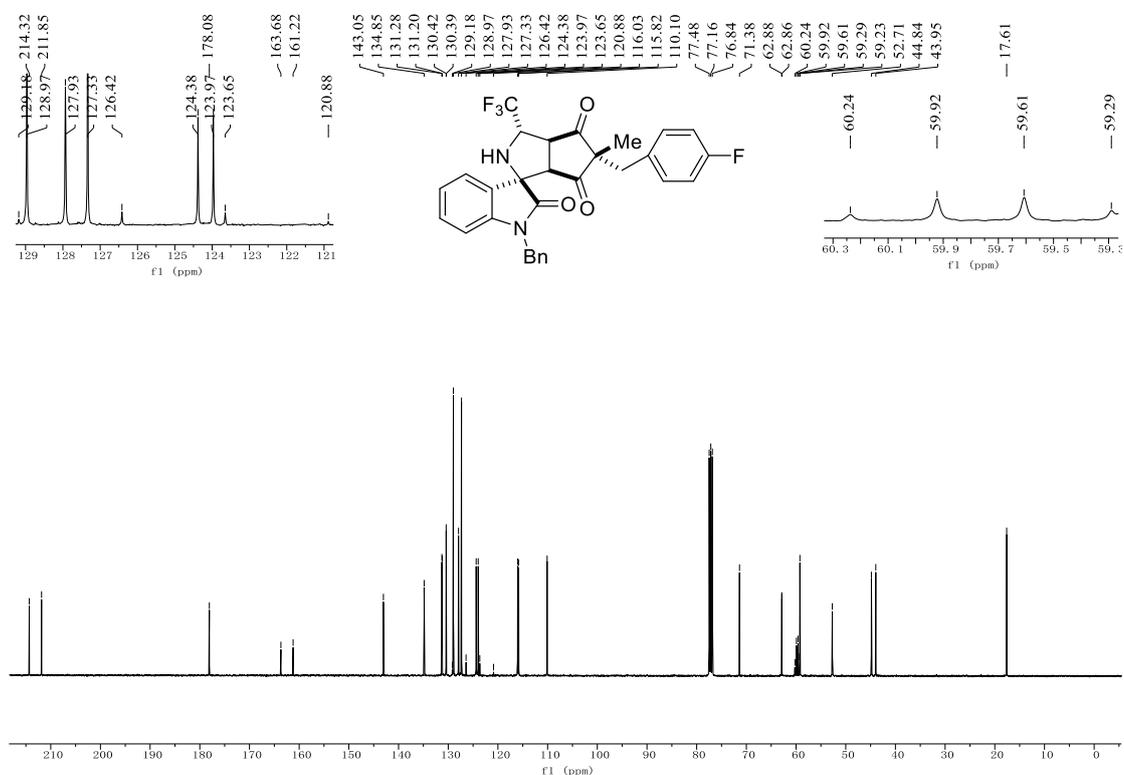
¹³C{¹H} NMR (101 MHz, CDCl₃) of **3ad**



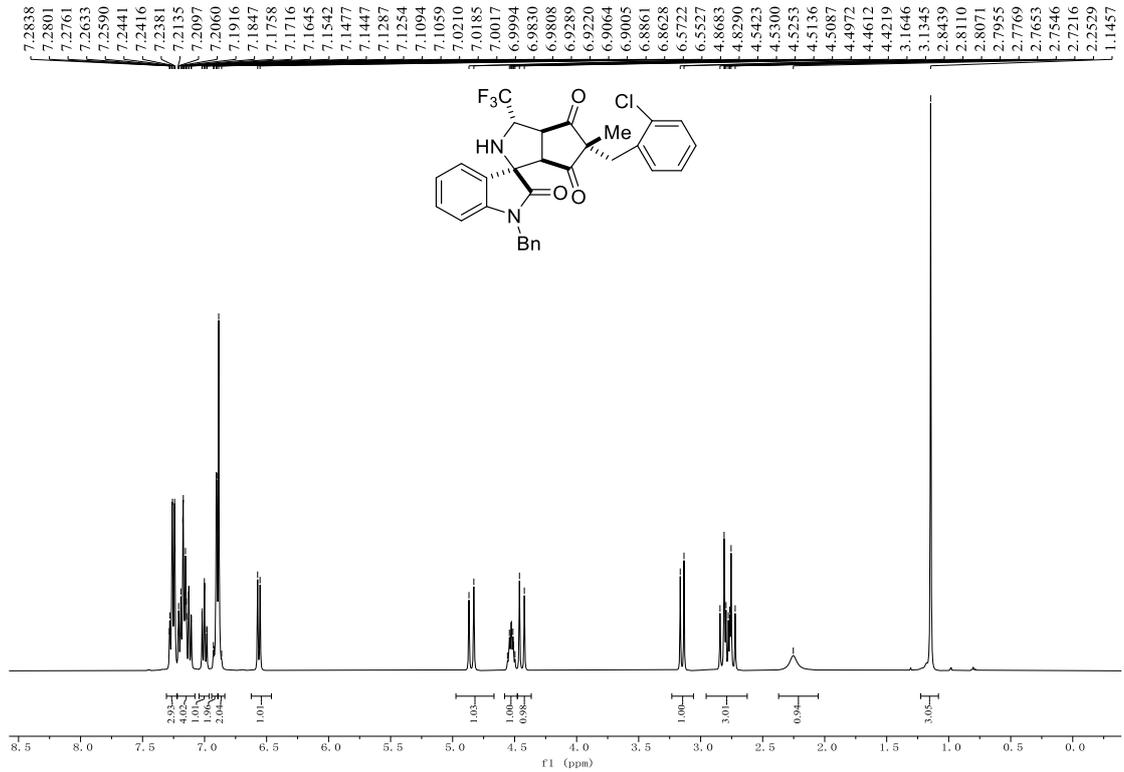
¹H NMR (400 MHz, CDCl₃) of **3ae**



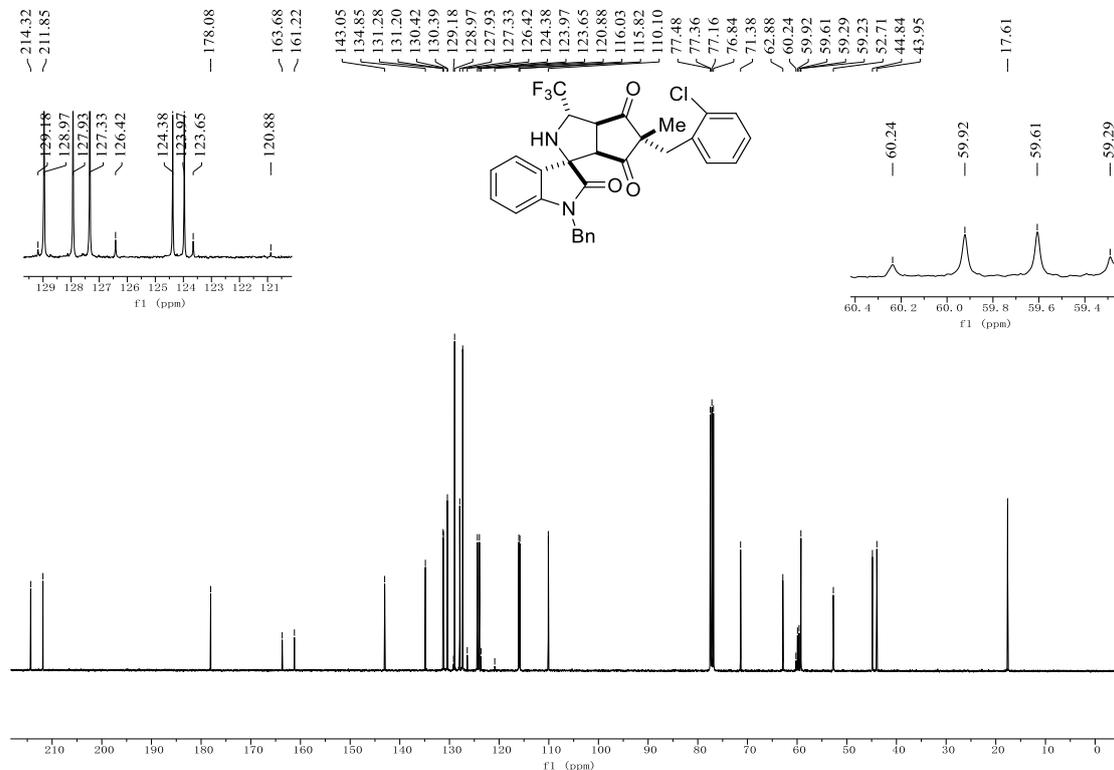
¹³C{¹H} NMR (101 MHz, CDCl₃) of **3ae**



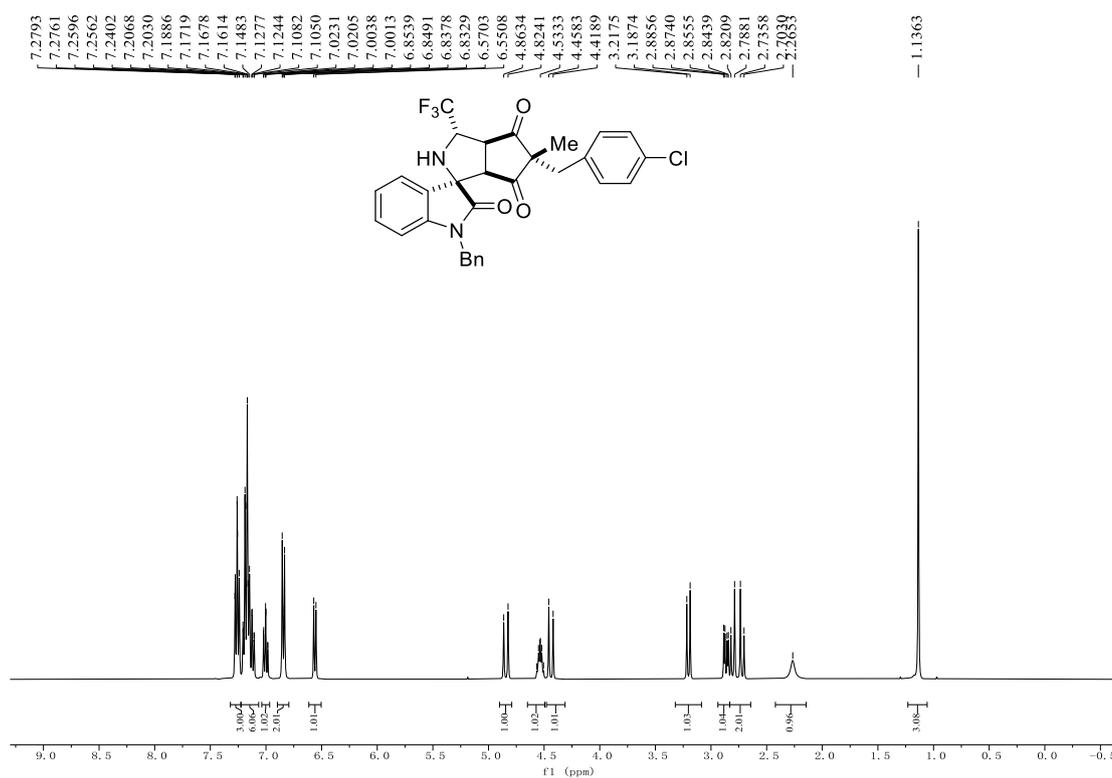
^1H NMR (400 MHz, CDCl_3) of **3af**



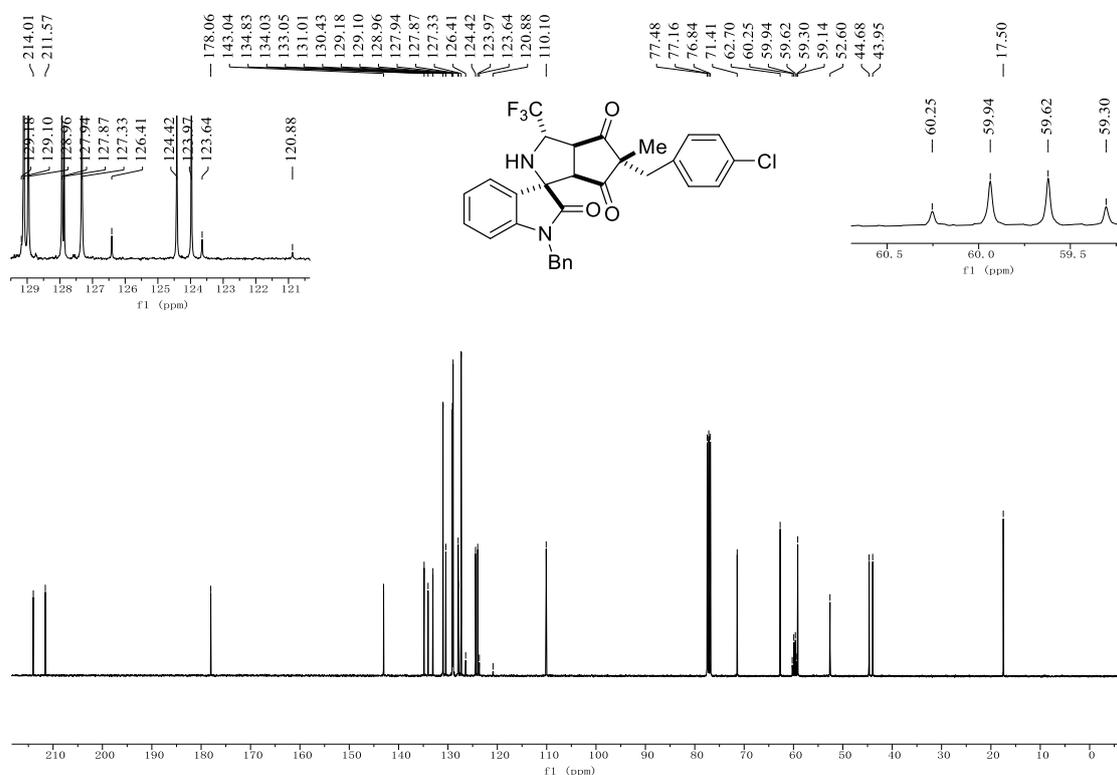
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of **3af**



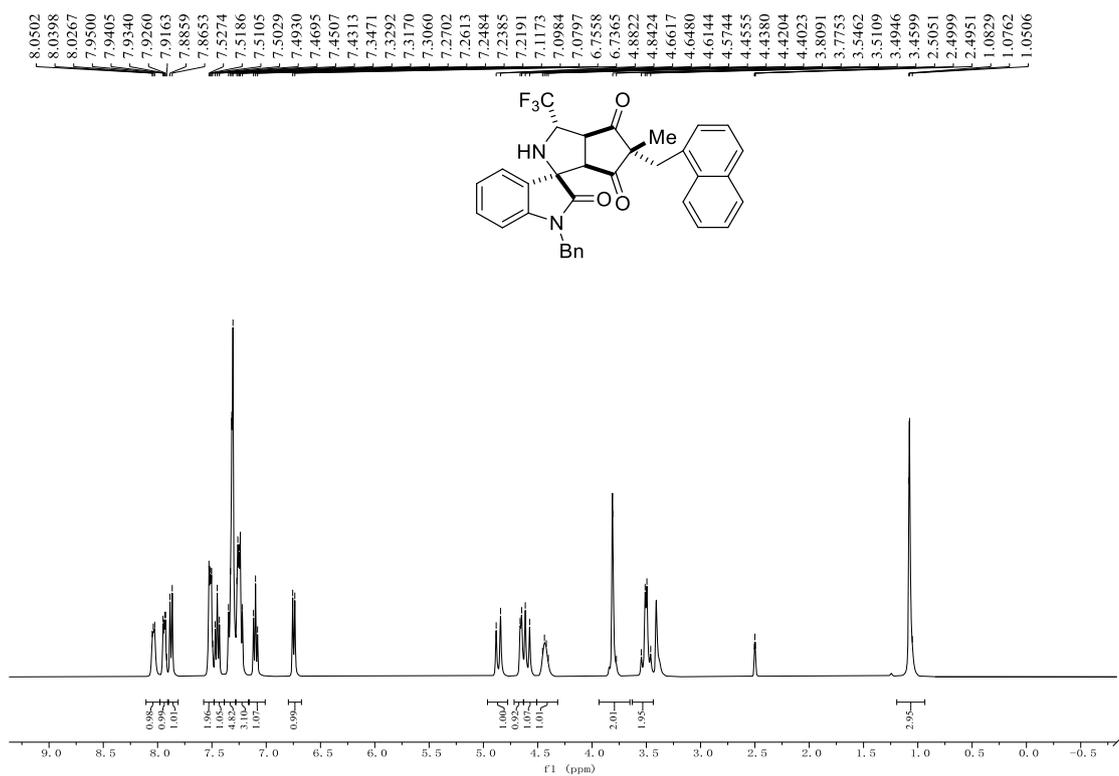
¹H NMR (400 MHz, CDCl₃) of **3ag**



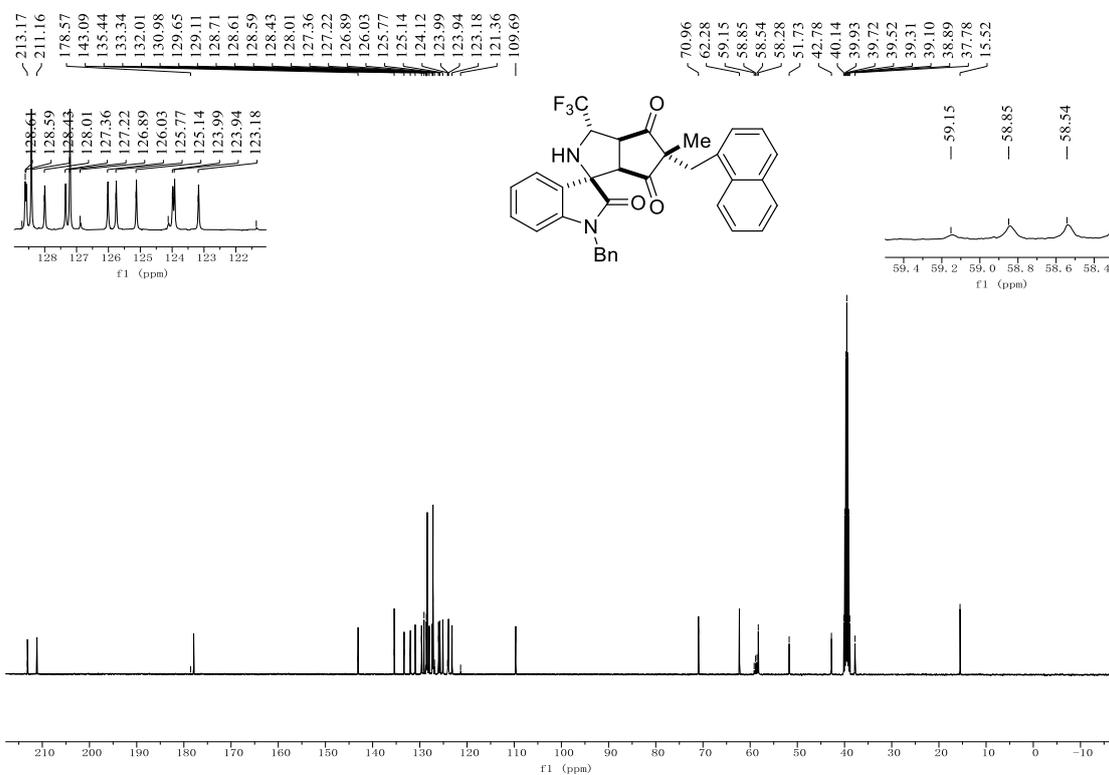
¹³C{¹H} NMR (101 MHz, CDCl₃) of **3ag**



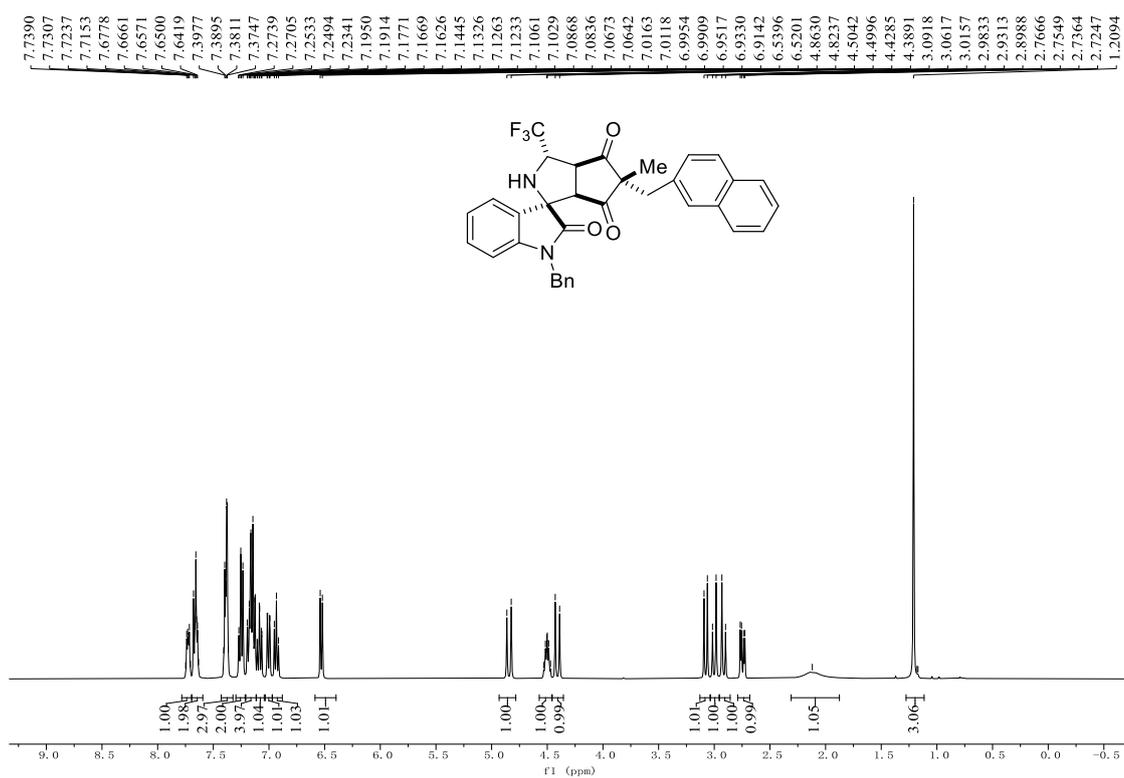
¹H NMR (400 MHz, DMSO-d₆) of 3aj



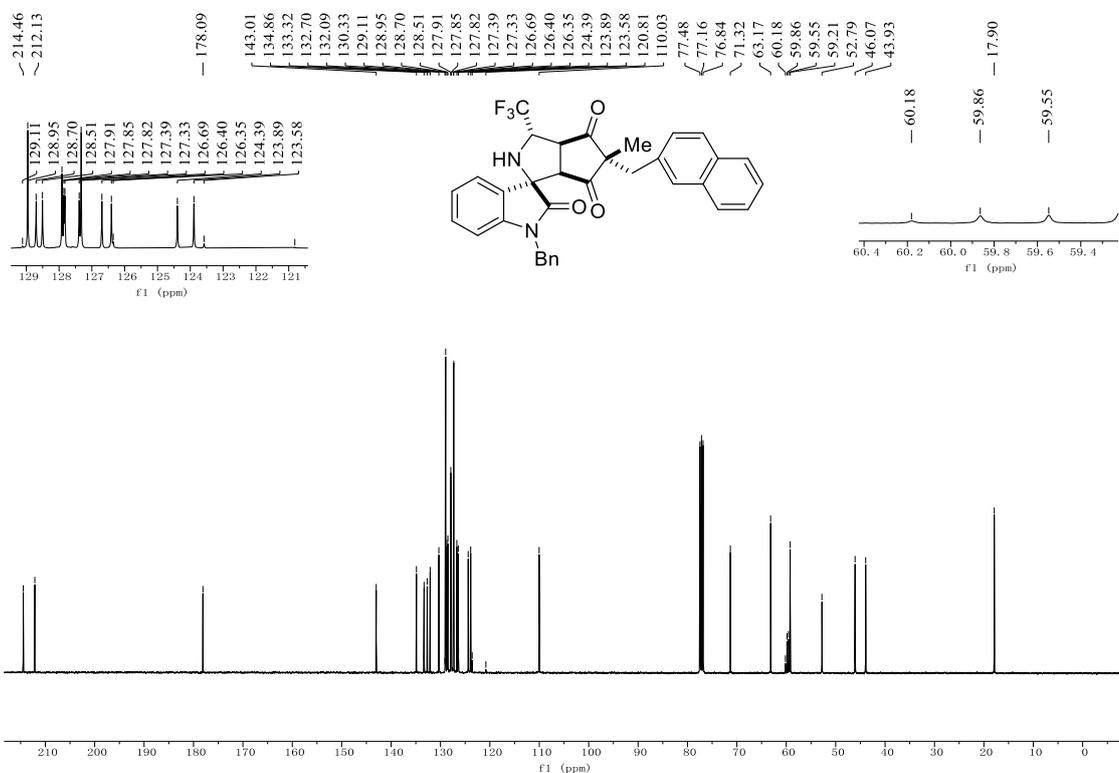
¹³C{¹H} NMR (101 MHz, DMSO-d₆) of 3aj



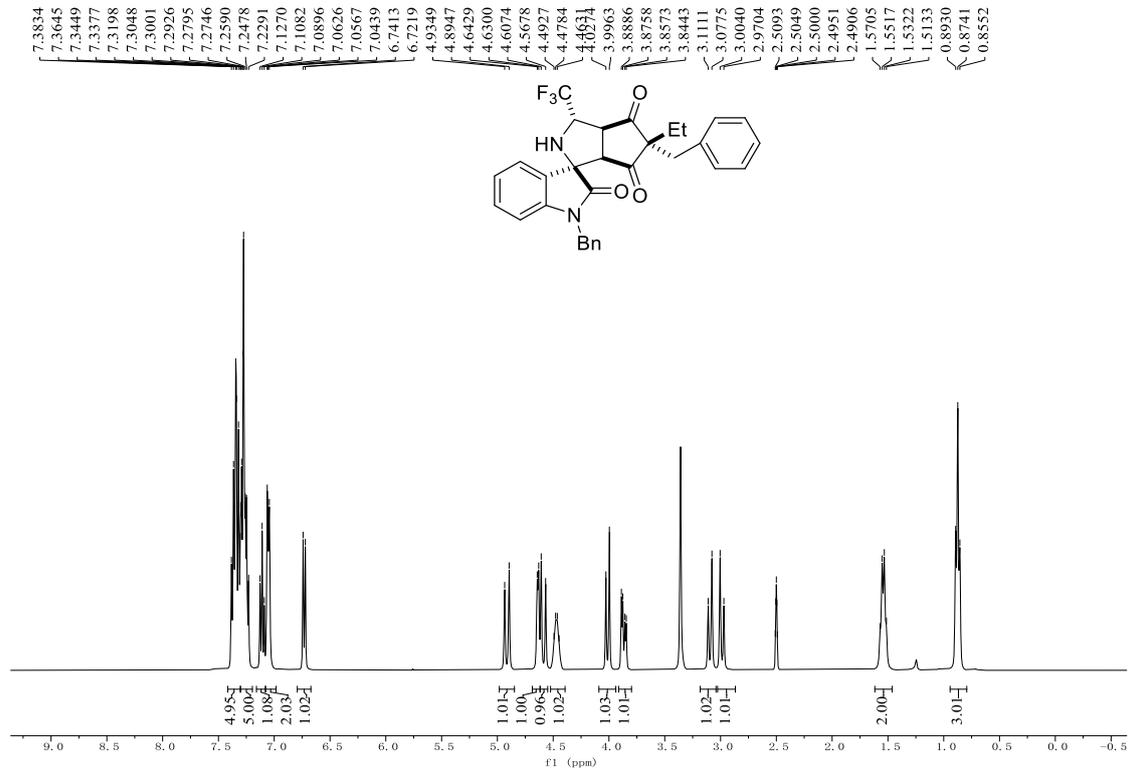
¹H NMR (400 MHz, CDCl₃) of **3ak**



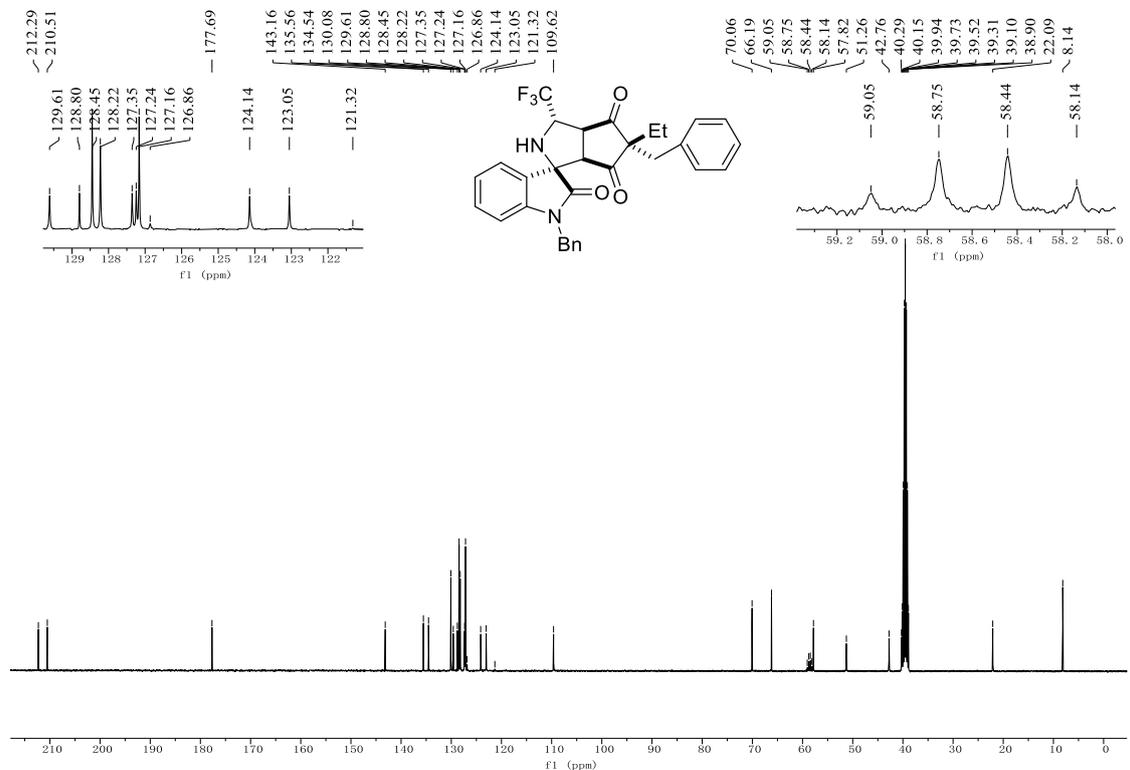
¹³C{¹H} NMR (101 MHz, CDCl₃) of **3ak**



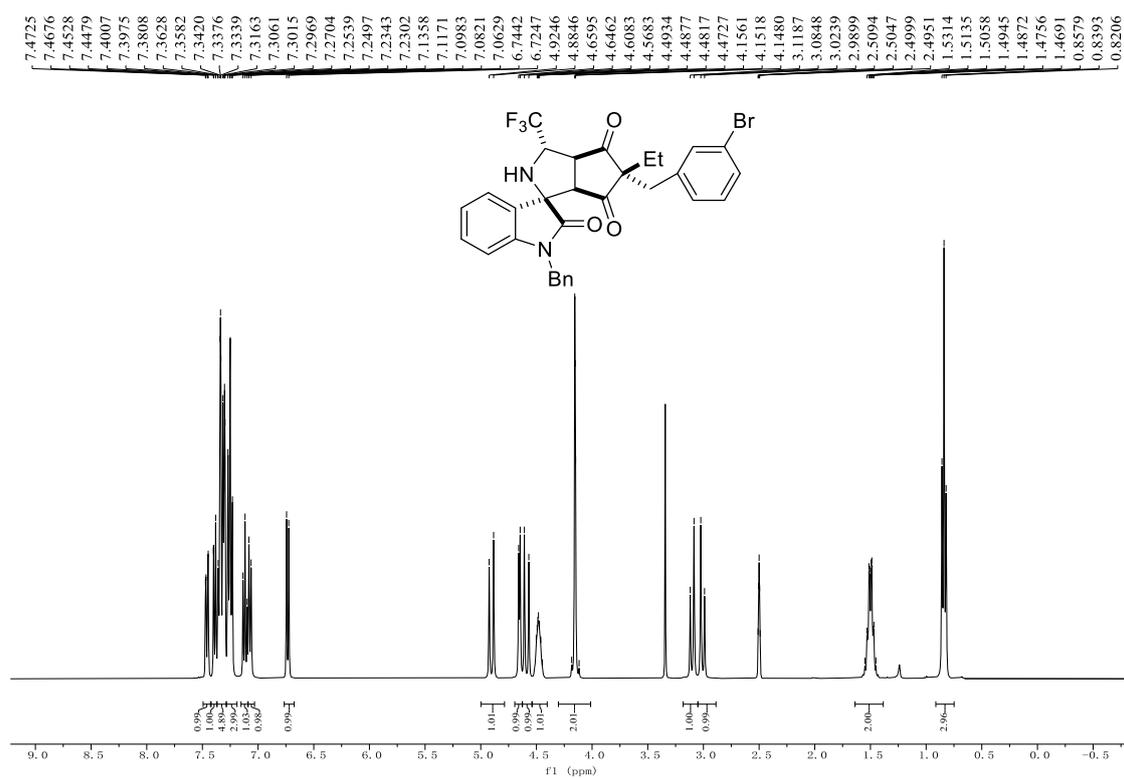
¹H NMR (400 MHz, DMSO-d₆) of **3al**



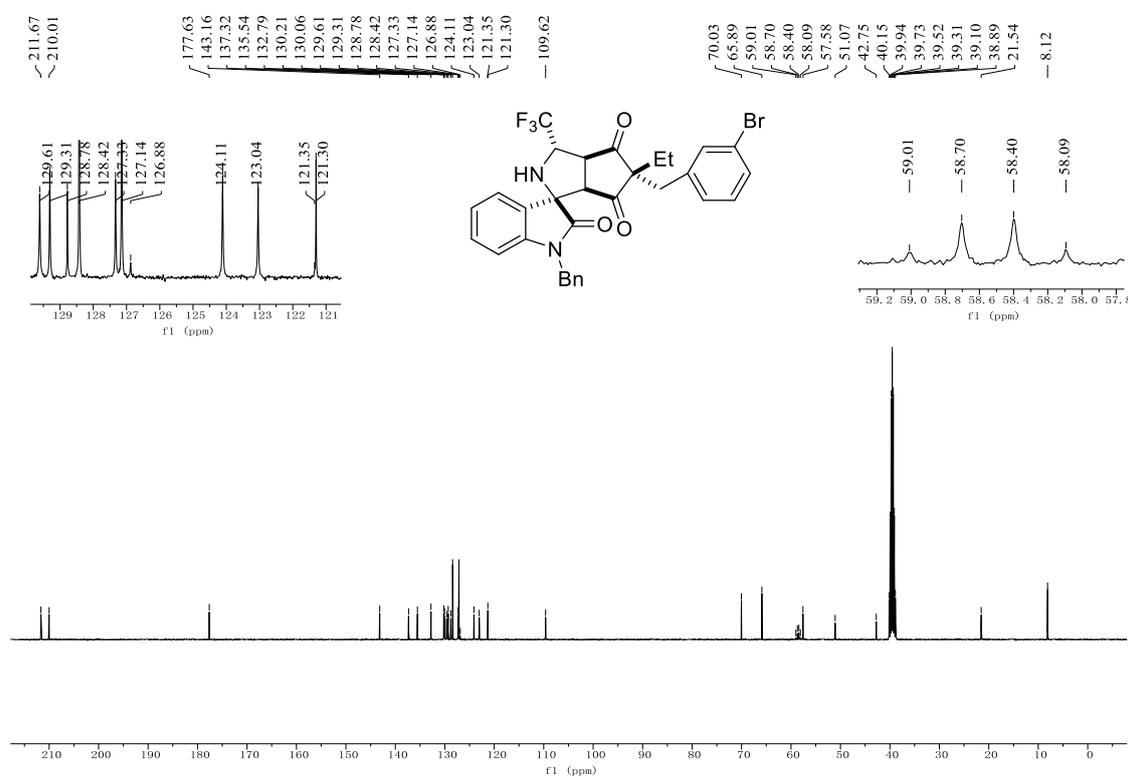
¹³C{¹H} NMR (101 MHz, DMSO-d₆) of **3al**



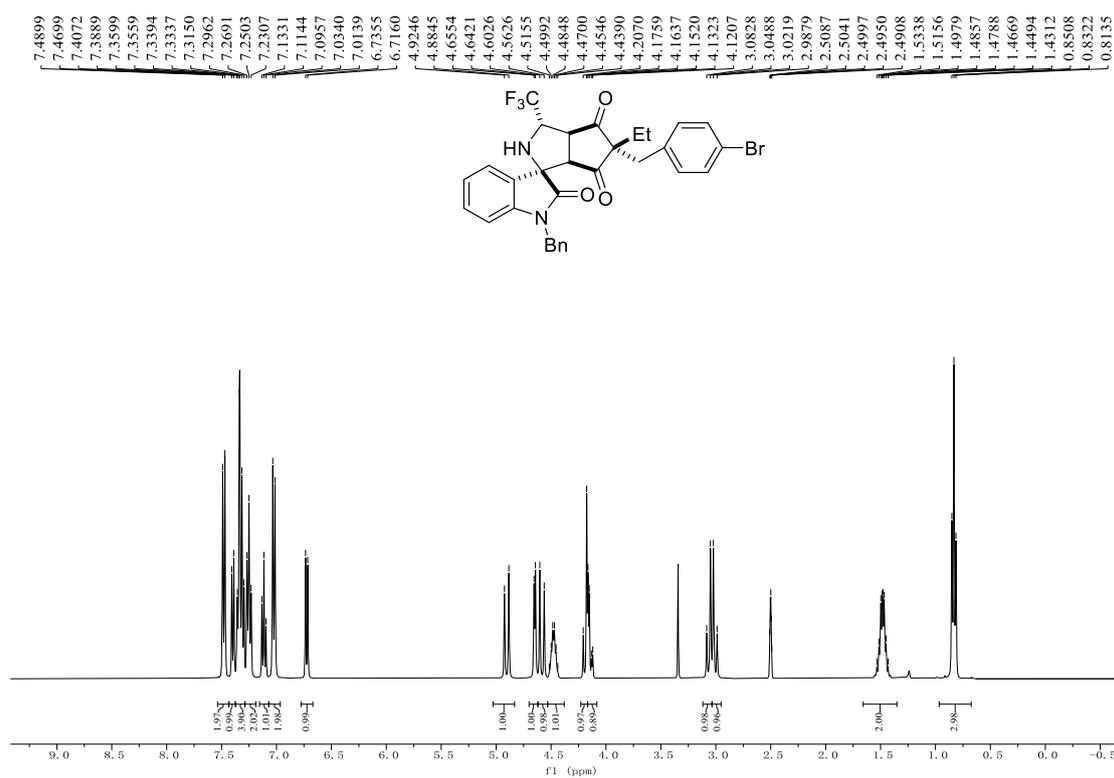
¹H NMR (400 MHz, DMSO-*d*₆) of **3am**



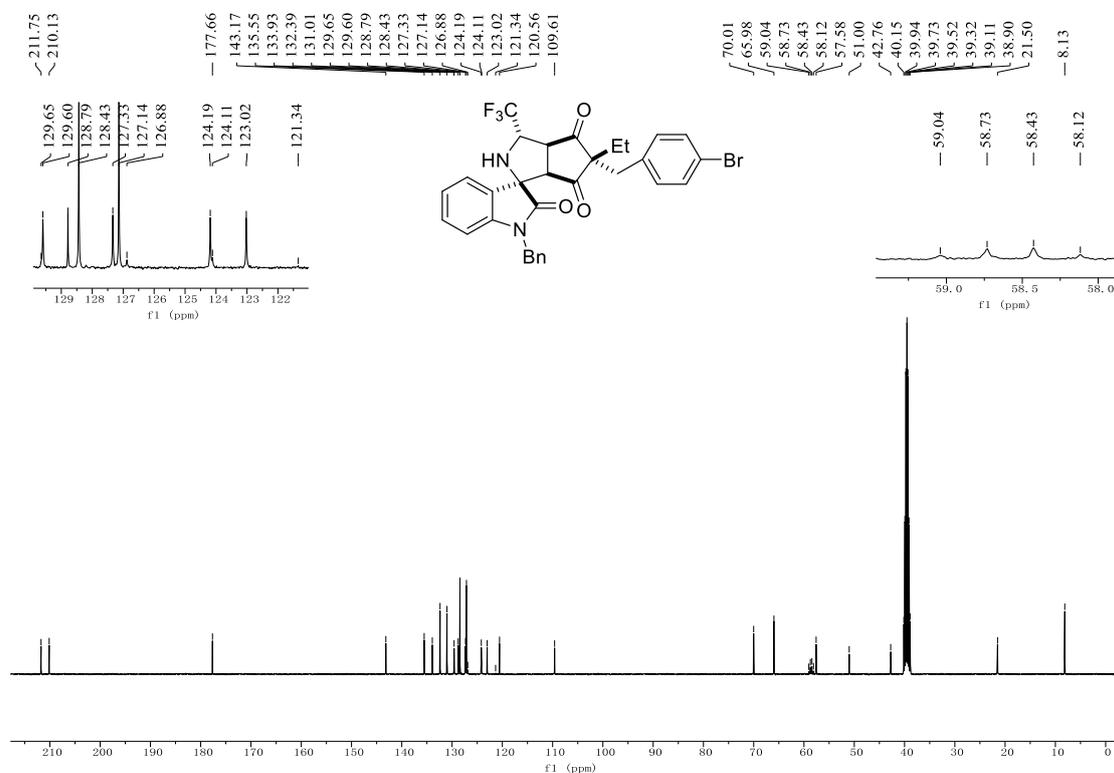
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **3am**



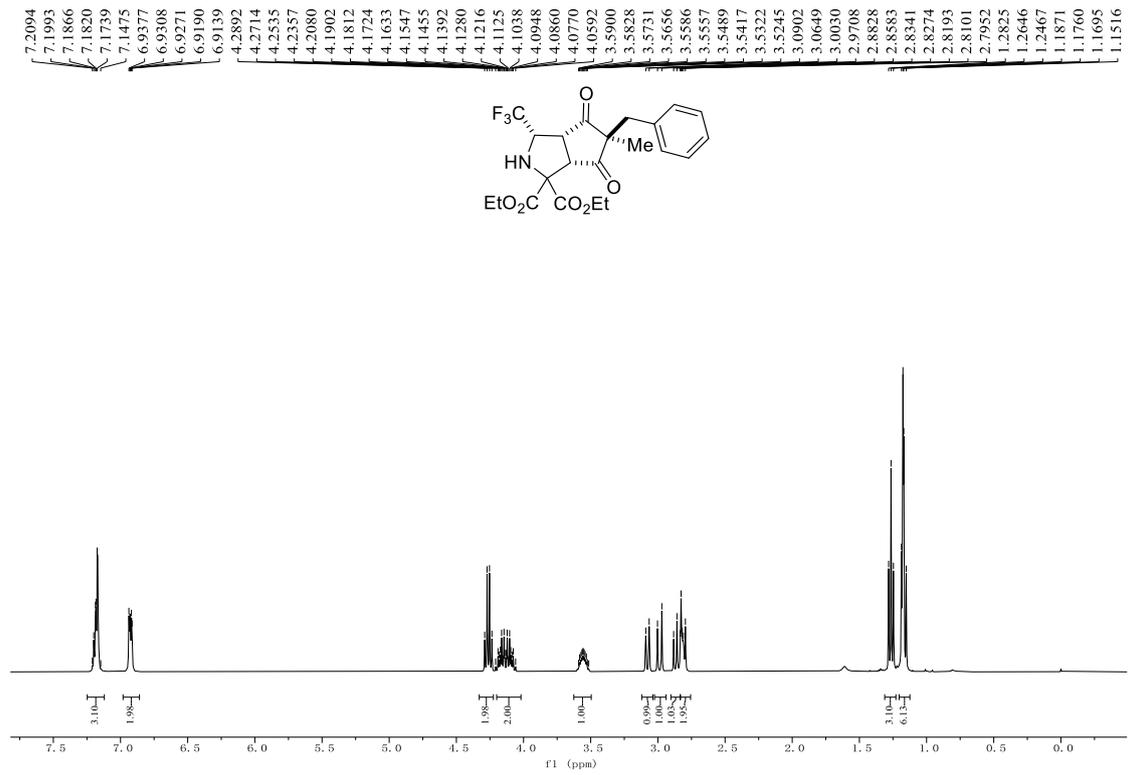
¹H NMR (400 MHz, DMSO-*d*₆) of **3an**



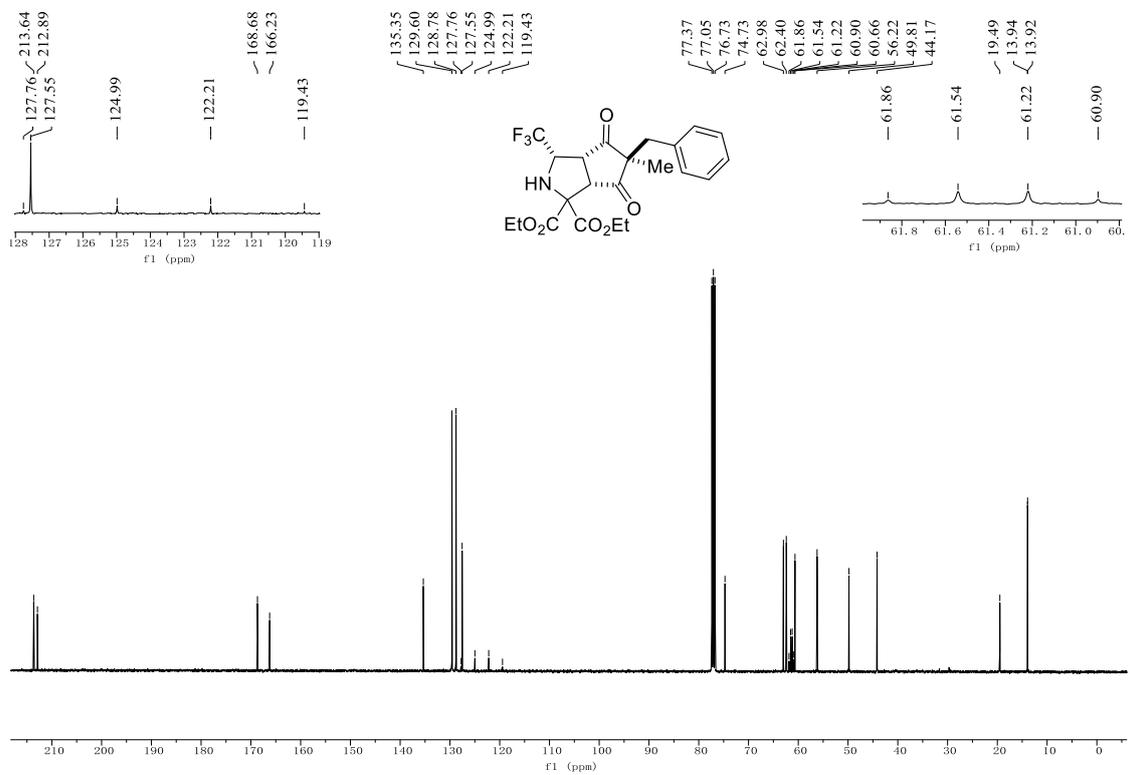
¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **3an**



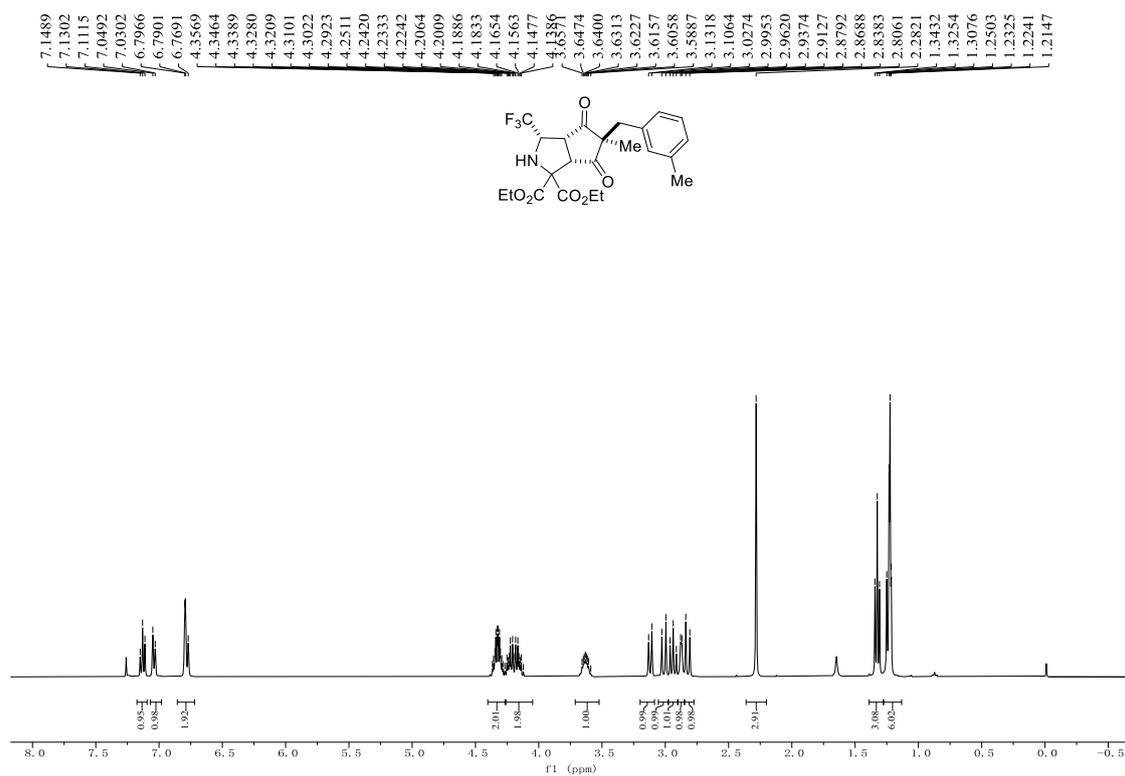
^1H NMR (400 MHz, CDCl_3) of **5a**



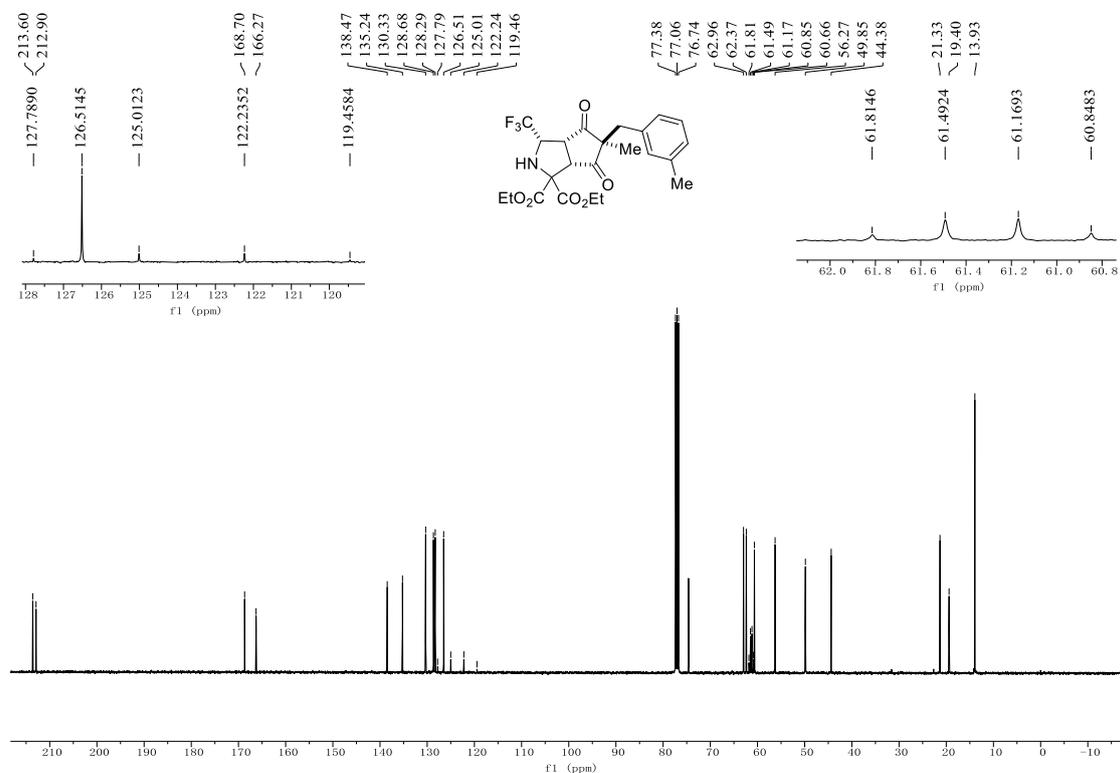
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of **5a**



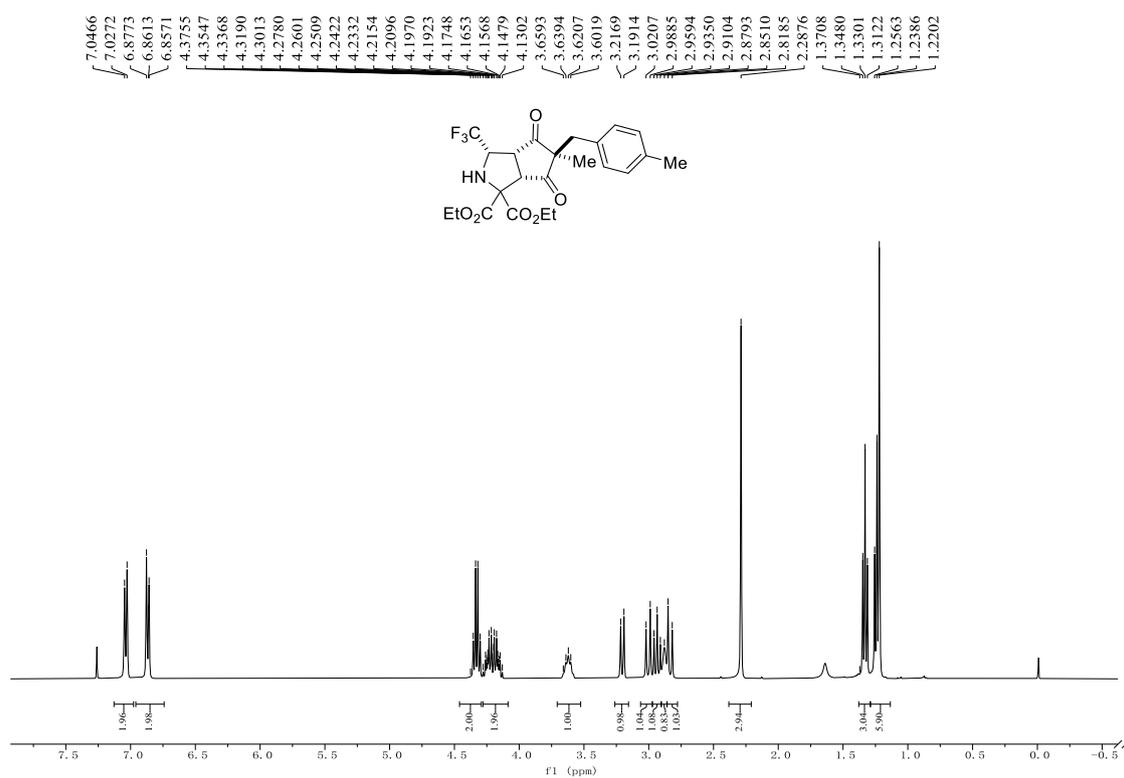
¹H NMR (400 MHz, CDCl₃) of **5b**



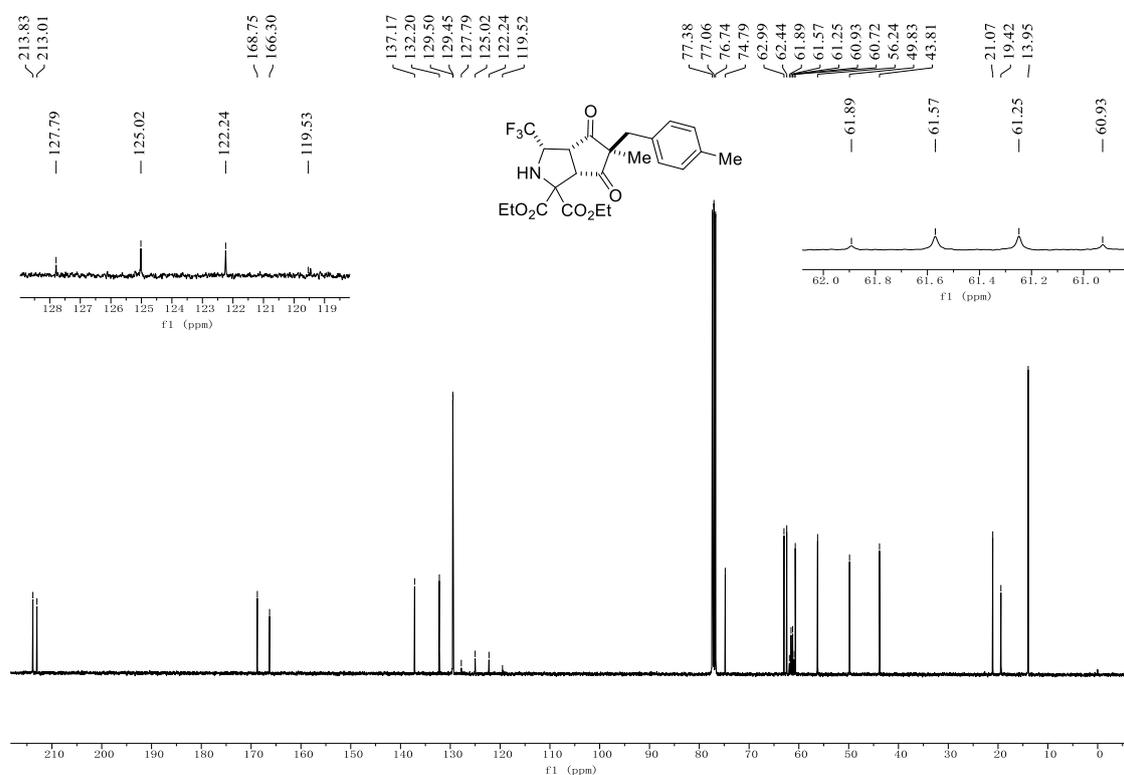
¹³C{¹H} NMR (101 MHz, CDCl₃) of **5b**



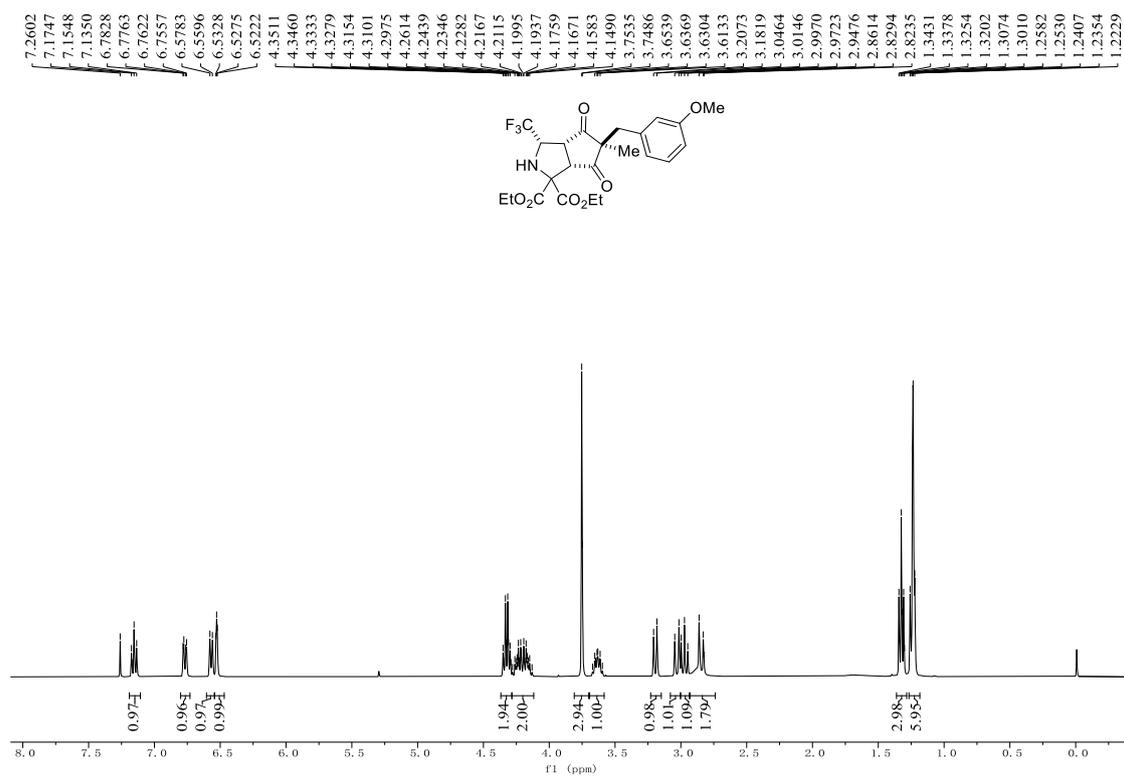
¹H NMR (400 MHz, CDCl₃) of **5c**



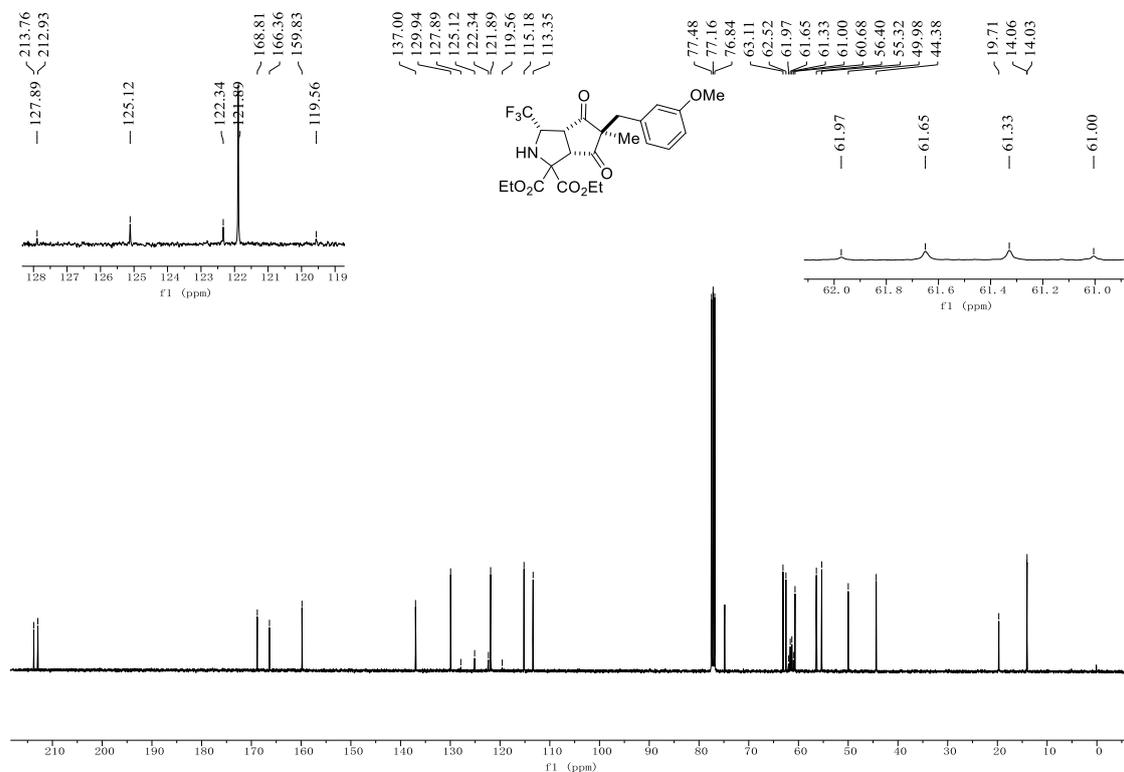
¹³C{¹H} NMR (101 MHz, CDCl₃) of **5c**



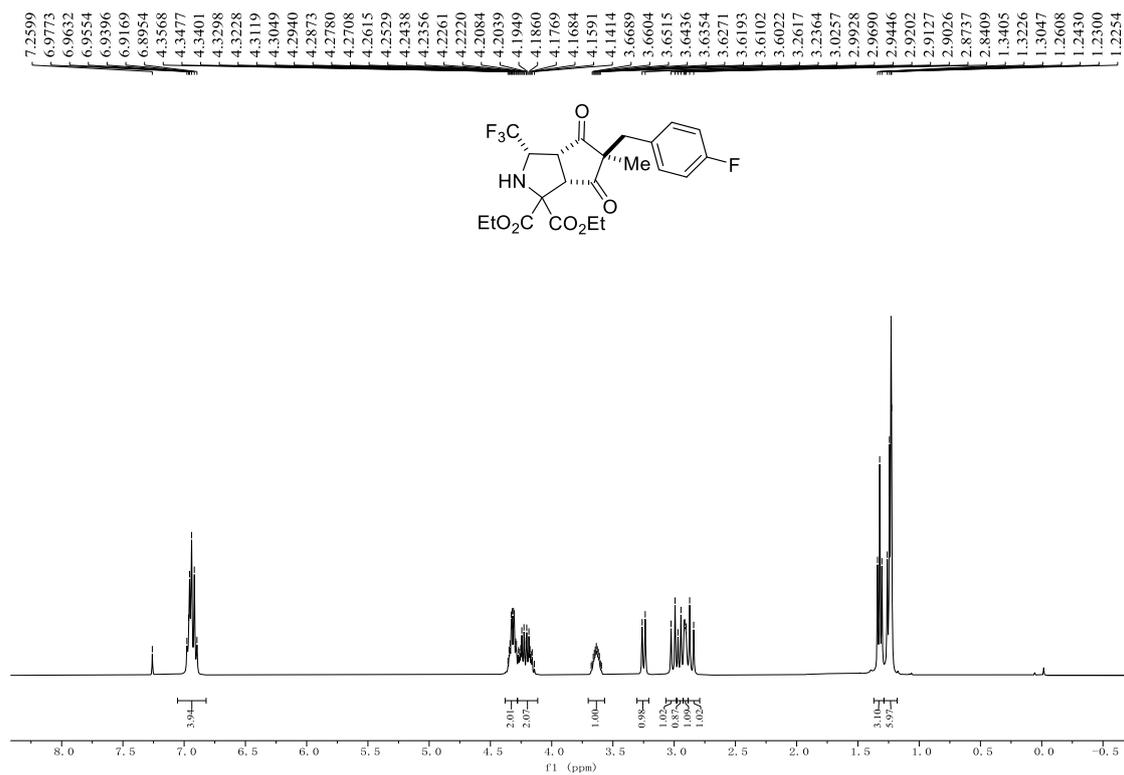
¹H NMR (400 MHz, CDCl₃) of **5d**



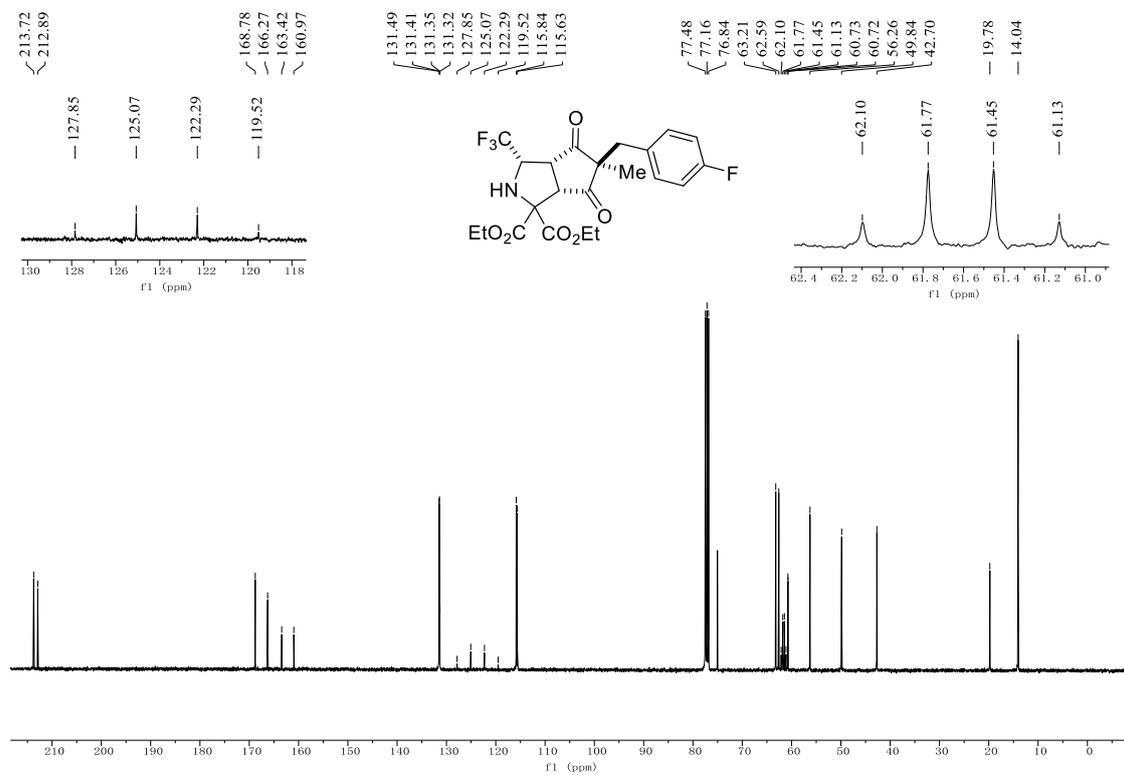
¹³C{¹H} NMR (101 MHz, CDCl₃) of **5d**



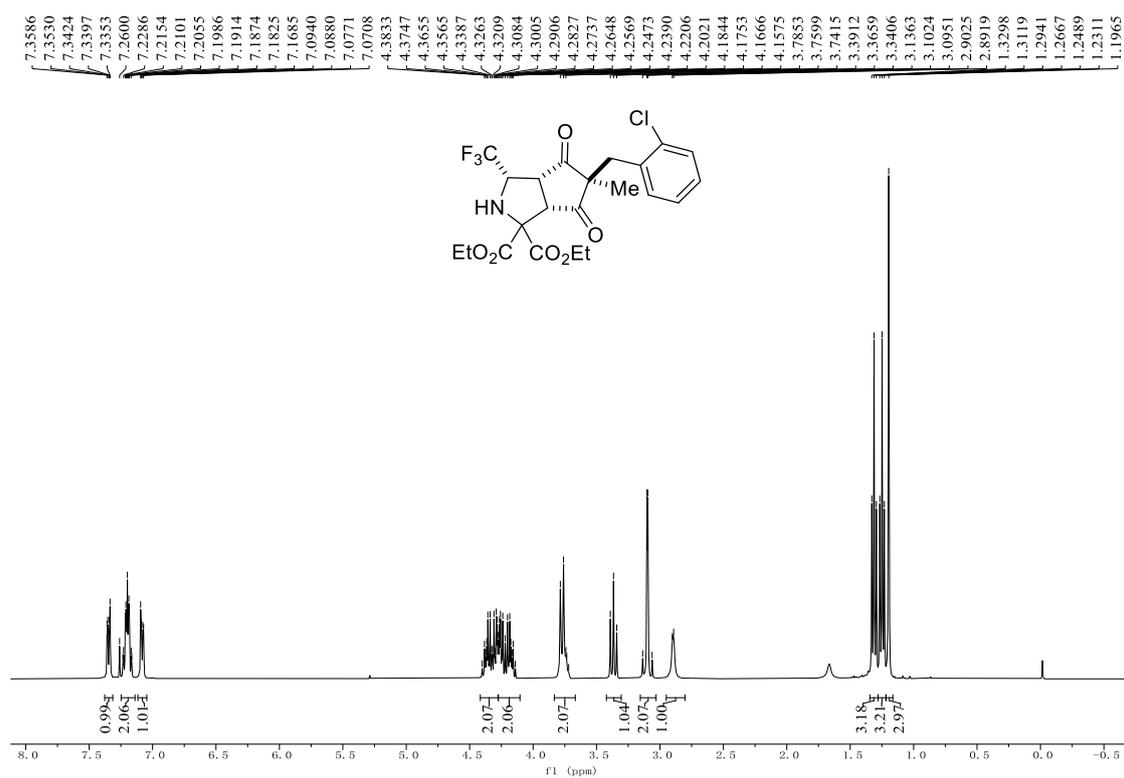
¹H NMR (400 MHz, CDCl₃) of **5e**



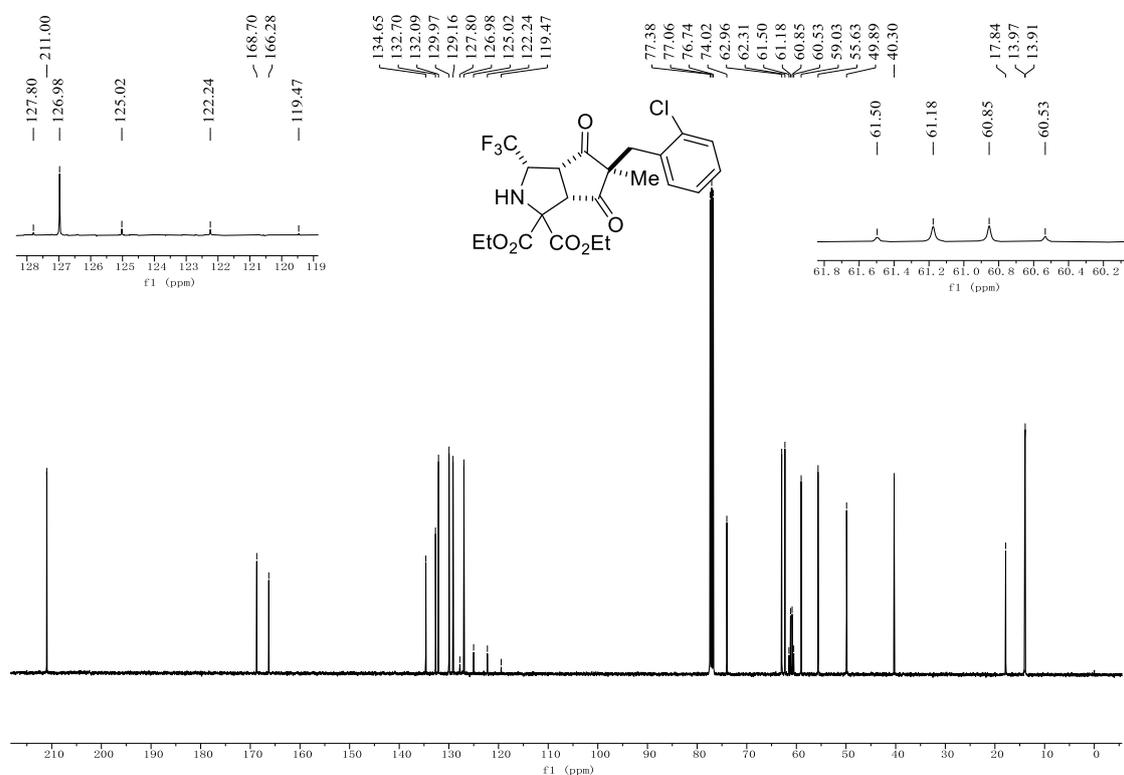
¹³C{¹H} NMR (101 MHz, CDCl₃) of 5e



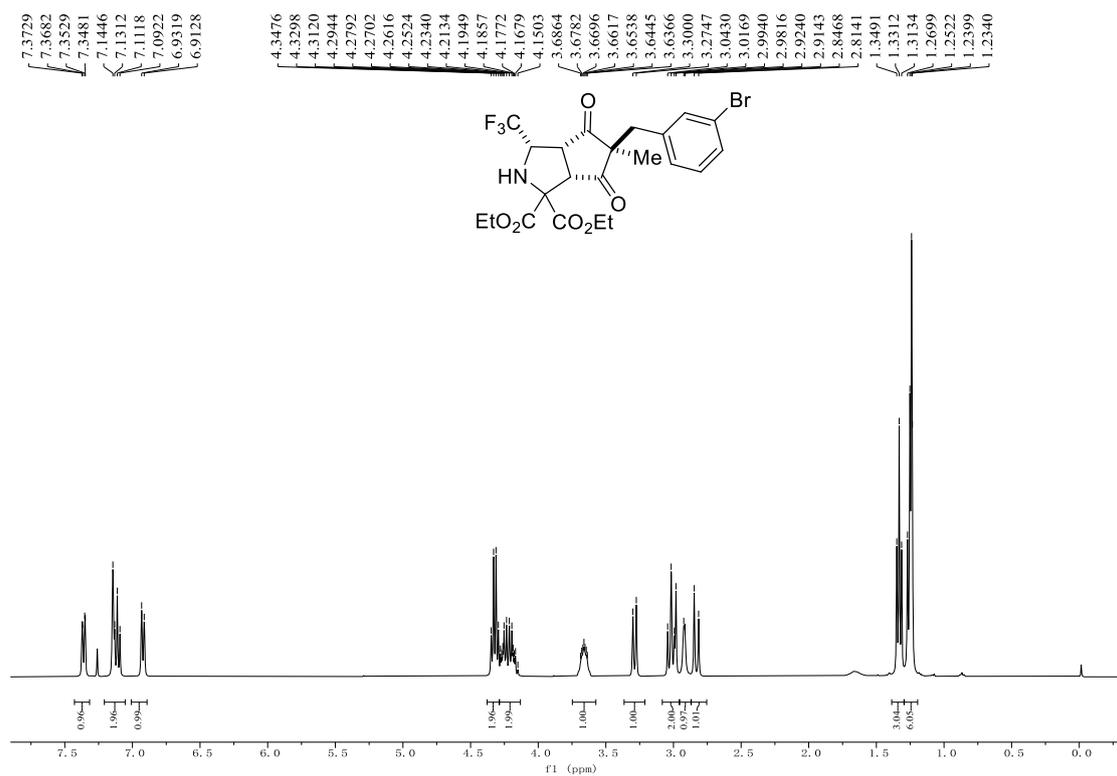
^1H NMR (400 MHz, CDCl_3) of **5f**



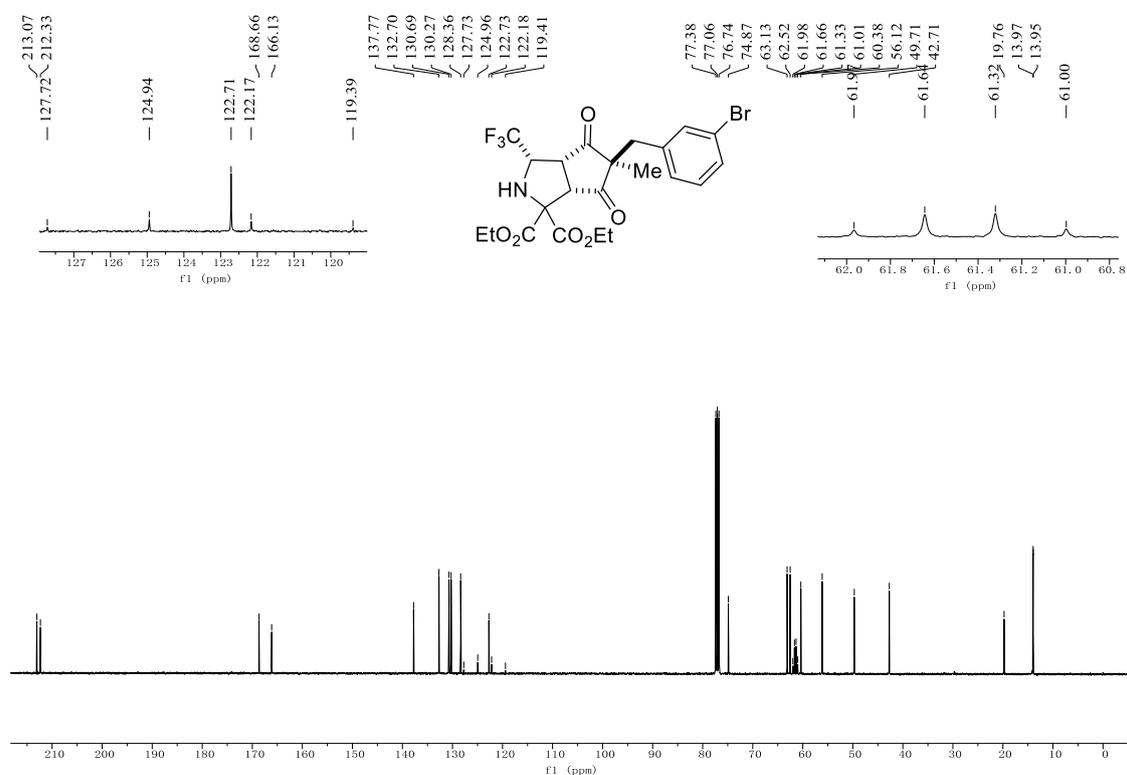
$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of **5f**



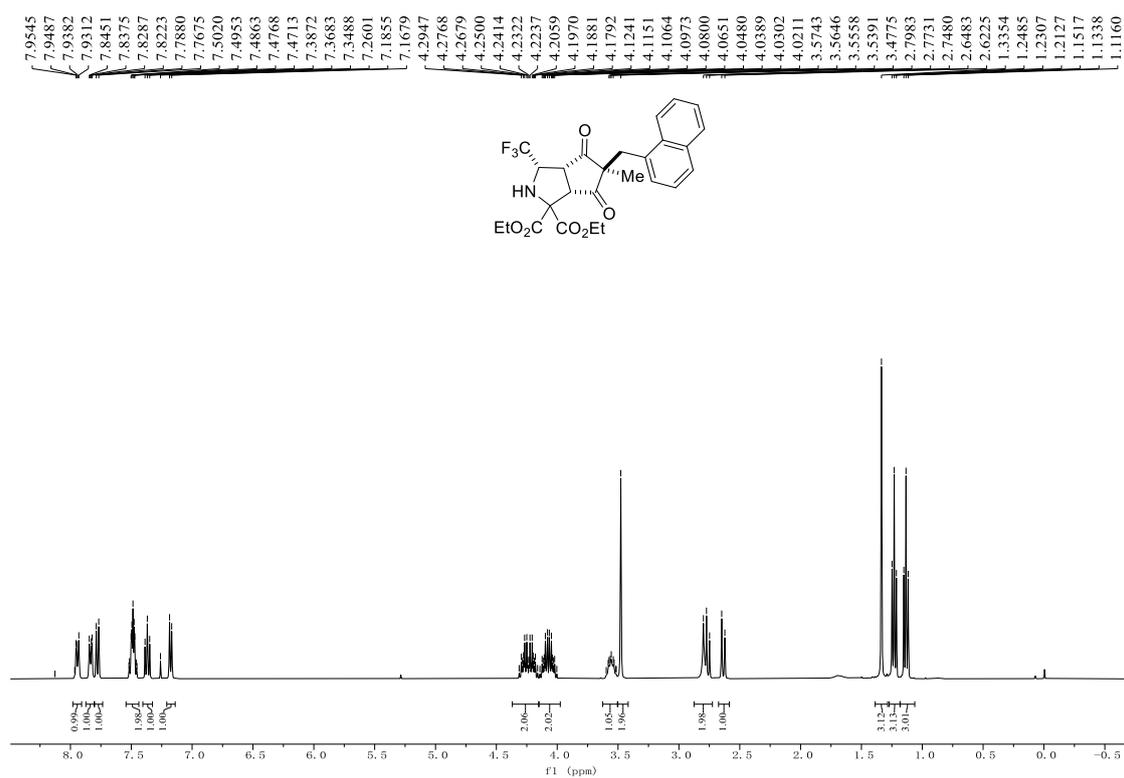
¹H NMR (400 MHz, CDCl₃) of **5g**



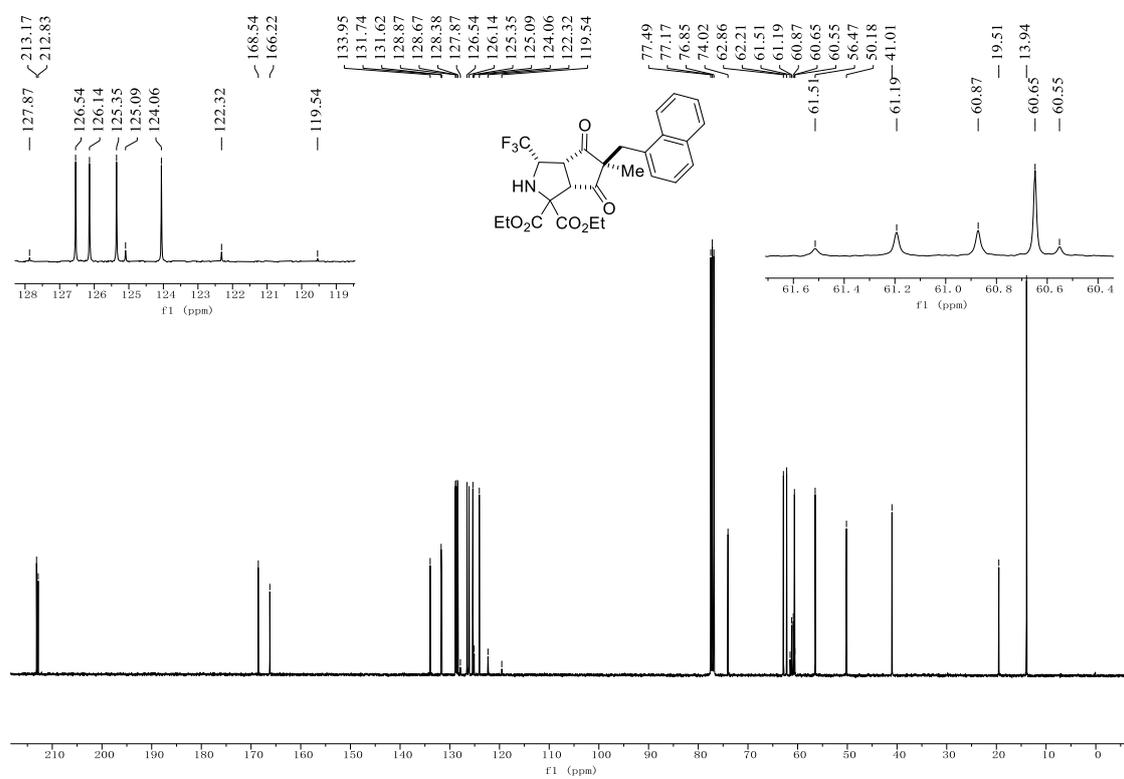
¹³C{¹H} NMR (101 MHz, CDCl₃) of **5g**



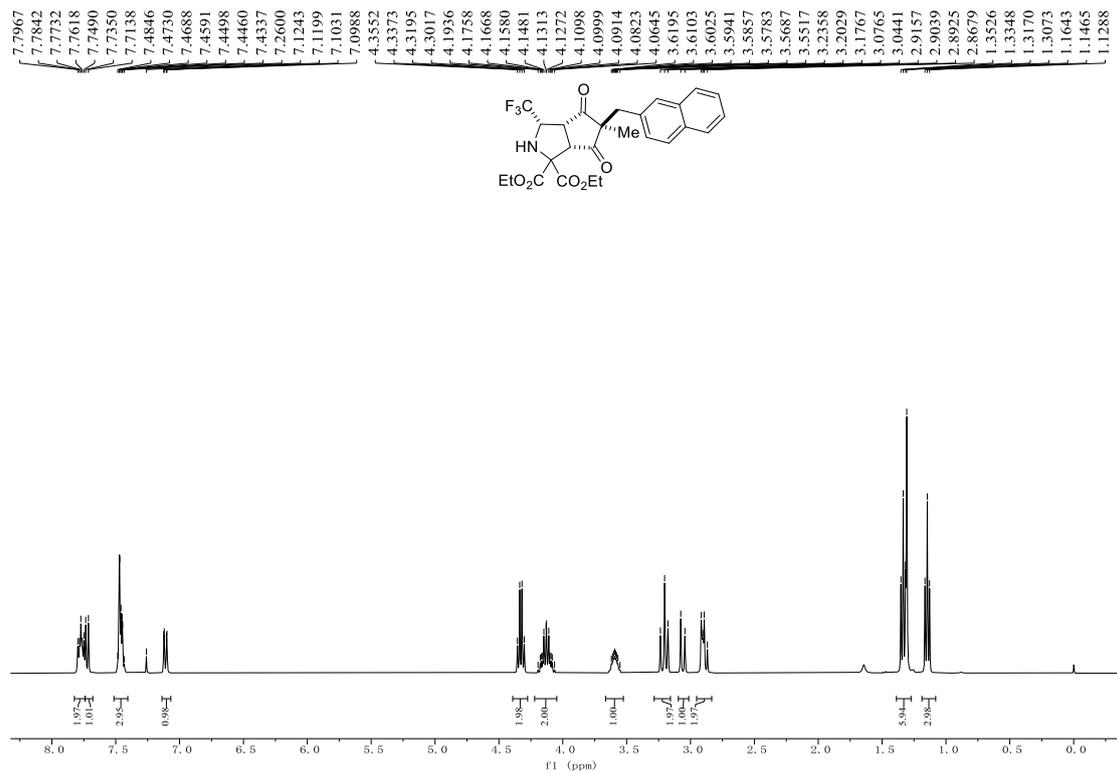
¹H NMR (400 MHz, CDCl₃) of **5h**



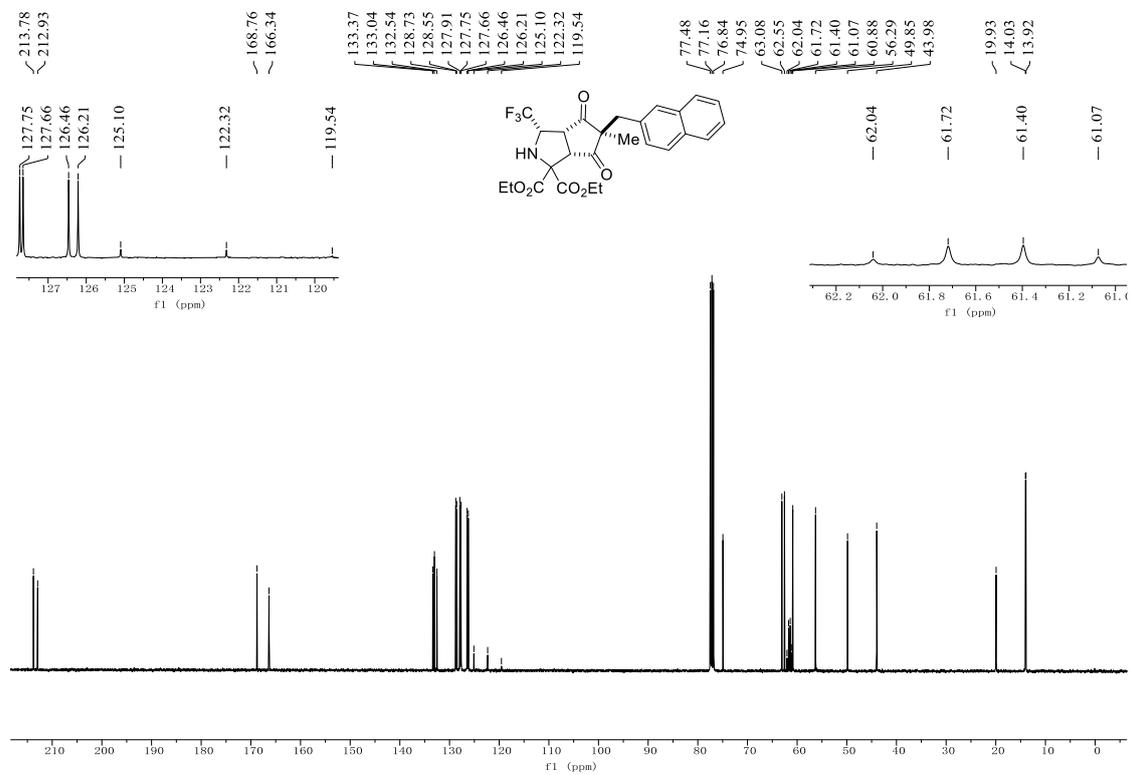
¹³C{¹H} NMR (101 MHz, CDCl₃) of **5h**



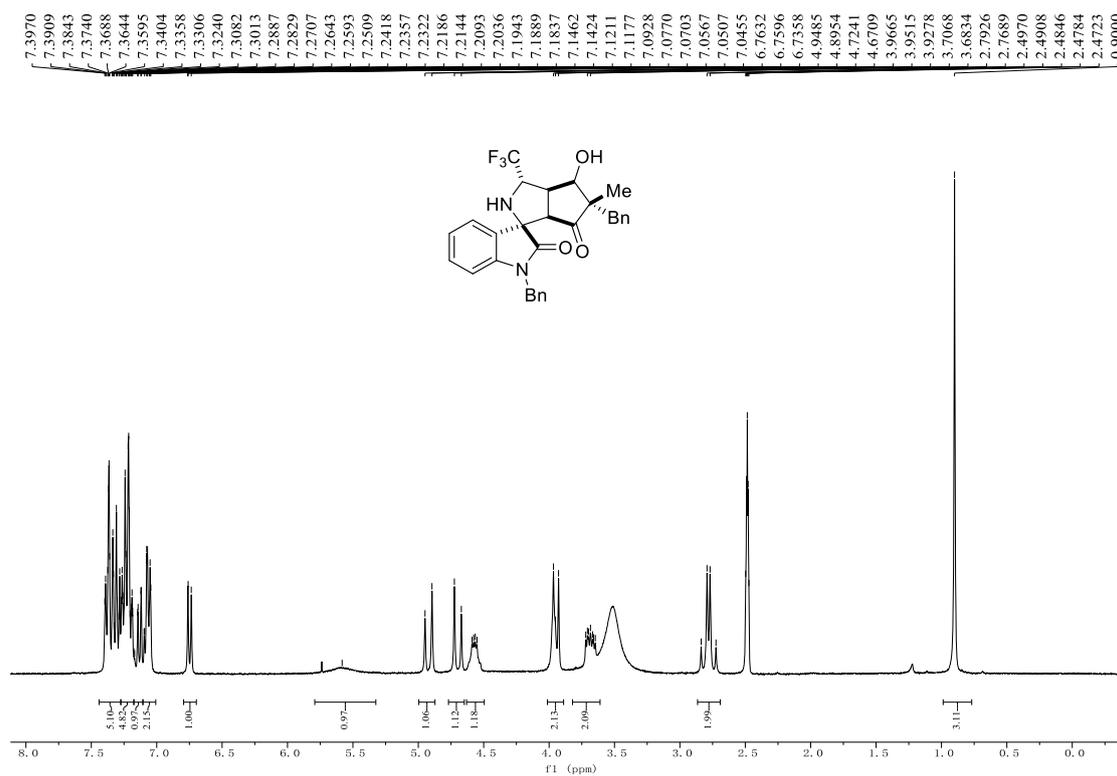
¹H NMR (400 MHz, CDCl₃) of **5i**



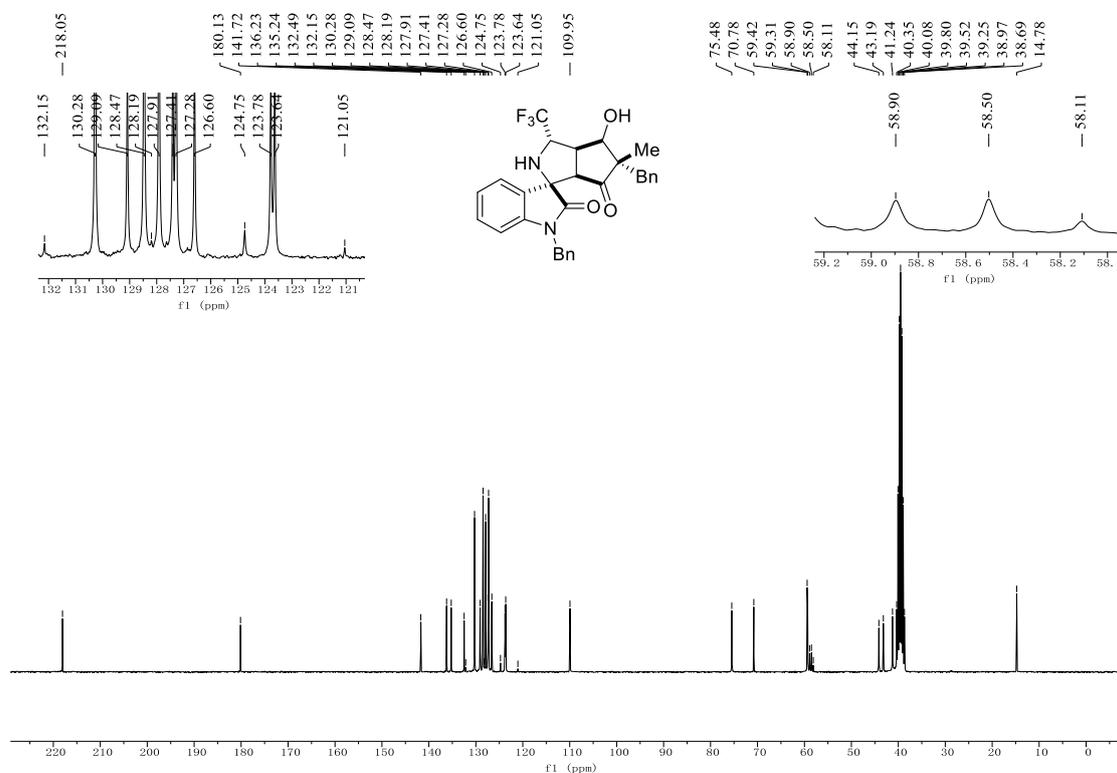
¹³C{¹H} NMR (101 MHz, CDCl₃) of **5i**



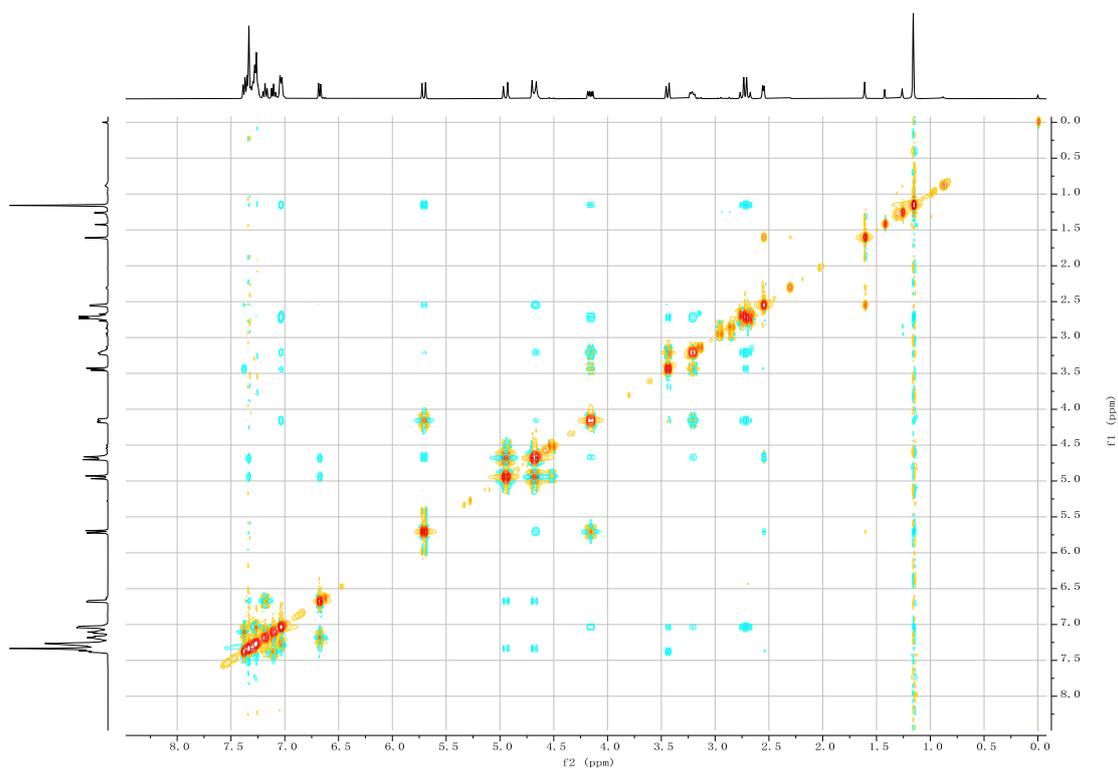
¹H NMR (300 MHz, DMSO-d₆) of 6



¹³C{¹H} NMR (75 MHz, CDCl₃) of 6

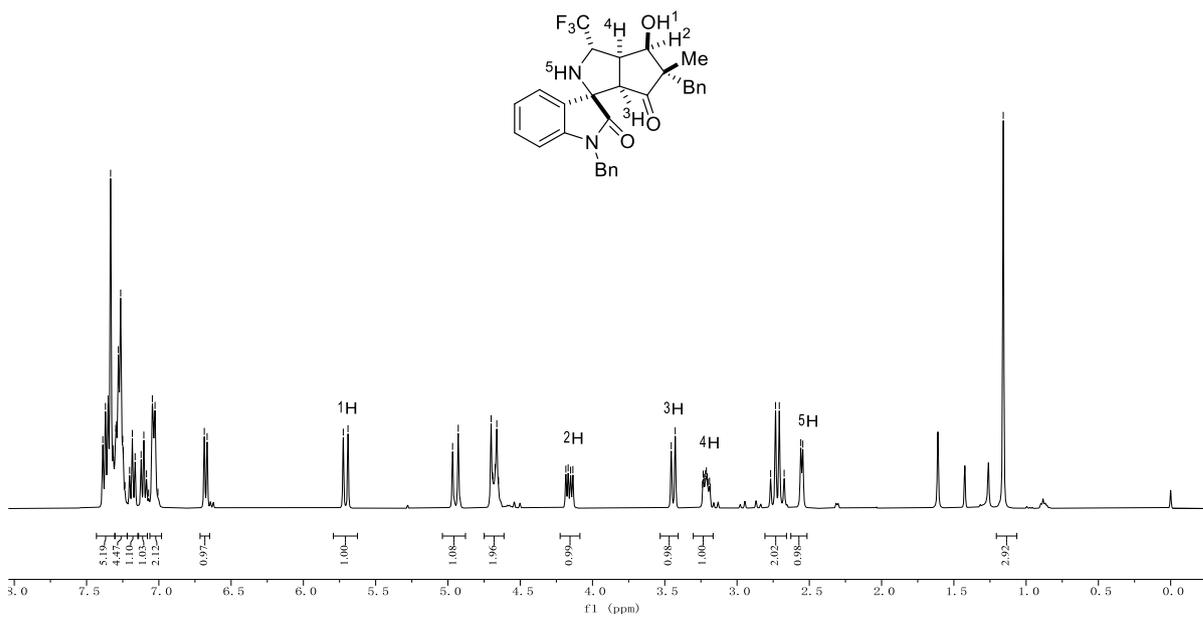


^1H - ^1H COSY spectra for stereochemistry of product **6**

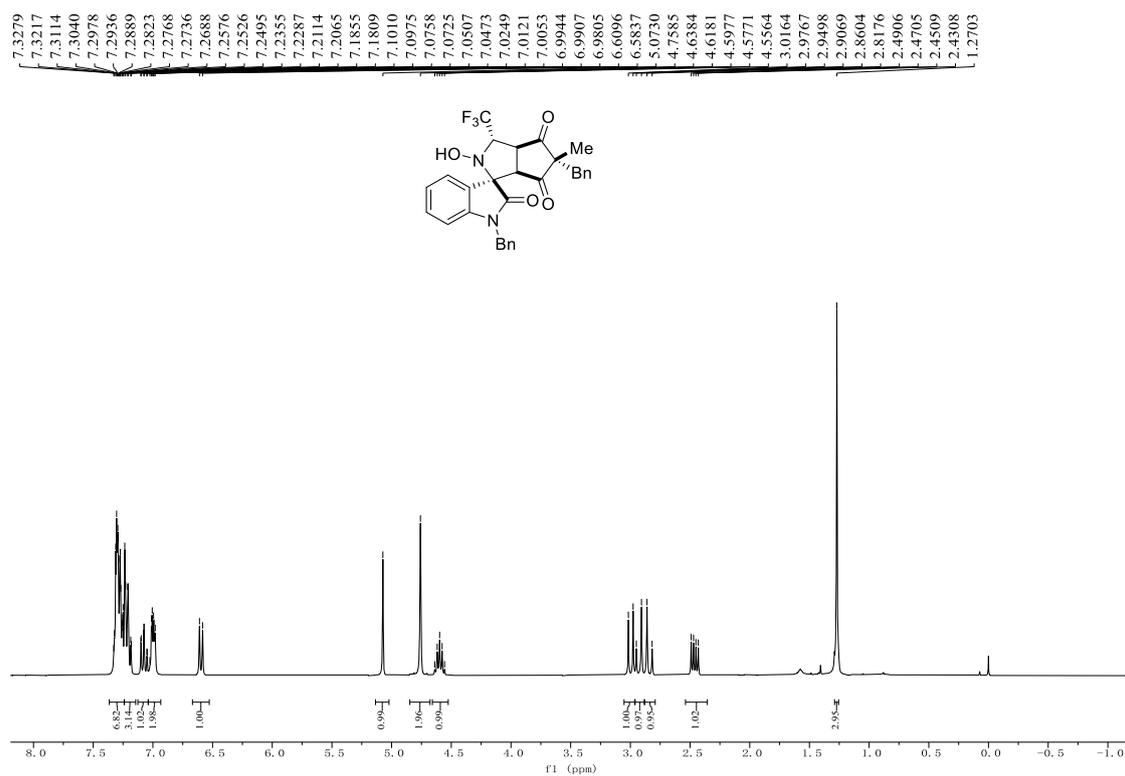


Attribution of hydrogen in compound **6**

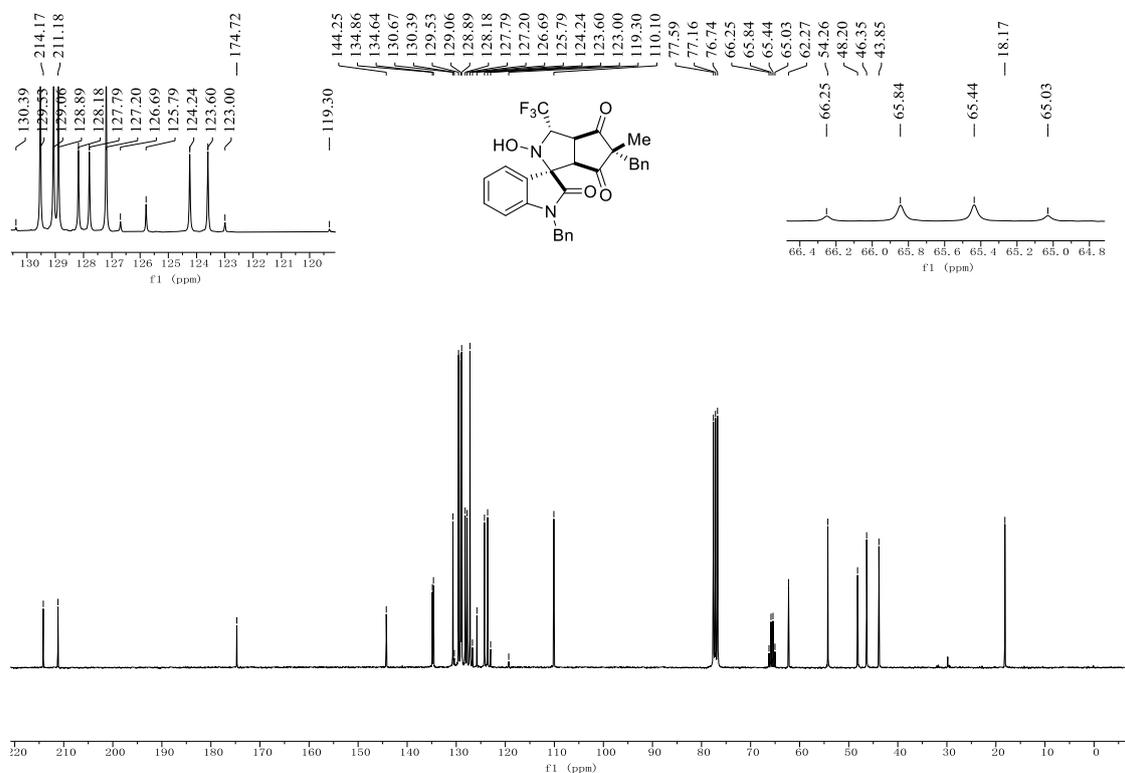
7.39
7.37
7.35
7.33
7.31
7.30
7.29
7.28
7.26
7.25
7.25
7.23
7.20
7.18
7.16
7.12
7.10
7.09
7.07
7.04
7.04
7.03
7.01
7.01
6.69
6.67
5.72
5.69
4.97
4.93
4.70
4.69
4.67
4.66
4.65
4.18
4.17
4.15
4.14
4.14
3.43
3.24
3.23
3.23
3.22
3.21
3.21
3.20
3.19
3.18
2.77
2.73
2.71
2.67
2.56
2.55
1.16



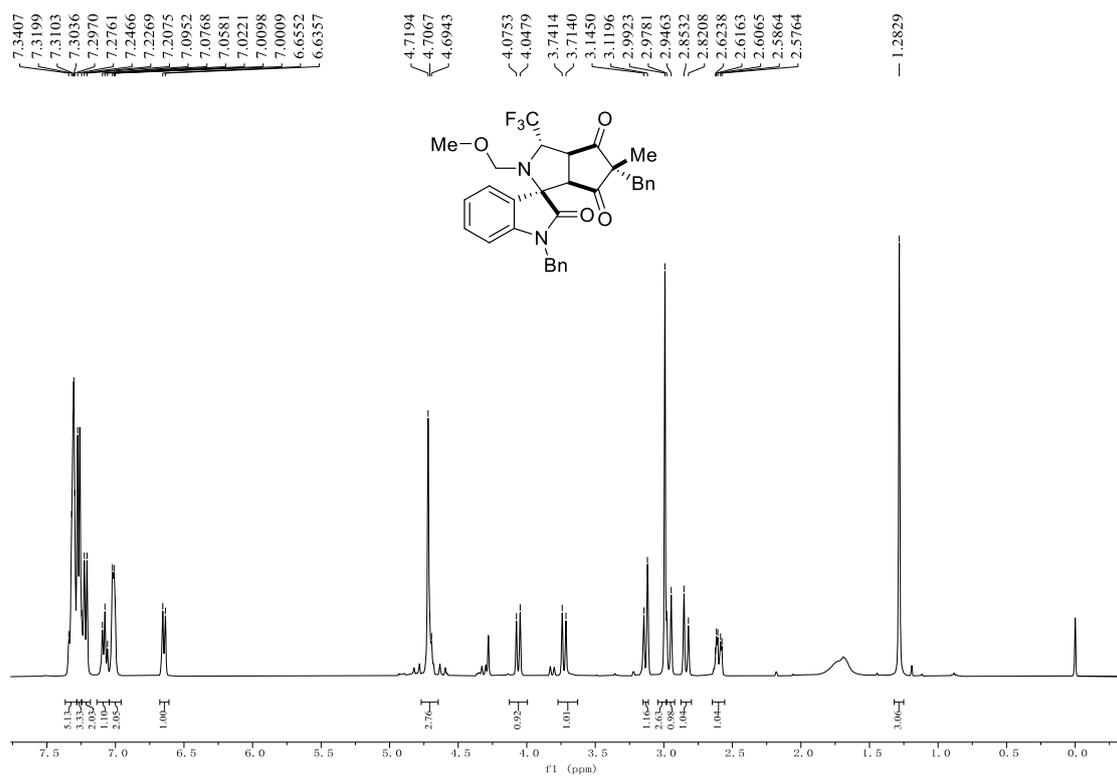
¹H NMR (300 MHz, CDCl₃) of 7



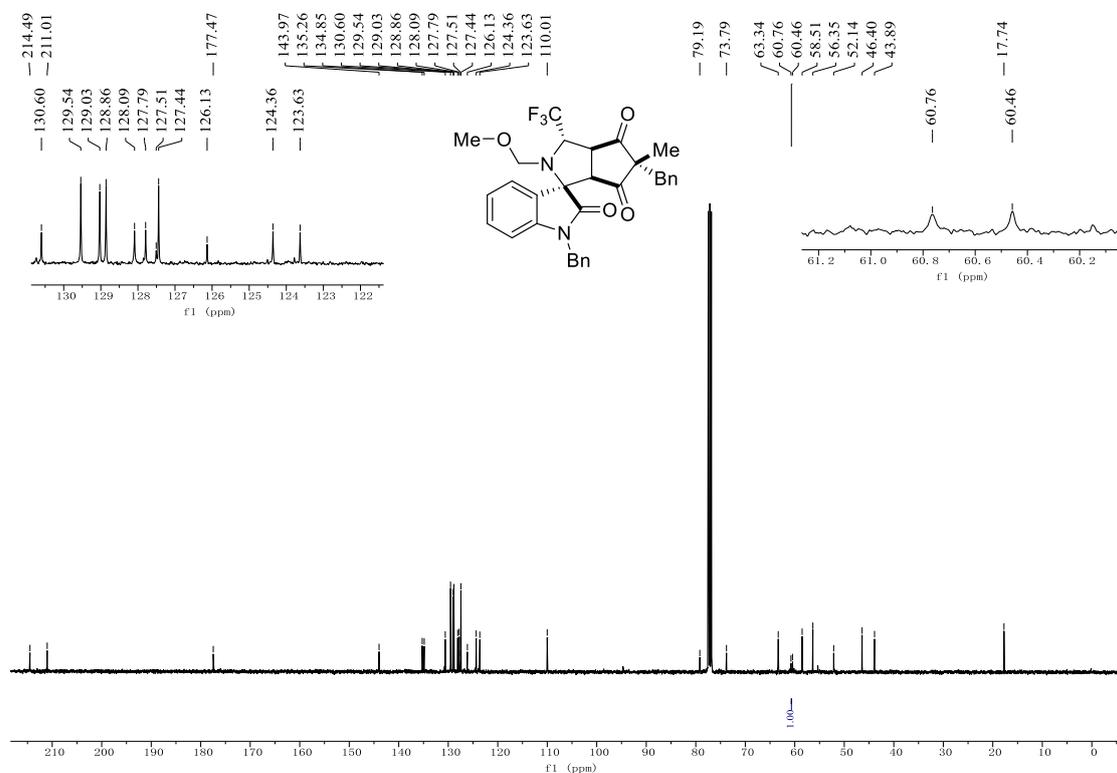
¹³C{¹H} NMR (75 MHz, CDCl₃) of 7



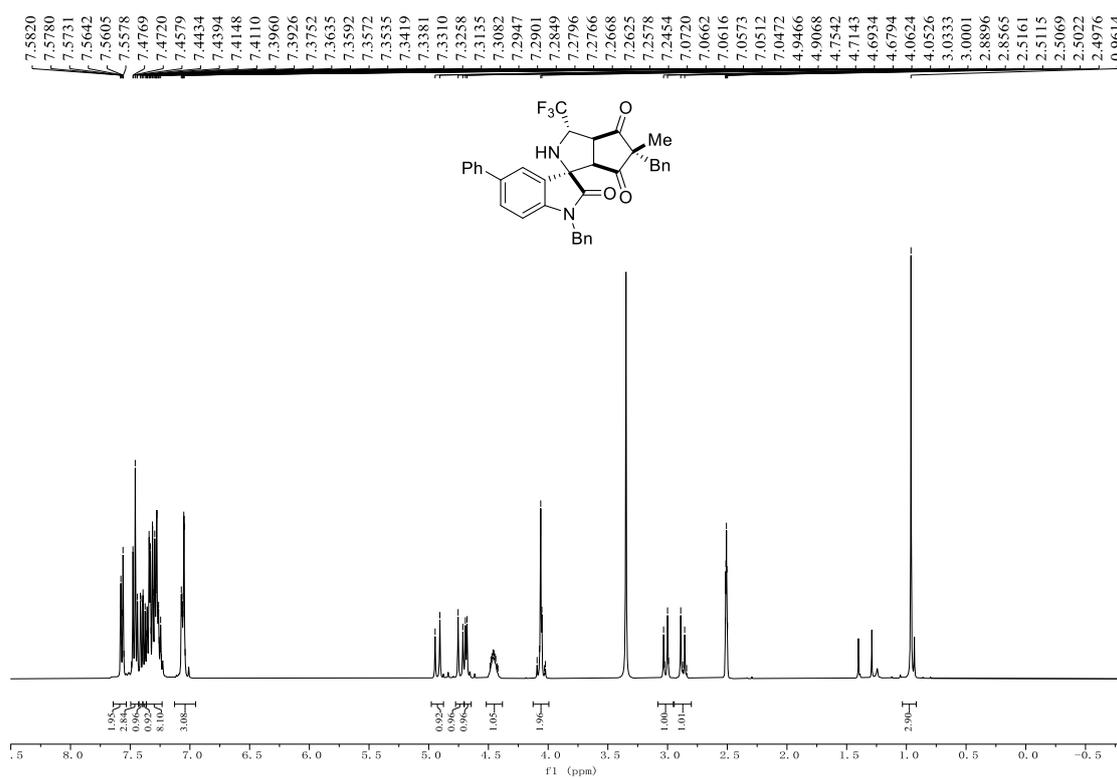
¹H NMR (400 MHz, CDCl₃) of **8**



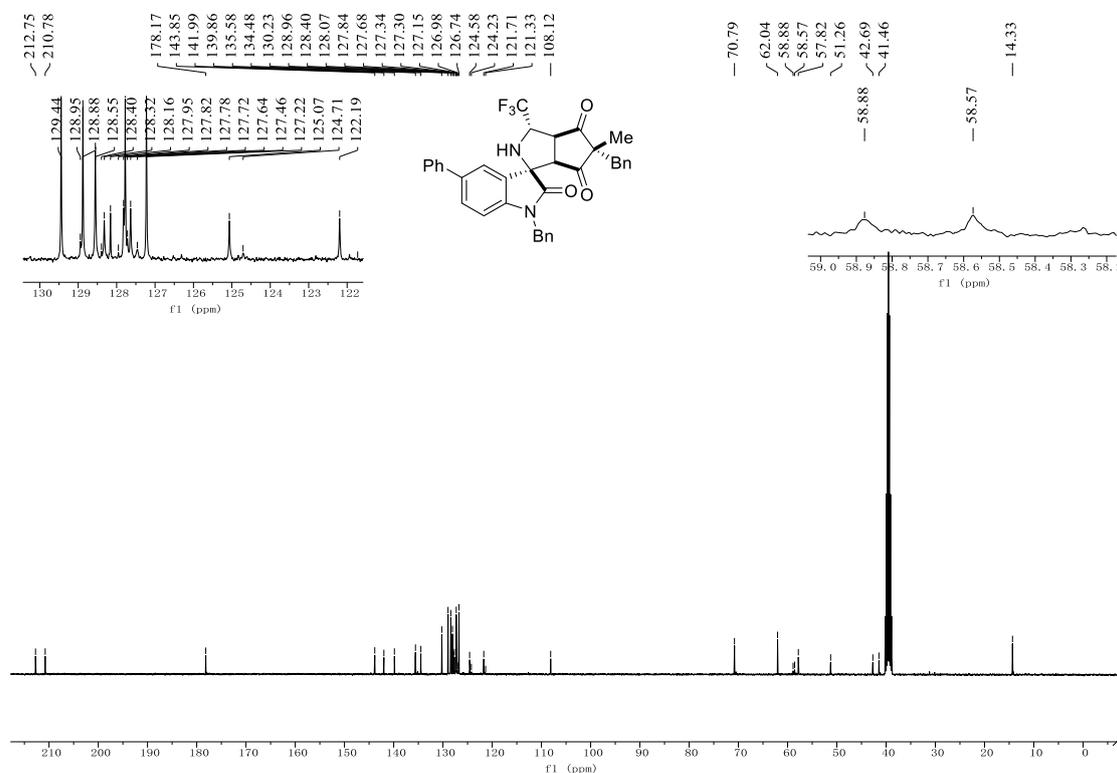
¹³C{¹H} NMR (101 MHz, CDCl₃) of **8**



¹H NMR (400 MHz, DMSO-*d*₆) of **9**



¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) of **9**



11. MS spectra for compounds 3, 5, 6, 7, 8, 9.

MS spectra of 3aa

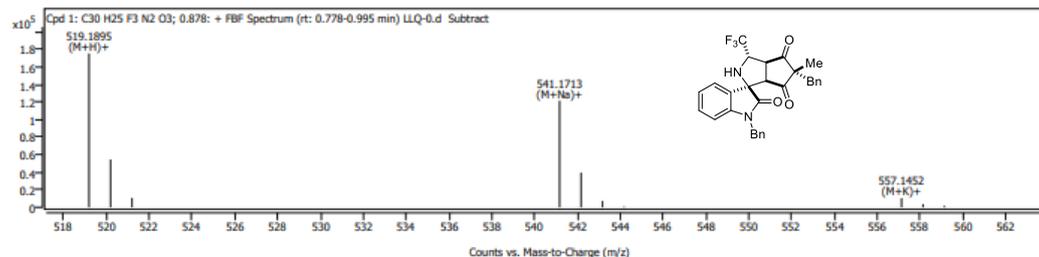
Custom Workflow Report



Compound Details

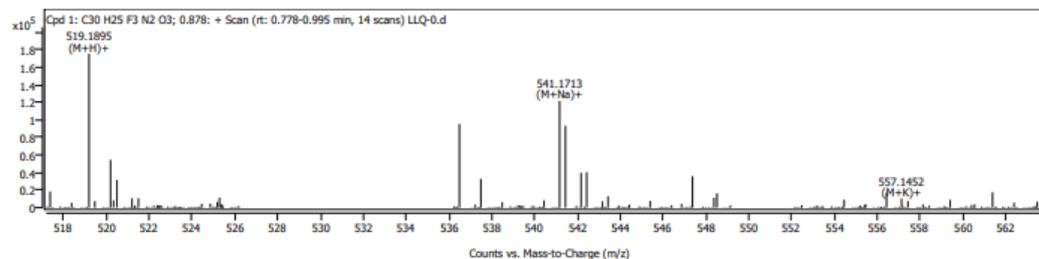
Cpd. 1: C30 H25 F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 519.1895 | 519.1890 | 1.03 | 175394 | 100.00 | 100.00 | (M+H)+ | 1 |
| 520.1925 | 520.1923 | 0.56 | 54535 | 31.09 | 33.59 | (M+H)+ | 1 |
| 521.1969 | 521.1953 | 3.16 | 10699 | 6.10 | 6.08 | (M+H)+ | 1 |
| 541.1713 | 541.1709 | 0.63 | 121518 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 542.1744 | 542.1742 | 0.38 | 39595 | 32.58 | 33.58 | (M+Na)+ | 1 |
| 543.1776 | 543.1772 | 0.66 | 7280 | 5.99 | 6.08 | (M+Na)+ | 1 |
| 544.1809 | 544.1801 | 1.51 | 933 | 0.77 | 0.78 | (M+Na)+ | 1 |
| 557.1452 | 557.1449 | 0.49 | 10442 | 100.00 | 100.00 | (M+K)+ | 1 |
| 558.1490 | 558.1481 | 1.56 | 3617 | 34.64 | 33.59 | (M+K)+ | 1 |
| 559.1466 | 559.1467 | -0.17 | 1795 | 17.19 | 13.30 | (M+K)+ | 1 |



Spectrum Peaks

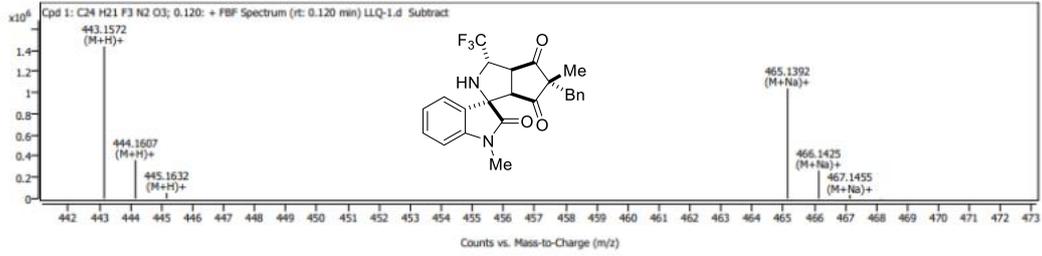
| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 519.1895 | 519.1890 | 1.03 | 175394 | 100.00 | 100.00 | (M+H)+ | 1 |
| 520.1925 | 520.1923 | 0.56 | 54535 | 31.09 | 33.59 | (M+H)+ | 1 |
| 521.1969 | 521.1953 | 3.16 | 10699 | 6.10 | 6.08 | (M+H)+ | 1 |
| 541.1713 | 541.1709 | 0.63 | 121518 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 542.1744 | 542.1742 | 0.38 | 39595 | 32.58 | 33.58 | (M+Na)+ | 1 |
| 543.1776 | 543.1772 | 0.66 | 7280 | 5.99 | 6.08 | (M+Na)+ | 1 |
| 544.1809 | 544.1801 | 1.51 | 933 | 0.77 | 0.78 | (M+Na)+ | 1 |
| 557.1452 | 557.1449 | 0.49 | 10442 | 100.00 | 100.00 | (M+K)+ | 1 |
| 558.1490 | 558.1481 | 1.56 | 3617 | 34.64 | 33.59 | (M+K)+ | 1 |
| 559.1466 | 559.1467 | -0.17 | 1795 | 17.19 | 13.30 | (M+K)+ | 1 |

MS spectra of **3ba**

Custom Workflow Report

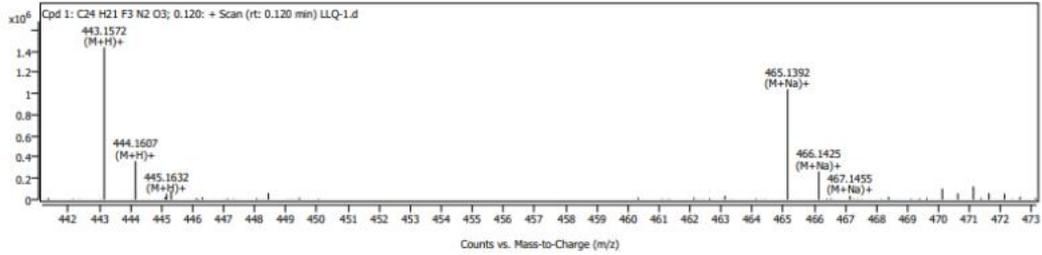


Compound Details
Cpd. 1: C24 H21 F3 N2 O3
 Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|---------|----------|-----------------|-------------|---|
| 443.1572 | 443.1577 | -1.12 | 1437005 | 100.00 | 100.00 | (M+H)+ | 1 |
| 444.1607 | 444.1609 | -0.53 | 364258 | 25.35 | 27.06 | (M+H)+ | 1 |
| 445.1632 | 445.1638 | -1.33 | 54690 | 3.81 | 4.13 | (M+H)+ | 1 |
| 465.1392 | 465.1396 | -0.87 | 1042003 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 466.1425 | 466.1429 | -0.77 | 266375 | 25.56 | 27.04 | (M+Na)+ | 1 |
| 467.1455 | 467.1457 | -0.46 | 35954 | 3.45 | 4.13 | (M+Na)+ | 1 |
| 468.1471 | 468.1485 | -3.06 | 4482 | 0.43 | 0.46 | (M+Na)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|---------|----------|-----------------|-------------|---|
| 443.1572 | 443.1577 | -1.12 | 1437005 | 100.00 | 100.00 | (M+H)+ | 1 |
| 444.1607 | 444.1609 | -0.53 | 364258 | 25.35 | 27.06 | (M+H)+ | 1 |
| 445.1632 | 445.1638 | -1.33 | 54690 | 3.81 | 4.13 | (M+H)+ | 1 |
| 465.1392 | 465.1396 | -0.87 | 1042003 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 466.1425 | 466.1429 | -0.77 | 266375 | 25.56 | 27.04 | (M+Na)+ | 1 |
| 467.1455 | 467.1457 | -0.46 | 35954 | 3.45 | 4.13 | (M+Na)+ | 1 |
| 468.1471 | 468.1485 | -3.06 | 4482 | 0.43 | 0.46 | (M+Na)+ | 1 |

MS spectra of 3ca

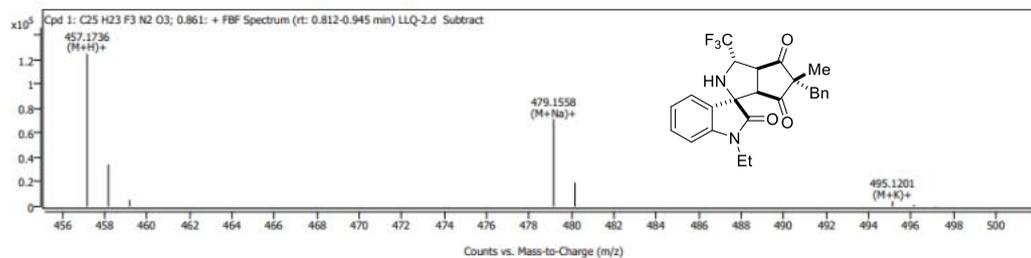
Custom Workflow Report



Compound Details

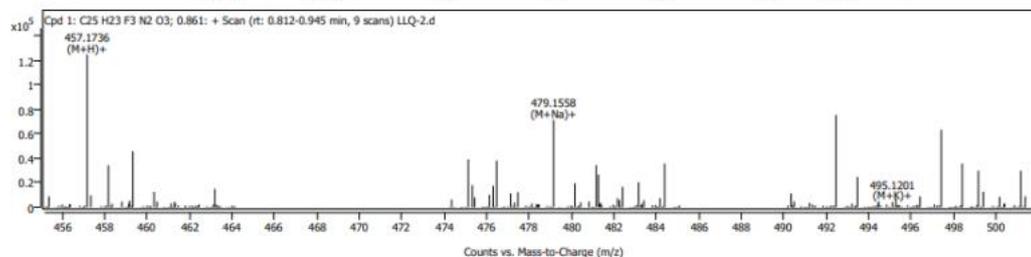
Cpd. 1: C₂₅H₂₃F₃N₂O₃

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 457.1736 | 457.1734 | 0.61 | 125137 | 100.00 | 100.00 | (M+H)+ | 1 |
| 458.1768 | 458.1766 | 0.44 | 34441 | 27.52 | 28.16 | (M+H)+ | 1 |
| 459.1791 | 459.1795 | -0.75 | 5439 | 4.35 | 4.43 | (M+H)+ | 1 |
| 479.1558 | 479.1553 | 0.99 | 71603 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 480.1593 | 480.1585 | 1.56 | 19577 | 27.34 | 28.15 | (M+Na)+ | 1 |
| 495.1201 | 495.1292 | -18.36 | 4328 | 100.00 | 100.00 | (M+K)+ | 1 |
| 496.1332 | 496.1325 | 1.47 | 1424 | 32.90 | 28.16 | (M+K)+ | 1 |
| 497.1351 | 497.1304 | 9.40 | 314 | 7.26 | 11.65 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 457.1736 | 457.1734 | 0.61 | 125137 | 100.00 | 100.00 | (M+H)+ | 1 |
| 458.1768 | 458.1766 | 0.44 | 34441 | 27.52 | 28.16 | (M+H)+ | 1 |
| 459.1791 | 459.1795 | -0.75 | 5439 | 4.35 | 4.43 | (M+H)+ | 1 |
| 479.1558 | 479.1553 | 0.99 | 71603 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 480.1593 | 480.1585 | 1.56 | 19577 | 27.34 | 28.15 | (M+Na)+ | 1 |
| 495.1201 | 495.1292 | -18.36 | 4328 | 100.00 | 100.00 | (M+K)+ | 1 |
| 496.1332 | 496.1325 | 1.47 | 1424 | 32.90 | 28.16 | (M+K)+ | 1 |
| 497.1351 | 497.1304 | 9.40 | 314 | 7.26 | 11.65 | (M+K)+ | 1 |

MS spectra of 3da

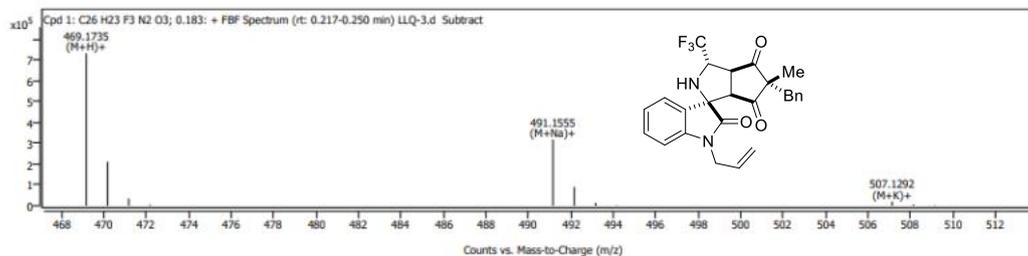
Custom Workflow Report



Compound Details

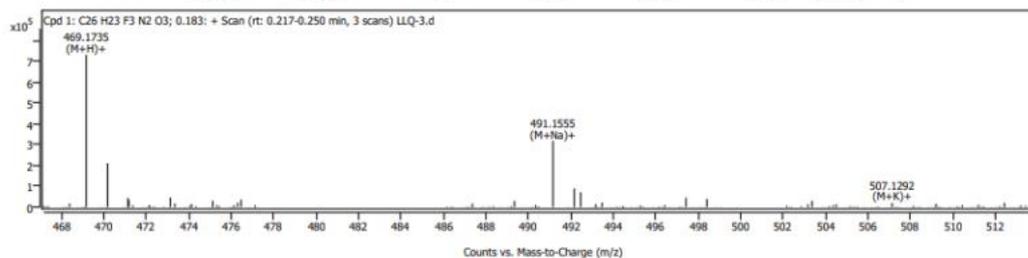
Cpd. 1: C26 H23 F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 469.1735 | 469.1734 | 0.36 | 734519 | 100.00 | 100.00 | (M+H)+ | 1 |
| 470.1767 | 470.1766 | 0.16 | 212012 | 28.86 | 29.24 | (M+H)+ | 1 |
| 471.1788 | 471.1795 | -1.56 | 34966 | 4.76 | 4.74 | (M+H)+ | 1 |
| 472.1811 | 472.1823 | -2.58 | 4588 | 0.62 | 0.55 | (M+H)+ | 1 |
| 491.1555 | 491.1553 | 0.34 | 319411 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 492.1584 | 492.1585 | -0.19 | 90504 | 28.33 | 29.23 | (M+Na)+ | 1 |
| 493.1615 | 493.1615 | 0.00 | 14136 | 4.43 | 4.74 | (M+Na)+ | 1 |
| 494.1635 | 494.1642 | -1.44 | 2121 | 0.66 | 0.55 | (M+Na)+ | 1 |
| 507.1292 | 507.1292 | -0.07 | 20384 | 100.00 | 100.00 | (M+K)+ | 1 |
| 508.1323 | 508.1325 | -0.40 | 6441 | 31.60 | 29.24 | (M+K)+ | 1 |
| 509.1310 | 509.1305 | 0.86 | 2394 | 11.74 | 11.96 | (M+K)+ | 1 |



Spectrum Peaks

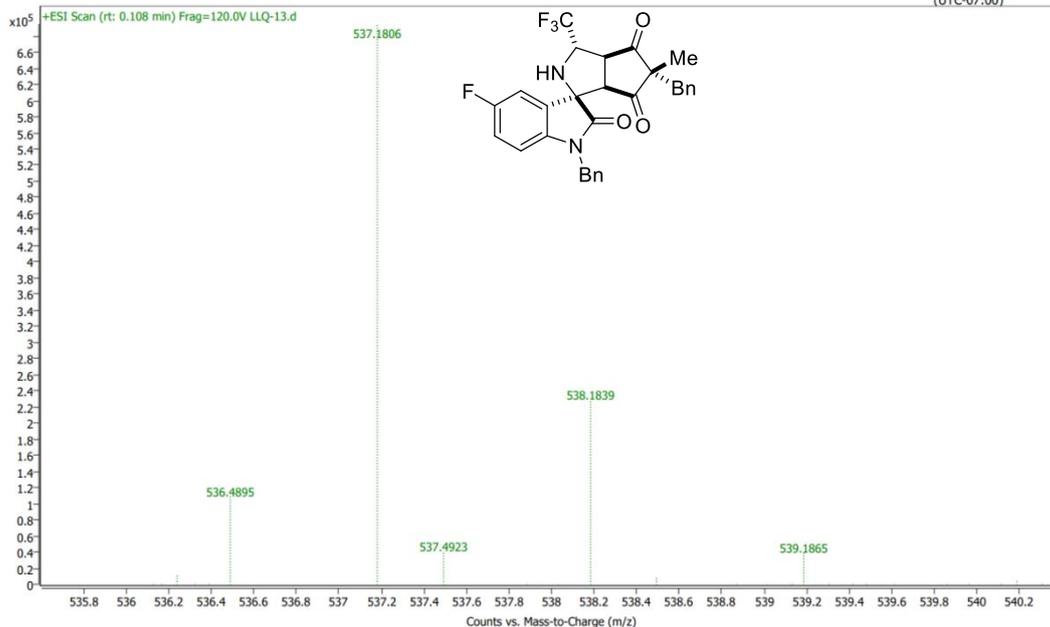
| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 469.1735 | 469.1734 | 0.36 | 734519 | 100.00 | 100.00 | (M+H)+ | 1 |
| 470.1767 | 470.1766 | 0.16 | 212012 | 28.86 | 29.24 | (M+H)+ | 1 |
| 471.1788 | 471.1795 | -1.56 | 34966 | 4.76 | 4.74 | (M+H)+ | 1 |
| 472.1811 | 472.1823 | -2.58 | 4588 | 0.62 | 0.55 | (M+H)+ | 1 |
| 491.1555 | 491.1553 | 0.34 | 319411 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 492.1584 | 492.1585 | -0.19 | 90504 | 28.33 | 29.23 | (M+Na)+ | 1 |
| 493.1615 | 493.1615 | 0.00 | 14136 | 4.43 | 4.74 | (M+Na)+ | 1 |
| 494.1635 | 494.1642 | -1.44 | 2121 | 0.66 | 0.55 | (M+Na)+ | 1 |
| 507.1292 | 507.1292 | -0.07 | 20384 | 100.00 | 100.00 | (M+K)+ | 1 |
| 508.1323 | 508.1325 | -0.40 | 6441 | 31.60 | 29.24 | (M+K)+ | 1 |
| 509.1310 | 509.1305 | 0.86 | 2394 | 11.74 | 11.96 | (M+K)+ | 1 |

MS spectra of 3ea

User Spectrum Plot Report



| | | | | | |
|----------------|----------|--------------|------------|------------------|--|
| Name | LLQ-13 | Rack Pos. | Instrument | Instrument 1 | Operator |
| Inj. Vol. (ul) | 10 | Plate Pos. | IRM Status | Some ions missed | |
| Data File | LLQ-13.d | Method (Acq) | 1367.m | Comment | Acq. Time (Local) 4/15/2022 2:01:27 AM (UTC-07:00) |

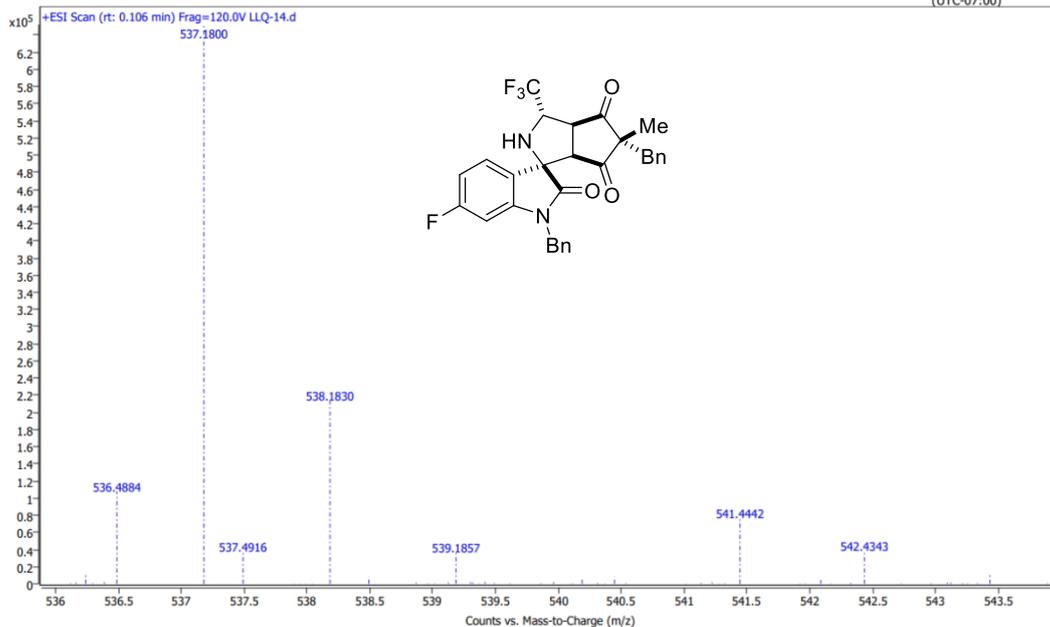


MS spectra of 3fa

User Spectrum Plot Report



| | | | | | |
|----------------|----------|--------------|------------|------------------|--|
| Name | LLQ-14 | Rack Pos. | Instrument | Instrument 1 | Operator |
| Inj. Vol. (ul) | 10 | Plate Pos. | IRM Status | Some ions missed | |
| Data File | LLQ-14.d | Method (Acq) | 1367.m | Comment | Acq. Time (Local) 4/15/2022 2:03:33 AM (UTC-07:00) |



MS spectra of 3ga

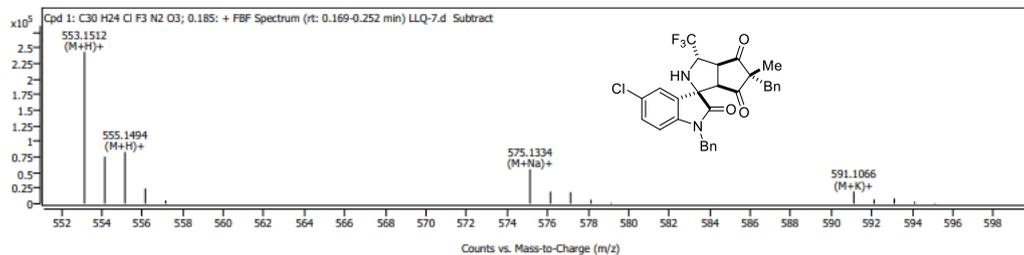
Custom Workflow Report



Compound Details

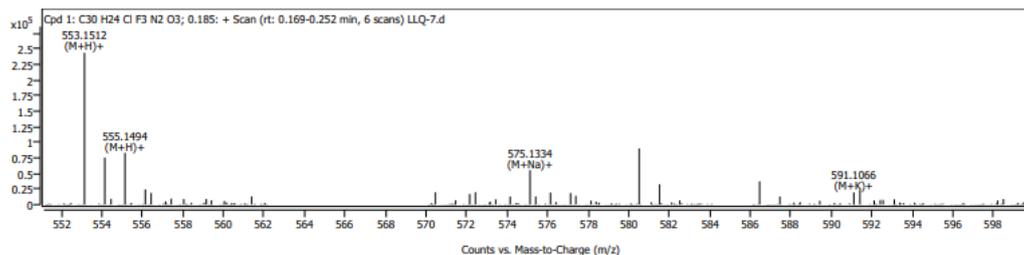
Cpd. 1: C30 H24 Cl F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 553.1512 | 553.1500 | 2.04 | 243609 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1541 | 554.1533 | 1.49 | 75418 | 30.96 | 33.58 | (M+H)+ | 1 |
| 555.1494 | 555.1486 | 1.49 | 83021 | 34.08 | 38.07 | (M+H)+ | 1 |
| 556.1521 | 556.1509 | 2.04 | 24430 | 10.03 | 11.52 | (M+H)+ | 1 |
| 557.1545 | 557.1537 | 1.50 | 5195 | 2.13 | 2.02 | (M+H)+ | 1 |
| 575.1334 | 575.1320 | 2.47 | 55249 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 576.1414 | 576.1352 | 10.75 | 19313 | 34.96 | 33.57 | (M+Na)+ | 1 |
| 577.1330 | 577.1305 | 4.38 | 18540 | 33.56 | 38.07 | (M+Na)+ | 1 |
| 578.1371 | 578.1329 | 7.30 | 6338 | 11.47 | 11.52 | (M+Na)+ | 1 |
| 579.1373 | 579.1356 | 2.94 | 1482 | 2.68 | 2.02 | (M+Na)+ | 1 |
| 591.1066 | 591.1059 | 1.09 | 19544 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1097 | 592.1092 | 0.89 | 6651 | 34.03 | 33.58 | (M+K)+ | 1 |
| 593.1050 | 593.1044 | 1.05 | 8365 | 42.80 | 45.29 | (M+K)+ | 1 |
| 594.1074 | 594.1069 | 0.90 | 3015 | 15.43 | 13.95 | (M+K)+ | 1 |
| 595.1078 | 595.1055 | 3.88 | 1057 | 5.41 | 4.77 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 553.1512 | 553.1500 | 2.04 | 243609 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1541 | 554.1533 | 1.49 | 75418 | 30.96 | 33.58 | (M+H)+ | 1 |
| 555.1494 | 555.1486 | 1.49 | 83021 | 34.08 | 38.07 | (M+H)+ | 1 |
| 556.1521 | 556.1509 | 2.04 | 24430 | 10.03 | 11.52 | (M+H)+ | 1 |
| 557.1545 | 557.1537 | 1.50 | 5195 | 2.13 | 2.02 | (M+H)+ | 1 |
| 575.1334 | 575.1320 | 2.47 | 55249 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 576.1414 | 576.1352 | 10.75 | 19313 | 34.96 | 33.57 | (M+Na)+ | 1 |
| 577.1330 | 577.1305 | 4.38 | 18540 | 33.56 | 38.07 | (M+Na)+ | 1 |
| 578.1371 | 578.1329 | 7.30 | 6338 | 11.47 | 11.52 | (M+Na)+ | 1 |
| 579.1373 | 579.1356 | 2.94 | 1482 | 2.68 | 2.02 | (M+Na)+ | 1 |
| 591.1066 | 591.1059 | 1.09 | 19544 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1097 | 592.1092 | 0.89 | 6651 | 34.03 | 33.58 | (M+K)+ | 1 |
| 593.1050 | 593.1044 | 1.05 | 8365 | 42.80 | 45.29 | (M+K)+ | 1 |
| 594.1074 | 594.1069 | 0.90 | 3015 | 15.43 | 13.95 | (M+K)+ | 1 |
| 595.1078 | 595.1055 | 3.88 | 1057 | 5.41 | 4.77 | (M+K)+ | 1 |

MS spectra of 3ha

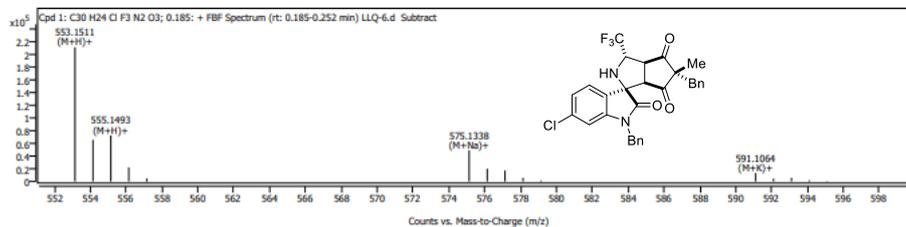
Custom Workflow Report



Compound Details

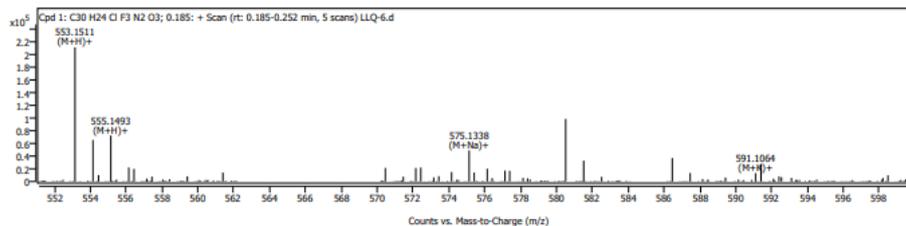
Cpd. 1: C30 H24 Cl F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 553.1511 | 553.1500 | 1.91 | 211201 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1541 | 554.1533 | 1.51 | 65510 | 31.02 | 33.58 | (M+H)+ | 1 |
| 555.1493 | 555.1486 | 1.37 | 72373 | 34.27 | 38.07 | (M+H)+ | 1 |
| 556.1518 | 556.1509 | 1.53 | 22089 | 10.46 | 11.52 | (M+H)+ | 1 |
| 557.1548 | 557.1537 | 1.99 | 4463 | 2.11 | 2.02 | (M+H)+ | 1 |
| 575.1338 | 575.1320 | 3.14 | 48986 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 576.1426 | 576.1352 | 12.82 | 20223 | 41.28 | 33.57 | (M+Na)+ | 1 |
| 577.1326 | 577.1305 | 3.62 | 17236 | 35.18 | 38.07 | (M+Na)+ | 1 |
| 578.1378 | 578.1329 | 8.45 | 5728 | 11.69 | 11.52 | (M+Na)+ | 1 |
| 579.1418 | 579.1356 | 10.76 | 1576 | 3.22 | 2.02 | (M+Na)+ | 1 |
| 591.1064 | 591.1059 | 0.79 | 13277 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1099 | 592.1092 | 1.30 | 4359 | 32.83 | 33.58 | (M+K)+ | 1 |
| 593.1050 | 593.1044 | 1.09 | 5706 | 42.98 | 45.29 | (M+K)+ | 1 |
| 594.1089 | 594.1069 | 3.46 | 1867 | 14.06 | 13.95 | (M+K)+ | 1 |
| 595.1029 | 595.1055 | -4.42 | 891 | 6.71 | 4.77 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 553.1511 | 553.1500 | 1.91 | 211201 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1541 | 554.1533 | 1.51 | 65510 | 31.02 | 33.58 | (M+H)+ | 1 |
| 555.1493 | 555.1486 | 1.37 | 72373 | 34.27 | 38.07 | (M+H)+ | 1 |
| 556.1518 | 556.1509 | 1.53 | 22089 | 10.46 | 11.52 | (M+H)+ | 1 |
| 557.1548 | 557.1537 | 1.99 | 4463 | 2.11 | 2.02 | (M+H)+ | 1 |
| 575.1338 | 575.1320 | 3.14 | 48986 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 576.1426 | 576.1352 | 12.82 | 20223 | 41.28 | 33.57 | (M+Na)+ | 1 |
| 577.1326 | 577.1305 | 3.62 | 17236 | 35.18 | 38.07 | (M+Na)+ | 1 |
| 578.1378 | 578.1329 | 8.45 | 5728 | 11.69 | 11.52 | (M+Na)+ | 1 |
| 579.1418 | 579.1356 | 10.76 | 1576 | 3.22 | 2.02 | (M+Na)+ | 1 |
| 591.1064 | 591.1059 | 0.79 | 13277 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1099 | 592.1092 | 1.30 | 4359 | 32.83 | 33.58 | (M+K)+ | 1 |
| 593.1050 | 593.1044 | 1.09 | 5706 | 42.98 | 45.29 | (M+K)+ | 1 |
| 594.1089 | 594.1069 | 3.46 | 1867 | 14.06 | 13.95 | (M+K)+ | 1 |
| 595.1029 | 595.1055 | -4.42 | 891 | 6.71 | 4.77 | (M+K)+ | 1 |

MS spectra of 3ia

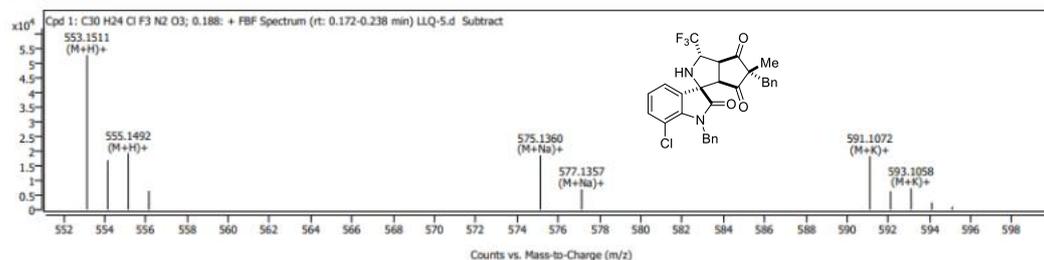
Custom Workflow Report



Compound Details

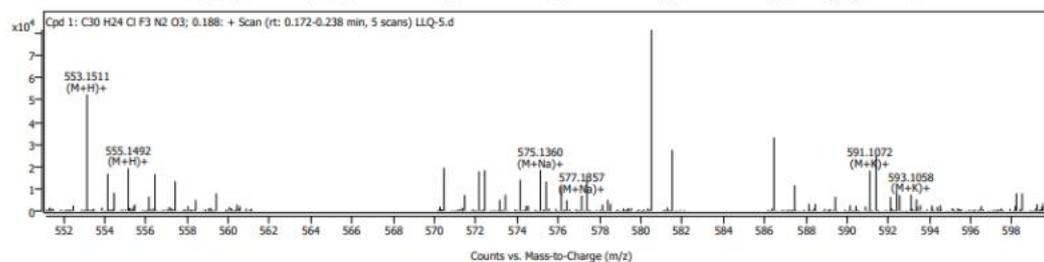
Cpd. 1: C30 H24 Cl F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 553.1511 | 553.1500 | 2.01 | 52565 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1546 | 554.1533 | 2.34 | 16787 | 31.94 | 33.58 | (M+H)+ | 1 |
| 555.1492 | 555.1486 | 1.15 | 19212 | 36.55 | 38.07 | (M+H)+ | 1 |
| 556.1526 | 556.1509 | 2.94 | 6427 | 12.23 | 11.52 | (M+H)+ | 1 |
| 575.1360 | 575.1320 | 6.92 | 18502 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 577.1357 | 577.1305 | 9.07 | 6943 | 37.53 | 38.07 | (M+Na)+ | 1 |
| 591.1072 | 591.1059 | 2.10 | 18238 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1108 | 592.1092 | 2.79 | 6278 | 34.42 | 33.58 | (M+K)+ | 1 |
| 593.1058 | 593.1044 | 2.41 | 7312 | 40.09 | 45.29 | (M+K)+ | 1 |
| 594.1090 | 594.1069 | 3.60 | 2471 | 13.55 | 13.95 | (M+K)+ | 1 |
| 595.1030 | 595.1055 | -4.29 | 1039 | 5.70 | 4.77 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 553.1511 | 553.1500 | 2.01 | 52565 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1546 | 554.1533 | 2.34 | 16787 | 31.94 | 33.58 | (M+H)+ | 1 |
| 555.1492 | 555.1486 | 1.15 | 19212 | 36.55 | 38.07 | (M+H)+ | 1 |
| 556.1526 | 556.1509 | 2.94 | 6427 | 12.23 | 11.52 | (M+H)+ | 1 |
| 575.1360 | 575.1320 | 6.92 | 18502 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 577.1357 | 577.1305 | 9.07 | 6943 | 37.53 | 38.07 | (M+Na)+ | 1 |
| 591.1072 | 591.1059 | 2.10 | 18238 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1108 | 592.1092 | 2.79 | 6278 | 34.42 | 33.58 | (M+K)+ | 1 |
| 593.1058 | 593.1044 | 2.41 | 7312 | 40.09 | 45.29 | (M+K)+ | 1 |
| 594.1090 | 594.1069 | 3.60 | 2471 | 13.55 | 13.95 | (M+K)+ | 1 |
| 595.1030 | 595.1055 | -4.29 | 1039 | 5.70 | 4.77 | (M+K)+ | 1 |

MS spectra of 3ja

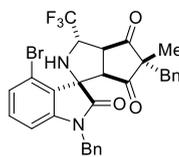
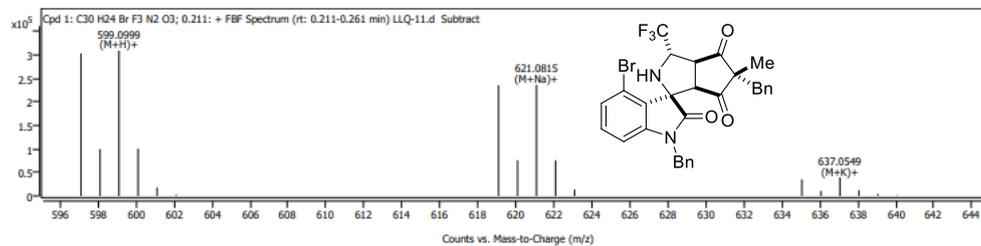
Custom Workflow Report



Compound Details

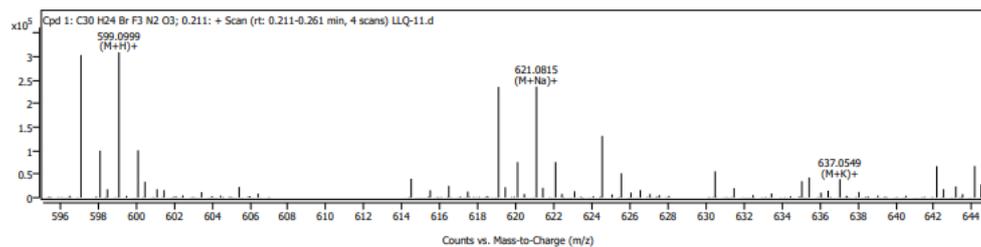
Cpd. 1: C30 H24 Br F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 597.1014 | 597.0995 | 3.18 | 303368 | 98.12 | 96.75 | (M+H)+ | 1 |
| 598.1044 | 598.1028 | 2.72 | 99940 | 32.33 | 32.49 | (M+H)+ | 1 |
| 599.0999 | 599.0980 | 3.18 | 309167 | 100.00 | 100.00 | (M+H)+ | 1 |
| 600.1024 | 600.1009 | 2.58 | 100665 | 32.56 | 32.36 | (M+H)+ | 1 |
| 601.1055 | 601.1038 | 2.77 | 18138 | 5.87 | 5.80 | (M+H)+ | 1 |
| 602.1082 | 602.1067 | 2.57 | 2120 | 0.69 | 0.74 | (M+H)+ | 1 |
| 619.0831 | 619.0815 | 2.61 | 235798 | 99.80 | 96.76 | (M+Na)+ | 1 |
| 620.0862 | 620.0847 | 2.35 | 75780 | 32.07 | 32.48 | (M+Na)+ | 1 |
| 621.0815 | 621.0799 | 2.63 | 236277 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 622.0841 | 622.0828 | 2.03 | 75675 | 32.03 | 32.35 | (M+Na)+ | 1 |
| 623.0868 | 623.0858 | 1.63 | 13552 | 5.74 | 5.79 | (M+Na)+ | 1 |
| 635.0566 | 635.0554 | 1.86 | 35115 | 89.59 | 90.44 | (M+K)+ | 1 |
| 636.0599 | 636.0586 | 1.94 | 10573 | 26.98 | 30.37 | (M+K)+ | 1 |
| 637.0549 | 637.0538 | 1.67 | 39194 | 100.00 | 100.00 | (M+K)+ | 1 |
| 638.0577 | 638.0568 | 1.37 | 12190 | 31.10 | 32.44 | (M+K)+ | 1 |
| 639.0574 | 639.0554 | 3.14 | 4295 | 10.96 | 12.15 | (M+K)+ | 1 |
| 640.0591 | 640.0567 | 3.72 | 1102 | 2.81 | 2.87 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 597.1014 | 597.0995 | 3.18 | 303368 | 98.12 | 96.75 | (M+H)+ | 1 |
| 598.1044 | 598.1028 | 2.72 | 99940 | 32.33 | 32.49 | (M+H)+ | 1 |
| 599.0999 | 599.0980 | 3.18 | 309167 | 100.00 | 100.00 | (M+H)+ | 1 |
| 600.1024 | 600.1009 | 2.58 | 100665 | 32.56 | 32.36 | (M+H)+ | 1 |
| 601.1055 | 601.1038 | 2.77 | 18138 | 5.87 | 5.80 | (M+H)+ | 1 |
| 602.1082 | 602.1067 | 2.57 | 2120 | 0.69 | 0.74 | (M+H)+ | 1 |
| 619.0831 | 619.0815 | 2.61 | 235798 | 99.80 | 96.76 | (M+Na)+ | 1 |
| 620.0862 | 620.0847 | 2.35 | 75780 | 32.07 | 32.48 | (M+Na)+ | 1 |
| 621.0815 | 621.0799 | 2.63 | 236277 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 622.0841 | 622.0828 | 2.03 | 75675 | 32.03 | 32.35 | (M+Na)+ | 1 |
| 623.0868 | 623.0858 | 1.63 | 13552 | 5.74 | 5.79 | (M+Na)+ | 1 |
| 635.0566 | 635.0554 | 1.86 | 35115 | 89.59 | 90.44 | (M+K)+ | 1 |
| 636.0599 | 636.0586 | 1.94 | 10573 | 26.98 | 30.37 | (M+K)+ | 1 |
| 637.0549 | 637.0538 | 1.67 | 39194 | 100.00 | 100.00 | (M+K)+ | 1 |
| 638.0577 | 638.0568 | 1.37 | 12190 | 31.10 | 32.44 | (M+K)+ | 1 |
| 639.0574 | 639.0554 | 3.14 | 4295 | 10.96 | 12.15 | (M+K)+ | 1 |
| 640.0591 | 640.0567 | 3.72 | 1102 | 2.81 | 2.87 | (M+K)+ | 1 |

MS spectra of 3ka

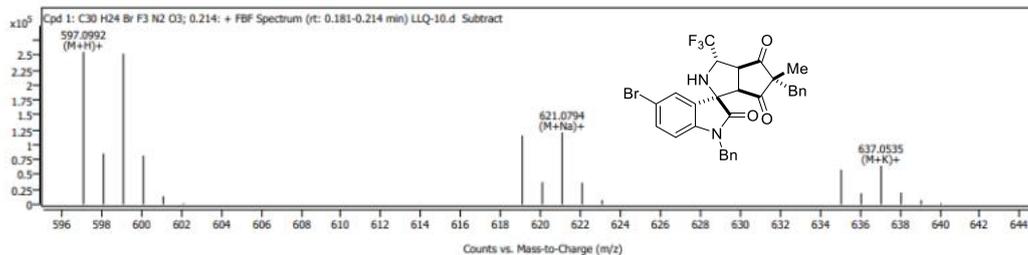
Custom Workflow Report



Compound Details

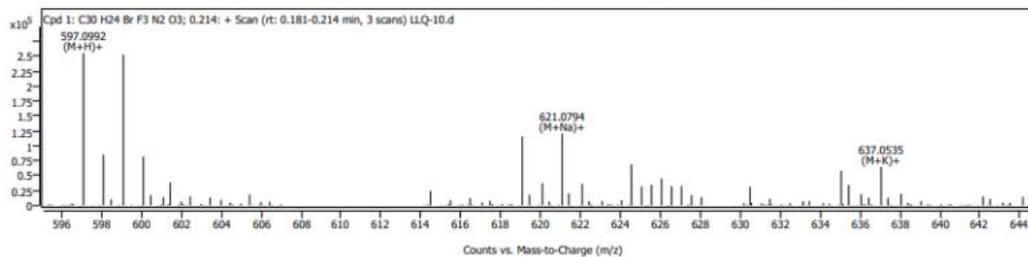
Cpd. 1: C30 H24 Br F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 597.0992 | 597.0995 | -0.61 | 255553 | 100.00 | 96.75 | (M+H)+ | 1 |
| 598.1021 | 598.1028 | -1.09 | 85199 | 33.34 | 32.49 | (M+H)+ | 1 |
| 599.0977 | 599.0980 | -0.49 | 252830 | 98.93 | 100.00 | (M+H)+ | 1 |
| 600.1003 | 600.1009 | -0.98 | 81816 | 32.02 | 32.36 | (M+H)+ | 1 |
| 601.1033 | 601.1038 | -0.87 | 13869 | 5.43 | 5.80 | (M+H)+ | 1 |
| 602.1068 | 602.1067 | 0.19 | 1872 | 0.73 | 0.74 | (M+H)+ | 1 |
| 619.0810 | 619.0815 | -0.75 | 115690 | 95.80 | 96.76 | (M+Na)+ | 1 |
| 620.0839 | 620.0847 | -1.23 | 37375 | 30.95 | 32.48 | (M+Na)+ | 1 |
| 621.0794 | 621.0799 | -0.85 | 120767 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 622.0821 | 622.0828 | -1.16 | 36341 | 30.09 | 32.35 | (M+Na)+ | 1 |
| 623.0844 | 623.0858 | -2.24 | 7433 | 6.15 | 5.79 | (M+Na)+ | 1 |
| 635.0552 | 635.0554 | -0.34 | 58299 | 90.13 | 90.44 | (M+K)+ | 1 |
| 636.0582 | 636.0586 | -0.63 | 18747 | 28.98 | 30.37 | (M+K)+ | 1 |
| 637.0535 | 637.0538 | -0.54 | 64681 | 100.00 | 100.00 | (M+K)+ | 1 |
| 638.0563 | 638.0568 | -0.68 | 19686 | 30.43 | 32.44 | (M+K)+ | 1 |
| 639.0558 | 639.0554 | 0.67 | 7218 | 11.16 | 12.16 | (M+K)+ | 1 |
| 640.0556 | 640.0567 | -1.80 | 2018 | 3.12 | 2.87 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 597.0992 | 597.0995 | -0.61 | 255553 | 100.00 | 96.75 | (M+H)+ | 1 |
| 598.1021 | 598.1028 | -1.09 | 85199 | 33.34 | 32.49 | (M+H)+ | 1 |
| 599.0977 | 599.0980 | -0.49 | 252830 | 98.93 | 100.00 | (M+H)+ | 1 |
| 600.1003 | 600.1009 | -0.98 | 81816 | 32.02 | 32.36 | (M+H)+ | 1 |
| 601.1033 | 601.1038 | -0.87 | 13869 | 5.43 | 5.80 | (M+H)+ | 1 |
| 602.1068 | 602.1067 | 0.19 | 1872 | 0.73 | 0.74 | (M+H)+ | 1 |
| 619.0810 | 619.0815 | -0.75 | 115690 | 95.80 | 96.76 | (M+Na)+ | 1 |
| 620.0839 | 620.0847 | -1.23 | 37375 | 30.95 | 32.48 | (M+Na)+ | 1 |
| 621.0794 | 621.0799 | -0.85 | 120767 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 622.0821 | 622.0828 | -1.16 | 36341 | 30.09 | 32.35 | (M+Na)+ | 1 |
| 623.0844 | 623.0858 | -2.24 | 7433 | 6.15 | 5.79 | (M+Na)+ | 1 |
| 635.0552 | 635.0554 | -0.34 | 58299 | 90.13 | 90.44 | (M+K)+ | 1 |
| 636.0582 | 636.0586 | -0.63 | 18747 | 28.98 | 30.37 | (M+K)+ | 1 |
| 637.0535 | 637.0538 | -0.54 | 64681 | 100.00 | 100.00 | (M+K)+ | 1 |
| 638.0563 | 638.0568 | -0.68 | 19686 | 30.43 | 32.44 | (M+K)+ | 1 |
| 639.0558 | 639.0554 | 0.67 | 7218 | 11.16 | 12.16 | (M+K)+ | 1 |
| 640.0556 | 640.0567 | -1.80 | 2018 | 3.12 | 2.87 | (M+K)+ | 1 |

MS spectra of 3la

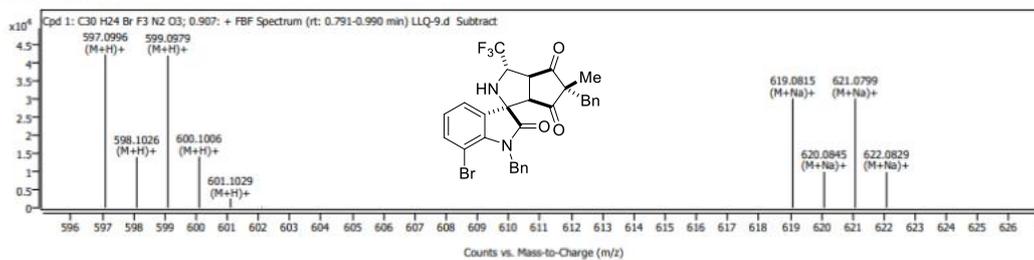
Custom Workflow Report



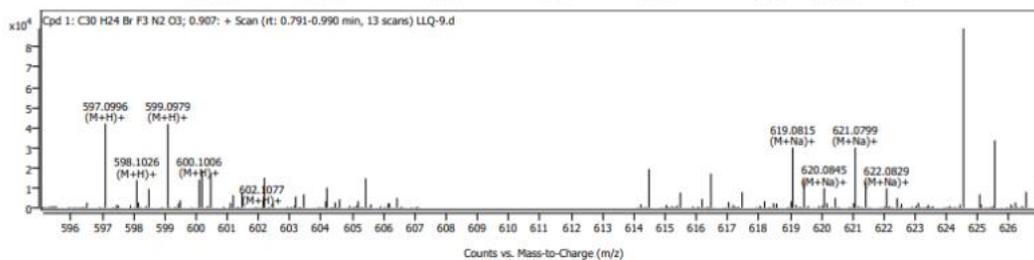
Compound Details

Cpd. 1: C30 H24 Br F3 N2 O3

Compound Spectra



| Spectrum Peaks | m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------------|----------|------------|------------|-------|----------|-----------------|-------------|---|
| | 597.0996 | 597.0995 | 0.20 | 42059 | 100.00 | 96.75 | (M+H)+ | 1 |
| | 598.1026 | 598.1028 | -0.20 | 13880 | 33.00 | 32.49 | (M+H)+ | 1 |
| | 599.0979 | 599.0980 | -0.17 | 41789 | 99.36 | 100.00 | (M+H)+ | 1 |
| | 600.1006 | 600.1009 | -0.44 | 14077 | 33.47 | 32.36 | (M+H)+ | 1 |
| | 601.1029 | 601.1038 | -1.48 | 2532 | 6.02 | 5.80 | (M+H)+ | 1 |
| | 602.1077 | 602.1067 | 1.78 | 197 | 0.47 | 0.74 | (M+H)+ | 1 |
| | 619.0815 | 619.0815 | 0.01 | 30024 | 100.00 | 96.76 | (M+Na)+ | 1 |
| | 620.0845 | 620.0847 | -0.31 | 9883 | 32.92 | 32.48 | (M+Na)+ | 1 |
| | 621.0799 | 621.0799 | 0.04 | 30021 | 99.99 | 100.00 | (M+Na)+ | 1 |
| | 622.0829 | 622.0828 | 0.02 | 9794 | 32.62 | 32.35 | (M+Na)+ | 1 |



| Spectrum Peaks | m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------------|----------|------------|------------|-------|----------|-----------------|-------------|---|
| | 597.0996 | 597.0995 | 0.20 | 42059 | 100.00 | 96.75 | (M+H)+ | 1 |
| | 598.1026 | 598.1028 | -0.20 | 13880 | 33.00 | 32.49 | (M+H)+ | 1 |
| | 599.0979 | 599.0980 | -0.17 | 41789 | 99.36 | 100.00 | (M+H)+ | 1 |
| | 600.1006 | 600.1009 | -0.44 | 14077 | 33.47 | 32.36 | (M+H)+ | 1 |
| | 601.1029 | 601.1038 | -1.48 | 2532 | 6.02 | 5.80 | (M+H)+ | 1 |
| | 602.1077 | 602.1067 | 1.78 | 197 | 0.47 | 0.74 | (M+H)+ | 1 |
| | 619.0815 | 619.0815 | 0.01 | 30024 | 100.00 | 96.76 | (M+Na)+ | 1 |
| | 620.0845 | 620.0847 | -0.31 | 9883 | 32.92 | 32.48 | (M+Na)+ | 1 |
| | 621.0799 | 621.0799 | 0.04 | 30021 | 99.99 | 100.00 | (M+Na)+ | 1 |
| | 622.0829 | 622.0828 | 0.02 | 9794 | 32.62 | 32.35 | (M+Na)+ | 1 |

MS spectra of 3ma

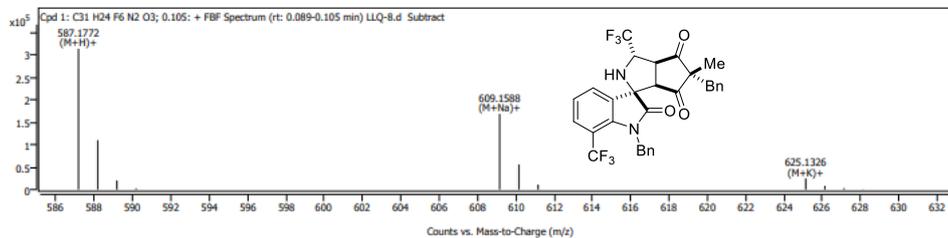
Custom Workflow Report



Compound Details

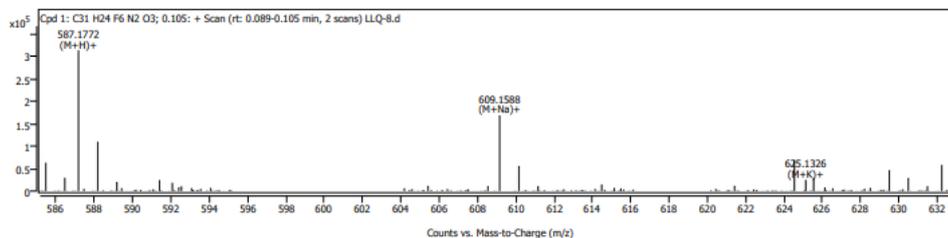
Cpd. 1: C31 H24 F6 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 587.1772 | 587.1764 | 1.31 | 313107 | 100.00 | 100.00 | (M+H)+ | 1 |
| 588.1801 | 588.1796 | 0.77 | 109910 | 35.10 | 34.66 | (M+H)+ | 1 |
| 589.1832 | 589.1827 | 0.91 | 20259 | 6.47 | 6.44 | (M+H)+ | 1 |
| 590.1821 | 590.1856 | -5.82 | 2818 | 0.90 | 0.85 | (M+H)+ | 1 |
| 609.1588 | 609.1583 | 0.75 | 168291 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 610.1630 | 610.1616 | 0.62 | 55804 | 33.16 | 34.65 | (M+Na)+ | 1 |
| 611.1657 | 611.1646 | 1.85 | 10917 | 6.49 | 6.44 | (M+Na)+ | 1 |
| 625.1326 | 625.1323 | 0.61 | 24811 | 100.00 | 100.00 | (M+K)+ | 1 |
| 626.1361 | 626.1355 | 0.98 | 8215 | 33.11 | 34.66 | (M+K)+ | 1 |
| 627.1330 | 627.1342 | -1.98 | 3277 | 13.21 | 13.66 | (M+K)+ | 1 |
| 628.1326 | 628.1356 | -4.83 | 613 | 2.47 | 3.35 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 587.1772 | 587.1764 | 1.31 | 313107 | 100.00 | 100.00 | (M+H)+ | 1 |
| 588.1801 | 588.1796 | 0.77 | 109910 | 35.10 | 34.66 | (M+H)+ | 1 |
| 589.1832 | 589.1827 | 0.91 | 20259 | 6.47 | 6.44 | (M+H)+ | 1 |
| 590.1821 | 590.1856 | -5.82 | 2818 | 0.90 | 0.85 | (M+H)+ | 1 |
| 609.1588 | 609.1583 | 0.75 | 168291 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 610.1630 | 610.1616 | 0.62 | 55804 | 33.16 | 34.65 | (M+Na)+ | 1 |
| 611.1657 | 611.1646 | 1.85 | 10917 | 6.49 | 6.44 | (M+Na)+ | 1 |
| 625.1326 | 625.1323 | 0.61 | 24811 | 100.00 | 100.00 | (M+K)+ | 1 |
| 626.1361 | 626.1355 | 0.98 | 8215 | 33.11 | 34.66 | (M+K)+ | 1 |
| 627.1330 | 627.1342 | -1.98 | 3277 | 13.21 | 13.66 | (M+K)+ | 1 |
| 628.1326 | 628.1356 | -4.83 | 613 | 2.47 | 3.35 | (M+K)+ | 1 |

MS spectra of 3na

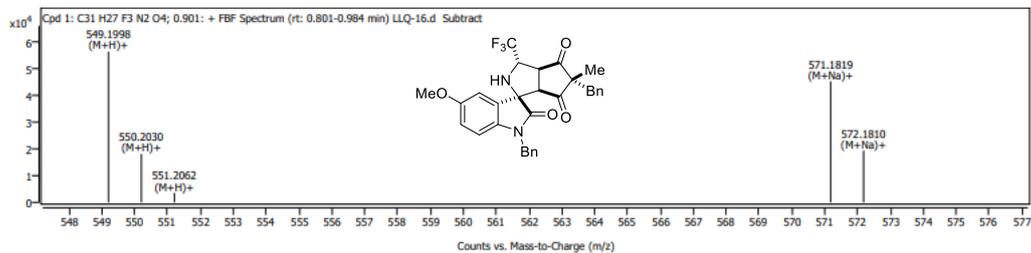
Custom Workflow Report



Compound Details

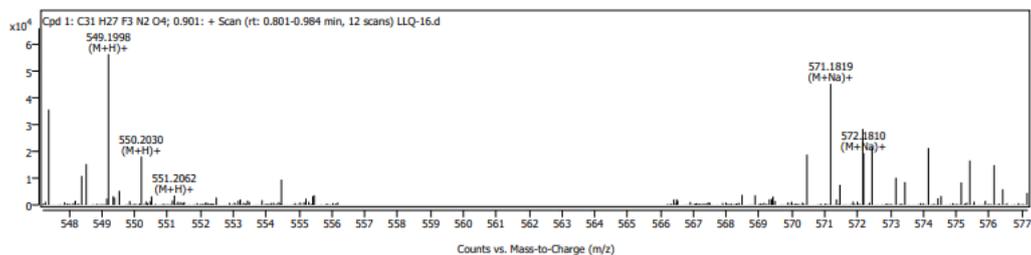
Cpd. 1: C31 H27 F3 N2 O4

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 549.1998 | 549.1996 | 0.36 | 56027 | 100.00 | 100.00 | (M+H)+ | 1 |
| 550.2030 | 550.2028 | 0.27 | 18008 | 32.14 | 34.73 | (M+H)+ | 1 |
| 551.2062 | 551.2058 | 0.79 | 3524 | 6.29 | 6.67 | (M+H)+ | 1 |
| 571.1819 | 571.1815 | 0.66 | 44962 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 572.1810 | 572.1848 | -6.59 | 19238 | 42.79 | 34.72 | (M+Na)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 549.1998 | 549.1996 | 0.36 | 56027 | 100.00 | 100.00 | (M+H)+ | 1 |
| 550.2030 | 550.2028 | 0.27 | 18008 | 32.14 | 34.73 | (M+H)+ | 1 |
| 551.2062 | 551.2058 | 0.79 | 3524 | 6.29 | 6.67 | (M+H)+ | 1 |
| 571.1819 | 571.1815 | 0.66 | 44962 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 572.1810 | 572.1848 | -6.59 | 19238 | 42.79 | 34.72 | (M+Na)+ | 1 |

MS spectra of 30a

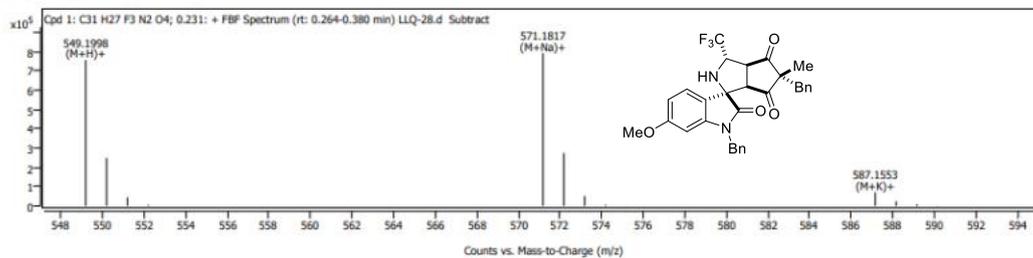
Custom Workflow Report



Compound Details

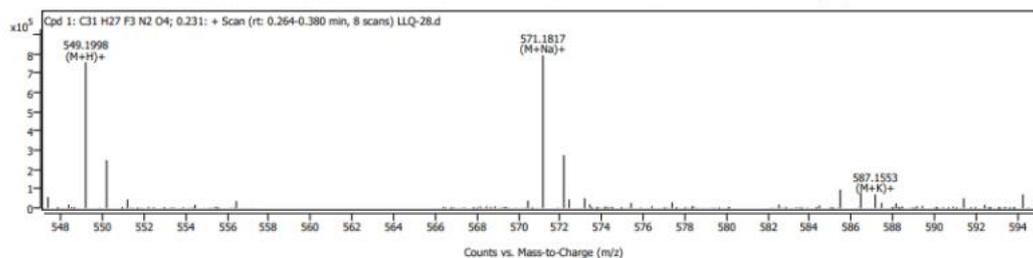
Cpd. 1: C31 H27 F3 N2 O4

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 549.1998 | 549.1996 | 0.51 | 757256 | 100.00 | 100.00 | (M+H)+ | 1 |
| 550.2030 | 550.2028 | 0.34 | 249121 | 32.90 | 34.73 | (M+H)+ | 1 |
| 551.2056 | 551.2058 | -0.39 | 44769 | 5.91 | 6.67 | (M+H)+ | 1 |
| 552.2086 | 552.2086 | 0.03 | 6303 | 0.83 | 0.92 | (M+H)+ | 1 |
| 571.1817 | 571.1815 | 0.41 | 792780 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 572.1849 | 572.1848 | 0.21 | 274659 | 34.65 | 34.72 | (M+Na)+ | 1 |
| 573.1877 | 573.1877 | 0.01 | 51065 | 6.44 | 6.67 | (M+Na)+ | 1 |
| 574.1900 | 574.1906 | -0.97 | 6765 | 0.85 | 0.92 | (M+Na)+ | 1 |
| 575.1910 | 575.1933 | -4.09 | 879 | 0.11 | 0.10 | (M+Na)+ | 1 |
| 587.1553 | 587.1555 | -0.18 | 70701 | 100.00 | 100.00 | (M+K)+ | 1 |
| 588.1586 | 588.1587 | -0.11 | 24685 | 34.91 | 34.73 | (M+K)+ | 1 |
| 589.1586 | 589.1575 | 1.93 | 9009 | 12.74 | 13.89 | (M+K)+ | 1 |
| 590.1596 | 590.1589 | 1.28 | 2361 | 3.34 | 3.43 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 549.1998 | 549.1996 | 0.51 | 757256 | 100.00 | 100.00 | (M+H)+ | 1 |
| 550.2030 | 550.2028 | 0.34 | 249121 | 32.90 | 34.73 | (M+H)+ | 1 |
| 551.2056 | 551.2058 | -0.39 | 44769 | 5.91 | 6.67 | (M+H)+ | 1 |
| 552.2086 | 552.2086 | 0.03 | 6303 | 0.83 | 0.92 | (M+H)+ | 1 |
| 571.1817 | 571.1815 | 0.41 | 792780 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 572.1849 | 572.1848 | 0.21 | 274659 | 34.65 | 34.72 | (M+Na)+ | 1 |
| 573.1877 | 573.1877 | 0.01 | 51065 | 6.44 | 6.67 | (M+Na)+ | 1 |
| 574.1900 | 574.1906 | -0.97 | 6765 | 0.85 | 0.92 | (M+Na)+ | 1 |
| 575.1910 | 575.1933 | -4.09 | 879 | 0.11 | 0.10 | (M+Na)+ | 1 |
| 587.1553 | 587.1555 | -0.18 | 70701 | 100.00 | 100.00 | (M+K)+ | 1 |
| 588.1586 | 588.1587 | -0.11 | 24685 | 34.91 | 34.73 | (M+K)+ | 1 |
| 589.1586 | 589.1575 | 1.93 | 9009 | 12.74 | 13.89 | (M+K)+ | 1 |
| 590.1596 | 590.1589 | 1.28 | 2361 | 3.34 | 3.43 | (M+K)+ | 1 |

MS spectra of 3pa

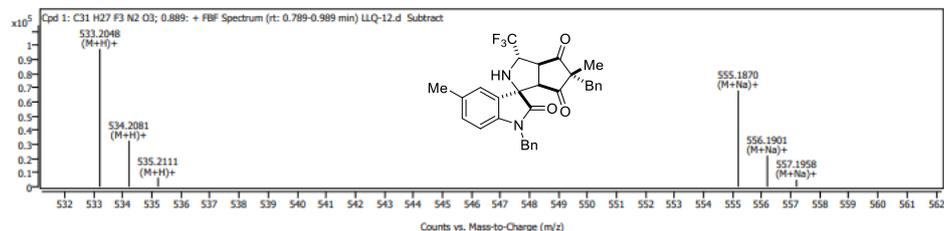
Custom Workflow Report



Compound Details

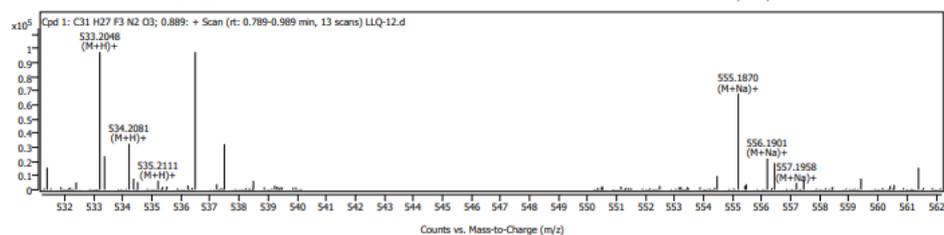
Cpd. 1: C31 H27 F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 533.2048 | 533.2047 | 0.30 | 97366 | 100.00 | 100.00 | (M+H)+ | 1 |
| 534.2081 | 534.2079 | 0.38 | 32648 | 33.53 | 34.70 | (M+H)+ | 1 |
| 535.2111 | 535.2109 | 0.34 | 6469 | 6.64 | 6.45 | (M+H)+ | 1 |
| 555.1870 | 555.1866 | 0.72 | 67999 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 556.1901 | 556.1898 | 0.40 | 22122 | 32.53 | 34.68 | (M+Na)+ | 1 |
| 557.1958 | 557.1929 | 5.30 | 4942 | 7.27 | 6.45 | (M+Na)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 533.2048 | 533.2047 | 0.30 | 97366 | 100.00 | 100.00 | (M+H)+ | 1 |
| 534.2081 | 534.2079 | 0.38 | 32648 | 33.53 | 34.70 | (M+H)+ | 1 |
| 535.2111 | 535.2109 | 0.34 | 6469 | 6.64 | 6.45 | (M+H)+ | 1 |
| 555.1870 | 555.1866 | 0.72 | 67999 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 556.1901 | 556.1898 | 0.40 | 22122 | 32.53 | 34.68 | (M+Na)+ | 1 |
| 557.1958 | 557.1929 | 5.30 | 4942 | 7.27 | 6.45 | (M+Na)+ | 1 |

MS spectra of 3qa

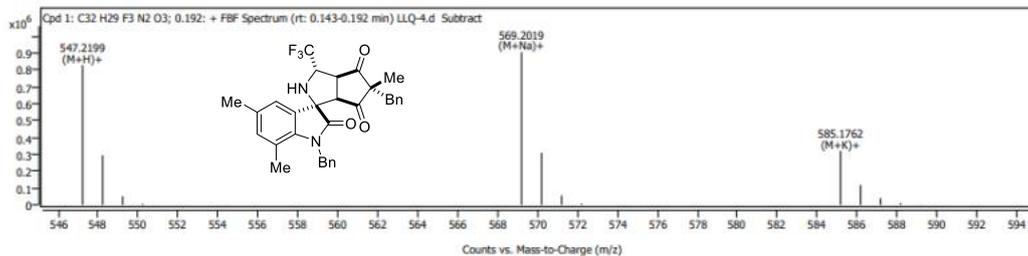
Custom Workflow Report



Compound Details

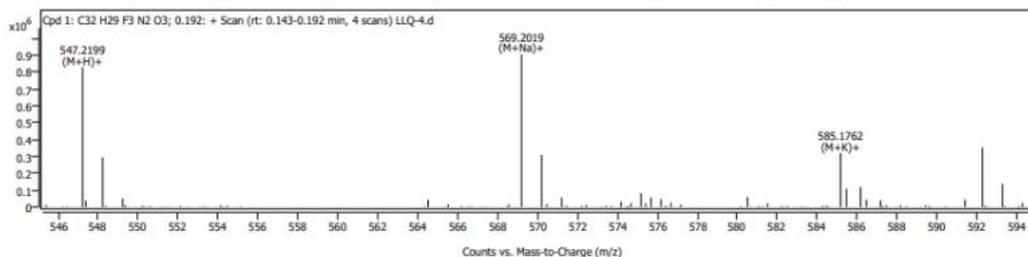
Cpd. 1: C32 H29 F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 547.2199 | 547.2203 | -0.69 | 830104 | 100.00 | 100.00 | (M+H)+ | 1 |
| 548.2234 | 548.2236 | -0.21 | 294391 | 35.46 | 35.80 | (M+H)+ | 1 |
| 549.2260 | 549.2266 | -1.03 | 50994 | 6.14 | 6.84 | (M+H)+ | 1 |
| 550.2289 | 550.2295 | -1.10 | 6975 | 0.84 | 0.92 | (M+H)+ | 1 |
| 569.2019 | 569.2022 | -0.56 | 906449 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 570.2054 | 570.2055 | -0.20 | 309395 | 34.13 | 35.79 | (M+Na)+ | 1 |
| 571.2079 | 571.2086 | -1.07 | 56075 | 6.19 | 6.83 | (M+Na)+ | 1 |
| 572.2113 | 572.2115 | -0.31 | 7156 | 0.79 | 0.92 | (M+Na)+ | 1 |
| 585.1762 | 585.1762 | -0.06 | 320930 | 100.00 | 100.00 | (M+K)+ | 1 |
| 586.1792 | 586.1794 | -0.36 | 117808 | 36.71 | 35.80 | (M+K)+ | 1 |
| 587.1784 | 587.1783 | 0.21 | 39781 | 12.40 | 14.05 | (M+K)+ | 1 |
| 588.1795 | 588.1796 | -0.22 | 9833 | 3.06 | 3.50 | (M+K)+ | 1 |
| 589.1821 | 589.1819 | 0.38 | 1761 | 0.55 | 0.59 | (M+K)+ | 1 |
| 590.1844 | 590.1844 | 0.12 | 334 | 0.10 | 0.07 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 547.2199 | 547.2203 | -0.69 | 830104 | 100.00 | 100.00 | (M+H)+ | 1 |
| 548.2234 | 548.2236 | -0.21 | 294391 | 35.46 | 35.80 | (M+H)+ | 1 |
| 549.2260 | 549.2266 | -1.03 | 50994 | 6.14 | 6.84 | (M+H)+ | 1 |
| 550.2289 | 550.2295 | -1.10 | 6975 | 0.84 | 0.92 | (M+H)+ | 1 |
| 569.2019 | 569.2022 | -0.56 | 906449 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 570.2054 | 570.2055 | -0.20 | 309395 | 34.13 | 35.79 | (M+Na)+ | 1 |
| 571.2079 | 571.2086 | -1.07 | 56075 | 6.19 | 6.83 | (M+Na)+ | 1 |
| 572.2113 | 572.2115 | -0.31 | 7156 | 0.79 | 0.92 | (M+Na)+ | 1 |
| 585.1762 | 585.1762 | -0.06 | 320930 | 100.00 | 100.00 | (M+K)+ | 1 |
| 586.1792 | 586.1794 | -0.36 | 117808 | 36.71 | 35.80 | (M+K)+ | 1 |
| 587.1784 | 587.1783 | 0.21 | 39781 | 12.40 | 14.05 | (M+K)+ | 1 |
| 588.1795 | 588.1796 | -0.22 | 9833 | 3.06 | 3.50 | (M+K)+ | 1 |
| 589.1821 | 589.1819 | 0.38 | 1761 | 0.55 | 0.59 | (M+K)+ | 1 |
| 590.1844 | 590.1844 | 0.12 | 334 | 0.10 | 0.07 | (M+K)+ | 1 |

MS spectra of **3ab**

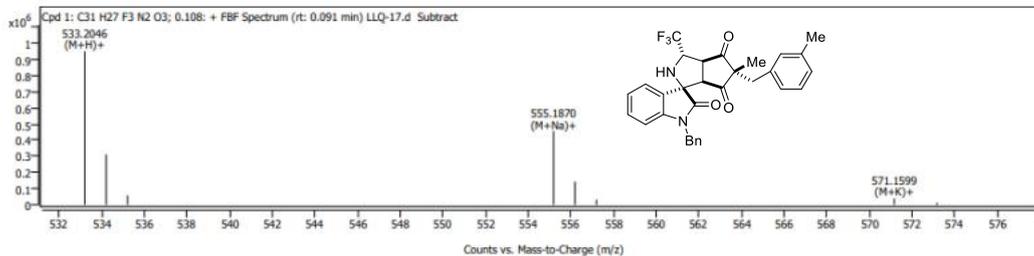
Custom Workflow Report



Compound Details

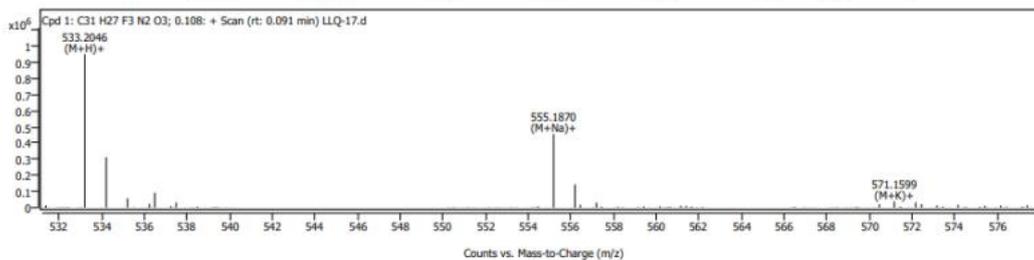
Cpd. 1: C31 H27 F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 533.2046 | 533.2047 | -0.05 | 951190 | 100.00 | 100.00 | (M+H)+ | 1 |
| 534.2080 | 534.2079 | 0.17 | 312435 | 32.85 | 34.70 | (M+H)+ | 1 |
| 535.2108 | 535.2109 | -0.17 | 58263 | 6.13 | 6.45 | (M+H)+ | 1 |
| 555.1870 | 555.1866 | 0.72 | 456690 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 556.1897 | 556.1898 | -0.19 | 143636 | 31.45 | 34.68 | (M+Na)+ | 1 |
| 557.1931 | 557.1929 | 0.39 | 31059 | 6.80 | 6.45 | (M+Na)+ | 1 |
| 571.1599 | 571.1605 | -1.16 | 39104 | 100.00 | 100.00 | (M+K)+ | 1 |
| 573.1604 | 573.1625 | -3.62 | 13165 | 33.67 | 13.67 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 533.2046 | 533.2047 | -0.05 | 951190 | 100.00 | 100.00 | (M+H)+ | 1 |
| 534.2080 | 534.2079 | 0.17 | 312435 | 32.85 | 34.70 | (M+H)+ | 1 |
| 535.2108 | 535.2109 | -0.17 | 58263 | 6.13 | 6.45 | (M+H)+ | 1 |
| 555.1870 | 555.1866 | 0.72 | 456690 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 556.1897 | 556.1898 | -0.19 | 143636 | 31.45 | 34.68 | (M+Na)+ | 1 |
| 557.1931 | 557.1929 | 0.39 | 31059 | 6.80 | 6.45 | (M+Na)+ | 1 |
| 571.1599 | 571.1605 | -1.16 | 39104 | 100.00 | 100.00 | (M+K)+ | 1 |
| 573.1604 | 573.1625 | -3.62 | 13165 | 33.67 | 13.67 | (M+K)+ | 1 |

MS spectra of 3ac

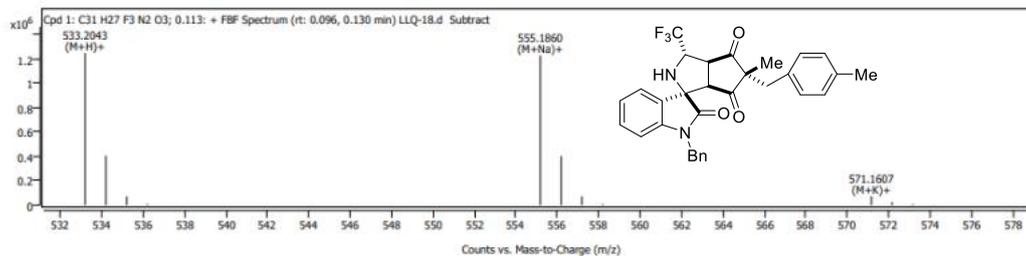
Custom Workflow Report



Compound Details

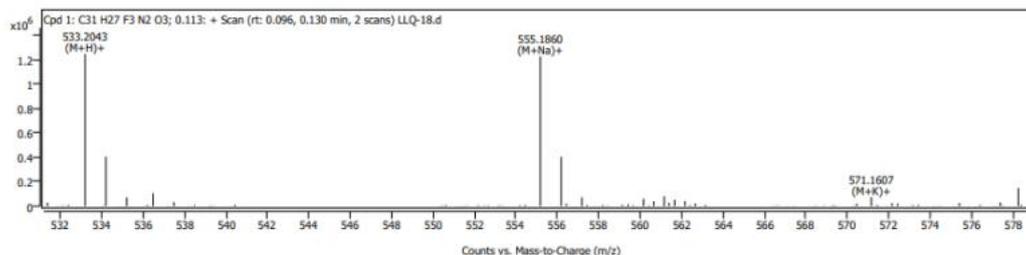
Cpd. 1: C31 H27 F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|---------|----------|-----------------|-------------|---|
| 533.2043 | 533.2047 | -0.75 | 1249956 | 100.00 | 100.00 | (M+H)+ | 1 |
| 534.2077 | 534.2079 | -0.36 | 406279 | 32.50 | 34.70 | (M+H)+ | 1 |
| 535.2102 | 535.2109 | -1.42 | 71651 | 5.73 | 6.45 | (M+H)+ | 1 |
| 536.2131 | 536.2138 | -1.41 | 9869 | 0.79 | 0.85 | (M+H)+ | 1 |
| 555.1860 | 555.1866 | -1.09 | 1229229 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 556.1895 | 556.1898 | -0.64 | 404334 | 32.89 | 34.68 | (M+Na)+ | 1 |
| 557.1921 | 557.1929 | -1.48 | 72708 | 5.91 | 6.45 | (M+Na)+ | 1 |
| 558.1950 | 558.1958 | -1.34 | 9147 | 0.74 | 0.85 | (M+Na)+ | 1 |
| 571.1607 | 571.1605 | 0.32 | 74153 | 100.00 | 100.00 | (M+K)+ | 1 |
| 572.1640 | 572.1638 | 0.36 | 24006 | 32.37 | 34.70 | (M+K)+ | 1 |
| 573.1623 | 573.1625 | -0.40 | 8471 | 11.42 | 13.67 | (M+K)+ | 1 |
| 574.1649 | 574.1639 | 1.71 | 2420 | 3.26 | 3.35 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|---------|----------|-----------------|-------------|---|
| 533.2043 | 533.2047 | -0.75 | 1249956 | 100.00 | 100.00 | (M+H)+ | 1 |
| 534.2077 | 534.2079 | -0.36 | 406279 | 32.50 | 34.70 | (M+H)+ | 1 |
| 535.2102 | 535.2109 | -1.42 | 71651 | 5.73 | 6.45 | (M+H)+ | 1 |
| 536.2131 | 536.2138 | -1.41 | 9869 | 0.79 | 0.85 | (M+H)+ | 1 |
| 555.1860 | 555.1866 | -1.09 | 1229229 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 556.1895 | 556.1898 | -0.64 | 404334 | 32.89 | 34.68 | (M+Na)+ | 1 |
| 557.1921 | 557.1929 | -1.48 | 72708 | 5.91 | 6.45 | (M+Na)+ | 1 |
| 558.1950 | 558.1958 | -1.34 | 9147 | 0.74 | 0.85 | (M+Na)+ | 1 |
| 571.1607 | 571.1605 | 0.32 | 74153 | 100.00 | 100.00 | (M+K)+ | 1 |
| 572.1640 | 572.1638 | 0.36 | 24006 | 32.37 | 34.70 | (M+K)+ | 1 |
| 573.1623 | 573.1625 | -0.40 | 8471 | 11.42 | 13.67 | (M+K)+ | 1 |
| 574.1649 | 574.1639 | 1.71 | 2420 | 3.26 | 3.35 | (M+K)+ | 1 |

MS spectra of 3ad

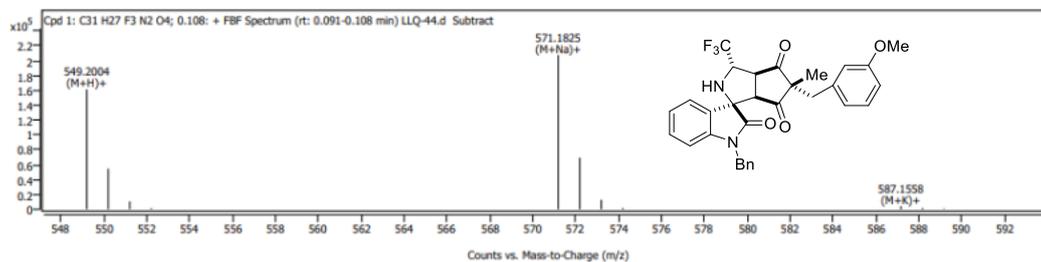
Custom Workflow Report



Compound Details

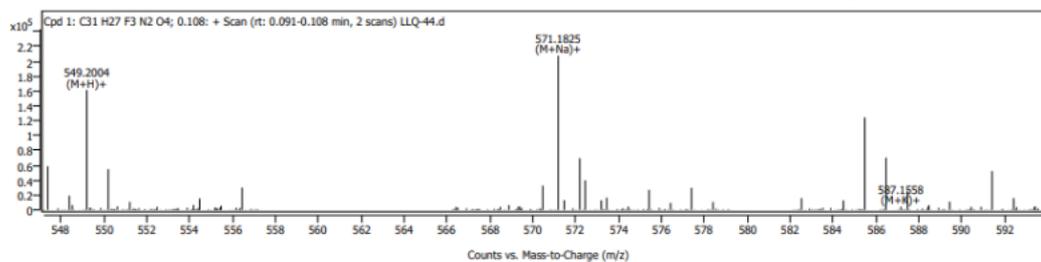
Cpd. 1: C31 H27 F3 N2 O4

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 549.2004 | 549.1996 | 1.50 | 161291 | 100.00 | 100.00 | (M+H)+ | 1 |
| 550.2034 | 550.2028 | 1.11 | 54645 | 33.88 | 34.73 | (M+H)+ | 1 |
| 551.2064 | 551.2058 | 1.13 | 10644 | 6.60 | 6.67 | (M+H)+ | 1 |
| 552.2094 | 552.2086 | 1.35 | 1491 | 0.92 | 0.92 | (M+H)+ | 1 |
| 571.1825 | 571.1815 | 1.70 | 207364 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 572.1856 | 572.1848 | 1.44 | 69409 | 33.47 | 34.72 | (M+Na)+ | 1 |
| 573.1888 | 573.1877 | 1.93 | 12746 | 6.15 | 6.67 | (M+Na)+ | 1 |
| 574.1906 | 574.1906 | 0.05 | 1875 | 0.90 | 0.92 | (M+Na)+ | 1 |
| 587.1558 | 587.1555 | 0.66 | 4241 | 100.00 | 100.00 | (M+K)+ | 1 |
| 588.1603 | 588.1587 | 2.76 | 1799 | 42.42 | 34.73 | (M+K)+ | 1 |
| 589.1601 | 589.1575 | 4.41 | 874 | 20.62 | 13.89 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 549.2004 | 549.1996 | 1.50 | 161291 | 100.00 | 100.00 | (M+H)+ | 1 |
| 550.2034 | 550.2028 | 1.11 | 54645 | 33.88 | 34.73 | (M+H)+ | 1 |
| 551.2064 | 551.2058 | 1.13 | 10644 | 6.60 | 6.67 | (M+H)+ | 1 |
| 552.2094 | 552.2086 | 1.35 | 1491 | 0.92 | 0.92 | (M+H)+ | 1 |
| 571.1825 | 571.1815 | 1.70 | 207364 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 572.1856 | 572.1848 | 1.44 | 69409 | 33.47 | 34.72 | (M+Na)+ | 1 |
| 573.1888 | 573.1877 | 1.93 | 12746 | 6.15 | 6.67 | (M+Na)+ | 1 |
| 574.1906 | 574.1906 | 0.05 | 1875 | 0.90 | 0.92 | (M+Na)+ | 1 |
| 587.1558 | 587.1555 | 0.66 | 4241 | 100.00 | 100.00 | (M+K)+ | 1 |
| 588.1603 | 588.1587 | 2.76 | 1799 | 42.42 | 34.73 | (M+K)+ | 1 |
| 589.1601 | 589.1575 | 4.41 | 874 | 20.62 | 13.89 | (M+K)+ | 1 |

Header
Data

MS spectra of 3ae

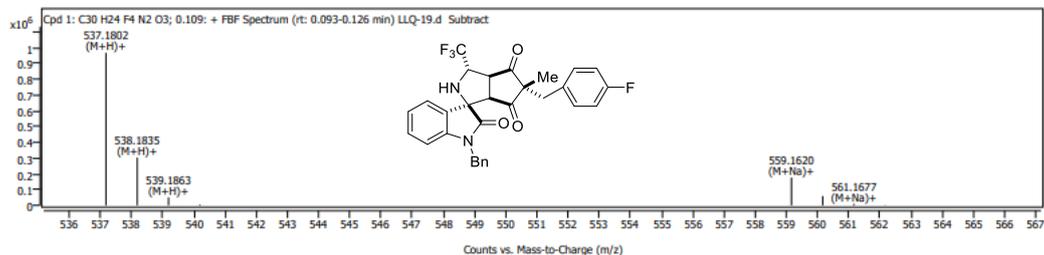
Custom Workflow Report



Compound Details

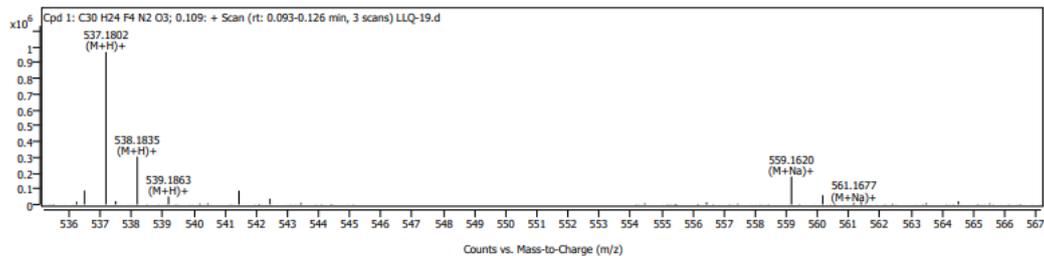
Cpd. 1: C30 H24 F4 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 537.1802 | 537.1796 | 1.14 | 967172 | 100.00 | 100.00 | (M+H)+ | 1 |
| 538.1835 | 538.1828 | 1.28 | 303638 | 31.39 | 33.58 | (M+H)+ | 1 |
| 539.1863 | 539.1858 | 0.82 | 50820 | 5.25 | 6.08 | (M+H)+ | 1 |
| 540.1898 | 540.1887 | 1.98 | 5759 | 0.60 | 0.78 | (M+H)+ | 1 |
| 559.1620 | 559.1615 | 0.76 | 176686 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 560.1650 | 560.1648 | 0.44 | 59109 | 33.45 | 33.57 | (M+Na)+ | 1 |
| 561.1677 | 561.1678 | -0.14 | 10244 | 5.80 | 6.07 | (M+Na)+ | 1 |
| 562.1677 | 562.1707 | -5.33 | 1864 | 1.06 | 0.78 | (M+Na)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 537.1802 | 537.1796 | 1.14 | 967172 | 100.00 | 100.00 | (M+H)+ | 1 |
| 538.1835 | 538.1828 | 1.28 | 303638 | 31.39 | 33.58 | (M+H)+ | 1 |
| 539.1863 | 539.1858 | 0.82 | 50820 | 5.25 | 6.08 | (M+H)+ | 1 |
| 540.1898 | 540.1887 | 1.98 | 5759 | 0.60 | 0.78 | (M+H)+ | 1 |
| 559.1620 | 559.1615 | 0.76 | 176686 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 560.1650 | 560.1648 | 0.44 | 59109 | 33.45 | 33.57 | (M+Na)+ | 1 |
| 561.1677 | 561.1678 | -0.14 | 10244 | 5.80 | 6.07 | (M+Na)+ | 1 |
| 562.1677 | 562.1707 | -5.33 | 1864 | 1.06 | 0.78 | (M+Na)+ | 1 |

MS spectra of 3af

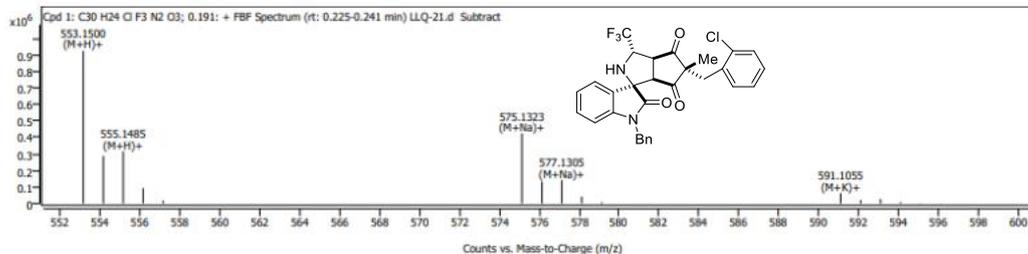
Custom Workflow Report



Compound Details

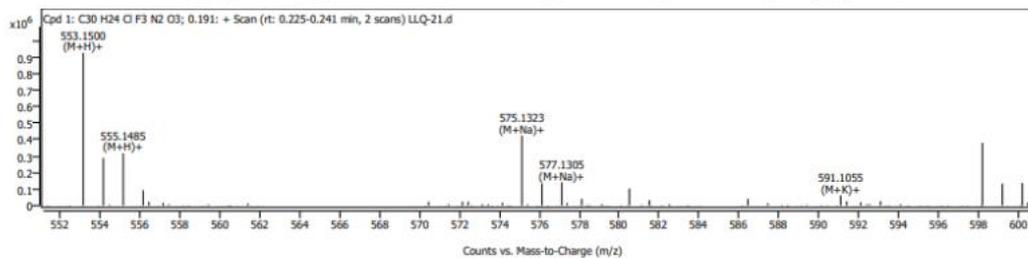
Cpd. 1: C30 H24 Cl F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 553.1500 | 553.1500 | -0.01 | 924458 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1533 | 554.1533 | -0.01 | 288363 | 31.19 | 33.58 | (M+H)+ | 1 |
| 555.1485 | 555.1486 | -0.02 | 316246 | 34.21 | 38.07 | (M+H)+ | 1 |
| 556.1508 | 556.1509 | -0.14 | 93362 | 10.10 | 11.52 | (M+H)+ | 1 |
| 557.1528 | 557.1537 | -1.53 | 17738 | 1.92 | 2.02 | (M+H)+ | 1 |
| 575.1323 | 575.1320 | 0.57 | 424342 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 576.1358 | 576.1352 | 0.98 | 133305 | 31.41 | 33.57 | (M+Na)+ | 1 |
| 577.1305 | 577.1305 | 0.02 | 141336 | 33.31 | 38.07 | (M+Na)+ | 1 |
| 578.1331 | 578.1329 | 0.34 | 42062 | 9.91 | 11.52 | (M+Na)+ | 1 |
| 579.1355 | 579.1356 | -0.14 | 8025 | 1.89 | 2.02 | (M+Na)+ | 1 |
| 591.1055 | 591.1059 | -0.74 | 61998 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1091 | 592.1092 | -0.14 | 20432 | 32.96 | 33.58 | (M+K)+ | 1 |
| 593.1035 | 593.1044 | -1.55 | 26998 | 43.55 | 45.29 | (M+K)+ | 1 |
| 594.1063 | 594.1069 | -1.03 | 8530 | 13.76 | 13.95 | (M+K)+ | 1 |
| 595.1063 | 595.1055 | 1.30 | 2317 | 3.74 | 4.77 | (M+K)+ | 1 |
| 596.1077 | 596.1067 | 1.72 | 614 | 0.99 | 1.09 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 553.1500 | 553.1500 | -0.01 | 924458 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1533 | 554.1533 | -0.01 | 288363 | 31.19 | 33.58 | (M+H)+ | 1 |
| 555.1485 | 555.1486 | -0.02 | 316246 | 34.21 | 38.07 | (M+H)+ | 1 |
| 556.1508 | 556.1509 | -0.14 | 93362 | 10.10 | 11.52 | (M+H)+ | 1 |
| 557.1528 | 557.1537 | -1.53 | 17738 | 1.92 | 2.02 | (M+H)+ | 1 |
| 575.1323 | 575.1320 | 0.57 | 424342 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 576.1358 | 576.1352 | 0.98 | 133305 | 31.41 | 33.57 | (M+Na)+ | 1 |
| 577.1305 | 577.1305 | 0.02 | 141336 | 33.31 | 38.07 | (M+Na)+ | 1 |
| 578.1331 | 578.1329 | 0.34 | 42062 | 9.91 | 11.52 | (M+Na)+ | 1 |
| 579.1355 | 579.1356 | -0.14 | 8025 | 1.89 | 2.02 | (M+Na)+ | 1 |
| 591.1055 | 591.1059 | -0.74 | 61998 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1091 | 592.1092 | -0.14 | 20432 | 32.96 | 33.58 | (M+K)+ | 1 |
| 593.1035 | 593.1044 | -1.55 | 26998 | 43.55 | 45.29 | (M+K)+ | 1 |
| 594.1063 | 594.1069 | -1.03 | 8530 | 13.76 | 13.95 | (M+K)+ | 1 |
| 595.1063 | 595.1055 | 1.30 | 2317 | 3.74 | 4.77 | (M+K)+ | 1 |
| 596.1077 | 596.1067 | 1.72 | 614 | 0.99 | 1.09 | (M+K)+ | 1 |

MS spectra of 3ag

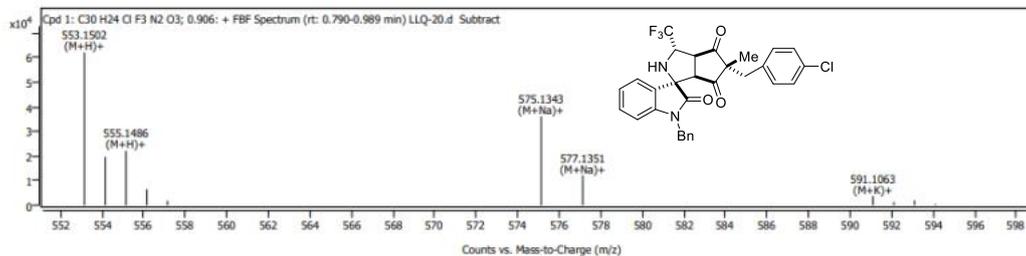
Custom Workflow Report



Compound Details

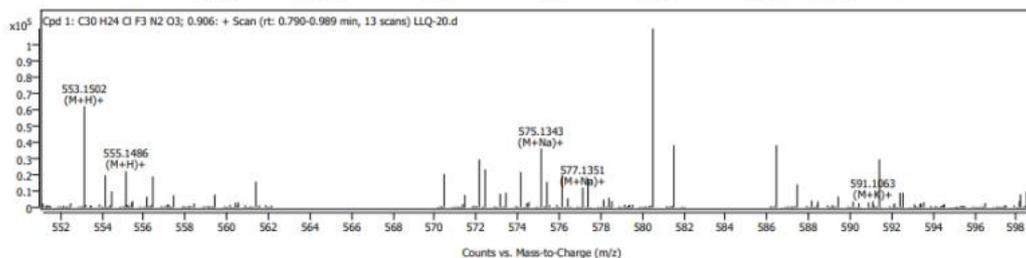
Cpd. 1: C30 H24 Cl F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 553.1502 | 553.1500 | 0.39 | 62205 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1534 | 554.1533 | 0.28 | 19713 | 31.69 | 33.58 | (M+H)+ | 1 |
| 555.1486 | 555.1486 | 0.02 | 22174 | 35.65 | 38.07 | (M+H)+ | 1 |
| 556.1516 | 556.1509 | 1.16 | 6497 | 10.44 | 11.52 | (M+H)+ | 1 |
| 557.1539 | 557.1537 | 0.33 | 1829 | 2.94 | 2.02 | (M+H)+ | 1 |
| 575.1343 | 575.1320 | 3.98 | 36214 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 577.1351 | 577.1305 | 7.91 | 12213 | 33.72 | 38.07 | (M+Na)+ | 1 |
| 591.1063 | 591.1059 | 0.63 | 3754 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1090 | 592.1092 | -0.32 | 1362 | 36.29 | 33.58 | (M+K)+ | 1 |
| 593.1048 | 593.1044 | 0.75 | 1992 | 53.07 | 45.29 | (M+K)+ | 1 |
| 594.1063 | 594.1069 | -0.99 | 476 | 12.69 | 13.95 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 553.1502 | 553.1500 | 0.39 | 62205 | 100.00 | 100.00 | (M+H)+ | 1 |
| 554.1534 | 554.1533 | 0.28 | 19713 | 31.69 | 33.58 | (M+H)+ | 1 |
| 555.1486 | 555.1486 | 0.02 | 22174 | 35.65 | 38.07 | (M+H)+ | 1 |
| 556.1516 | 556.1509 | 1.16 | 6497 | 10.44 | 11.52 | (M+H)+ | 1 |
| 557.1539 | 557.1537 | 0.33 | 1829 | 2.94 | 2.02 | (M+H)+ | 1 |
| 575.1343 | 575.1320 | 3.98 | 36214 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 577.1351 | 577.1305 | 7.91 | 12213 | 33.72 | 38.07 | (M+Na)+ | 1 |
| 591.1063 | 591.1059 | 0.63 | 3754 | 100.00 | 100.00 | (M+K)+ | 1 |
| 592.1090 | 592.1092 | -0.32 | 1362 | 36.29 | 33.58 | (M+K)+ | 1 |
| 593.1048 | 593.1044 | 0.75 | 1992 | 53.07 | 45.29 | (M+K)+ | 1 |
| 594.1063 | 594.1069 | -0.99 | 476 | 12.69 | 13.95 | (M+K)+ | 1 |

MS spectra of 3ah

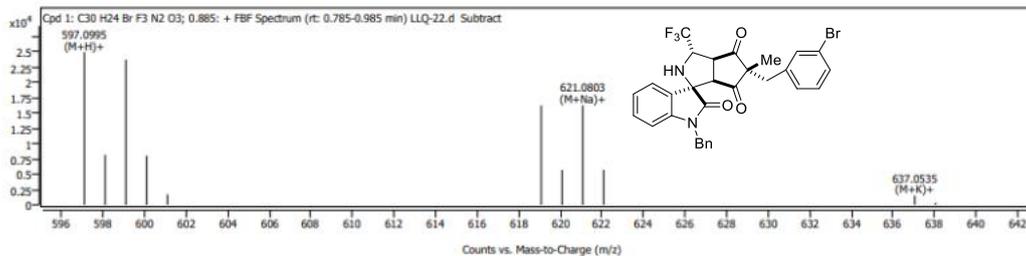
Custom Workflow Report



Compound Details

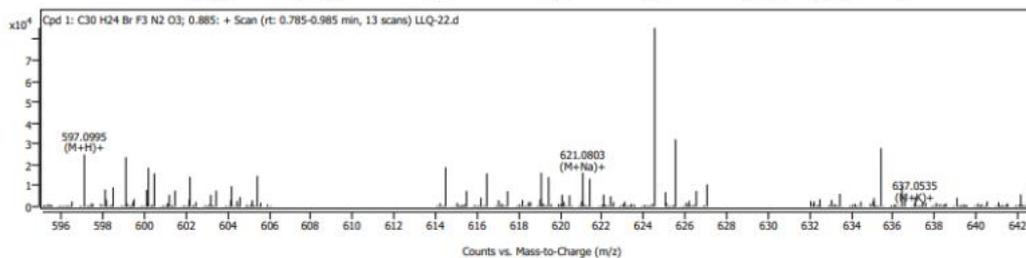
Cpd. 1: C30 H24 Br F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 597.0995 | 597.0995 | -0.04 | 24938 | 100.00 | 96.75 | (M+H)+ | 1 |
| 598.1027 | 598.1028 | -0.13 | 8163 | 32.73 | 32.49 | (M+H)+ | 1 |
| 599.0981 | 599.0980 | 0.23 | 23722 | 95.12 | 100.00 | (M+H)+ | 1 |
| 600.1008 | 600.1009 | -0.21 | 8023 | 32.17 | 32.36 | (M+H)+ | 1 |
| 601.1036 | 601.1038 | -0.43 | 1678 | 6.73 | 5.80 | (M+H)+ | 1 |
| 619.0813 | 619.0815 | -0.28 | 16249 | 99.93 | 96.76 | (M+Na)+ | 1 |
| 620.0847 | 620.0847 | -0.03 | 5695 | 35.03 | 32.48 | (M+Na)+ | 1 |
| 621.0803 | 621.0799 | 0.63 | 16260 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 622.0829 | 622.0828 | 0.09 | 5729 | 35.24 | 32.35 | (M+Na)+ | 1 |
| 637.0535 | 637.0538 | -0.50 | 1513 | 100.00 | 100.00 | (M+K)+ | 1 |
| 638.0540 | 638.0568 | -4.38 | 302 | 19.97 | 32.44 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 597.0995 | 597.0995 | -0.04 | 24938 | 100.00 | 96.75 | (M+H)+ | 1 |
| 598.1027 | 598.1028 | -0.13 | 8163 | 32.73 | 32.49 | (M+H)+ | 1 |
| 599.0981 | 599.0980 | 0.23 | 23722 | 95.12 | 100.00 | (M+H)+ | 1 |
| 600.1008 | 600.1009 | -0.21 | 8023 | 32.17 | 32.36 | (M+H)+ | 1 |
| 601.1036 | 601.1038 | -0.43 | 1678 | 6.73 | 5.80 | (M+H)+ | 1 |
| 619.0813 | 619.0815 | -0.28 | 16249 | 99.93 | 96.76 | (M+Na)+ | 1 |
| 620.0847 | 620.0847 | -0.03 | 5695 | 35.03 | 32.48 | (M+Na)+ | 1 |
| 621.0803 | 621.0799 | 0.63 | 16260 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 622.0829 | 622.0828 | 0.09 | 5729 | 35.24 | 32.35 | (M+Na)+ | 1 |
| 637.0535 | 637.0538 | -0.50 | 1513 | 100.00 | 100.00 | (M+K)+ | 1 |
| 638.0540 | 638.0568 | -4.38 | 302 | 19.97 | 32.44 | (M+K)+ | 1 |

MS spectra of 3ai

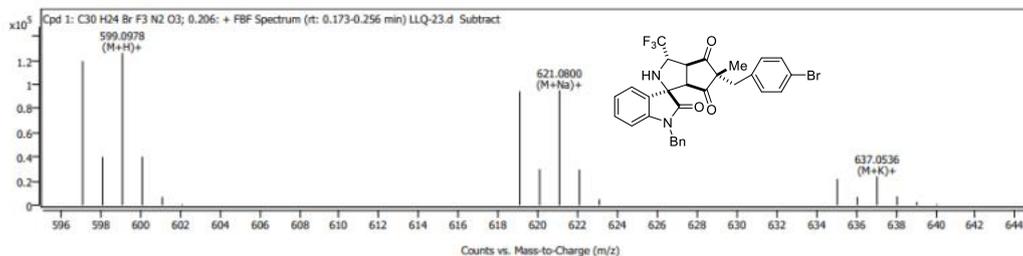
Custom Workflow Report



Compound Details

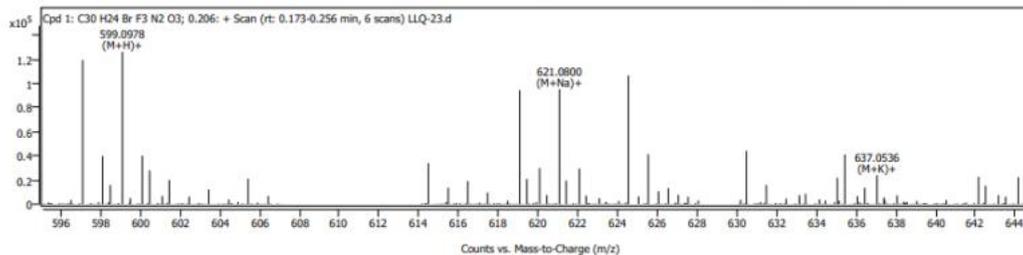
Cpd. 1: C₃₀H₂₄BrF₃N₂O₃

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 597.0995 | 597.0995 | 0.04 | 119468 | 94.78 | 96.75 | (M+H)+ | 1 |
| 598.1026 | 598.1028 | -0.26 | 39986 | 31.72 | 32.49 | (M+H)+ | 1 |
| 599.0978 | 599.0980 | -0.28 | 126047 | 100.00 | 100.00 | (M+H)+ | 1 |
| 600.1007 | 600.1009 | -0.27 | 40211 | 31.90 | 32.36 | (M+H)+ | 1 |
| 601.1034 | 601.1038 | -0.74 | 6793 | 5.39 | 5.80 | (M+H)+ | 1 |
| 602.1060 | 602.1067 | -1.13 | 792 | 0.63 | 0.74 | (M+H)+ | 1 |
| 619.0815 | 619.0815 | 0.04 | 94233 | 98.93 | 96.76 | (M+Na)+ | 1 |
| 620.0846 | 620.0847 | -0.24 | 29844 | 31.33 | 32.48 | (M+Na)+ | 1 |
| 621.0800 | 621.0799 | 0.12 | 95251 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 622.0829 | 622.0828 | 0.04 | 29519 | 30.99 | 32.35 | (M+Na)+ | 1 |
| 623.0856 | 623.0858 | -0.33 | 4931 | 5.18 | 5.79 | (M+Na)+ | 1 |
| 635.0552 | 635.0554 | -0.32 | 21773 | 90.91 | 90.44 | (M+K)+ | 1 |
| 636.0581 | 636.0586 | -0.92 | 6745 | 28.16 | 30.37 | (M+K)+ | 1 |
| 637.0536 | 637.0538 | -0.32 | 23949 | 100.00 | 100.00 | (M+K)+ | 1 |
| 638.0570 | 638.0568 | 0.35 | 7323 | 30.58 | 32.44 | (M+K)+ | 1 |
| 639.0566 | 639.0554 | 1.85 | 2610 | 10.90 | 12.16 | (M+K)+ | 1 |
| 640.0568 | 640.0567 | 0.02 | 834 | 3.48 | 2.87 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 597.0995 | 597.0995 | 0.04 | 119468 | 94.78 | 96.75 | (M+H)+ | 1 |
| 598.1026 | 598.1028 | -0.26 | 39986 | 31.72 | 32.49 | (M+H)+ | 1 |
| 599.0978 | 599.0980 | -0.28 | 126047 | 100.00 | 100.00 | (M+H)+ | 1 |
| 600.1007 | 600.1009 | -0.27 | 40211 | 31.90 | 32.36 | (M+H)+ | 1 |
| 601.1034 | 601.1038 | -0.74 | 6793 | 5.39 | 5.80 | (M+H)+ | 1 |
| 602.1060 | 602.1067 | -1.13 | 792 | 0.63 | 0.74 | (M+H)+ | 1 |
| 619.0815 | 619.0815 | 0.04 | 94233 | 98.93 | 96.76 | (M+Na)+ | 1 |
| 620.0846 | 620.0847 | -0.24 | 29844 | 31.33 | 32.48 | (M+Na)+ | 1 |
| 621.0800 | 621.0799 | 0.12 | 95251 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 622.0829 | 622.0828 | 0.04 | 29519 | 30.99 | 32.35 | (M+Na)+ | 1 |
| 623.0856 | 623.0858 | -0.33 | 4931 | 5.18 | 5.79 | (M+Na)+ | 1 |
| 635.0552 | 635.0554 | -0.32 | 21773 | 90.91 | 90.44 | (M+K)+ | 1 |
| 636.0581 | 636.0586 | -0.92 | 6745 | 28.16 | 30.37 | (M+K)+ | 1 |
| 637.0536 | 637.0538 | -0.32 | 23949 | 100.00 | 100.00 | (M+K)+ | 1 |
| 638.0570 | 638.0568 | 0.35 | 7323 | 30.58 | 32.44 | (M+K)+ | 1 |
| 639.0566 | 639.0554 | 1.85 | 2610 | 10.90 | 12.16 | (M+K)+ | 1 |
| 640.0568 | 640.0567 | 0.02 | 834 | 3.48 | 2.87 | (M+K)+ | 1 |

MS spectra of 3aj

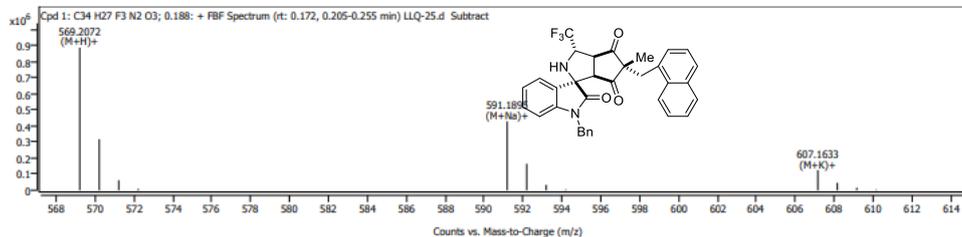
Custom Workflow Report



Compound Details

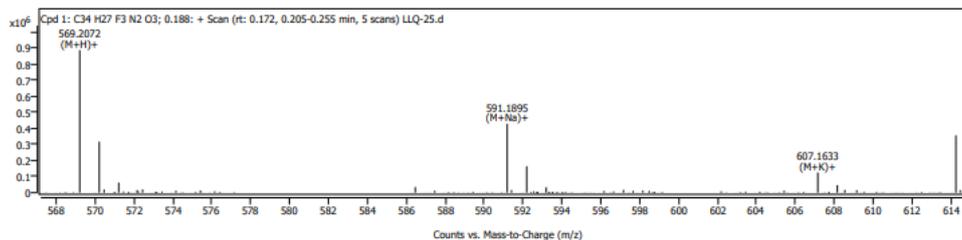
Cpd. 1: C₃₄H₂₇F₃N₂O₃

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 569.2072 | 569.2047 | 4.56 | 886025 | 100.00 | 100.00 | (M+H)+ | 1 |
| 570.2107 | 570.2079 | 4.96 | 317127 | 35.79 | 37.94 | (M+H)+ | 1 |
| 571.2134 | 571.2110 | 4.20 | 62585 | 7.06 | 7.61 | (M+H)+ | 1 |
| 572.2160 | 572.2139 | 3.68 | 8611 | 0.97 | 1.07 | (M+H)+ | 1 |
| 591.1895 | 591.1866 | 4.92 | 428151 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 592.1924 | 592.1899 | 4.32 | 164430 | 38.40 | 37.93 | (M+Na)+ | 1 |
| 593.1954 | 593.1929 | 4.22 | 33447 | 7.81 | 7.61 | (M+Na)+ | 1 |
| 594.1976 | 594.1959 | 2.86 | 4683 | 1.09 | 1.07 | (M+Na)+ | 1 |
| 607.1633 | 607.1605 | 4.56 | 124773 | 100.00 | 100.00 | (M+K)+ | 1 |
| 608.1663 | 608.1638 | 4.16 | 46378 | 37.17 | 37.94 | (M+K)+ | 1 |
| 609.1658 | 609.1629 | 4.86 | 15524 | 12.44 | 14.83 | (M+K)+ | 1 |
| 610.1675 | 610.1641 | 5.57 | 4336 | 3.47 | 3.81 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 569.2072 | 569.2047 | 4.56 | 886025 | 100.00 | 100.00 | (M+H)+ | 1 |
| 570.2107 | 570.2079 | 4.96 | 317127 | 35.79 | 37.94 | (M+H)+ | 1 |
| 571.2134 | 571.2110 | 4.20 | 62585 | 7.06 | 7.61 | (M+H)+ | 1 |
| 572.2160 | 572.2139 | 3.68 | 8611 | 0.97 | 1.07 | (M+H)+ | 1 |
| 591.1895 | 591.1866 | 4.92 | 428151 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 592.1924 | 592.1899 | 4.32 | 164430 | 38.40 | 37.93 | (M+Na)+ | 1 |
| 593.1954 | 593.1929 | 4.22 | 33447 | 7.81 | 7.61 | (M+Na)+ | 1 |
| 594.1976 | 594.1959 | 2.86 | 4683 | 1.09 | 1.07 | (M+Na)+ | 1 |
| 607.1633 | 607.1605 | 4.56 | 124773 | 100.00 | 100.00 | (M+K)+ | 1 |
| 608.1663 | 608.1638 | 4.16 | 46378 | 37.17 | 37.94 | (M+K)+ | 1 |
| 609.1658 | 609.1629 | 4.86 | 15524 | 12.44 | 14.83 | (M+K)+ | 1 |
| 610.1675 | 610.1641 | 5.57 | 4336 | 3.47 | 3.81 | (M+K)+ | 1 |

MS spectra of 3ak

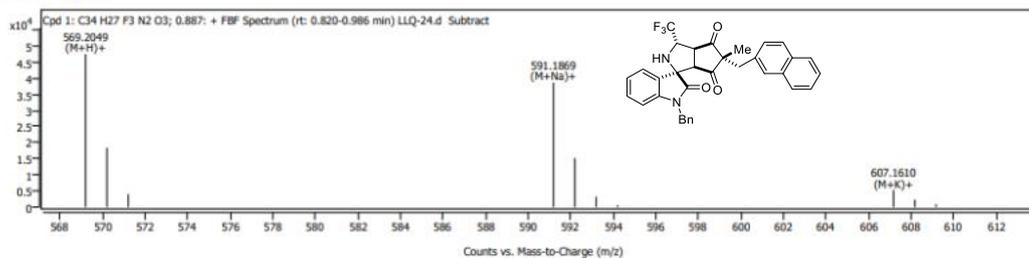
Custom Workflow Report



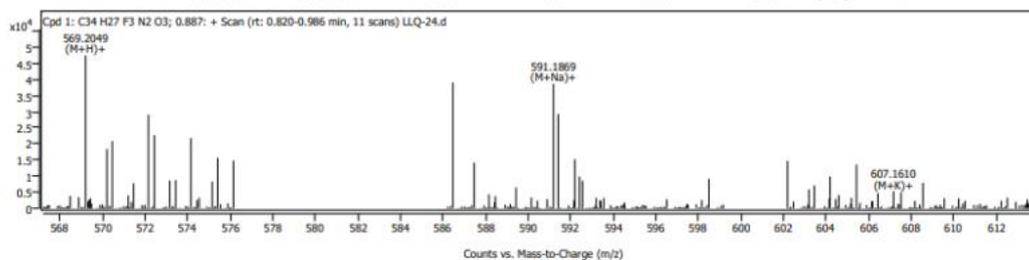
Compound Details

Cpd. 1: C₃₄H₂₇F₃N₂O₃

Compound Spectra



| Spectrum Peaks | | | | | | | |
|----------------|------------|------------|-------|----------|-----------------|-------------|---|
| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
| 569.2049 | 569.2047 | 0.35 | 47470 | 100.00 | 100.00 | (M+H)+ | 1 |
| 570.2081 | 570.2079 | 0.32 | 18422 | 38.81 | 37.94 | (M+H)+ | 1 |
| 571.2108 | 571.2110 | -0.25 | 4035 | 8.50 | 7.61 | (M+H)+ | 1 |
| 591.1869 | 591.1866 | 0.45 | 38621 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 592.1900 | 592.1899 | 0.23 | 15245 | 39.47 | 37.93 | (M+Na)+ | 1 |
| 593.1933 | 593.1929 | 0.64 | 3223 | 8.35 | 7.61 | (M+Na)+ | 1 |
| 594.1998 | 594.1959 | 6.63 | 632 | 1.64 | 1.07 | (M+Na)+ | 1 |
| 607.1610 | 607.1605 | 0.72 | 5308 | 100.00 | 100.00 | (M+K)+ | 1 |
| 608.1647 | 608.1638 | 1.42 | 2312 | 43.55 | 37.94 | (M+K)+ | 1 |
| 609.1623 | 609.1629 | -1.01 | 907 | 17.10 | 14.83 | (M+K)+ | 1 |



| Spectrum Peaks | | | | | | | |
|----------------|------------|------------|-------|----------|-----------------|-------------|---|
| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
| 569.2049 | 569.2047 | 0.35 | 47470 | 100.00 | 100.00 | (M+H)+ | 1 |
| 570.2081 | 570.2079 | 0.32 | 18422 | 38.81 | 37.94 | (M+H)+ | 1 |
| 571.2108 | 571.2110 | -0.25 | 4035 | 8.50 | 7.61 | (M+H)+ | 1 |
| 591.1869 | 591.1866 | 0.45 | 38621 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 592.1900 | 592.1899 | 0.23 | 15245 | 39.47 | 37.93 | (M+Na)+ | 1 |
| 593.1933 | 593.1929 | 0.64 | 3223 | 8.35 | 7.61 | (M+Na)+ | 1 |
| 594.1998 | 594.1959 | 6.63 | 632 | 1.64 | 1.07 | (M+Na)+ | 1 |
| 607.1610 | 607.1605 | 0.72 | 5308 | 100.00 | 100.00 | (M+K)+ | 1 |
| 608.1647 | 608.1638 | 1.42 | 2312 | 43.55 | 37.94 | (M+K)+ | 1 |
| 609.1623 | 609.1629 | -1.01 | 907 | 17.10 | 14.83 | (M+K)+ | 1 |

MS spectra of 3aI

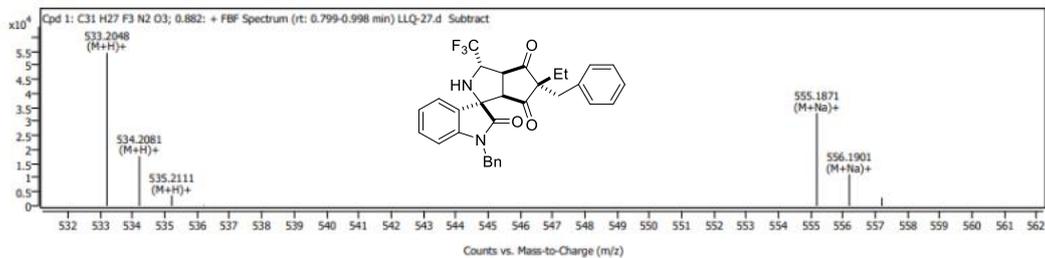
Custom Workflow Report



Compound Details

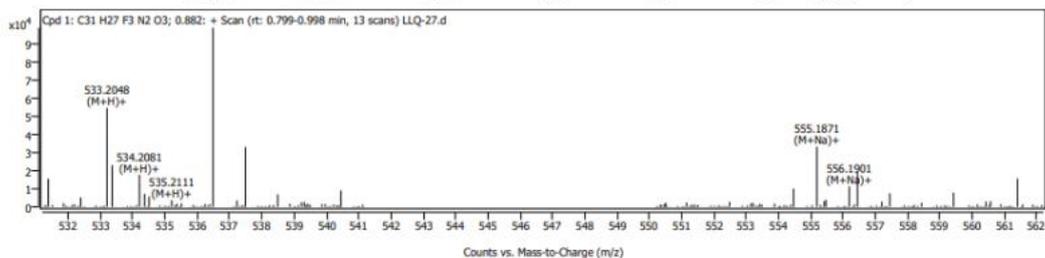
Cpd. 1: C31 H27 F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 533.2048 | 533.2047 | 0.26 | 54477 | 100.00 | 100.00 | (M+H)+ | 1 |
| 534.2081 | 534.2079 | 0.45 | 17702 | 32.49 | 34.70 | (M+H)+ | 1 |
| 535.2111 | 535.2109 | 0.24 | 3723 | 6.83 | 6.45 | (M+H)+ | 1 |
| 536.2122 | 536.2138 | -3.13 | 189 | 0.35 | 0.85 | (M+H)+ | 1 |
| 555.1871 | 555.1866 | 0.91 | 33120 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 556.1901 | 556.1898 | 0.53 | 11242 | 33.94 | 34.68 | (M+Na)+ | 1 |
| 557.1988 | 557.1929 | 10.68 | 2914 | 8.80 | 6.45 | (M+Na)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 533.2048 | 533.2047 | 0.26 | 54477 | 100.00 | 100.00 | (M+H)+ | 1 |
| 534.2081 | 534.2079 | 0.45 | 17702 | 32.49 | 34.70 | (M+H)+ | 1 |
| 535.2111 | 535.2109 | 0.24 | 3723 | 6.83 | 6.45 | (M+H)+ | 1 |
| 536.2122 | 536.2138 | -3.13 | 189 | 0.35 | 0.85 | (M+H)+ | 1 |
| 555.1871 | 555.1866 | 0.91 | 33120 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 556.1901 | 556.1898 | 0.53 | 11242 | 33.94 | 34.68 | (M+Na)+ | 1 |
| 557.1988 | 557.1929 | 10.68 | 2914 | 8.80 | 6.45 | (M+Na)+ | 1 |

MS spectra of 3am

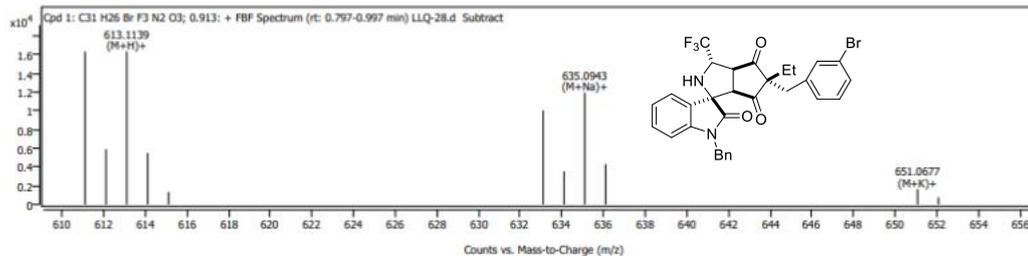
Custom Workflow Report



Compound Details

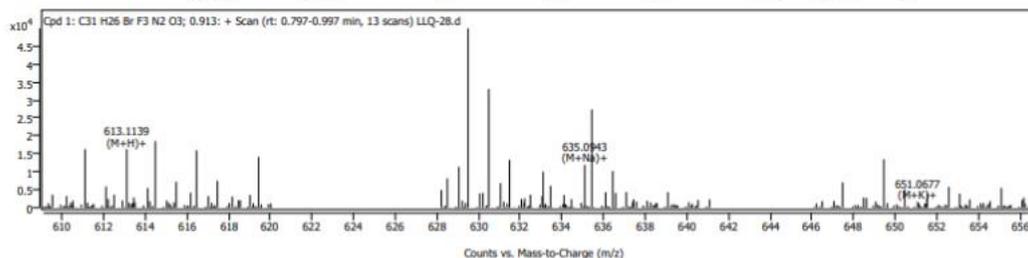
Cpd. 1: C31 H26 Br F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 611.1149 | 611.1152 | -0.36 | 16313 | 99.88 | 96.41 | (M+H)+ | 1 |
| 612.1180 | 612.1184 | -0.75 | 5900 | 36.13 | 33.44 | (M+H)+ | 1 |
| 613.1139 | 613.1136 | 0.36 | 16333 | 100.00 | 100.00 | (M+H)+ | 1 |
| 614.1165 | 614.1166 | -0.18 | 5487 | 33.60 | 33.34 | (M+H)+ | 1 |
| 615.1214 | 615.1195 | 3.07 | 1330 | 8.14 | 6.13 | (M+H)+ | 1 |
| 633.0968 | 633.0971 | -0.57 | 10034 | 84.04 | 96.41 | (M+Na)+ | 1 |
| 634.1001 | 634.1004 | -0.39 | 3547 | 29.71 | 33.43 | (M+Na)+ | 1 |
| 635.0943 | 635.0956 | -2.07 | 11940 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 636.0973 | 636.0985 | -1.95 | 4297 | 35.99 | 33.33 | (M+Na)+ | 1 |
| 651.0677 | 651.0695 | -2.75 | 1642 | 100.00 | 100.00 | (M+K)+ | 1 |
| 652.0729 | 652.0724 | 0.76 | 760 | 46.29 | 33.43 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 611.1149 | 611.1152 | -0.36 | 16313 | 99.88 | 96.41 | (M+H)+ | 1 |
| 612.1180 | 612.1184 | -0.75 | 5900 | 36.13 | 33.44 | (M+H)+ | 1 |
| 613.1139 | 613.1136 | 0.36 | 16333 | 100.00 | 100.00 | (M+H)+ | 1 |
| 614.1165 | 614.1166 | -0.18 | 5487 | 33.60 | 33.34 | (M+H)+ | 1 |
| 615.1214 | 615.1195 | 3.07 | 1330 | 8.14 | 6.13 | (M+H)+ | 1 |
| 633.0968 | 633.0971 | -0.57 | 10034 | 84.04 | 96.41 | (M+Na)+ | 1 |
| 634.1001 | 634.1004 | -0.39 | 3547 | 29.71 | 33.43 | (M+Na)+ | 1 |
| 635.0943 | 635.0956 | -2.07 | 11940 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 636.0973 | 636.0985 | -1.95 | 4297 | 35.99 | 33.33 | (M+Na)+ | 1 |
| 651.0677 | 651.0695 | -2.75 | 1642 | 100.00 | 100.00 | (M+K)+ | 1 |
| 652.0729 | 652.0724 | 0.76 | 760 | 46.29 | 33.43 | (M+K)+ | 1 |

MS spectra of 3an

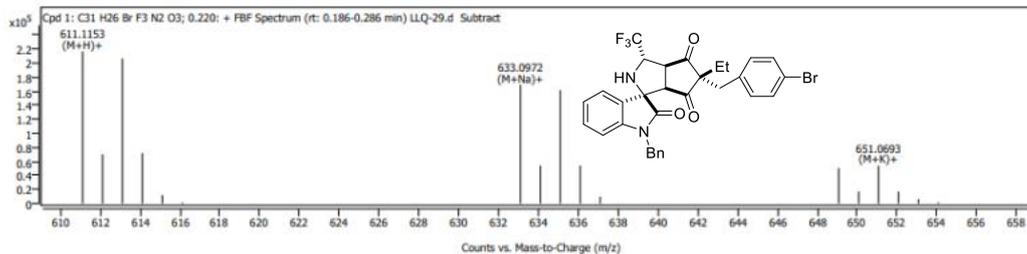
Custom Workflow Report



Compound Details

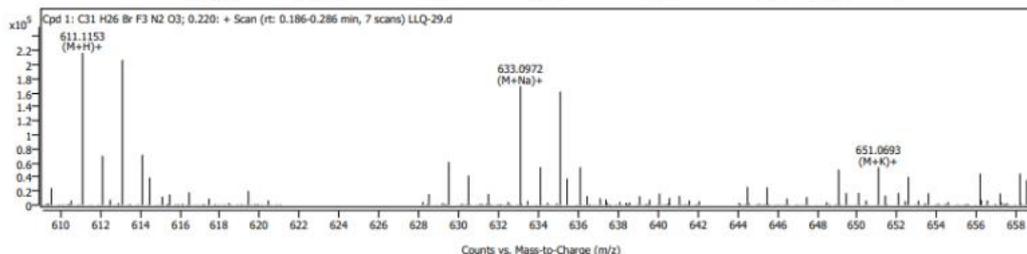
Cpd. 1: C31 H26 Br F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 611.1153 | 611.1152 | 0.29 | 216361 | 100.00 | 96.41 | (M+H)+ | 1 |
| 612.1184 | 612.1184 | -0.05 | 70057 | 32.38 | 33.44 | (M+H)+ | 1 |
| 613.1138 | 613.1136 | 0.20 | 206466 | 95.43 | 100.00 | (M+H)+ | 1 |
| 614.1165 | 614.1166 | -0.12 | 71674 | 33.13 | 33.34 | (M+H)+ | 1 |
| 615.1194 | 615.1195 | -0.12 | 11955 | 5.53 | 6.13 | (M+H)+ | 1 |
| 616.1229 | 616.1224 | 0.88 | 1633 | 0.75 | 0.80 | (M+H)+ | 1 |
| 633.0972 | 633.0971 | 0.08 | 169227 | 100.00 | 96.41 | (M+Na)+ | 1 |
| 634.1003 | 634.1004 | -0.12 | 53984 | 31.90 | 33.43 | (M+Na)+ | 1 |
| 635.0956 | 635.0956 | 0.00 | 161508 | 95.44 | 100.00 | (M+Na)+ | 1 |
| 636.0986 | 636.0985 | 0.07 | 53971 | 31.89 | 33.33 | (M+Na)+ | 1 |
| 637.1010 | 637.1015 | -0.70 | 9759 | 5.77 | 6.13 | (M+Na)+ | 1 |
| 649.0710 | 649.0710 | -0.14 | 50521 | 93.62 | 90.14 | (M+K)+ | 1 |
| 650.0741 | 650.0743 | -0.33 | 17269 | 32.00 | 31.26 | (M+K)+ | 1 |
| 651.0693 | 651.0695 | -0.24 | 53963 | 100.00 | 100.00 | (M+K)+ | 1 |
| 652.0722 | 652.0724 | -0.40 | 17167 | 31.81 | 33.43 | (M+K)+ | 1 |
| 653.0720 | 653.0712 | 1.29 | 6342 | 11.75 | 12.48 | (M+K)+ | 1 |
| 654.0721 | 654.0725 | -0.55 | 1996 | 3.70 | 3.00 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 611.1153 | 611.1152 | 0.29 | 216361 | 100.00 | 96.41 | (M+H)+ | 1 |
| 612.1184 | 612.1184 | -0.05 | 70057 | 32.38 | 33.44 | (M+H)+ | 1 |
| 613.1138 | 613.1136 | 0.20 | 206466 | 95.43 | 100.00 | (M+H)+ | 1 |
| 614.1165 | 614.1166 | -0.12 | 71674 | 33.13 | 33.34 | (M+H)+ | 1 |
| 615.1194 | 615.1195 | -0.12 | 11955 | 5.53 | 6.13 | (M+H)+ | 1 |
| 616.1229 | 616.1224 | 0.88 | 1633 | 0.75 | 0.80 | (M+H)+ | 1 |
| 633.0972 | 633.0971 | 0.08 | 169227 | 100.00 | 96.41 | (M+Na)+ | 1 |
| 634.1003 | 634.1004 | -0.12 | 53984 | 31.90 | 33.43 | (M+Na)+ | 1 |
| 635.0956 | 635.0956 | 0.00 | 161508 | 95.44 | 100.00 | (M+Na)+ | 1 |
| 636.0986 | 636.0985 | 0.07 | 53971 | 31.89 | 33.33 | (M+Na)+ | 1 |
| 637.1010 | 637.1015 | -0.70 | 9759 | 5.77 | 6.13 | (M+Na)+ | 1 |
| 649.0710 | 649.0710 | -0.14 | 50521 | 93.62 | 90.14 | (M+K)+ | 1 |
| 650.0741 | 650.0743 | -0.33 | 17269 | 32.00 | 31.26 | (M+K)+ | 1 |
| 651.0693 | 651.0695 | -0.24 | 53963 | 100.00 | 100.00 | (M+K)+ | 1 |
| 652.0722 | 652.0724 | -0.40 | 17167 | 31.81 | 33.43 | (M+K)+ | 1 |
| 653.0720 | 653.0712 | 1.29 | 6342 | 11.75 | 12.48 | (M+K)+ | 1 |
| 654.0721 | 654.0725 | -0.55 | 1996 | 3.70 | 3.00 | (M+K)+ | 1 |

MS spectra of 5a

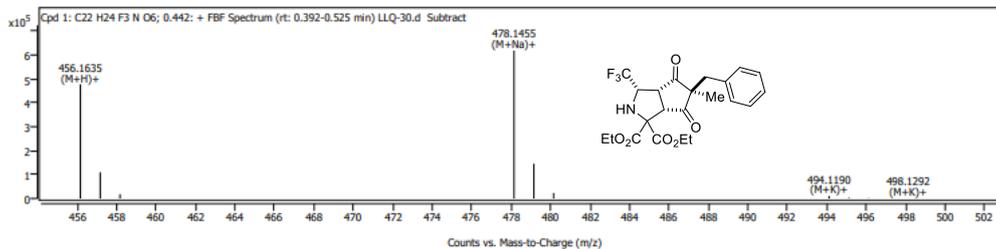
Custom Workflow Report



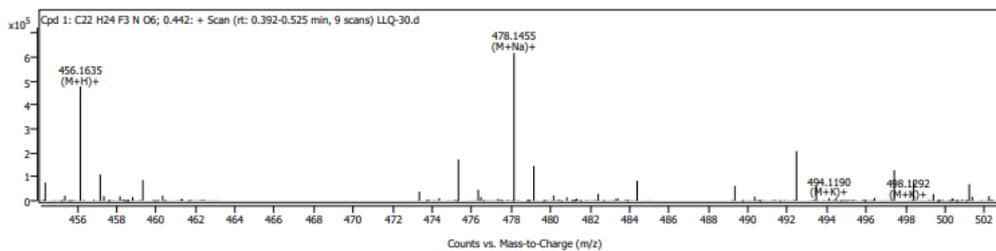
Compound Details

Cpd. 1: C22 H24 F3 N O6

Compound Spectra



| Spectrum Peaks | m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------------|----------|------------|------------|--------|----------|-----------------|-------------|---|
| | 456.1635 | 456.1628 | 1.42 | 478204 | 100.00 | 100.00 | (M+H)+ | 1 |
| | 457.1665 | 457.1662 | 0.79 | 109749 | 22.95 | 24.68 | (M+H)+ | 1 |
| | 458.1691 | 458.1688 | 0.83 | 18224 | 3.81 | 4.15 | (M+H)+ | 1 |
| | 478.1455 | 478.1448 | 1.53 | 619194 | 100.00 | 100.00 | (M+Na)+ | 1 |
| | 479.1487 | 479.1481 | 1.18 | 145815 | 23.55 | 24.66 | (M+Na)+ | 1 |
| | 480.1513 | 480.1507 | 1.28 | 22963 | 3.71 | 4.15 | (M+Na)+ | 1 |
| | 494.1190 | 494.1187 | 0.56 | 10602 | 100.00 | 100.00 | (M+K)+ | 1 |
| | 495.1223 | 495.1220 | 0.63 | 2895 | 27.30 | 24.68 | (M+K)+ | 1 |
| | 496.1200 | 496.1197 | 0.63 | 1254 | 11.83 | 11.37 | (M+K)+ | 1 |
| | 498.1292 | 498.1238 | 10.71 | 54 | 0.51 | 0.35 | (M+K)+ | 1 |



| Spectrum Peaks | m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------------|----------|------------|------------|--------|----------|-----------------|-------------|---|
| | 456.1635 | 456.1628 | 1.42 | 478204 | 100.00 | 100.00 | (M+H)+ | 1 |
| | 457.1665 | 457.1662 | 0.79 | 109749 | 22.95 | 24.68 | (M+H)+ | 1 |
| | 458.1691 | 458.1688 | 0.83 | 18224 | 3.81 | 4.15 | (M+H)+ | 1 |
| | 478.1455 | 478.1448 | 1.53 | 619194 | 100.00 | 100.00 | (M+Na)+ | 1 |
| | 479.1487 | 479.1481 | 1.18 | 145815 | 23.55 | 24.66 | (M+Na)+ | 1 |
| | 480.1513 | 480.1507 | 1.28 | 22963 | 3.71 | 4.15 | (M+Na)+ | 1 |
| | 494.1190 | 494.1187 | 0.56 | 10602 | 100.00 | 100.00 | (M+K)+ | 1 |
| | 495.1223 | 495.1220 | 0.63 | 2895 | 27.30 | 24.68 | (M+K)+ | 1 |
| | 496.1200 | 496.1197 | 0.63 | 1254 | 11.83 | 11.37 | (M+K)+ | 1 |
| | 498.1292 | 498.1238 | 10.71 | 54 | 0.51 | 0.35 | (M+K)+ | 1 |

MS spectra of 5b

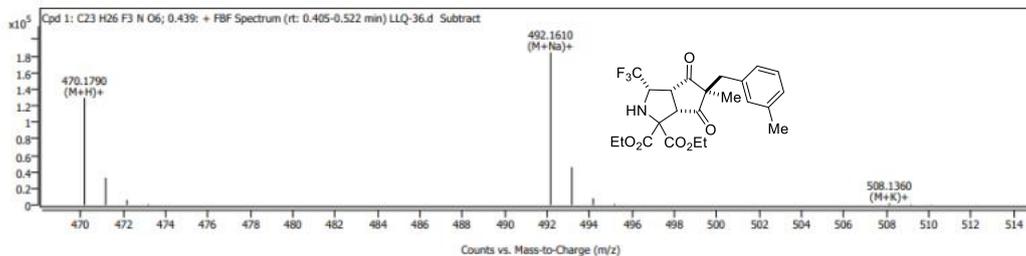
Custom Workflow Report



Compound Details

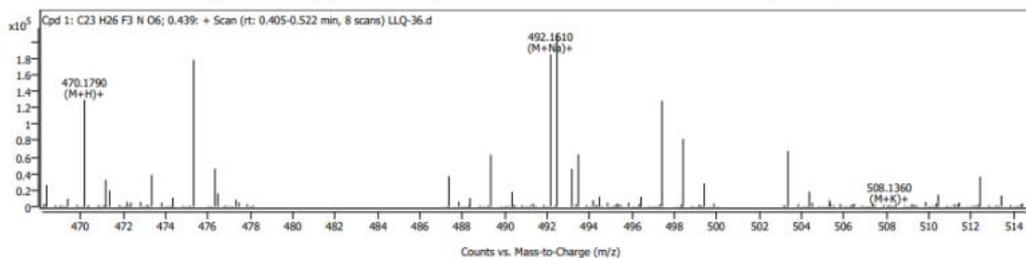
Cpd. 1: C23 H26 F3 N O6

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 470.1790 | 470.1785 | 1.16 | 129387 | 100.00 | 100.00 | (M+H)+ | 1 |
| 471.1819 | 471.1818 | 0.30 | 32758 | 25.32 | 25.78 | (M+H)+ | 1 |
| 472.1845 | 472.1845 | 0.07 | 6056 | 4.68 | 4.42 | (M+H)+ | 1 |
| 473.1891 | 473.1871 | 4.29 | 1011 | 0.78 | 0.57 | (M+H)+ | 1 |
| 492.1610 | 492.1604 | 1.22 | 184478 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 493.1642 | 493.1638 | 0.96 | 45706 | 24.78 | 25.77 | (M+Na)+ | 1 |
| 494.1668 | 494.1664 | 0.77 | 8016 | 4.35 | 4.42 | (M+Na)+ | 1 |
| 495.1714 | 495.1690 | 4.77 | 1259 | 0.68 | 0.57 | (M+Na)+ | 1 |
| 508.1360 | 508.1344 | 3.16 | 2260 | 100.00 | 100.00 | (M+K)+ | 1 |
| 509.1418 | 509.1377 | 8.02 | 834 | 36.88 | 25.78 | (M+K)+ | 1 |
| 510.1344 | 510.1355 | -2.19 | 486 | 21.50 | 11.64 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 470.1790 | 470.1785 | 1.16 | 129387 | 100.00 | 100.00 | (M+H)+ | 1 |
| 471.1819 | 471.1818 | 0.30 | 32758 | 25.32 | 25.78 | (M+H)+ | 1 |
| 472.1845 | 472.1845 | 0.07 | 6056 | 4.68 | 4.42 | (M+H)+ | 1 |
| 473.1891 | 473.1871 | 4.29 | 1011 | 0.78 | 0.57 | (M+H)+ | 1 |
| 492.1610 | 492.1604 | 1.22 | 184478 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 493.1642 | 493.1638 | 0.96 | 45706 | 24.78 | 25.77 | (M+Na)+ | 1 |
| 494.1668 | 494.1664 | 0.77 | 8016 | 4.35 | 4.42 | (M+Na)+ | 1 |
| 495.1714 | 495.1690 | 4.77 | 1259 | 0.68 | 0.57 | (M+Na)+ | 1 |
| 508.1360 | 508.1344 | 3.16 | 2260 | 100.00 | 100.00 | (M+K)+ | 1 |
| 509.1418 | 509.1377 | 8.02 | 834 | 36.88 | 25.78 | (M+K)+ | 1 |
| 510.1344 | 510.1355 | -2.19 | 486 | 21.50 | 11.64 | (M+K)+ | 1 |

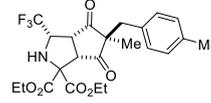
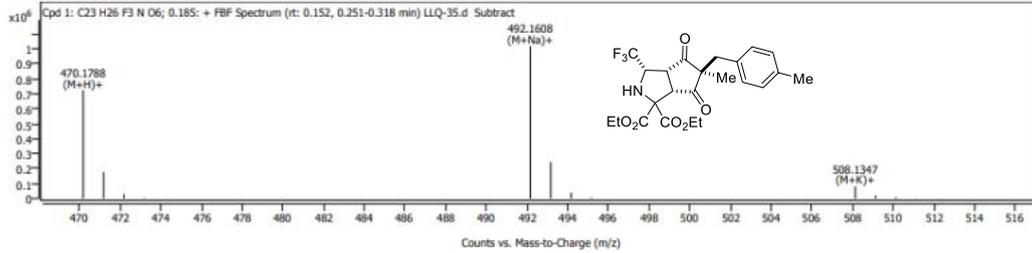
Custom Workflow Report



Compound Details

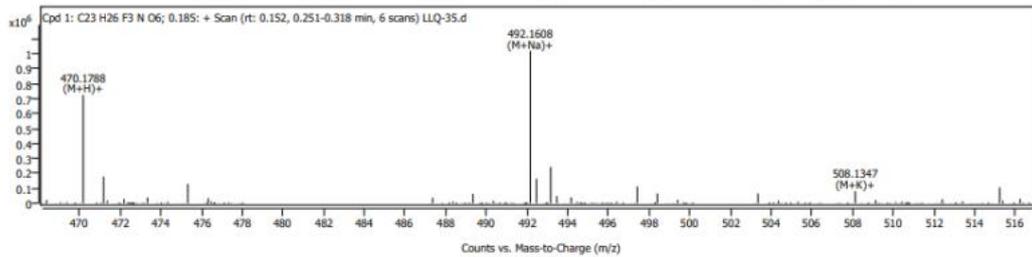
Cpd. 1: C23 H26 F3 N O6

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|---------|----------|-----------------|-------------|---|
| 470.1788 | 470.1785 | 0.63 | 723910 | 100.00 | 100.00 | (M+H)+ | 1 |
| 471.1820 | 471.1818 | 0.39 | 177929 | 24.58 | 25.78 | (M+H)+ | 1 |
| 472.1846 | 472.1845 | 0.37 | 28781 | 3.98 | 4.42 | (M+H)+ | 1 |
| 473.1874 | 473.1871 | 0.57 | 4052 | 0.56 | 0.57 | (M+H)+ | 1 |
| 492.1608 | 492.1604 | 0.69 | 1018487 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 493.1640 | 493.1638 | 0.43 | 242763 | 23.84 | 25.77 | (M+Na)+ | 1 |
| 494.1665 | 494.1664 | 0.25 | 39401 | 3.87 | 4.42 | (M+Na)+ | 1 |
| 495.1695 | 495.1690 | 1.02 | 5249 | 0.52 | 0.57 | (M+Na)+ | 1 |
| 508.1347 | 508.1344 | 0.65 | 80836 | 100.00 | 100.00 | (M+K)+ | 1 |
| 509.1378 | 509.1377 | 0.18 | 20636 | 25.53 | 25.78 | (M+K)+ | 1 |
| 510.1355 | 510.1355 | 0.06 | 8481 | 10.49 | 11.64 | (M+K)+ | 1 |
| 511.1362 | 511.1375 | -2.53 | 1862 | 2.30 | 2.43 | (M+K)+ | 1 |
| 512.1335 | 512.1396 | -11.85 | 222 | 0.27 | 0.38 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|---------|----------|-----------------|-------------|---|
| 470.1788 | 470.1785 | 0.63 | 723910 | 100.00 | 100.00 | (M+H)+ | 1 |
| 471.1820 | 471.1818 | 0.39 | 177929 | 24.58 | 25.78 | (M+H)+ | 1 |
| 472.1846 | 472.1845 | 0.37 | 28781 | 3.98 | 4.42 | (M+H)+ | 1 |
| 473.1874 | 473.1871 | 0.57 | 4052 | 0.56 | 0.57 | (M+H)+ | 1 |
| 492.1608 | 492.1604 | 0.69 | 1018487 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 493.1640 | 493.1638 | 0.43 | 242763 | 23.84 | 25.77 | (M+Na)+ | 1 |
| 494.1665 | 494.1664 | 0.25 | 39401 | 3.87 | 4.42 | (M+Na)+ | 1 |
| 495.1695 | 495.1690 | 1.02 | 5249 | 0.52 | 0.57 | (M+Na)+ | 1 |
| 508.1347 | 508.1344 | 0.65 | 80836 | 100.00 | 100.00 | (M+K)+ | 1 |
| 509.1378 | 509.1377 | 0.18 | 20636 | 25.53 | 25.78 | (M+K)+ | 1 |
| 510.1355 | 510.1355 | 0.06 | 8481 | 10.49 | 11.64 | (M+K)+ | 1 |
| 511.1362 | 511.1375 | -2.53 | 1862 | 2.30 | 2.43 | (M+K)+ | 1 |
| 512.1335 | 512.1396 | -11.85 | 222 | 0.27 | 0.38 | (M+K)+ | 1 |

MS spectra of 5d

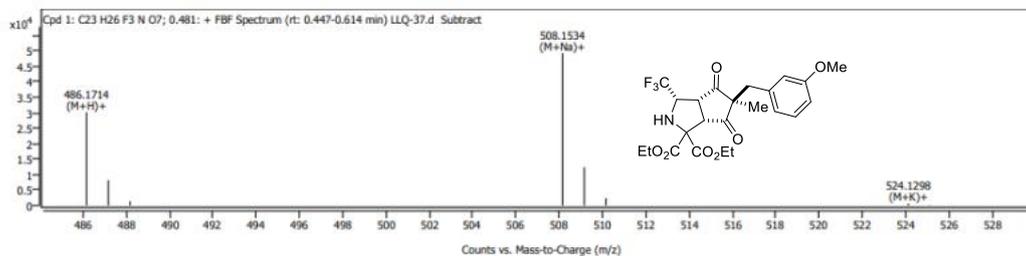
Custom Workflow Report



Compound Details

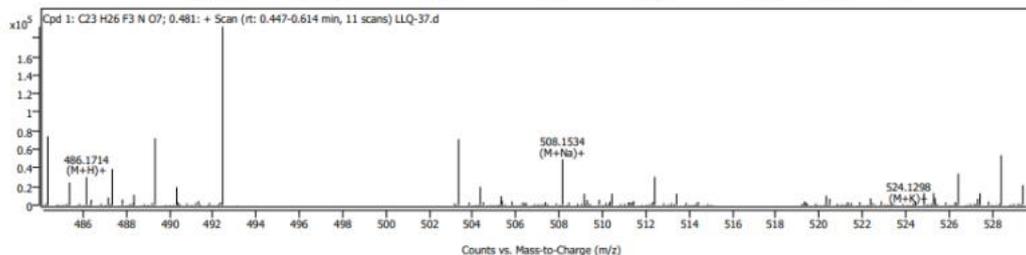
Cpd. 1: C23 H26 F3 N O7

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 486.1714 | 486.1734 | -4.18 | 30213 | 100.00 | 100.00 | (M+H)+ | 1 |
| 487.1751 | 487.1767 | -3.42 | 8180 | 27.07 | 25.82 | (M+H)+ | 1 |
| 488.1784 | 488.1793 | -1.81 | 1359 | 4.50 | 4.64 | (M+H)+ | 1 |
| 508.1534 | 508.1554 | -3.87 | 49310 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 509.1571 | 509.1587 | -3.16 | 12408 | 25.16 | 25.81 | (M+Na)+ | 1 |
| 510.1600 | 510.1612 | -2.36 | 2342 | 4.75 | 4.63 | (M+Na)+ | 1 |
| 524.1298 | 524.1293 | 0.96 | 694 | 100.00 | 100.00 | (M+K)+ | 1 |
| 525.1235 | 525.1326 | -17.43 | 153 | 22.07 | 25.82 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 486.1714 | 486.1734 | -4.18 | 30213 | 100.00 | 100.00 | (M+H)+ | 1 |
| 487.1751 | 487.1767 | -3.42 | 8180 | 27.07 | 25.82 | (M+H)+ | 1 |
| 488.1784 | 488.1793 | -1.81 | 1359 | 4.50 | 4.64 | (M+H)+ | 1 |
| 508.1534 | 508.1554 | -3.87 | 49310 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 509.1571 | 509.1587 | -3.16 | 12408 | 25.16 | 25.81 | (M+Na)+ | 1 |
| 510.1600 | 510.1612 | -2.36 | 2342 | 4.75 | 4.63 | (M+Na)+ | 1 |
| 524.1298 | 524.1293 | 0.96 | 694 | 100.00 | 100.00 | (M+K)+ | 1 |
| 525.1235 | 525.1326 | -17.43 | 153 | 22.07 | 25.82 | (M+K)+ | 1 |

Header
Data

MS spectra of 5e

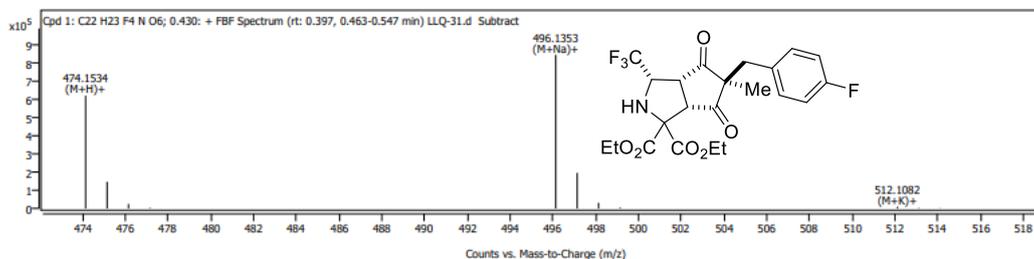
Custom Workflow Report



Compound Details

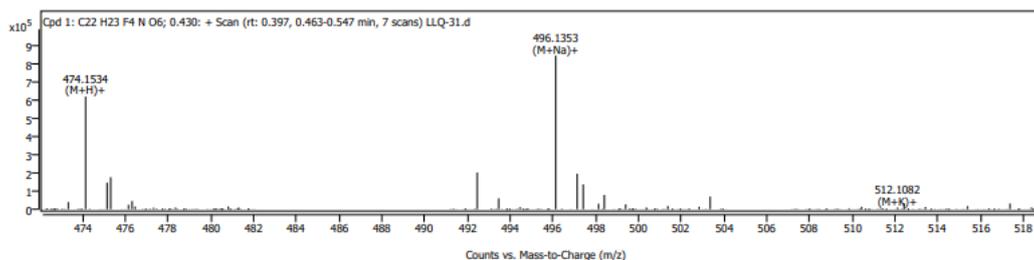
Cpd. 1: C22 H23 F4 N O6

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 474.1534 | 474.1534 | -0.05 | 621233 | 100.00 | 100.00 | (M+H)+ | 1 |
| 475.1567 | 475.1567 | -0.16 | 146644 | 23.61 | 24.66 | (M+H)+ | 1 |
| 476.1590 | 476.1593 | -0.72 | 24736 | 3.98 | 4.15 | (M+H)+ | 1 |
| 477.1613 | 477.1620 | -1.37 | 3595 | 0.58 | 0.52 | (M+H)+ | 1 |
| 496.1353 | 496.1354 | -0.10 | 846512 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 497.1387 | 497.1387 | -0.01 | 195950 | 23.15 | 24.65 | (M+Na)+ | 1 |
| 498.1408 | 498.1413 | -1.02 | 30778 | 3.64 | 4.14 | (M+Na)+ | 1 |
| 499.1505 | 499.1439 | 13.19 | 4712 | 0.56 | 0.52 | (M+Na)+ | 1 |
| 512.1082 | 512.1093 | -2.13 | 9629 | 100.00 | 100.00 | (M+K)+ | 1 |
| 513.1130 | 513.1126 | 0.70 | 2841 | 29.50 | 24.67 | (M+K)+ | 1 |
| 514.1099 | 514.1103 | -0.65 | 1529 | 15.88 | 11.36 | (M+K)+ | 1 |



Spectrum Peaks

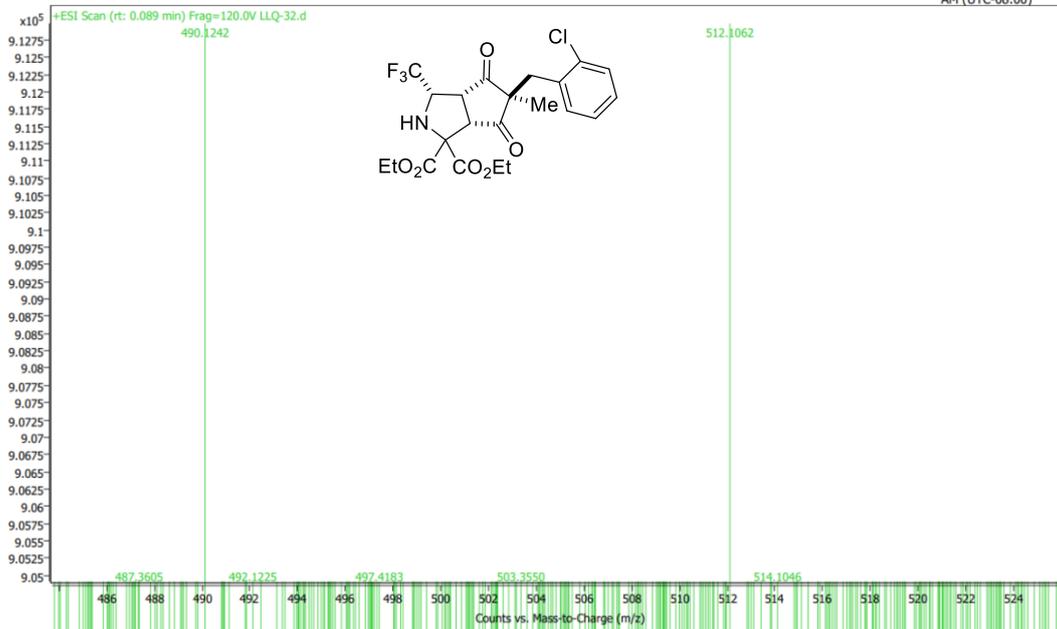
| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 474.1534 | 474.1534 | -0.05 | 621233 | 100.00 | 100.00 | (M+H)+ | 1 |
| 475.1567 | 475.1567 | -0.16 | 146644 | 23.61 | 24.66 | (M+H)+ | 1 |
| 476.1590 | 476.1593 | -0.72 | 24736 | 3.98 | 4.15 | (M+H)+ | 1 |
| 477.1613 | 477.1620 | -1.37 | 3595 | 0.58 | 0.52 | (M+H)+ | 1 |
| 496.1353 | 496.1354 | -0.10 | 846512 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 497.1387 | 497.1387 | -0.01 | 195950 | 23.15 | 24.65 | (M+Na)+ | 1 |
| 498.1408 | 498.1413 | -1.02 | 30778 | 3.64 | 4.14 | (M+Na)+ | 1 |
| 499.1505 | 499.1439 | 13.19 | 4712 | 0.56 | 0.52 | (M+Na)+ | 1 |
| 512.1082 | 512.1093 | -2.13 | 9629 | 100.00 | 100.00 | (M+K)+ | 1 |
| 513.1130 | 513.1126 | 0.70 | 2841 | 29.50 | 24.67 | (M+K)+ | 1 |
| 514.1099 | 514.1103 | -0.65 | 1529 | 15.88 | 11.36 | (M+K)+ | 1 |

MS spectra of 5f

User Spectrum Plot Report



| Name | LLQ-32 | Rack Pos. | Instrument | Instrument 1 | Operator |
|----------------|----------|--------------|------------|-----------------|-----------------------------------|
| Inj. Vol. (ul) | 10 | Plate Pos. | IRM Status | All ions missed | |
| Data File | LLQ-32.d | Method (Acq) | 1367.m | Comment | Acq. Time (Local) |
| | | | | | 11/11/2022 2:54:38 AM (UTC-08:00) |



MS spectra of 5g

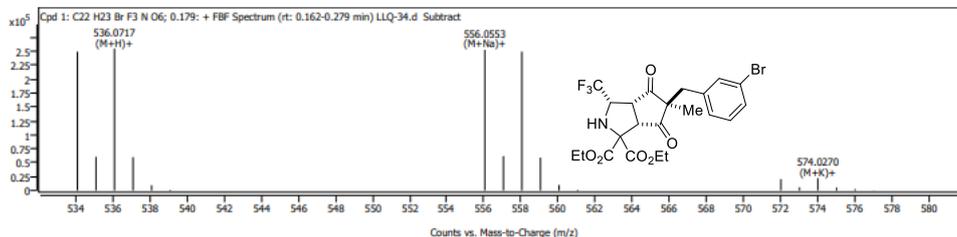
Custom Workflow Report



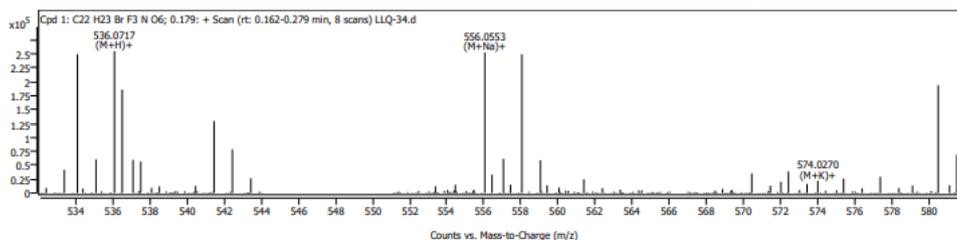
Compound Details

Cpd. 1: C22 H23 Br F3 N O6

Compound Spectra



| Spectrum Peaks | | | | | | | |
|----------------|------------|------------|--------|----------|-----------------|-------------|---|
| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
| 534.0732 | 534.0734 | -0.23 | 249547 | 97.87 | 98.60 | (M+H)+ | 1 |
| 535.0763 | 535.0767 | -0.72 | 60417 | 23.69 | 24.32 | (M+H)+ | 1 |
| 536.0717 | 536.0716 | 0.05 | 254979 | 100.00 | 100.00 | (M+H)+ | 1 |
| 537.0745 | 537.0748 | -0.50 | 59885 | 23.49 | 24.17 | (M+H)+ | 1 |
| 538.0768 | 538.0773 | -0.92 | 9460 | 3.71 | 4.03 | (M+H)+ | 1 |
| 539.0788 | 539.0799 | -2.09 | 1325 | 0.52 | 0.51 | (M+H)+ | 1 |
| 556.0553 | 556.0553 | 0.03 | 252877 | 100.00 | 98.60 | (M+Na)+ | 1 |
| 557.0583 | 557.0586 | -0.63 | 61675 | 24.39 | 24.31 | (M+Na)+ | 1 |
| 558.0535 | 558.0536 | -0.22 | 249600 | 98.70 | 100.00 | (M+Na)+ | 1 |
| 559.0565 | 559.0567 | -0.39 | 59086 | 23.37 | 24.16 | (M+Na)+ | 1 |
| 560.0593 | 560.0593 | 0.01 | 9815 | 3.88 | 4.03 | (M+Na)+ | 1 |
| 561.0622 | 561.0619 | 0.53 | 1481 | 0.59 | 0.51 | (M+Na)+ | 1 |
| 572.0287 | 572.0292 | -0.88 | 20300 | 91.59 | 92.05 | (M+K)+ | 1 |
| 573.0317 | 573.0325 | -1.49 | 5399 | 24.36 | 22.70 | (M+K)+ | 1 |
| 574.0270 | 574.0275 | -0.83 | 22163 | 100.00 | 100.00 | (M+K)+ | 1 |
| 575.0300 | 575.0307 | -1.05 | 5016 | 22.63 | 24.20 | (M+K)+ | 1 |
| 576.0291 | 576.0283 | 1.40 | 2519 | 11.37 | 10.50 | (M+K)+ | 1 |
| 577.0370 | 577.0303 | 11.47 | 454 | 2.05 | 2.10 | (M+K)+ | 1 |



| Spectrum Peaks | | | | | | | |
|----------------|------------|------------|--------|----------|-----------------|-------------|---|
| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
| 534.0732 | 534.0734 | -0.23 | 249547 | 97.87 | 98.60 | (M+H)+ | 1 |
| 535.0763 | 535.0767 | -0.72 | 60417 | 23.69 | 24.32 | (M+H)+ | 1 |
| 536.0717 | 536.0716 | 0.05 | 254979 | 100.00 | 100.00 | (M+H)+ | 1 |
| 537.0745 | 537.0748 | -0.50 | 59885 | 23.49 | 24.17 | (M+H)+ | 1 |
| 538.0768 | 538.0773 | -0.92 | 9460 | 3.71 | 4.03 | (M+H)+ | 1 |
| 539.0788 | 539.0799 | -2.09 | 1325 | 0.52 | 0.51 | (M+H)+ | 1 |
| 556.0553 | 556.0553 | 0.03 | 252877 | 100.00 | 98.60 | (M+Na)+ | 1 |
| 557.0583 | 557.0586 | -0.63 | 61675 | 24.39 | 24.31 | (M+Na)+ | 1 |
| 558.0535 | 558.0536 | -0.22 | 249600 | 98.70 | 100.00 | (M+Na)+ | 1 |
| 559.0565 | 559.0567 | -0.39 | 59086 | 23.37 | 24.16 | (M+Na)+ | 1 |
| 560.0593 | 560.0593 | 0.01 | 9815 | 3.88 | 4.03 | (M+Na)+ | 1 |
| 561.0622 | 561.0619 | 0.53 | 1481 | 0.59 | 0.51 | (M+Na)+ | 1 |
| 572.0287 | 572.0292 | -0.88 | 20300 | 91.59 | 92.05 | (M+K)+ | 1 |
| 573.0317 | 573.0325 | -1.49 | 5399 | 24.36 | 22.70 | (M+K)+ | 1 |
| 574.0270 | 574.0275 | -0.83 | 22163 | 100.00 | 100.00 | (M+K)+ | 1 |
| 575.0300 | 575.0307 | -1.05 | 5016 | 22.63 | 24.20 | (M+K)+ | 1 |
| 576.0291 | 576.0283 | 1.40 | 2519 | 11.37 | 10.50 | (M+K)+ | 1 |
| 577.0370 | 577.0303 | 11.47 | 454 | 2.05 | 2.10 | (M+K)+ | 1 |

MS spectra of 5h

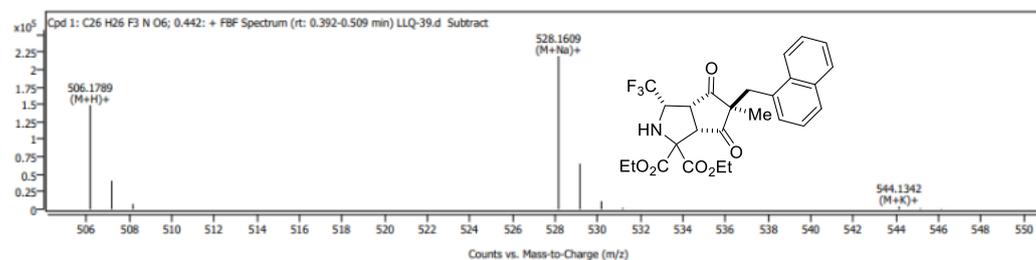
Custom Workflow Report



Compound Details

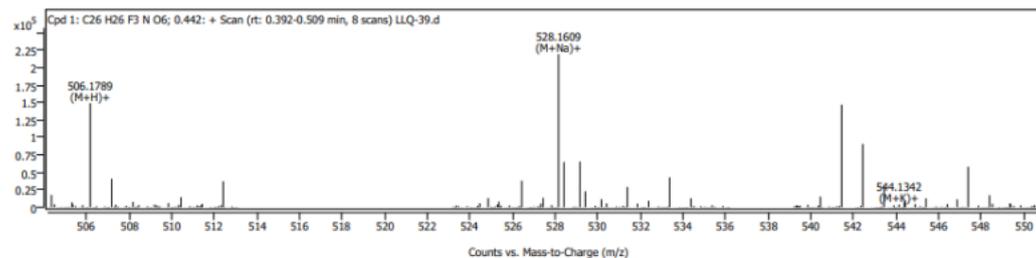
Cpd. 1: C₂₆H₂₆F₃N O₆

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 506.1789 | 506.1785 | 0.84 | 149107 | 100.00 | 100.00 | (M+H)+ | 1 |
| 507.1818 | 507.1818 | 0.02 | 40963 | 27.47 | 29.03 | (M+H)+ | 1 |
| 508.1846 | 508.1846 | 0.11 | 7736 | 5.19 | 5.29 | (M+H)+ | 1 |
| 528.1609 | 528.1604 | 0.80 | 219260 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 529.1640 | 529.1638 | 0.54 | 65329 | 29.80 | 29.01 | (M+Na)+ | 1 |
| 530.1671 | 530.1665 | 1.03 | 11653 | 5.31 | 5.29 | (M+Na)+ | 1 |
| 531.1723 | 531.1692 | 5.92 | 1940 | 0.88 | 0.72 | (M+Na)+ | 1 |
| 544.1342 | 544.1344 | -0.34 | 3950 | 100.00 | 100.00 | (M+K)+ | 1 |
| 545.1378 | 545.1377 | 0.21 | 1465 | 37.08 | 29.03 | (M+K)+ | 1 |
| 546.1329 | 546.1359 | -5.51 | 895 | 22.66 | 12.51 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 506.1789 | 506.1785 | 0.84 | 149107 | 100.00 | 100.00 | (M+H)+ | 1 |
| 507.1818 | 507.1818 | 0.02 | 40963 | 27.47 | 29.03 | (M+H)+ | 1 |
| 508.1846 | 508.1846 | 0.11 | 7736 | 5.19 | 5.29 | (M+H)+ | 1 |
| 528.1609 | 528.1604 | 0.80 | 219260 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 529.1640 | 529.1638 | 0.54 | 65329 | 29.80 | 29.01 | (M+Na)+ | 1 |
| 530.1671 | 530.1665 | 1.03 | 11653 | 5.31 | 5.29 | (M+Na)+ | 1 |
| 531.1723 | 531.1692 | 5.92 | 1940 | 0.88 | 0.72 | (M+Na)+ | 1 |
| 544.1342 | 544.1344 | -0.34 | 3950 | 100.00 | 100.00 | (M+K)+ | 1 |
| 545.1378 | 545.1377 | 0.21 | 1465 | 37.08 | 29.03 | (M+K)+ | 1 |
| 546.1329 | 546.1359 | -5.51 | 895 | 22.66 | 12.51 | (M+K)+ | 1 |

MS spectra of 5i

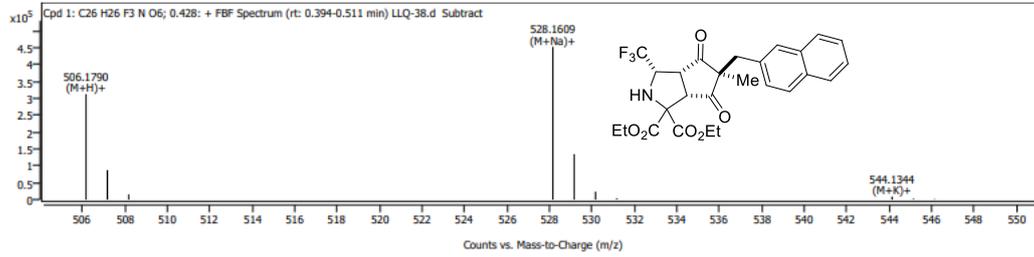
Custom Workflow Report



Compound Details

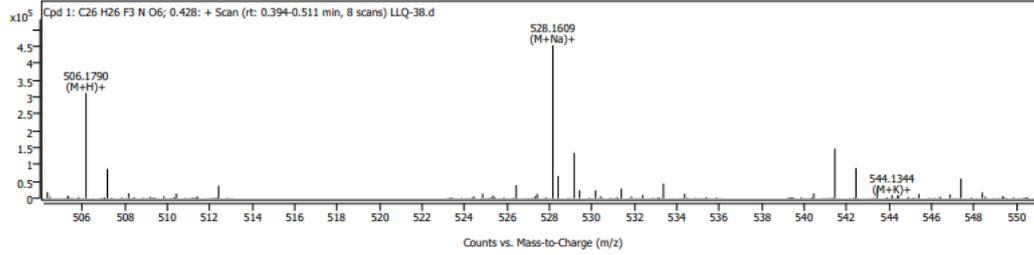
Cpd. 1: C26 H26 F3 N O6

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 506.1790 | 506.1785 | 0.94 | 312723 | 100.00 | 100.00 | (M+H)+ | 1 |
| 507.1818 | 507.1818 | -0.01 | 87332 | 27.93 | 29.03 | (M+H)+ | 1 |
| 508.1846 | 508.1846 | 0.01 | 15353 | 4.91 | 5.29 | (M+H)+ | 1 |
| 528.1609 | 528.1604 | 0.87 | 453006 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 529.1639 | 529.1638 | 0.30 | 134582 | 29.71 | 29.01 | (M+Na)+ | 1 |
| 530.1668 | 530.1665 | 0.56 | 23509 | 5.19 | 5.29 | (M+Na)+ | 1 |
| 531.1711 | 531.1692 | 3.50 | 3579 | 0.79 | 0.72 | (M+Na)+ | 1 |
| 544.1344 | 544.1344 | -0.05 | 8885 | 100.00 | 100.00 | (M+K)+ | 1 |
| 545.1373 | 545.1377 | -0.76 | 2667 | 30.02 | 29.03 | (M+K)+ | 1 |
| 546.1365 | 546.1359 | 1.18 | 1417 | 15.95 | 12.51 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 506.1790 | 506.1785 | 0.94 | 312723 | 100.00 | 100.00 | (M+H)+ | 1 |
| 507.1818 | 507.1818 | -0.01 | 87332 | 27.93 | 29.03 | (M+H)+ | 1 |
| 508.1846 | 508.1846 | 0.01 | 15353 | 4.91 | 5.29 | (M+H)+ | 1 |
| 528.1609 | 528.1604 | 0.87 | 453006 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 529.1639 | 529.1638 | 0.30 | 134582 | 29.71 | 29.01 | (M+Na)+ | 1 |
| 530.1668 | 530.1665 | 0.56 | 23509 | 5.19 | 5.29 | (M+Na)+ | 1 |
| 531.1711 | 531.1692 | 3.50 | 3579 | 0.79 | 0.72 | (M+Na)+ | 1 |
| 544.1344 | 544.1344 | -0.05 | 8885 | 100.00 | 100.00 | (M+K)+ | 1 |
| 545.1373 | 545.1377 | -0.76 | 2667 | 30.02 | 29.03 | (M+K)+ | 1 |
| 546.1365 | 546.1359 | 1.18 | 1417 | 15.95 | 12.51 | (M+K)+ | 1 |

MS spectra of 6

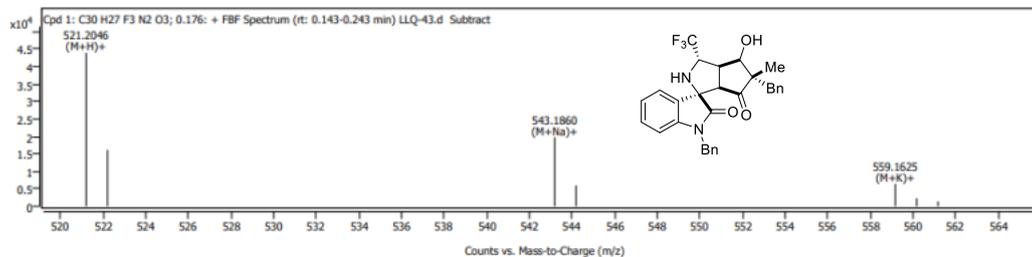
Custom Workflow Report



Compound Details

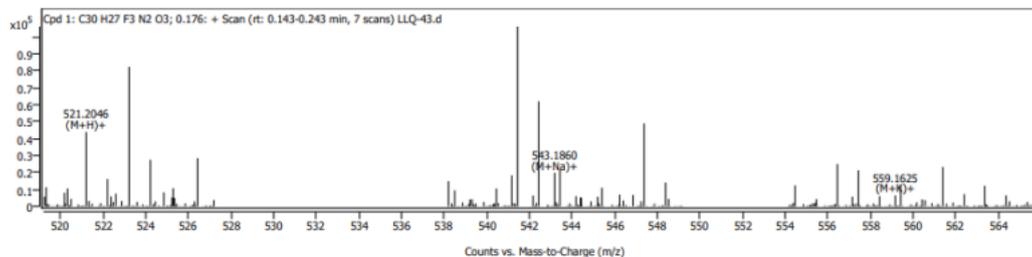
Cpd. 1: C30 H27 F3 N2 O3

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 521.2046 | 521.2047 | -0.09 | 43941 | 100.00 | 100.00 | (M+H)+ | 1 |
| 522.2081 | 522.2079 | 0.37 | 16182 | 36.83 | 33.61 | (M+H)+ | 1 |
| 543.1860 | 543.1866 | -1.18 | 19771 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 544.1895 | 544.1898 | -0.59 | 5979 | 30.24 | 33.60 | (M+Na)+ | 1 |
| 559.1625 | 559.1605 | 3.45 | 6441 | 100.00 | 100.00 | (M+K)+ | 1 |
| 560.1669 | 560.1638 | 5.49 | 2305 | 35.79 | 33.62 | (M+K)+ | 1 |
| 561.1661 | 561.1624 | 6.61 | 1391 | 21.60 | 13.31 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 521.2046 | 521.2047 | -0.09 | 43941 | 100.00 | 100.00 | (M+H)+ | 1 |
| 522.2081 | 522.2079 | 0.37 | 16182 | 36.83 | 33.61 | (M+H)+ | 1 |
| 543.1860 | 543.1866 | -1.18 | 19771 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 544.1895 | 544.1898 | -0.59 | 5979 | 30.24 | 33.60 | (M+Na)+ | 1 |
| 559.1625 | 559.1605 | 3.45 | 6441 | 100.00 | 100.00 | (M+K)+ | 1 |
| 560.1669 | 560.1638 | 5.49 | 2305 | 35.79 | 33.62 | (M+K)+ | 1 |
| 561.1661 | 561.1624 | 6.61 | 1391 | 21.60 | 13.31 | (M+K)+ | 1 |

Header
Data

MS spectra of 7

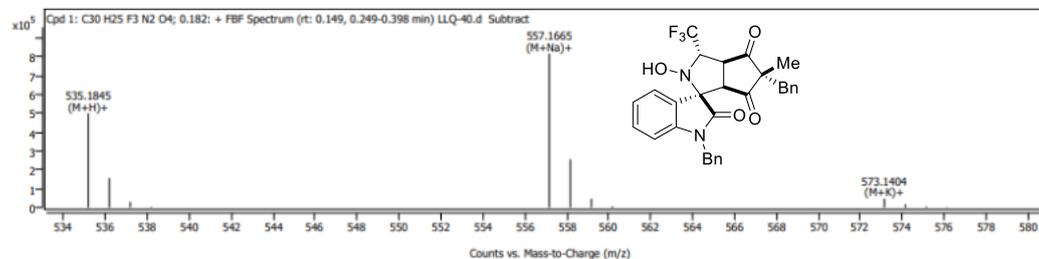
Custom Workflow Report



Compound Details

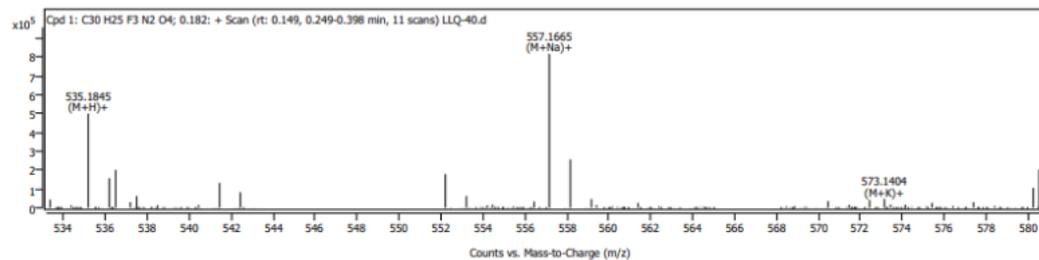
Cpd. 1: C30 H25 F3 N2 O4

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 535.1845 | 535.1839 | 1.11 | 499625 | 100.00 | 100.00 | (M+H)+ | 1 |
| 536.1876 | 536.1872 | 0.78 | 156286 | 31.28 | 33.63 | (M+H)+ | 1 |
| 537.1906 | 537.1901 | 0.81 | 29855 | 5.98 | 6.30 | (M+H)+ | 1 |
| 538.1934 | 538.1929 | 0.89 | 3873 | 0.78 | 0.85 | (M+H)+ | 1 |
| 557.1665 | 557.1659 | 1.07 | 816319 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 558.1697 | 558.1691 | 1.10 | 255837 | 31.34 | 33.62 | (M+Na)+ | 1 |
| 559.1724 | 559.1721 | 0.67 | 46112 | 5.65 | 6.30 | (M+Na)+ | 1 |
| 560.1755 | 560.1749 | 1.09 | 6473 | 0.79 | 0.85 | (M+Na)+ | 1 |
| 573.1404 | 573.1398 | 1.10 | 47321 | 100.00 | 100.00 | (M+K)+ | 1 |
| 574.1441 | 574.1430 | 1.88 | 16274 | 34.39 | 33.63 | (M+K)+ | 1 |
| 575.1437 | 575.1417 | 3.42 | 6286 | 13.28 | 13.52 | (M+K)+ | 1 |
| 576.1480 | 576.1431 | 8.49 | 2228 | 4.71 | 3.28 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 535.1845 | 535.1839 | 1.11 | 499625 | 100.00 | 100.00 | (M+H)+ | 1 |
| 536.1876 | 536.1872 | 0.78 | 156286 | 31.28 | 33.63 | (M+H)+ | 1 |
| 537.1906 | 537.1901 | 0.81 | 29855 | 5.98 | 6.30 | (M+H)+ | 1 |
| 538.1934 | 538.1929 | 0.89 | 3873 | 0.78 | 0.85 | (M+H)+ | 1 |
| 557.1665 | 557.1659 | 1.07 | 816319 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 558.1697 | 558.1691 | 1.10 | 255837 | 31.34 | 33.62 | (M+Na)+ | 1 |
| 559.1724 | 559.1721 | 0.67 | 46112 | 5.65 | 6.30 | (M+Na)+ | 1 |
| 560.1755 | 560.1749 | 1.09 | 6473 | 0.79 | 0.85 | (M+Na)+ | 1 |
| 573.1404 | 573.1398 | 1.10 | 47321 | 100.00 | 100.00 | (M+K)+ | 1 |
| 574.1441 | 574.1430 | 1.88 | 16274 | 34.39 | 33.63 | (M+K)+ | 1 |
| 575.1437 | 575.1417 | 3.42 | 6286 | 13.28 | 13.52 | (M+K)+ | 1 |
| 576.1480 | 576.1431 | 8.49 | 2228 | 4.71 | 3.28 | (M+K)+ | 1 |

MS spectra of 8

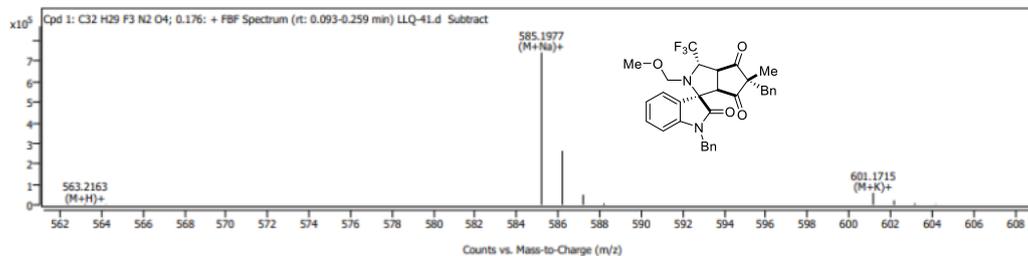
Custom Workflow Report



Compound Details

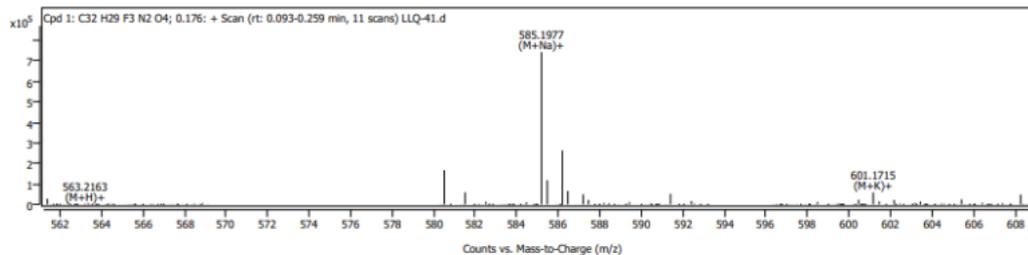
Cpd. 1: C32 H29 F3 N2 O4

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 563.2163 | 563.2152 | 1.90 | 4693 | 100.00 | 100.00 | (M+H)+ | 1 |
| 564.2198 | 564.2185 | 2.28 | 1732 | 36.91 | 35.84 | (M+H)+ | 1 |
| 585.1977 | 585.1972 | 0.93 | 743671 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 586.2011 | 586.2004 | 1.20 | 263711 | 35.46 | 35.83 | (M+Na)+ | 1 |
| 587.2037 | 587.2034 | 0.47 | 49381 | 6.64 | 7.05 | (M+Na)+ | 1 |
| 588.2062 | 588.2063 | -0.05 | 6684 | 0.90 | 0.99 | (M+Na)+ | 1 |
| 601.1715 | 601.1711 | 0.72 | 58570 | 100.00 | 100.00 | (M+K)+ | 1 |
| 602.1751 | 602.1744 | 1.23 | 21619 | 36.91 | 35.84 | (M+K)+ | 1 |
| 603.1754 | 603.1732 | 3.57 | 7725 | 13.19 | 14.27 | (M+K)+ | 1 |
| 604.1790 | 604.1746 | 7.23 | 2286 | 3.90 | 3.58 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|--------|----------|-----------------|-------------|---|
| 563.2163 | 563.2152 | 1.90 | 4693 | 100.00 | 100.00 | (M+H)+ | 1 |
| 564.2198 | 564.2185 | 2.28 | 1732 | 36.91 | 35.84 | (M+H)+ | 1 |
| 585.1977 | 585.1972 | 0.93 | 743671 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 586.2011 | 586.2004 | 1.20 | 263711 | 35.46 | 35.83 | (M+Na)+ | 1 |
| 587.2037 | 587.2034 | 0.47 | 49381 | 6.64 | 7.05 | (M+Na)+ | 1 |
| 588.2062 | 588.2063 | -0.05 | 6684 | 0.90 | 0.99 | (M+Na)+ | 1 |
| 601.1715 | 601.1711 | 0.72 | 58570 | 100.00 | 100.00 | (M+K)+ | 1 |
| 602.1751 | 602.1744 | 1.23 | 21619 | 36.91 | 35.84 | (M+K)+ | 1 |
| 603.1754 | 603.1732 | 3.57 | 7725 | 13.19 | 14.27 | (M+K)+ | 1 |
| 604.1790 | 604.1746 | 7.23 | 2286 | 3.90 | 3.58 | (M+K)+ | 1 |

Header
Data

MS spectra of 9

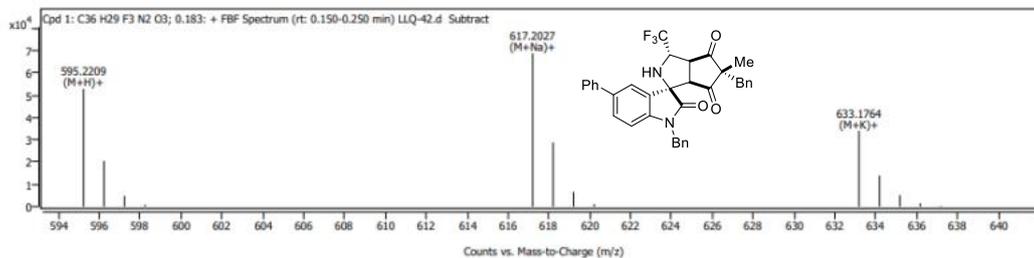
Custom Workflow Report



Compound Details

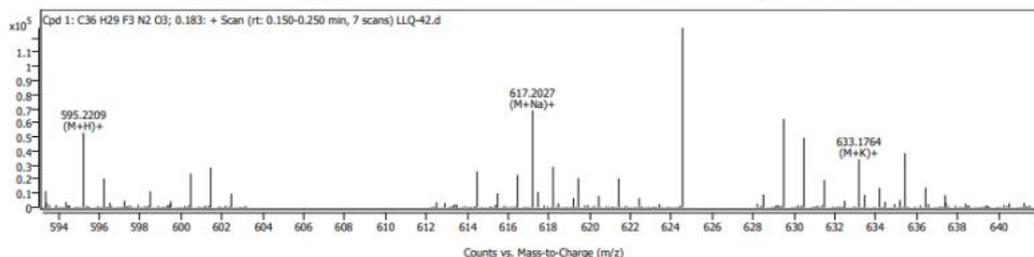
Cpd. 1: C₃₆H₂₉F₃N₂O₃

Compound Spectra



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 595.2209 | 595.2203 | 0.94 | 52887 | 100.00 | 100.00 | (M+H)+ | 1 |
| 596.2241 | 596.2236 | 0.87 | 20525 | 38.81 | 40.13 | (M+H)+ | 1 |
| 597.2284 | 597.2267 | 2.89 | 4818 | 9.11 | 8.46 | (M+H)+ | 1 |
| 598.2320 | 598.2296 | 4.00 | 838 | 1.58 | 1.24 | (M+H)+ | 1 |
| 617.2027 | 617.2022 | 0.78 | 68885 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 618.2062 | 618.2055 | 1.03 | 28814 | 41.83 | 40.12 | (M+Na)+ | 1 |
| 619.2099 | 619.2086 | 2.06 | 6634 | 9.63 | 8.45 | (M+Na)+ | 1 |
| 620.2156 | 620.2116 | 6.47 | 1132 | 1.64 | 1.24 | (M+Na)+ | 1 |
| 633.1764 | 633.1762 | 0.39 | 34057 | 100.00 | 100.00 | (M+K)+ | 1 |
| 634.1800 | 634.1795 | 0.91 | 13924 | 40.88 | 40.13 | (M+K)+ | 1 |
| 635.1800 | 635.1788 | 1.92 | 5160 | 15.15 | 15.67 | (M+K)+ | 1 |
| 636.1814 | 636.1800 | 2.27 | 1511 | 4.44 | 4.14 | (M+K)+ | 1 |
| 637.1883 | 637.1821 | 9.69 | 385 | 1.13 | 0.75 | (M+K)+ | 1 |



Spectrum Peaks

| m/z | m/z (Calc) | Diff (ppm) | Abund | Height % | Height % (Calc) | Ion Species | Z |
|----------|------------|------------|-------|----------|-----------------|-------------|---|
| 595.2209 | 595.2203 | 0.94 | 52887 | 100.00 | 100.00 | (M+H)+ | 1 |
| 596.2241 | 596.2236 | 0.87 | 20525 | 38.81 | 40.13 | (M+H)+ | 1 |
| 597.2284 | 597.2267 | 2.89 | 4818 | 9.11 | 8.46 | (M+H)+ | 1 |
| 598.2320 | 598.2296 | 4.00 | 838 | 1.58 | 1.24 | (M+H)+ | 1 |
| 617.2027 | 617.2022 | 0.78 | 68885 | 100.00 | 100.00 | (M+Na)+ | 1 |
| 618.2062 | 618.2055 | 1.03 | 28814 | 41.83 | 40.12 | (M+Na)+ | 1 |
| 619.2099 | 619.2086 | 2.06 | 6634 | 9.63 | 8.45 | (M+Na)+ | 1 |
| 620.2156 | 620.2116 | 6.47 | 1132 | 1.64 | 1.24 | (M+Na)+ | 1 |
| 633.1764 | 633.1762 | 0.39 | 34057 | 100.00 | 100.00 | (M+K)+ | 1 |
| 634.1800 | 634.1795 | 0.91 | 13924 | 40.88 | 40.13 | (M+K)+ | 1 |
| 635.1800 | 635.1788 | 1.92 | 5160 | 15.15 | 15.67 | (M+K)+ | 1 |
| 636.1814 | 636.1800 | 2.27 | 1511 | 4.44 | 4.14 | (M+K)+ | 1 |
| 637.1883 | 637.1821 | 9.69 | 385 | 1.13 | 0.75 | (M+K)+ | 1 |

Header
Data