Supplementary Information

Visible-Light-Induced Smiles Rearrangement without Release of SO_2: Rapid Access to Alkyl Sulfonyl Derivatives

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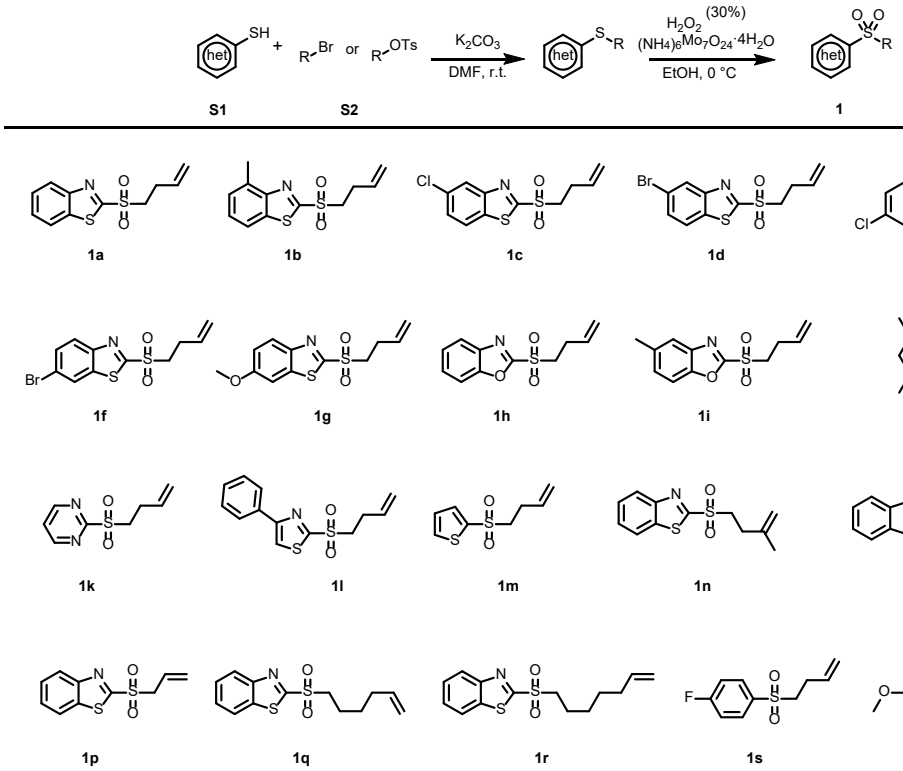
General Information

All commercially available reagents were used without further purification unless mentioned otherwise. ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) spectra were recorded on Bruker Avance 400 Ultrashield NMR spectrometer. Chemical shifts (δ) were given in parts per million (ppm) and were measured downfield from internal tetramethylsilane. High-resolution mass spectrometry (HRMS) data were obtained on an FTICR-MS instrument (Ionspec 7.0 T, ESI/ Quadrupole Mass Analyzer, ESI-QMA). The melting points were determined on an X-4 microscope melting point apparatus and are uncorrected. Conversion was monitored by thin layer chromatography (TLC). Flash column chromatography was performed over silica gel (100-200 mesh). 200 mesh). Blue LED (30 W, λ max = 470nm) was purchased from JIADENG (LS) was used for blue light irradiation. A fan attached to the apparatus was used to maintain the reaction temperature at room temperature.

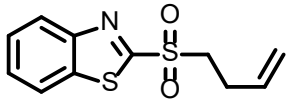
1.Preparation of substrates

General procedure 1 for the preparation of butenyl heteroaryl sulfone



According to literature reports,[1, 2]to a 100 mL round-bottom flask was added compound **S1** (5.0 mmol), compound **S2**(7.5 mmol, 1.5 equiv), K_2CO_3 (1.0 g, 7.5 mmol, 1.5 equiv), and 30 mL DMF. The resulting solution was stirred at room temperature for 3 ~ 10 h, quenched with H_2O (50 mL), extracted with EA (50 mL × 3). The combined organic layer was washed with brine (30 mL × 3), dried over Na_2SO_4, and concentrated. The crude sulfide product was used in the next step without further purification. The sulfide was dissolved (5.0 mmol, 1 equiv) in EtOH (30 mL), $(NH_4)_6Mo_7O_{24}·4H_2O$ (0.5 mmol, 0.1 equiv), and 30% H_2O_2(15.0 mmol) was added at 0 ºC. The resulting mixture was stirred at room temperature for 8 ~16 h. quenched with H_2O (50 mL), extracted with EA (50 mL × 3). The combined organic layer was washed with brine (30 mL × 3), dried over Na_2SO_4, and concentrated.The residue was purified by flash chromatography on a silica gel using petroleum ether and ethyl acetate (20/1~2/1, v/v) as the eluent to give substrate **1**.

2-(but-3-en-1-ylsulfonyl)benzo[*d*]thiazole(1a)



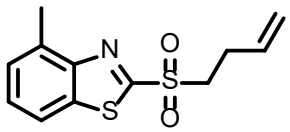
White solid, yield 70% (0.88 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 7.7 Hz, 1H), 8.02 (d, J = 7.6 Hz, 1H), 7.70 – 7.55 (m, 2H), 5.77 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.19 – 4.99 (m, 2H), 3.64 – 3.57 (m, 2H), 2.71 – 2.60 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 152.9, 136.9, 133.3, 128.2, 127.8, 125.6, 122.5, 117.8, 54.0, 26.7.

The data are in accord with the previous literature.[3]

2-(but-3-en-1-ylsulfonyl)-4-methylbenzo[*d*]thiazole(1b)



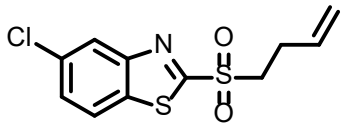
White solid,yield 80% (1.06 g). M.p. = 64–65 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.1 Hz, 1H), 7.45 (t, J = 7.7 Hz, 1H), 7.39 (d, J = 7.3 Hz, 1H), 5.84 – 5.72 (m, 1H), 5.15 – 5.04 (m, 2H), 3.62 – 3.57 (m, 2H), 2.77 (s, 3H), 2.68 – 2.62 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 152.3, 136.7, 135.8, 133.4, 128.1, 128.0, 119.6, 117.6, 53.8, 26.6, 18.3.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{12}H_{14}NO_2S_2^+$268.0460;found268.0462

2-(but-3-en-1-ylsulfonyl)-5-chlorobenzo[*d*]thiazole(1c)



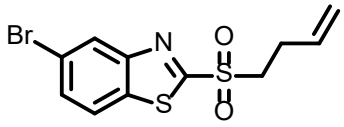
White solid,yield 75% (1.07 g). M.p. = 97–98 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, J = 1.7 Hz, 1H), 7.95 (d, J = 8.7 Hz, 1H), 7.58 (dd, J = 8.7, 2.0 Hz, 1H), 5.77 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.13 (ddd, J = 17.1, 2.8, 1.5 Hz, 1H), 5.08 (ddd, J = 10.2, 2.4, 1.1 Hz, 1H), 3.64 – 3.57 (m, 2H), 2.68 – 2.61 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 153.6, 135.1, 134.1, 133.2, 129.0, 125.2, 123.3, 117.9, 53.9, 26.6.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{11}H_{11}ClNO_2S_2^+$287.9914;found 287.9918

5-bromo-2-(but-3-en-1-ylsulfonyl)benzo[*d*]thiazole(1d)



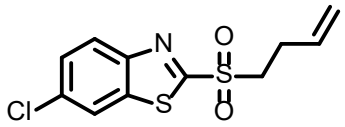
White solid,yield 73% (1.21 g). M.p. = 91–92 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, J = 1.8 Hz, 1H), 7.89 (d, J = 8.7 Hz, 1H), 7.70 (dd, J = 8.7, 1.8 Hz, 1H), 5.76 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.15 – 5.05 (m, 2H), 3.62 – 3.57 (m, 2H), 2.67 – 2.60 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 153.8, 135.6, 133.1, 131.5, 128.3, 123.6, 121.6, 117.9, 53.9, 26.6.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{11}H_{11}BrNO_2S_2^+$331.9409;found 331.9412

2-(but-3-en-1-ylsulfonyl)-6-chlorobenzo[*d*]thiazole(1e)



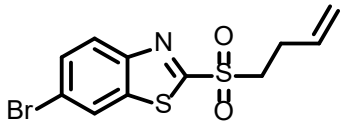
White solid,yield 74% (1.06 g). M.p. = 98–99 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.8 Hz, 1H), 8.00 (d, J = 1.9 Hz, 1H), 7.60 (dd, J = 8.8, 2.0 Hz, 1H), 5.76 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.15 – 5.03 (m, 2H), 3.62 – 3.56 (m, 2H), 2.68 – 2.60 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 151.3, 138.0, 134.6, 133.2, 129.0, 126.4, 122.0, 117.9, 54.0, 26.6.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{11}H_{11}ClNO_2S_2^+$287.9914;found 287.9918

6-bromo-2-(but-3-en-1-ylsulfonyl)benzo[*d*]thiazole(1f)



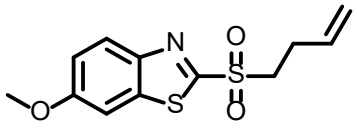
White solid,yield 69% (1.14 g). M.p. = 112–114 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 1.6 Hz, 1H), 8.07 (d, J = 8.8 Hz, 1H), 7.74 (dd, J = 8.8, 1.7 Hz, 1H), 5.77 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.16 – 5.03 (m, 2H), 3.66 – 3.56 (m, 2H), 2.69 – 2.59 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 151.6, 138.4, 133.2, 131.6, 126.6, 125.0, 122.4, 117.9, 54.0, 26.6.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{11}H_{11}BrNO_2S_2^+$331.9409;found 311.9412

2-(but-3-en-1-ylsulfonyl)-6-methoxybenzo[*d*]thiazole(1g)



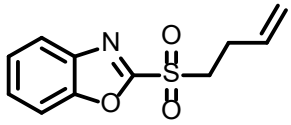
White solid,yield 77% (1.09 g). M.p. = 72–74 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 9.1 Hz, 1H), 7.39 (d, J = 2.4 Hz, 1H), 7.23 (dd, J = 9.1, 2.5 Hz, 1H), 5.77 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.16 – 5.01 (m, 2H), 3.92 (s, 3H), 3.58 – 3.51 (m, 2H), 2.66 – 2.60 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 160.0, 147.4, 139.0, 133.4, 126.3, 118.5, 117.7, 103.6, 56.1, 54.2, 26.7.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{12}H_{14}NO_3S_2^+$284.0410;found 284.0412

2-(but-3-en-1-ylsulfonyl)benzo[*d*]oxazole(1h)



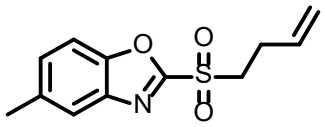
White solid, yield 52% (0.62 g). M.p. = 71–73 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 8.3 Hz, 1H), 7.58 (t, J = 7.8 Hz, 1H), 7.51 (t, J = 7.7 Hz, 1H), 5.78 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.14 (dd, J = 17.1, 1.2 Hz, 1H), 5.07 (dd, J = 10.2, 0.8 Hz, 1H), 3.66 – 3.60 (m, 2H), 2.73 – 2.65 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 151.0, 139.5, 132.9, 128.7, 126.3, 122.2, 118.0, 112.0, 54.0, 26.3.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{11}H_{12}NO_3S^+$238.0532;found 238.0537

2-(but-3-en-1-ylsulfonyl)-5-methylbenzo[*d*]oxazole (1i)



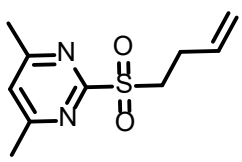
White solid,yield 50% (0.63 g). M.p. = 69–71 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.53 (d, J = 8.5 Hz, 1H), 7.36 (d, J = 8.4 Hz, 1H), 5.76 (ddt, J = 13.1, 10.2, 6.5 Hz, 1H), 5.09 (dd, J = 27.5, 13.6 Hz, 2H), 3.66 – 3.52 (m, 2H), 2.66 (dd, J = 15.0, 7.0 Hz, 2H), 2.50 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 149.4, 139.8, 136.6, 133.0, 130.1, 121.9, 118.0, 111.4, 54.1, 26.3, 21.6.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{12}H_{14}NO_3S^+$252.0689;found 252.0691

2-(but-3-en-1-ylsulfonyl)-4,6-dimethylpyrimidine(1j)



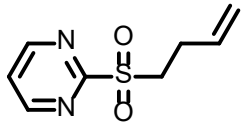
White solid,yield 61% (0.68 g). M.p. = 64–75 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (s, 1H), 5.82 (ddt, J = 16.8, 10.1, 6.6 Hz, 1H), 5.17 – 5.04 (m, 2H), 3.64 – 3.57 (m, 2H), 2.67 – 2.60 (m, 8H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 165.0, 134.1, 123.0, 117.2, 50.4, 26.4, 24.1.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{10}H_{15}N_2O_2S^+$227.0849; found 227.0849

2-(but-3-en-1-ylsulfonyl)pyrimidine (1k)



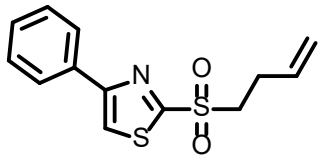
Colorless oil, yield 56% (0.55 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, J = 4.9 Hz, 2H), 7.58 (t, J = 4.9 Hz, 1H), 5.77 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.12 – 5.01 (m, 2H), 3.63 – 3.57 (m, 2H), 2.64 – 2.57 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 158.8, 133.8, 124.0, 117.4, 50.6, 26.4.

HRMS (ESI)m/z:$[M+H]^+$calcd. for $C_8H_{11}N_2O_2S^+$199.0536, found 199.0538.

2-(but-3-en-1-ylsulfonyl)-4-phenylthiazole(1l)



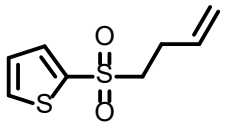
Colorless oil, yield 50% (0.70 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 7.4 Hz, 2H), 7.84 (s, 1H), 7.49 – 7.38 (m, 3H), 5.77 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.17 – 5.03 (m, 2H), 3.61 – 3.52 (m, 2H), 2.69 – 2.59 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 158.3, 133.4, 132.8, 129.4, 129.1, 126.7, 119.3, 117.7, 54.1, 26.7.

HRMS (ESI)m/z:$[M+H]^+$calcd. for $C_{13}H_{14}NO_2S_2^+$ 280.0460, found 280.0460

2-(but-3-en-1-ylsulfonyl)thiophene(1m)



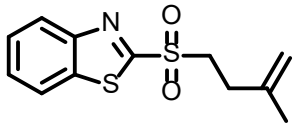
Colorless oil, yield 57% (0.57 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, J = 5.0, 1.3 Hz, 1H), 7.70 (dd, J = 3.8, 1.3 Hz, 1H), 7.17 (dd, J = 5.0, 3.8 Hz, 1H), 5.74 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.10 – 5.04 (m, 2H), 3.29 – 3.25 (m, 2H), 2.56 – 2.49 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 134.3, 134.2, 133.7, 128.1, 117.4, 56.9, 27.4.

HRMS (ESI) m/z: $[M+H]^+$calcd. for $C_8H_{11}O_2S_2^+$203.0195, found 203.0196

2-((3-methylbut-3-en-1-yl)sulfonyl)benzo[*d*]thiazole(1n)



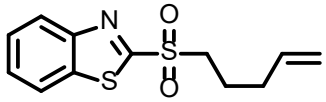
White solid,yield 76% (1.01 g). M.p. = 56–58 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (dd, J = 7.6, 1.3 Hz, 1H), 8.03 (dd, J = 7.2, 1.0 Hz, 1H), 7.68 – 7.58 (m, 2H), 4.77 (d, J = 26.3 Hz, 2H), 3.68 – 3.61 (m, 2H), 2.62 – 2.54 (m, 2H), 1.74 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 152.9, 141.0, 136.9, 128.2, 127.8, 125.6, 122.5, 112.6, 53.3, 30.1, 22.4.

HRMS (ESI)m/z: $[M+H]^+$calcd. for $C_{12}H_{14}NO_2S_2^+$268.0460, found 268.0462

2-(pent-4-en-1-ylsulfonyl)benzo[*d*]thiazole(1o)



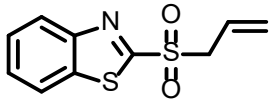
Colorless oil, yield 80% (1.07 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 8.0 Hz, 1H), 8.02 (d, J = 7.9 Hz, 1H), 7.67 – 7.57 (m, 2H), 5.72 (ddt, J = 13.4, 10.5, 6.7 Hz, 1H), 5.09 – 4.99 (m, 2H), 3.55 – 3.48 (m, 2H), 2.26 – 2.18 (m, 2H), 2.03 – 1.95 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 152.9, 136.9, 136.1, 128.2, 127.8, 125.6, 122.5, 117.0, 54.1, 32.1, 21.6.

The data are in accord with the previous literature.[4]

2-(allylsulfonyl)benzo[*d*]thiazole(1p)



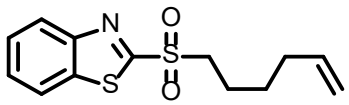
White solid,yield 71% (0.85 g). M.p. = 65–66 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 7.9 Hz, 1H), 8.01 (d, J = 7.7 Hz, 1H), 7.68 – 7.56 (m, 2H), 5.96 – 5.82 (m, 1H), 5.41 (d, J = 10.1 Hz, 1H), 5.35 (d, J = 17.1 Hz, 1H), 4.25 (d, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 152.5, 136.7, 128.1, 127.6, 126.2, 125.3, 123.0, 122.3, 59.0.

HRMS (ESI)m/z:$[M+H]^+$calcd. for $C_{10}H_{10}NO_2S_2^+$240.0147, found 240.0149

2-(hex-5-en-1-ylsulfonyl)benzo[*d*]thiazole(1q)



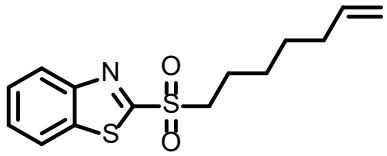
Colorless oil, yield 79% (1.01 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 8.2 Hz, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.67 – 7.58 (m, 2H), 5.73 (ddt, J = 16.9, 10.1, 6.7 Hz, 1H), 5.02 – 4.92 (m, 2H), 3.54 – 3.49 (m, 2H), 2.10 – 2.05 (m, 2H), 1.94 – 1.86 (m, 2H), 1.58 – 1.53 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 152.9, 137.5, 136.9, 128.2, 127.8, 125.6, 122.5, 115.7, 54.7, 33.1, 27.5, 21.9.

HRMS (ESI)m/z:$[M+H]^+$calcd. for$C_{13}H_{16}NO_2S_2^+$282.0617, found 282.0619

2-(hept-6-en-1-ylsulfonyl)benzo[*d*]thiazole(1r)



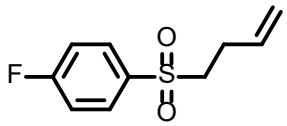
Colorless oil, yield 76% (1.12 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 7.8 Hz, 1H), 8.03 (d, J = 7.9 Hz, 1H), 7.65 (t, J = 7.1 Hz, 1H), 7.60 (t, J = 7.1 Hz, 1H), 5.74 (ddt, J = 16.9, 10.2, 6.7 Hz, 1H), 5.02 – 4.89 (m, 2H), 3.54 – 3.48 (m, 2H), 2.03 (q, J = 6.7 Hz, 2H), 1.93 – 1.85 (m, 2H), 1.48 – 1.38 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 152.8, 138.3, 136.9, 128.1, 127.8, 125.6, 122.5, 115.0, 54.8, 33.3, 28.2, 27.8, 22.3.

HRMS (ESI)m/z:$[M+H]^+$calcd. for$C_{14}H_{18}NO_2S_2^+$296.0773, found 296.0775

1-(but-3-en-1-ylsulfonyl)-4-fluorobenzene(1s)



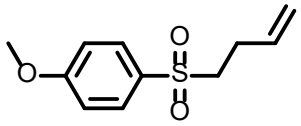
Colorless oil, yield 86% (0.92 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.92 (m, 2H), 7.27 (t, J = 8.5 Hz, 2H), 5.74 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.10 – 5.02 (m, 2H), 3.22 – 3.17 (m, 2H), 2.50 – 2.43 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8 (d, J = 256.1 Hz), 135.0 (d, J = 3.0 Hz), 133.6 (s), 131.0 (d, J = 9.7 Hz), 117.1, 116.6 (d, J = 22.6 Hz), 55.3, 26.8.

The data are in accord with the previous literature.[5]

1-(but-3-en-1-ylsulfonyl)-4-methoxybenzene(1t)



Colorless oil, yield 90% (1.02 g).

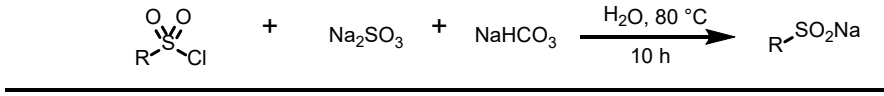
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.9 Hz, 2H), 7.02 (d, J = 8.9 Hz, 2H), 5.72 (ddt, J = 16.8, 10.2, 6.5 Hz, 1H), 5.09 – 4.99 (m, 2H), 3.88 (s, 3H), 3.16 – 3.10 (m, 2H), 2.48 – 2.40 (m, 2H).

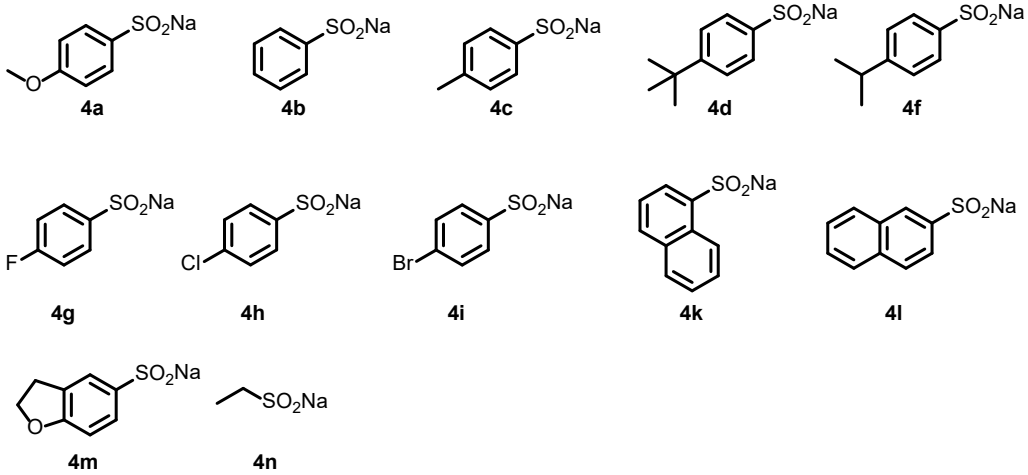
^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 134.0, 130.6, 130.4, 117.2, 114.6, 55.8, 55.8, 27.2.

The data are in accord with the previous literature.[5]

General procedure 2 for the preparation of Sodium Sulfinates

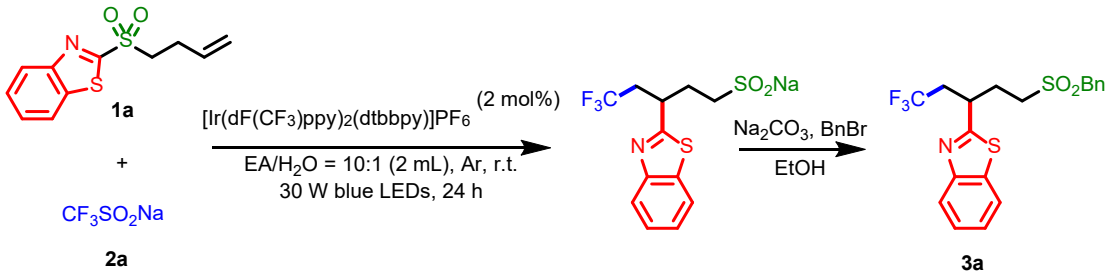
General procedure: The sodium sulfinates were synthesized according to a published procedure.[6] Sulfonic acid chloride (5 mmol) was added to a mixture of Na_2SO_3 (10 mmol) and $NaHCO_3$ (10 mmol) in water (8 mL) and the result mixture was stirred at 80 °C for 10 h. After cooling down to room temperature, the water was removed in vacuum and the residue was extracted in ethanol. Recrystallization from ethanolfurnished sodium sulfinate as a white or light yellow solid.





2.Reaction optimization

Table S1: Screening ofreaction A[a]

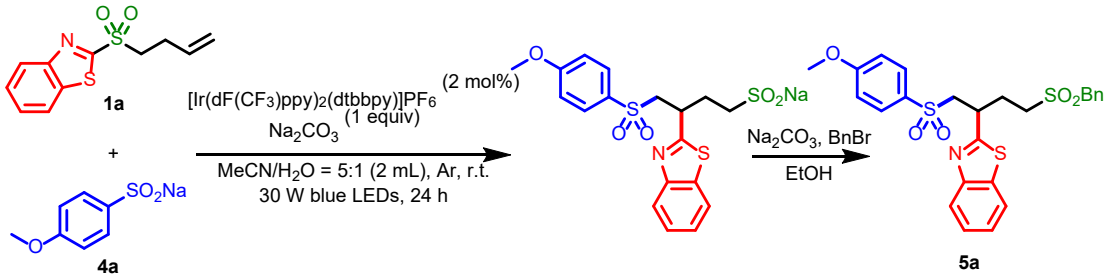


Entry	Variation from standard conditions	Yield(%)[b]
1	None	57
2	4CzIPN (5 mol%) as photocatalyst	47
3	*fac*-Ir(ppy)$_3$ as photocatalyst	trace
4	Eosin Y (5 mol%) as photocatalyst	0
5	Ru(bpy)$_3$Cl$_2$·6H$_2$O as photocatalyst	0
6	Added Na_2CO_3 (100 mol%)	75 (71[c])
7	Added $NaHCO_3$ (100 mol%)	62
8	Added K_2CO_3 (100 mol%)	59
9	Added Cs_2CO_3 (100 mol%)	60
10	Added acetic acid (100 mol%)	53
11	10:1 acetone/H_2O as solvent	67[d]
12	10:1 MeCN/H_2O as solvent	65[d]
13	10:1 THF/H_2O as solvent	40[d]
14	H_2O as solvent	0
15	No photocatalyst	0
16	No light	0

[a]Reaction conditions, unless otherwise noted: **1a** (0.2 mmol), **2a** (0.6 mmol, 3 equiv), and [Ir(dF(CF$_3$)ppy)$_2$(dtbbpy)]PF$_6$ (2 mol%) in 10:1 (v/v) ethyl acetate (EA)/H_2O (2 mL) were irradiated with 30 W blue LEDs at room temperature under an argon atmosphere for 24 h; then Na_2CO_3 (3 equiv), EtOH (1 mL), and benzyl bromide

(BnBr, 3 equiv) were added; and the mixture was stirred at room temperature for another 12 h.[b]Yields were determined by ^{19}F NMR spectroscopy with trifluoromethylbenzene as an internal standard. [c] Isolated yield. [d] The reaction was performed with 1 equiv of Na_2CO_3.

Table S2: Screening of reaction B[a]

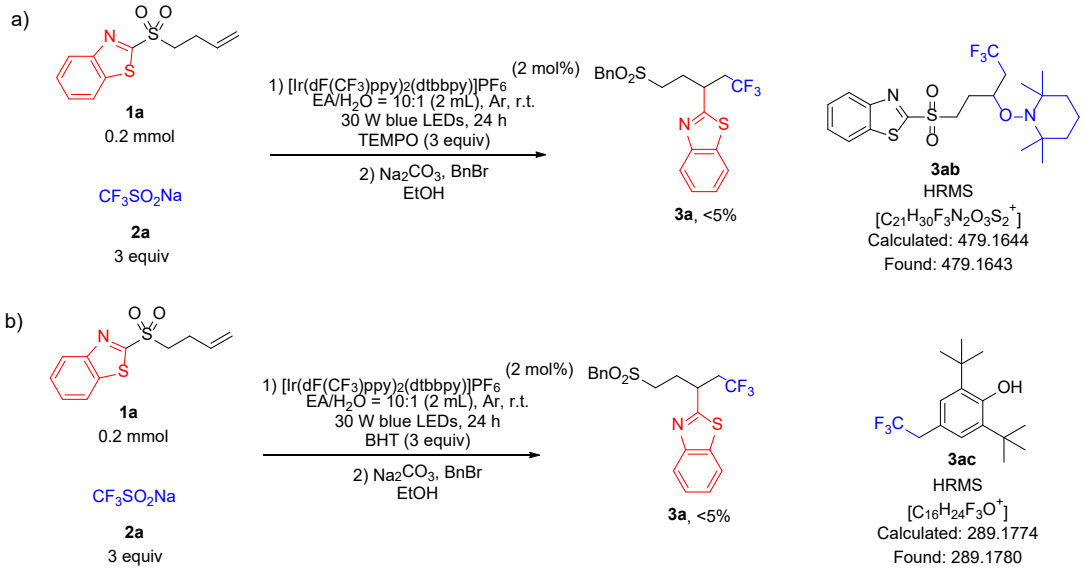


Entry	Variation from standard conditions	Yield(%)[b]
1	None	81
2	10:1 MeCN/H_2O as solvent	67
3	10:1 acetone/H_2O as solvent	53
4	10:1 EA/H_2O as solvent	49
5	EAas solvent	trace
6	H_2O as solvent	0
7	MeCNas solvent	trace

[a]Reaction conditions, unless otherwise noted: **1a** (0.2 mmol), **4a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv) and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 5:1 (v/v) MeCN/H_2O (2 mL) were irradiated with 30 W blue LEDs at room temperature under an argon atmosphere for 24 h; then Na_2CO_3 (3 equiv), EtOH (1 mL), and benzyl bromide (BnBr, 3 equiv) were added; and the mixture was stirred at room temperature for another 12 h.[b] Isolated yield.

3.Investigation of the mechanism

General procedure 3



To a 4 mL glass vial equipped with a magnetic stir bar was added **1a** (0.2 mmol), **2a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv) and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 10:1 (v/v) ethyl acetate (EA)/H_2O (2 mL)and additive (TEMPO (93.8 mg, 0.6 mmol) or BHT(132 mg, 0.6 mmol).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL), and benzyl bromide (BnBr, 3 equiv) were added; and the mixture was stirred at room temperature for another 12 h.

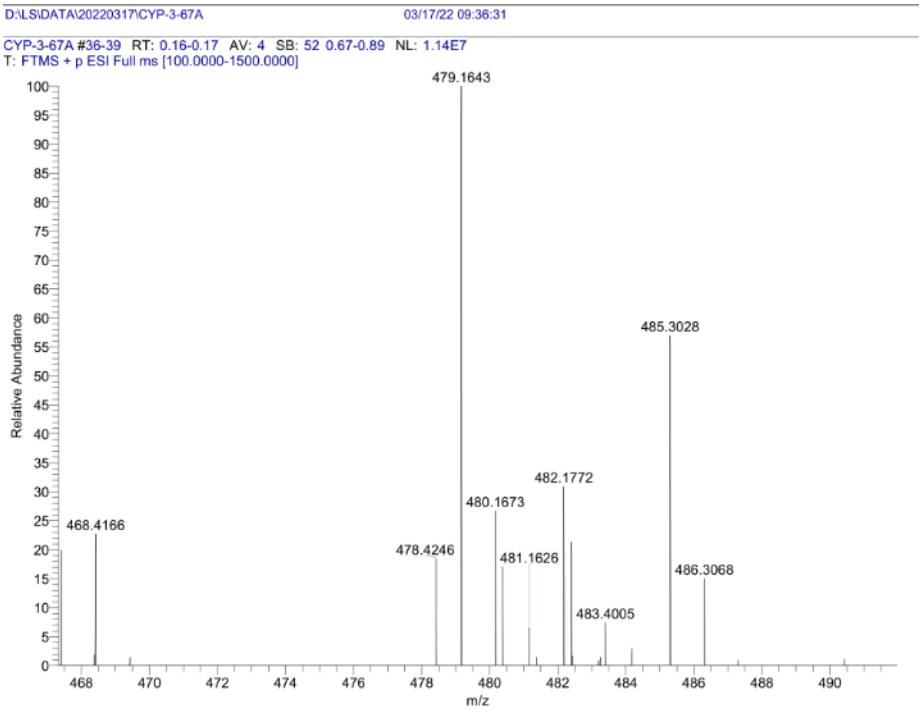


Figure S1 High resolution mass spectrum of TEMPO capture product.

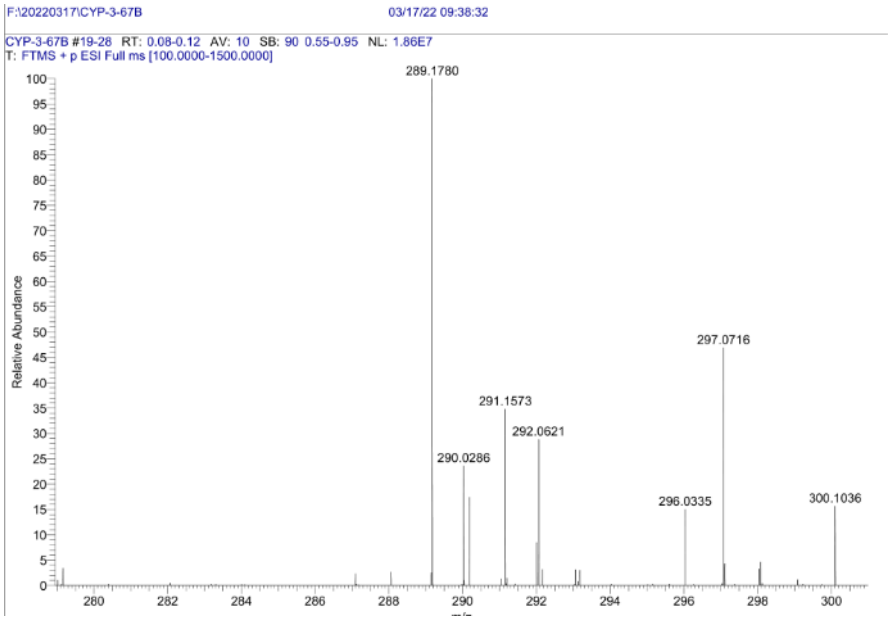
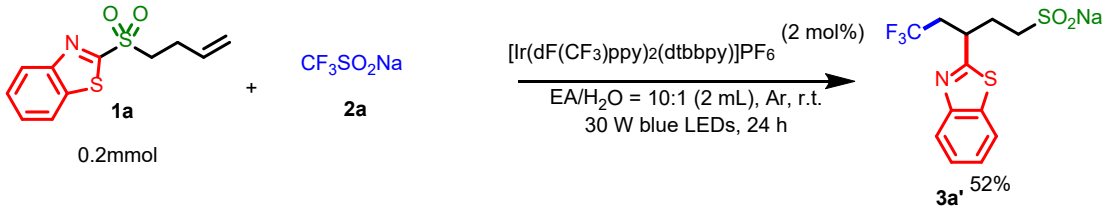


Figure S2 High resolution mass spectrum of BHT capture product.

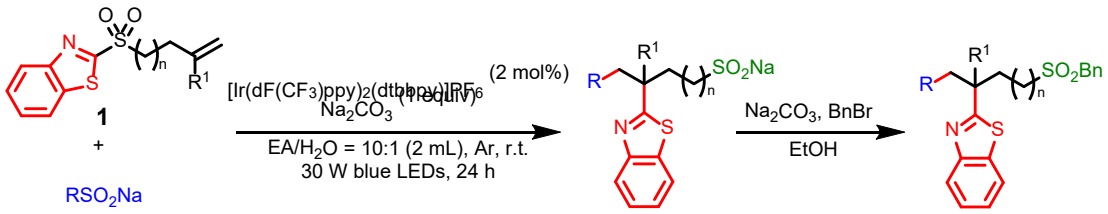
4.Experimental procedures and product characterization.

General procedure for 3a'



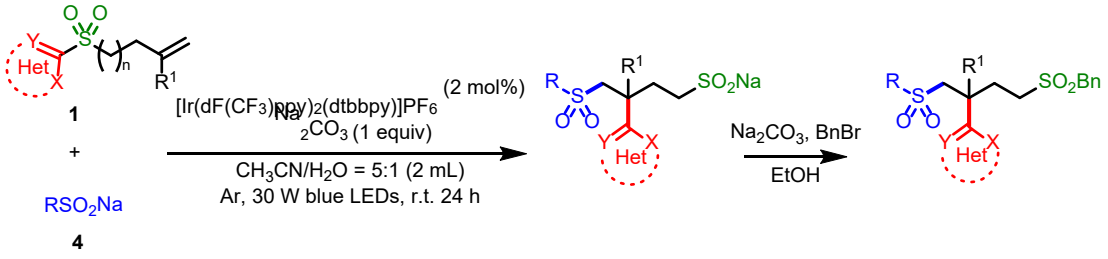
To a 4 mL glass vial equipped with a magnetic stir bar was added 1 (0.2 mmol), 2 (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv) and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 10:1 (v/v) ethyl acetate (EA)/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h**.**The solvent wasconcentrated in vacuo, and purified by column chromatography (DCM/MeOH = 10:1-5:1) to afford the target compound**3a'** (36 mg, 52%).

General procedure for 3a – 3p and 6l – 6m



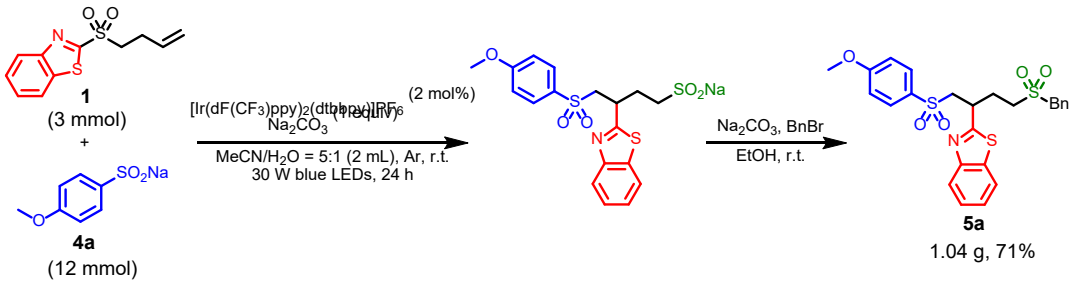
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **2** (0.6 mmol, 3 equiv),Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 10:1 (v/v) ethyl acetate (EA)/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL), and benzyl bromide (BnBr, 3 equiv) were added; and the mixture was stirred at room temperature for another 12 h.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate) to afford thecorresponding target compounds.

General procedure5a – 5p, 6j, 6k, and 6n



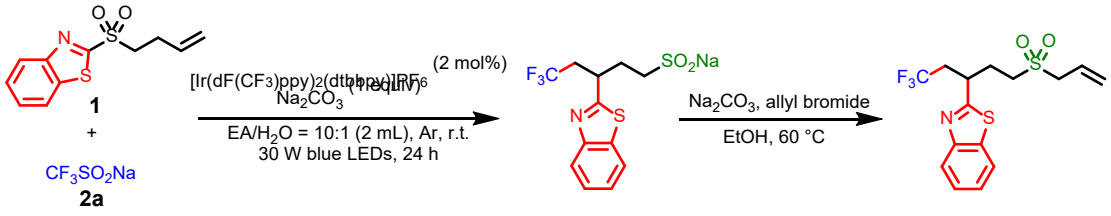
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **4** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 10:1 (v/v) EA/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL), and benzyl bromide (BnBr, 3 equiv) were added; and the mixture was stirred at room temperature for another 12 h.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate) to afford thecorresponding target compounds.

General procedure：procedure for 5a in gram scale



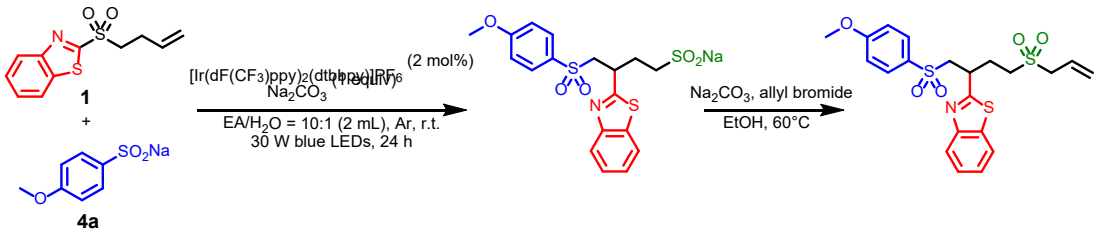
To an oven-dried 100 mL Schlenk Tube with a stirring bar was added **1** (3 mmol), **4a** (12 mmol, 3 equiv), Na_2CO_3 (3 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%).Then, air was withdrawn and backfilled with Ar (three times). 5:1 (v/v) MeCN/H_2O (30 mL) was added andthe mixture was irradiated under 30 W× 2blue LED at room temperature for 24 h. Then Na_2CO_3 (3 equiv), EtOH (15 mL),andethyl bromoacetate(3 equiv) were added.The reaction mixture stirred at room temperature for 8 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 10:1~5:1, v/v) to afford thecorresponding target compound**5a** (1.04g, 71%).

procedure for 6a



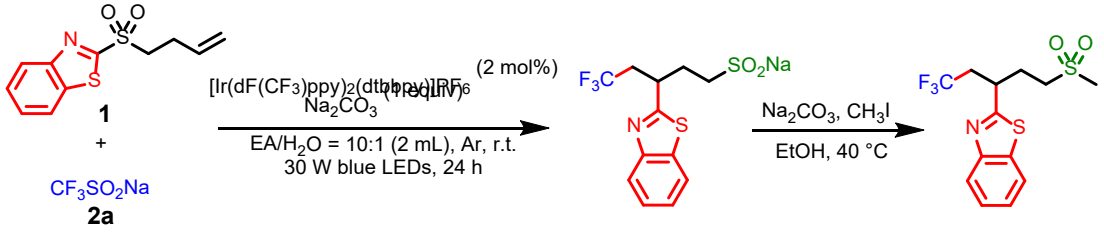
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **2a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 10:1 (v/v) EA/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL),andallyl bromide(3 equiv) were added.The reaction mixture stirred at 60 ºC for 10 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 10:1 ~ 5:1, v/v) to afford thecorresponding target compounds.

procedure for 6b



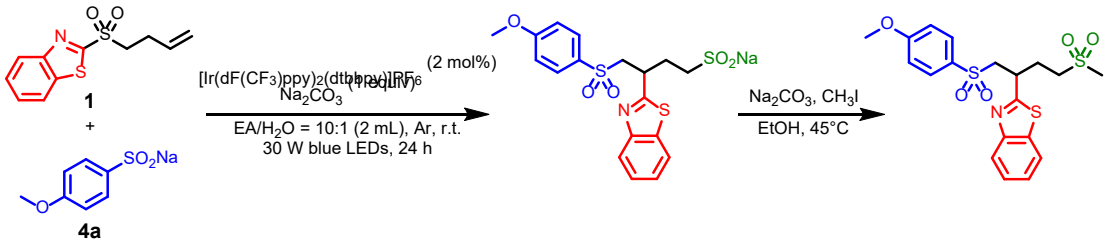
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **4a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 5:1 (v/v) MeCN/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL),andallyl bromide(3 equiv) were added.The reaction mixture stirred at 60 ºC for 10 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 8:1 ~ 4:1, v/v) to afford thecorresponding target compounds.

procedure for 6c



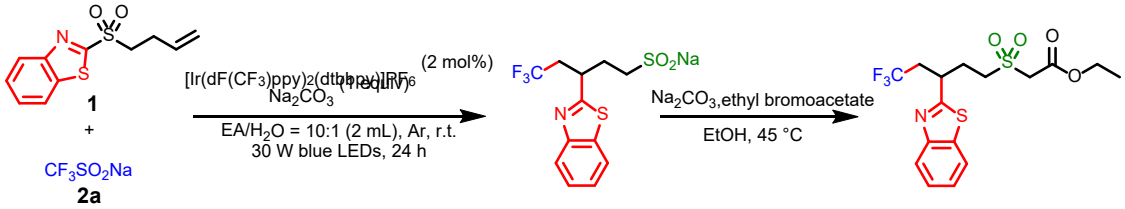
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **2a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 10:1 (v/v) EA/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL),andmethyl iodide (3 equiv) were added.The reaction mixture stirred at 45 ºC for 16 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 10:1 ~ 4:1, v/v) to afford thecorresponding target compounds.

procedure for 6d



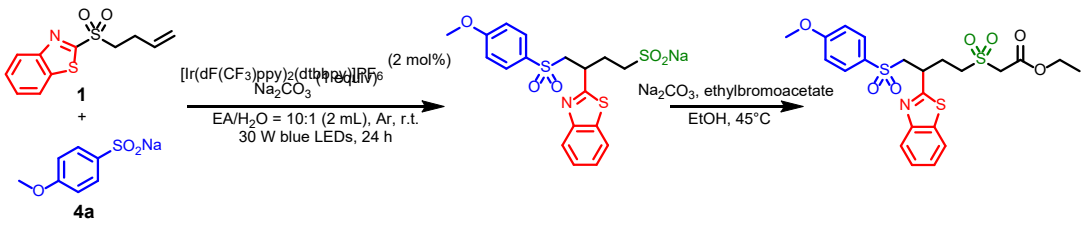
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **4a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 5:1 (v/v) MeCN/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL),andmethyl iodide (3 equiv) were added.The reaction mixture stirred at 45 ºC for 16 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 5:1 ~ 2:1, v/v) to afford thecorresponding target compounds.

procedure for 6e



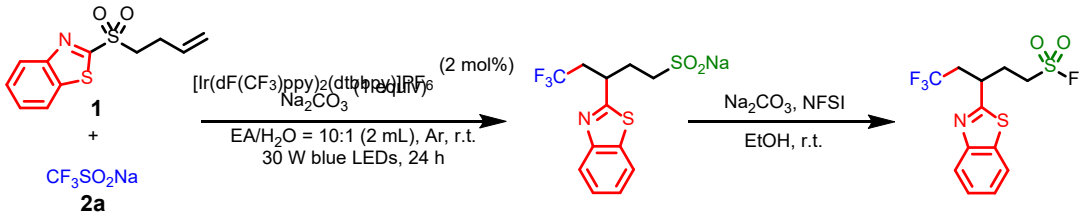
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **2a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 10:1 (v/v) EA/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL),andethyl bromoacetate(3 equiv) were added.The reaction mixture stirred at 45 ºC for 16 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 10:1 ~ 5:1, v/v) to afford thecorresponding target compounds.

procedure for 6f



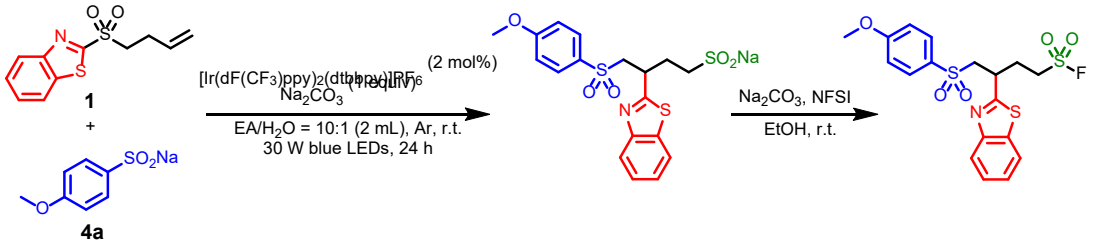
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **4a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 5:1 (v/v) MeCN/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL),andethyl bromoacetate(3 equiv) were added.The reaction mixture stirred at 45 ºC for 16 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 8:1 ~ 4:1, v/v) to afford thecorresponding target compounds.

procedure for 6g



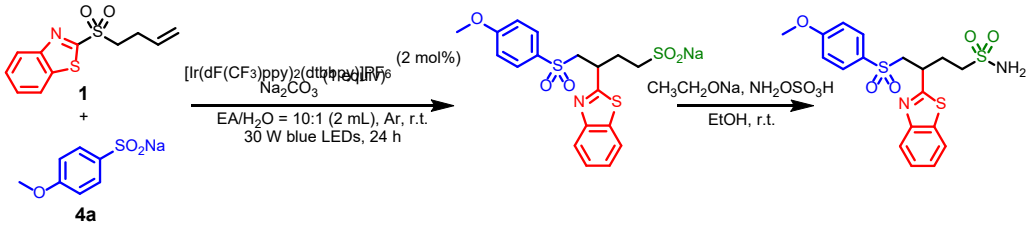
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **2a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 10:1 (v/v) EA/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL),and NFSI(3 equiv) were added.The reaction mixture stirred at room temperature for 8 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 10:1 ~ 5:1, v/v) to afford thecorresponding target compounds.

procedure for 6h



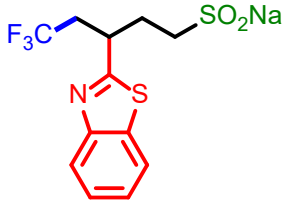
To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **4a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 5:1 (v/v) MeCN/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then Na_2CO_3 (3 equiv), EtOH (1 mL),andethyl bromoacetate(3 equiv) were added.The reaction mixture stirred at room temperature for 8 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 8:1 ~ 4:1, v/v) to afford thecorresponding target compounds.

procedure for 6i



To a 4 mL glass vial equipped with a magnetic stir bar was added **1** (0.2 mmol), **4a** (0.6 mmol, 3 equiv), Na_2CO_3 (0.2 mmol, 1 equiv)and $[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$ (2 mol%) in 5:1 (v/v) MeCN/H_2O (2 mL).Thereaction mixture was degassed by bubbling with argon for 10 s with an outlet needle and the vial was sealedwith PTFE cap. The mixture was then stirred rapidly and irradiated with a 30 W Blue LED at room temperature for 24 h.Then CH_3CH_2ONa (3 equiv), EtOH (1 mL),andhydroxylamine-O-sulfonic acid(3 equiv) were added.The reaction mixture stirred at room temperature for 8 hours.When the reaction is completed, extracted with ethyl acetate, washed with brine, dried over anhydroussodiumsulfate,concentrated in vacuo, and purified by columnchromatography (hexane/ethyl acetate = 5:1 ~ 2:1, v/v) to afford thecorresponding target compounds.

sodium 3-(benzo[*d*]thiazol-2-yl)-5,5,5-trifluoropentane-1-sulfinate (3a')



White solid, yield 52% (36 mg). M.p.> 300 °C.

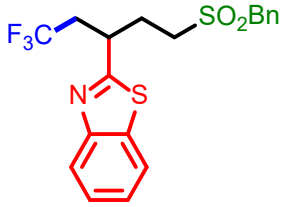
^{1}H NMR (400 MHz, D_2O) δ 7.85 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 3.77 – 3.69 (m, 1H), 2.93 – 2.84 (m, 1H), 2.82 – 2.69 (m, 3H), 2.35 – 2.21 (m, 2H).

^{13}C NMR (100 MHz, D_2O) δ 174.0, 151.5, 134.0, 126.6, 126.1 (q, *J* = 277.3 Hz), 125.6, 122.1, 121.6, 48.1, 38.3 (q, *J* = 28.2 Hz), 37.0 (q, *J* = 2.2 Hz), 30.5.

^{19}F NMR (376 MHz, D_2O) δ -64.13 (t, *J* = 10.7 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{12}H_{12}F_3NNaO_2S_2^+$346.0154; found 346.0158.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)benzo[*d*]thiazole(3a)



White solid, yield 70% (57.5 mg). M.p. = 72–73 °C.

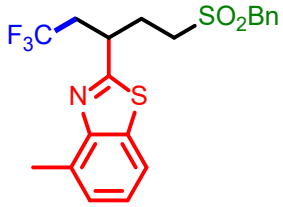
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.32 – 7.14 (m, 5H), 4.16 (s, 2H), 3.69 – 3.54 (m, 1H), 2.94 – 2.77 (m, 3H), 2.61 – 2.48 (m, 1H), 2.43 – 2.34 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 153.1, 134.7, 130.5, 129.2, 129.1, 127.8, 125.9 (q, *J* = 277.4 Hz), 126.6, 125.7, 123.3, 121.9, 59.7, 48.1, 39.1 (q, *J* = 28.7 Hz), 37.2 (q, *J* = 2.2 Hz). 28.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -64.00 (t, *J* = 10.3 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{19}H_{19}F_3NO_2S_2^+$414.0804;found 414.0808.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-4-methylbenzo[*d*]thiazole(3b)



White solid, yield 70% (74 mg). M.p. = 75–76 °C.

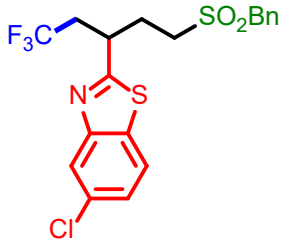
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.65 (m, 1H), 7.31 – 7.17 (m, 7H), 4.15 (s, 2H), 3.64 – 3.56 (m, 1H), 2.89 – 2.81 (m, 3H), 2.69 (s, 3H), 2.57 – 2.50 (m, 1H), 2.40 – 2.34 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 152.5, 134.6, 133.4, 131.0, 130.5, 129.1, 129.1, 127.8, 127.0, 126.0 (q, J = 277.4 Hz), 125.5, 119.2, 59.5, 48.1, 38.9 (q, J = 28.8 Hz), 37.2 (q, J = 2.5 Hz), 28.0, 18.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.91 (t, J = 10.5 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{20}H_{21}F_3NO_2S_2^+$428.0960; found 428.0963.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-5-chlorobenzo[*d*]thiazole(3c)



White solid, yield 51% (45.6 mg). M.p. = 86–88 °C.

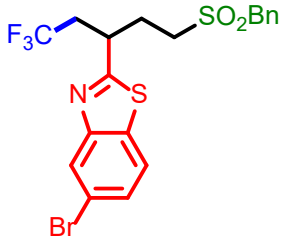
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 1.9 Hz, 1H), 7.76 (d, J = 8.6 Hz, 1H), 7.39 (dd, J = 8.6, 1.9 Hz, 1H), 7.31 – 7.22 (m, 5H), 4.17 (s, 2H), 3.67 – 3.58 (m, 1H), 2.88 – 2.78 (m, 3H), 2.58 – 2.48 (m, 1H), 2.39 – 2.33 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 153.9, 133.0, 132.6, 130.5, 129.2, 129.1, 127.7, 126.1, 125.8 (q, J = 277.4 Hz), 123.1, 122.6, 59.7, 47.9, 38.9 (q, J = 28.7 Hz), 37.2 (q, J = 2.5 Hz), 27.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.97 (t, J = 10.4 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{19}H_{18}ClF_3NO_2S_2^+$; found 448.0417.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-5-bromobenzo[*d*]thiazole(3d)



White solid, yield 73% (71.6 mg). M.p. = 87–89 °C.

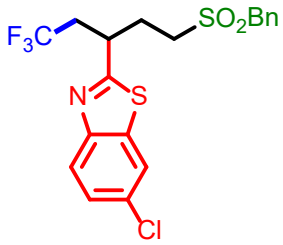
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.71 (d, J = 8.5 Hz, 1H), 7.53 (d, J = 8.5 Hz, 1H), 7.31 – 7.22 (m, 5H), 4.17 (s, 2H), 3.67 – 3.59 (m, 1H), 2.90 – 2.77 (m, 3H), 2.58 – 2.45 (m, 1H), 2.36 (dd, J = 15.1, 7.5 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 154.2, 133.5, 130.5, 129.2, 129.1, 128.8, 127.7, 126.2, 125.8 (q, *J* = 277.6 Hz), 122.9, 120.2, 59.8, 47.9, 38.9 (q, *J* = 29.0 Hz), 37.2 (q, *J* = 2.3 Hz), 27.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.97 (t, *J* = 10.4 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{19}H_{18}BrF_3NO_2S_2^+$491.9909; found 491.9912.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-6-chlorobenzo[*d*]thiazole(3e)



White solid, yield 78% (70.0 mg). M.p. = 70–72 °C.

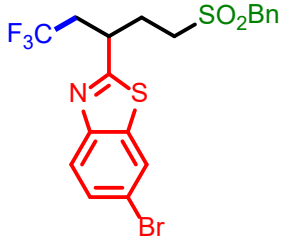
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.83 (d, *J* = 2.0 Hz, 1H), 7.47 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.32 – 7.22 (m, 5H), 4.18 (s, 2H), 3.66 – 3.57 (m, 1H), 2.90 – 2.78 (m, 3H), 2.58 – 2.46 (m, 1H), 2.37 (dd, *J* = 15.2, 7.3 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 151.6, 135.9, 131.6, 130.5, 129.2, 129.1, 127.7, 127.3, 125.8 (q, *J* = 277.5 Hz), 123.9, 121.5, 59.7, 47.9, 38.9 (q, *J* = 29.0 Hz), 37.1 (q, *J* = 2.6 Hz), 27.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.97 (t, *J* = 10.3 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{19}H_{18}ClF_3NO_2S_2^+$448.0414; found 448.0419

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-6-bromobenzo[*d*]thiazole(3f)



White solid, yield 73% (71.7 mg). M.p. = 92–94 °C.

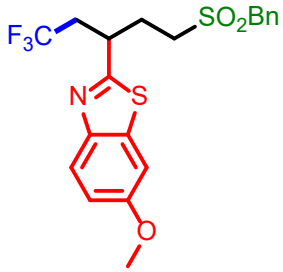
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 1.8 Hz, 1H), 7.82 (d, *J* = 8.7 Hz, 1H), 7.60 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.34 – 7.21 (m, 5H), 4.17 (s, 2H), 3.67 – 3.56 (m, 1H), 2.93 – 2.76 (m, 3H), 2.60 – 2.45 (m, 1H), 2.42 – 2.31 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 153.9, 132.7, 131.0, 130.6, 129.3, 129.2, 127.8, 126.2, 125.8 (q, *J* = 277.1 Hz), 123.2, 122.6, 59.9, 47.9, 39.0 (q, *J* = 29.1 Hz), 37.3 (q, *J* = 2.0 Hz), 27.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.95 (t, *J* = 10.5 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{19}H_{18}BrF_3NO_2S_2^+$491.9909; found 491.9907.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-6-methoxybenzo[*d*]thiazole(3g)



White solid, yield 52% (45.8 mg). M.p. = 82–83 °C.

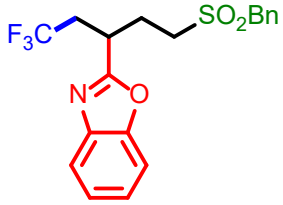
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.9 Hz, 1H), 7.31 – 7.22 (m, 6H), 7.11 (dd, *J* = 9.0, 2.5 Hz, 1H), 4.16 (s, 2H), 3.88 (s, 3H), 3.60 – 3.52 (m, 1H), 2.89 – 2.80 (m, 3H), 2.57 – 2.48 (m, 1H), 2.39 – 2.33 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 158.0, 147.5, 136.1, 130.5, 129.2, 129.1, 127.7, 125.9 (q, *J* = 277.5 Hz), 123.6, 115.9, 104.3, 59.6, 55.9, 48.1, 39.0 (q, *J* = 28.8 Hz), 37.1 (q, *J* = 2.6 Hz), 27.9.

^{19}F NMR (376 MHz, $CDCl_3$)*δ* -63.97 (t, *J* = 10.5 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{20}H_{21}F_3NO_3S_2^+$444.0909;found 444.0915.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)benzo[*d*]oxazole(3h)



White solid, yield 63% (50.0 mg). M.p. = 103–105 °C.

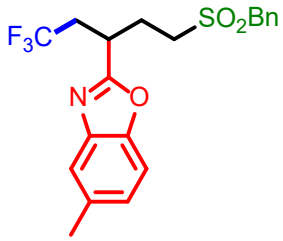
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.67 (m, 1H), 7.54 – 7.48 (m, 1H), 7.40 – 7.35 (m, 2H), 7.33 – 7.25 (m, 5H), 4.20 (s, 2H), 3.61 – 3.46 (m, 1H), 2.96 – 2.81 (m, 3H), 2.58 – 2.44 (m, 1H), 2.41 – 2.31 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 150.8, 140.8, 130.5, 129.3, 129.2, 127.7, 125.8 (q, *J* = 277.2 Hz), 125.6, 124.8, 120.2, 110.9, 59.8, 48.2, 37.1 (q, *J* = 29.3 Hz), 33.1 (q, *J* = 2.8 Hz), 25.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -64.56 (t, *J* = 10.3 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{19}H_{19}F_3NO_3S^+$398.1032; found 398.1033.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-5-methylbenzo[*d*]oxazole(3i)



White solid, yield 60% (49.4 mg). M.p. = 120–122 °C.

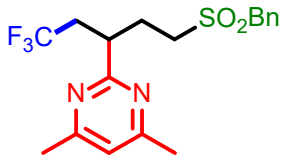
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (s, 1H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.33 – 7.25 (m, 5H), 7.18 (d, *J* = 8.2 Hz, 1H), 4.19 (s, 2H), 3.54 – 3.44 (m, 1H), 2.92 – 2.80 (m, 3H), 2.55 – 2.44 (m, 4H), 2.38 – 2.32 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 149.0, 141.0, 134.7, 130.6, 129.3, 129.2, 127.7, 126.6, 125.8 (q, *J* = 277.0 Hz), 120.1, 110.2, 59.8, 48.3, 37.0 (q, *J* = 29.2 Hz), 33.1 (q, *J* = 2.5 Hz), 25.8, 21.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -64.57 (t, *J* = 10.3 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{20}H_{21}F_3NO_3S^+$412.1189; found 412.1191.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-4,6-dimethylpyrimidine(3j)



White solid, yield 60% (45.8 mg). M.p. = 111–113 °C.

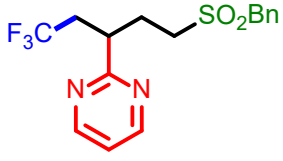
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.27 (m, 5H), 6.87 (s, 1H), 4.16 (s, 2H), 3.29 – 3.19 (m, 1H), 2.93 – 2.80 (m, 2H), 2.66 – 2.57 (m, 1H), 2.44 – 2.32 (m, 7H), 2.30 – 2.18 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 167.1, 130.5, 129.1, 128.0, 126.5 (q, *J* = 277.0 Hz), 118.5, 59.2, 48.8, 41.4 (q, *J* = 2.3 Hz), 37.7 (q, *J* = 28.2 Hz), 27.2, 24.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -64.14 (t, *J* = 10.8 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{18}H_{22}F_3N_2O_2S^+$387.1349; found 387.1353.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)pyrimidine(3k)



White solid, yield 75% (58.7 mg). M.p. = 69–70 °C.

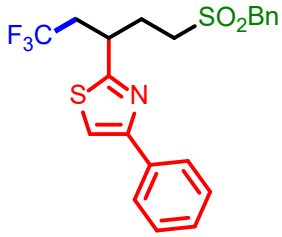
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.9 Hz, 2H), 7.26 – 7.19 (m, 5H), 7.07 (t, *J* = 4.9 Hz, 1H), 4.06 (s, 2H), 3.30 – 3.21 (m, 1H), 2.83 – 2.69 (m, 2H), 2.55 – 2.46 (m, 1H), 2.36 – 2.25 (m, 1H), 2.22 – 2.10 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 157.4, 130.6, 129.1, 127.9, 126.4 (q, *J* = 277.1 Hz), 119.7, 59.3, 48.6, 41.6 (q, *J* = 2.3 Hz), 37.8 (q, *J* = 28.5 Hz), 27.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -64.23 (t, *J* = 10.7 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{16}H_{18}F_3N_2O_2S^+$359.1036; found 359.1037.

2-(5-(benzylsulfonyl)-1,1,1-trifluoropentan-3-yl)-4-phenylthiazole(3l)



White solid, yield 69% (60.6 mg). M.p. = 58–60°C.

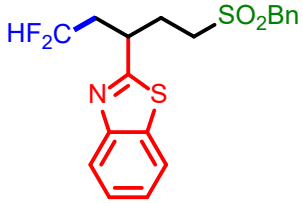
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.5 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.37 – 7.34 (m, 2H), 7.30 – 7.22 (m, 5H), 4.17 (d, *J* = 2.3 Hz, 2H), 3.61 – 3.52 (m, 1H), 2.87 – 2.78 (m, 3H), 2.57 – 2.46 (m, 1H), 2.36 (dd, *J* = 15.7, 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 155.9, 134.2, 130.5, 129.2, 129.2, 128.9, 128.5, 127.8, 126.5, 126.0 (q, *J* = 277.3 Hz), 112.6, 59.7, 48.2, 39.4 (q, *J* = 28.5 Hz), 36.6 (q, *J* = 2.3 Hz), 28.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.90 (t, *J* = 10.4 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{21}H_{21}F_3NO_2S_2^+$440.0960; found 440.0966.

2-(5-(benzylsulfonyl)-1,1-difluoropentan-3-yl)benzo[*d*]thiazole(3m)



White solid, yield 70% (55.2 mg). M.p. = 87–88 °C.

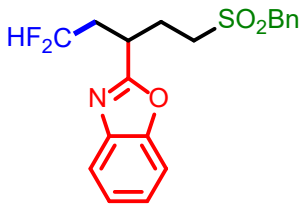
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.2 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.33 – 7.18 (m, 5H), 5.99 – 5.66 (m, 1H), 4.16 (s, 2H), 3.59 – 3.45 (m, 1H), 2.85 (t, *J* = 8.0 Hz, 2H), 2.59 – 2.44 (m, 1H), 2.41 – 2.18 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 153.1, 134.7, 130.5, 129.1, 129.1, 127.8, 126.5, 125.6, 123.2, 121.9, 115.5 (t, *J* = 239.9 Hz), 59.6, 48.3, 39.3 (t, *J* = 22.0 Hz), 37.6 (dd, *J* = 6.9, 4.2 Hz), 28.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -113.56 – -118.63 (m, 2F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{19}H_{20}F_2NO_2S_2^+$396.0898; found 396.0901.

2-(5-(benzylsulfonyl)-1,1-difluoropentan-3-yl)benzo[*d*]oxazole(3n)



White solid, yield 57% (43.5 mg). M.p. = 98–100 °C.

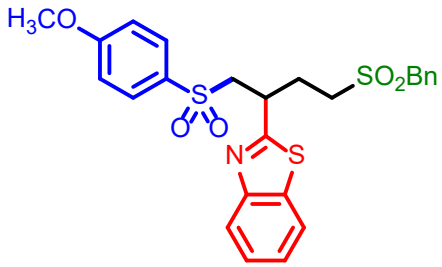
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.66 (m, 1H), 7.53 – 7.47 (m, 1H), 7.39 – 7.35 (m, 2H), 7.34 – 7.26 (m, 5H), 6.08 – 5.77 (m, 1H), 4.21 (s, 2H), 3.48 – 3.37 (m, 1H), 2.97 – 2.89 (m, 2H), 2.60 – 2.44 (m, 1H), 2.39 – 2.16 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 150.8, 140.8, 130.6, 129.2, 129.2, 127.7, 125.5, 124.8, 120.1, 115.4 (t, J = 240.0 Hz), 110.8, 59.7, 48.4, 37.2 (t, J = 22.1 Hz), 33.0 (dd, J = 6.3, 4.9 Hz), 25.93.

^{19}F NMR (376 MHz, $CDCl_3$) δ -114.54 – -117.63 (m, 2F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{19}H_{20}F_2NO_3S^+$380.1126; found 380.1130.

2-(4-(benzylsulfonyl)-1-((4-methoxyphenyl)sulfonyl)butan-2-yl)benzo[*d*]thiazole(5a)



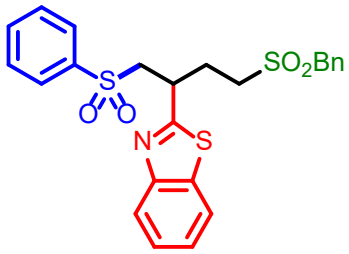
White solid, yield 81% (83.4 mg). M.p. = 162–163 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (t, J = 7.9 Hz, 2H), 7.73 – 7.66 (m, 2H), 7.46 (td, J = 7.3, 1.3 Hz, 1H), 7.39 (td, J = 7.3, 1.3 Hz, 1H), 7.30 – 7.26 (m, 3H), 7.25 – 7.19 (m, 2H), 6.83 – 6.73 (m, 2H), 4.19 (s, 2H), 3.94 – 3.85 (m, 2H), 3.70 (s, 3H), 3.54 – 3.43 (m, 1H), 2.93 – 2.79 (m, 2H), 2.55 – 2.35 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 163.8, 152.8, 134.8, 130.6, 130.4, 130.3, 129.1, 129.1, 127.7, 126.4, 125.6, 123.1, 121.8, 114.4, 60.0, 59.3, 55.7, 47.9, 37.9, 28.3.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{25}H_{26}NO_5S_3^+$516.0968; found 516.0973.

2-(4-(benzylsulfonyl)-1-(phenylsulfonyl)butan-2-yl)benzo[*d*]thiazole(5b)



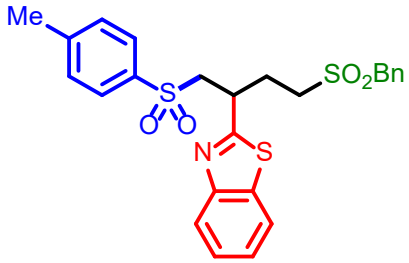
White solid, yield 51% (49.5 mg). M.p. = 100–102 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.58 (m, 4H), 7.35 – 7.29 (m, 2H), 7.28 – 7.20 (m, 3H), 7.17 – 7.12 (m, 3H), 7.12 – 7.00 (m, 2H), 4.05 (s, 2H), 3.84 – 3.73 (m, 2H), 3.43 – 3.33 (m, 1H), 2.73 (t, *J* = 7.9 Hz, 2H), 2.43 – 2.25 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 152.8, 139.1, 134.8, 133.9, 130.6, 129.2, 129.1, 128.0, 127.7, 126.4, 125.7, 123.1, 121.8, 59.8, 59.3, 47.9, 37.7, 28.2.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{24}H_{24}NO_4S_3^+$486.0862; found 486.0863.

2-(4-(benzylsulfonyl)-1-tosylbutan-2-yl)benzo[*d*]thiazole(5c)



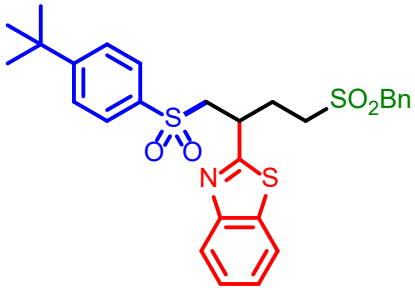
White solid, yield 60% (61.2 mg). M.p. = 142–143 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (t, *J* = 7.2 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.30 – 7.25 (m, 3H), 7.25 – 7.18 (m, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 4.18 (s, 2H), 3.95 – 3.85 (m, 2H), 3.48 (dd, *J* = 17.0, 8.4 Hz, 1H), 2.92 – 2.79 (m, 2H), 2.54 – 2.37 (m, 2H), 2.26 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 152.8, 145.0, 136.1, 134.8, 130.6, 129.8, 129.1, 128.0, 127.8, 126.4, 125.6, 123.1, 121.8, 59.8, 59.3, 47.9, 37.8, 28.2, 21.6.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{25}H_{26}NO_4S_3^+$500.1018; found 500.1020.

2-(4-(benzylsulfonyl)-1-((4-(tert-butyl)phenyl)sulfonyl)butan-2-yl)benzo[*d*]thiazol e(5d)



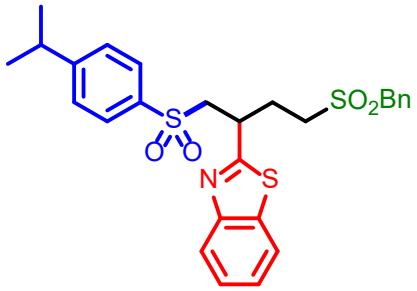
White solid, yield 60% (64.0 mg). M.p. = 160–161 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.40 – 7.33 (m, 3H), 7.30 – 7.25 (m, 3H), 7.25 – 7.18 (m, 2H), 4.19 (s, 2H), 3.98 – 3.89 (m, 2H), 3.49 (q, *J* = 8.3 Hz, 1H), 2.92 – 2.78 (m, 2H), 2.55 – 2.37 (m, 2H), 1.20 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 157.9, 152.8, 135.9, 134.8, 130.6, 129.1, 127.9, 127.8, 126.5, 126.2, 125.6, 123.1, 121.8, 59.8, 59.3, 47.9, 37.9, 35.2, 31.0, 28.4.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{28}H_{32}NO_4S_3^+$542.1488; found 542.1488.

2-(4-(benzylsulfonyl)-1-((4-isopropylphenyl)sulfonyl)butan-2-yl)benzo[*d*]thiazole(5e)



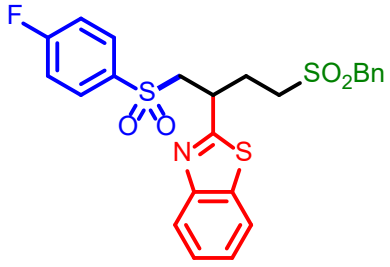
White solid, yield 58% (61.3 mg). M.p. = 138–140°C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.44 (td, *J* = 7.2, 1.1 Hz, 1H), 7.37 (td, *J* = 7.2 Hz, 1H), 7.29 – 7.24 (m, 3H), 7.24 – 7.16 (m, 4H), 4.18 (s, 2H), 3.98 – 3.89 (m, 2H), 3.59 – 3.39 (m, 1H), 2.92 – 2.78 (m, 3H), 2.55 – 2.37 (m, 2H), 1.15 – 1.10 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 155.6, 152.7, 136.3, 134.7, 130.6, 129.1, 129.1, 128.2, 127.7, 127.3, 126.4, 125.6, 123.1, 121.8, 59.8, 59.3, 47.9, 37.8, 34.2, 28.4, 23.5.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{27}H_{30}NO_4S_3^+$528.1331; found 528.1337.

2-(4-(benzylsulfonyl)-1-((4-fluorophenyl)sulfonyl)butan-2-yl)benzo[*d*]thiazole(5f)



White solid, yield 43% (43.0 mg). M.p. = 74–75 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.76 (m, 4H), 7.47 (td, *J* = 8.3, 1.1 Hz, 1H), 7.40 (td, *J* = 8.3, 1.1 Hz, 1H), 7.31 – 7.21 (m, 5H), 7.00 (t, *J* = 8.5 Hz, 2H), 4.19 (s,

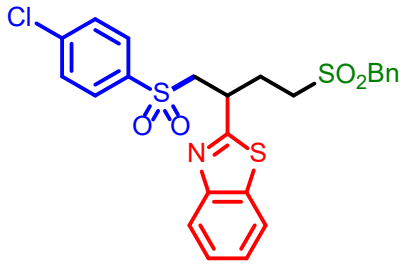
2H), 3.98 – 3.89 (m, 2H), 3.51 (dd, *J* = 17.2, 8.4 Hz, 1H), 2.91 – 2.81 (m, 2H), 2.55 – 2.39 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 165.9 (d, *J* = 257.2 Hz), 152.8, 135.2 (d, *J* = 3.1 Hz), 134.7, 131.0 (d, *J* = 9.8 Hz), 130.6, 129.2, 127.8, 126.6, 125.8, 123.1, 121.8, 116.5 (d, *J* = 22.8 Hz), 60.0, 59.5, 47.8, 37.8, 28.2.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{24}H_{23}FNO_4S_3^+$504.0768; found 504.0772.

2-(4-(benzylsulfonyl)-1-((4-chlorophenyl)sulfonyl)butan-2-yl)benzo[d]thiazole(5g

)



White solid, yield 34% (35.8 mg). M.p. = 82–83 °C.

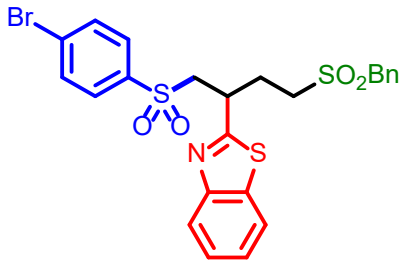
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 5.6 Hz, 1H), 7.79 (d, *J* = 6.0 Hz, 1H), 7.71 – 7.62 (m, 2H), 7.48 (t, *J* = 8.3 Hz, 1H), 7.40 (t, *J* = 8.1 Hz, 1H), 7.29 – 7.20 (m, 7H), 4.19 (s, 2H), 3.98 – 3.88 (m, 2H), 3.50 (dd, *J* = 13.2, 4.1 Hz, 1H), 2.92 – 2.80 (m, 2H), 2.53 – 2.35 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 152.7, 140.7, 137.5, 134.7, 130.6, 129.5, 129.4, 129.2, 129.1, 127.7, 126.6, 125.8, 123.1, 121.8, 59.9, 59.5, 47.8, 37.8, 28.2.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{24}H_{23}ClNO_4S_3^+$520.0472; found 520.0478.

2-(4-(benzylsulfonyl)-1-((4-bromophenyl)sulfonyl)butan-2-yl)benzo[*d*]thiazole(5h

)



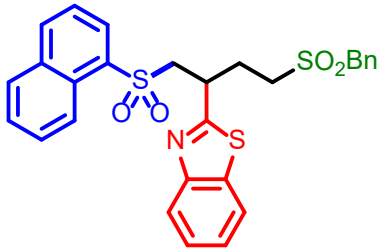
White solid, yield 27% (30.0 mg). M.p. = 79–81 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (t, *J* = 7.4 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.45 – 7.38 (m, 3H), 7.29 – 7.20 (m, 5H), 4.19 (s, 2H), 3.99 – 3.89 (m, 2H), 3.49 (dd, *J* = 13.4, 4.2 Hz, 1H), 2.91 – 2.79 (m, 2H), 2.52 – 2.35 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 152.7, 138.1, 134.7, 132.4, 130.6, 129.5, 129.3, 129.2, 129.2, 127.7, 126.7, 125.9, 123.1, 121.8, 59.9, 59.5, 47.8, 37.8, 28.2.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{24}H_{23}BrNO_4S_3^+$563.9967; found 563.9972.

2-(4-(benzylsulfonyl)-1-(naphthalen-1-ylsulfonyl)butan-2-yl)benzo[*d*]thiazole(5i)



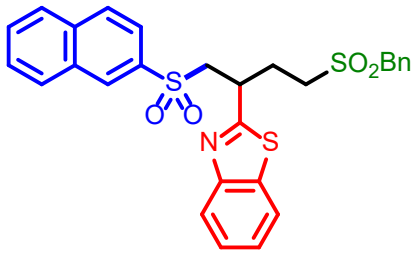
White solid, yield 43% (46.4 mg). M.p. = 145–146 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.6 Hz, 1H), 8.14 (d, *J* = 7.3 Hz, 1H), 7.84 (d, *J* = 8.2 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 1H), 7.74 – 7.66 (m, 2H), 7.60 – 7.53 (m, 2H), 7.39 – 7.31 (m, 3H), 7.26 – 7.23 (m, 3H), 7.22 – 7.14 (m, 2H), 4.22 (dd, *J* = 14.3, 7.4 Hz, 1H), 4.15 (s, 2H), 3.98 – 3.89 (m, 1H), 3.64 (dd, *J* = 14.4, 5.3 Hz, 1H), 2.91 – 2.77 (m, 2H), 2.52 – 2.33 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 152.6, 135.3, 134.7, 134.1, 133.8, 130.8, 130.6, 129.3, 129.1, 129.1, 129.1, 128.7, 127.7, 127.1, 126.3, 125.6, 124.2, 123.9, 123.0, 121.6, 59.4, 47.9, 37.9, 28.4.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{28}H_{26}NO_4S_3^+$536.1018; found 536.1025.

2-(4-(benzylsulfonyl)-1-(naphthalen-2-ylsulfonyl)butan-2-yl)benzo[*d*]thiazole(5j)



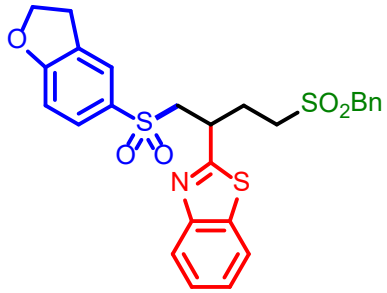
White solid, yield 47% (50.4 mg). M.p. = 133–135 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.82 – 7.77 (m, 2H), 7.74 (t, *J* = 7.5 Hz, 2H), 7.65 (t, *J* = 7.1 Hz, 2H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.33 – 7.25 (m, 5H), 7.23 – 7.18 (m, 2H), 4.18 (s, 2H), 4.05 – 3.94 (m, 2H), 3.57 (dd, *J* = 13.7, 4.8 Hz, 1H), 2.90 – 2.80 (m, 2H), 2.54 – 2.39 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 152.6, 135.8, 135.2, 134.6, 132.0, 130.6, 130.1, 129.6, 129.4, 129.1, 129.1, 127.9, 127.7, 126.4, 125.6, 122.9, 122.4, 121.6, 59.8, 59.4, 47.9, 37.9, 28.3.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{28}H_{26}NO_4S_3^+$536.1018; found 536.1021.

2-(4-(benzylsulfonyl)-1-((2,3-dihydrobenzofuran-5-yl)sulfonyl)butan-2-yl)benzo[*d*]thiazole(5k)



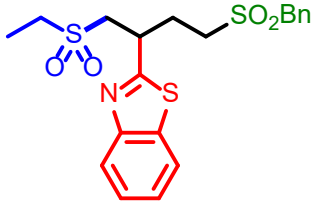
White solid, yield 65% (68.5 mg). M.p. = 146–148 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 – 7.77 (m, 2H), 7.59 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.50 – 7.43 (m, 2H), 7.43 – 7.37 (m, 1H), 7.31 – 7.27 (m, 2H), 7.25 – 7.17 (m, 2H), 6.70 (d, *J* = 8.5 Hz, 1H), 4.55 – 4.38 (m, 2H), 4.18 (s, 2H), 3.99 – 3.81 (m, 2H), 3.53 – 3.42 (m, 1H), 3.03 – 2.93 (m, 1H), 2.92 – 2.71 (m, 3H), 2.52 – 2.31 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 164.7, 152.9, 134.9, 130.6, 130.3, 129.9, 129.2, 129.1, 128.6, 127.7, 126.5, 125.6, 125.3, 123.1, 121.8, 109.8, 72.4, 60.2, 59.4, 47.9, 38.1, 28.7, 28.3.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{26}H_{26}NO_5S_3^+$ 528.0968; found 528.0972.

2-(4-(benzylsulfonyl)-1-(ethylsulfonyl)butan-2-yl)benzo[*d*]thiazole(5l)



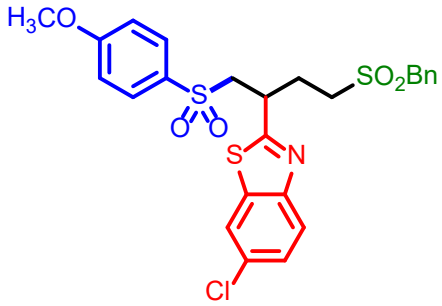
White solid, yield 50% (44.0 mg). M.p. = 125–127 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.32 – 7.22 (m, 5H), 4.21 (s, 2H), 4.06 – 3.98 (m, 1H), 3.81 (dd, *J* = 14.3, 6.9 Hz, 1H), 3.33 (dd, *J* = 14.3, 6.1 Hz, 1H), 3.03 – 2.77 (m, 4H), 2.58 – 2.40 (m, 2H), 1.33 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 152.9, 134.9, 130.6, 129.1, 129.1, 127.7, 126.7, 125.8, 123.2, 122.0, 59.3, 55.3, 48.7, 47.9, 37.1, 28.3, 6.6.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{20}H_{24}NO_4S_3^+$438.0862; found 438.0866.

2-(4-(benzylsulfonyl)-1-((4-methoxyphenyl)sulfonyl)butan-2-yl)-6-chlorobenzo[*d*]thiazole(5m)



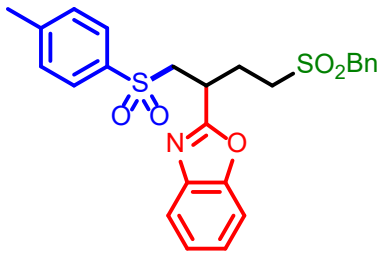
White solid, yield 57% (62.6 mg). M.p. = 139–141 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 2.0 Hz, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.68 (d, *J* = 8.9 Hz, 2H), 7.42 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.33 – 7.26 (m, 5H), 6.79 (d, *J* = 8.9 Hz, 2H), 4.20 (s, 2H), 3.91 – 3.82 (m, 2H), 3.74 (s, 3H), 3.45 (dd, *J* = 13.4, 4.5 Hz, 1H), 2.89 – 2.80 (m, 2H), 2.51 – 2.35 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 163.9, 151.4, 136.0, 131.6, 130.6, 130.4, 130.3, 129.2, 129.2, 127.7, 127.2, 123.9, 121.3, 114.4, 60.0, 59.5, 55.7, 47.9, 37.9, 28.0.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{25}H_{25}ClNO_5S_3^+$550.0578; found 550.0580.

2-(4-(benzylsulfonyl)-1-tosylbutan-2-yl)benzo[*d*]oxazole(5n)



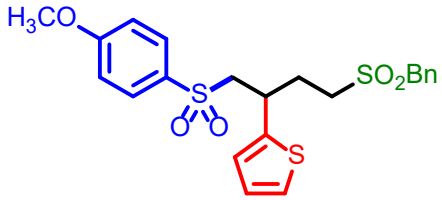
White solid, yield 59% (57.0 mg). M.p. = 139–141 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.9 Hz, 2H), 7.59 – 7.52 (m, 1H), 7.37 – 7.24 (m, 8H), 7.10 (d, *J* = 7.9 Hz, 2H), 4.19 (s, 2H), 3.87 (dd, *J* = 14.3, 7.9 Hz, 1H), 3.79 – 3.70 (m, 1H), 3.44 (dd, *J* = 14.3, 4.9 Hz, 1H), 2.98 – 2.79 (m, 2H), 2.49 – 2.32 (m, 2H), 2.22 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 150.5, 145.1, 140.6, 135.4, 130.6, 129.8, 129.1, 129.1, 128.1, 127.7, 125.4, 124.7, 120.0, 110.8, 59.4, 58.0, 48.0, 34.0, 26.1, 21.5.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{25}H_{26}NO_5S_2^+$484.1247; found 484.1252.

2-(4-(benzylsulfonyl)-1-((4-methoxyphenyl)sulfonyl)butan-2-yl)thiophene(5o)



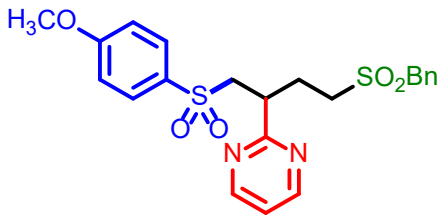
White solid, yield 38% (35.3 mg). M.p. = 38–40 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.71 (m, 2H), 7.40 – 7.35 (m, 5H), 7.13 (dd, *J* = 5.1, 0.8 Hz, 1H), 6.97 – 6.92 (m, 2H), 6.83 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.71 (dd, *J* = 3.4, 0.8 Hz, 1H), 4.21 (s, 2H), 3.86 (s, 3H), 3.73 – 3.65 (m, 1H), 3.43 – 3.35 (m, 2H), 2.78 – 2.68 (m, 2H), 2.64 – 2.56 (m, 1H), 2.11 – 2.01 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 143.4, 131.0, 130.7, 130.2, 129.2, 129.2, 127.9, 127.2, 125.9, 125.0, 114.7, 62.8, 59.3, 55.9, 48.7, 34.9, 29.8.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{22}H_{25}O_5S_3^+$465.0859; found 465.0860.

2-(4-(benzylsulfonyl)-1-((4-methoxyphenyl)sulfonyl)butan-2-yl)pyrimidine(5p)



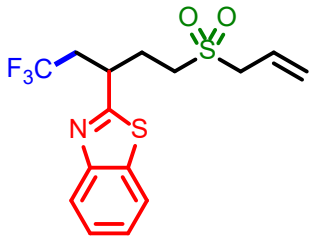
White solid, yield 43% (39.8 mg). M.p. = 161–163 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.9 Hz, 2H), 7.73 (d, *J* = 8.9 Hz, 2H), 7.38 – 7.32 (m, 5H), 7.11 (t, *J* = 4.9 Hz, 1H), 6.93 (d, *J* = 8.9 Hz, 2H), 4.17 (s, 2H), 3.97 (dd, *J* = 14.3, 8.0 Hz, 1H), 3.85 (s, 3H), 3.59 – 3.50 (m, 1H), 3.31 (dd, *J* = 14.3, 5.0 Hz, 1H), 2.89 – 2.78 (m, 1H), 2.71 – 2.60 (m, 1H), 2.40 – 2.24 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 163.8, 157.3, 130.7, 130.7, 130.4, 129.2, 127.9, 119.6, 114.5, 59.3, 59.2, 55.8, 48.4, 42.3, 27.4.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{22}H_{25}N_2O_5S_2^+$461.1199; found 461.1203.

2-(5-(allylsulfonyl)-1,1,1-trifluoropentan-3-yl)benzo[*d*]thiazole(6a)



Colorless oil, yield 75% (54.5 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 5.91 – 5.77 (m, 1H), 5.41 – 5.31 (m, 2H),

3.74 – 3.65 (m, 3H), 2.99 – 2.85 (m, 3H), 2.65 – 2.56 (m, 1H), 2.51 – 2.41 (m, 2H).

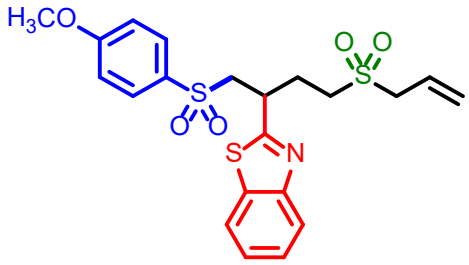
^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 153.1, 134.7, 126.6, 125.9 (q, *J* = 277.2 Hz), 125.7, 125.0, 124.8, 123.2, 121.9, 57.9, 48.3, 39.1 (q, *J* = 28.9 Hz), 37.3 (q, *J* = 2.5 Hz), 27.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.96 (t, *J* = 10.4 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{15}H_{17}F_3NO_2S_2^+$364.0647;found 364.0650.

2-(4-(allylsulfonyl)-1-((4-methoxyphenyl)sulfonyl)butan-2-yl)benzo[*d*]thiazole(6b

)



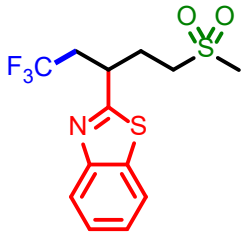
Light yellow solid, yield 71% (66.3 mg). M.p. = 111–112 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (t, *J* = 7.6 Hz, 2H), 7.72 – 7.63 (m, 2H), 7.43 (td, *J* = 8.2, 1.3 Hz, 1H), 7.36 (td, *J* = 8.2, 1.3 Hz, 1H), 6.83 – 6.72 (m, 2H), 5.89 – 5.77 (m, 1H), 5.42 – 5.33 (m, 2H), 3.98 – 3.86 (m, 2H), 3.73 – 3.64 (m, 5H), 3.52 (dd, *J* = 13.9, 5.4 Hz, 1H), 3.05 – 2.93 (m, 2H), 2.58 – 2.39 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 163.8, 152.8, 134.8, 130.4, 130.2, 126.4, 125.6, 125.1, 124.7, 123.0, 121.8, 114.4, 60.0, 57.6, 55.6, 48.1, 38.0, 27.9.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{21}H_{24}NO_5S_3^+$ 466.0811; found 466.0813.

2-(1,1,1-trifluoro-5-(methylsulfonyl)pentan-3-yl)benzo[*d*]thiazole(6c)



White solid, yield 60% (40.4 mg). M.p. = 121–123 °C.

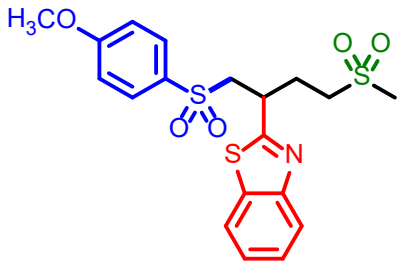
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 3.78 – 3.68 (m, 1H), 3.08 – 2.92 (m, 3H), 2.88 (s, 3H), 2.67 – 2.58 (m, 1H), 2.53 – 2.44 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 153.1, 134.7, 126.6, 125.9 (q, *J* = 277.2 Hz), 125.8, 123.3, 122.0, 51.8, 40.9, 39.1 (q, *J* = 28.8 Hz), 37.3 (q, *J* = 2.4 Hz), 27.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.98 (t, *J* = 10.3 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{13}H_{15}F_3NO_2S_2^+$338.0491;found 338.0493.

2-(1-((4-methoxyphenyl)sulfonyl)-4-(methylsulfonyl)butan-2-yl)benzo[*d*]thiazole(6d)



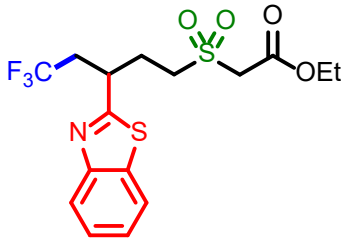
White solid, yield 66% (57.7 mg). M.p. = 95–97 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (t, *J* = 8.9 Hz, 2H), 7.70 (d, *J* = 8.9 Hz, 2H), 7.43 (td, *J* = 7.4, 1.1 Hz, 1H), 7.36 (td, *J* = 7.4, 1.1 Hz, 1H), 6.78 (d, *J* = 8.9 Hz, 2H), 4.04 – 3.95 (m, 1H), 3.89 (dd, *J* = 14.3, 7.0 Hz, 1H), 3.70 (s, 3H), 3.55 (dd, *J* = 14.3, 6.0 Hz, 1H), 3.11 – 2.98 (m, 2H), 2.87 (s, 3H), 2.61 – 2.44 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 163.8, 152.8, 134.8, 130.4, 130.2, 126.4, 125.6, 123.1, 121.8, 114.4, 59.8, 55.7, 51.4, 40.7, 37.9, 28.1.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{19}H_{22}NO_5S_3^+$440.0655; found 440.0660.

ethyl 2-((3-(benzo[*d*]thiazol-2-yl)-5,5,5-trifluoropentyl)sulfonyl)acetate(6e)



Colorless oil, yield 73% (60.0 mg).

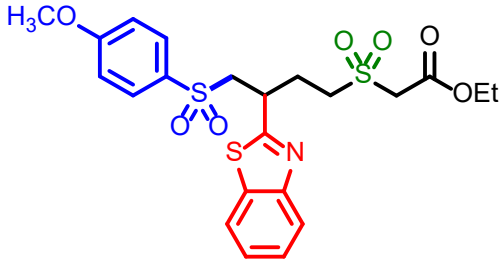
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.93 (s, 2H), 3.77 – 3.69 (m, 1H), 3.32 – 3.23 (m, 2H), 2.99 – 2.88 (m, 1H), 2.68 – 2.58 (m, 1H), 2.54 – 2.47 (m, 2H), 1.20 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 162.8, 153.1, 134.8, 126.6, 125.9 (q, *J* = 277.6 Hz), 125.7, 123.3, 121.9, 62.9, 57.7, 50.7, 39.0 (q, *J* = 28.7 Hz), 37.2 (q, *J* = 2.5 Hz), 27.6, 13.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.97 (t, *J* = 10.4 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{16}H_{19}F_3NO_4S_2^+$410.0702;found 410.0704.

Ethyl2-((3-(benzo[*d*]thiazol-2-yl)-4-((4-methoxyphenyl)sulfonyl)butyl)sulfonyl)acetate(6f)



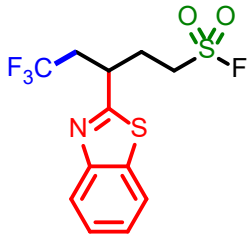
Colorless oil, yield 69% (70.3 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (t, *J* = 8.7 Hz, 1H), 7.70 (d, *J* = 8.9 Hz, 2H), 7.44 (td, *J* = 7.4, 1.1 Hz, 1H), 7.37 (td, *J* = 7.4, 1.1 Hz, 1H), 6.78 (d, *J* = 8.9 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 4.04 – 3.88 (m, 4H), 3.70 (s, 3H), 3.56 (dd, *J* = 14.2, 5.7 Hz, 1H), 3.38 – 3.23 (m, 2H), 2.64 – 2.46 (m, 2H), 1.21 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 163.8, 162.9, 152.8, 134.8, 130.4, 130.3, 126.4, 125.6, 123.1, 121.8, 114.4, 62.8, 59.9, 57.3, 55.7, 50.4, 37.9, 27.8, 13.9.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{22}H_{26}NO_7S_3^+$512.0866; found512.0863.

3-(benzo[*d*]thiazol-2-yl)-5,5,5-trifluoropentane-1-sulfonyl fluoride(6g)



Colorless oil, yield 60% (40.9 mg).

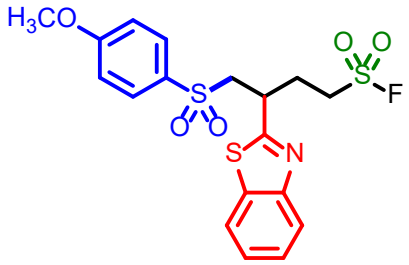
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.1 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 8.3 Hz, 1H), 7.44 (t, *J* = 8.2 Hz, 1H), 3.77 – 3.70 (m, 1H), 3.47 – 3.37 (m, 2H), 2.96 – 2.86 (m, 1H), 2.67 – 2.55 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 153.1, 134.7, 126.8, 126.0, 125.8 (q, *J* = 277.7 Hz), 123.4, 122.0, 48.2 (q, *J* = 17.9 Hz), 39.1 (q, *J* = 29.2 Hz), 36.7 (q, *J* = 2.1 Hz), 28.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ 53.81 (t, *J* = 5.0 Hz, 1F), -63.95 (t, *J* = 10.9 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{12}H_{12}F_4NO_2S_2^+$342.0240; found 342.0243.

3-(benzo[*d*]thiazol-2-yl)-4-((4-methoxyphenyl)sulfonyl)butane-1-sulfonyl fluoride(6h)



White solid, yield 47% (41.6 mg). M.p. = 120–121 °C.

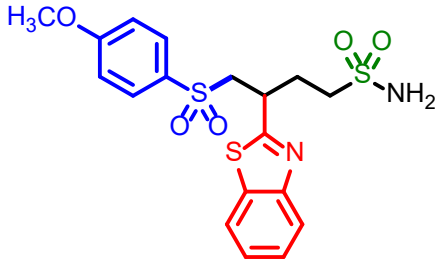
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.8 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.9 Hz, 2H), 7.47 (td, *J* = 7.3, 1.2 Hz, 1H), 7.40 (td, *J* = 7.3, 1.2 Hz, 1H), 6.83 (d, *J* = 8.9 Hz, 2H), 4.04 – 3.95 (m, 1H), 3.86 (dd, *J* = 14.4, 6.5 Hz, 1H), 3.74 (s, 3H), 3.52 (dd, *J* = 14.4, 6.5 Hz, 1H), 3.48 – 3.40 (m, 2H), 2.70 – 2.60 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 164.1, 152.9, 134.8, 130.3, 126.7, 125.9, 123.3, 121.9, 114.6, 60.0, 55.7, 48.0 (d, *J* = 18.2 Hz), 37.6, 28.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ 53.79 (t, *J* = 4.4 Hz, 1F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{18}H_{19}FNO_5S_3^+$444.0404; found444.0408.

3-(benzo[*d*]thiazol-2-yl)-4-((4-methoxyphenyl)sulfonyl)butane-1-sulfonamide(6i)



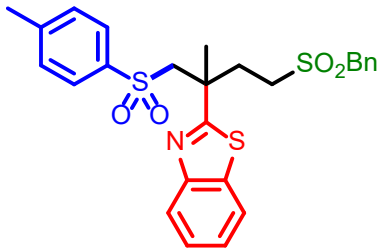
White solid, yield 54% (47.3 mg). M.p. = 70–72 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 7.5 Hz, 1H), 7.64 (d, *J* = 8.9 Hz, 2H), 7.43 – 7.36 (m, 1H), 7.35 – 7.28 (m, 1H), 6.70 (d, *J* = 8.9 Hz, 2H), 5.41 (s, 2H), 4.05 – 3.97 (m, 1H), 3.94 – 3.86 (m, 1H), 3.70 – 3.57 (m, 4H), 3.24 – 3.07 (m, 2H), 2.62 – 2.40 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 163.7, 152.7, 134.8, 130.3, 130.2, 126.3, 125.4, 123.0, 121.8, 114.3, 60.0, 55.6, 51.9, 37.9, 30.0.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{18}H_{21}N_2O_5S_3^+$441.0607; found 441.0611.

2-(4-(benzylsulfonyl)-2-methyl-1-tosylbutan-2-yl)benzo[*d*]thiazole(6j)



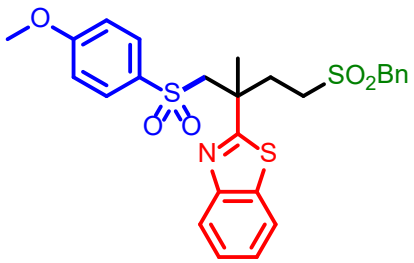
White solid, yield 56% (57.5 mg). M.p. = 132–133 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.0,, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.46 (td, *J* = 7.3, 1.2 Hz, 1H), 7.38 (td, *J* = 7.3, 1.2 Hz, 1H), 7.29 – 7.26 (m, 3H), 7.22 – 7.17 (m, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.19 (s, 2H), 3.85 (d, *J* = 14.5 Hz, 1H), 3.65 (d, *J* = 14.5 Hz, 1H), 2.93 – 2.86 (m, 2H), 2.71 – 2.62 (m, 1H), 2.43 – 2.35 (m, 1H), 2.28 (s, 3H), 1.87 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 152.7, 144.8, 137.6, 134.8, 130.7, 129.7, 129.1, 129.0, 127.8, 127.6, 126.4, 125.5, 123.2, 121.8, 64.2, 59.0, 47.2, 43.4, 35.0, 25.1, 21.6.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{26}H_{28}NO_4S_3^+$514.1175; found514.1179.

2-(4-(benzylsulfonyl)-1-((4-methoxyphenyl)sulfonyl)-2-methylbutan-2-yl)benzo[*d*]thiazole(6k)



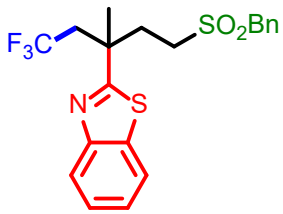
White solid, yield 58% (61.4 mg). M.p. = 73–75 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (t, *J* = 8.7 Hz, 2H), 7.66 (d, *J* = 8.9 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.30 – 7.26 (m, 3H), 7.23 – 7.15 (m, 2H), 6.76 (d, *J* = 8.9 Hz, 2H), 4.19 (s, 2H), 3.85 (d, *J* = 14.5 Hz, 1H), 3.72 (s, 3H), 3.65 (d, *J* = 14.5 Hz, 1H), 2.93 – 2.84 (m, 2H), 2.72 – 2.59 (m, 1H), 2.43 – 2.33 (m, 1H), 1.86 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 163.7, 152.8, 134.9, 132.1, 130.7, 130.0, 129.1, 129.0, 127.6, 126.4, 125.5, 123.2, 121.8, 114.2, 64.5, 59.0, 55.7, 47.2, 43.3, 35.0, 25.0.

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{26}H_{28}NO_5S_3^+$530.1124; found 530.1127.

2-(5-(benzylsulfonyl)-1,1,1-trifluoro-3-methylpentan-3-yl)benzo[*d*]thiazole(6l)



Colorless oil, yield 74% (63.0 mg).

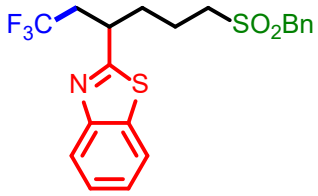
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 8.2 Hz, 1H), 7.41 (t, *J* = 8.2 Hz, 1H), 7.26 – 7.20 (m, 3H), 7.20 – 7.10 (m, 2H), 4.14 (s, 2H), 3.01 – 2.90 (m, 1H), 2.88 – 2.71 (m, 2H), 2.67 – 2.55 (m, 1H), 2.48 (td, *J* = 13.1, 4.5 Hz, 1H), 2.21 (td, *J* = 13.1, 4.4 Hz, 1H), 1.65 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 152.9, 134.8, 130.5, 129.1, 129.0, 127.7, 126.4, 125.9 (q, *J* = 278.7 Hz), 125.5, 123.3, 121.8, 59.2, 46.8, 43.7 (q, *J* = 27.4 Hz), 41.2 (q, *J* = 1.5 Hz), 34.9, 24.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -59.41 (t, *J* = 10.9 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{20}H_{21}F_3NO_2S_2^+$428.0960; found 428.0965.

2-(6-(benzylsulfonyl)-1,1,1-trifluorohexan-3-yl)benzo[*d*]thiazole(6m)



Colorless oil, yield 74% (63.2 mg).

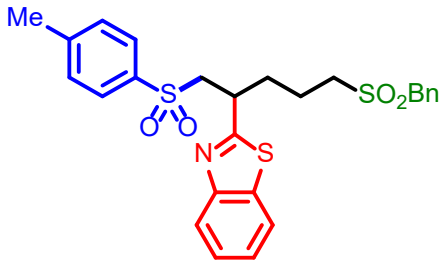
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.1 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.34 – 7.27 (m, 5H), 4.15 (s, 2H), 3.54 – 3.44 (m, 1H), 2.93 – 2.77 (m, 3H), 2.61 – 2.48 (m, 1H), 2.05 – 1.94 (m, 2H), 1.84 – 1.70 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 153.1, 134.7, 130.5, 129.2, 128.0, 126.5, 126.1 (q, *J* = 277.5 Hz), 125.5, 123.2, 121.9, 59.9, 50.6, 39.1 (q, *J* = 28.4 Hz), 38.4 (q, *J* = 2.7 Hz), 34.3, 19.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -64.03 (t, *J* = 10.6 Hz, 3F).

HRMS(ESI) m/z: $[M+H]^+$Calcd for $C_{20}H_{21}F_3NO_2S_2^+$428.0960; found 428.0966.

2-(5-(benzylsulfonyl)-1-tosylpentan-2-yl)benzo[*d*]thiazole(6n)



White solid, yield 49% (50.7 mg). M.p. = 159–160 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.78 (m, 2H), 7.64 (d, *J* = 8.1 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.33 – 7.27 (m, 5H), 7.12 (d, *J* = 8.1 Hz, 2H), 4.15 (s, 2H), 3.89 (dd, *J* = 14.2, 7.2 Hz, 1H), 3.80 – 3.72 (m, 1H), 3.47 (dd, *J* = 14.2, 5.6 Hz, 1H), 2.83 – 2.72 (m, 2H), 2.25 (s, 3H), 2.08 – 2.02 (m, 2H), 1.82 – 1.70 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 152.9, 144.9, 136.3, 134.8, 130.5, 129.8, 129.2, 128.0, 128.0, 126.3, 125.4, 123.0, 121.8, 60.0, 59.8, 50.6, 39.1, 34.3, 21.6, 19.3.

HRMS(ESI) m/z: $[M+H]^+$Calcd for$C_{26}H_{28}NO_4S_3^+$514.1175; found 514.1178.

5.Reference

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2. H. V. Trinh, L. Perrin, P. G. Goekjian and D. Gueyrard, *Eur. J. Org. Chem.*, **2016**, *2016*, 2944-2953.
3. 3. X.-Y. Liu, S.-Y. Tian, Y.-F. Jiang, W. Rao and S.-Y. Wang, *Org. Lett*., **2021**, *23*, 8246-8251.
4. M. Rehman, S. Surendran, N. Siddavatam and G. Rajendar, *Org & Biom. Chem.*, **2022**, *20*, 329-333.
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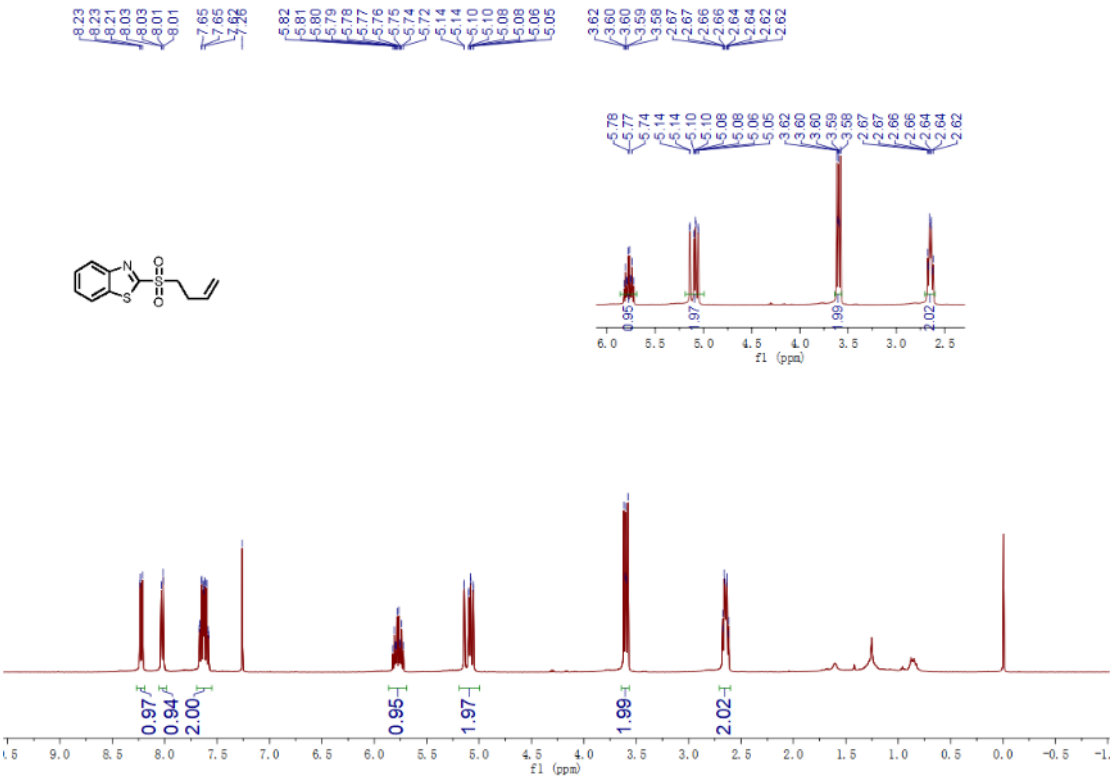
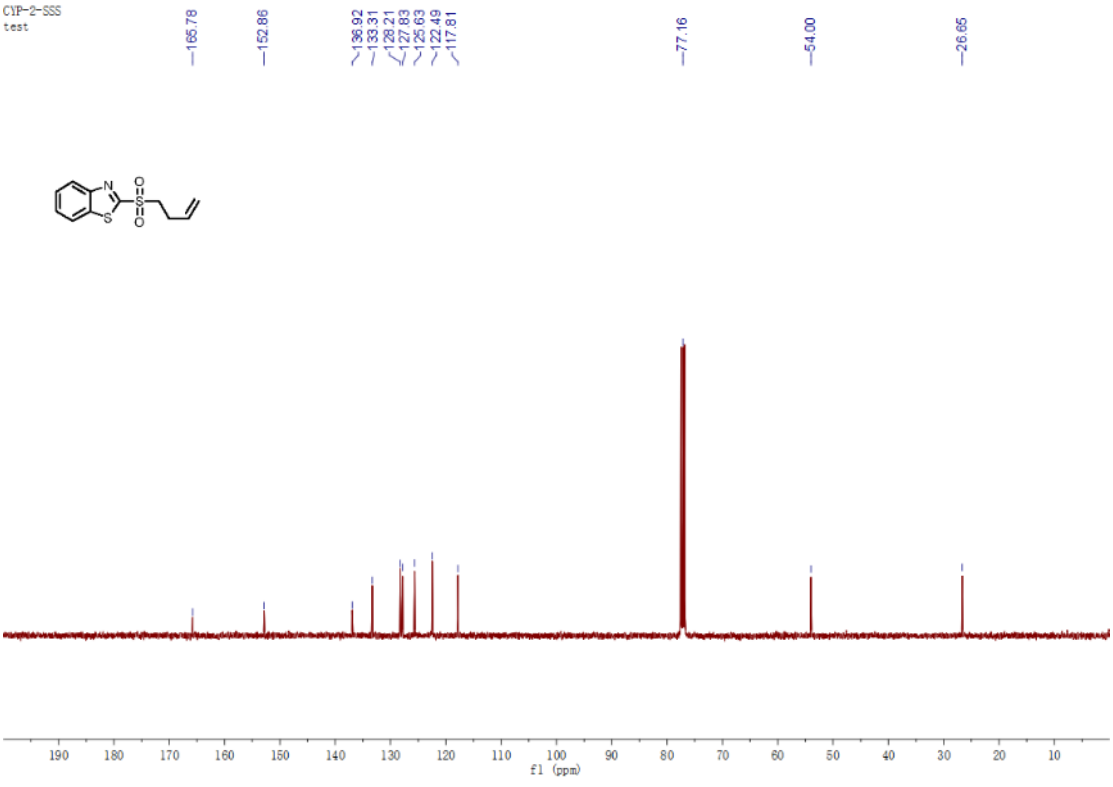
6.NMR spectra

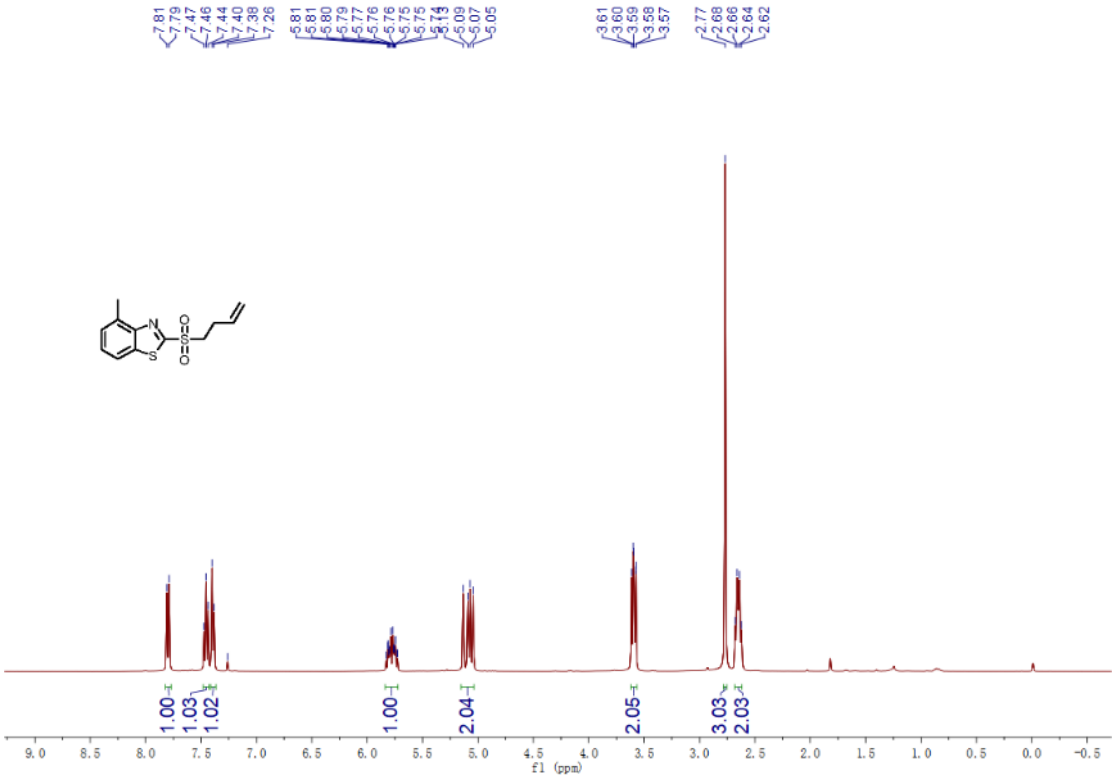
^{1}H NMR spectrum(400MHz, $CDCl_3$) of compound 1a



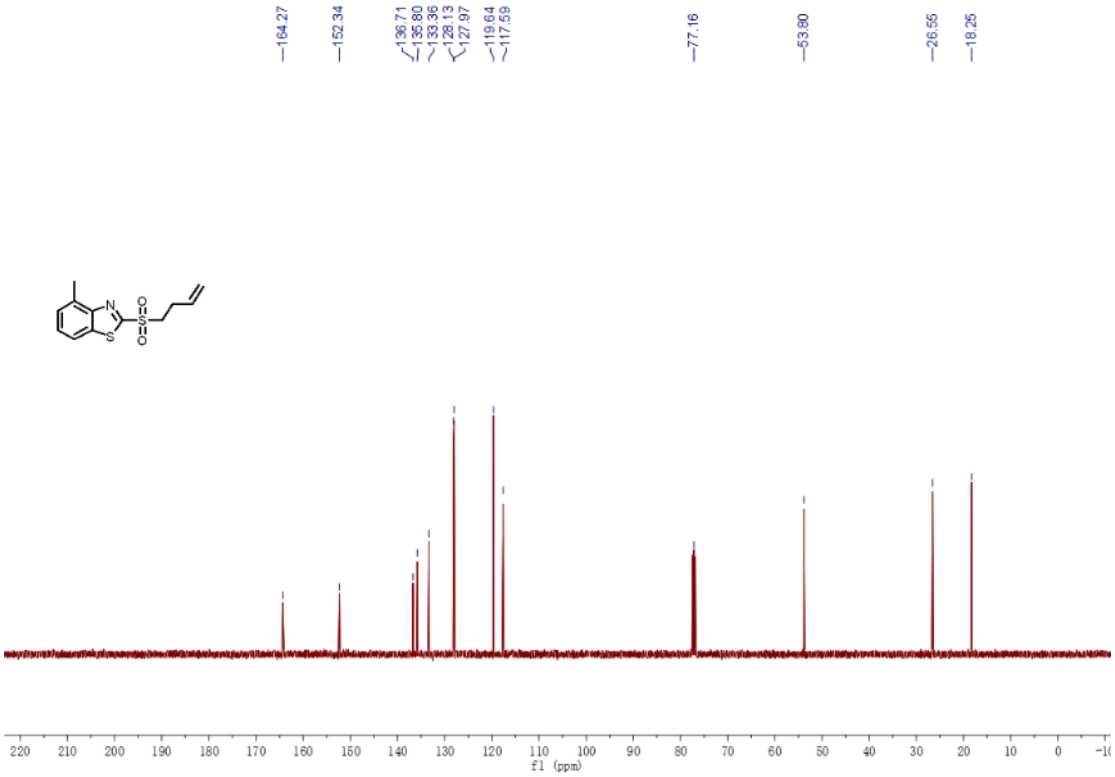
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1a



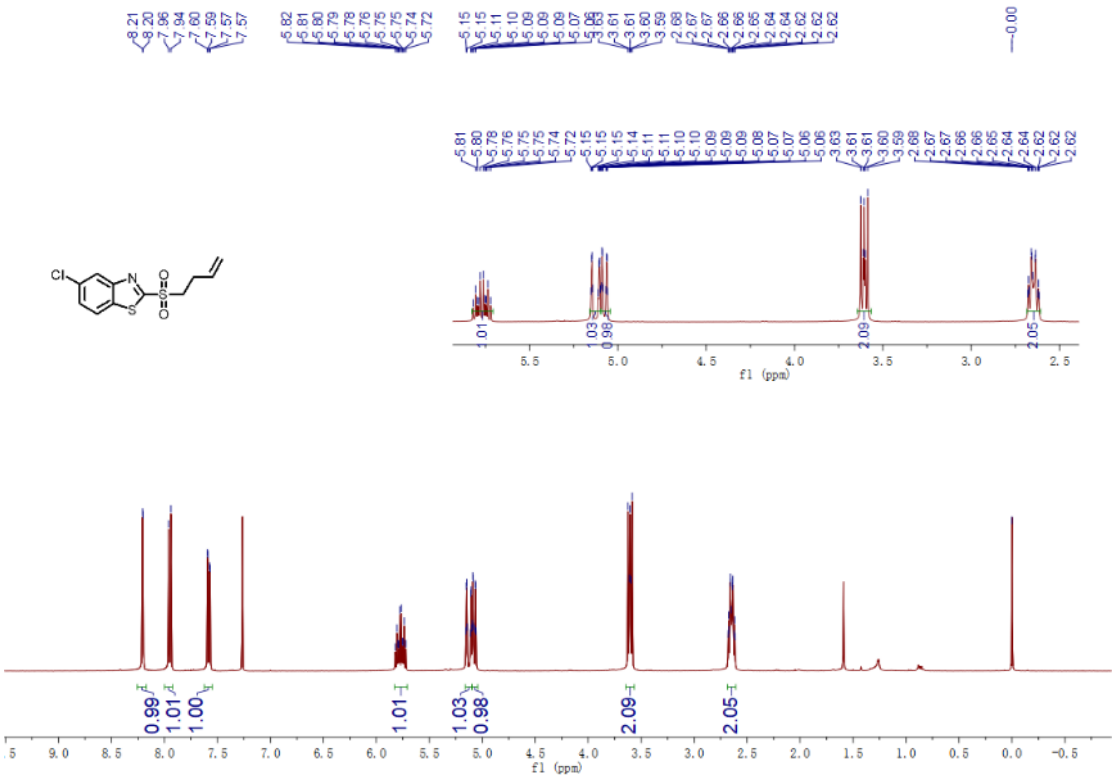
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1b



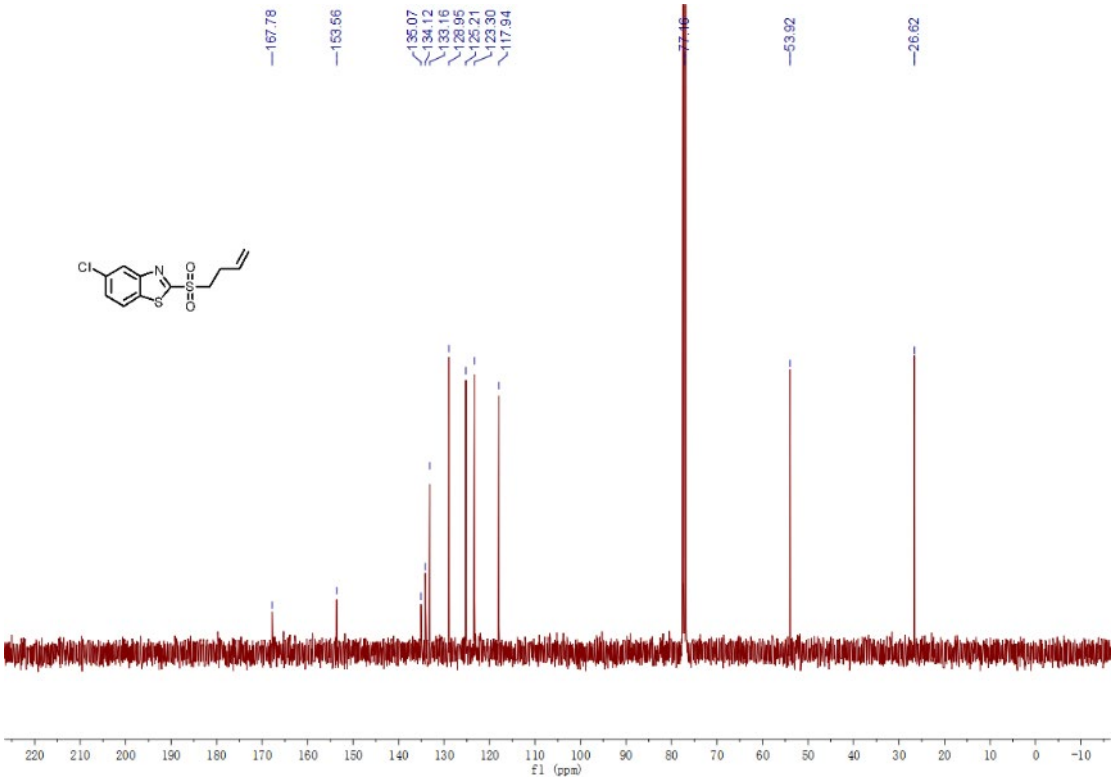
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1b



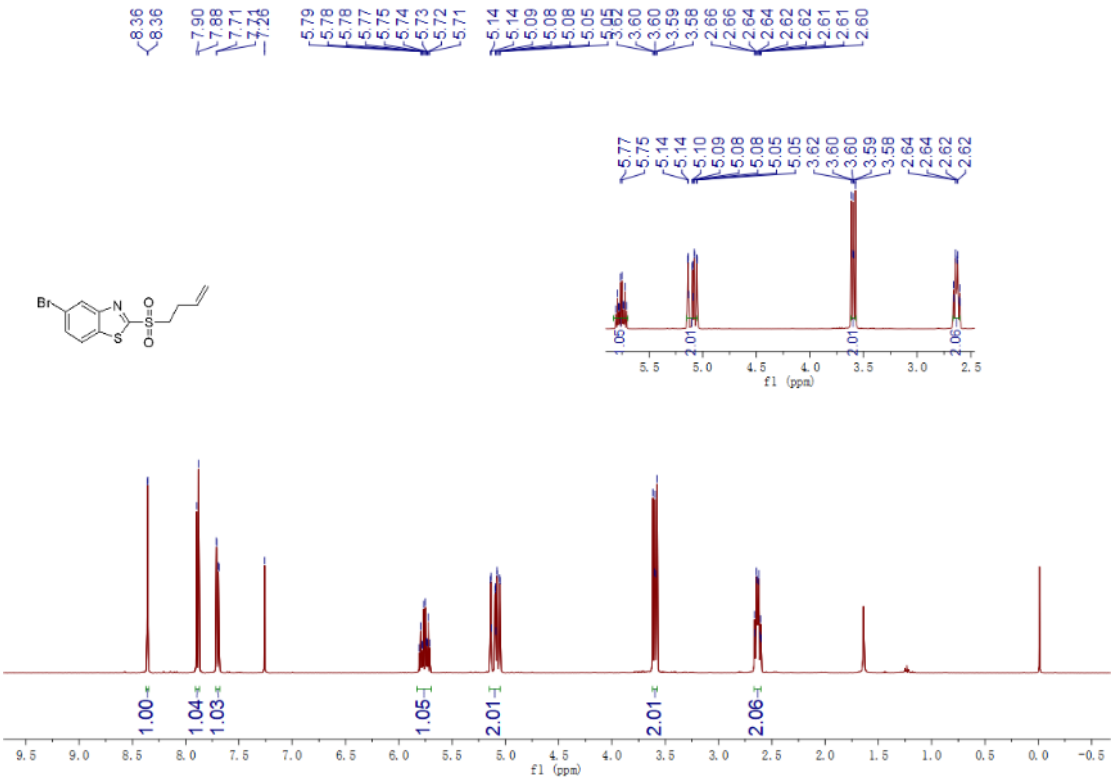
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1c



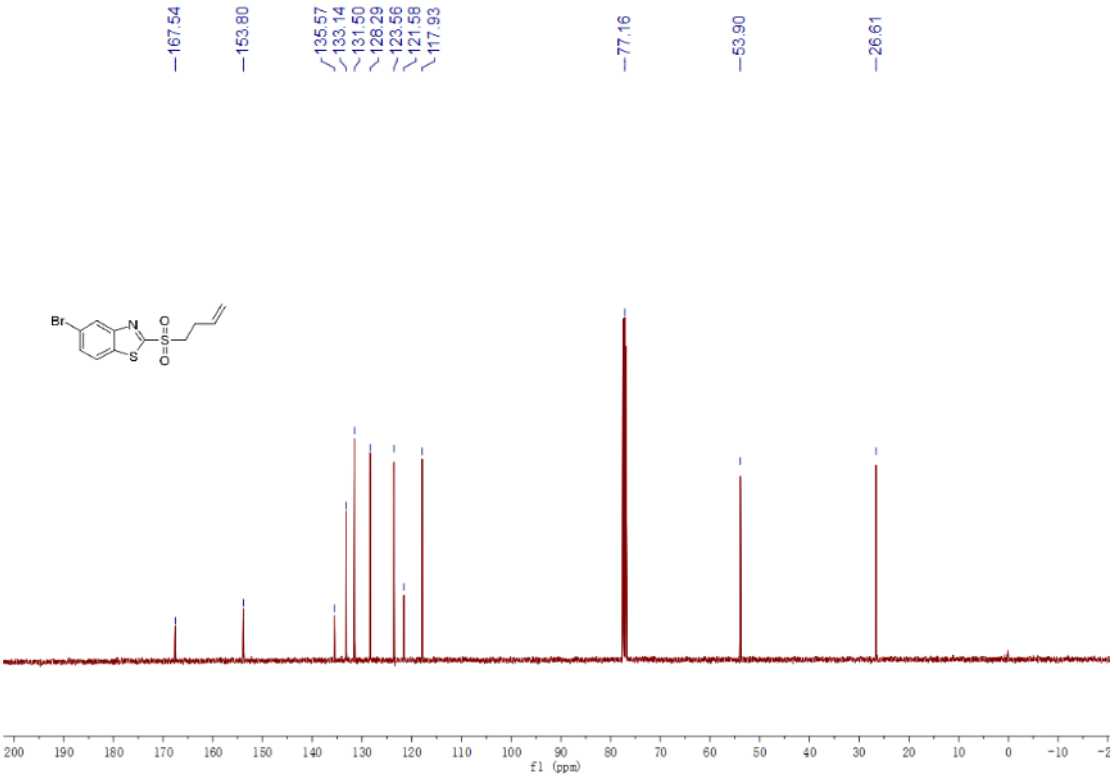
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1c



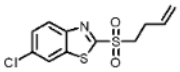
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1d

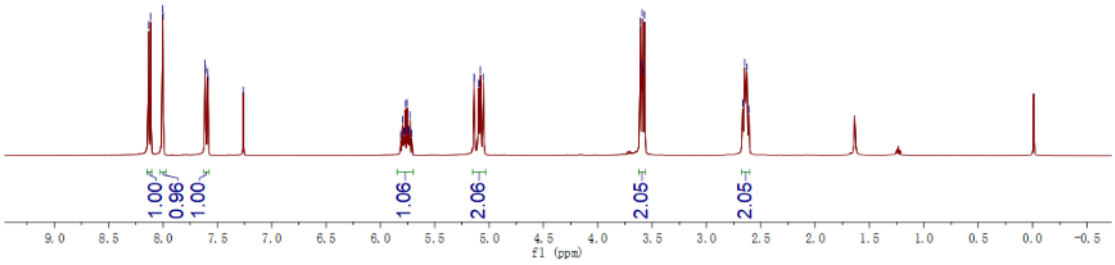


^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1d

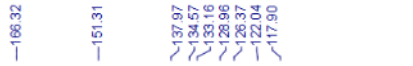


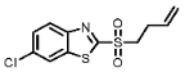
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1e

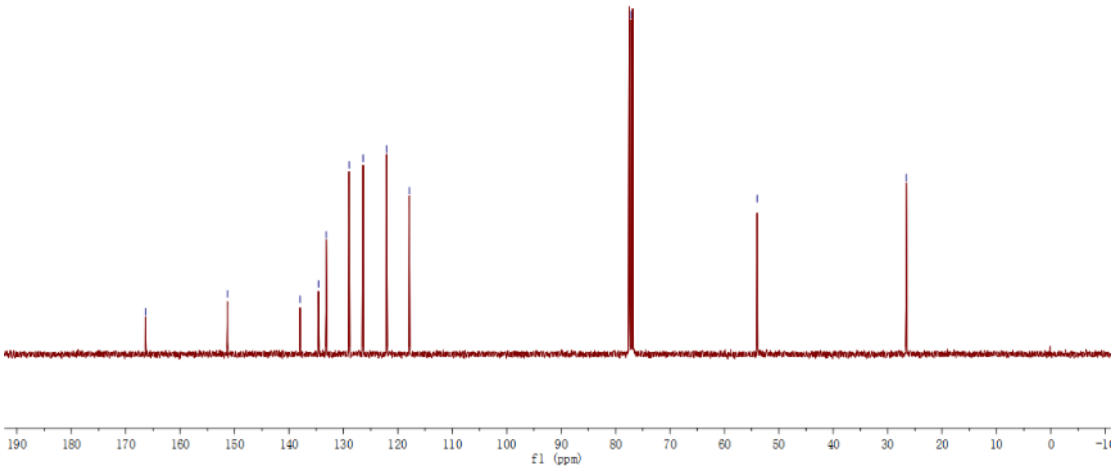




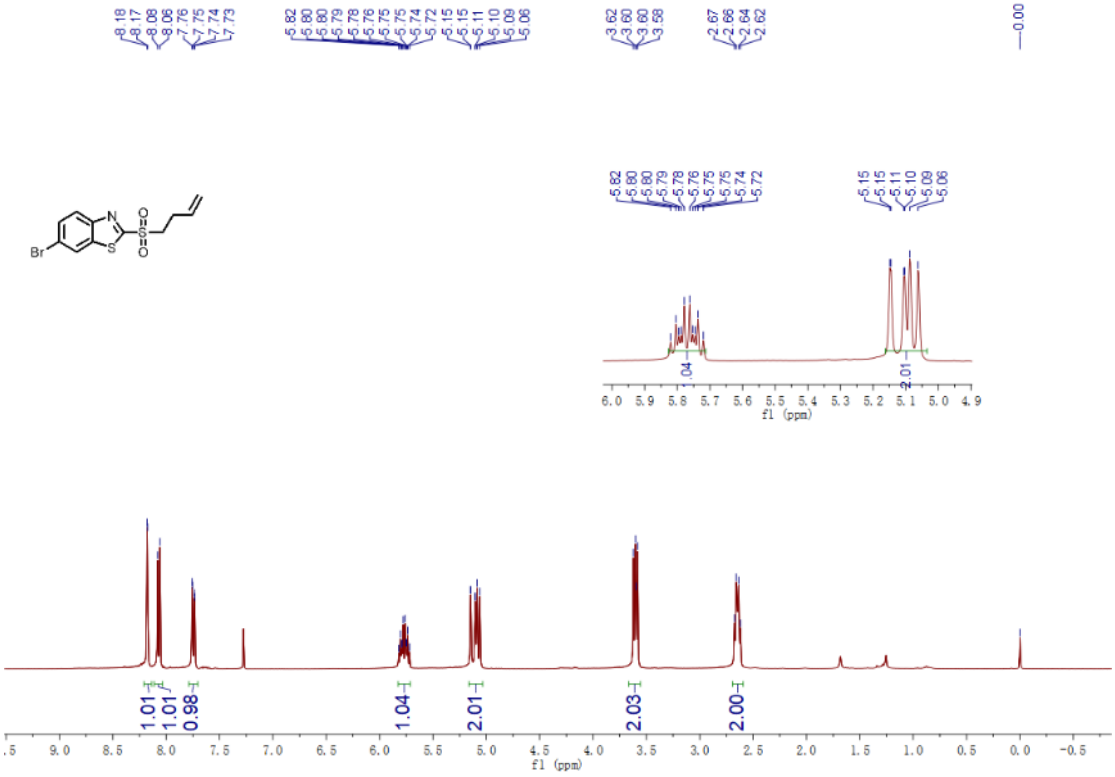
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1e



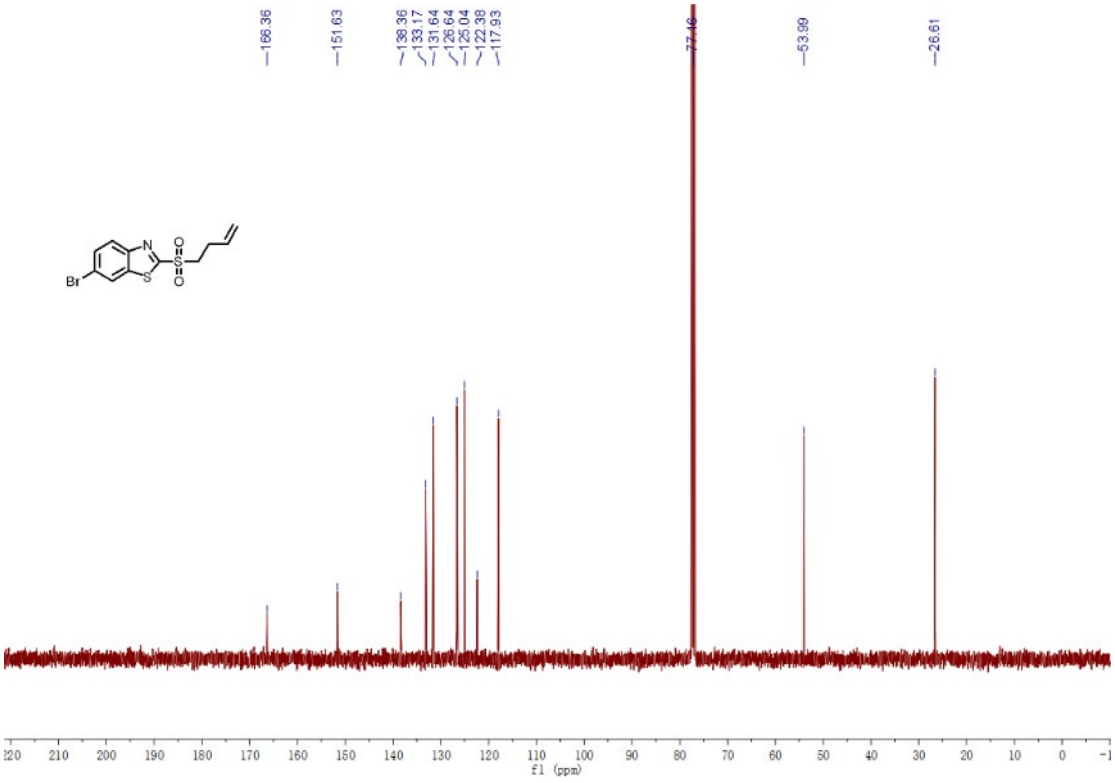




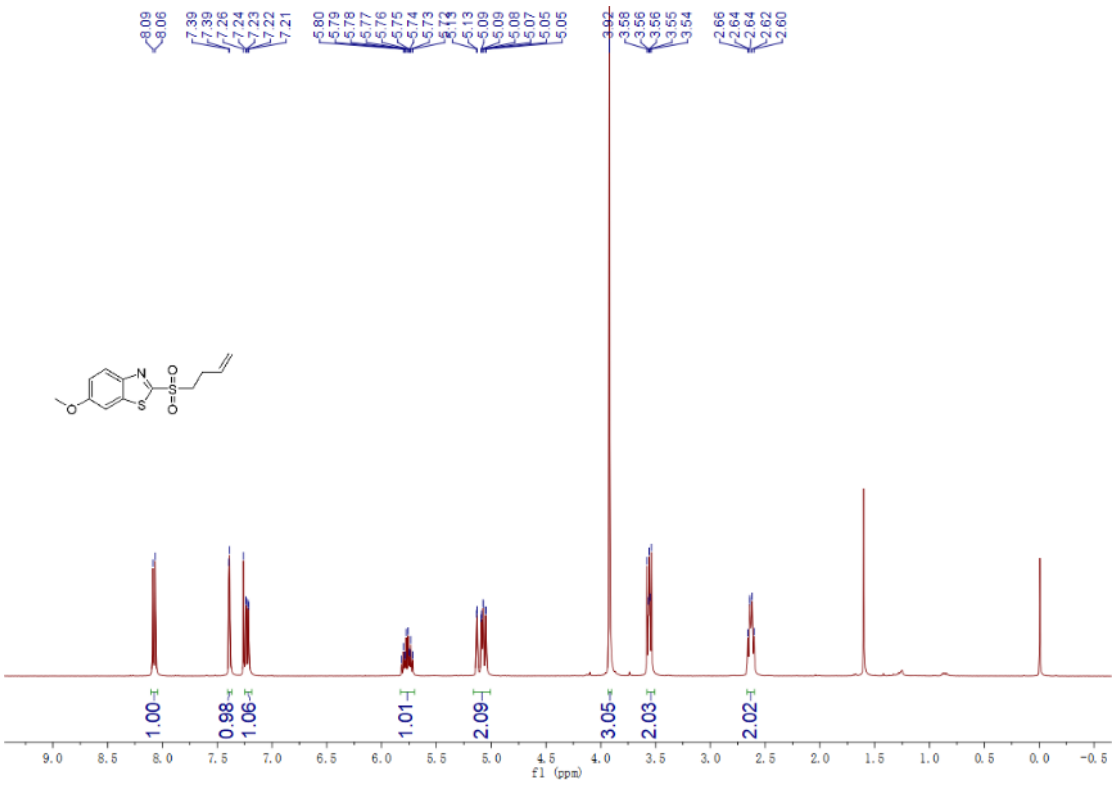
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1f



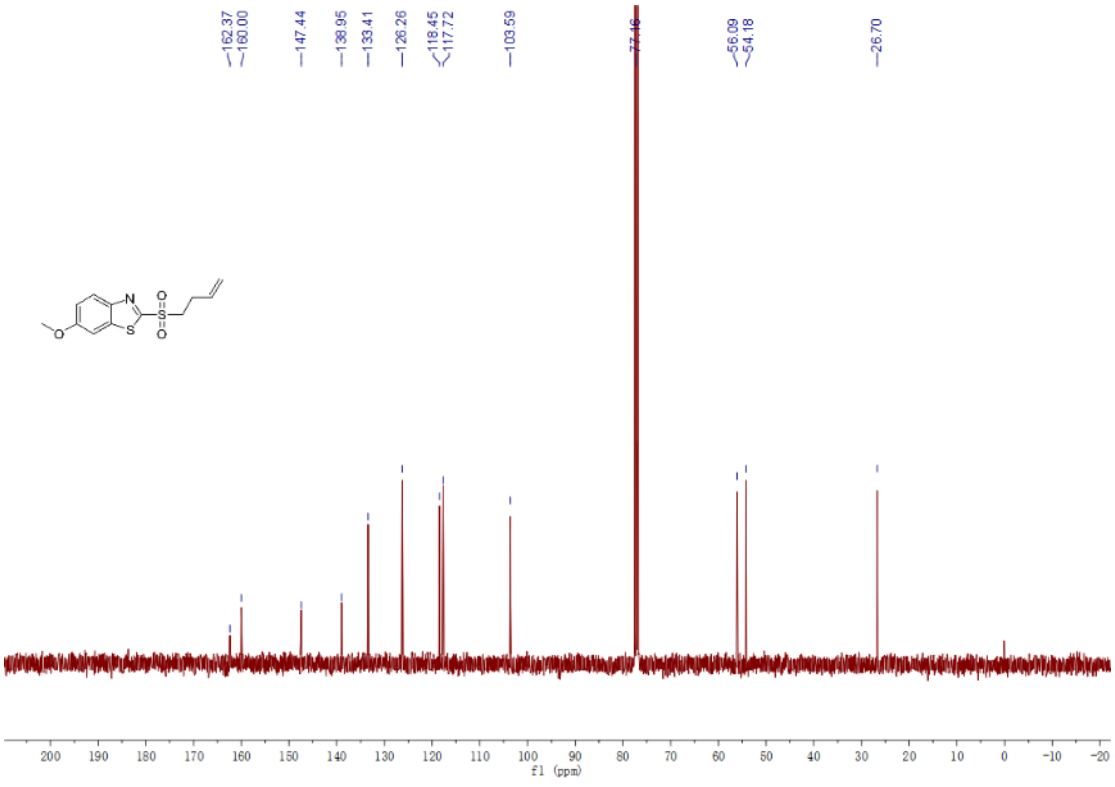
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1f



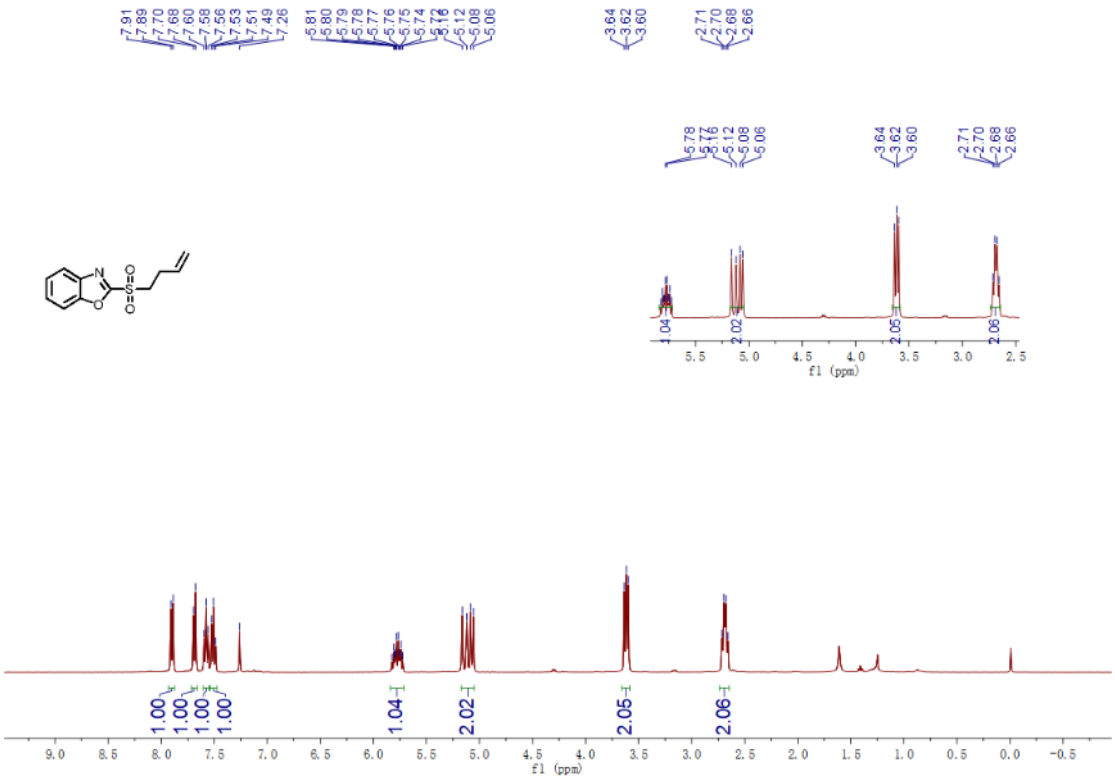
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1g



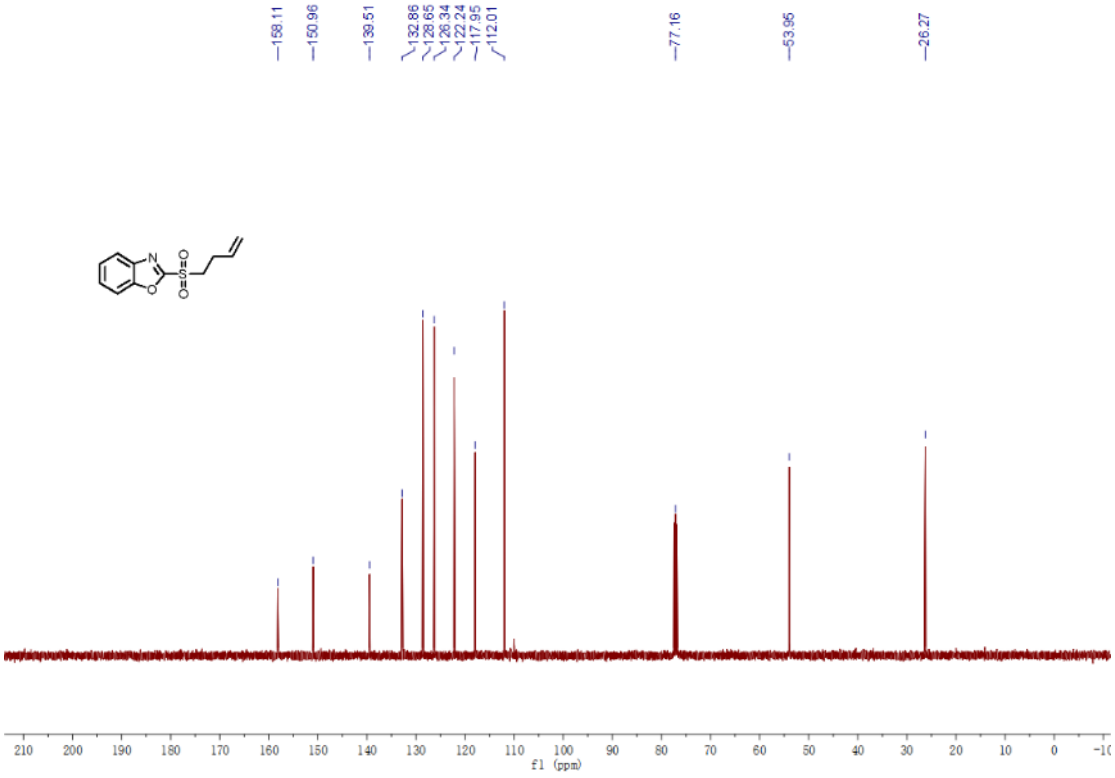
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1g



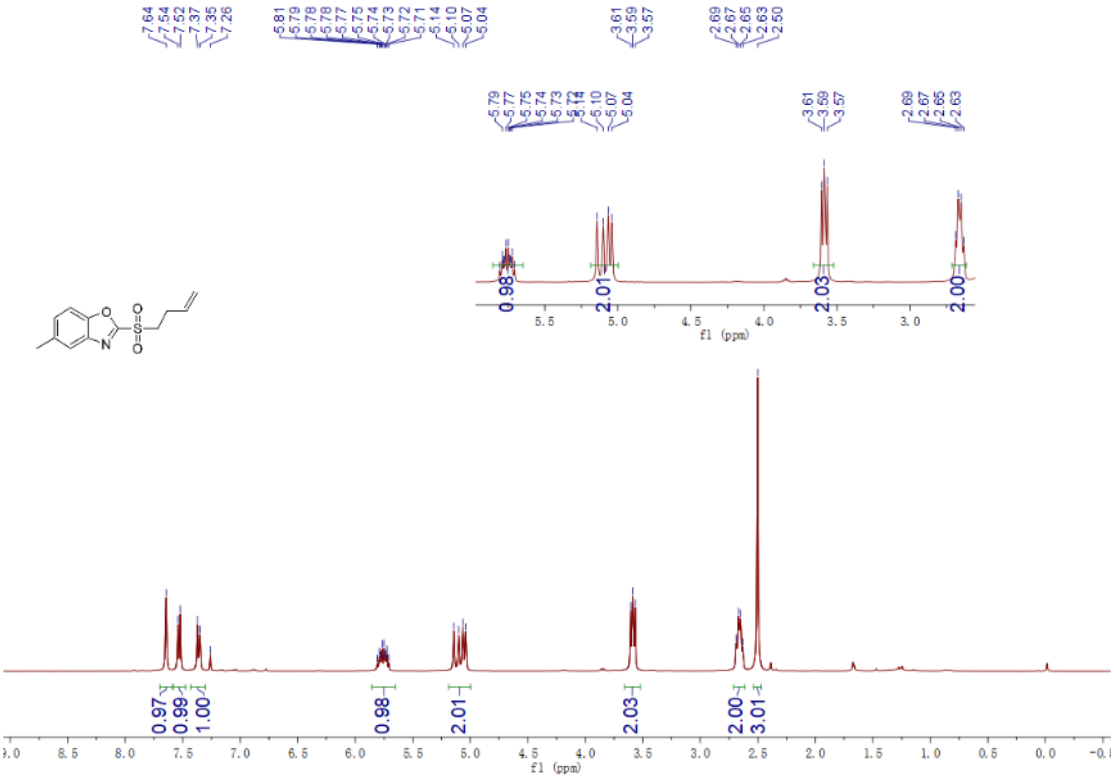
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1h



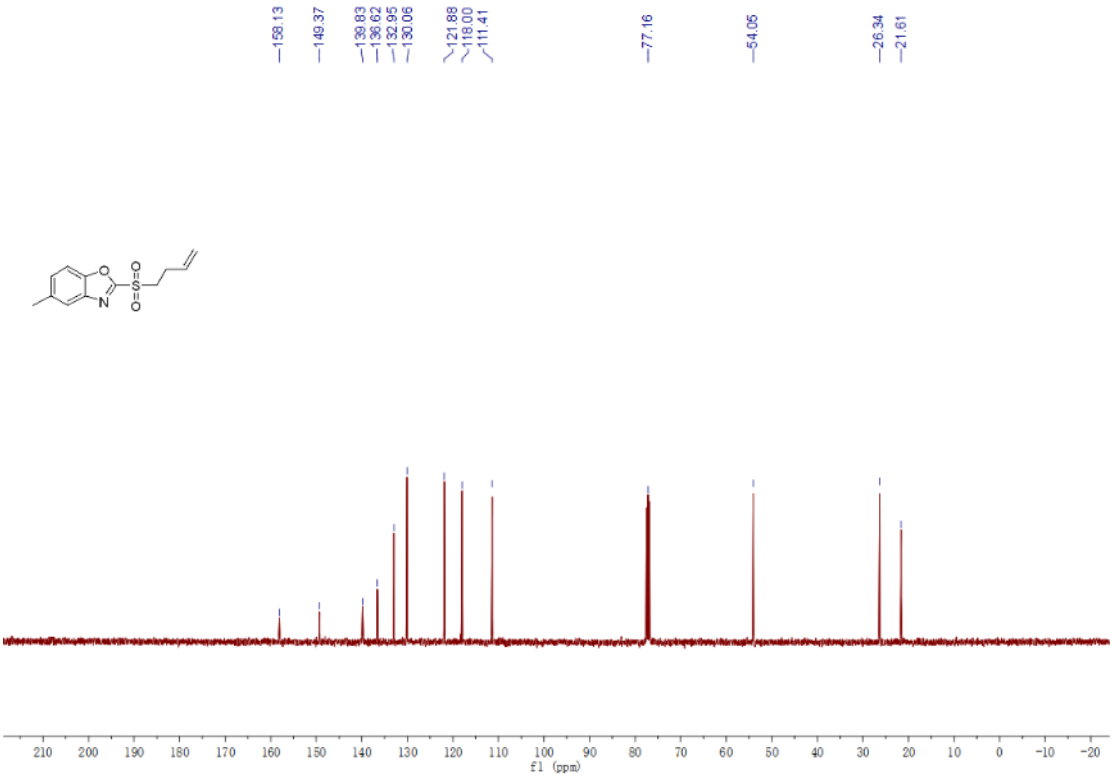
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1h



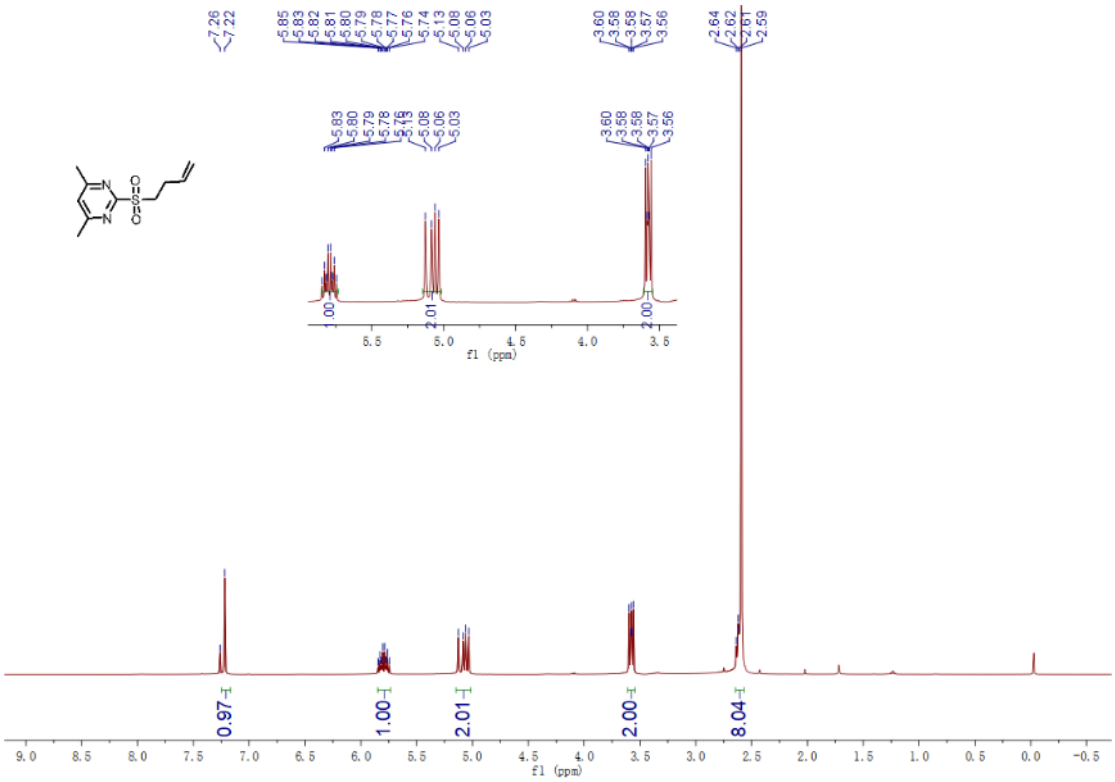
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1i



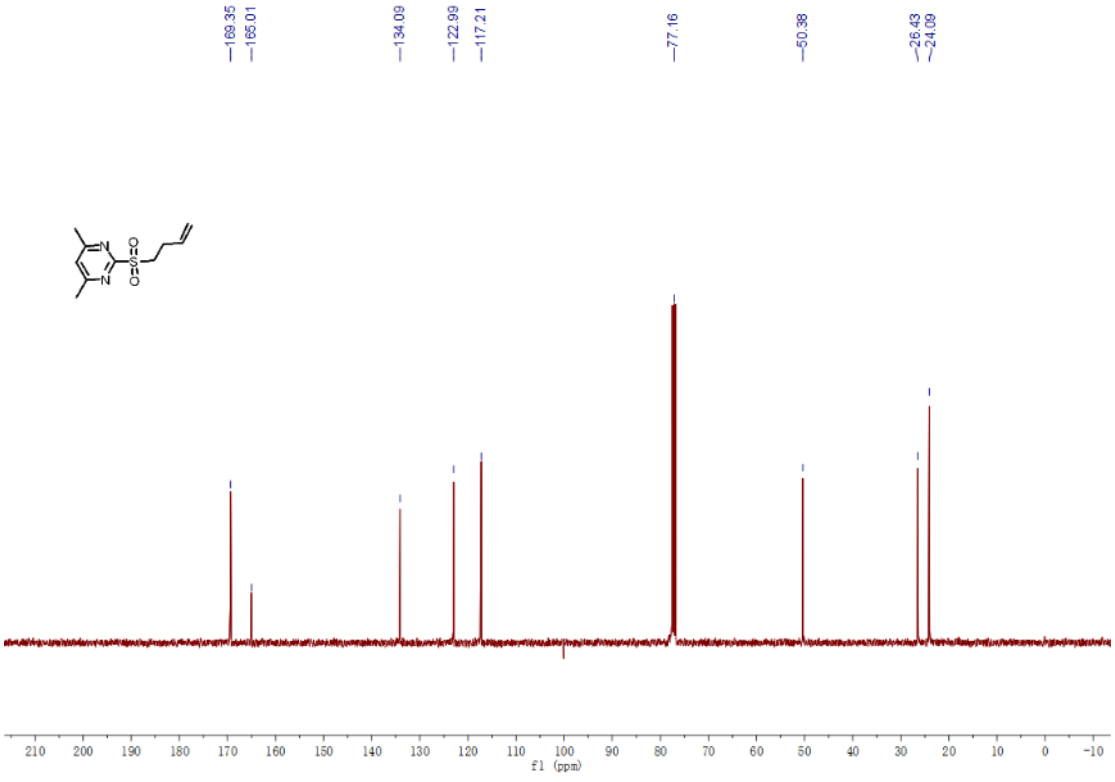
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1i



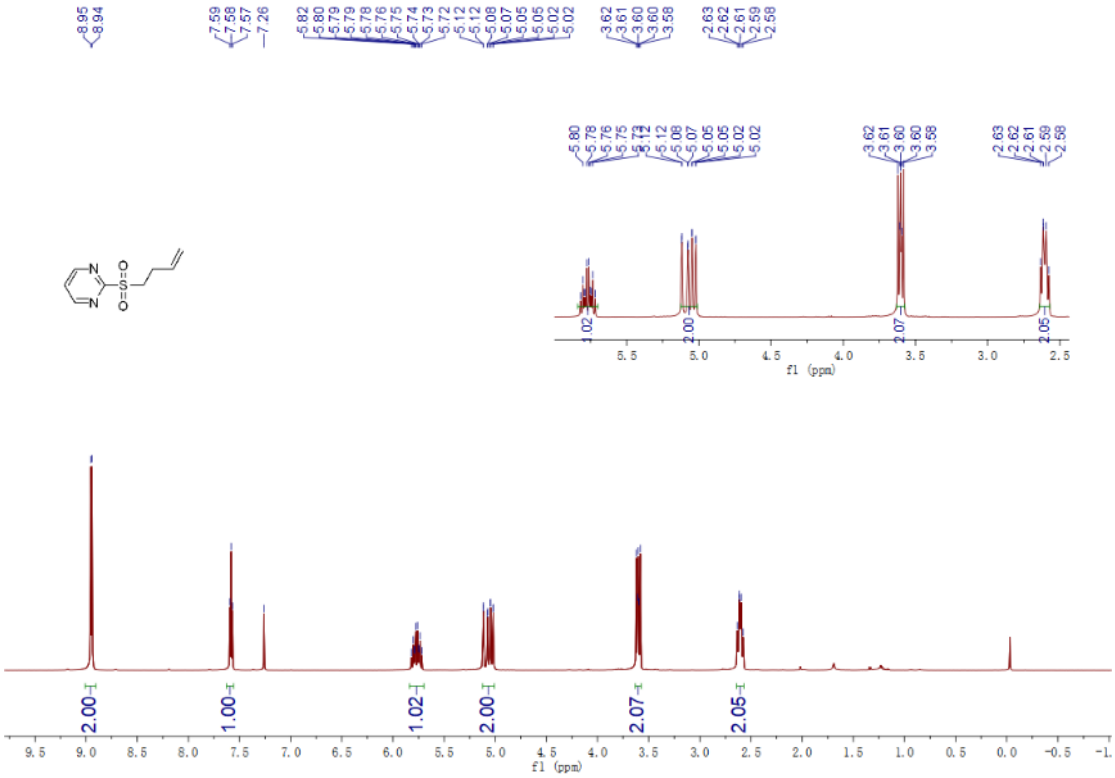
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1j



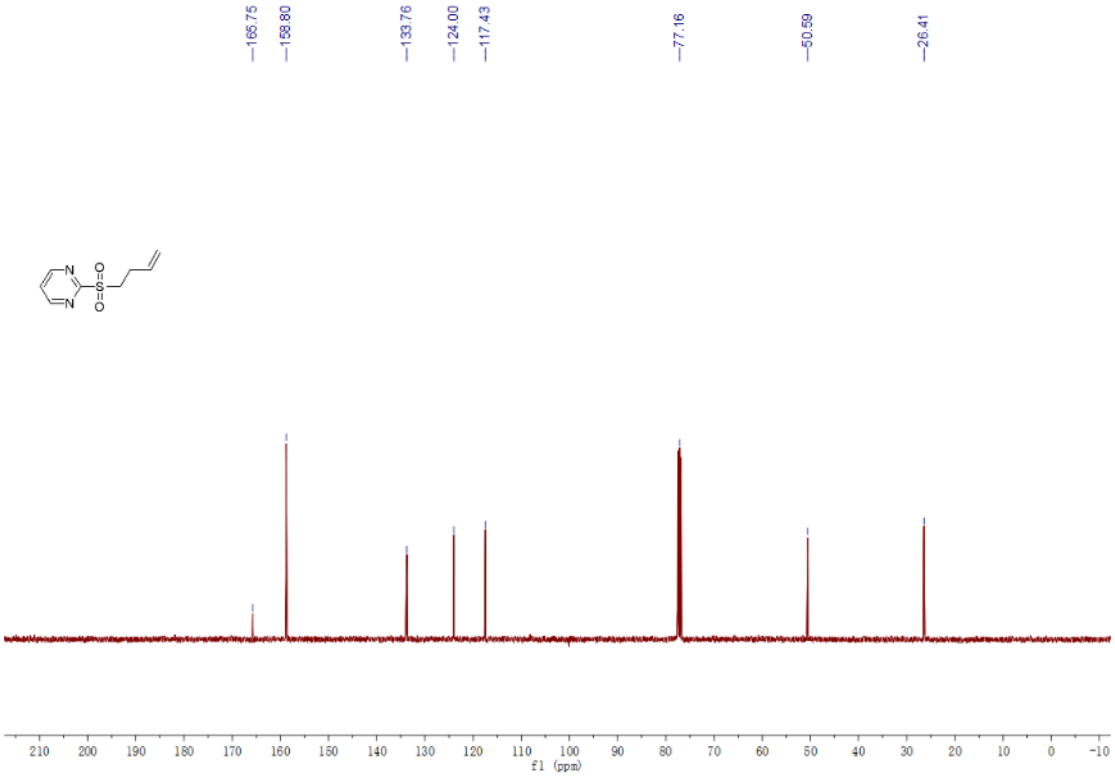
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1j



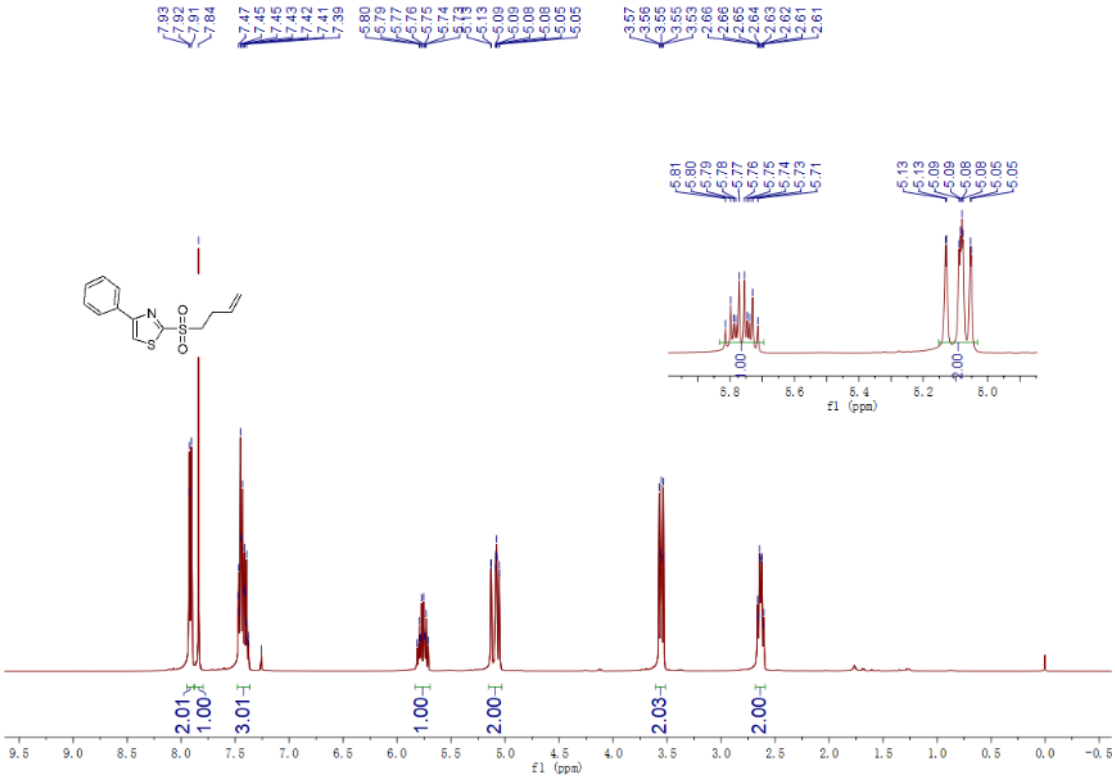
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1k



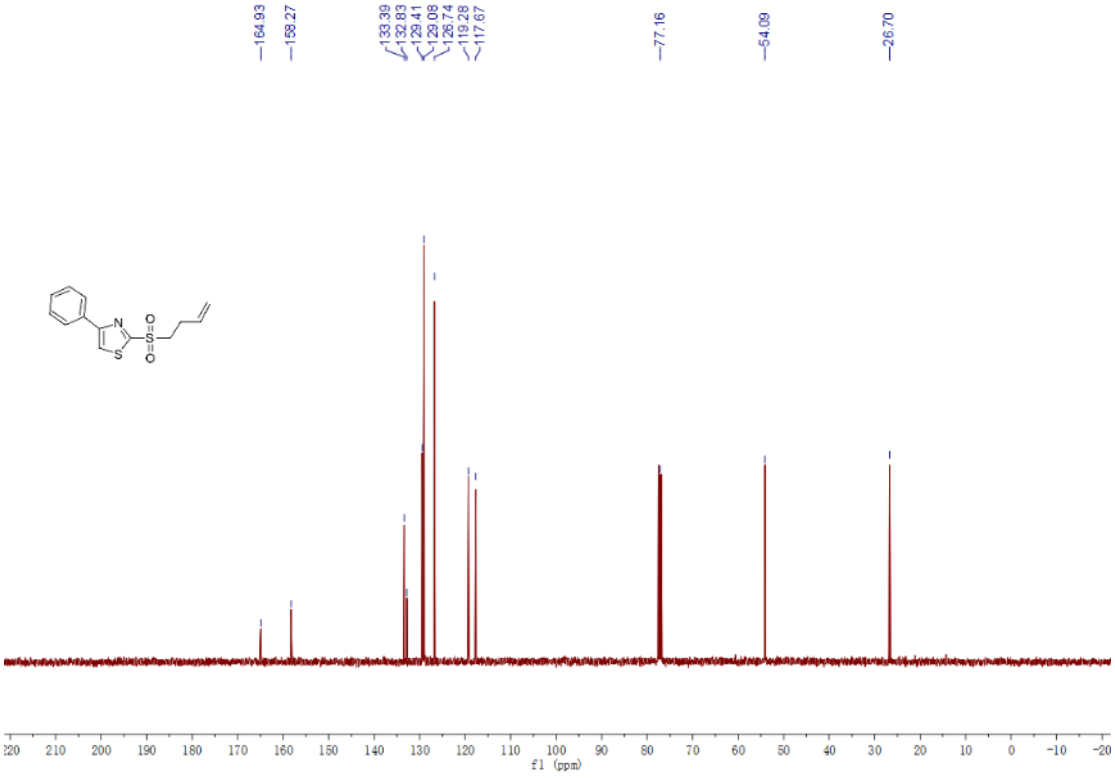
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1k



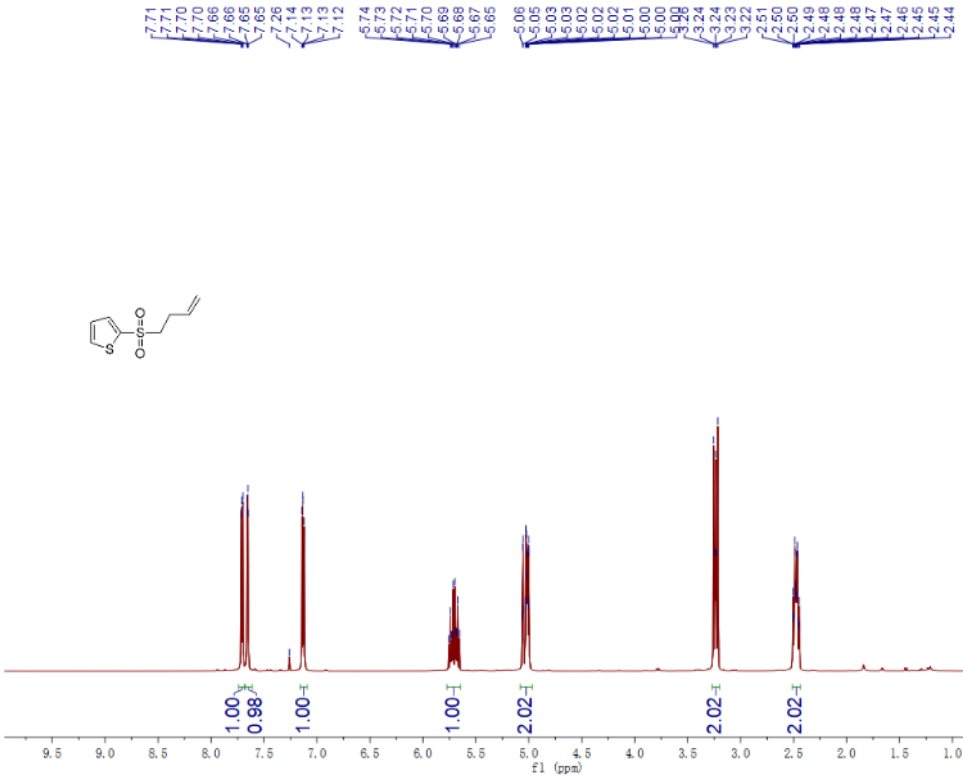
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1l



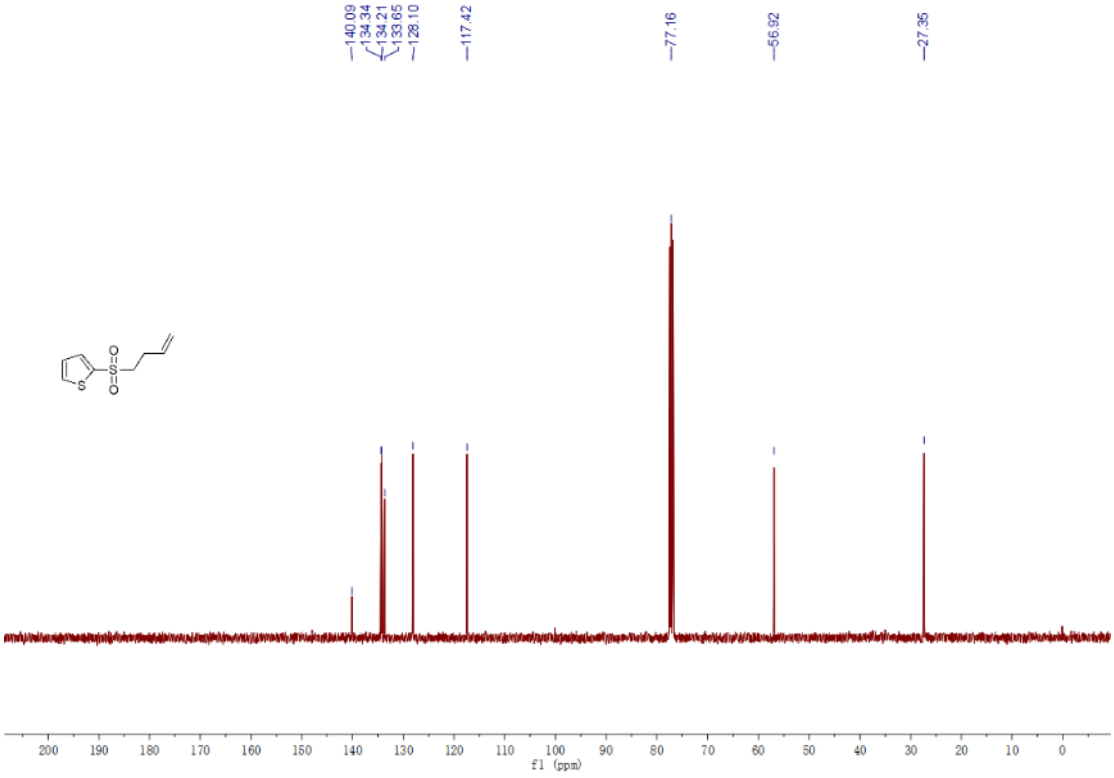
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1l



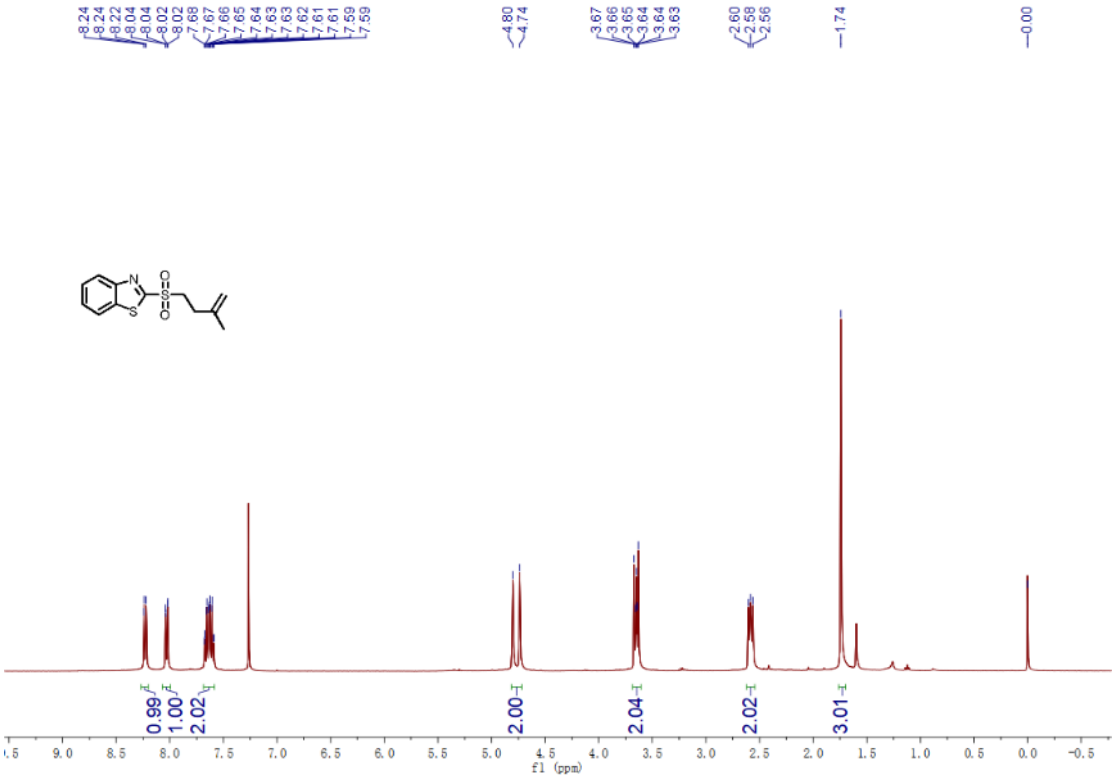
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1m



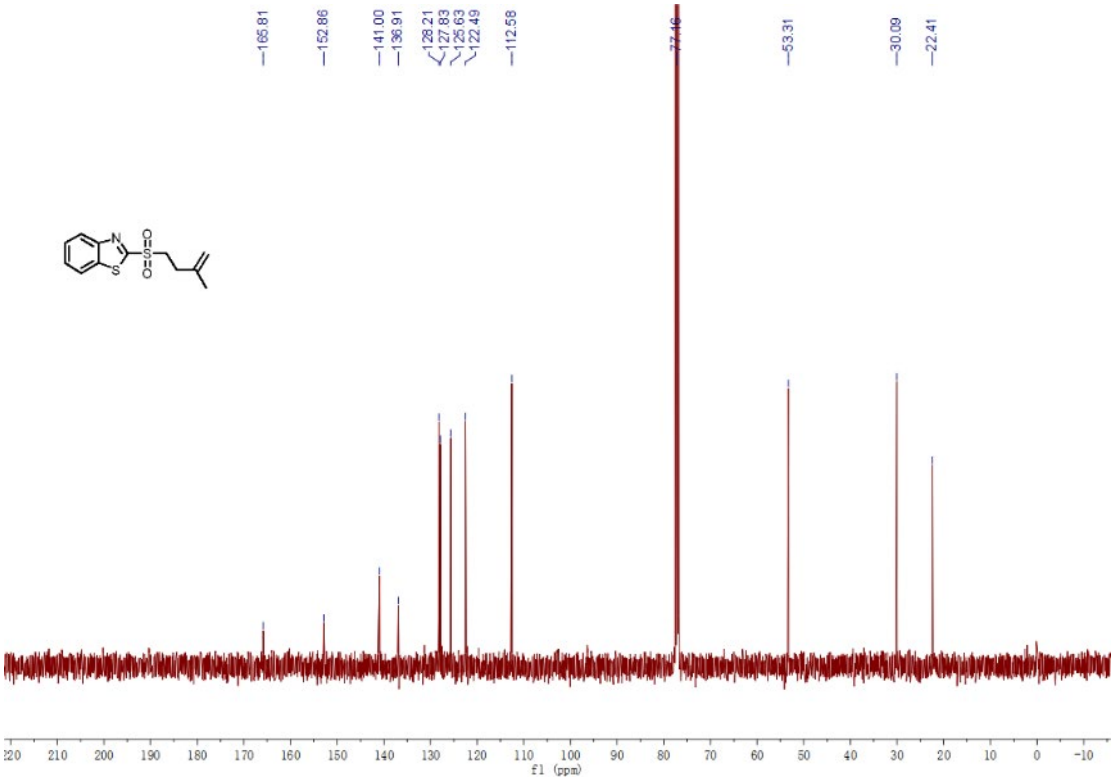
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1m



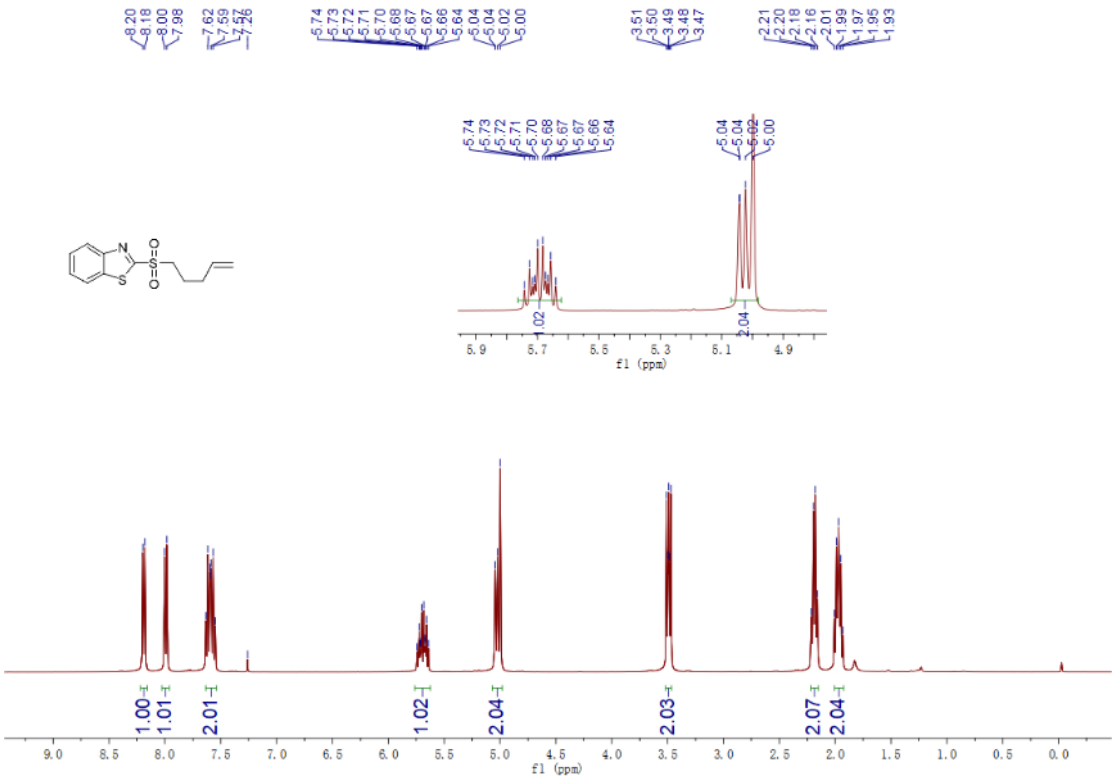
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1n



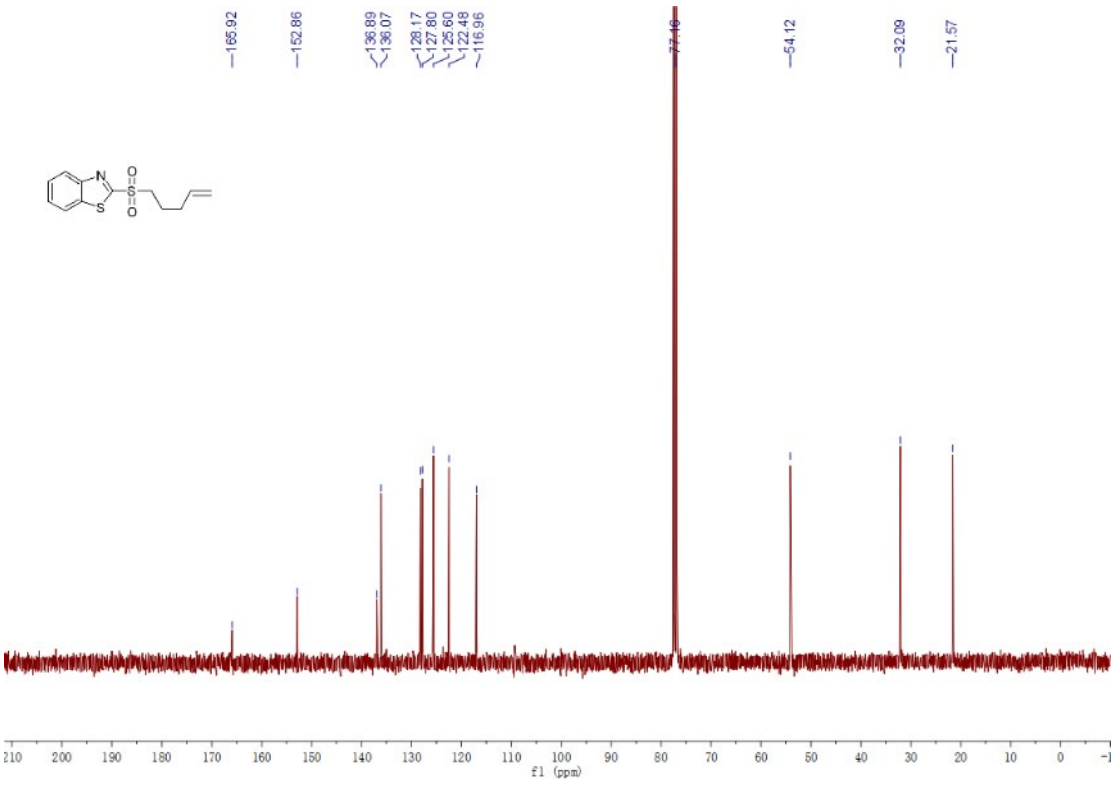
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1n



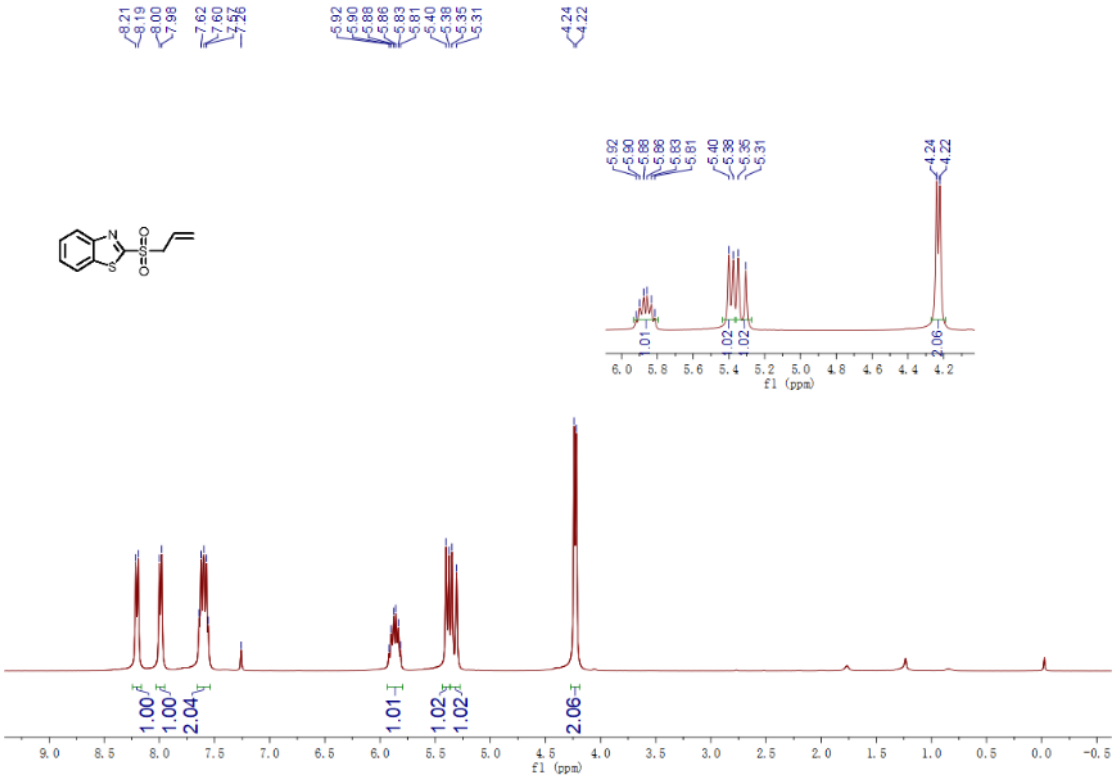
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1o



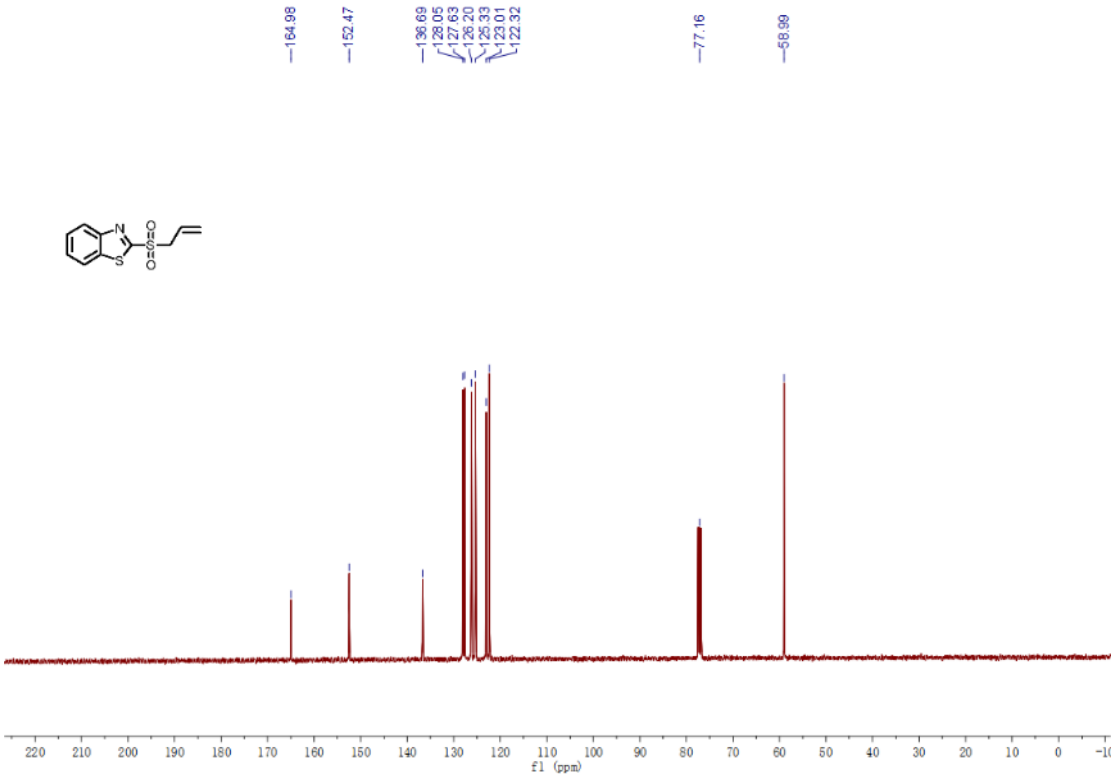
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1o



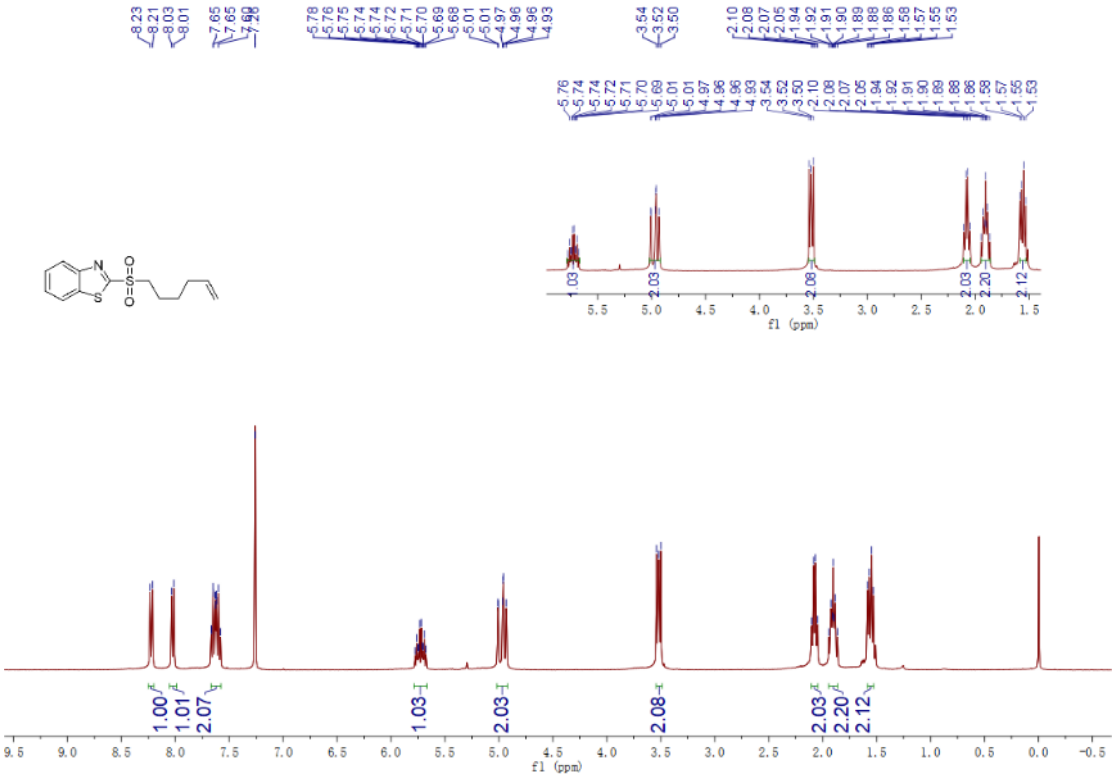
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1p



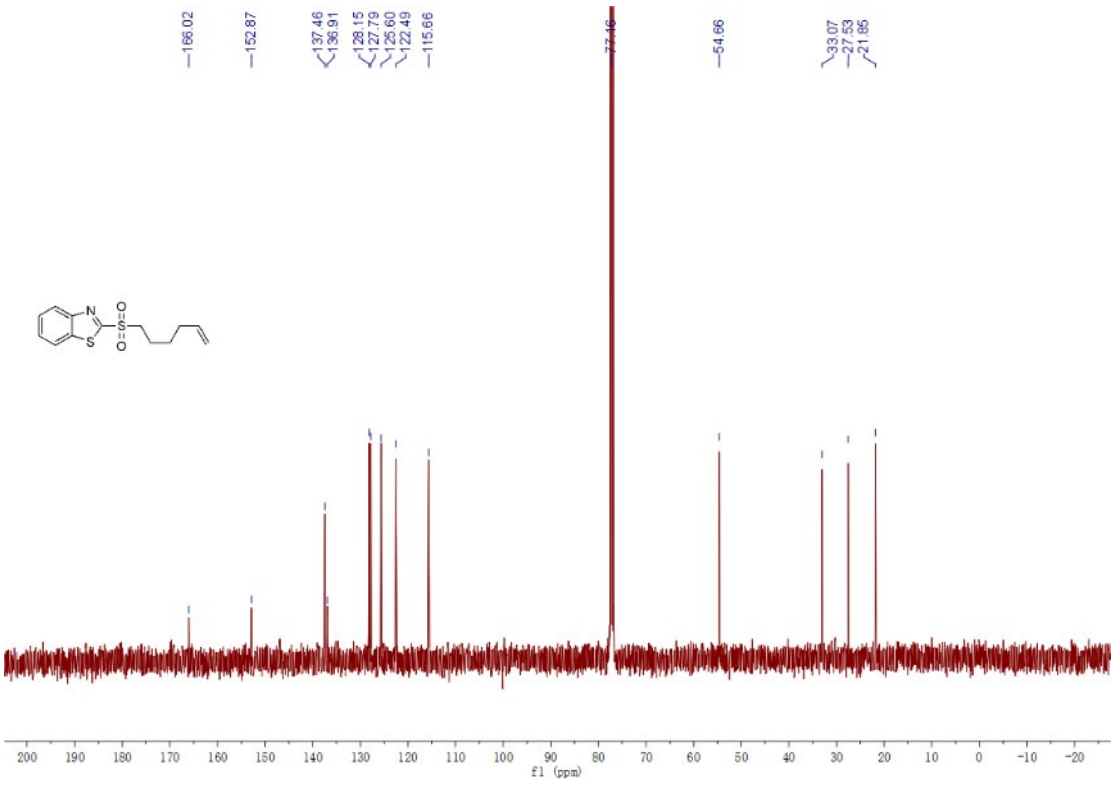
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1p



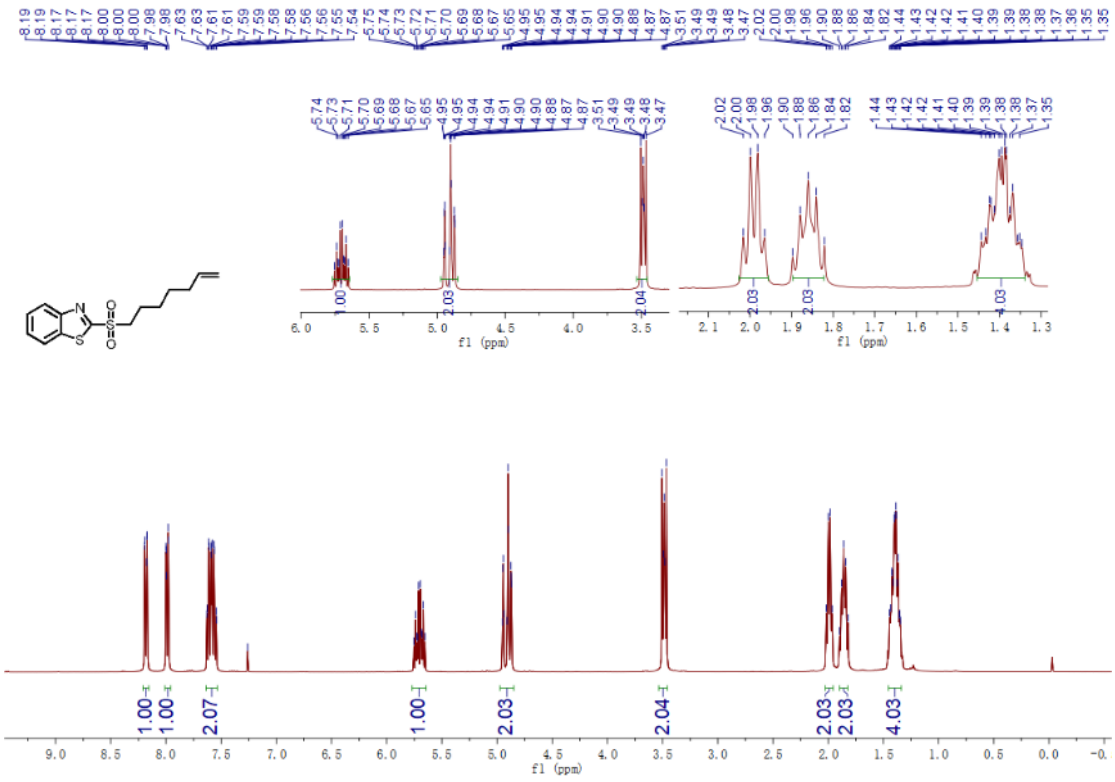
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1q



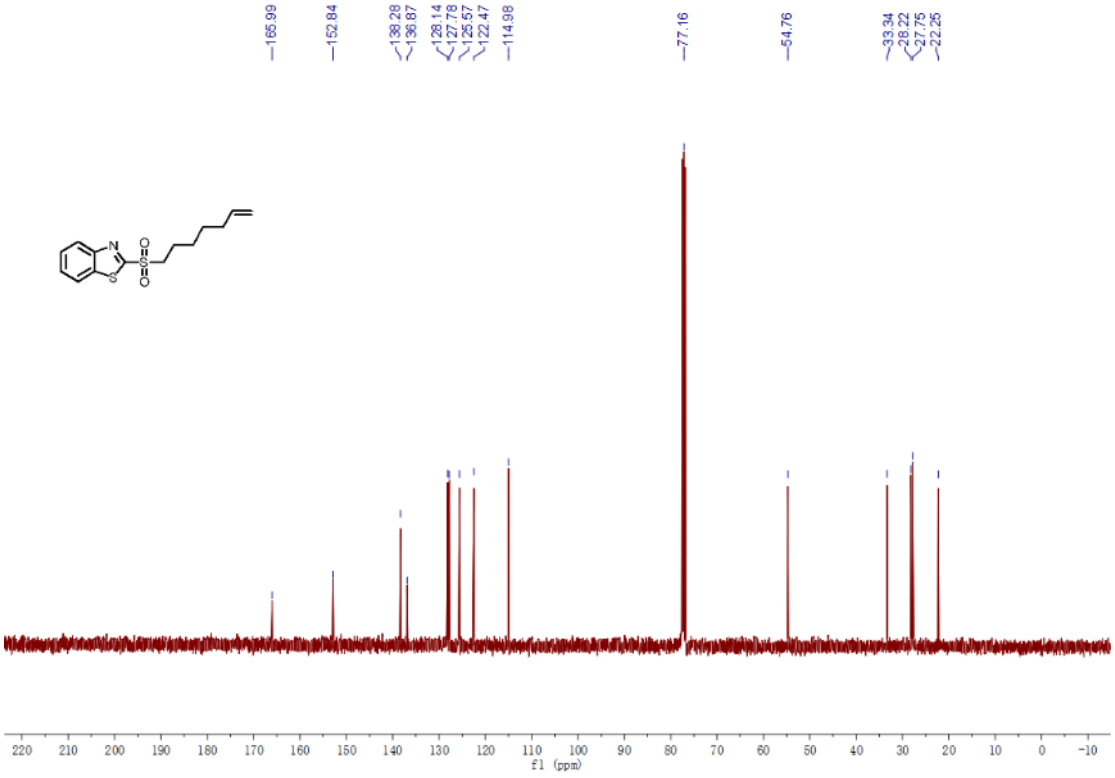
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1q



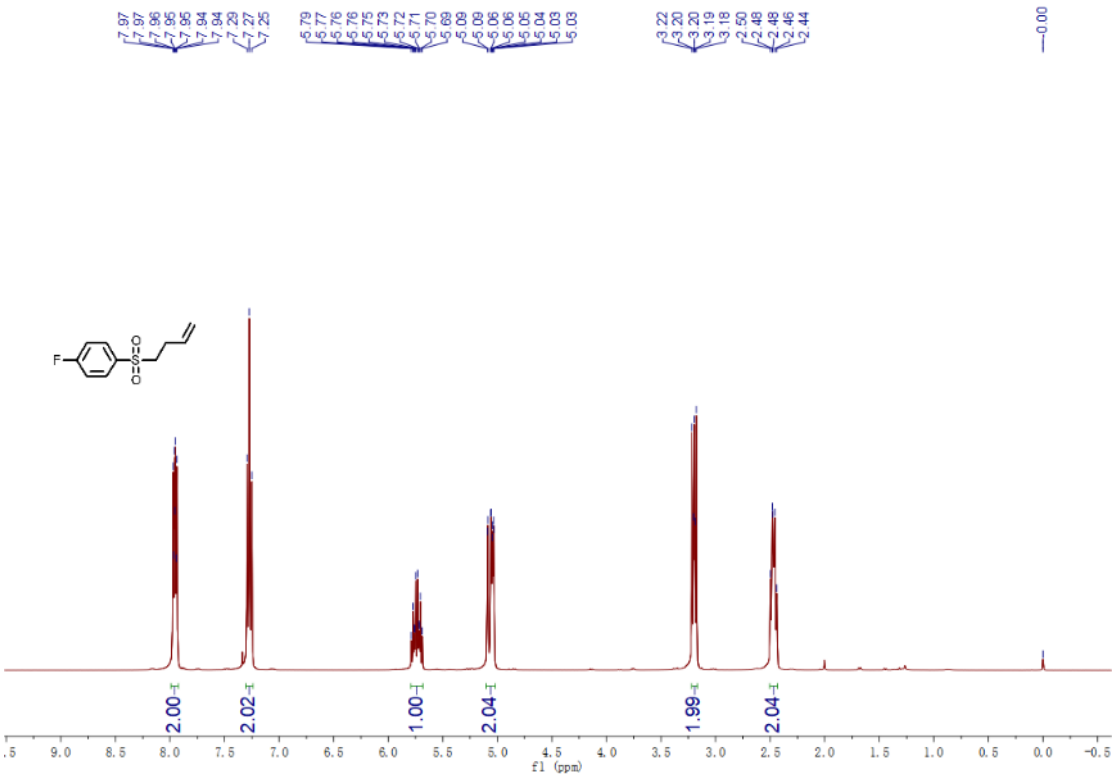
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1r



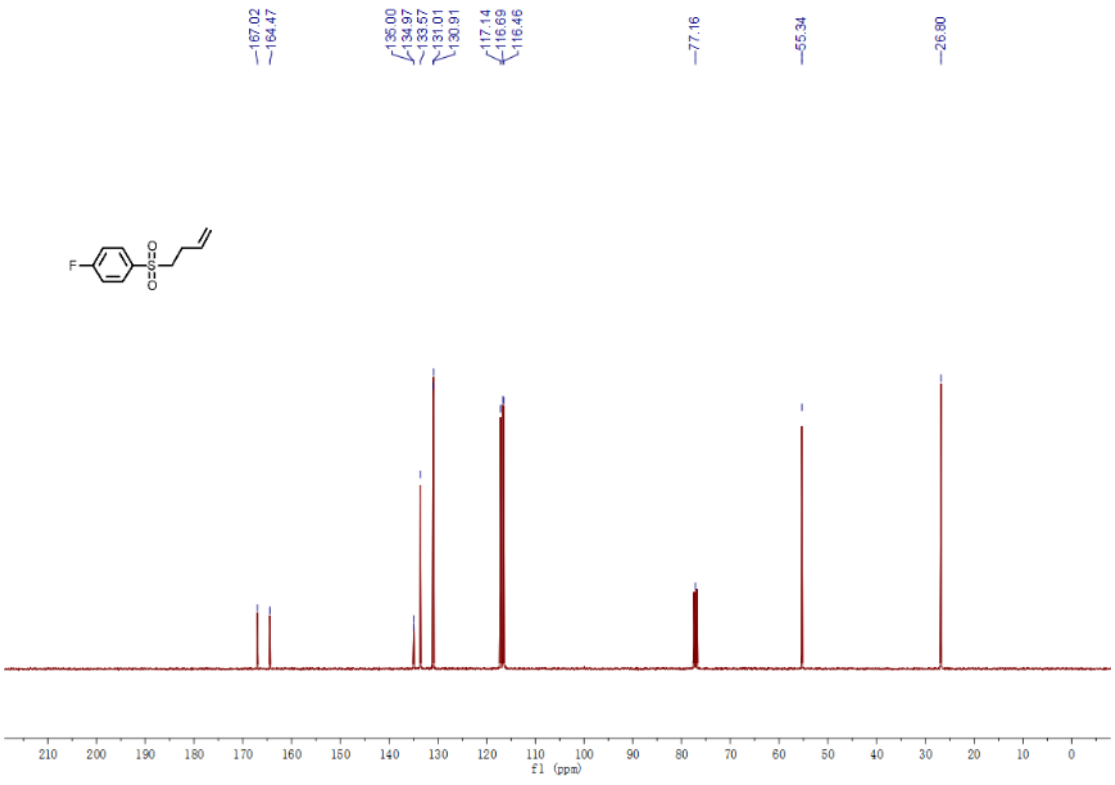
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1r



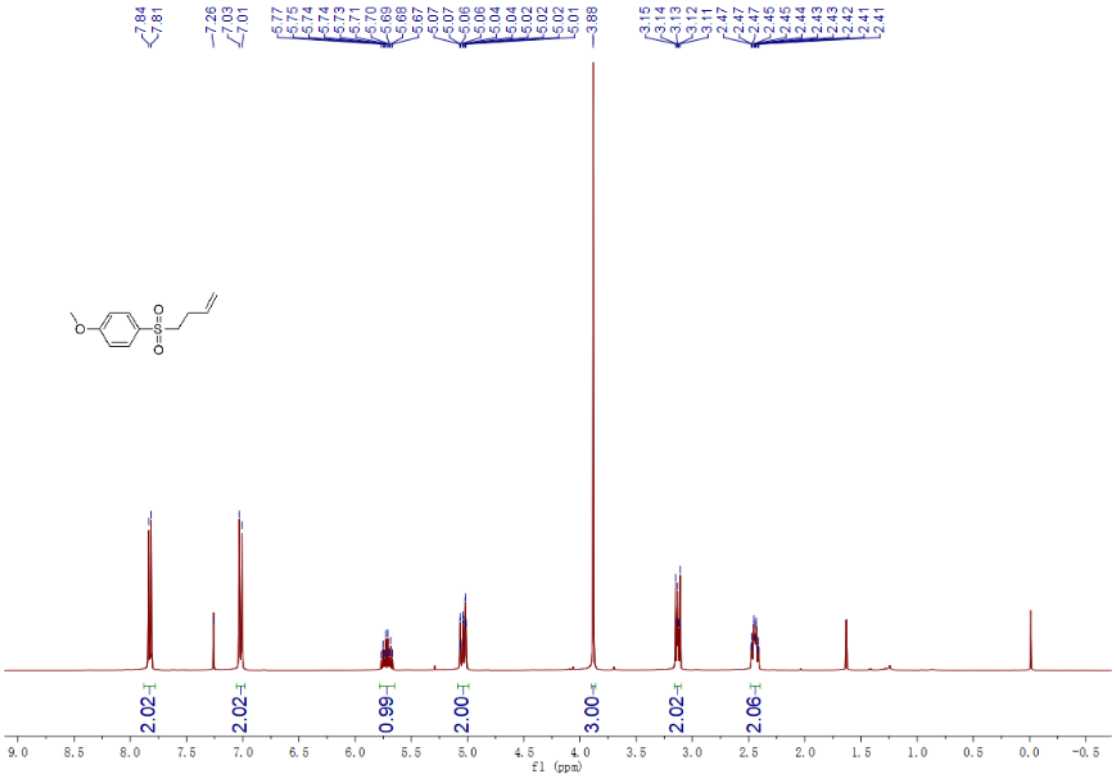
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1s



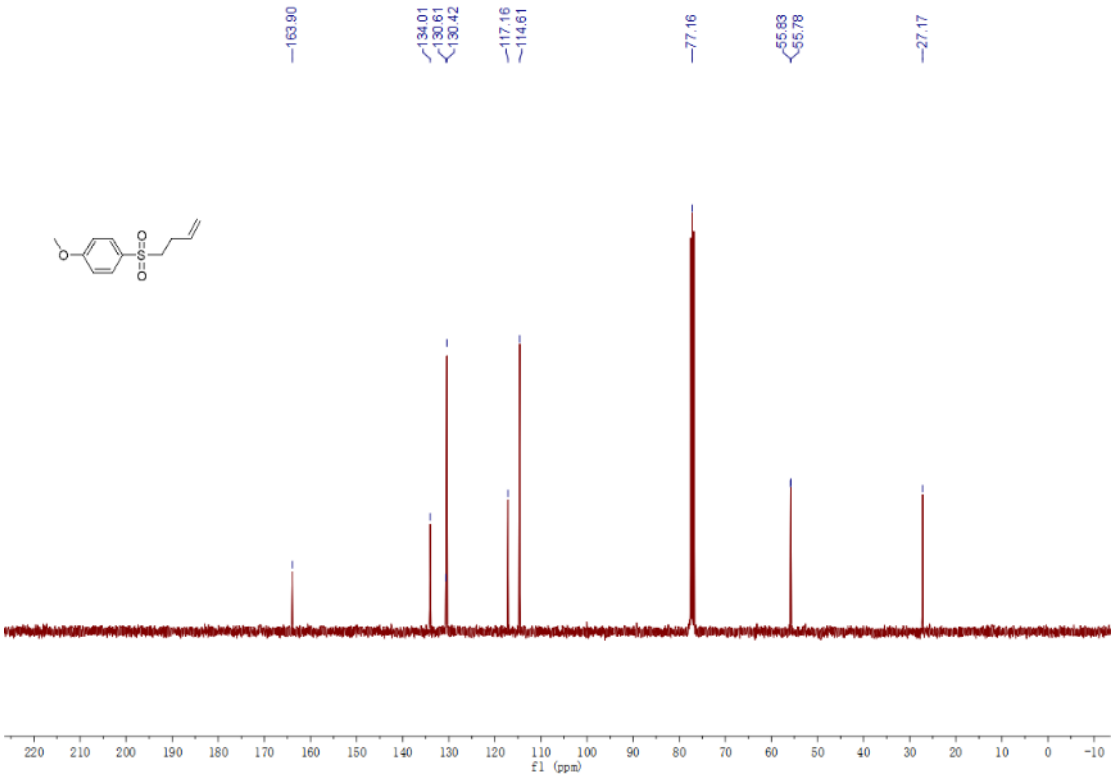
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1s



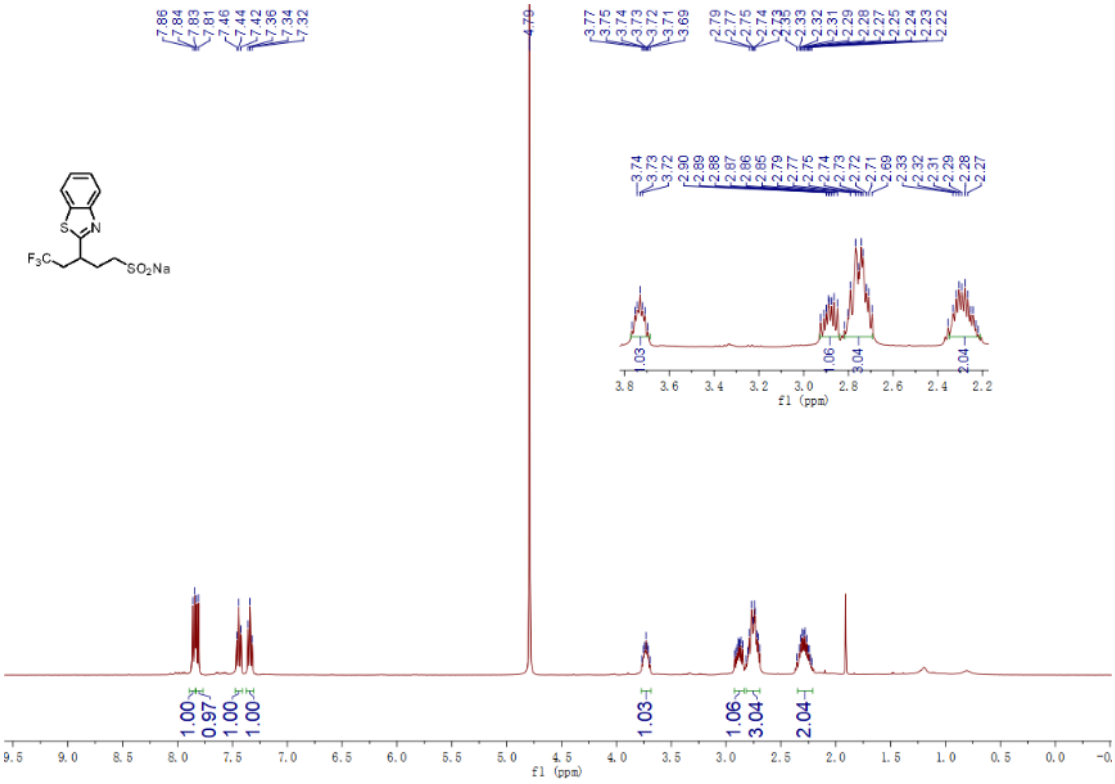
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 1t



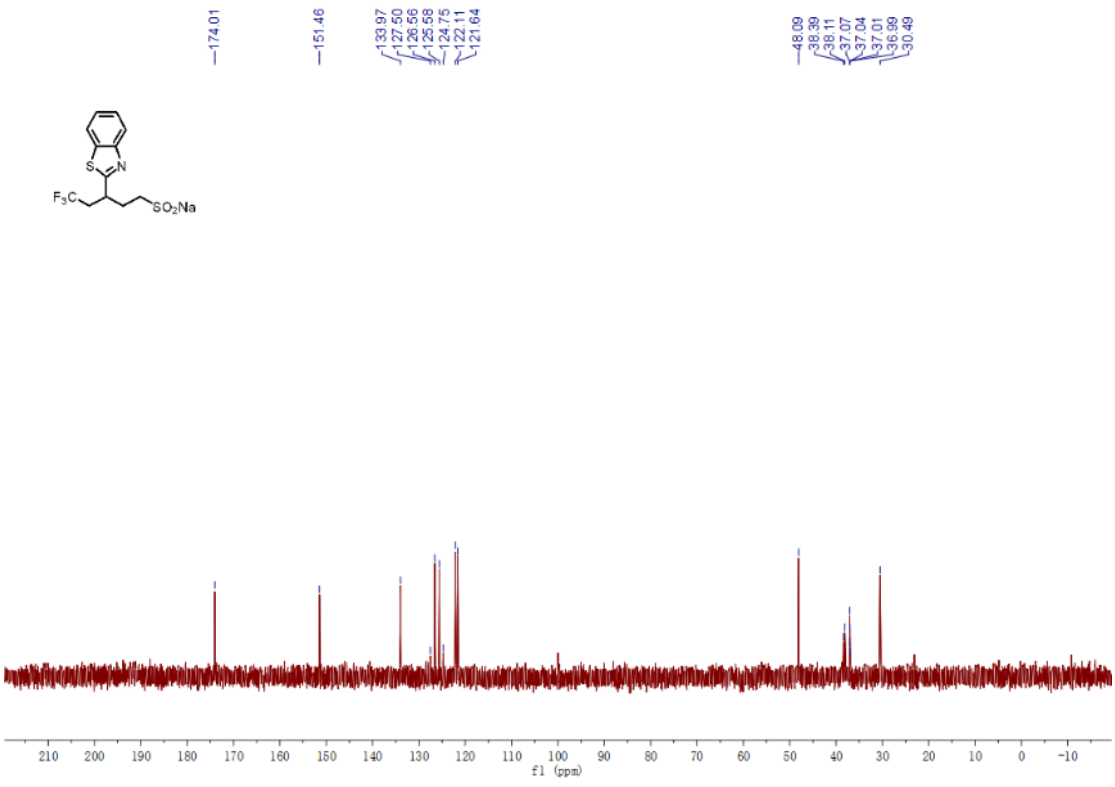
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 1t



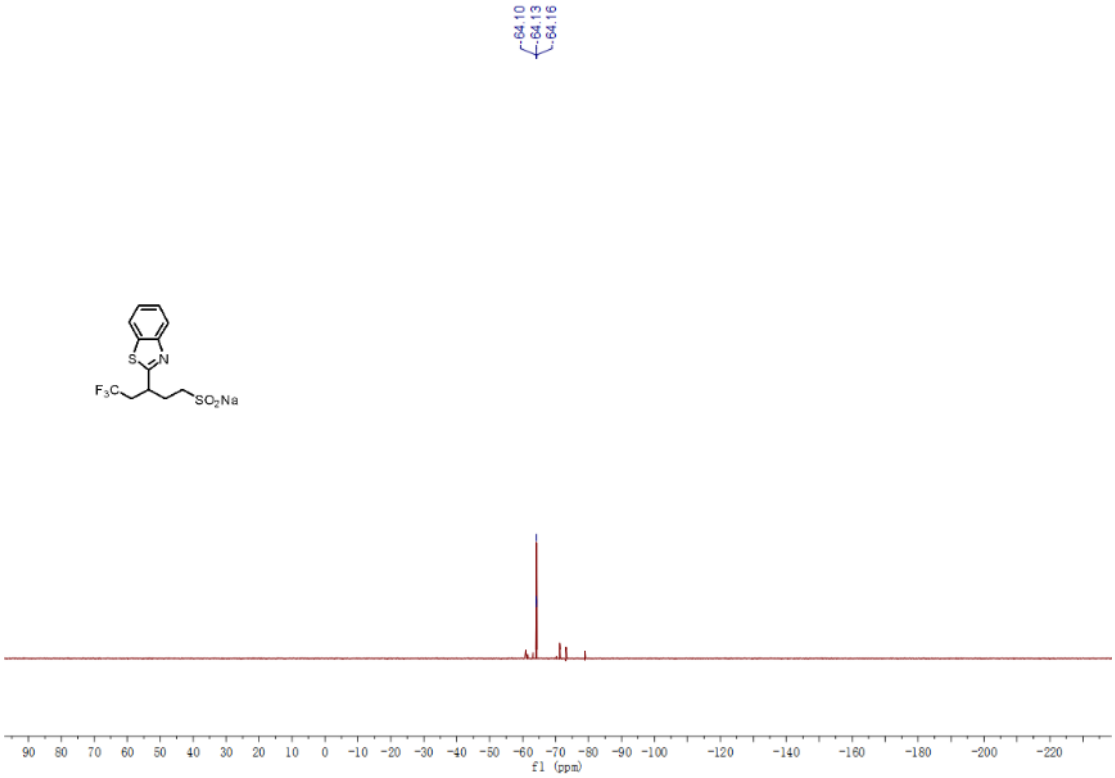
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3a'



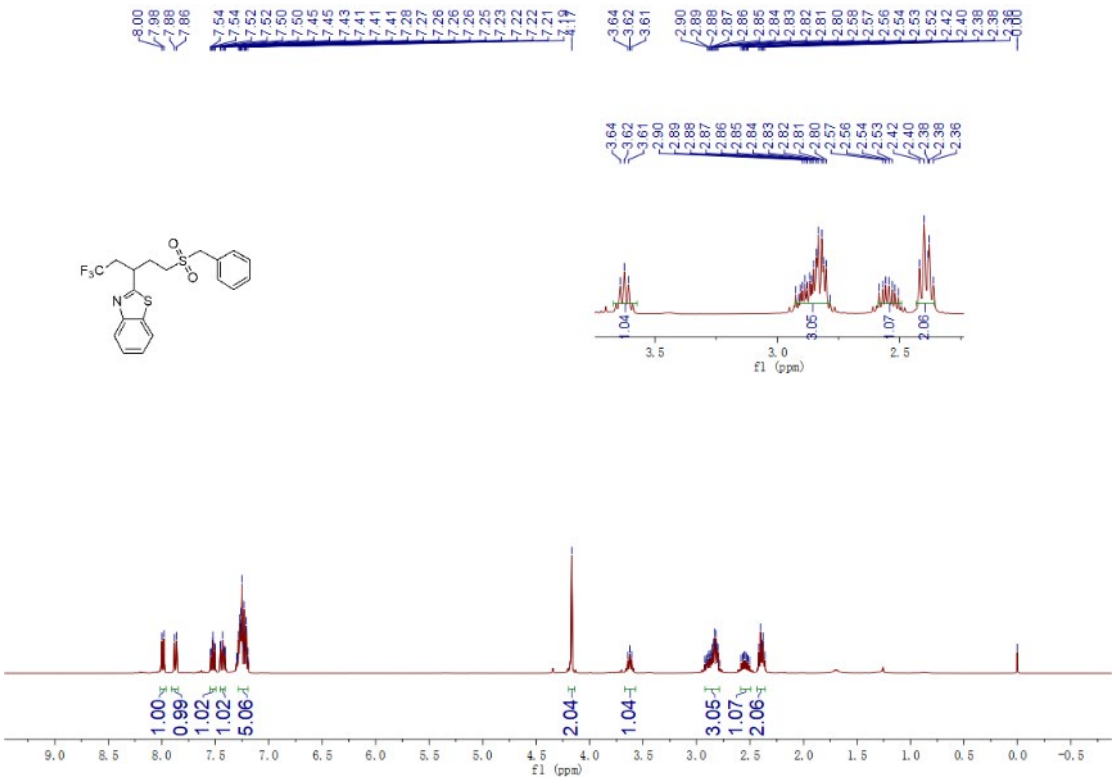
^{13}C NMR spectrum (100MHz, $CDCl_3$) of compound 3a'



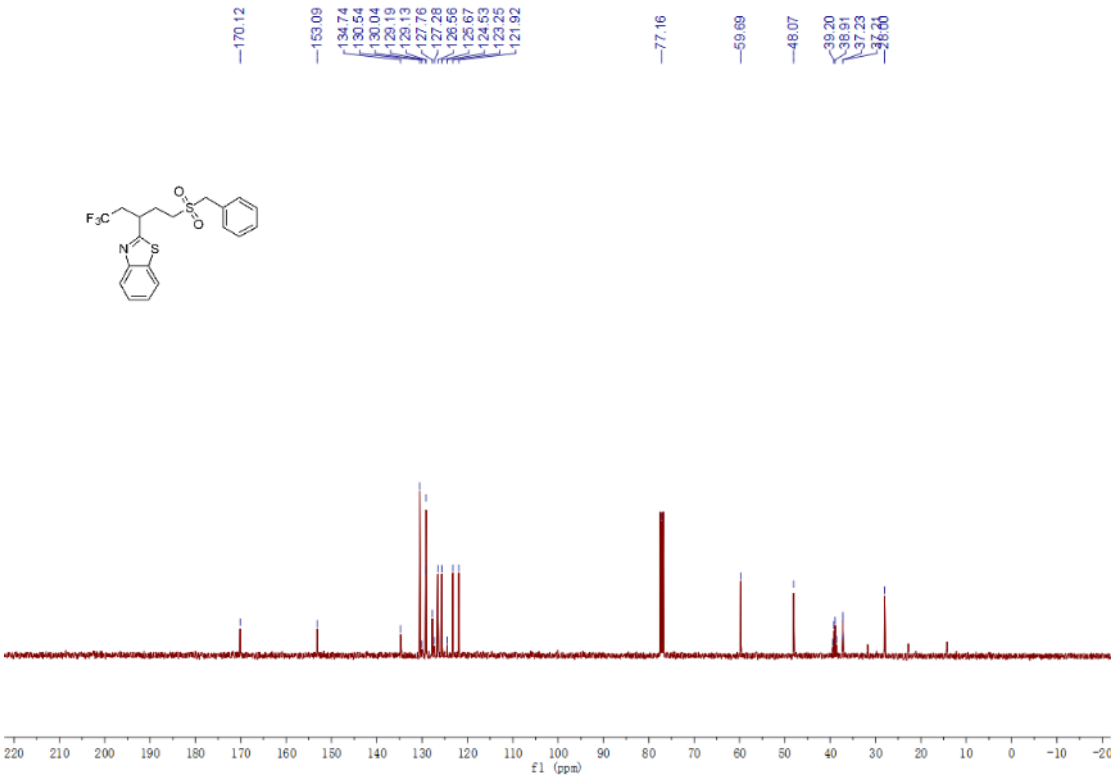
^{19}F NMR spectrum (376MHz, $CDCl_3$) of compound 3a'



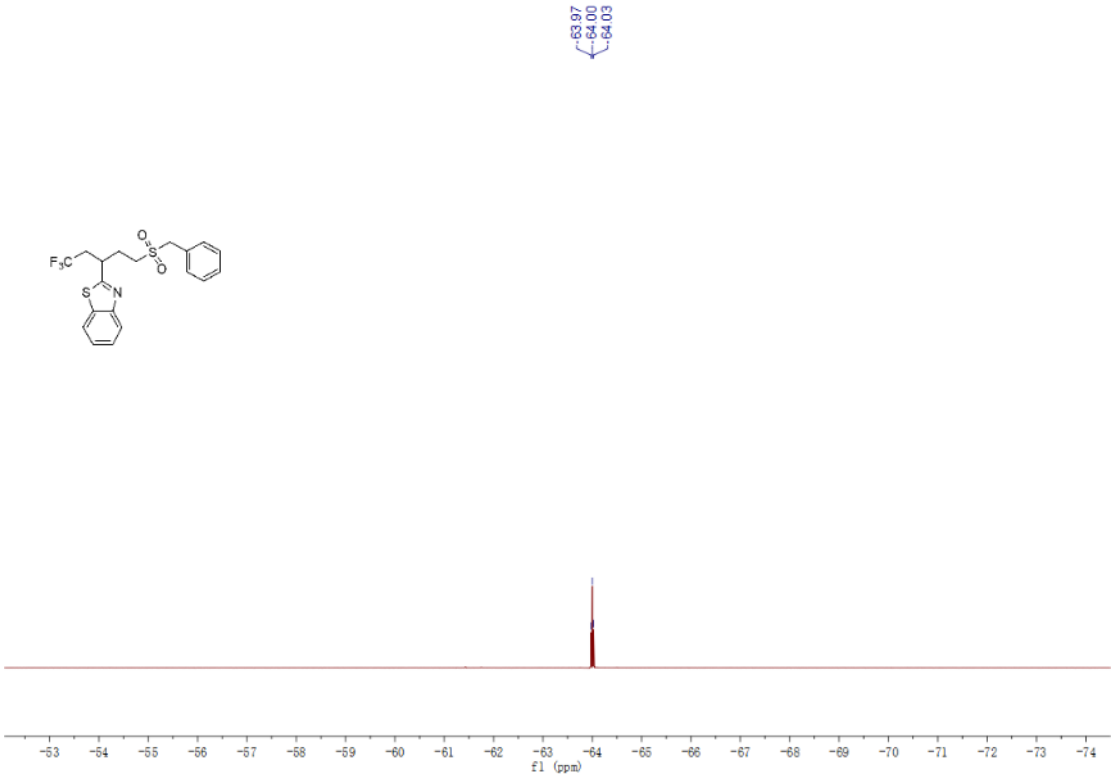
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3a



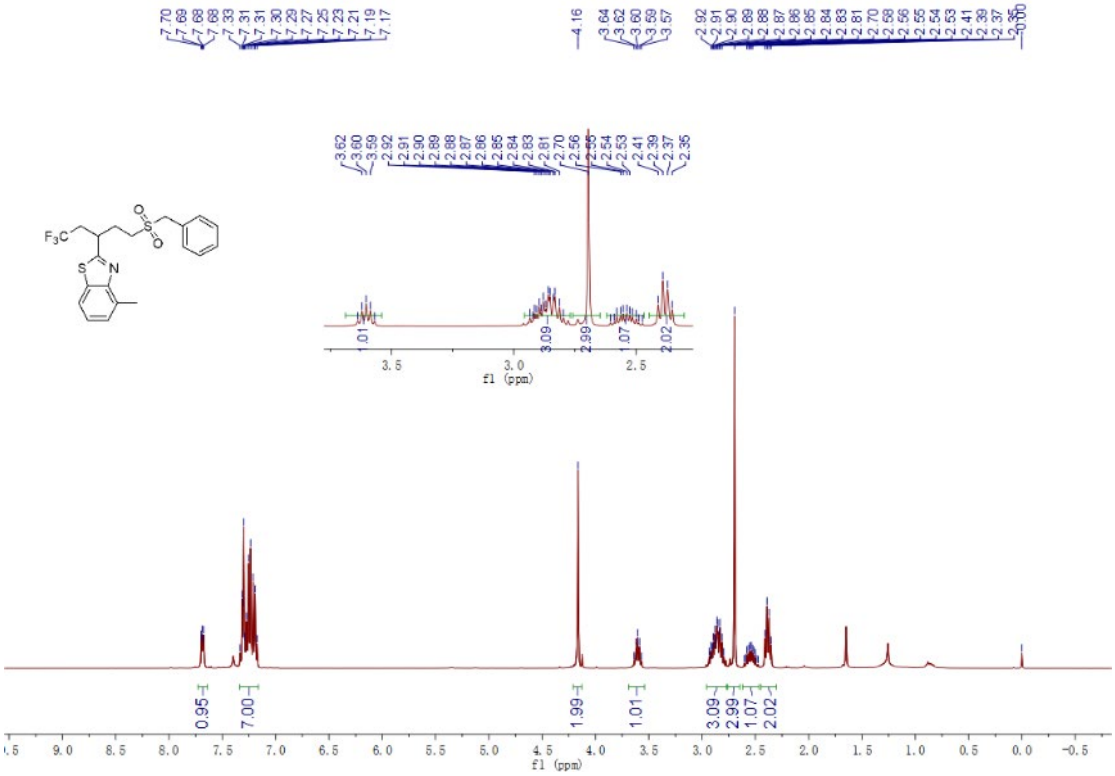
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3a



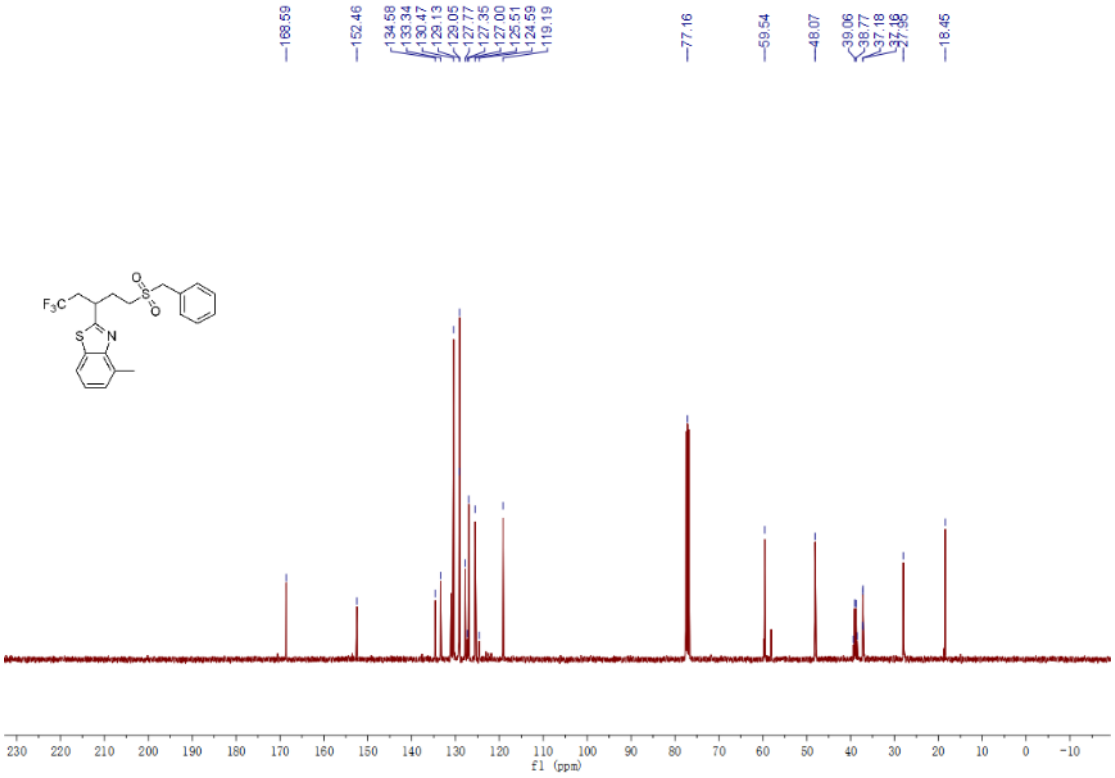
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3a



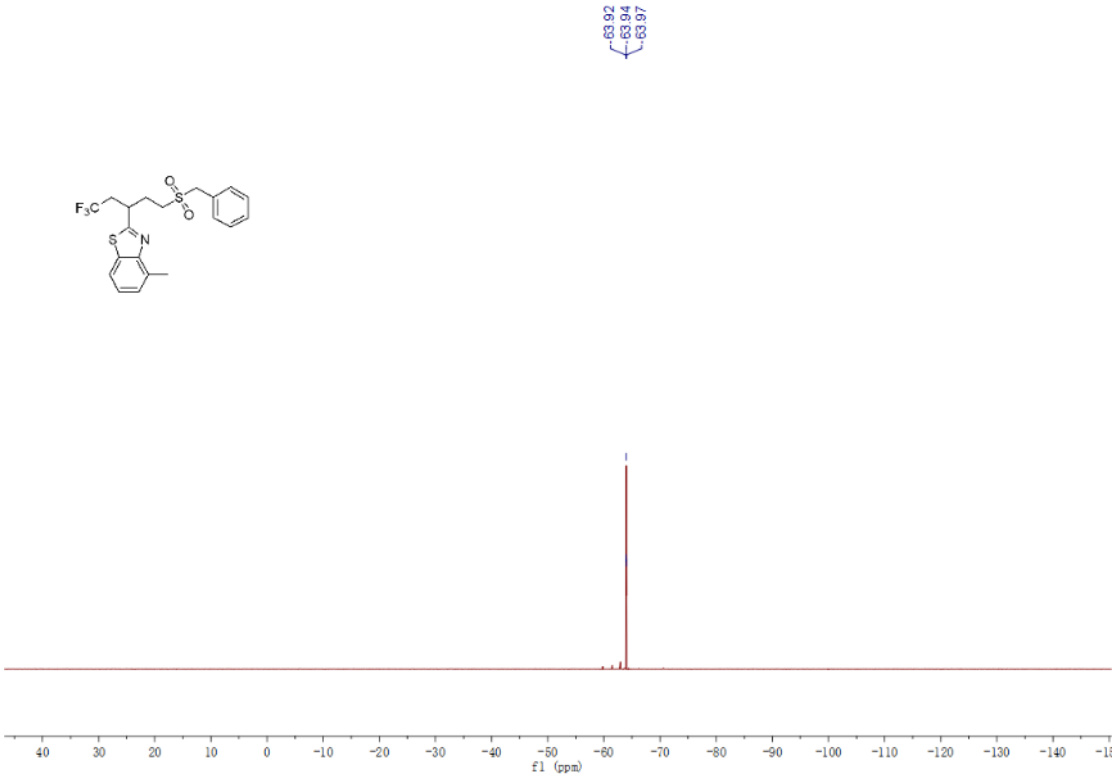
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3b



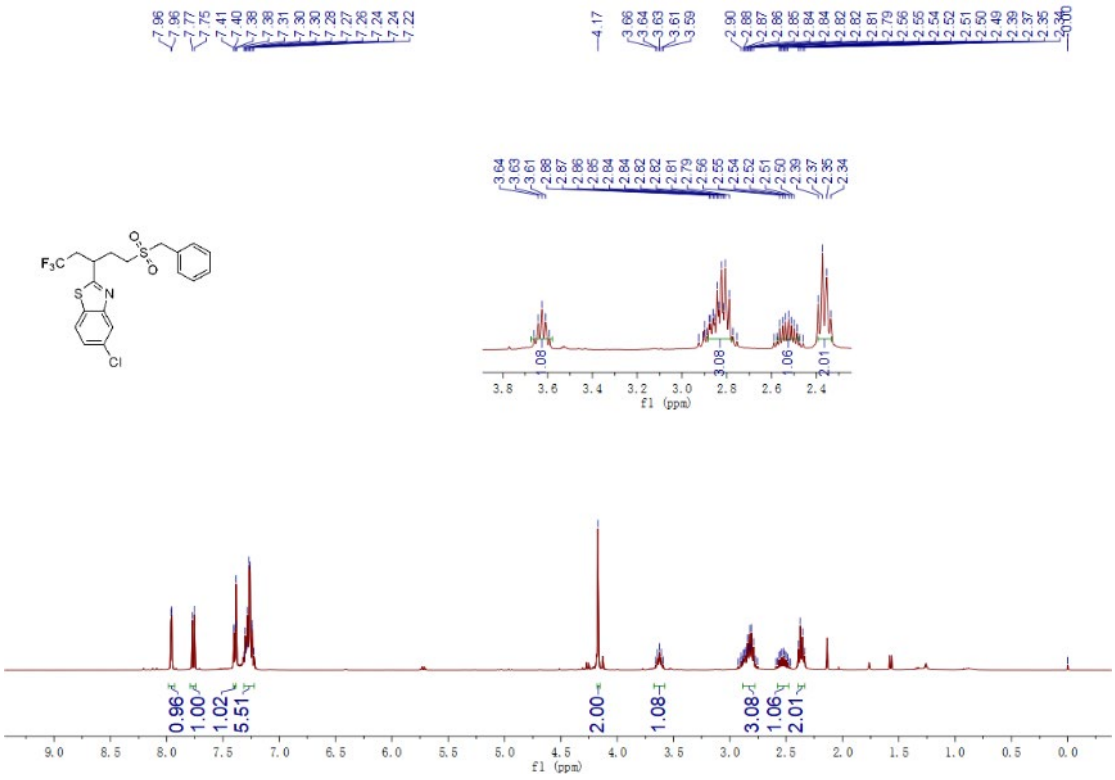
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3b



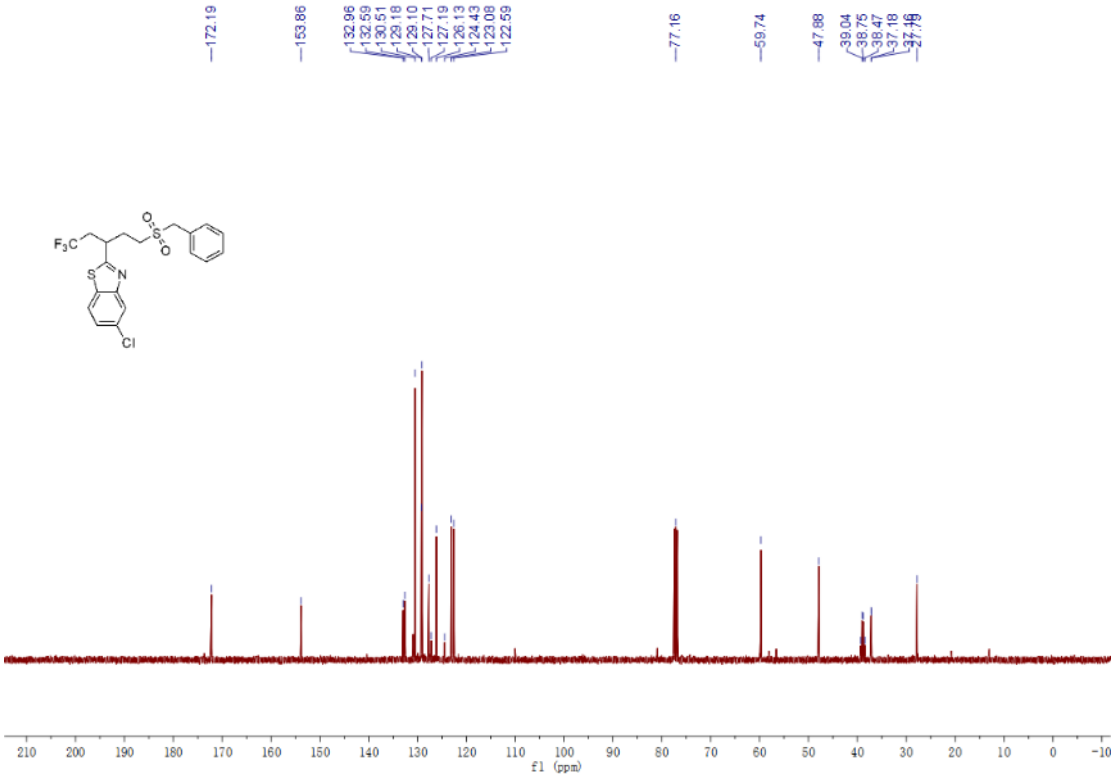
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3b



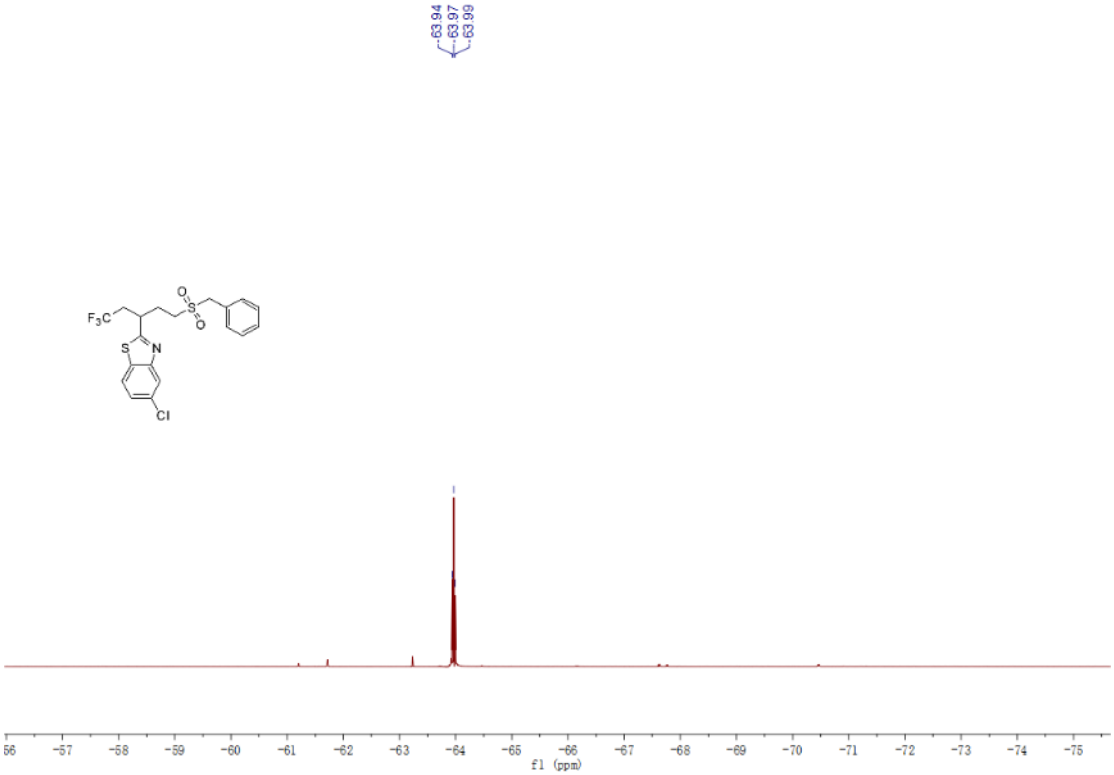
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3c



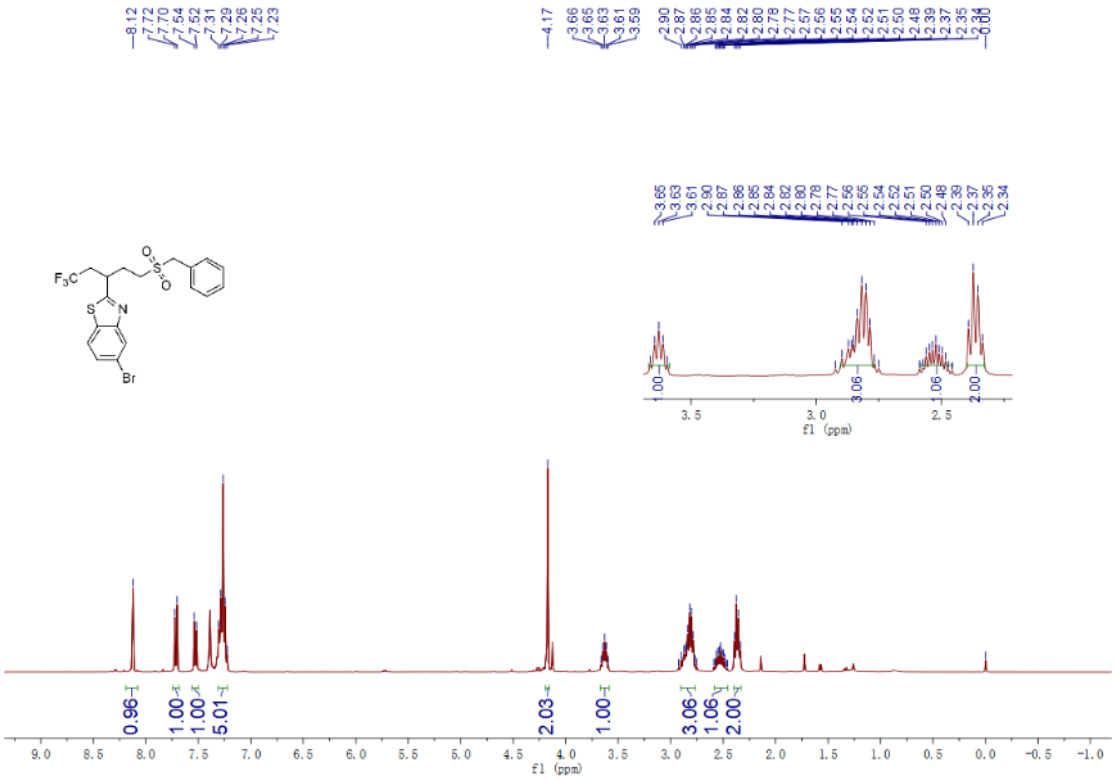
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3c



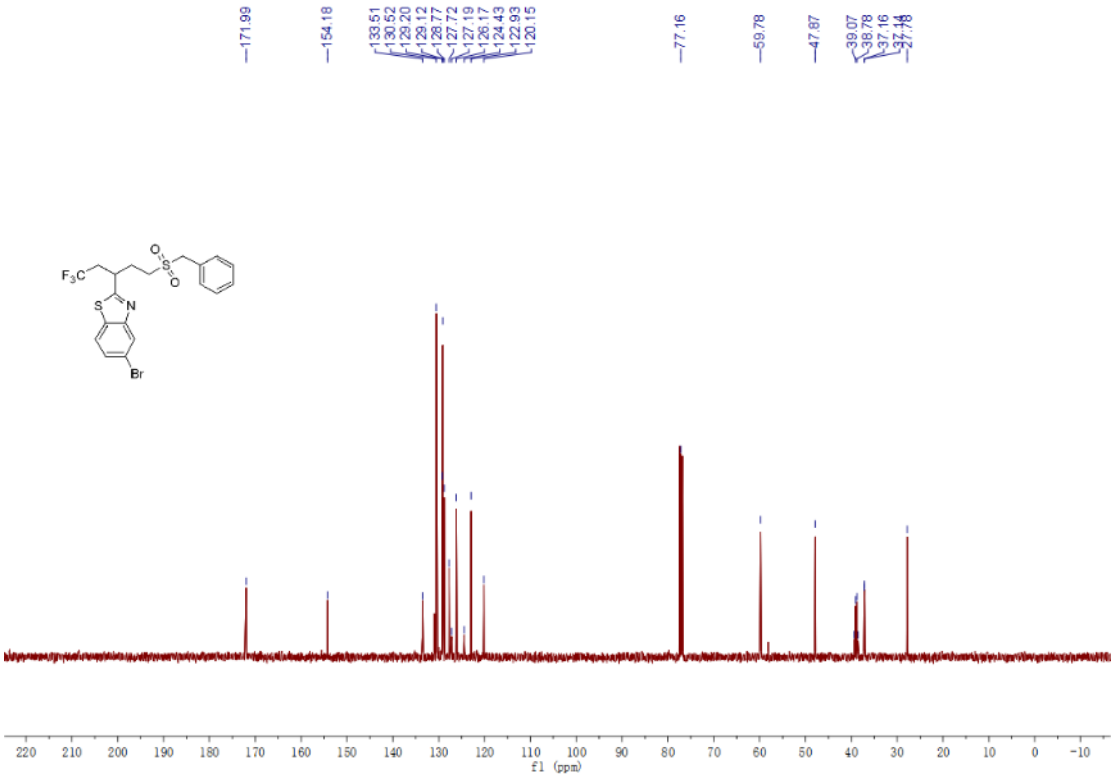
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3c



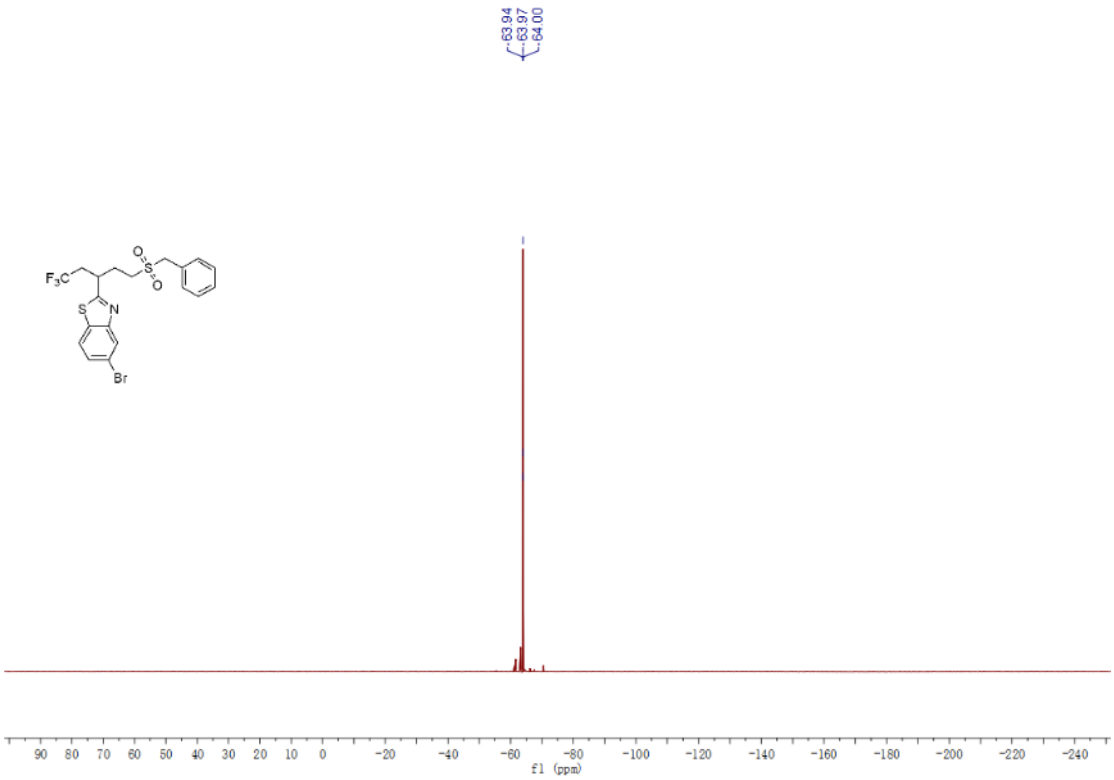
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3d



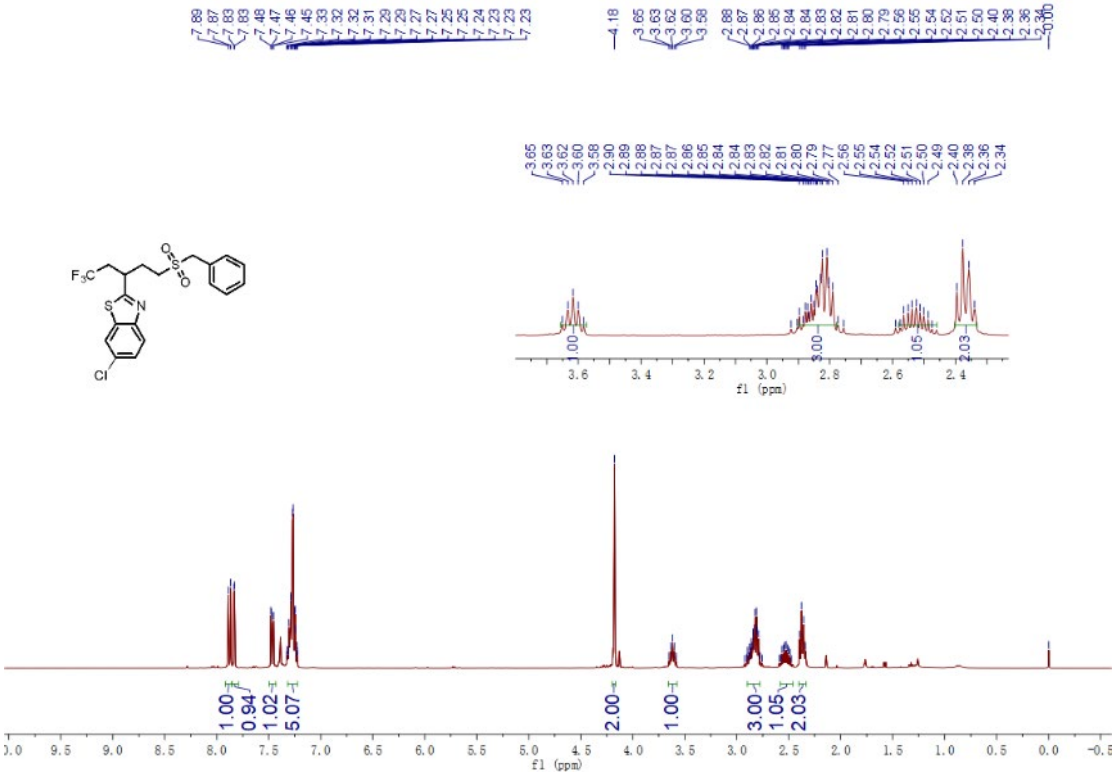
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3d



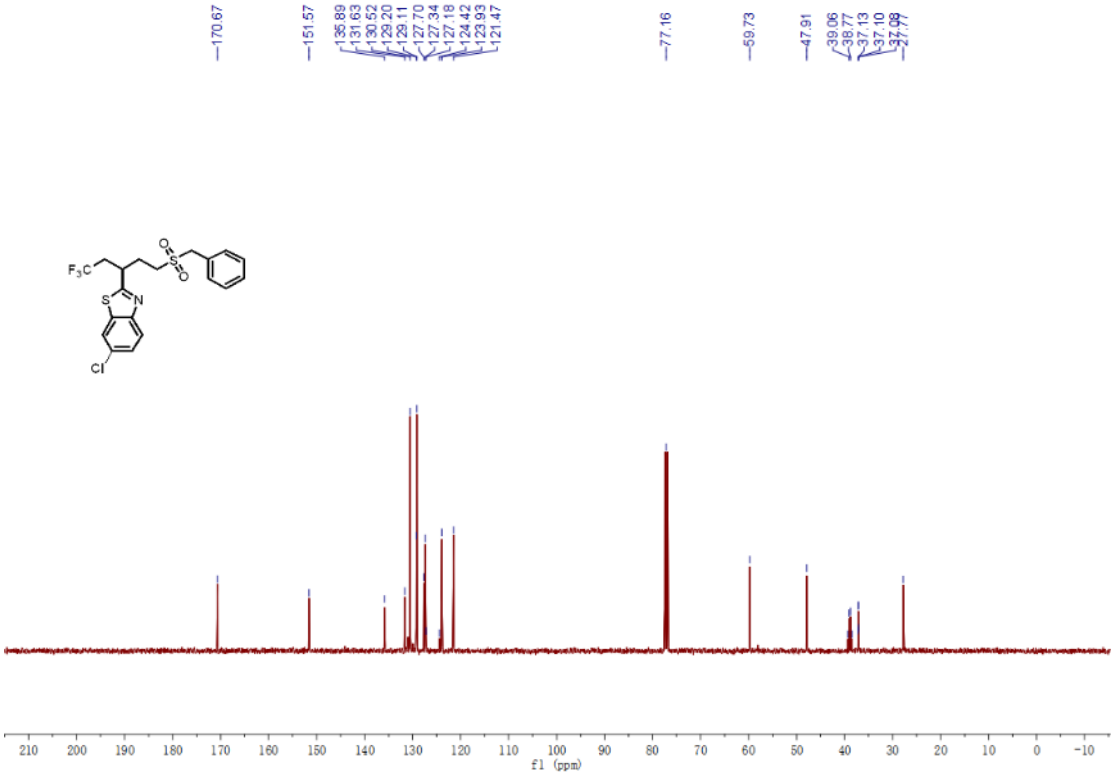
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3d



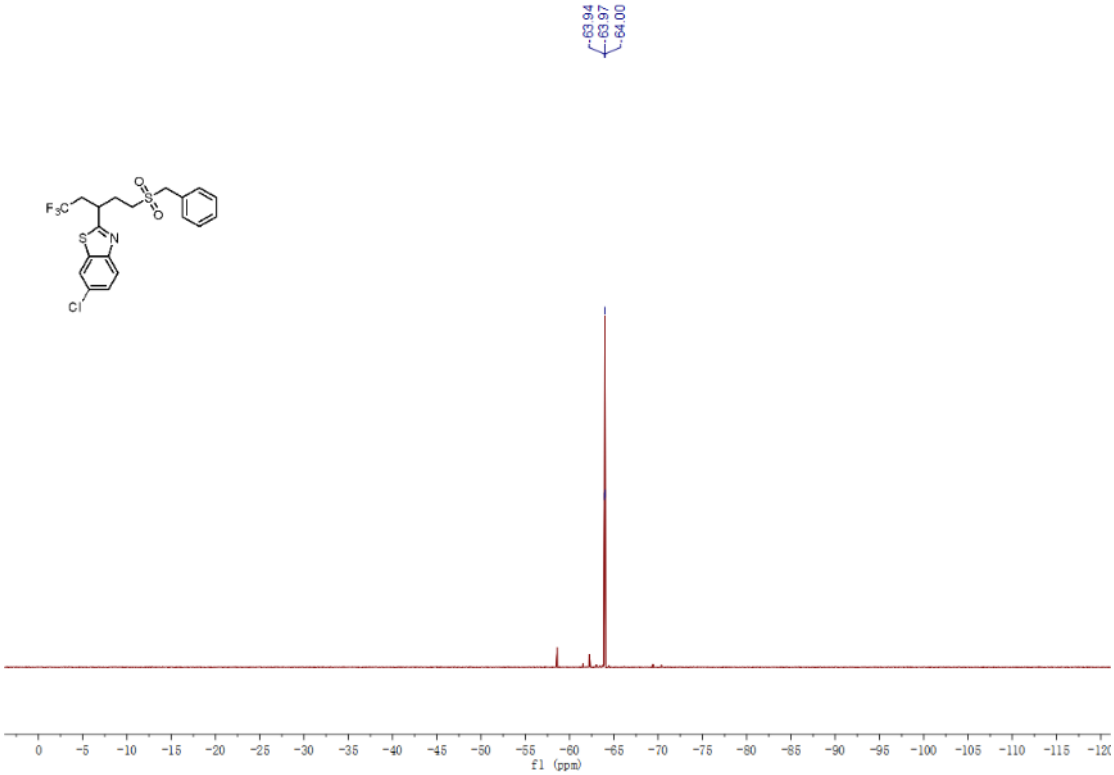
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3e



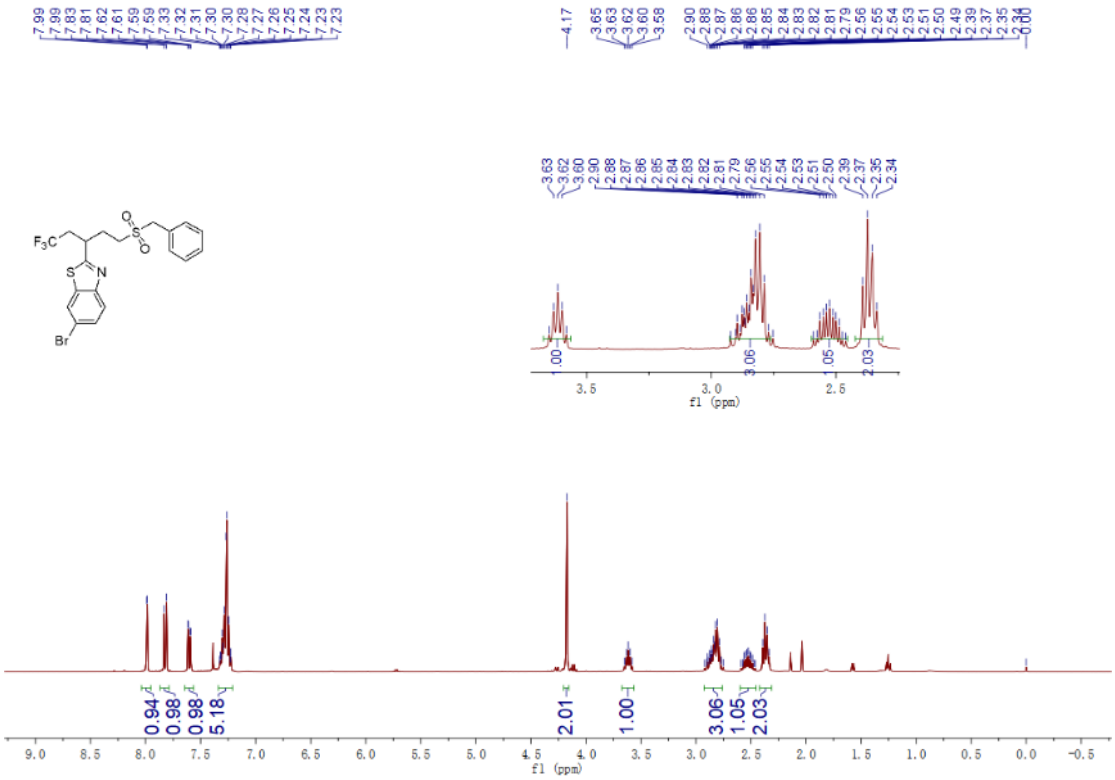
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3e



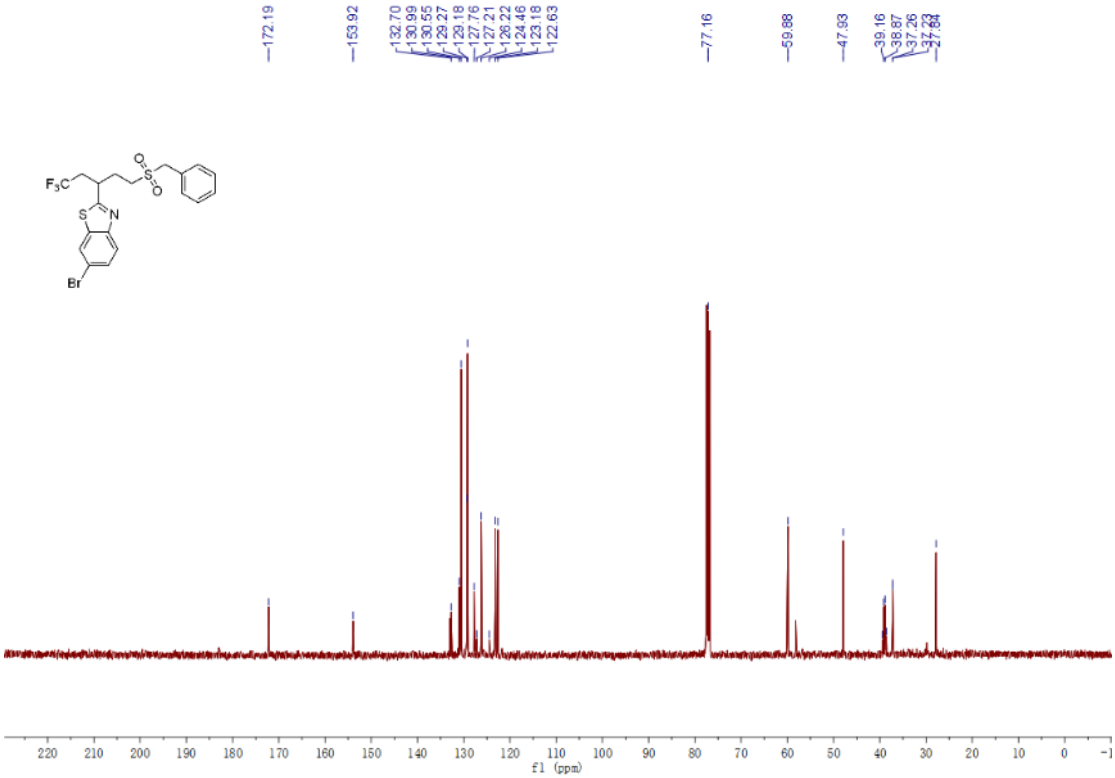
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3f



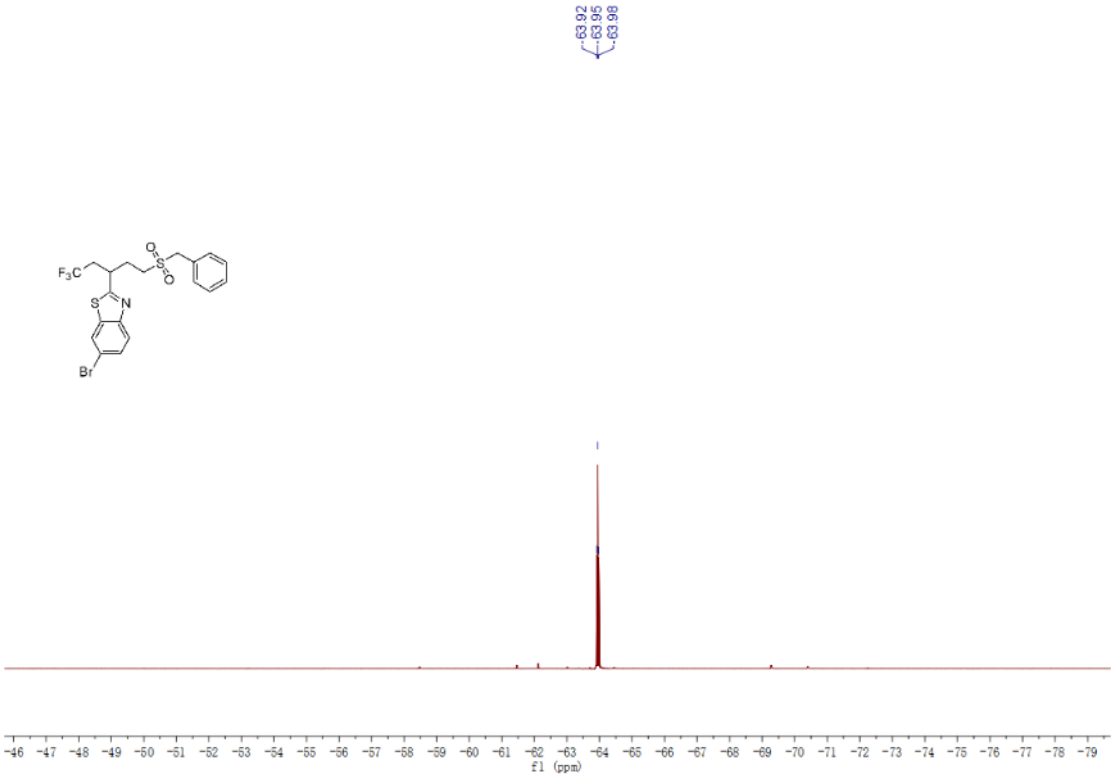
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3f



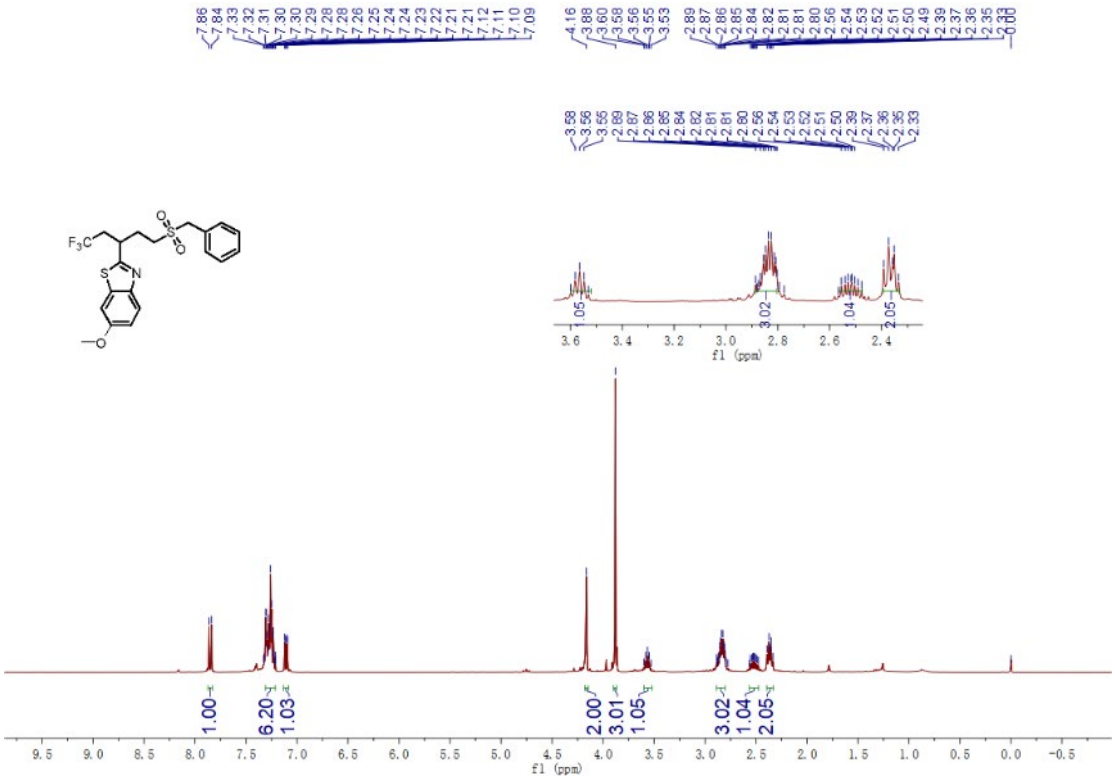
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3f



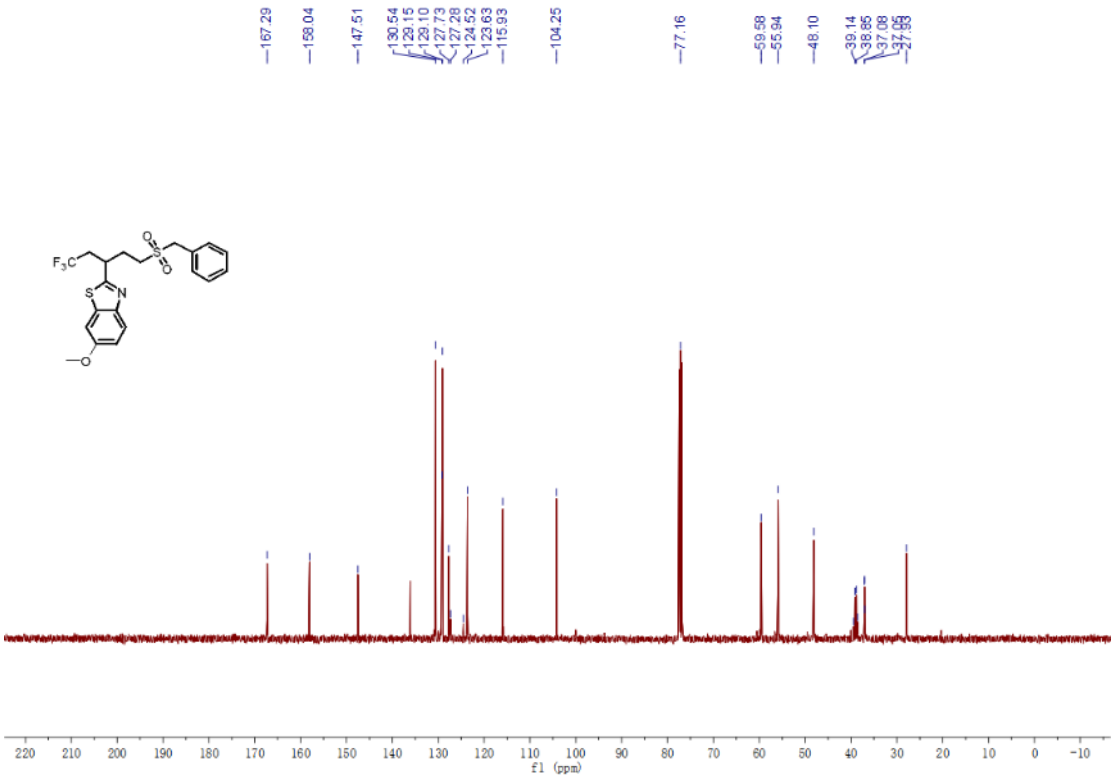
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3f



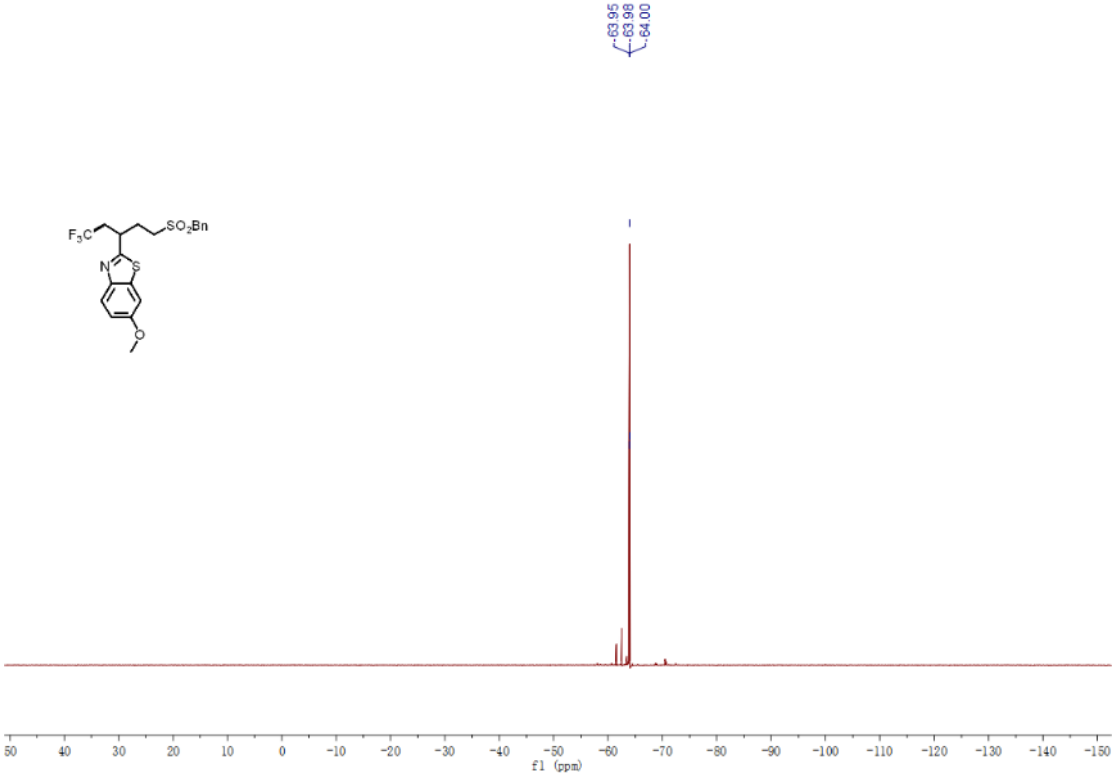
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3g



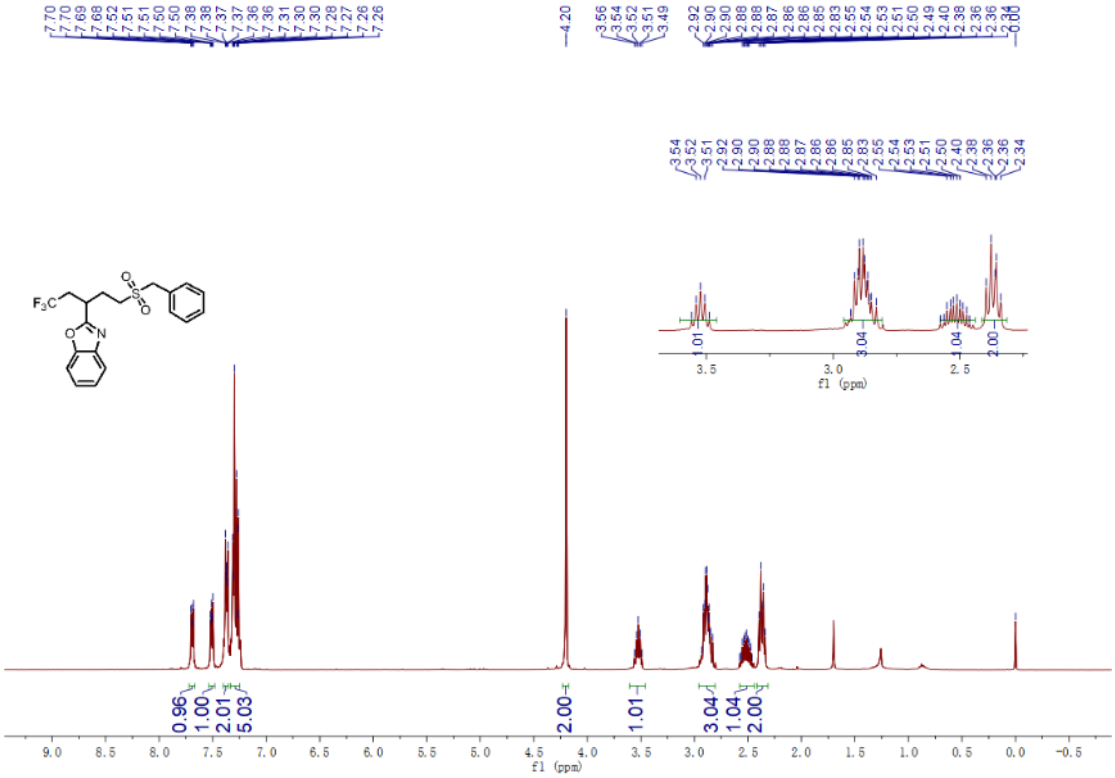
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3g



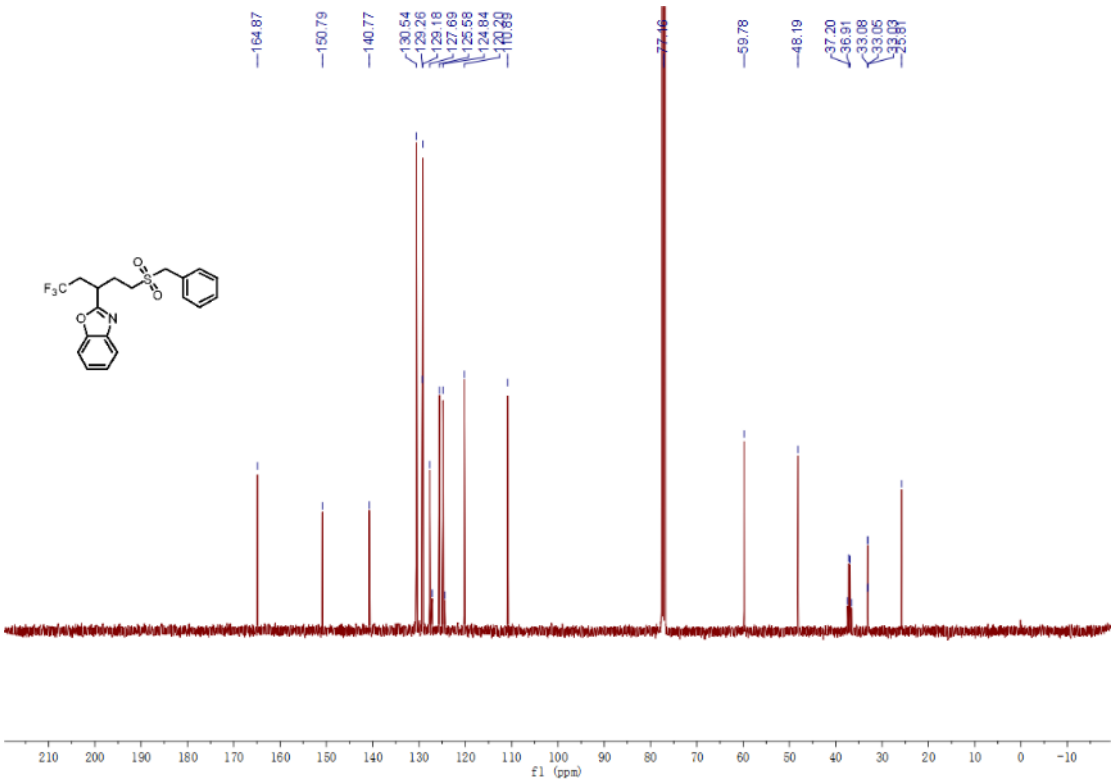
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3g



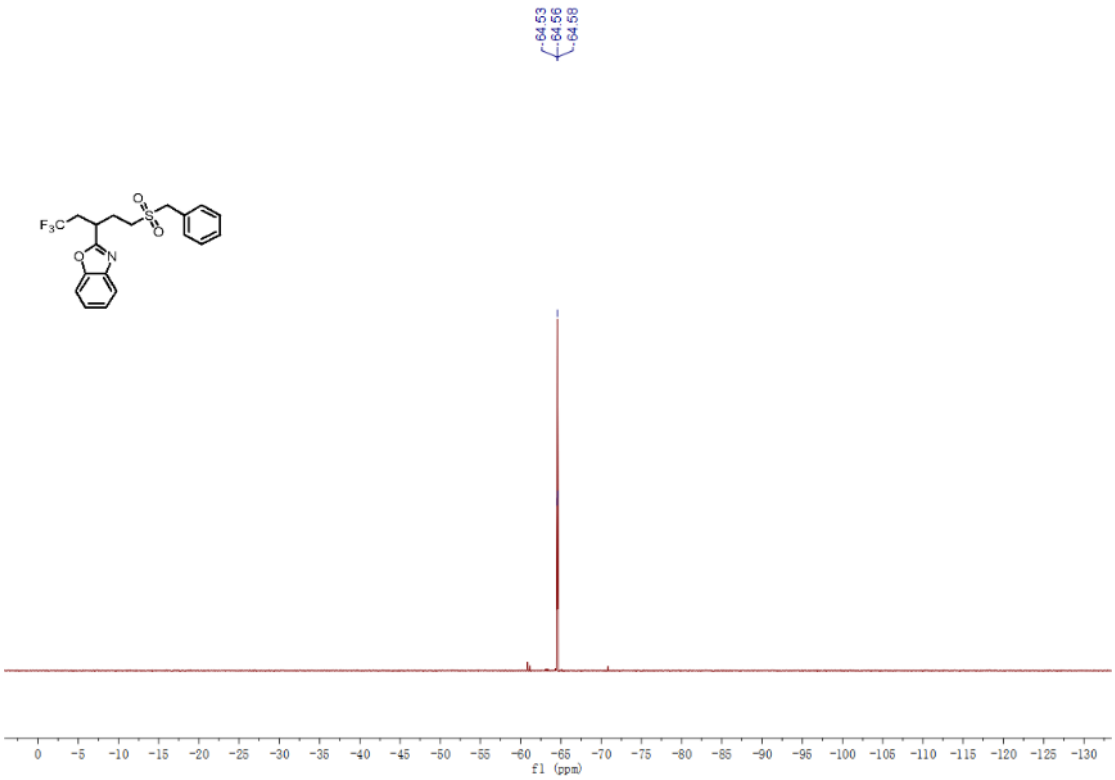
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3h



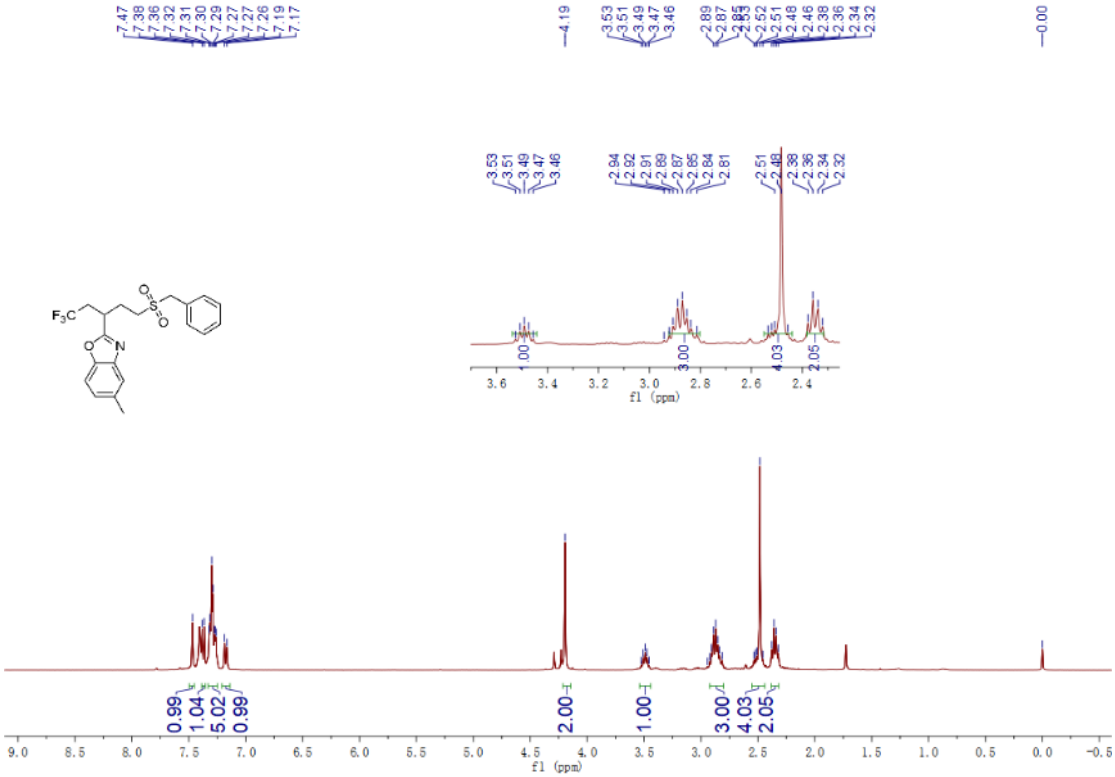
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3h



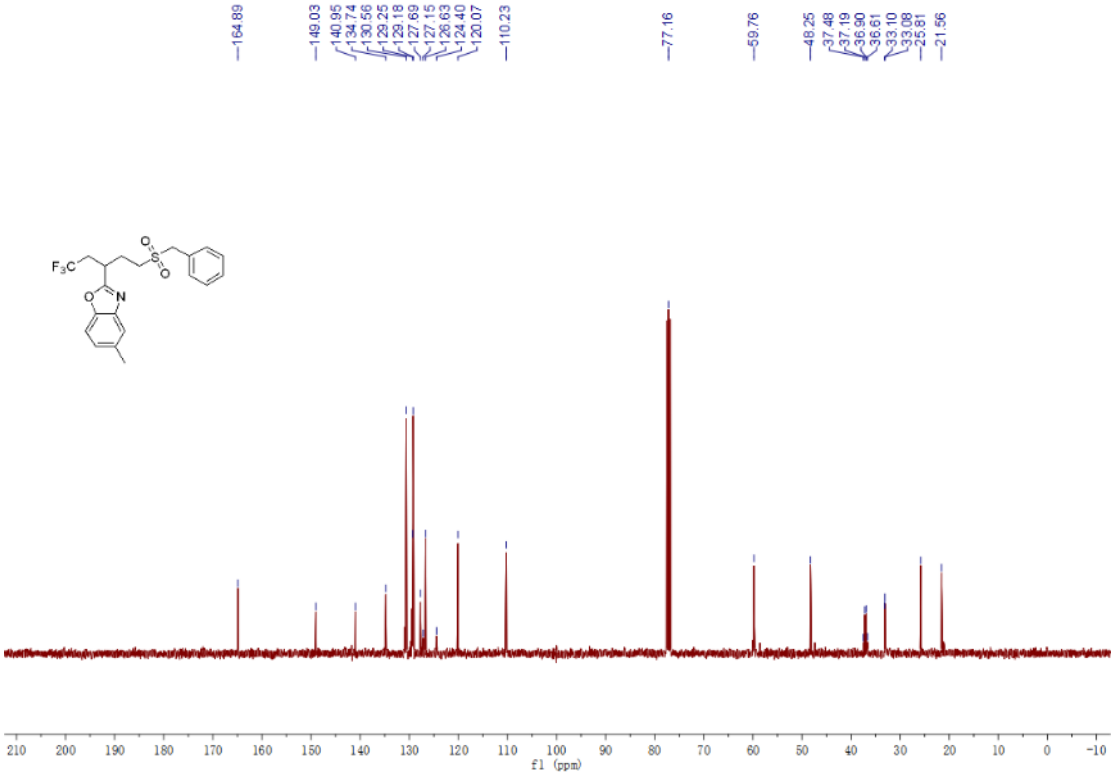
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3h



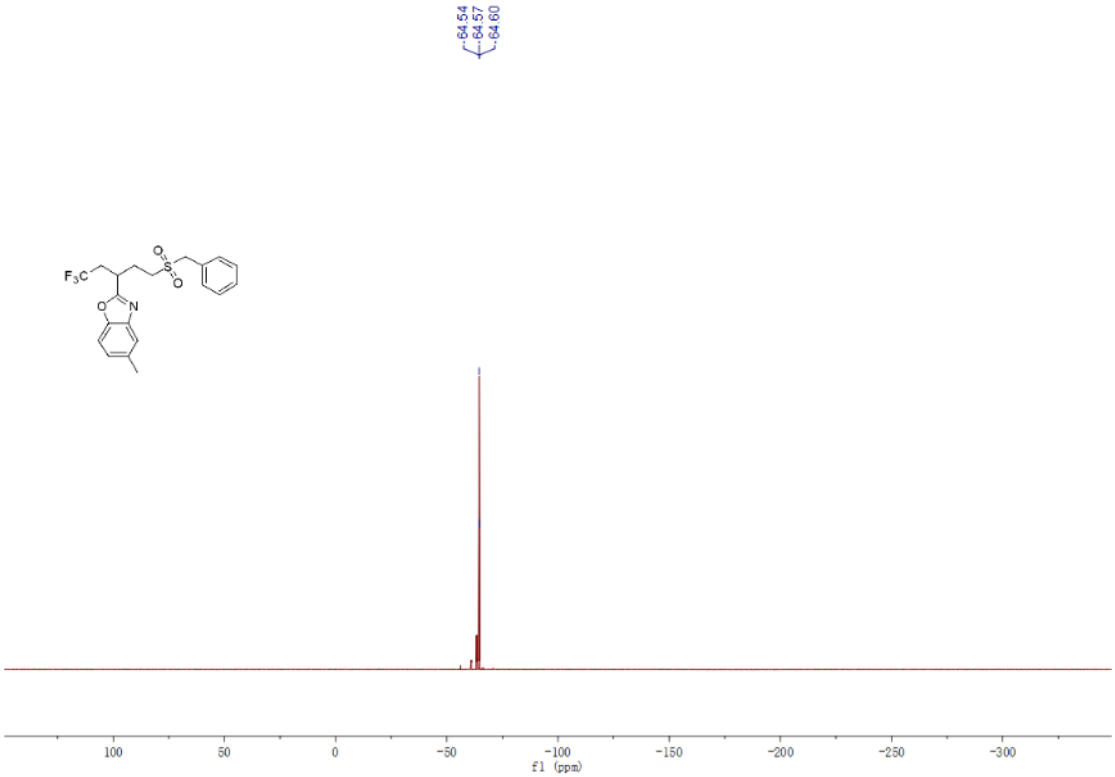
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3i



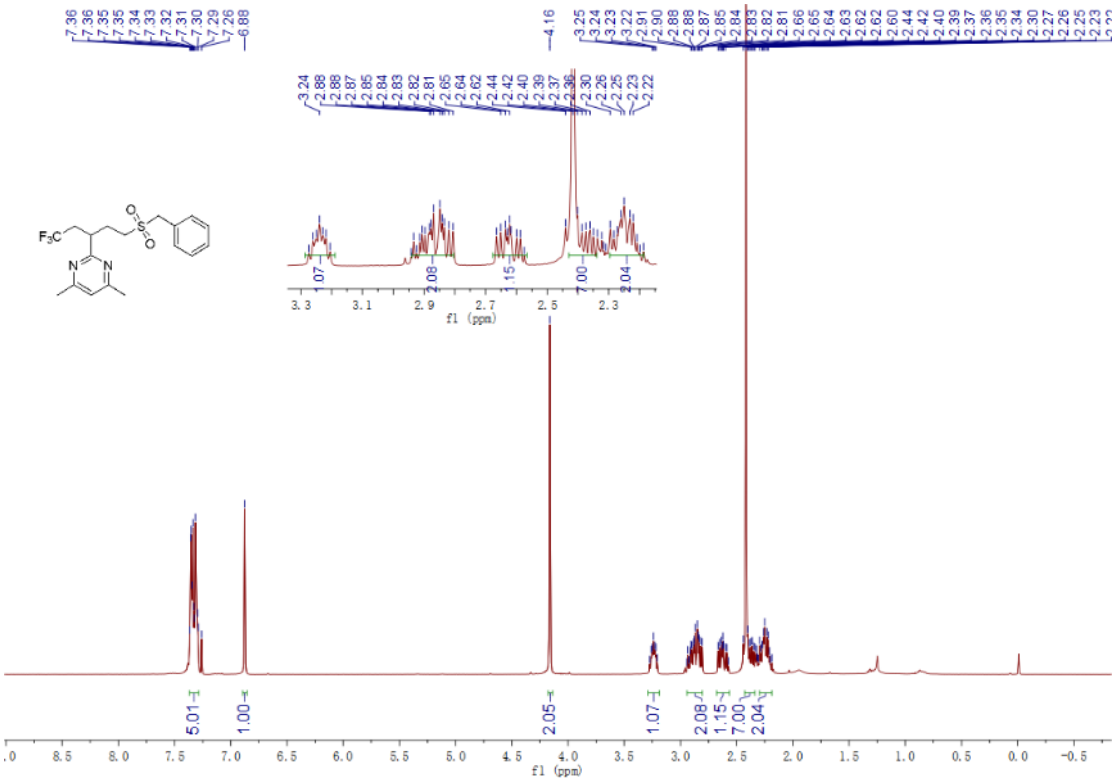
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3i



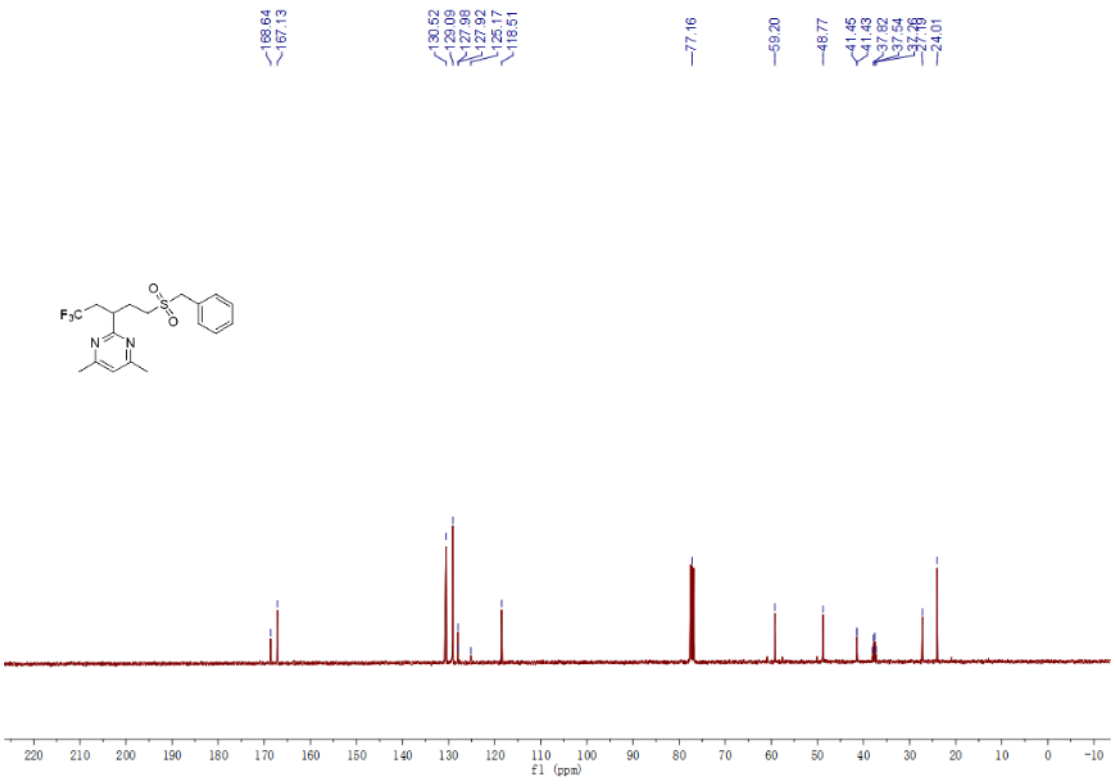
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3i



^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3j



^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3j



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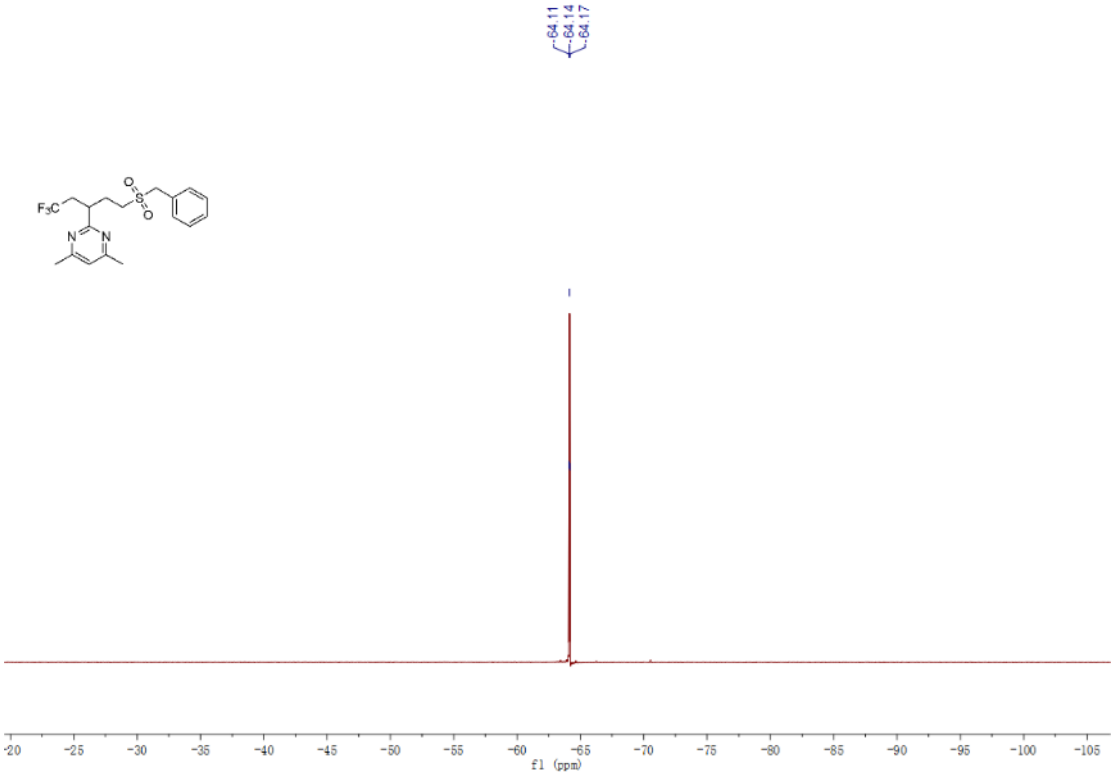

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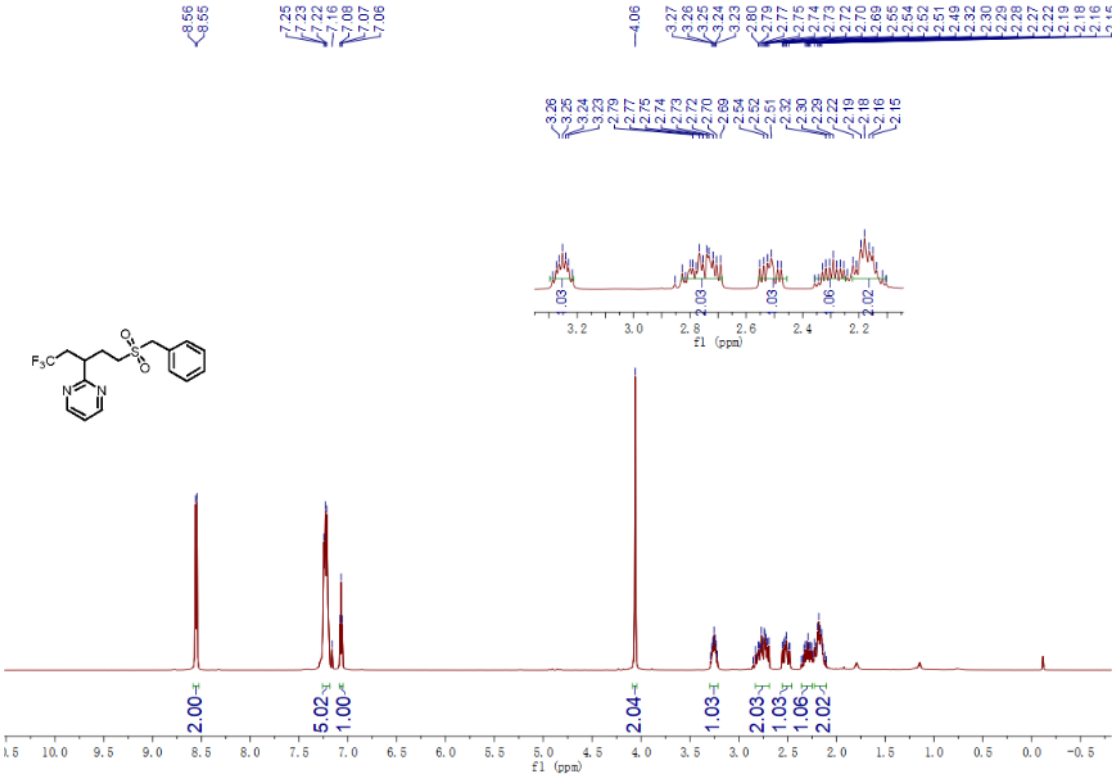
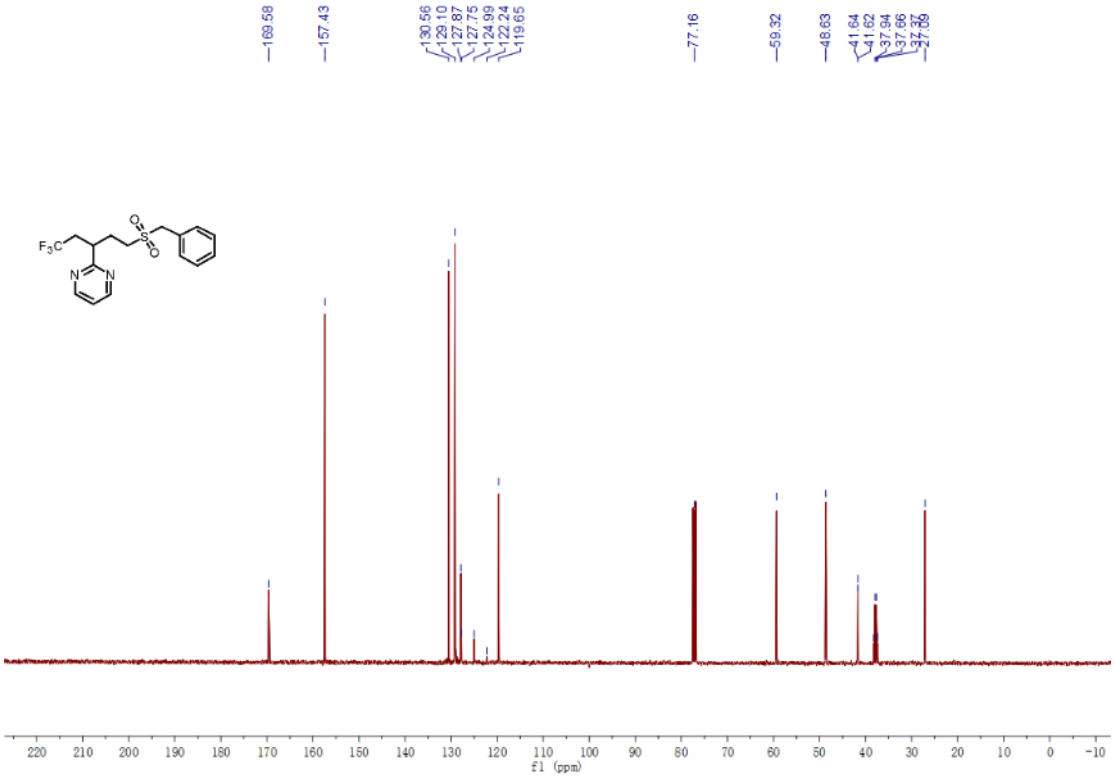
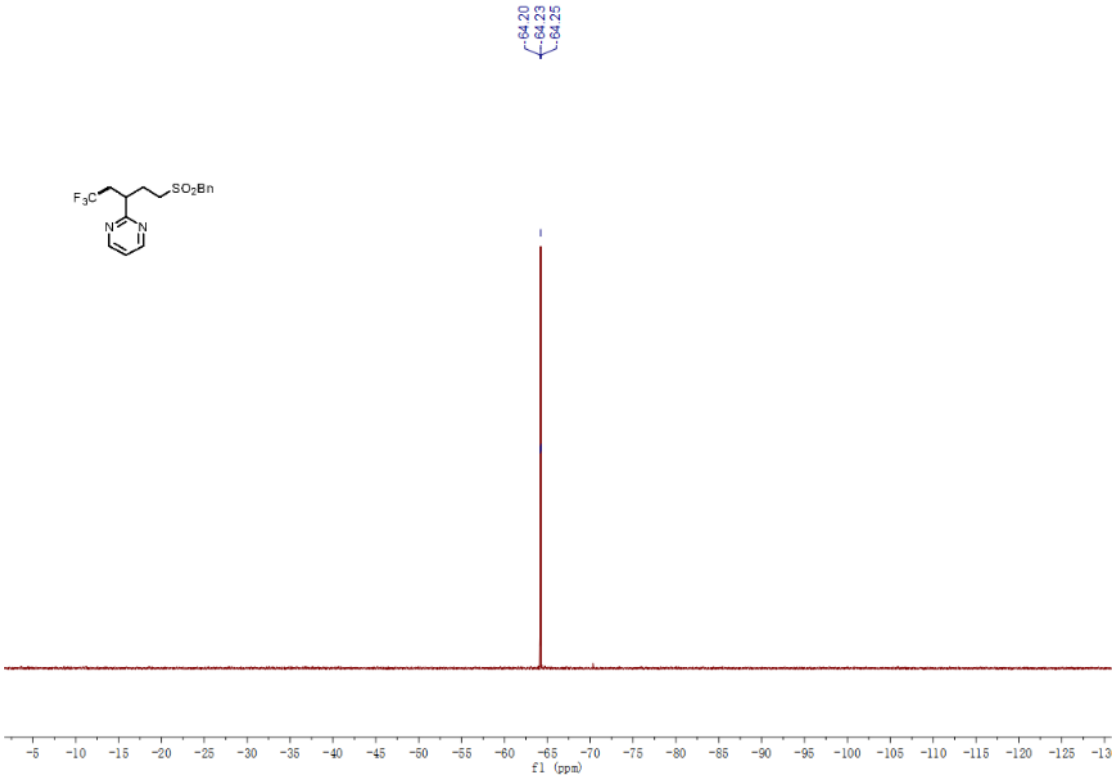


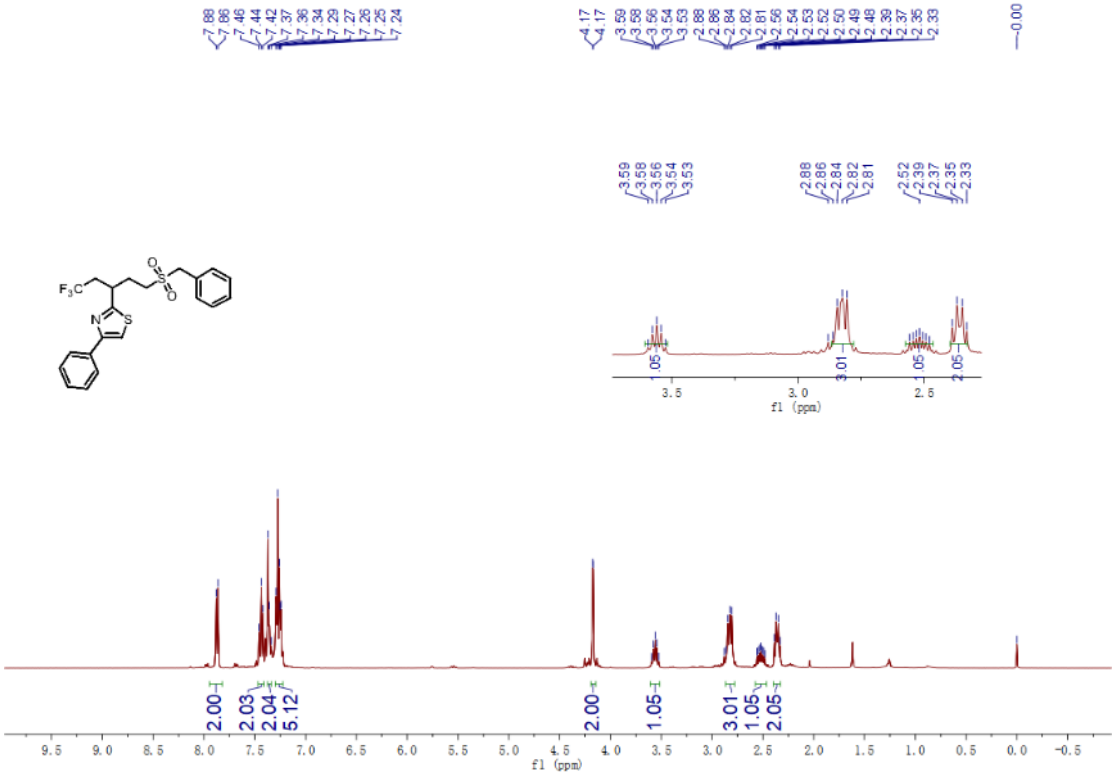
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3k



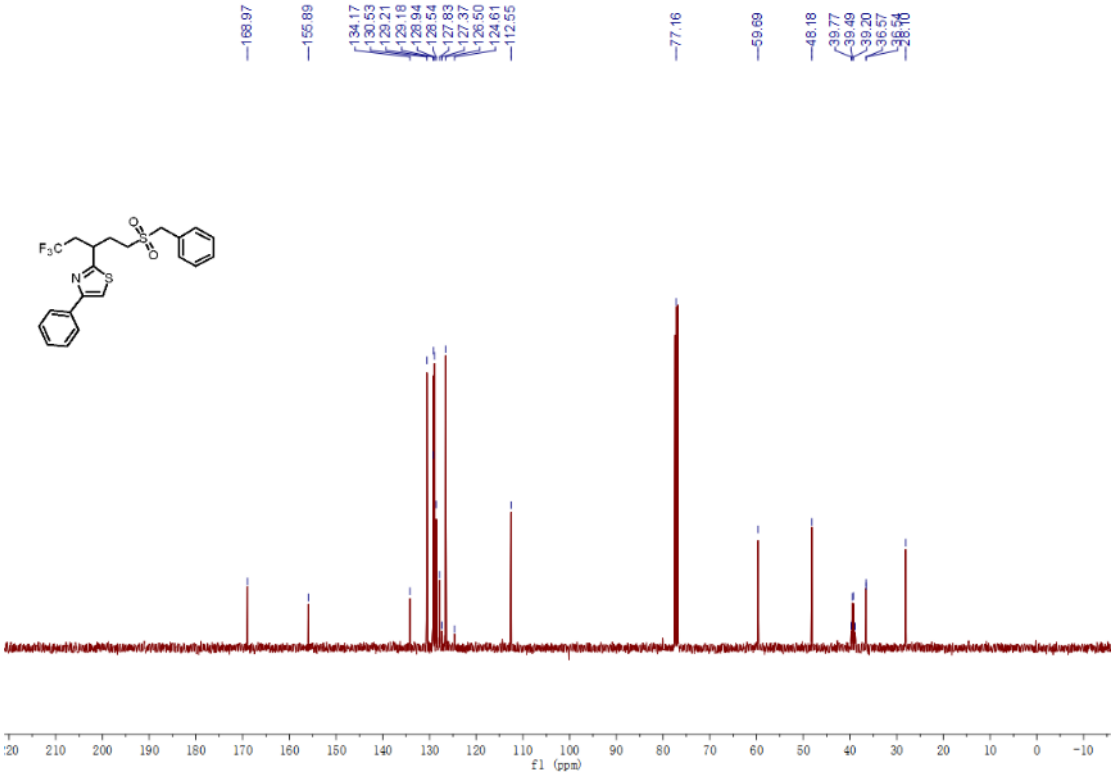
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3k



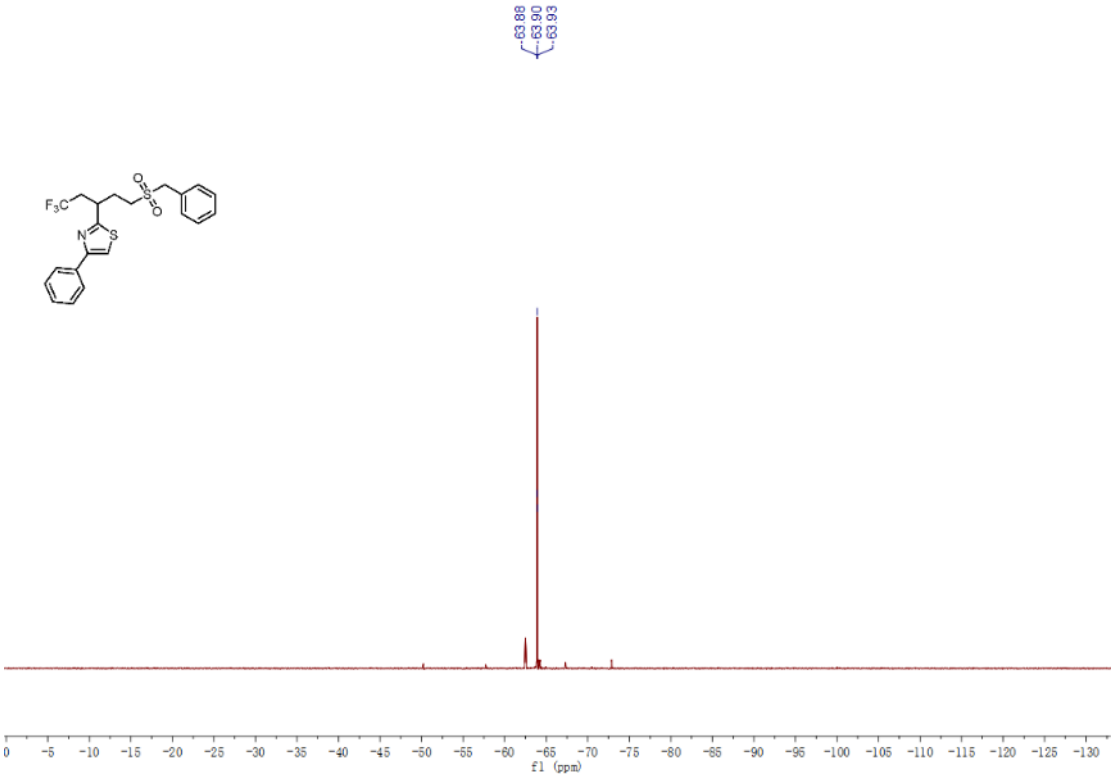
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3l



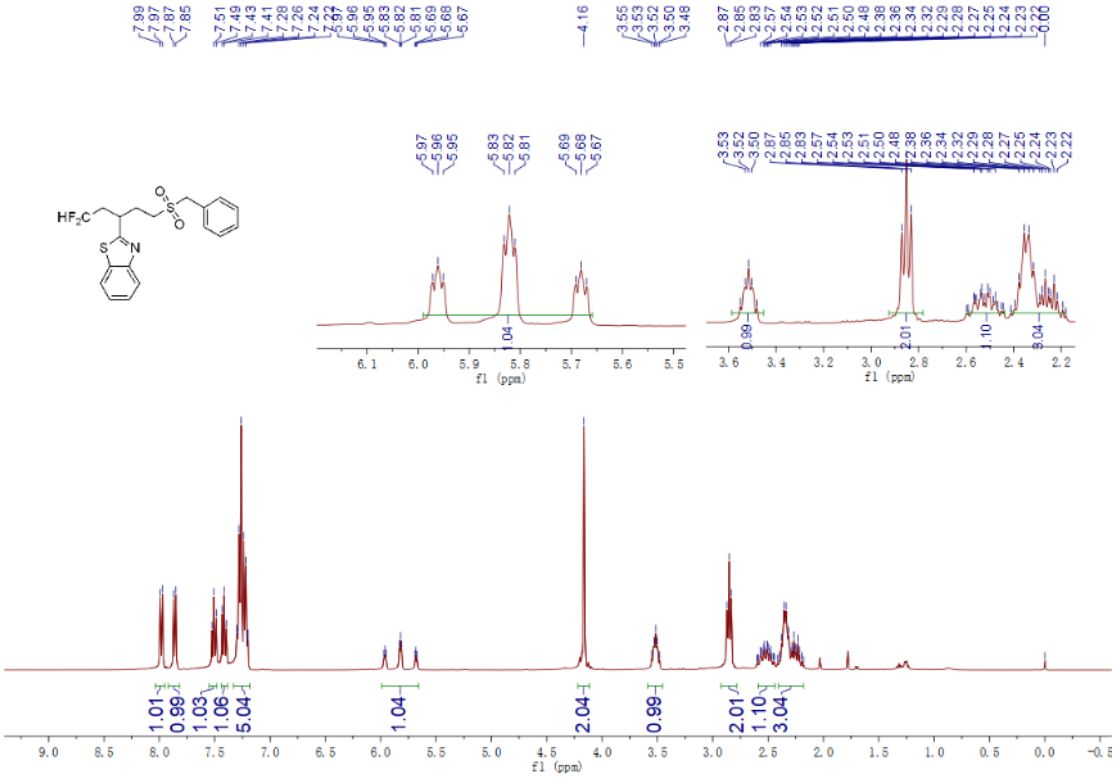
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3l



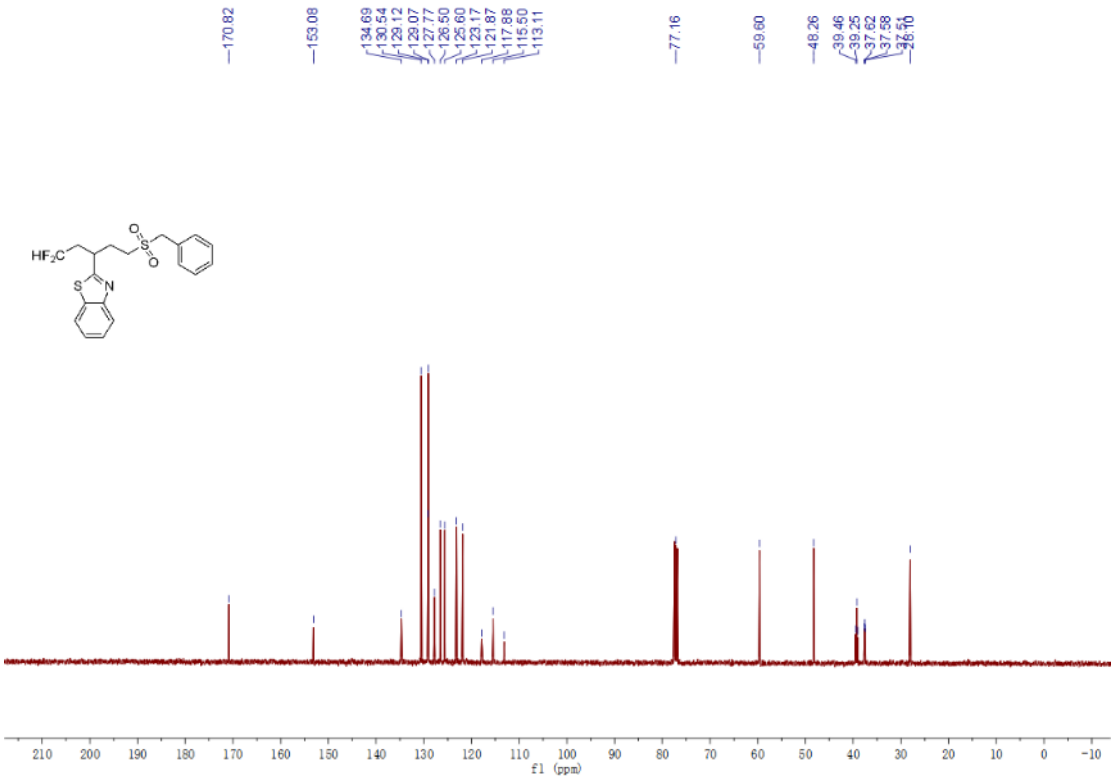
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3l



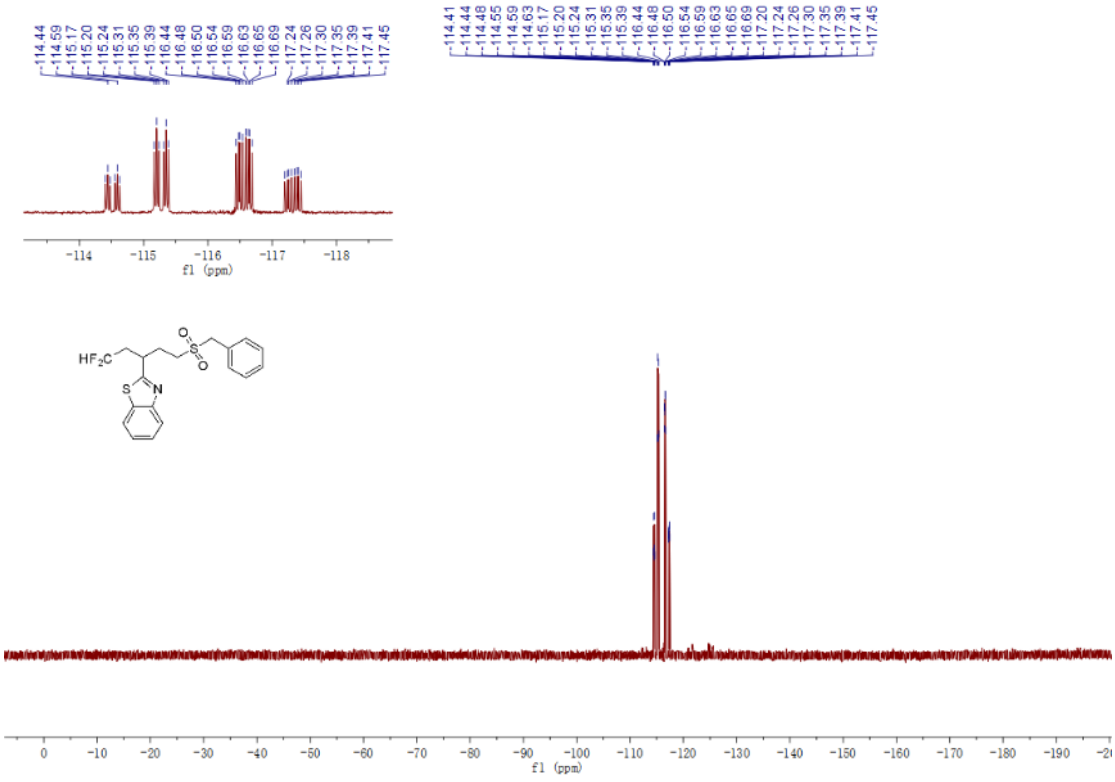
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3m



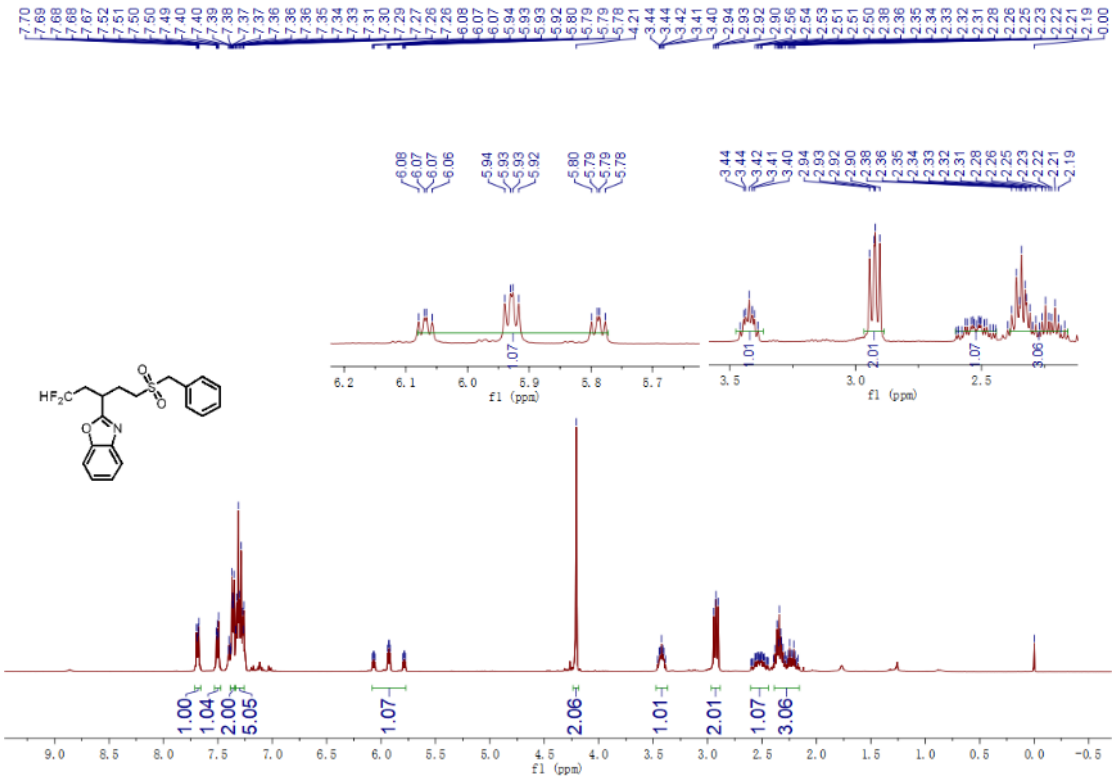
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3m



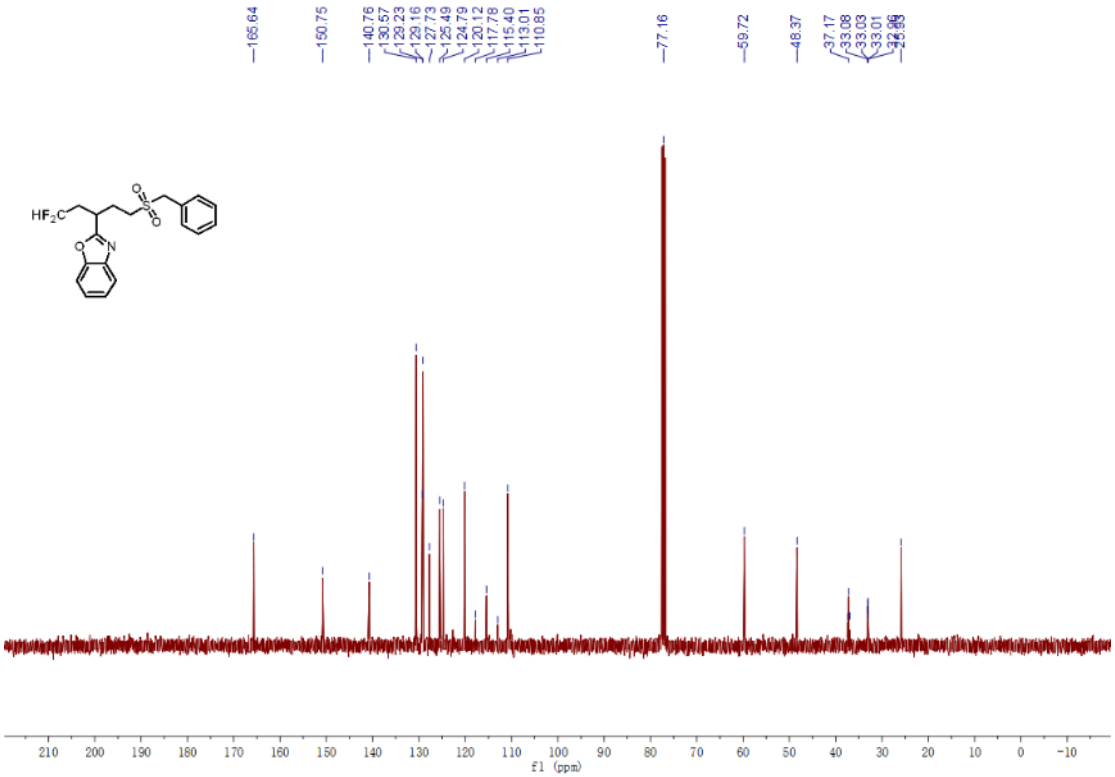
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3m



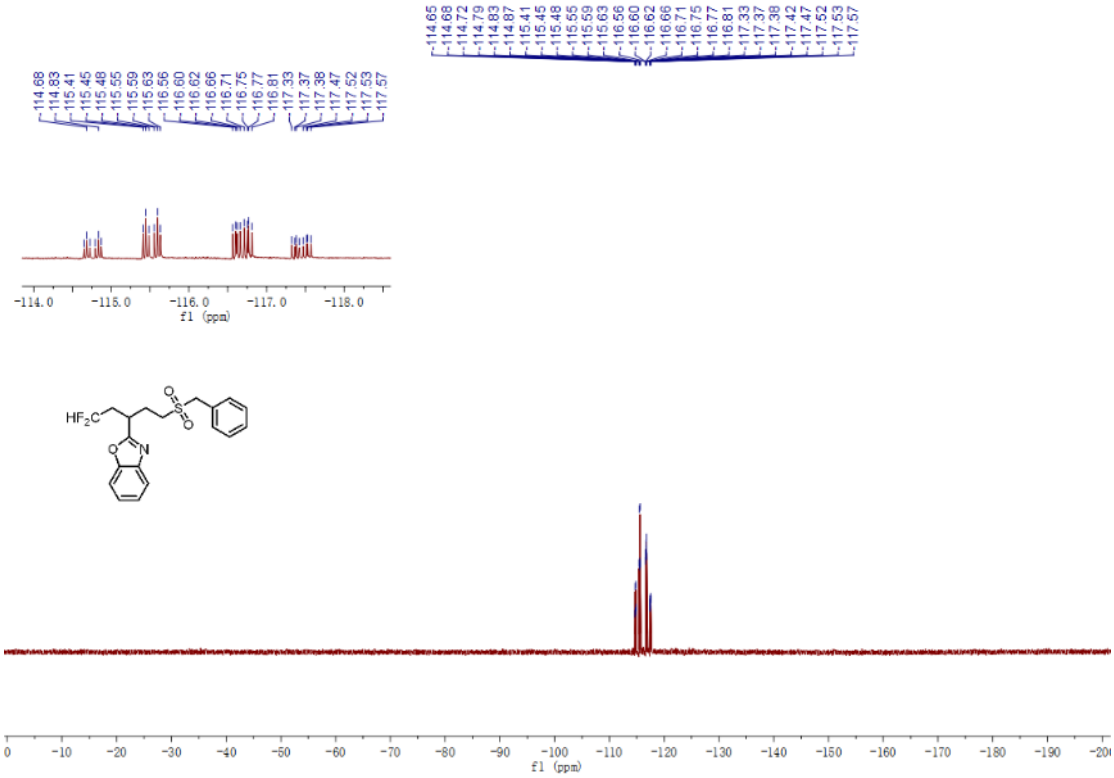
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 3n



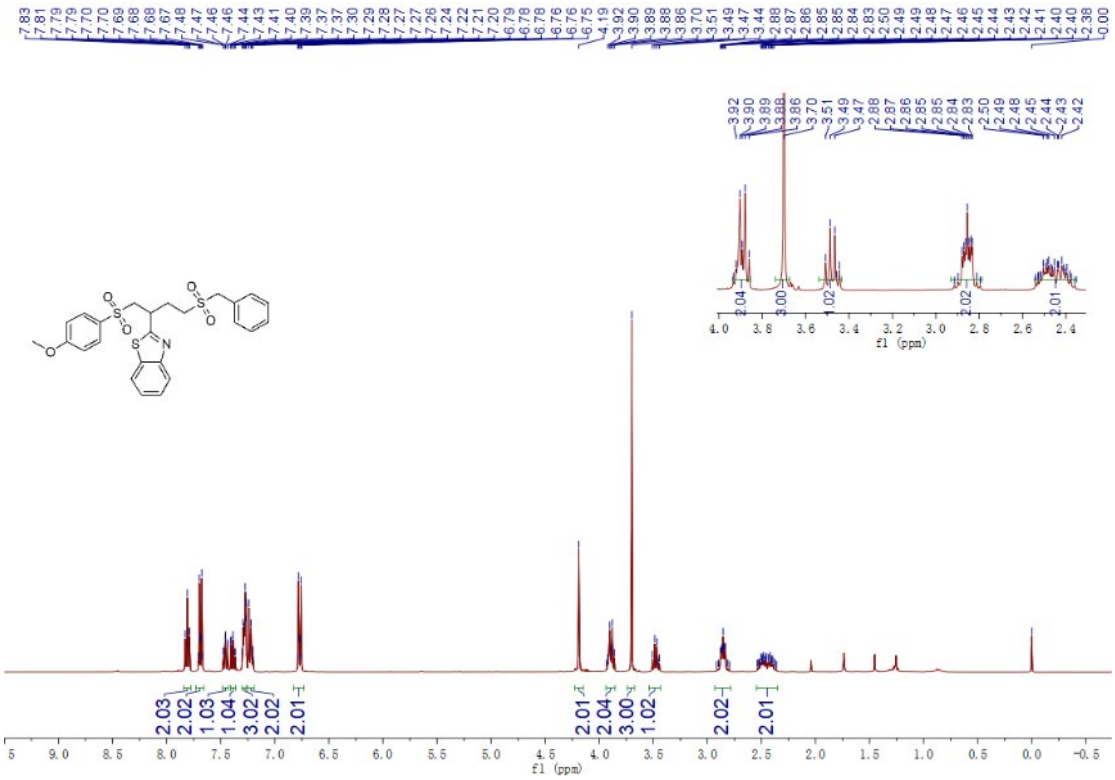
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 3n



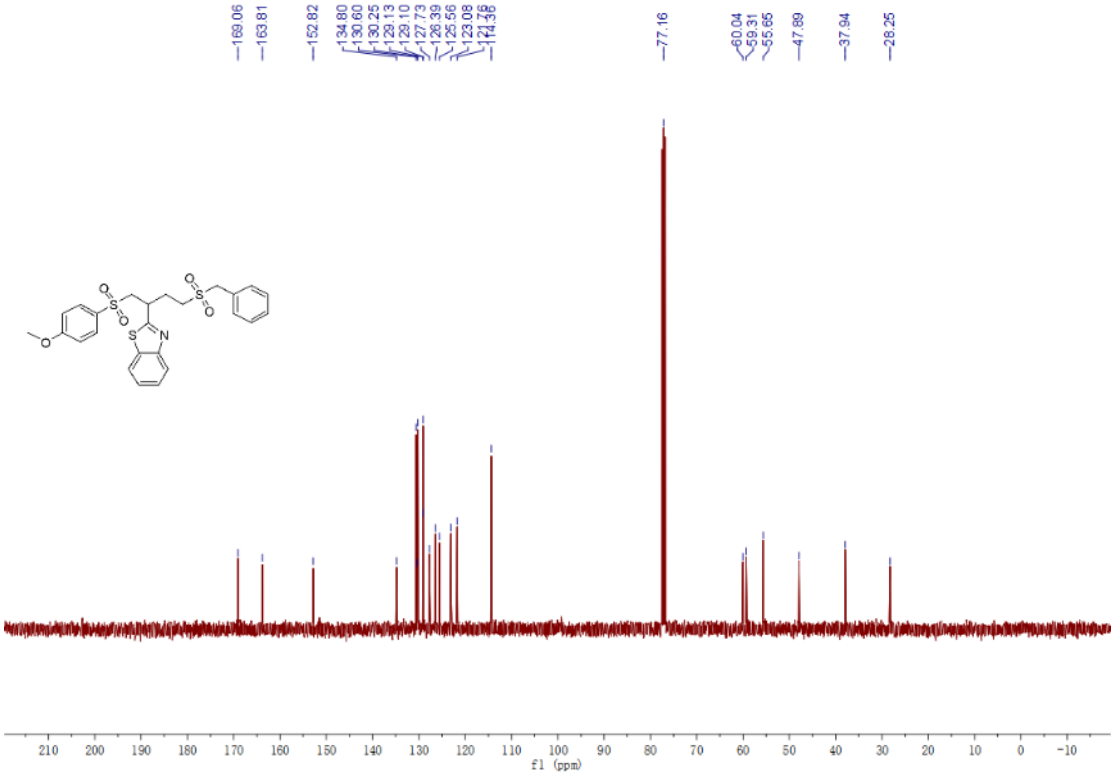
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 3n



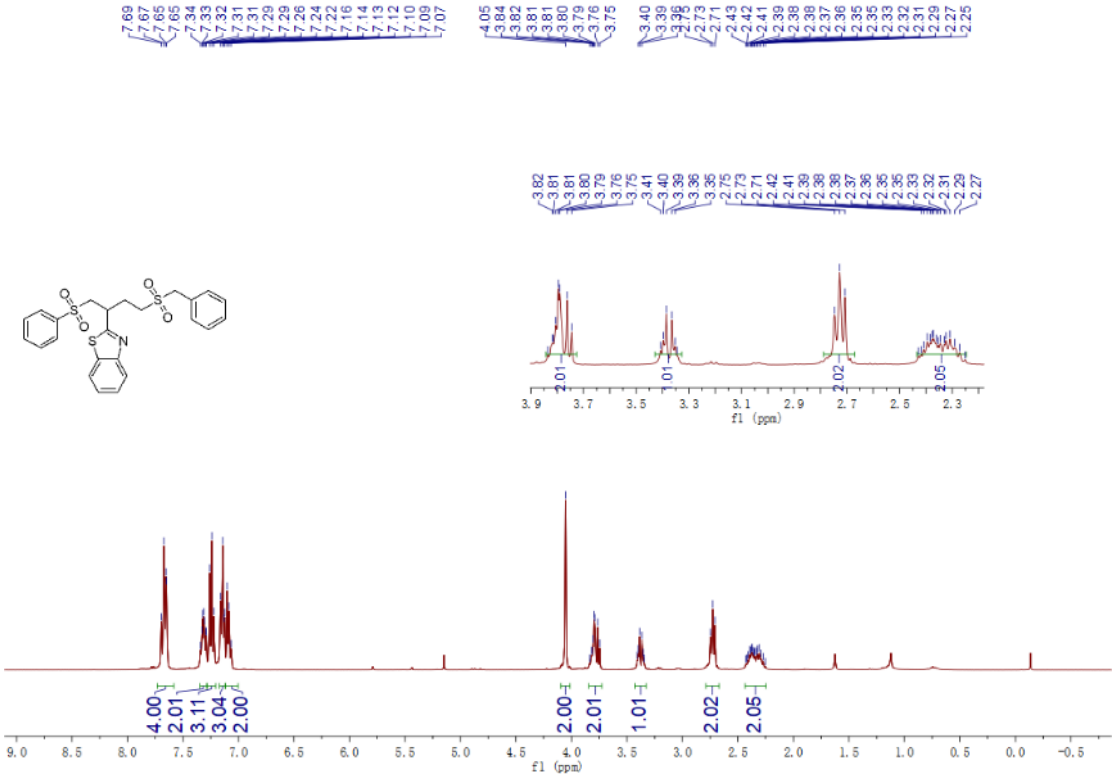
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5a



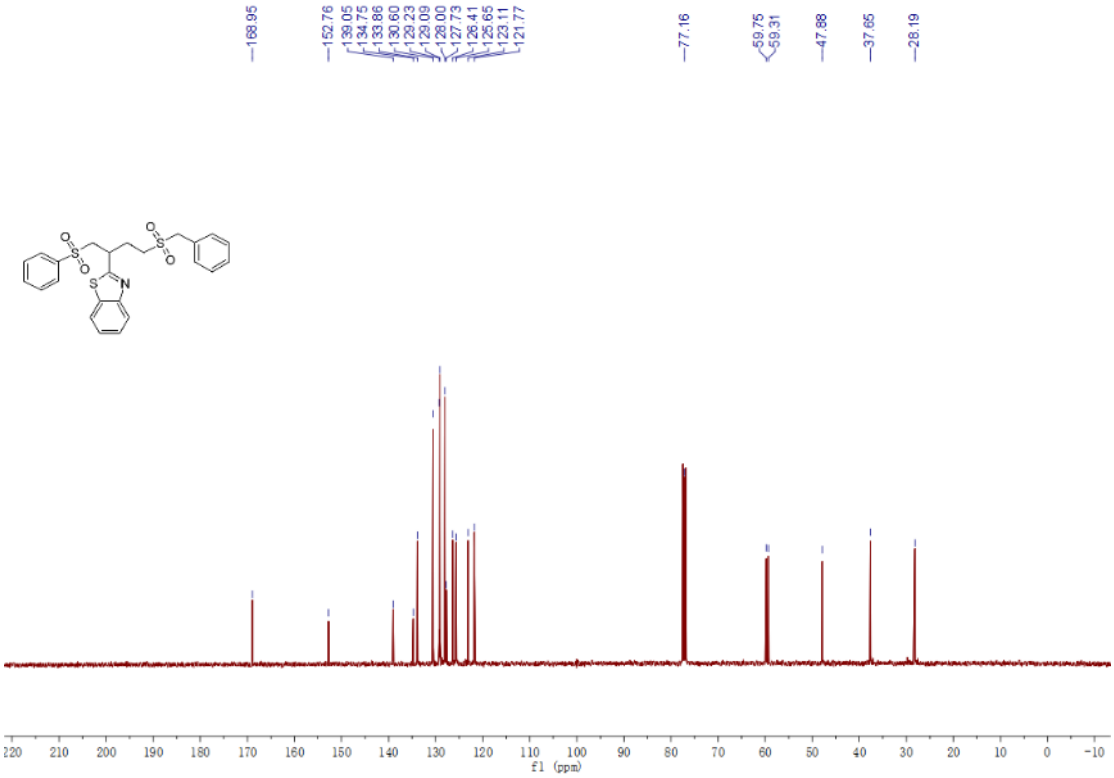
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5a



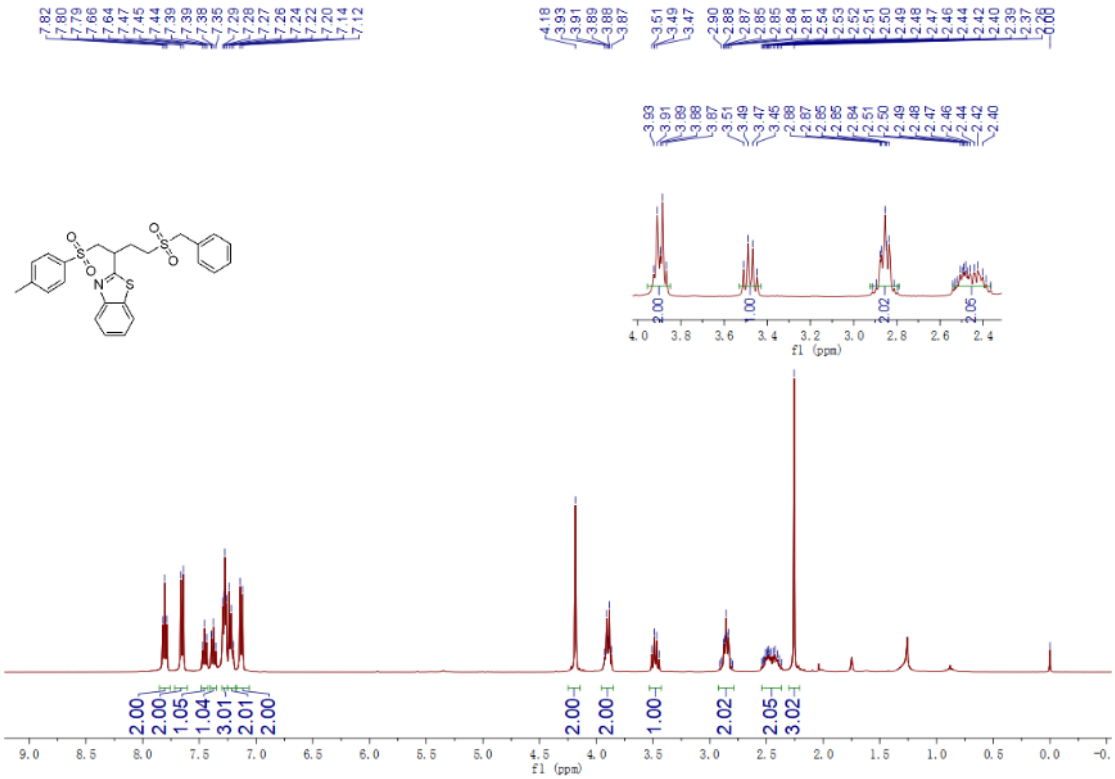
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5b



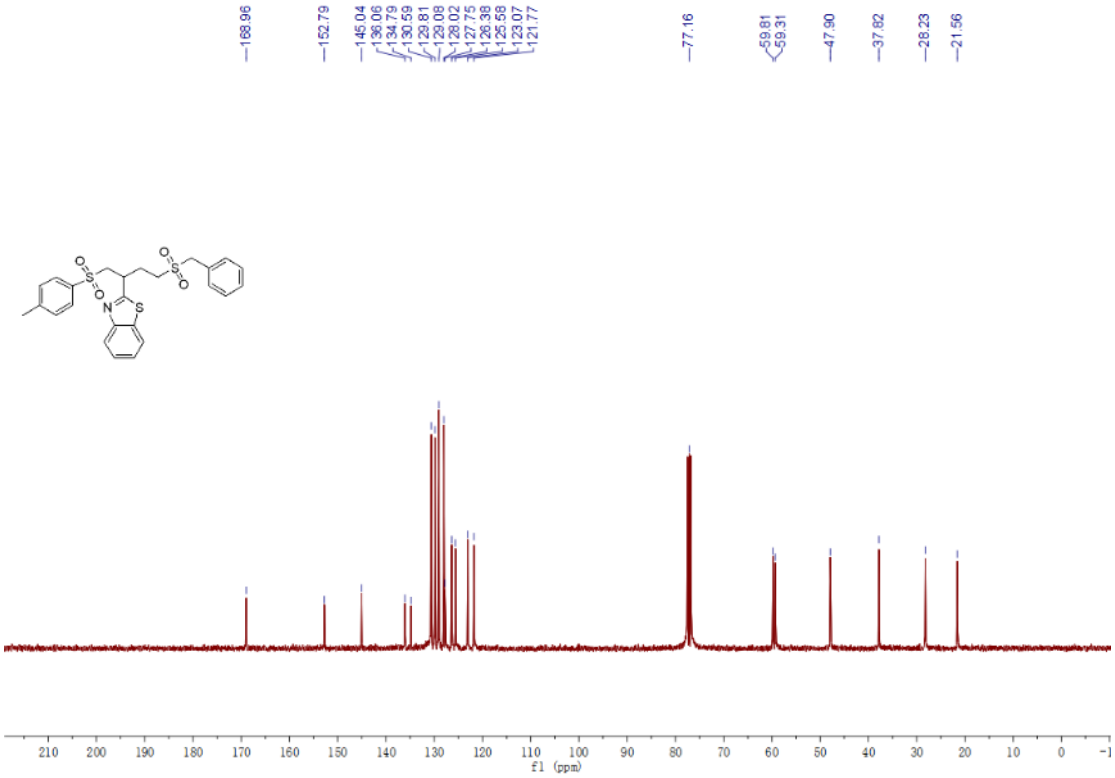
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5b



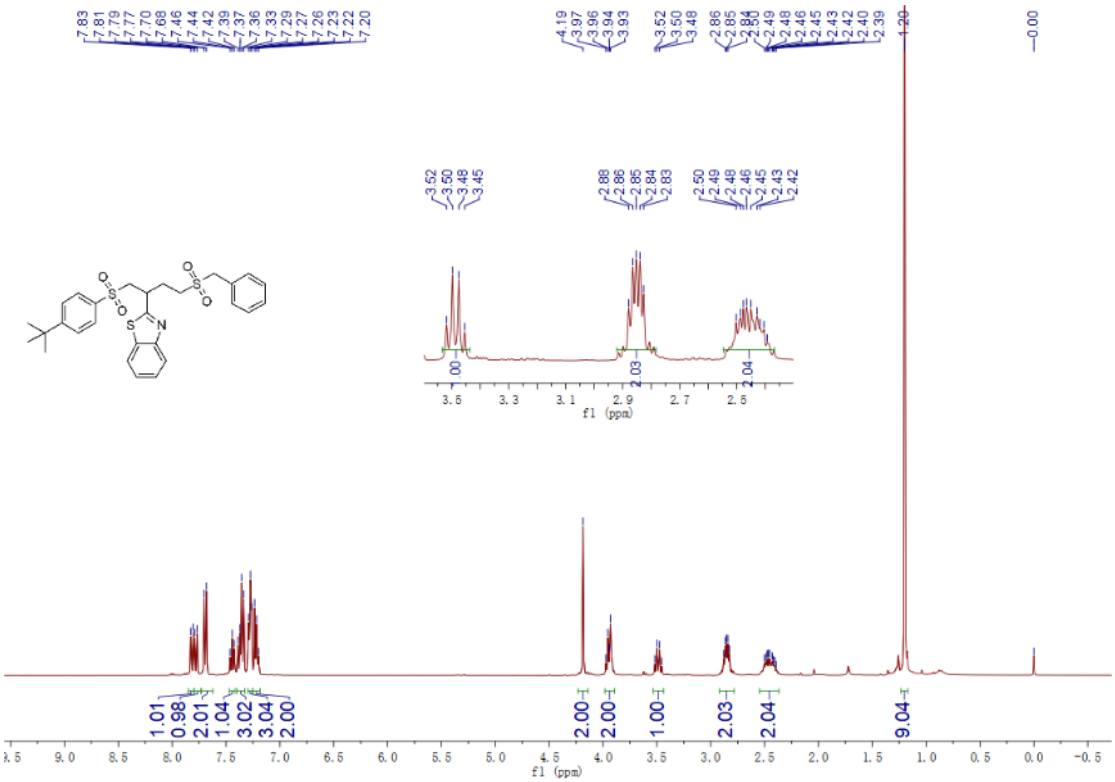
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5c



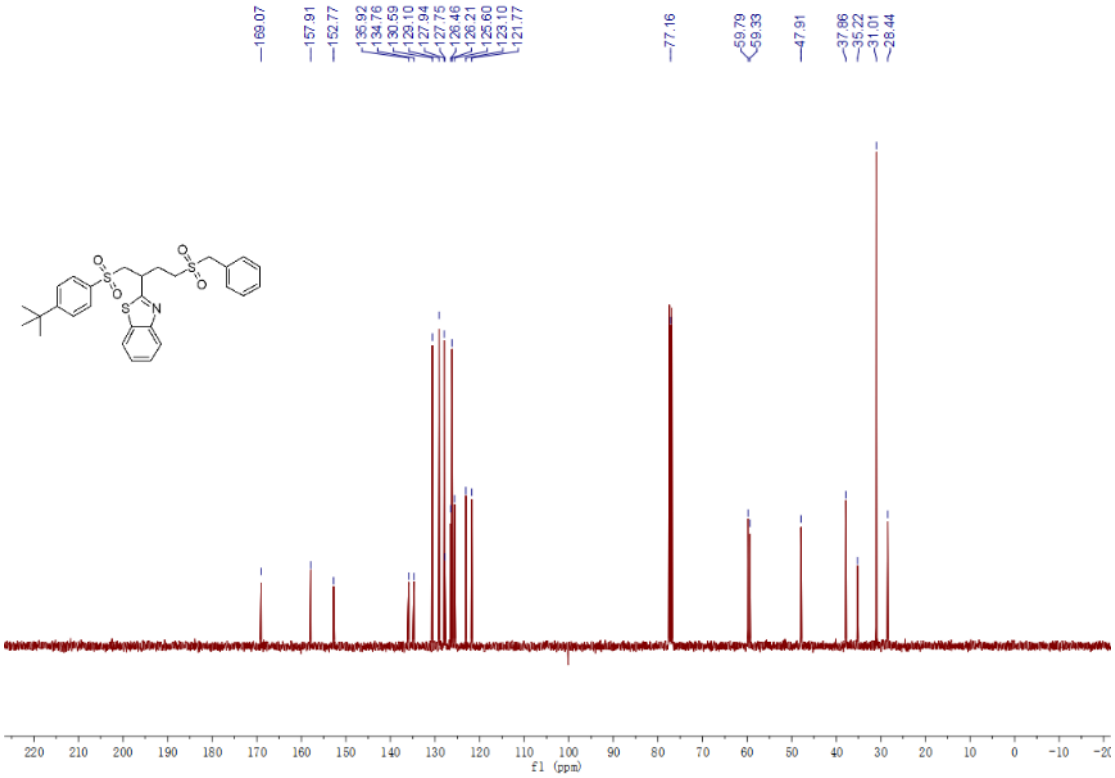
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5c



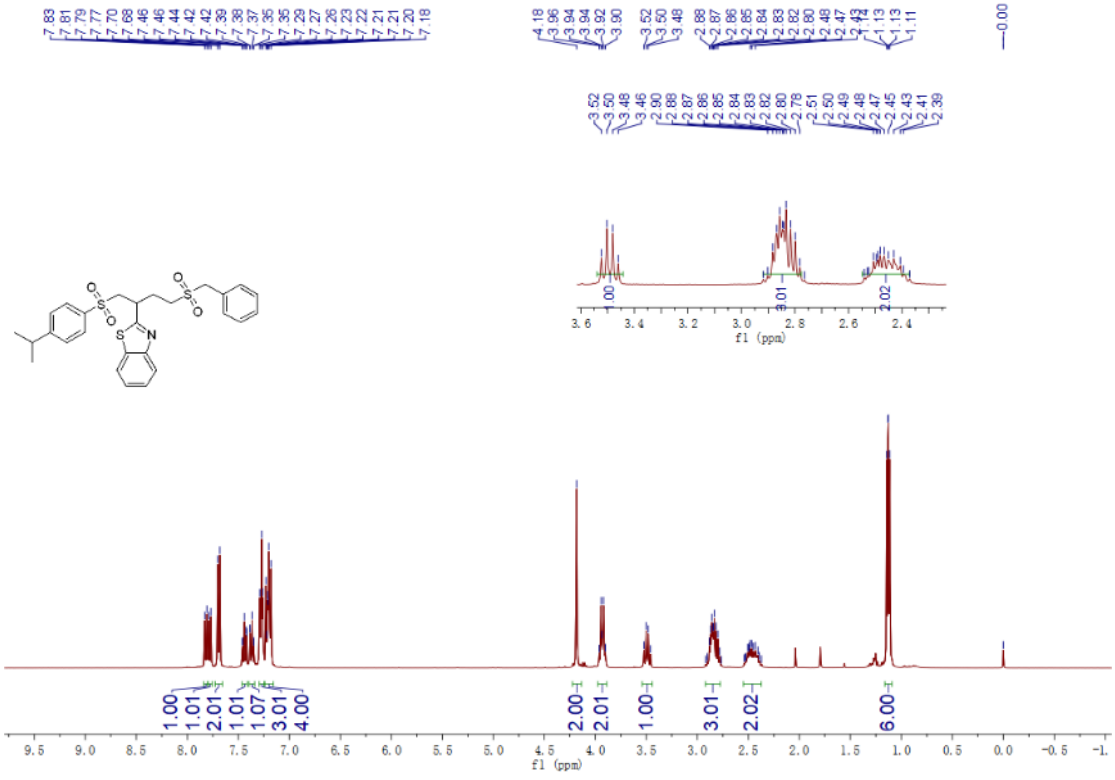
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5d



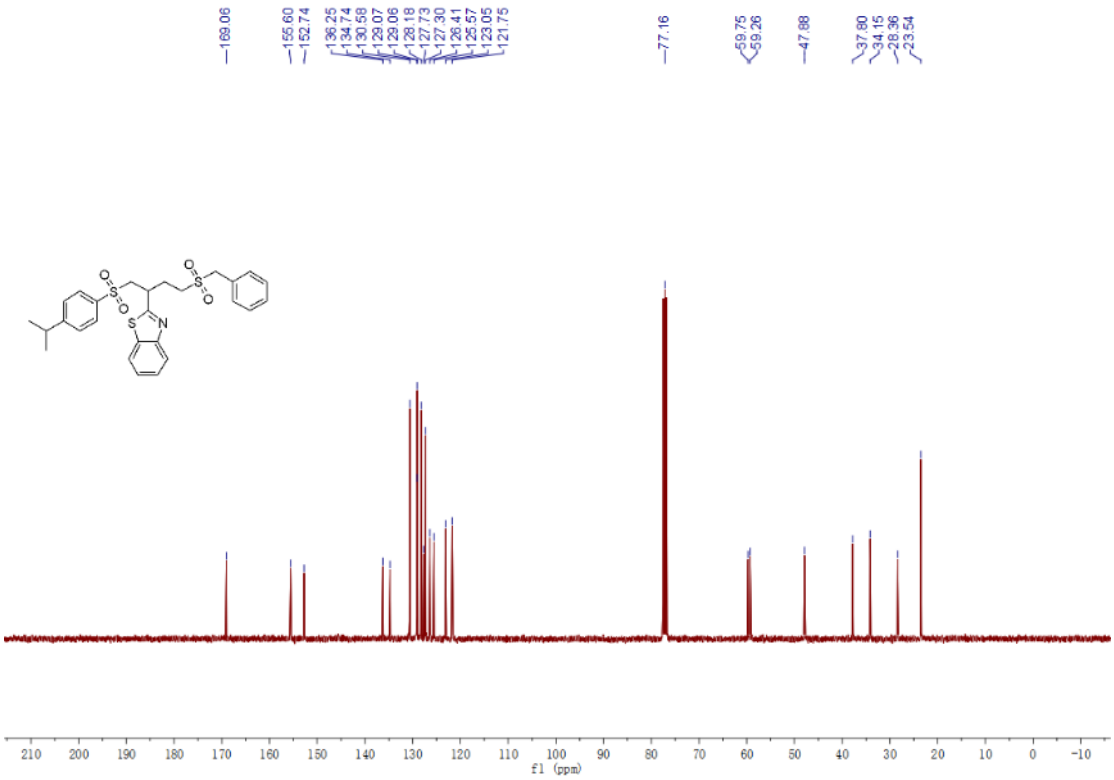
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5d



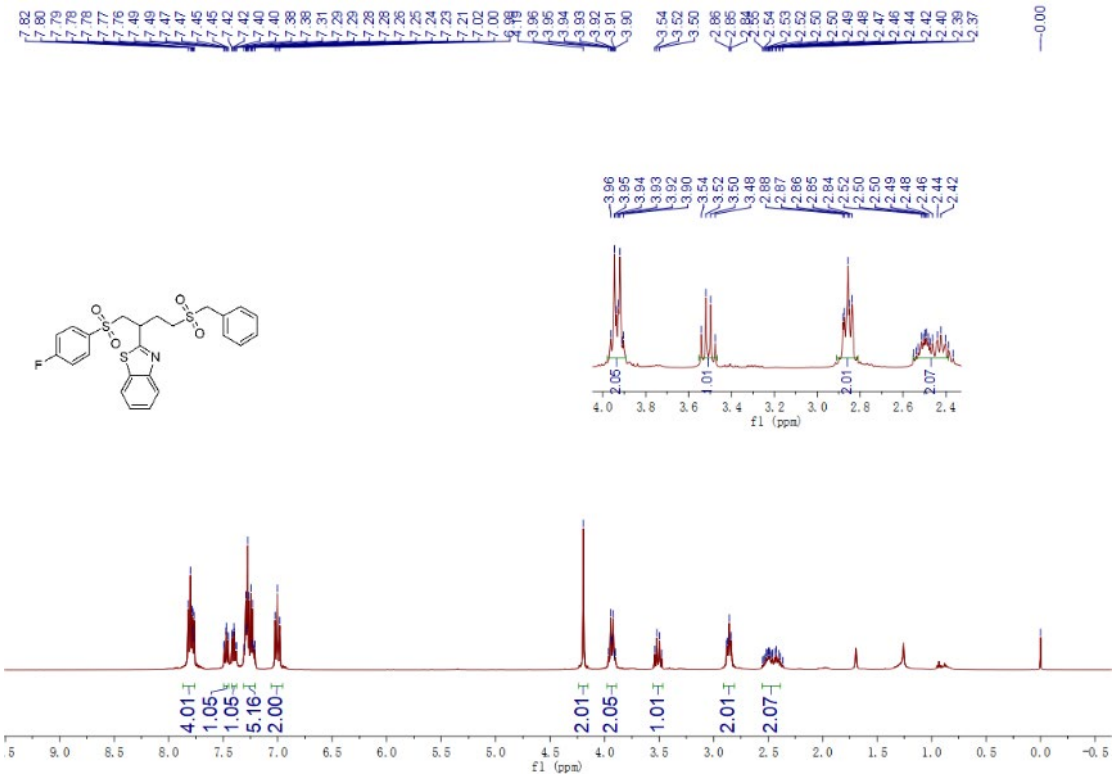
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5e



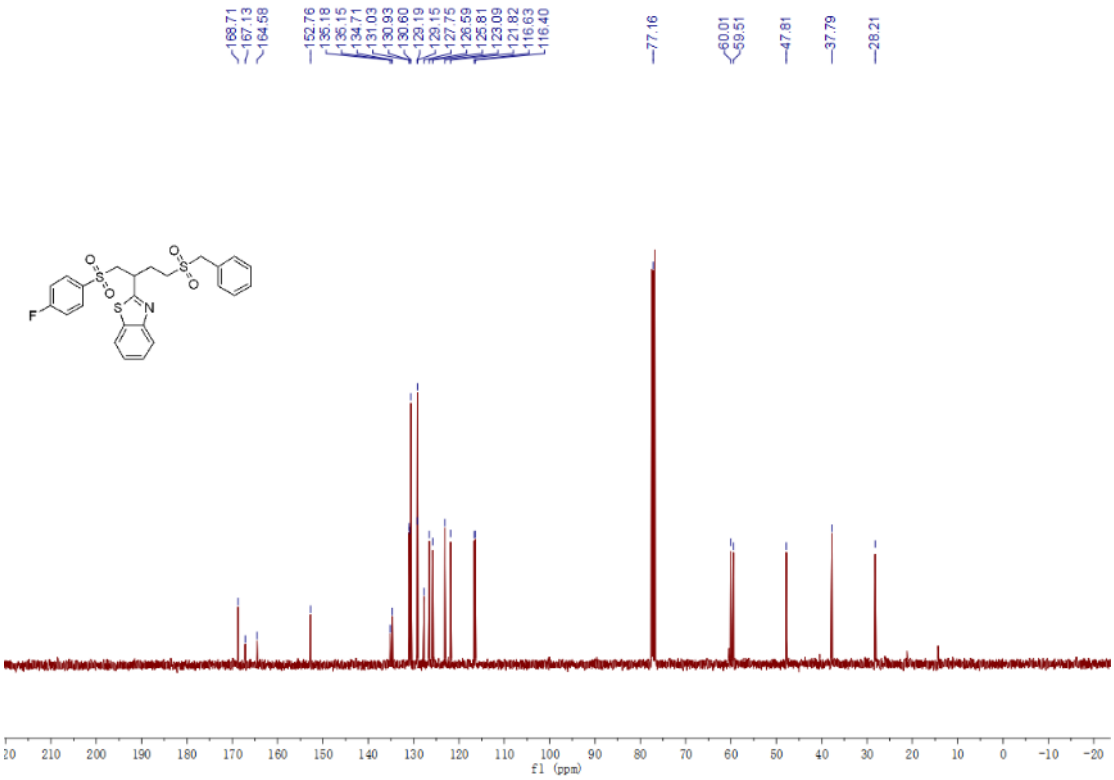
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5e



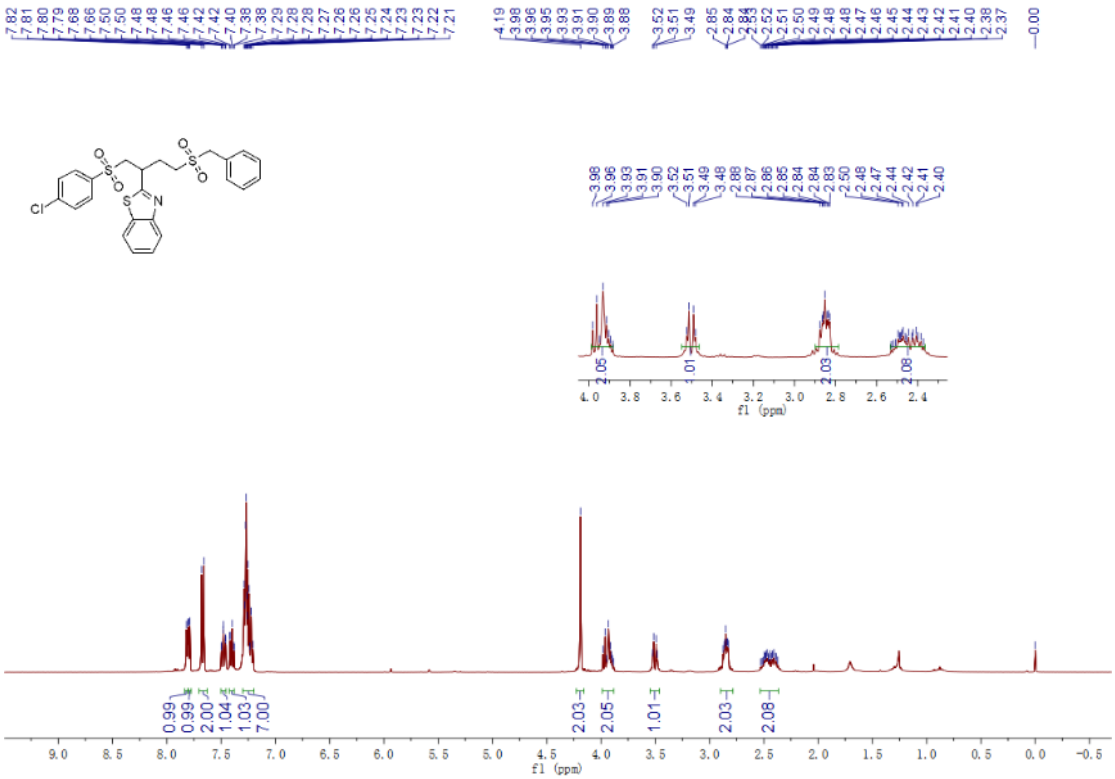
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5f



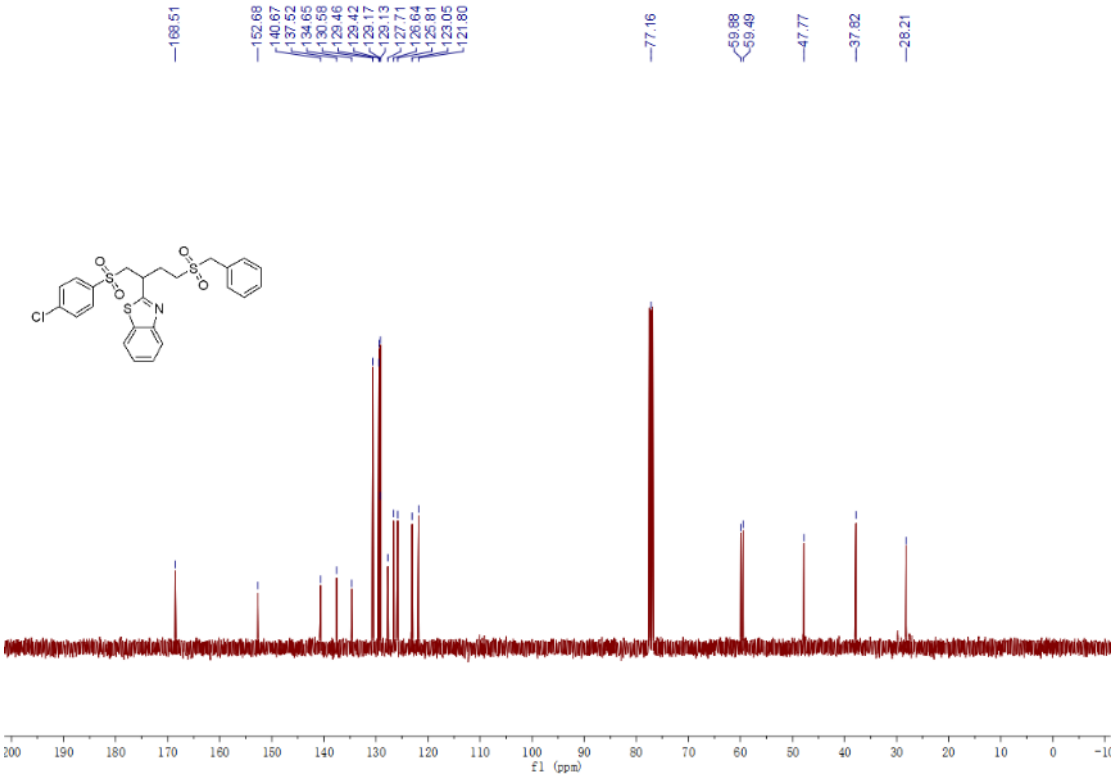
^{13}C NMR spectrum (100MHz, $CDCl_3$) of compound 5f



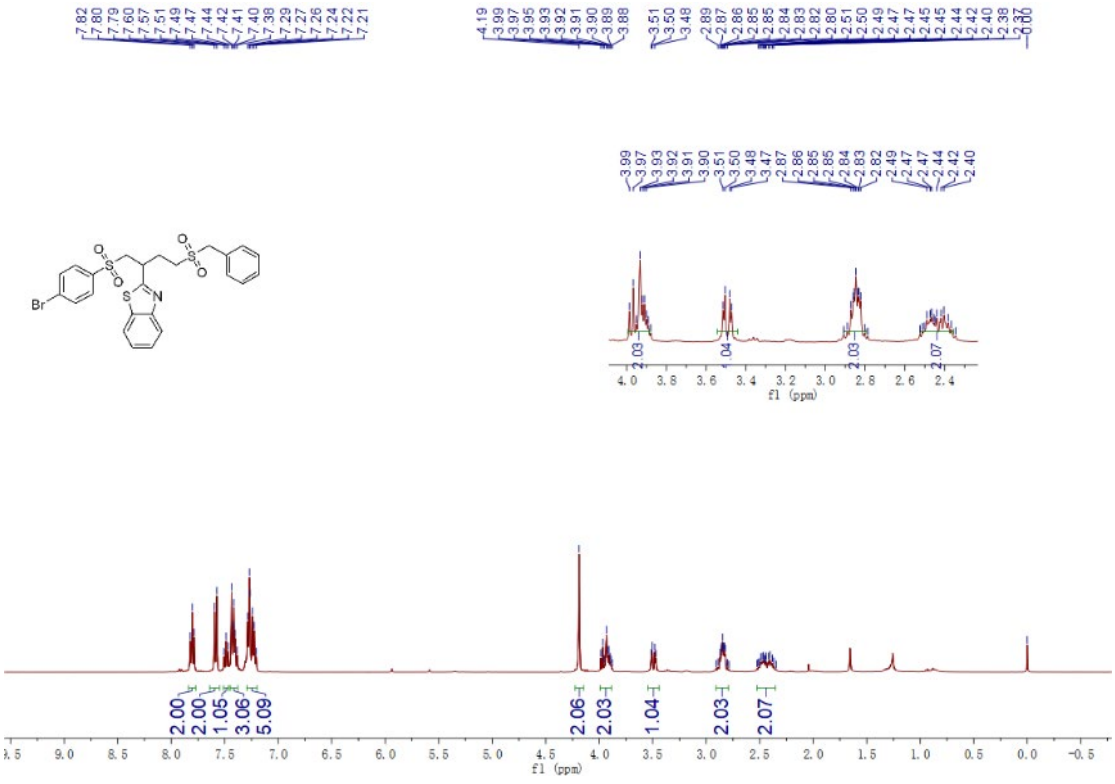
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5g



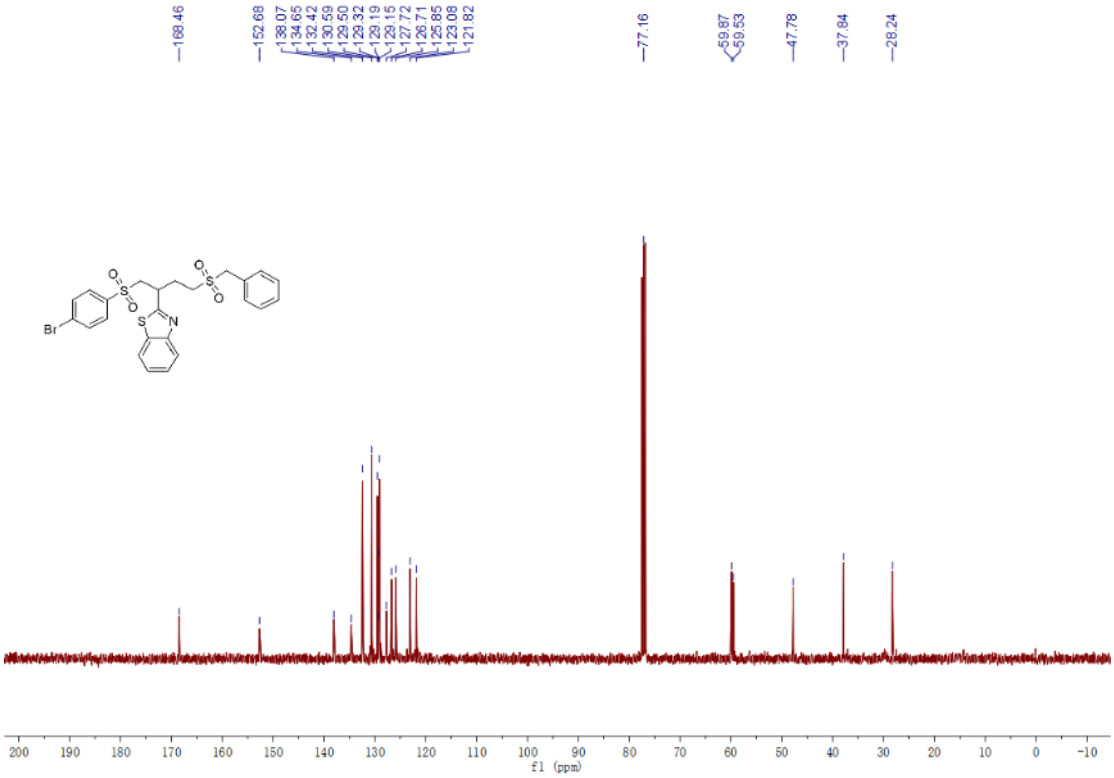
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5g



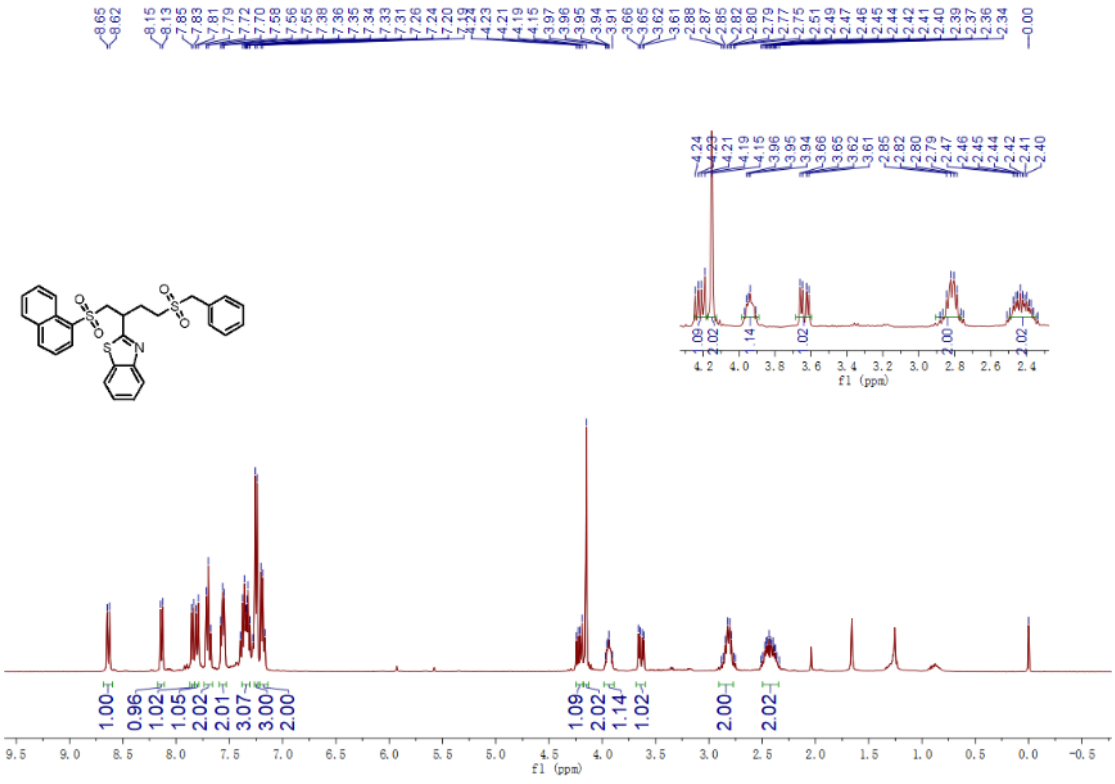
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5h



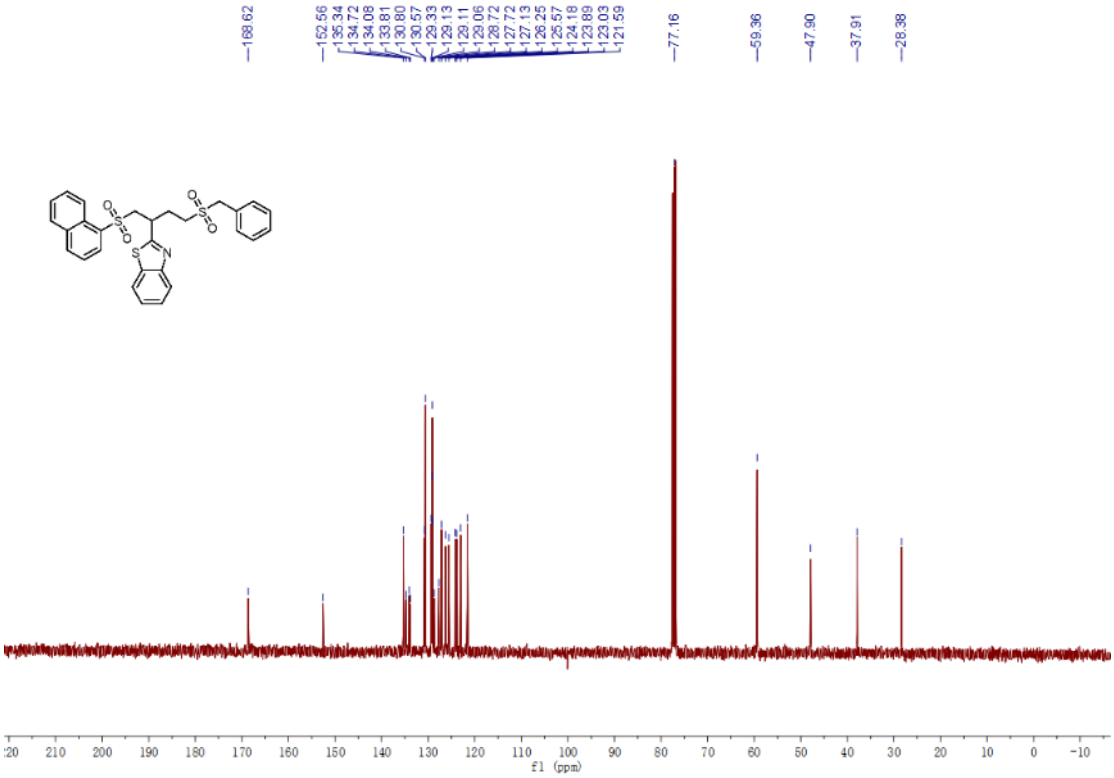
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5h



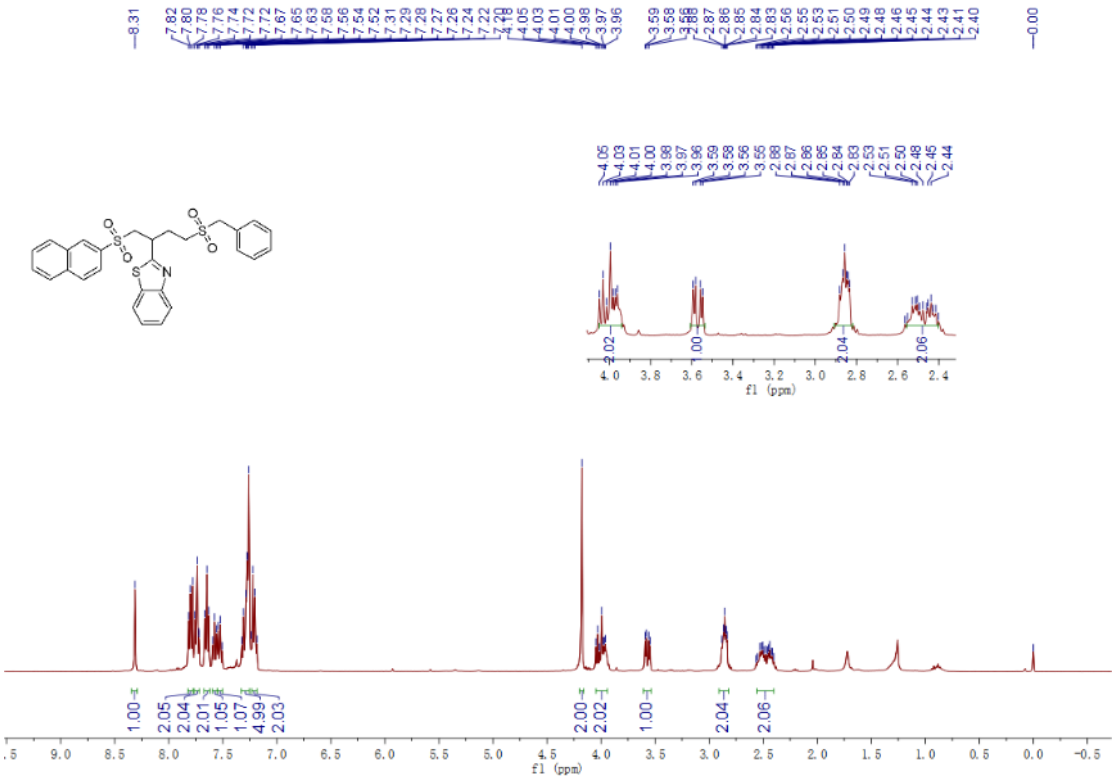
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5i



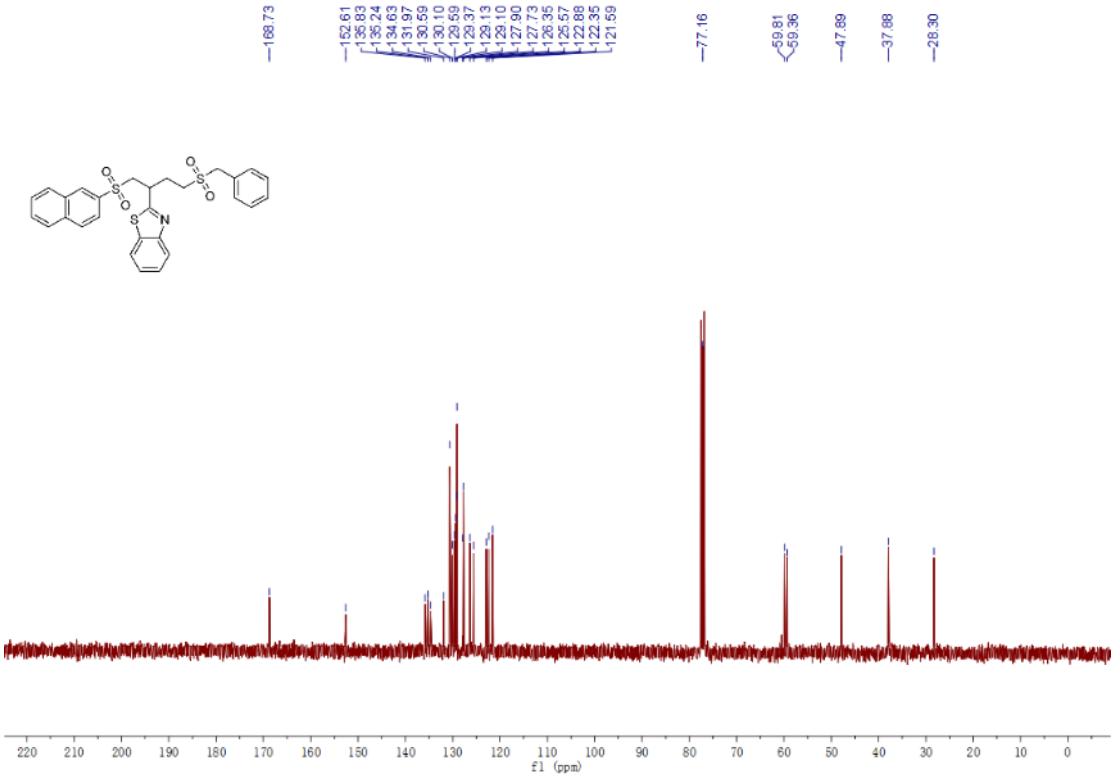
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5i



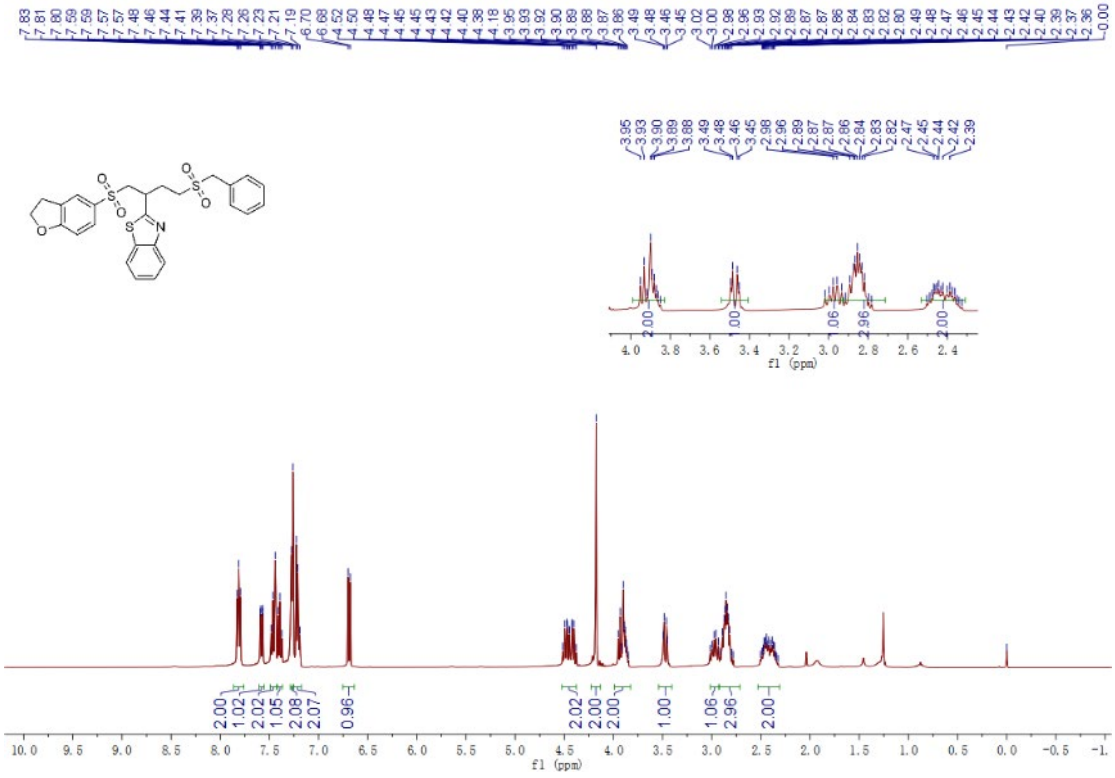
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5j



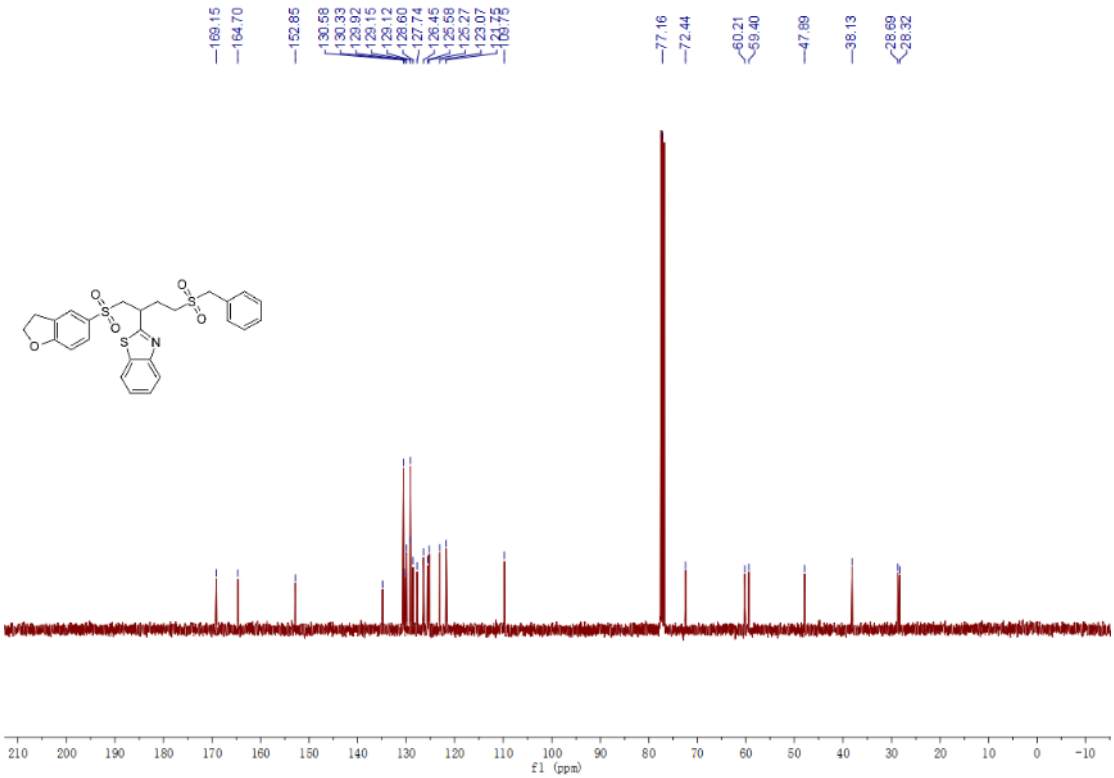
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5j



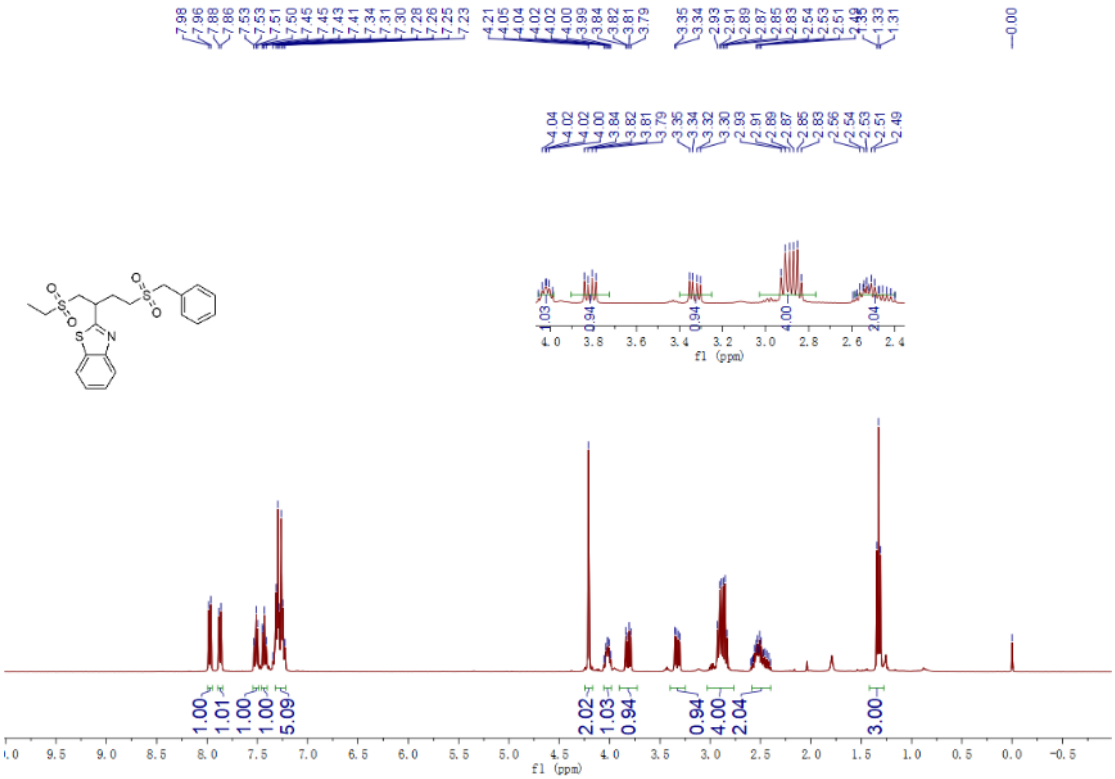
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5k



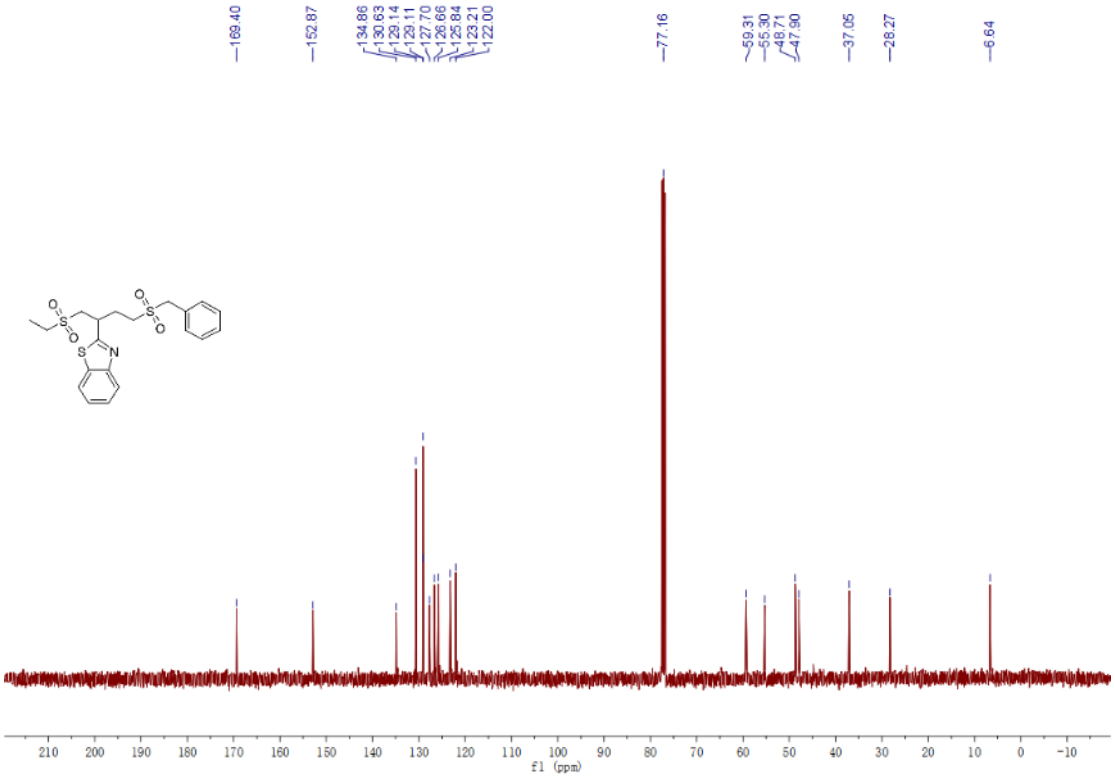
^{13}C NMR spectrum (100MHz, $CDCl_3$) of compound 5k



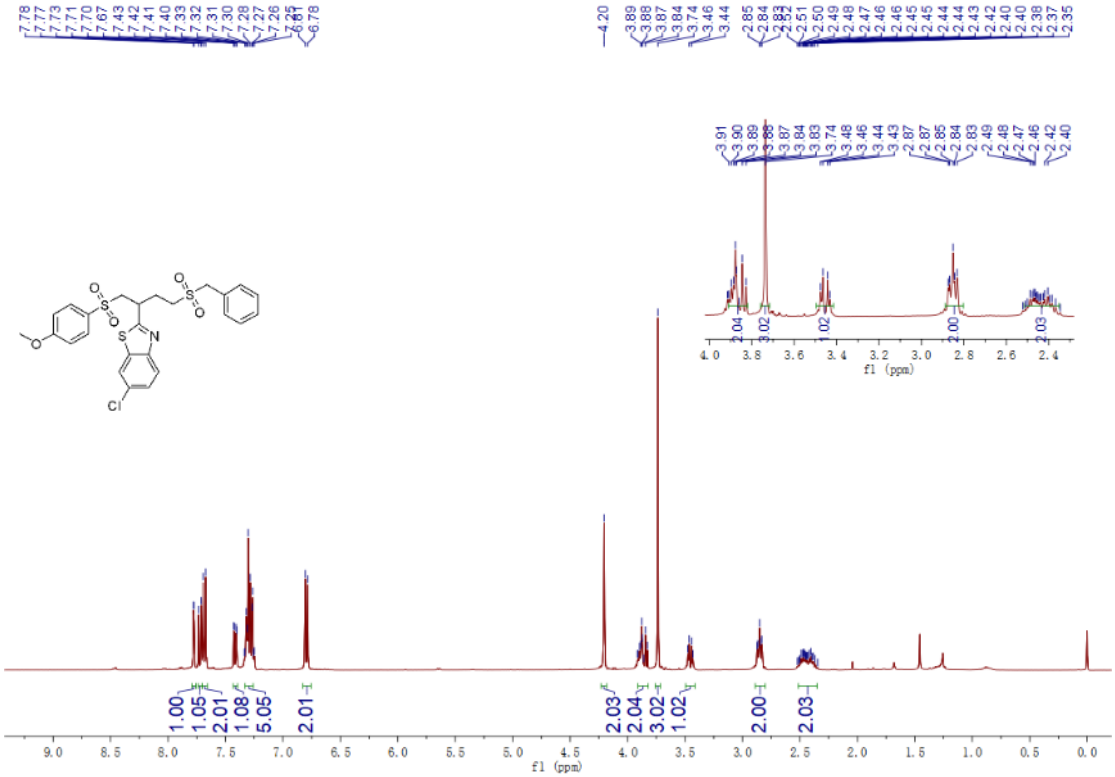
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5l



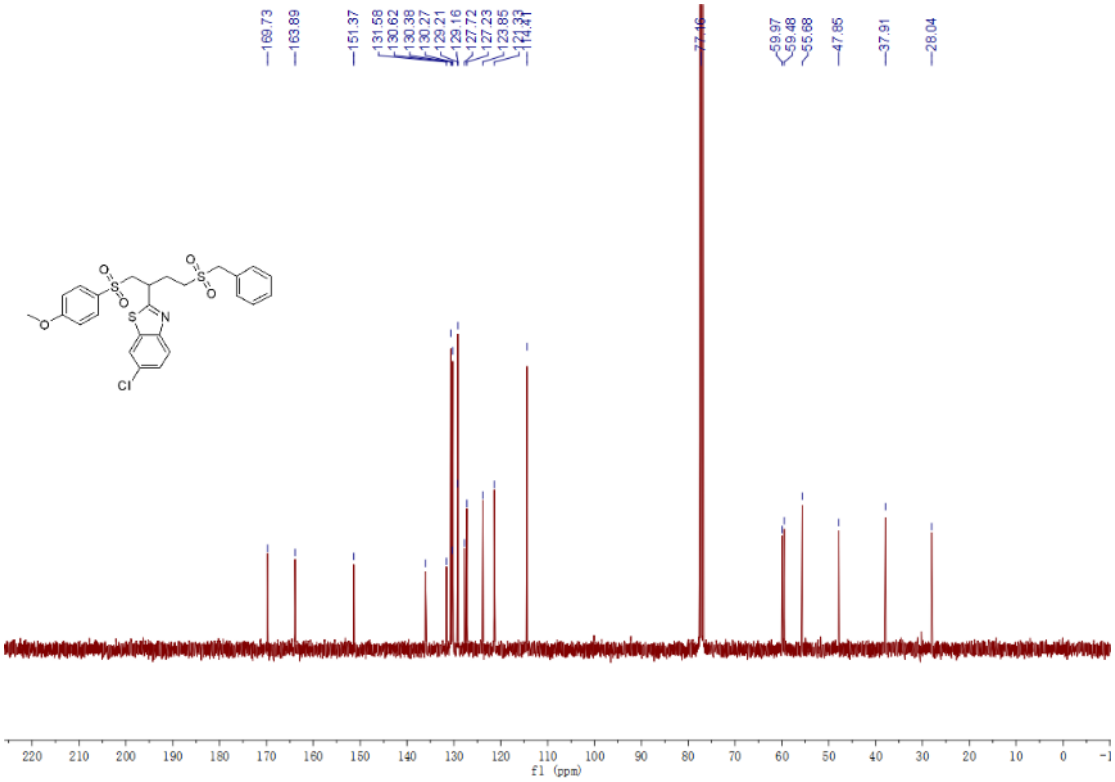
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5l



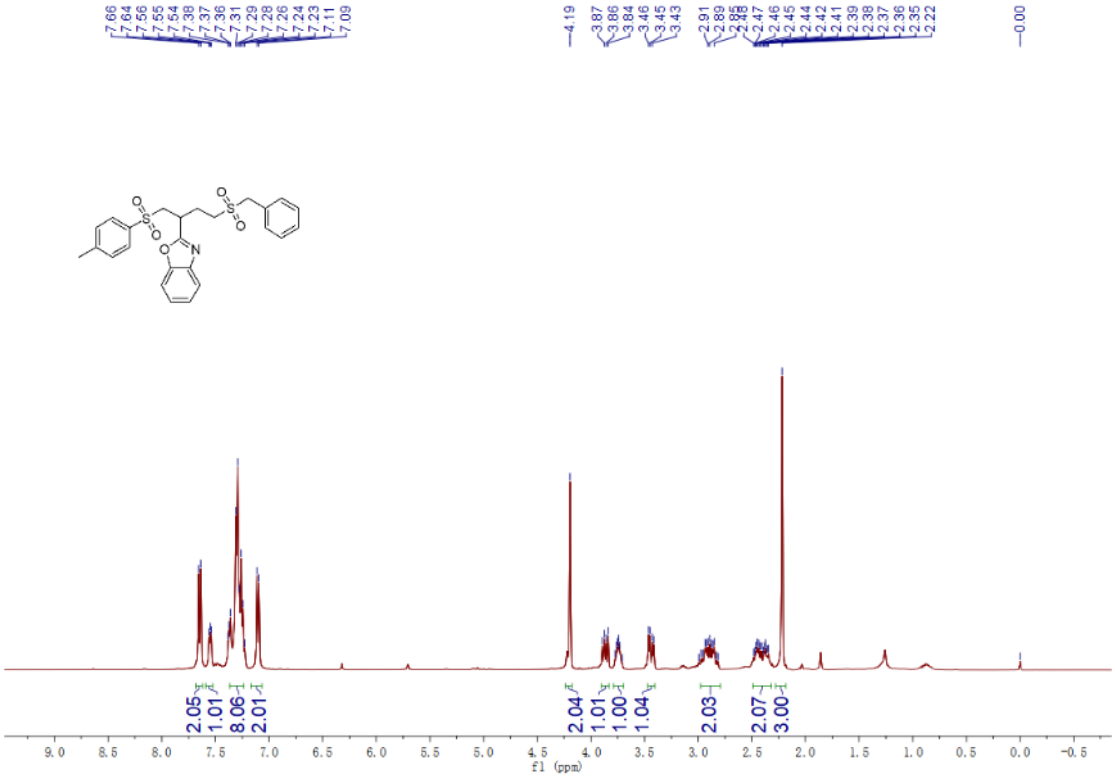
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5m



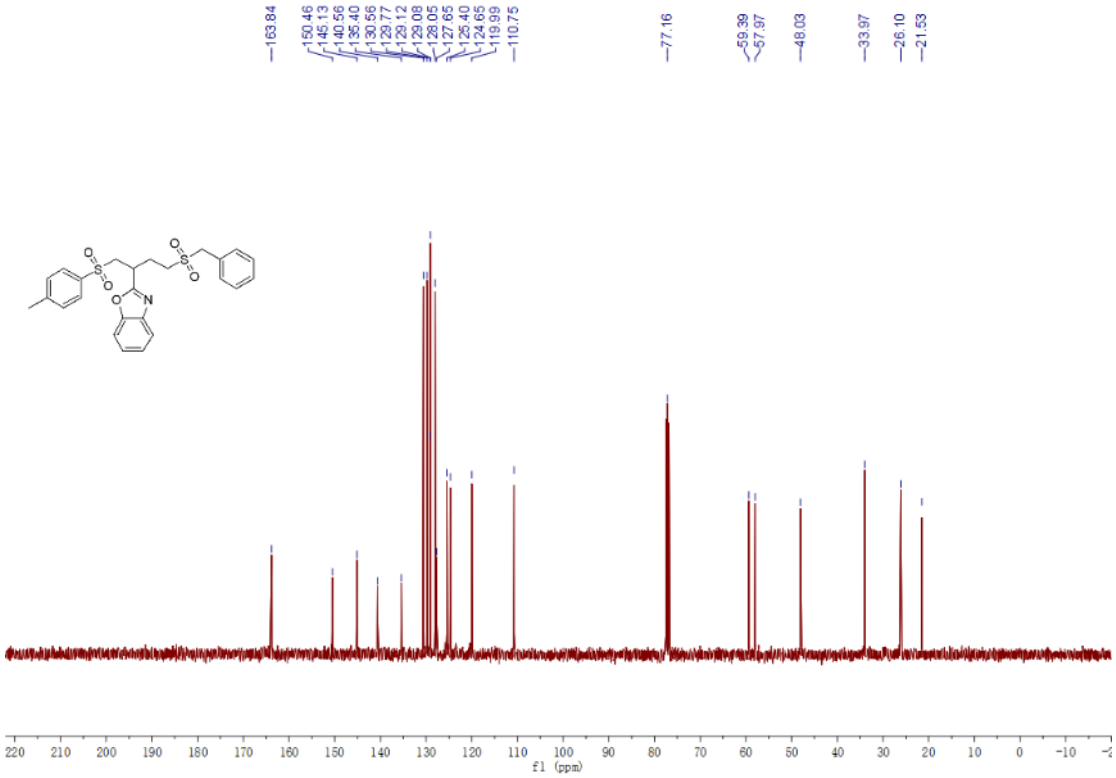
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5m



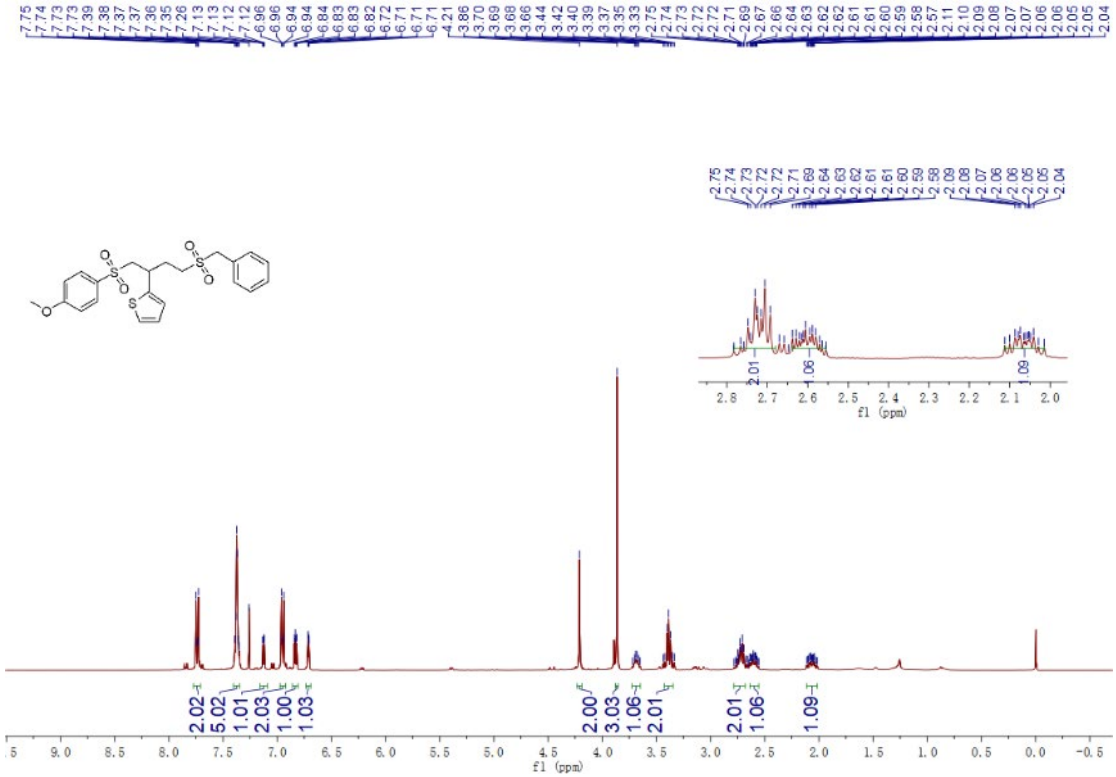
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5n



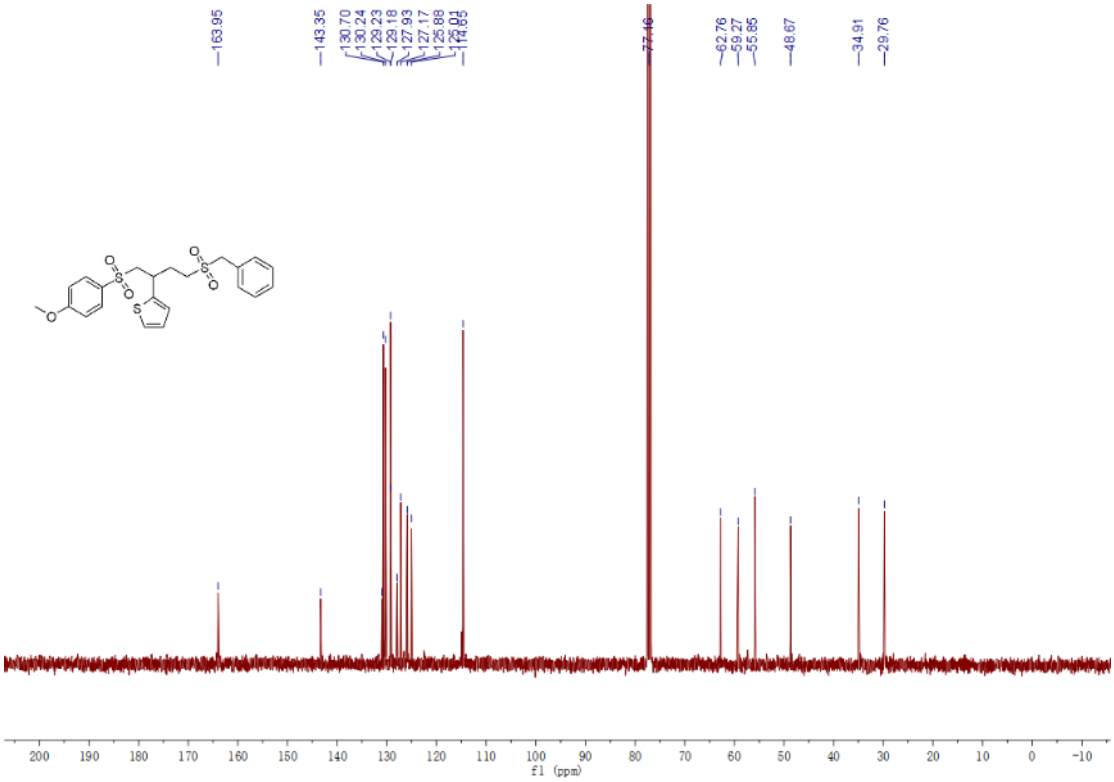
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5n



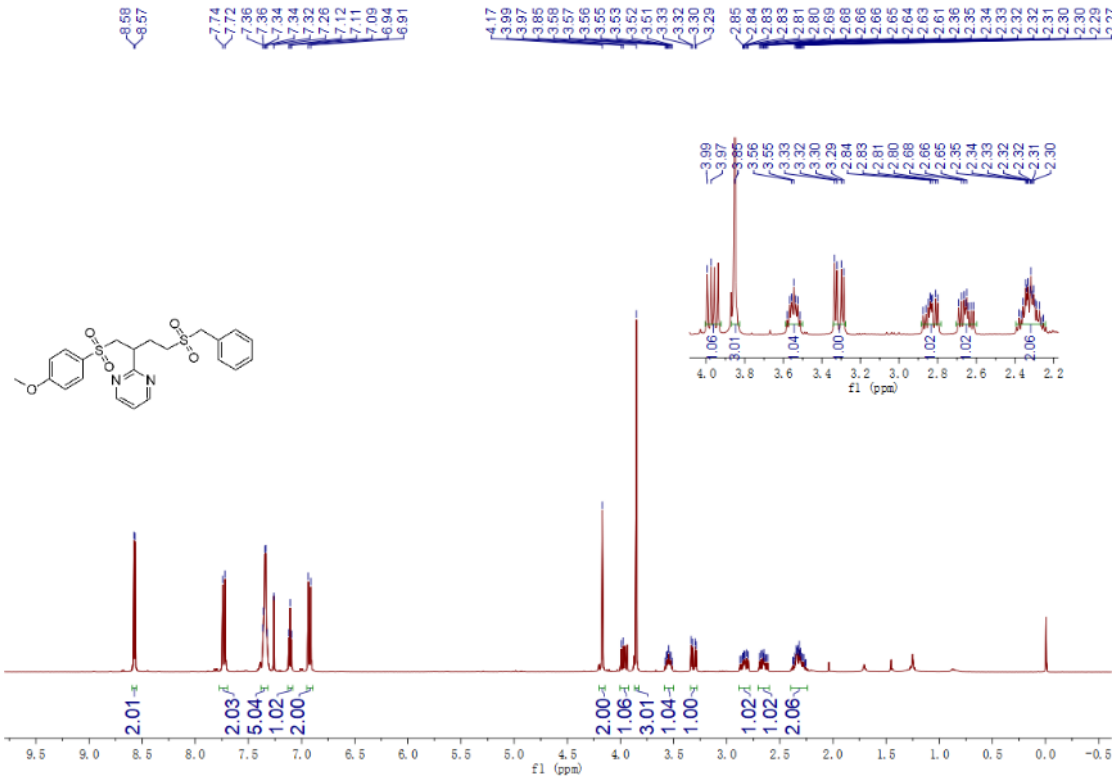
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5o



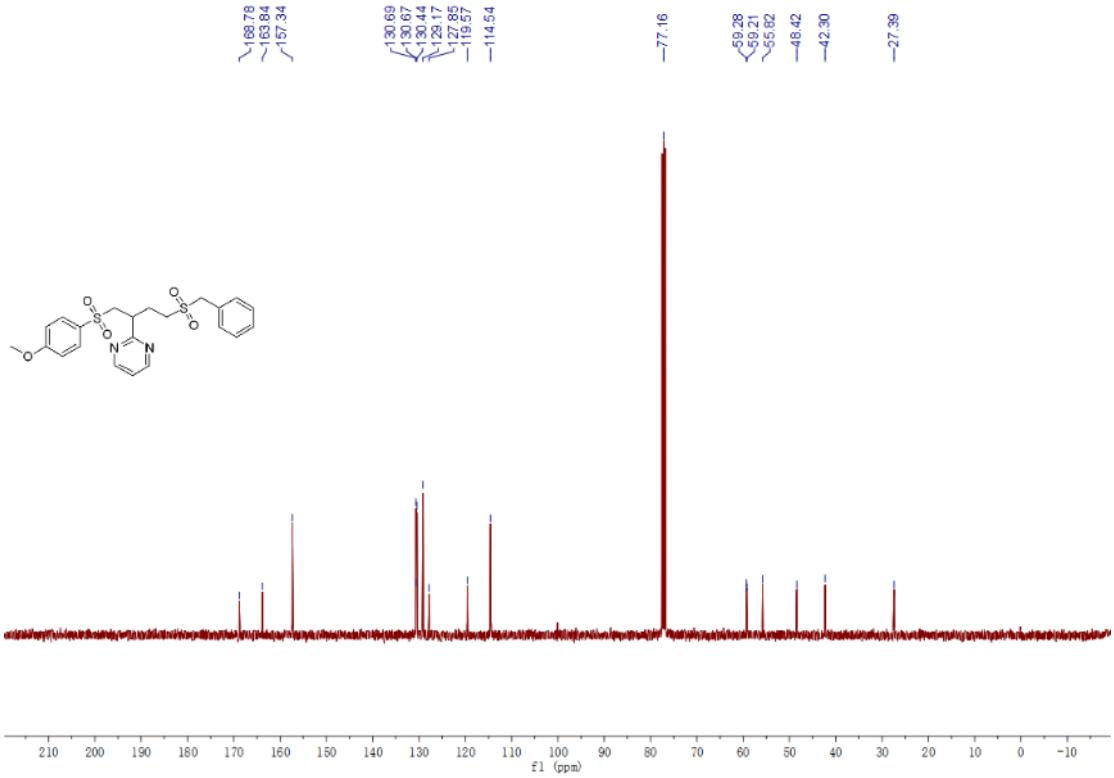
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5o



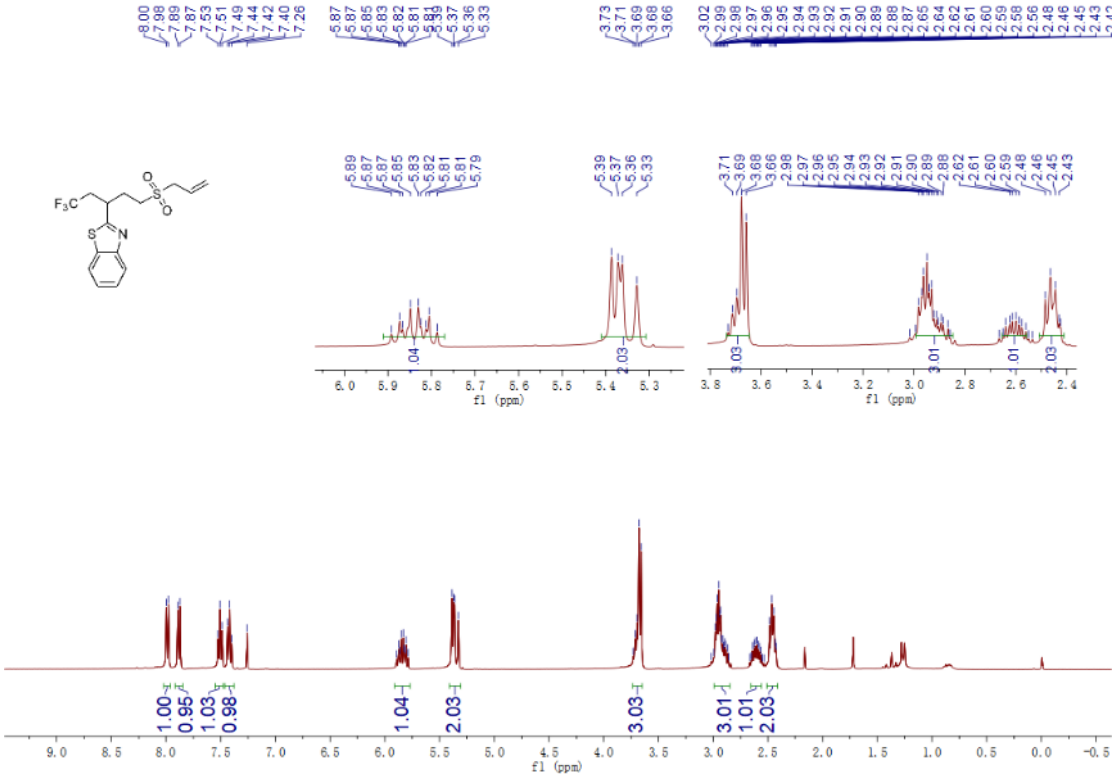
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 5p



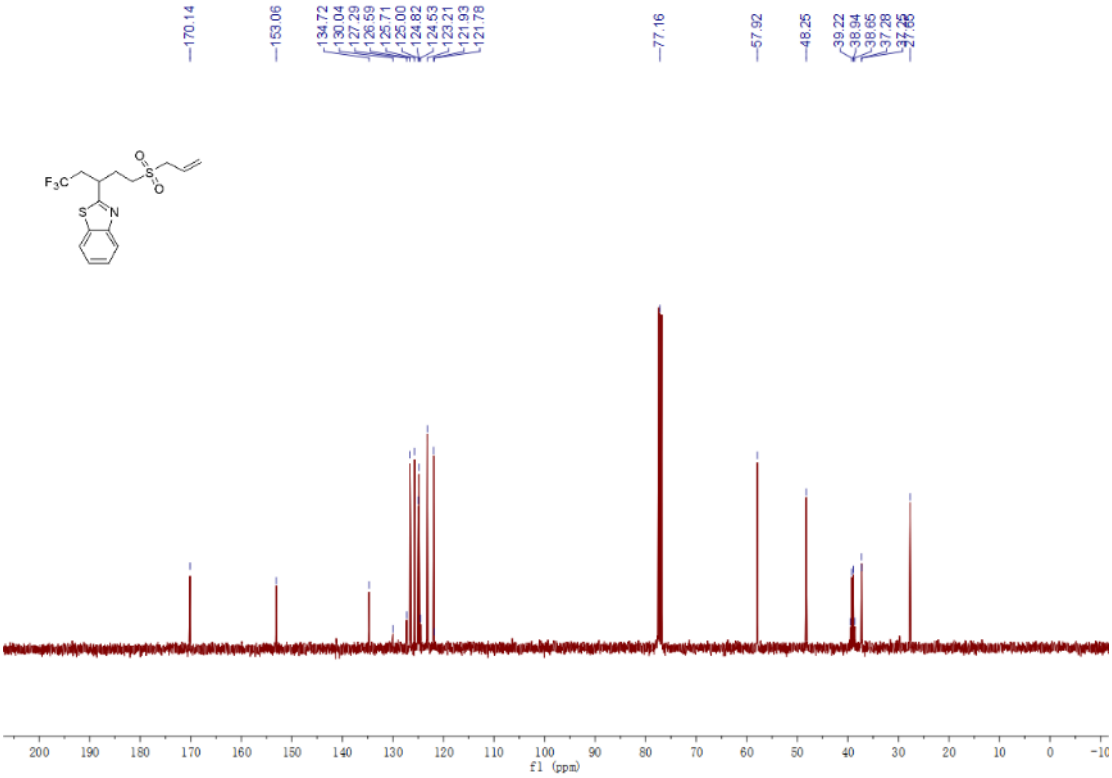
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 5p



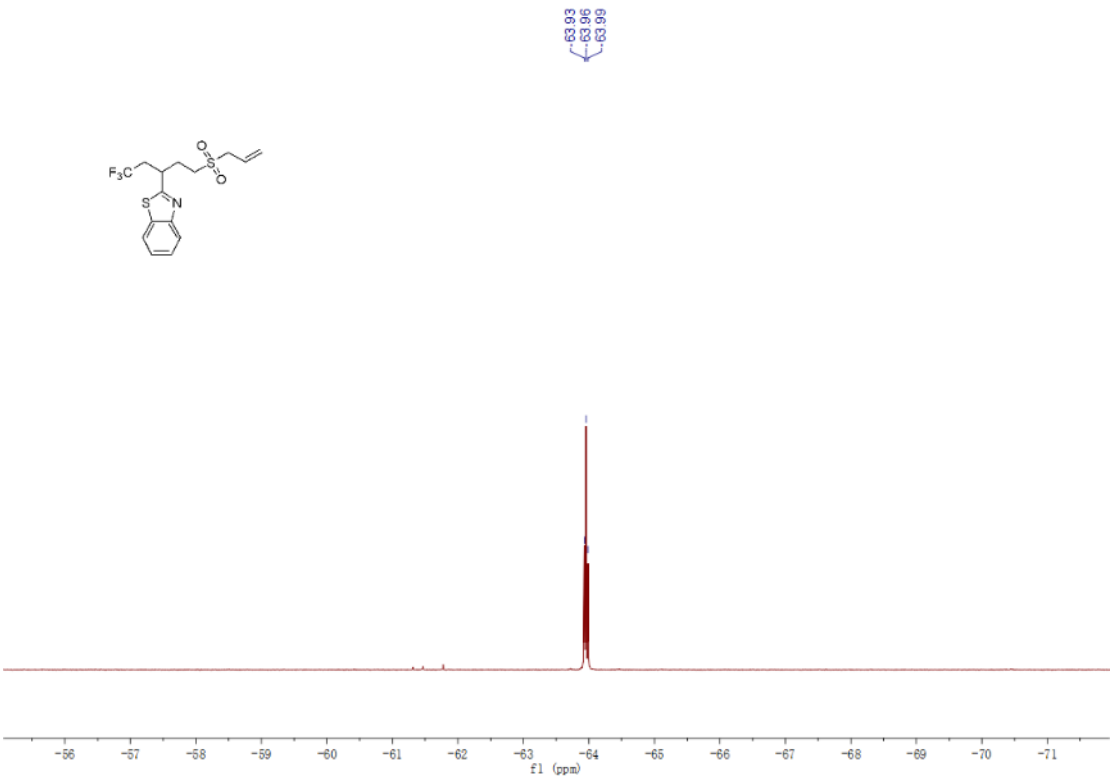
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6a



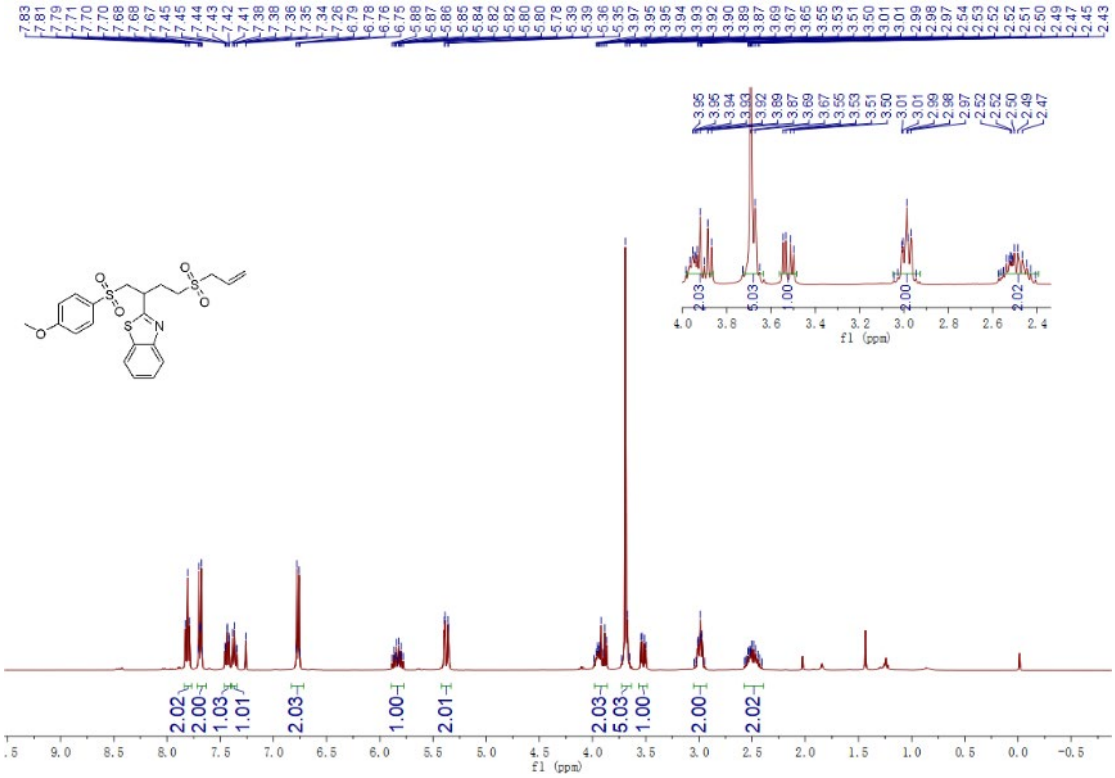
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6a



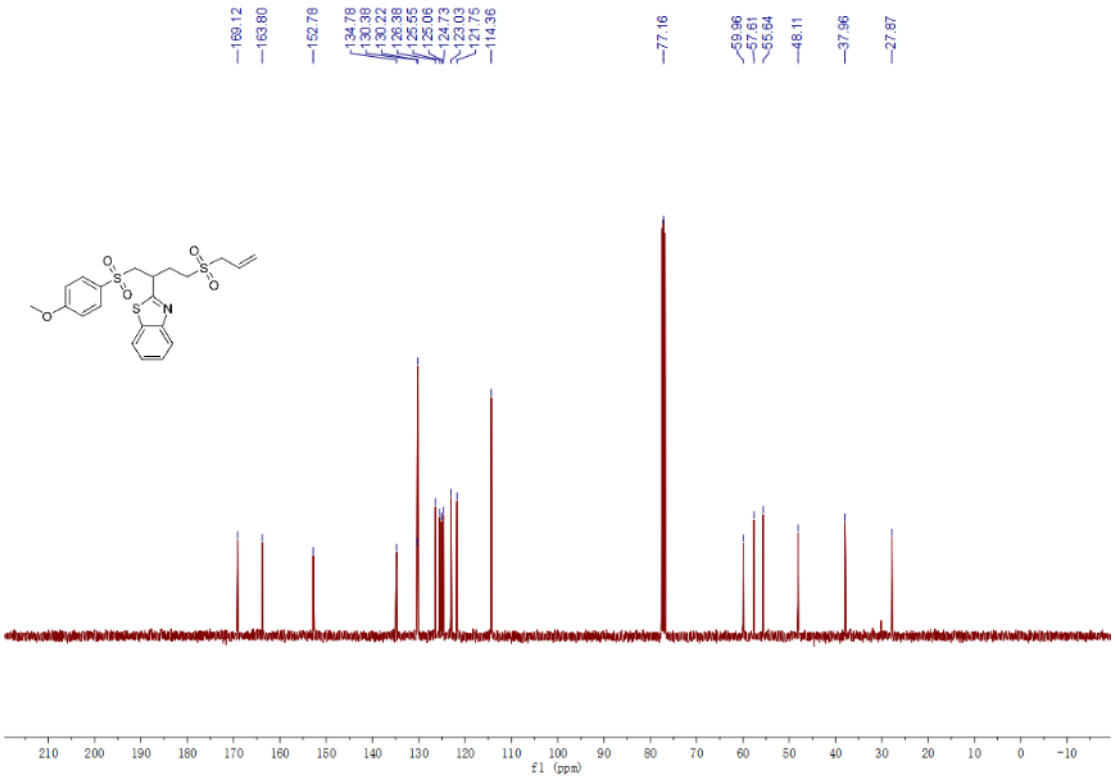
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound6a



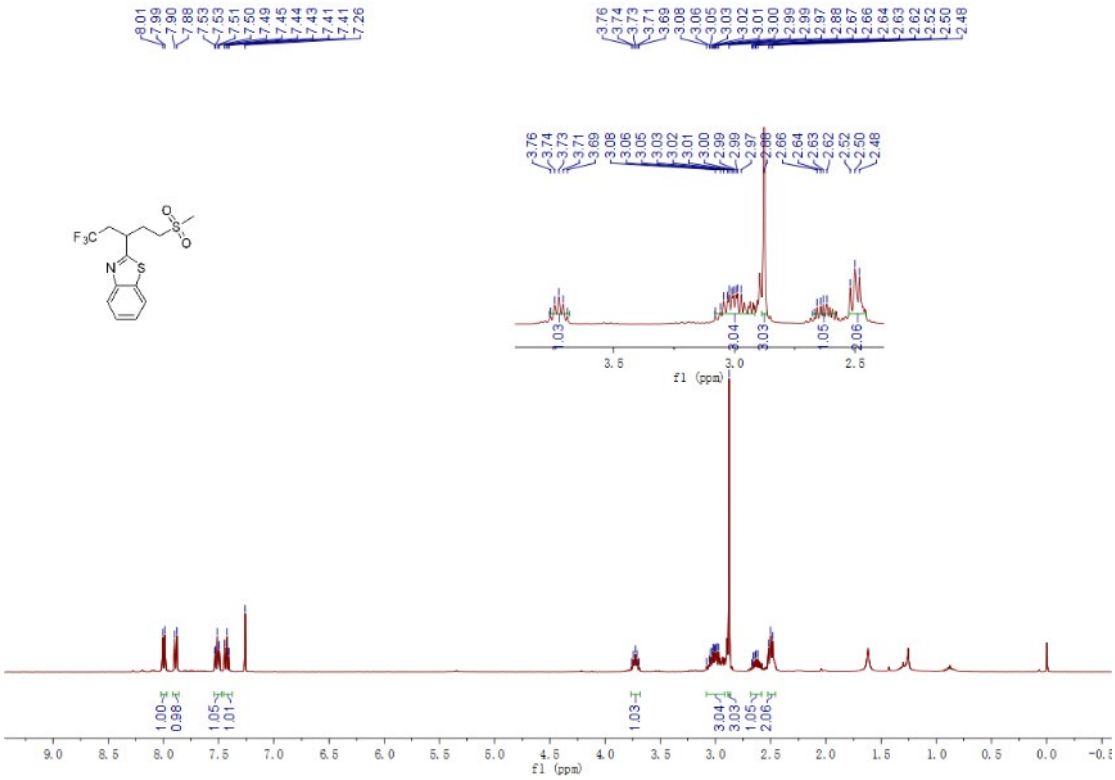
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6b



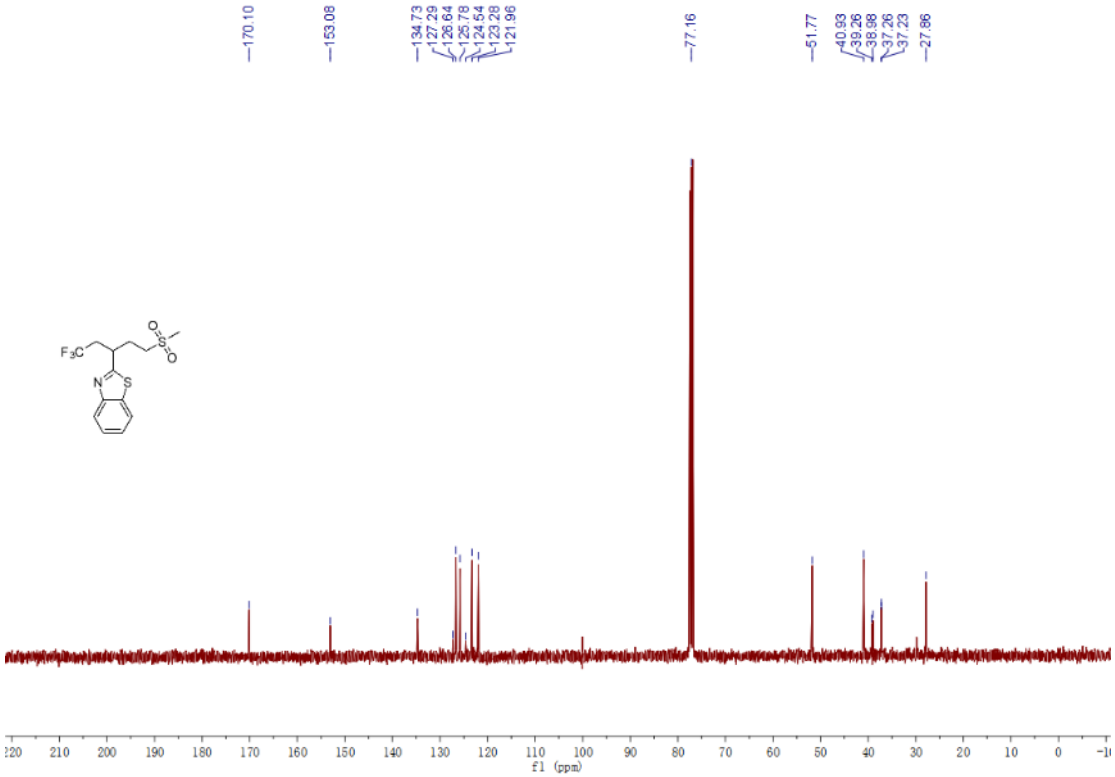
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6b



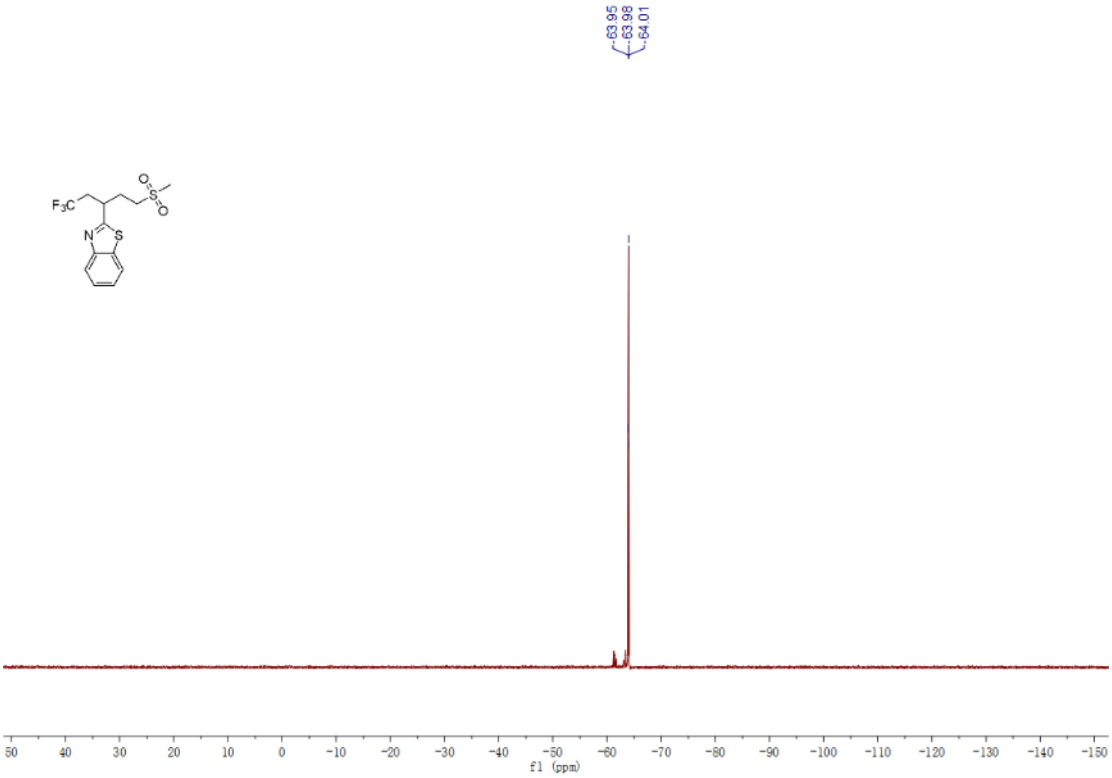
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6c



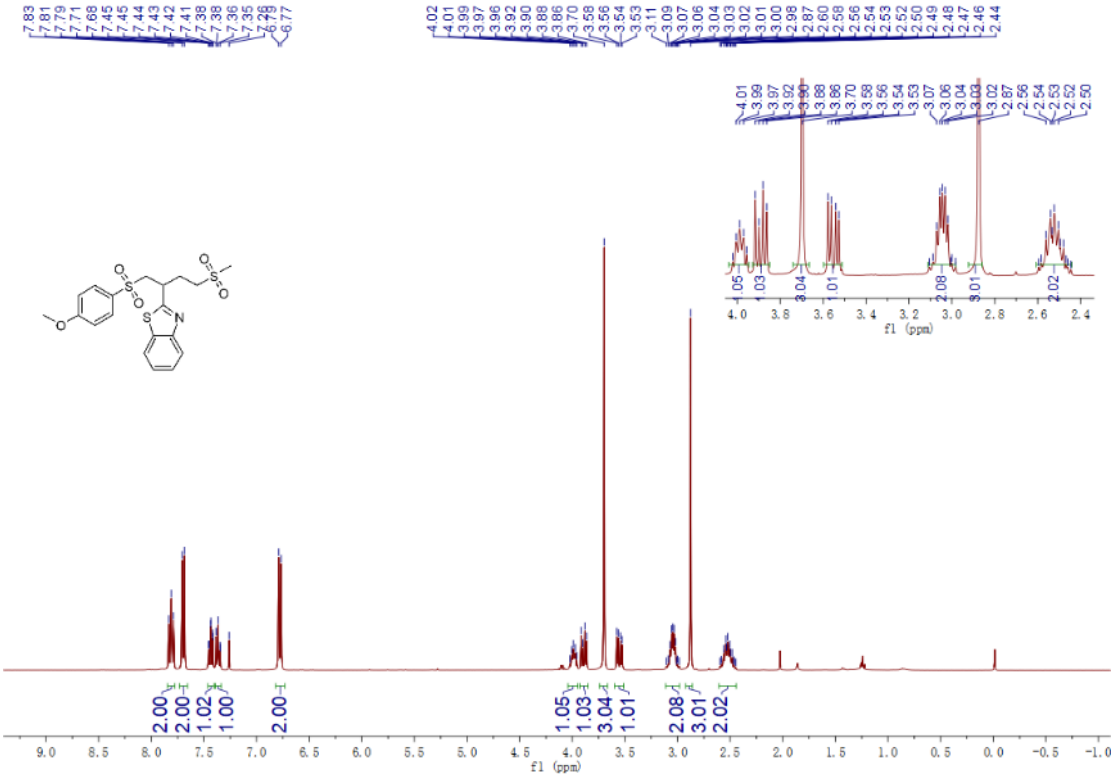
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6c



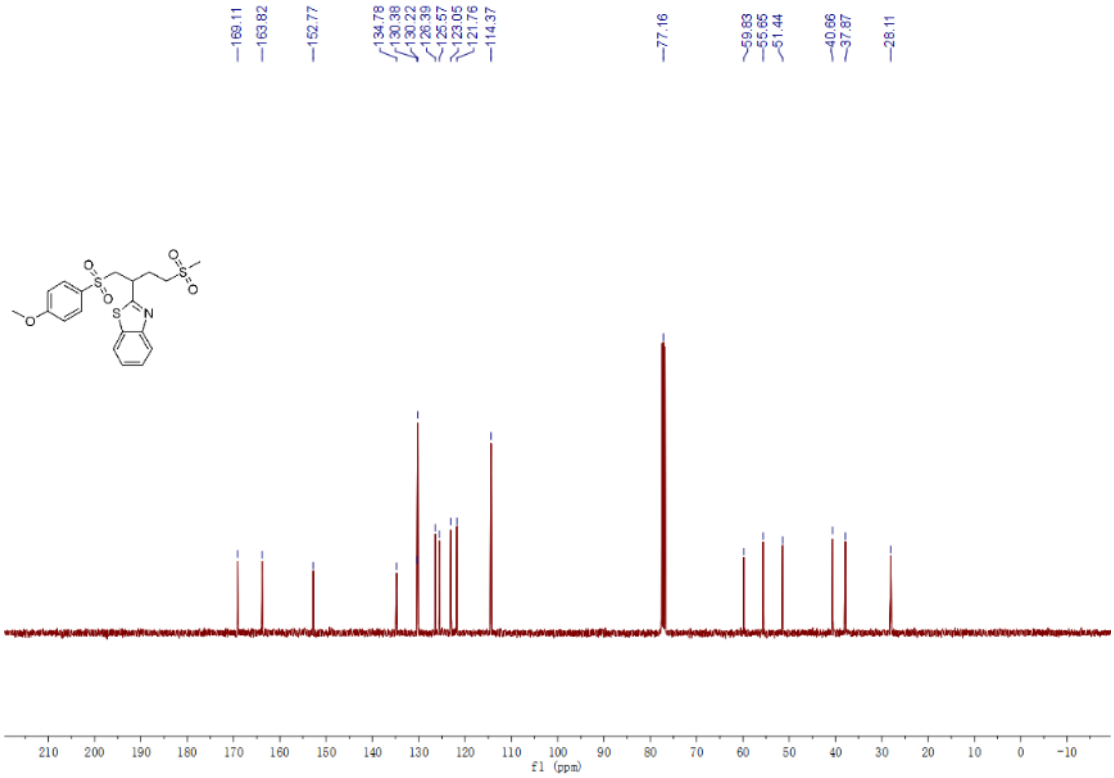
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 6c



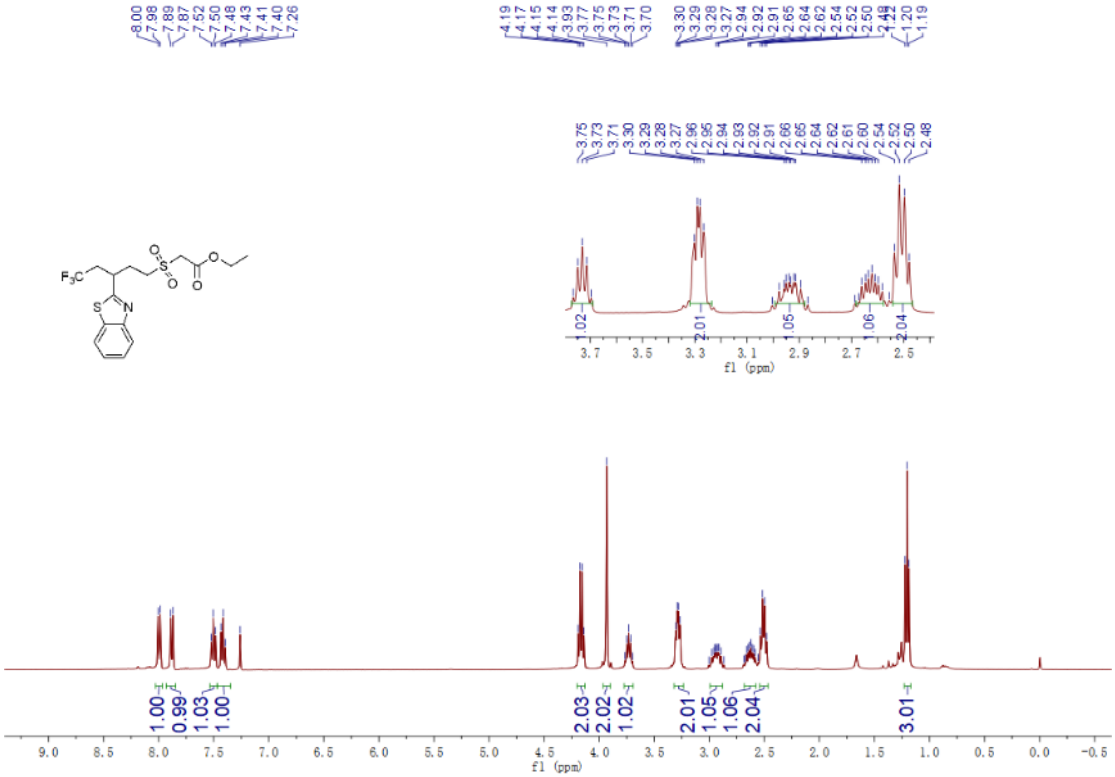
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6d



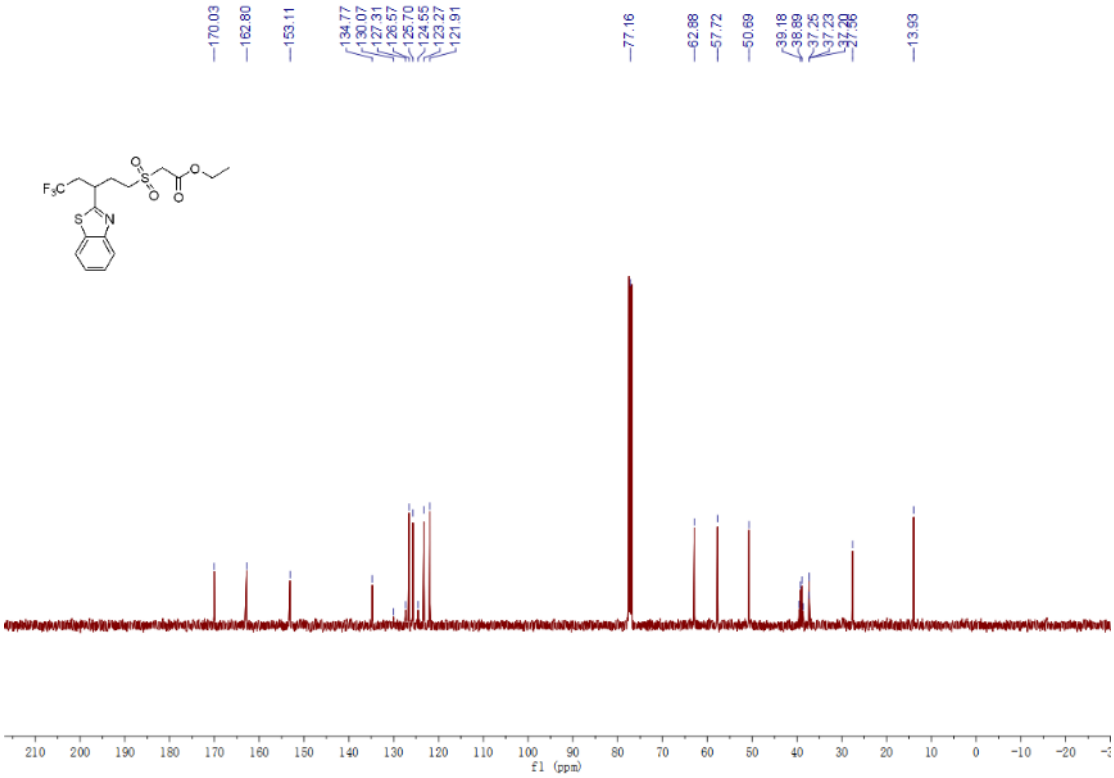
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6d



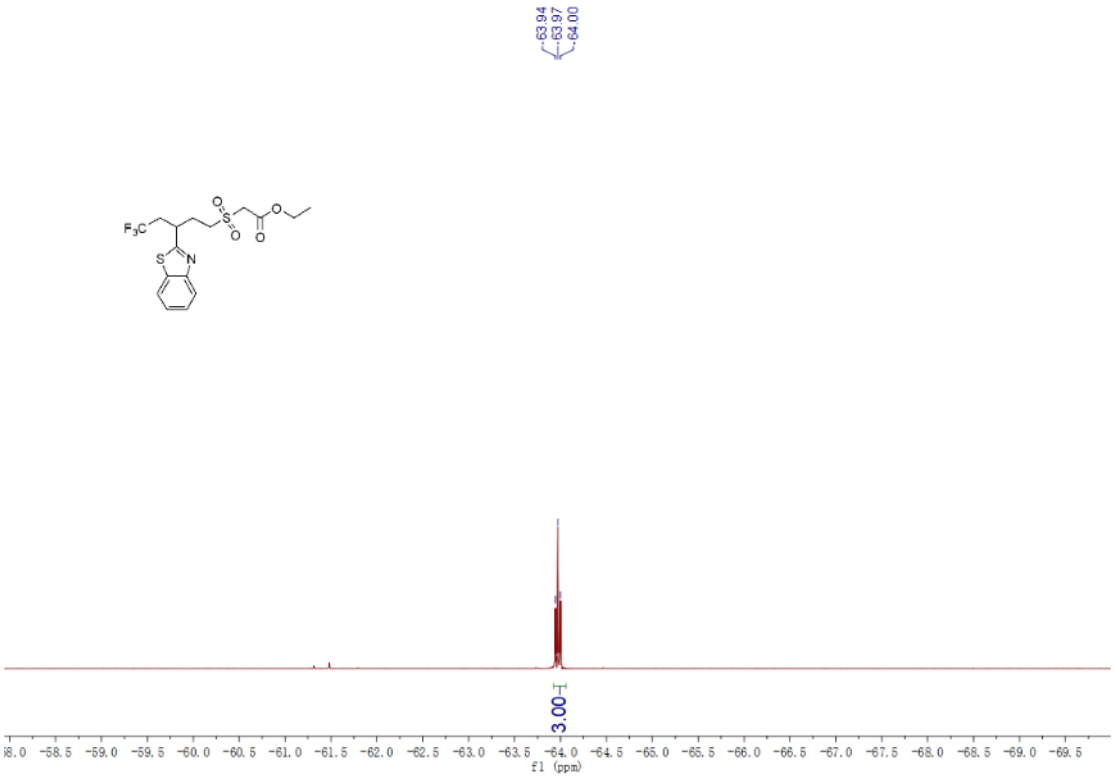
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6e



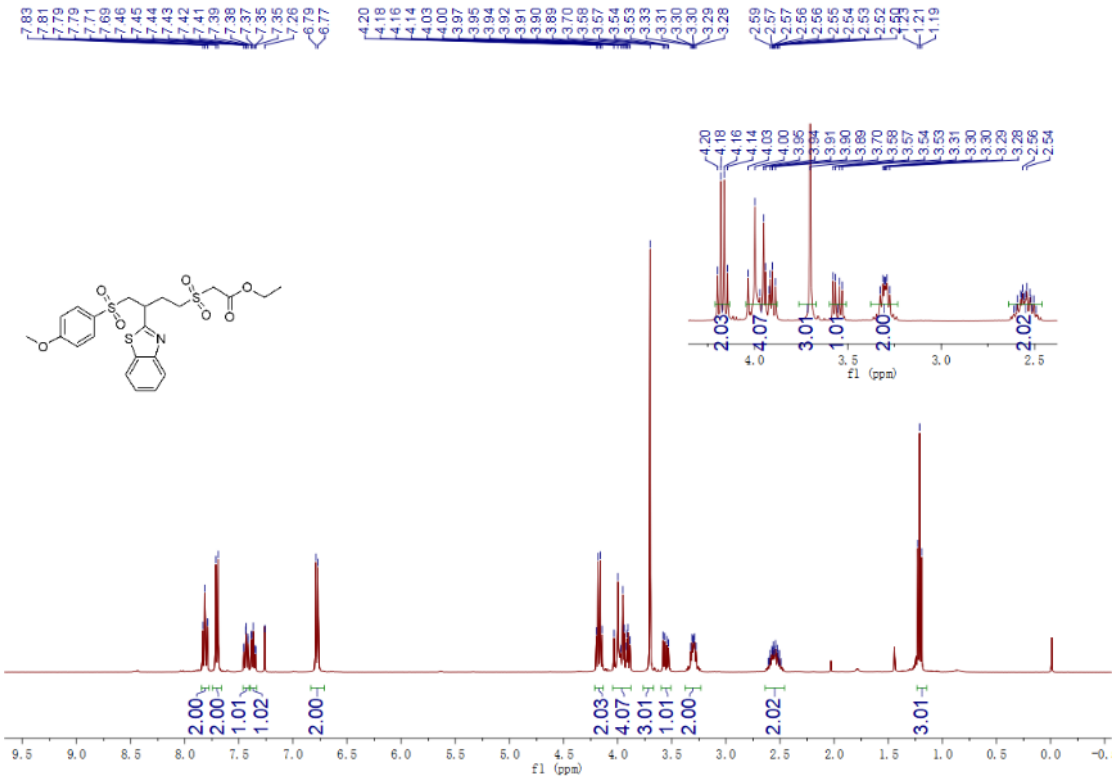
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6e



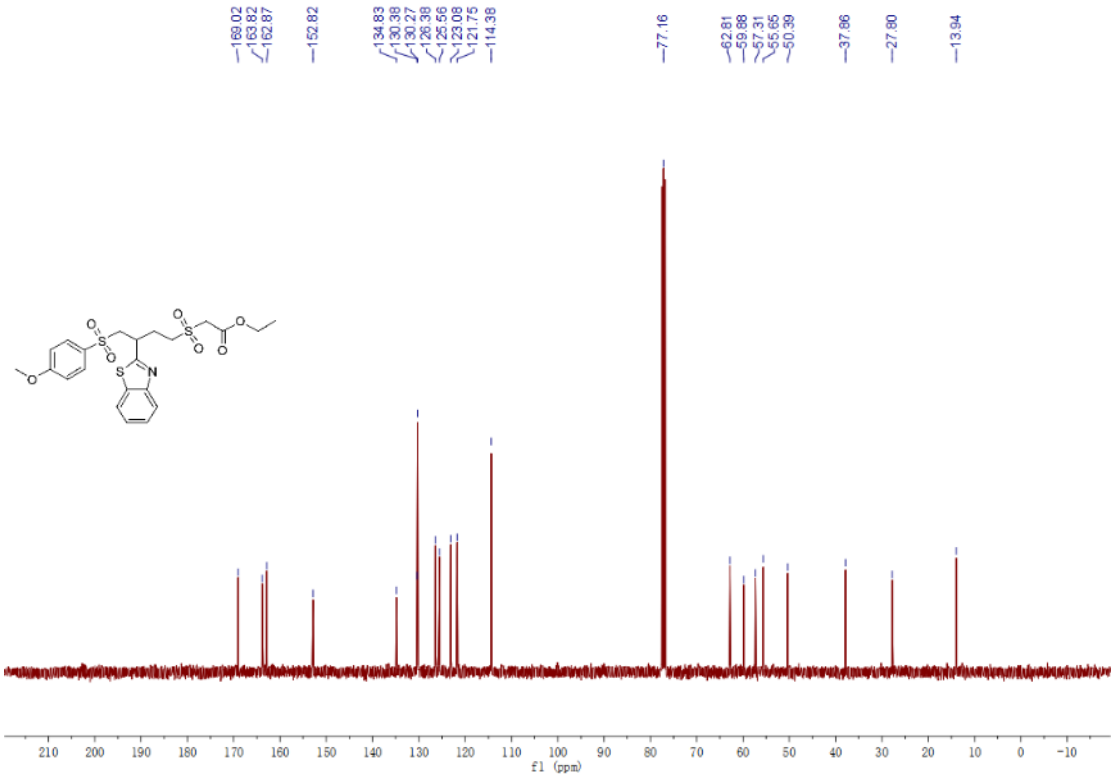
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 6e



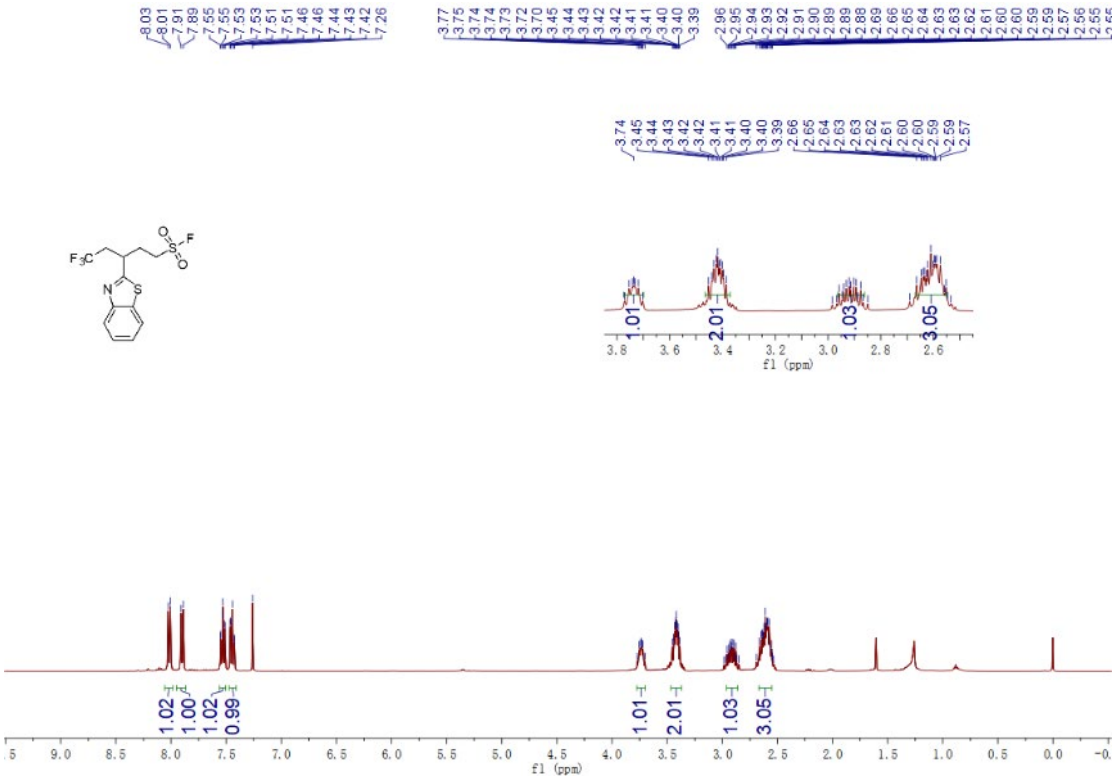
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6f



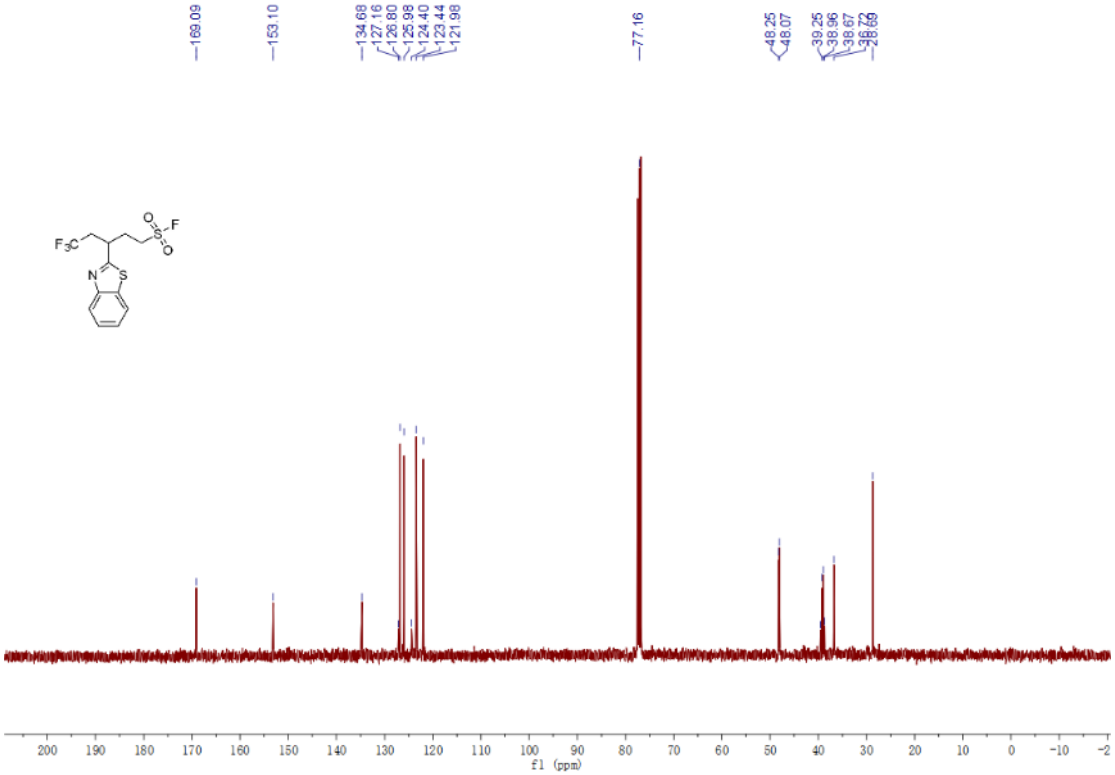
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6f



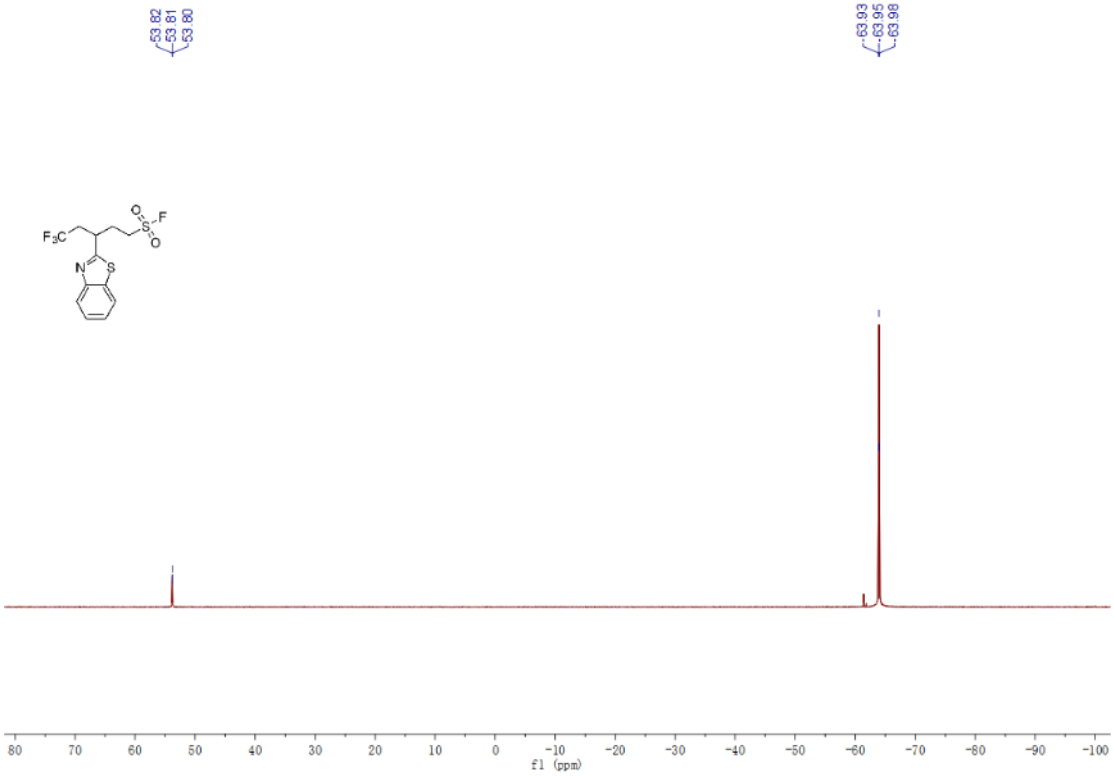
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6g



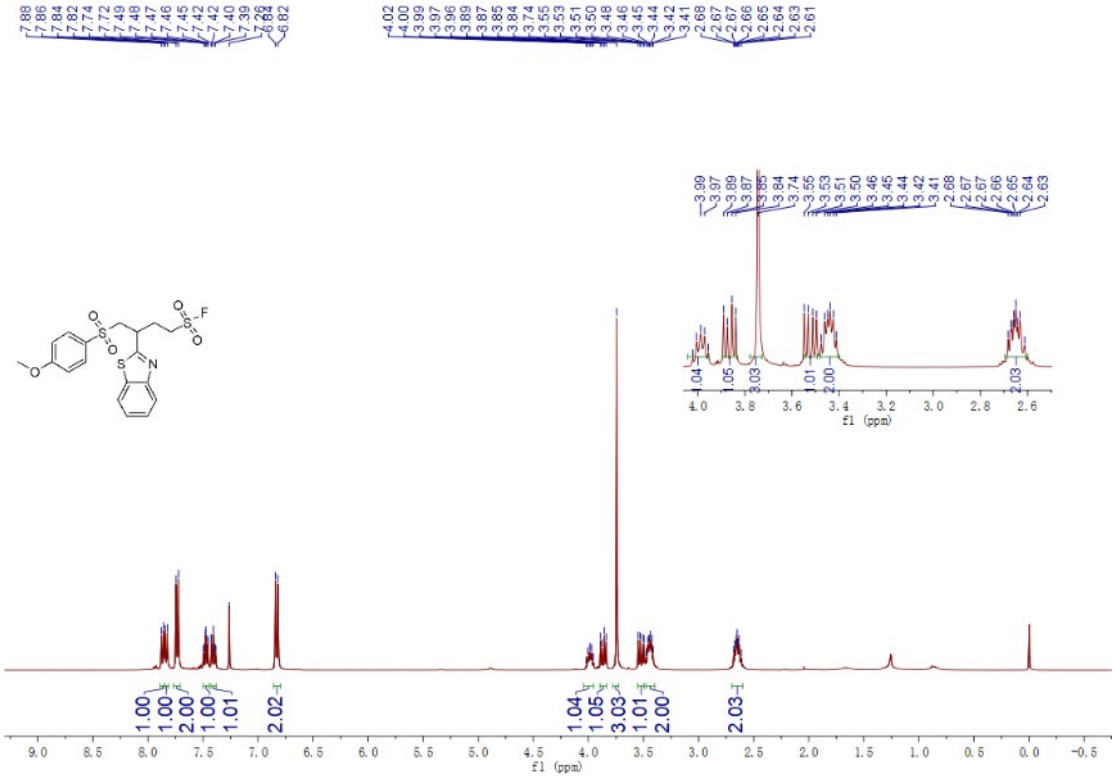
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6g



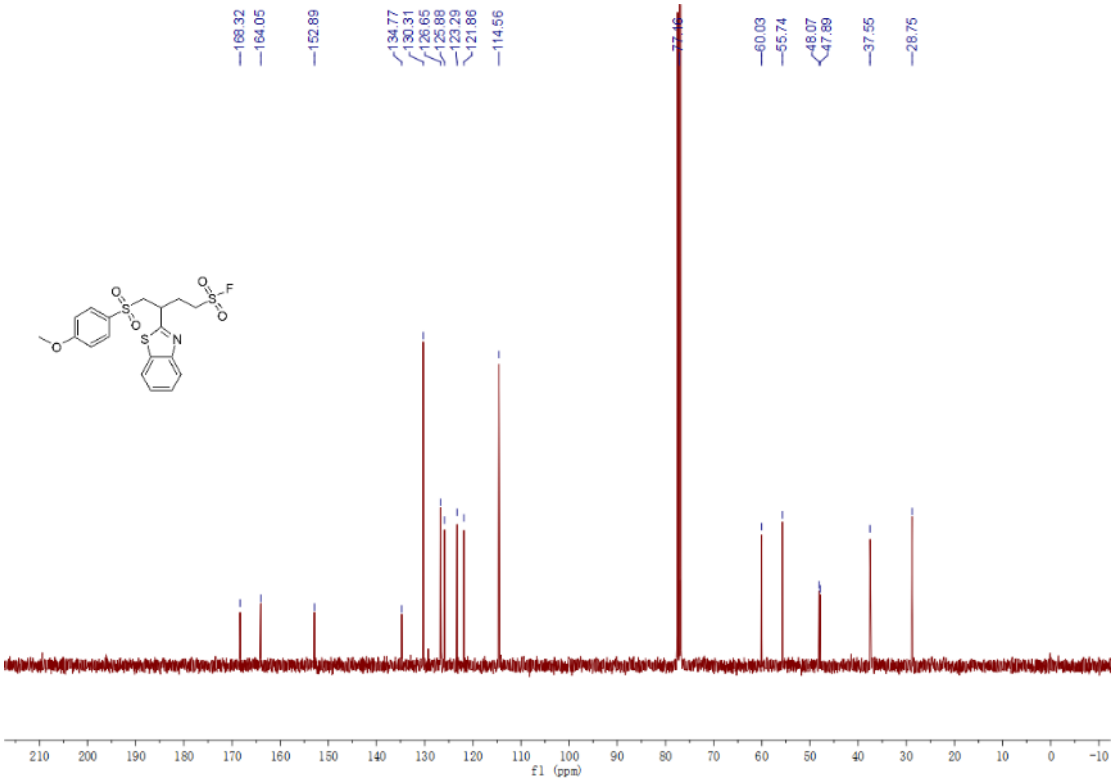
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 6g



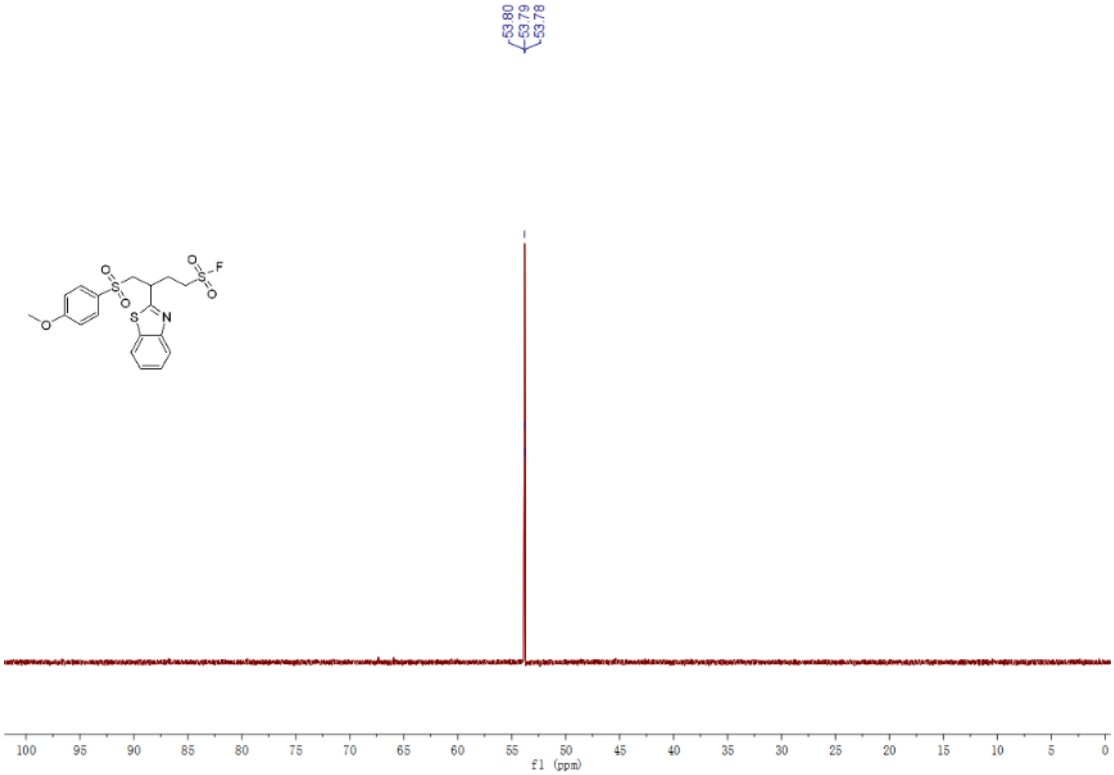
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6h



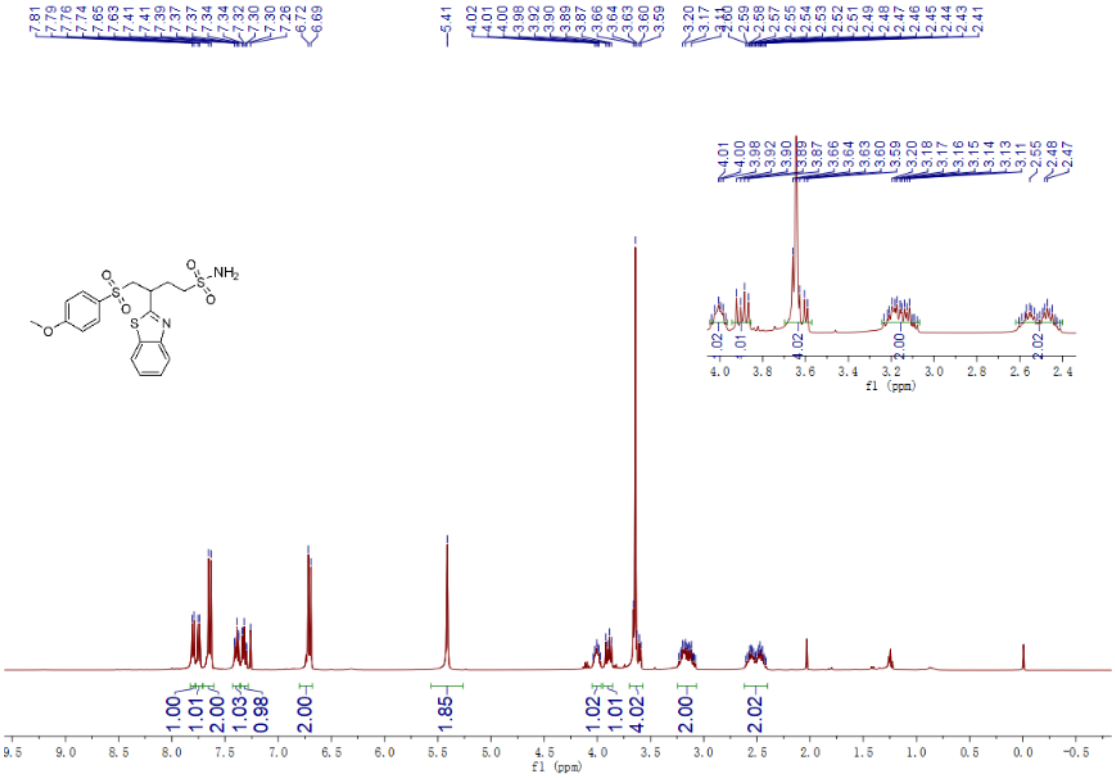
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6h



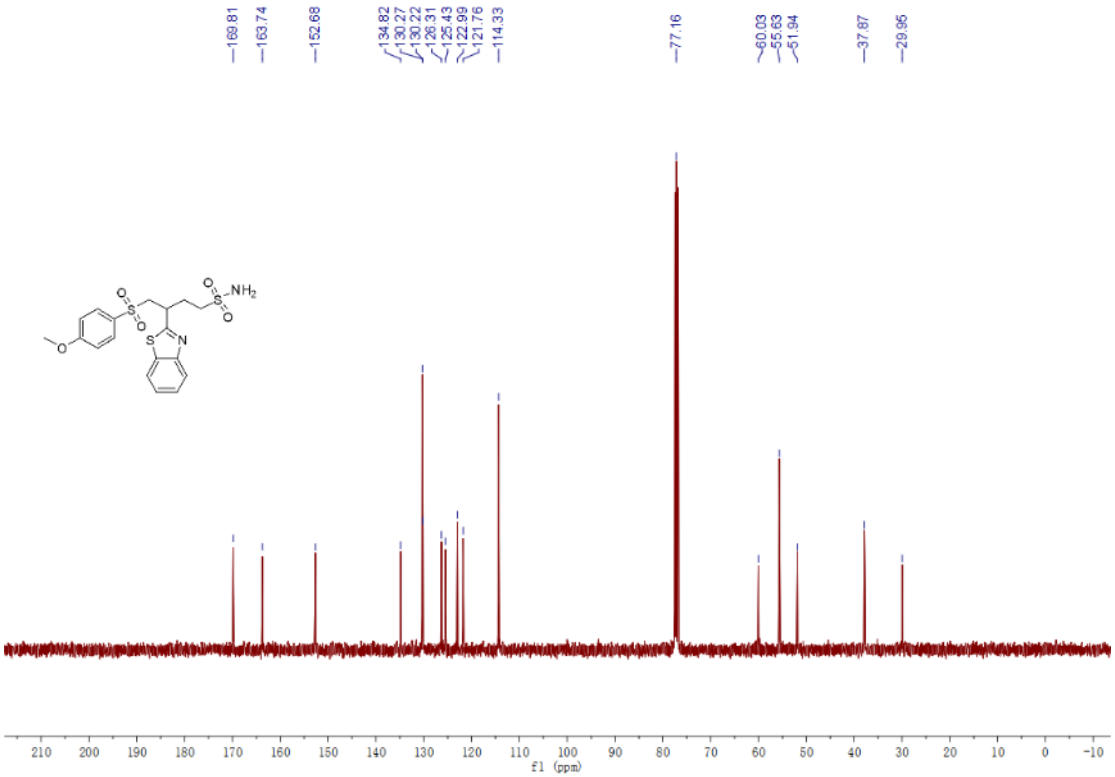
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 6h



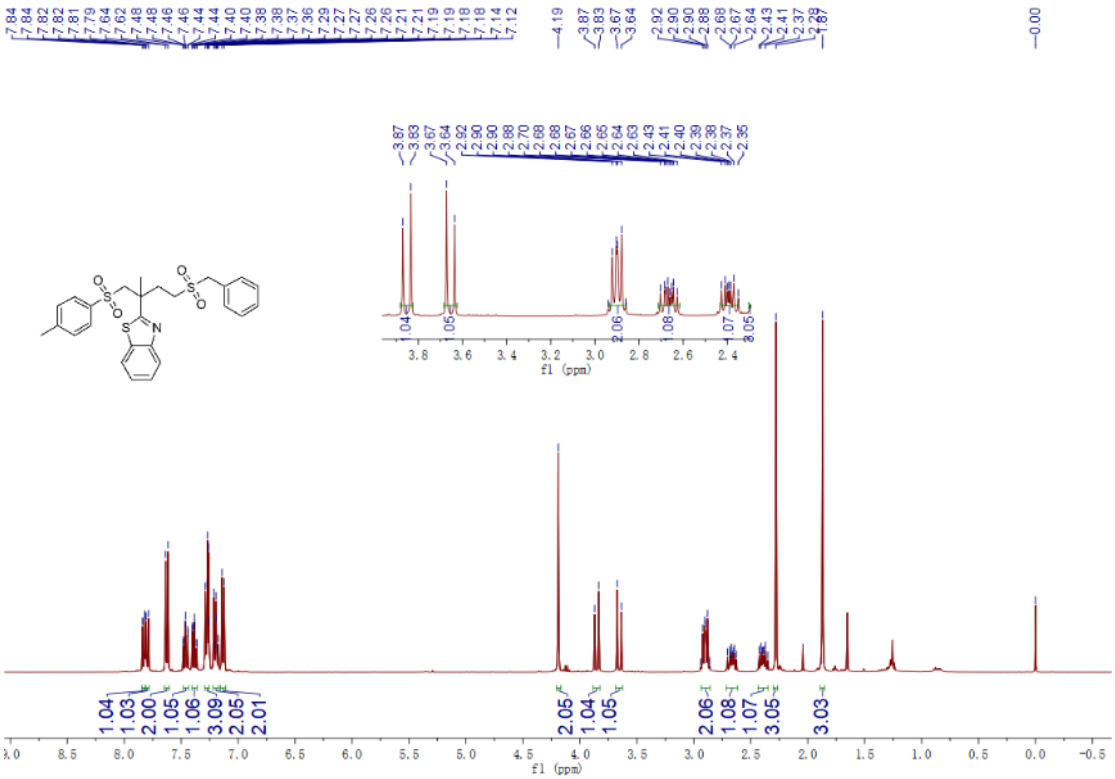
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6i



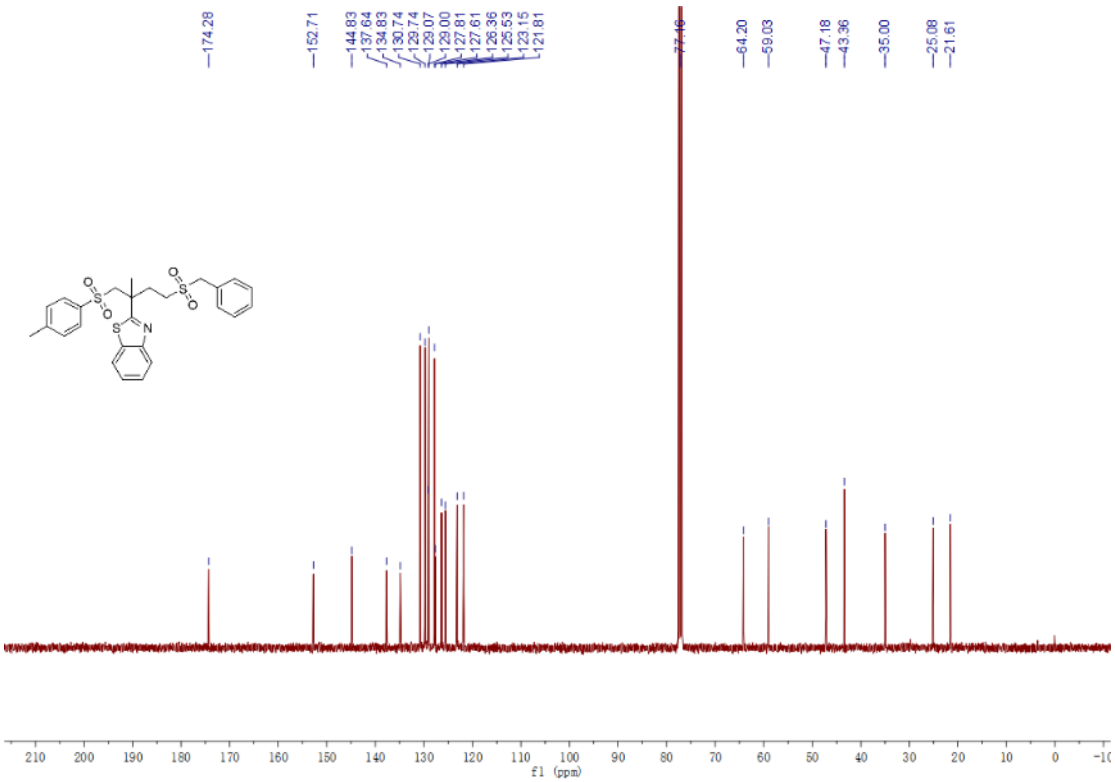
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6i



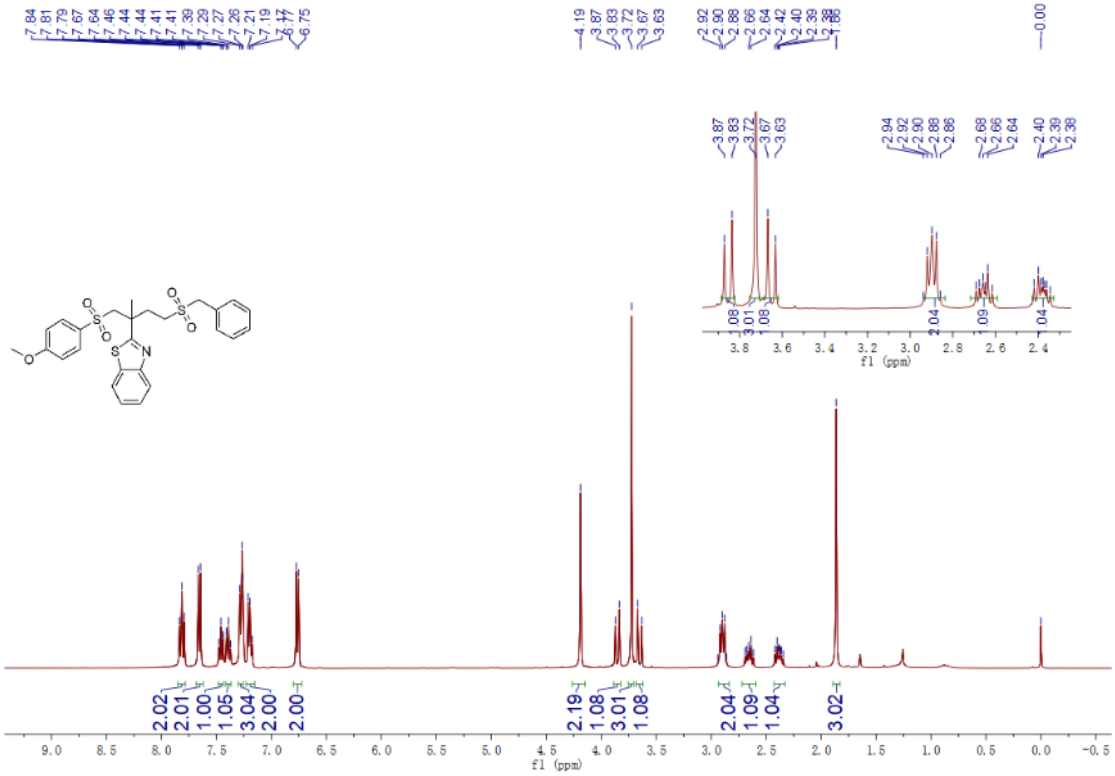
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6j



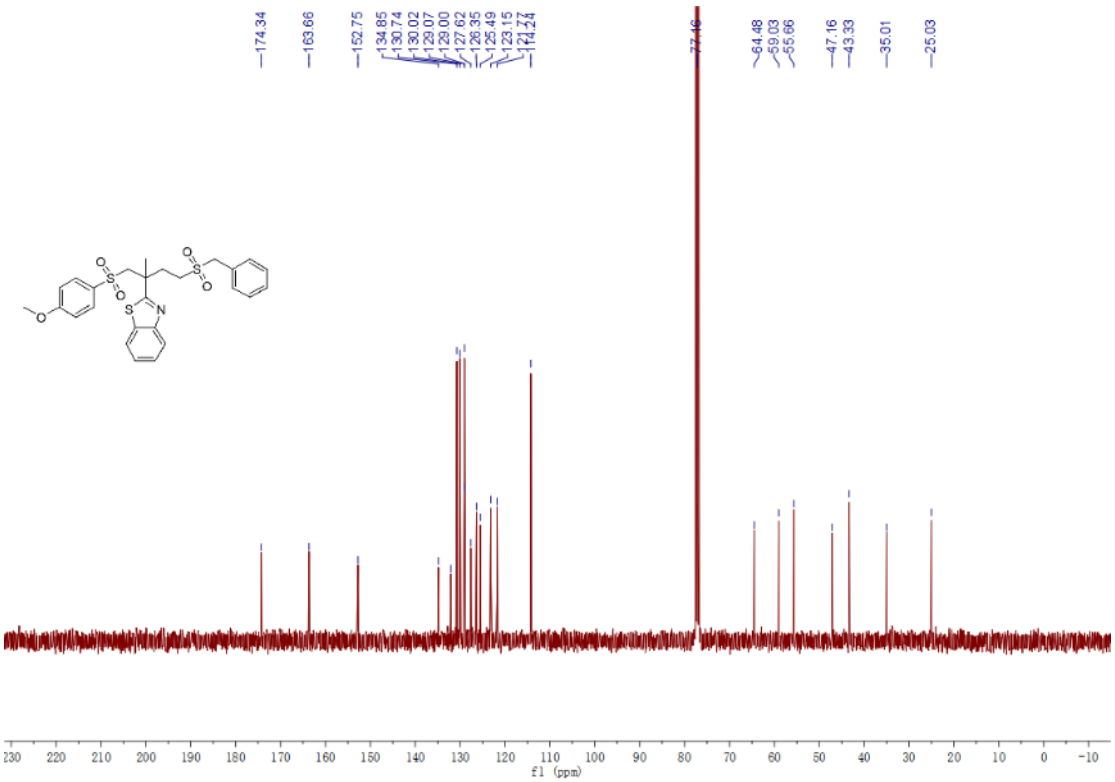
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6j



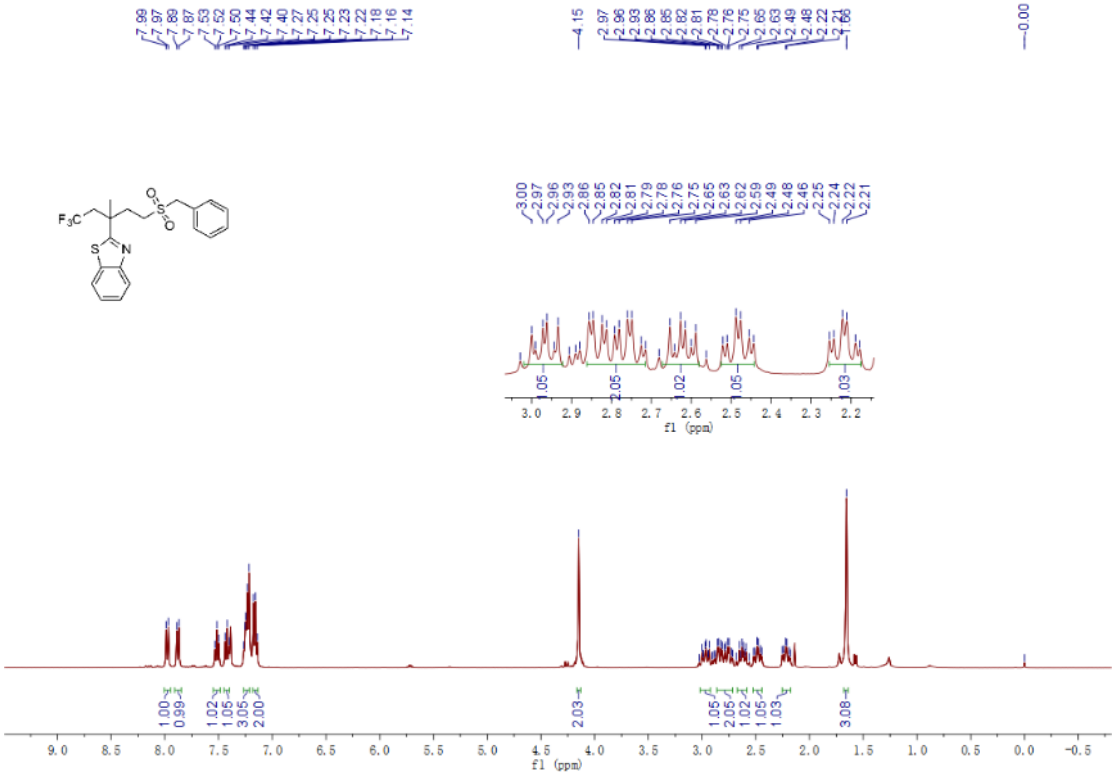
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6k



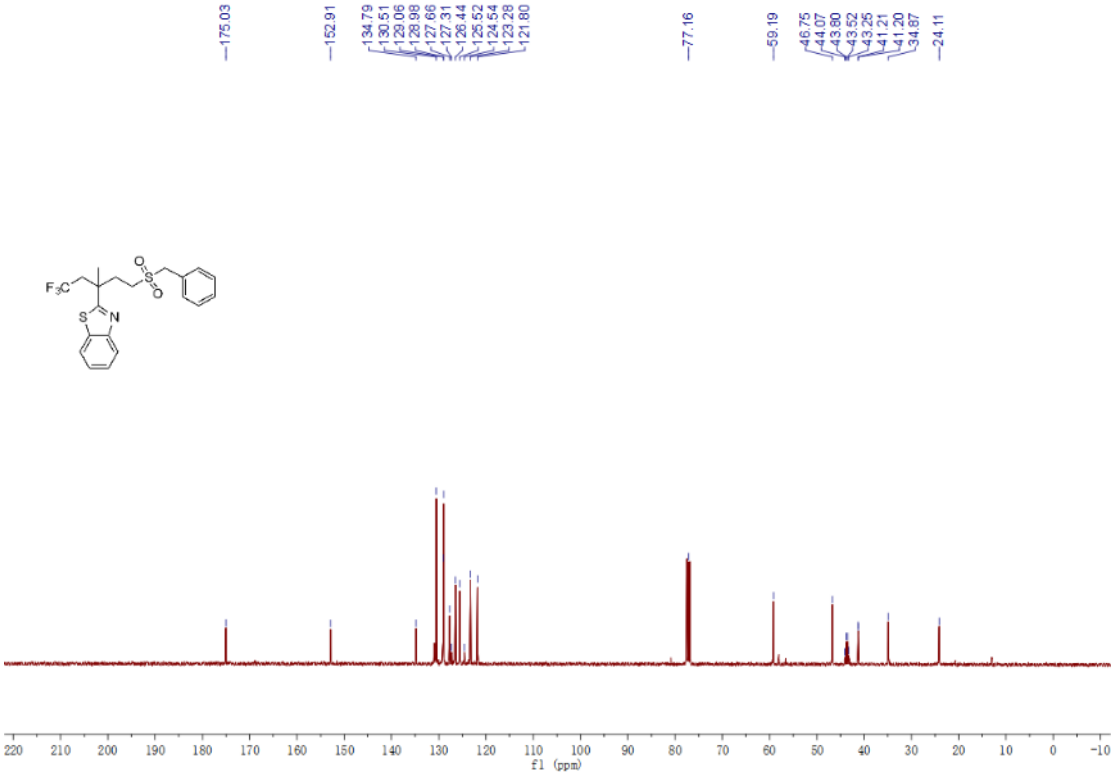
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6k



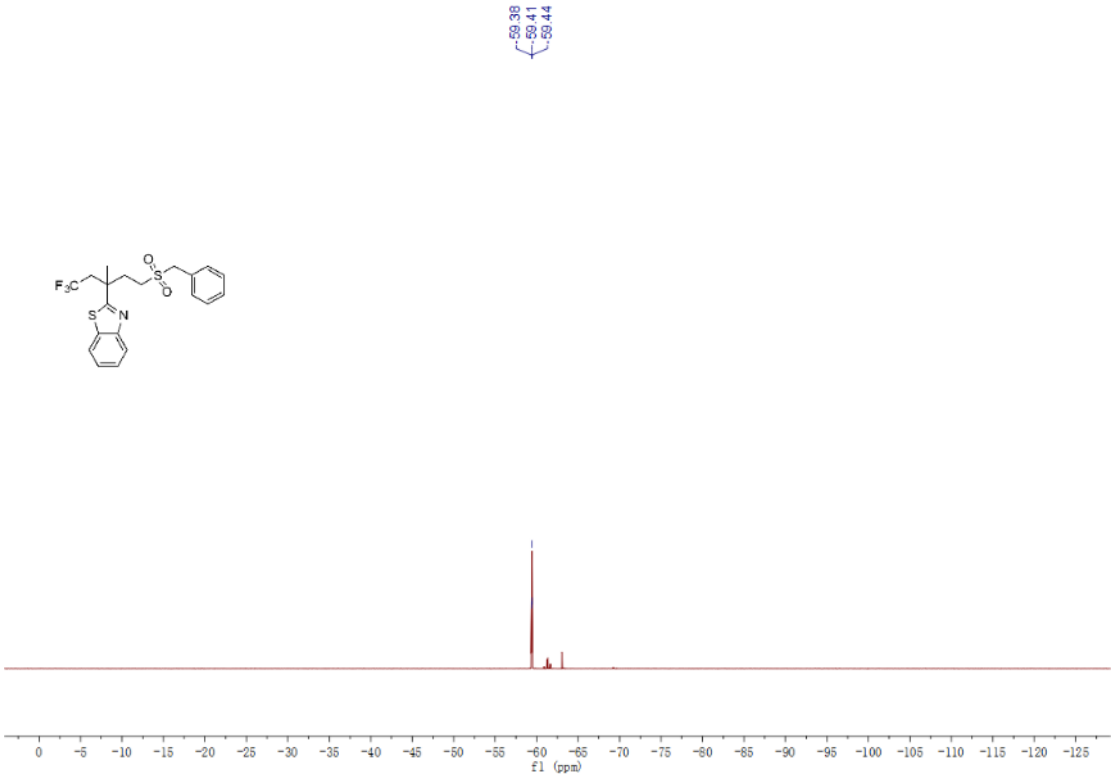
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6l



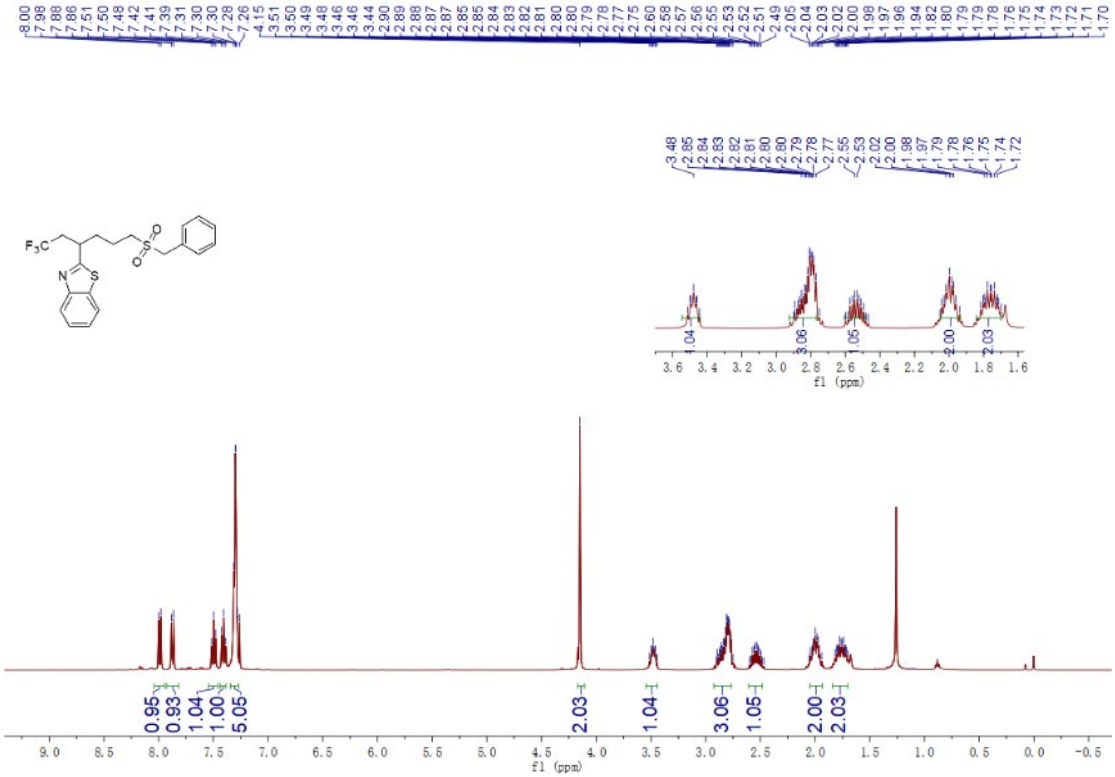
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6l



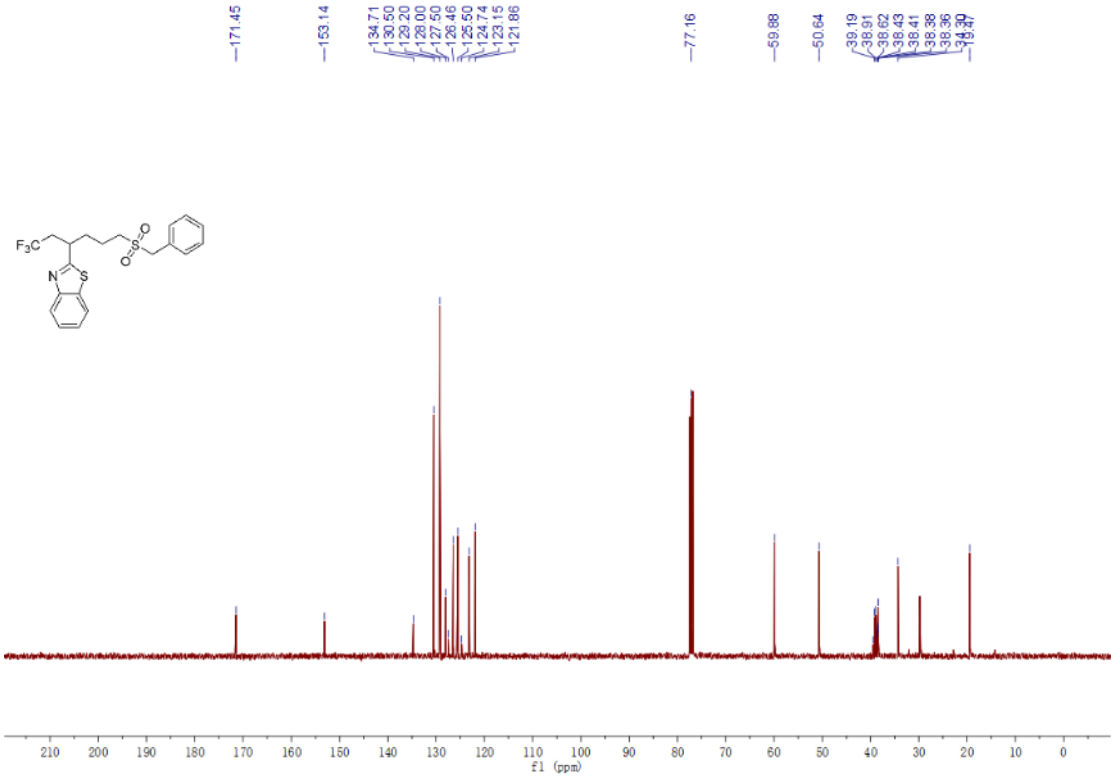
^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 6l



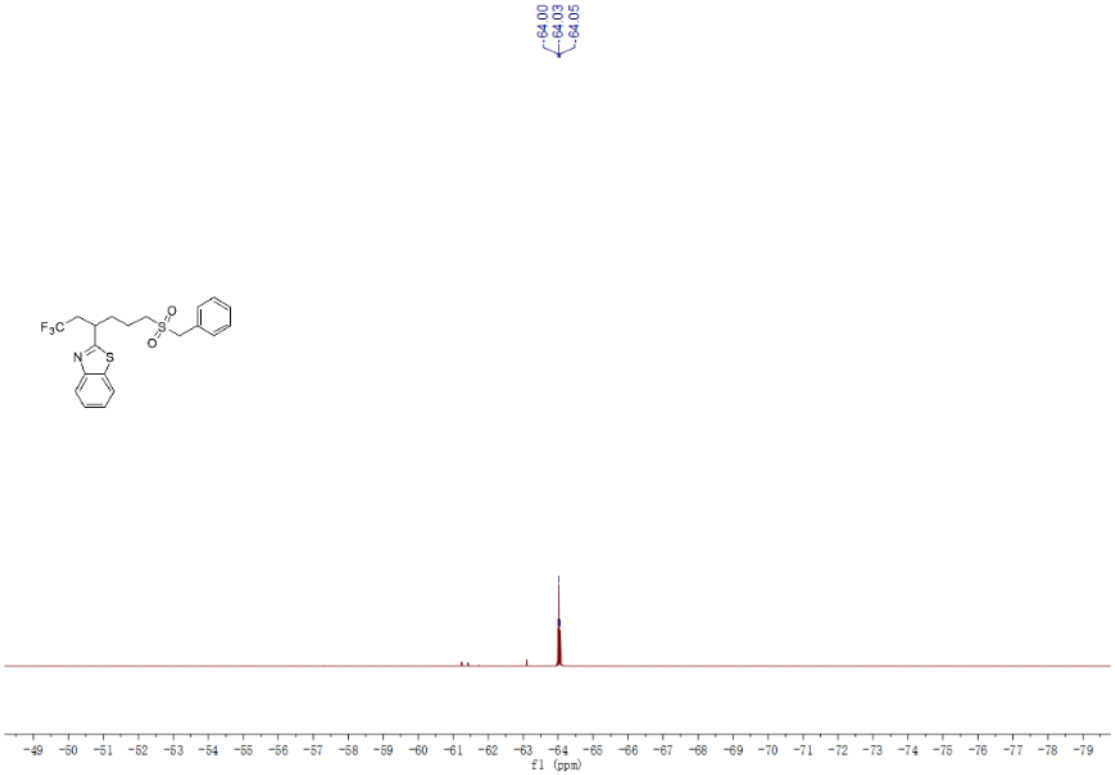
^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6m



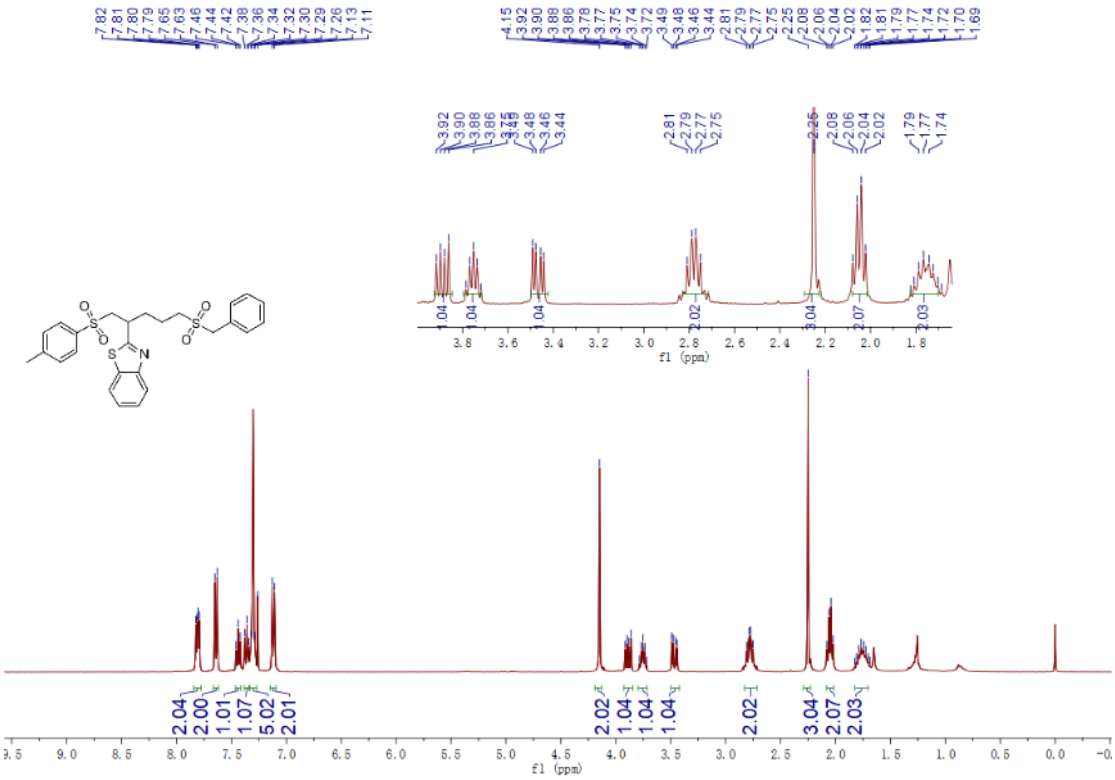
^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6m



^{19}F NMR spectrum(376MHz, $CDCl_3$) of compound 6m



^{1}H NMR spectrum (400MHz, $CDCl_3$) of compound 6n



^{13}C NMR spectrum(100MHz, $CDCl_3$) of compound 6n