Supporting Information

Self-photocatalyzed regulable alkylation of 2*H*-benzothiazoles with diverse aliphatic C–H donors

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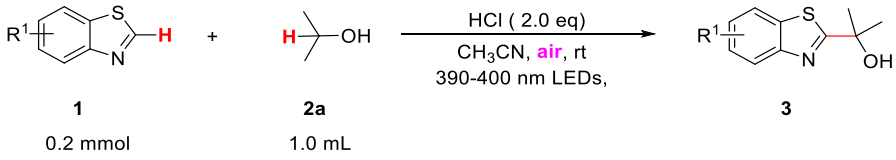
1.General method.

The reagents and solvents were purchased from commercial suppliers and used without further purification unless noted. All reactions were monitored by TLC with silica gel-coated plates. ^{1}H (400 MHz or 600 MHz) NMR and ^{13}C (101 MHz or 151 MHz) NMR spectra were recorded on a Varian spectrometer in $CDCl_3$ or DMSO-d_6 using tetramethylsilane (TMS) as internal standards. Data are reported as follows: Chemical shift (number of protons, multiplicity, coupling constants). Coupling constants were quoted to the nearest 0.1 Hz and multiplicity reported according to the following convention: s = singlet, d = doublet, t = triplet, q = quartet, hept = heptet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets, ddd = doublet of doublet of doublets, br s = broad singlet. Mass spectra were measured with a HRMS-APCI instrument using ESI ionization. Fluorescence quenching experiments were performed on Hitachi F7000 FL Spectrophotometer and F97Pro Spectrophotometer.

2.General procedure

2.1 Representative procedure for the synthesis of 3



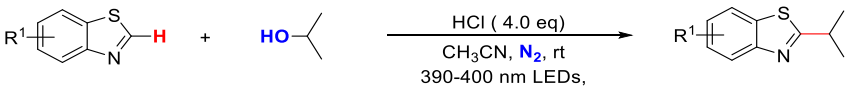
1 0.2 mmol

2a 1.0 mL

3

General procedure A. A mixture of compound **1** (0.2 mmol, 1.0 equiv.), alcohol **2** (1.0 mL), HCl (36wt%, 35 μL, 2.0 equiv.) in a 10 mL Schlenk tube was added CH_3CN (2.0 mL). The reaction mixture was open to the air and stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 24 h. The reaction mixture was quenched by $NaHCO_3$ and then extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated under reduced pressure and purified by column chromatography (petroleum ether/ethyl acetate = 30/1 – 3/1) on silica get to give the products **3**.

2.2 Representative procedure for the synthesis of 11

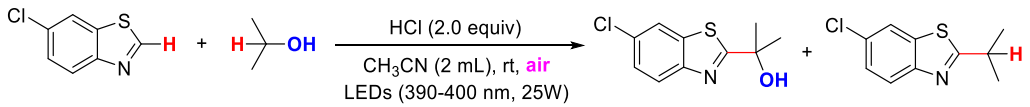


1 0.2 mmol **2a** 1.0 mL **11**

General procedure B. To a 10 mL Schlenk tube equipped with a magnetic stirring bar was added compound **1** (0.2 mmol, 1.0 equiv.). After three cycles of evacuation and backfilling of the reaction flask with N_2, alcohol **2** (1.0 mL), HCl (36wt%, 70 μL, 4.0 equiv.) and CH_3CN (2.0 mL) was added. The reaction mixture stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 48 h. The reaction mixture was quenched by $NaHCO_3$ and then extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated under reduced pressure and purified by column chromatography (petroleum ether/ethyl acetate = 60/1 – 30/1) on silica get to give the products **11**.

3. Additional optimization studies

Table S1. Additional optimization of reaction conditions.[a]



1a **2a** **"standard conditions"** **3a** **11a**

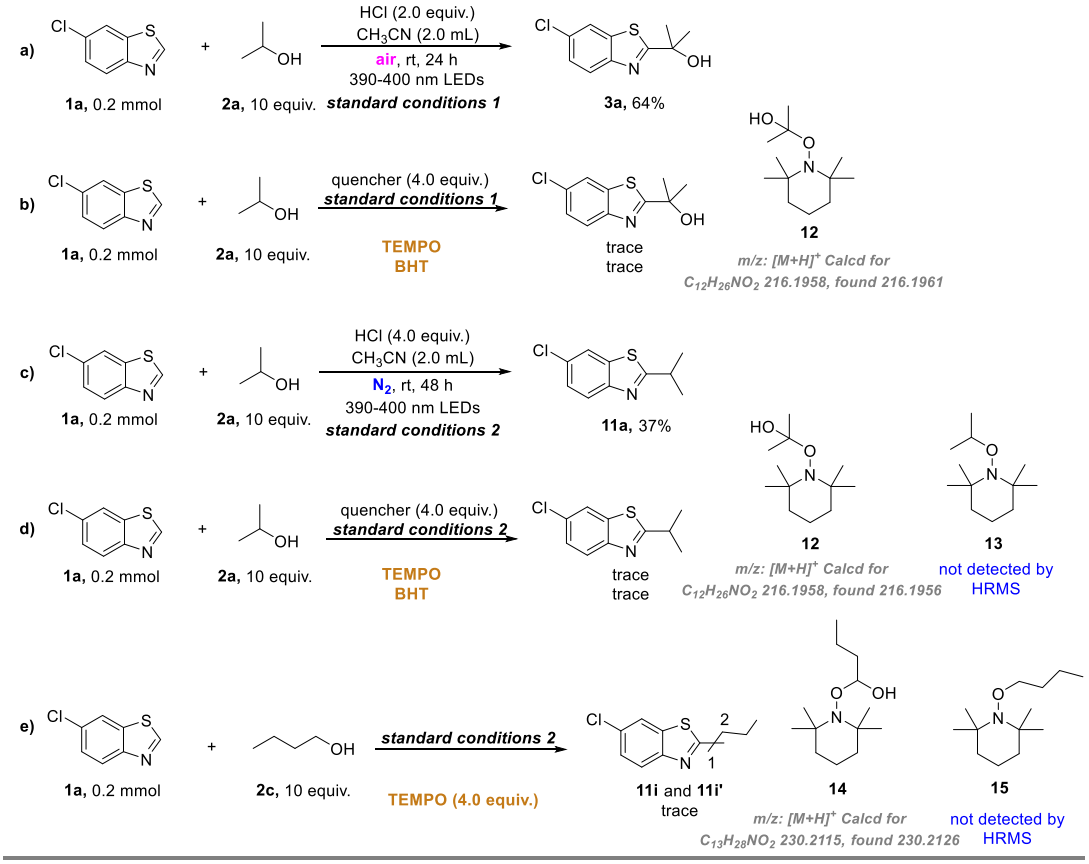
Entry	Deviation from standard conditions	Yield **3a** (%)[b]	Yield **11a** (%)[b]
1	40 mol% TBAB and TFA instead of HCl	37	0
2	40 mol% TBAI and TFA instead of HCl	0	0
3	40 mol% TBAC without HCl	22	0
3	25W Bule LEDs (450 – 460 nm) instead of Purple LEDs	15	0
4	25W White LEDs instead of Purple LEDs	18	0
5	Reaction at 60℃ in the dark instead of light irradiation	0	0
6	5 equiv of **2a**	41	0
7	10 equiv of **2a**	64	0
8	0.2 mL (13 equiv) of **2a**	66	0
9	0.5 mL (32 equiv) of **2a**	71	0
10	1 equiv of HCl	62	0
11	3 equiv of HCl	86	0
12	4 equiv of TFA, under a N_2 atmosphere, 48 h	trace	42
13	4 equiv of HCl, under a N_2 atmosphere, 48 h, 60℃	trace	68

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (1.0 mL), HCl (2.0 equiv.), CH_3CN (2.0 mL), 2 × 25W Purple LEDs

(390 – 400 nm), 24 h, under an air atmosphere. [b] Isolated yields based on **1a**.

4. The mechanistic studies

4.1 Radical quenching experiment



A mixture of compound **1a** (0.2 mmol, 1.0 equiv.), IPA **2a** (2.0 mmol, 10 equiv.), HCl (36wt%, 35 μL, 2.0 equiv.) and a radical quencher (TEMPO or BHT, 0.8 mmol, 4.0 equiv.) in a 10 mL Schlenk tube was added CH_3CN (2.0 mL). The reaction mixture was open to the air and stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 24 h. After the reaction was completed, only a trace amount of **3a** was observed by TLC.

To a 10 mL Schlenk tube equipped with a magnetic stirring bar was added compound **1a** (0.2 mmol, 1.0 equiv.) and a radical quencher (TEMPO or BHT, 0.8 mmol, 4.0 equiv.). After three cycles of evacuation and backfilling of the reaction flask with N_2, IPA **2a** (2.0 mmol, 10 equiv.), HCl (36wt%,

70 μL, 4.0 equiv.) and CH_3CN (2.0 mL) was added. The reaction mixture stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 48 h. After the reaction was completed, only a trace amount of **11a** was observed by TLC.

To a 10 mL Schlenk tube equipped with a magnetic stirring bar was added compound **1a** (0.2 mmol, 1.0 equiv.) and TEMPO (0.8 mmol, 4.0 equiv.). After three cycles of evacuation and backfilling of the reaction flask with N_2, 1-butanol **2c** (2.0 mmol, 10 equiv.), HCl (36wt%, 70 μL, 4.0 equiv.) and CH_3CN (2.0 mL) was added. The reaction mixture stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 48 h. After the reaction was completed, only a trace amount of **11i** and **11i′** was observed by TLC.

The formation of **3a**, **11a, 11i** and **11i′** was significantly suppressed by radical quenchers, which suggested that both dehydrogenative alkylation and dehydrative alkylation proceed through a radical-involved pathway.

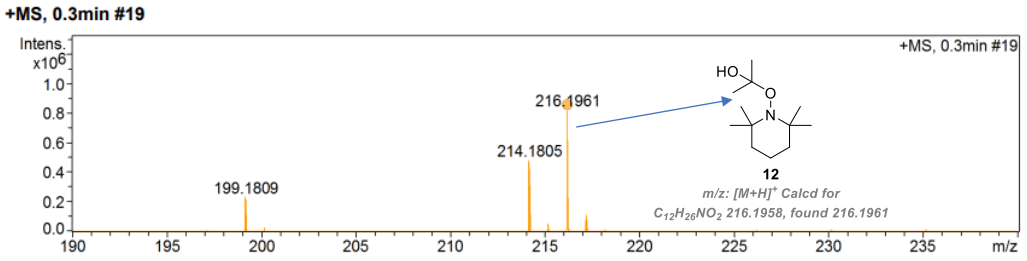


Figure S1. The HRMS analysis of radical quenching experiment **b**

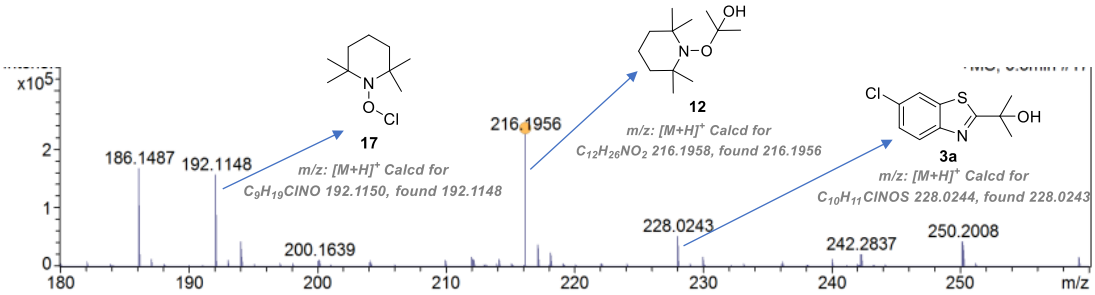


Figure S2. The HRMS analysis of radical quenching experiment **d**

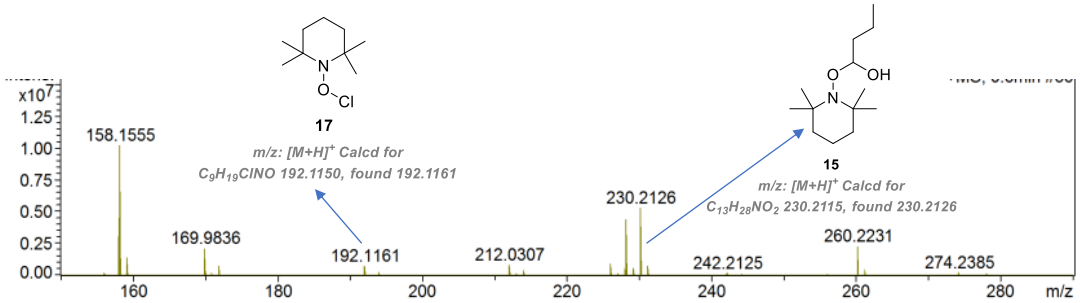
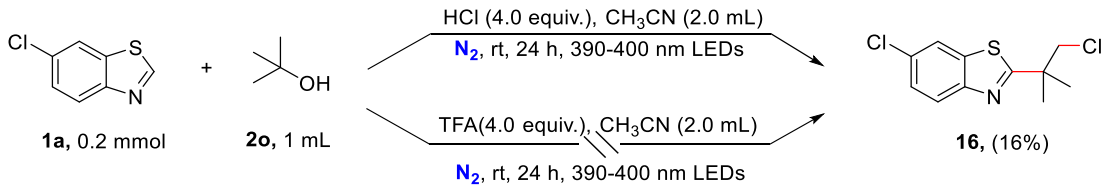
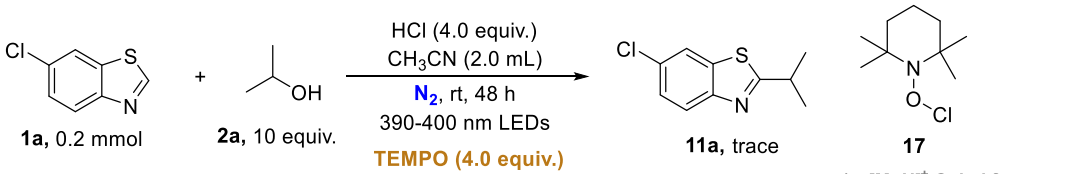


Figure S3. The HRMS analysis of radical quenching experiment **e**

4.2 Chlorine radical trapping experiment



To a 10 mL Schlenk tube equipped with a magnetic stirring bar was added compound **1a** (0.2 mmol, 1.0 equiv.). After three cycles of evacuation and backfilling of the reaction flask with N_2, *t*-BuOH **2o** (1.0 mL), HCl (36wt%, 70 μL, 4.0 equiv.) and CH_3CN (2.0 mL) was added. The reaction mixture stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 24 h. The reaction mixture was quenched by $NaHCO_3$ and then extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated under reduced pressure to obtain the crude product. The isolated **16** was obtained in 16% yield by preparative thin-layer chromatography using petroleum ether/ethyl acetate (50:1) as the eluent. On the contrary, no chloroalkylated product **16** was formed in the absence of chlorine anion.



m/z: $[M+H]^+$ Calcd for $C_9H_{19}ClNO$ 192.1150, found 192.1148

To a 10 mL Schlenk tube equipped with a magnetic stirring bar was added compound **1a** (0.2 mmol, 1.0 equiv.) and TEMPO (0.8 mmol, 4.0 equiv.). After three cycles of evacuation and backfilling of the reaction flask with N_2, IPA **2a** (2.0 mmol, 10 equiv.), HCl (36wt%, 70 μL, 4.0 equiv.) and CH_3CN (2.0 mL) was added. The reaction mixture stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 48 h. After the reaction was completed, a chlorine radical adduct **17** was detected by ESI-HRMS, which indicated the formation of $Cl^{\cdot}$ in our case (see Figure S2).

4.3 Light on/off experiment

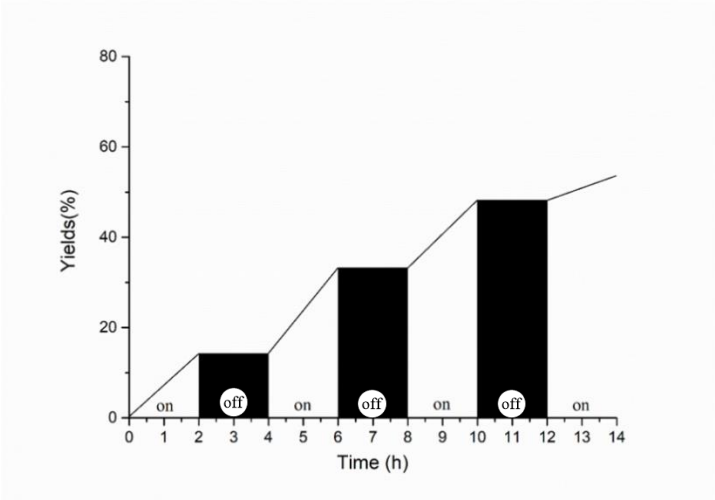
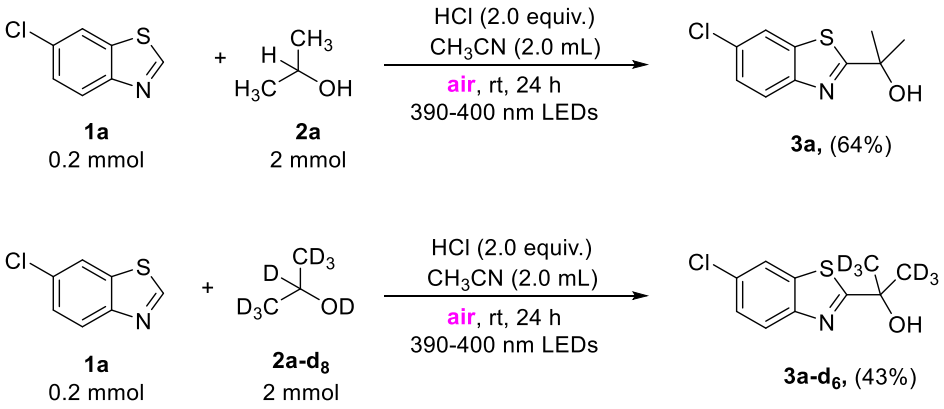
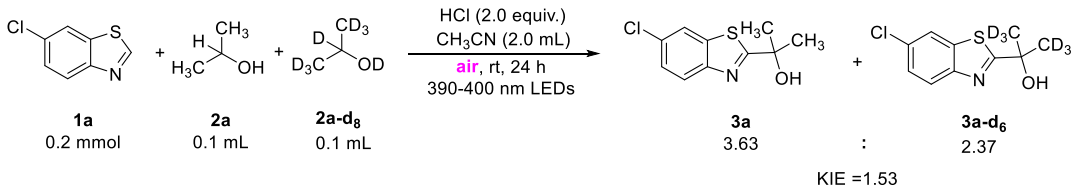


Figure S4. On/off light experiments for the model reaction under air atmosphere

4.4 Kinetic isotope effect (KIE) experiment



Parallel reactions. Two 10 mL Schlenk tubes were added **2a** (2 mmol) and **2a-d$_8$** (2 mmol), separately. The mixtures were then sequentially added compound **1a** (0.2 mmol, 1.0 equiv.), HCl (36wt%, 35 μL, 2.0 equiv.), CH_3CN (2.0 mL). The reaction tubes were open to the air and stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 24 h. The reaction mixtures were quenched by $NaHCO_3$ and then extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated under reduced pressure and purified by column chromatography (petroleum ether/ethyl acetate = 10/1) on silica get to give the products **3a** and **3a-d$_6$** in 64% and 43% yields, respectively. k_H/k_D = 1.48.



Intermolecular competition. A mixture of compound **1a** (0.2 mmol, 1.0 equiv.), **2a** (0.1 mL), **2a-d$_8$** (0.1 mL), HCl (36wt%, 35 μL, 2.0 equiv.) in a 10 mL Schlenk tube was added CH_3CN (2.0 mL). The reaction mixture was open to the air and stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 24 h. The reaction mixture was quenched by $NaHCO_3$ and then extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated under reduced pressure and purified by column chromatography (petroleum ether/ethyl acetate = 10/1) on silica get to give the products **3a** and **3a-d$_6$**, with a ratio of 3.63:2.37, k_H/k_D = 1.53.

Kinetic isotope effect experiment suggesting that the alkyl C–H cleavage might not be the rate-determine step.

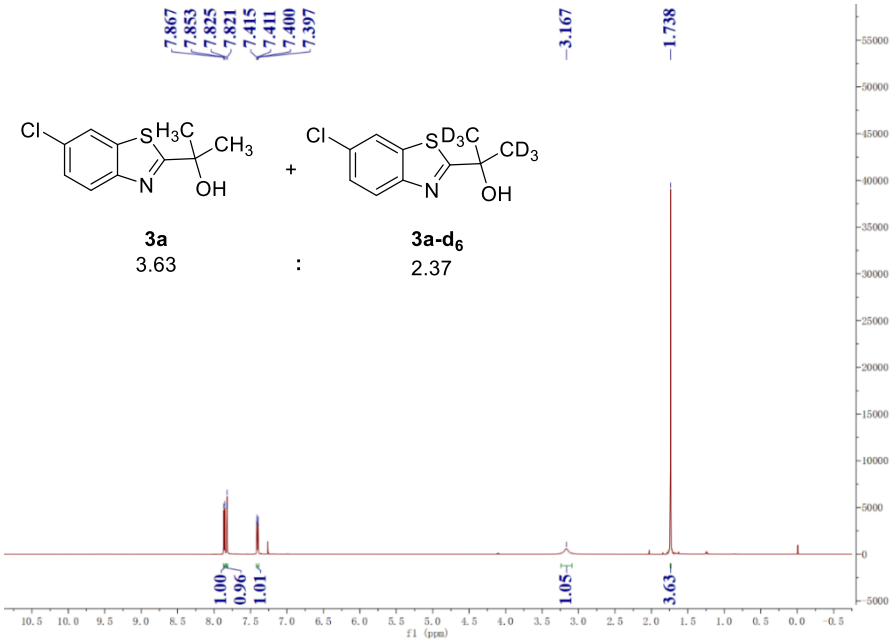


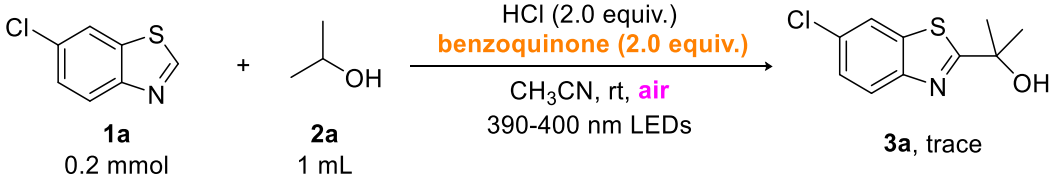
Figure S5. Determination of the ratio of **3a** and **3a-d$_6$** by ^{1}H NMR

4.5 Singlet oxygen quenching experiment

1a 0.2 mmol | **2a** 1 mL | **3a** 39%

A mixture of compound **1a** (0.2 mmol, 1.0 equiv.), **2a** (IPA, 1.0 mL), HCl (36wt%, 35 μL, 2.0 equiv.) and DABCO (0.4 mmol, 2.0 equiv.) in a 10 mL Schlenk tube was added H_2O (2.0 mL). The reaction tubes was open to the air and stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 24 h. The reaction mixtures were quenched by $NaHCO_3$ and then extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were washed by brine, dried over Na_2SO_4, filtered, concentrated under reduced pressure and purified by column chromatography (petroleum ether/ethyl acetate = 10/1) on silica get to give the products **3a** in 39% yields.

4.6 Superoxide radical quenching experiment



1a 0.2 mmol | **2a** 1 mL | **3a**, trace

A mixture of compound **1a** (0.2 mmol, 1.0 equiv.), **2a** (IPA, 1.0 mL), HCl (36wt%, 35 μL, 2.0 equiv.) and benzoquinone (0.4 mmol, 2.0 equiv.) in a 10 mL Schlenk tube was added CH_3CN (2.0 mL). The reaction tubes was open to the air and stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 24 h. After the reaction was completed, only a trace amount of **3a** was observed by TLC.

4.7 Fluorescence quenching Screening Studies

Preparation. Four formulated solutions were prepared with CH_3CN in 10 mL volumetric flasks. For flask A, 6-chlorobenzo[d]thiazole (**1a**, 0.5 mmol, 84.5 mg) was added; for flask B, 6-chlorobenzo[d]thiazole (**1a**, 0.5 mmol, 84.5 mg) and TFA (0.75 mmol, 57 μL) were added; for the flask C, Bu_4NCl (0.5 mmol, 139 mg) was added; for the flask D, isopropyl alcohol (**2a**, IPA, 0.5

mmol, 38 μL). All these flasks were diluted to 10 mL to set the concentration to be 0.05 M.

Fluorescence quenching experiments of 1a with Cl^-. A quartz cuvette (1 cm ×1 cm ×3.5 cm) was added 60 μL of the formulated solution from flask A and was diluted to 3 mL as a 1 μM **1a** solution, which was then irradiated at 350 nm. Duplicate experiments were performed with the addition of 0, 60, 90, 120, 180, 240 μL 0.05 M Bu_4NCl solution from flask C before diluted to 3 mL, emission spectra of the sample were collected instantly after each addition. The resulting fluorescence emission spectra are shown in Figure S6**.** No significant fluorescence quenching between excited **1a** and Bu_4NCl was observed.

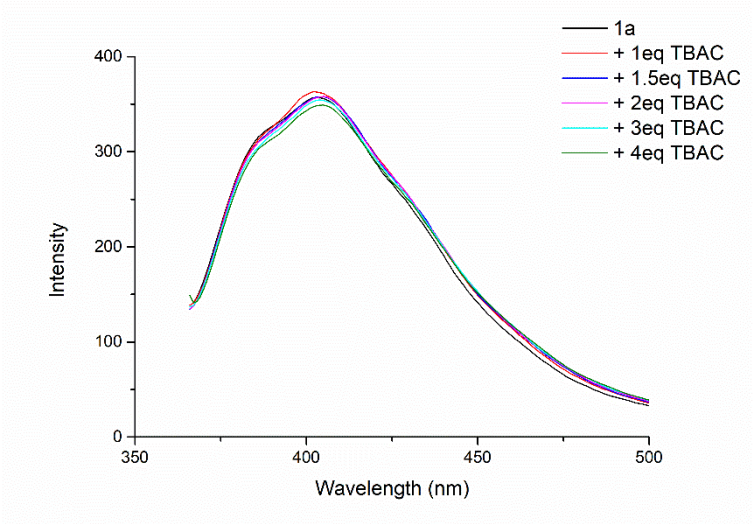


Figure S6. Emission intensity of 1 μM **1a** in CH_3CN, with varied amount of Bu_4NCl

Fluorescence quenching experiments of 1a-H^+ with Cl^-. A quartz cuvette (1 cm ×1 cm ×3.5 cm) was added 60 μL of the formulated solution from flask B and was diluted to 3 mL as a 1 μM **1a** solution, which was then irradiated at 350 nm. Duplicate experiments were performed with the addition of 0, 60, 120, 180, 240, 360 μL 0.05 M Bu_4NCl solution from flask C before diluted to 3 mL, emission spectra of the sample were collected instantly after each addition. The resulting fluorescence emission spectra are shown in Figure S7.

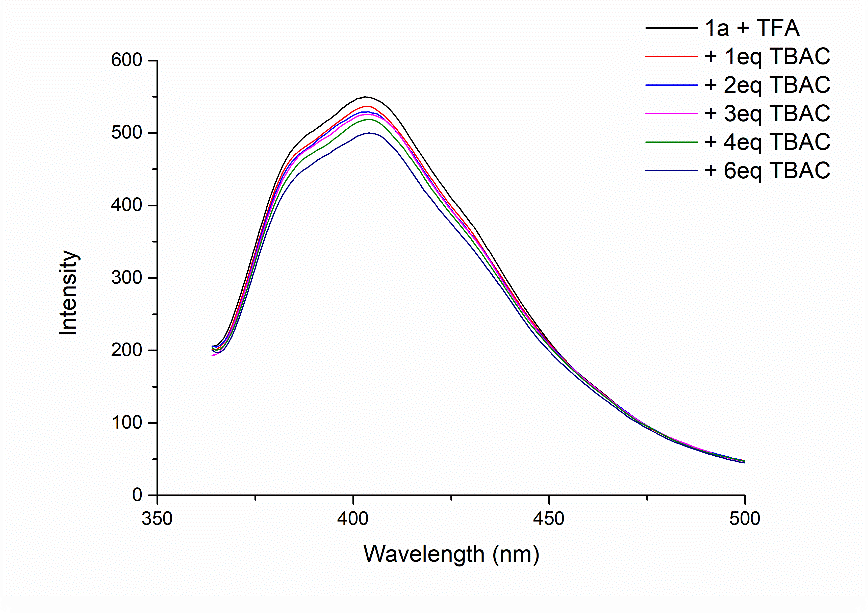


Figure S7. Emission intensity of 1 μM **1a-H**$^+$ in CH_3CN, with varied amount of Bu_4NCl

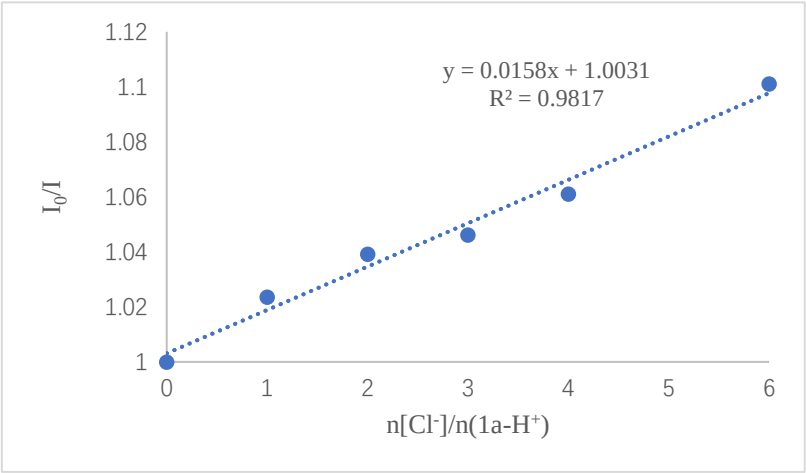


Figure S8. Stern-Volmer plot of **1a-H**$^+$ and Bu_4NCl

Fluorescence quenching experiments of 1a with IPA. A quartz cuvette (1 cm ×1 cm ×3.5 cm) was added 60 μL of the formulated solution from flask A and was diluted to 3 mL as a 1 μM **1a** solution, which was then irradiated at 365 nm. Duplicate experiments were performed with the addition of 0, 60, 120, 180, 240, 360μL 0.05 M IPA solution from flask D before diluted to 3 mL, emission spectra of the sample were collected instantly after each addition. The resulting fluorescence emission spectra are shown in Figure S9. No significant fluorescence quenching between excited **1a** and IPA was observed.

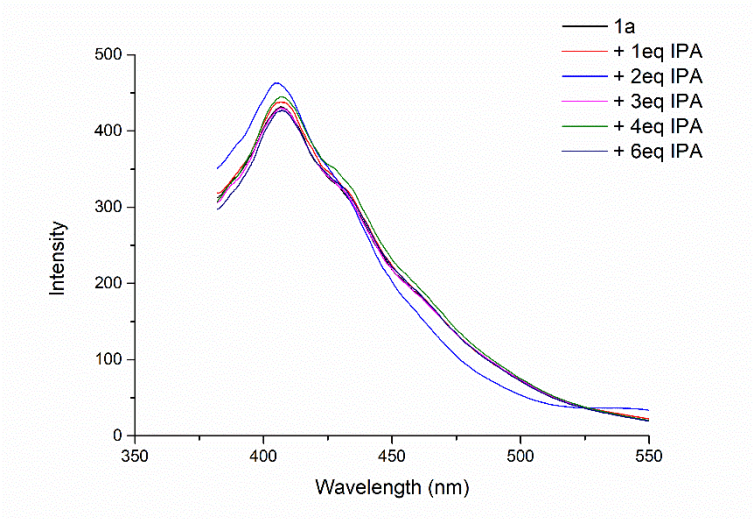


Figure S9. Emission intensity of 1 μM **1a** in CH_3CN, with varied amount of IPA

Fluorescence quenching experiments of 1a-H$^+$ with IPA. A quartz cuvette (1 cm ×1 cm ×3.5 cm) was added 60 μL of the formulated solution from flask B and was diluted to 3 mL as a 1 μM **1a** solution, which was then irradiated at 350 nm. Duplicate experiments were performed with the addition of 0, 60, 120, 180, 240, 360 μL 0.05 M IPA solution from flask D before diluted to 3 mL, emission spectra of the sample were collected instantly after each addition. The resulting fluorescence emission spectra are shown in Figure S10.

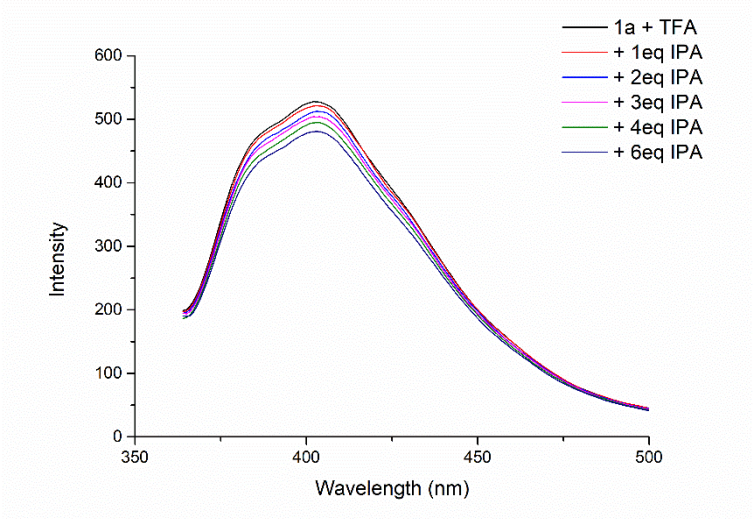


Figure S10. Emission intensity of 1 μM **1a-H$^+$** in CH_3CN, with varied amount of IPA

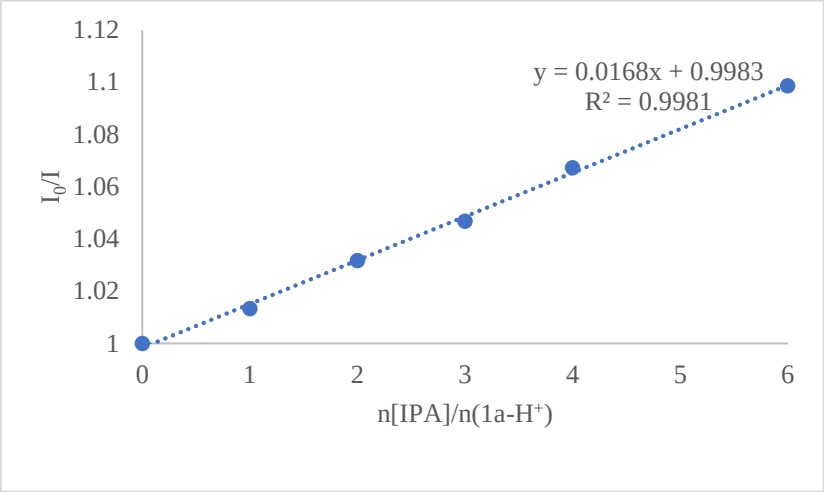


Figure S11. Stern-Volmer plot of **1a-H**$^+$ and IPA

4.8 Isomerization experiment of alcohols

Three 10 mL Schlenk tubes were added IPA (1.0 mL), 1-butanol (1.0 mL) and 3-pentanol (1.0 mL). After three cycles of evacuation and backfilling of the reaction flask with N_2. The mixtures were then sequentially added HCl (36wt%, 70 μL) and CH_3CN (2.0 mL). The reaction mixture stirred under the irradiation of 2×25 W Purple LEDs (λ = 390 – 400 nm) at room temperature for 48 h. After the reaction was completed, the reaction mixture was directly detected by ^{1}H NMR. The results of ^{1}H NMR spectrogram showed that no isomers formed in our conditions.

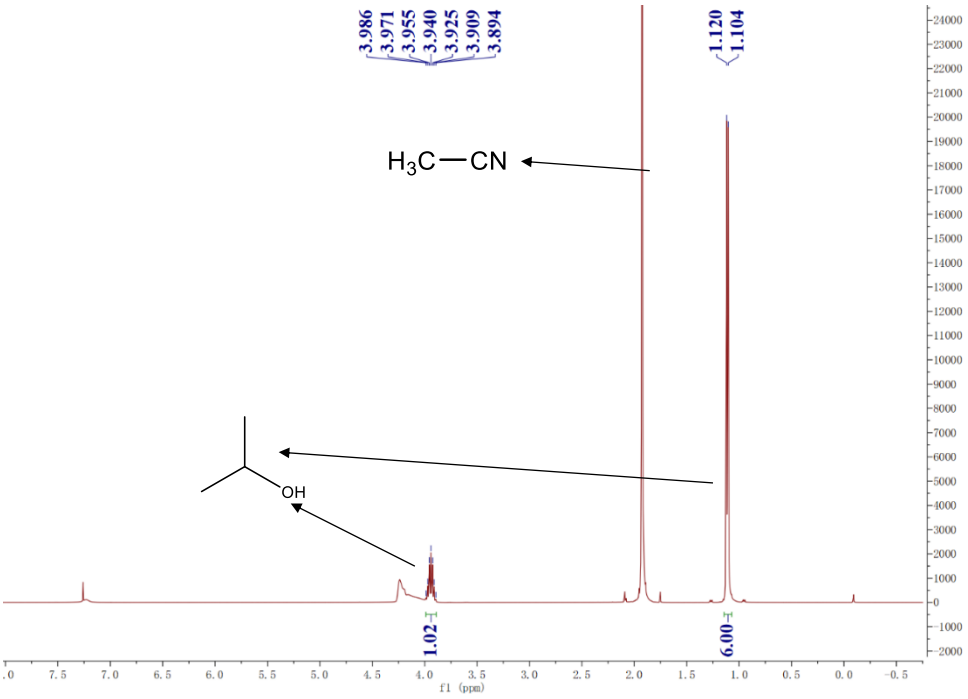


Figure S12. ^{1}H NMR (400 MHz, $CDCl_3$) spectrogram of IPA under acidic condition in CH_3CN

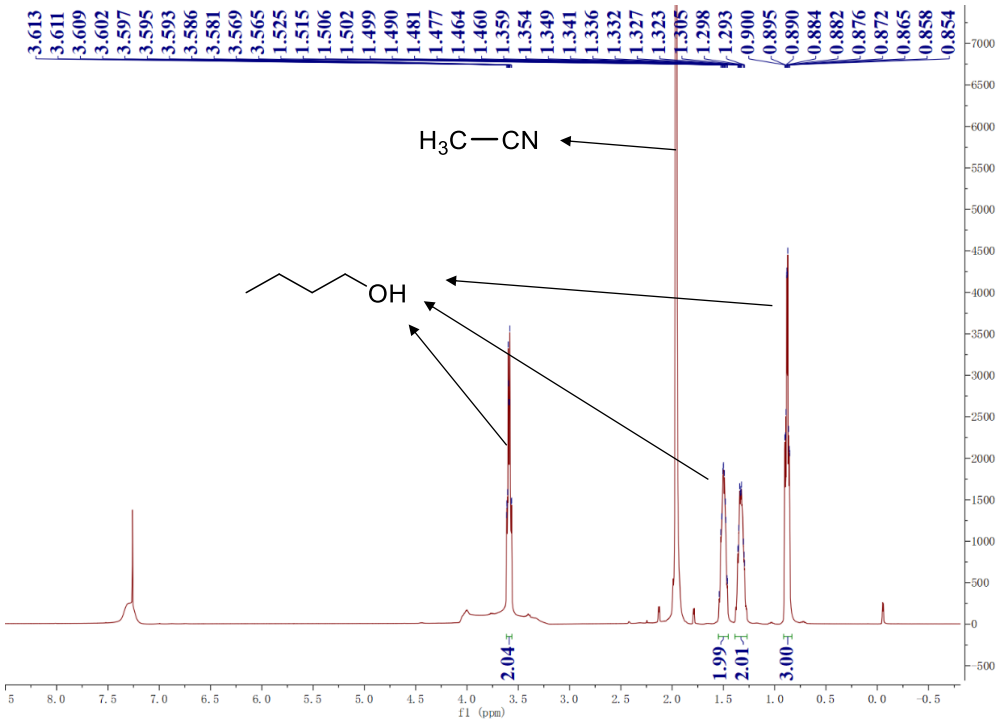


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) spectrogram of 1-butanol under acidic condition in CH_3CN

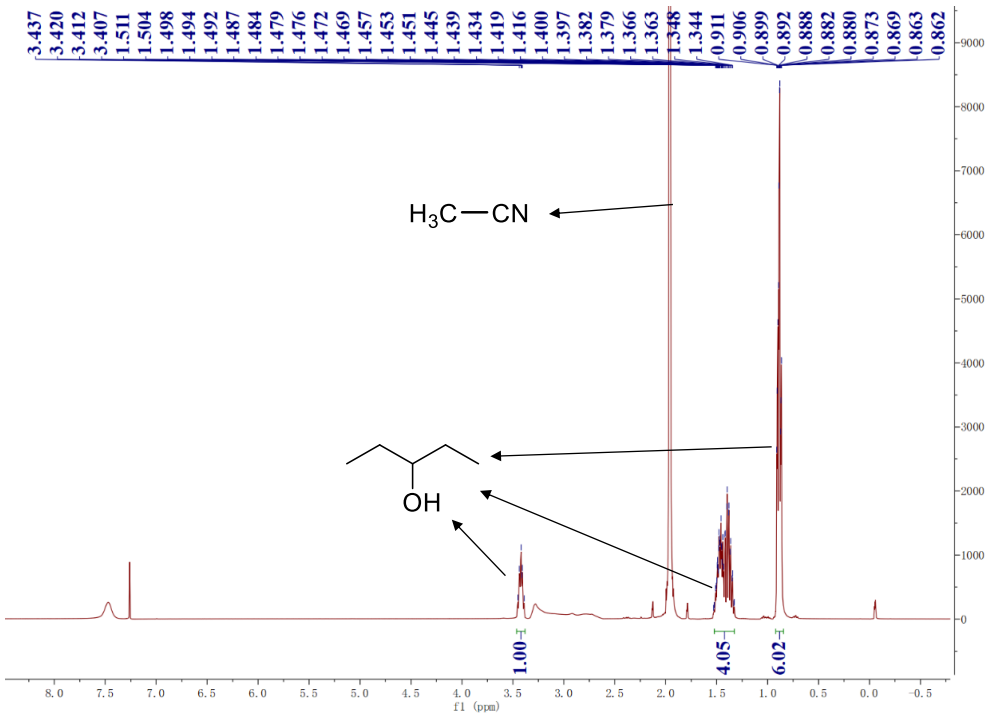
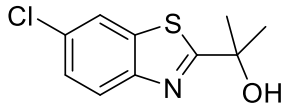
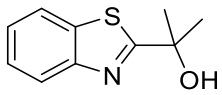


Figure S14. ^{1}H NMR (400 MHz, $CDCl_3$) spectrogram of 3-pentanol under acidic condition in CH_3CN

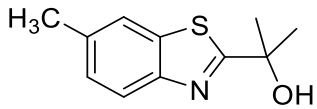
5. Characterization data for compounds



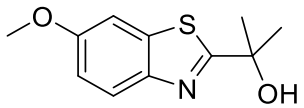
2-(6-chlorobenzo[d]thiazol-2-yl)propan-2-ol (3a). Yield = 82%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.85 (d, *J* = 2.1 Hz, 1H), 7.43 (dd, *J* = 8.7, 2.0 Hz, 1H), 2.77 (br, 1H), 1.75 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 180.69, 151.63, 136.51, 130.86, 126.88, 123.62, 121.41, 73.71, 30.74. **HRMS** (ESI) calcd for $C_{10}H_{11}ClNOS$ $[M+H]^+$: 228.0244, found 228.0243.



2-(benzo[d]thiazol-2-yl)propan-2-ol (3b). Yield = 65%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.2 Hz, 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.38 – 7.34 (m, 1H), 3.26 (br, 1H), 1.75 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.28, 152.96, 135.26, 126.09, 124.97, 122.83, 121.81, 73.63, 30.82.

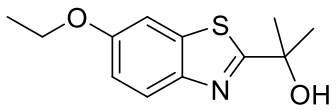


2-(6-methylbenzo[d]thiazol-2-yl)propan-2-ol (3c). Yield = 81%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.3 Hz, 1H), 7.59 (s, 1H), 7.23 (d, *J* = 8.3 Hz, 1H), 3.87 (br, 1H), 2.44 (s, 3H), 1.73 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.24, 151.15, 135.42, 134.92, 127.56, 122.29, 121.48, 73.52, 30.78, 21.48.

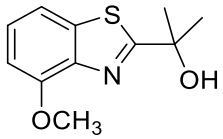


2-(6-methoxybenzo[d]thiazol-2-yl)propan-2-ol (3d). Yield = 67%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.9 Hz, 1H), 7.33 – 7.29 (m, 1H), 7.05 (dd, *J* = 8.9, 2.4 Hz, 1H), 3.86 (s, 3H), 3.18 (br, 1H), 1.73 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 177.51, 157.45, 147.45, 136.58, 123.29, 115.33,

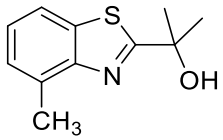
104.29, 73.46, 55.80, 30.77.



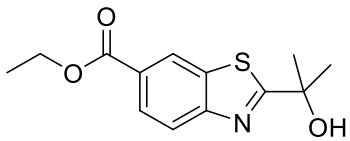
2-(6-ethoxybenzo[d]thiazol-2-yl)propan-2-ol (3e). Yield = 75%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.9 Hz, 1H), 7.31 (d, *J* = 2.5 Hz, 1H), 7.05 (dd, *J* = 8.9, 2.5 Hz, 1H), 4.08 (q, *J* = 7.0 Hz, 2H), 3.15 (br, 1H), 1.73 (s, 6H), 1.45 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 177.31, 156.82, 147.30, 136.55, 123.26, 115.80, 105.02, 73.45, 64.13, 30.79, 14.83. **HRMS** (ESI) calcd for $C_{12}H_{16}NO_2S$ $[M+H]^+$: 238.0896, found 238.0903.



2-(4-methoxybenzo[d]thiazol-2-yl)propan-2-ol (3f). Yield = 68%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.44 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.29 (td, *J* = 8.0, 0.9 Hz, 1H), 6.89 (dd, *J* = 8.0, 1.1 Hz, 1H), 4.01 (s, 3H), 3.29 (br, 1H), 1.76 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 178.89, 153.13, 143.14, 136.97, 125.82, 113.78, 106.56, 73.69, 56.00, 30.80.

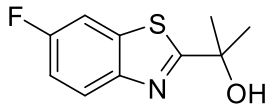


2-(4-methylbenzo[d]thiazol-2-yl)propan-2-ol (3g). Yield = 83%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.72 – 7.70 (m, 1H), 7.29 – 7.26 (m, 2H), 3.62 (br, 1H), 2.75 (s, 3H), 1.76 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 178.11, 152.05, 135.38, 132.97, 126.59, 124.86, 119.12, 73.42, 31.04, 18.30.

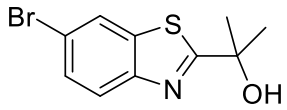


ethyl 2-(2-hydroxypropan-2-yl)benzo[d]thiazole-6-carboxylate (3h). Yield = 79%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.58 (d, *J* = 1.3 Hz, 1H), 8.12 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.97 (d, *J* = 8.6 Hz,

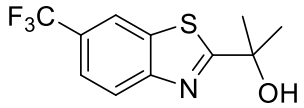
1H), 4.41 (q, *J* = 7.1 Hz, 2H), 3.22 (br, 1H), 1.76 (s, 6H), 1.41 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 184.17, 166.27, 156.11, 135.21, 127.21, 126.99, 123.99, 122.50, 73.88, 61.34, 30.67, 14.35. **HRMS** (ESI) calcd for $C_{13}H_{16}NO_3S$ $[M+H]^+$: 266.0845, found 266.0854.



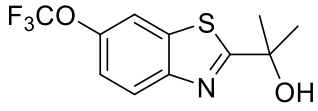
2-(6-fluorobenzo[d]thiazol-2-yl)propan-2-ol (3i). Yield = 71%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8.9, 4.8 Hz, 1H), 7.55 (dd, *J* = 8.1, 2.6 Hz, 1H), 7.20 (td, *J* = 8.9, 2.6 Hz, 1H), 2.86 (br, 1H), 1.74 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.78 (d, *J* = 3.1 Hz), 160.25 (d, *J* = 245.3 Hz), 149.70 (d, *J* = 1.3 Hz), 136.31 (d, *J* = 11.1 Hz), 123.79 (d, *J* = 9.4 Hz), 114.68 (d, *J* = 24.7 Hz), 107.94 (d, *J* = 26.6 Hz), 73.65, 30.74.



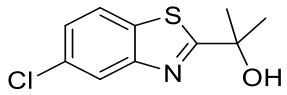
2-(6-bromobenzo[d]thiazol-2-yl)propan-2-ol (3j). Yield = 89%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 1.9 Hz, 1H), 7.82 (d, *J* = 8.7 Hz, 1H), 7.56 (dd, *J* = 8.7, 1.9 Hz, 1H), 2.93 (br, 1H), 1.74 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 180.74, 152.00, 137.01, 129.55, 124.34, 124.00, 118.47, 73.71, 30.73. **HRMS** (ESI) calcd for $C_{10}H_{11}BrNOS$ $[M+H]^+$: 273.9719, found 273.9719.



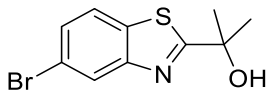
2-(6-(trifluoromethyl)benzo[d]thiazol-2-yl)propan-2-ol (3k). Yield = 78%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.18 (d, *J* = 1.5Hz, 1H), 8.06 (d, *J* = 8.6 Hz, 1H), 7.71 (dd, *J* = 8.6, 1.5 Hz, 1H), 2.87 (br, 1H), 1.77 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 183.57, 155.26, 135.46, 127.14 (q, *J* = 32.7 Hz), 125.08 (q, *J* = 270.7 Hz), 123.25, 123.02 (q, *J* = 3.4 Hz), 119.51 (q, *J* = 4.2 Hz), 73.94, 30.71. **HRMS** (ESI) calcd for $C_{11}H_{11}F_3NOS$ $[M+H]^+$: 262.0508, found 262.0514.



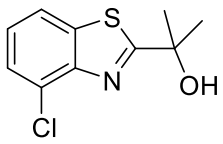
2-(6-(trifluoromethoxy)benzo[d]thiazol-2-yl)propan-2-ol (3l). Yield = 78%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.9 Hz, 1H), 7.75 – 7.72 (m, 1H), 7.35 – 7.31 (m, 1H), 3.17 (br, 1H), 1.75 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 181.67, 151.68, 146.23 (q, *J* = 2.0 Hz), 136.13, 123.66, 120.53 (q, *J* = 257.3 Hz), 119.98, 114.37, 73.76, 30.67. **HRMS** (ESI) calcd for $C_{11}H_{11}F_3NO_2S$ $[M+H]^+$: 278.0457, found 278.0466.



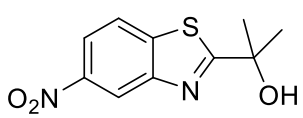
2-(5-chlorobenzo[d]thiazol-2-yl)propan-2-ol (3m). Yield = 84%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 2.0 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.34 (dd, *J* = 8.5, 2.0 Hz, 1H), 3.01 (br, 1H), 1.74 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 182.24, 153.96, 133.57, 132.05, 125.44, 122.76, 122.50, 73.75, 30.73.



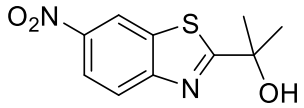
2-(5-bromobenzo[d]thiazol-2-yl)propan-2-ol (3n). Yield = 84%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 1.8 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.47 (dd, *J* = 8.5, 1.9 Hz, 1H), 2.92 (br, 1H), 1.74 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 182.00, 154.31, 134.13, 128.05, 125.83, 122.84, 119.60, 73.73, 30.74. **HRMS** (ESI) calcd for $C_{10}H_{11}BrNOS$ $[M+H]^+$: 273.9719, found 273.9729.



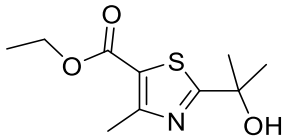
2-(4-chlorobenzo[d]thiazol-2-yl)propan-2-ol (3o). Yield = 80%; Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.76 – 7.71 (m, 1H), 7.48 – 7.44 (m, 1H), 7.29 – 7.24 (m, 1H), 3.83 (br, 1H), 1.78 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 181.35, 150.12, 136.78, 127.55, 126.24, 125.38, 120.33, 73.81, 30.73. **HRMS** (ESI) calcd for $C_{10}H_{11}ClNOS$ $[M+H]^+$: 228.0244, found 228.0246.



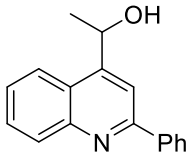
2-(5-nitrobenzo[d]thiazol-2-yl)propan-2-ol (3p). Yield = 35%; Yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 2.1 Hz, 1H), 8.23 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.99 (d, *J* = 8.8 Hz, 1H), 3.10 (br, 1H), 1.77 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 184.34, 153.18, 146.63, 142.09, 122.28, 119.35, 118.43, 74.00, 30.61.



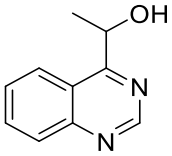
2-(6-nitrobenzo[d]thiazol-2-yl)propan-2-ol (3q). Yield = 28%; Yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 2.3 Hz, 1H), 8.30 (dd, *J* = 9.0, 2.3 Hz, 1H), 8.02 (d, *J* = 9.0 Hz, 1H), 3.29 (br, 1H), 1.77 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 186.99, 157.22, 144.70, 135.71, 123.13, 121.47, 118.42, 74.21, 30.58.



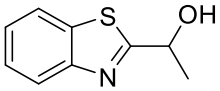
ethyl 2-(2-hydroxypropan-2-yl)-4-methylthiazole-5-carboxylate (3r). Yield = 75%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 4.30 (q, *J* = 7.1 Hz, 2H), 3.16 (br, 1H), 2.67 (s, 3H), 1.64 (s, 6H), 1.34 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 181.92, 162.41, 159.86, 121.98, 73.37, 61.16, 30.72, 17.41, 14.29. **HRMS** (ESI) calcd for $C_{10}H_{16}NO_3S$ $[M+H]^+$: 230.0845, found 230.0856.



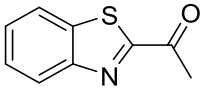
1-(2-phenylquinolin-4-yl)ethan-1-ol (3s). Yield = 43%; Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.4 Hz, 1H), 8.12 – 8.08 (m, 2H), 7.97 (s, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.70 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.52 – 7.42 (m, 4H), 5.59 (q, *J* = 6.5 Hz, 1H), 2.60 (br, 1H), 1.64 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.22, 152.10, 148.12, 139.34, 130.34, 129.44, 129.34, 128.78, 127.55, 126.23, 124.26, 122.71, 114.44, 66.37, 24.58.



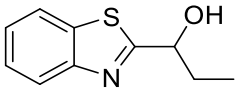
1-(quinazolin-4-yl)ethan-1-ol (3t). Yield = 56%; White solid; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.80 (s, 1H), 8.11 (dd, J = 7.9, 1.2 Hz, 1H), 7.84 – 7.76 (m, 1H), 7.64 (d, J = 8.1 Hz, 1H), 7.53 – 7.45 (m, 1H), 5.66 (s, 1H), 4.60 (q, J = 6.3 Hz, 1H), 1.43 (d, J = 6.6 Hz, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ 162.00, 160.20, 148.93, 134.84, 127.43, 126.77, 126.29, 121.67, 67.62, 22.06.



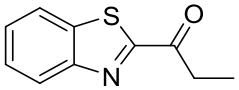
1-(benzo[d]thiazol-2-yl)ethan-1-ol (4a). Yield = 33%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.92 (d, J = 8.2 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.43 – 7.40 (m, 1H), 7.34 – 7.31 (m, 1H), 5.25 (q, J = 6.6 Hz, 1H), 4.41 (br, 1H), 1.68 (d, J = 6.6 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 177.80, 152.73, 134.67, 126.10, 125.00, 122.67, 121.83, 68.34, 24.05.



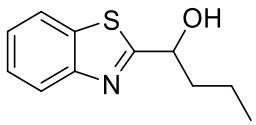
1-(benzo[d]thiazol-2-yl)ethan-1-one (4a′). Yield = 21%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.18 (d, J = 8.2 Hz, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.58 – 7.55 (m, 1H), 7.53 – 7.50 (m, 1H), 2.82 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 193.13, 166.50, 153.58, 137.44, 127.70, 126.98, 125.45, 122.44, 26.16.



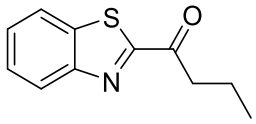
1-(benzo[d]thiazol-2-yl)propan-1-ol (4b). Yield = 31%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98 (d, J = 8.1 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.48 – 7.46 (m, 1H), 7.39 – 7.36 (m, 1H), 5.05 (dd, J = 7.3, 4.9 Hz, 1H), 3.07 (br, 1H), 2.13 – 1.92 (m, 2H), 1.06 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 176.13, 152.58, 134.78, 126.13, 125.06, 122.80, 121.84, 73.39, 31.14, 9.38.



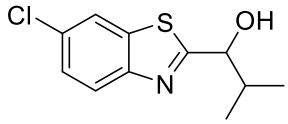
1-(benzo[d]thiazol-2-yl)propan-1-one (4b′). Yield = 17%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.58 – 7.55 (m, 1H), 7.53 – 7.50 (m, 1H), 3.30 (q, *J* = 7.3 Hz, 2H), 1.30 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.98, 166.36, 153.59, 137.21, 127.56, 126.91, 125.36, 122.42, 32.09, 7.89.



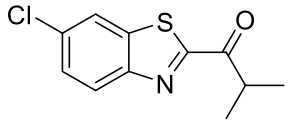
1-(benzo[d]thiazol-2-yl)butan-1-ol (4c). Yield = 40%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.37 – 7.34 (m, 1H), 5.09 (dd, *J* = 7.9, 4.7 Hz, 1H), 3.35 (br, 1H), 2.06 – 1.84 (m, 2H), 1.63 – 1.44 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.83, 152.70, 134.73, 126.09, 125.01, 122.78, 121.84, 72.06, 40.18, 18.50, 13.83.



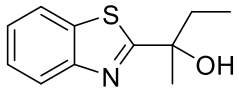
1-(benzo[d]thiazol-2-yl)butan-1-one (4c′). Yield = 26%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 7.9 Hz, 1H), 7.58 – 7.48 (m, 2H), 3.24 (t, *J* = 7.4 Hz, 2H), 1.89 – 1.79 (m, 2H), 1.04 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 195.47, 166.63, 153.59, 137.24, 127.58, 126.92, 125.38, 122.43, 40.49, 17.51, 13.79.



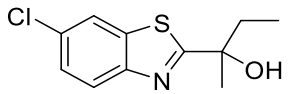
1-(6-chlorobenzo[d]thiazol-2-yl)-2-methylpropan-1-ol (4d). Yield = 42%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.7 Hz, 1H), 7.81 (d, *J* = 2.1 Hz, 1H), 7.39 (dd, *J* = 8.7, 2.1 Hz, 1H), 4.85 (d, *J* = 4.9 Hz, 1H), 3.61 (br, 1H), 2.28 – 2.20 (m, 1H), 1.03 (d, *J* = 6.9 Hz, 3H), 0.96 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 176.64, 151.16, 135.95, 130.94, 126.84, 123.50, 121.36, 76.79, 35.13, 18.97, 16.48. **HRMS** (ESI) calcd for $C_{11}H_{13}ClNOS$ $[M+H]^+$: 242.0401, found 242.0400.



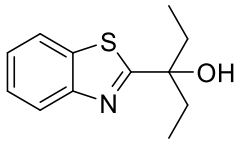
1-(6-chlorobenzo[d]thiazol-2-yl)-2-methylpropan-1-one (4d′). Yield = 23%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.8 Hz, 1H), 7.93 (d, *J* = 2.0 Hz, 1H), 7.50 (dd, *J* = 8.8, 2.1 Hz, 1H), 3.92 (hept, *J* = 6.9 Hz, 1H), 1.31 (d, *J* = 7.0 Hz, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 198.86, 166.52, 152.12, 138.40, 133.85, 127.91, 126.17, 121.94, 36.40, 18.63.



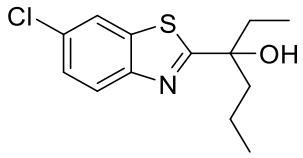
2-(benzo[d]thiazol-2-yl)butan-2-ol (4e). Yield = 59%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.45 (m, 1H), 7.38 – 7.35 (m, 1H), 3.31 (br, 1H), 2.09 – 1.97 (m, 2H), 1.71 (s, 3H), 0.93 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.44, 152.89, 135.41, 126.01, 124.88, 122.84, 121.76, 76.09, 36.29, 29.14, 8.02.



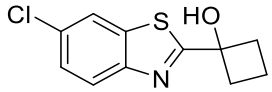
2-(6-chlorobenzo[d]thiazol-2-yl)butan-2-ol (4e'). Yield = 78%; Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.84 (d, *J* = 2.1 Hz, 1H), 7.42 (dd, *J* = 8.7, 2.1 Hz, 1H), 2.90 (br, 1H), 2.11 – 1.93 (m, 2H), 1.69 (s, 3H), 0.92 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.11, 151.60, 136.61, 130.79, 126.77, 123.60, 121.35, 76.16, 36.18, 28.94, 7.95.



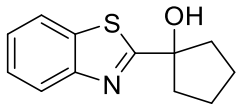
3-(benzo[d]thiazol-2-yl)pentan-3-ol (4f). Yield = 61%; Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.40 – 7.34 (m, 1H), 3.38 (br, 1H), 2.00 (dq, *J* = 14.1, 7.1 Hz, 4H), 0.88 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 178.32, 152.69, 135.59, 125.95, 124.83, 122.83, 121.75, 78.73, 35.14, 7.72. **HRMS** (ESI) calcd for $C_{12}H_{16}NOS$ $[M+H]^+$: 222.0947, found 222.0955.



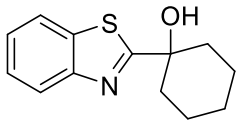
3-(6-chlorobenzo[d]thiazol-2-yl)hexan-3-ol (4g). Yield = 43%; Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.7 Hz, 1H), 7.84 (d, *J* = 2.0 Hz, 1H), 7.42 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.12 (br, 1H), 2.06 – 1.90 (m, 4H), 1.53 – 1.45 (m, 1H), 1.17 – 1.09 (m, 1H), 0.89 – 0.86 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.42, 151.40, 136.69, 130.73, 126.73, 123.56, 121.33, 78.64, 44.46, 35.30, 16.71, 14.26, 7.66. **HRMS** (ESI) calcd for $C_{13}H_{17}ClNOS$ $[M+H]^+$: 270.0714, found 270.0721.



1-(6-chlorobenzo[d]thiazol-2-yl)cyclobutan-1-ol (4h). Yield = 52%; Pale yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.7 Hz, 1H), 7.84 (d, *J* = 2.0 Hz, 1H), 7.43 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.23 (br, 1H), 2.80 – 2.71 (m, 2H), 2.56 – 2.47 (m, 2H), 2.14 – 2.01 (m, 2H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 178.52, 151.35, 136.41, 130.91, 126.92, 123.62, 121.40, 76.74, 37.82, 12.81. **HRMS** (ESI) calcd for $C_{11}H_{11}ClNOS$ $[M+H]^+$: 240.0244, found 240.0253.

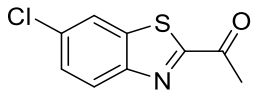


1-(benzo[d]thiazol-2-yl)cyclopentan-1-ol (4i). Yield = 54%; Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 3.31 (br, 1H), 2.34 – 2.29 (m, 2H), 2.12 – 2.09 (m, 2H), 2.05 – 1.89 (m, 4H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.45, 153.16, 135.32, 126.00, 124.80, 122.75, 121.71, 83.92, 42.72, 24.24.

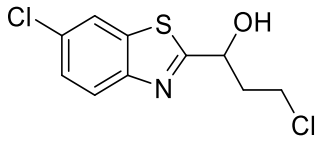


1-(benzo[d]thiazol-2-yl)cyclohexan-1-ol (4j). Yield = 66%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.33 (m, 1H), 3.09 (br,

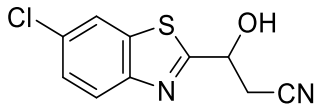
1H), 2.10 – 2.05 (m, 2H), 1.98 – 1.93 (m, 2H), 1.80 – 1.66 (m, 5H), 1.42 – 1.36 (m, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 180.91, 153.07, 135.08, 125.96, 124.82, 122.83, 121.77, 74.81, 38.41, 25.13, 21.73.



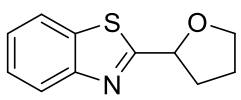
1-(6-chlorobenzo[d]thiazol-2-yl)ethan-1-one (4k). Yield = 41%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.8 Hz, 1H), 7.94 (d, *J* = 2.0 Hz, 1H), 7.52 (dd, *J* = 8.8, 2.1 Hz, 1H), 2.80 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 192.80, 166.92, 152.05, 138.54, 134.03, 128.06, 126.22, 122.00, 26.09.



3-chloro-1-(6-chlorobenzo[d]thiazol-2-yl)propan-1-ol (4l). Yield = 31%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.86 (d, *J* = 1.9 Hz, 1H), 7.44 (dd, *J* = 8.7, 2.0 Hz, 1H), 5.34 (dd, *J* = 9.0, 3.8 Hz, 1H), 3.89 – 3.83 (m, 1H), 3.78 – 3.74 (m, 1H), 2.86 (br, 1H), 2.51 – 2.46 (m, 1H), 2.37 – 2.32 (m, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 175.61, 151.40, 135.99, 131.23, 127.12, 123.72, 121.50, 69.38, 40.78, 40.04. **HRMS** (ESI) calcd for $C_{10}H_{10}Cl_2NOS$ $[M+H]^+$: 261.9855, found 261.9863.

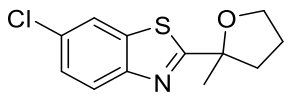


3-(6-chlorobenzo[d]thiazol-2-yl)-3-hydroxypropanenitrile (4m). Yield = 32%; Yellow solid; **^{1}H NMR** (600 MHz, DMSO-d_6) δ 8.28 (d, *J* = 2.1 Hz, 1H), 7.98 (d, *J* = 8.7 Hz, 1H), 7.55 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.24 – 7.19 (m, 1H), 5.32 – 5.28 (m, 1H), 3.21 – 3.11 (m, 2H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 177.00, 152.18, 136.66, 130.15, 127.22, 124.34, 122.59, 118.39, 67.09, 26.15. **HRMS** (ESI) calcd for $C_{10}H_8ClN_2OS$ $[M+H]^+$: 239.0040, found 239.0045.

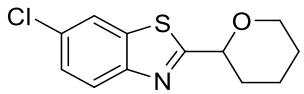


2-(tetrahydrofuran-2-yl)benzo[d]thiazole (6a). Yield = 55%; Yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.36 – 7.34 (m, 1H), 5.34 (dd,

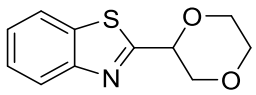
J = 7.8, 5.4 Hz, 1H), 4.16 – 4.13 (m, 1H), 4.01 – 3.91 (m, 1H), 2.54 – 2.48 (m, 1H), 2.30 – 2.21 (m, 1H), 2.05 – 1.99 (m, 2H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 176.41, 153.60, 134.71, 125.94, 124.79, 122.77, 121.77, 78.75, 69.46, 33.39, 25.71.



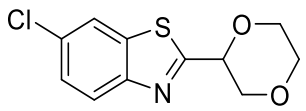
6-chloro-2-(2-methyltetrahydrofuran-2-yl)benzo[d]thiazole (6b). Yield = 50%; Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.7 Hz, 1H), 7.83 (d, *J* = 2.0 Hz, 1H), 7.40 (dd, *J* = 8.7, 2.1 Hz, 1H), 4.07 (dd, *J* = 7.3, 6.2 Hz, 2H), 2.62 – 2.55 (m, 1H), 2.18 – 2.11 (m, 1H), 2.09 – 1.99 (m, 1H), 1.97 – 1.90 (m, 1H), 1.72 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 181.46, 152.50, 136.48, 130.57, 126.60, 123.50, 121.35, 84.92, 69.10, 39.19, 27.83, 26.15. **HRMS** (ESI) calcd for $C_{12}H_{13}ClNOS$ $[M+H]^+$: 254.0401, found 254.0409.



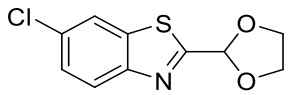
6-chloro-2-(tetrahydro-2H-pyran-2-yl)benzo[d]thiazole (6c). Yield = 58%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.7 Hz, 1H), 7.87 (d, *J* = 2.0 Hz, 1H), 7.42 (dd, *J* = 8.7, 2.1 Hz, 1H), 4.76 (dd, *J* = 10.2, 2.6 Hz, 1H), 4.22 – 4.16 (m, 1H), 3.69 (td, *J* = 11.5, 2.5 Hz, 1H), 2.31 – 2.23 (m, 1H), 2.01 – 1.97 (m, 1H), 1.76 – 1.69 (m, 3H), 1.66 – 1.60 (m, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.67, 151.47, 135.90, 130.78, 126.73, 123.61, 121.39, 77.68, 69.02, 32.35, 25.56, 22.93. **HRMS** (ESI) calcd for $C_{12}H_{13}ClNOS$ $[M+H]^+$: 254.0401, found 254.0406.



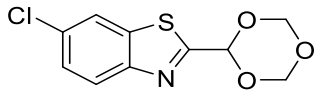
2-(1,4-dioxan-2-yl)benzo[d]thiazole (6d). Yield = 64%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.9 Hz, 1H), 7.90 (d, *J* = 7.7 Hz, 1H), 7.48 – 7.46 (m, 1H), 7.39 – 7.36 (m, 1H), 5.08 – 5.02 (m, 1H), 4.29 (d, *J* = 11.6 Hz, 1H), 4.02 – 3.94 (m, 2H), 3.86 – 3.66 (m, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 169.02, 152.98, 134.55, 126.13, 125.15, 123.11, 121.79, 75.43, 70.49, 66.99, 66.40.



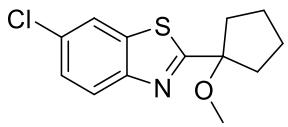
6-chloro-2-(1,4-dioxan-2-yl)benzo[d]thiazole (6d'). Yield = 73%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.92 – 7.87 (m, 2H), 7.44 (dd, *J* = 8.7, 2.1 Hz, 1H), 5.03 (dd, *J* = 9.7, 3.1 Hz, 1H), 4.29 (dd, *J* = 11.6, 3.1 Hz, 1H), 4.05 – 3.93 (m, 2H), 3.87 – 3.73 (m, 2H), 3.69 (dd, *J* = 11.6, 9.7 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.67, 151.60, 135.84, 131.16, 126.96, 123.88, 121.40, 75.24, 70.33, 66.98, 66.39.



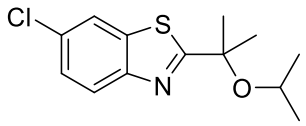
6-chloro-2-(1,3-dioxolan-2-yl)benzo[d]thiazole (6e). Yield = 52%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.7 Hz, 1H), 7.87 (d, *J* = 2.0 Hz, 1H), 7.44 (dd, *J* = 8.7, 2.1 Hz, 1H), 6.20 (s, 1H), 4.19 – 4.11 (m, 4H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 169.79, 151.84, 136.16, 131.72, 127.14, 124.57, 121.52, 100.32, 65.81.



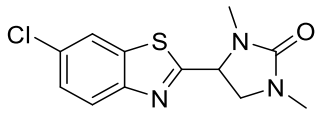
6-chloro-2-(1,3,5-trioxan-2-yl)benzo[d]thiazole (6f). Yield = 77%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 – 7.94 (m, 1H), 7.91 – 7.88 (m, 1H), 7.47 – 7.43 (m, 1H), 6.24 – 6.21 (m, 1H), 5.42 – 5.37 (m, 2H), 5.37 – 5.32 (m, 2H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 165.99, 151.15, 136.08, 132.01, 127.31, 124.71, 121.57, 97.80, 93.40. **HRMS** (ESI) calcd for $C_{10}H_9ClNO_3S$ $[M+H]^+$: 257.9986, found 257.9993.



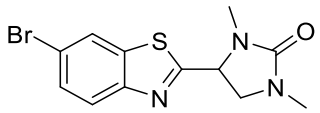
6-chloro-2-(1-methoxycyclopentyl)benzo[d]thiazole (6g). Yield = 63%; Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.84 (d, *J* = 2.0 Hz, 1H), 7.40 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.24 (s, 3H), 2.26 – 2.18 (m, 4H), 1.91 – 1.82 (m, 4H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 177.96, 151.60, 137.05, 130.89, 126.57, 123.75, 121.33, 89.25, 52.31, 37.55, 23.66. **HRMS** (ESI) calcd for $C_{13}H_{15}ClNOS$ $[M+H]^+$: 268.0557, found 268.0559.



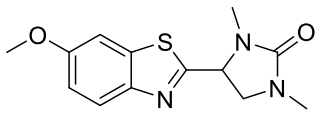
6-chloro-2-(2-isopropoxypropan-2-yl)benzo[d]thiazole (6h). Yield = 32%; Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.83 (d, *J* = 2.1 Hz, 1H), 7.39 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.86 (hept, *J* = 6.1 Hz, 1H), 1.70 (s, 6H), 1.17 (d, *J* = 6.1 Hz, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 180.54, 151.50, 136.86, 130.75, 126.48, 123.73, 121.27, 78.00, 66.46, 28.19, 24.77. **HRMS** (ESI) calcd for $C_{13}H_{17}ClNOS$ $[M+H]^+$: 270.0714, found 270.0718.



4-(6-chlorobenzo[d]thiazol-2-yl)-1,3-dimethylimidazolidin-2-one (8a). Yield = 68%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.7 Hz, 1H), 7.79 (d, *J* = 2.0 Hz, 1H), 7.36 (dd, *J* = 8.7, 2.1 Hz, 1H), 4.81 (dd, *J* = 9.1, 7.3 Hz, 1H), 3.75 (t, *J* = 9.2 Hz, 1H), 3.28 (dd, *J* = 9.0, 7.3 Hz, 1H), 2.78 (s, 3H), 2.75 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.33, 160.74, 151.47, 136.19, 131.56, 127.16, 123.90, 121.64, 58.75, 51.89, 31.16, 30.78. **HRMS** (ESI) calcd for $C_{12}H_{13}ClN_3OS$ $[M+H]^+$: 282.0462, found 282.0476.

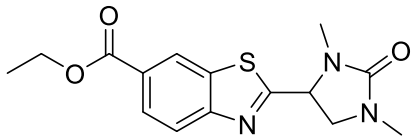


4-(6-bromobenzo[d]thiazol-2-yl)-1,3-dimethylimidazolidin-2-one (8b). Yield = 76%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 1.9 Hz, 1H), 7.86 (d, *J* = 8.7 Hz, 1H), 7.62 (dd, *J* = 8.7, 1.9 Hz, 1H), 4.90 (dd, *J* = 9.3, 7.2 Hz, 1H), 3.84 (t, *J* = 9.2 Hz, 1H), 3.36 (dd, *J* = 9.2, 7.2 Hz, 1H), 2.87 (s, 3H), 2.84 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.66, 160.83, 151.61, 136.60, 130.07, 124.68, 124.25, 119.48, 58.79, 51.97, 31.22, 30.89. **HRMS** (ESI) calcd for $C_{12}H_{13}BrN_3OS$ $[M+H]^+$: 327.9937, found 327.9937.

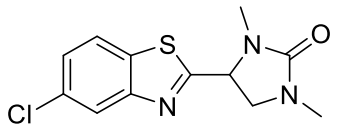


4-(6-methoxybenzo[d]thiazol-2-yl)-1,3-dimethylimidazolidin-2-one (8c). Yield = 51%; White solid;

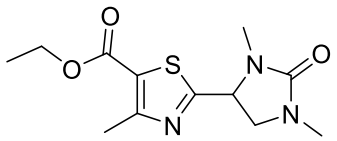
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.9 Hz, 1H), 7.33 (d, *J* = 2.5 Hz, 1H), 7.08 (dd, *J* = 8.9, 2.5 Hz, 1H), 4.86 (dd, *J* = 9.2, 7.4 Hz, 1H), 3.87 (s, 3H), 3.80 (t, *J* = 9.2 Hz, 1H), 3.35 (dd, *J* = 9.2, 7.4 Hz, 1H), 2.85 (s, 3H), 2.81 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 168.84, 160.91, 158.07, 147.22, 136.46, 123.63, 115.89, 104.37, 58.84, 55.84, 52.12, 31.20, 30.66. **HRMS** (ESI) calcd for $C_{13}H_{16}N_3O_2S$ $[M+H]^+$: 278.0958, found 278.0960.



ethyl 2-(1,3-dimethyl-2-oxoimidazolidin-4-yl)benzo[d]thiazole-6-carboxylate (8d). Yield = 74%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.58 (d, *J* = 1.4 Hz, 1H), 8.12 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.97 (d, *J* = 8.6 Hz, 1H), 4.88 (dd, *J* = 9.3, 7.1 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.81 (t, *J* = 9.3 Hz, 1H), 3.34 (dd, *J* = 9.2, 7.1 Hz, 1H), 2.82 (s, 3H), 2.81 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 175.41, 165.80, 160.75, 155.76, 134.89, 127.80, 127.48, 124.13, 122.85, 61.34, 58.91, 51.90, 31.13, 30.84, 14.31. **HRMS** (ESI) calcd for $C_{15}H_{18}N_3O_3S$ $[M+H]^+$: 320.1063, found 320.1064.

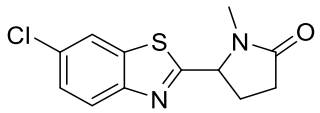


4-(5-chlorobenzo[d]thiazol-2-yl)-1,3-dimethylimidazolidin-2-one (8e). Yield = 65%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 1.9 Hz, 1H), 7.80 (d, *J* = 8.6 Hz, 1H), 7.38 (dd, *J* = 8.6, 2.0 Hz, 1H), 4.88 (dd, *J* = 9.3, 7.1 Hz, 1H), 3.82 (t, *J* = 9.3 Hz, 1H), 3.34 (dd, *J* = 9.2, 7.1 Hz, 1H), 2.85 (s, 3H), 2.83 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 173.90, 160.81, 153.83, 133.28, 132.45, 126.20, 123.05, 122.79, 58.84, 51.99, 31.18, 30.82. **HRMS** (ESI) calcd for $C_{12}H_{13}ClN_3OS$ $[M+H]^+$: 282.0462, found 282.0468.

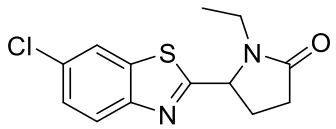


ethyl 2-(1,3-dimethyl-2-oxoimidazolidin-4-yl)-4-methylthiazole-5-carboxylate (8f). Yield = 48%;

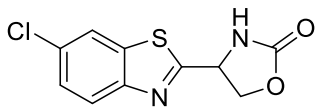
White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 4.70 (dd, *J* = 9.1, 7.0 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 3.74 (t, *J* = 9.2 Hz, 1H), 3.23 (dd, *J* = 6.5, 2.5 Hz, 1H), 2.81 (s, 3H), 2.79 (s, 3H), 2.68 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 173.31, 161.83, 160.74, 160.10, 123.04, 61.41, 58.33, 52.34, 31.13, 30.65, 17.25, 14.25. **HRMS** (ESI) calcd for $C_{12}H_{18}N_3O_3S$ $[M+H]^+$: 284.1063, found 284.1069.



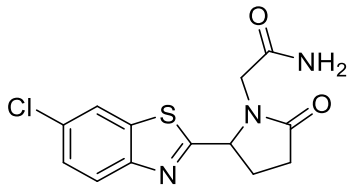
5-(6-chlorobenzo[d]thiazol-2-yl)-1-methylpyrrolidin-2-one (8g). Yield = 44%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.85 (d, *J* = 2.0 Hz, 1H), 7.44 (dd, *J* = 8.7, 2.1 Hz, 1H), 4.98 (dd, *J* = 8.7, 4.2 Hz, 1H), 2.85 (s, 3H), 2.68 – 2.58 (m, 2H), 2.50 – 2.43 (m, 1H), 2.21 – 2.14 (m, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 175.07, 172.87, 151.59, 136.00, 131.65, 127.30, 124.02, 121.60, 62.65, 29.29, 28.94, 26.60. **HRMS** (ESI) calcd for $C_{12}H_{12}ClN_2OS$ $[M+H]^+$: 267.0353, found 267.0358.



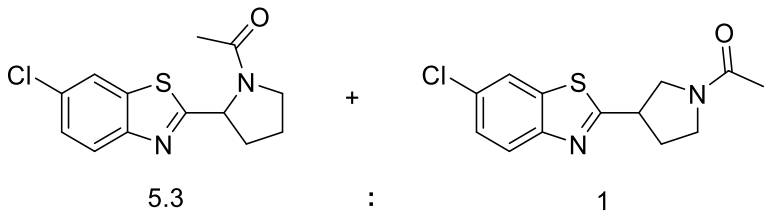
5-(6-chlorobenzo[d]thiazol-2-yl)-1-ethylpyrrolidin-2-one (8h). Yield = 46%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.7 Hz, 1H), 7.86 (d, *J* = 2.0 Hz, 1H), 7.46 (dd, *J* = 8.7, 2.1 Hz, 1H), 5.13 (dd, *J* = 8.6, 3.9 Hz, 1H), 3.81 (dq, *J* = 14.6, 7.3 Hz, 1H), 2.96 – 2.90 (m, 1H), 2.71 – 2.59 (m, 2H), 2.52 – 2.46 (m, 1H), 2.22 – 2.17 (m, 1H), 1.09 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.72, 173.31, 151.55, 136.03, 131.67, 127.30, 124.02, 121.60, 59.86, 36.43, 29.61, 26.80, 12.45. **HRMS** (ESI) calcd for $C_{13}H_{14}ClN_2OS$ $[M+H]^+$: 281.0510, found 281.0515.



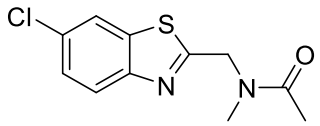
4-(6-chlorobenzo[d]thiazol-2-yl)oxazolidin-2-one (8i). Yield = 63%; Yellow solid; **^{1}H NMR** (600 MHz, DMSO-d_6) δ 8.76 (s, 1H), 8.33 – 8.30 (m, 1H), 8.00 (d, *J* = 8.7 Hz, 1H), 7.58 (dd, *J* = 8.7, 2.0 Hz, 1H), 5.41 (ddd, *J* = 9.0, 4.7, 1.4 Hz, 1H), 4.78 (t, *J* = 8.9 Hz, 1H), 4.41 (dd, *J* = 8.8, 4.8 Hz, 1H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 174.62, 158.90, 152.09, 136.35, 130.49, 127.51, 124.49, 122.80, 69.76, 54.15. **HRMS** (ESI) calcd for $C_{10}H_8ClN_2O_2S$ $[M+H]^+$: 254.9990, found 255.0001.



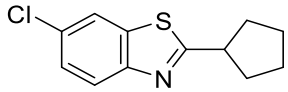
2-(2-(6-chlorobenzo[d]thiazol-2-yl)-5-oxopyrrolidin-1-yl)acetamide (8j). Yield = 28%; White solid; **^{1}H NMR** (600 MHz, DMSO-d_6) δ 8.30 (d, J = 2.1 Hz, 1H), 8.00 (d, J = 8.7 Hz, 1H), 7.57 (dd, J = 8.7, 2.2 Hz, 1H), 7.39 (s, 1H), 7.10 (s, 1H), 5.22 (dd, J = 8.6, 4.6 Hz, 1H), 4.23 (d, J = 16.9 Hz, 1H), 3.33 (d, J = 16.9 Hz, 1H), 2.68 – 2.61 (m, 1H), 2.54 – 2.40 (m, 2H), 2.12 – 2.07 (m, 1H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 175.38, 174.15, 169.40, 151.91, 136.55, 130.50, 127.41, 124.51, 122.71, 60.39, 43.90, 29.25, 26.72. **HRMS** (ESI) calcd for $C_{13}H_{13}ClN_3O_2S$ $[M+H]^+$: 310.0412, found 310.0420.



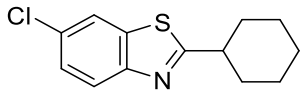
1-(2-(6-chlorobenzo[d]thiazol-2-yl)pyrrolidin-1-yl)ethan-1-one, 1:0.54 rotamers (8k) and **1-(3-(6-chlorobenzo[d]thiazol-2-yl)pyrrolidin-1-yl)ethan-1-one (8k′).** Yield = 22%; Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.08 (d, J = 8.8 Hz, 0.29H), 7.96 (d, J = 1.9 Hz, 0.29H), 7.90 – 7.86 (m, 1.54H), 7.85 (d, J = 2.0 Hz, 0.54H), 7.78 (d, J = 2.0 Hz, 1H), 7.54 (dd, J = 8.8, 2.1 Hz, 0.29H), 7.46 (dd, J = 8.7, 2.1 Hz, 0.54H), 7.40 (dd, J = 8.7, 2.1 Hz, 1H), 5.53 (dd, J = 8.1, 2.0 Hz, 1H), 5.29 (dd, J = 8.2, 1.9 Hz, 0.54H), 4.32 (dd, J = 7.5, 4.7 Hz, 0.29H), 3.82 – 3.74 (m, 1.54H), 3.72 – 3.65 (m, 0.58H), 3.62 – 3.52 (m, 1.54H), 3.51 – 3.49 (m, 0.29H), 3.41 – 3.37 (m, 0.29H), 2.69 – 2.63 (m, 0.29H), 2.55 – 2.49 (m, 0.29H), 2.47 – 2.43 (m, 1.08H), 2.37 – 2.28 (m, 2H), 2.23 – 2.18 (m, 1.08H), 2.16 (s, 3H), 2.12 – 2.07 (m, 2H), 2.01 (s, 1.62H), 1.96 (s, 0.87H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 175.30, 174.54, 173.30, 170.26, 170.15, 170.09, 152.13, 151.98, 151.67, 138.28, 136.23, 135.89, 134.29, 131.38, 130.81, 128.26, 127.27, 126.73, 126.36, 123.84, 123.63, 122.01, 121.49, 121.15, 61.00, 58.74, 53.86, 48.10, 46.64, 39.83, 38.79, 34.92, 34.24, 31.99, 24.55, 23.30, 22.74, 22.60, 22.48. **HRMS** (ESI) calcd for $C_{13}H_{14}ClN_2OS$ $[M+H]^+$: 281.0510, found 281.0522.



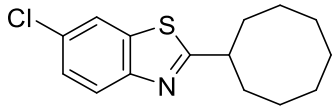
N-((6-chlorobenzo[d]thiazol-2-yl)methyl)-N-methylacetamide, 1:0.3 rotamers (8l). Yield = 18%; Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.91 – 7.86 (m, 1+0.3H), 7.85 (d, *J* = 2.0 Hz, 0.3H), 7.81 (d, *J* = 2.0 Hz, 1H), 7.45 (dd, *J* = 8.7, 2.0 Hz, 0.3H), 7.42 (dd, *J* = 8.7, 2.1 Hz, 1H), 4.93 (s, 2H), 4.85 (s, 0.6H), 3.12 (s, 3H), 3.08 (s, 0.9H), 2.21 (s, 0.9H), 2.18 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 170.99, 170.81, 168.65, 168.43, 151.87, 151.20, 136.89, 136.02, 131.56, 131.23, 127.31, 126.90, 123.91, 123.67, 121.49, 121.33, 53.00, 49.39, 36.51, 34.45, 21.54, 21.50.



6-chloro-2-cyclopentylbenzo[d]thiazole (10a). Yield = 52%; Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.7 Hz, 1H), 7.79 (d, *J* = 2.1 Hz, 1H), 7.39 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.55 – 3.50 (m, 1H), 2.30 – 2.19 (m, 2H), 1.98 – 1.82 (m, 4H), 1.79 – 1.70 (m, 2H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 177.73, 151.66, 136.00, 130.43, 126.60, 123.19, 121.10, 44.73, 34.00, 22.59. **HRMS** (ESI) calcd for $C_{12}H_{13}ClNS$ $[M+H]^+$: 238.0452, found 238.0457.

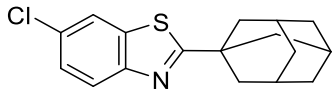


6-chloro-2-cyclohexylbenzo[d]thiazole (10b). Yield = 58%; Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.7 Hz, 1H), 7.81 (d, *J* = 1.8 Hz, 1H), 7.39 (dd, *J* = 8.6, 1.7 Hz, 1H), 3.11 – 3.06 (m, 1H), 2.21 – 2.18 (m, 2H), 1.90 – 1.87 (m, 2H), 1.78 – 1.75 (m, 1H), 1.65 – 1.59 (m, 2H), 1.48 – 1.40 (m, 2H), 1.35 – 1.27 (m, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 178.26, 151.48, 135.69, 130.47, 126.63, 123.24, 121.17, 43.36, 33.33, 26.00, 25.73.

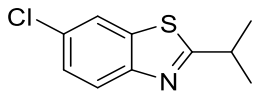


6-chloro-2-cyclooctylbenzo[d]thiazole (10c); Yield = 44%; Yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.7 Hz, 1H), 7.81 – 7.79 (m, 1H), 7.41 – 7.37 (m, 1H), 3.38 – 3.33 (m, 1H), 2.17 – 2.12 (m,

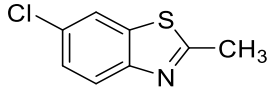
2H), 1.99 – 1.91 (m, 2H), 1.85 – 1.78 (m, 2H), 1.68 – 1.60 (m, 8H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.68, 151.51, 135.92, 130.38, 126.55, 123.25, 121.11, 43.68, 32.79, 26.89, 26.09, 25.38. **HRMS** (ESI) calcd for $C_{15}H_{19}ClNS$ $[M+H]^+$: 280.0921, found 280.0928.



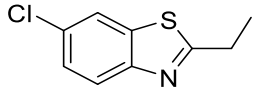
2-(adamantan-1-yl)-6-chlorobenzo[d]thiazole (10d). Yield = 65%; White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.81 (d, *J* = 2.0 Hz, 1H), 7.38 (dd, *J* = 8.7, 2.1 Hz, 1H), 2.12 (s, 8H), 2.04 – 1.94 (m, 1H), 1.81 (s, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 182.72, 151.74, 135.63, 130.26, 126.45, 123.40, 121.17, 42.94, 40.28, 38.46, 37.50, 36.47, 32.58, 32.51, 28.53, 27.80, 27.54. **HRMS** (ESI) calcd for $C_{17}H_{19}ClNS$ $[M+H]^+$: 304.0921, found 304.0929.



6-chloro-2-isopropylbenzo[d]thiazole (11a). Yield = 62%; Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.41 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.41 (hept, *J* = 7.0 Hz, 1H), 1.48 (d, *J* = 6.9 Hz, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 179.38, 151.35, 135.77, 130.61, 126.74, 123.24, 121.20, 34.05, 22.81.

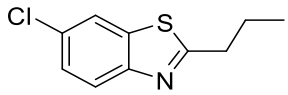


6-chloro-2-methylbenzo[d]thiazole (11b). Yield = 41%; Pale yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.7 Hz, 1H), 7.80 (d, *J* = 2.0 Hz, 1H), 7.41 (dd, *J* = 8.7, 2.1 Hz, 1H), 2.83 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 167.62, 151.68, 136.72, 130.72, 126.77, 123.06, 121.05, 20.06.

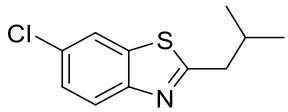


6-chloro-2-ethylbenzo[d]thiazole (11c). Yield = 53%; Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.7 Hz, 1H), 7.80 (d, *J* = 2.1 Hz, 1H), 7.40 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.13 (q, *J* = 7.5 Hz, 2H),

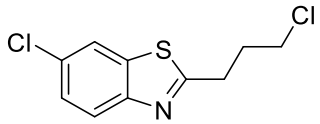
1.46 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.12, 151.72, 136.22, 130.57, 126.68, 123.20, 121.12, 27.74, 13.64.



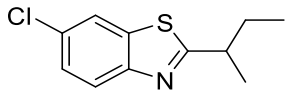
6-chloro-2-propylbenzo[d]thiazole (11d). Yield = 45%; Yellow solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.7 Hz, 1H), 7.80 (d, *J* = 2.0 Hz, 1H), 7.40 (dd, *J* = 8.7, 2.0 Hz, 1H), 3.07 (t, *J* = 7.6 Hz, 2H), 1.93 – 1.87 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 172.76, 151.75, 136.32, 130.57, 126.65, 123.22, 121.10, 36.19, 22.98, 13.69.



6-chloro-2-isobutylbenzo[d]thiazole (11e). Yield = 40%; Yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.6 Hz, 1H), 7.81 (d, *J* = 2.0 Hz, 1H), 7.41 (dd, *J* = 8.7, 2.0 Hz, 1H), 2.97 (d, *J* = 7.2 Hz, 2H), 2.25 – 2.18 (m, 1H), 1.04 (d, *J* = 6.6 Hz, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 171.92, 151.72, 136.41, 130.61, 126.66, 123.27, 121.08, 43.18, 29.71, 22.38. **HRMS** (ESI) calcd for $C_{11}H_{13}ClNS$ $[M+H]^+$: 226.0452, found 226.0462.

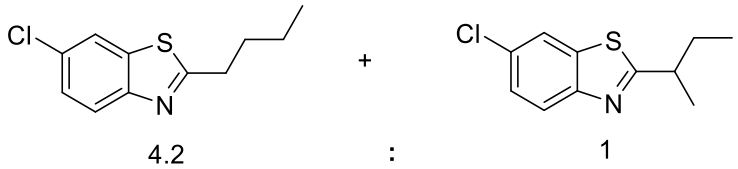


6-chloro-2-(3-chloropropyl)benzo[d]thiazole (11f). Yield = 30%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.82 (d, *J* = 2.1 Hz, 1H), 7.42 (dd, *J* = 8.6, 2.1 Hz, 1H), 3.68 (t, *J* = 6.3 Hz, 2H), 3.29 (t, *J* = 7.4 Hz, 2H), 2.37 (dt, *J* = 13.6, 6.5 Hz, 2H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 170.60, 151.70, 136.24, 130.91, 126.88, 123.34, 121.16, 43.73, 31.65, 31.14.



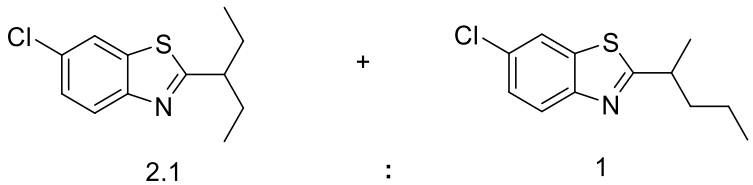
2-(sec-butyl)-6-chlorobenzo[d]thiazole (11g). Yield = 42%; Yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.40 (dd, *J* = 8.7, 2.0 Hz, 1H), 3.23 – 3.17 (m, 1H),

1.94 – 1.74 (m, 2H), 1.44 (d, *J* = 6.9 Hz, 3H), 0.97 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 178.49, 151.55, 135.87, 130.51, 126.60, 123.30, 121.17, 41.04, 30.53, 20.56, 11.77. **HRMS** (ESI) calcd for $C_{11}H_{13}ClNS$ $[M+H]^+$: 226.0452, found 226.0458.



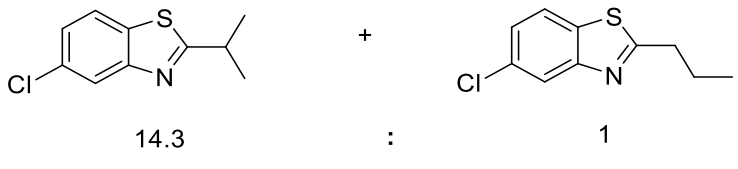
4.2 : 1

2-butyl-6-chlorobenzo[d]thiazole (11i) and **2-(sec-butyl)-6-chlorobenzo[d]thiazole (11i′).** Yield = 38%; Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 – 7.85 (m, 1H+0.24H), 7.82 – 7.80 (m, 1H+0.24H), 7.40 (dd, *J* = 8.7, 2.1 Hz, 1H+0.24H), 3.24 – 3.15 (m, 0.24H), 3.10 (t, *J* = 8.0 Hz, 2H), 1.93 – 1.73 (m, 2H+0.48H), 1.51 – 1.41 (m, 2H+0.72H), 0.97 (t, *J* = 7.4 Hz, 3H+0.72H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.55, 173.07, 151.67, 151.51, 136.27, 135.84, 130.55, 130.49, 126.68, 126.62, 123.29, 123.18, 121.20, 121.12, 41.05, 34.02, 31.67, 30.58, 22.31, 20.62, 13.79, 11.82. **HRMS** (ESI) calcd for $C_{11}H_{13}ClNS$ $[M+H]^+$: 226.0452, found 226.0453.



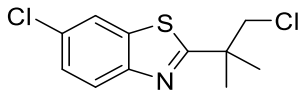
2.1 : 1

6-chloro-2-(pentan-3-yl)benzo[d]thiazole (11j) and **6-chloro-2-(pentan-2-yl)benzo[d]thiazole (11j′).** Yield = 43%; Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 – 7.86 (m, 1H+0.48H), 7.83 – 7.82 (m, 1H+0.48H), 7.42 – 7.39 (m, 1H+0.48H), 3.33 – 3.24 (m, 0.48H), 3.02 – 2.94 (m, 1H), 1.89 – 1.72 (m, 4H), 1.76 – 1.65 (m, 0.95H), 1.44 (d, *J* = 6.9 Hz, 1.43H), 1.41 – 1.32 (m, 0.95H), 0.94 – 0.90 (m, 6H+1.43H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.77, 177.57, 151.51, 151.47, 135.90, 135.83, 130.51, 130.49, 126.61, 126.57, 123.31, 123.29, 121.20, 48.69, 39.73, 39.28, 28.93, 21.07, 20.50, 13.98, 11.92. **HRMS** (ESI) calcd for $C_{12}H_{15}ClNS$ $[M+H]^+$: 240.0608, found 240.0614.

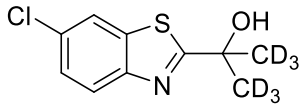


14.3 : 1

6-chloro-2-isopropylbenzo[d]thiazole (11k) and **6-chloro-2-propylbenzo[d]thiazole (11k′).** Yield = 56%; Pale yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 – 7.93 (m, 1H+0.07H), 7.73 – 7.70 (m, 1H+0.07H), 7.29 (dd, *J* = 8.5, 2.0 Hz, 1H+0.07H), 3.40 (hept, *J* = 6.9 Hz, 1H), 3.07 (t, *J* = 7.6 Hz, 0.14H), 1.94 – 1.84 (m, 0.14H), 1.46 (d, *J* = 6.9 Hz, 6H), 1.04 (t, *J* = 7.4 Hz, 0.21H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.66, 174.25, 154.08, 154.01, 133.39, 132.97, 131.88, 131.83, 125.11, 125.05, 122.48, 122.40, 122.24, 122.17, 36.29, 34.19, 23.05, 22.83, 13.72. **HRMS** (ESI) calcd for $C_{10}H_{11}ClNS$ $[M+H]^+$: 212.0295, found 212.0299.



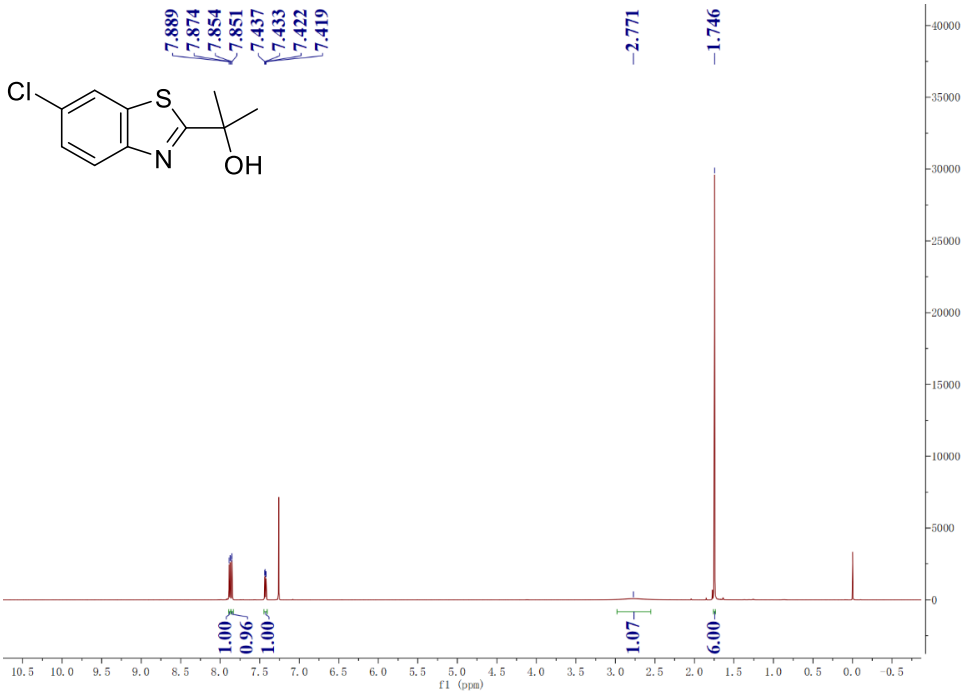
6-chloro-2-(1-chloro-2-methylpropan-2-yl)benzo[d]thiazole (16). Yield = 16%; Yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.7 Hz, 1H), 7.85 (d, *J* = 2.0 Hz, 1H), 7.43 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.89 (s, 2H), 1.60 (s, 6H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 177.77, 151.64, 136.05, 130.88, 126.84, 123.70, 121.14, 54.26, 43.17, 26.45. **HRMS** (ESI) calcd for $C_{11}H_{12}Cl_2NS$ $[M+H]^+$: 260.0062, found 260.0073.



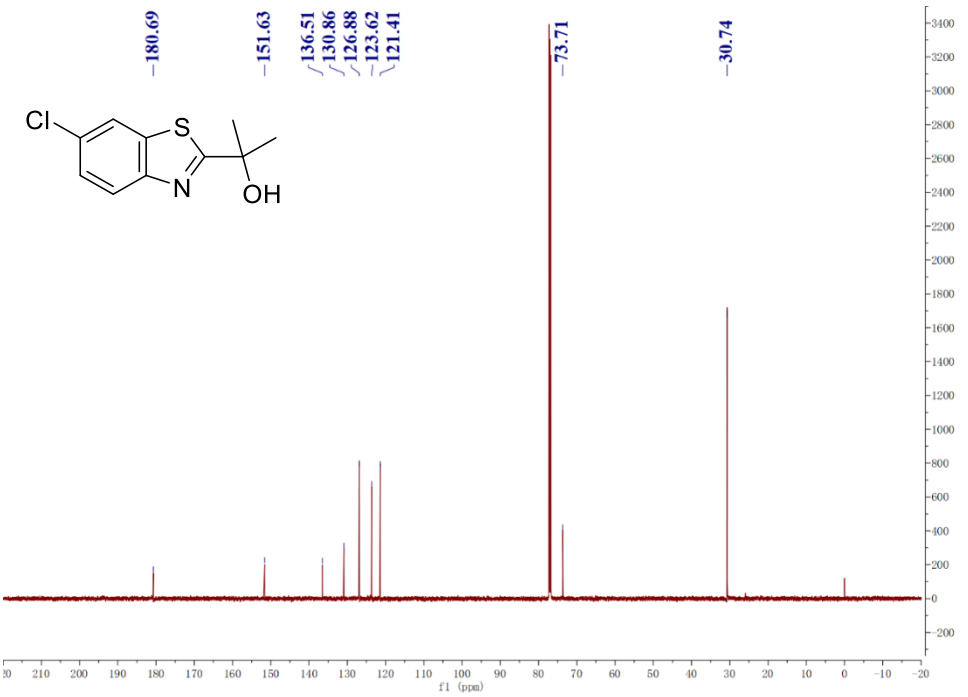
2-(6-chlorobenzo[d]thiazol-2-yl)propan-1,1,1,3,3,3-d$_6$-2-ol (3a-d$_6$). Yield = 43%; White solid; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.7 Hz, 1H), 7.86 (d, *J* = 2.1 Hz, 1H), 7.43 (dd, *J* = 8.7, 2.1 Hz, 1H), 2.70 (br, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 180.65, 151.71, 136.54, 130.82, 126.85, 123.64, 121.40, 73.45, 29.66. **HRMS** (ESI) calcd for $C_{10}H_5D_6ClNOS$ $[M+H]^+$: 234.0621, found 234.0623.

6. NMR spectra

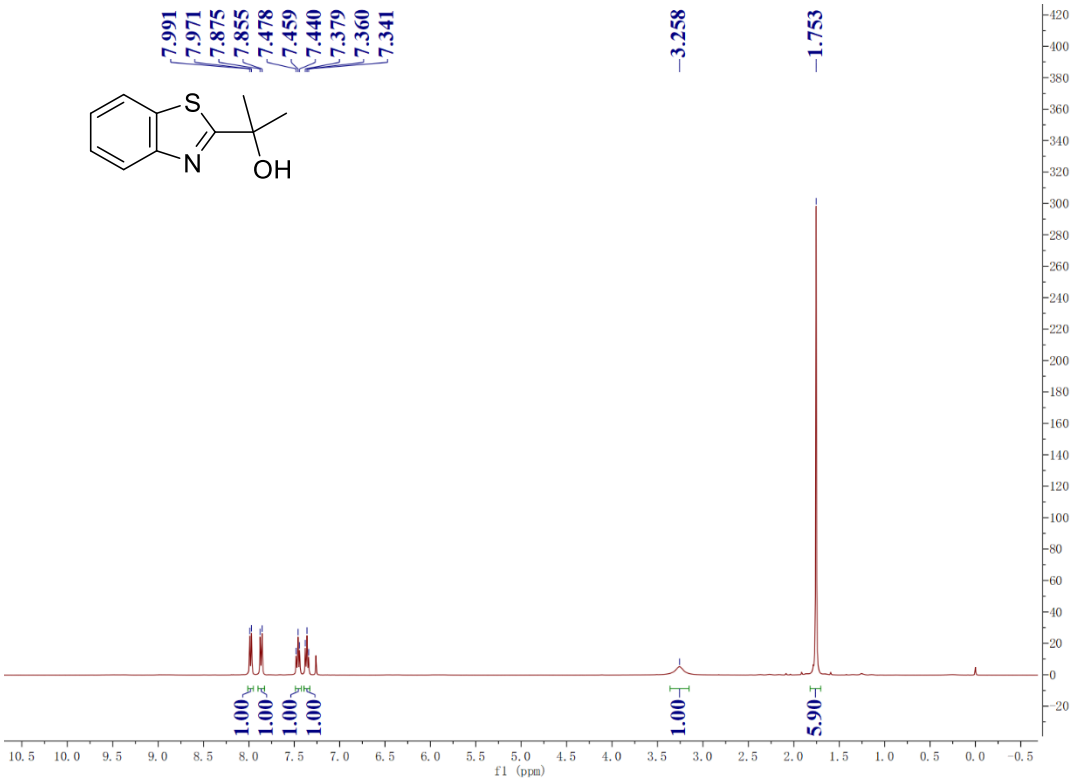
^{1}H NMR (600 MHz, $CDCl_3$) of 3a



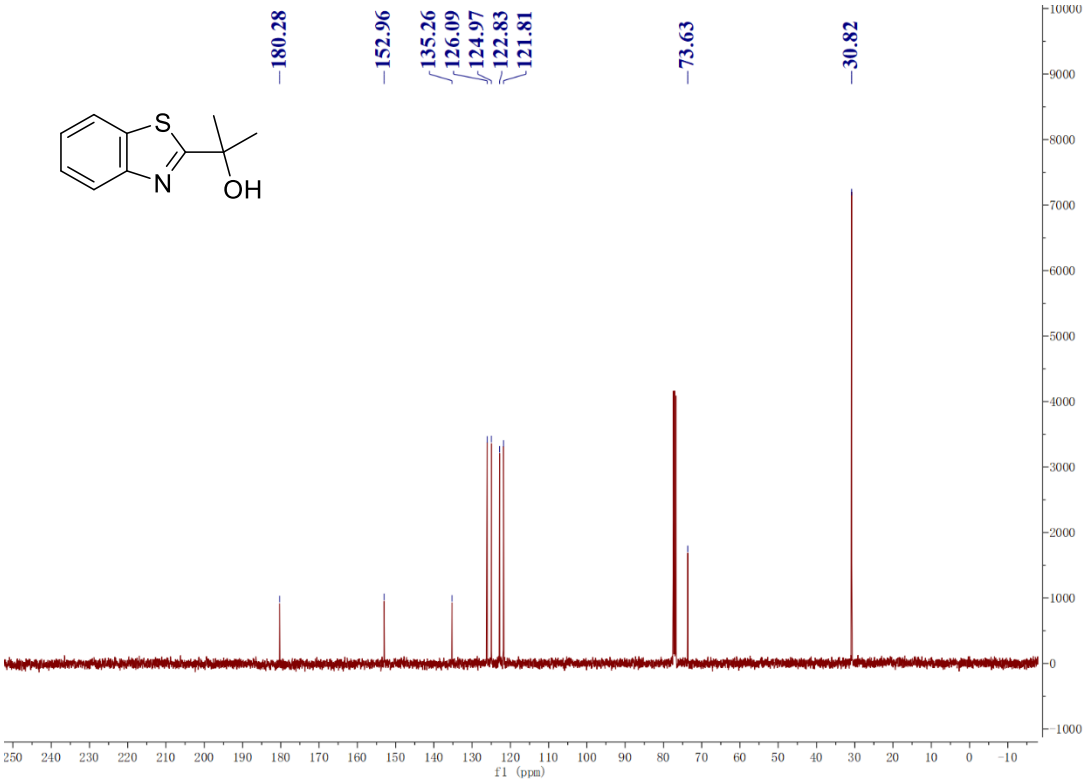
^{13}C NMR (151 MHz, $CDCl_3$) of 3a



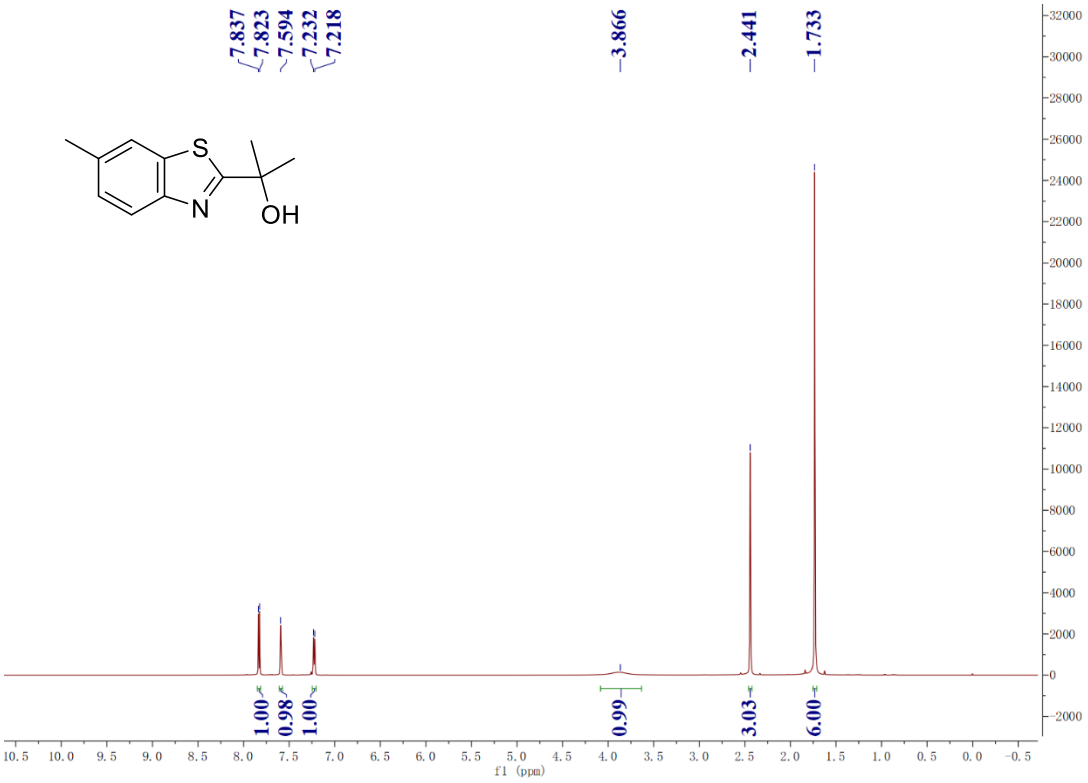
^{1}H NMR (400 MHz, $CDCl_3$) of 3b



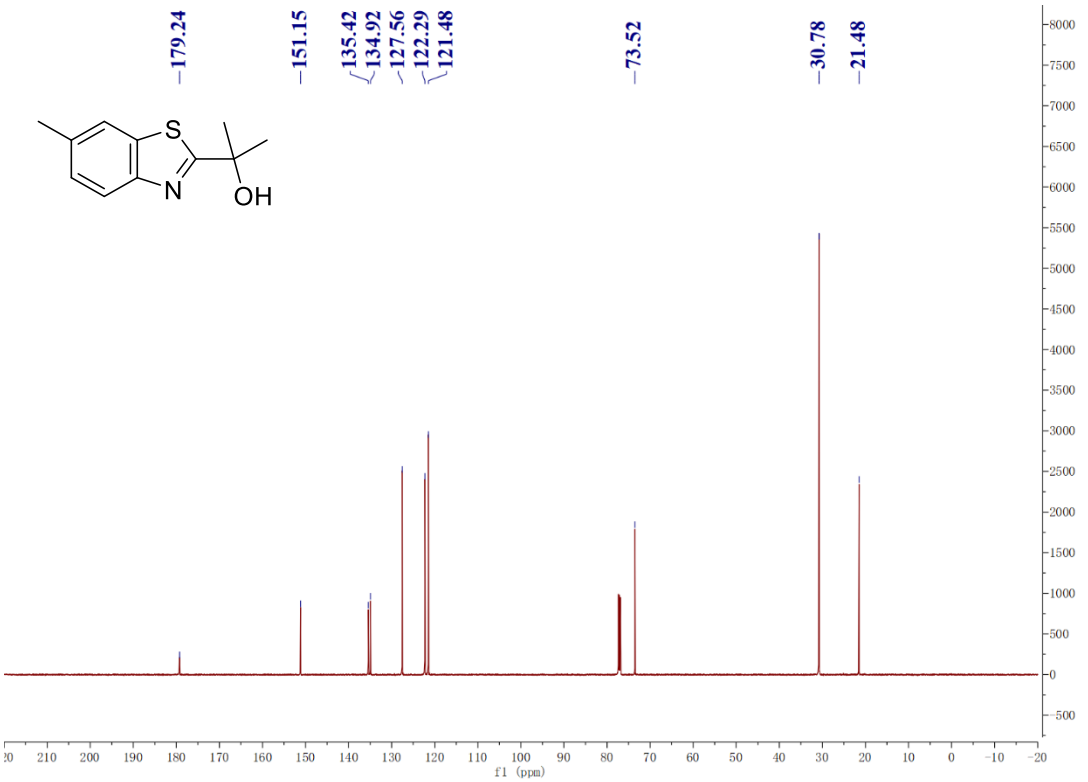
^{13}C NMR (101 MHz, $CDCl_3$) of 3b



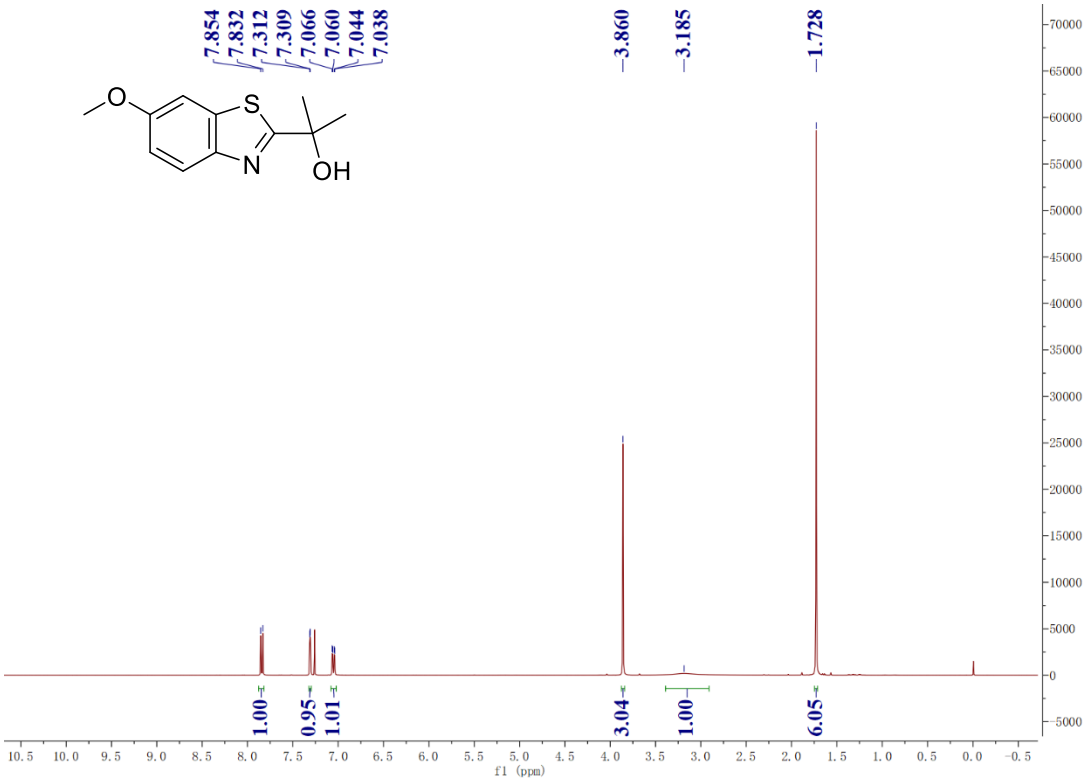
^{1}H NMR (600 MHz, $CDCl_3$) of 3c



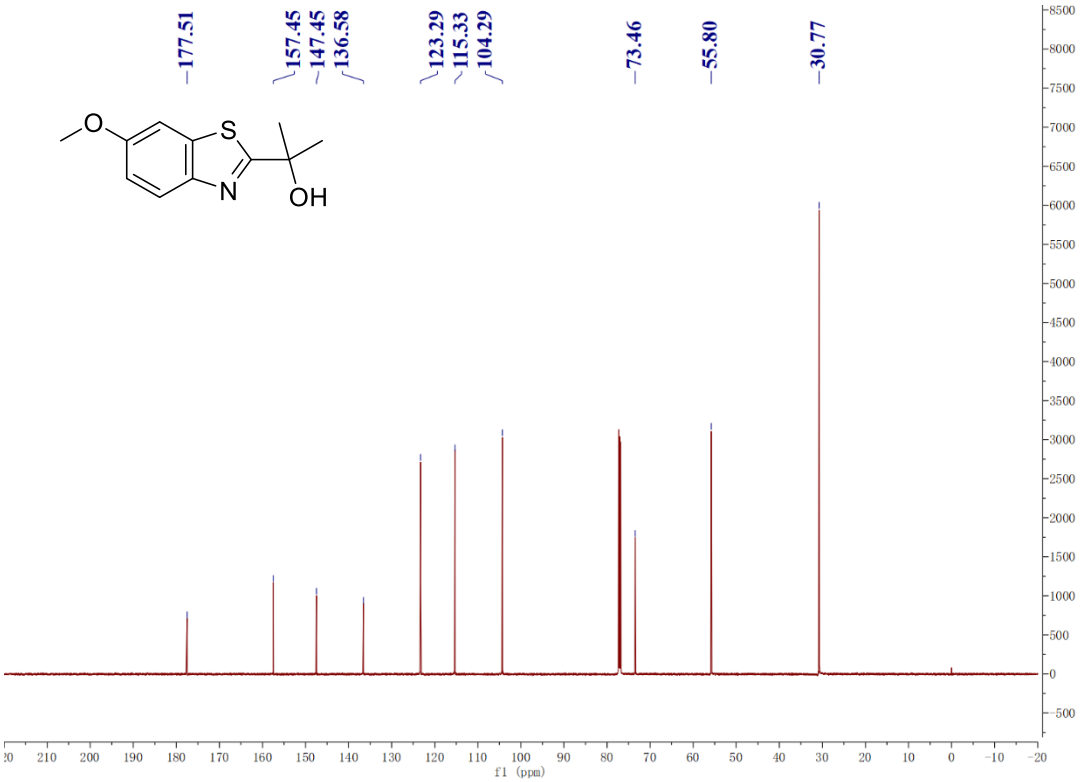
^{13}C NMR (151 MHz, $CDCl_3$) of 3c



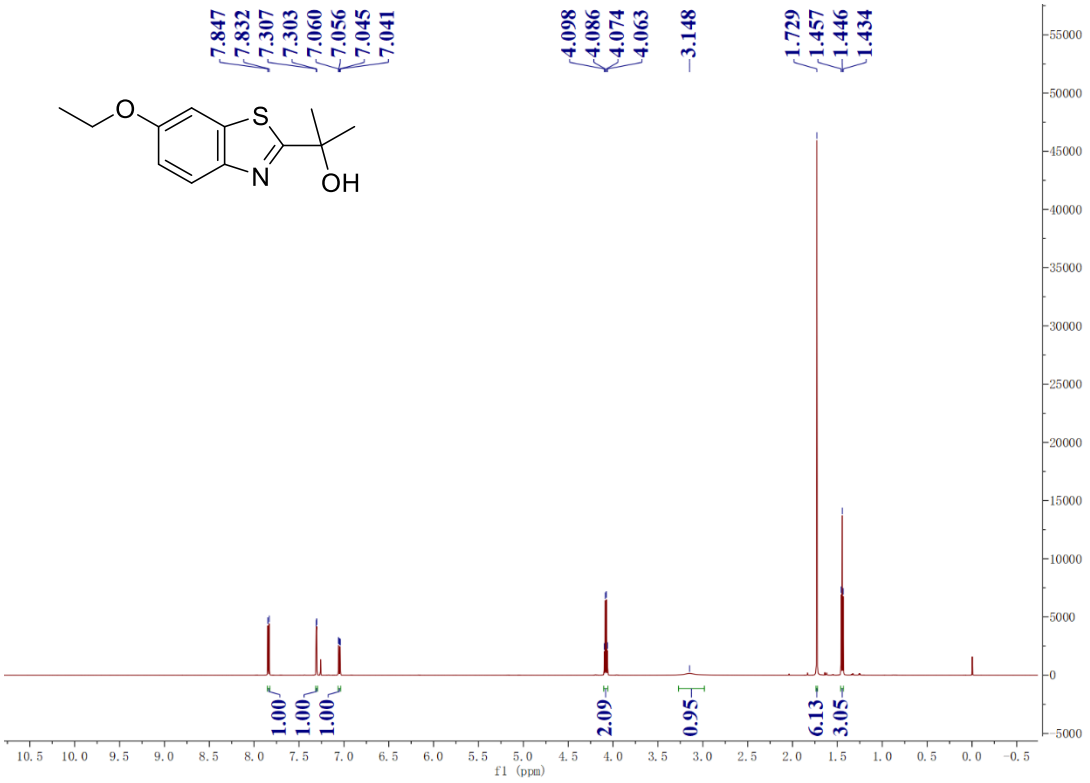
^{1}H NMR (400 MHz, $CDCl_3$) of 3d



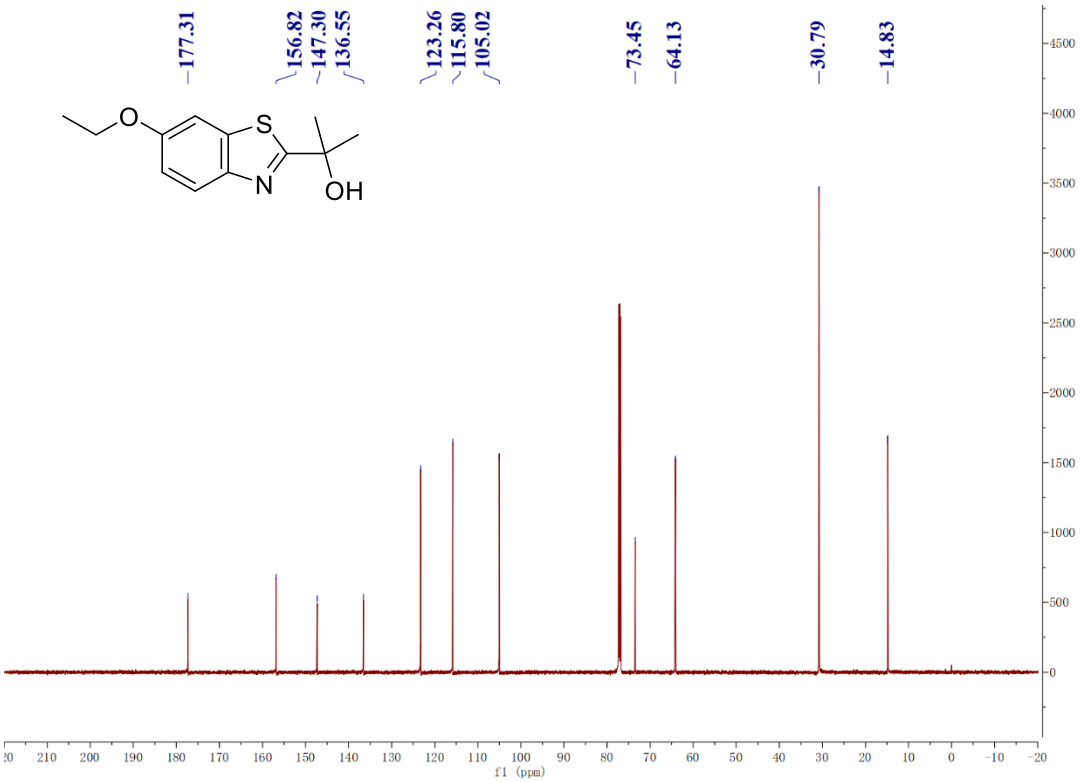
^{13}C NMR (151 MHz, $CDCl_3$) of 3d



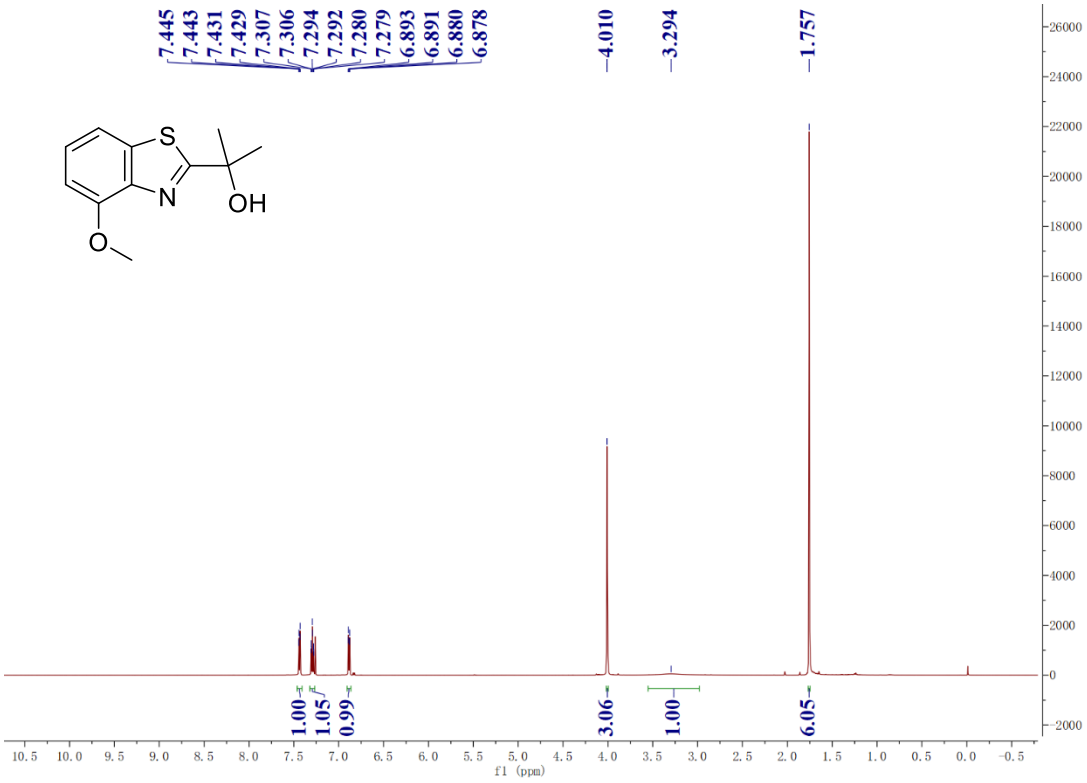
^{1}H NMR (600 MHz, $CDCl_3$) of 3e



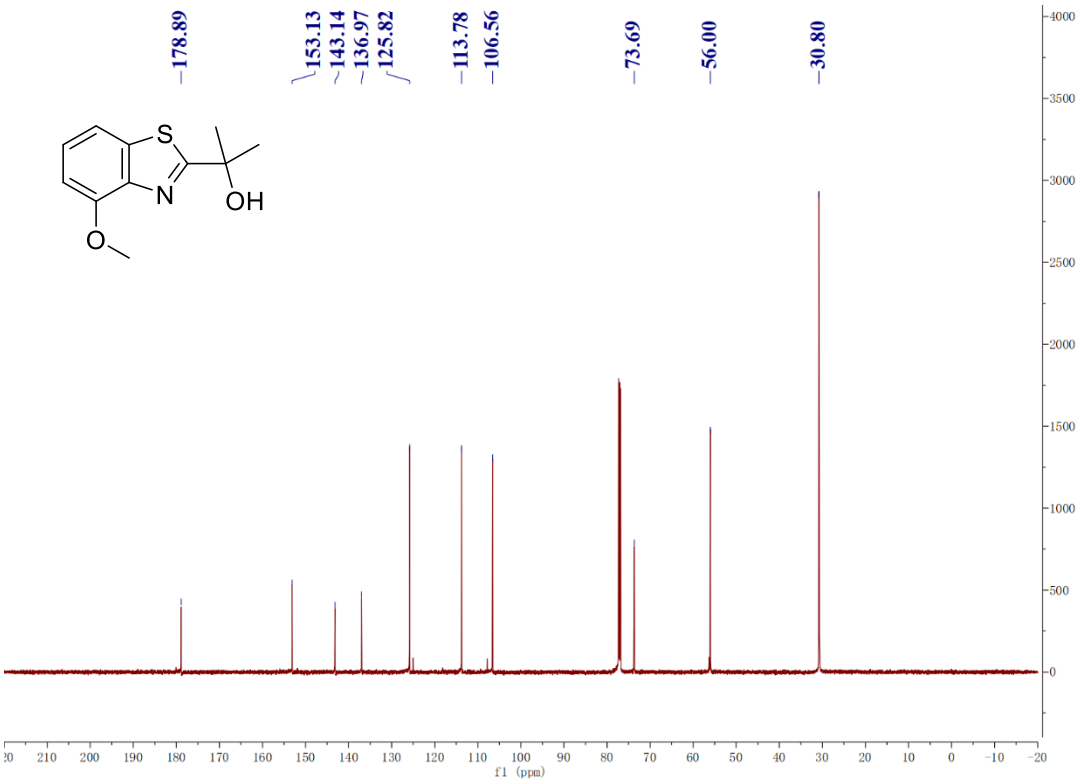
^{13}C NMR (151 MHz, $CDCl_3$) of 3e



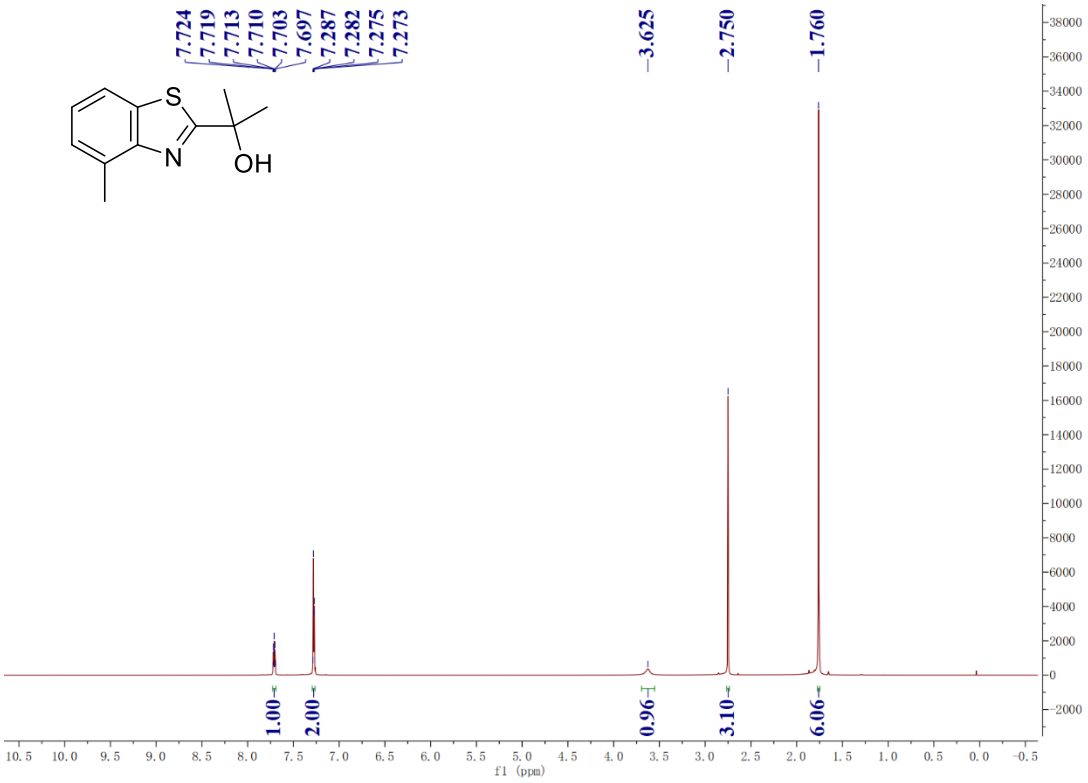
^{1}H NMR (600 MHz, $CDCl_3$) of 3f



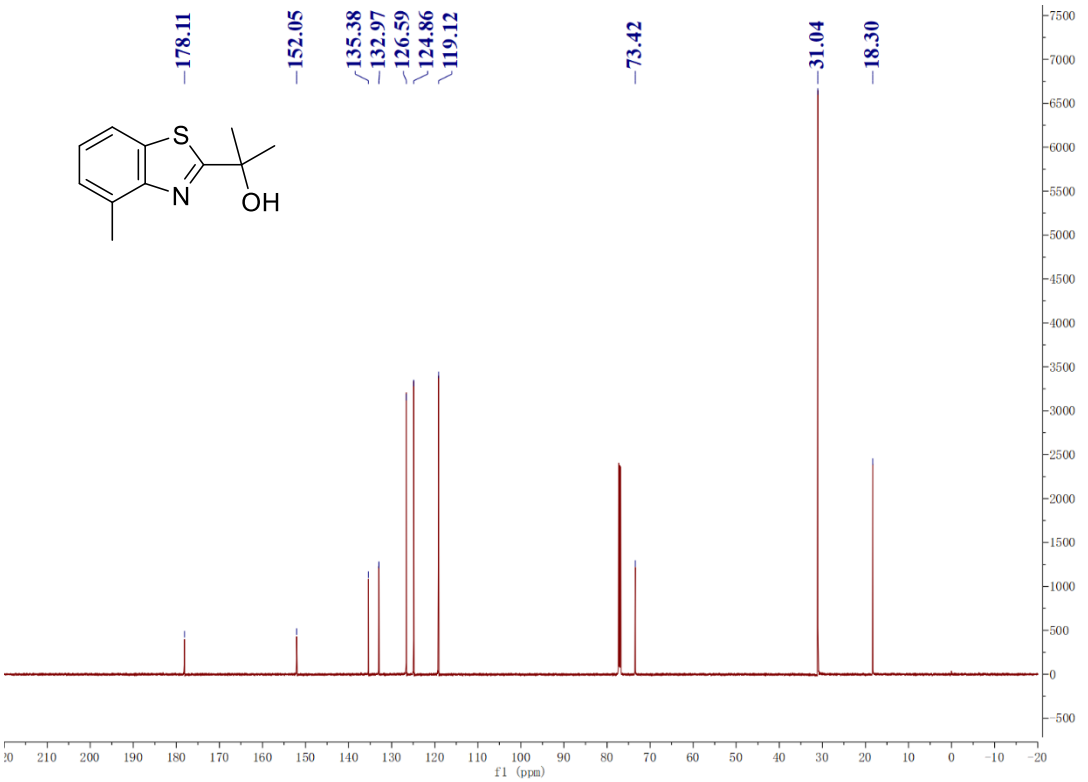
^{13}C NMR (151 MHz, $CDCl_3$) of 3f



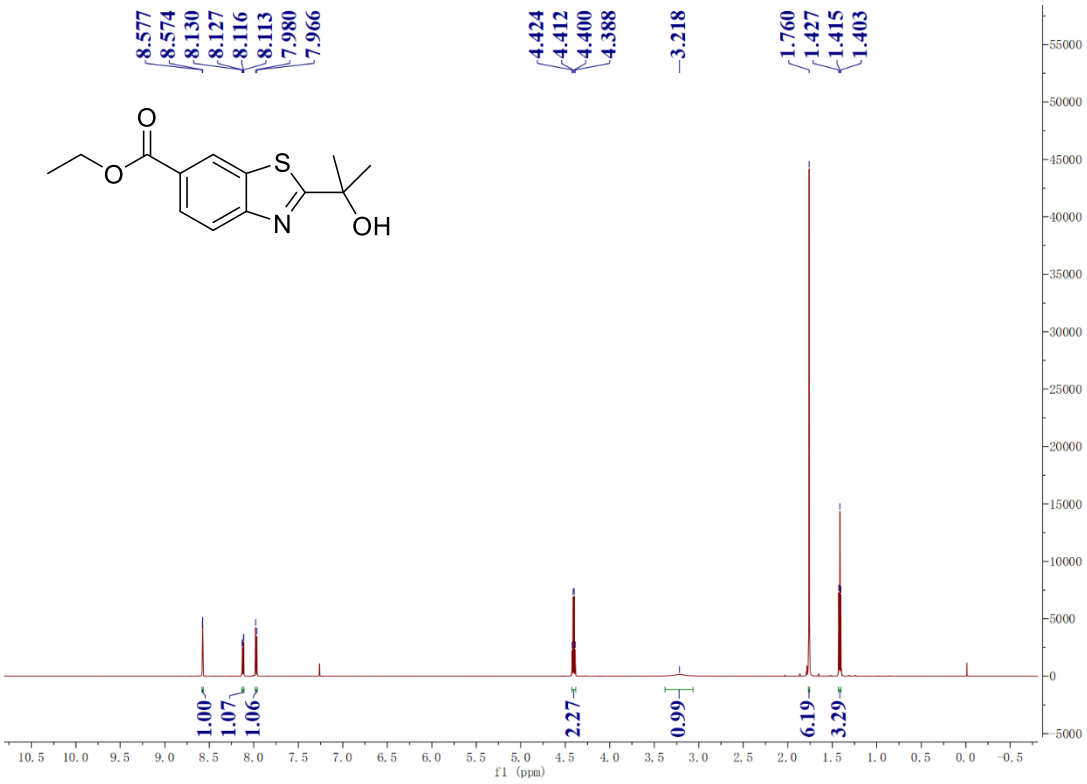
^{1}H NMR (600 MHz, $CDCl_3$) of 3g



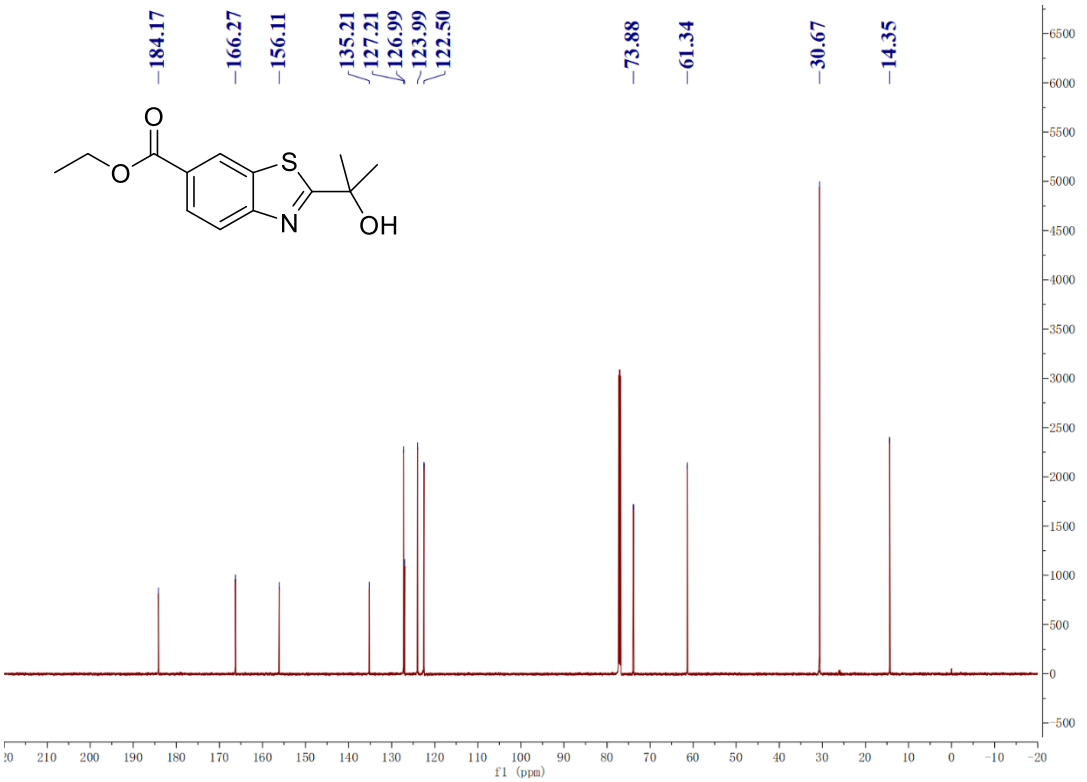
^{13}C NMR (151 MHz, $CDCl_3$) of 3g



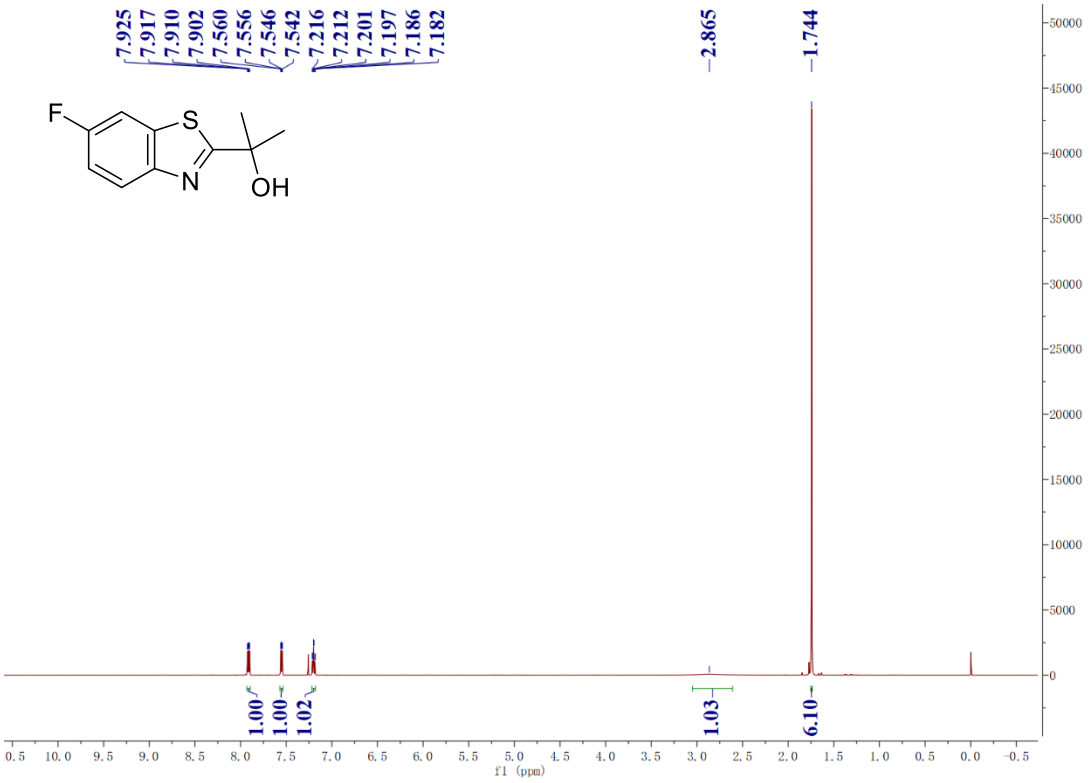
^{1}H NMR (600 MHz, $CDCl_3$) of 3h



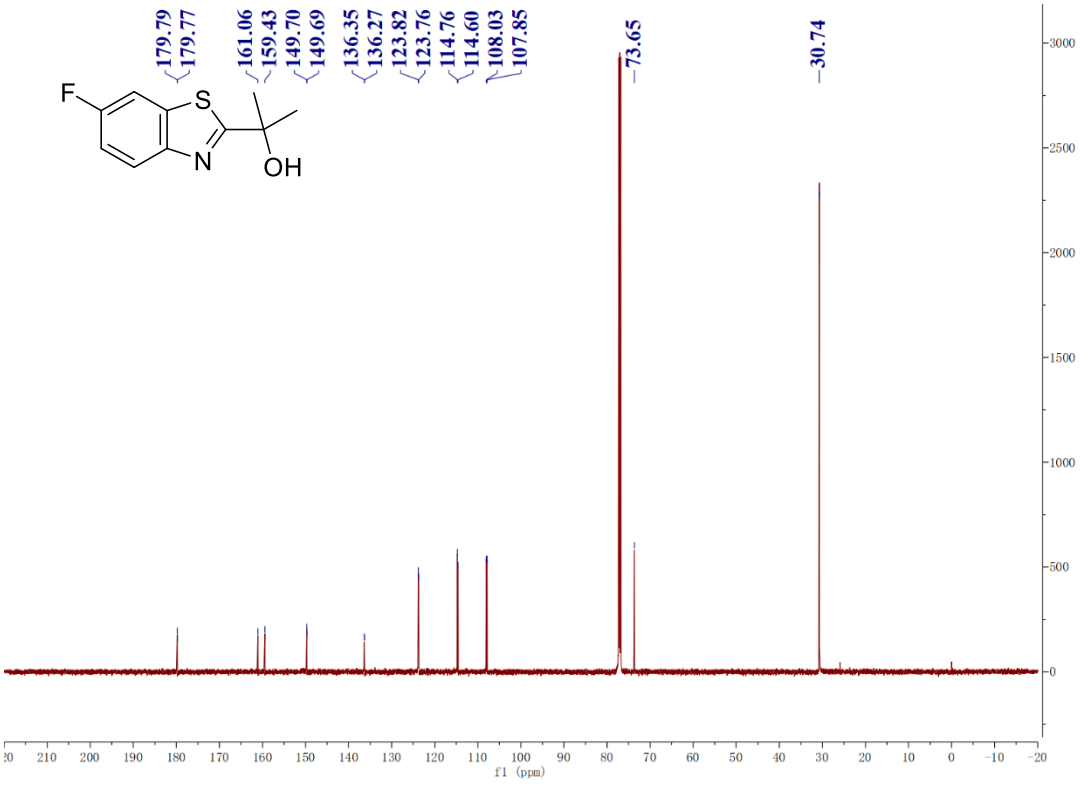
^{13}C NMR (151 MHz, $CDCl_3$) of 3h



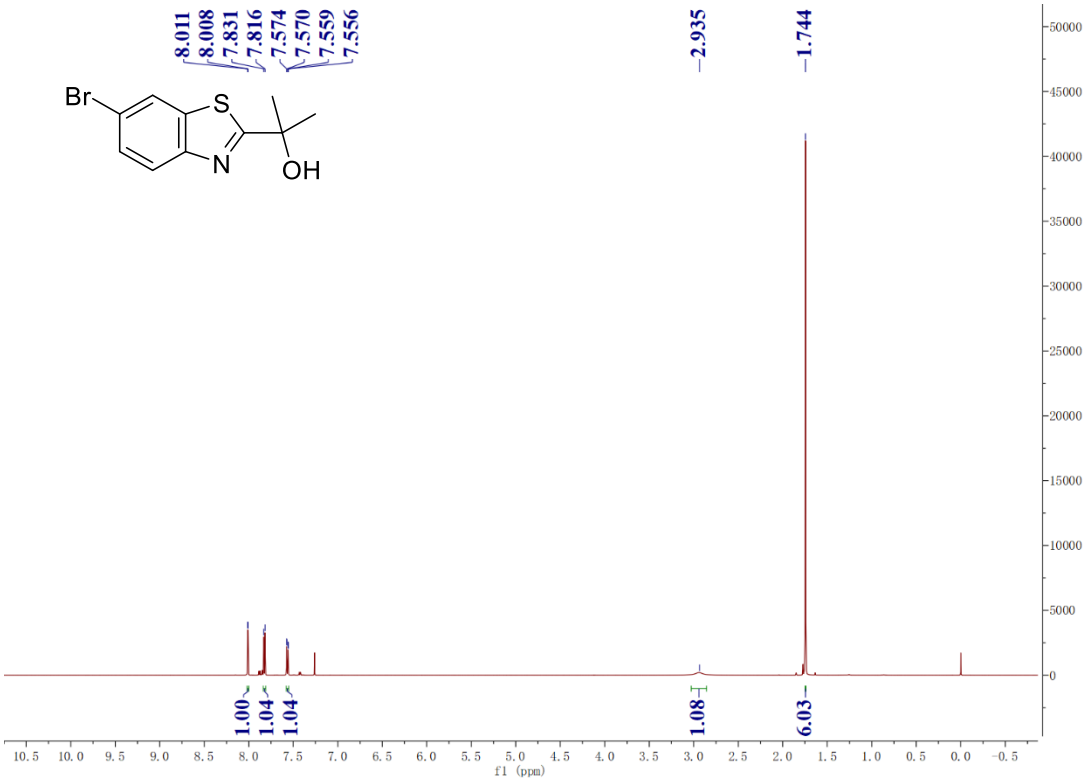
^{1}H NMR (600 MHz, $CDCl_3$) of 3i



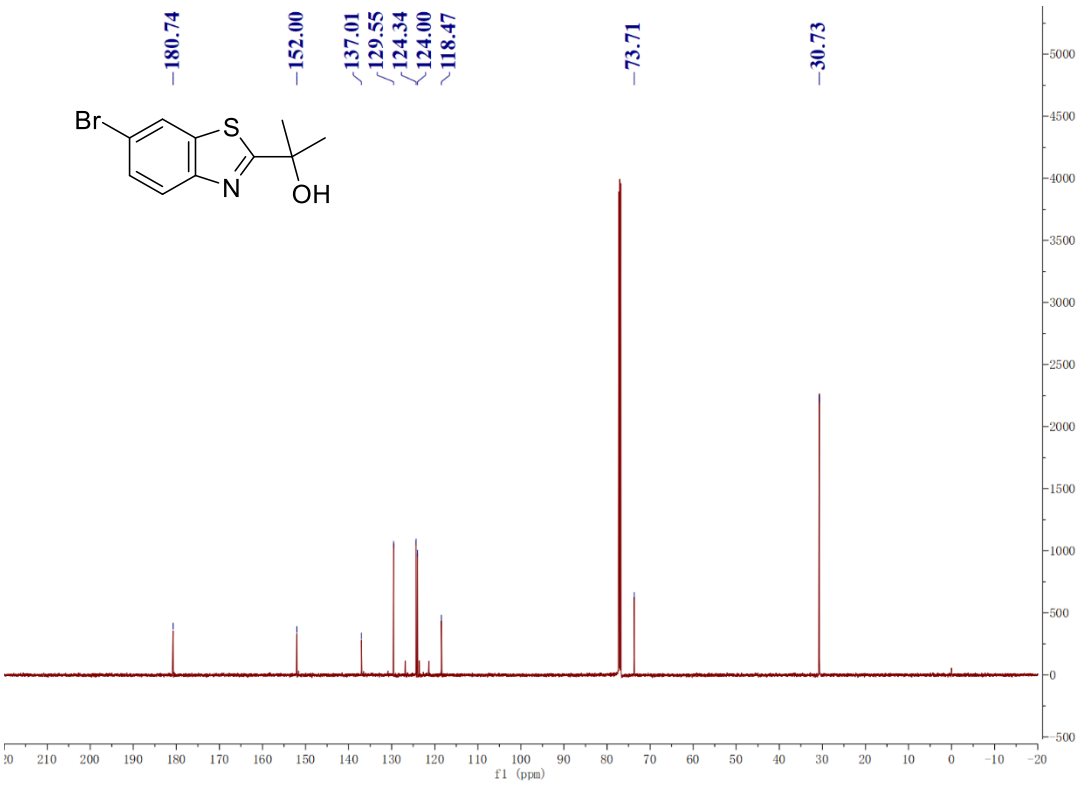
^{13}C NMR (151 MHz, $CDCl_3$) of 3i



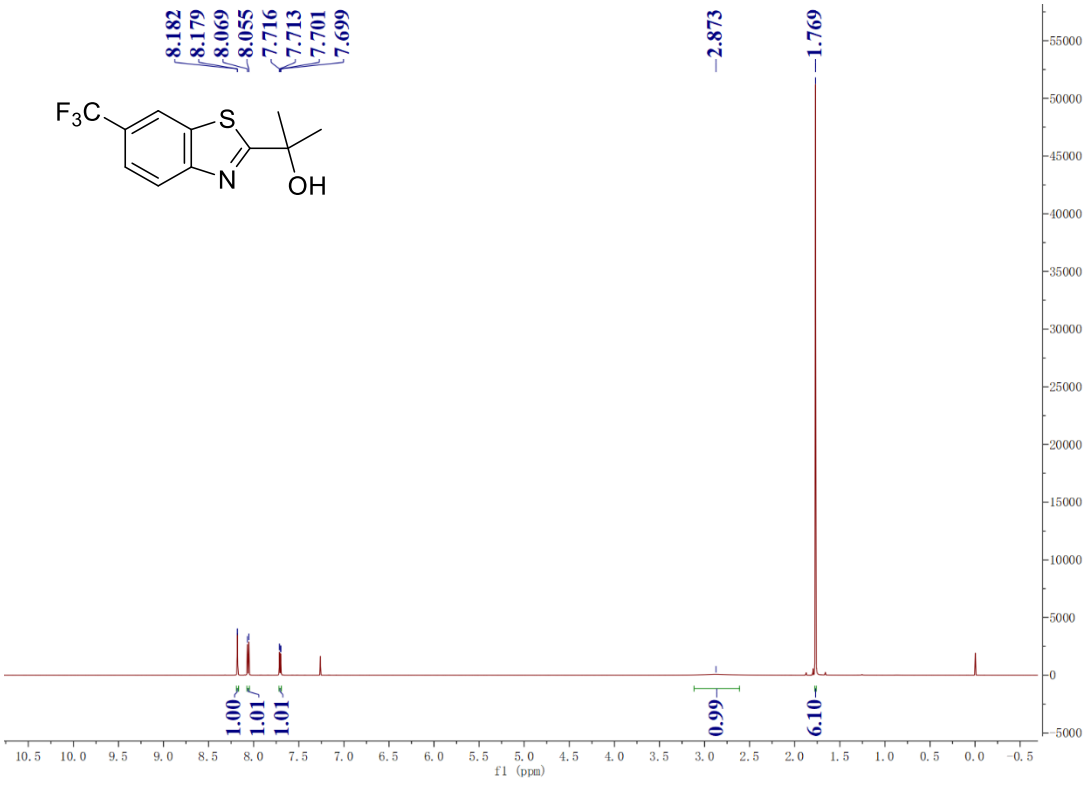
^{1}H NMR (600 MHz, $CDCl_3$) of 3j



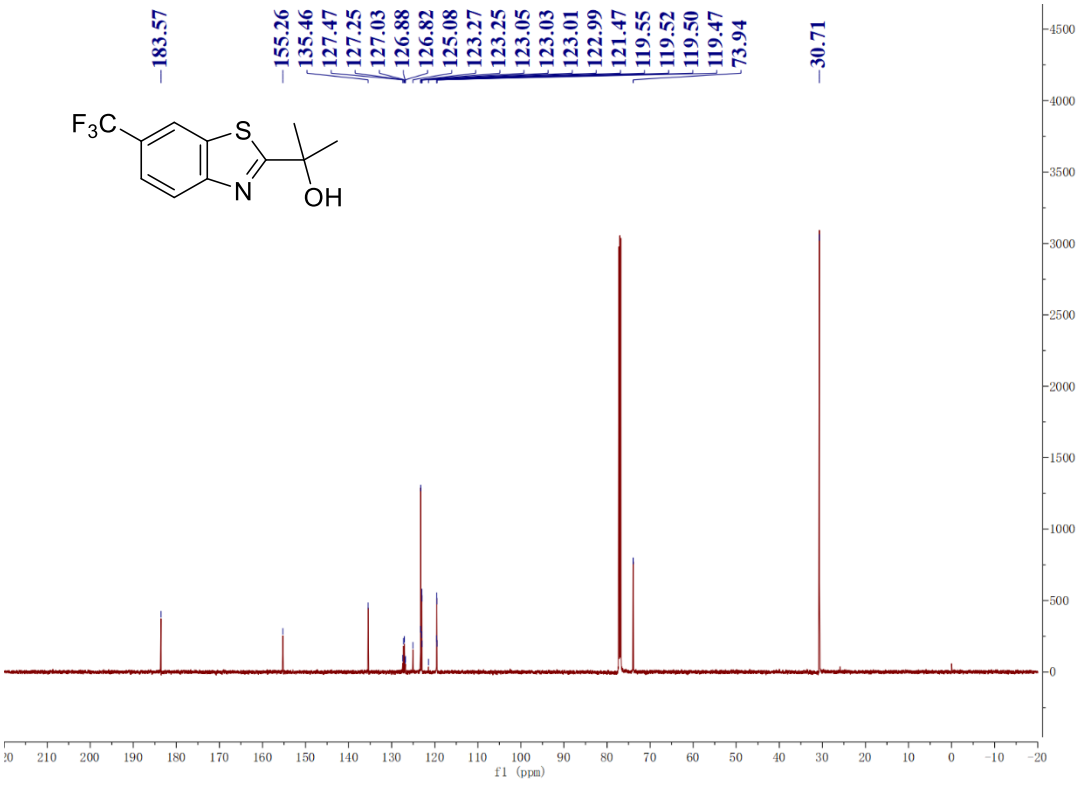
^{13}C NMR (151 MHz, $CDCl_3$) of 3j



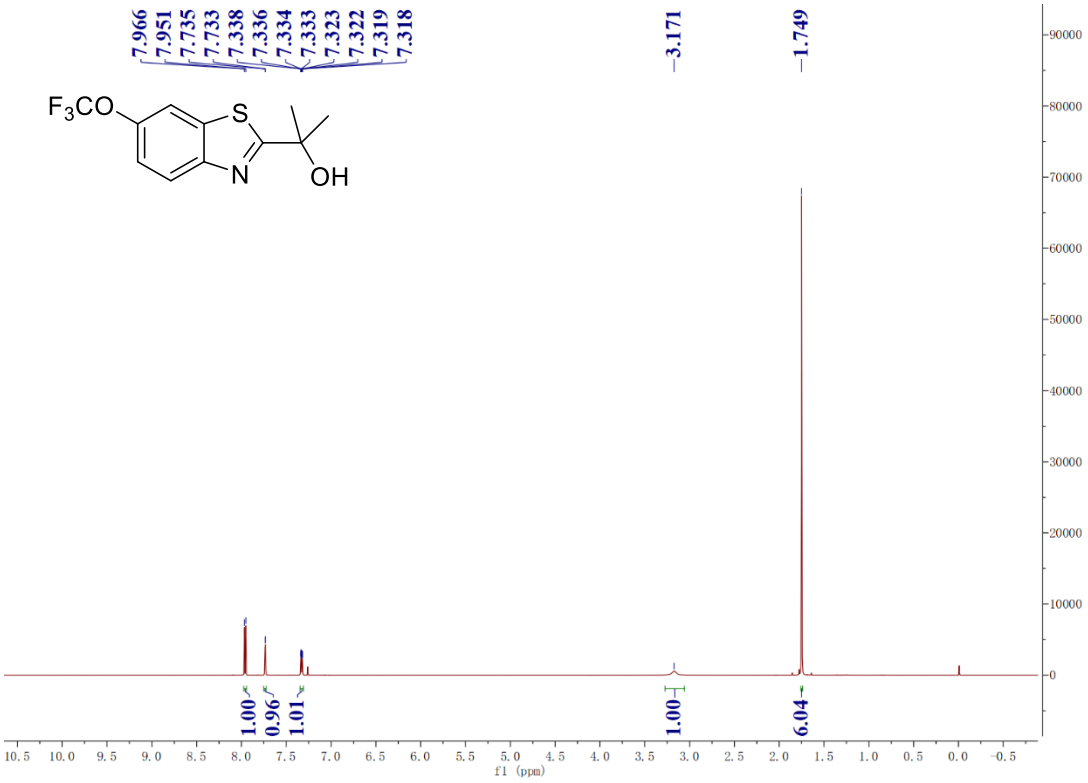
^{1}H NMR (600 MHz, $CDCl_3$) of 3k



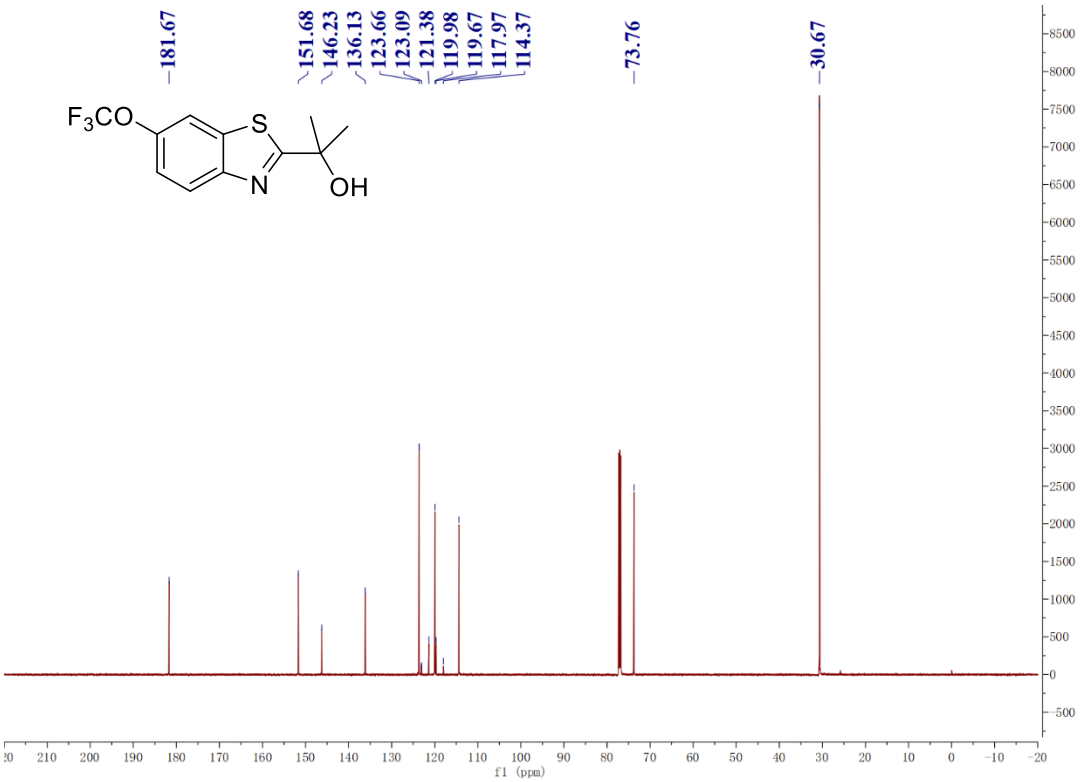
^{13}C NMR (151 MHz, $CDCl_3$) of 3k



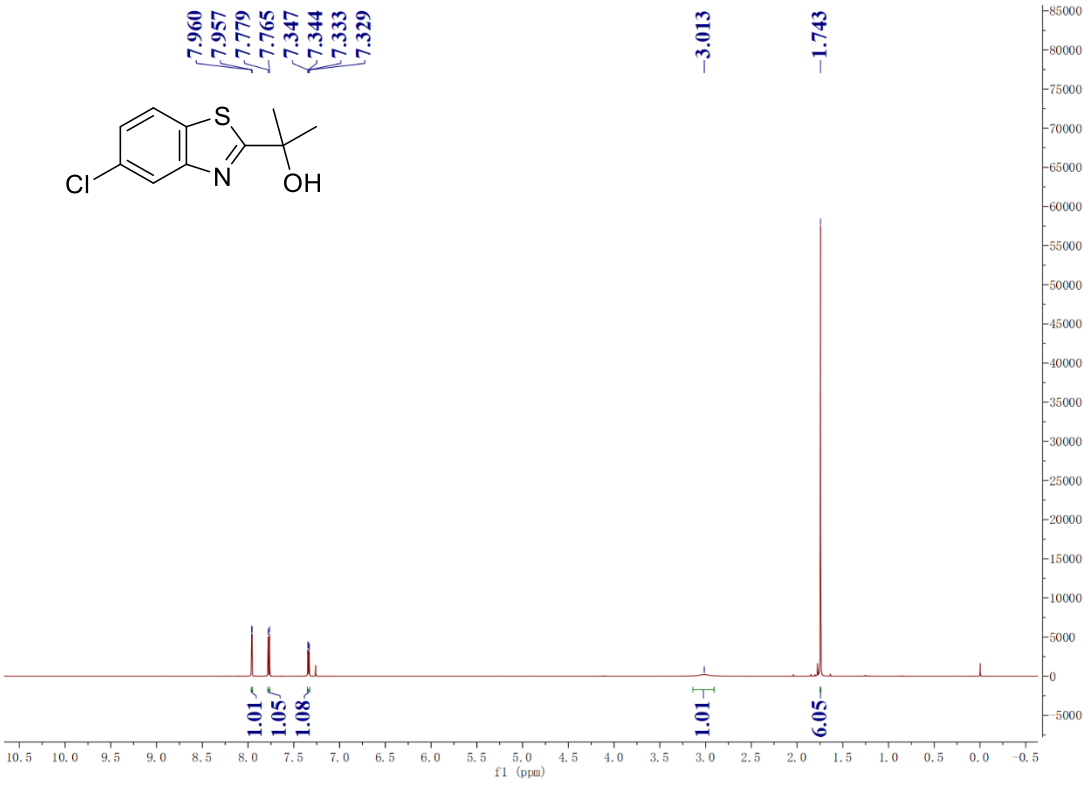
^{1}H NMR (600 MHz, $CDCl_3$) of 3l



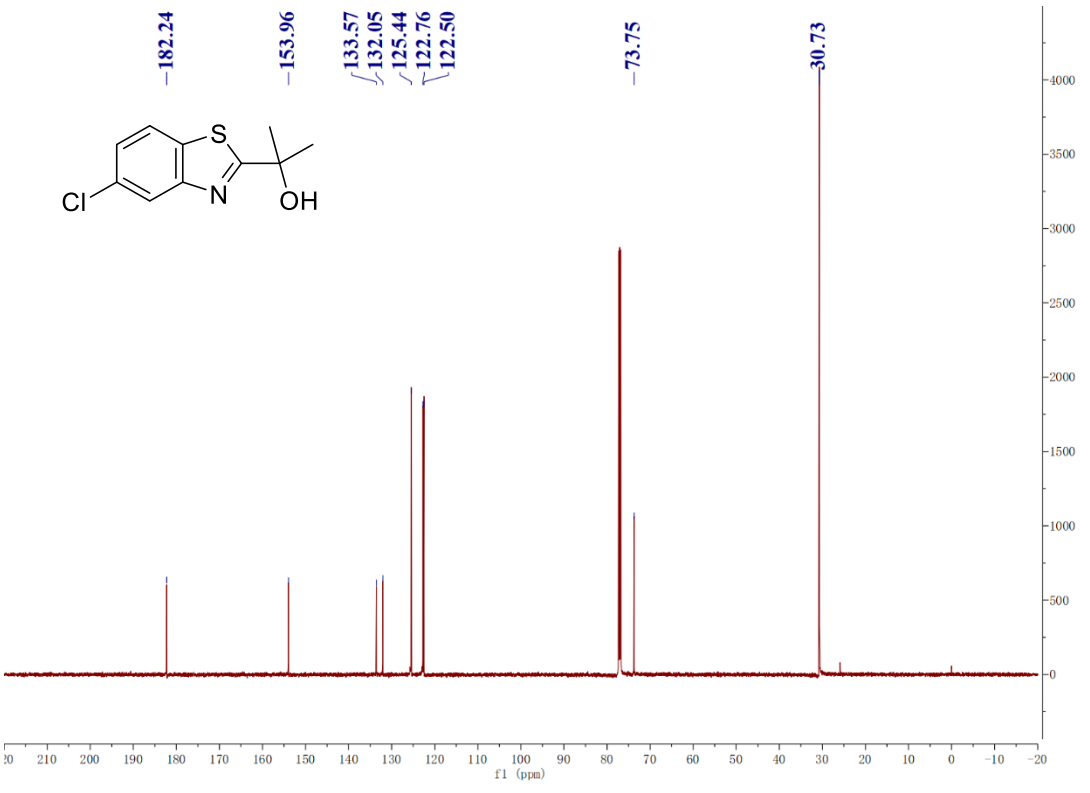
^{13}C NMR (151 MHz, $CDCl_3$) of 3l



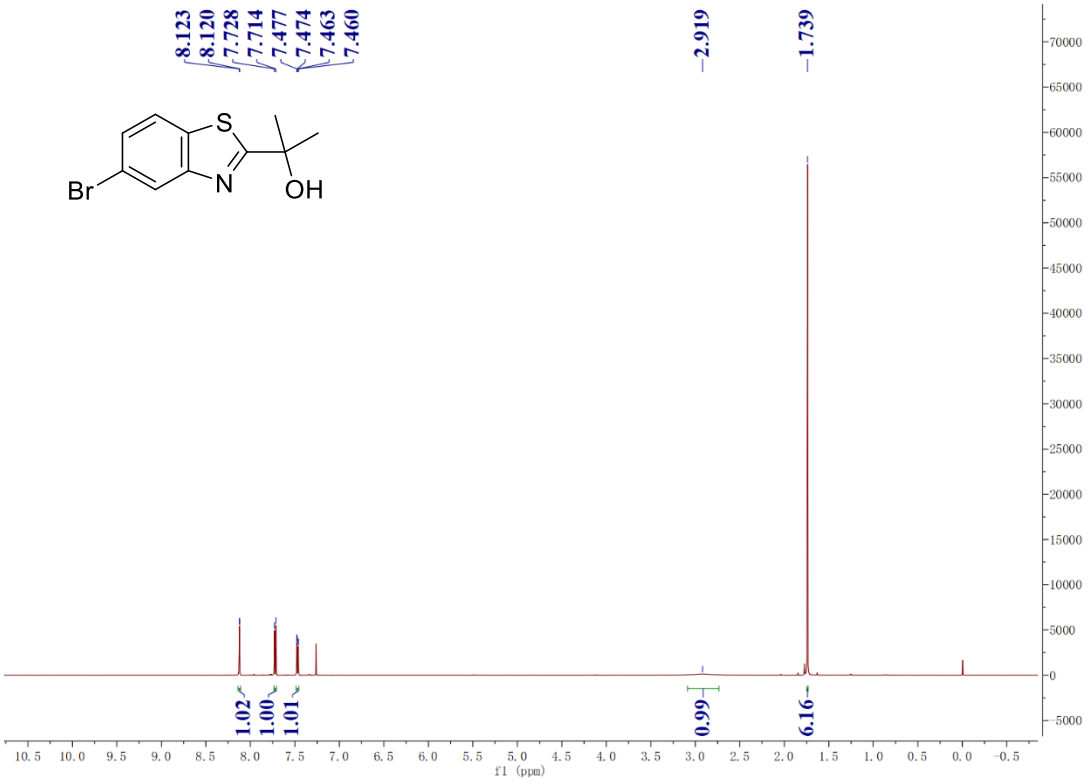
^{1}H NMR (600 MHz, $CDCl_3$) of 3m



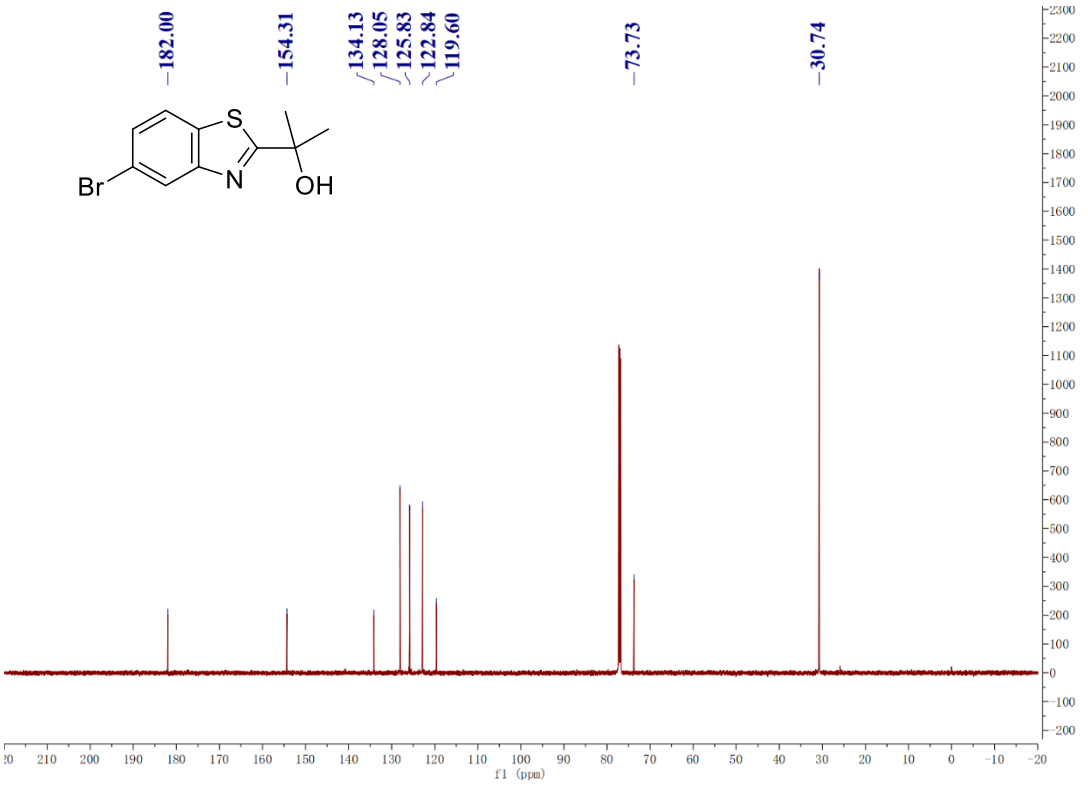
^{13}C NMR (151 MHz, $CDCl_3$) of 3m



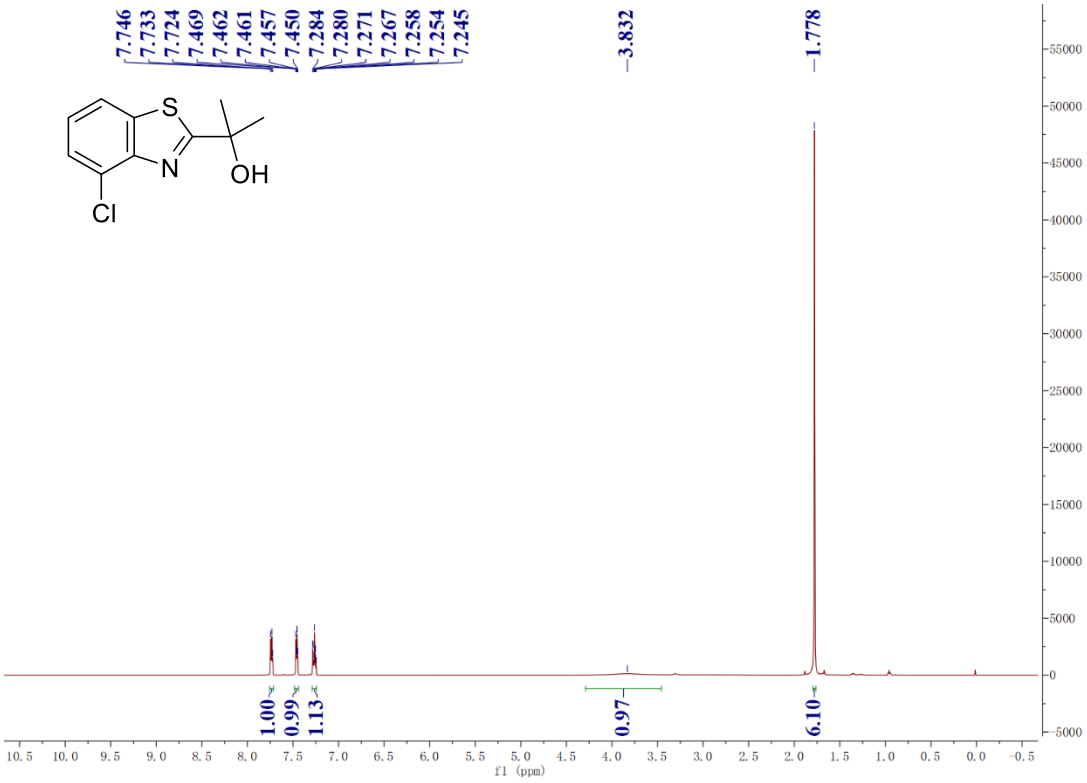
^{1}H NMR (600 MHz, $CDCl_3$) of 3n



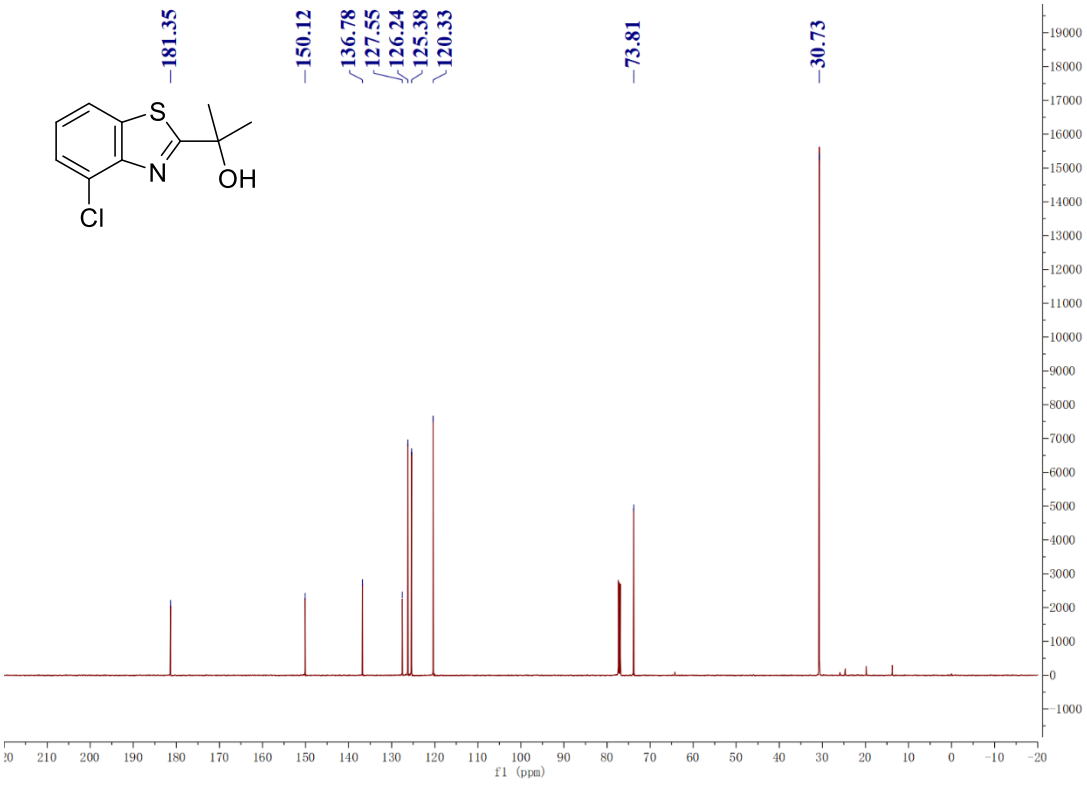
^{13}C NMR (151 MHz, $CDCl_3$) of 3n



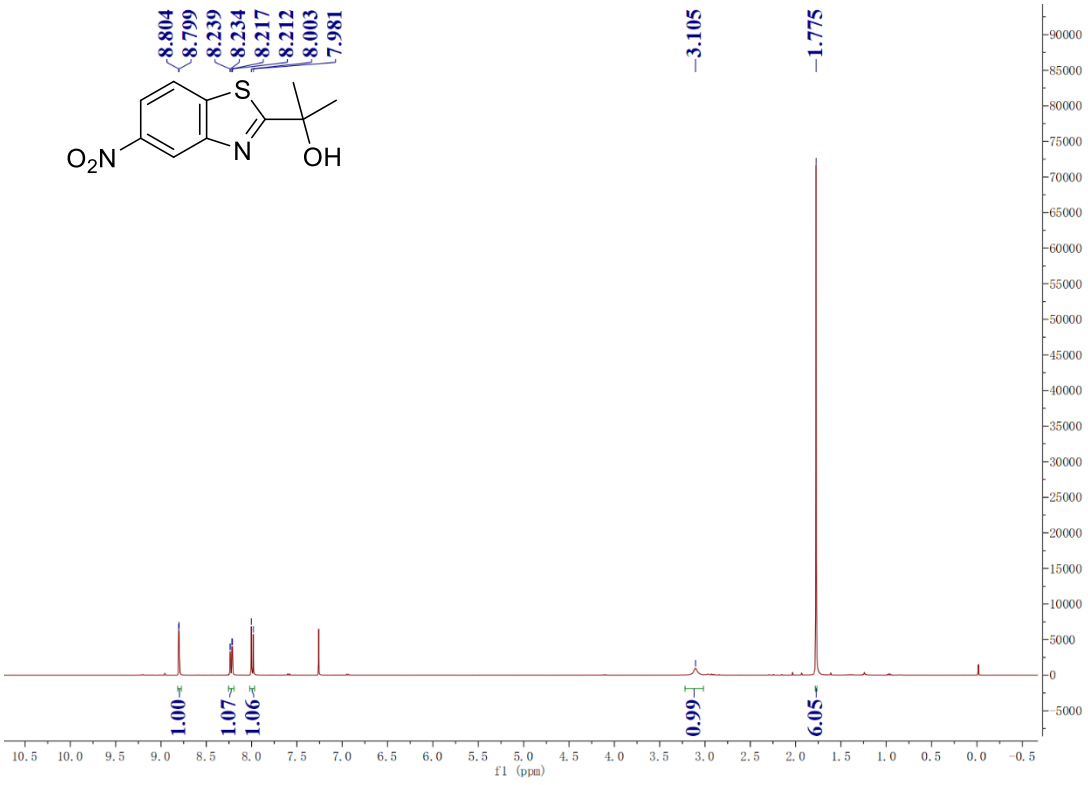
^{1}H NMR (600 MHz, $CDCl_3$) of 3o



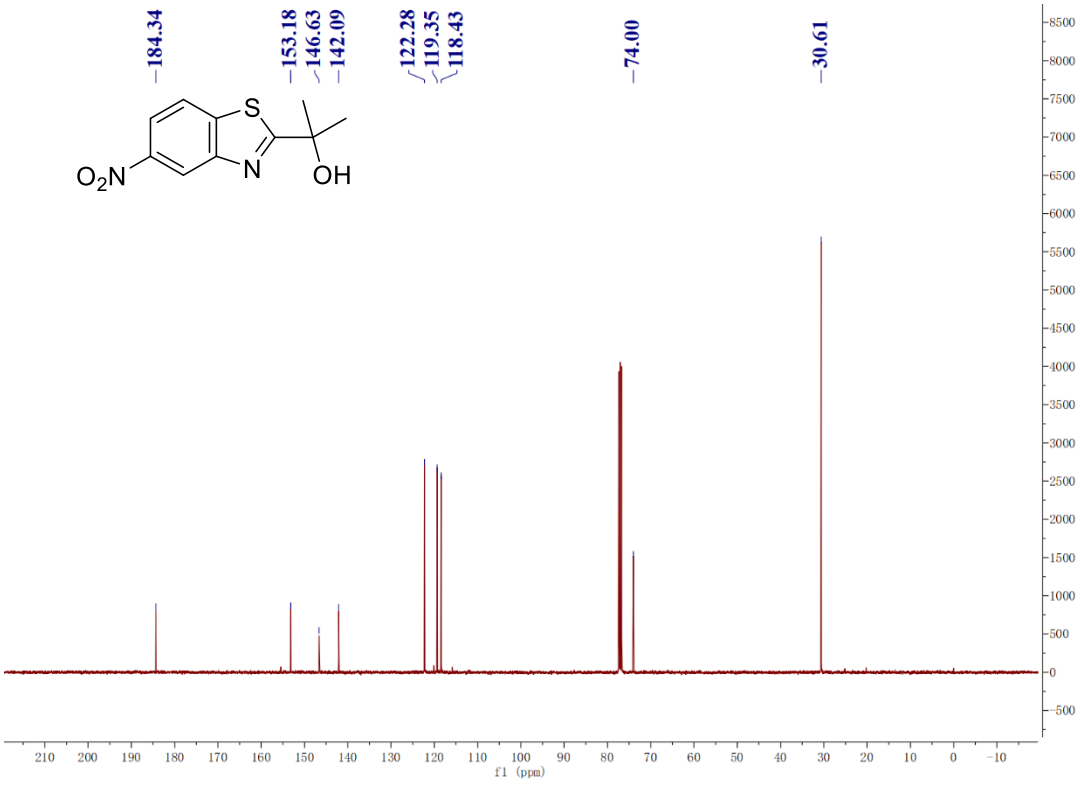
^{13}C NMR (151 MHz, $CDCl_3$) of 3o



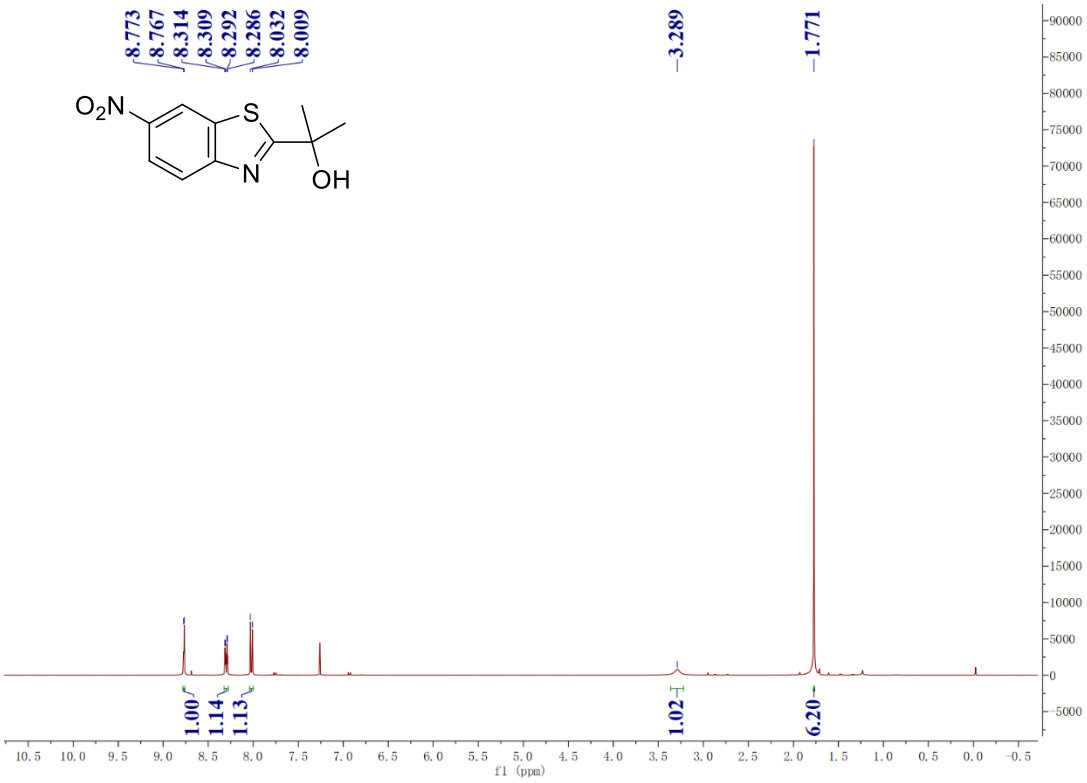
^{1}H NMR (400 MHz, $CDCl_3$) of 3p



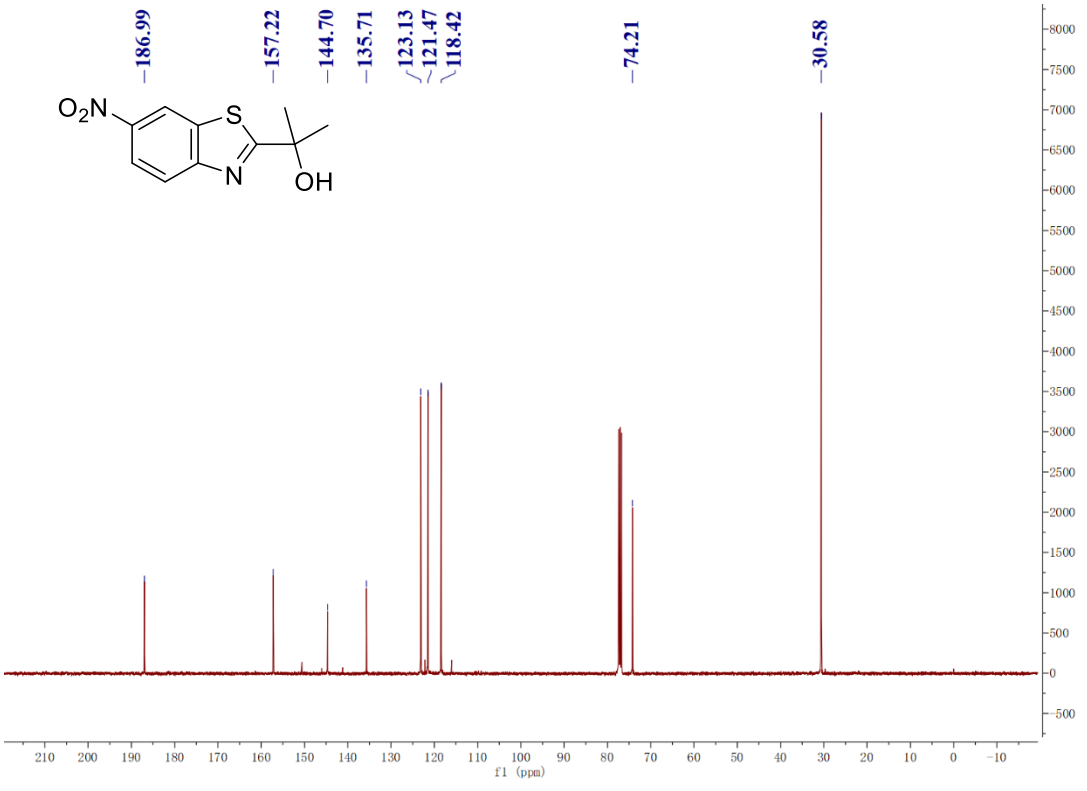
^{13}C NMR (101 MHz, $CDCl_3$) of 3p



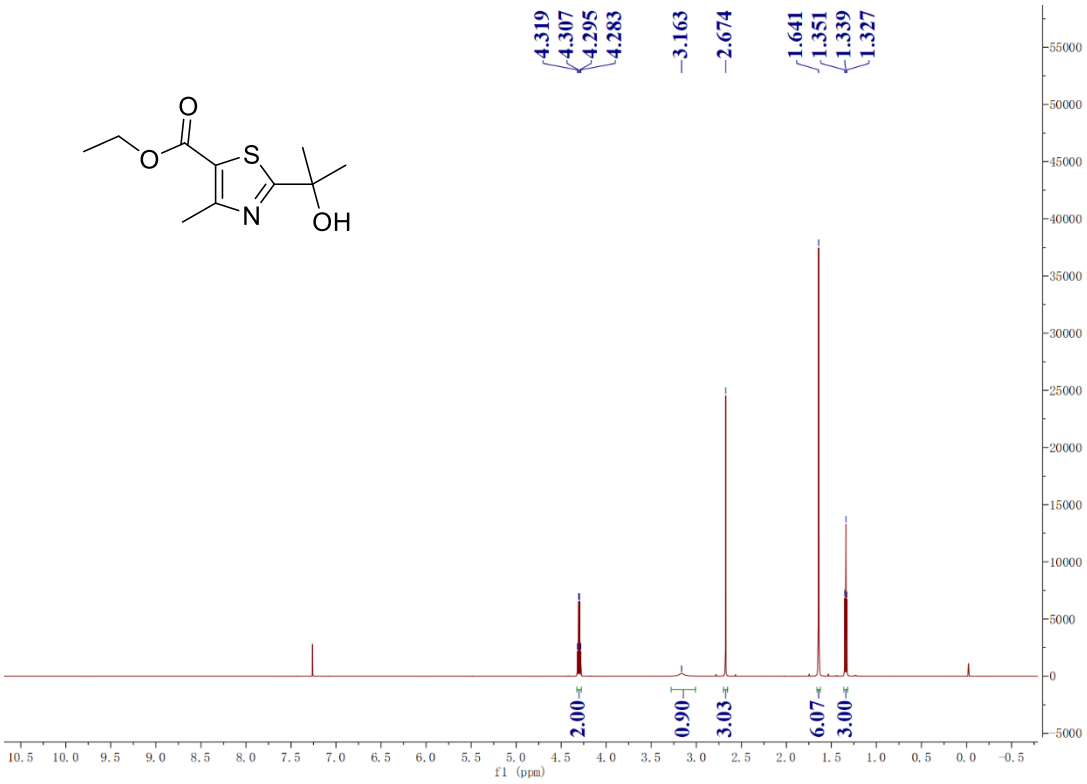
^{1}H NMR (400 MHz, $CDCl_3$) of 3q



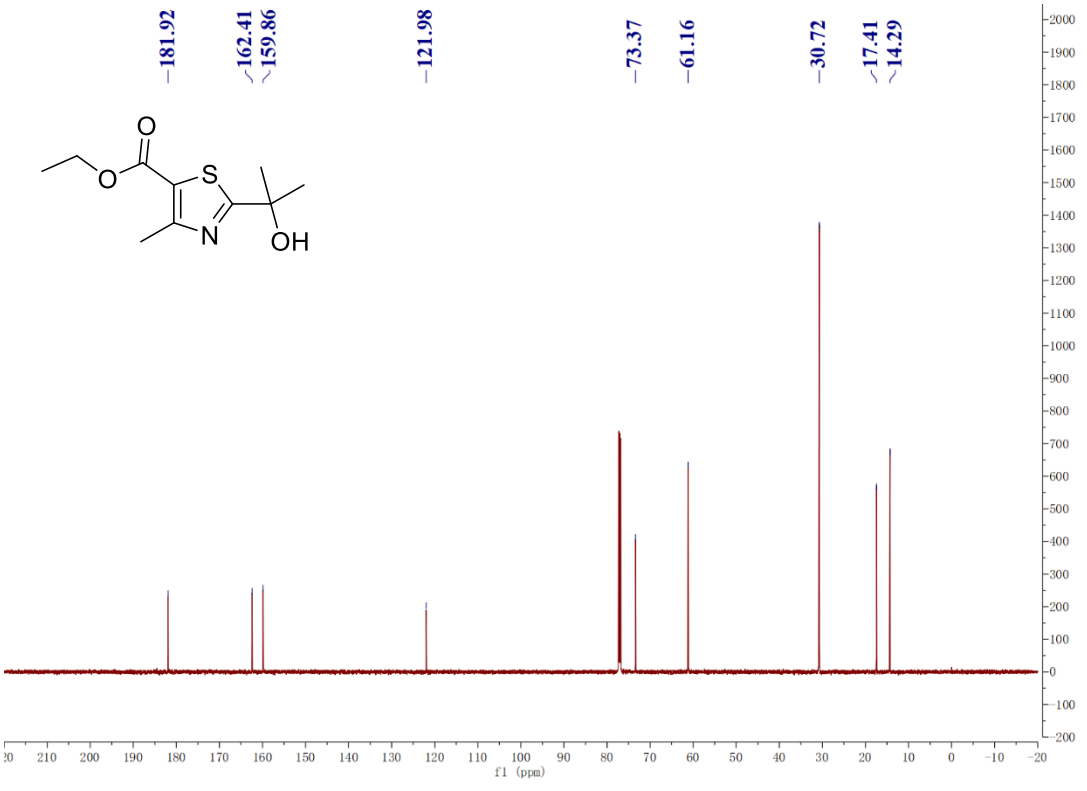
^{13}C NMR (101 MHz, $CDCl_3$) of 3q



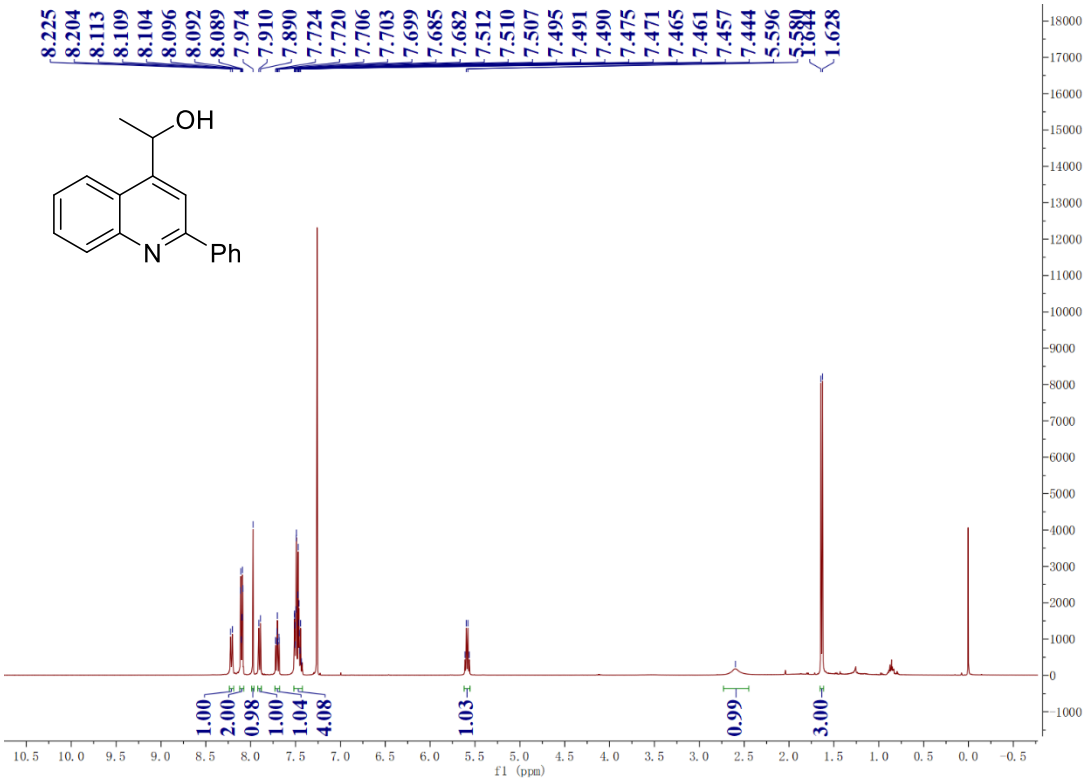
^{1}H NMR (600 MHz, $CDCl_3$) of 3r



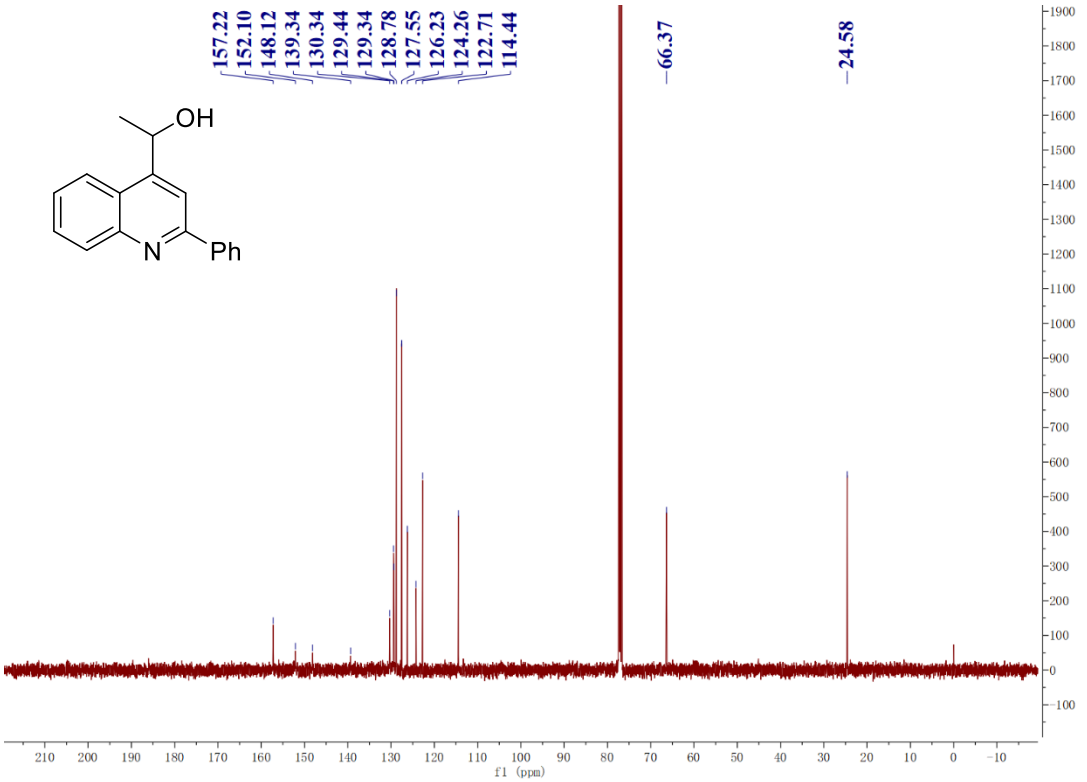
^{13}C NMR (151 MHz, $CDCl_3$) of 3r



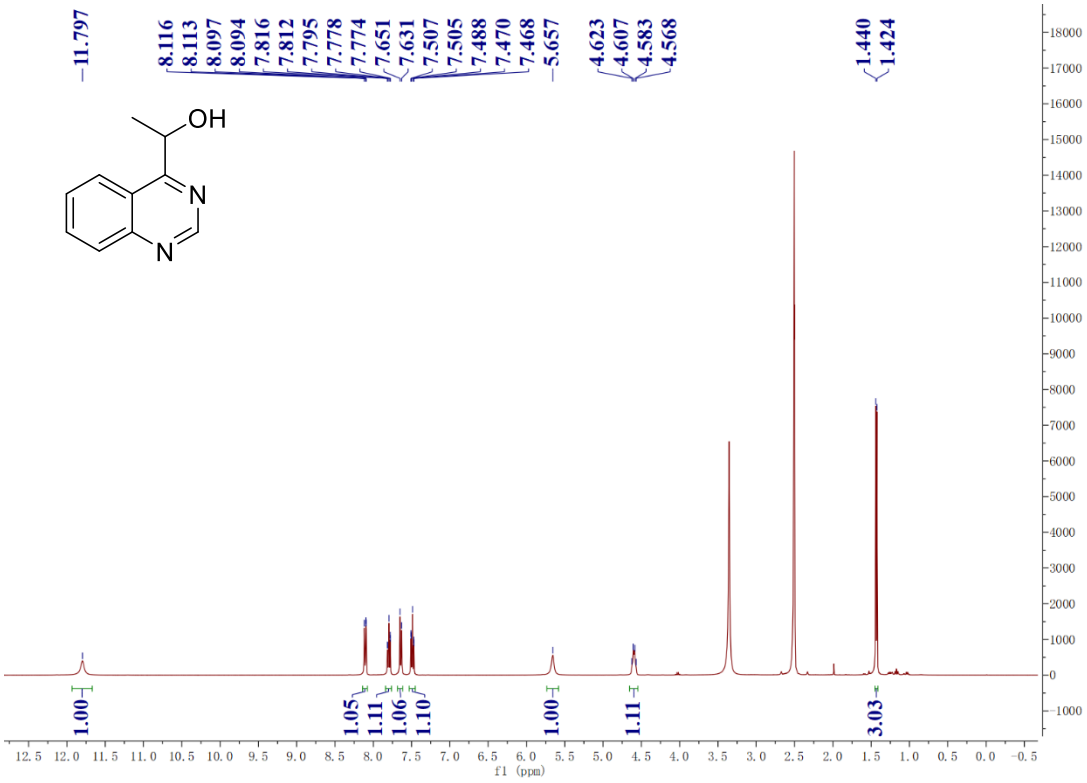
^{1}H NMR (400 MHz, $CDCl_3$) of 3s



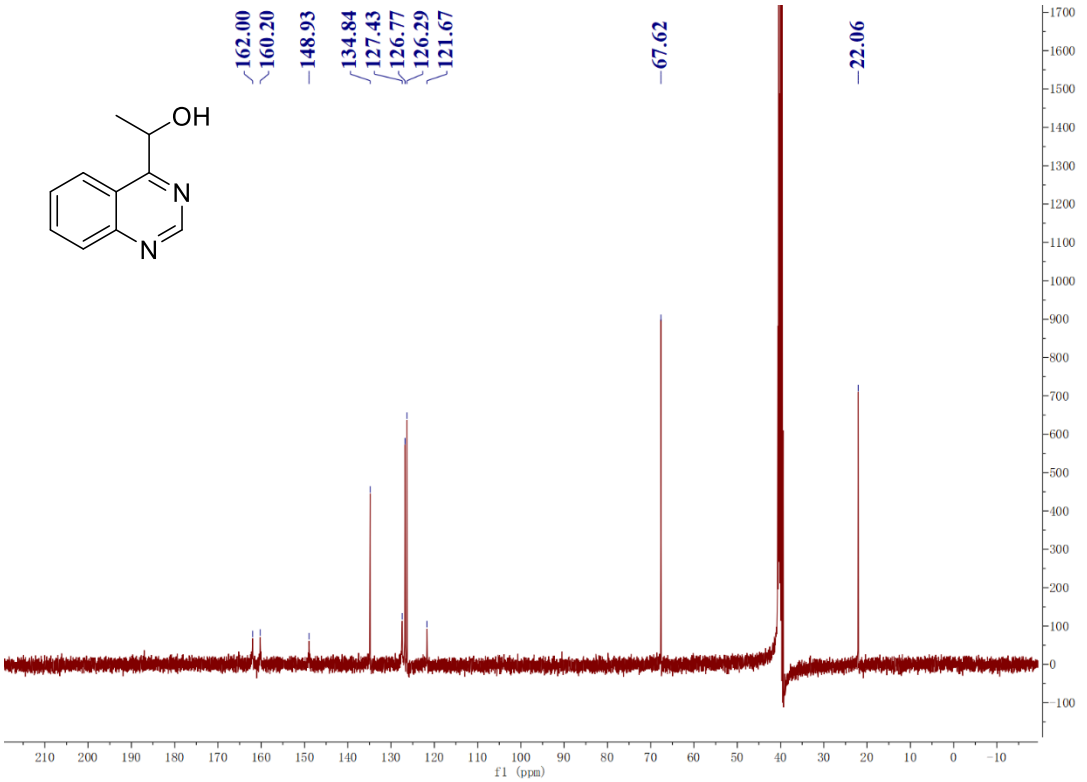
^{13}C NMR (101 MHz, $CDCl_3$) of 3s



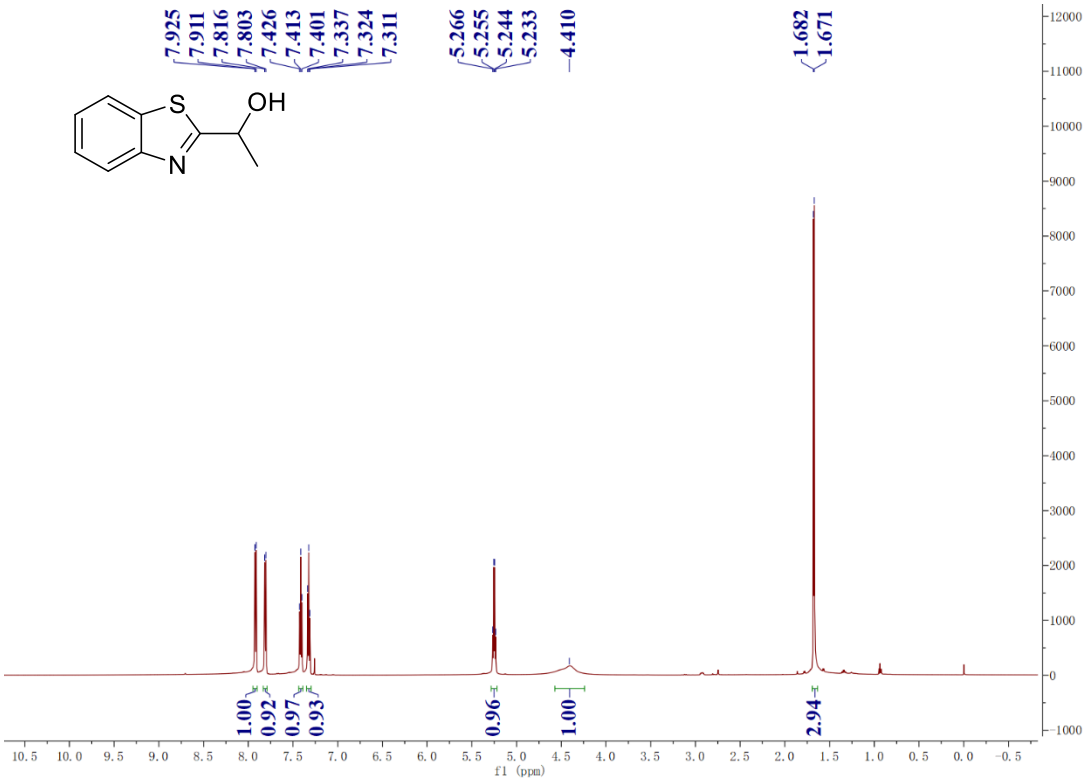
^{1}H NMR (400 MHz, DMSO-d_6) of 3t



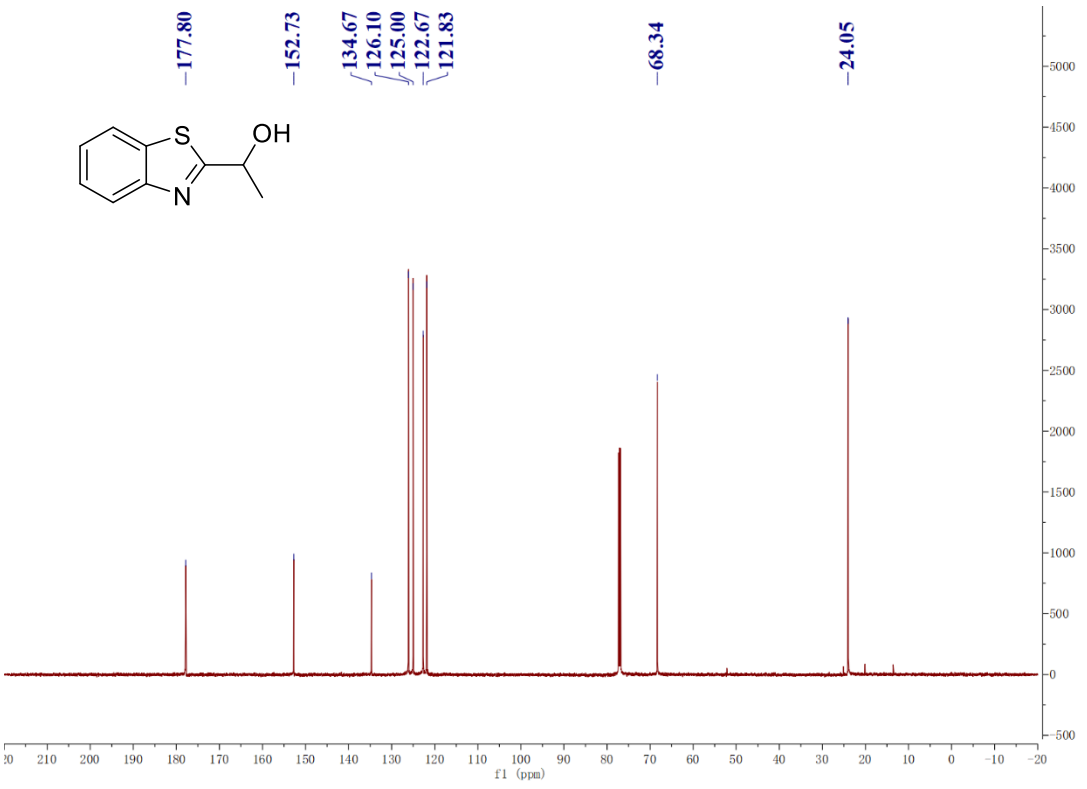
^{13}C NMR (101 MHz, DMSO-d_6) of 3t



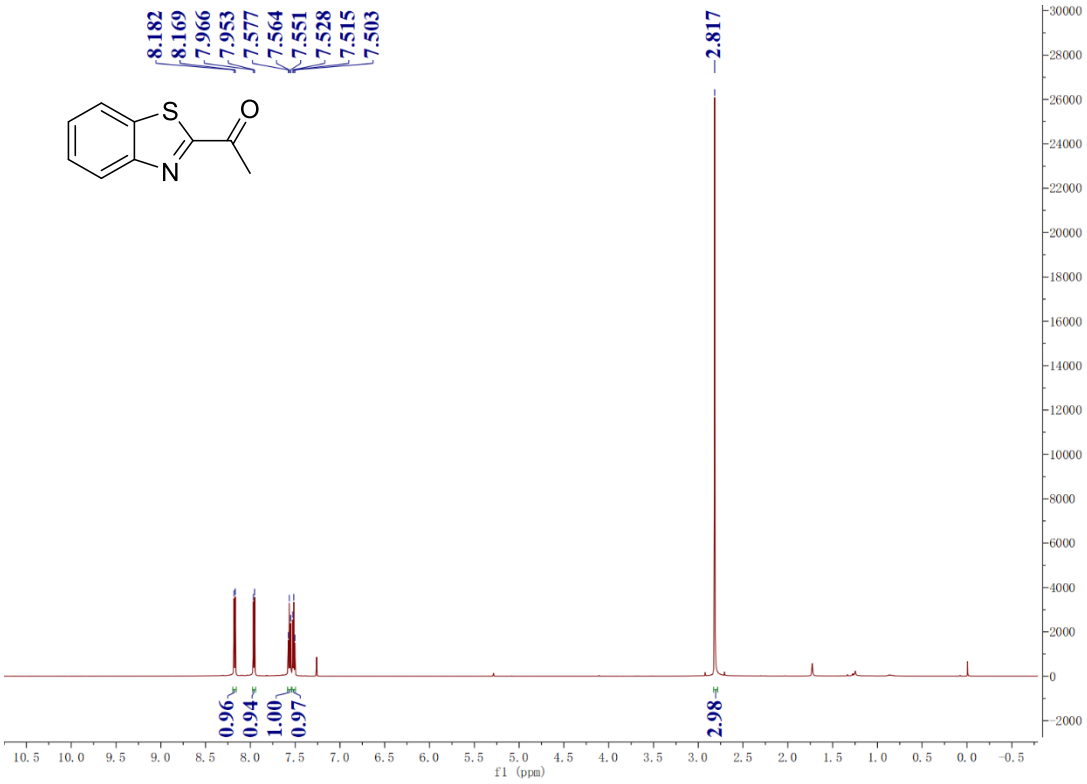
^{1}H NMR (600 MHz, $CDCl_3$) of 4a



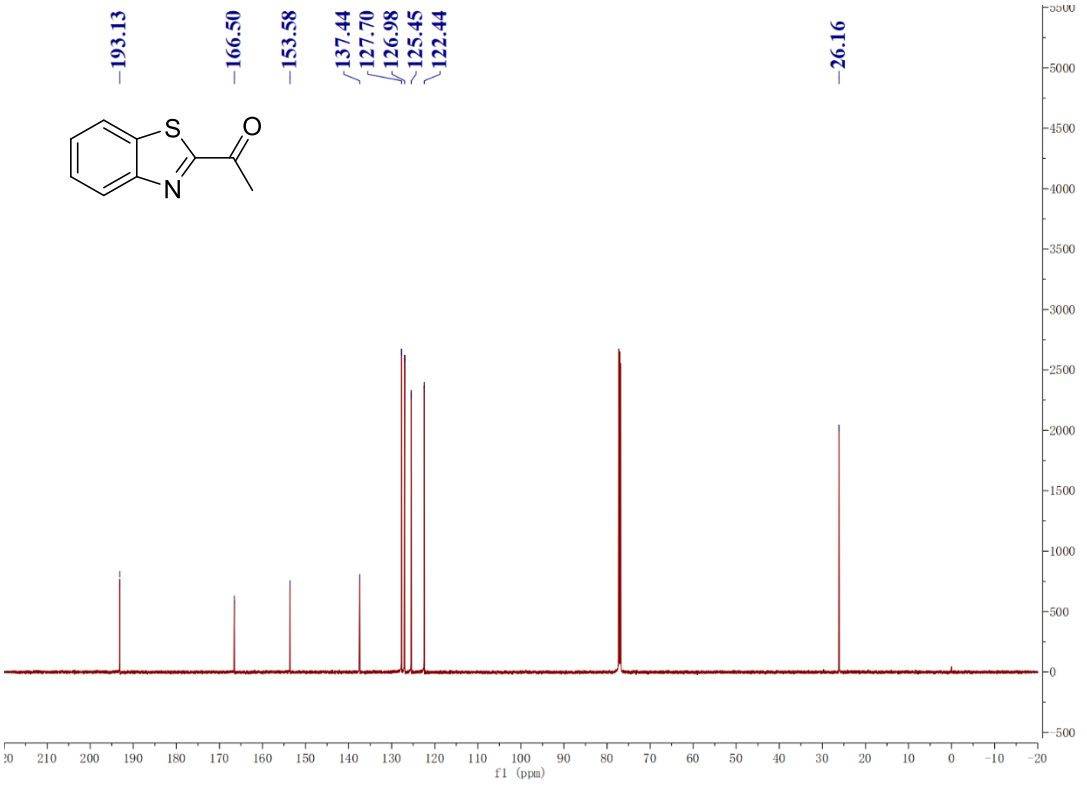
^{13}C NMR (151 MHz, $CDCl_3$) of 4a



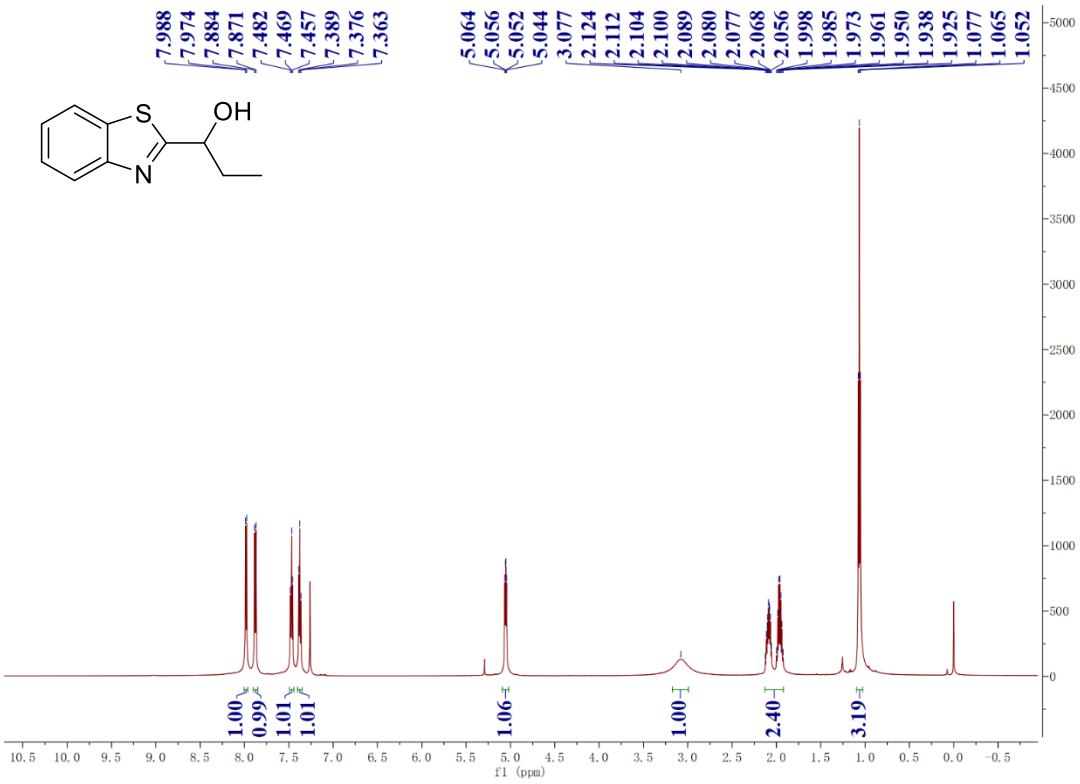
^{1}H NMR (600 MHz, $CDCl_3$) of 4a′



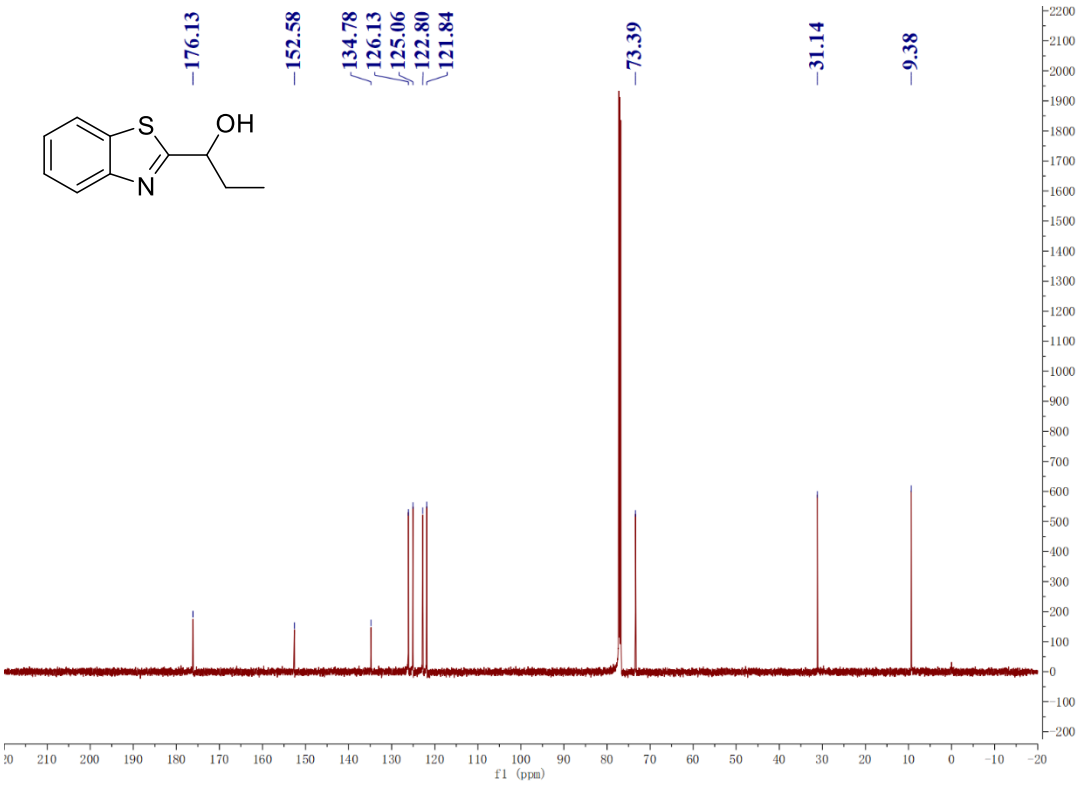
^{13}C NMR (151 MHz, $CDCl_3$) of 4a′



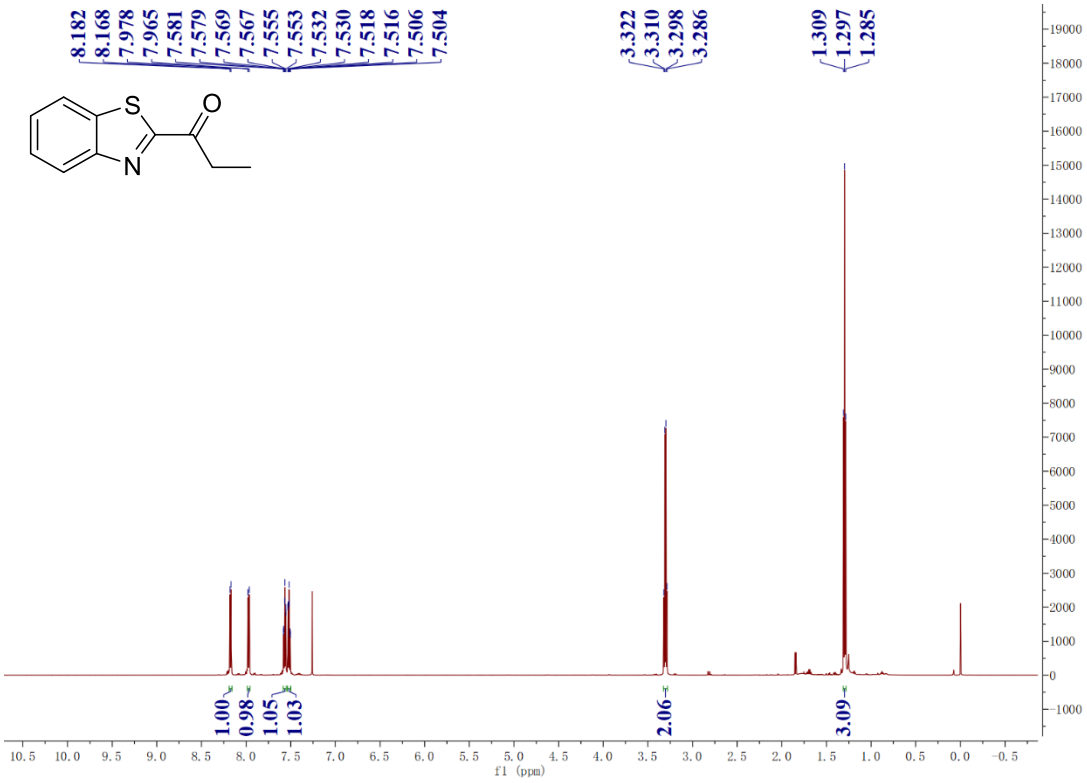
^{1}H NMR (600 MHz, $CDCl_3$) of 4b



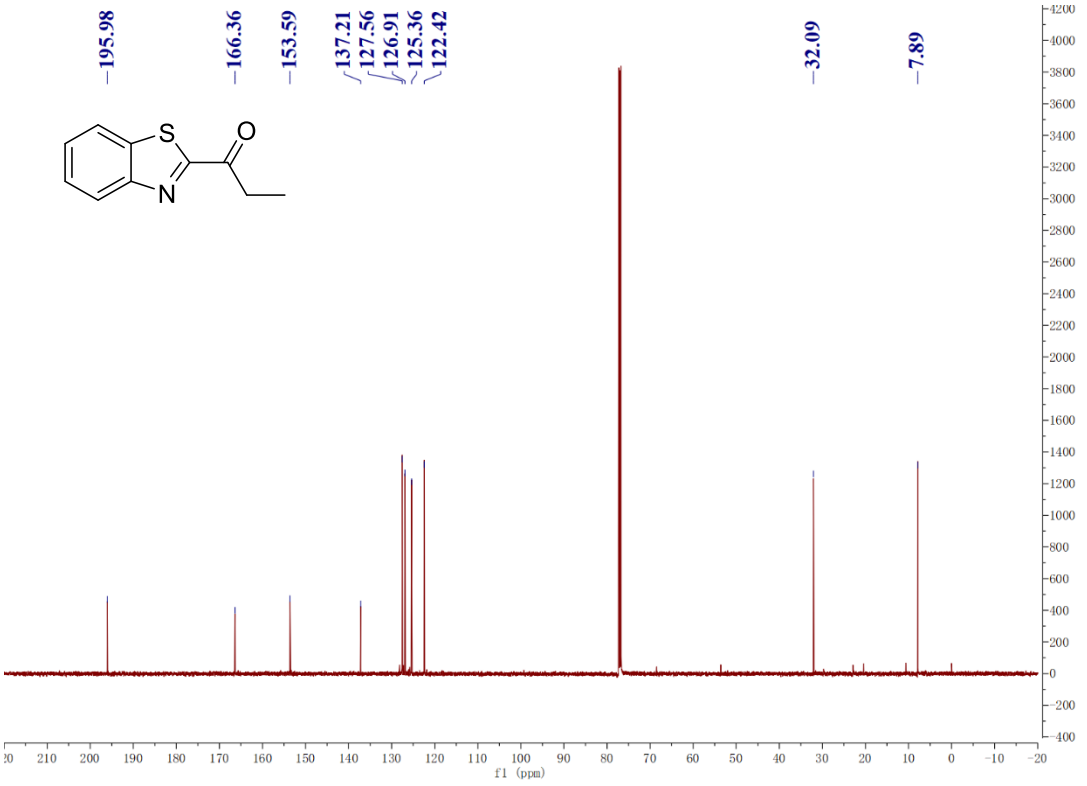
^{13}C NMR (151 MHz, $CDCl_3$) of 4b



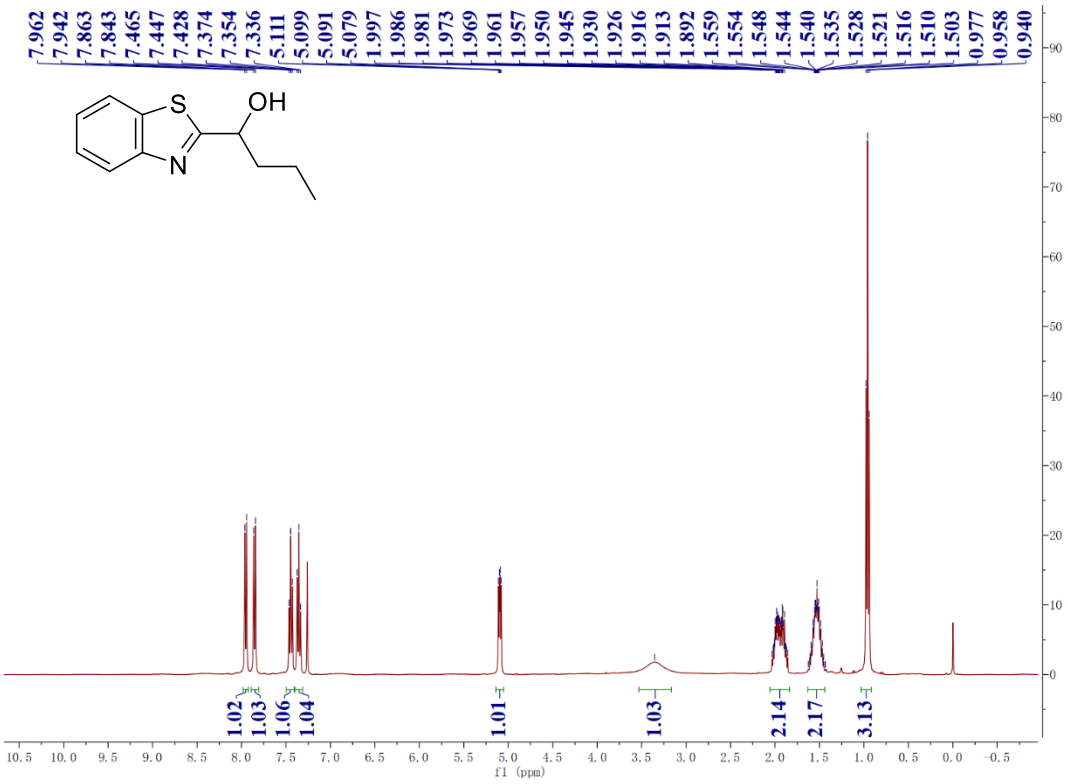
^{1}H NMR (600 MHz, $CDCl_3$) of 4b′



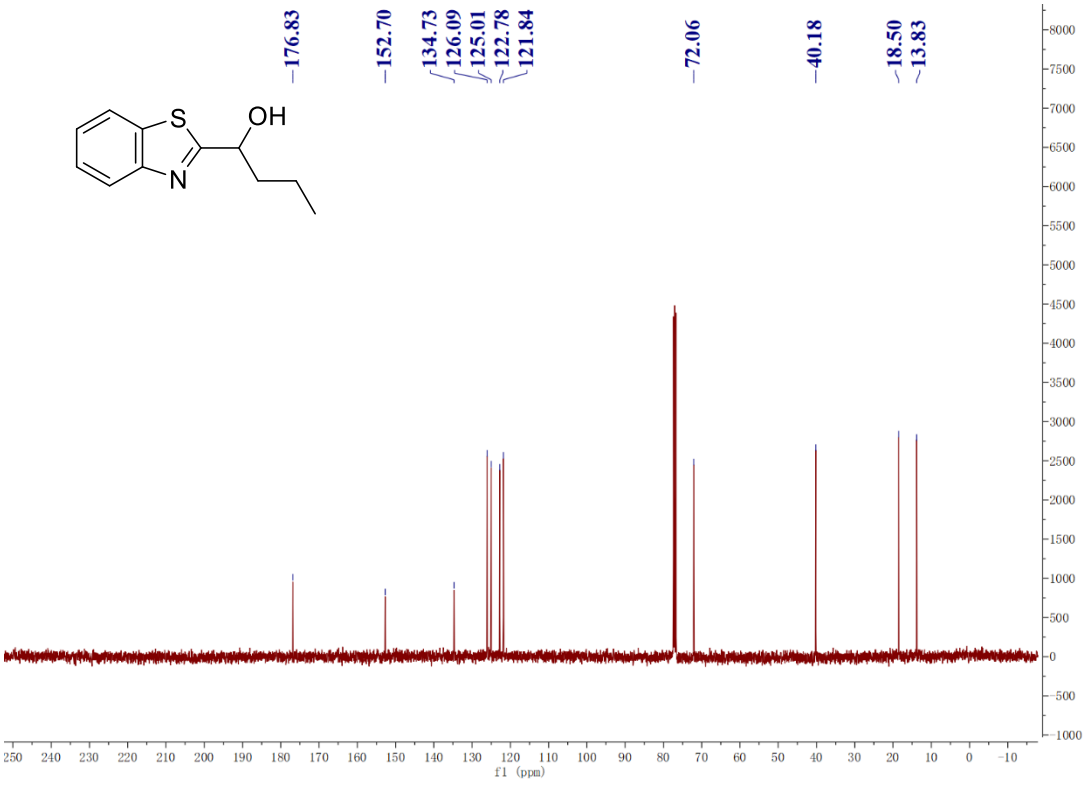
^{13}C NMR (151 MHz, $CDCl_3$) of 4b′



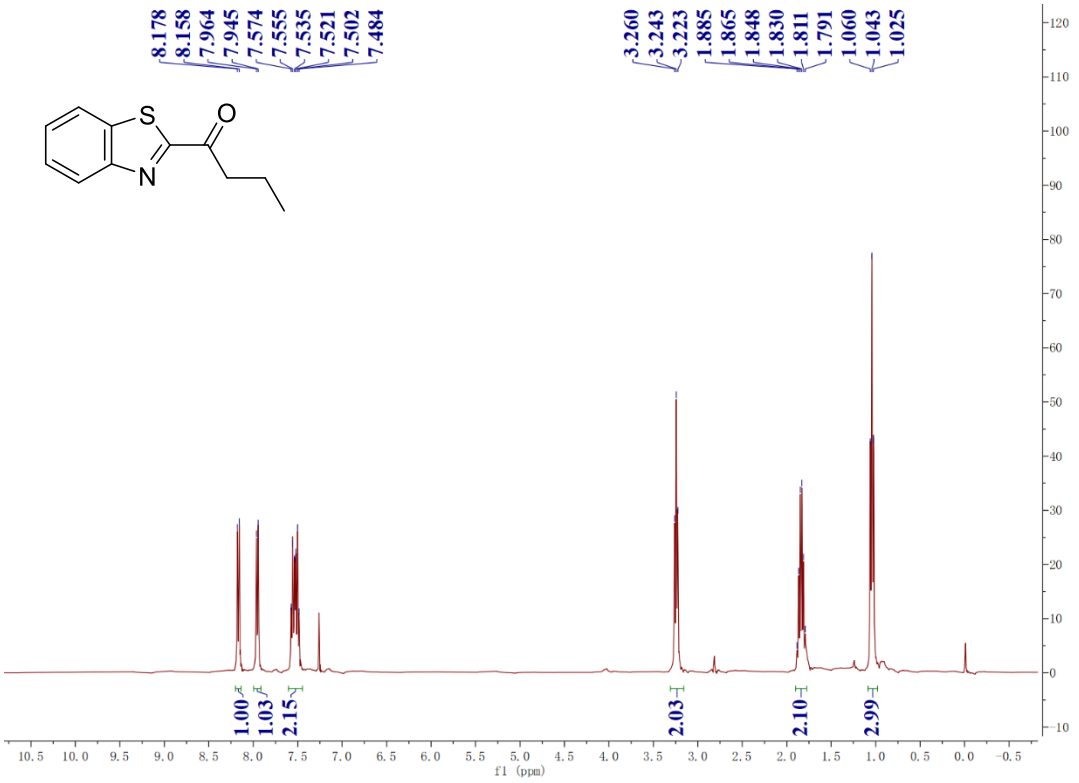
^{1}H NMR (400 MHz, $CDCl_3$) of 4c



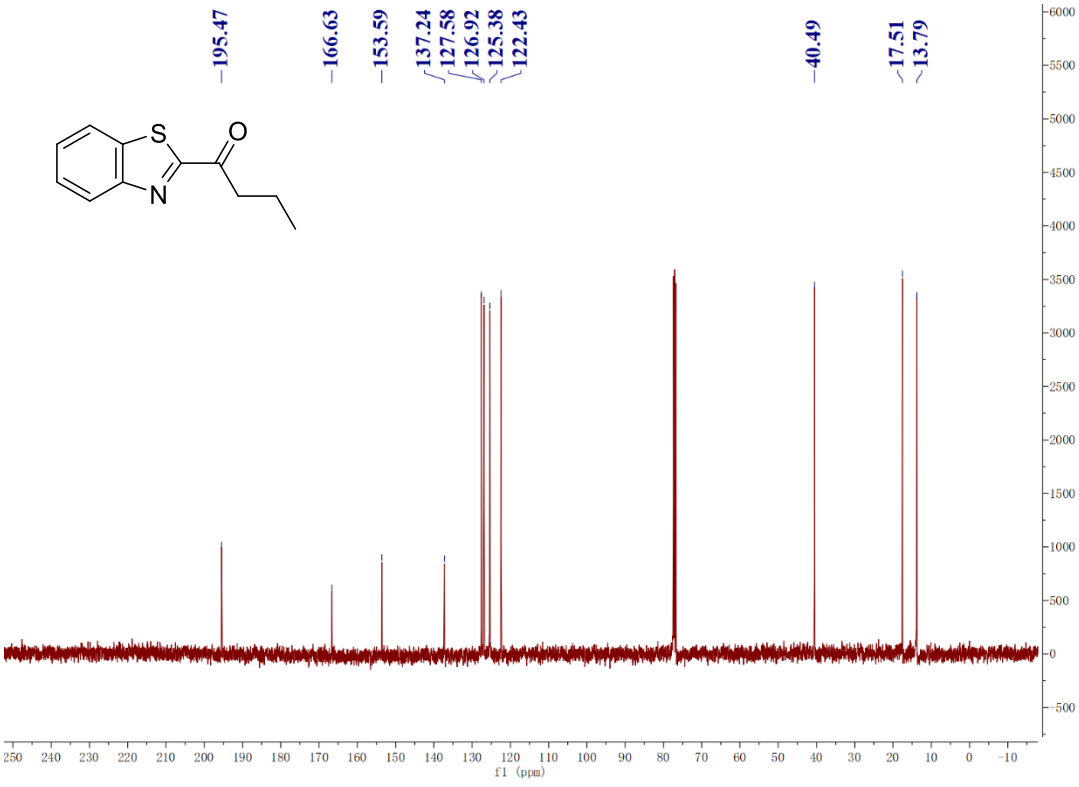
^{13}C NMR (101 MHz, $CDCl_3$) of 4c



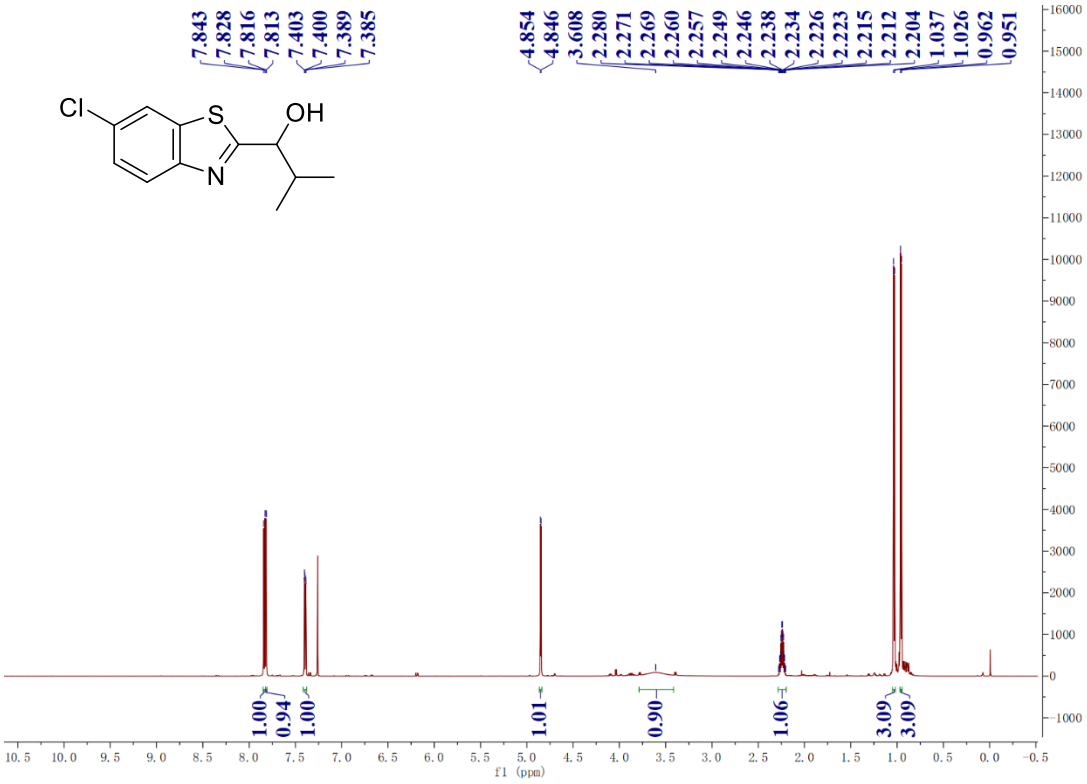
^{1}H NMR (400 MHz, $CDCl_3$) of 4c′



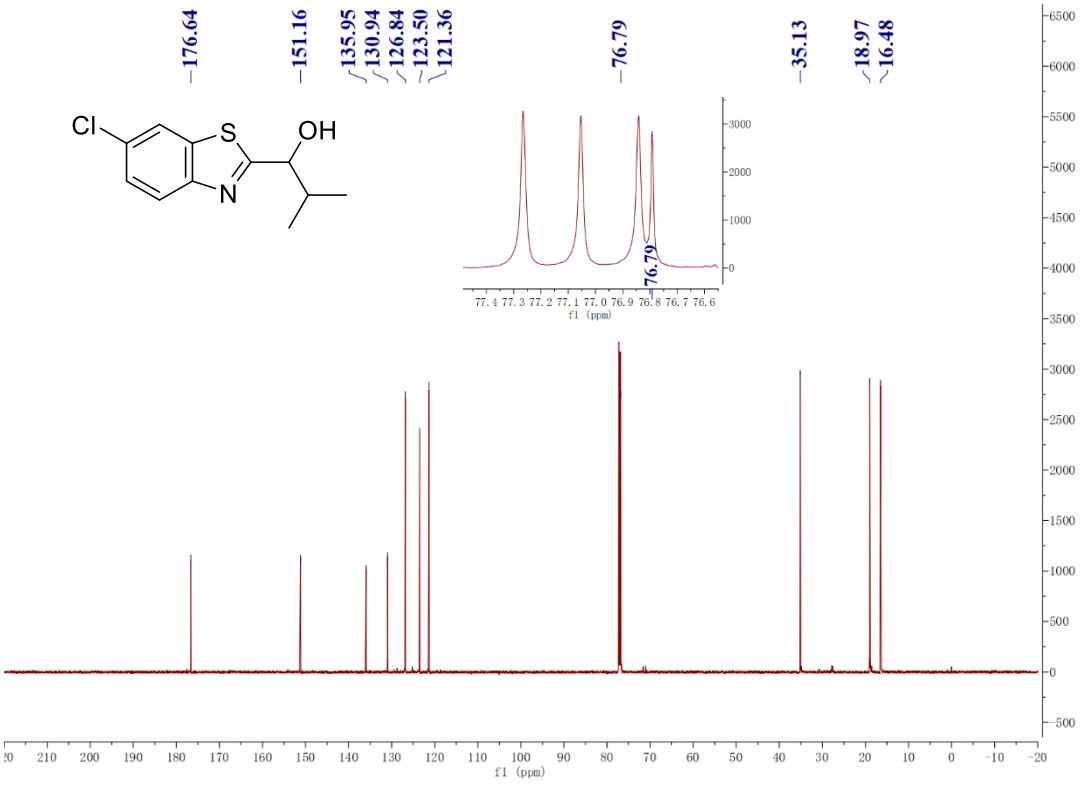
^{13}C NMR (101 MHz, $CDCl_3$) of 4c′



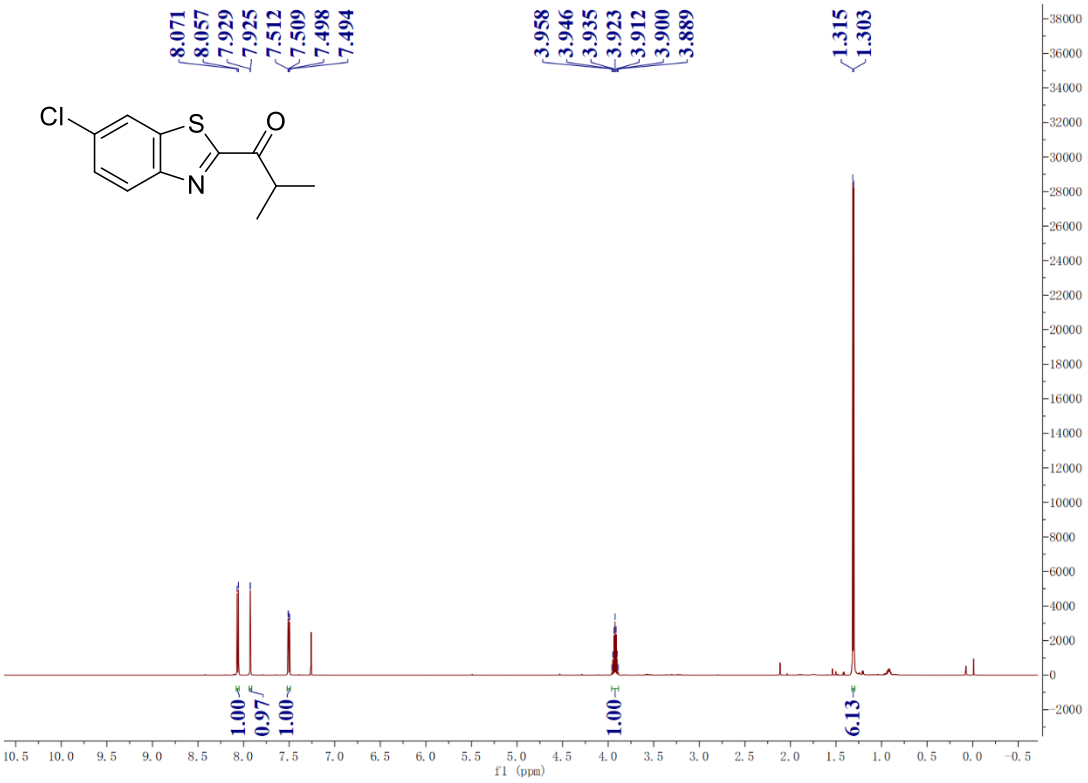
^{1}H NMR (600 MHz, $CDCl_3$) of 4d



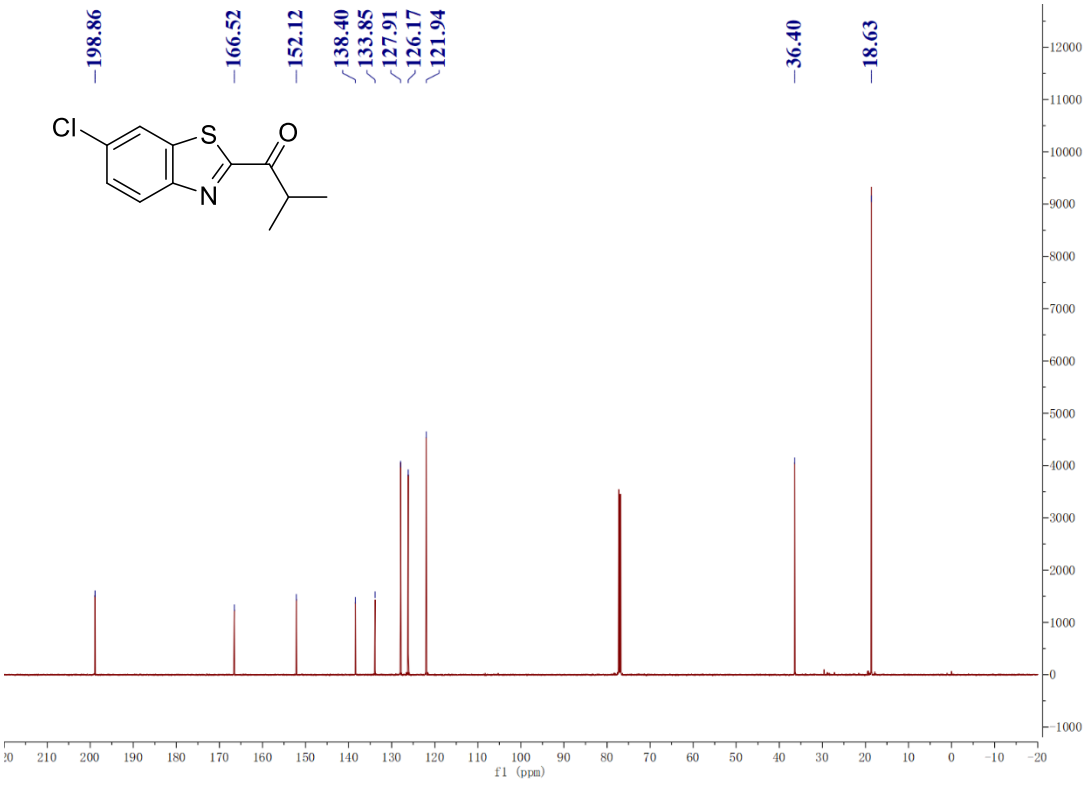
^{13}C NMR (151 MHz, $CDCl_3$) of 4d



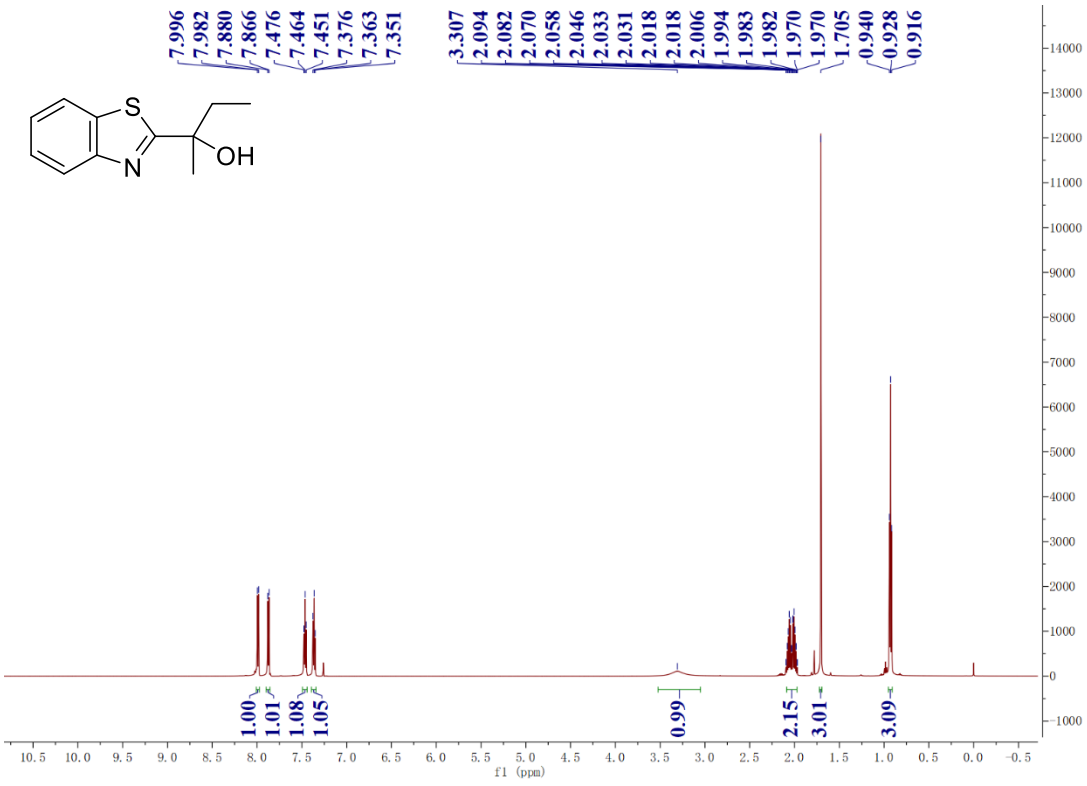
^{1}H NMR (600 MHz, $CDCl_3$) of 4d′



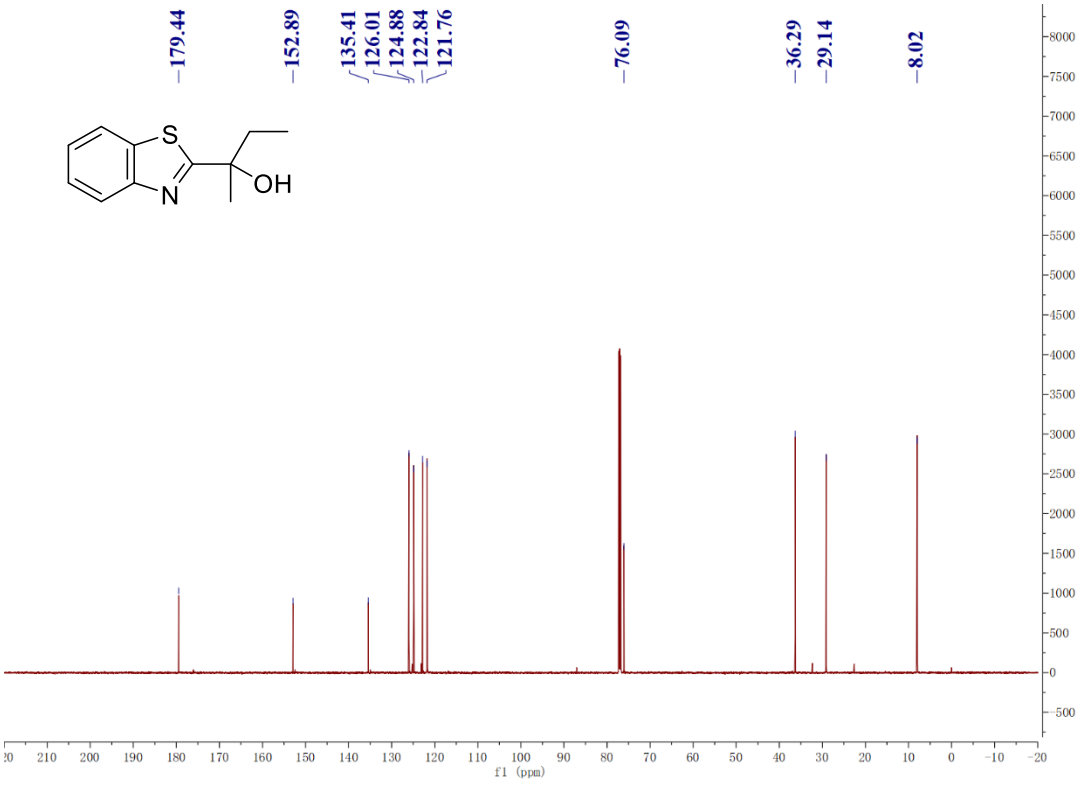
^{13}C NMR (151 MHz, $CDCl_3$) of 4d′



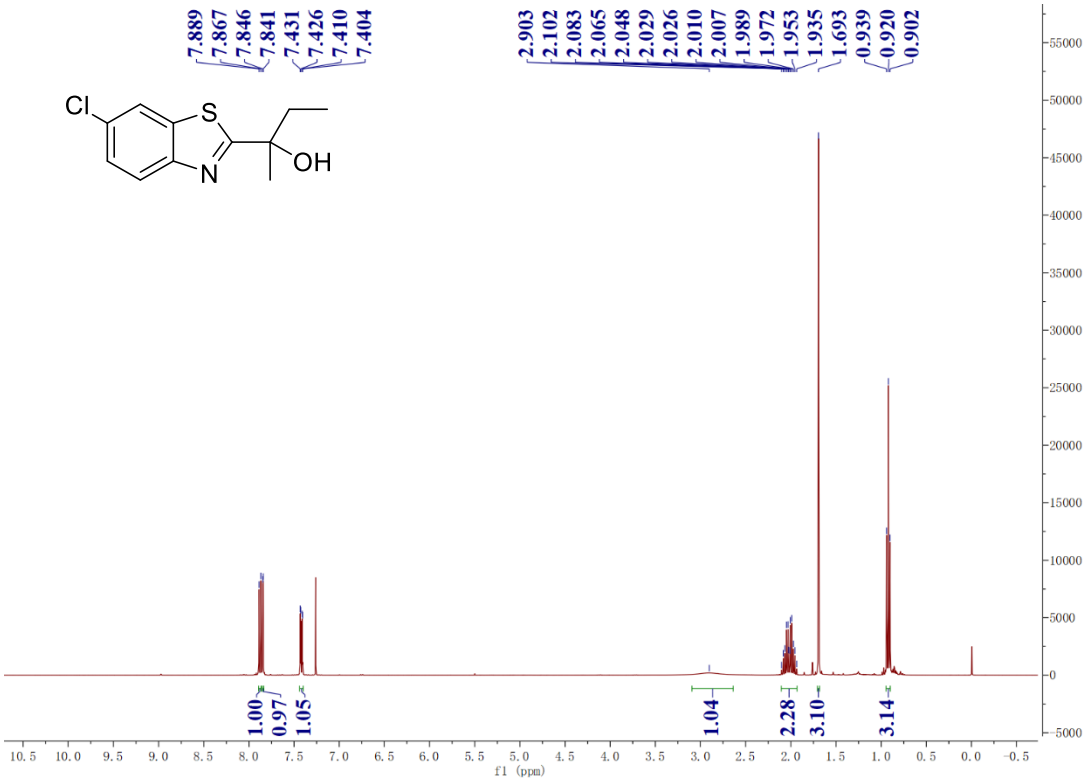
^{1}H NMR (600 MHz, $CDCl_3$) of 4e



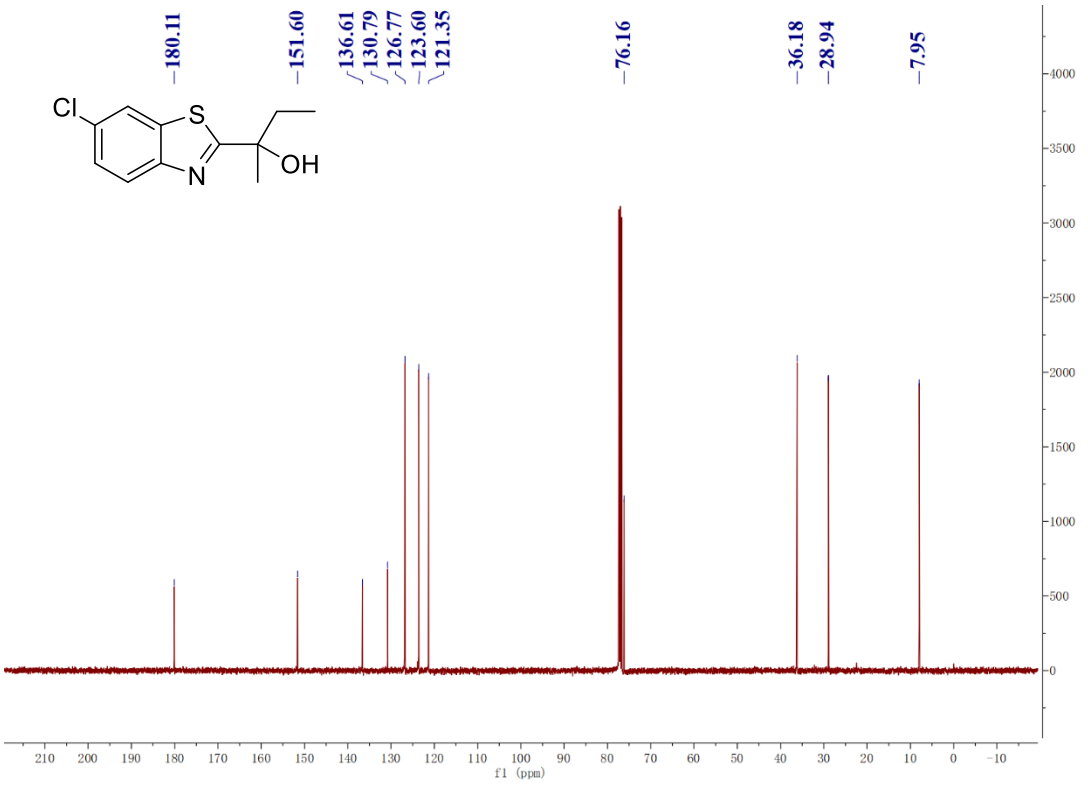
^{13}C NMR (151 MHz, $CDCl_3$) of 4e



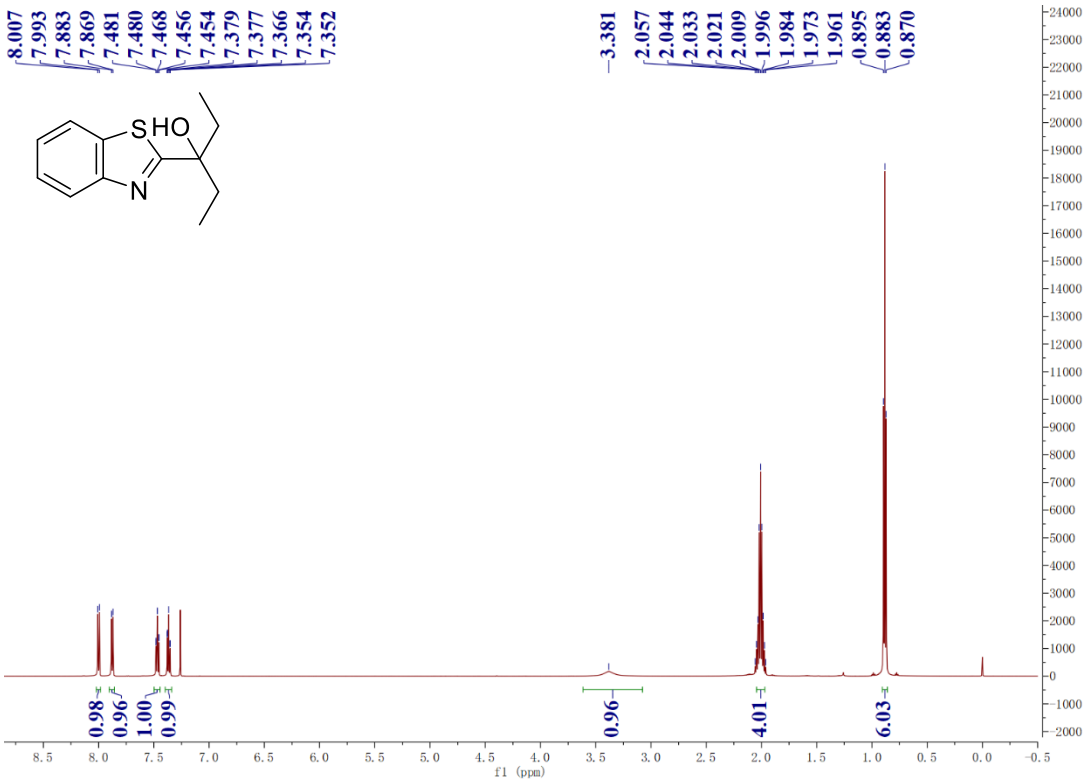
^{1}H NMR (400 MHz, $CDCl_3$) of 4e′



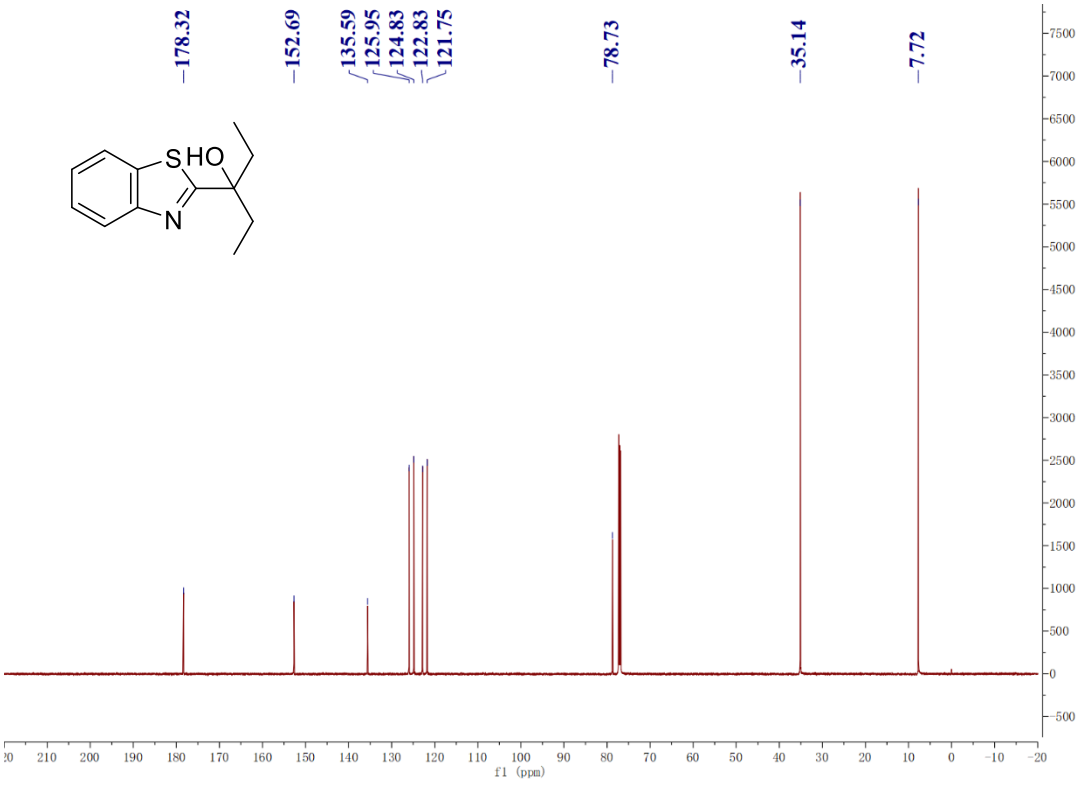
^{13}C NMR (101 MHz, $CDCl_3$) of 4e′



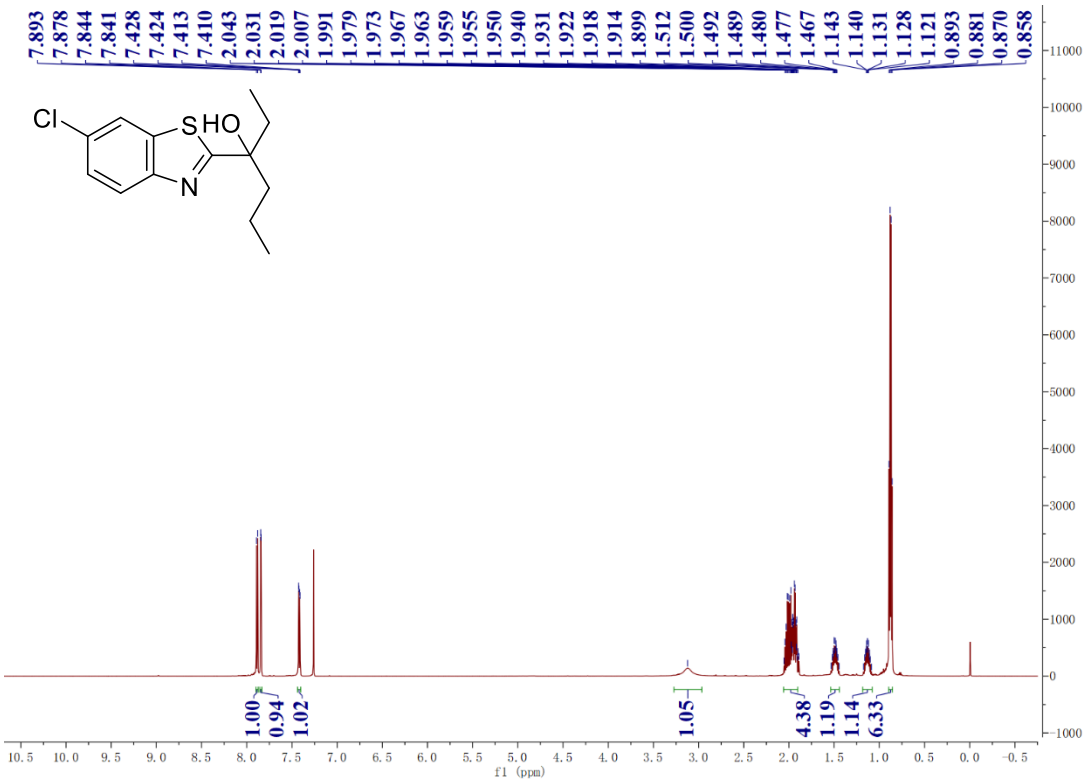
^{1}H NMR (600 MHz, $CDCl_3$) of 4f



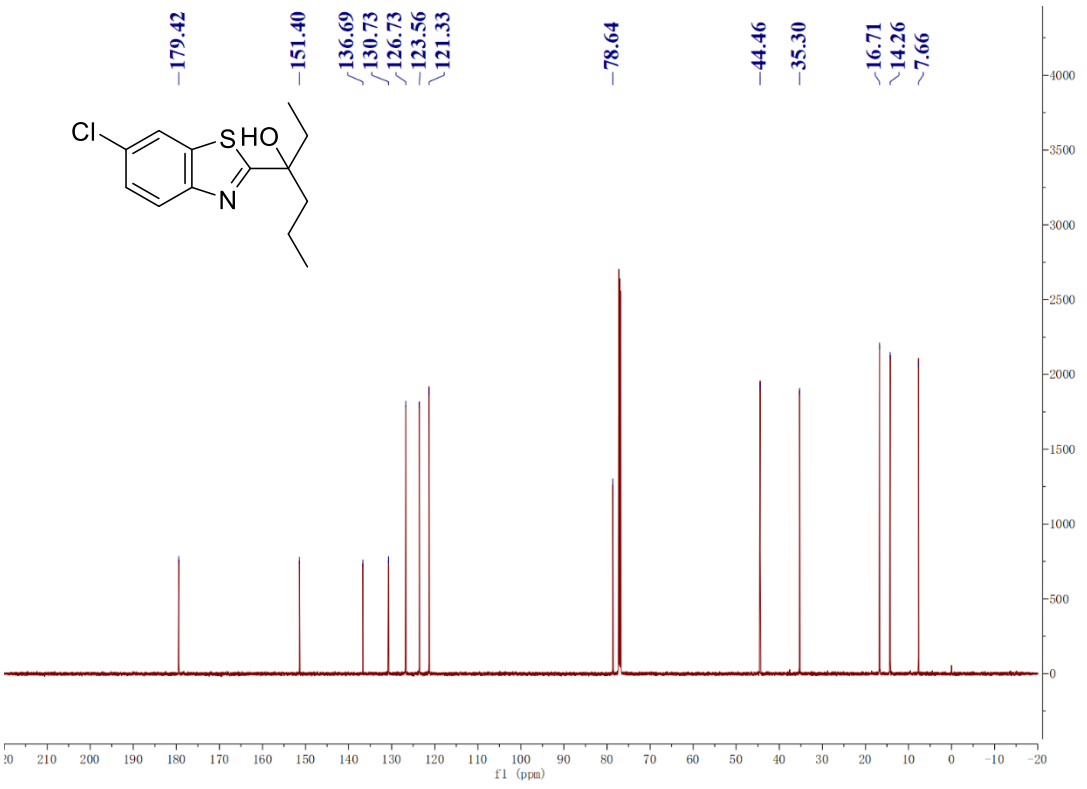
^{13}C NMR (151 MHz, $CDCl_3$) of 4f



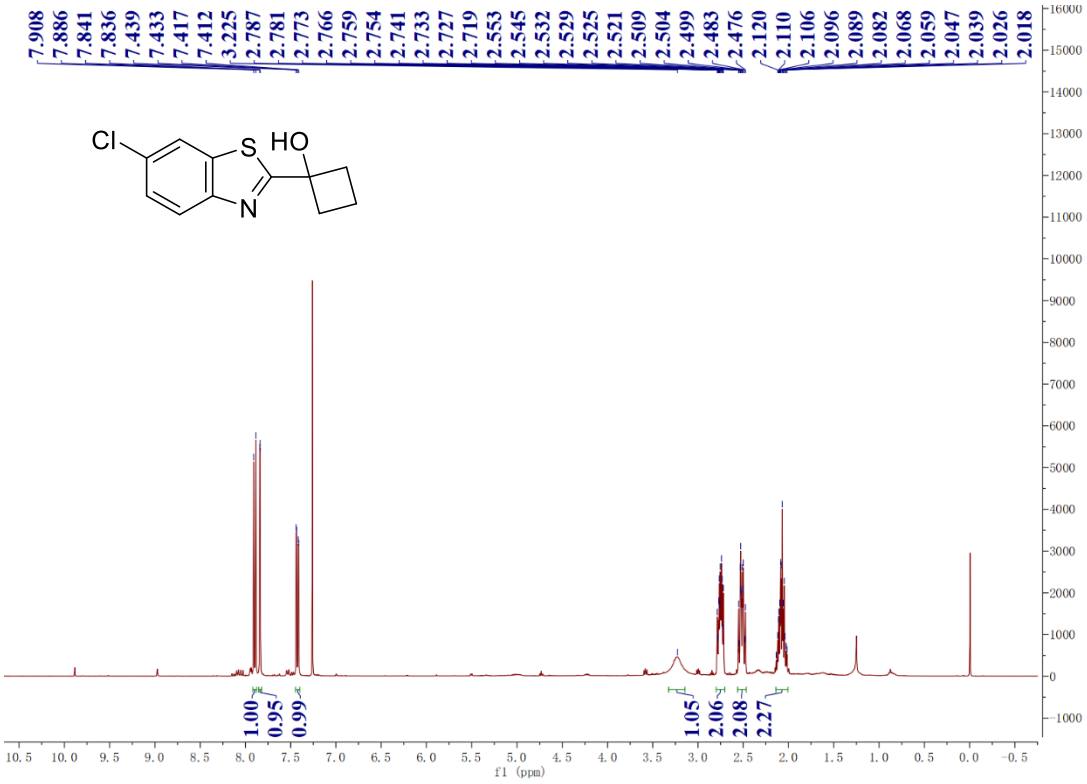
^{1}H NMR (600 MHz, $CDCl_3$) of 4g



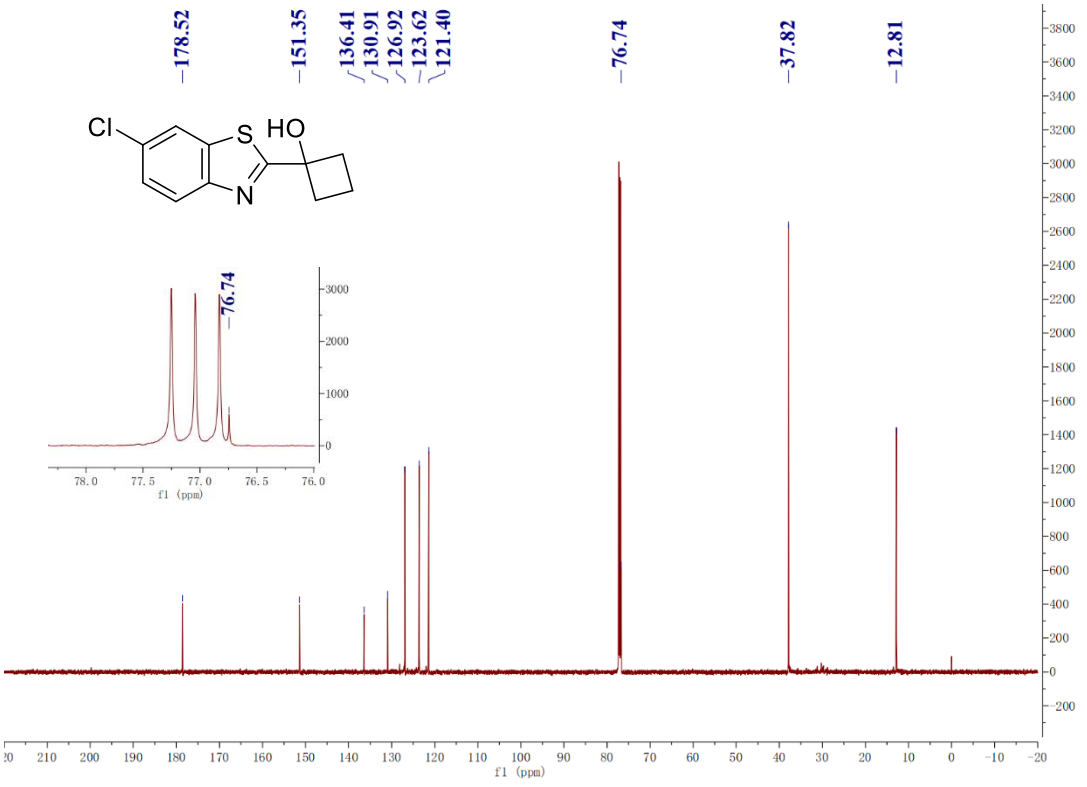
^{13}C NMR (151 MHz, $CDCl_3$) of 4g



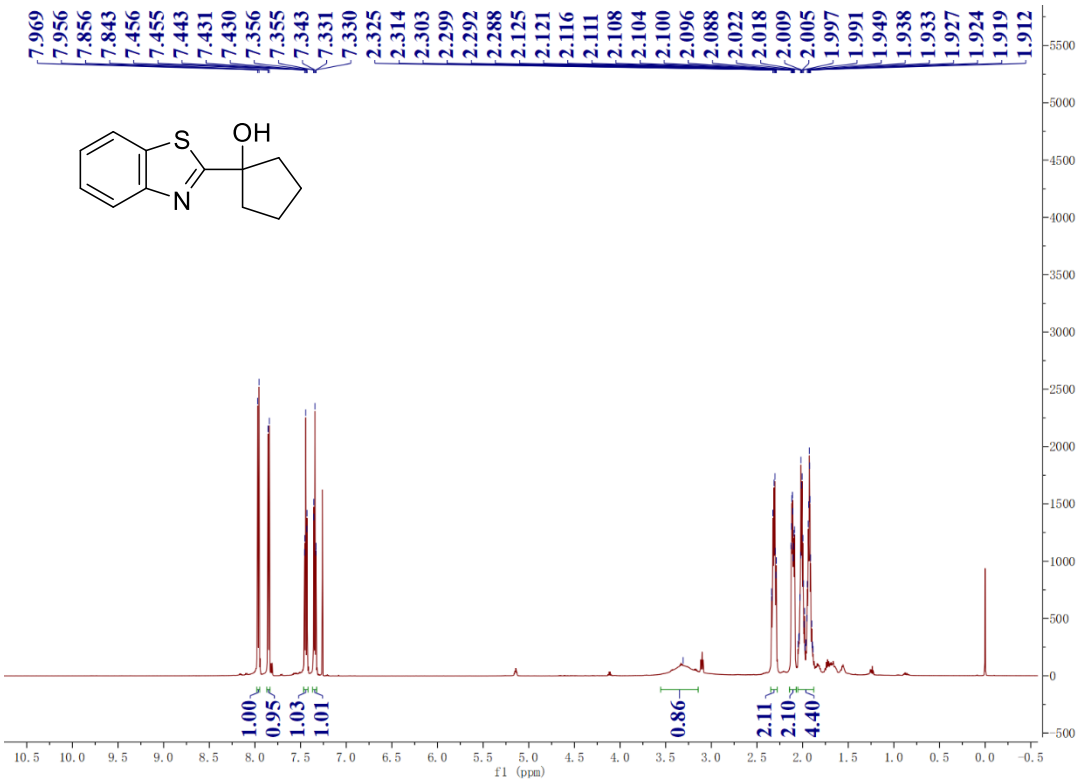
^{1}H NMR (400 MHz, $CDCl_3$) of 4h



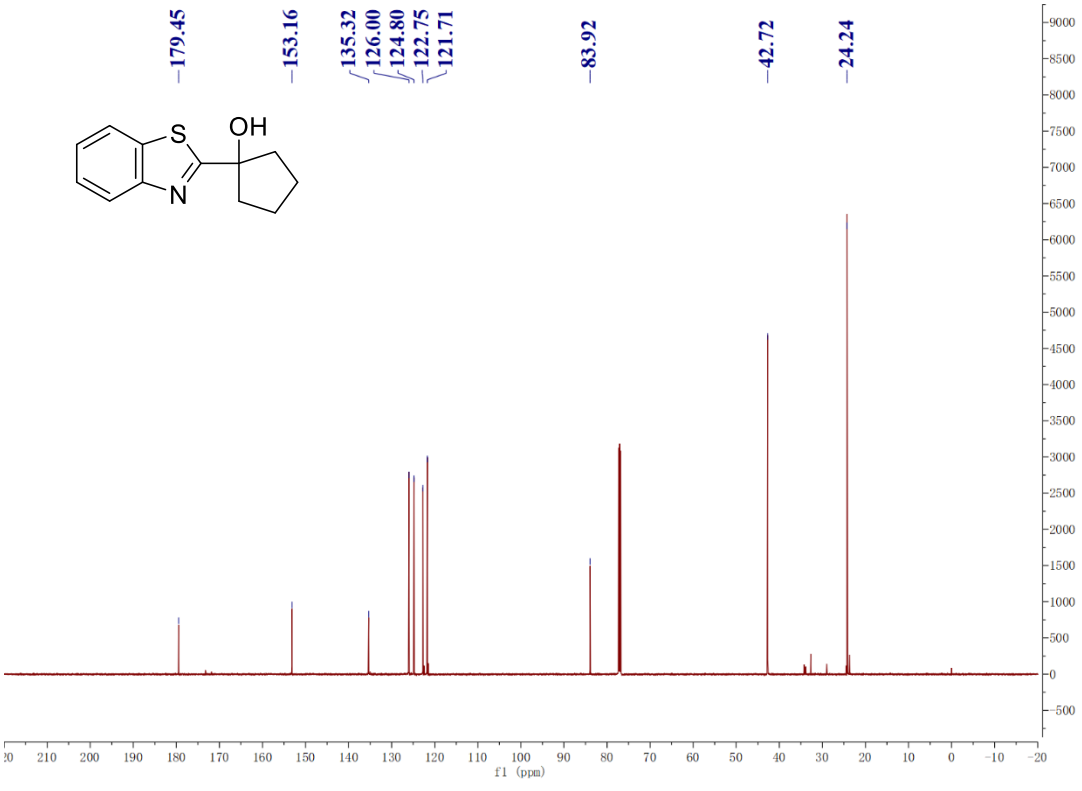
^{13}C NMR (151 MHz, $CDCl_3$) of 4h



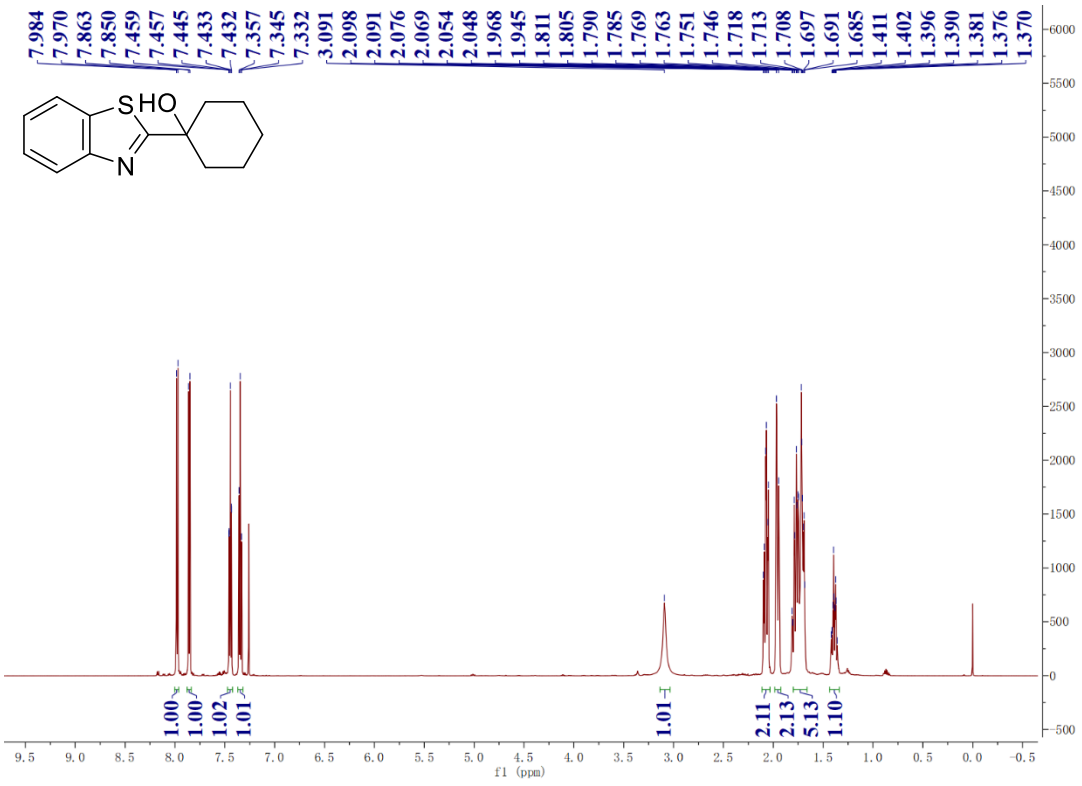
^{1}H NMR (600 MHz, $CDCl_3$) of 4i



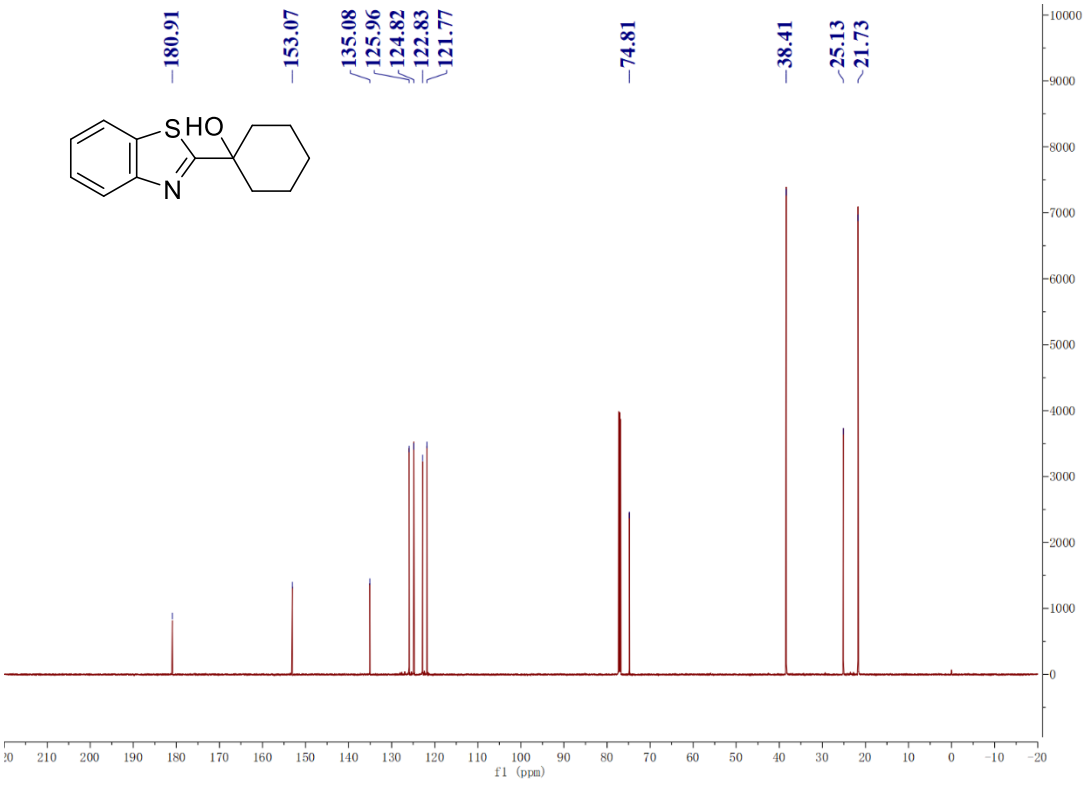
^{13}C NMR (151 MHz, $CDCl_3$) of 4i



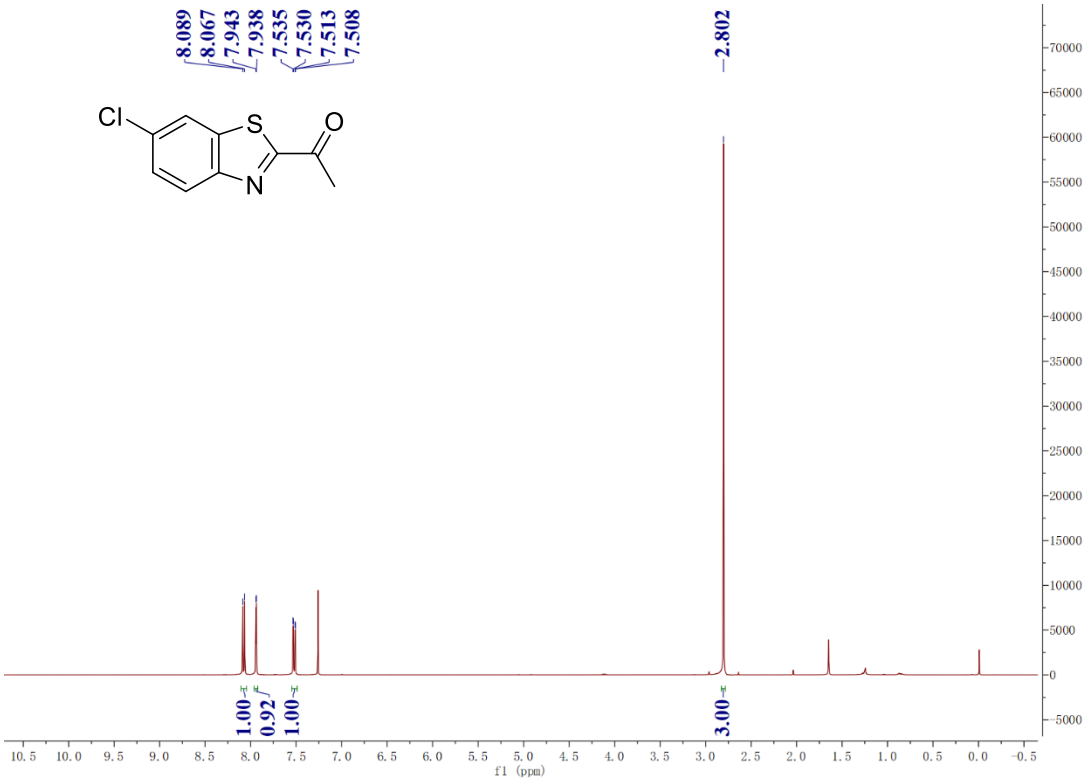
^{1}H NMR (600 MHz, $CDCl_3$) of 4j



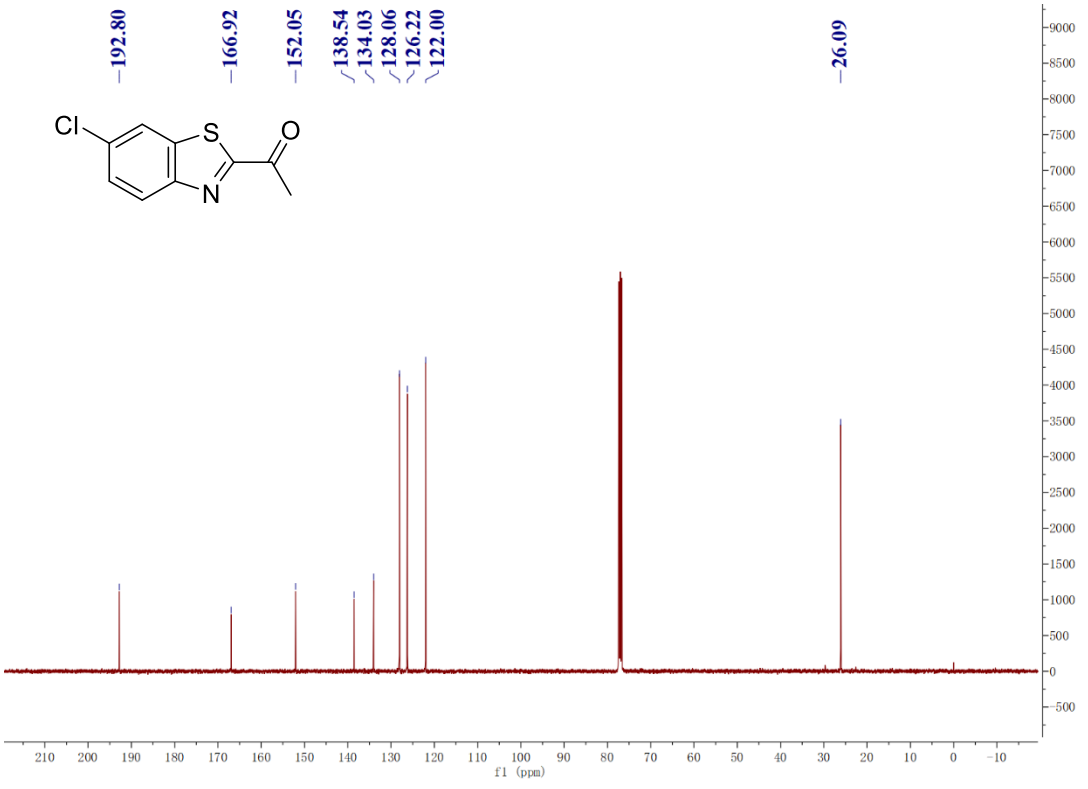
^{13}C NMR (151 MHz, $CDCl_3$) of 4j



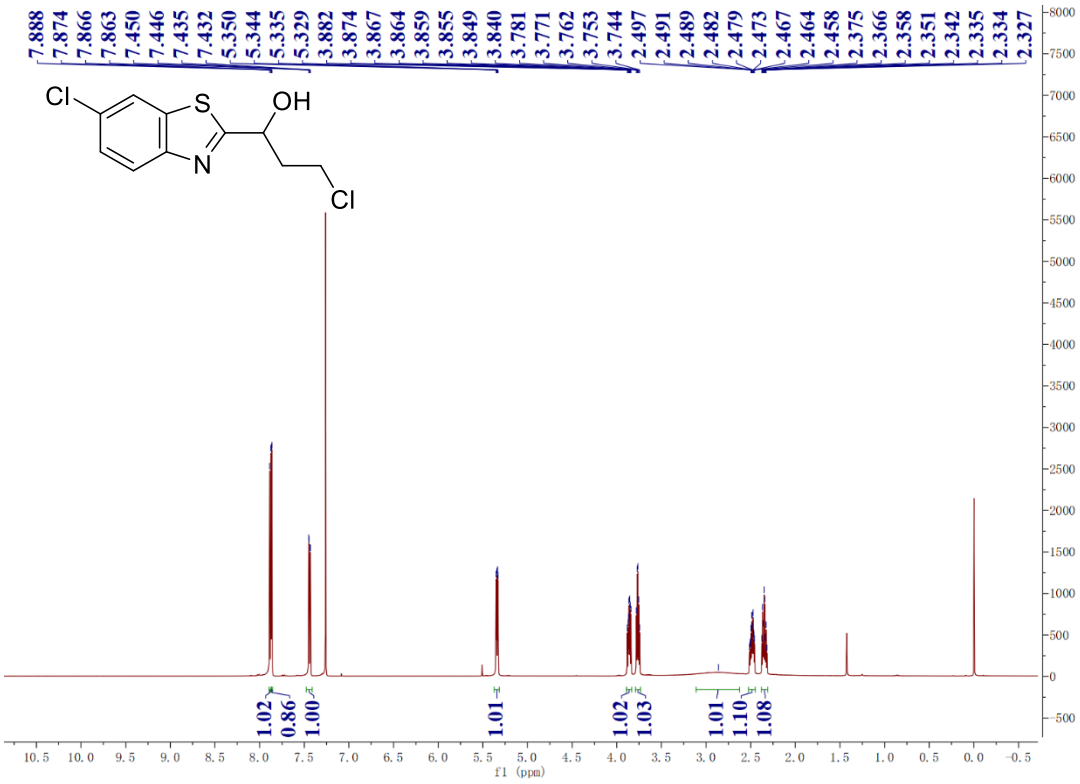
^{1}H NMR (400 MHz, $CDCl_3$) of 4k



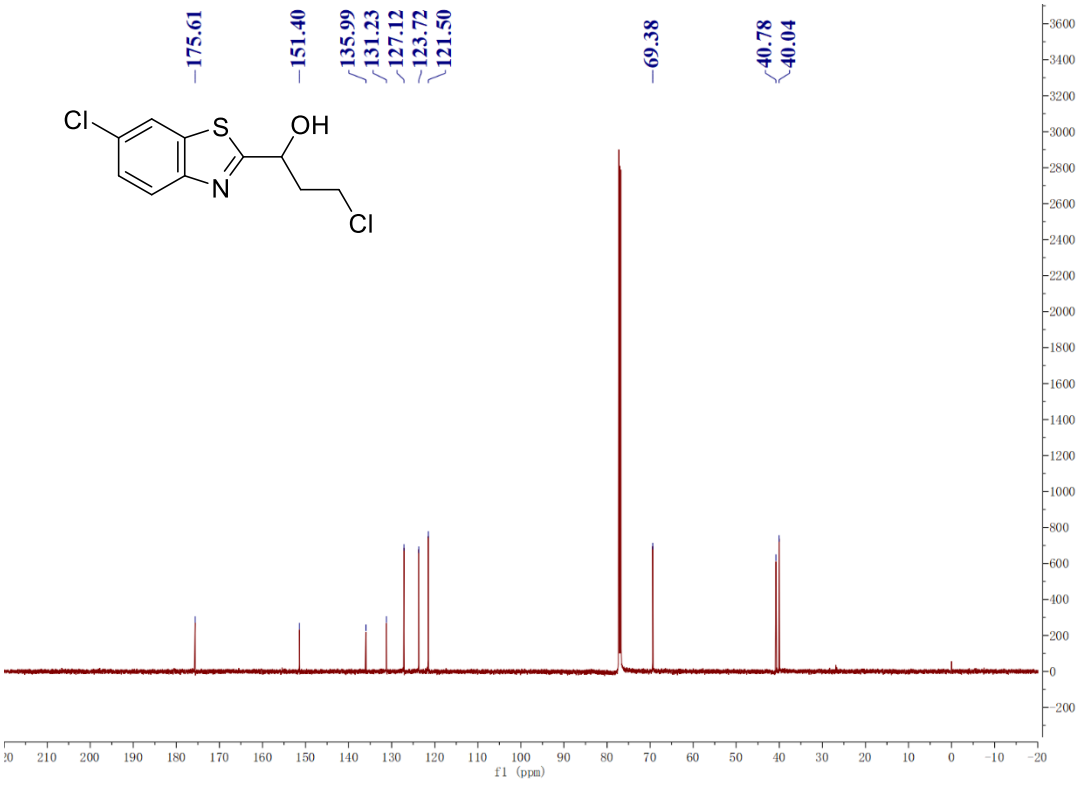
^{13}C NMR (101 MHz, $CDCl_3$) of 4k



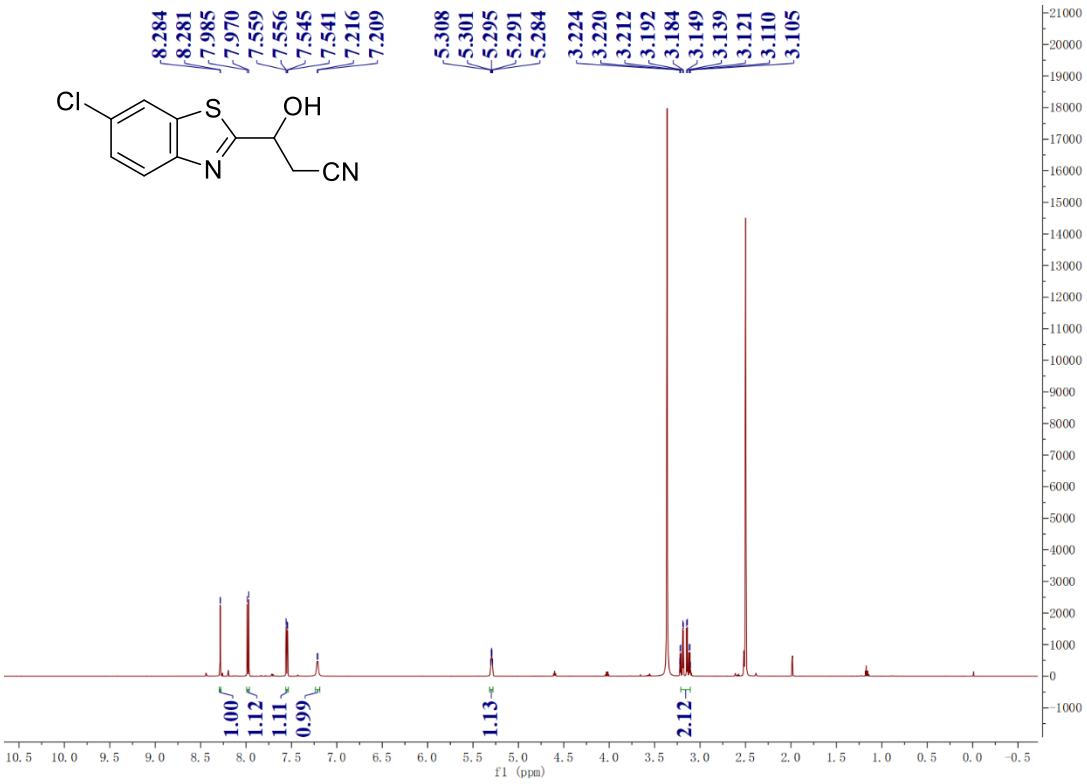
^{1}H NMR (600 MHz, $CDCl_3$) of 4l



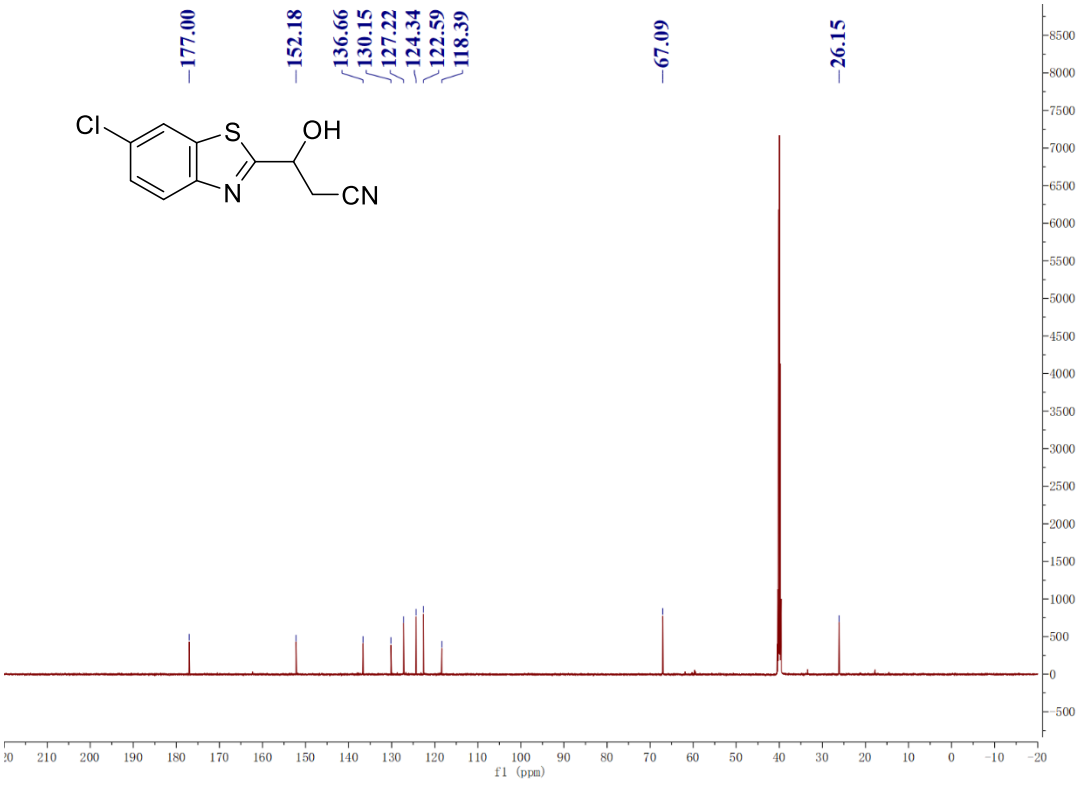
^{13}C NMR (151 MHz, $CDCl_3$) of 4l



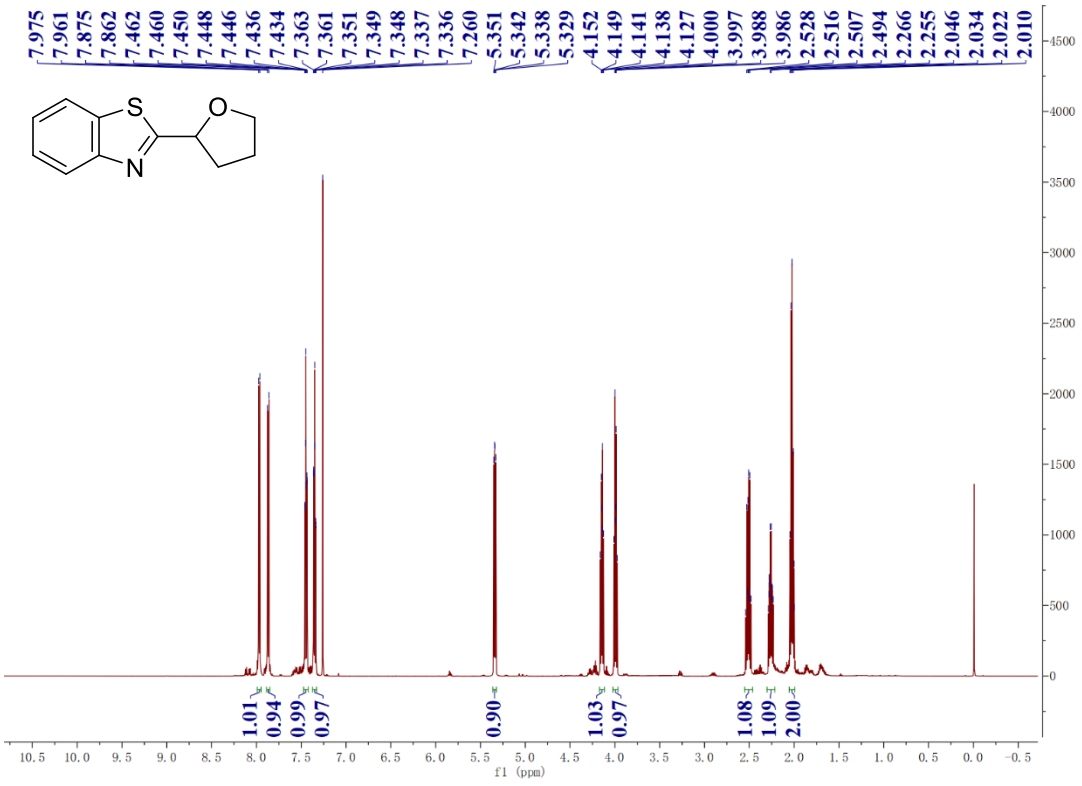
^{1}H NMR (600 MHz, DMSO-d_6) of 4m



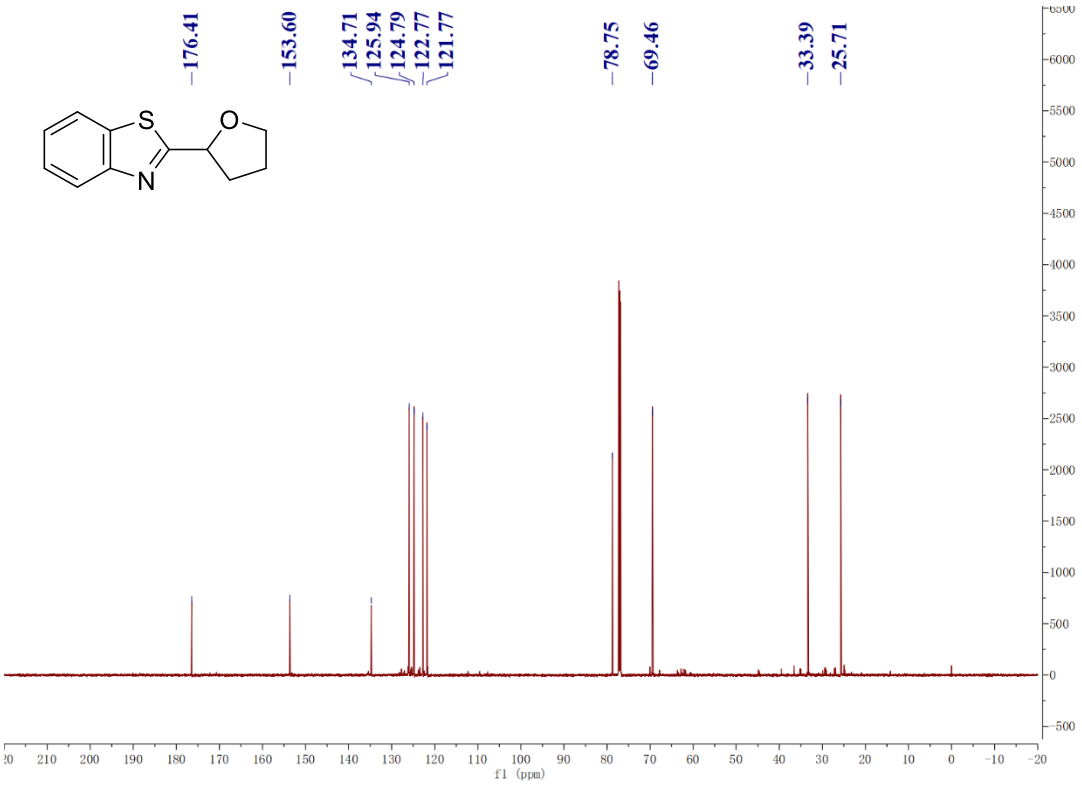
^{13}C NMR (151 MHz, DMSO-d_6) of 4m



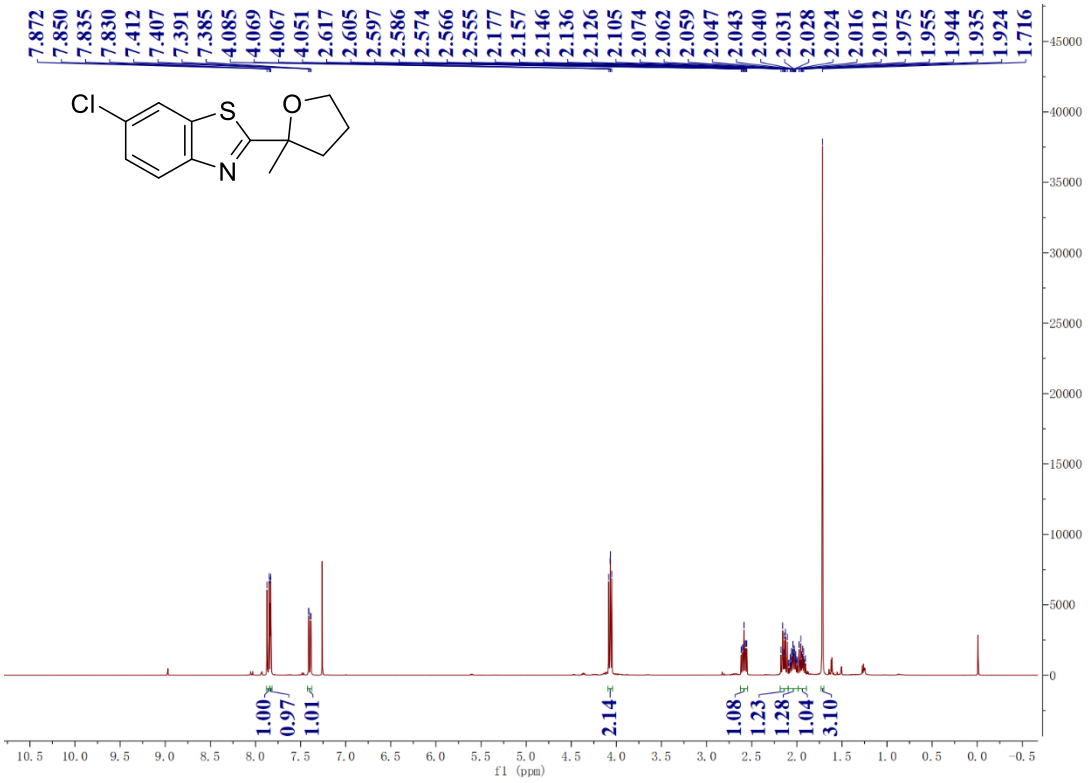
^{1}H NMR (600 MHz, $CDCl_3$) of 6a



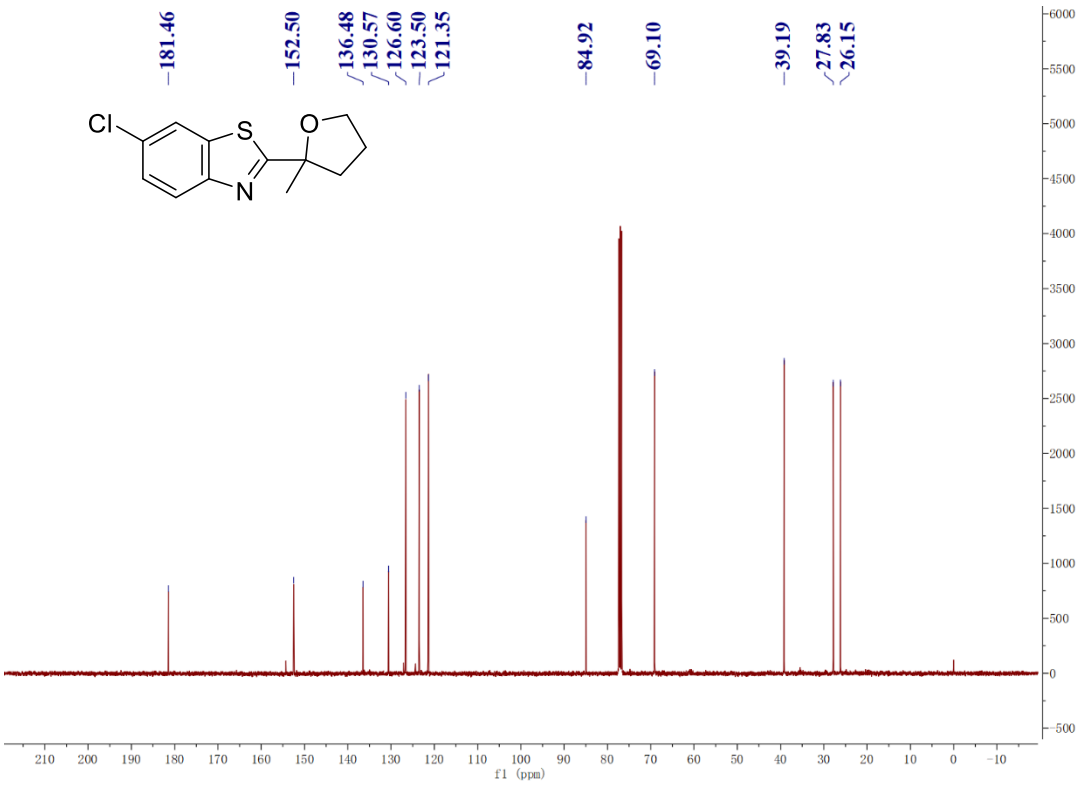
^{13}C NMR (151 MHz, $CDCl_3$) of 6a



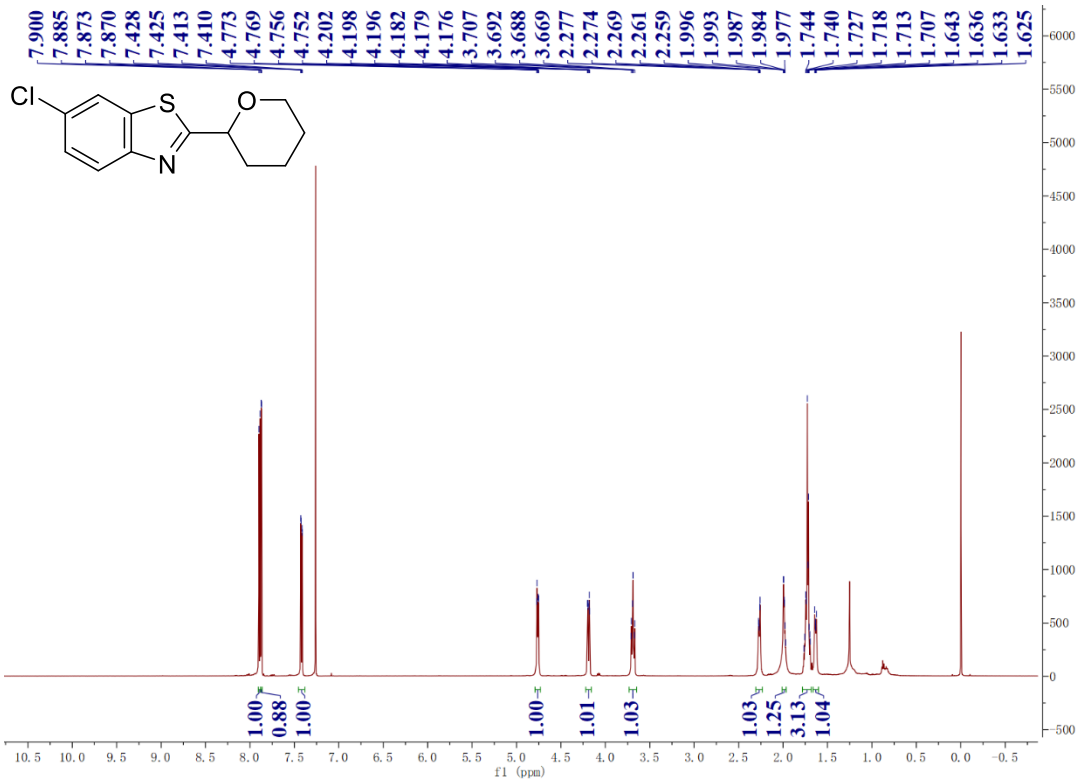
^{1}H NMR (400 MHz, $CDCl_3$) of 6b



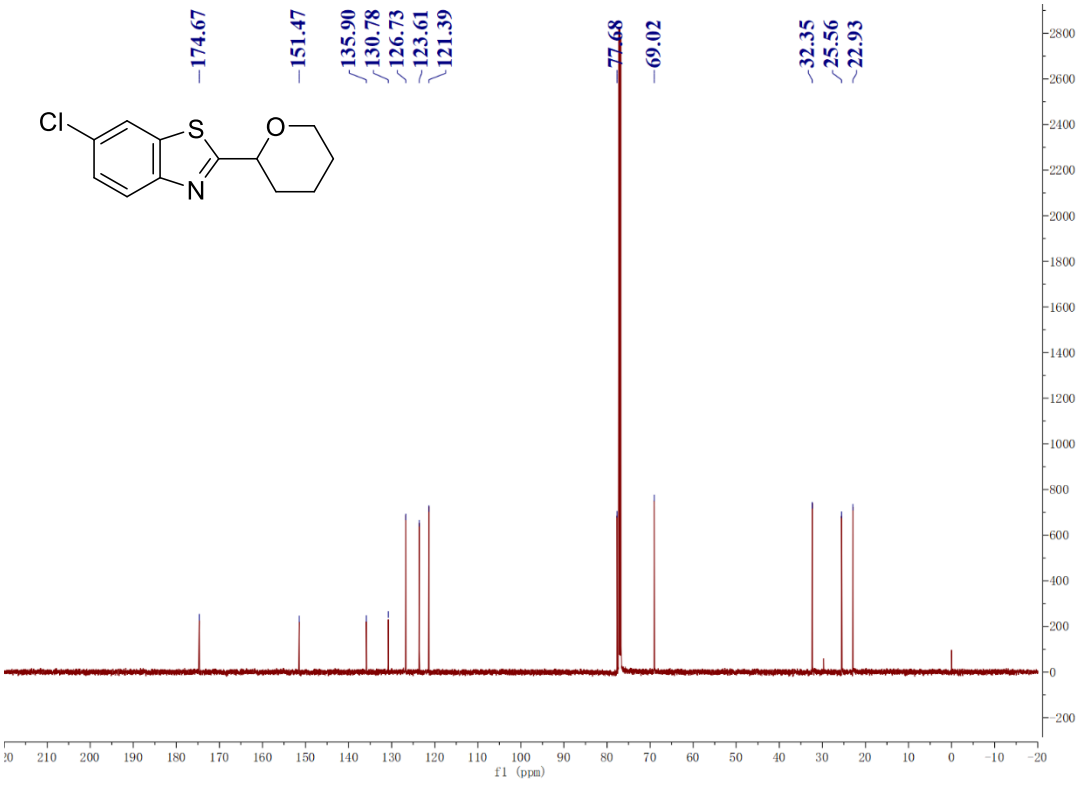
^{13}C NMR (101 MHz, $CDCl_3$) of 6b



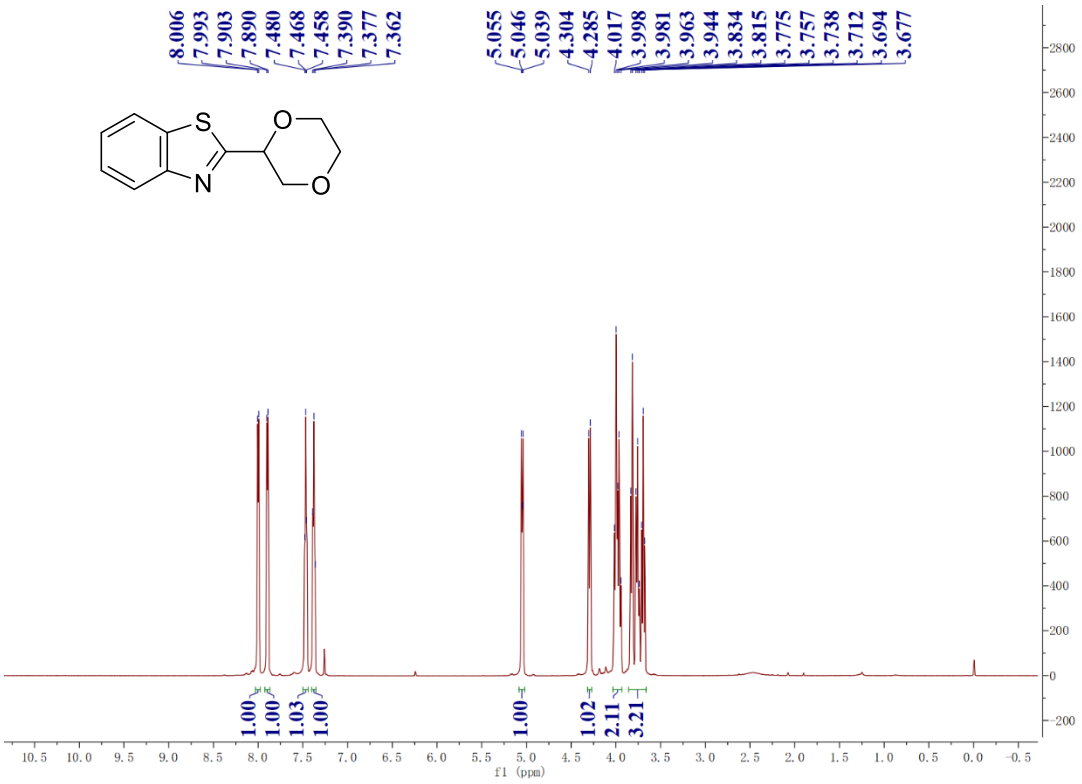
^{1}H NMR (600 MHz, $CDCl_3$) of 6c



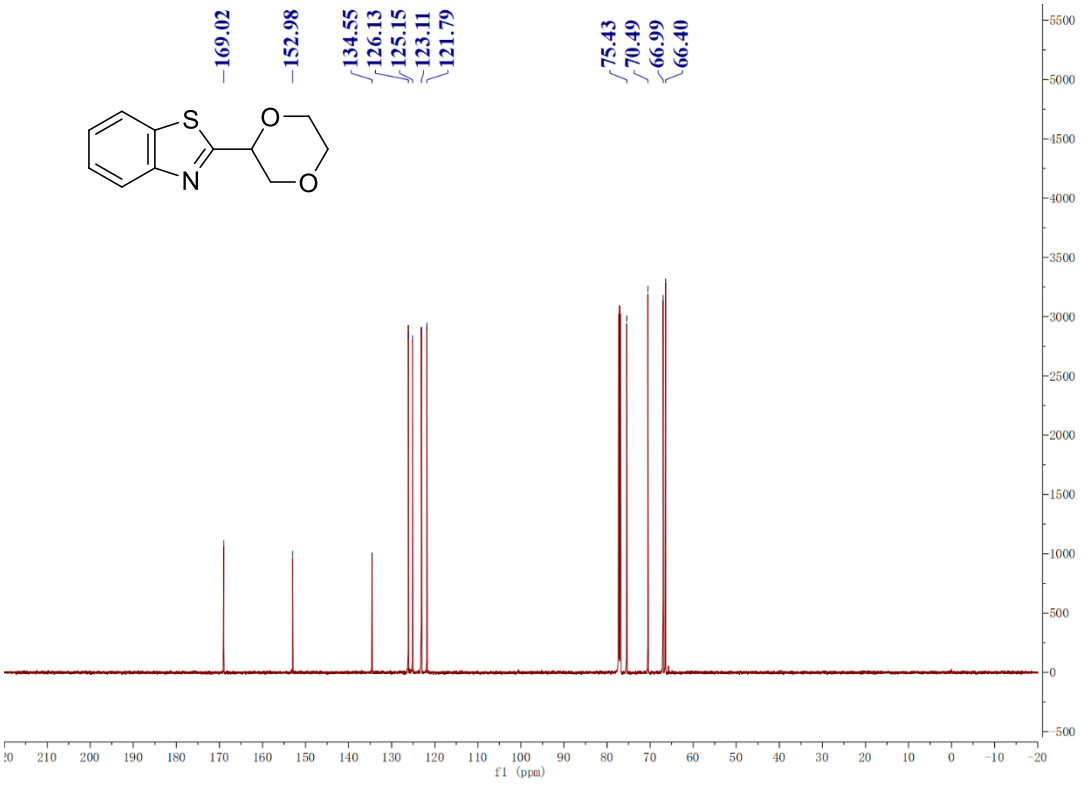
^{13}C NMR (151 MHz, $CDCl_3$) of 6c



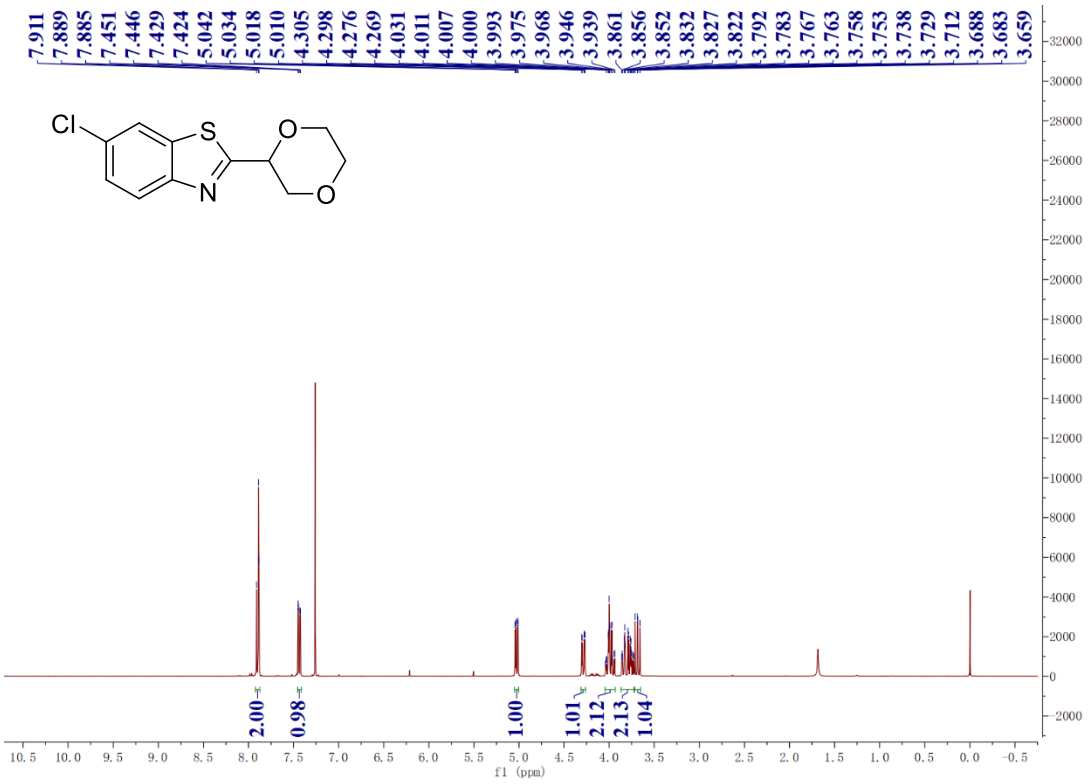
^{1}H NMR (600 MHz, $CDCl_3$) of 6d



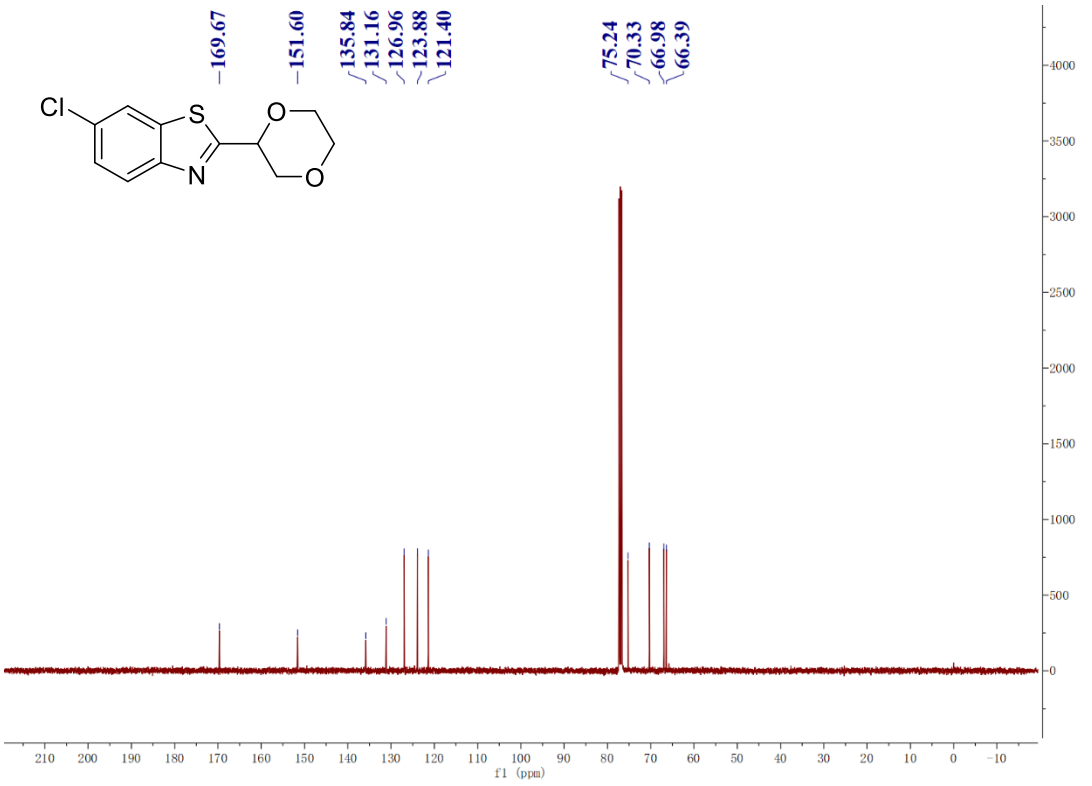
^{13}C NMR (151 MHz, $CDCl_3$) of 6d



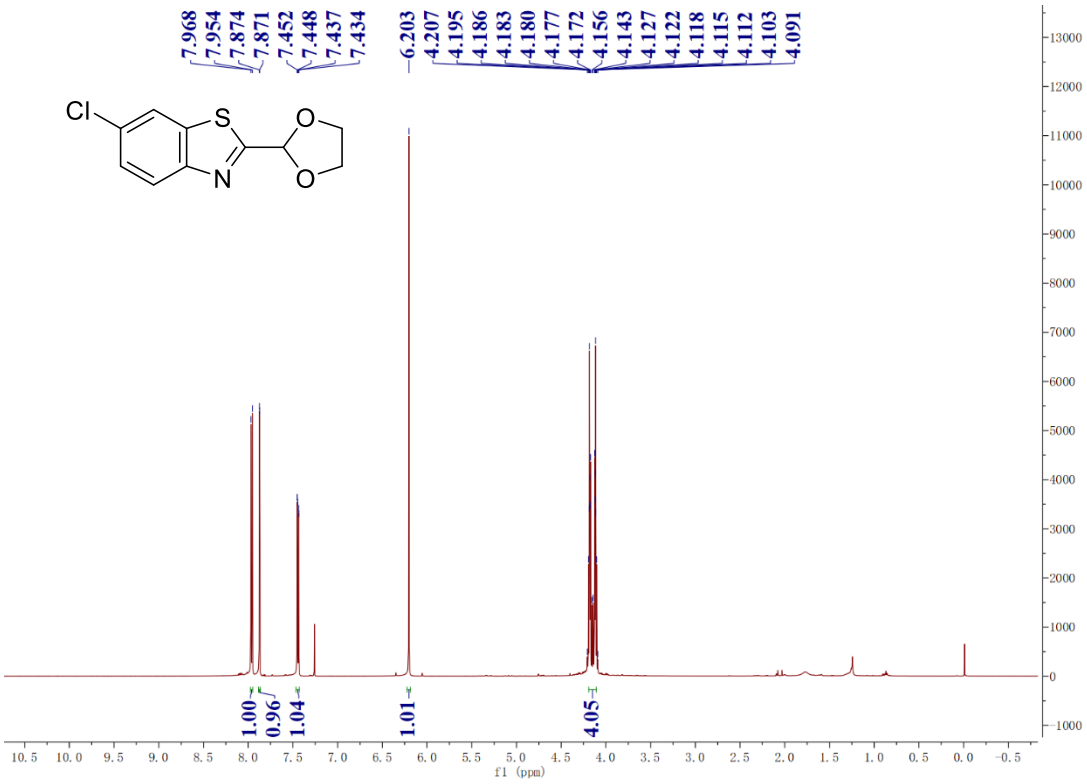
^{1}H NMR (400 MHz, $CDCl_3$) of 6d′



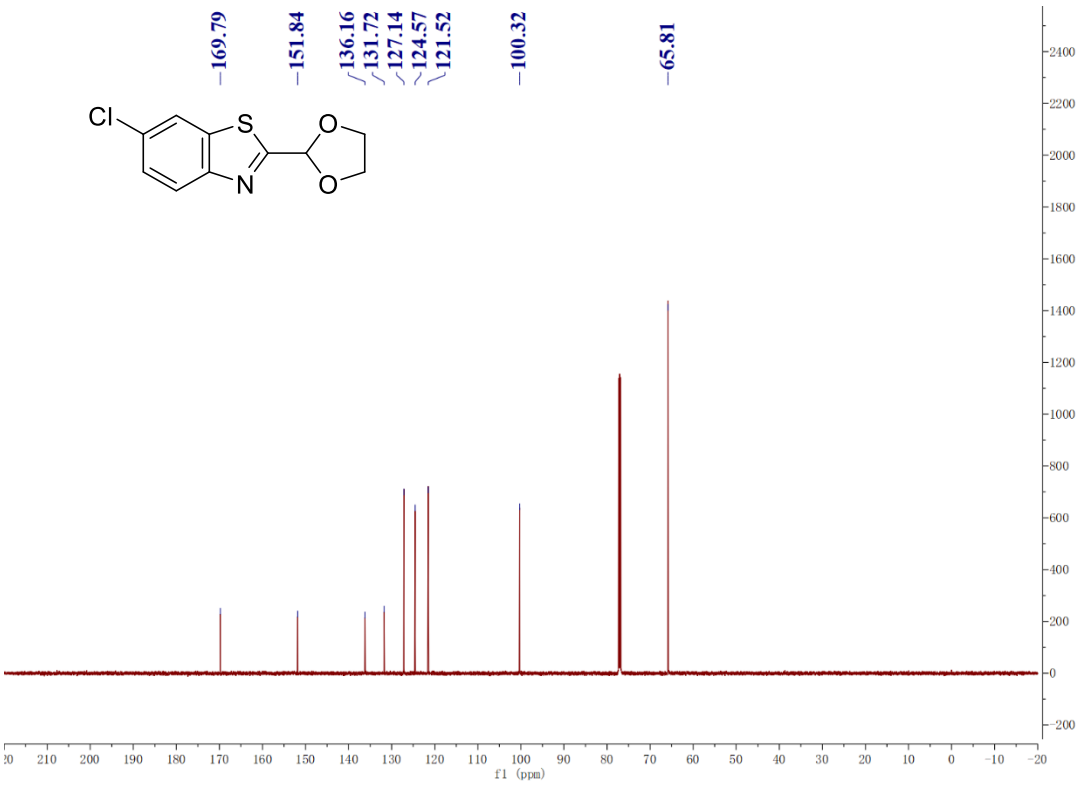
^{13}C NMR (101 MHz, $CDCl_3$) of 6d′



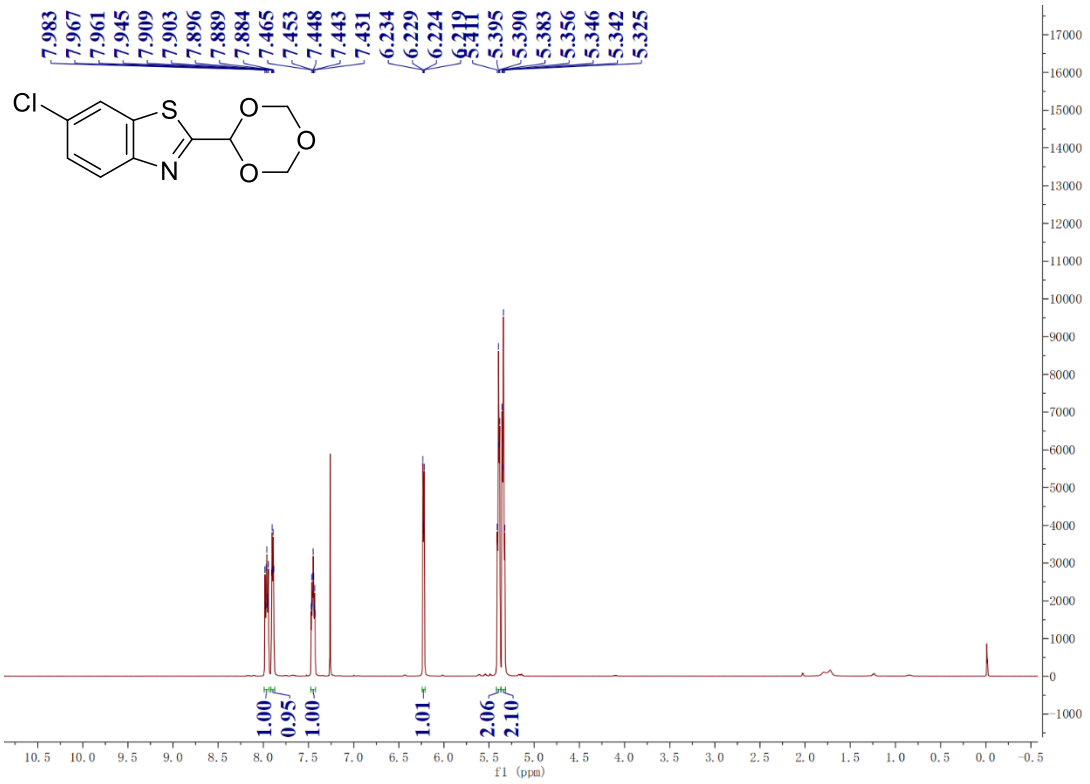
^{1}H NMR (600 MHz, $CDCl_3$) of 6e



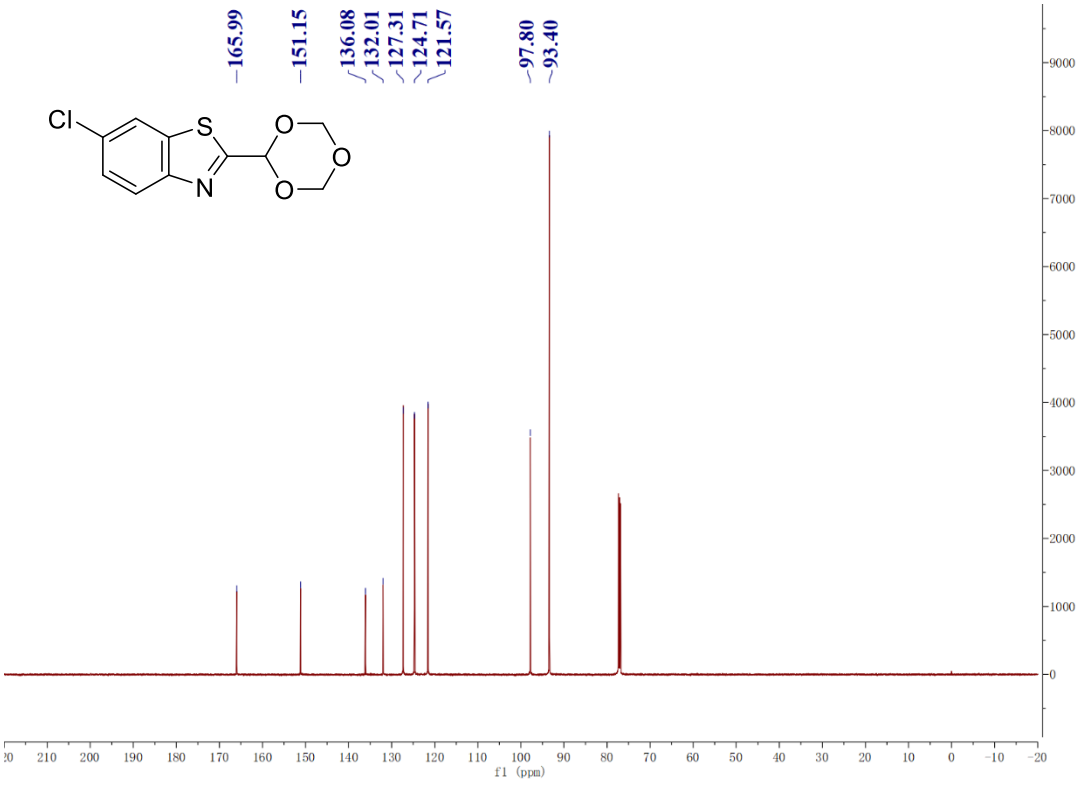
^{13}C NMR (151 MHz, $CDCl_3$) of 6e



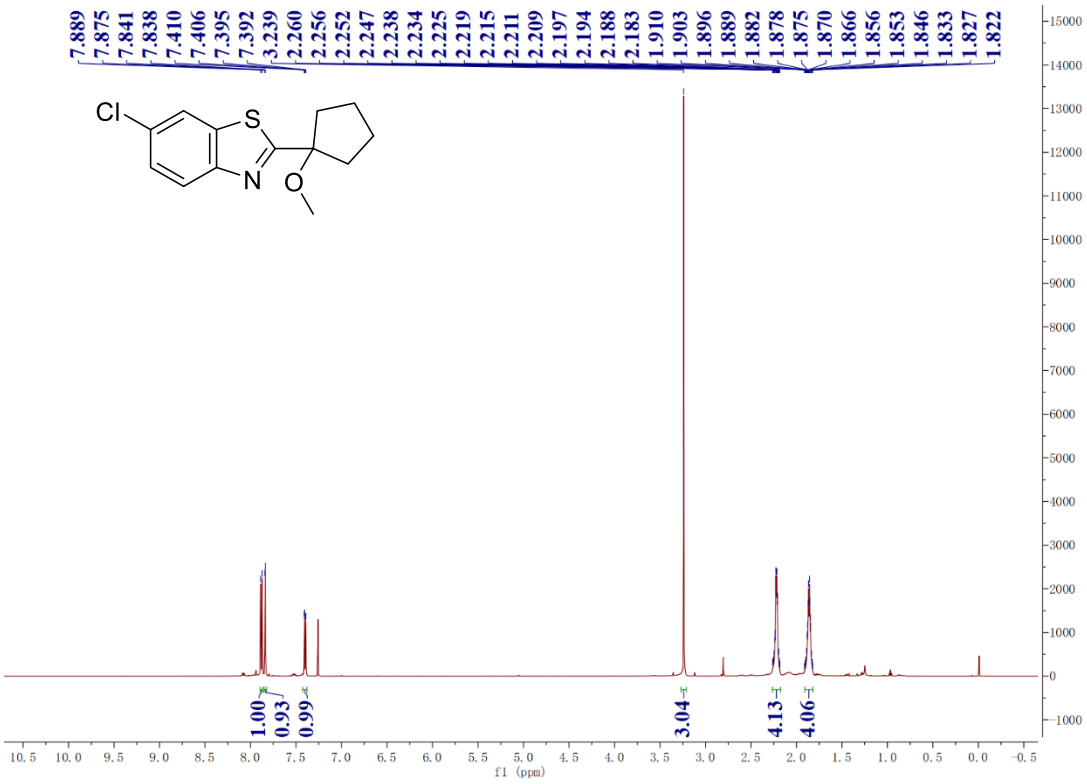
^{1}H NMR (400 MHz, $CDCl_3$) of 6f



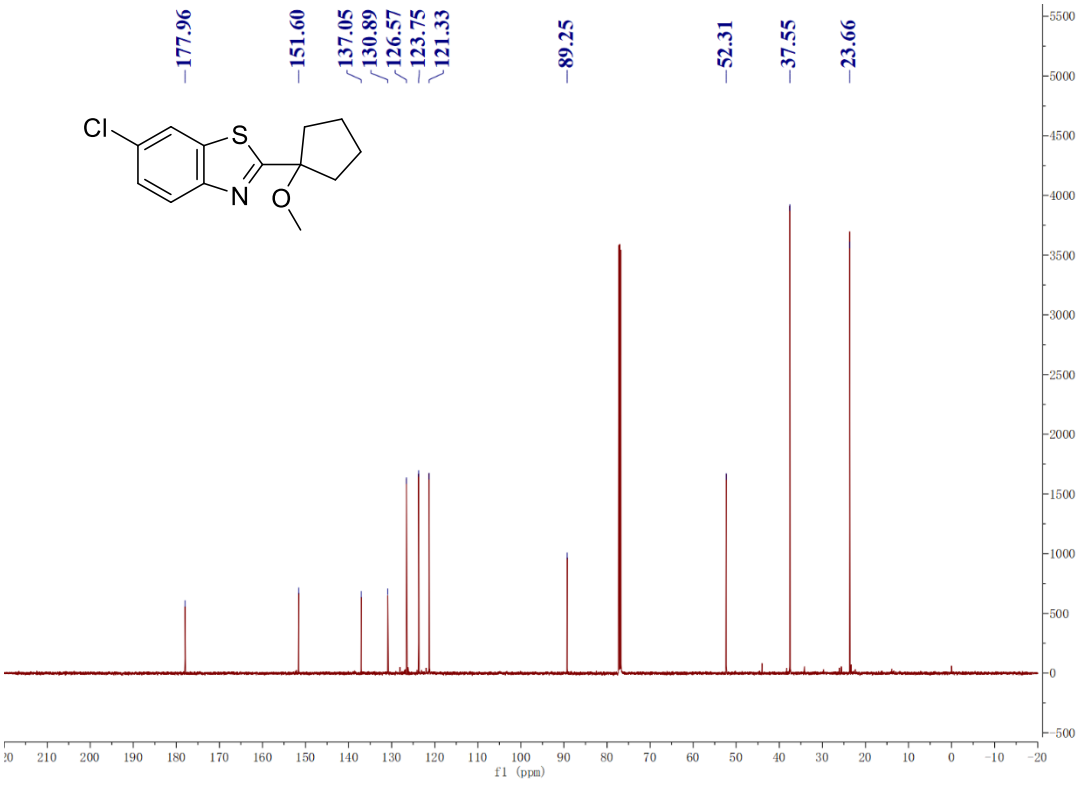
^{13}C NMR (151 MHz, $CDCl_3$) of 6f



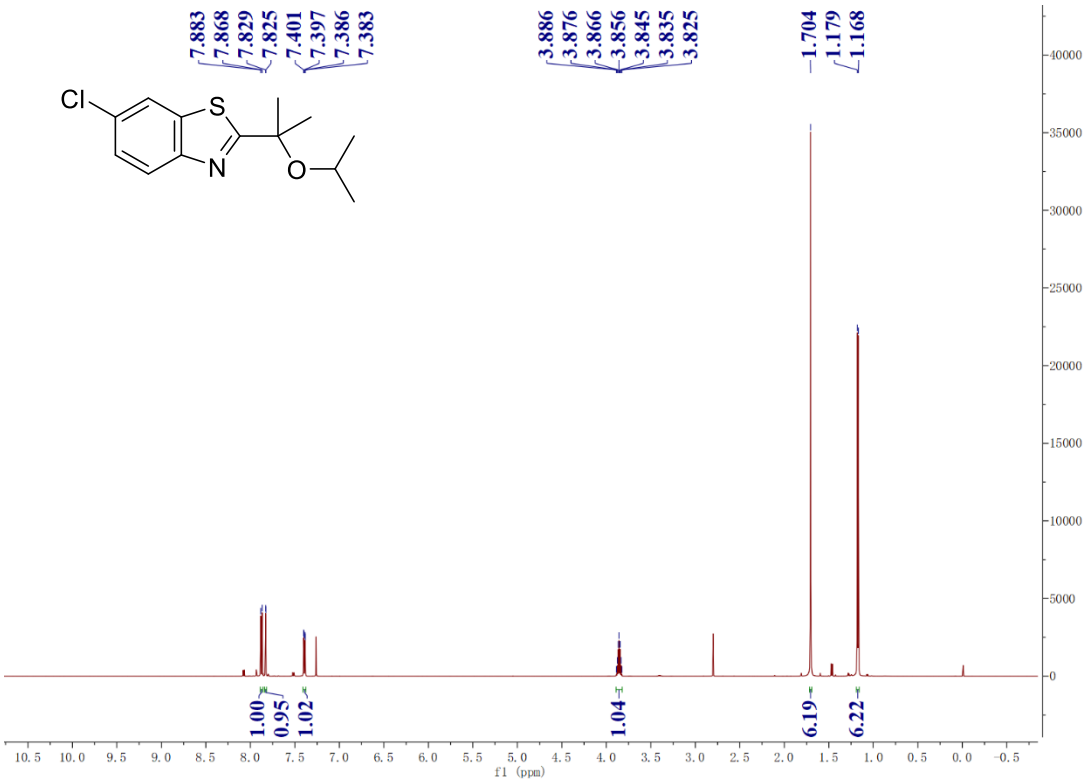
^{1}H NMR (600 MHz, $CDCl_3$) of 6g



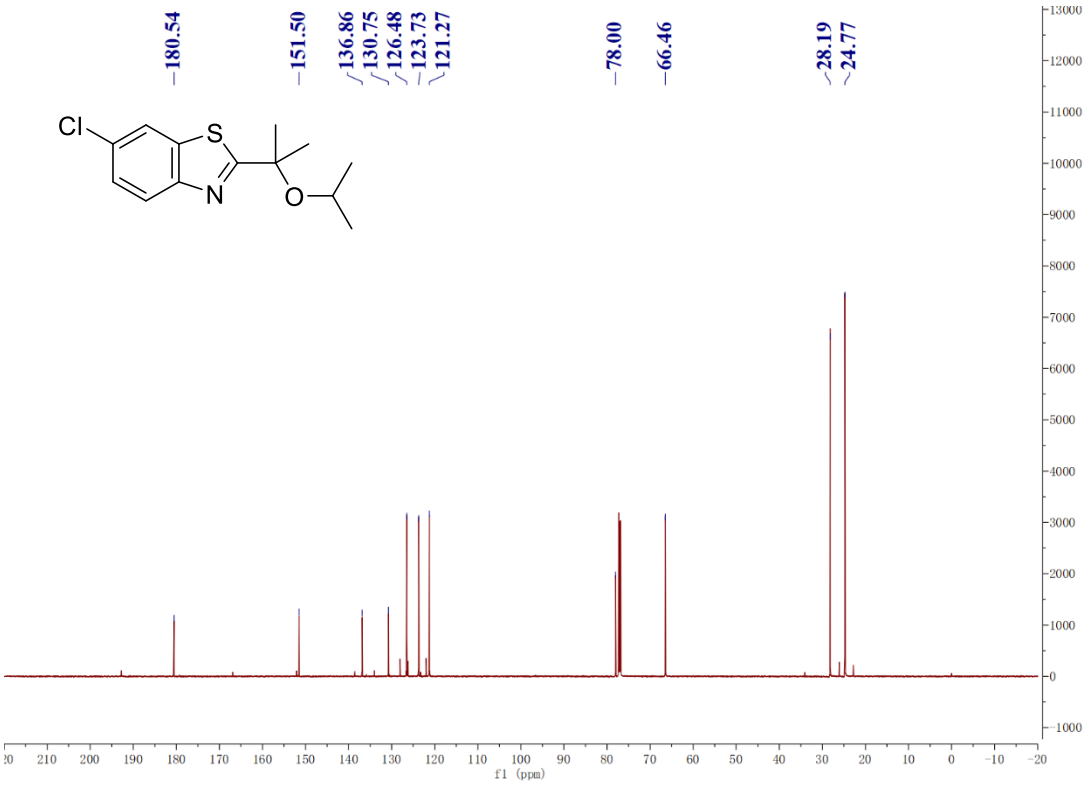
^{13}C NMR (151 MHz, $CDCl_3$) of 6g



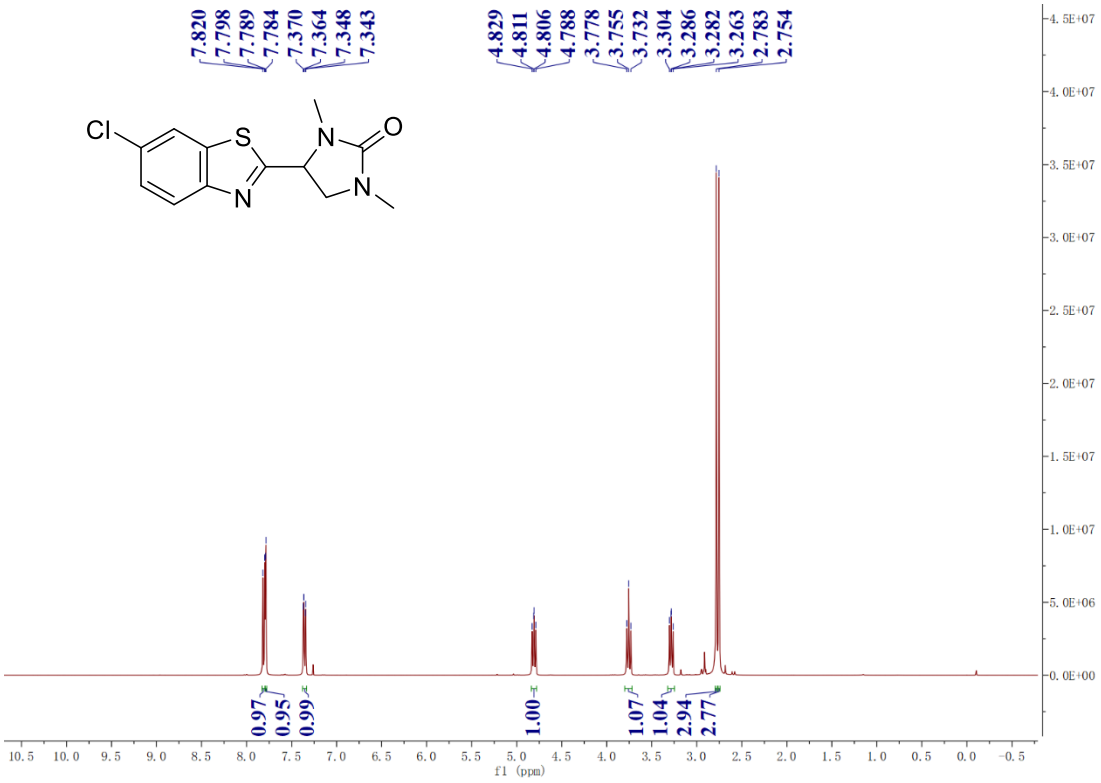
^{1}H NMR (600 MHz, $CDCl_3$) of 6h



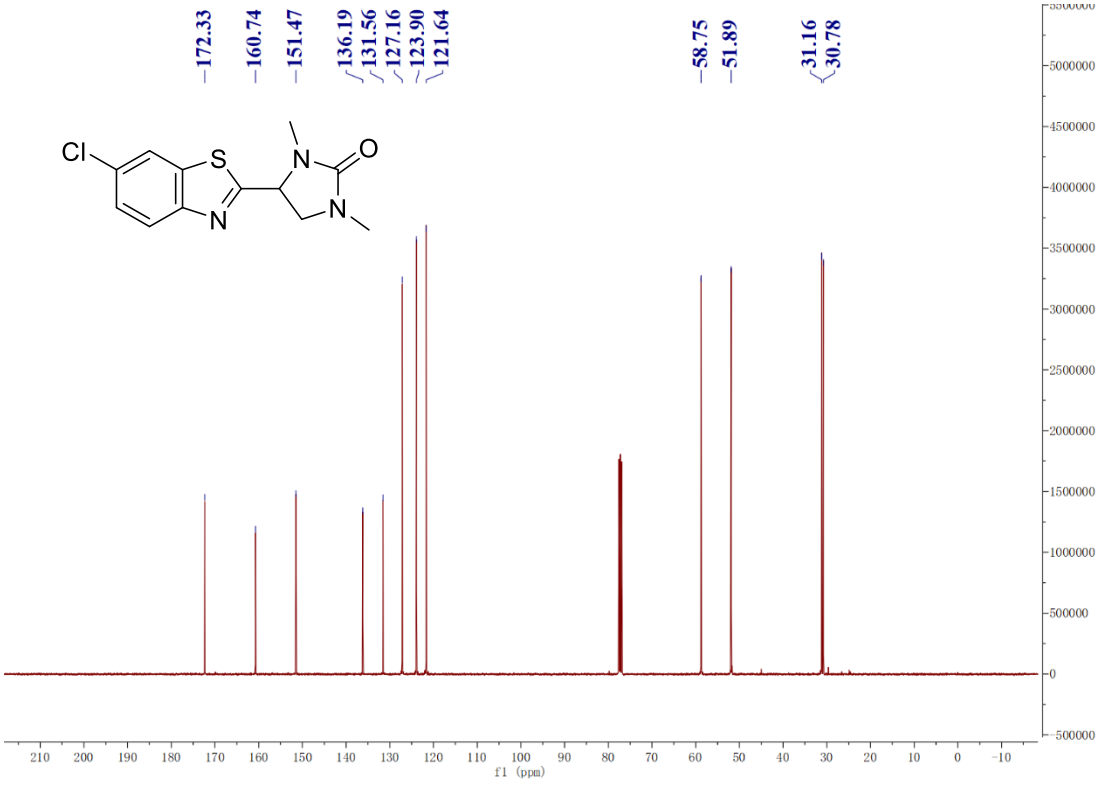
^{13}C NMR (151 MHz, $CDCl_3$) of 6h



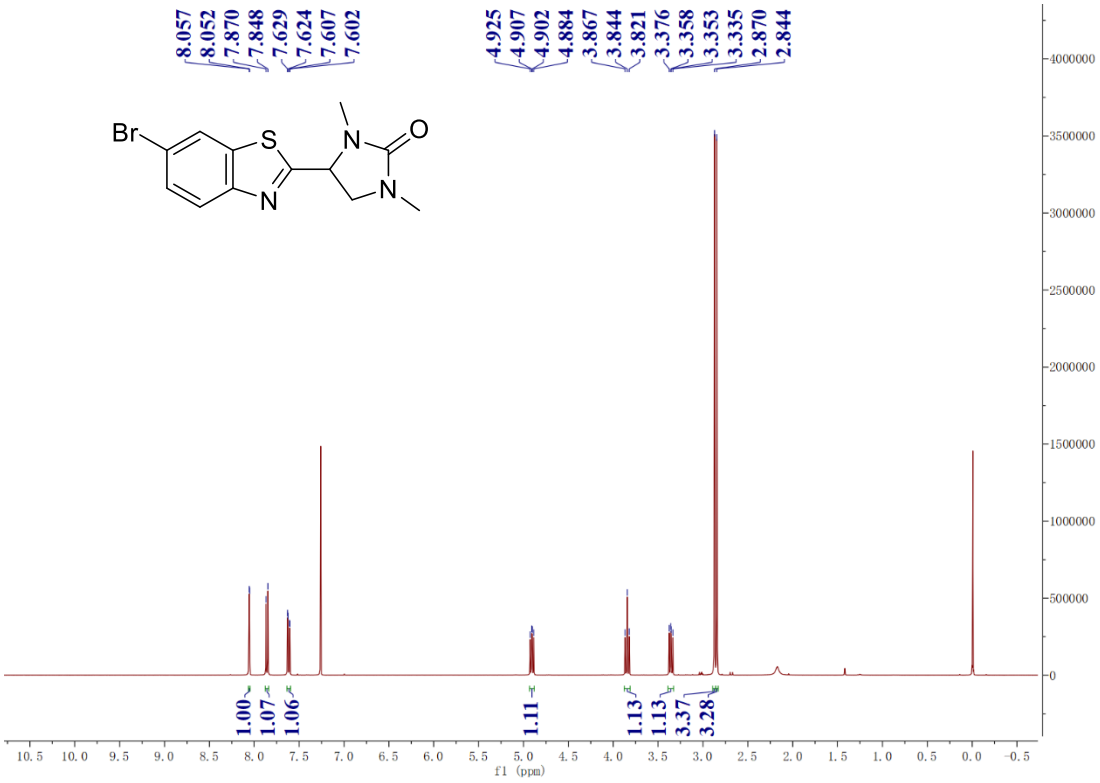
^{1}H NMR (400 MHz, $CDCl_3$) of 8a



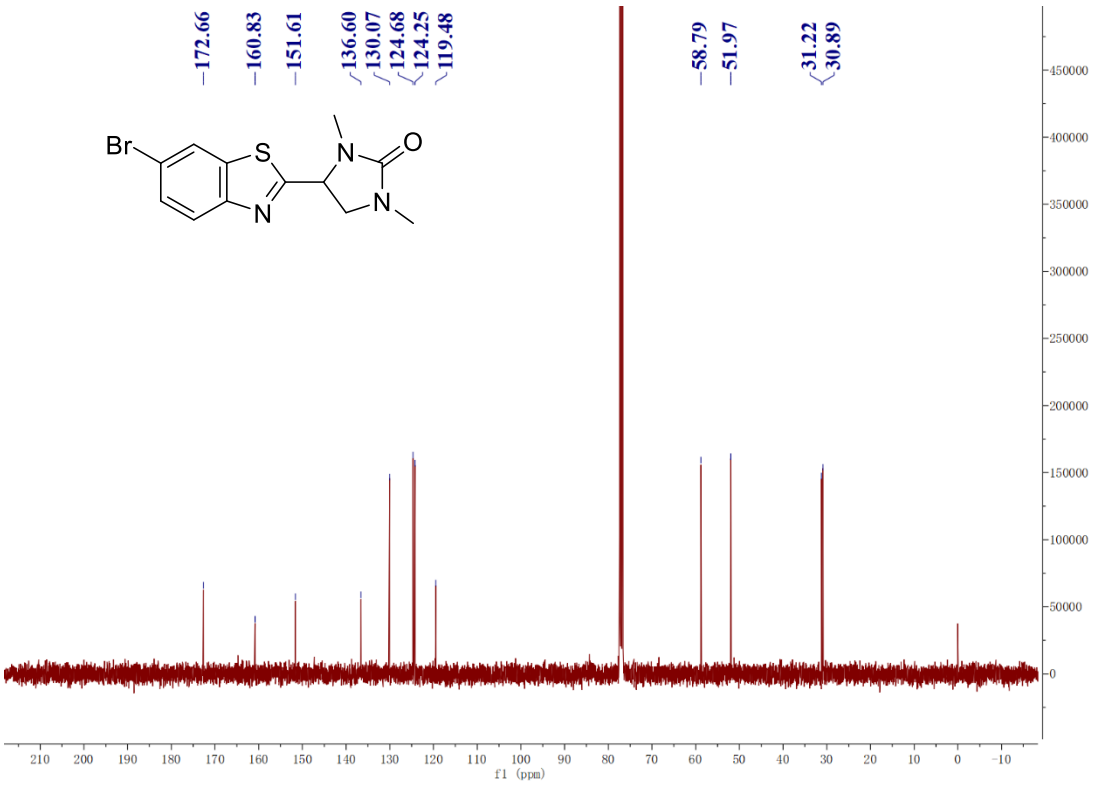
^{13}C NMR (101 MHz, $CDCl_3$) of 8a



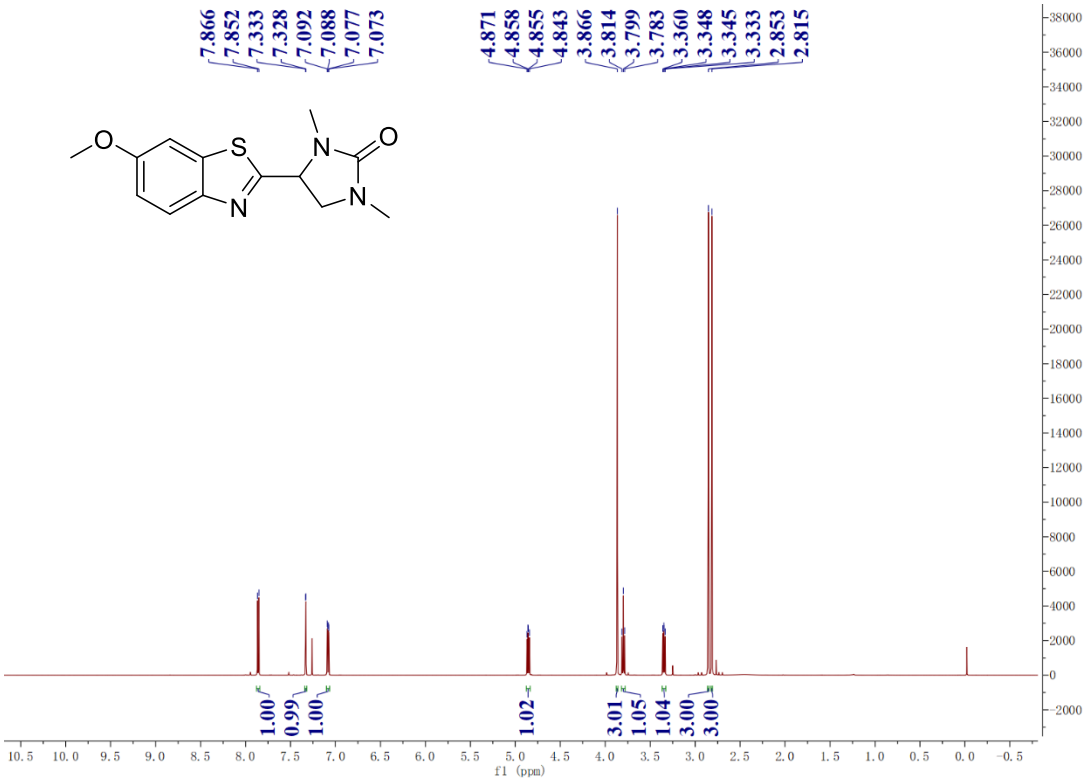
^{1}H NMR (400 MHz, $CDCl_3$) of 8b



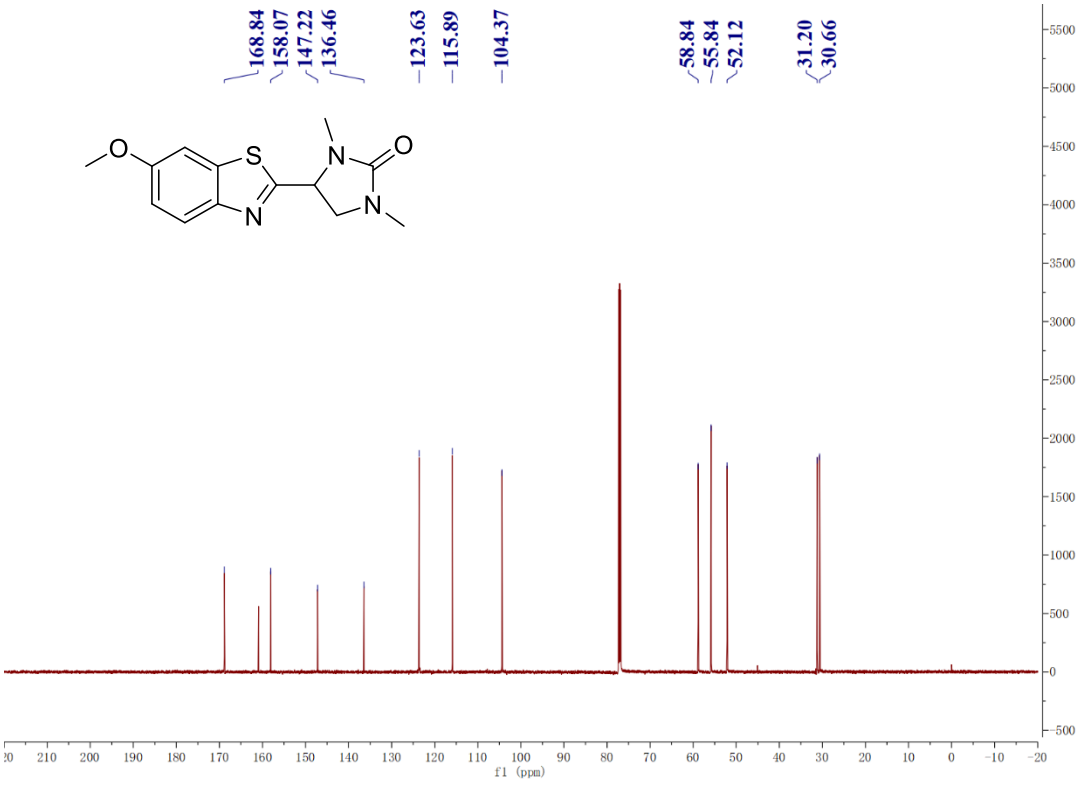
^{13}C NMR (101 MHz, $CDCl_3$) of 8b



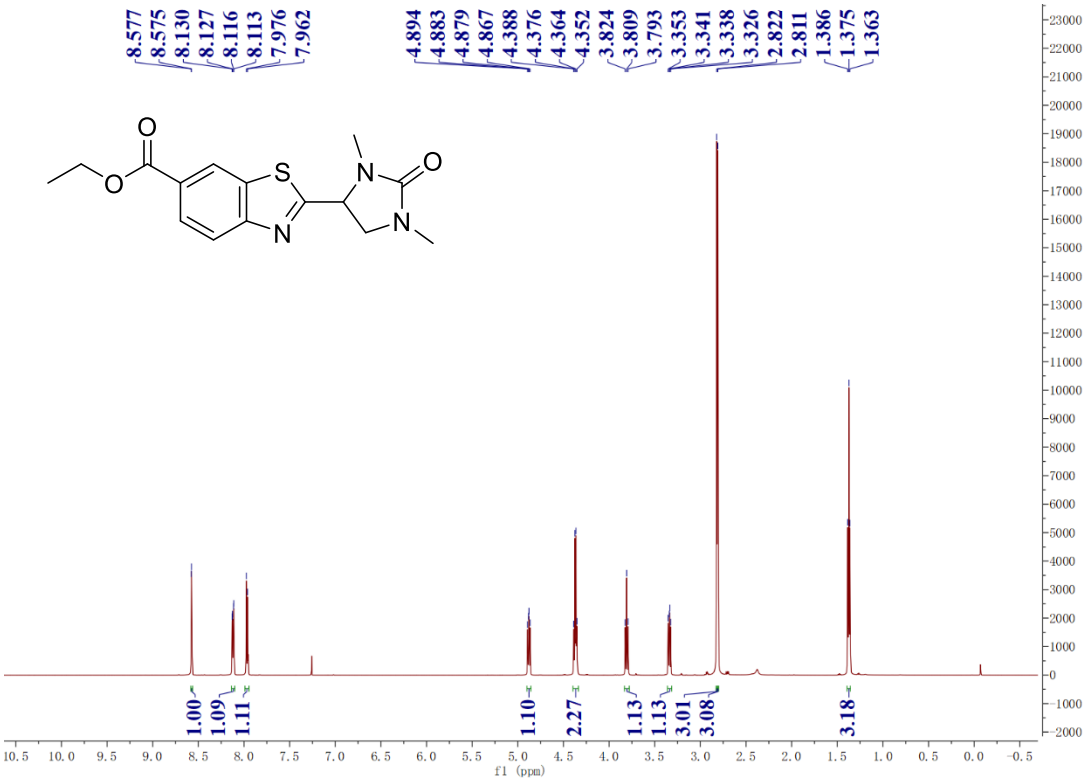
^{1}H NMR (600 MHz, $CDCl_3$) of 8c



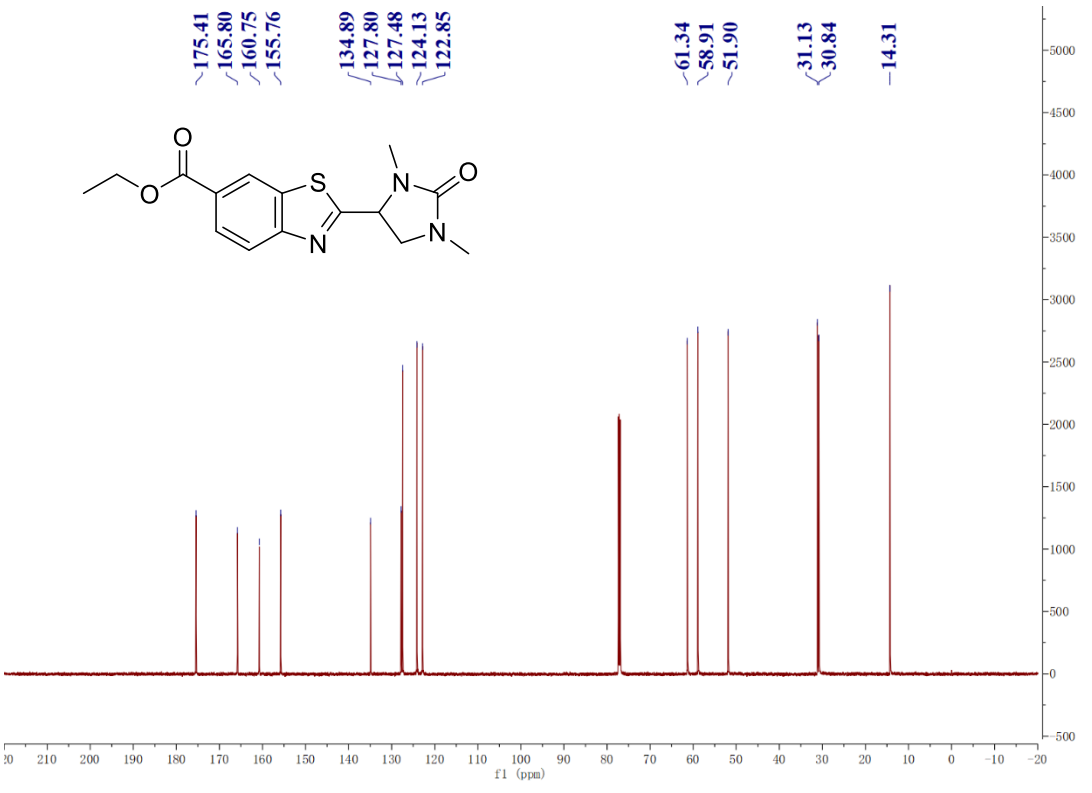
^{13}C NMR (151 MHz, $CDCl_3$) of 8c



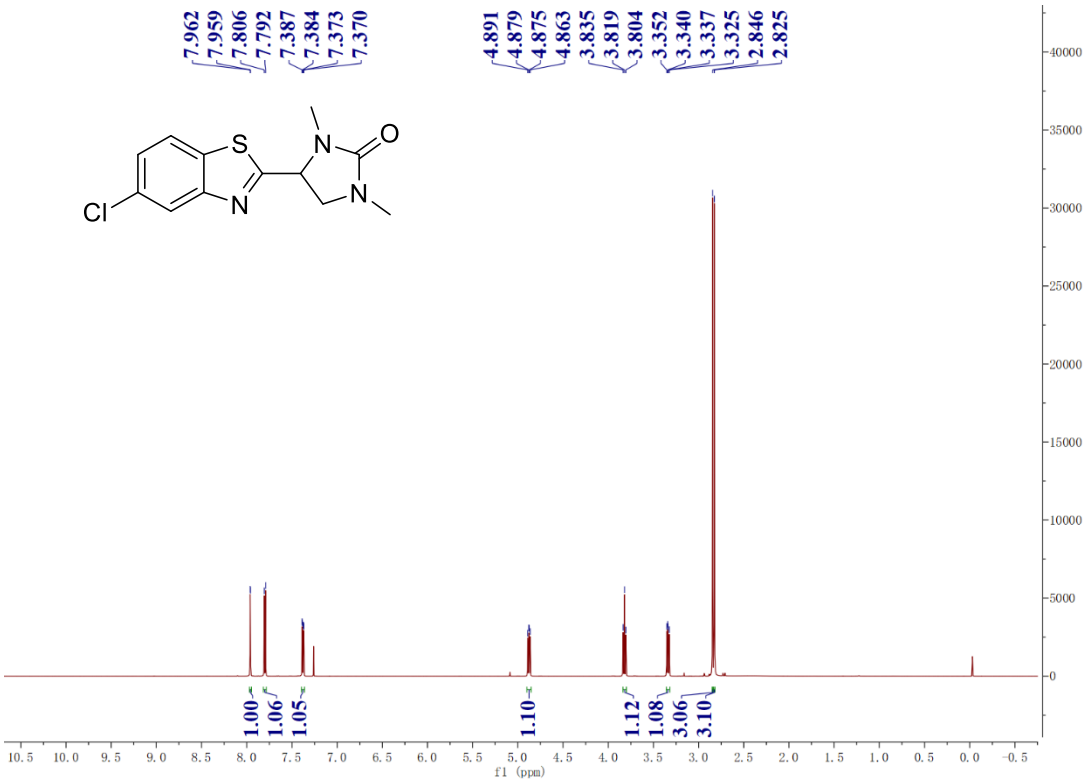
^{1}H NMR (600 MHz, $CDCl_3$) of 8d



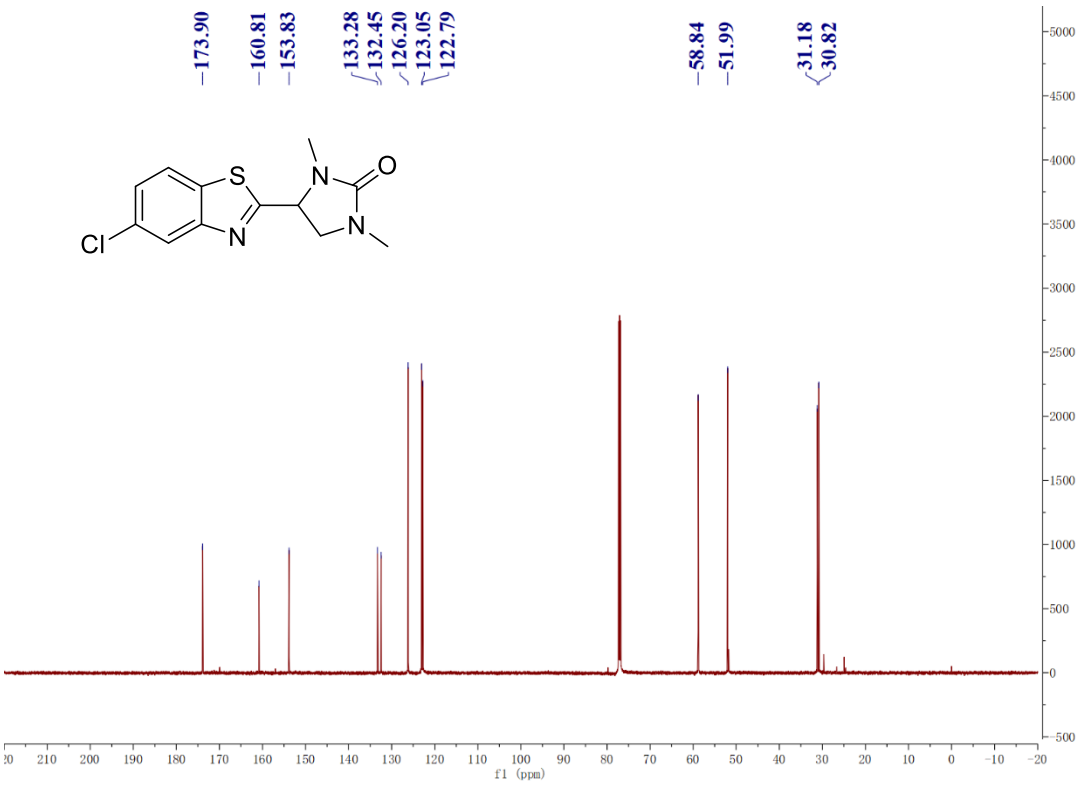
^{13}C NMR (151 MHz, $CDCl_3$) of 8d



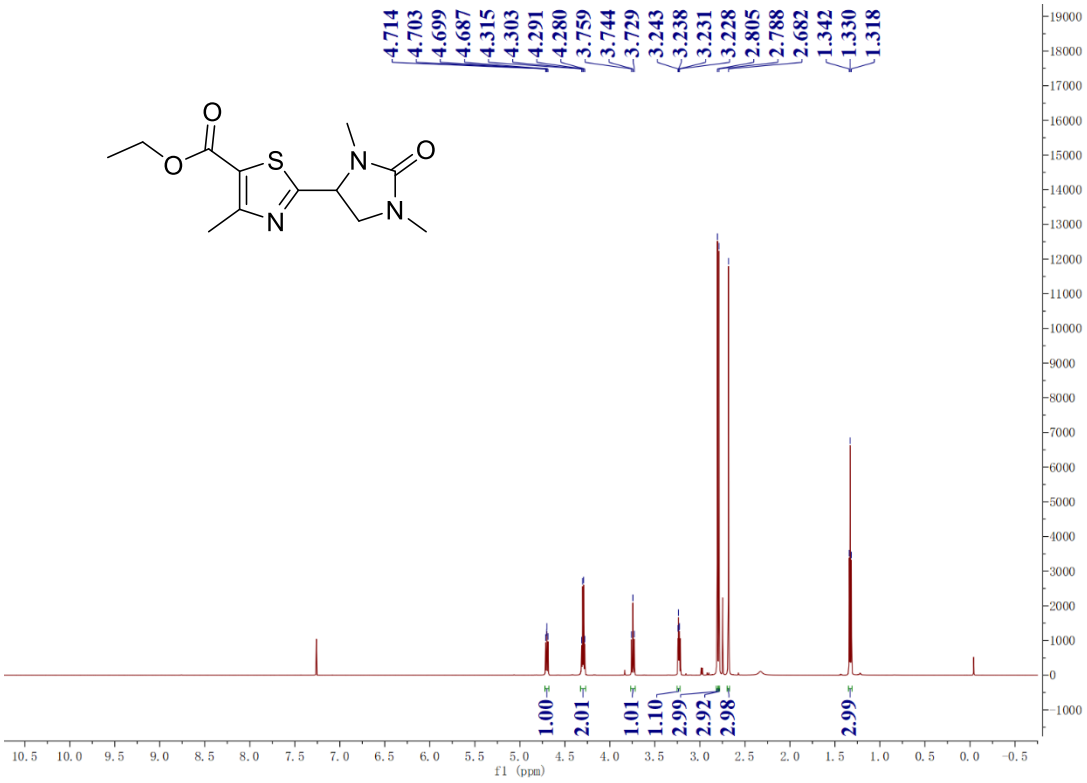
^{1}H NMR (600 MHz, $CDCl_3$) of 8e



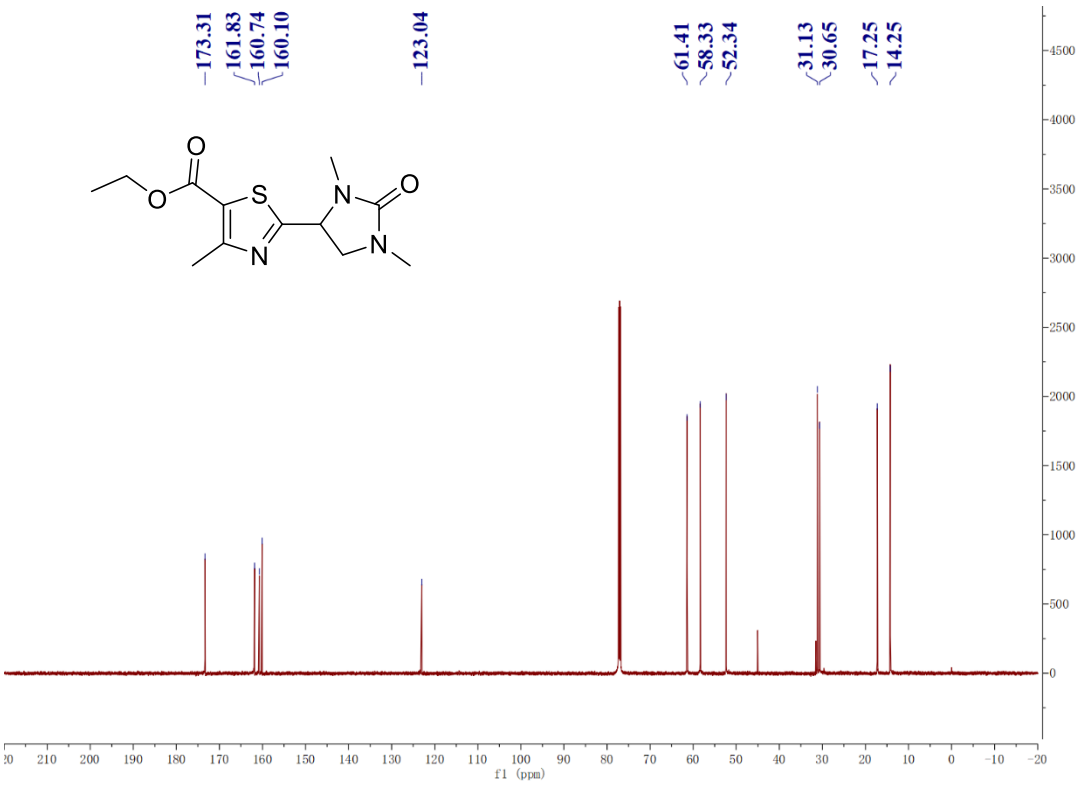
^{13}C NMR (151 MHz, $CDCl_3$) of 8e



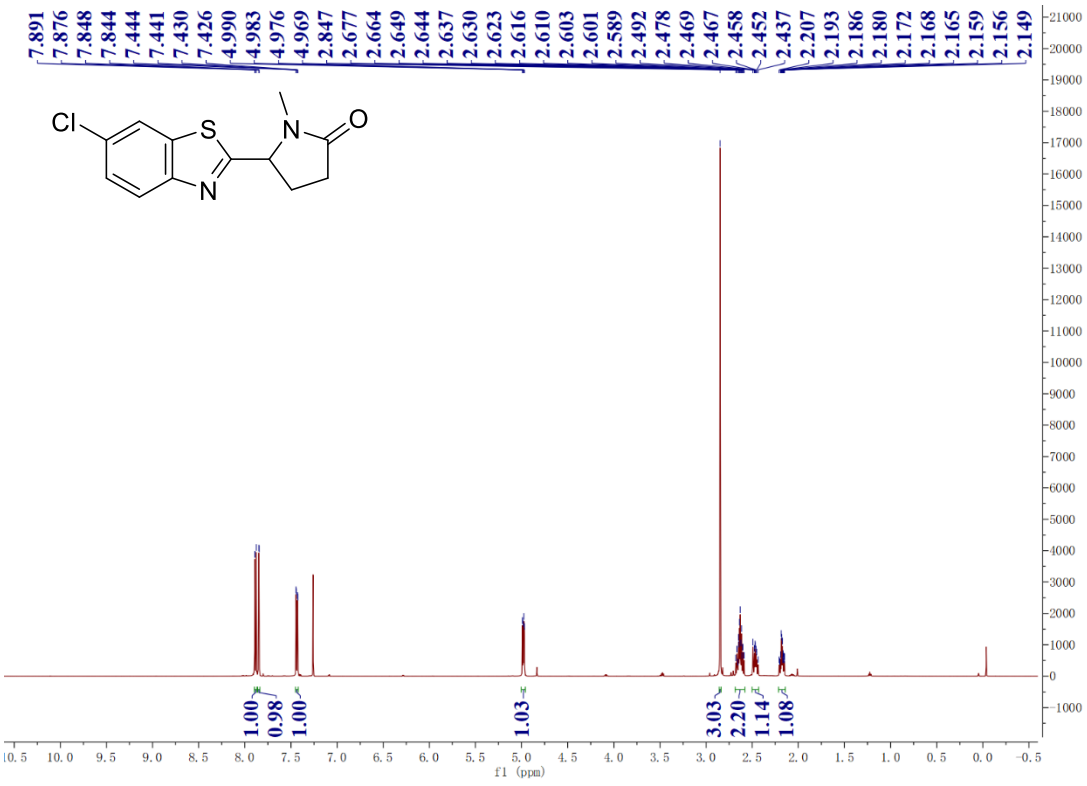
^{1}H NMR (600 MHz, $CDCl_3$) of 8f



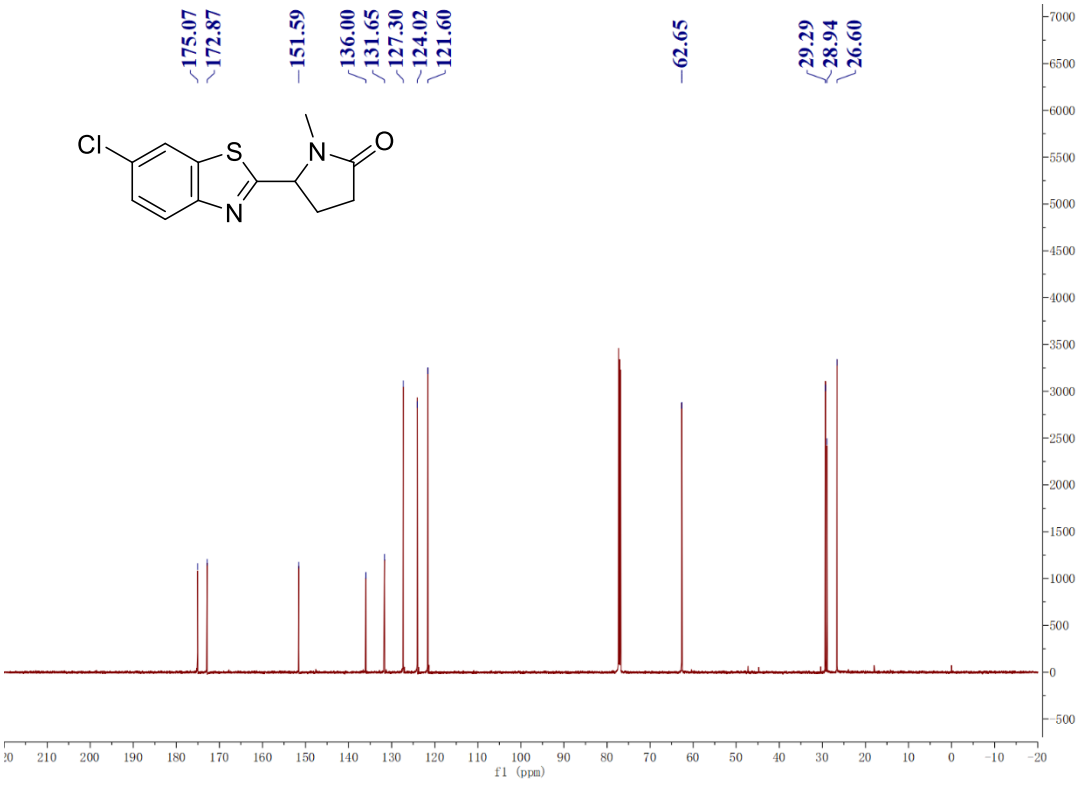
^{13}C NMR (151 MHz, $CDCl_3$) of 8f



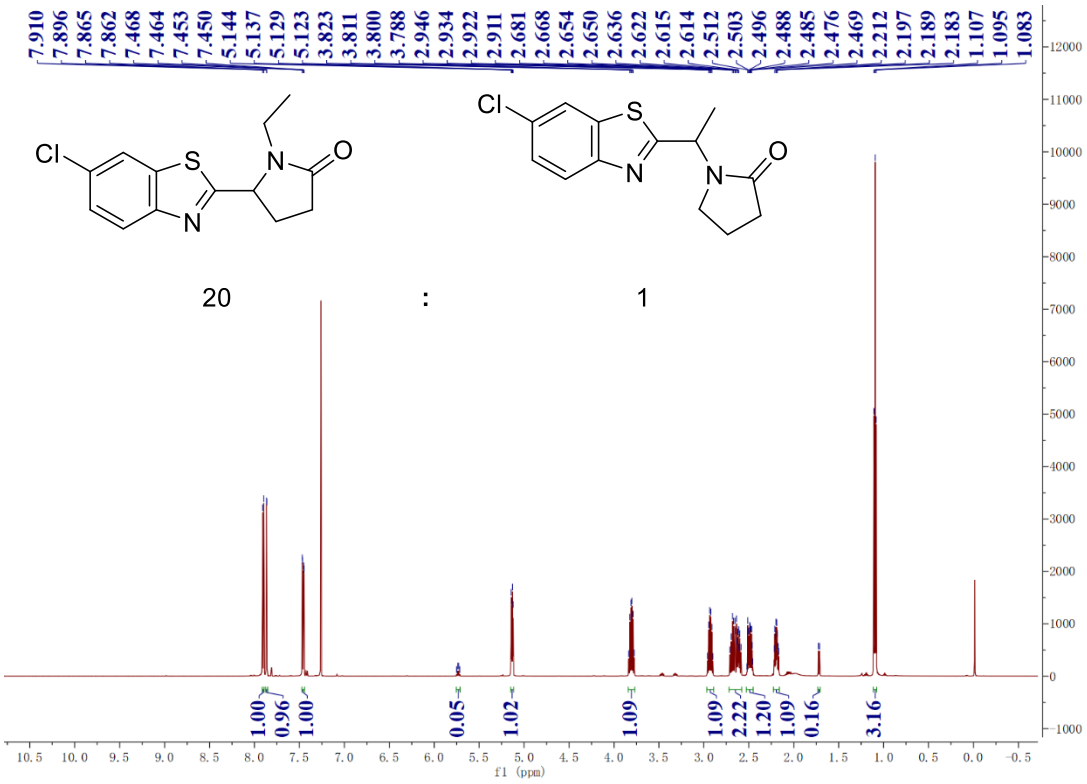
^{1}H NMR (600 MHz, $CDCl_3$) of 8g



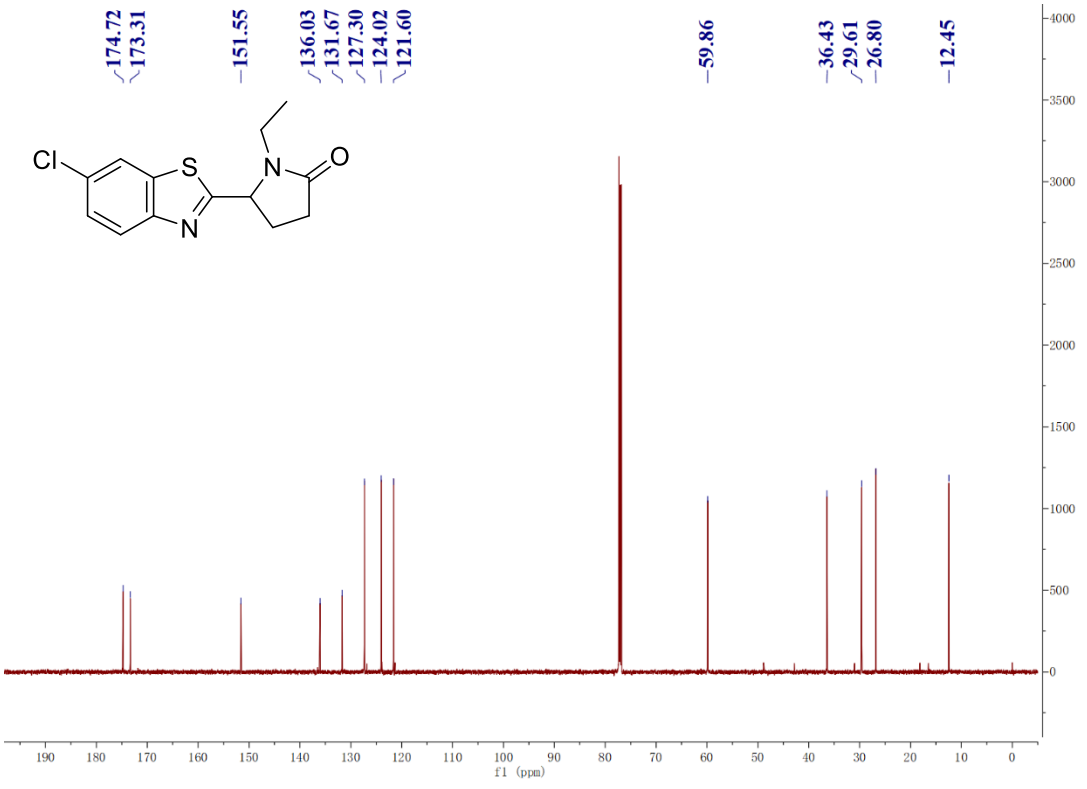
^{13}C NMR (151 MHz, $CDCl_3$) of 8g



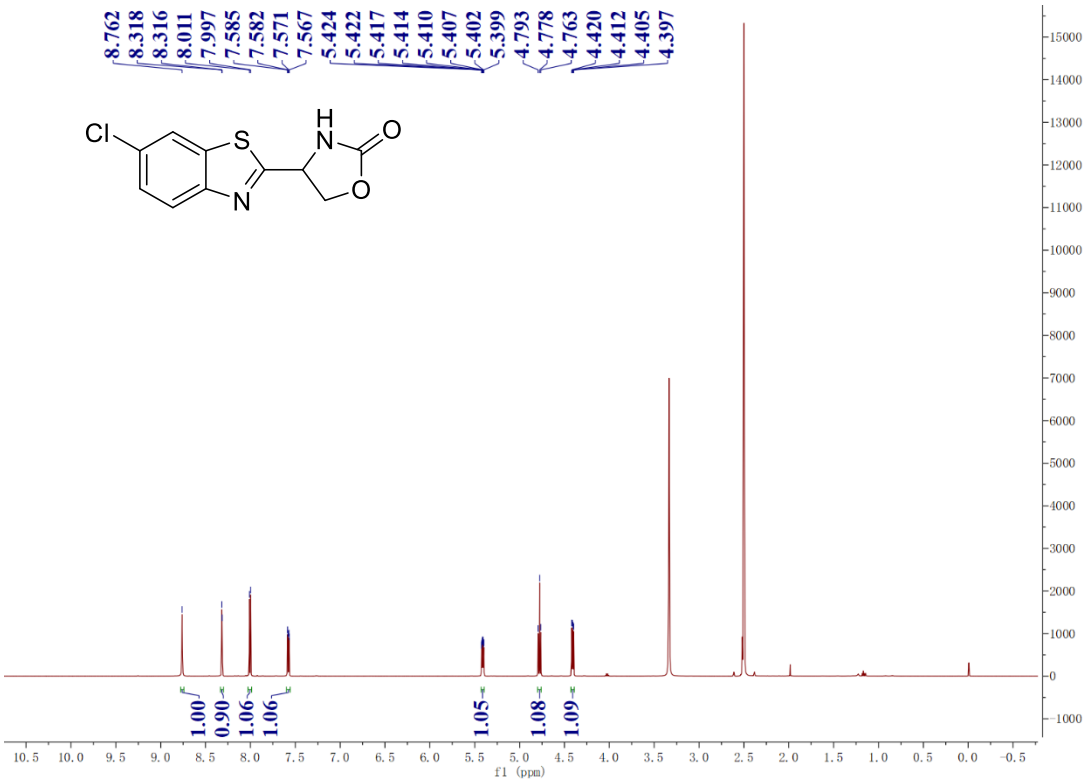
^{1}H NMR (600 MHz, $CDCl_3$) of 8h



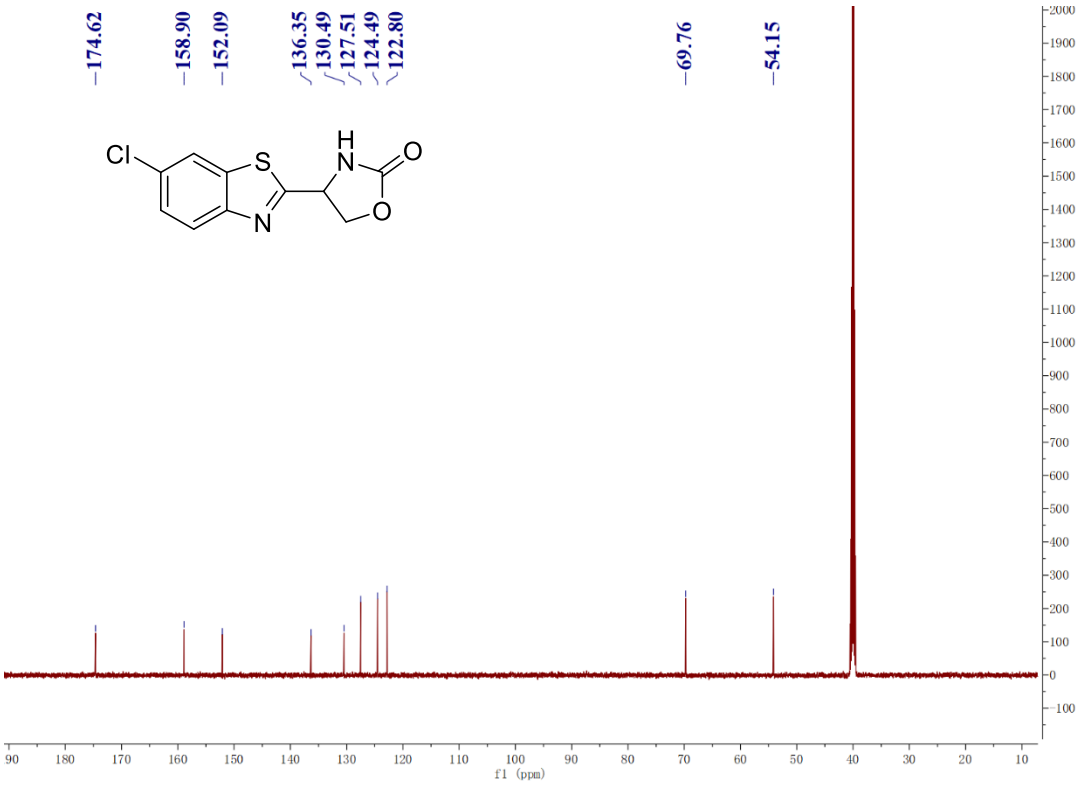
^{13}C NMR (151 MHz, $CDCl_3$) of 8h



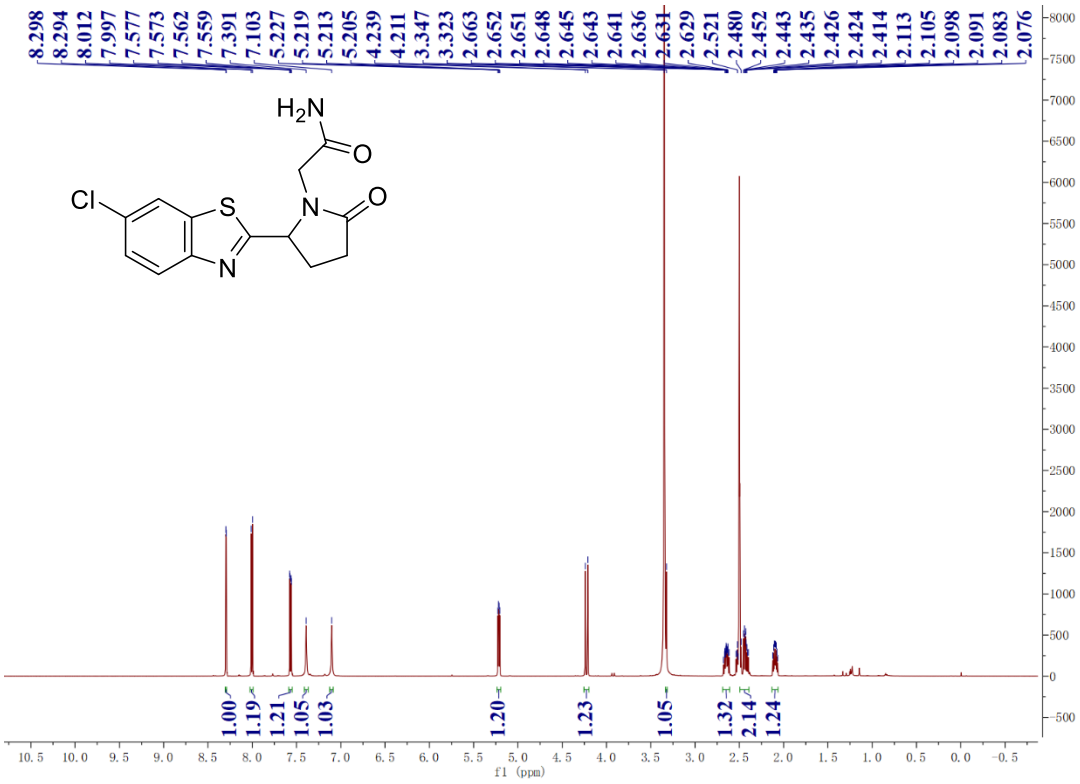
^{1}H NMR (600 MHz, DMSO-d_6) of 8i



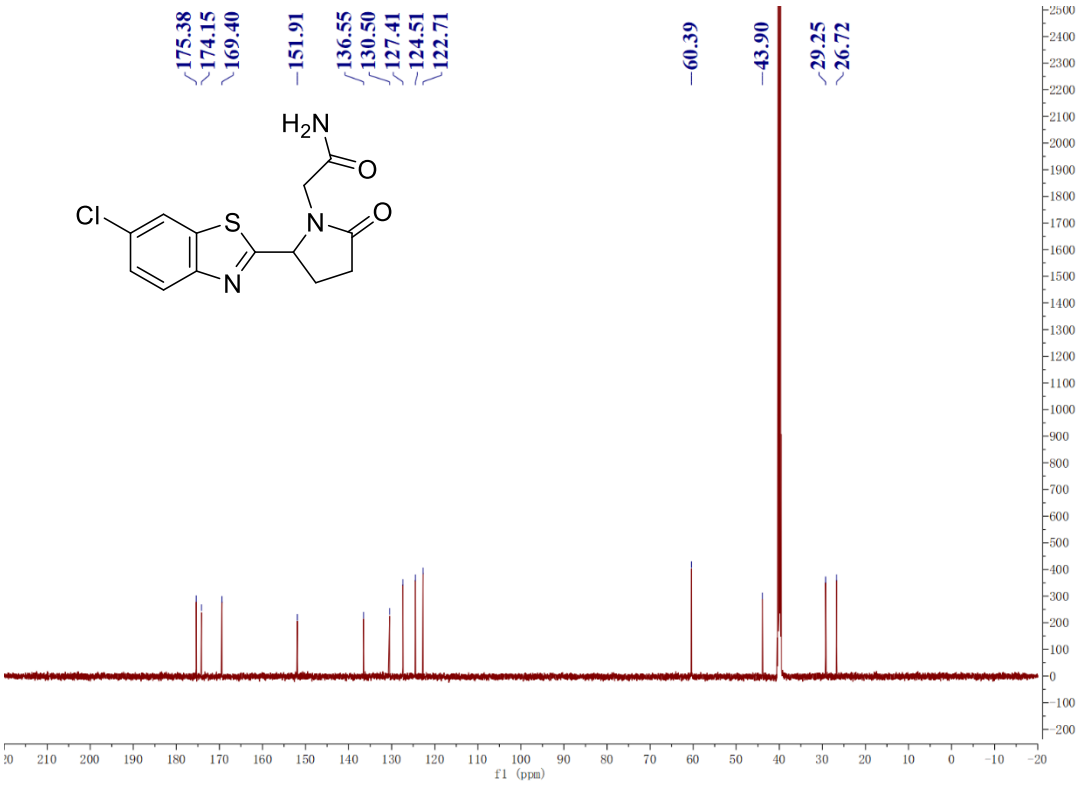
^{13}C NMR (151 MHz, DMSO-d_6) of 8i



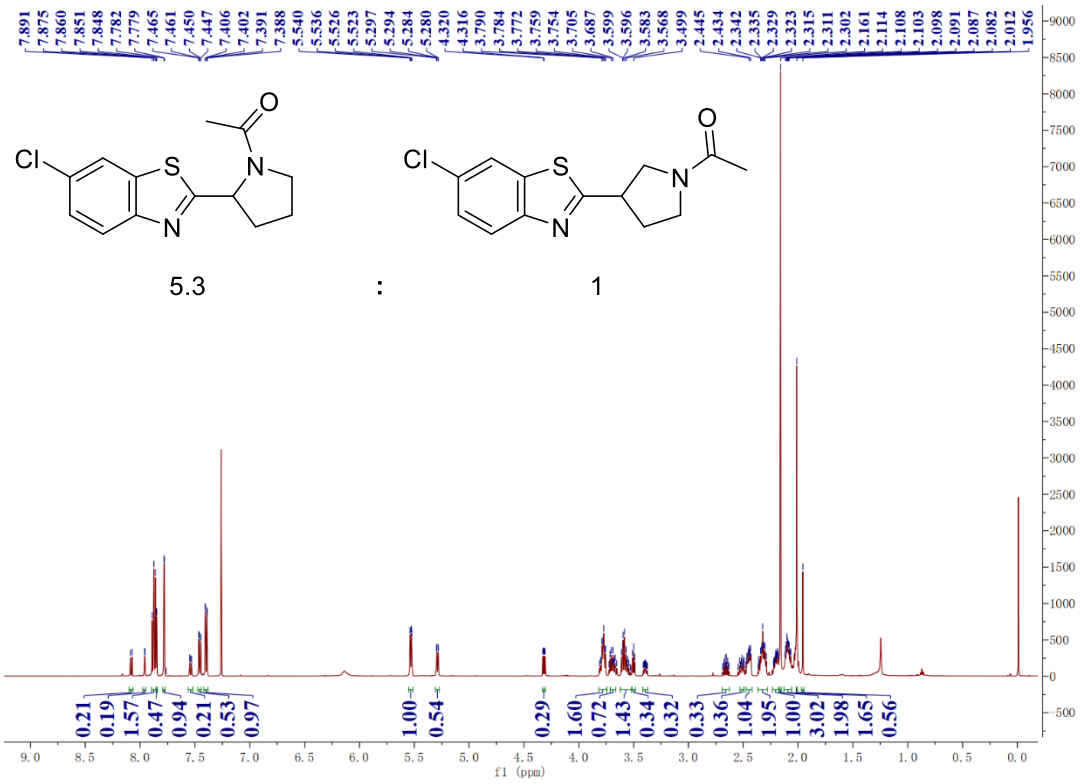
^{1}H NMR (600 MHz, DMSO-d_6) of 8j



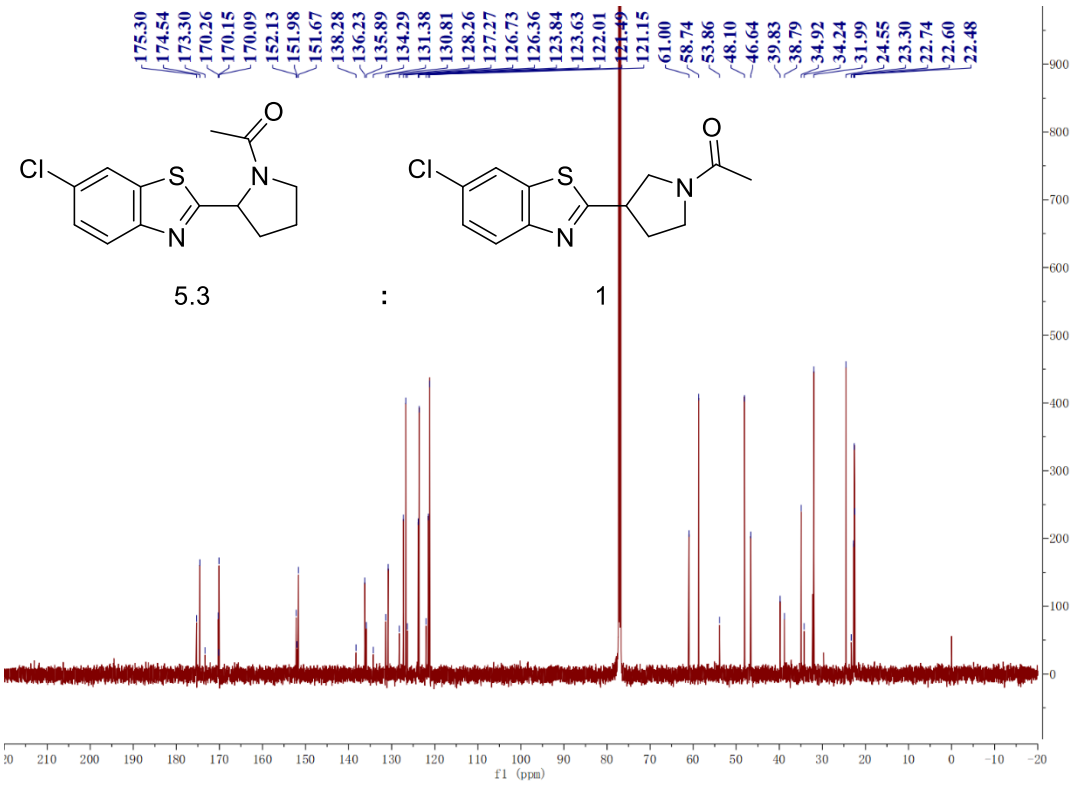
^{13}C NMR (151 MHz, DMSO-d_6) of 8j



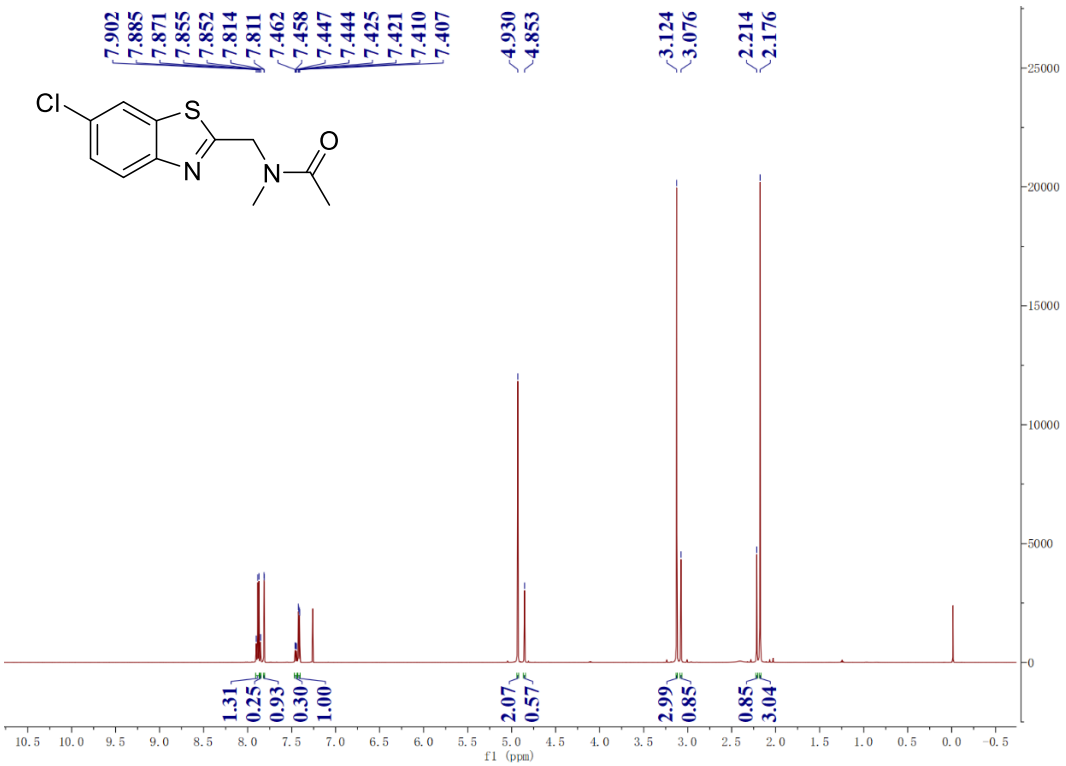
^{1}H NMR (600 MHz, $CDCl_3$) of 8k and 8k′



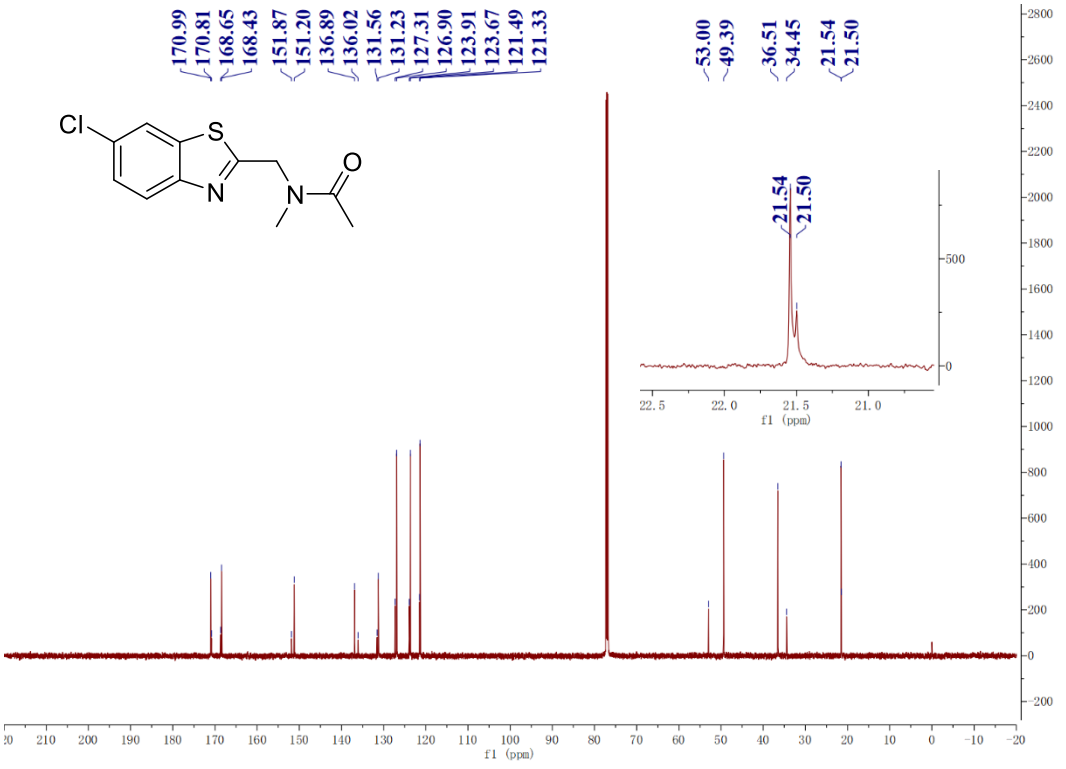
^{13}C NMR (151 MHz, $CDCl_3$) of 8k and 8k′



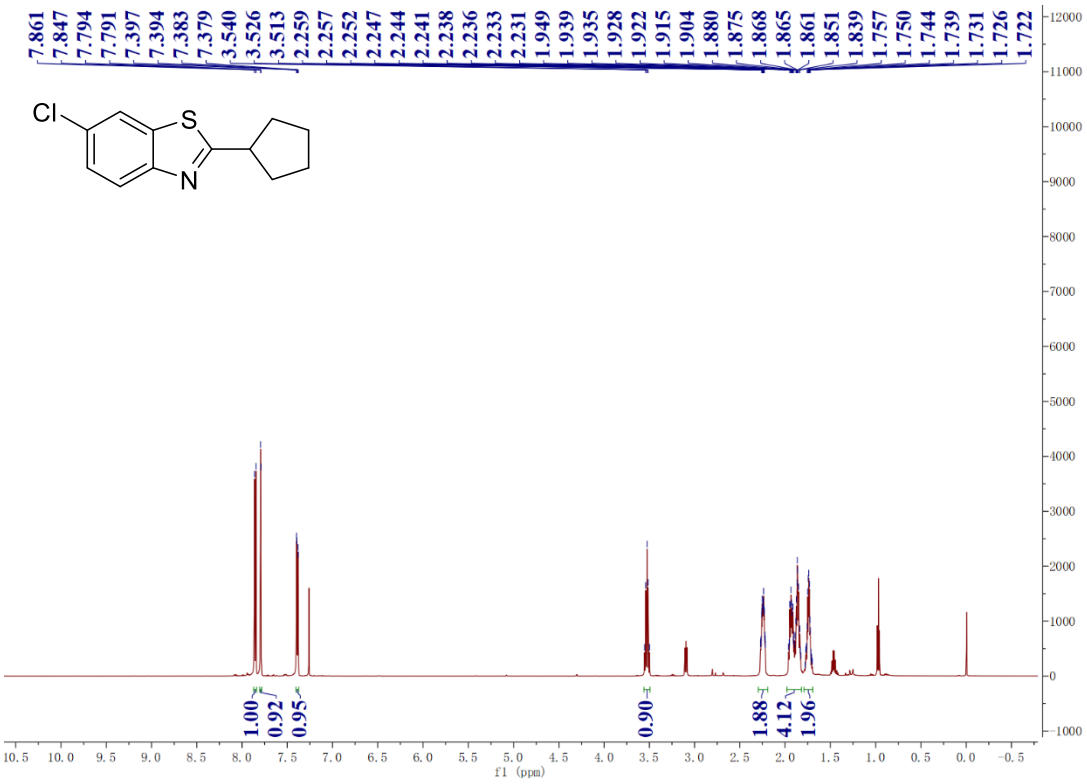
^{1}H NMR (600 MHz, $CDCl_3$) of 8l



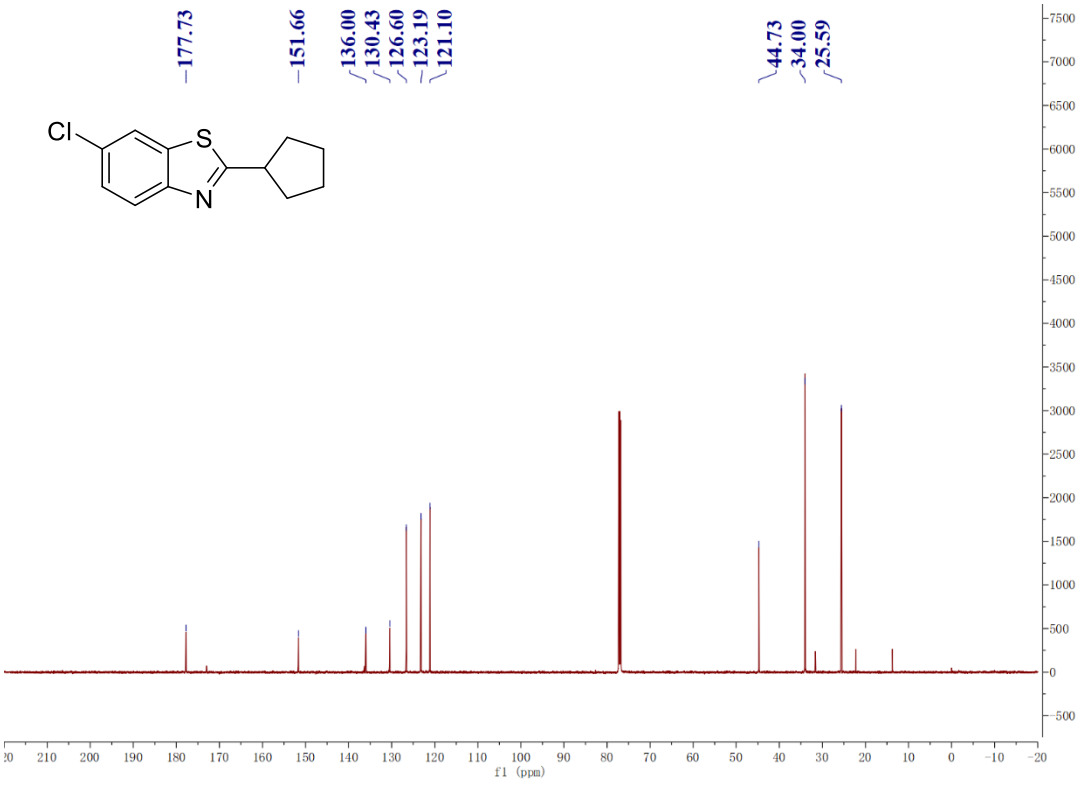
^{13}C NMR (151 MHz, $CDCl_3$) of 8l



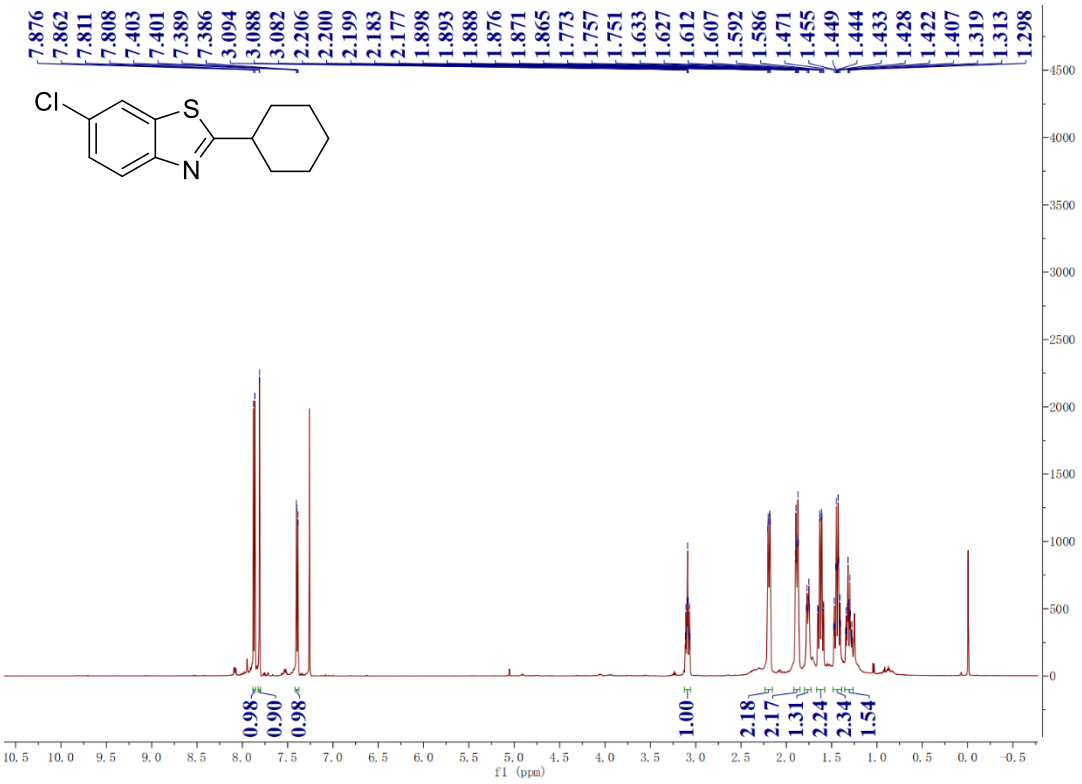
^{1}H NMR (600 MHz, $CDCl_3$) of 10a



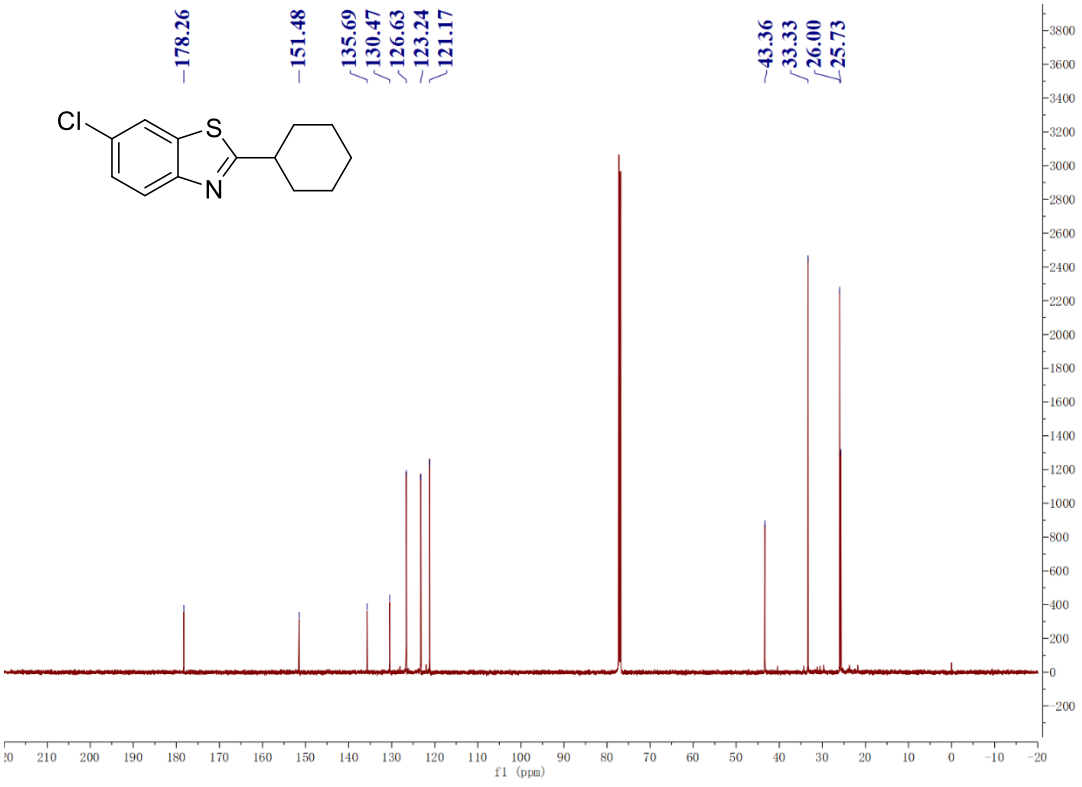
^{13}C NMR (151 MHz, $CDCl_3$) of 10a



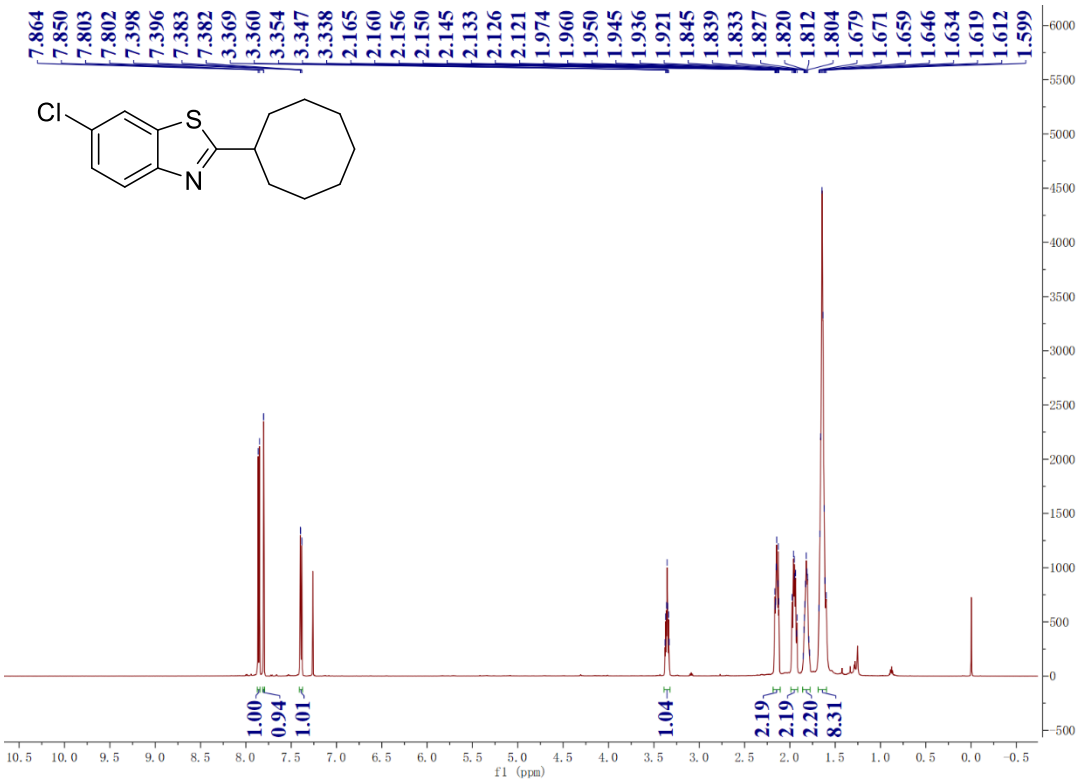
^{1}H NMR (600 MHz, $CDCl_3$) of 10b



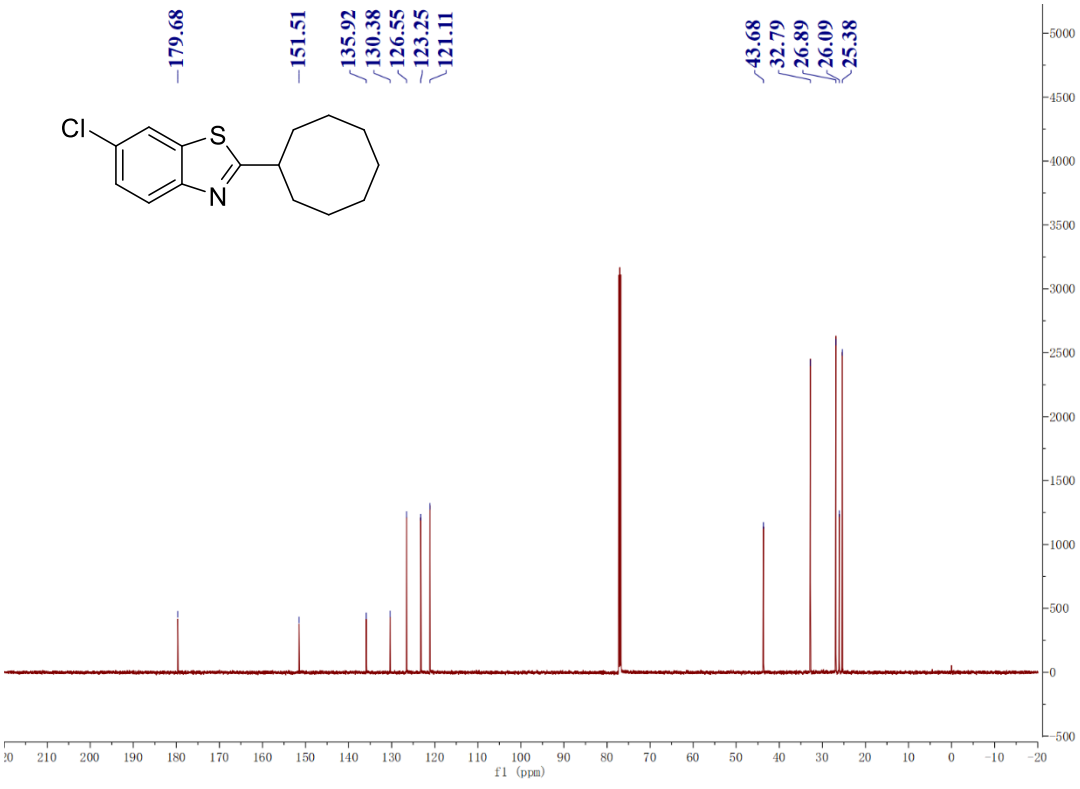
^{13}C NMR (151 MHz, $CDCl_3$) of 10b



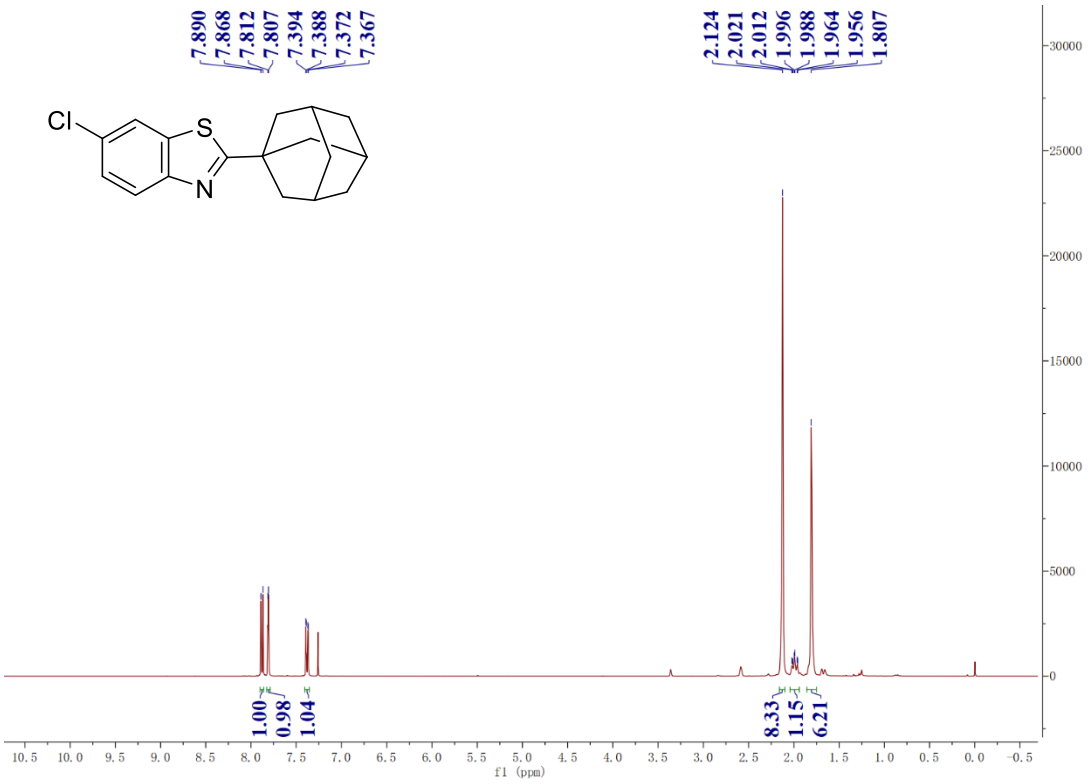
^{1}H NMR (600 MHz, $CDCl_3$) of 10c



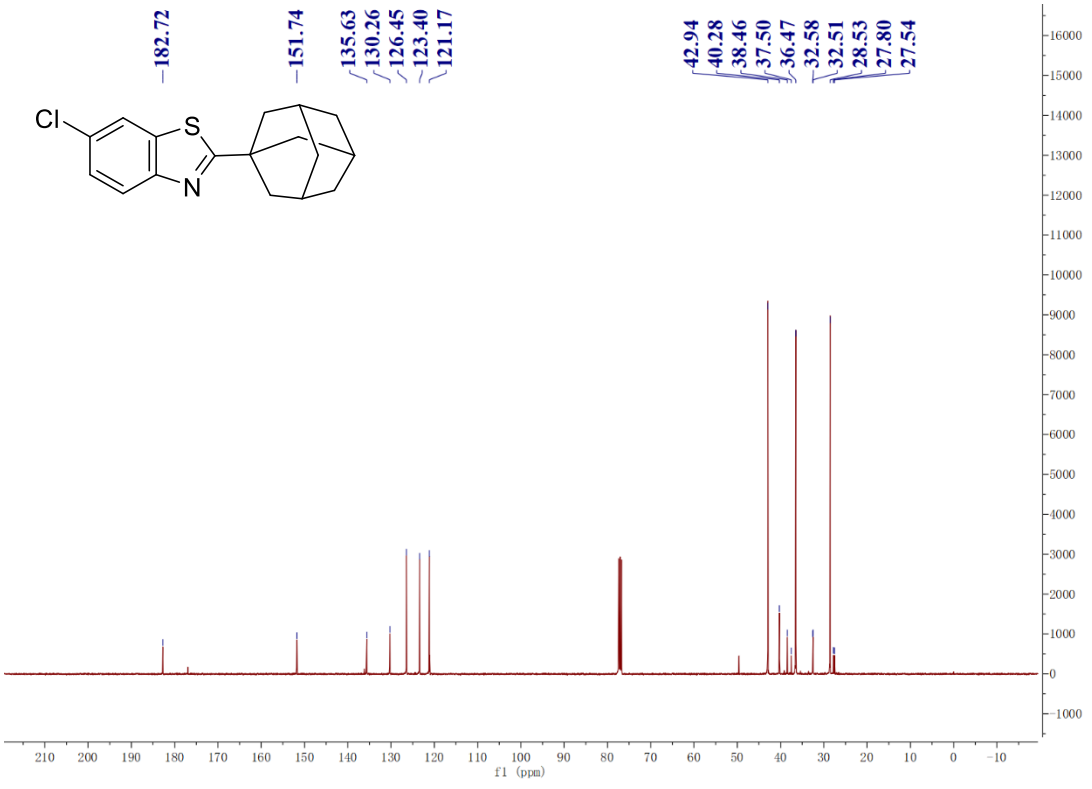
^{13}C NMR (151 MHz, $CDCl_3$) of 10c



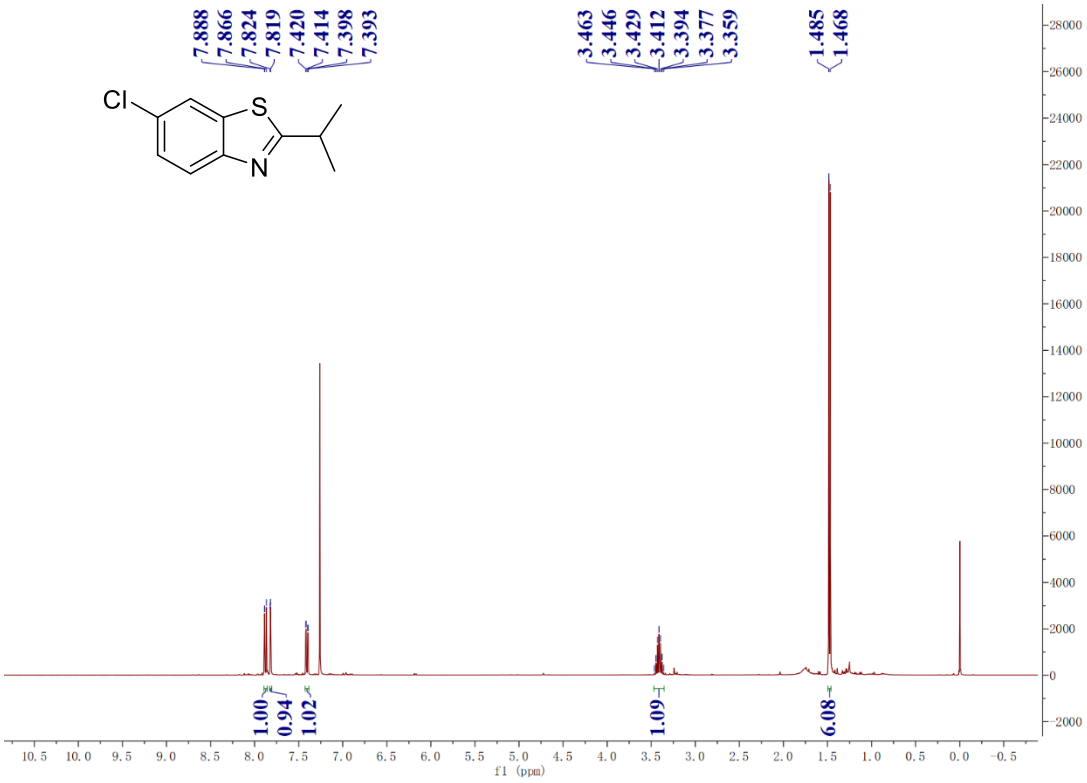
^{1}H NMR (400 MHz, $CDCl_3$) of 10d



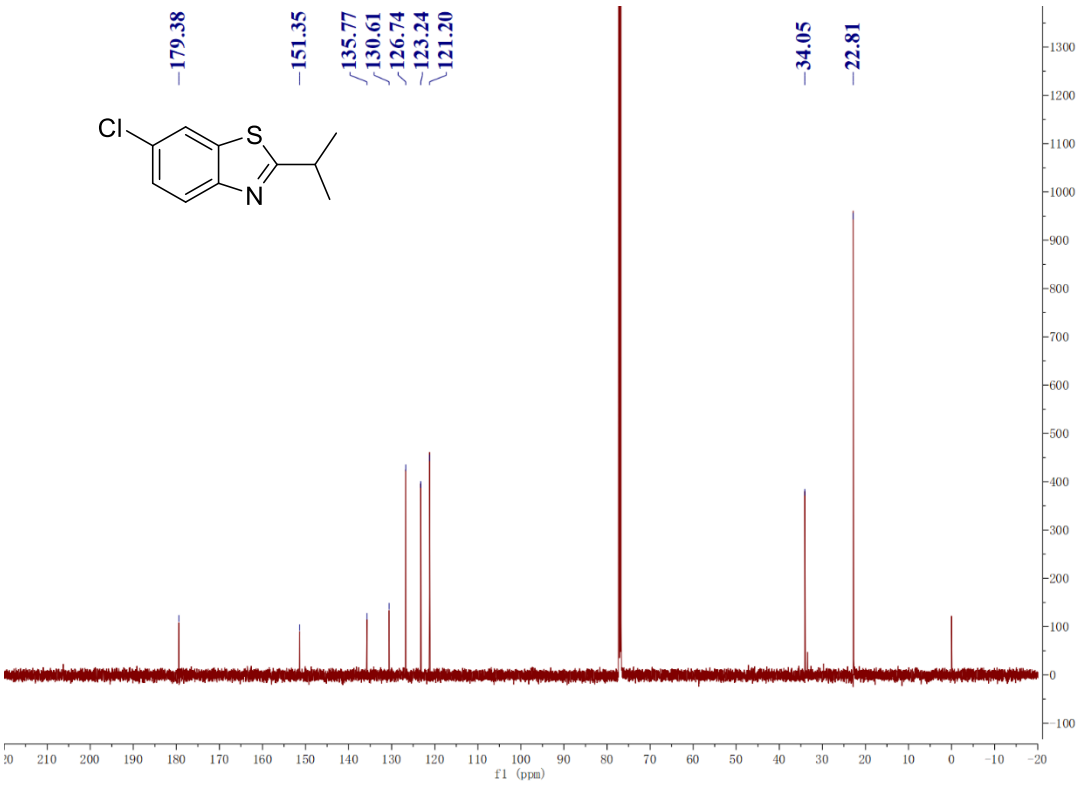
^{13}C NMR (101 MHz, $CDCl_3$) of 10d



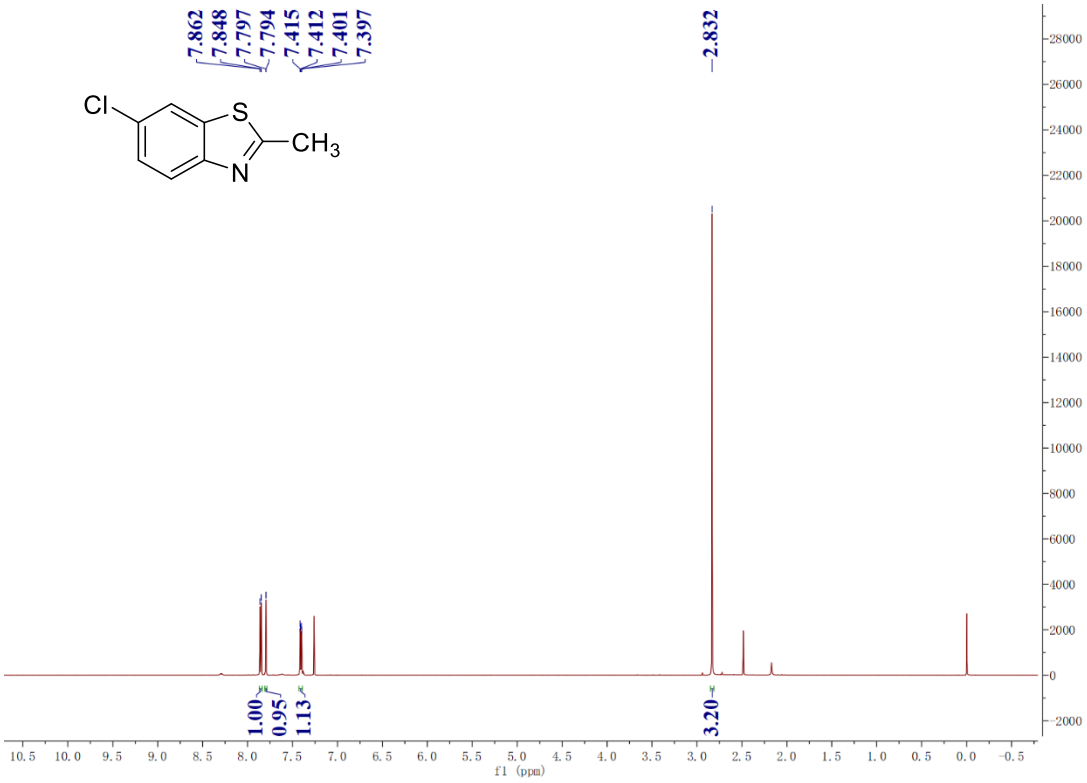
^{1}H NMR (400 MHz, $CDCl_3$) of 11a



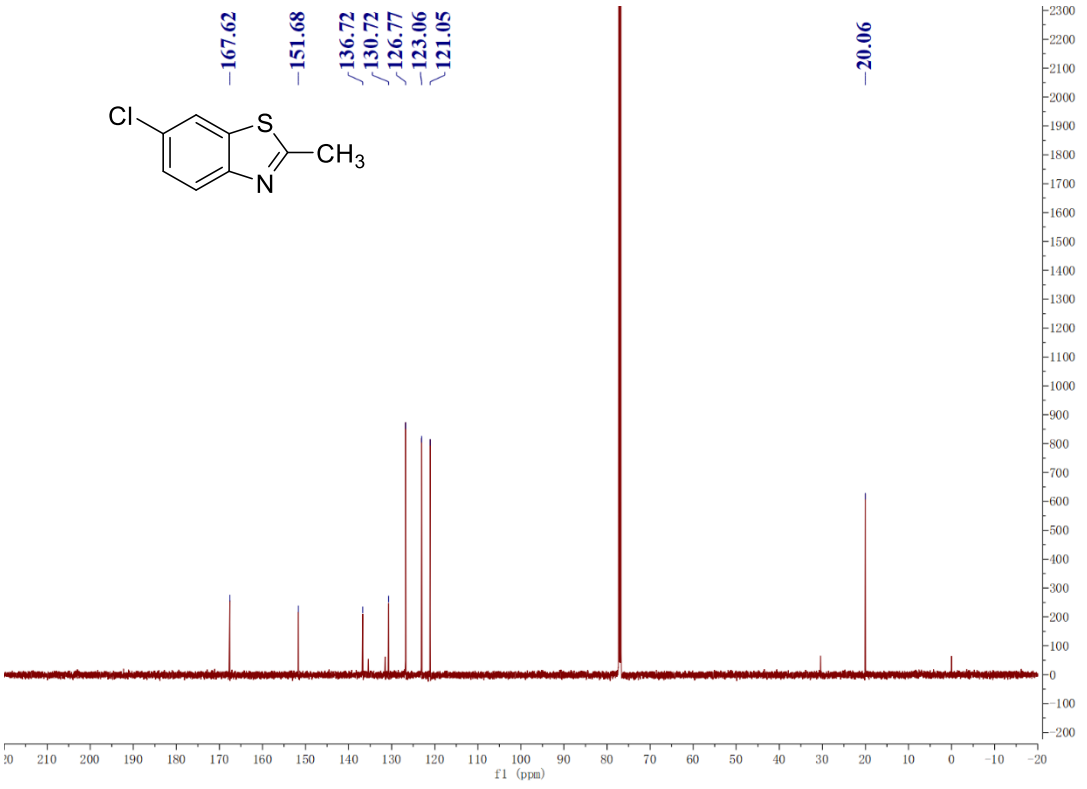
^{13}C NMR (151 MHz, $CDCl_3$) of 11a



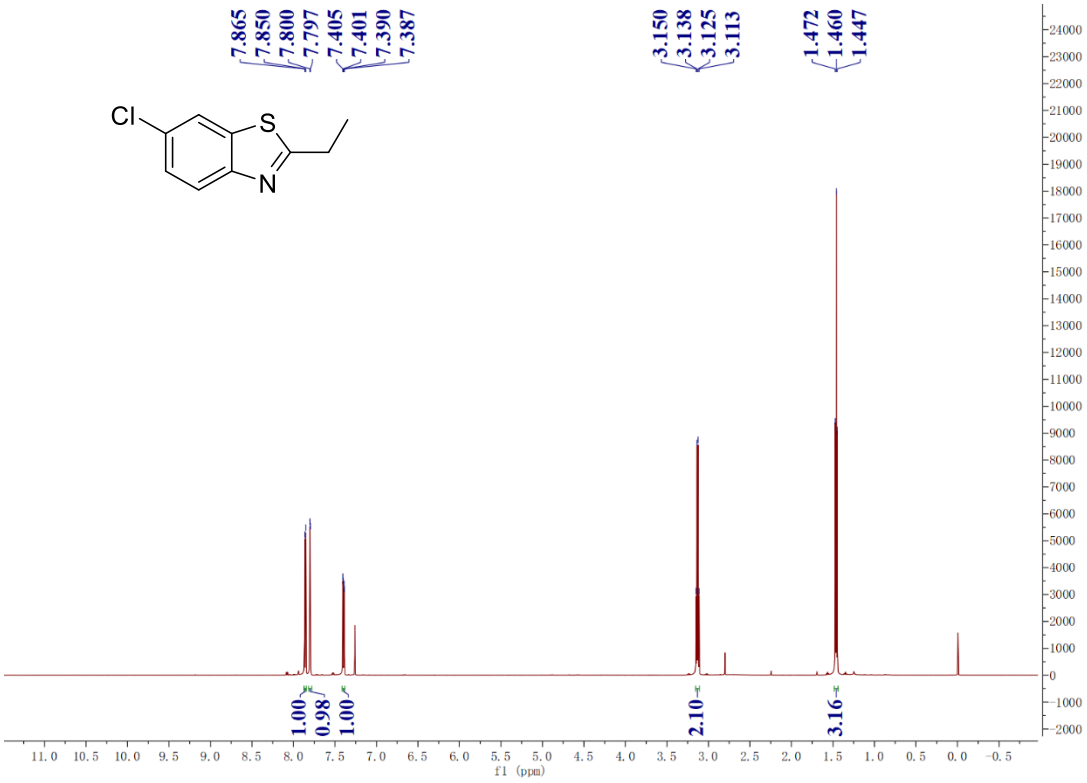
^{1}H NMR (600 MHz, $CDCl_3$) of 11b



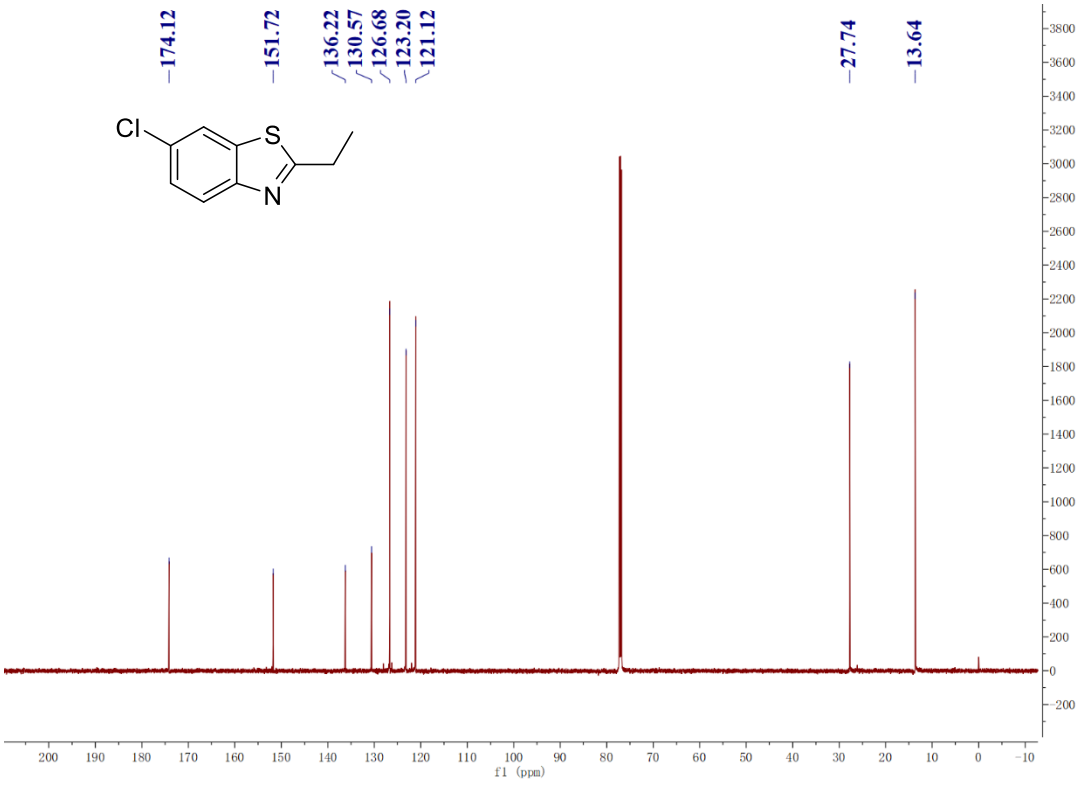
^{13}C NMR (151 MHz, $CDCl_3$) of 11b



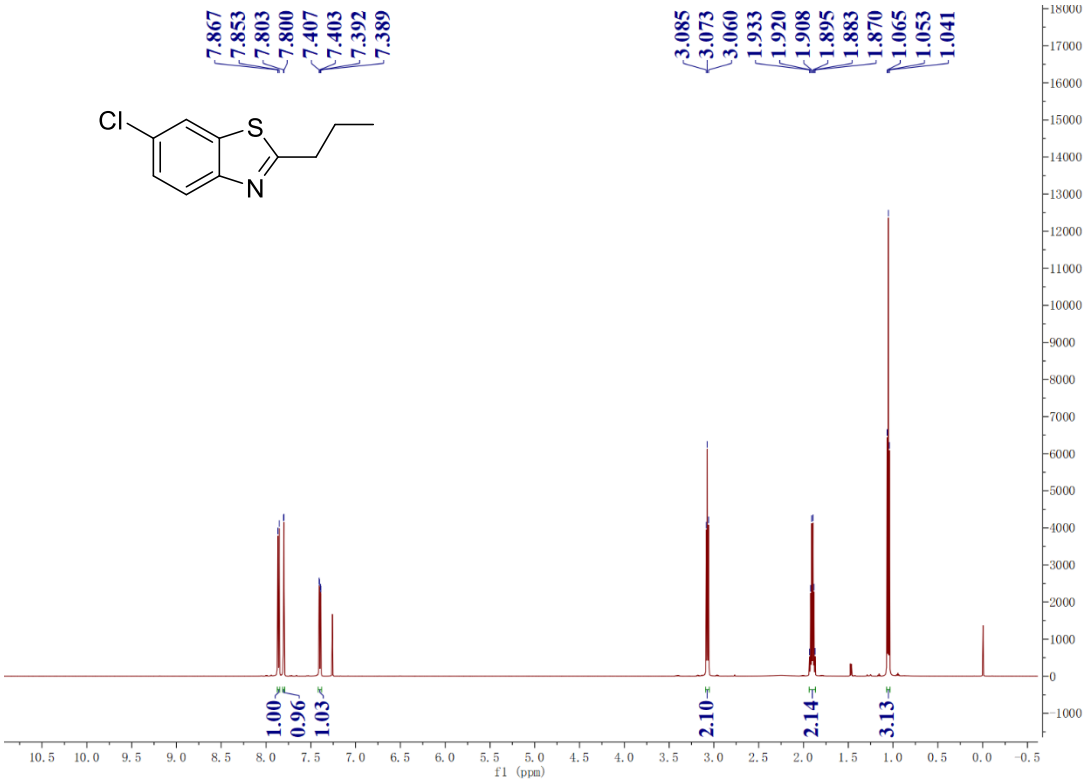
^{1}H NMR (600 MHz, $CDCl_3$) of 11c



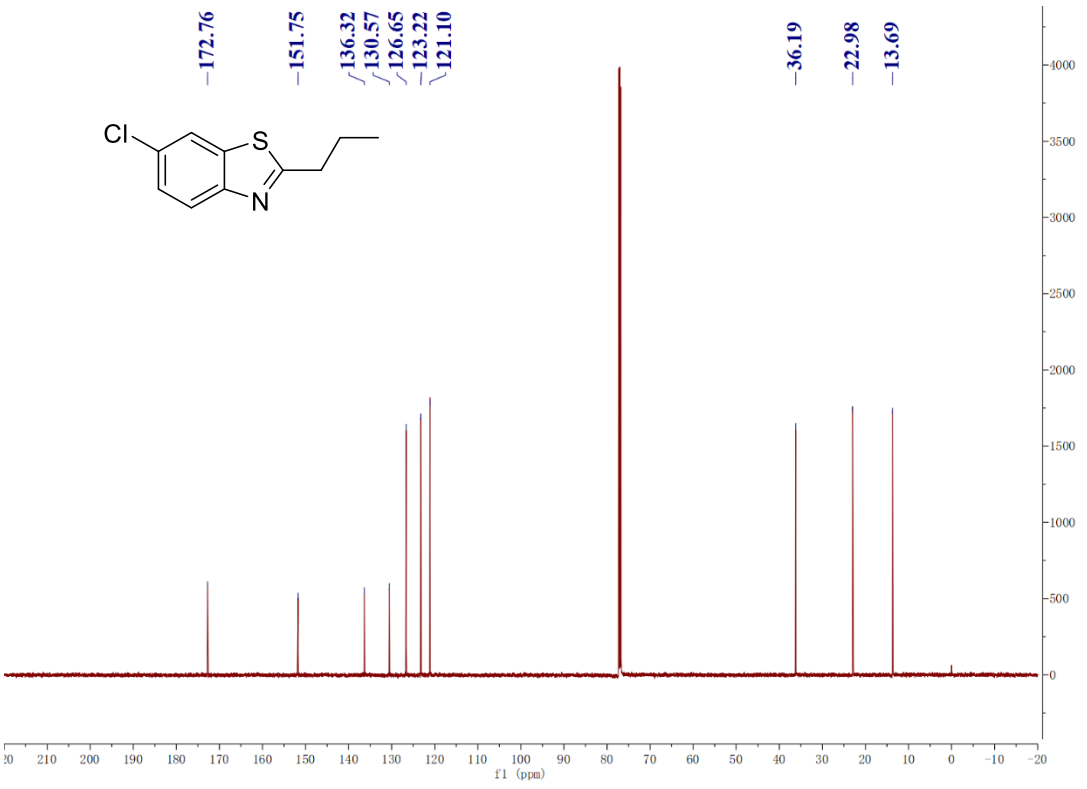
^{13}C NMR (151 MHz, $CDCl_3$) of 11c



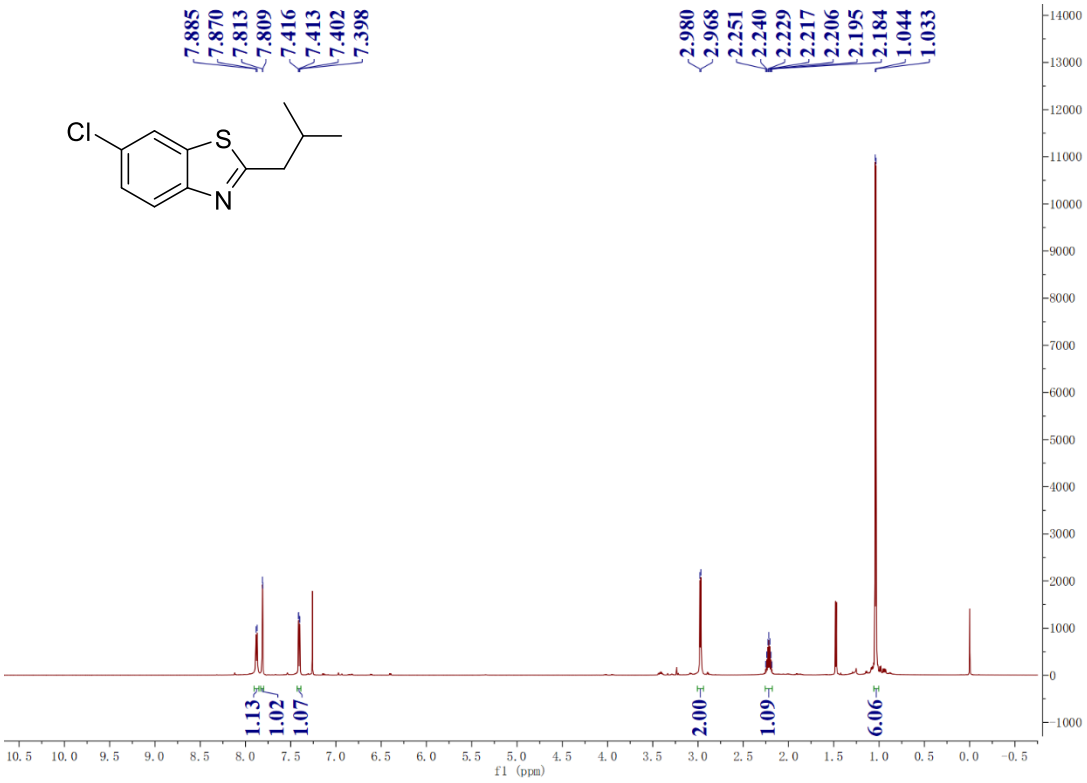
^{1}H NMR (600 MHz, $CDCl_3$) of 11d



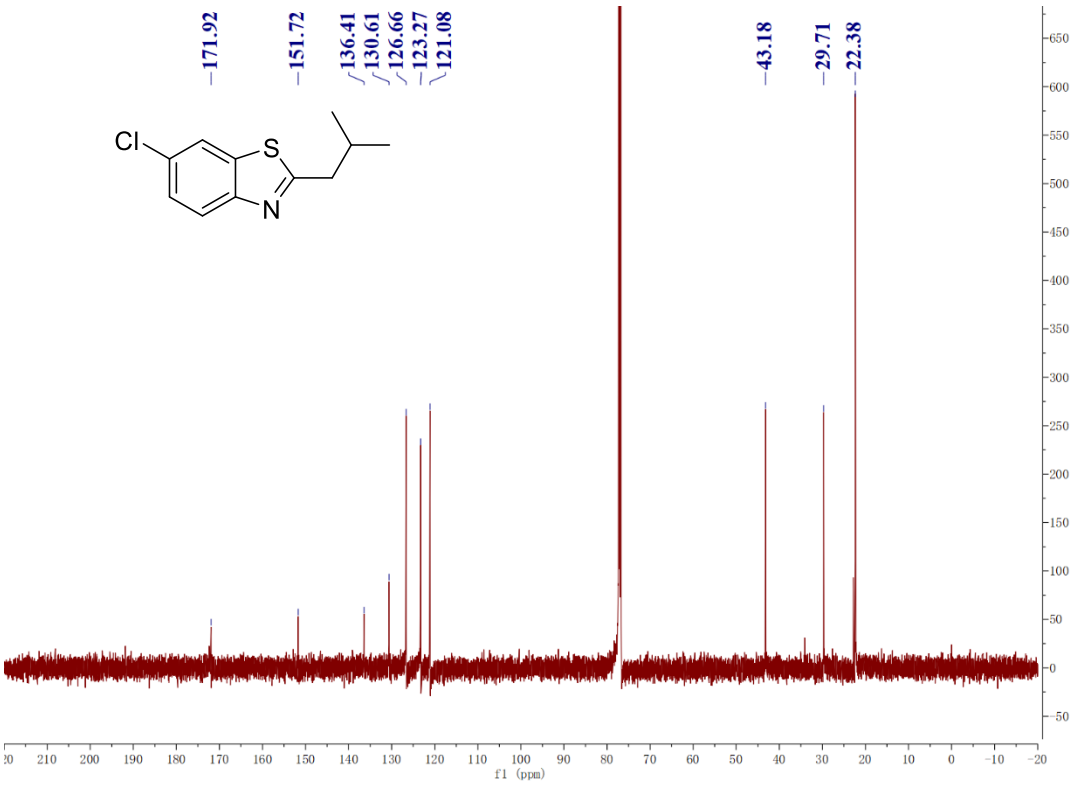
^{13}C NMR (151 MHz, $CDCl_3$) of 11d



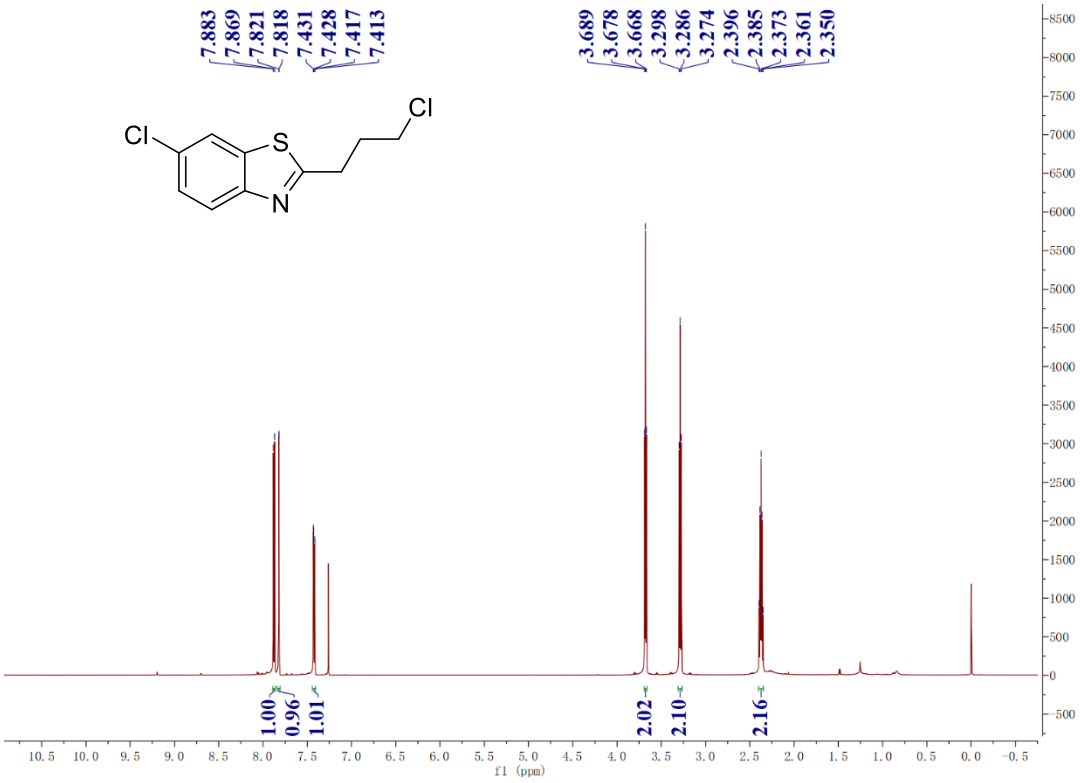
^{1}H NMR (600 MHz, $CDCl_3$) of 11e



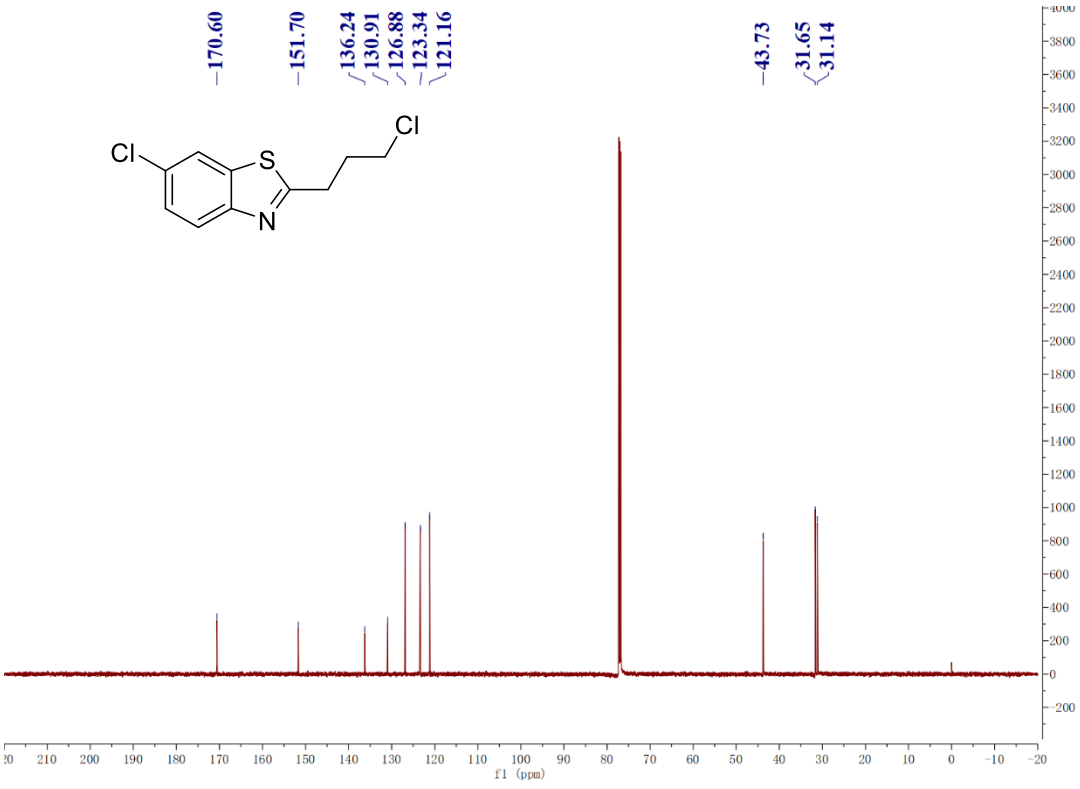
^{13}C NMR (151 MHz, $CDCl_3$) of 11e



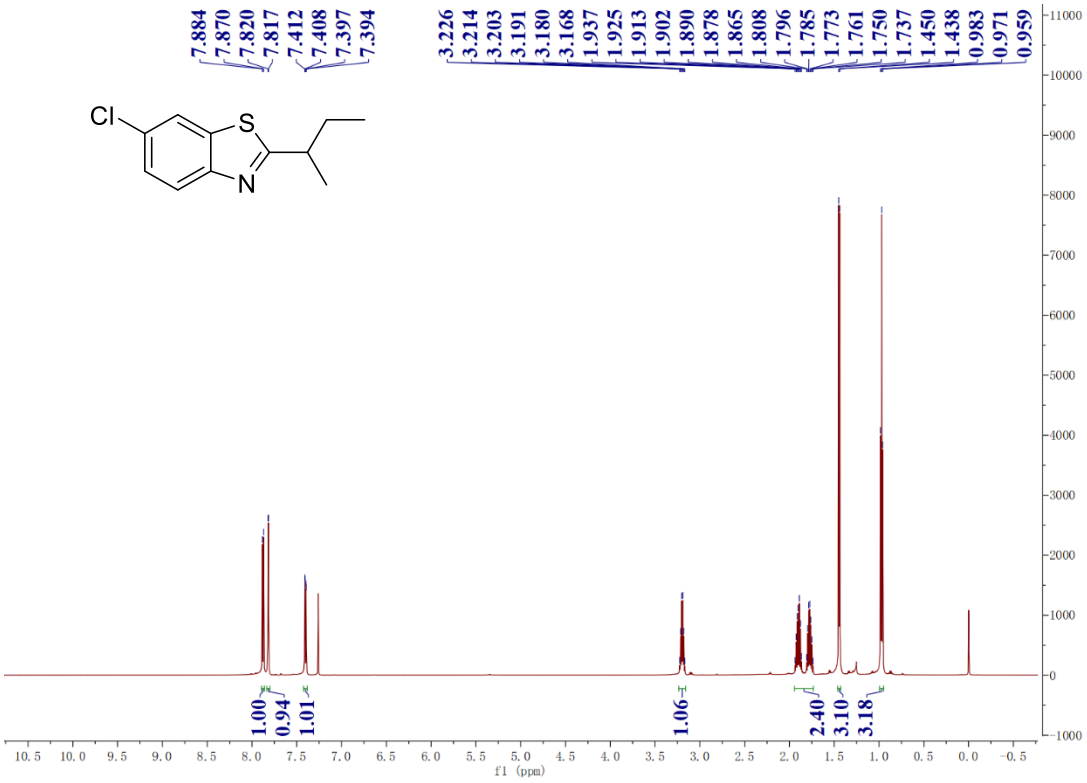
^{1}H NMR (600 MHz, $CDCl_3$) of 11f



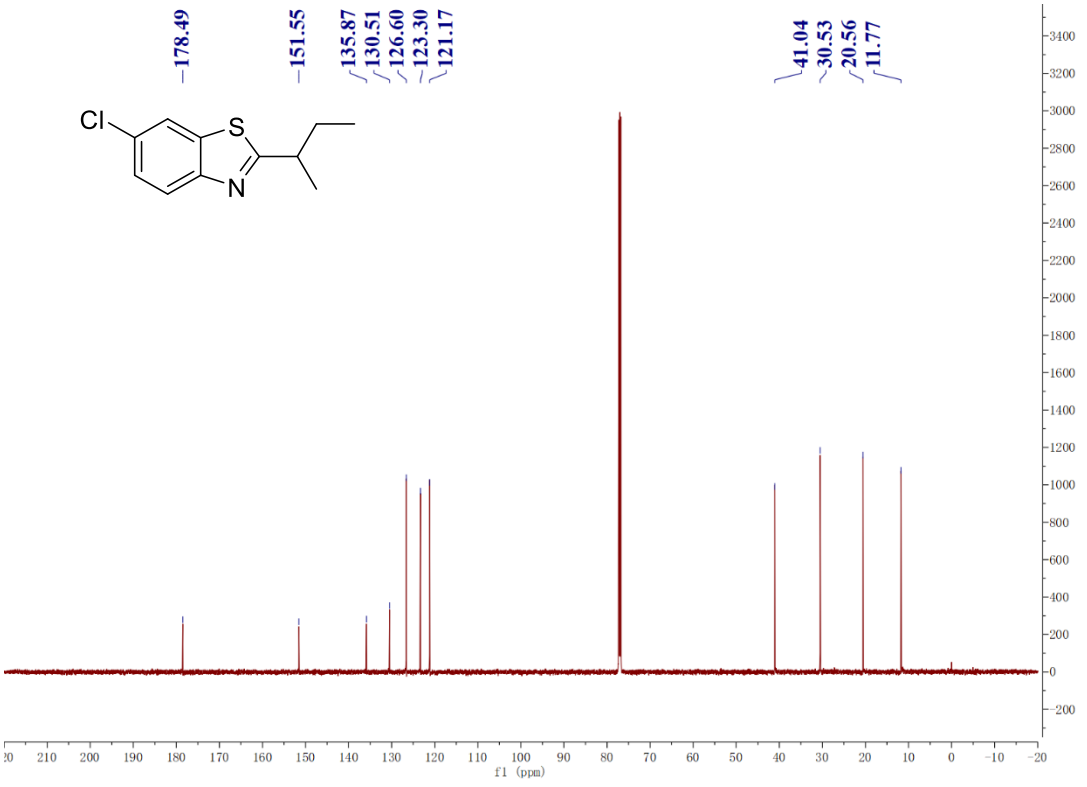
^{13}C NMR (151 MHz, $CDCl_3$) of 11f



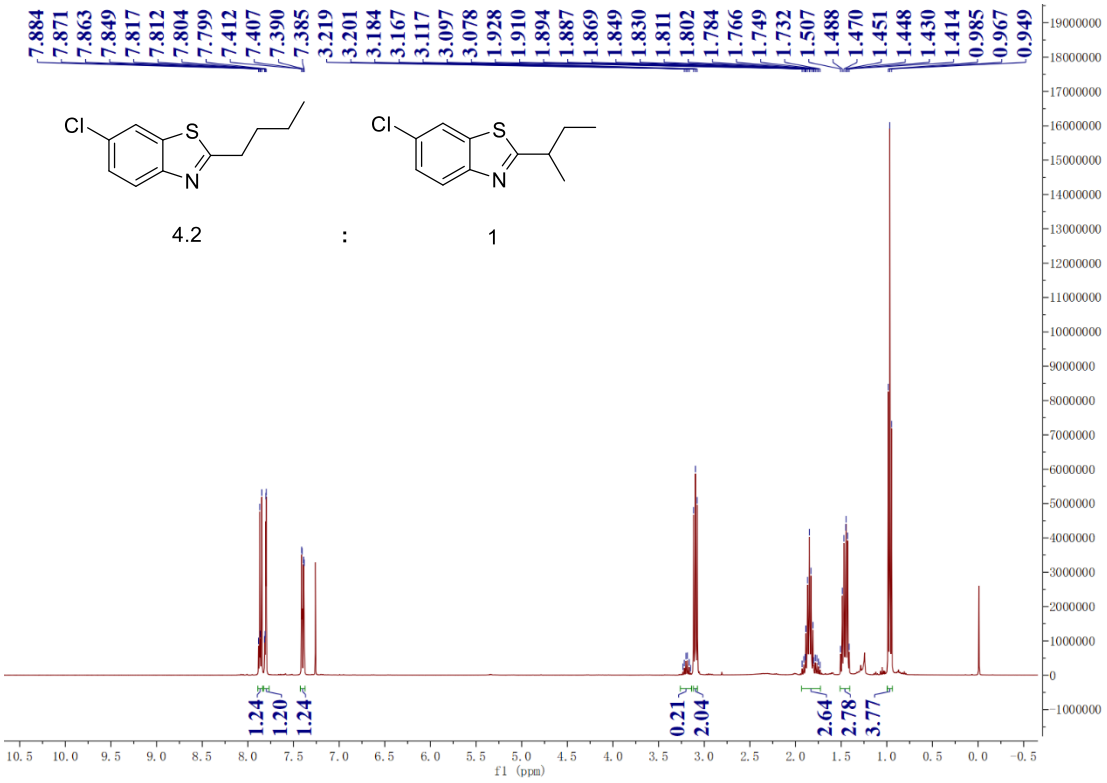
^{1}H NMR (600 MHz, $CDCl_3$) of 11g



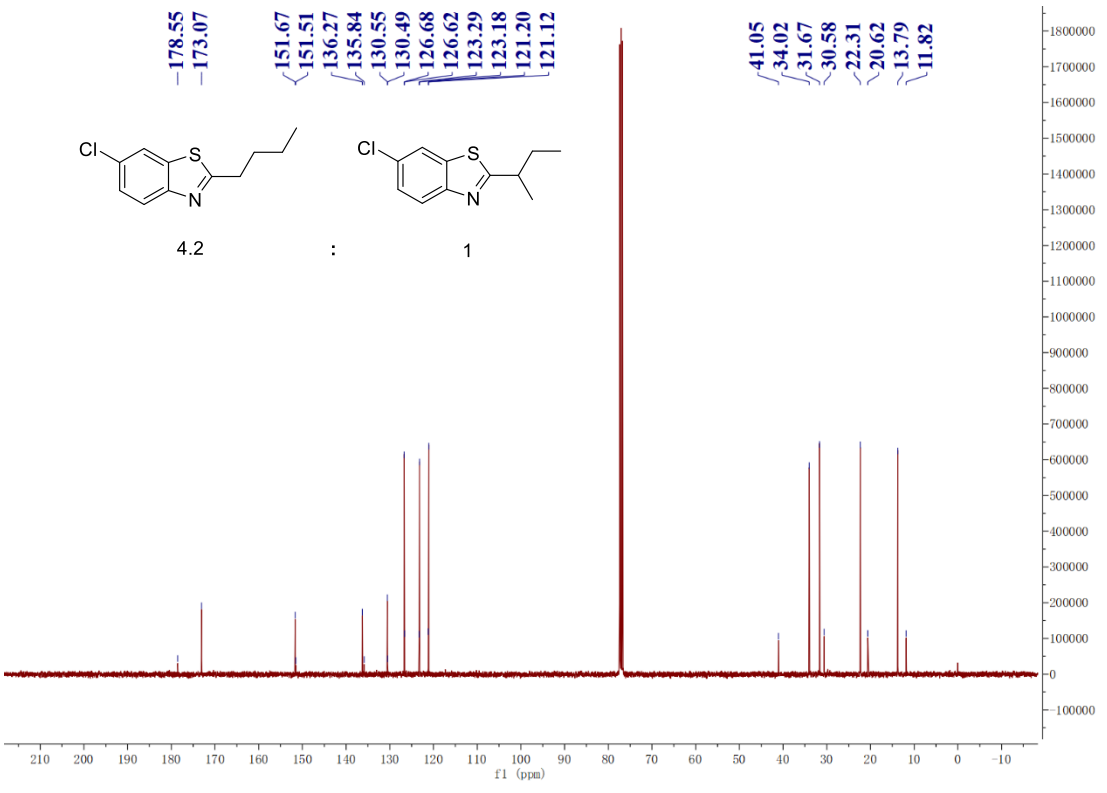
^{13}C NMR (151 MHz, $CDCl_3$) of 11g



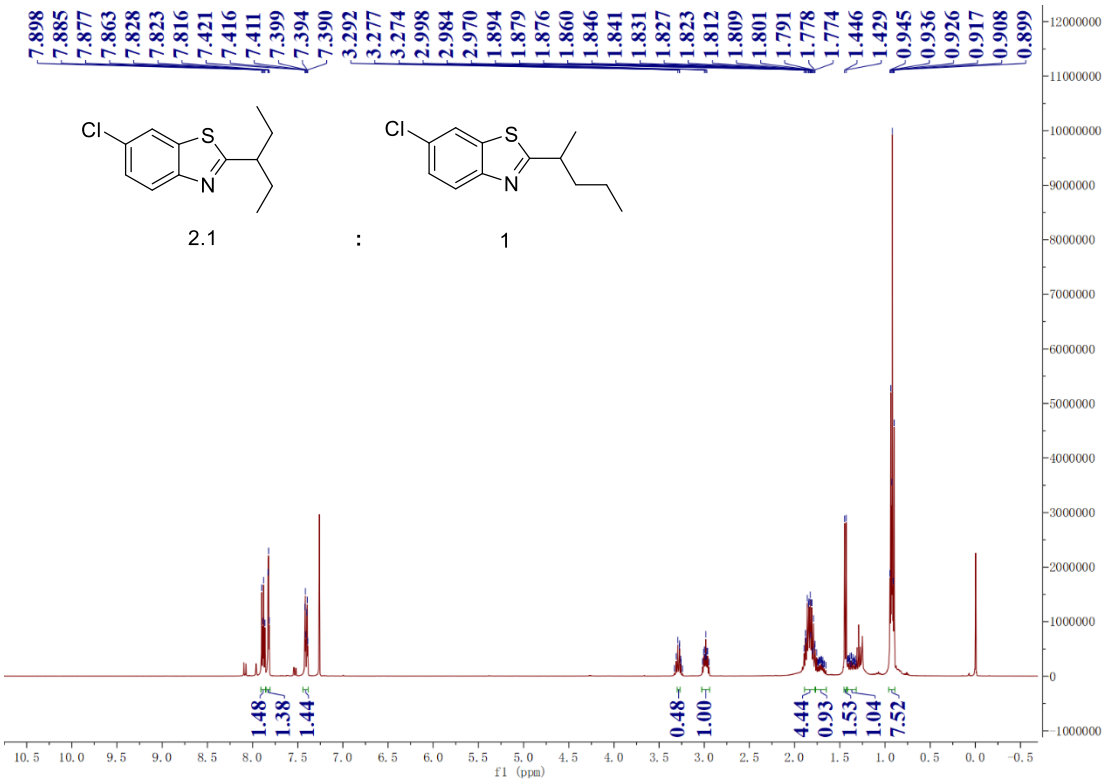
^{1}H NMR (400 MHz, $CDCl_3$) of 11i and 11i′



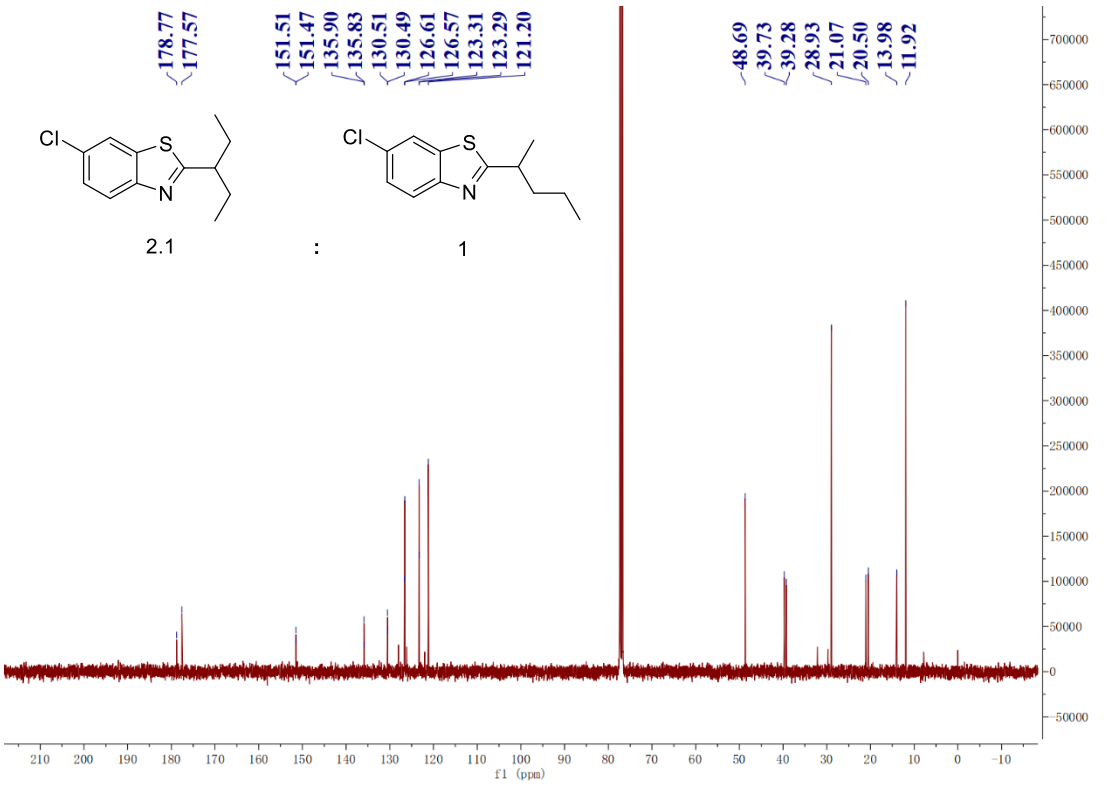
^{13}C NMR (101 MHz, $CDCl_3$) of 11i and 11i′



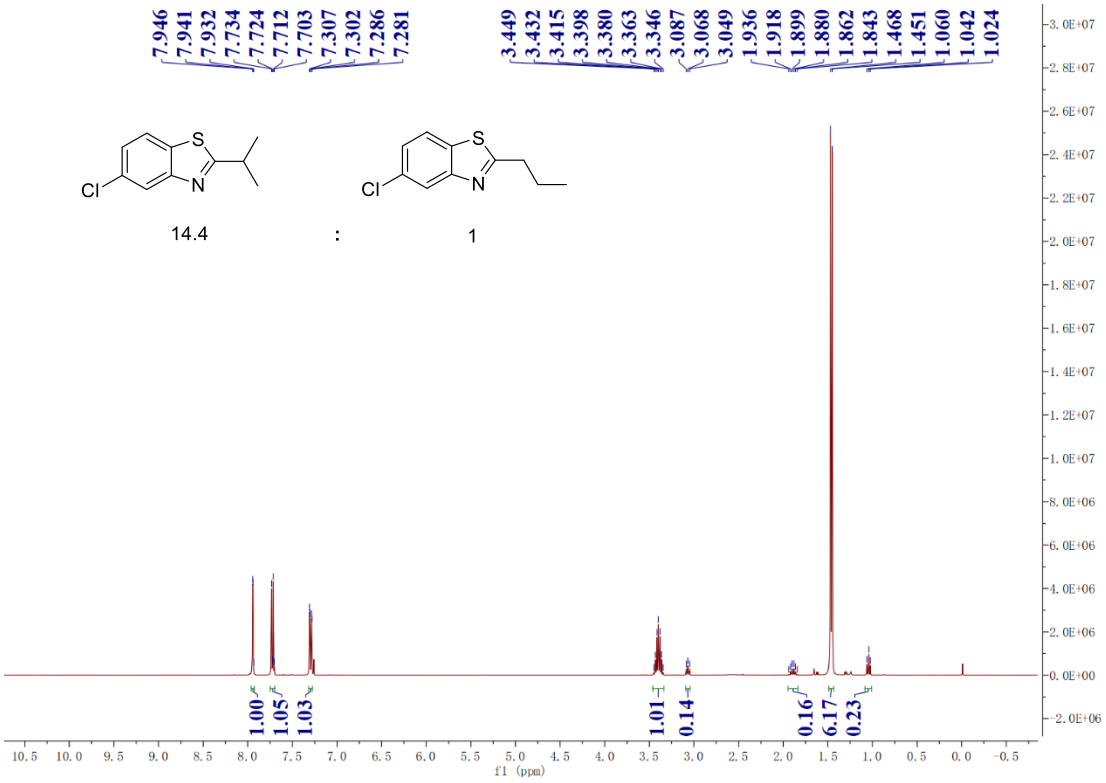
^{1}H NMR (400 MHz, $CDCl_3$) of 11j and 11j′



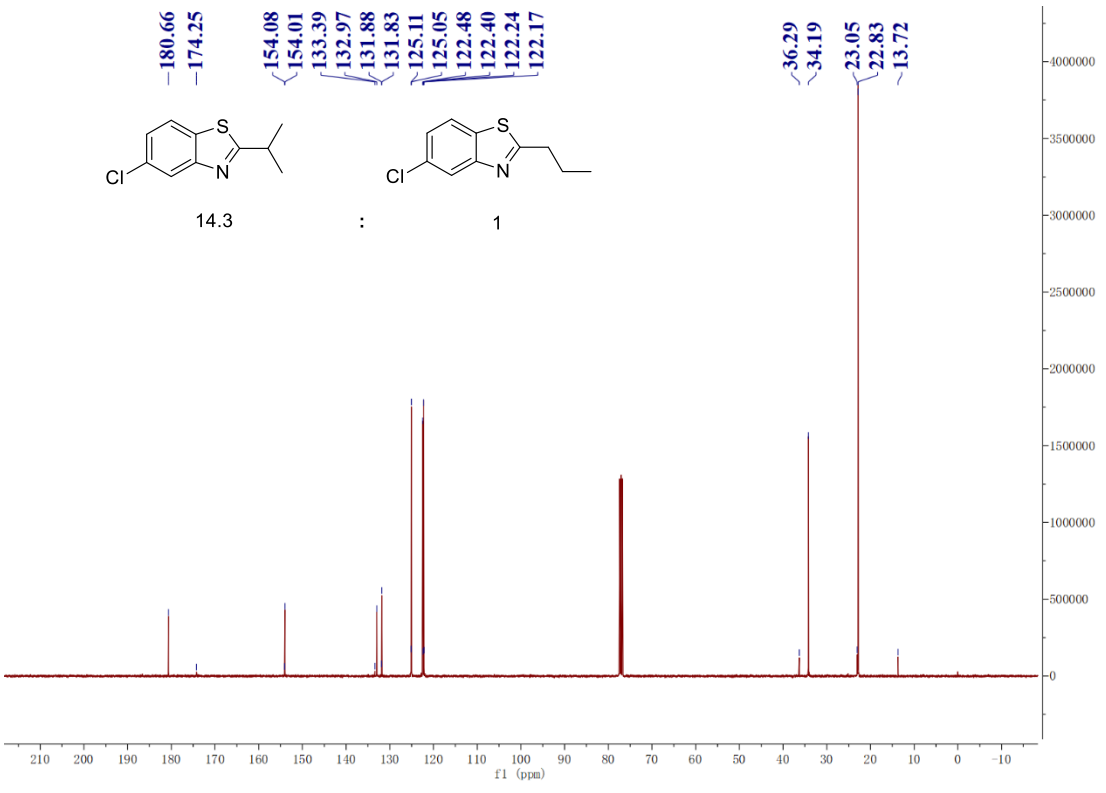
^{13}C NMR (101 MHz, $CDCl_3$) of 11j and 11j′



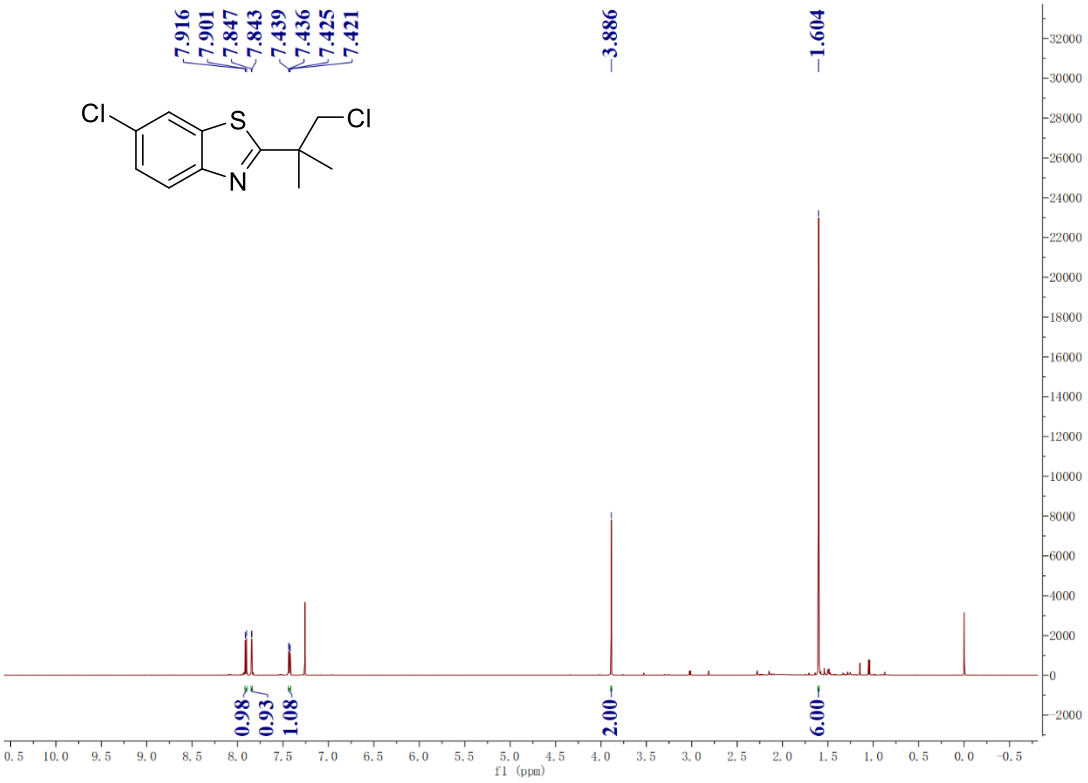
^{1}H NMR (400 MHz, $CDCl_3$) of 11k and 11k′



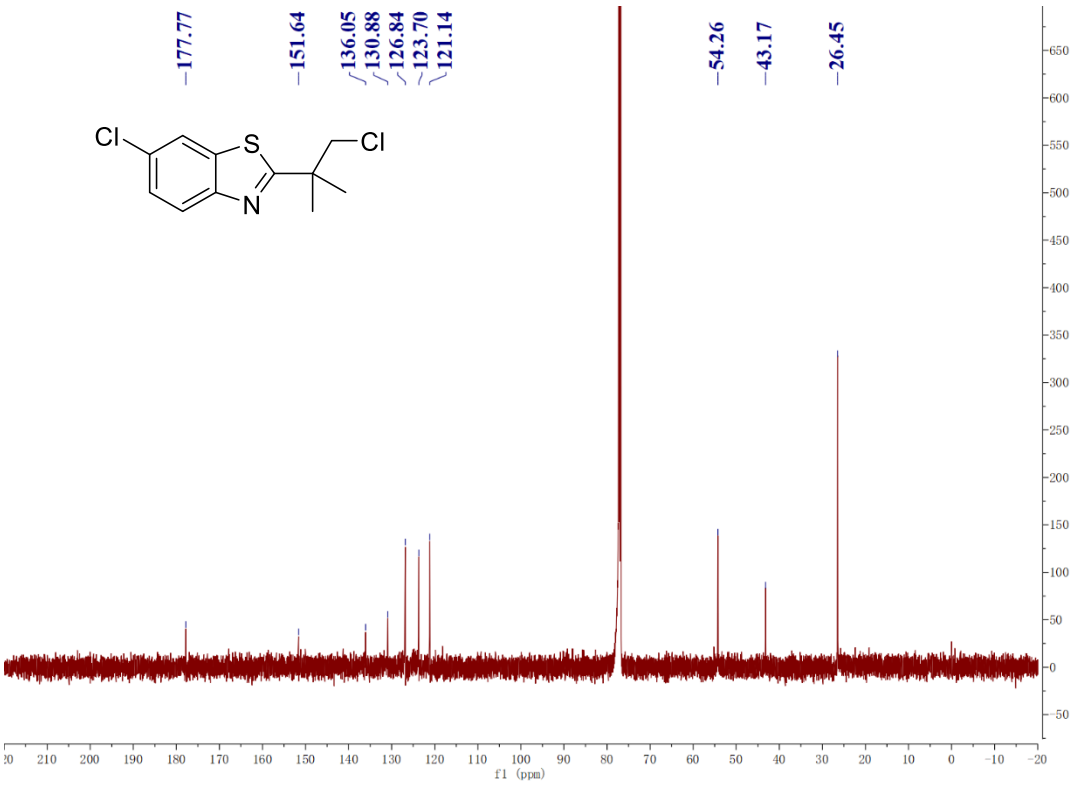
^{13}C NMR (101 MHz, $CDCl_3$) of 11k and 11k′



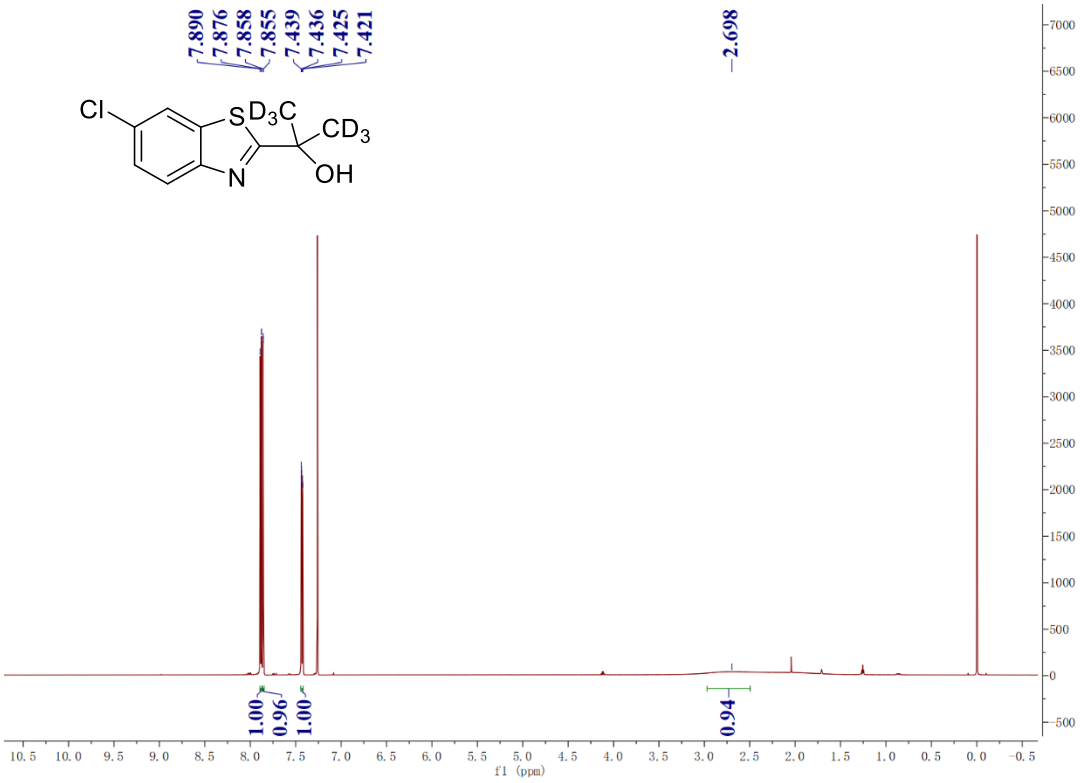
^{1}H NMR (600 MHz, $CDCl_3$) of 16



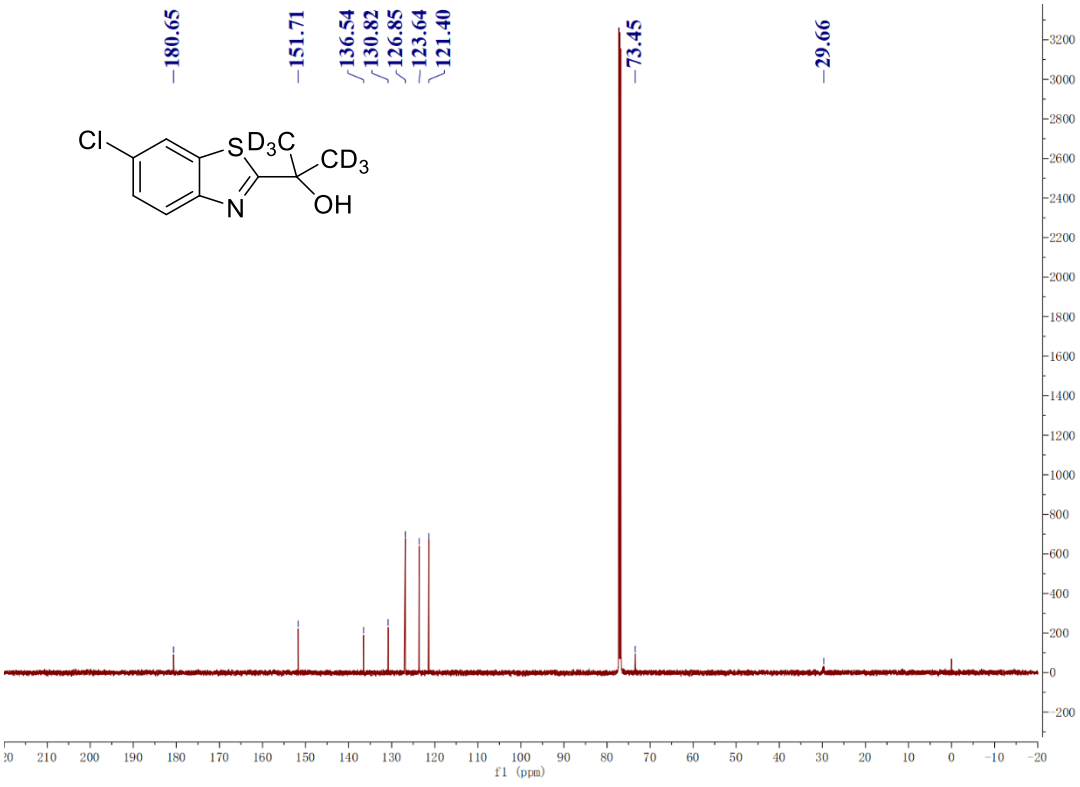
^{13}C NMR (151 MHz, $CDCl_3$) of 16



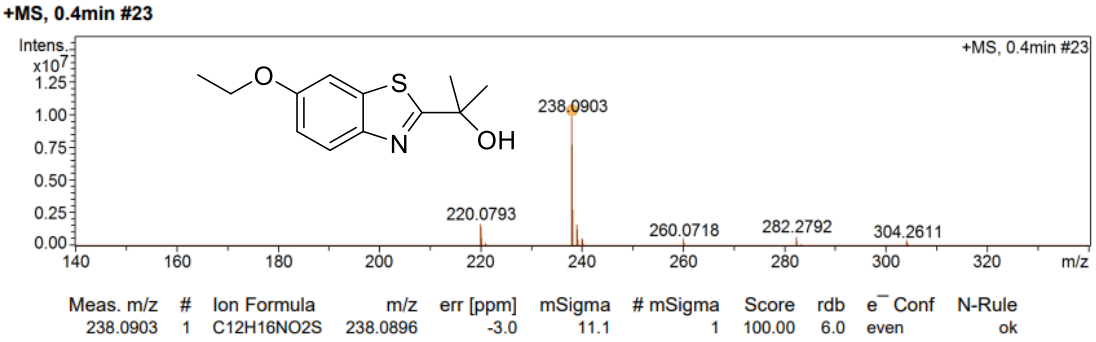
^{1}H NMR (600 MHz, $CDCl_3$) of 3a-d_6



^{13}C NMR (151 MHz, $CDCl_3$) of 3a-d_6

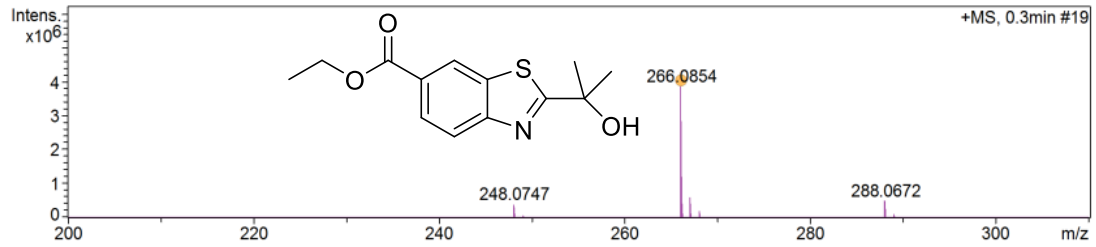


7. HRMS spectra



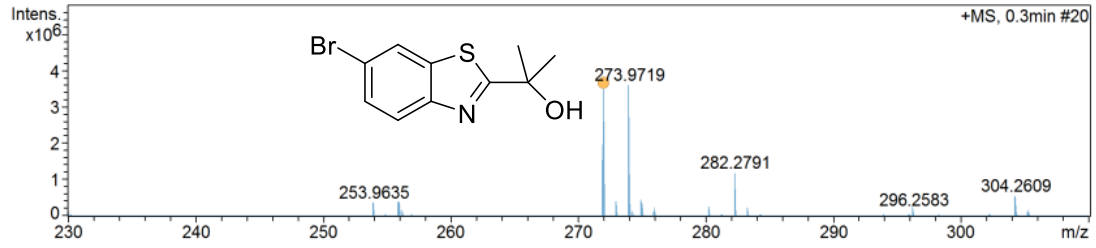
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
238.0903	1	C12H16NO2S	238.0896	-3.0	11.1	1	100.00	6.0	even	ok

HRMS spectra of 3d



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
266.0854	1	C13H16NO3S	266.0845	-3.3	4.4	1	100.00	7.0	even	ok

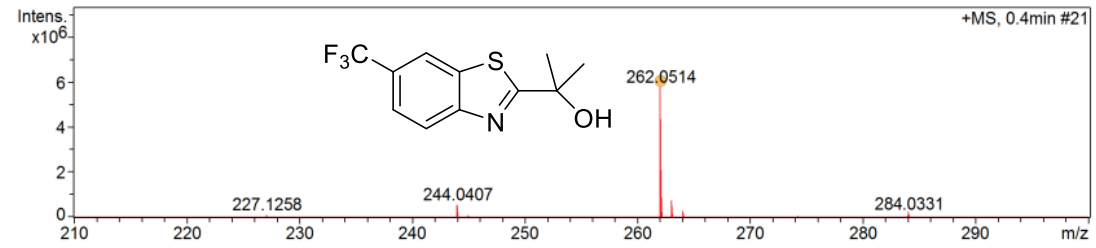
HRMS spectra of 3h



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
271.9740	1	C10H11BrNOS	271.9739	-0.5	4.3	1	100.00	6.0	even	ok

HRMS spectra of 3j

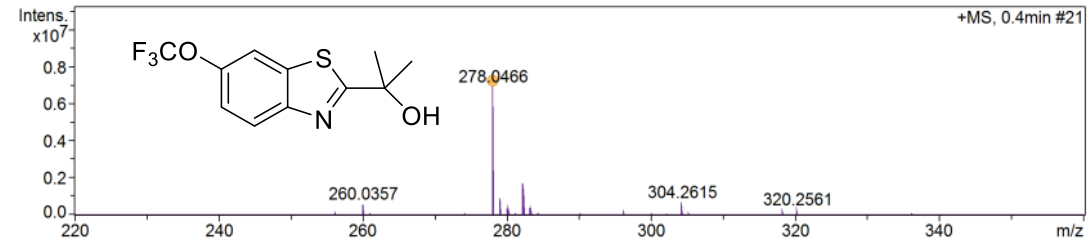
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
262.0514	1	C11H11F3NOS	262.0508	-2.4	3.5	1	100.00	6.0	even	ok

HRMS spectra of 3k

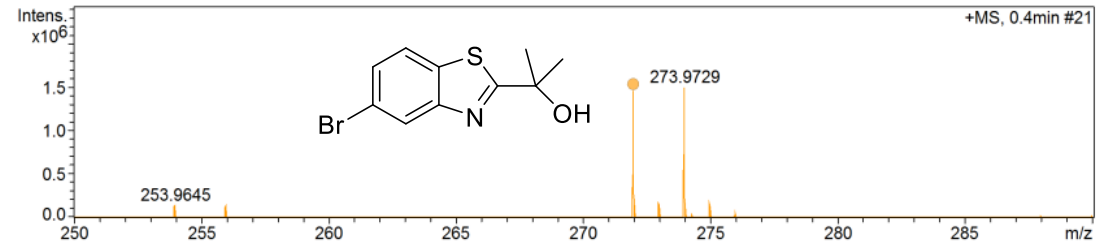
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
278.0466	1	C11H11F3NO2S	278.0457	-3.1	4.2	1	100.00	6.0	even	ok

HRMS spectra of 3i

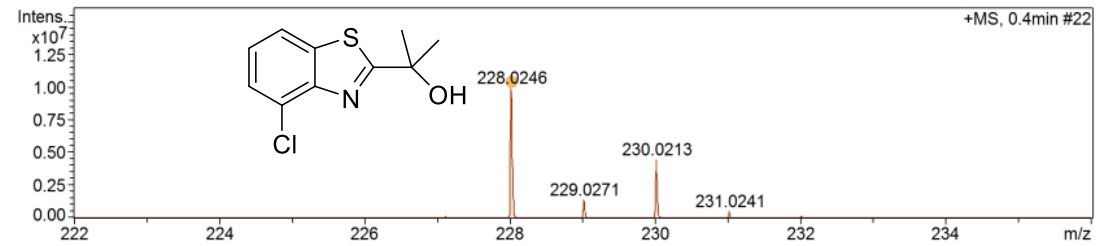
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
271.9750	1	C10H11BrNOS	271.9739	-4.1	6.5	1	100.00	6.0	even	ok

HRMS spectra of 3n

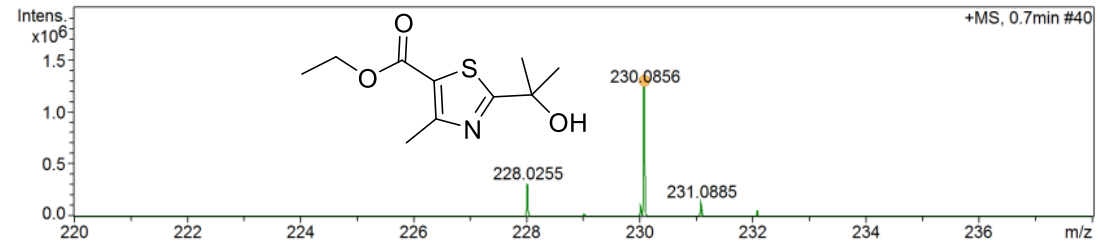
+MS, 0.4min #22



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
228.0246	1	C10H11ClNOS	228.0244	-0.8	36.3	1	100.00	6.0	even	ok

HRMS spectra of 3o

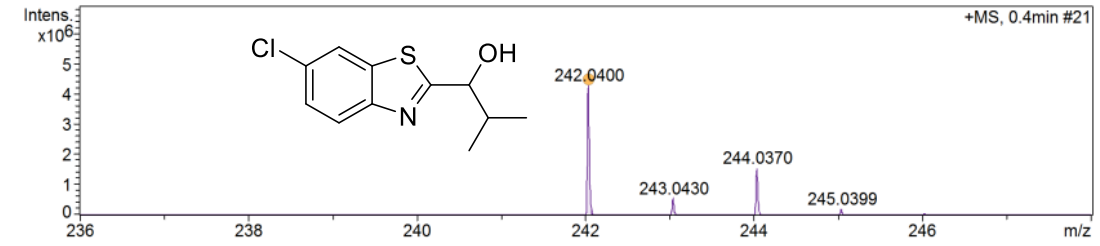
+MS, 0.7min #40



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
230.0856	1	C10H16NO3S	230.0845	-4.7	8.6	1	100.00	4.0	even	ok

HRMS spectra of 3r

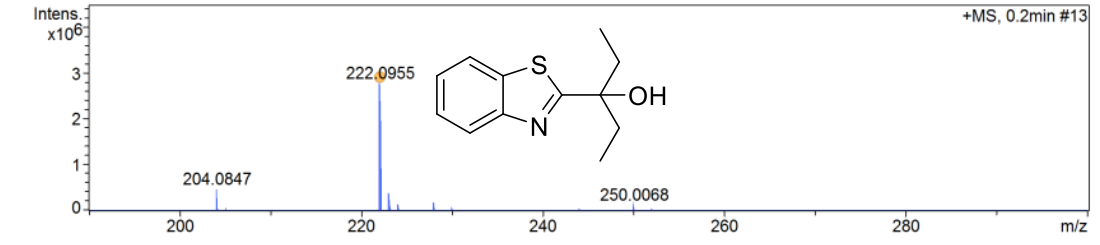
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
242.0400	1	C11H13ClNOS	242.0401	0.2	6.2	1	100.00	6.0	even	ok

HRMS spectra of 4d

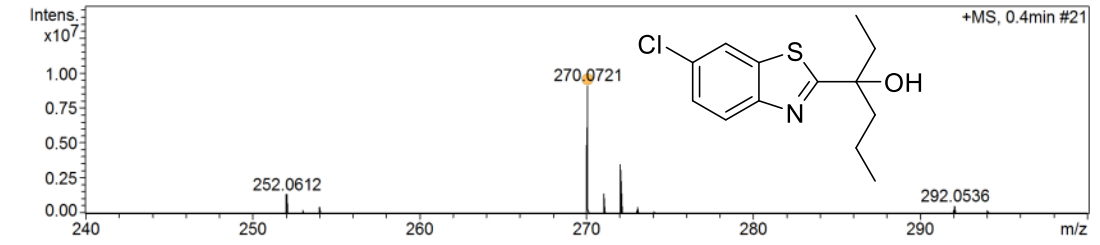
+MS, 0.2min #13



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
222.0955	1	C12H16NOS	222.0947	-3.4	4.4	1	100.00	6.0	even	ok

HRMS spectra of 4f

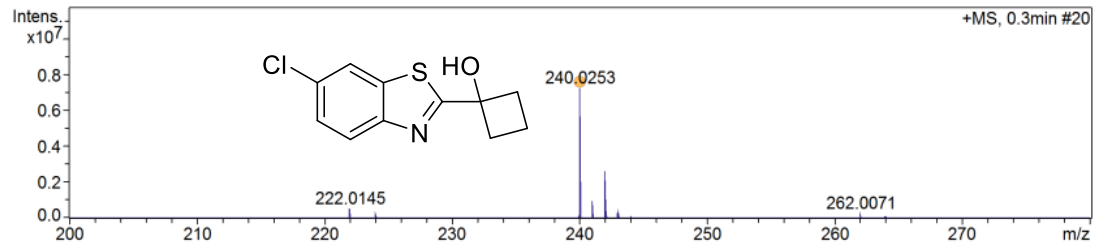
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
270.0721	1	C13H17ClNOS	270.0714	-2.6	4.9	1	100.00	6.0	even	ok

HRMS spectra of 4g

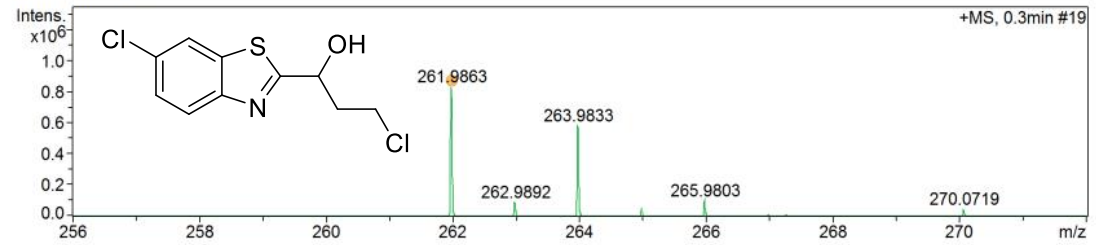
+MS, 0.3min #20



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
240.0253	1	C11H11ClNOS	240.0244	-3.5	5.9	1	100.00	7.0	even	ok

HRMS spectra of 4h

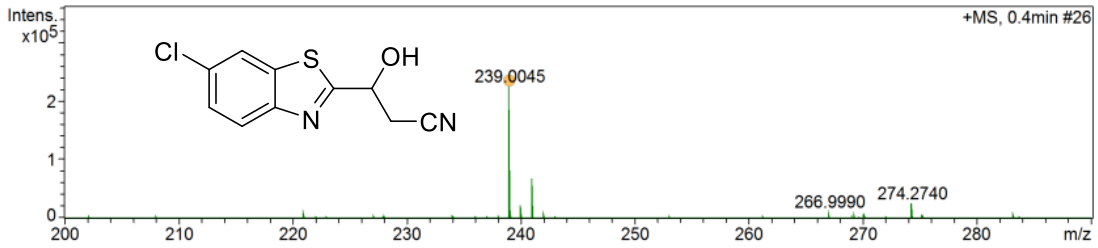
+MS, 0.3min #19



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
261.9863	1	C10H10Cl2NOS	261.9855	-3.1	10.3	1	100.00	6.0	even	ok

HRMS spectra of 4l

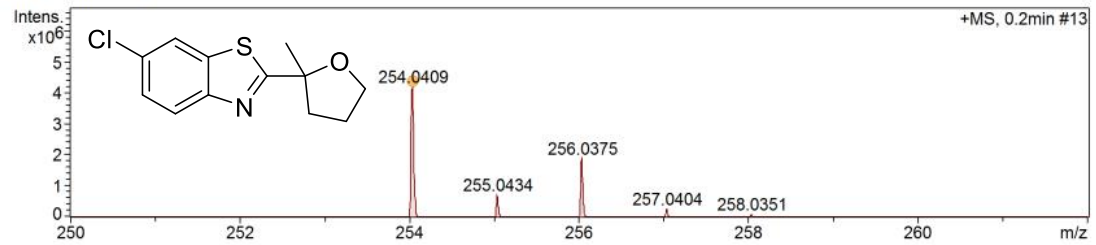
+MS, 0.4min #26



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
239.0045	1	C10H8ClN2OS	239.0040	-2.0	37.9	1	100.00	8.0	even	ok

HRMS spectra of 4m

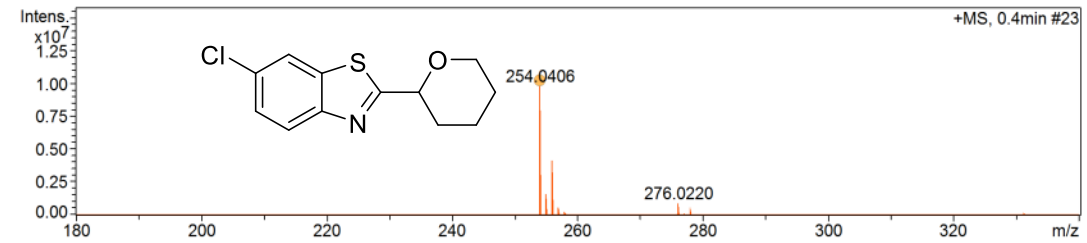
+MS, 0.2min #13



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
254.0409	1	C12H13ClNOS	254.0401	-3.2	35.6	1	100.00	7.0	even	ok

HRMS spectra of 6b

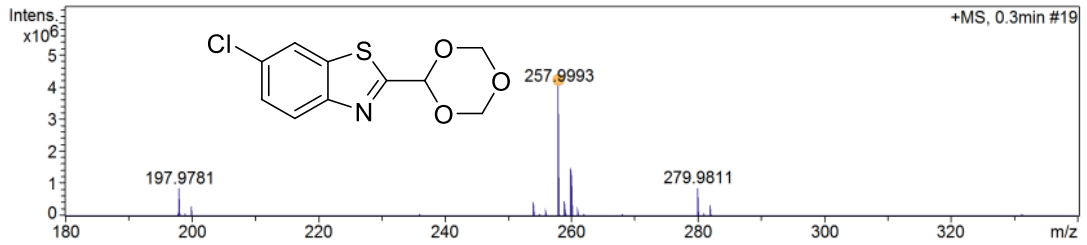
+MS, 0.4min #23



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
254.0406	1	C12H13ClNOS	254.0401	-1.9	23.5	1	100.00	7.0	even	ok

HRMS spectra of 6c

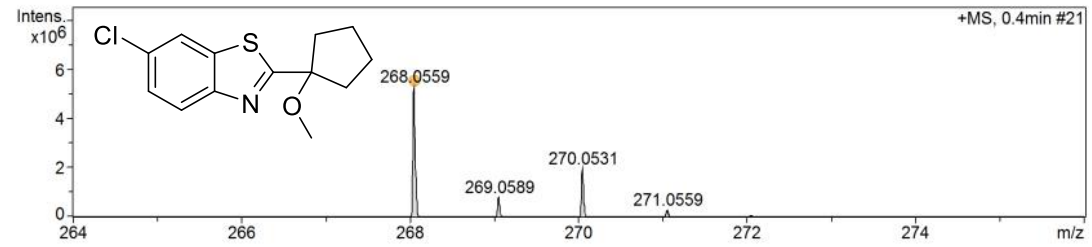
+MS, 0.3min #19



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
257.9993	1	C10H9ClNO3S	257.9986	-2.7	4.6	1	100.00	7.0	even	ok

HRMS spectra of 6f

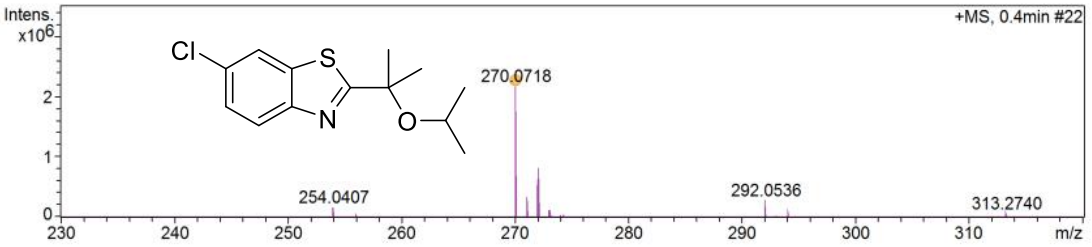
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
268.0559	1	C13H15ClNOS	268.0557	-0.7	3.6	1	100.00	7.0	even	ok

HRMS spectra of 6g

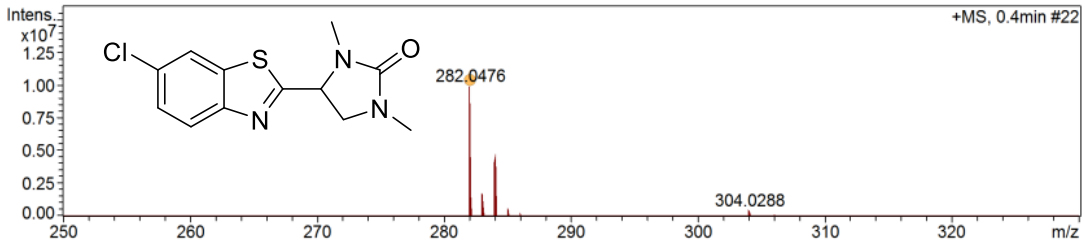
+MS, 0.4min #22



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
270.0718	1	C13H17ClNOS	270.0714	-1.6	4.2	1	100.00	6.0	even	ok

HRMS spectra of 6h

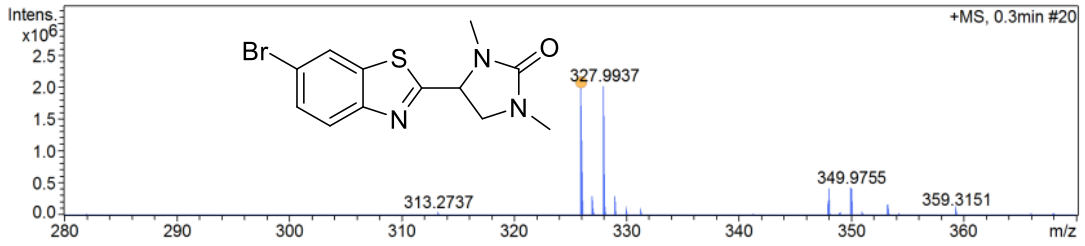
+MS, 0.4min #22



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
282.0476	1	C12H13ClN3OS	282.0462	-4.8	37.5	1	100.00	8.0	even	ok

HRMS spectra of 8a

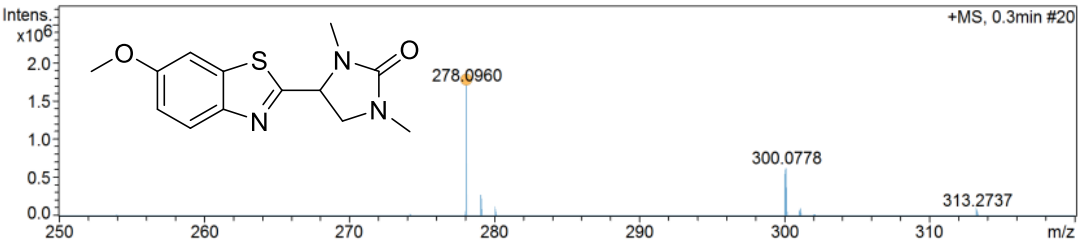
+MS, 0.3min #20



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
325.9958	1	C12H13BrN3OS	325.9957	-0.4	7.0	1	100.00	8.0	even	ok

HRMS spectra of 8b

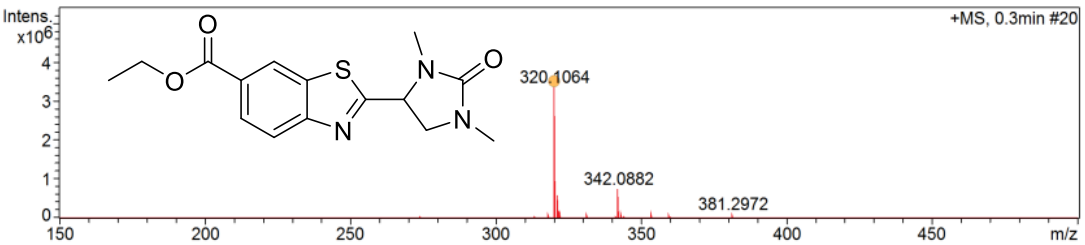
+MS, 0.3min #20



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
278.0960	1	C13H16N3O2S	278.0958	-0.8	7.3	1	100.00	8.0	even	ok

HRMS spectra of 8c

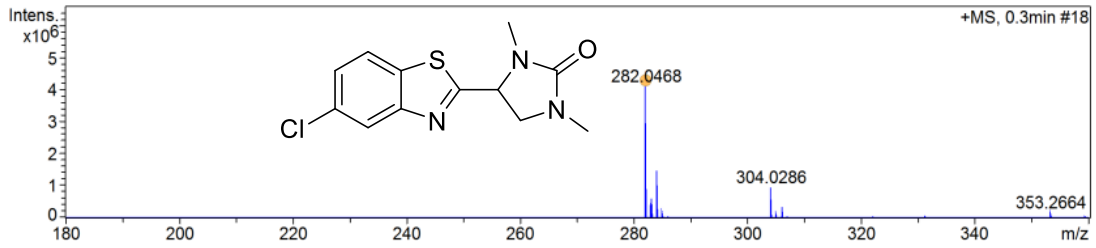
+MS, 0.3min #20



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
320.1064	1	C15H18N3O3S	320.1063	-0.2	4.4	1	100.00	9.0	even	ok

HRMS spectra of 8d

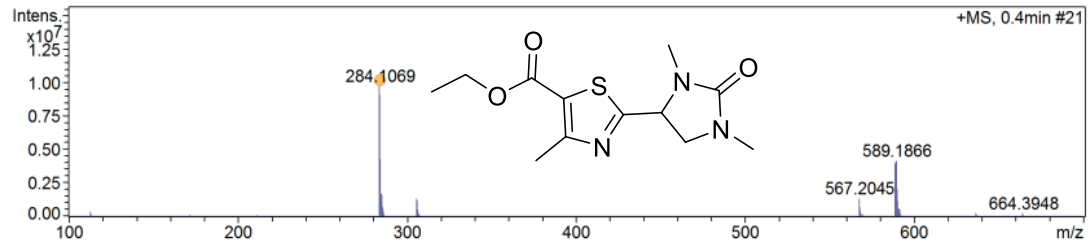
+MS, 0.3min #18



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
282.0468	1	C12H13ClN3OS	282.0462	-2.1	5.7	1	100.00	8.0	even	ok

HRMS spectra of 8e

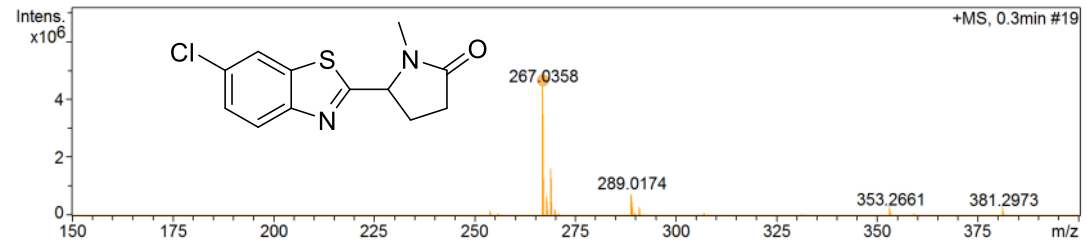
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
284.1069	1	C12H18N3O3S	284.1063	-1.8	13.3	1	100.00	6.0	even	ok

HRMS spectra of 8f

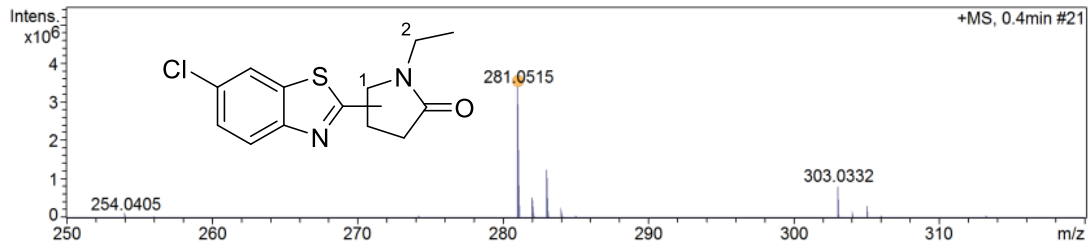
+MS, 0.3min #19



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
267.0358	1	C12H12ClN2OS	267.0353	-1.7	4.7	1	100.00	8.0	even	ok

HRMS spectra of 8g

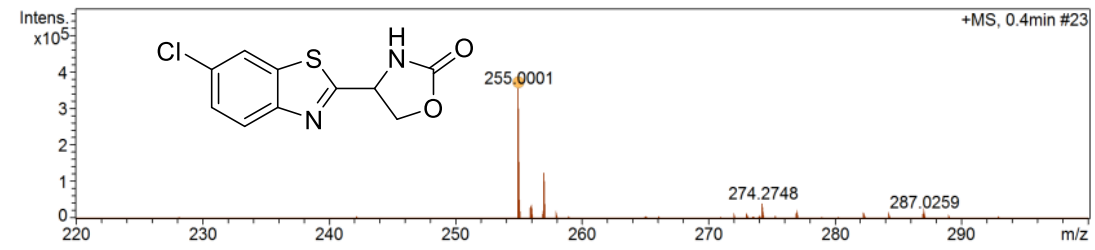
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
281.0515	1	C13H14ClN2OS	281.0510	-1.8	5.5	1	100.00	8.0	even	ok

HRMS spectra of 8h

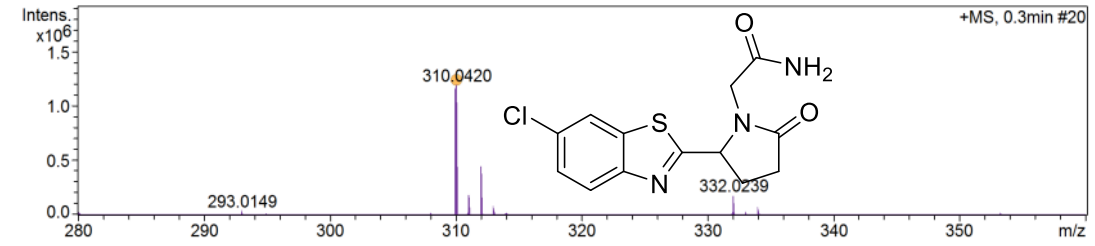
+MS, 0.4min #23



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
255.0001	1	C10H8ClN2O2S	254.9990	-4.6	18.3	1	100.00	8.0	even	ok

HRMS spectra of 8i

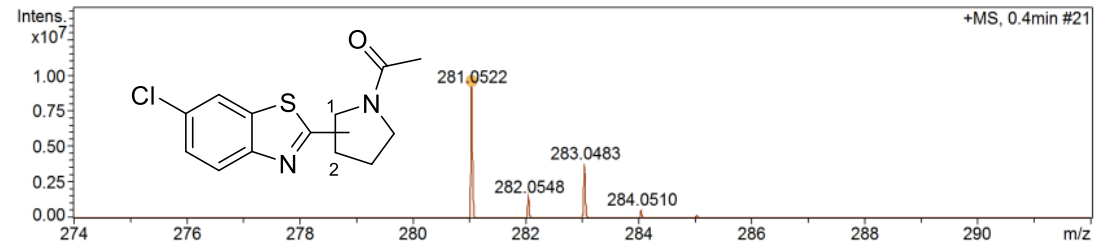
+MS, 0.3min #20



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
310.0420	1	C13H13ClN3O2S	310.0412	-2.9	7.9	1	100.00	9.0	even	ok

HRMS spectra of 8j

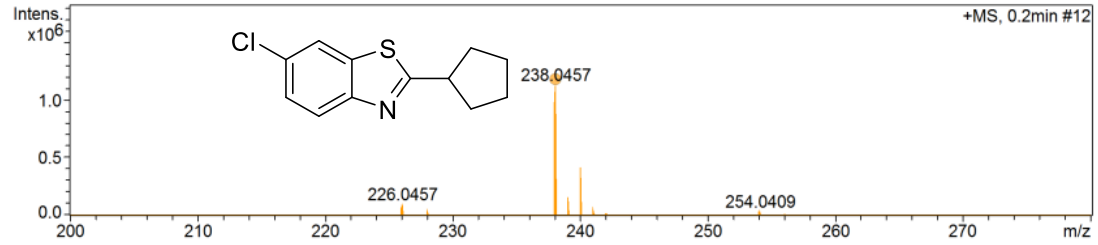
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
281.0522	1	C13H14ClN2OS	281.0510	-4.4	17.6	2	100.00	8.0	even	ok

HRMS spectra of 8k

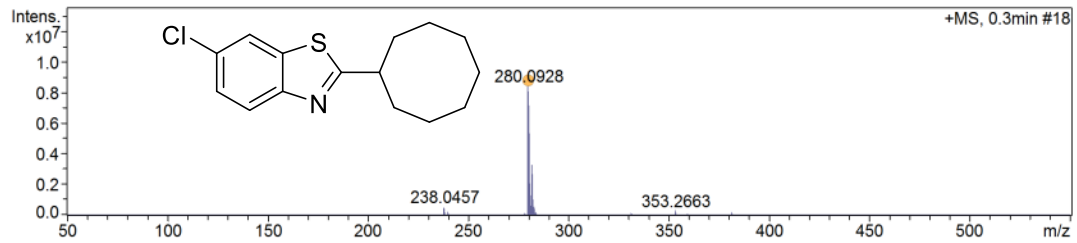
+MS, 0.2min #12



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
238.0457	1	C12H13ClNS	238.0452	-2.3	2.9	1	100.00	7.0	even	ok

HRMS spectra of 10a

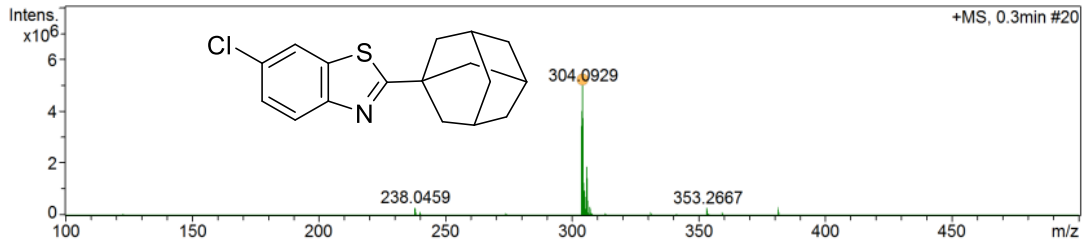
+MS, 0.3min #18



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
280.0928	1	C15H19ClNS	280.0921	-2.5	9.2	1	100.00	7.0	even	ok

HRMS spectra of 10c

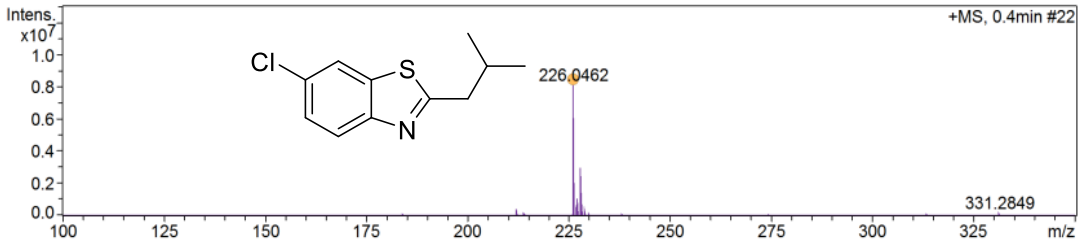
+MS, 0.3min #20



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
304.0929	1	C17H19ClNS	304.0921	-2.6	4.2	1	100.00	9.0	even	ok

HRMS spectra of 10d

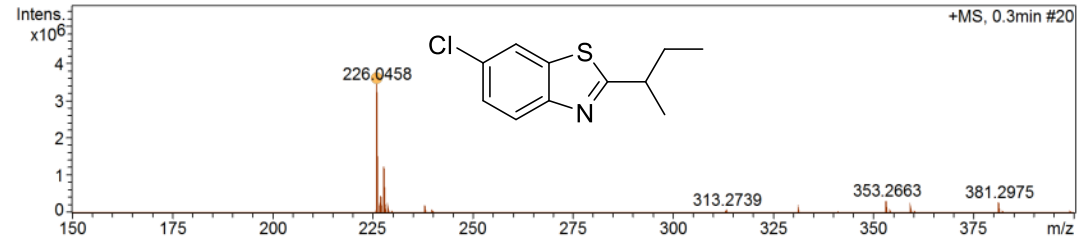
+MS, 0.4min #22



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
226.0462	1	C11H13ClNS	226.0452	-4.7	2.0	1	100.00	6.0	even	ok

HRMS spectra of 11e

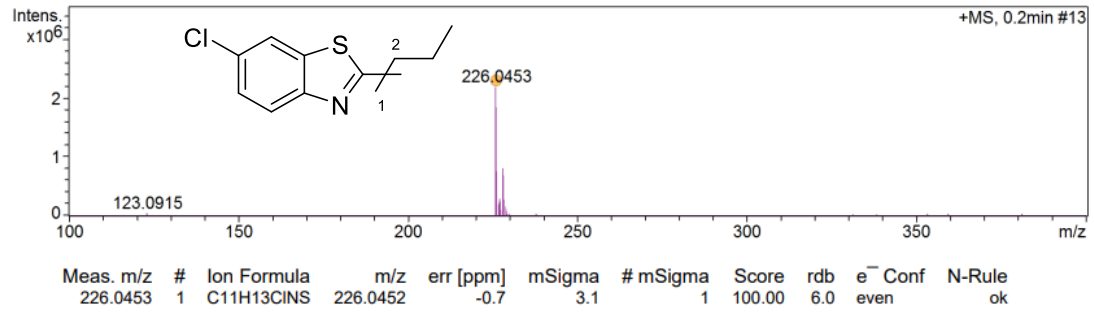
+MS, 0.3min #20



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
226.0458	1	C11H13ClNS	226.0452	-2.6	6.5	1	100.00	6.0	even	ok

HRMS spectra of 11g

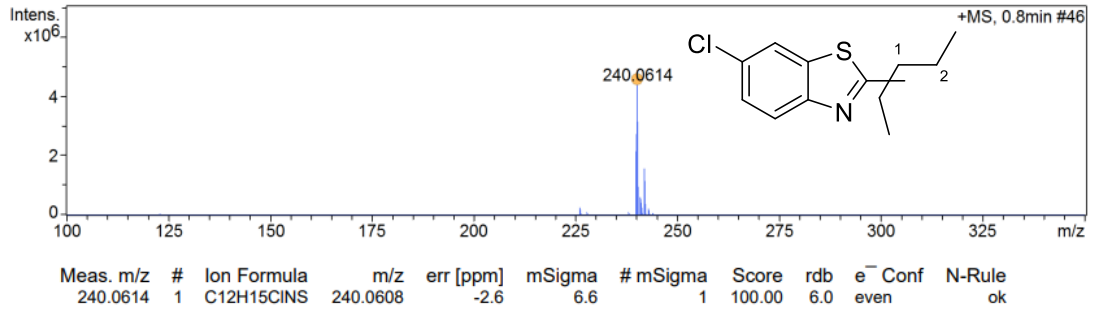
+MS, 0.2min #13



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
226.0453	1	C11H13ClNS	226.0452	-0.7	3.1	1	100.00	6.0	even	ok

HRMS spectra of 11i and 11i′

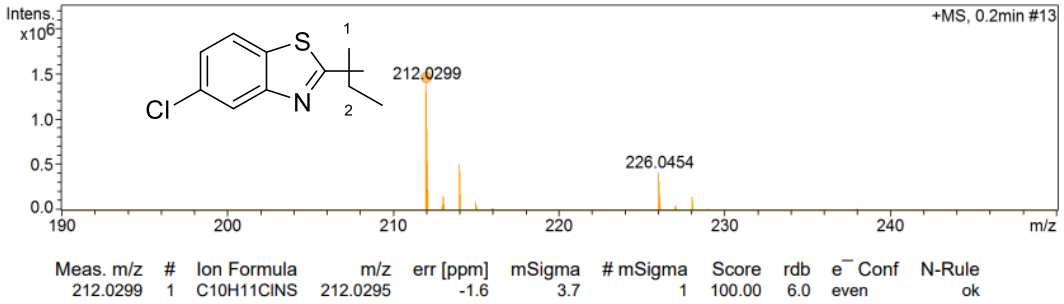
+MS, 0.8min #46



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
240.0614	1	C12H15ClNS	240.0608	-2.6	6.6	1	100.00	6.0	even	ok

HRMS spectra of 11j and 11j′

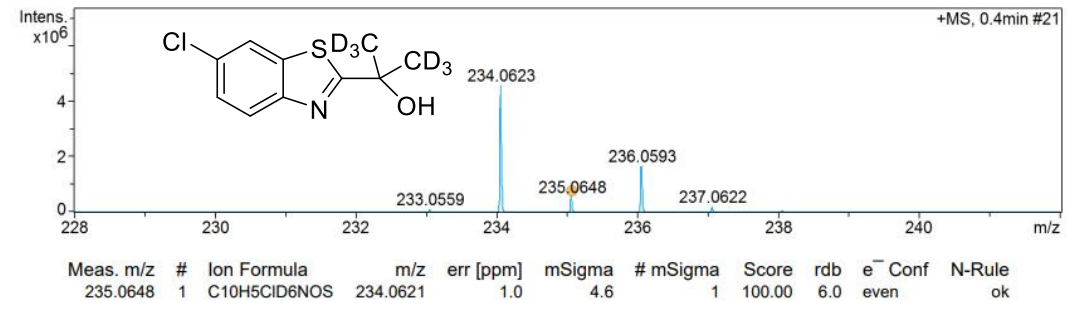
+MS, 0.2min #13



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
212.0299	1	C10H11ClNS	212.0295	-1.6	3.7	1	100.00	6.0	even	ok

HRMS spectra of 11k and 11k′

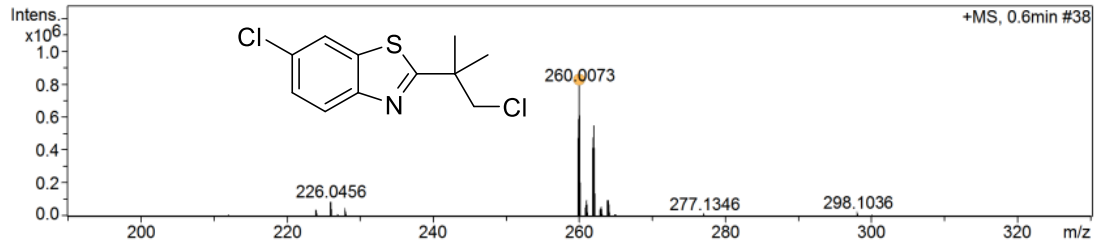
+MS, 0.4min #21



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
235.0648	1	C10H5ClD6NOS	234.0621	1.0	4.6	1	100.00	6.0	even	ok

HRMS spectra of 3a-d$_6$

+MS, 0.6min #38



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
260.0073	1	C11H12Cl2NS	260.0062	-4.4	9.0	1	100.00	6.0	even	ok

HRMS spectra of 16