
Supplementary information

Enantioselective aza-Mislow-Evans rearrangement through S -allenylation of sulfenamides with alkynyl carbenes

Bin Wei, Yue Shi, Jiangtao Wang, Wenjie Zhang, Jichao Xiao, Ruijie Mi, Xihe Bi, Genping Huang, Xingwei Li

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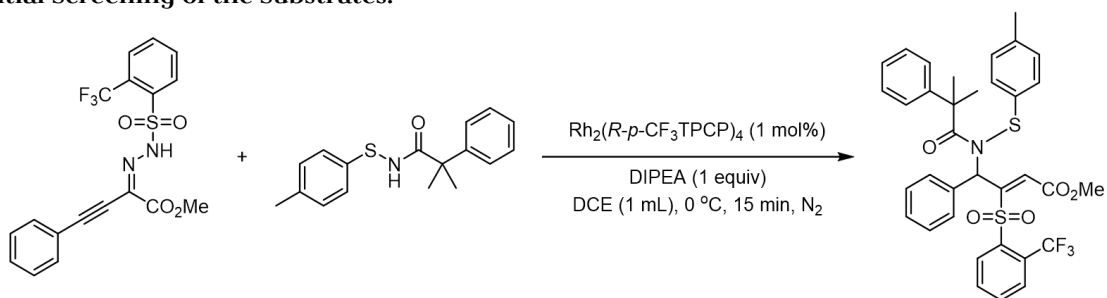
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1. General Information

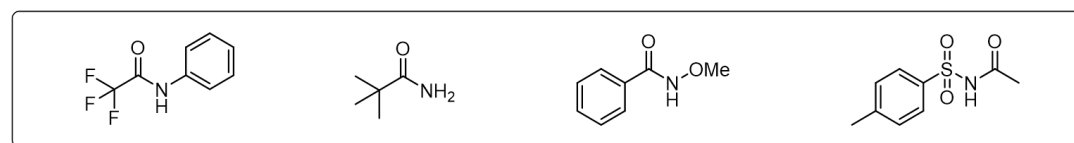
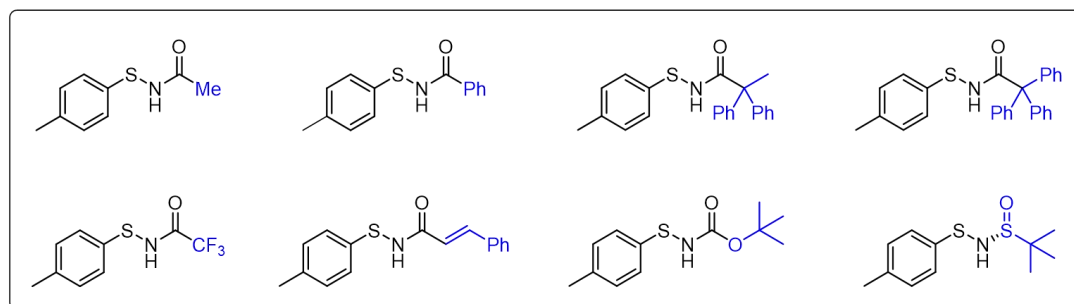
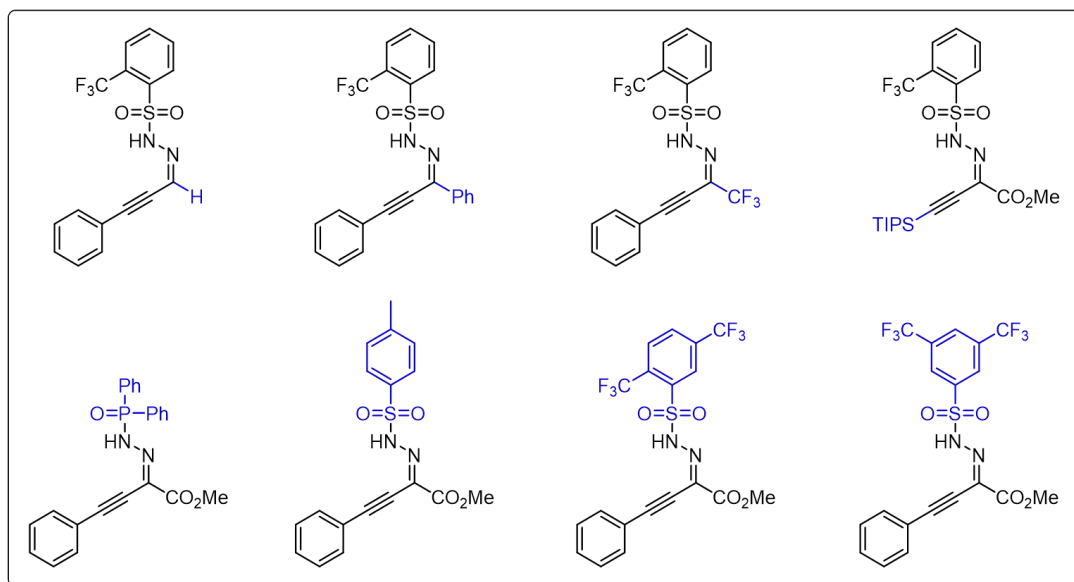
Commercially available chemicals were obtained from Adamas, Acros Organics, Aldrich Chemical Co., Alfa Aesar and TCI and were used as received unless otherwise stated. Anhydrous solvent, purchased from Adamas, Acros Organics and J&K Chemical, were used as received. All reactions were carried out using schlenk tube at N₂ atmosphere unless stated otherwise. NMR Spectra were recorded on a 400 or 600 MHz NMR spectrometer in the solvent indicated. The chemical shift is given in dimensionless δ values and is frequency referenced relative to TMS in ¹H and ¹³C NMR spectroscopy. HRMS data were obtained on a Thermo Scientific LTQ Orbitrap Discovery spectrometer (Bremen, Germany). Column chromatography was performed on silica gel (200-300 mesh) using ethyl acetate/hexanes. The enantiomeric excess (e.e.) of the products were determined by high-performance liquid chromatography (HPLC) with a chiral stationary phase in comparison with the authenticated racemate. All the chiral stationary phases including Chiralcel AD-3, OD-3, IC, AS-H and OJ-H used were purchased from Daicel Chiral Technologies. Optical rotations were reported as follows: $[\alpha]_D^{25}$ = (c: g/100 mL, in CHCl₃). Chiral rhodium catalysts¹, Ar₂SO₂NHNH₂², 2-oxo-3-butynoates³, thiosuccinimide⁴ and sulfenamide⁵ were prepared according to published procedures.

2. Optimization Studies

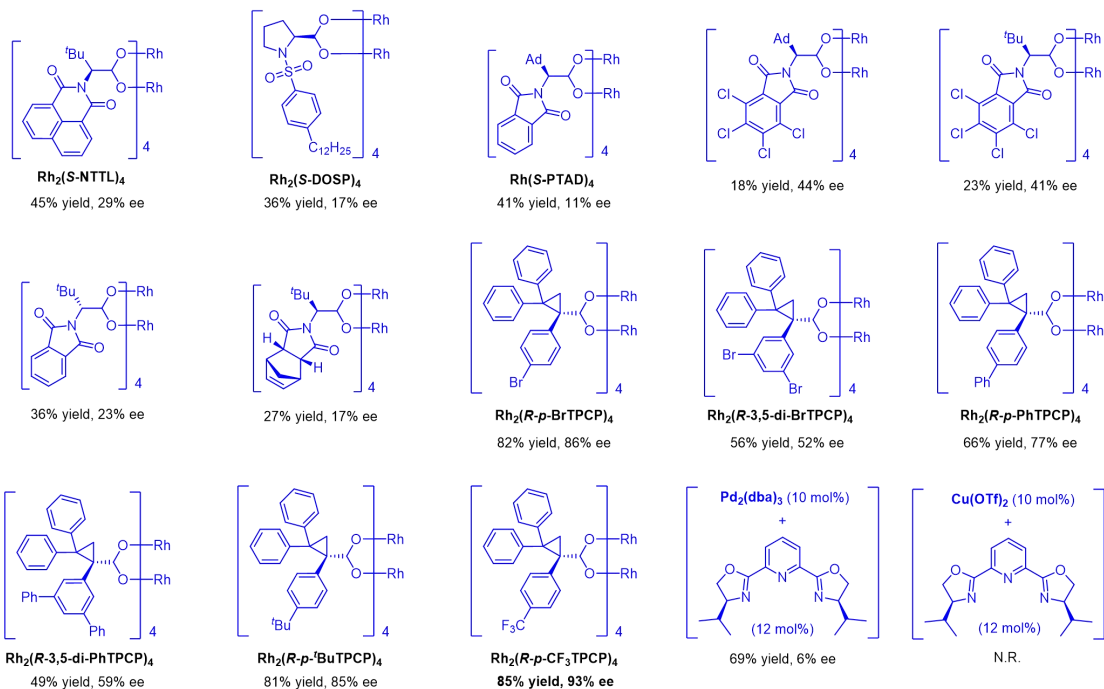
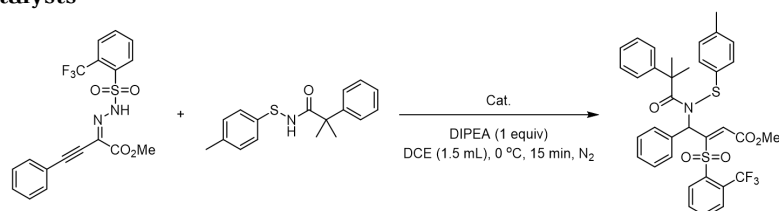
2.1 Initial Screening of the Substrates.



The substrates given below had no reactivity:

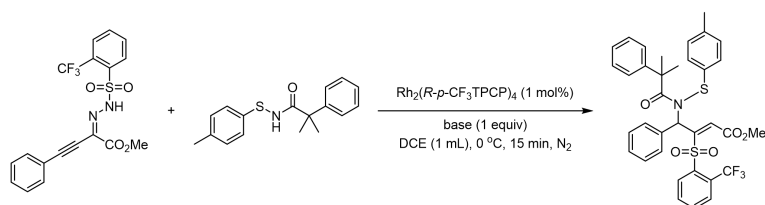


2.2 Screening of catalysts



Reaction conditions: **2a** (0.15 mmol), **1a** (1.25 equiv), DIPEA (1 equiv), and a dimeric rhodium catalyst (1 mol %) in DCE (1.5 mL) at 0 °C for 15 min, N₂ atmosphere.

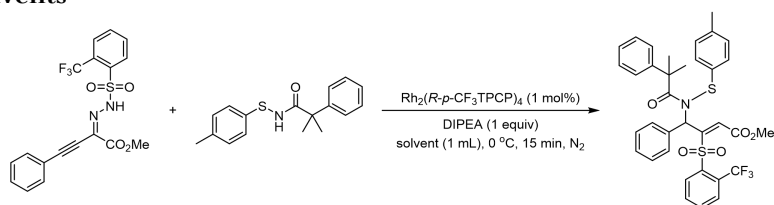
2.3 Screening of bases



Entry	Base	Yield (%)	Ee (%)
1	4-cyclohexylmorpholine	80	87
2	DIPEA	85	93
3	CyNEt ₂	61	85
4	2,6-lutidine	18	66
5	DMAP	trace	n.d.
6	NaH	< 3	n.d.
7	LiO ^t Bu	trace	n.d.
8	KOAc	48	53
9	K ₃ PO ₄	37	53

Reaction conditions: **2a** (0.15 mmol), **1a** (1.25 equiv), base (1 equiv), and Rh₂(R-p-CF₃TPCP)₄ (1 mol%) in DCE (1.5 mL) at 0 °C for 15 min, N₂ atmosphere.

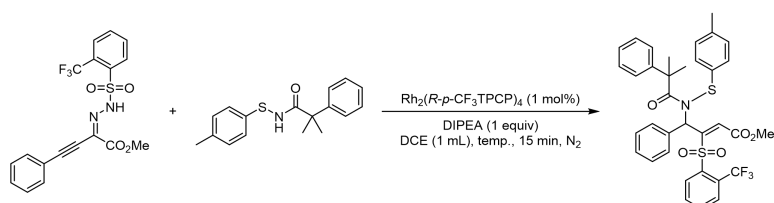
2.4 Screening of solvents



Entry	solvent	Yield (%)	Ee (%)
1	DCM	80	90
2	CHCl ₃	32	80
3	CCl ₄	44	75
4	TCE	20	80
5	Tol	75	78
6	PhCl	78	79
7	PhCF ₃	69	80

Reaction conditions: **2a** (0.15 mmol), **1a** (1.25 equiv), DIPEA (1 equiv), and Rh₂(R-p-CF₃TPCP)₄ (1 mol%) in solvent (1.5 mL) at 0 °C for 15 min, N₂ atmosphere.

2.5 Screening of temperature

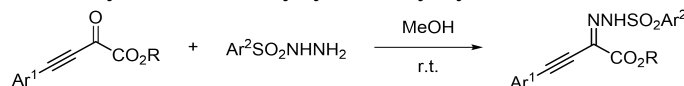


Entry	Temp.	Yield (%)	Ee (%)
1	-20 °C	34	94
2	-10 °C	56	91
3	20 °C	82	89

Reaction conditions: **2a** (0.15 mmol), **1a** (1.25 equiv), DIPEA (1 equiv), and Rh₂(R-p-CF₃TPCP)₄ (1 mol%) in DCE (1.5 mL) at a specific temperature for 15 min under N₂ atmosphere.

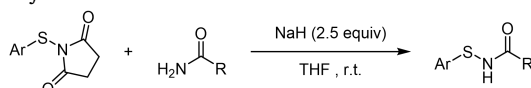
3. General Procedure and Characterization of Products

3.1 General Procedure for the Synthesis of alkynyl sulfonylhydrazones



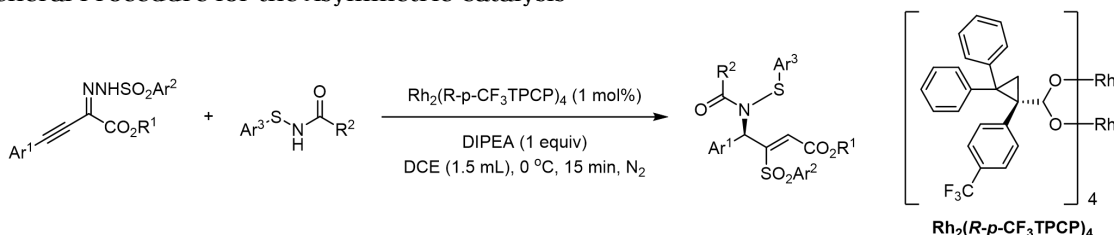
To a stirred solution of $\text{ArSO}_2\text{NHNH}_2$ (2.0 mmol, 1.0 equiv) in methanol (2 mL) was added carbonyl compound (2.2 mmol, 1.1 equiv), and the mixture was stirred for 1–12 h at room temperature. If the hydrazone precipitated, the mixture was filtered and the resulting solid was washed with ice cold diethyl ether and dried under reduced pressure to give pure alkynyl sulfonylhydrazones. If not, the solvent was removed in vacuo and the residue was purified by flash chromatography on silica gel to obtain the alkynyl sulfonylhydrazone. The yields were around 80% in general.

3.2 General Procedure for the Synthesis of Sulfenamides^{4,5}



To a 2-neck round bottom flask under nitrogen with a stir bar was added the amine (1 mmol, 1.0 equiv). THF (0.15 M) was added and the solution was cooled to 0 °C. NaH (2.5 equiv) was added, then the solution was warmed to room temperature and stirred for 30 minutes. The flask was charged with a solution of the indicated thiosuccinimide (1 mmol, 1.0 equiv) in THF (0.3 M), which was added dropwise over one hour. The reaction mixture was stirred at rt for 30 minutes and was then quenched with saturated aqueous ammonium chloride and extracted with ethyl acetate. The combined organic layers were washed with brine, dried over sodium sulfate, and concentrated. The crude residue was purified by the corresponding chromatographic method to afford the desired sulfenamide product.

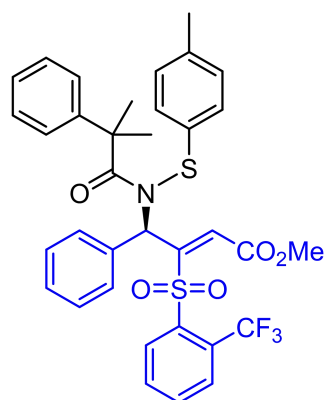
3.3 General Procedure for the Asymmetric Catalysis



Under nitrogen atmosphere, sulfenamide (0.15 mmol), $\text{Rh}_2(\text{R-}p\text{-CF}_3\text{TPCP})_4$ (1 mol%), DCE (0.5 mL), and DIPEA (1.0 equiv) were sequentially added to a screw-capped vial (8 mL) with a stir bar. Then the vial was cooled to 0 °C using ice bath. A solution of alkynyl sulfonylhydrazone (1.25 equiv) in DCE (1 mL) was added dropwise to the mixture using a syringe and stirred for 15 minutes. After the reaction completed, the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate to provide product. The enantiomeric excess was determined by chiral HPLC analysis. The corresponding racemic samples were obtained by carrying out the reactions under the identical conditions except using $\text{Rh}_2(\text{OAc})_4$ as the catalyst.

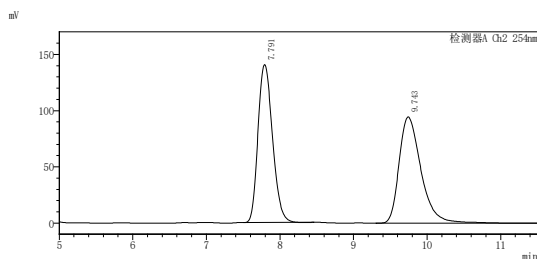
3.4 Characterization (NMR, HRMS, and HPLC) of Products

methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (3), White solid (85 mg, 85%), ^1H NMR (400 MHz, CDCl_3) δ

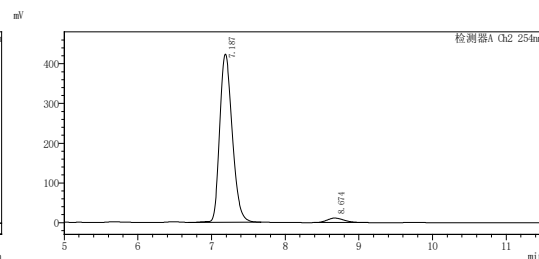


8.20 (dt, $J = 7.9, 3.8$ Hz, 1H), 7.73 (dt, $J = 7.8, 3.8$ Hz, 1H), 7.68 – 7.57(m, 2H), 7.31 (t, $J = 7.5$ Hz, 2H), 7.25 – 7.20 (m, 1H), 7.20 – 7.14 (m, 2H), 6.93 – 6.82 (m, 3H), 6.79 (t, $J = 7.5$ Hz, 2H), 6.71 (d, $J = 8.0$ Hz, 2H), 6.49 (d, $J = 6.2$ Hz, 2H), 6.35 (d, $J = 8.0$ Hz, 2H), 3.89 (s, 3H), 2.15 (s, 3H), 1.68 (s, 3H), 1.53 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.93, 164.88, 146.02, 144.60, 137.29, 135.65, 134.60, 133.79, 133.15, 131.90, 131.84, 131.36, 129.47 (q, $J = 33.9$ Hz), 128.48, 128.39, 128.36, 128.00 (q, $J = 6.3$ Hz), 127.06, 126.43, 125.65, 123.35, 122.25 (q, $J = 274.7$ Hz), 61.59, 52.64, 48.54, 31.93, 24.72, 20.70; ^{19}F NMR (376 MHz, CDCl_3) δ -56.20; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{33}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 668.1747, found 668.1745.

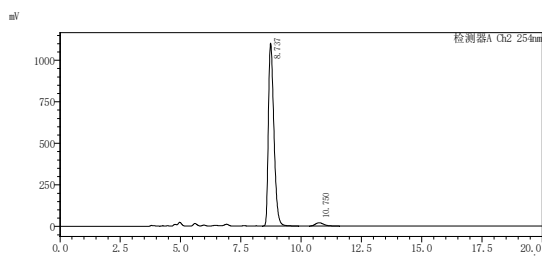
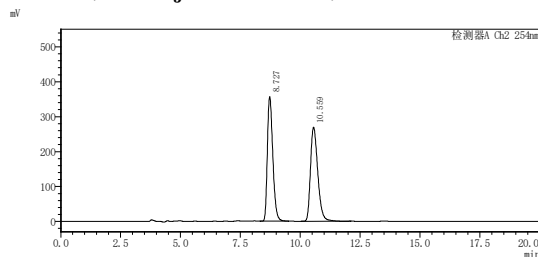
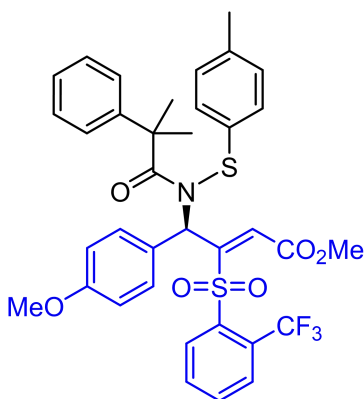
$[\alpha]_{\text{D}}^{20} = -172$ ($c = 0.1$, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.2 min, tr (minor) = 8.7 min, 93% e.e.



NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.791	1921839	49.480	1	7.187	5004572	96.475
2	9.743	1962225	50.520	2	8.674	182860	3.525

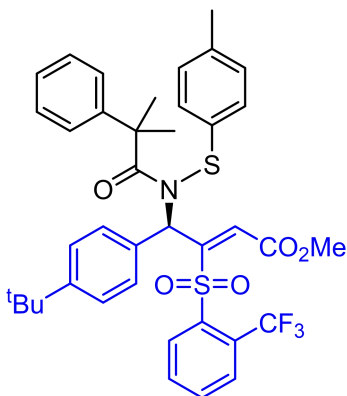


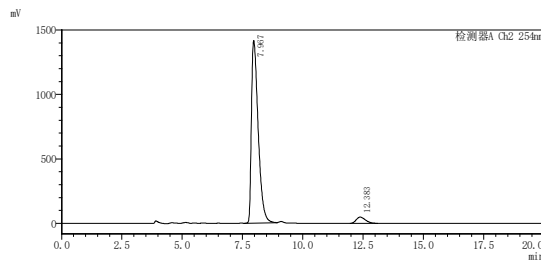
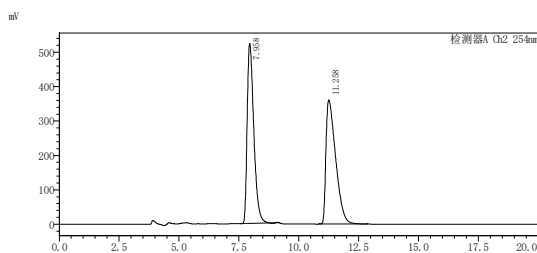
methyl (*R,Z*)-4-(4-methoxyphenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (4), White solid (91 mg, 87%), ^1H NMR (400 MHz, CDCl_3) δ 8.24 – 8.13 (m, 1H), 7.82 – 7.71 (m, 1H), 7.71 – 7.60 (m, 2H), 7.35 – 7.27 (m, 2H), 7.25 – 7.19 (m, 1H), 7.19 – 7.13 (m, 2H), 6.82 – 6.66 (m, 4H), 6.41 (d, J = 4.5 Hz, 2H), 6.38 – 6.33 (m, 2H), 6.32 – 6.24 (m, 2H), 3.89 (s, 3H), 3.56 (s, 3H), 2.15 (s, 3H), 1.70 (s, 3H), 1.51 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.89, 164.95, 159.54, 146.41, 144.69, 137.46, 135.56, 134.84, 133.70, 133.12, 132.87, 131.86, 129.51 (d, J = 33.9 Hz), 128.40, 127.99 (d, J = 6.0 Hz), 127.55, 126.45, 125.70, 125.03 (d, J = 274.7 Hz), 123.67, 123.55, 112.51, 61.01, 55.00, 52.68, 48.57, 32.22, 24.41, 20.70; ^{19}F NMR (376 MHz, CDCl_3) δ -56.21; **HRMS** (ESI-TOF). (m/z): Calcd for $\text{C}_{36}\text{H}_{35}\text{F}_3\text{NO}_6\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 698.1853, found 698.1853. $[\alpha]_{\text{D}}^{20}$ = -125 (c = 0.1, CHCl_3). **HPLC** conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); t_{r} (major) = 8.4 min, t_{r} (minor) = 10.8 min, 95% e.e.



NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	8.727	5640956	49.782	1	8.737	17477105	97.376
2	10.559	5690297	50.218	2	10.750	470938	2.624

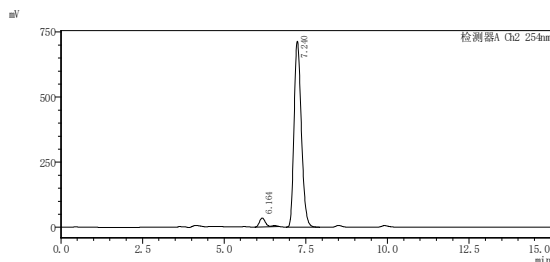
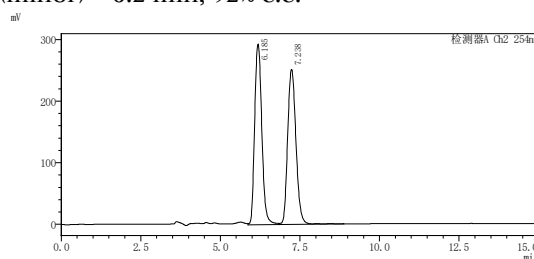
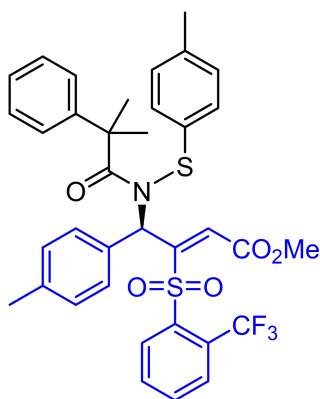
methyl (*R,Z*)-4-(4-(tert-butyl)phenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (5), White solid (96 mg, 89%), ^1H NMR (400 MHz, CDCl_3) δ 8.20 (dd, J = 7.3, 1.9 Hz, 1H), 7.68 – 7.56 (m, 3H), 7.32 (t, J = 7.5 Hz, 2H), 7.25 – 7.21 (m, 1H), 7.20 – 7.15 (m, 2H), 6.77 – 6.67 (m, 4H), 6.65 (d, J = 8.1 Hz, 2H), 6.48 (d, J = 8.3 Hz, 2H), 6.35 – 6.27 (m, 2H), 3.91 (s, 3H), 2.10 (s, 3H), 1.71 (s, 3H), 1.52 (s, 3H), 1.04 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.87, 165.01, 151.03, 146.07, 144.73, 137.32, 136.68, 135.25, 134.70, 134.66, 133.67, 133.22, 131.82, 131.37, 130.20 (q, J = 8.6 Hz), 129.48 (q, J = 33.9 Hz), 128.40, 128.31, 128.24, 127.85 (q, J = 6.2 Hz), 127.62, 126.43, 125.65, 125.58, 123.82, 123.32, 122.21 (q, J = 274.4 Hz), 60.75, 52.66, 48.54, 34.07, 32.43, 30.85, 24.13, 20.62; ^{19}F NMR (376 MHz, CDCl_3) δ -56.20; **HRMS** (ESI-TOF). (m/z): Calcd for $\text{C}_{39}\text{H}_{41}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 724.2373, found 724.2370. $[\alpha]_{\text{D}}^{20}$ = -72 (c = 0.1, CHCl_3). **HPLC** conditions: Daicel Chiralpak AS-H column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); t_{r} (major) = 7.9 min, t_{r} (minor) = 12.4 min, 91% e.e.





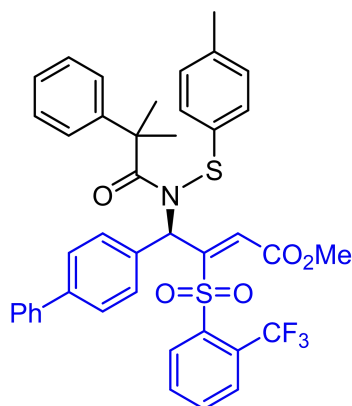
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
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2	11.258	10193737	50.346	2	12.383	1277751	4.432

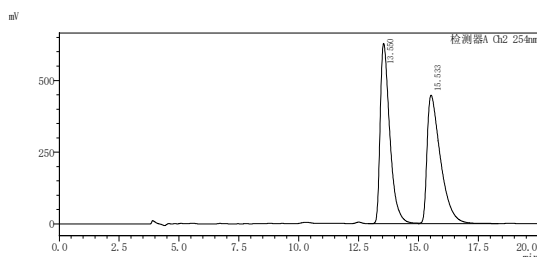
methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-(*p*-tolyl)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (6), White solid (88 mg, 86%), ^1H NMR (400 MHz, CDCl_3) δ 8.24 – 8.14 (m, 1H), 7.82 – 7.73 (m, 1H), 7.72 – 7.62 (m, 2H), 7.31 (t, J = 7.4 Hz, 2H), 7.22 (t, J = 7.3 Hz, 1H), 7.16 (d, J = 7.6 Hz, 2H), 6.78 – 6.66 (m, 4H), 6.57 (d, J = 7.8 Hz, 2H), 6.46 (s, 1H), 6.42 (s, 1H), 6.35 (d, J = 8.0 Hz, 2H), 3.88 (s, 3H), 2.16 (s, 3H), 2.03 (s, 3H), 1.69 (s, 3H), 1.51 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.94, 164.96, 146.13, 144.73, 138.31, 137.43, 135.64, 134.72, 133.66, 133.18, 131.88, 131.27, 129.59 (q, J = 33.7 Hz), 128.92, 128.42, 128.33, 128.16, 128.00 (q, J = 6.2 Hz), 127.81, 126.43, 125.69, 123.74, 122.32 (q, J = 274.3 Hz), 61.25, 52.66, 48.58, 31.99, 24.74, 20.80, 20.74; ^{19}F NMR (376 MHz, CDCl_3) δ -56.23; **HRMS** (ESI-TOF). (m/z): Calcd for $\text{C}_{36}\text{H}_{35}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 682.1904, found 682.1903. $[\alpha]_{\text{D}}^{20}$ = -42 (c = 0.1, CHCl_3). **HPLC** conditions: Daicel Chiralpak AD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.2 min, tr (minor) = 6.2 min, 92% e.e.



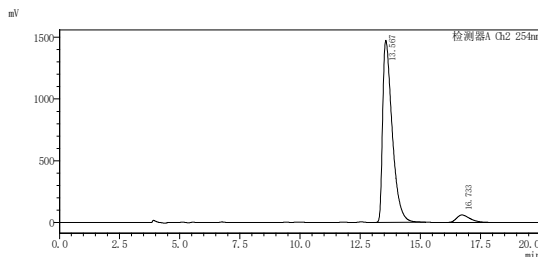
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	6.185	4601267	50.166	1	6.164	460744	3.995
2	7.238	4570897	49.834	2	7.240	11072594	96.005

methyl (*R,Z*)-4-([1,1'-biphenyl]-4-yl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (7), White solid (97 mg, 87%), ^1H NMR (400 MHz, CDCl_3) δ 8.26 – 8.16 (m, 1H), 7.75 – 7.67 (m, 1H), 7.67 – 7.58 (m, 2H), 7.38 – 7.27 (m, 5H), 7.25 – 7.20 (m, 3H), 7.19 – 7.15 (m, 2H), 6.95 – 6.83 (m, 4H), 6.65 (d, J = 8.0 Hz, 2H), 6.50 (d, J = 2.9 Hz, 2H), 6.38 – 6.29 (m, 2H), 3.89 (s, 3H), 2.08 (s, 3H), 1.72 (s, 3H), 1.51 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.88, 164.92, 145.89, 144.65, 141.24, 140.45, 137.30, 135.71, 134.57, 133.77, 133.22, 131.92, 131.86, 130.74, 129.57 (q, J = 33.7 Hz), 128.53, 128.43, 128.10, 128.00 (q, J = 6.1 Hz), 127.27, 126.91, 126.50, 125.77, 125.70, 123.82, 122.29 (q, J = 274.4 Hz), 61.02, 52.71, 48.57, 32.26, 24.41, 20.6; ^{19}F NMR (376 MHz, CDCl_3) δ -56.13; **HRMS** (ESI-TOF). (m/z): Calcd for $\text{C}_{41}\text{H}_{37}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 744.2060, found 744.2055. $[\alpha]_{\text{D}}^{20}$ = -67 (c = 0.1, CHCl_3). **HPLC** conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 13.6 min, tr (minor) = 16.7 min, 89% e.e.



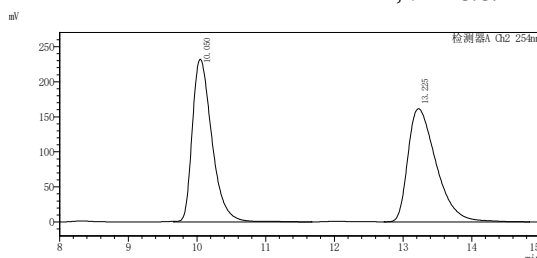


NO.	Time	Area	Area (%)
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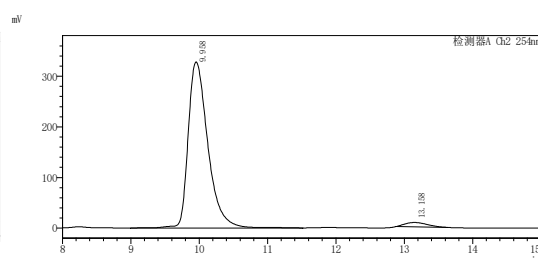


NO.	Time	Area	Area (%)
1	13.567	40591705	94.536
2	16.733	2346321	5.464

methyl (*R,Z*)-4-(4-fluorophenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (8), White solid (84 mg, 82%), ^1H NMR (400 MHz, CDCl_3) δ 8.18 – 8.08 (m, 1H), 7.73 – 7.66 (m, 1H), 7.64 – 7.56 (m, 2H), 7.23 (t, J = 7.4 Hz, 2H), 7.14 (t, J = 7.3 Hz, 1H), 7.10 – 7.05 (m, 2H), 6.82 – 6.71 (m, 2H), 6.66 (d, J = 7.9 Hz, 2H), 6.43 – 6.32 (m, 4H), 6.27 (d, J = 8.0 Hz, 2H), 3.81 (s, 3H), 2.08 (s, 3H), 1.62 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.88, 164.79, 163.74, 161.26, 146.10, 144.48, 137.32, 136.04, 134.47, 133.88, 133.37 (d, J = 8.6 Hz), 133.09, 131.96, 129.53 (q, J = 33.9 Hz), 128.50 (d, J = 13.3 Hz), 128.07 (q, J = 7.9 Hz), 127.68, 126.54, 125.69, 123.45, 122.26 (q, J = 274.4 Hz), 113.94 (d, J = 21.8 Hz), 60.75, 52.73, 48.54, 32.20, 24.35, 20.70; ^{19}F NMR (376 MHz, CDCl_3) δ -56.20, -112.88 (tt, J = 8.7, 5.2 Hz); HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{32}\text{F}_4\text{NO}_5\text{S}_2^+$, ([M + H] $^+$), 686.1653, found 686.1654. [α] $_{\text{D}}^{20}$ = -84 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 $^\circ\text{C}$, 254 nm); tr (major) = 9.9 min, tr (minor) = 13.2 min, 94% e.e.

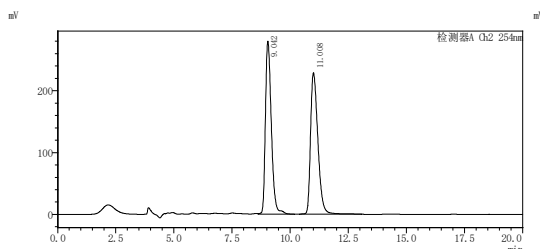


NO.	Time	Area	Area (%)
1	10.050	4594025	49.945
2	13.225	4604064	50.055

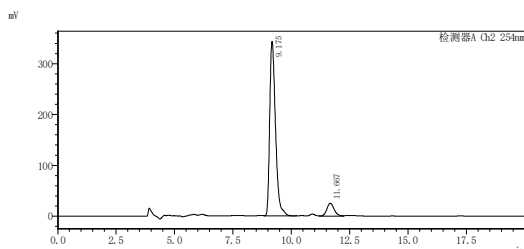


NO.	Time	Area	Area (%)
1	9.958	6554498	96.985
2	13.158	203776	3.015

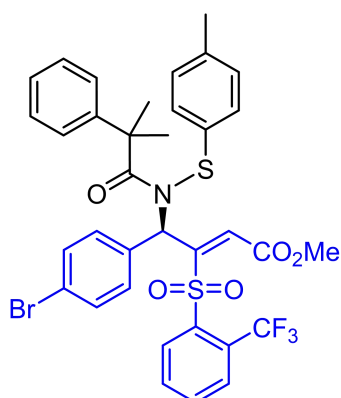
methyl (*R,Z*)-4-(4-chlorophenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (9), White solid (85 mg, 81%), ^1H NMR (400 MHz, CDCl_3) δ 8.20 (dd, J = 7.2, 2.1 Hz, 1H), 7.80 (dd, J = 7.3, 2.1 Hz, 1H), 7.75 – 7.65 (m, 2H), 7.35 – 7.29 (m, 2H), 7.26 – 7.21 (m, 1H), 7.20 – 7.13 (m, 2H), 6.82 – 6.71 (m, 6H), 6.46 (s, 1H), 6.43 (s, 1H), 6.39 – 6.32 (m, 2H), 3.90 (s, 3H), 2.19 (s, 3H), 1.72 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.85, 164.76, 145.73, 144.50, 137.29, 136.32, 134.70, 134.30, 133.90, 133.14, 132.66, 131.99, 130.57, 129.60 (q, J = 33.9 Hz), 128.61, 128.48, 128.39, 128.13 (q, J = 6.2 Hz), 127.22, 126.58, 125.72, 123.95, 122.28 (q, J = 274.5 Hz), 60.78, 52.76, 48.55, 32.16, 24.49, 20.78; ^{19}F NMR (376 MHz, CDCl_3) δ -56.20; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{32}\text{ClF}_3\text{NO}_5\text{S}_2^+$, ([M + H] $^+$), 702.1358, found 702.1353. [α] $_{\text{D}}^{20}$ = -30 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 $^\circ\text{C}$, 254 nm); tr (major) = 9.2 min, tr (minor) = 11.7 min, 93% e.e.



NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	9.042	4940821	49.665	1	9.175	5936837	91.561
2	11.008	5007555	50.335	2	11.667	547201	8.439

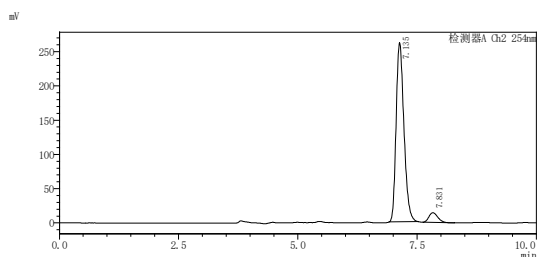
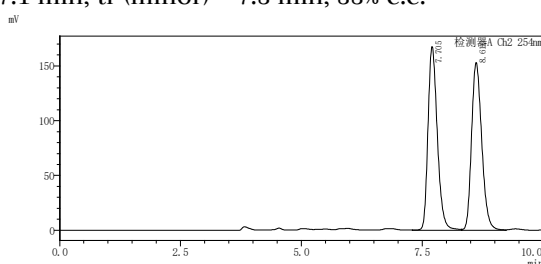


methyl (*R,Z*)-4-(4-bromophenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (10), White solid (94 mg, 84%), ^1H NMR (400 MHz, CDCl_3) δ



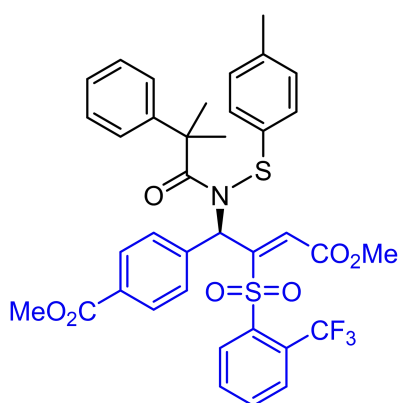
8.19 (dd, $J = 7.4, 1.8$ Hz, 1H), 7.81 (dd, $J = 7.4, 1.8$ Hz, 1H), 7.76 – 7.65 (m, 2H), 7.32 (t, $J = 7.5$ Hz, 2H), 7.26 – 7.21 (m, 1H), 7.16 (d, $J = 7.1$ Hz, 2H), 6.88 (d, $J = 8.2$ Hz, 2H), 6.80 – 6.67 (m, 4H), 6.46 (s, 1H), 6.41 (s, 1H), 6.35 (d, $J = 8.0$ Hz, 2H), 3.90 (s, 3H), 2.21 (s, 3H), 1.73 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.87, 164.77, 145.64, 144.52, 137.32, 136.41, 134.27, 133.90, 133.18, 132.92, 132.00, 131.13, 130.22, 129.65 (q, $J = 34.1$ Hz), 128.65, 128.50, 128.16 (q, $J = 6.2$ Hz), 126.60, 125.75, 124.10, 123.17, 122.29 (q, $J = 274.7$ Hz), 60.83, 52.78, 48.58, 32.18, 24.53, 20.84; ^{19}F NMR (376 MHz, CDCl_3) δ -56.21; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{32}\text{BrF}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 746.0852, found 746.0851.

$[\alpha]_{\text{D}}^{20} = -91$ (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.1 min, tr (minor) = 7.8 min, 88% e.e.

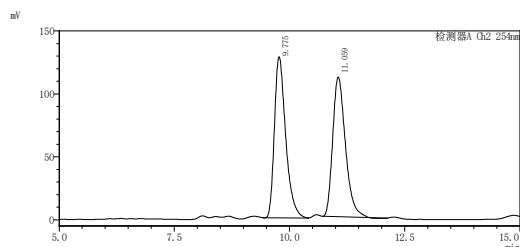


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.705	2261420	50.013	1	7.135	2982772	94.230
2	8.616	2260203	49.987	2	7.831	182630	5.770

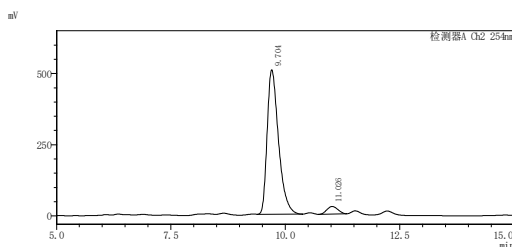
methyl (*R,Z*)-4-(4-methoxy-1-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-oxo-2-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-en-1-yl)benzoate (11), White solid (65 mg, 60%), ^1H NMR (400 MHz, CDCl_3) δ



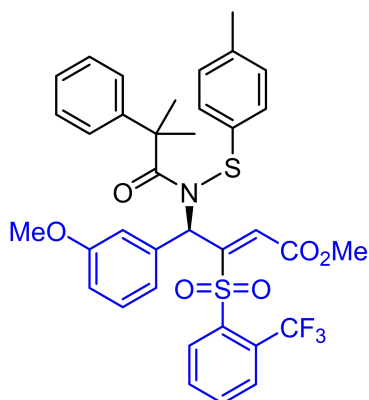
8.17 – 8.10 (m, 1H), 7.75 – 7.69 (m, 1H), 7.66 – 7.59 (m, 2H), 7.39 (d, $J = 8.2$ Hz, 2H), 7.25 (t, $J = 7.5$ Hz, 2H), 7.18 – 7.14 (m, 1H), 7.11 – 7.05 (m, 2H), 6.88 (d, $J = 8.0$ Hz, 2H), 6.63 (d, $J = 8.0$ Hz, 2H), 6.45 (s, 1H), 6.42 (s, 1H), 6.28 (d, $J = 8.2$ Hz, 2H), 3.82 (s, 3H), 3.76 (s, 3H), 2.07 (s, 3H), 1.63 (s, 3H), 1.44 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.97, 166.35, 164.79, 145.45, 144.54, 137.31, 136.40, 134.20, 134.01, 133.27, 132.10, 131.22, 129.94, 129.26, 128.73, 128.57, 128.40, 128.22 (d, $J = 6.1$ Hz), 126.65, 125.77, 124.18, 61.37, 52.82, 52.08, 48.63, 31.93, 24.93, 20.78; ^{19}F NMR (376 MHz, CDCl_3) δ -56.23; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{37}\text{H}_{35}\text{F}_3\text{NO}_7\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 726.1802, found 726.1797. $[\alpha]_{\text{D}}^{20} = -75$ (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 9.7 min, tr (minor) = 11.0 min, 90% e.e.



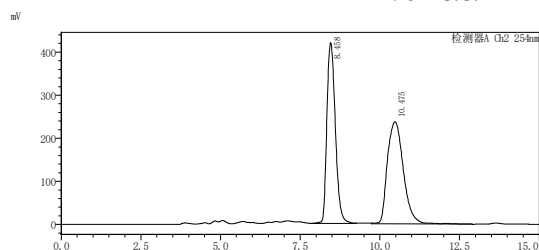
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	9.775	2180000	50.627	1	9.704	8789793	95.147
2	11.059	2126033	49.373	2	11.026	448278	4.853



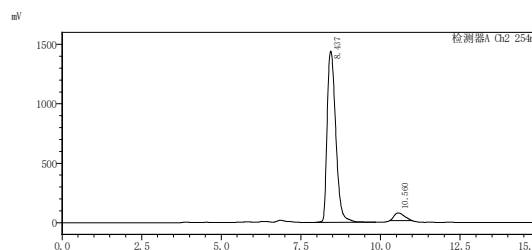
methyl (*R,Z*)-4-(3-methoxyphenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (12), White solid (77 mg, 74%), ¹H NMR (400 MHz, CDCl₃) δ



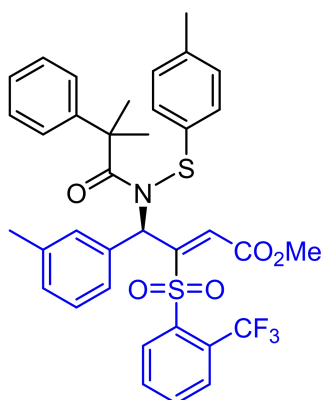
8.27 – 8.20 (m, 1H), 7.76 – 7.76 (m, 1H), 7.68 – 7.62 (m, 2H), 7.33 – 7.28 (m, 2H), 7.25 – 7.20 (m, 1H), 7.20 – 7.15 (m, 2H), 6.77 – 6.70 (m, 3H), 6.53 – 6.47 (m, 2H), 6.46 (s, 1H), 6.43 – 6.36 (m, 3H), 6.30 (t, *J* = 2.1 Hz, 1H), 3.88 (s, 3H), 3.51 (s, 3H), 2.15 (s, 3H), 1.71 (s, 3H), 1.53 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 180.97, 164.92, 158.31, 145.82, 144.66, 137.36, 135.80, 134.58, 133.75, 133.42, 133.27, 131.90, 129.54 (q, *J* = 34.0 Hz), 128.68, 128.48, 128.43, 128.18, 128.00 (q, *J* = 6.2 Hz), 126.48, 125.72, 123.82, 122.30 (q, *J* = 274.4 Hz), 116.87, 114.21, 61.43, 54.83, 52.68, 48.61, 31.91, 24.92, 20.75; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.19; HRMS (ESI-TOF). (*m/z*): Calcd for C₃₆H₃₅F₃NO₆S₂⁺, ([*M* + *H*]⁺), 698.1852, found 698.1855. [α]_D²⁰ = -79 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 8.4 min, tr (minor) = 10.6 min, 90% e.e.



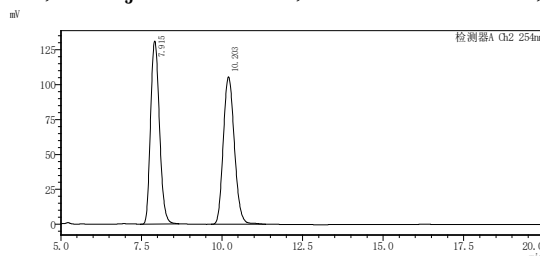
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	8.458	7763928	48.445	1	8.437	27146251	94.995
2	10.475	8262475	51.555	2	10.560	1430201	5.005

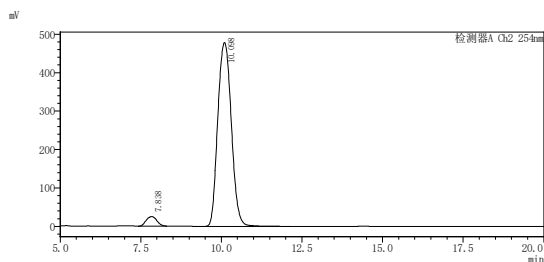


methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-(*m*-tolyl)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (13), White solid (79 mg, 77%), ¹H NMR (400 MHz, CDCl₃) δ



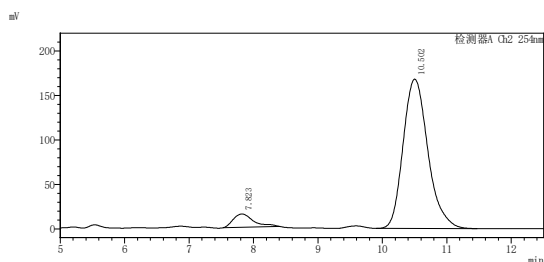
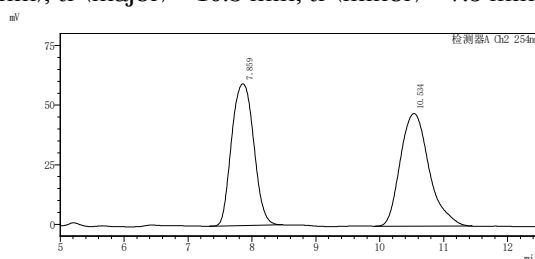
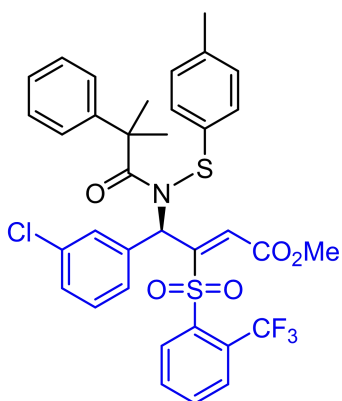
8.25 – 8.19 (m, 1H), 7.72 – 7.68 (m, 1H), 7.67 – 7.60 (m, 2H), 7.33 – 7.28 (m, 2H), 7.25 – 7.20 (m, 1H), 7.19 – 7.15 (m, 2H), 6.73 (s, 1H), 6.72 – 6.66 (m, 3H), 6.64 – 6.60 (m, 1H), 6.51 – 6.46 (m, 2H), 6.45 (s, 1H), 6.41 – 6.35 (m, 2H), 3.89 (s, 3H), 2.15 (s, 3H), 1.92 (s, 3H), 1.71 (s, 3H), 1.53 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 180.89, 164.97, 145.94, 144.68, 137.40, 136.44, 135.65, 134.63, 133.65, 133.21, 132.30, 131.79, 131.63, 129.49 (q, *J* = 33.8 Hz), 128.94, 128.40, 128.37, 128.34, 127.92 (q, *J* = 6.3 Hz), 127.07, 126.45, 125.72, 123.75, 122.26 (q, *J* = 274.2 Hz), 61.49, 52.66, 48.57, 31.99, 24.77, 20.75, 20.71; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.25; HRMS (ESI-TOF). (*m/z*): Calcd for C₃₆H₃₅F₃NO₅S₂⁺, ([*M* + *H*]⁺), 682.1903, found 682.1903. [α]_D²⁰ = -21 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 10.0 min, tr (minor) = 7.8 min, 92% e.e.





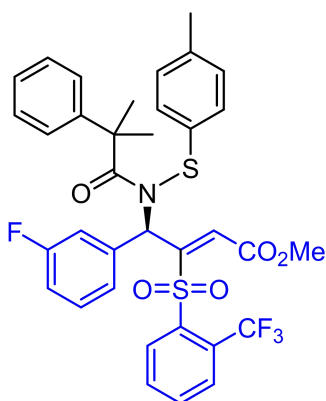
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.915	2517634	49.847	1	7.838	570286	3.923
2	10.203	2533087	50.153	2	10.098	13967257	96.077

methyl (*R,Z*)-4-(3-chlorophenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (14), White solid (65 mg, 62%), ^1H NMR (400 MHz, CDCl_3) δ 8.20 – 8.12 (m, 1H), 7.70 – 7.66 (m, 1H), 7.62 (td, J = 6.9, 5.7, 3.8 Hz, 2H), 7.25 (t, J = 7.5 Hz, 2H), 7.16 (t, J = 7.2 Hz, 1H), 7.09 (d, J = 7.6 Hz, 2H), 6.78 (d, J = 7.6 Hz, 1H), 6.74 – 6.66 (m, 4H), 6.59 (s, 1H), 6.40 (s, 1H), 6.35 (s, 1H), 6.31 (d, J = 8.0 Hz, 2H), 3.84 (s, 3H), 2.10 (s, 3H), 1.65 (s, 3H), 1.44 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.85, 164.80, 145.42, 144.51, 137.22, 136.32, 134.14, 133.97, 133.23, 132.98, 132.00, 131.63, 129.79, 129.46, 128.80, 128.68, 128.53, 128.43, 128.34, 128.09 (d, J = 6.2 Hz), 126.63, 125.75, 123.95, 122.25 (d, J = 274.0 Hz), 60.93, 52.80, 48.59, 32.15, 24.56, 20.79; ^{19}F NMR (376 MHz, CDCl_3) δ -56.23; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{32}\text{ClF}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 702.1357, found 702.1359. $[\alpha]_{\text{D}}^{20}$ = -20 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 10.5 min, tr (minor) = 7.8 min, 86% e.e.

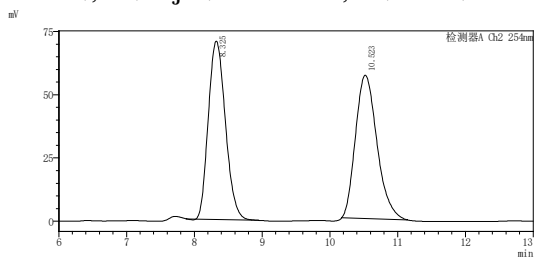


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.859	1434449	49.218	1	7.823	327217	6.783
2	10.534	1480016	50.782	2	10.502	4497108	93.217

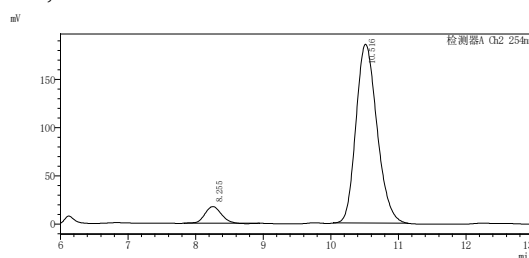
methyl (*R,Z*)-4-(3-fluorophenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (15), White solid (68 mg, 66%), ^1H NMR (400 MHz, CDCl_3) δ 8.28 – 8.21 (m, 1H), 7.80 – 7.75 (m, 1H), 7.74 – 7.67 (m, 2H), 7.34 – 7.29 (m, 2H), 7.23 (td, J = 7.1, 6.7, 1.4 Hz, 1H), 7.19 – 7.14 (m, 2H), 6.81 – 6.74 (m, 3H), 6.69 (d, J = 7.7 Hz, 1H), 6.59 – 6.52 (m, 2H), 6.50 (s, 1H), 6.46 (s, 1H), 6.40 (d, J = 8.2 Hz, 2H), 3.89 (s, 3H), 2.16 (s, 3H), 1.70 (s, 3H), 1.51 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.93, 164.78, 162.72, 160.28, 145.54, 144.51, 137.26, 136.15, 134.56 (d, J = 6.9 Hz), 134.26, 133.94, 133.22, 132.02, 129.62 (q, J = 33.8 Hz), 128.89, 128.68, 128.65, 128.60, 128.51, 128.12 (q, J = 6.4 Hz), 127.06, 126.59, 125.69, 123.74, 122.27 (q, J = 274.4 Hz), 118.35 (d, J = 22.5 Hz), 115.31 (d, J = 21.0 Hz), 60.88, 52.77, 48.58, 31.98, 24.71, 20.76; ^{19}F NMR (376 MHz, CDCl_3) δ -56.24, -114.12 (q, J = 8.3 Hz); HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{32}\text{F}_4\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 686.1653, found 686.1655. $[\alpha]_{\text{D}}^{20}$ = -88 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C,



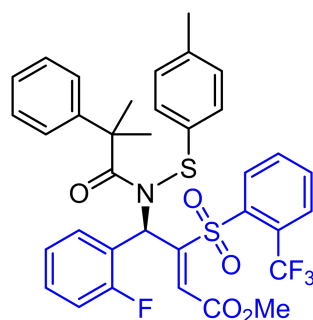
254 nm); tr (major) = 10.5 min, tr (minor) = 8.3 min, 86% e.e.



NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	8.325	1236387	49.647	1	8.255	290411	6.732
2	10.523	1253957	50.353	2	10.516	4023303	93.268

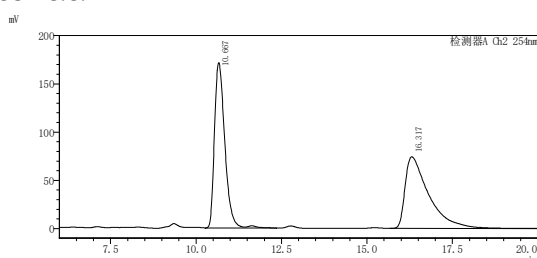


methyl (*R,Z*)-4-(2-fluorophenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (16), White solid (56 mg, 54%), ¹H NMR (400 MHz, CDCl₃) δ

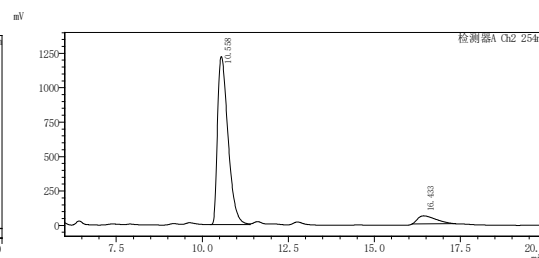


8.26 – 8.20 (m, 1H), 7.81 – 7.75 (m, 1H), 7.74 – 7.67 (m, 2H), 7.35 – 7.28 (m, 2H), 7.25 – 7.19 (m, 2H), 7.18 – 7.14 (m, 2H), 6.87 – 6.80 (m, 1H), 6.80 – 6.74 (m, 2H), 6.72 (d, *J* = 7.9 Hz, 2H), 6.43 (s, 1H), 6.38 (d, *J* = 8.0 Hz, 2H), 6.30 – 6.21 (m, 1H), 3.95 (s, 3H), 2.14 (s, 3H), 1.69 (s, 3H), 1.49 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 180.65, 164.76, 161.68, 159.21, 145.38, 144.67, 136.76, 135.79, 134.36, 134.00, 133.22, 133.07, 131.99, 130.81 (d, *J* = 8.7 Hz), 129.87 (q, *J* = 33.9 Hz), 128.52 (d, *J* = 10.8 Hz), 128.32, 128.14 (q, *J* = 6.2 Hz), 126.53, 125.72, 122.87, 122.36 (q, *J* = 274.3 Hz), 119.75 (d, *J* = 13.6 Hz), 114.04 (d, *J* = 21.9 Hz), 53.27, 52.82, 48.51, 32.52, 23.91, 20.75; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.35, -114.81 (d, *J* = 9.6 Hz); HRMS (ESI-TOF). (*m/z*): Calcd for C₃₅H₃₂F₄NO₅S₂⁺, ([*M* + *H*]⁺), 686.1653, found 686.1653. [α]_D²⁰ = -69 (*c* = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OD-3

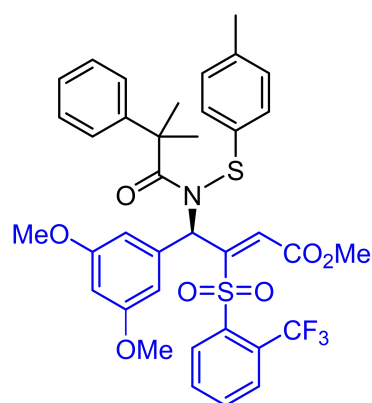
column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 16.4 min, tr (minor) = 10.5 min, 85% e.e.



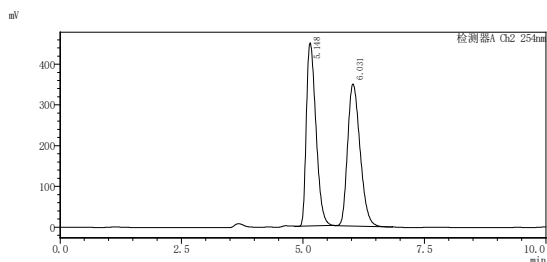
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	10.667	3626886	50.232	1	10.558	26001930	92.424
2	16.317	3593358	49.768	2	16.433	2131286	7.576



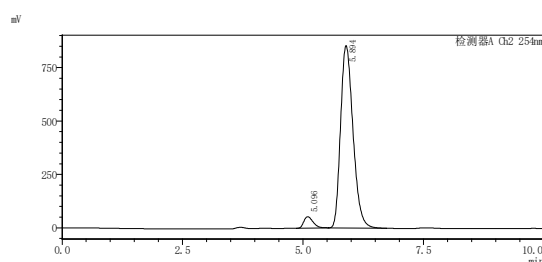
methyl (*R,Z*)-4-(3,5-dimethoxyphenyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (17), White solid (71 mg, 65%), ¹H NMR (400 MHz, CDCl₃) δ



8.33 – 8.20 (m, 1H), 7.77 – 7.71 (m, 1H), 7.70 – 7.59 (m, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.25 – 7.14 (m, 3H), 6.75 (d, *J* = 7.9 Hz, 2H), 6.53 – 6.42 (m, 4H), 5.98 (s, 2H), 5.90 (t, *J* = 2.2 Hz, 1H), 3.87 (s, 3H), 3.51 (s, 6H), 2.16 (s, 3H), 1.73 (s, 3H), 1.54 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 181.01, 164.97, 159.57, 145.63, 144.76, 137.43, 135.98, 134.54, 134.29, 133.80, 133.41, 131.95, 129.56 (q, *J* = 33.7 Hz), 129.05, 128.51, 128.02 (q, *J* = 6.3 Hz), 126.55, 125.78, 124.25, 122.38 (q, *J* = 274.2 Hz), 109.66, 100.67, 61.37, 55.06, 52.74, 48.71, 31.93, 25.14, 20.83; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.15; HRMS (ESI-TOF). (*m/z*): Calcd for C₃₇H₃₇F₃NO₇S₂⁺, ([*M* + *H*]⁺), 728.1958, found 728.1959. [α]_D²⁰ = -33 (*c* = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak AD-3 column (80: 20 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 5.9 min, tr (minor) = 5.1 min, 91% e.e.

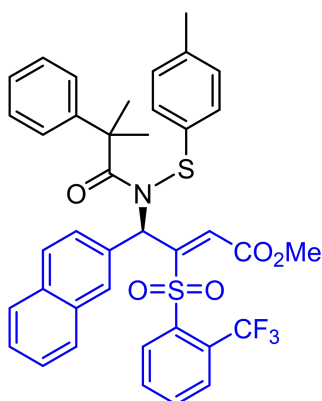


NO.	Time	Area	Area (%)
1	5.148	6163786	49.698
2	6.031	6238739	50.302

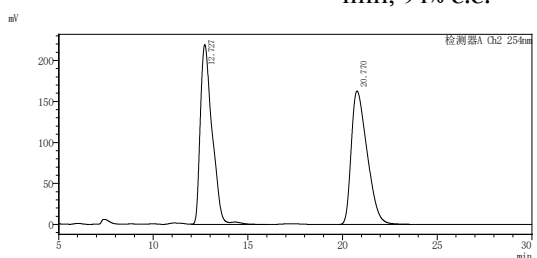


NO.	Time	Area	Area (%)
1	5.096	714211	4.446
2	5.894	15350441	95.554

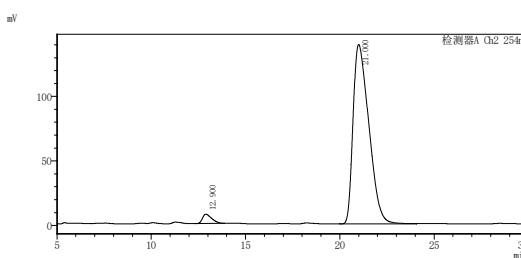
methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-(naphthalen-2-yl)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (18), White solid (96 mg, 89%), ^1H NMR (400 MHz, CDCl_3) δ



8.17 (d, J = 7.8 Hz, 1H), 7.62 – 7.53 (m, 2H), 7.49 (t, J = 7.5 Hz, 2H), 7.39 (d, J = 7.5 Hz, 1H), 7.35 – 7.26 (m, 5H), 7.19 (d, J = 7.6 Hz, 3H), 7.15 (s, 1H), 7.00 (d, J = 8.5 Hz, 1H), 6.63 (s, 1H), 6.56 (s, 1H), 6.41 (d, J = 7.8 Hz, 2H), 6.26 (d, J = 7.9 Hz, 2H), 3.91 (s, 3H), 1.87 (s, 3H), 1.74 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.92, 165.05, 145.79, 144.77, 137.36, 135.95, 134.24, 133.76, 133.26, 132.88, 131.92, 131.89, 131.83, 129.53 (q, J = 35.0 Hz), 129.36, 128.73, 128.56, 128.16, 127.96 (q, J = 6.2 Hz), 127.85, 127.09, 126.91, 126.62, 126.42, 125.89, 125.53, 124.02, 122.38 (q, J = 274.5 Hz), 77.31, 61.79, 52.81, 48.68, 32.14, 24.88, 20.58; ^{19}F NMR (376 MHz, CDCl_3) δ -56.19; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{39}\text{H}_{35}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 718.1903, found 718.1904. $[\alpha]_{\text{D}}^{20}$ = -81 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 21.0 min, tr (minor) = 12.9 min, 94% e.e.

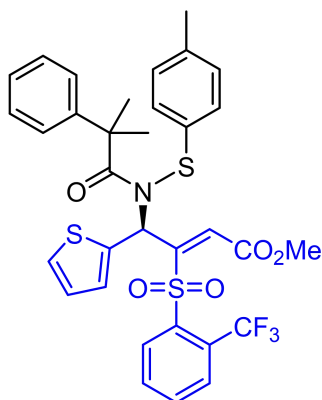


NO.	Time	Area	Area (%)
1	12.727	9550378	50.173
2	20.770	9484339	49.827

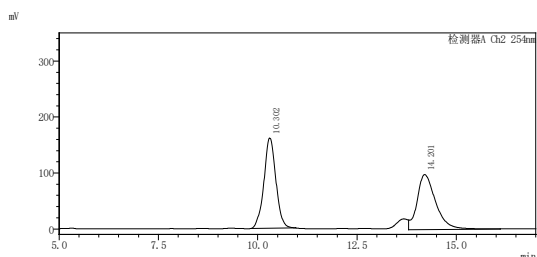


NO.	Time	Area	Area (%)
1	12.900	244790	2.928
2	21.000	8114390	97.072

methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-(thiophen-2-yl)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (19), White solid (70 mg, 69%), ^1H NMR (400 MHz, CDCl_3) δ

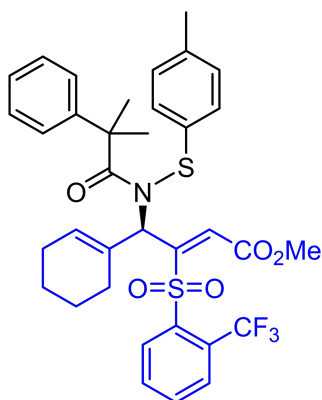


8.28 – 8.19 (m, 1H), 7.79 – 7.72 (m, 1H), 7.71 – 7.63 (m, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.24 – 7.14 (m, 3H), 6.79 (d, J = 8.0 Hz, 2H), 6.75 – 6.65 (m, 2H), 6.55 (d, J = 13.2 Hz, 2H), 6.50 (d, J = 5.0 Hz, 1H), 6.45 (d, J = 8.0 Hz, 2H), 3.86 (s, 3H), 2.19 (s, 3H), 1.69 (s, 3H), 1.53 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.80, 164.87, 146.54, 144.65, 137.49, 135.83, 134.66, 133.76, 133.46, 133.10, 131.97, 129.39 (q, J = 34.0 Hz), 129.16, 128.72, 128.47, 128.27, 128.09 (q, J = 6.1 Hz), 126.48, 125.64, 124.26, 122.33 (q, J = 276.0 Hz), 123.34, 56.87, 52.68, 48.57, 31.65, 25.03, 20.81; ^{19}F NMR (376 MHz, CDCl_3) δ -56.24; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{33}\text{H}_{31}\text{F}_3\text{NO}_5\text{S}_3^+$, ($[\text{M} + \text{H}]^+$), 674.1311, found 674.1312. $[\alpha]_{\text{D}}^{20}$ = -91 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 10.4 min, tr (minor) = 14.4 min, 94% e.e.

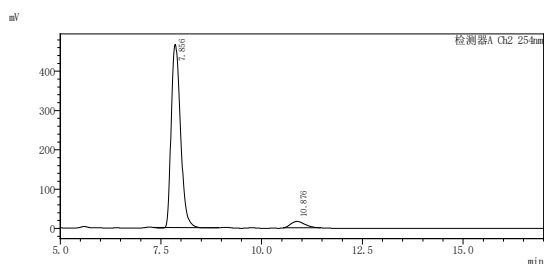
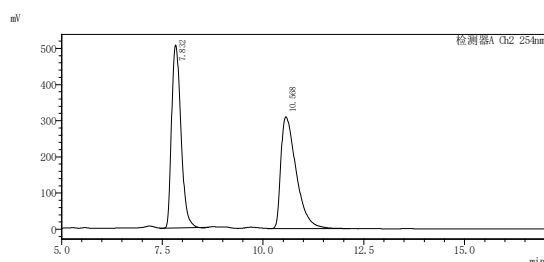


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	10.302	3377995	51.140	1	10.365	4646908	97.118
2	14.201	3227435	48.860	2	14.431	137898	2.882

methyl (R,Z)-4-(cyclohex-1-en-1-yl)-4-(2-methyl-2-phenyl-N-(p-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (20), Colorless oil (63 mg, 62%), ¹H NMR (400 MHz, CDCl₃)

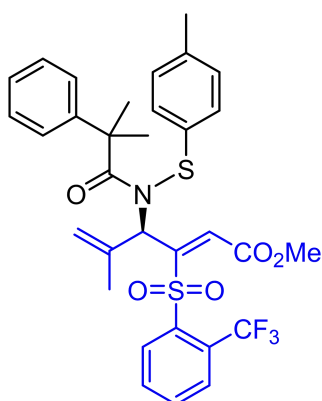


δ 8.47 – 8.37 (m, 1H), 7.94 – 7.87 (m, 1H), 7.80 – 7.72 (m, 2H), 7.30 (t, J = 7.5 Hz, 2H), 7.23 – 7.18 (m, 1H), 7.18 – 7.13 (m, 2H), 7.00 (d, J = 8.0 Hz, 2H), 6.77 (d, J = 8.3 Hz, 2H), 6.31 (s, 1H), 5.76 (s, 1H), 5.51 (d, J = 3.5 Hz, 1H), 3.82 (s, 3H), 2.26 (s, 3H), 1.74 (s, 3H), 1.60 – 1.50 (m, 4H), 1.50 (s, 3H), 1.09 – 1.01 (m, 1H), 1.01 – 0.89 (m, 2H), 0.73 – 0.48 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 181.51, 164.91, 145.90, 144.84, 138.14, 136.23, 135.92, 135.35, 133.61, 132.97, 131.98, 129.51 (q, J = 33.7 Hz), 129.46, 129.08, 128.37, 128.06 (q, J = 6.1 Hz), 127.84, 126.35, 125.61, 124.01, 122.42 (q, J = 274.4 Hz), 62.16, 52.52, 48.69, 31.90, 28.27, 25.29, 25.13, 21.57, 20.86, 20.77; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.28; HRMS (ESI-TOF). (m/z): Calcd for C₃₅H₃₇F₃NO₅S₂⁺, ([M + H]⁺), 672.2060, found 672.2059. [α]_D²⁰ = -140 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.9 min, tr (minor) = 10.9 min, 90% e.e.

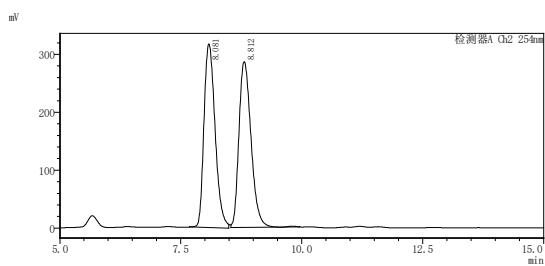


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.832	8156687	49.930	1	7.856	7476354	94.945
2	10.568	8179685	50.070	2	10.876	398048	5.055

methyl (R,Z)-5-methyl-4-(2-methyl-2-phenyl-N-(p-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)hexa-2,5-dienoate (21), Colorless oil (65 mg, 68%), ¹H NMR (400 MHz, CDCl₃) δ 8.44 (dd, J = 7.2, 2.1 Hz, 1H), 7.92 (dd, J = 7.1, 2.2 Hz, 1H), 7.78 (tt, J = 7.6, 5.8 Hz, 2H), 7.29 (d, J = 7.9 Hz, 2H), 7.18 (td, J = 7.3, 1.4 Hz, 3H), 6.99 (d, J = 8.0 Hz, 2H), 6.77 (d, J = 8.3 Hz, 2H), 6.53 (s, 1H), 5.86 (s, 1H), 4.87 (s, 1H), 4.74 (s, 1H), 3.71 (s, 3H), 2.28 (s, 3H), 1.67 (s, 3H), 1.59 (s, 3H), 1.33 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 181.35, 164.73, 144.77, 144.14, 138.55, 137.97, 136.77, 136.58, 134.93, 134.83, 133.75, 133.47, 133.36, 132.25, 131.46, 130.29, 129.60 (q, J = 33.8 Hz), 129.18, 128.43, 128.18 (q, J = 6.2 Hz), 126.35, 125.65, 125.00, 122.41 (q, J = 274.4 Hz), 119.22, 62.48, 52.39, 48.74, 29.34, 27.97, 21.44, 20.96; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.23; HRMS (ESI-TOF). (m/z):

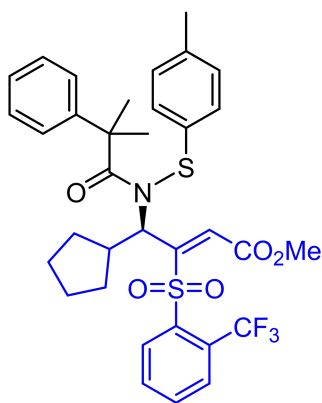


Calcd for C₃₂H₃₃F₃NO₅S₂⁺, ([M + H]⁺), 632.1747, found 632.1747. [α]_D²⁰ = -12 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.4 min, tr (minor) = 8.0 min, 88% e.e.

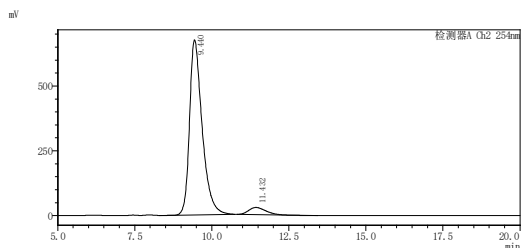
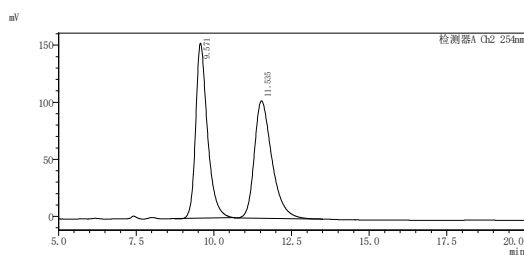


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	8.081	5058664	50.324	1	7.443	4009939	93.886
2	8.812	4993483	49.676	2	8.024	261117	6.114

methyl (R,Z)-4-cyclopentyl-4-(2-methyl-2-phenyl-N-(p-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (22), Colorless oil (66 mg, 67%), ¹H NMR (400 MHz, CDCl₃)

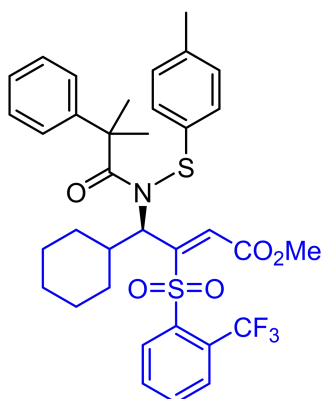


δ 8.57 (s, 1H), 7.95 – 7.86 (m, 2H), 7.80 (t, J = 7.6 Hz, 1H), 7.30 – 7.16 (m, 4H), 7.09 (t, J = 7.2 Hz, 1H), 6.95 (d, J = 7.8 Hz, 2H), 6.76 (s, 2H), 6.60 (s, 1H), 5.46 (d, J = 10.9 Hz, 1H), 3.61 (s, 3H), 2.27 (s, 3H), 1.71 (s, 3H), 1.65 (s, 3H), 1.46 – 1.14 (m, 7H), 1.04 (s, 1H), 0.39 (s, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 181.23, 164.57, 144.57, 141.59, 136.51, 134.86, 133.99, 132.34, 129.69 (q, J = 33.8 Hz), 129.21, 128.28 (q, J = 4.5 Hz), 126.01, 125.96, 122.39 (q, J = 274.5 Hz), 52.11, 48.85, 42.77, 30.99, 29.73, 29.52, 26.95, 24.74, 24.53, 20.92; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.22; HRMS (ESI-TOF). (m/z): Calcd for C₃₄H₃₇F₃NO₅S₂⁺, ([M + H]⁺), 660.2060, found 660.2063. [α]_D²⁰ = 59 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak IG column (95: 5 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 9.4 min, tr (minor) = 11.4 min, 90% e.e.

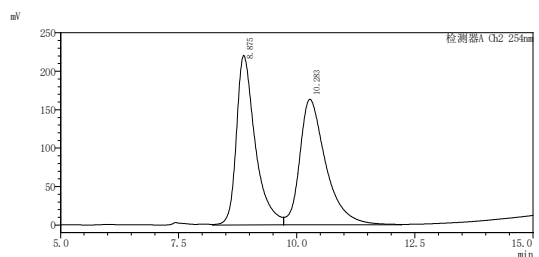


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	9.571	4051143	49.973	1	9.440	19210886	94.991
2	11.535	4055453	50.027	2	11.432	1013109	5.009

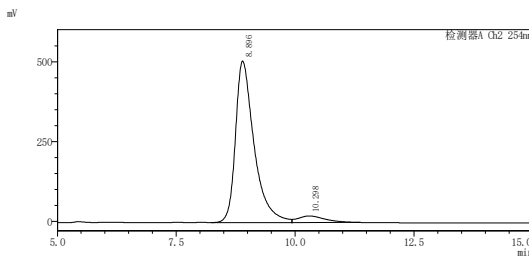
methyl (R,Z)-4-cyclohexyl-4-(2-methyl-2-phenyl-N-(p-tolylthio)propanamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (23), Colorless oil (76 mg, 75%), ¹H NMR (400 MHz, CDCl₃)



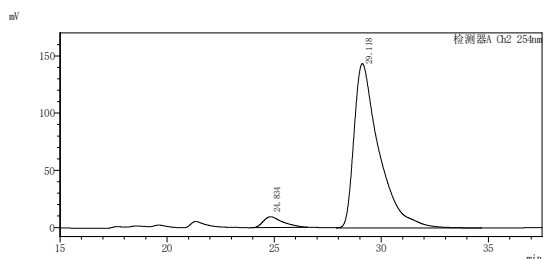
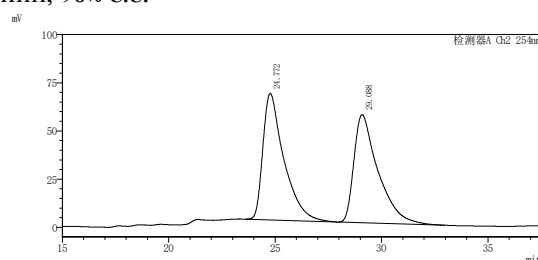
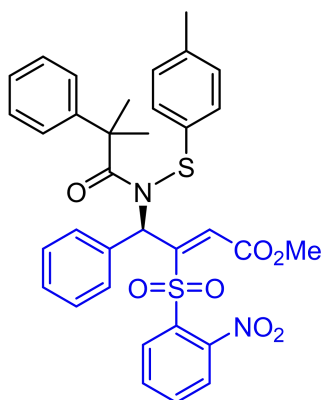
δ 8.56 (s, 1H), 7.94 – 7.84 (m, 2H), 7.79 (t, J = 7.6 Hz, 1H), 7.26 (d, J = 3.4 Hz, 2H), 7.21 (t, J = 7.5 Hz, 2H), 7.11 (t, J = 7.6 Hz, 1H), 6.96 (d, J = 7.9 Hz, 2H), 6.75 (s, 2H), 6.61 (s, 1H), 5.38 (d, J = 10.4 Hz, 1H), 3.62 (s, 3H), 2.27 (s, 3H), 1.72 (s, 3H), 1.66 (s, 3H), 1.54 – 1.26 (m, 6H), 1.01 – 0.74 (m, 3H), 0.72 – 0.61 (m, 1H), 0.20 – 0 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 181.21, 164.63, 144.34, 140.56, 136.40, 134.87, 133.96, 132.72, 132.30, 129.67 (q, J = 33.7 Hz), 129.22, 128.24 (q, J = 6.2 Hz), 126.11, 122.36 (q, J = 274.6 Hz), 52.09, 48.82, 39.51, 31.03, 29.02, 28.84, 26.94, 25.67, 25.55, 25.21, 20.91; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.18; HRMS (ESI-TOF). (m/z): Calcd for C₃₅H₃₉F₃NO₅S₂⁺, ([M + H]⁺), 674.2216, found 674.2214. [α]_D²⁰ = 70 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak IG column (95: 5 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 8.9 min, tr (minor) = 10.3 min, 89% e.e.



NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	8.875	6125521	49.310	1	8.896	13856755	94.451
2	10.283	6297041	50.690	2	10.298	814146	5.549

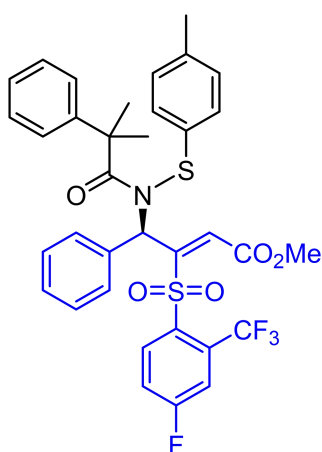


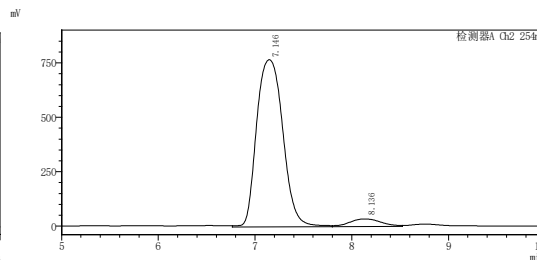
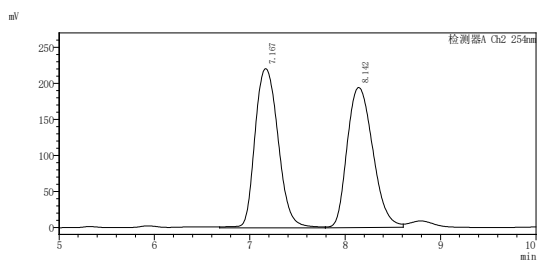
methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-3-((2-nitrophenyl)sulfonyl)-4-phenylbut-2-enoate (24), White solid (75 mg, 78%), ¹H NMR (400 MHz, CDCl₃) δ 8.11 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.75 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.73 – 7.63 (m, 2H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.25 – 7.19 (m, 3H), 7.00 (d, *J* = 7.1 Hz, 2H), 6.91 – 6.86 (m, 1H), 6.86 – 6.79 (m, 2H), 6.73 (s, 1H), 6.70 (d, *J* = 4.2 Hz, 2H), 6.53 (s, 1H), 6.42 – 6.33 (m, 2H), 3.87 (s, 3H), 2.15 (s, 3H), 1.69 (s, 3H), 1.51 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 181.24, 164.82, 148.43, 145.95, 144.71, 135.83, 134.95, 134.61, 132.68, 132.41, 132.25, 131.39, 129.15, 128.66, 128.54, 128.52, 127.32, 126.56, 125.85, 124.81, 123.63, 61.89, 52.81, 48.70, 31.91, 25.06, 20.85; HRMS (ESI-TOF). (*m/z*): Calcd for C₃₄H₃₃N₂O₇S₂⁺, ([*M* + *H*]⁺), 645.1724, found 645.1727. [α]_D²⁰ = -15 (*c* = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 29.1 min, tr (minor) = 24.8 min, 90% e.e.



NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	24.772	4500183	50.458	1	24.834	599650	4.902
2	29.088	4418524	49.542	2	29.118	11632151	95.098

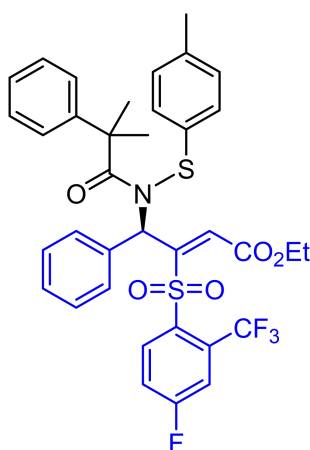
methyl (*R,Z*)-3-((4-fluoro-2-(trifluoromethyl)phenyl)sulfonyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-phenylbut-2-enoate (25), White solid (55 mg, 53%), ¹H NMR (400 MHz, CDCl₃) δ 8.24 (dd, *J* = 8.9, 5.2 Hz, 1H), 7.40 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.30 (t, *J* = 7.4 Hz, 3H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.15 (d, *J* = 7.4 Hz, 2H), 6.91 – 6.83 (m, 3H), 6.80 (t, *J* = 7.4 Hz, 2H), 6.71 (d, *J* = 7.8 Hz, 2H), 6.48 (s, 1H), 6.40 (s, 1H), 6.34 (d, *J* = 7.9 Hz, 2H), 3.92 (s, 3H), 2.15 (s, 3H), 1.68 (s, 3H), 1.51 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 181.02, 164.97, 145.84, 144.58, 136.57 (d, *J* = 9.6 Hz), 135.77, 134.62, 131.67, 131.53, 128.53, 128.51 (d, *J* = 9.8 Hz), 127.14, 126.54, 125.72, 123.40, 118.62 (d, *J* = 21.1 Hz), 61.63, 52.81, 48.58, 32.12, 24.57, 20.78; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.72, -101.25 (dt, *J* = 12.3, 6.0 Hz); HRMS (ESI-TOF). (*m/z*): Calcd for C₃₅H₃₂F₄NO₅S₂⁺, ([*M* + *H*]⁺), 686.1653, found 686.1653. [α]_D²⁰ = -43 (*c* = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.1 min, tr (minor) = 8.1min, 90% e.e.



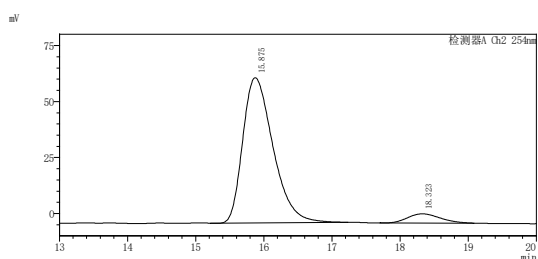
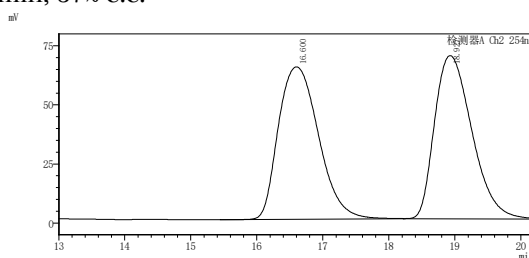


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.167	3746113	50.676	1	7.146	14507834	94.740
2	8.142	3646168	49.324	2	8.136	805415	5.260

ethyl (*R,Z*)-3-((4-fluoro-2-(trifluoromethyl)phenyl)sulfonyl)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-phenylbut-2-enoate (26), White solid (58 mg, 55%), ¹H NMR (400 MHz, CDCl₃) δ

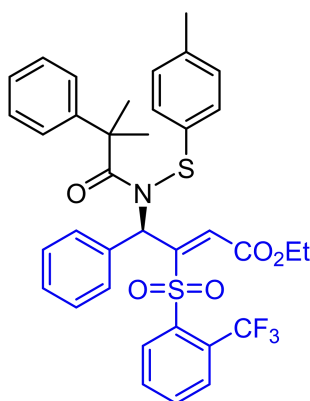


8.26 (dd, *J* = 9.0, 5.3 Hz, 1H), 7.40 (dd, *J* = 9.0, 2.6 Hz, 1H), 7.33 – 7.28 (m, 3H), 7.25 – 7.20 (m, 1H), 7.15 (d, *J* = 7.5 Hz, 2H), 6.92 – 6.83 (m, 3H), 6.80 (t, *J* = 7.5 Hz, 2H), 6.72 (d, *J* = 7.9 Hz, 2H), 6.49 (s, 1H), 6.43 (s, 1H), 6.36 (d, *J* = 8.4 Hz, 2H), 4.39 (q, *J* = 7.2 Hz, 2H), 2.15 (s, 3H), 1.68 (s, 3H), 1.51 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 181.06, 166.22, 164.61, 163.65, 145.34, 144.70, 136.60 (d, *J* = 9.1 Hz), 135.78, 134.71, 133.56, 131.83, 131.54, 129.02, 128.55 (d, *J* = 10.7 Hz), 128.53, 127.17, 126.55, 125.74, 123.40, 118.63 (d, *J* = 21.2 Hz), 116.29 (d, *J* = 26.4 Hz), 62.18, 61.60, 48.62, 32.18, 24.62, 20.82, 14.05; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.66, -101.41 (q, *J* = 7.1, 6.4 Hz); HRMS (ESI-TOF). (*m/z*): Calcd for C₃₆H₃₄F₄NO₅S₂⁺, ([*M* + *H*]⁺), 700.1809, found 700.1808. [α]_D²⁰ = -36 (*c* = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OD-3 column (98: 2 hexane: 2-propanol, 0.5 mL/min, 40 °C, 254 nm); tr (major) = 15.9 min, tr (minor) = 18.3 min, 87% e.e.



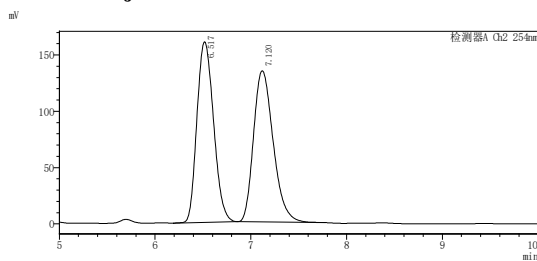
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	16.600	2729429	50.154	1	15.875	2002464	93.536
2	18.927	2712652	49.846	2	18.323	138374	6.464

ethyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (27), White solid (91 mg, 89%), ¹H NMR (400 MHz, CDCl₃) δ

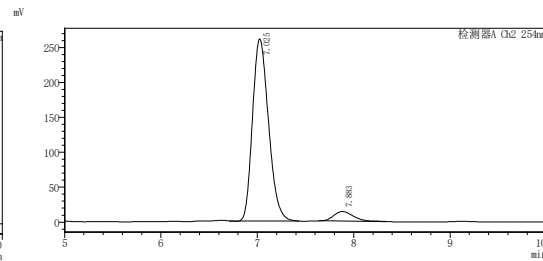


8.26 – 8.19 (m, 1H), 7.76 – 7.69 (m, 1H), 7.68 – 7.62 (m, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.25 – 7.20 (m, 1H), 7.16 (d, *J* = 7.3 Hz, 2H), 6.90 – 6.82 (m, 3H), 6.82 – 6.76 (m, 2H), 6.72 (d, *J* = 7.9 Hz, 2H), 6.50 (d, *J* = 3.5 Hz, 2H), 6.36 (d, *J* = 8.0 Hz, 2H), 4.36 (q, *J* = 7.1 Hz, 2H), 2.15 (s, 3H), 1.67 (s, 3H), 1.52 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 181.02, 164.55, 145.46, 144.74, 137.56, 135.66, 134.74, 133.68, 133.23, 132.07, 131.89, 131.36, 129.54 (q, *J* = 33.9 Hz), 129.09, 128.55, 128.44, 128.36, 128.01 (q, *J* = 6.1 Hz), 127.11, 126.45, 125.70, 123.39, 122.30 (q, *J* = 274.7 Hz), 62.03, 61.55, 48.60, 31.97, 24.85, 20.77, 13.97; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.20; HRMS (ESI-TOF). (*m/z*): Calcd for C₃₆H₃₅F₃NO₅S₂⁺, ([*M* + *H*]⁺), 682.1903, found 682.1901. [α]_D²⁰ = -67 (*c* = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254

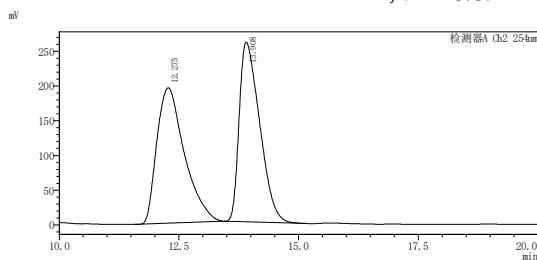
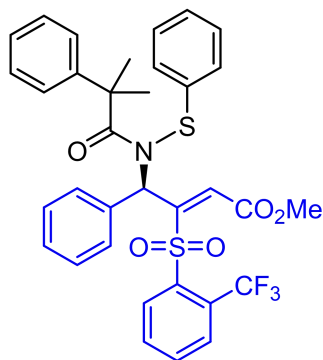
nm); tr (major) = 7.0 min, tr (minor) = 7.9 min, 88% e.e.



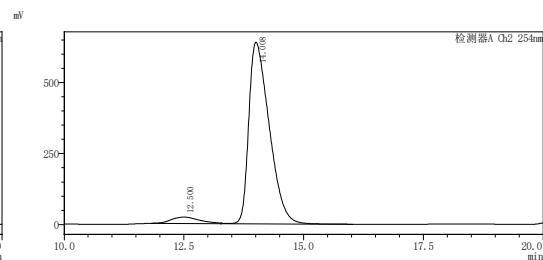
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	6.517	1938355	50.262	1	7.025	3014198	93.953
2	7.120	1918160	49.738	2	7.883	193983	6.047



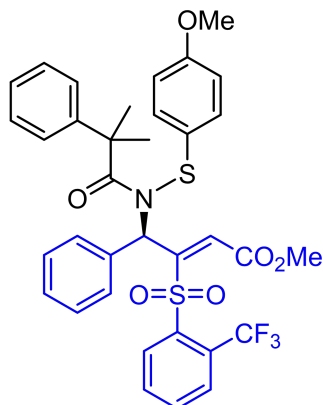
methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(phenylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (28), White solid (78 mg, 80%), ^1H NMR (400 MHz, CDCl_3) δ 8.25 – 8.15 (m, 1H), 7.79 – 7.70 (m, 1H), 7.70 – 7.61 (m, 2H), 7.33 – 7.27 (m, 2H), 7.23 – 7.19 (m, 1H), 7.19 – 7.13 (m, 2H), 6.97 – 6.86 (m, 5H), 6.85 – 6.81 (m, 1H), 6.81 – 6.75 (m, 2H), 6.53 (s, 1H), 6.49 (s, 1H), 6.48 – 6.39 (m, 2H), 3.89 (s, 3H), 1.67 (s, 3H), 1.53 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.98, 164.86, 145.98, 144.48, 138.16, 137.25, 133.83, 133.20, 131.91, 131.66, 131.46, 129.55 (q, J = 33.8 Hz), 128.48, 128.41, 128.25, 128.05 (q, J = 6.1 Hz), 127.72, 127.10, 126.48, 125.67, 125.59, 122.82, 122.27 (q, J = 274.3 Hz), 61.31, 52.68, 48.58, 31.90, 24.70; ^{19}F NMR (376 MHz, CDCl_3) δ -56.22; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{34}\text{H}_{31}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[M + H]^+$), 654.1590, found 654.1591. $[\alpha]_D^{20}$ = -57 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 14.0 min, tr (minor) = 12.5 min, 91% e.e.

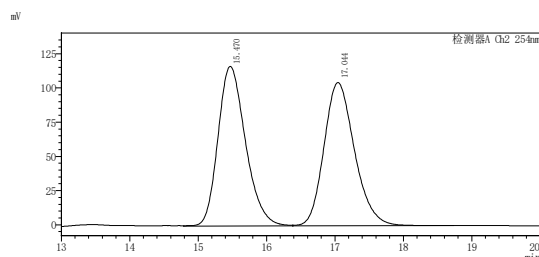


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	12.275	7804962	50.303	1	12.500	912940	4.592
2	13.908	7710959	49.697	2	14.008	18966390	95.408

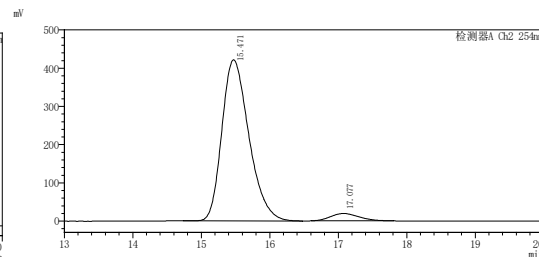


methyl (*R,Z*)-4-(*N*-((4-methoxyphenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (29), White solid (90 mg, 88%), ^1H NMR (400 MHz, CDCl_3) δ 8.20 (dt, J = 8.7, 4.2 Hz, 1H), 7.75 – 7.70 (m, 1H), 7.68 – 7.61 (m, 2H), 7.31 (t, J = 7.5 Hz, 2H), 7.23 (t, J = 7.3 Hz, 1H), 7.18 (d, J = 7.4 Hz, 2H), 6.91 – 6.86 (m, 1H), 6.85 – 6.77 (m, 4H), 6.51 (s, 1H), 6.46 (d, J = 8.7 Hz, 2H), 6.42 – 6.35 (m, 3H), 3.88 (s, 3H), 3.66 (s, 3H), 1.73 (s, 3H), 1.54 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.69, 164.94, 158.46, 146.02, 144.71, 137.43, 133.75, 133.14, 132.23, 131.92, 131.10, 129.45 (q, J = 33.7 Hz), 128.86, 128.46, 128.37, 128.01 (q, J = 6.3 Hz), 127.16, 126.61, 126.46, 125.74, 122.26 (q, J = 274.4 Hz), 113.63, 62.22, 55.26, 52.68, 48.57, 31.80, 25.11; ^{19}F NMR (376 MHz, CDCl_3) δ -56.22; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{33}\text{F}_3\text{NO}_6\text{S}_2^+$, ($[M + H]^+$), 684.1696, found 684.1700. $[\alpha]_D^{20}$ = -3 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 15.5 min, tr (minor) = 17.1 min, 91% e.e.



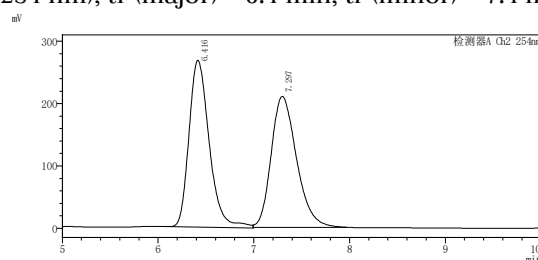
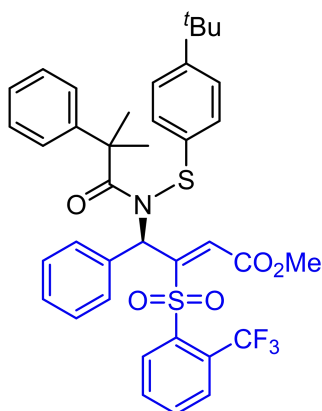


NO.	Time	Area	Area (%)
1	15.470	3265859	50.092
2	17.044	3253905	49.908



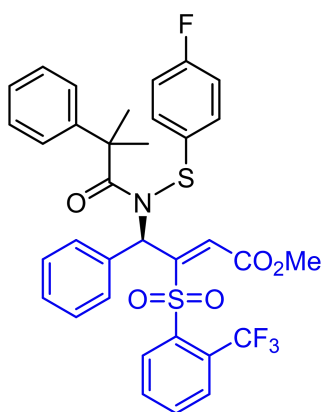
NO.	Time	Area	Area (%)
1	15.471	11573915	95.401
2	17.077	557962	4.599

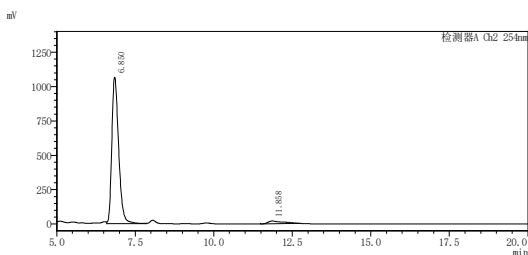
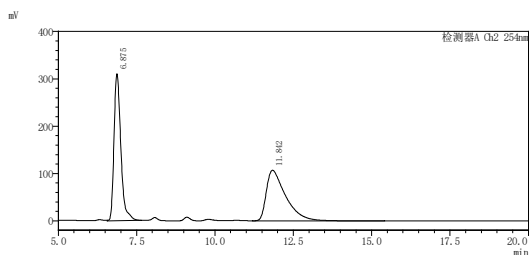
methyl (*R,Z*)-4-(*N*-((4-(*tert*-butyl)phenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (30), White solid (91 mg, 86%), ^1H NMR (400 MHz, CDCl_3) δ 8.24 – 8.17 (m, 1H), 7.77 – 7.70 (m, 1H), 7.69 – 7.62 (m, 2H), 7.32 – 7.27 (m, 2H), 7.25 – 7.21 (m, 1H), 7.19 – 7.15 (m, 2H), 6.92 – 6.87 (m, 2H), 6.87 – 6.82 (m, 2H), 6.81 – 6.76 (m, 1H), 6.76 – 6.71 (m, 2H), 6.52 – 6.45 (m, 2H), 6.42 – 6.35 (m, 2H), 3.90 (s, 3H), 1.75 (s, 3H), 1.53 (s, 3H), 1.18 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.95, 164.93, 149.10, 146.01, 144.69, 137.30, 134.77, 134.49, 133.78, 133.18, 131.88, 131.67, 131.48, 129.56 (q, J = 33.8 Hz), 128.50, 128.40, 128.35, 128.19, 128.02 (q, J = 6.1 Hz), 127.00, 126.63, 126.45, 125.71, 124.72, 123.67, 122.30 (q, J = 278.8 Hz), 61.37, 52.69, 48.58, 34.21, 32.20, 31.08, 24.58; ^{19}F NMR (376 MHz, CDCl_3) δ -56.22; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{38}\text{H}_{39}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 710.2216, found 710.2215. $[\alpha]_{\text{D}}^{20}$ = -48 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-H column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 6.4 min, tr (minor) = 7.4 min, 92% e.e.



NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	6.416	3927139	50.376	1	6.431	11537991	95.953
2	7.297	3868486	49.624	2	7.365	486626	4.047

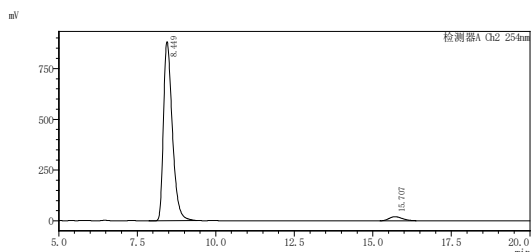
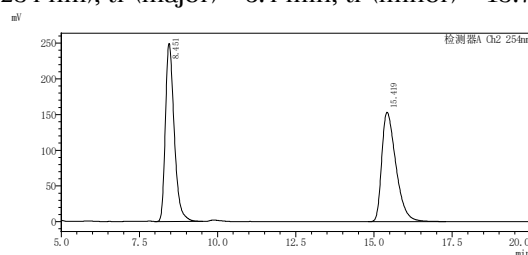
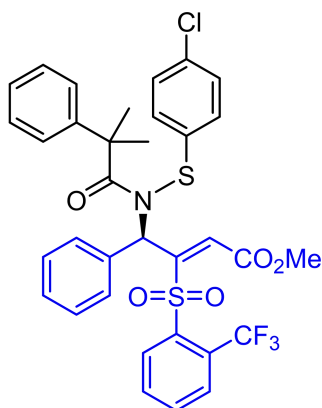
methyl (*R,Z*)-4-(*N*-((4-fluorophenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (31), White solid (84 mg, 83%), ^1H NMR (400 MHz, CDCl_3) δ 8.23 – 8.17 (m, 1H), 7.76 – 7.70 (m, 1H), 7.70 – 7.63 (m, 2H), 7.31 – 7.26 (m, 2H), 7.21 (dd, J = 7.5, 1.7 Hz, 1H), 7.19 – 7.15 (m, 2H), 6.91 – 6.79 (m, 5H), 6.64 – 6.56 (m, 2H), 6.48 (d, J = 2.4 Hz, 2H), 6.45 – 6.37 (m, 2H), 3.88 (s, 3H), 1.69 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.73, 164.82, 162.30, 159.85, 145.84, 144.32, 137.22, 133.88, 133.21, 133.09 (d, J = 3.2 Hz), 131.93 (d, J = 5.0 Hz), 131.24, 129.55 (q, J = 33.8 Hz), 128.70, 128.56 (d, J = 5.4 Hz), 128.48, 128.08 (q, J = 6.2 Hz), 127.26, 126.55, 125.69, 125.33 (d, J = 8.1 Hz), 122.26 (q, J = 274.5 Hz), 114.93 (d, J = 22.4 Hz), 61.51, 52.72, 48.59, 31.57, 25.07; ^{19}F NMR (376 MHz, CDCl_3) δ -56.22, -116.02; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{34}\text{H}_{30}\text{F}_4\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 672.1496, found 672.1492. $[\alpha]_{\text{D}}^{20}$ = -37 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-H column (80: 20 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 6.9 min, tr (minor) = 11.8 min, 92% e.e.





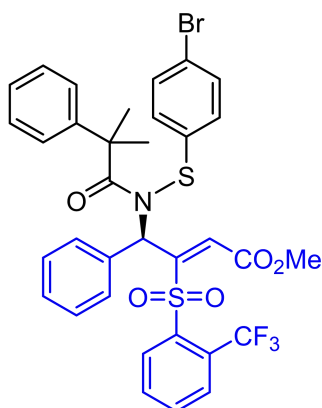
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	6.875	4695869	50.522	1	6.850	16057278	95.906
2	11.842	4598830	49.478	2	11.858	685367	4.094

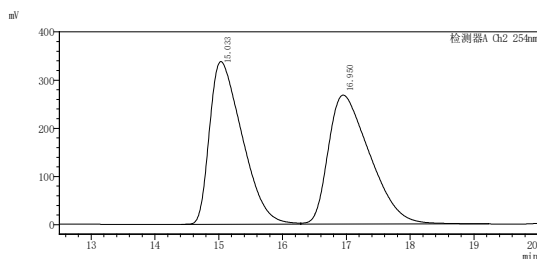
methyl (*R,Z*)-4-(*N*-((4-chlorophenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (32), White solid (91 mg, 88%), ^1H NMR (400 MHz, CDCl_3) δ 8.20 (dd, $J = 5.7, 3.4$ Hz, 1H), 7.76 – 7.71 (m, 1H), 7.71 – 7.63 (m, 2H), 7.28 (t, $J = 7.3$ Hz, 2H), 7.20 (d, $J = 7.1$ Hz, 1H), 7.16 (d, $J = 7.6$ Hz, 2H), 6.93 – 6.81 (m, 7H), 6.53 (s, 1H), 6.47 (s, 1H), 6.38 (d, $J = 8.2$ Hz, 2H), 3.87 (s, 3H), 1.65 (s, 3H), 1.54 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.73, 164.73, 145.73, 144.17, 137.09, 136.68, 133.93, 133.22, 131.97, 131.80, 131.39, 131.23, 129.53 (q, $J = 33.7$ Hz), 128.63, 128.47, 128.09 (q, $J = 6.1$ Hz), 127.82, 127.31, 126.55, 125.62, 124.20, 122.24 (q, $J = 274.4$ Hz), 61.25, 52.69, 48.56, 31.42, 25.05; ^{19}F NMR (376 MHz, CDCl_3) δ -56.20; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{34}\text{H}_{30}\text{ClF}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 688.1201, found 688.1205. $[\alpha]_{\text{D}}^{20} = -78$ ($c = 0.1$, CHCl_3). HPLC conditions: Daicel Chiralpak OD-H column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 8.4 min, tr (minor) = 15.7 min, 93% e.e.



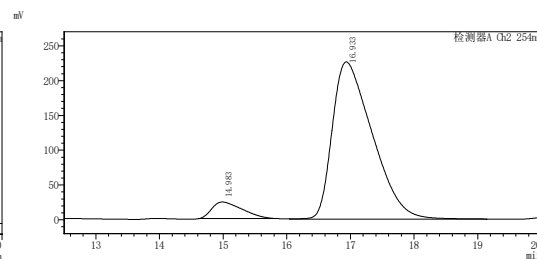
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	8.451	4895977	50.357	1	8.449	17301456	96.724
2	15.419	4826586	49.643	2	15.707	586003	3.276

methyl (*R,Z*)-4-(*N*-((4-bromophenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (33), White solid (90 mg, 82%), ^1H NMR (400 MHz, CDCl_3) δ 8.25 – 8.17 (m, 1H), 7.78 – 7.72 (m, 1H), 7.71 – 7.64 (m, 2H), 7.30 – 7.26 (m, 2H), 7.20 (d, $J = 7.2$ Hz, 1H), 7.18 – 7.13 (m, 2H), 7.01 (d, $J = 8.3$ Hz, 2H), 6.93 – 6.89 (m, 1H), 6.89 – 6.80 (m, 4H), 6.53 (s, 1H), 6.46 (s, 1H), 6.33 (d, $J = 8.3$ Hz, 2H), 3.87 (s, 3H), 1.64 (s, 3H), 1.54 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.75, 164.74, 145.70, 144.16, 137.40, 137.10, 133.93, 133.25, 132.67, 131.98, 131.22, 130.72, 129.57 (q, $J = 33.9$ Hz), 128.66, 128.49, 128.11 (q, $J = 6.2$ Hz), 127.35, 126.57, 125.63, 124.43, 122.25 (q, $J = 273.9$ Hz), 119.19, 61.23, 52.72, 48.58, 31.40, 25.10; ^{19}F NMR (376 MHz, CDCl_3) δ -56.21; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{34}\text{H}_{30}\text{BrF}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 732.0695, found 732.0703. $[\alpha]_{\text{D}}^{20} = -78$ ($c = 0.1$, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 16.9 min, tr (minor) = 15.0 min, 85% e.e.

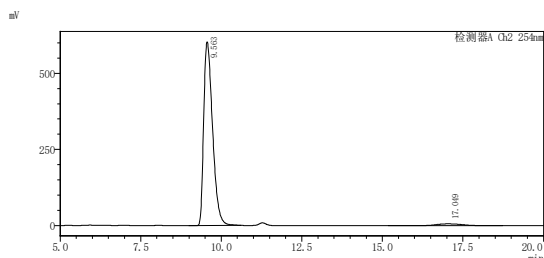
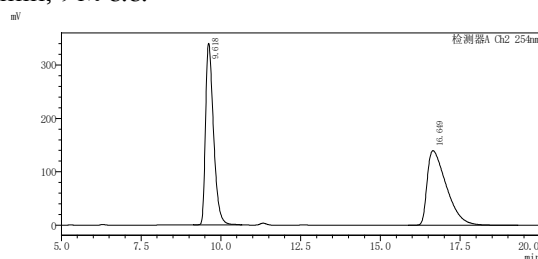
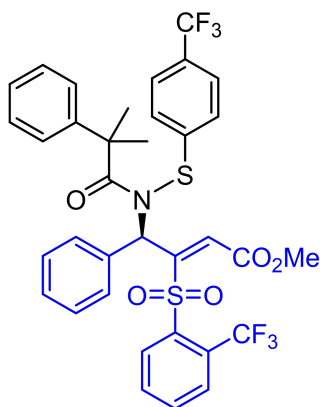




NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	15.033	12013164	49.772	1	14.983	783757	7.365
2	16.950	12123294	50.228	2	16.933	9857855	92.635

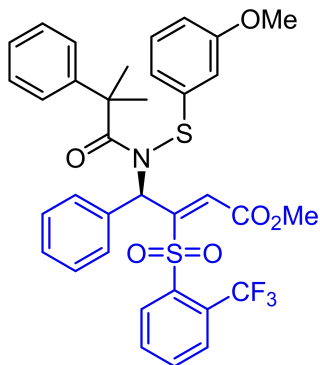


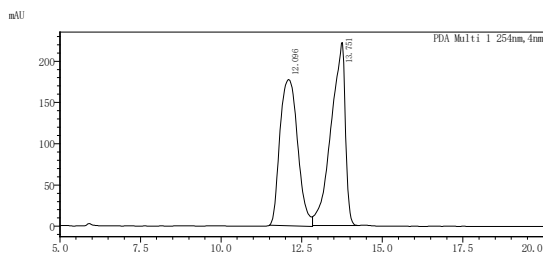
methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-((4-(trifluoromethyl)phenyl)thio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (34), White solid (79 mg, 73%), ^1H NMR (400 MHz, CDCl_3) δ 8.28 – 8.15 (m, 1H), 7.79 – 7.73 (m, 1H), 7.72 – 7.65 (m, 2H), 7.28 – 7.24 (m, 2H), 7.20 – 7.10 (m, 5H), 6.93 – 6.78 (m, 5H), 6.67 – 6.50 (m, 3H), 6.48 (s, 1H), 3.85 (s, 3H), 1.64 (s, 3H), 1.56 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.75, 164.70, 143.95, 143.11, 137.08, 134.01, 133.35, 132.02, 129.67 (q, J = 33.8 Hz), 128.77, 128.55, 128.19 (q, J = 6.2 Hz), 127.78, 127.45 (q, J = 2.3 Hz), 126.64, 125.66, 125.13, 124.56 (q, J = 4.0 Hz), 122.49, 121.67 (q, J = 152.1 Hz), 61.07, 52.72, 48.65; ^{19}F NMR (376 MHz, CDCl_3) δ -56.25, -62.55; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{30}\text{F}_6\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 722.1464, found 722.1465. $[\alpha]_{\text{D}}^{20}$ = -85 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 9.6 min, tr (minor) = 17.0 min, 94% e.e.



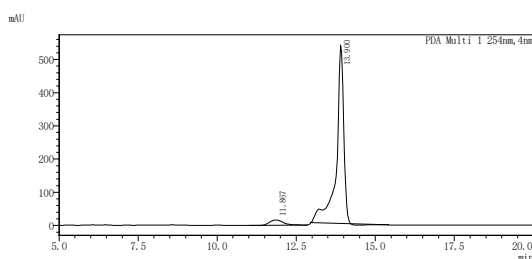
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	9.618	5903024	50.214	1	9.563	11540545	97.034
2	16.649	5852822	49.786	2	17.049	352720	2.966

methyl (*R,Z*)-4-(*N*-((3-methoxyphenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (35), White solid (73 mg, 71%), ^1H NMR (400 MHz, CDCl_3) δ 8.26 – 8.20 (m, 1H), 7.78 – 7.71 (m, 1H), 7.70 – 7.63 (m, 2H), 7.30 (t, J = 7.5 Hz, 2H), 7.23 – 7.19 (m, 1H), 7.16 (dd, J = 7.1, 1.7 Hz, 2H), 6.92 – 6.85 (m, 3H), 6.82 (t, J = 7.8 Hz, 3H), 6.54 (s, 1H), 6.49 (s, 1H), 6.42 (dd, J = 8.3, 2.4 Hz, 1H), 6.09 (dd, J = 7.7, 1.8 Hz, 1H), 5.99 (s, 1H), 3.88 (s, 3H), 3.63 (s, 3H), 1.67 (s, 3H), 1.53 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 181.07, 164.91, 158.97, 145.88, 144.53, 139.69, 137.30, 133.89, 133.35, 131.99, 131.46, 129.70 (q, J = 33.8 Hz), 128.75, 128.53, 128.49, 128.15 (q, J = 6.1 Hz), 127.21, 126.55, 125.75, 122.34 (q, J = 274.4 Hz), 115.13, 111.63, 108.68, 61.29, 55.19, 52.76, 48.67, 31.87, 25.01; ^{19}F NMR (376 MHz, CDCl_3) δ -56.26; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{33}\text{F}_3\text{NO}_6\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 684.1696, found 684.1696. $[\alpha]_{\text{D}}^{20}$ = -73 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 13.9 min, tr (minor) = 11.8 min, 90% e.e.

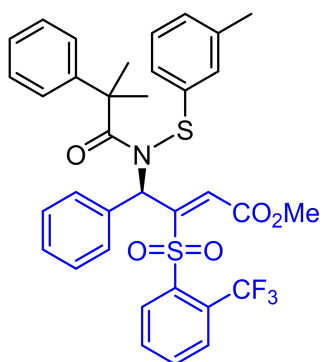




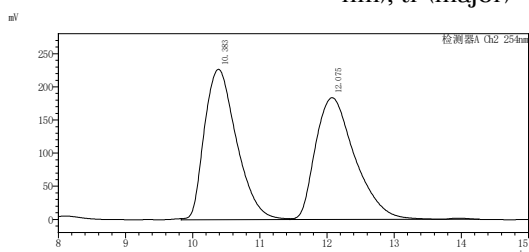
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	12.096	6818973	50.035	1	11.867	472829	5.116
2	13.751	6809363	49.965	2	13.900	8769370	94.884



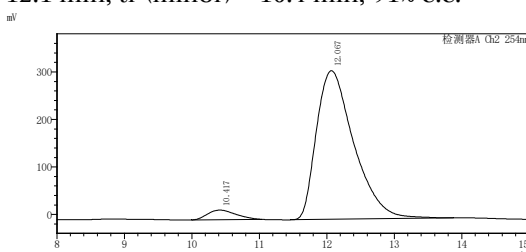
methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(*m*-tolylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (36), White solid (76 mg, 76%), ^1H NMR (400 MHz, CDCl_3) δ



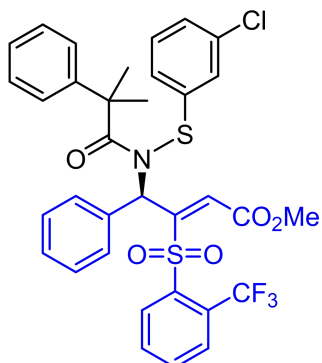
8.28 – 8.16 (m, 1H), 7.76 – 7.71 (m, 1H), 7.71 – 7.62 (m, 2H), 7.30 (t, $J = 7.4$ Hz, 2H), 7.22 (d, $J = 7.2$ Hz, 1H), 7.20 – 7.15 (m, 2H), 6.91 – 6.83 (m, 3H), 6.83 – 6.75 (m, 3H), 6.67 (d, $J = 7.6$ Hz, 1H), 6.52 (d, $J = 10.0$ Hz, 2H), 6.30 (d, $J = 7.9$ Hz, 1H), 6.18 (s, 1H), 3.89 (s, 3H), 2.07 (s, 3H), 1.67 (s, 3H), 1.54 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 181.13, 164.97, 146.02, 144.62, 137.91, 137.57, 137.35, 133.91, 133.31, 132.01, 131.90, 131.47, 129.63 (q, $J = 33.8$ Hz), 128.47, 128.45, 128.13 (q, $J = 6.1$ Hz), 127.67, 127.08, 126.53, 126.50, 125.76, 123.65, 122.35 (q, $J = 274.5$ Hz), 119.89, 61.42, 52.77, 48.67, 31.94, 24.90, 21.12; ^{19}F NMR (376 MHz, CDCl_3) δ -56.23; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{33}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 668.1747, found 668.1746. $[\alpha]_{\text{D}}^{20} = -51$ (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 12.1 min, tr (minor) = 10.4 min, 91% e.e.



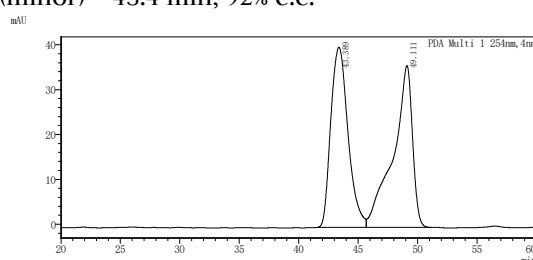
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	10.383	7534417	49.976	1	10.417	587665	4.645
2	12.075	7541554	50.024	2	12.067	12064240	95.355

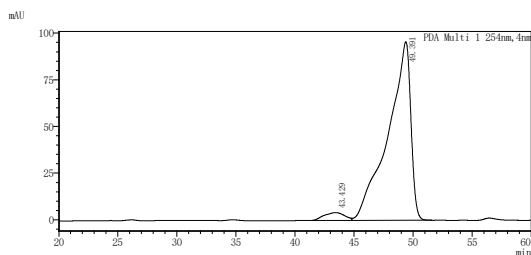


methyl (*R,Z*)-4-(*N*-((3-chlorophenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (37), White solid (65 mg, 63%), ^1H NMR (400 MHz, CDCl_3) δ



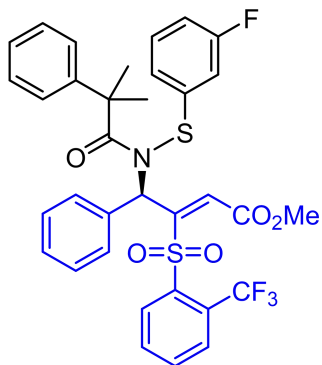
8.19 (dt, $J = 7.6, 3.9$ Hz, 1H), 7.78 – 7.70 (m, 1H), 7.70 – 7.63 (m, 2H), 7.30 – 7.25 (m, 2H), 7.21 – 7.12 (m, 3H), 6.94 – 6.75 (m, 7H), 6.55 (s, 1H), 6.47 (s, 1H), 6.38 – 6.26 (m, 2H), 3.88 (s, 3H), 1.65 (s, 3H), 1.56 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.72, 164.74, 145.84, 144.05, 140.04, 137.09, 133.95, 133.75, 133.27, 131.97, 131.38, 129.61 (q, $J = 33.8$ Hz), 128.72, 128.69, 128.49, 128.12 (q, $J = 6.2$ Hz), 127.24, 126.56, 125.63, 125.58, 122.81, 122.27 (q, $J = 274.5$ Hz), 120.32, 61.21, 52.74, 48.60, 31.40, 25.05; ^{19}F NMR (376 MHz, CDCl_3) δ -56.23; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{34}\text{H}_{30}\text{ClF}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 688.1201, found 688.1204. $[\alpha]_{\text{D}}^{20} = -95$ (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak IC column (98: 2 hexane: 2-propanol, 0.5 mL/min, 40 °C, 254 nm); tr (major) = 49.4 min, tr (minor) = 43.4 min, 92% e.e.





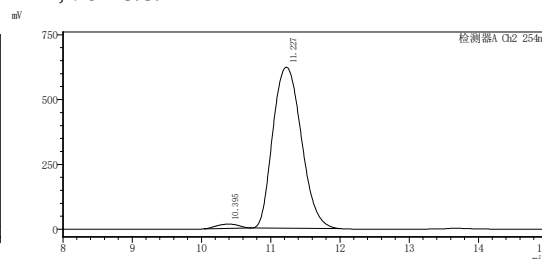
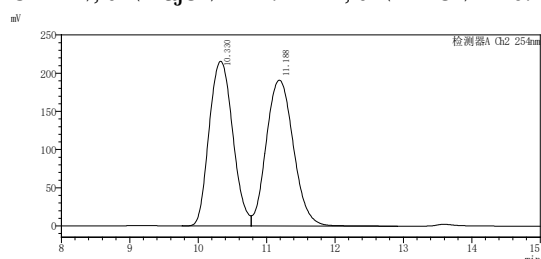
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	43.389	4049656	49.785	1	43.429	498428	3.742
2	49.111	4084708	50.215	2	49.391	12822951	96.258

methyl (*R,Z*)-4-(*N*-((3-fluorophenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (38), White solid (68 mg, 67%), ¹H NMR (400 MHz, CDCl₃) δ



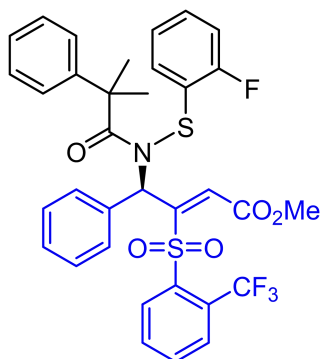
8.20 (dd, J = 5.7, 3.5 Hz, 1H), 7.78 – 7.71 (dt, J = 7.7, 3.7 Hz, 1H), 7.71 – 7.64 (m, 2H), 7.29 (t, J = 7.5 Hz, 2H), 7.22 – 7.14 (m, 3H), 6.93 – 6.80 (m, 6H), 6.59 – 6.50 (m, 2H), 6.47 (s, 1H), 6.25 (dd, J = 7.8, 1.8 Hz, 1H), 6.12 (dt, J = 9.4, 2.2 Hz, 1H), 3.88 (s, 3H), 1.65 (s, 3H), 1.55 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 180.73, 164.74, 163.11, 160.64, 145.85, 144.13, 140.68, 140.61, 137.09, 133.94, 133.25, 131.96, 131.43, 129.60 (q, J = 33.8 Hz), 129.14 (d, J = 8.4 Hz), 128.80 (d, J = 5.5 Hz), 128.66, 128.47, 128.11 (q, J = 6.2 Hz), 127.22, 126.57, 125.64, 122.26 (q, J = 274.4 Hz), 118.03 (d, J = 3.0 Hz), 112.48 (d, J = 21.4 Hz), 110.13 (d, J = 25.0 Hz), 61.21, 52.71, 48.58, 31.58, 24.88; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.23, -112.63 (td, J = 8.9, 5.6 Hz); HRMS (ESI-TOF). (m/z): Calcd for C₃₄H₃₀F₄NO₅S₂⁺, ([M + H]⁺), 672.1496, found 672.1495. [α]_D²⁰ = -23 (c = 0.1, CHCl₃). HPLC conditions:

Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 11.2 min, tr (minor) = 10.4 min, 96% e.e.

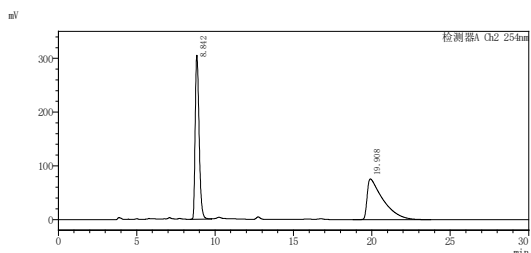


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	10.330	5182905	49.452	1	10.395	374153	2.052
2	11.188	5297820	50.548	2	11.227	17861827	97.948

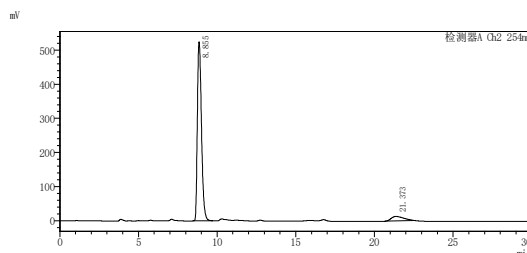
methyl (*R,Z*)-4-(*N*-((2-fluorophenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (39), White solid (63 mg, 62%), ¹H NMR (400 MHz, CDCl₃) δ



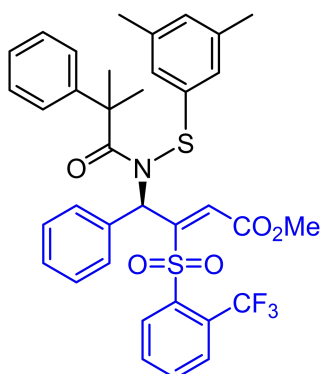
8.31 – 8.24 (m, 1H), 7.84 – 7.79 (m, 1H), 7.77 – 7.69 (m, 2H), 7.39 – 7.30 (m, 3H), 7.25 – 7.22 (m, 2H), 6.99 (d, J = 7.4 Hz, 2H), 6.95 – 6.85 (m, 4H), 6.78 (t, J = 7.6 Hz, 1H), 6.67 – 6.52 (m, 4H), 3.94 (s, 3H), 1.73 (s, 3H), 1.61 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 181.05, 164.80, 157.21, 154.79, 145.74, 144.03, 137.23, 133.88, 133.26, 131.97, 131.23, 129.59 (q, J = 34.2 Hz), 128.63, 128.49, 128.09 (q, J = 6.3 Hz), 127.21, 126.97 (d, J = 7.5 Hz), 126.60, 125.91 (d, J = 2.4 Hz), 125.69, 125.27 (d, J = 15.1 Hz), 123.41 (d, J = 3.3 Hz), 122.27 (q, J = 274.3 Hz), 114.60 (d, J = 20.3 Hz), 61.04, 52.72, 48.66, 31.57, 24.95; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.23, -114.87 (d, J = 11.4 Hz); HRMS (ESI-TOF). (m/z): Calcd for C₃₄H₃₀F₄NO₅S₂⁺, ([M + H]⁺), 672.1496, found 672.1495. [α]_D²⁰ = -43 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 21.3 min, tr (minor) = 8.8 min, 86% e.e.



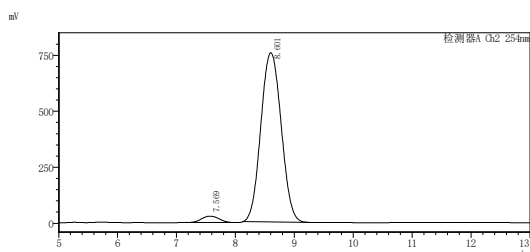
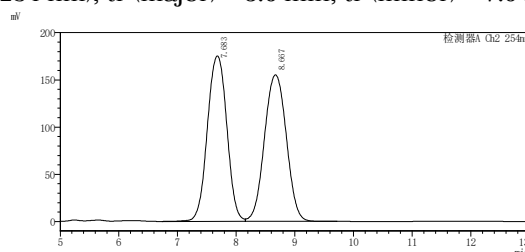
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	8.842	5316872	50.034	1	8.855	9512140	92.632
2	19.908	5309649	49.966	2	21.373	756648	7.368



methyl (*R,Z*)-4-(*N*-((3,5-dimethylphenyl)thio)-2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (40), White solid (79 mg, 77%), ^1H NMR (400 MHz, CDCl_3) δ

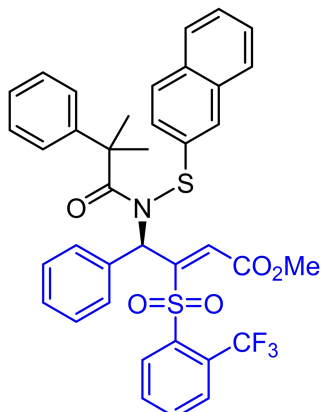


8.20 (dd, $J = 5.7, 3.5$ Hz, 1H), 7.77 – 7.70 (m, 1H), 7.69 – 7.26 (m, 2H), 7.30 (t, $J = 7.5$ Hz, 2H), 7.24 – 7.15 (m, 3H), 6.92 – 6.77 (m, 5H), 6.54 (d, $J = 3.2$ Hz, 2H), 6.48 (s, 1H), 6.03 (s, 2H), 3.88 (s, 3H), 2.04 (s, 6H), 1.67 (s, 3H), 1.54 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 181.06, 164.88, 145.93, 144.57, 137.54, 137.30, 137.24, 133.81, 133.18, 131.92, 131.31, 129.46 (q, $J = 33.9$ Hz), 128.80, 128.46, 128.34, 128.26, 128.01 (q, $J = 6.1$ Hz), 127.40, 126.88, 126.39, 125.63, 122.25 (q, $J = 274.5$ Hz), 120.58, 61.43, 52.63, 48.55, 31.77, 24.90, 20.88; ^{19}F NMR (376 MHz, CDCl_3) δ -56.21; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{36}\text{H}_{35}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 682.1903, found 682.1904. $[\alpha]_{\text{D}}^{20} = -25$ (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 8.6 min, tr (minor) = 7.6 min, 94% e.e.

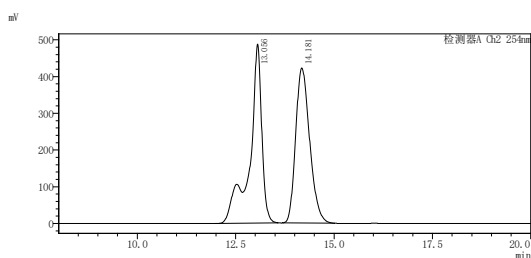


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.683	4051465	50.060	1	7.569	596390	3.178
2	8.667	4041711	49.940	2	8.601	18172694	96.822

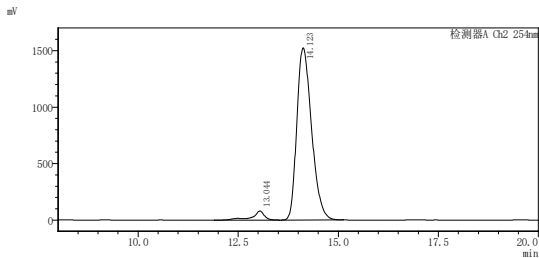
methyl (*R,Z*)-4-(2-methyl-*N*-(naphthalen-2-ylthio)-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (41), White solid (88 mg, 83%), ^1H NMR (400 MHz, CDCl_3) δ



8.24 (dd, $J = 5.8, 3.4$ Hz, 1H), 7.74 (dd, $J = 5.8, 3.6$ Hz, 1H), 7.69 – 7.60 (m, 3H), 7.49 (d, $J = 8.0$ Hz, 1H), 7.41 – 7.33 (m, 3H), 7.29 (t, $J = 7.7$ Hz, 2H), 7.22 – 7.15 (m, 3H), 6.91 (d, $J = 5.1$ Hz, 2H), 6.86 (s, 1H), 6.74 – 6.65 (m, 3H), 6.65 – 6.55 (m, 3H), 3.80 (s, 3H), 1.70 (s, 3H), 1.59 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 181.09, 164.84, 145.74, 144.42, 137.19, 135.48, 133.87, 133.32, 132.61, 131.97, 131.37, 131.06, 129.57 (q, $J = 34.2$ Hz), 128.78, 128.45, 128.41, 128.08 (q, $J = 6.2$ Hz), 127.47, 127.12, 126.85, 126.50, 126.47, 125.69, 125.49, 122.28 (q, $J = 274.9$ Hz), 121.52, 120.52, 61.40, 52.61, 48.67, 31.53, 25.21; ^{19}F NMR (376 MHz, CDCl_3) δ -56.19; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{38}\text{H}_{33}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 704.1747, found 704.1746. $[\alpha]_{\text{D}}^{20} = -41$ (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 14.1 min, tr (minor) = 13.0 min, 92% e.e.

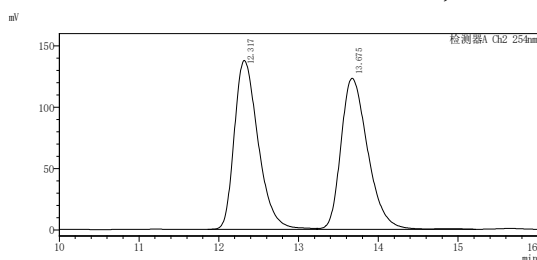


NO.	Time	Area	Area (%)
1	13.056	10446334	49.908
2	14.181	10484847	50.092

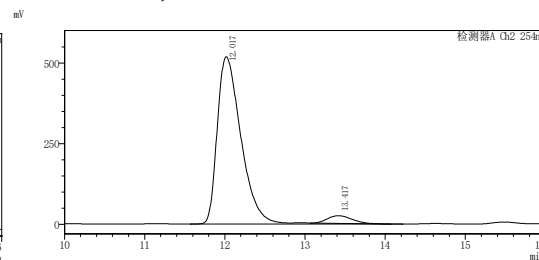


NO.	Time	Area	Area (%)
1	13.044	1672714	4.104
2	14.123	39084346	95.896

methyl (*R,Z*)-4-(2-methyl-2-phenyl-*N*-(thiophen-2-ylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (42), White solid (52 mg, 52%), ^1H NMR (400 MHz, CDCl_3) δ 8.23 (dd, J = 5.7, 3.5 Hz, 1H), 7.78 – 7.69 (m, 1H), 7.69 – 7.60 (m, 2H), 7.38 – 7.32 (m, 2H), 7.31 – 7.27 (m, 1H), 7.25 – 7.19 (m, 3H), 7.02 (t, J = 7.3 Hz, 1H), 6.93 (t, J = 7.6 Hz, 2H), 6.74 (s, 2H), 6.60 (dd, J = 5.3, 3.6 Hz, 1H), 6.56 (d, J = 1.0 Hz, 1H), 6.21 (s, 1H), 6.17 (dd, J = 3.7, 1.3 Hz, 1H), 3.85 (s, 3H), 1.84 (s, 3H), 1.61 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 179.61, 164.95, 146.09, 144.97, 137.82, 134.65, 134.47, 133.66, 133.00, 132.02, 131.53, 130.86, 130.15, 129.25 (q, J = 33.8 Hz), 128.80, 128.14, 128.01 (q, J = 6.4 Hz), 127.56, 126.63, 125.71, 122.26 (q, J = 274.5 Hz), 64.63, 52.71, 48.56, 31.31, 26.57; ^{19}F NMR (376 MHz, CDCl_3) δ -56.20; **HRMS** (ESI-TOF). (m/z): Calcd for $\text{C}_{32}\text{H}_{29}\text{F}_3\text{NO}_5\text{S}_3^+$, ($[\text{M} + \text{H}]^+$), 660.1154, found 660.1154. $[\alpha]_{\text{D}}^{20}$ = -51 (c = 0.1, CHCl_3). **HPLC** conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 12.0 min, tr (minor) = 13.4 min, 90% e.e.

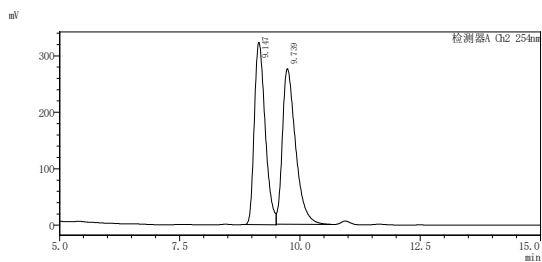


NO.	Time	Area	Area (%)
1	12.317	2859312	49.921
2	13.675	2868313	50.079

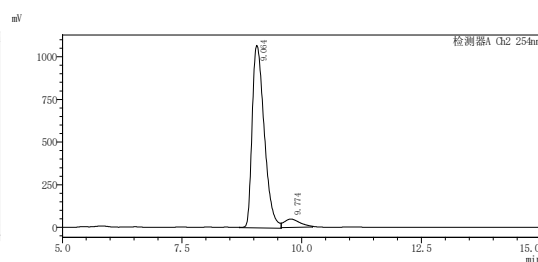


NO.	Time	Area	Area (%)
1	12.017	10747174	95.342
2	13.417	525112	4.658

methyl (*R,Z*)-4-(2-methyl-2-(*p*-tolyl)-*N*-(*p*-tolylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (43), White solid (74 mg, 72%), ^1H NMR (400 MHz, CDCl_3) δ 8.21 (dd, J = 5.7, 3.6 Hz, 1H), 7.75 – 7.70 (m, 1H), 7.69 – 7.62 (m, 2H), 7.10 (d, J = 8.1 Hz, 2H), 7.07 – 7.03 (m, 2H), 6.90 – 6.83 (m, 3H), 6.83 – 6.75 (m, 2H), 6.71 (d, J = 8.0 Hz, 2H), 6.49 (d, J = 11.3 Hz, 2H), 6.39 – 6.30 (m, 2H), 3.89 (s, 3H), 2.32 (s, 3H), 2.15 (s, 3H), 1.67 (s, 3H), 1.52 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 181.07, 164.92, 146.08, 141.55, 137.31, 135.95, 135.54, 134.78, 134.70, 133.77, 133.13, 131.89, 131.38, 130.22, 129.83 (q, J = 19.1 Hz), 129.04 (q, J = 44.6 Hz), 129.03, 128.42, 128.34, 127.99 (q, J = 6.2 Hz), 127.04, 125.56, 123.29, 122.24 (q, J = 274.4 Hz), 61.70, 52.64, 48.19, 31.84, 24.88, 20.96, 20.71; ^{19}F NMR (376 MHz, CDCl_3) δ -56.22; **HRMS** (ESI-TOF). (m/z): Calcd for $\text{C}_{36}\text{H}_{35}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 682.1903, found 682.1904. $[\alpha]_{\text{D}}^{20}$ = -14 (c = 0.1, CHCl_3). **HPLC** conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 9.1 min, tr (minor) = 9.8 min, 89% e.e.

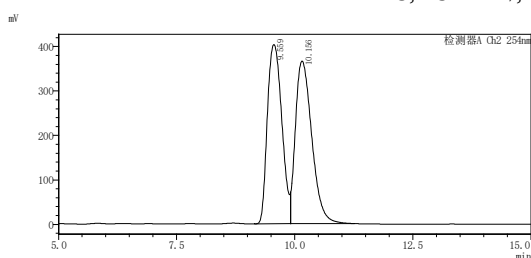
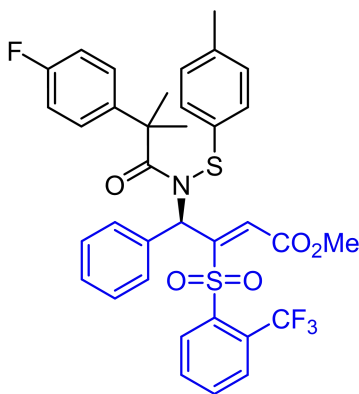


NO.	Time	Area	Area (%)
1	9.147	5092072	49.171
2	9.739	5263762	50.829

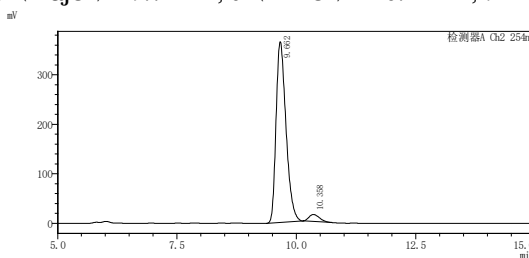


NO.	Time	Area	Area (%)
1	9.064	18850343	94.315
2	9.774	1136325	5.685

methyl (*R,Z*)-4-(2-(4-fluorophenyl)-2-methyl-*N*-(*p*-tolylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (44), White solid (72 mg, 70%), ^1H NMR (400 MHz, CDCl_3) δ 8.22 – 8.15 (m, 1H), 7.78 – 7.71 (m, 1H), 7.70 – 7.61 (m, 2H), 7.12 (dd, J = 8.6, 5.2 Hz, 2H), 7.00 – 6.93 (m, 2H), 6.92 – 6.85 (m, 3H), 6.85 – 6.78 (m, 2H), 6.72 (d, J = 7.9 Hz, 2H), 6.47 (d, J = 2.4 Hz, 2H), 6.34 (d, J = 8.0 Hz, 2H), 3.88 (s, 3H), 2.15 (s, 3H), 1.66 (s, 3H), 1.52 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.71, 164.79, 162.57, 160.13, 146.12, 140.32 (d, J = 3.3 Hz), 137.14, 135.73, 134.43, 133.88, 133.17, 131.86 (d, J = 10.4 Hz), 131.28, 129.57 (q, J = 34.0 Hz), 128.50 (d, J = 5.8 Hz), 128.22, 128.07 (q, J = 6.3 Hz), 127.28 (q, J = 8.0 Hz), 127.17, 123.14, 122.27 (q, J = 274.4 Hz), 115.16 (q, J = 21.4 Hz), 61.59, 52.69, 48.10, 31.72, 25.21, 20.70; ^{19}F NMR (376 MHz, CDCl_3) δ -56.22, -116.29 (td, J = 8.7, 4.4 Hz); HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{32}\text{F}_4\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 686.1653, found 686.1654. $[\alpha]_{\text{D}}^{20}$ = -22 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 $^\circ\text{C}$, 254 nm); tr (major) = 9.7 min, tr (minor) = 10.4 min, 92% e.e.

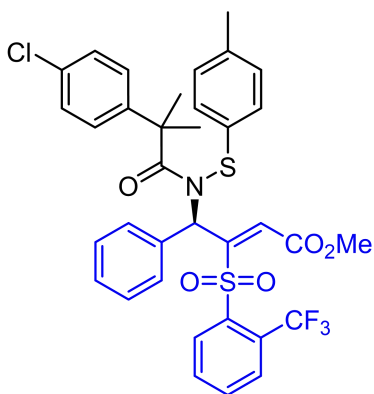


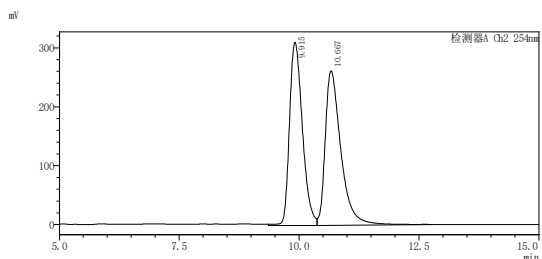
NO.	Time	Area	Area (%)
1	9.559	8617992	49.545
2	10.156	8776390	50.455



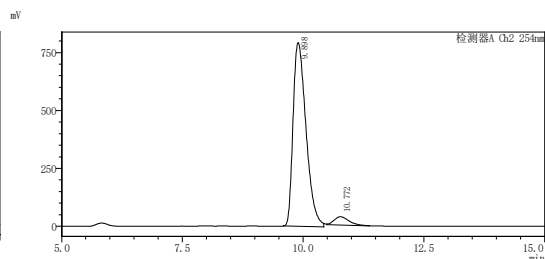
NO.	Time	Area	Area (%)
1	9.662	5275705	96.059
2	10.358	216449	3.941

methyl (*R,Z*)-4-(2-(4-chlorophenyl)-2-methyl-*N*-(*p*-tolylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (45), White solid (72 mg, 68%), ^1H NMR (400 MHz, CDCl_3) δ 8.25 – 8.15 (m, 1H), 7.77 – 7.72 (m, 1H), 7.71 – 7.63 (m, 2H), 7.25 – 7.19 (m, 2H), 7.10 – 7.04 (m, 2H), 6.94 – 6.87 (m, 3H), 6.87 – 6.80 (m, 2H), 6.71 (d, J = 8.0 Hz, 2H), 6.49 (d, J = 12.1 Hz, 2H), 6.32 (d, J = 8.3 Hz, 2H), 3.87 (s, 3H), 2.15 (s, 3H), 1.64 (s, 3H), 1.52 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.55, 164.76, 146.20, 143.10, 137.20, 135.78, 134.33, 133.86, 133.19, 132.15, 131.92, 131.23, 129.59 (q, J = 33.8 Hz), 128.55, 128.52, 128.34, 128.09 (q, J = 6.2 Hz), 127.26, 127.07, 123.09, 122.28 (q, J = 274.7 Hz), 61.71, 52.73, 48.26, 31.30, 25.37, 20.74; ^{19}F NMR (376 MHz, CDCl_3) δ -56.24; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{32}\text{ClF}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 702.1357, found 702.1357. $[\alpha]_{\text{D}}^{20}$ = -42 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 $^\circ\text{C}$, 254 nm); tr (major) = 9.9 min, tr (minor) = 10.8 min, 90% e.e.



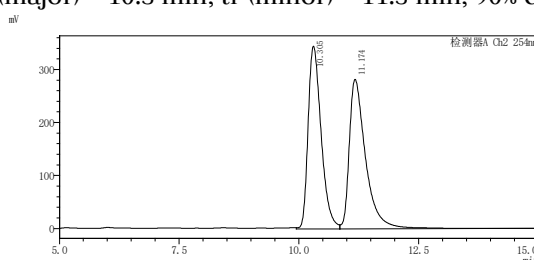
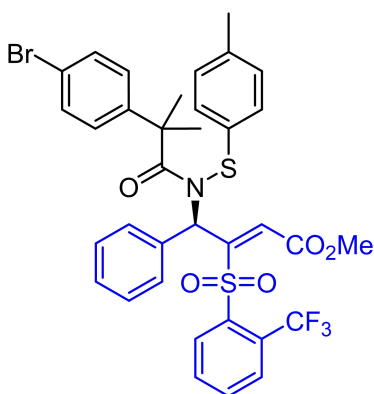


NO.	Time	Area	Area (%)
1	9.915	5829099	49.513
2	10.667	5943741	50.487

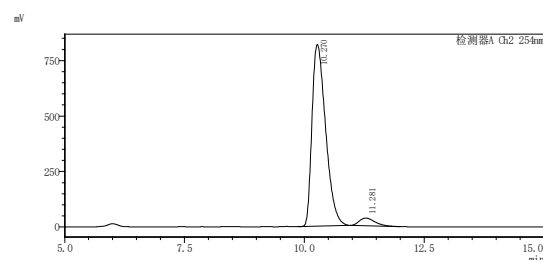


NO.	Time	Area	Area (%)
1	9.898	14785484	95.053
2	10.772	769533	4.947

methyl (*R,Z*)-4-(2-(4-bromophenyl)-2-methyl-N-(p-tolylthio)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (46), White solid (72 mg, 64%), ^1H NMR (400 MHz, CDCl_3) δ 8.24 – 8.15 (m, 1H), 7.78 – 7.71 (m, 1H), 7.70 – 7.63 (m, 2H), 7.39 – 7.32 (m, 2H), 7.04 – 6.97 (m, 2H), 6.94 – 6.87 (m, 3H), 6.87 – 6.80 (m, 2H), 6.71 (d, J = 8.2 Hz, 2H), 6.51 (s, 1H), 6.47 (s, 1H), 6.31 (d, J = 8.2 Hz, 2H), 3.87 (s, 3H), 2.16 (s, 3H), 1.63 (s, 3H), 1.52 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 180.50, 164.76, 146.21, 143.61, 137.23, 135.80, 134.32, 133.85, 133.20, 131.93, 131.47, 131.21, 129.61 (q, J = 33.8 Hz), 128.56, 128.54, 128.40, 128.10 (q, J = 6.2 Hz), 127.45, 127.29, 123.08, 122.28 (q, J = 274.3 Hz), 120.26, 61.76, 52.75, 48.35, 31.15, 25.46, 20.78; ^{19}F NMR (376 MHz, CDCl_3) δ -56.25; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{32}\text{BrF}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 746.0852, found 746.0851. $[\alpha]_{\text{D}}^{20}$ = -48 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 10.3 min, tr (minor) = 11.3 min, 90% e.e.

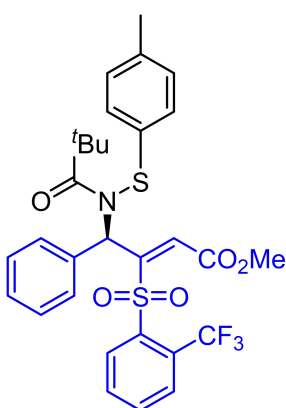


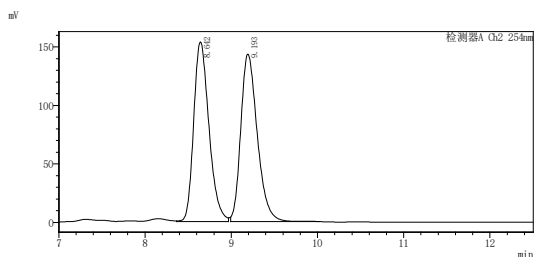
NO.	Time	Area	Area (%)
1	10.305	6525253	49.173
2	11.174	6744789	50.827



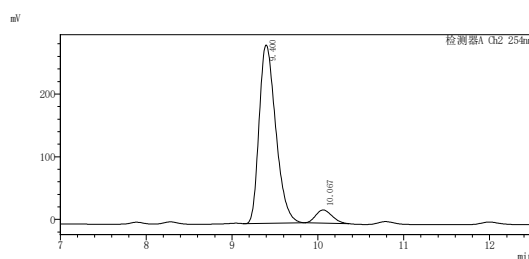
NO.	Time	Area	Area (%)
1	10.270	16197235	95.299
2	11.281	799028	4.701

methyl (*R,Z*)-4-phenyl-4-(*N*-(p-tolylthio)pivalamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (47), White solid (76 mg, 84%), ^1H NMR (400 MHz, CDCl_3) δ 8.24 – 8.17 (m, 1H), 7.78 – 7.72 (m, 1H), 7.69 – 7.62 (m, 2H), 7.01 – 6.96 (m, 3H), 6.95 – 6.90 (m, 2H), 6.85 (d, J = 7.9 Hz, 2H), 6.70 (s, 1H), 6.59 (d, J = 7.9 Hz, 2H), 6.49 (s, 1H), 3.76 (s, 3H), 2.20 (s, 3H), 1.39 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.99, 164.77, 147.25, 137.55, 135.85, 135.22, 133.68, 133.03, 132.74, 131.94, 130.89, 129.29 (q, J = 33.7 Hz), 128.91, 128.62, 128.37, 128.13, 128.04 (q, J = 6.1 Hz), 127.40, 123.23, 122.29 (q, J = 274.6 Hz), 62.75, 52.58, 41.52, 28.28, 20.81; ^{19}F NMR (376 MHz, CDCl_3) δ -56.36; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{30}\text{H}_{31}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 606.1590, found 606.1594. $[\alpha]_{\text{D}}^{20}$ = -71 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 10.1 min, tr (minor) = 9.4 min, 84% e.e.

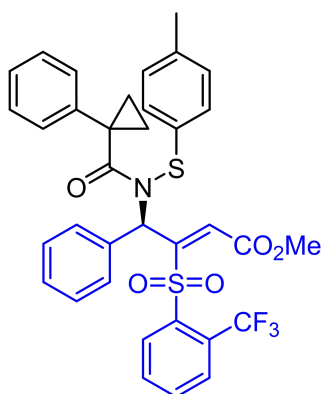




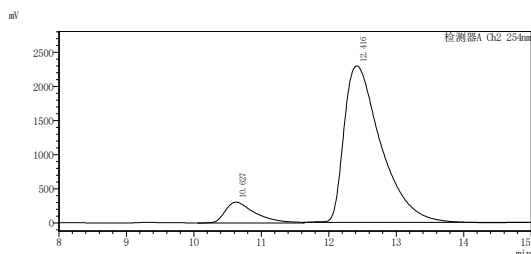
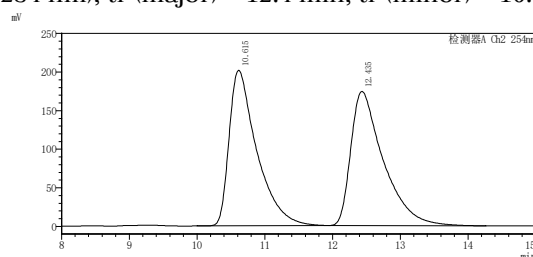
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	8.642	1887632	49.815	1	9.400	3834626	93.282
2	9.193	1901617	50.185	2	10.067	276150	6.718



methyl (R,Z)-4-phenyl-4-(1-phenyl-N-(p-tolylthio)cyclopropane-1-carboxamido)-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (48), White solid (69 mg, 69%), ^1H NMR (400 MHz, CDCl_3) δ



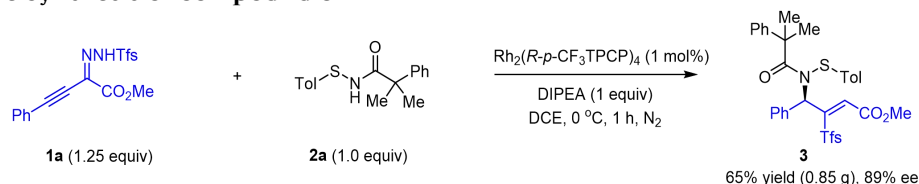
8.22 – 8.12 (m, 1H), 7.73 – 7.66 (m, 1H), 7.66 – 7.59 (m, 2H), 7.37 – 7.14 (m, 6H), 6.96 (t, J = 7.3 Hz, 1H), 6.86 (t, J = 7.5 Hz, 2H), 6.77 (d, J = 8.0 Hz, 3H), 6.54 (s, 1H), 6.45 – 6.30 (m, 3H), 3.81 (s, 3H), 2.18 (s, 3H), 1.64 – 1.54 (m, 1H), 1.49 – 1.34 (m, 1H), 1.15 (dt, J = 10.2, 6.2 Hz, 1H), 0.90 – 0.83 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 164.75, 146.19, 139.64, 137.47, 134.29, 133.76, 133.24, 132.69, 132.00, 130.73, 129.37, 128.89, 128.54, 128.40, 128.00 (q, J = 21.8 Hz), 127.72, 127.44, 126.80, 122.20 (q, J = 272.2 Hz), 61.63, 52.63, 31.12, 20.87, 15.10, 12.40; ^{19}F NMR (376 MHz, CDCl_3) δ -56.26; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{30}\text{F}_3\text{NO}_5\text{S}_2^+$, ($[\text{M} + \text{H}]^+$), 665.1517, found 665.1516. $[\alpha]_{\text{D}}^{20}$ = -17 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 12.4 min, tr (minor) = 10.6 min, 81% e.e.



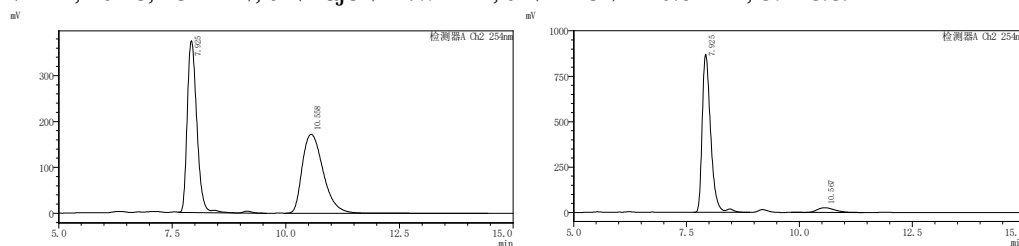
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	10.615	5714261	49.573	1	10.627	8925129	9.349
2	12.435	5812664	50.427	2	12.416	86546002	90.651

4. Synthetic Applications

4.1 Gram-scale Synthesis of Compound 3

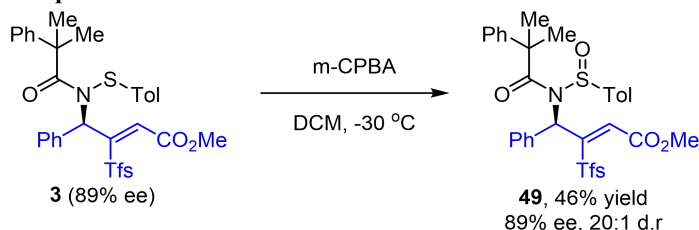


In nitrogen atmosphere, sulfenamide (2.0 mmol), $\text{Rh}_2(\text{R-}p\text{-CF}_3\text{TPCP})_4$ (1 mol%), DCE (7 mL), and DIPEA (1.0 equiv) were sequentially added to a schlenk tube (50 mL) with a stir bar. Then the vial was cooled to 0 °C using ice bath. A solution of alkynyl sulfonylhydrazone (1.25 equiv) in DCE (14 mL) was added dropwise to the mixture using a syringe and stirred for 30–60 minutes. After the reaction completed, the reaction mixture was washed with aqueous NH_4Cl solution and diluted with EtOAc. The organic layer was dried over Na_2SO_4 , filtered, and concentrated. The residue was purified with silica gel chromatography to give the products 3 (65% yield). HPLC conditions: Daicel Chiralpak OD-3 column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.9 min, tr (minor) = 10.6 min, 89% e.e.



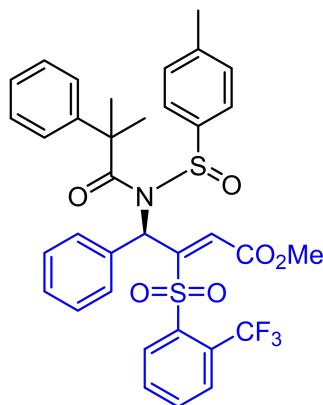
NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.925	5577397	50.023	1	7.925	11376471	94.408
2	10.558	5572279	49.977	2	10.567	673830	5.592

4.2 Transformation of Compound 3

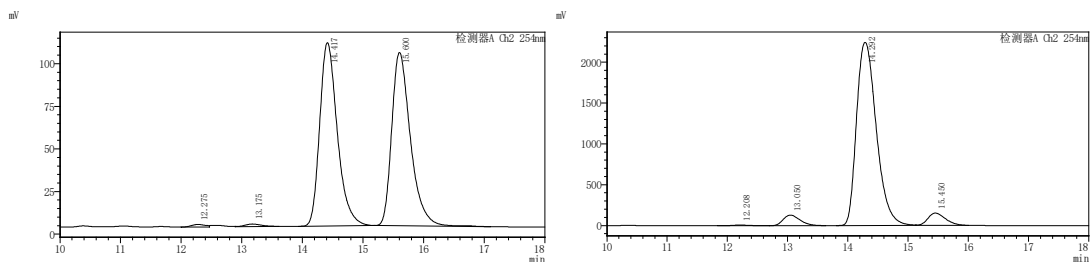


A dry reaction tube was charged with 3 (0.1 mmol, 1.0 equiv) and CH_2Cl_2 (1 mL) was added. The reaction was stirred at -30 °C for 10 min. To this was added *m*-CPBA (0.12 mmol, 1.2 equiv), and the reaction was stirred for a further 3 h. The residue was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate = 2:1) to afford the product 49.

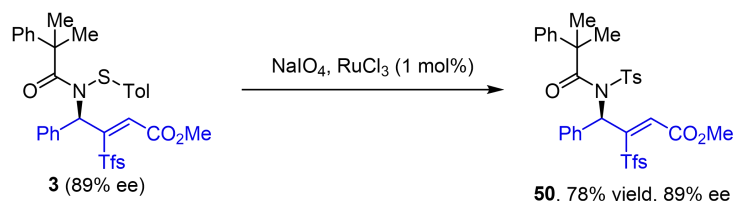
methyl (4*R*,*Z*)-4-(2-methyl-2-phenyl-*N*-(*p*-tolylsulfinyl)propanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (49), White solid (32 mg, 46%), ^1H NMR (400 MHz, CDCl_3) δ



8.28 (d, J = 7.6 Hz, 1H), 7.68 (d, J = 7.3 Hz, 1H), 7.64 – 7.55 (m, 2H), 7.29 (d, J = 7.3 Hz, 1H), 7.24 – 7.19 (m, 1H), 7.18 – 7.06 (m, 3H), 6.91 (t, J = 7.3 Hz, 1H), 6.86 – 6.75 (m, 4H), 6.67 (s, 1H), 6.47 (d, J = 7.7 Hz, 2H), 6.31 (d, J = 7.9 Hz, 2H), 5.41 (s, 1H), 3.60 (s, 3H), 2.11 (s, 3H), 1.91 (s, 3H), 1.44 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 177.10, 164.73, 145.43, 144.52, 143.02, 138.64, 136.43, 135.47, 134.52, 133.11, 132.44, 132.02, 129.39, 129.00, 128.59 (q, J = 11.0 Hz), 128.20, 127.77 (q, J = 6.2 Hz), 127.40, 127.28, 127.02, 126.13, 125.53, 122.32 (q, J = 274.9 Hz), 56.39, 52.40, 49.20, 32.37, 24.47, 21.17; ^{19}F NMR (376 MHz, CDCl_3) δ -56.46; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{35}\text{H}_{33}\text{F}_3\text{NO}_6\text{S}_2^+$, ($[M + H]^+$), 684.1696, found 684.1697. [α] $_{\text{D}}^{20}$ = -87 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak OD-3 column (95: 5 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 14.3 min, tr (minor) = 15.5 min, 89% e.e., 20:1 d.r.

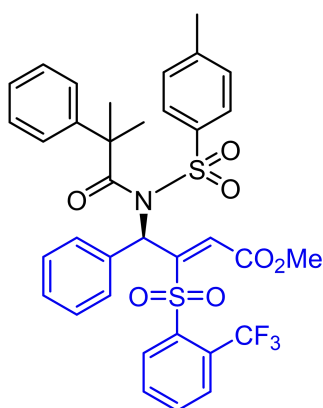


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	12.275	22953	0.521	1	12.208	161357	0.284
2	13.175	27042	0.614	2	13.050	2530397	4.446
3	14.417	2173377	49.336	3	14.292	51141028	89.856
4	15.600	2181857	49.529	4	15.450	3081746	5.415

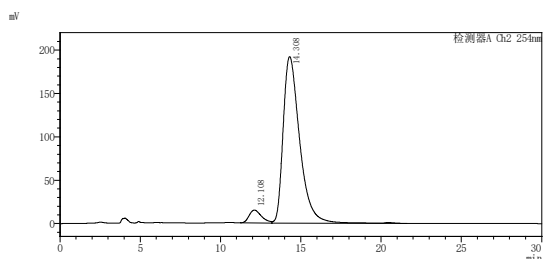
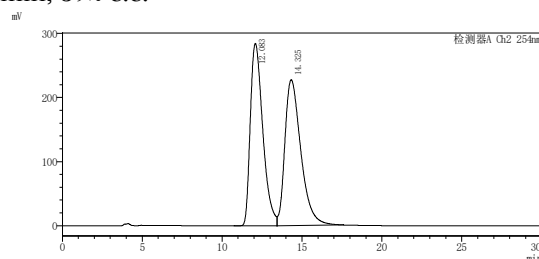


Prepared according to the modified literature procedure.⁶ In a round-bottomed flask with a stir bar, **3** (0.1 mmol, 1.0 equiv) was dissolved in MeCN (0.5 mL), CCl₄ (0.5 mL) and H₂O (1 mL). To this mixture were added NaIO₄ (3.0 equiv), and RuCl₃ (1 mol%). After stirring for 1 h at room temperature under a N₂ atmosphere. The mixture was extracted with CH₂Cl₂ three times. The combined organic layers were washed with brine and then passed through a short silica gel/Na₂SO₄ plug eluting with a CH₂Cl₂. The obtained solution was concentrated and the residue was purified by column chromatography on silica gel (petroleum ether: ethyl acetate = 3: 1) to afford the product **50**.

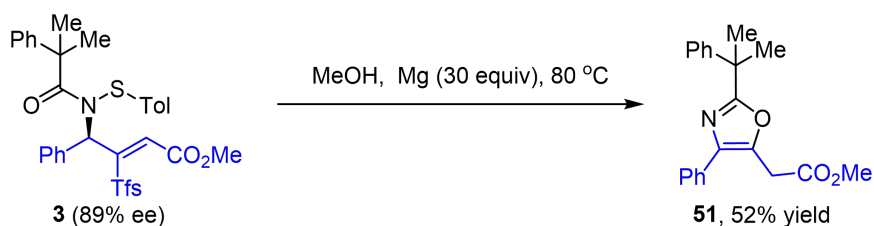
methyl (R,Z)-4-(2-methyl-2-phenyl-N-tosylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (50), White solid (55 mg, 78%), ¹H NMR (400 MHz, CDCl₃) δ



8.19 (dd, *J* = 6.8, 2.5 Hz, 1H), 7.57 – 7.48 (m, 2H), 7.48 – 7.41 (m, 2H), 7.41 – 7.28 (m, 5H), 6.98 (d, *J* = 8.2 Hz, 2H), 6.89 (t, *J* = 7.4 Hz, 1H), 6.86 – 6.80 (m, 2H), 6.60 (t, *J* = 7.8 Hz, 2H), 6.24 (d, *J* = 1.8 Hz, 1H), 6.11 (d, *J* = 8.2 Hz, 2H), 3.93 (s, 3H), 2.31 (s, 3H), 1.77 (s, 3H), 1.51 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 177.43, 165.39, 144.32, 144.28, 141.93, 138.78, 136.02, 134.86, 133.39, 132.94, 132.08 (d, *J* = 15.1 Hz), 131.25, 129.14, 128.68 (d, *J* = 5.8 Hz), 128.51, 128.17, 127.42 (q, *J* = 3.3 Hz), 126.69, 126.12, 121.67 (q, *J* = 274.5 Hz), 63.06, 52.76, 50.16, 32.26, 23.76, 21.47; ¹⁹F NMR (376 MHz, CDCl₃) δ -56.23; HRMS (ESI-TOF). (*m/z*): Calcd for (C₃₅H₃₃F₃NO₇S₂⁺ NH₄)⁺, ([*M* + NH₄]⁺), 717.1911, found 717.1903. [*α*]_D²⁰ = -79 (*c* = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OJ-H column (90: 10 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 14.3 min, tr (minor) = 12.1 min, 89% e.e.

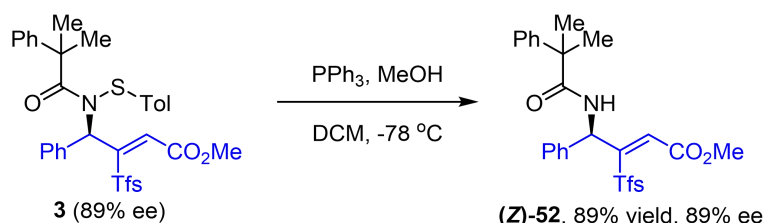
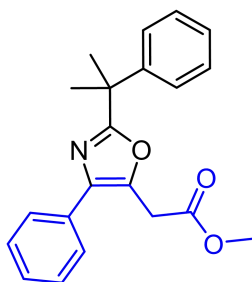


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	12.083	15455282	49.311	1	12.108	794887	5.474
2	14.325	15886876	50.689	2	14.308	13727171	94.526

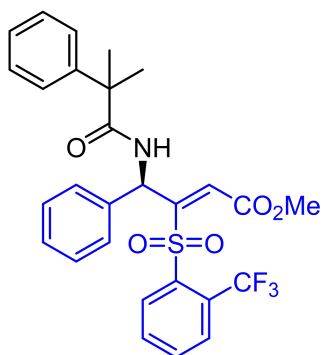


A dry reaction tube was charged with **3** (0.1 mmol, 1.0 equiv), Mg (30 equiv) and MeOH (4 mL) was added. The reaction was stirred at 40 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate = 2:1) to afford the oxazole product **51**.

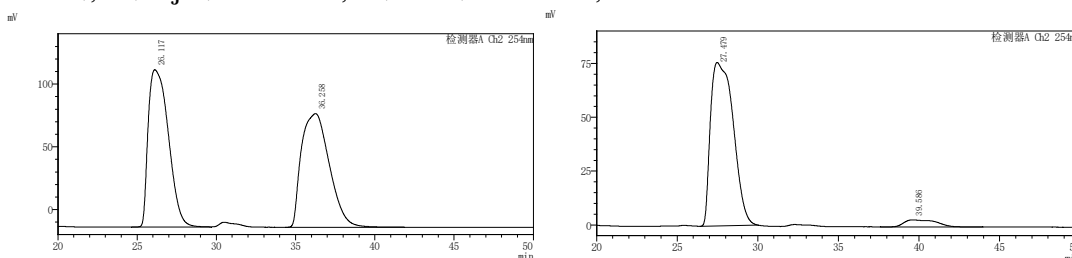
methyl 2-(4-phenyl-2-(2-phenylpropan-2-yl)oxazol-5-yl)acetate (51), White solid (18 mg, 52%), ^1H NMR (400 MHz, CDCl_3) δ 7.70 – 7.64 (m, 2H), 7.46 – 7.40 (m, 2H), 7.36 – 7.27 (m, 5H), 7.26 – 7.19 (m, 1H), 3.83 (s, 2H), 3.70 (s, 3H), 1.82 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 169.20, 168.44, 146.15, 139.56, 136.88, 131.73, 128.66, 128.33, 127.77, 127.12, 126.51, 125.72, 52.40, 41.30, 32.00, 28.01; **HRMS** (ESI-TOF). (m/z): Calcd for $\text{C}_{21}\text{H}_{22}\text{NO}_3^+$, ($[\text{M} + \text{H}]^+$), 336.1594, found 336.1596.



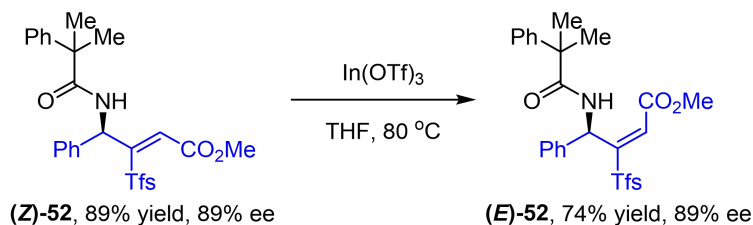
Prepared according to the modified literature procedure.⁷ A dry reaction tube was charged with **3** (0.1 mmol, 1.0 equiv.) and then CH_2Cl_2 (1 mL) was added. The reaction was stirred at -78 °C for 10 min. To this was added Ph_3P (0.11 mmol, 1.1 equiv.) and MeOH (10 μL), and the reaction was stirred for a further 3 h. The residue was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate = 2:1) to afford the product **(Z)-52**.



methyl (R,Z)-4-(2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate ((Z)-52), White solid (49 mg, 89%), ^1H NMR (400 MHz, CDCl_3) δ 8.04 (dd, J = 7.6, 1.6 Hz, 1H), 7.70 (dd, J = 7.7, 1.7 Hz, 1H), 7.63 – 7.51 (m, 2H), 7.25 – 7.14 (m, 5H), 7.10 – 7.04 (m, 3H), 6.86 – 6.78 (m, 2H), 6.02 (s, 1H), 5.94 (d, J = 7.9 Hz, 1H), 5.74 (d, J = 7.9 Hz, 1H), 3.50 (s, 3H), 1.44 (s, 3H), 1.38 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 175.78, 164.33, 148.15, 144.29, 137.43, 136.83, 134.06, 132.46 (d, J = 10.3 Hz), 130.75, 129.14, 128.86 (d, J = 1.7 Hz), 128.37 (q, J = 6.2 Hz), 128.13, 127.29, 126.95, 126.25, 122.56 (q, J = 274.5 Hz), 53.92, 52.62, 46.78, 26.87, 26.21; ^{19}F NMR (376 MHz, CDCl_3) δ -56.20; **HRMS** (ESI-TOF). (m/z): Calcd for $\text{C}_{28}\text{H}_{27}\text{F}_3\text{NO}_5\text{S}^+$, ($[\text{M} + \text{H}]^+$), 546.1557, found 546.1557. $[\alpha]_{\text{D}}^{20}$ = +19 (c = 0.1, CHCl_3). **HPLC** conditions: Daicel Chiralpak AD-3 column (90: 10 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 27.5 min, tr (minor) = 39.5 min, 89% e.e.

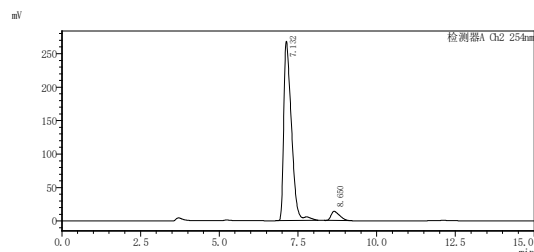
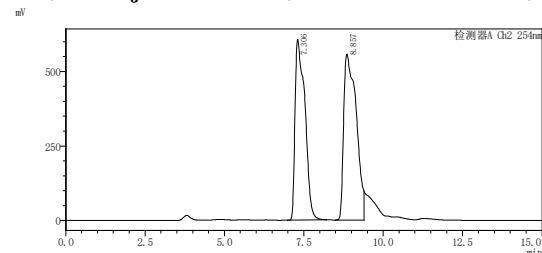
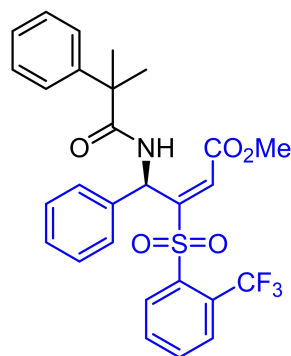


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	26.117	11106070	50.002	1	27.479	7442993	94.279
2	36.258	11105058	49.998	2	39.586	451662	5.721

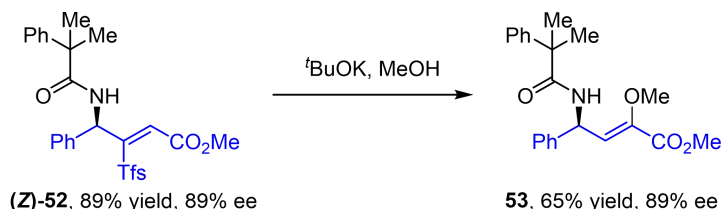


A dry reaction tube was charged with **Z-52** (0.1 mmol, 1.0 equiv), $\text{In}(\text{OTf})_3$ (1 equiv) and THF (1 mL) was added. The reaction was stirred at 80 °C for 12 h. The residue was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate = 2:1) to afford the product (**E-52**).

methyl (*R,E*)-4-(2-methyl-2-phenylpropanamido)-4-phenyl-3-((2-(trifluoromethyl)phenyl)sulfonyl)but-2-enoate (E-52**)**, White solid (41 mg, 74%), ^1H NMR (400 MHz, CDCl_3) δ 8.33 (dd, J = 7.2, 2.1 Hz, 1H), 7.81 (dd, J = 6.8, 2.3 Hz, 1H), 7.77 – 7.68 (m, 2H), 7.28 – 7.23 (m, 2H), 7.20 – 7.18 (m, 1H), 7.17 – 7.14 (m, 2H), 7.11 – 7.03 (m, 4H), 7.00 (d, J = 9.9 Hz, 1H), 6.94 – 6.86 (m, 2H), 6.24 (d, J = 9.8 Hz, 1H), 3.29 (s, 3H), 1.42 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 175.53, 164.54, 155.46, 144.35, 137.54, 135.35, 135.12, 134.38, 132.90, 129.69, 129.16 (q, J = 33.6 Hz), 128.60, 128.46 (q, J = 6.2 Hz), 128.08, 127.35, 126.94, 126.20, 125.83, 122.60 (q, J = 274.3 Hz), 52.56, 48.23, 46.73, 26.55, 26.48; ^{19}F NMR (376 MHz, CDCl_3) δ -56.19; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{28}\text{H}_{27}\text{F}_3\text{NO}_5\text{S}^+$, ($[\text{M} + \text{H}]^+$), 546.1557, found 546.1555. $[\alpha]_{\text{D}}^{20}$ = +38 (c = 0.1, CHCl_3). HPLC conditions: Daicel Chiralpak AD-3 column (80: 20 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.1 min, tr (minor) = 8.6 min, 89% e.e.

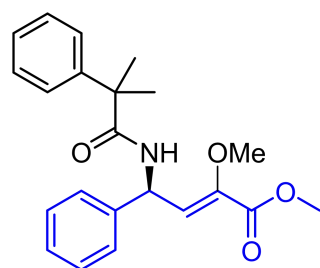


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.306	13119877	46.119	1	7.132	4542767	94.576
2	8.857	15328142	53.881	2	8.650	260521	5.424

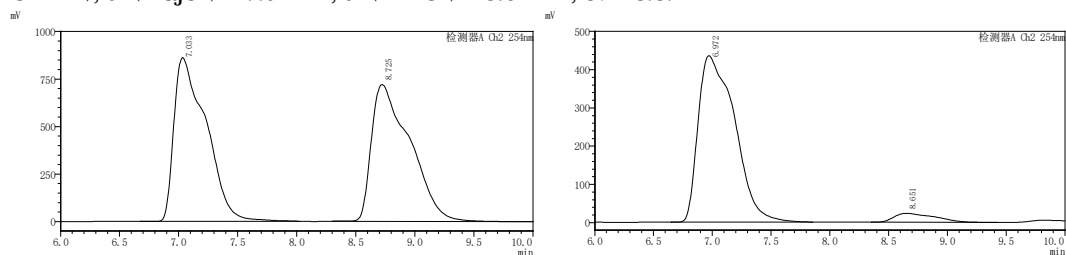


A dry reaction tube was charged with **Z-52** (0.1 mmol, 1.0 equiv), $t\text{BuOK}$ (1 equiv) and MeOH (1 mL) was added. The reaction was stirred at 40 °C for 8 h. The residue was purified by column chromatography on silica gel (petroleum ether/ ethyl acetate = 2:1) to afford the product **53**.

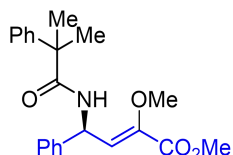
methyl (*R,Z*)-3-methoxy-4-(2-methyl-2-phenylpropanamido)-4-phenylbut-2-enoate (53**)**, White solid (24 mg, 65%), ^1H NMR (400 MHz, CDCl_3) δ 7.28 – 7.23 (m, 4H), 7.19 – 7.11 (m, 4H), 7.05 – 7.01 (m, 2H), 6.06 (d, J = 8.6 Hz, 1H), 5.99 (d, J = 7.8 Hz, 1H), 5.84 (t, J = 8.2 Hz, 1H), 3.62 (s, 3H), 3.50 (s, 3H), 1.49 (s, 3H), 1.47 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 176.37, 163.49, 146.06, 144.79, 140.24, 128.55, 128.54, 127.39, 126.91, 126.23, 126.15, 125.19, 59.79, 51.90, 49.79, 46.86, 26.85, 26.73; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{22}\text{H}_{26}\text{NO}_4^+$, ($[\text{M} + \text{H}]^+$), 368.1856, found 368.1856. $[\alpha]_{\text{D}}^{20}$ = +39



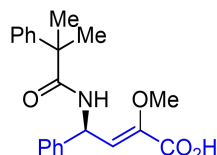
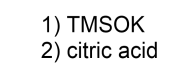
(c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak AD-3 column (80: 20 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 7.0 min, tr (minor) = 8.6 min, 89% e.e.



NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.033	16357940	50.010	1	6.972	9402471	94.350
2	8.725	16351426	49.990	2	8.651	563055	5.650



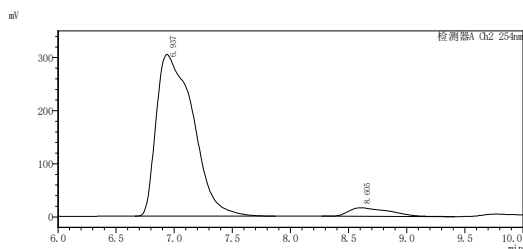
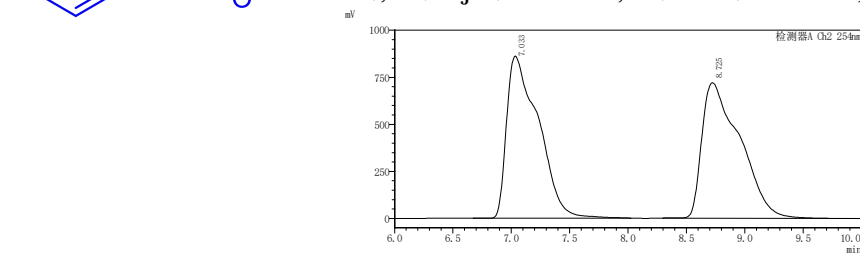
53, 65% yield, 89% ee



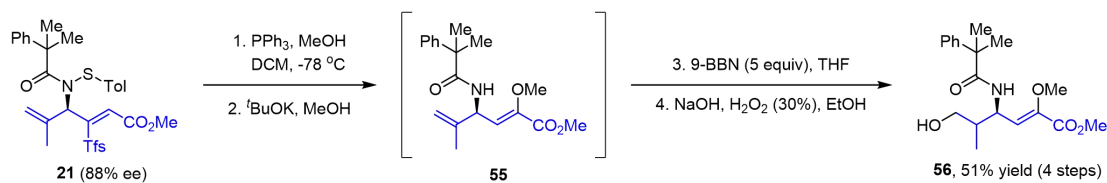
54, 64% yield, 89% ee

Prepared according to the modified literature procedure.^{1h} An oven-dried roundbottom flask at room temperature under argon atmosphere was 53 (0.1 mmol) in anhydrous THF (1 mL), and then potassium trimethylsilanolate (10.0 equiv) was added. The reaction mixture was stirred overnight and monitored by TLC technique until the starting material was consumed completely. The reaction mixture was quenched by adding a 0.5 M citric acid solution (0.5 mL) and stirring for 30 min. The resulting cloudy mixture was transferred to a separatory funnel and extracted with ethyl acetate, washed with brine dried over anhydrous MgSO₄ and filtered. Then the filtrate was concentrated in vacuo. The crude material was purified using flash column chromatography (hexanes: ethyl acetate = 1/2) to provide the desired product **50**. To test the % e.e. of the acid, a small sample was converted back to the corresponding methyl ester using K₂CO₃ and dimethyl sulfate in acetone at room temperature.

(R,Z)-3-methoxy-4-(2-methyl-2-phenylpropanamido)-4-phenylbut-2-enoic acid (54), White solid (23 mg, 64%), ¹H NMR (400 MHz, CDCl₃) δ 7.52 – 7.31 (m, 4H), 7.27 – 7.15 (m, 4H), 7.09 (d, J = 7.3 Hz, 2H), 7.01 (s, 1H), 5.53 (d, J = 9.2 Hz, 1H), 4.19 (d, J = 9.1 Hz, 1H), 3.28 (s, 3H), 1.67 (s, 3H), 1.65 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 178.10, 170.81, 143.63, 138.76, 136.01, 129.39, 129.19, 128.66, 127.82, 126.23, 126.01, 117.36, 76.29, 57.27, 47.66, 26.52, 26.49; HRMS (ESI-TOF). (m/z): Calcd for C₂₁H₂₄NO₄⁺, ([M + H]⁺), 354.1700, found 354.1703. [α]_D²⁰ = +29 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak AD-3 column (80: 20 hexane: ethanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 6.9 min, tr (minor) = 8.6 min, 89% e.e.

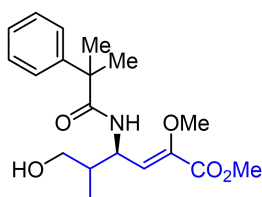
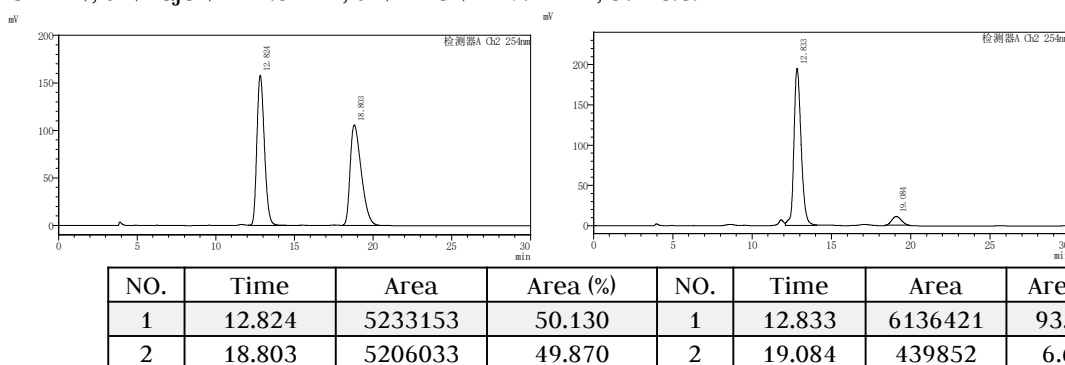


NO.	Time	Area	Area (%)	NO.	Time	Area	Area (%)
1	7.033	16357940	50.010	1	6.937	6719086	94.670
2	8.725	16351426	49.990	2	8.605	378260	5.330



Following a modified literature procedure⁸, 55 (75.3 mg, 0.3 mmol, 1 equiv) was dissolved in tetrahydrofuran (5 mL) under an argon atmosphere at 0 °C. After stirring for 15 minutes, 9-BBN (3 mL, 1.5 mmol, 5 equiv, 0.5 M in tetrahydrofuran) was added slowly. The resulting mixture was stirred overnight at room temperature. Then the reaction mixture was cooled down to 0 °C, ethanol (1 mL), NaOH (1 mL, 2 M) and H₂O₂ (1 mL, 30% in H₂O) were added slowly in sequence. The resulting mixture was stirred 3 h at room temperature. The reaction mixture was diluted with dichloromethane. After extraction with dichloromethane (20 mL $\times$ 3), the combined organic phase was dried over Na₂SO₄, concentrated under vacuum, and purified on silica gel chromatography (ethyl acetate/petroleum ether = 1:8) to afford product 56 as a colorless oil. (The preparation of 55 is the same as that of 53)

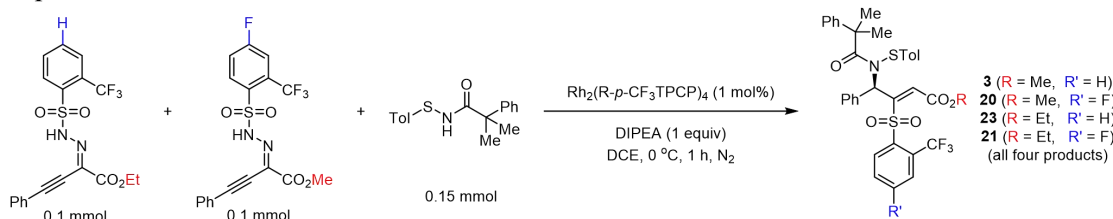
methyl (4R,Z)-6-hydroxy-2-methoxy-5-methyl-4-(2-methyl-2-phenylpropanamido)hex-2-enoate (56), colorless oil (18 mg, 51%), ¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.34 (m, 4H), 7.31 – 7.26 (m, 1H), 6.08 (d, J = 8.2 Hz, 1H), 6.01 (d, J = 8.8 Hz, 1H), 4.70 (q, J = 8.4 Hz, 1H), 3.77 (s, 3H), 3.60 (s, 3H), 3.57 (dd, J = 11.8, 3.0 Hz, 1H), 3.33 (dd, J = 11.6, 3.9 Hz, 1H), 2.78 (s, 1H), 1.59 (s, 3H), 1.57 (s, 3H), 0.88 (d, J = 7.0 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 178.06, 163.50, 146.97, 144.80, 128.71, 127.09, 126.42, 125.06, 64.21, 59.89, 52.14, 48.49, 47.06, 40.17, 27.11, 26.77, 14.03; HRMS (ESI-TOF). (m/z): Calcd for C₁₉H₂₈NO₅⁺, ([M + H]⁺), 350.1962, found 350.1961. [α]_D²⁰ = +92 (c = 0.1, CHCl₃). HPLC conditions: Daicel Chiralpak OJ-H column (90: 10 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); tr (major) = 12.8 min, tr (minor) = 19.1 min, 87% e.e.



5. Mechanistic Studies

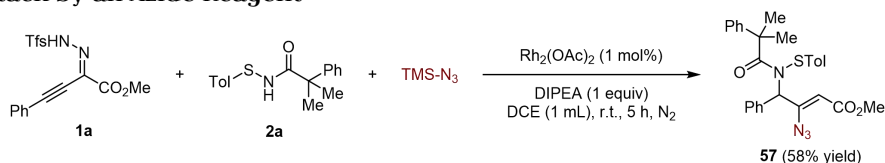
5.1 Crossover

Experiments



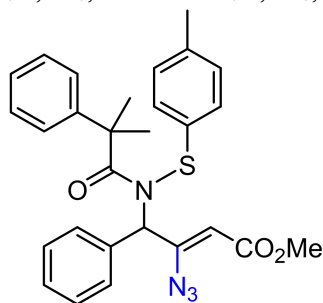
In nitrogen atmosphere, sulfenamide (0.15 mmol), $\text{Rh}_2(\text{R-p-CF}_3\text{TPCP})_4$ (1 mol%), DCE (0.5 mL), and DIPEA (1.0 equiv) were sequentially added to a screw-capped vial (8 mL) with a stir bar. Then the vial was cooled to $0\text{ }^\circ\text{C}$ using ice bath. A solution of two alkynyl sulfonylhydrazones (0.1 mmol each) in DCE (1 mL) was added dropwise to the mixture using a syringe and stirred for 15 minutes. After the reaction completed, the residue was purified by preparative TLC (petroleum ether/ethyl acetate = 3:1) to afford the four products 3 (22% yield), 20 (16% yield), 20 (22% yield) and 23 (15% yield).

5.2 External Attack by an Azide Reagent

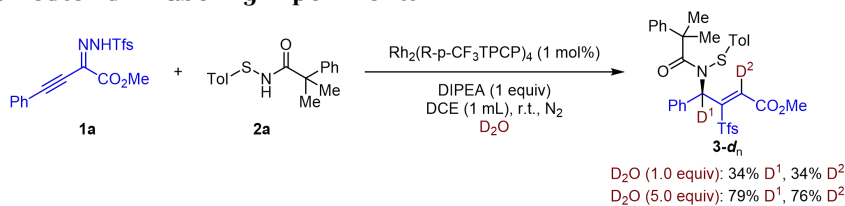


In nitrogen atmosphere, sulfenamide (0.15 mmol), $\text{Rh}_2(\text{OAc})_4$ (1 mol%), DCE (0.5 mL), DIPEA (1.0 equiv) and TMS- N_3 (1.5 equiv) were sequentially added to a screw-capped vial (8 mL) with a stir bar. Then the vial was cooled to $0\text{ }^\circ\text{C}$ using ice bath. A solution of alkynyl sulfonylhydrazone (1.25 equiv) in DCE (1 mL) was added dropwise to the mixture using a syringe and stirred for 15 minutes. After the reaction completed, the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate to provide product 57.

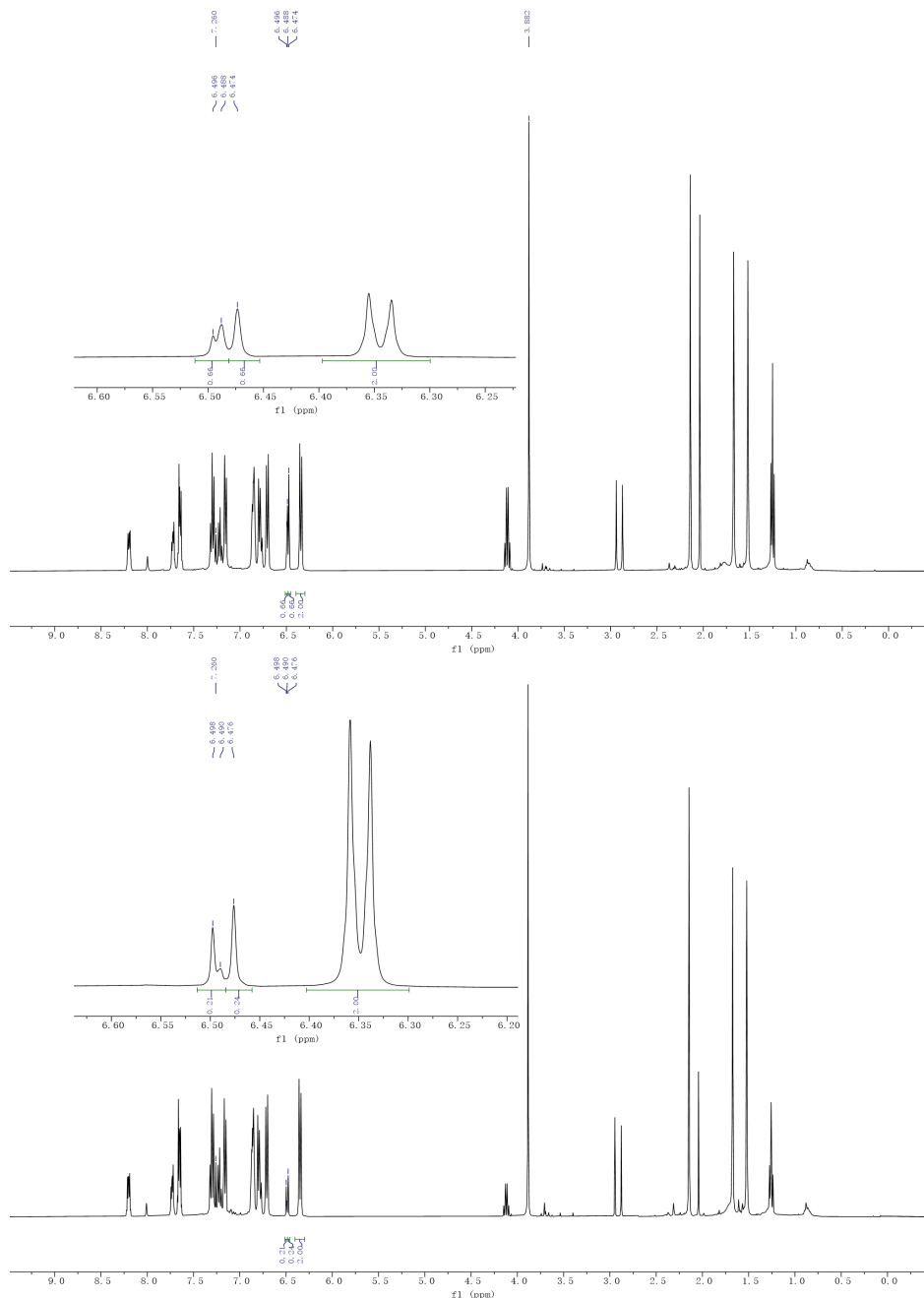
methyl (Z)-3-azido-4-(2-methyl-2-phenyl-*N*-(*p*-tolylthio)propanamido)-4-phenylbut-2-enoate (57), White solid (44 mg, 58%), ^1H NMR (400 MHz, CDCl_3) δ 7.23 (d, $J = 8.1$ Hz, 2H), 7.19 – 7.14 (m, 3H), 7.13 – 7.08 (m, 2H), 7.08 – 7.01 (m, 3H), 6.78 (d, $J = 8.0$ Hz, 2H), 6.50 (d, $J = 7.9$ Hz, 2H), 6.02 (s, 1H), 5.32 (s, 1H), 3.68 (s, 3H), 2.17 (s, 3H), 1.66 (s, 3H), 1.62 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 164.67, 152.06, 144.59, 136.26, 134.36, 133.68, 130.81, 128.85, 128.55, 127.98, 126.46, 125.59, 124.38, 106.19, 67.14, 51.35, 48.70, 30.60, 26.66, 20.91; IR (neat, cm^{-1}): 2100, 1700, 1200; HRMS (ESI-TOF). (m/z): Calcd for $\text{C}_{28}\text{H}_{29}\text{N}_4\text{O}_3\text{S}^+$, ($[\text{M} + \text{H}]^+$), 501.1955, found 501.1949.



5.3 Deuterium Labeling Experiments

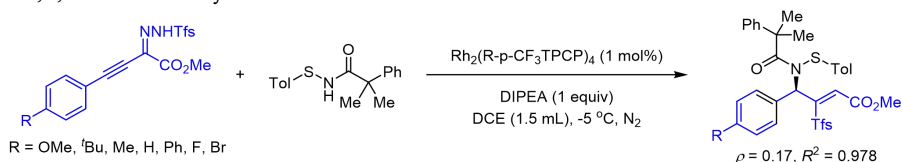


In nitrogen atmosphere, sulfenamide (0.15 mmol), $\text{Rh}_2(\text{R-p-CF}_3\text{TPCP})_4$ (1 mol%), DCE (0.5 mL), DIPEA (1.0 equiv) and D_2O (1.0 equiv or 3.3 equiv) were sequentially added to a screw-capped vial (8 mL) with a stir bar. Then the vial was cooled to $0\text{ }^\circ\text{C}$ using ice bath. A solution of alkynyl sulfonylhydrazone (1.25 equiv) in DCE (1 mL) was added dropwise to the mixture using a syringe and stirred for 15 minutes. After the reaction completed, the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate to provide product 3- d_n . And the deuterated ratio was determined by ^1H NMR analysis.

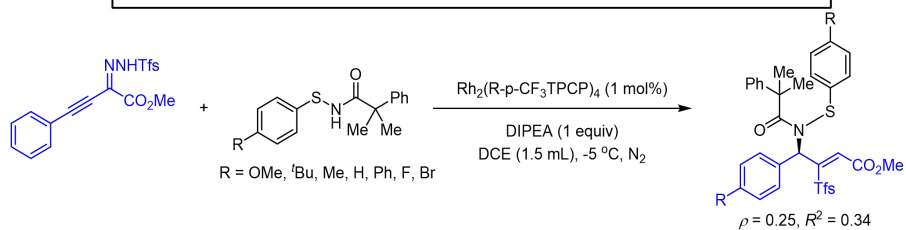
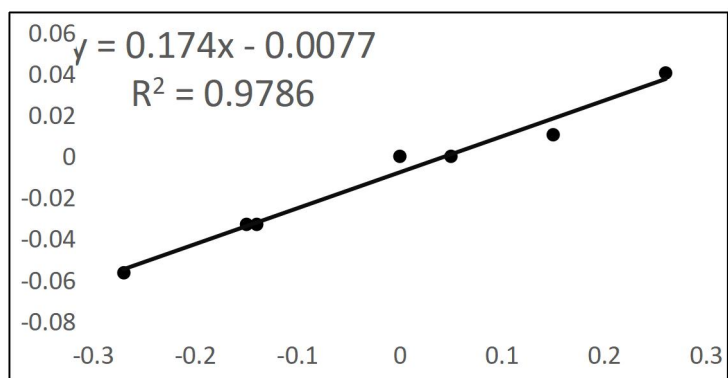


5.4 Hammett Studies

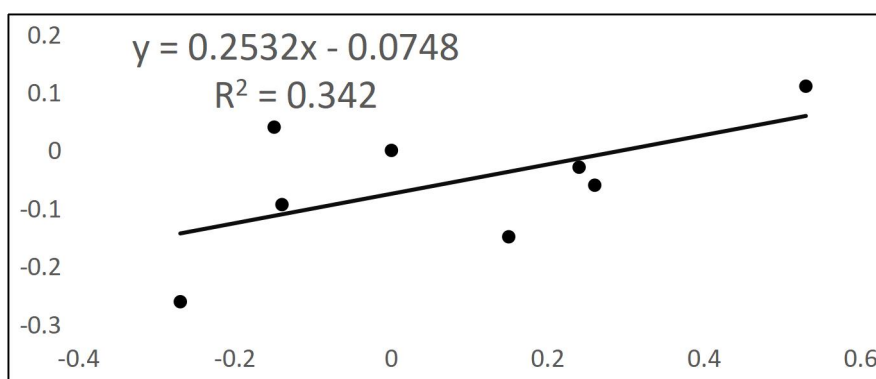
In nitrogen atmosphere, sulfenamide (0.15 mmol), $\text{Rh}_2(\text{R-}p\text{-CF}_3\text{TPCP})_4$ (1 mol%), DCE (0.5 mL), and DIPEA (1.0 equiv) were sequentially added to a screw-capped vial (8 mL) with a stir bar. Then the vial was cooled to 0 °C using ice bath. A solution of alkynyl sulfonylhydrazone (1.25 equiv) in DCE (1 mL) was added dropwise to the mixture using a syringe and stirred for 15 seconds. The reaction mixture was then quenched with 0.5 mL HCl (1 M) and extracted with EtOAc (10 mL $\times$ 3). The organic layer was collected, dried over Na_2SO_4 , filtered and concentrated under reduced pressure. The conversions were determined by ^1H NMR with 1,3,5- trimethoxybenzene as an internal standard.



<i>para</i> -substituent	σ	$\log(k_{\text{R}}/k_{\text{H}})$
OMe	-0.27	-0.05648
H	0	0
F	0.15	0.010465
$t\text{Bu}$	-0.15	-0.033
Br	0.26	0.040429
Ph	0.05	0
Me	-0.14	-0.033



<i>para</i> -substituent	σ	$\log(k_R/k_H)$
H	0	0
OMe	-0.27	-0.26091
tBu	-0.15	0.040117
Me	-0.14	-0.09342
Br	0.26	-0.06
Cl	0.24	-0.02896
F	0.15	-0.14894
CF ₃	0.53	0.110698



6. DFT Calculations

1. Computational details

All of the calculations were performed using the Gaussian 09 package.¹ The geometry optimizations were carried out using the B3LYP-D3(BJ)²⁻⁵ functional with a mixed basis set of SDD for the Rh and the 6-31G(d) for all other atoms. Frequencies were computed analytically at the same level of theory to confirm whether the structures are minima (no imaginary frequencies) or transition states (only one imaginary frequency). Selected transition-state structures were confirmed to connect the correct reactants and products by intrinsic reaction coordinate (IRC) calculations.^{6,7} Thorough conformation search of key transition states and intermediates was performed with the ConformerRotamer Ensemble Sampling Tool (CREST) developed by Grimme and co-worker.⁸⁻¹¹ To obtain better accuracy, solution-phase single-point energies for the optimized geometries were recalculated using B3LYP-D3(BJ) functional with a larger basis set of SDD for Rh and 6-311+G(d,p) for all other atoms. Solvation effects (Dichloromethane, $\epsilon = 8.93$) were taken into account by performing single-point calculations using the SMD model.¹² The final free energies reported in the article (ΔG_{sol}) are the large basis set single-point energies with Gibbs free energy correction (at 298.15 K). All 3D structures of the optimized geometries were generated using CYLview.¹³

References:

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Men-nucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Son-nenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Mont-gomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Nor-mand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochter-ski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Dan-iels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision E.01; Gaussian, Inc.: Wallingford, CT, 2013.
2. Lee, C.; Yang, W.; Parr, R. G. Development of the colle-salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B.* **1988**, 37, 785–789.
3. Becke, A. D. Density functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, 98, 5648–5652.
4. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate Ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H–Pu. *J. Chem. Phys.* **2010**, 132, 154104.
5. Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comp. Chem.* **2011**, 32, 1456–1465.
6. Fukui, K. Formulation of the reaction coordinate. *J. Phys. Chem.* **1970**, 74, 4161–4163.
7. Fukui, K. The path of chemical reactions – the IRC approach. *Acc. Chem. Res.* **1981**, 14, 363–368.
8. Grimme, S.; Bannwarth, C.; Shushkov, P. A robust and accurate tight-binding quantum chemical method for structures, vibrational frequencies, and noncovalent interactions of large molecular systems parametrized for all spd-block elements (Z = 1–86). *J. Chem. Theory Comput.* **2017**, 13, 1989–2009.
9. Grimme, S.; Bannwarth, C.; Dohm, S.; Hansen, A.; Pisarek, J.; Pracht, P.; Seibert, J.; Neese, F. Fully automated quantum-chemistry-based computation of spin-spin-coupled nuclear magnetic resonance spectra. *Angew. Chem. Int. Ed.* **2017**, 56, 14763–14769.
10. Grimme, S. Exploration of chemical compound, conformer, and reaction space with meta-dynamics simulations based on tight-binding quantum chemical calculations. *J. Chem. Theory Comput.* **2019**, 15, 2847–2862.
11. Bannwarth, C.; Ehlert, S.; Grimme, S. GFN2-xTB—an accurate and broadly parametrized selfconsistent tight-binding quantum chemical method with multipole electrostatics and densitydependent dispersion contributions. *J. Chem. Theory Comput.* **2019**, 15, 1652–1671.
12. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B.* **2009**, 113, 6378–6396.
13. Legault, C. Y. CYLview, ver. 1.0b, Université de Sherbrooke: 2009, <http://www.cylview.org>.

2. Deprotonation by DIPEA to form intermediate IM3

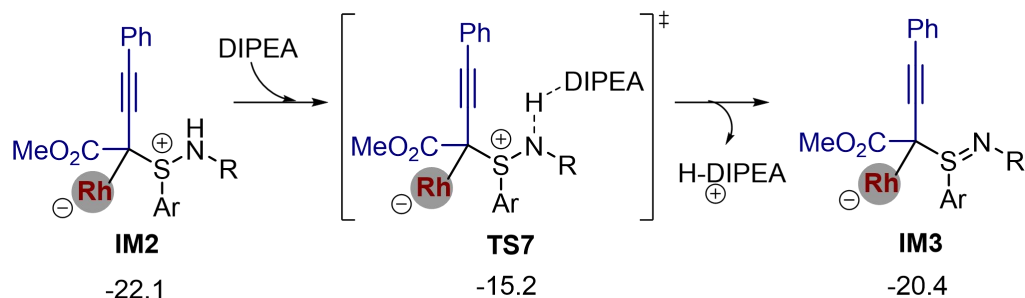


Figure S1. Deprotonation by DIPEA to form intermediate IM3.

3. Other possibilities to form Rh-allene intermediate

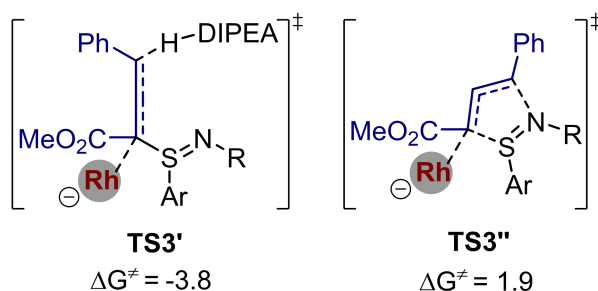


Figure S2. Other possibilities to form Rh-allene intermediate.

4. Other enantiomers for the enantioselectivity-determining protonation transition states

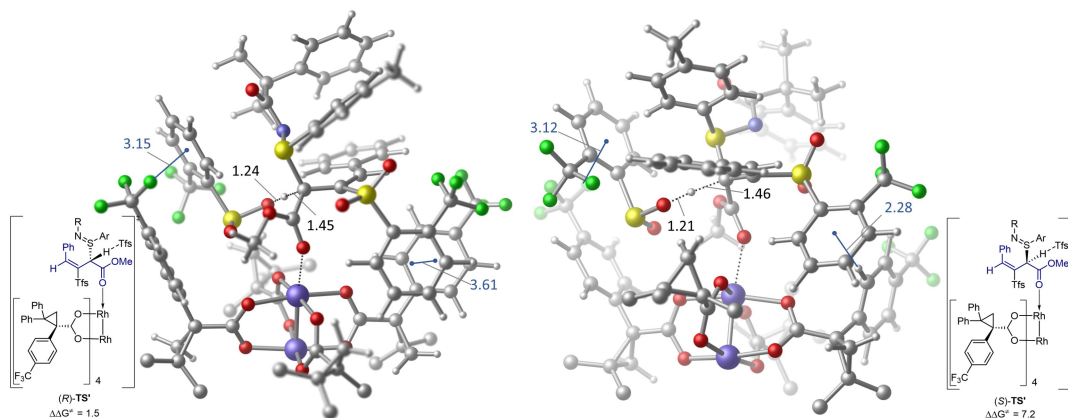


Figure S3. Other enantiomers for the enantioselectivity-determining protonation transition states with the $\text{Rh}_2(\text{R-}p\text{-CF}_3\text{TPCP})_4$ catalyst.

5. Table of Benchmark study using various DFT functionals for energy calculations. Values are in $\text{kcal}\cdot\text{mol}^{-1}$ unit.

	(R)-TS	(S)-TS
B3LYP-D3(BJ) _(SMD) /SDD&6-311+G(<i>d,p</i>)	0.0	4.3
PBE0-D3(BJ) _(SMD) /SDD&6-311+G(<i>d,p</i>)	0.0	5.5
ω B97XD _(SMD) /SDD&6-311+G(<i>d,p</i>)	0.0	5.5
MN15 _(SMD) /SDD&6-311+G(<i>d,p</i>)	0.0	5.7

6. Table of calculated energies and energy corrections

Stationary point	Single-point energy- B3LYP-D3(BJ)/6-311+G(<i>d,p</i>) (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
1a'	-684.0785498	0.124682

2a	-1187.7748075	0.273351
Rh ₂ (OAc) ₄	-1135.6473452	0.159124
3	-2880.5542850	0.524883
N2	-109.555146	-0.012849
DIPEA	-371.1983959	0.226878
DIPEA-H⁺	-371.6713795	0.243136
HTfs	-1118.1652534	0.075633
Tfs⁻	-1117.6954571	0.062844
IM1	-1710.2030897	0.295660
IM2	-2898.0161172	0.605379
IM3	-2897.5417553	0.590480
IM4	-2898.0118977	0.602705
IM5	-4015.7356822	0.700297
IM6	-4016.2047317	0.712255
TS1	-1819.7282528	0.303953
TS2	-2898.0095123	0.603184
TS3	-4015.7168207	0.690834
TS3'	-3269.2089278	0.855879
TS3'	-2897.5051986	0.589322
TS4	-4015.7174204	0.694973
TS5	-5133.9061639	0.795626
TS6	-4016.1995581	0.711448
TS7	-3269.2273106	0.856004
(R)-TS	-9565.92050947037	1.852922
(R)-TS'	-9565.91560032259	1.850420
(S)-TS	-9565.91201709459	1.851252
(S)-TS'	-9565.90626935432	1.850199

7. Cartesian coordinates

1a'

C	-12.61092100	1.62226900	-1.31130900
N	-12.21391500	2.68400200	-1.99548000
N	-11.87632100	3.59624700	-2.58321600
C	-11.64719600	0.69518700	-0.87339100
C	-10.81692200	-0.10702400	-0.49362600
C	-9.86926900	-1.06205300	-0.03547100
C	-8.49679600	-0.90123300	-0.30791600
C	-10.29607500	-2.18532700	0.70040300
C	-7.57825100	-1.84282900	0.14660800
H	-8.16617300	-0.03669500	-0.87465000
C	-9.36827600	-3.12001800	1.14945000
H	-11.35365400	-2.30820300	0.90979900
C	-8.00825500	-2.95404700	0.87568700
H	-6.52209200	-1.70879000	-0.06915400
H	-9.70810800	-3.98228600	1.71595400
H	-7.28788900	-3.68630000	1.22839900
C	-14.05496000	1.47757500	-1.04840600
O	-14.54024600	0.55177500	-0.43666800
O	-14.75579700	2.50798900	-1.57762700
C	-16.17473900	2.44450400	-1.36718600
H	-16.58761000	1.53820100	-1.81741500
H	-16.40301800	2.44790000	-0.29832700
H	-16.57953600	3.33370400	-1.85042200

2a

C	1.79859200	1.62056500	1.63667500
C	2.74297600	1.70861600	-0.57490200
C	3.09101600	3.04557900	-0.37548700
C	2.80274200	3.66801900	0.84222000

C	2.16132400	2.94468800	1.85953200
H	1.29576900	1.06562500	2.42544200
H	2.97626900	1.22976600	-1.52266400
H	3.58768400	3.60544100	-1.16227700
H	1.94856900	3.43445900	2.80327700
C	1.68205700	-0.45746600	0.19954100
H	2.10656400	-0.85505100	-0.72734900
H	0.59078700	-0.55627600	0.13542500
H	2.01402100	-1.09653000	1.02595800
C	2.08594700	0.97940300	0.42115600
S	3.31214600	5.36298400	1.11293600
N	1.80423000	6.19205700	1.19878800
H	1.43041600	6.54305800	0.32876800
C	1.03009900	6.25775400	2.34026700
C	-0.27223300	7.09583100	2.23397600
O	1.34132200	5.70965900	3.38337300
C	-1.38383300	6.22477800	2.84516200
C	-0.67672600	7.46448700	0.79009600
C	-0.02072900	8.39150300	3.01991100
C	1.06783900	9.20436600	2.66885400
C	-0.85104600	8.81282400	4.06270700
C	1.31480700	10.40303900	3.33325700
H	1.74152100	8.88787000	1.87722100
C	-0.60888200	10.01685900	4.72858600
H	-1.69323700	8.20411400	4.37092500
C	0.47259100	10.81760200	4.36695600
H	2.16832800	11.01107300	3.04650600
H	-1.26846700	10.32306400	5.53592500
H	0.66227400	11.75181800	4.88771800
H	-2.34357500	6.75067800	2.82884800
H	-1.49584200	5.30441400	2.26193800
H	-1.13709900	5.94680600	3.87124800
H	-1.62478000	8.01085200	0.81318400
H	0.05306000	8.12128700	0.30499700
H	-0.82271200	6.56943800	0.17303900

Rh₂(OAc)₄

O	0.28863800	-1.72036900	1.08939900
O	0.51077800	-2.19604300	-1.11668700
O	1.81300900	0.72236100	0.72022700
O	2.03703100	0.24566400	-1.48492300
O	-0.63763800	2.16787300	0.16146300
O	-0.41527600	1.69225100	-2.04461000
O	-2.16378200	-0.27392500	0.52979800
O	-1.93981900	-0.75038500	-1.67540900
Rh	-0.18149800	0.23519800	0.68394900
Rh	0.05472500	-0.26334500	-1.63914500
C	0.82275700	-3.94896600	0.45714200
H	1.23931700	-4.02435000	1.46324400
H	1.50630700	-4.37752400	-0.27872800
H	-0.11373100	-4.51797900	0.42550700
C	3.93418700	1.05003100	-0.29932000
H	4.34752200	0.84459300	0.69022600
H	3.99602300	2.12985200	-0.47837800
H	4.50882800	0.53843800	-1.07364300
C	-0.94962300	3.92083300	-1.41224400
H	-1.36273300	3.99675600	-2.41971400
H	-0.01385400	4.49076400	-1.37651300
H	-1.63624700	4.34803400	-0.67841500
C	-4.06100300	-1.07800000	-0.65615600

H	-4.12216100	-2.15943000	-0.48689900
H	-4.47638700	-0.86409400	-1.64309400
H	-4.63421400	-0.57324500	0.12364600
C	0.52693500	-2.50924700	0.11799400
C	2.48607800	0.63185100	-0.35732600
C	-0.65368300	2.48110300	-1.07322000
C	-2.61286800	-0.65995100	-0.59782100

3

C	0.69302800	0.50479800	4.52474200
C	1.87514200	0.77622800	3.64933500
O	2.37046600	1.87125500	3.49949900
O	2.27185500	-0.33396200	3.00895000
C	3.47417300	-0.18282700	2.22740700
H	4.28466500	0.16642600	2.86922000
H	3.68694200	-1.17548200	1.83200400
H	3.31303900	0.53255300	1.41729600
C	0.69117800	0.58332300	5.85650600
C	-0.53899100	0.43879100	6.72948400
C	-1.83150900	0.52858300	5.92960700
C	-2.66565800	-0.57290500	5.74081500
C	-2.19085400	1.75840800	5.36339400
C	-3.83749200	-0.45195100	4.99094600
H	-2.40374700	-1.52333200	6.18445100
C	-3.35891000	1.88167900	4.61499800
H	-1.54528000	2.62226400	5.50271100
C	-4.18782700	0.77254700	4.42443600
H	-4.47378900	-1.32161500	4.85210100
H	-3.62476700	2.84272100	4.18379800
H	-5.09962400	0.86672600	3.84152000
C	0.08479100	-3.36093900	3.43119600
C	-1.66013700	-4.33979100	4.76673700
C	-1.16067200	-3.70682700	5.90071700
C	-0.05030700	-2.86150900	5.79271000
C	0.58535200	-2.70714200	4.55605900
H	0.58274800	-3.22633100	2.47422700
H	-2.52899200	-4.98690400	4.86078400
H	-1.63058700	-3.86484400	6.85993100
H	1.46344700	-2.07822400	4.47309900
C	-1.62625800	-4.83408500	2.28490900
H	-0.86292100	-4.97741500	1.51359500
H	-2.42528700	-4.22215400	1.84562800
H	-2.06004700	-5.81130800	2.52234200
C	-1.05373000	-4.17161000	3.51323400
S	0.66050000	-2.03036900	7.20499000
N	-0.47773700	-0.77160400	7.58405900
C	-1.10656000	-0.60961100	8.81934900
C	-1.04285300	-1.70504200	9.91054500
O	-1.72728700	0.42757000	9.02061200
C	-1.87288200	-1.19405500	11.11313900
C	0.40347600	-1.89592500	10.41553400
C	-1.71953300	-2.97670900	9.39535300
C	-3.00006300	-2.87246600	8.82820800
C	-1.15511900	-4.24840900	9.53133300
C	-3.69691100	-4.00581000	8.41289600
H	-3.45080100	-1.89140100	8.70555800
C	-1.85035100	-5.38660600	9.11535900
H	-0.16382100	-4.35740200	9.95642300
C	-3.12385800	-5.27199200	8.55706100
H	-4.68486400	-3.89914800	7.97347100

H	-1.39035400	-6.36466600	9.22518500
H	-3.66238900	-6.15828400	8.23400700
H	-1.89356100	-1.97275400	11.88226900
H	-1.42481500	-0.28918400	11.53229100
H	-2.89843300	-0.95752400	10.82570800
H	0.39257200	-2.45323300	11.35843000
H	1.04132400	-2.42584900	9.70994700
H	0.85662200	-0.91851900	10.60693900
C	2.53603200	2.67202800	6.42464700
C	3.75766100	3.24889900	6.03945100
C	3.80138800	4.63053800	5.83014000
C	2.67312400	5.42771300	6.00878100
C	1.47741400	4.85169400	6.42778700
C	1.41671100	3.47730200	6.64062800
H	4.73824400	5.08247200	5.53110100
H	2.73752200	6.49694400	5.83330200
H	0.59557200	5.46255700	6.59372500
H	0.48891500	3.03364500	6.98020600
C	5.05184700	2.47794700	5.85700200
S	2.26418200	0.89905500	6.72362600
O	3.28768200	0.10699700	6.03438900
O	2.01413800	0.75215200	8.16491900
F	5.31368400	1.68844300	6.91368200
F	5.05981800	1.72400800	4.74289200
F	6.10110600	3.33064100	5.74419700
H	-0.54514500	1.27414500	7.43691000
H	-0.23163000	0.24757000	4.01474200

N2

N	-0.71444400	1.02503000	0.00000000
N	-1.81974900	1.02503000	0.00000000

DIPEA

N	-2.83358000	-0.78056600	-10.02269400
C	-2.88116800	-2.12155700	-10.59677000
H	-3.76818100	-2.69122800	-10.26228600
H	-2.97972300	-2.02497500	-11.68190200
C	-3.08313000	-0.73326600	-8.57551100
H	-2.64994500	-1.65824400	-8.17778200
C	-3.43015500	0.28984000	-10.83715200
H	-3.55118500	1.14819100	-10.16748800
C	-1.61235600	-2.92804800	-10.30685200
H	-1.66919500	-3.91862200	-10.77399800
H	-0.73608900	-2.40163300	-10.69887900
H	-1.45926800	-3.07841200	-9.23260200
C	-2.44817800	0.71315700	-11.93859700
H	-1.48927300	1.00240300	-11.49867900
H	-2.26243100	-0.10969700	-12.63963400
H	-2.84366600	1.55677000	-12.51685500
C	-4.81792400	-0.01591700	-11.43758200
H	-4.76581600	-0.81376200	-12.18696100
H	-5.53597800	-0.31985200	-10.67159200
H	-5.21393300	0.87500500	-11.93905300
C	-2.31636100	0.42402000	-7.92251200
H	-2.40326700	0.37608000	-6.83083800
H	-1.25803700	0.37645300	-8.19605700
H	-2.70542100	1.39935100	-8.23734600
C	-4.56699600	-0.71905100	-8.16162400
H	-5.11825900	-1.54410100	-8.62580000
H	-4.66208500	-0.82158800	-7.07420100

H	-5.05214700	0.22054400	-8.44823100
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DIPEA-H⁺

N	-2.73456300	-0.74921200	-10.04944000
C	-2.86596900	-2.13563200	-10.65105100
H	-3.85010100	-2.51433000	-10.37384200
H	-2.84555800	-2.00409600	-11.73352800
C	-3.00947700	-0.71087300	-8.53203500
H	-2.52917900	-1.61861700	-8.16123400
C	-3.44797500	0.35321300	-10.86915400
H	-3.61045600	1.15839500	-10.15117600
C	-1.74310000	-3.06805800	-10.21661100
H	-1.84742600	-4.01158400	-10.75999700
H	-0.75849200	-2.65513800	-10.46551800
H	-1.76705600	-3.30422500	-9.14978800
C	-2.48776800	0.83720500	-11.95349300
H	-1.55425300	1.22531600	-11.52968800
H	-2.24904500	0.04506300	-12.67173100
H	-2.95720400	1.65212600	-12.51109200
C	-4.79233700	-0.09484100	-11.43774000
H	-4.67870600	-0.81435900	-12.25297800
H	-5.45815600	-0.51668700	-10.68361800
H	-5.28521300	0.78883600	-11.85332900
C	-2.29960900	0.49534600	-7.92098400
H	-2.37923100	0.43353900	-6.83217000
H	-1.23180400	0.51136100	-8.16932500
H	-2.74695900	1.44621700	-8.22596300
C	-4.49523000	-0.76247400	-8.19944700
H	-5.00005800	-1.62437800	-8.64410400
H	-4.59200000	-0.85640400	-7.11408800
H	-5.01723100	0.15106300	-8.49609500
H	-1.73857100	-0.51826600	-10.12518900

HTfs

C	0.53346900	0.16564300	0.11223700
C	1.92196900	0.22491700	-0.06740600
C	2.55501400	1.46829500	-0.05307600
C	1.81004200	2.63308800	0.13715800
C	0.43082400	2.56114100	0.32935000
C	-0.20918300	1.32126300	0.32495100
H	3.62882800	1.51975400	-0.18800000
H	2.31333000	3.59498500	0.14439700
H	-0.14665100	3.46718100	0.48652700
H	-1.27720000	1.22622600	0.49326000
C	2.74025900	-1.03175600	-0.22089600
S	-0.39014700	-1.40908600	0.11700700
O	-1.68121200	-1.10620000	0.79367600
O	-0.61217100	-1.33743100	-1.56134900
F	2.67482800	-1.79479800	0.89533200
F	2.30130100	-1.80120000	-1.24277400
F	4.04097900	-0.76535300	-0.44914600
H	-0.82584200	-2.24482500	-1.84750600

Tfs⁻

C	0.60275000	0.11109000	-0.12241100
C	1.99468500	0.20646900	-0.01199800
C	2.62010100	1.45580700	0.10717900
C	1.85339900	2.61828300	0.13032500
C	0.46102100	2.53044500	0.01837900
C	-0.14920900	1.28574600	-0.11162600

H	3.70142200	1.51271200	0.18039900
H	2.34012600	3.58642700	0.22572700
H	-0.13985900	3.43913400	0.02715900
H	-1.22489000	1.17123000	-0.23691500
C	2.84300800	-1.03349800	-0.07305900
S	-0.41923500	-1.52175900	-0.18030400
O	-0.67678100	-1.71094900	1.30188500
O	-1.62900200	-1.00589900	-0.94616000
F	2.52515600	-1.94198400	0.87050500
F	2.74551400	-1.66419600	-1.27031300
F	4.17108100	-0.75645800	0.09540100

IM1

C	3.06275600	-1.15526400	-0.77277400
C	1.60596000	-0.11038600	2.48560600
C	-0.53504500	2.38992200	0.72684100
C	0.96741700	1.37638100	-2.52136000
O	0.70704600	-0.72119900	1.81527900
O	2.35247400	0.82239200	2.06549400
O	-0.97798100	1.22760500	0.43211300
O	0.67111700	2.77061000	0.69732700
O	0.20730600	0.44056800	-2.10025400
O	1.85240300	1.98300400	-1.84820900
O	1.84806800	-1.55083300	-0.73367900
O	3.48737900	0.00148000	-0.48279500
Rh	0.37432400	-0.22958200	-0.16144500
Rh	2.14343200	1.44762700	0.11625700
C	-1.03568400	-1.63298400	-0.38180100
C	0.77252900	1.78156100	-3.96330500
C	-1.57492400	3.40650200	1.14595500
C	1.78447600	-0.56805600	3.91450500
C	4.07193400	-2.19003900	-1.21373900
H	4.01558600	-3.05966800	-0.55120000
H	3.82455700	-2.52924800	-2.22481300
H	5.07997100	-1.77390300	-1.19713900
H	2.13359800	-1.60598100	3.91963900
H	2.50678500	0.06585400	4.43055100
H	0.82091000	-0.54332800	4.43211400
H	-1.09722300	4.34180600	1.44035300
H	-2.25842500	3.59256900	0.31032000
H	-2.16329500	3.00992400	1.97946600
H	-0.25692700	2.12368000	-4.10987200
H	1.47095900	2.57434800	-4.23438600
H	0.92296700	0.91069100	-4.60889500
C	-0.60393100	-2.97519200	-0.83945700
O	-0.62927200	-3.29202600	-2.01025700
O	-0.13949400	-3.72927100	0.16368300
C	0.47526800	-4.96613100	-0.23840900
H	-0.23758200	-5.59347400	-0.77920300
H	1.33677800	-4.75829800	-0.87756400
H	0.78766600	-5.44720200	0.68794000
C	-2.34314200	-1.33935600	-0.19067600
C	-3.50220700	-0.97026800	0.01624300
C	-4.72684500	-0.33459900	0.28665700
C	-4.71509700	1.04068000	0.62070300
C	-5.95489400	-1.02978100	0.23147800
C	-5.90762500	1.69743100	0.89316800
H	-3.75846800	1.54961800	0.65494300
C	-7.14156100	-0.36068500	0.50399800
H	-5.95341400	-2.08358500	-0.02646500

C	-7.11891200	0.99891500	0.83454600
H	-5.90007100	2.75238400	1.15014900
H	-8.08665400	-0.89306900	0.46066300
H	-8.05010700	1.51619700	1.04706200

IM2

C	1.52369500	-0.17109700	2.69662600
C	2.88432600	2.59469800	0.45553300
C	3.78493400	0.02567200	-2.06517900
C	2.44828200	-2.64648800	0.19429500
O	1.84991800	2.12777700	-0.11856900
O	3.82800600	1.91994300	0.97519600
O	2.51048500	0.03208300	-2.03709100
O	4.56031900	-0.01118000	-1.06151900
O	1.44672800	-1.98552600	-0.24429300
O	3.53391100	-2.16242400	0.63341000
O	0.75729600	0.10763700	1.70098100
O	2.77957300	-0.26457500	2.64704900
Rh	1.54981800	0.09502600	-0.22285300
Rh	3.74165000	-0.12766200	0.82127100
C	-0.51873300	0.49247900	-1.13120900
C	2.32107900	-4.15194700	0.20946600
C	4.41779600	0.04600700	-3.43739200
C	2.99962600	4.10113400	0.49377700
C	0.82807000	-0.43204000	4.00775400
H	0.08849000	0.35014900	4.20341900
H	0.29713300	-1.38711100	3.91827900
H	1.54953000	-0.48619600	4.82395000
H	2.01151000	4.55051900	0.61903100
H	3.67405700	4.41271400	1.29362800
H	3.40557600	4.44779800	-0.46352000
H	5.49186700	0.22115200	-3.36083600
H	4.24505800	-0.91900100	-3.92731500
H	3.94670800	0.82087700	-4.04868100
H	2.06658900	-4.51744000	-0.78980700
H	3.25474600	-4.60630500	0.54322900
H	1.51208400	-4.42755100	0.89367400
C	-0.21287900	0.49911800	-2.59288100
O	0.07870500	1.48845400	-3.22711200
O	-0.23758300	-0.75428800	-3.12368800
C	0.29037100	-0.85447900	-4.45195900
H	0.17921200	-1.90301200	-4.73106200
H	-0.26456500	-0.21082000	-5.13959300
H	1.34301200	-0.56483100	-4.44973000
C	-0.94140700	1.71829400	-0.55619100
C	-1.36276500	2.69335000	0.03206000
C	-1.87966800	3.82495600	0.72019400
C	-3.13541200	4.35761200	0.36822100
C	-1.15968700	4.41206900	1.77815000
C	-3.65495200	5.44798000	1.06039300
H	-3.68545700	3.90160700	-0.44783100
C	-1.68540300	5.50410800	2.46406300
H	-0.19359400	3.99541300	2.04554300
C	-2.93327600	6.02363400	2.10969200
H	-4.62204300	5.85550900	0.77784700
H	-1.12160300	5.95184800	3.27762000
H	-3.34013500	6.87569000	2.64686700
C	-4.67458200	1.28138200	1.02529200
C	-5.20957300	1.07410300	-1.31477600
C	-4.07260900	0.28978200	-1.51166000

C	-3.24358300	0.02099600	-0.42695800
C	-3.53388500	0.51040600	0.84611900
H	-4.89940200	1.67819000	2.01138700
H	-5.85986700	1.29055900	-2.15759100
H	-3.83764800	-0.10131500	-2.49672400
H	-2.87423200	0.29059500	1.67684600
C	-6.73390100	2.45701400	0.16284000
H	-7.29254700	2.60520400	-0.76590200
H	-6.43661400	3.44272500	0.54145600
H	-7.41618400	2.02068700	0.90218600
C	-5.52398000	1.58304300	-0.05078600
S	-1.72874800	-0.85801100	-0.77910500
N	-1.29509600	-1.44590500	0.75107800
H	-0.61009700	-0.85677700	1.25693900
C	-1.20159400	-2.80314400	1.06613600
C	-1.97247100	-3.83964500	0.21613400
O	-0.55310900	-3.11293200	2.05228600
C	-2.07091000	-5.14025800	1.04227200
C	-1.15350000	-4.14487200	-1.05851200
C	-3.39066600	-3.33885400	-0.07638000
C	-3.95827800	-3.37852900	-1.35530800
C	-4.17236600	-2.84821900	0.98002000
C	-5.26186400	-2.92921000	-1.57304800
H	-3.37978000	-3.74387300	-2.19592700
C	-5.47061400	-2.39292200	0.76550800
H	-3.74890000	-2.80017000	1.97989100
C	-6.02142400	-2.42983300	-0.51587300
H	-5.67907600	-2.96301400	-2.57569200
H	-6.04633800	-1.99693100	1.59667100
H	-7.02935300	-2.06517800	-0.68960200
H	-1.07551300	-5.52284600	1.28017800
H	-2.60253400	-4.97597200	1.98270400
H	-2.61620300	-5.89147800	0.46272500
H	-1.63175000	-4.95868400	-1.61296500
H	-1.04571100	-3.28472600	-1.72213100
H	-0.15386800	-4.47434800	-0.77749300

IM3

C	1.86159700	-1.44388200	-1.92060200
C	3.15514600	2.01840400	-1.18923300
C	3.88175600	0.96105800	2.30017300
C	2.59552800	-2.44569700	1.53828600
O	2.02857400	1.83485900	-0.62634000
O	4.15831400	1.24359900	-1.16177700
O	2.63345600	1.10730700	2.11187500
O	4.69833000	0.32555200	1.56512600
O	1.65236600	-1.60119300	1.63133300
O	3.67146800	-2.32272100	0.87149700
O	1.03550700	-0.92777000	-1.10690500
O	3.13055100	-1.41572000	-1.84152400
Rh	1.73080300	0.13161700	0.51969900
Rh	3.99295500	-0.56524400	-0.16430200
C	-0.33743700	0.65801000	1.14227300
C	2.38736100	-3.74622000	2.28541300
C	4.43651300	1.61854000	3.54804700
C	3.28387700	3.28784500	-2.00699700
C	1.26700100	-2.16596000	-3.11170800
H	1.56309900	-1.65046100	-4.03137000
H	0.17918100	-2.17815100	-3.04088800
H	1.66294200	-3.18548900	-3.15693200

H	4.33469400	3.55263300	-2.14095700
H	2.73725000	4.10321800	-1.52692300
H	2.83852900	3.11964100	-2.99530800
H	4.15139700	2.67521300	3.56342500
H	5.52306400	1.52276100	3.58573400
H	3.99214200	1.14454600	4.42988000
H	1.69492200	-4.37440100	1.71326800
H	1.92666300	-3.54563700	3.25597900
H	3.33394700	-4.27656500	2.40803400
C	-0.15494600	1.22544400	2.50911600
O	-0.17808900	0.59254400	3.54503600
O	0.10863600	2.55949700	2.46650300
C	0.46411400	3.14157300	3.71667000
H	-0.33200000	3.00044800	4.45396500
H	0.61211300	4.20399700	3.51407100
H	1.38684900	2.69042500	4.09116100
C	-1.08499700	-0.54808000	1.08976000
C	-1.70784100	-1.58031400	0.93599700
C	-2.47860100	-2.74796500	0.71587800
C	-3.11250500	-3.41799400	1.78254100
C	-2.66260900	-3.24077600	-0.59342600
C	-3.91137800	-4.53287500	1.54255900
H	-2.97458100	-3.03989900	2.79060900
C	-3.46871800	-4.35094700	-0.82400800
H	-2.17816100	-2.72337300	-1.41398600
C	-4.10026800	-5.00276200	0.23925600
H	-4.39616500	-5.03479500	2.37648700
H	-3.60771100	-4.70965900	-1.84106800
H	-4.73064900	-5.86882600	0.05529800
C	-0.49613400	0.82570700	-3.81262000
C	-2.40988100	-0.39605800	-3.01452700
C	-2.28305100	0.20156000	-1.76163000
C	-1.24323100	1.10087900	-1.54347300
C	-0.35792400	1.43222100	-2.56728600
H	0.19667600	1.07956600	-4.61245800
H	-3.23260400	-1.08574400	-3.18387700
H	-2.99134400	-0.01109000	-0.97278200
H	0.43813400	2.14088800	-2.37715100
C	-1.63609900	-0.78795700	-5.39204300
H	-0.96632900	-1.65724600	-5.45244000
H	-2.65541500	-1.14802800	-5.56798500
H	-1.36586900	-0.11476100	-6.21367600
C	-1.51761200	-0.10311700	-4.05236800
S	-1.07944900	1.95096900	0.04257400
N	-2.62622900	1.90985200	0.69706100
C	-3.50946800	2.65913700	0.01022400
C	-4.97185900	2.41523100	0.51771300
O	-3.30180800	3.37260600	-0.98566200
C	-5.01451800	2.33753400	2.05223800
C	-5.87349800	3.56905700	0.04949400
C	-5.36574700	1.08744600	-0.14564400
C	-5.30634600	-0.13456600	0.54117900
C	-5.67587900	1.05092500	-1.51388700
C	-5.55717600	-1.34407700	-0.10739900
H	-5.02350900	-0.15288100	1.58621400
C	-5.93454600	-0.15524000	-2.16559400
H	-5.67307400	1.97175400	-2.08540800
C	-5.87551900	-1.36107200	-1.46597900
H	-5.47616600	-2.27562000	0.44396400

H	-6.16189000	-0.15052600	-3.22922700
H	-6.05615200	-2.30596200	-1.97194700
H	-4.75972400	3.31588700	2.47429900
H	-4.28830600	1.62100300	2.43640100
H	-6.01926300	2.06511700	2.40090600
H	-5.61861600	4.48346100	0.59681000
H	-6.92825900	3.33461500	0.23709800
H	-5.73002800	3.78326800	-1.00998800

IM4

C	2.15783400	0.89858500	2.17620300
C	4.90302100	-1.47137100	1.14003200
C	4.50057000	-0.28508900	-2.39584900
C	1.76327000	2.05314400	-1.20193900
O	3.80313000	-1.91421500	0.67446800
O	5.32637000	-0.27510900	1.05303800
O	3.47904800	-0.98368600	-2.08339200
O	5.01521000	0.64138500	-1.69668500
O	1.39487300	0.83071400	-1.22873800
O	2.89370000	2.47100500	-0.80217700
O	1.72801500	-0.12002600	1.53670500
O	3.19333200	1.57191100	1.87211700
Rh	2.55125600	-0.59333300	-0.27978200
Rh	4.16529100	1.13584600	0.11323500
C	-1.16174600	-1.02340500	-1.32215000
C	0.74293100	3.07959200	-1.61951900
C	5.14590300	-0.59417800	-3.72633100
C	5.76896500	-2.45276600	1.89306600
C	1.32599200	1.35059200	3.34545000
H	0.43329200	1.84453400	2.94070200
H	1.88332100	2.04756200	3.97319600
H	0.99413500	0.48650400	3.92771900
H	5.46396200	-2.45437400	2.94607100
H	6.81740100	-2.15323900	1.83901000
H	5.63305000	-3.46117900	1.49665100
H	5.41320800	-1.65476300	-3.76662600
H	6.03450000	0.02060700	-3.87431200
H	4.42722100	-0.40334800	-4.53027200
H	0.02803700	2.64998800	-2.32349300
H	1.23102700	3.96149500	-2.03900000
H	0.19477800	3.37595200	-0.71670900
C	-0.03735000	-1.95750400	-1.51933000
O	0.83890600	-2.13946900	-0.67591000
O	-0.05924700	-2.57798800	-2.69224100
C	1.08010000	-3.43047500	-2.96343000
H	1.99988800	-2.84527300	-2.90258600
H	0.91207700	-3.80712400	-3.97151800
H	1.11260200	-4.24972500	-2.24165300
C	-2.21897400	-0.89890100	-2.07967400
C	-3.34731900	-0.64237200	-2.69505500
C	-4.65320400	-1.23225600	-2.37747200
C	-4.81135500	-2.15772500	-1.33197000
C	-5.78270500	-0.82453600	-3.10270000
C	-6.07097200	-2.65270200	-1.01764400
H	-3.94626100	-2.46816800	-0.75551500
C	-7.04508300	-1.32616400	-2.78795600
H	-5.66786700	-0.10716500	-3.91104000
C	-7.19316800	-2.24098000	-1.74441800
H	-6.17976900	-3.35833500	-0.19923000
H	-7.91132000	-1.00112000	-3.35676600

H	-8.17645300	-2.62927100	-1.49567900
C	-1.66201700	-2.58837400	3.14349800
C	-3.81665600	-1.78100000	2.41947100
C	-3.20669300	-0.96783100	1.46958800
C	-1.81603500	-0.98462800	1.36834500
C	-1.02741300	-1.77751400	2.20188900
H	-1.06110500	-3.21517100	3.79759200
H	-4.89968700	-1.76443100	2.50696500
H	-3.79143700	-0.32299300	0.82412800
H	0.05339100	-1.74762000	2.11647100
C	-3.73284700	-3.45294400	4.31446800
H	-3.94339700	-2.86738900	5.21901700
H	-4.68948900	-3.84633400	3.95420500
H	-3.10493200	-4.29904000	4.61098200
C	-3.05763400	-2.60233100	3.26699000
S	-0.99006100	0.06061900	0.14773000
N	-2.14149100	1.17171700	-0.29205500
C	-2.12106300	2.25272800	0.52551000
C	-3.32909900	3.19111200	0.23826400
O	-1.32754900	2.48120700	1.45352200
C	-3.17737600	4.49939100	1.03015700
C	-3.38579000	3.52172000	-1.26331600
C	-4.54430600	2.37874600	0.71304800
C	-4.72662000	2.14404100	2.08447900
C	-5.42094200	1.74904600	-0.18044000
C	-5.75221400	1.31965100	2.54631000
H	-4.03687900	2.58081500	2.79873200
C	-6.44128900	0.91350400	0.27545900
H	-5.29716700	1.88296900	-1.24800100
C	-6.61474800	0.69646600	1.64300100
H	-5.86490100	1.15209000	3.61412400
H	-7.08892000	0.42205900	-0.44389100
H	-7.40966900	0.04657800	1.99924300
H	-3.02790700	4.31936000	2.09530800
H	-4.06729600	5.12378900	0.89549400
H	-2.30376400	5.05423500	0.67355400
H	-2.50651400	4.11235800	-1.54236300
H	-4.27845900	4.11385900	-1.49604200
H	-3.38434100	2.61649800	-1.87266500
H	-3.32177400	0.10334200	-3.48988000

IM5

C	2.02917700	0.39906100	-2.23891100
C	1.96572500	3.02410000	0.11137700
C	4.51097000	1.27797900	2.32161600
C	4.60318200	-1.52646000	-0.08957700
O	1.50992800	2.04759000	0.78838000
O	3.09548000	3.05749000	-0.47649600
O	3.42894400	0.61573000	2.39742000
O	5.07961700	1.69133000	1.26164000
O	3.46137300	-1.56355700	0.46725300
O	5.15605900	-0.51785700	-0.62952200
O	1.51524700	-0.09658900	-1.18255000
O	3.18320000	0.93342000	-2.31752200
Rh	2.40864200	0.21114700	0.64435600
Rh	4.19061300	1.31422200	-0.56665000
C	-1.16529900	-0.98304000	0.44832800
C	5.40141700	-2.81510500	-0.10111700
C	5.17245700	1.63978400	3.63507900
C	1.04280200	4.20520600	-0.03837500

C	1.16460500	0.38719700	-3.47086300
H	0.51708900	1.27178700	-3.40887200
H	0.51165700	-0.48805800	-3.47840000
H	1.77620700	0.44523200	-4.37399500
H	0.52868300	4.40151300	0.90652500
H	0.28358200	3.92225500	-0.77984100
H	1.58615400	5.08881000	-0.37922500
H	4.73899400	2.57871200	3.99940600
H	6.24570900	1.78613000	3.49495800
H	4.98163200	0.86542600	4.38163200
H	4.80637800	-3.64159400	0.29025200
H	6.29658200	-2.68530700	0.51677900
H	5.73600500	-3.03656100	-1.11945000
C	-0.16795900	-1.42390500	1.30931100
O	0.79829400	-0.75373200	1.78891800
O	-0.33393800	-2.71526900	1.73938500
C	0.78607400	-3.28794400	2.41937500
H	0.51761900	-4.33557800	2.56926100
H	0.95516200	-2.79479300	3.38112000
H	1.69311700	-3.20840400	1.81462000
C	-2.19703400	-1.81951500	-0.13810900
C	-3.52364700	-1.80765300	0.06435900
C	-4.21125400	-1.02980800	1.10265300
C	-3.69318700	-0.91925100	2.40343300
C	-5.42855700	-0.40167600	0.80208600
C	-4.37695900	-0.19311100	3.37298000
H	-2.75593300	-1.41041200	2.63863000
C	-6.10065100	0.34405800	1.76801100
H	-5.82409300	-0.46800400	-0.20685800
C	-5.57930200	0.44541900	3.05839300
H	-3.95866800	-0.10564500	4.37155700
H	-7.02275100	0.85593500	1.50647000
H	-6.09988300	1.02898400	3.81352200
C	-1.72464500	2.46564900	3.60998200
C	-3.63408900	2.97545400	2.23776400
C	-3.08633000	2.24115800	1.18944900
C	-1.85172800	1.62486000	1.36399000
C	-1.15034800	1.74072300	2.56616700
H	-1.18948600	2.55394100	4.55340500
H	-4.60382100	3.44744300	2.09881200
H	-3.61496900	2.12372600	0.25344800
H	-0.18000800	1.27131300	2.67618300
C	-3.60593900	3.83356800	4.61397100
H	-2.85773900	4.16824900	5.34086100
H	-4.16078800	4.71291900	4.26706500
H	-4.32025000	3.19309500	5.15057600
C	-2.97023300	3.09084500	3.46389900
S	-1.07533800	0.73263500	-0.01709000
N	-2.26530600	0.80189200	-1.18645200
C	-2.03459600	1.74804400	-2.11528000
C	-3.20414600	1.79813400	-3.14915200
O	-1.09604000	2.56667700	-2.19280600
C	-2.79807900	2.67476800	-4.34690900
C	-3.52221900	0.37925800	-3.64497900
C	-4.37732000	2.44387700	-2.40111600
C	-4.20081500	3.70781500	-1.81321800
C	-5.61284400	1.80999800	-2.22689300
C	-5.21550200	4.30833500	-1.07122000
H	-3.23508500	4.19655700	-1.90097700

C	-6.63410800	2.40922800	-1.48510000
H	-5.78015000	0.82943300	-2.65783400
C	-6.44146200	3.66005000	-0.90025200
H	-5.04260800	5.27871200	-0.61238900
H	-7.58073900	1.88848400	-1.35969800
H	-7.23279600	4.12299300	-0.31613800
H	-2.49302900	3.67346700	-4.02970100
H	-3.63695500	2.76314900	-5.04758300
H	-1.94966200	2.22314800	-4.87138000
H	-4.31491700	0.39962000	-4.40429400
H	-3.82021600	-0.27079300	-2.82165900
H	-2.62904900	-0.06877000	-4.08759500
C	-0.22365600	-3.75545700	-1.07230700
C	-0.25642600	-4.96974500	-0.36566900
C	0.93986700	-5.66519000	-0.17320000
C	2.15056300	-5.15857500	-0.64629400
C	2.17775000	-3.93212100	-1.30076200
C	0.98975200	-3.23436700	-1.51251900
H	0.92091800	-6.60294000	0.36917400
H	3.06771800	-5.71753900	-0.48254200
H	3.11318600	-3.50651100	-1.64455800
H	0.99193100	-2.27233500	-2.00304700
C	-1.50875100	-5.58676200	0.21489100
S	-1.69102300	-2.80468800	-1.58871200
O	-1.18515500	-1.88865400	-2.63000000
O	-2.74457800	-3.77329200	-1.95259000
F	-2.36634300	-4.68391300	0.71080700
F	-2.16907800	-6.34433300	-0.68406800
F	-1.18804100	-6.41728700	1.24926200
H	-4.14909600	-2.39612700	-0.60357100

IM6

C	-1.09630400	1.26178700	1.68052200
C	2.25027800	1.85848700	0.25496900
C	2.35682800	5.24324700	1.80301700
C	-1.03046700	4.70398500	3.24464100
O	2.36158100	1.71272200	1.51707400
O	1.41505600	2.60991700	-0.33829800
O	2.46561200	4.36147000	2.71408800
O	1.49361800	5.25369600	0.86717600
O	-0.19398500	3.95285000	3.84849600
O	-1.14144700	4.83131800	1.98642400
O	-0.25462300	1.27953600	2.64323900
O	-1.21512100	2.15882600	0.79078700
Rh	1.12422500	2.80965800	2.74740000
Rh	0.11020600	3.74048300	0.77678500
C	0.32103800	0.67097600	5.60184600
C	-1.98910500	5.47792600	4.11576500
C	3.32231600	6.40299800	1.85620100
C	3.22203400	1.08752200	-0.60553000
C	-2.00439600	0.06141700	1.61387400
H	-1.40068000	-0.83257300	1.42597900
H	-2.49435100	-0.08515600	2.57936700
H	-2.74516000	0.18206500	0.82215300
H	3.41321000	0.10294000	-0.17177400
H	2.83864300	0.99135300	-1.62260200
H	4.17292300	1.63190500	-0.63792100
H	3.59074900	6.71727700	0.84510800
H	2.83127800	7.24888000	2.35162700
H	4.21270700	6.13089500	2.42547100

H	-1.45278000	5.93104500	4.95433000
H	-2.50419000	6.24426000	3.53505100
H	-2.72575200	4.78191400	4.53279600
C	1.67417000	0.72524400	4.93775700
O	2.16509400	1.76744400	4.51336600
O	2.25308200	-0.45182200	4.78509600
C	3.52284800	-0.44309900	4.08312800
H	4.24905100	0.11563400	4.67337500
H	3.80418800	-1.49224700	4.00395700
H	3.39488100	0.01893000	3.10279700
C	0.02218900	1.72283600	6.59033200
C	-1.22527800	2.00035300	7.02661400
C	-2.48689400	1.70458600	6.32774100
C	-3.56434300	1.16358200	7.04945700
C	-2.63475100	1.96469900	4.95863300
C	-4.75811100	0.86904800	6.39640800
H	-3.41962500	0.90158300	8.09342500
C	-3.84157600	1.68534400	4.31390700
H	-1.80743800	2.39691700	4.41108600
C	-4.90332800	1.13088300	5.02896100
H	-5.57908100	0.42888800	6.95520500
H	-3.94904600	1.90648000	3.25545100
H	-5.84113300	0.90788400	4.52775700
C	-0.77883200	-3.33844000	3.25502900
C	-2.86177300	-2.45216300	4.08022300
C	-2.18767800	-1.77081800	5.08730900
C	-0.79966200	-1.88225100	5.16365800
C	-0.08502700	-2.66371900	4.26153300
H	-0.22959900	-3.95979300	2.55246100
H	-3.94399700	-2.36931800	4.01506200
H	-2.71531400	-1.17457500	5.82376000
H	0.99062300	-2.76175100	4.35370700
C	-2.91727300	-3.95875600	2.04952800
H	-2.27710800	-4.68102800	1.53412700
H	-3.28866000	-3.24911000	1.29894300
H	-3.78784900	-4.49575100	2.44254400
C	-2.17056000	-3.24367600	3.14835100
S	0.08973200	-1.06421400	6.50721500
N	-1.08321700	-0.64123600	7.53666100
C	-1.20131300	-1.13952800	8.81398500
C	-0.29457100	-2.29876400	9.33107800
O	-2.06022000	-0.65890000	9.54888500
C	-0.90901900	-2.85964200	10.62871000
C	1.08296300	-1.68887600	9.66717700
C	-0.23701700	-3.41956600	8.29169000
C	-1.43711200	-3.89533500	7.73778000
C	0.96038600	-4.00666100	7.86500900
C	-1.44213800	-4.90770400	6.78245400
H	-2.37618600	-3.44104400	8.04218700
C	0.96032400	-5.02436000	6.90787100
H	1.90536800	-3.65671000	8.26556000
C	-0.23950100	-5.47723000	6.36015500
H	-2.38353400	-5.23821000	6.35307600
H	1.90390400	-5.45980600	6.58942800
H	-0.23853200	-6.26026500	5.60726900
H	-0.27744900	-3.66746700	11.01438300
H	-0.98982600	-2.07175100	11.38080900
H	-1.91195100	-3.25735400	10.45280500
H	1.71484800	-2.42652400	10.17447700

H	1.61878800	-1.31839500	8.79061600
H	0.94543400	-0.84219500	10.34639700
C	2.21579100	3.51063600	6.90338400
C	3.60947100	3.66816400	6.80881700
C	4.10746900	4.81473600	6.18398700
C	3.25211800	5.78658700	5.66990800
C	1.87584400	5.62696000	5.78236500
C	1.36225200	4.49316900	6.40433200
H	5.17946700	4.94289400	6.10642000
H	3.66696500	6.66192700	5.18039000
H	1.19710500	6.36998700	5.37611400
H	0.29161900	4.34965400	6.45994700
C	4.61704600	2.67014300	7.33777400
S	1.37450100	2.11496200	7.70396600
O	2.23216600	0.91399500	7.66445300
O	0.83495800	2.61906400	8.97455300
F	4.36773900	2.32472900	8.61244400
F	4.66381900	1.54231400	6.59390900
F	5.86928400	3.18735900	7.31320800
H	-1.30372100	2.51081500	7.98483500
H	-0.42625400	0.63835200	4.80931400

TS1

C	2.69691700	0.20768400	2.05321700
C	-0.11705300	2.53668900	1.39465200
C	-0.39909700	1.22031700	-2.08751700
C	2.42359500	-1.13723700	-1.39721700
O	-0.58869100	1.34943800	1.45084300
O	0.89265400	2.91066500	0.72814100
O	-0.80447000	0.32970500	-1.27041000
O	0.67053800	1.89675400	-1.99505900
O	1.40956900	-1.52231000	-0.72465700
O	2.86563900	0.04764200	-1.48145700
O	1.60580800	-0.45266600	1.97906000
O	3.10410000	1.07392500	1.22301900
Rh	0.34779100	-0.14046900	0.38366700
Rh	1.93168500	1.53667200	-0.40914200
C	-1.07007600	-1.61362700	1.03837100
N	-1.00570900	-1.38707500	2.74327200
N	-0.87454200	-0.76575700	3.65509500
C	3.17136200	-2.21624900	-2.14625500
C	-1.27454200	1.46598400	-3.29529200
C	-0.85896000	3.58103300	2.19592900
C	3.55747000	-0.06822100	3.26319800
H	3.08705300	0.38072800	4.14535700
H	3.62309300	-1.14588100	3.43488200
H	4.55159200	0.36107300	3.13039300
H	-1.85476300	3.72741200	1.76343700
H	-0.99570200	3.23036800	3.22310000
H	-0.31567400	4.52679600	2.18823300
H	-2.32413300	1.29270600	-3.04712000
H	-1.12593000	2.47966600	-3.67265900
H	-0.99194400	0.75854100	-4.08360700
H	2.46445200	-2.86121400	-2.67557800
H	3.88042500	-1.77389100	-2.84737300
H	3.71669100	-2.83715300	-1.42648100
C	-0.51518700	-3.00112600	0.92556600
O	0.14202500	-3.56052200	1.77638400
O	-0.77441500	-3.47820600	-0.29884600
C	-0.02314900	-4.64743500	-0.66554200

H	1.04272000	-4.40914100	-0.66509300
H	-0.22033300	-5.46457400	0.03220200
H	-0.36159700	-4.90355000	-1.66910100
C	-2.36250200	-1.28321700	0.63495100
C	-3.40957600	-0.88302700	0.15343000
C	-4.51899600	-0.25445300	-0.46617400
C	-4.39072200	1.08768800	-0.88352800
C	-5.72922200	-0.93756300	-0.68939500
C	-5.45496500	1.72613600	-1.51089400
H	-3.44746300	1.59427700	-0.70901000
C	-6.78853100	-0.28974300	-1.31792900
H	-5.82079700	-1.96988100	-0.36773500
C	-6.65361400	1.03922700	-1.72865400
H	-5.35313200	2.75846500	-1.83241700
H	-7.72060100	-0.81983300	-1.48950700
H	-7.48298700	1.54014400	-2.21962500

TS2

C	1.47308400	-0.28740700	2.64259800
C	2.98711700	2.62501800	0.70128000
C	3.99438300	0.22764500	-1.96336700
C	2.49544000	-2.56966200	-0.00705400
O	1.94545500	2.22756900	0.08265500
O	3.91144100	1.89505100	1.17286200
O	2.72146300	0.31252500	-1.99698100
O	4.71205600	0.06509600	-0.93186300
O	1.54398800	-1.84572400	-0.45850300
O	3.55083500	-2.15779900	0.55962500
O	0.75357800	0.04507300	1.62553400
O	2.72854600	-0.36410200	2.66031400
Rh	1.65170000	0.21388300	-0.24286100
Rh	3.79568600	-0.14195700	0.89727600
C	-0.14234400	0.65093500	-1.28540700
C	2.31916200	-4.06386500	-0.14170500
C	4.69568900	0.30291400	-3.30018000
C	3.13404500	4.12177600	0.85524000
C	0.70721300	-0.65156400	3.88948900
H	-0.09004400	0.07500100	4.07160000
H	0.24471100	-1.63163400	3.71935700
H	1.37557600	-0.70859100	4.74963200
H	2.15782400	4.58083100	1.02865800
H	3.82254900	4.35561100	1.66924900
H	3.53720800	4.53379300	-0.07705800
H	5.75010700	0.54870300	-3.16331900
H	4.62363700	-0.67313700	-3.79434100
H	4.20600100	1.04199300	-3.93897700
H	1.96903600	-4.31118800	-1.14771700
H	3.25693300	-4.57912900	0.07103500
H	1.55594500	-4.38386200	0.57573900
C	0.01720600	0.39088600	-2.74983500
O	0.20584300	1.27060900	-3.56463400
O	0.05095100	-0.92599800	-3.04807100
C	0.49480900	-1.23259000	-4.37550500
H	0.48118500	-2.32082300	-4.44158700
H	-0.17212300	-0.79192600	-5.12164600
H	1.50706200	-0.84905600	-4.52330600
C	-0.79575800	1.81379900	-0.90602100
C	-1.44688000	2.73979300	-0.44377500
C	-2.22780900	3.79717800	0.08003900
C	-3.13594400	4.49363200	-0.74284700

C	-2.14226300	4.13469100	1.44610400
C	-3.92508700	5.50993600	-0.21380400
H	-3.20515300	4.22325600	-1.79109600
C	-2.94195600	5.14514900	1.96993400
H	-1.44631200	3.58975800	2.07533800
C	-3.83170500	5.83756500	1.14228500
H	-4.61692900	6.04651100	-0.85656600
H	-2.86950300	5.39998900	3.02330400
H	-4.44903100	6.63156300	1.55288800
C	-4.17009100	1.30606100	1.62715600
C	-5.02856700	1.43895300	-0.61674700
C	-4.02556400	0.57987000	-1.05824800
C	-3.09144900	0.08905600	-0.14360000
C	-3.15498300	0.45851800	1.20259100
H	-4.22035700	1.59416000	2.67379600
H	-5.75688400	1.81873200	-1.32796900
H	-3.97750200	0.28527300	-2.10251200
H	-2.41864100	0.07932700	1.90141100
C	-6.17428100	2.78219900	1.19834300
H	-6.98732200	2.87268400	0.47140700
H	-5.74276500	3.78007200	1.34232400
H	-6.60443200	2.46822800	2.15579200
C	-5.11646300	1.81844900	0.72758900
S	-1.79324500	-0.92397600	-0.78976000
N	-1.17353800	-1.64713900	0.60275300
H	-0.43785800	-1.10346700	1.07655300
C	-1.17208000	-3.00022300	0.90531900
C	-2.07928000	-3.96001900	0.10650100
O	-0.45788800	-3.37918500	1.82361400
C	-2.16998800	-5.28780800	0.88669400
C	-1.39167200	-4.24194000	-1.24853700
C	-3.48509600	-3.36615900	-0.02454600
C	-4.17658100	-3.31001300	-1.23977500
C	-4.12033100	-2.86957000	1.12281000
C	-5.45505300	-2.75423800	-1.30970900
H	-3.71074200	-3.67778300	-2.14710400
C	-5.39384400	-2.30982000	1.05657900
H	-3.59865300	-2.89684600	2.07602100
C	-6.06717400	-2.24650200	-0.16384800
H	-5.96899300	-2.71285300	-2.26616000
H	-5.85272900	-1.90893800	1.95548400
H	-7.05510600	-1.79949800	-0.22187500
H	-1.17893800	-5.73051800	1.01204200
H	-2.59857600	-5.13694400	1.88048800
H	-2.80923600	-5.98489500	0.33600100
H	-1.94579400	-5.01219800	-1.79468800
H	-1.31110300	-3.35467700	-1.88078400
H	-0.38219700	-4.61971900	-1.07127600

TS3

C	3.93913800	0.26450800	0.95512300
C	2.25643700	-0.43823400	-2.37719100
C	0.93924300	-3.60375800	-1.00904200
C	2.60901900	-2.92516100	2.25377300
O	1.40291600	-0.12909700	-1.48645800
O	3.22072500	-1.25871400	-2.23535300
O	0.32904200	-2.64375300	-0.43979800
O	2.19575700	-3.72790800	-1.14443300
O	1.61864300	-2.14338500	2.10191800
O	3.52575900	-3.15571400	1.40408800

O	2.67977700	0.34916100	1.11240900
O	4.54193400	-0.66656900	0.32654900
Rh	1.43216900	-1.07398800	0.34825100
Rh	3.42291700	-2.22166700	-0.43047000
C	-0.41787800	0.13442400	1.33465100
C	2.67368600	-3.67314300	3.56652100
C	0.05951000	-4.69573700	-1.57845400
C	2.10787900	0.25321000	-3.70959400
C	4.76214400	1.35132700	1.59819300
H	5.60431400	1.61183200	0.95443500
H	4.13736500	2.22685800	1.78710800
H	5.15293800	0.97404000	2.55143100
H	2.26000100	1.32788900	-3.57014900
H	2.83783400	-0.13108800	-4.42411100
H	1.09007000	0.10383900	-4.08105300
H	-0.46299000	-5.20341900	-0.76041900
H	-0.70248800	-4.24667600	-2.22322400
H	0.65314100	-5.41938800	-2.13914200
H	2.23093600	-3.06968500	4.36181500
H	2.09606000	-4.60089500	3.47536400
H	3.70706200	-3.93333200	3.80521500
C	-0.81298500	-0.80052600	2.41666700
O	-0.55004100	-0.62253400	3.59074400
O	-1.49290200	-1.87250100	1.95774600
C	-1.81485600	-2.84926300	2.95067900
H	-0.89783800	-3.28118900	3.36091600
H	-2.40126400	-2.40243600	3.75740100
H	-2.39883200	-3.60930000	2.42960200
C	-1.07214800	0.22803100	0.14278800
C	-1.81327200	0.42687500	-0.86563800
C	-1.86298800	0.11597500	-2.28899600
C	-2.65040400	0.91021200	-3.13769000
C	-1.21170900	-1.00984700	-2.81940100
C	-2.76130700	0.60053500	-4.49211500
H	-3.19691400	1.74482100	-2.71552400
C	-1.32982200	-1.31720500	-4.17226300
H	-0.63869500	-1.63682700	-2.15174700
C	-2.10091200	-0.51219900	-5.01608100
H	-3.38195200	1.22001300	-5.13361800
H	-0.82327900	-2.19462700	-4.56853900
H	-2.19481800	-0.75779500	-6.07093900
C	-3.46319400	2.74405300	3.19427300
C	-1.88158500	4.33309300	4.06775300
C	-0.82959400	3.61223200	3.50688400
C	-1.11279900	2.45080900	2.77987800
C	-2.42579100	2.01326600	2.61999800
H	-4.47629000	2.37934000	3.05272900
H	-1.66524800	5.23908900	4.62996500
H	0.19720500	3.95186800	3.59685300
H	-2.68498900	1.12268600	2.06420100
C	-4.34740900	4.71741200	4.50293400
H	-4.01003300	5.34846100	5.33268700
H	-5.14859200	4.06727700	4.87137500
H	-4.79135500	5.37877300	3.74655400
C	-3.21030900	3.91263900	3.92083400
S	0.32821600	1.63290000	2.05238500
N	0.58005500	2.51631600	0.63883900
C	1.48061500	3.49155200	0.86008300
C	1.82257500	4.32333800	-0.41284400

O	2.03603400	3.79029300	1.93911000
C	1.78057000	5.80374400	-0.00314100
C	0.81394800	4.08959200	-1.55653400
C	3.21489200	3.87804100	-0.87237700
C	3.39128000	2.54578700	-1.27653600
C	4.32249700	4.73050800	-0.91849600
C	4.62358900	2.08334900	-1.73454400
H	2.55081200	1.86831400	-1.19500200
C	5.56343200	4.27142400	-1.37127300
H	4.22819400	5.76172600	-0.59681800
C	5.71932900	2.94987100	-1.78640300
H	4.73280800	1.04316200	-2.02665100
H	6.40981800	4.95422000	-1.39652300
H	6.68420900	2.59328500	-2.13833400
H	2.05493300	6.45372400	-0.84268600
H	0.76390300	6.06636000	0.30882100
H	2.44800200	5.99090700	0.84069300
H	1.10505700	4.68405500	-2.43229900
H	0.76124800	3.03816700	-1.84196500
H	-0.19051500	4.39009000	-1.24338000
H	-2.91111300	1.04024400	-0.49056200
C	-4.73882200	-0.91960900	-0.78460000
C	-5.10156300	-1.16267800	-2.11660800
C	-4.61153000	-2.29653600	-2.77044200
C	-3.74667300	-3.16815200	-2.11009700
C	-3.38835200	-2.92429200	-0.78494400
C	-3.90083900	-1.81018200	-0.12322300
H	-4.88860000	-2.47809600	-3.80191200
H	-3.34816900	-4.02976800	-2.63876800
H	-2.68419000	-3.57385900	-0.27381800
H	-3.63305300	-1.58935400	0.90259900
C	-6.06649200	-0.26247900	-2.83966600
S	-5.21384000	0.61347900	0.16664200
O	-4.92965200	0.20005900	1.59321800
O	-4.08722700	1.59025100	-0.36922200
F	-6.16461800	-0.56956300	-4.15669600
F	-7.31794600	-0.36903100	-2.32319900
F	-5.73518800	1.04342500	-2.76913900

TS3'

C	3.48552100	-2.41668400	-1.41069900
C	1.52777400	-3.35805500	1.57831000
C	1.95951500	0.14553100	2.92949800
C	3.90736300	1.04187600	-0.06198300
O	0.82398000	-2.55010300	0.88841000
O	2.74167100	-3.19462700	1.91383900
O	1.16855400	0.16445500	1.93255200
O	3.06156000	-0.48891200	2.99159100
O	2.70857700	0.85933200	-0.44897900
O	4.58700900	0.25366500	0.66913500
O	2.35552600	-1.83271900	-1.46544500
O	4.27547500	-2.43292500	-0.41760300
Rh	1.67461000	-0.80390200	0.19885300
Rh	3.70848600	-1.48071900	1.31688100
C	-0.52655700	-0.29771600	-0.90722200
C	4.56992700	2.32788500	-0.48965900
C	1.56008700	0.97527800	4.12341000
C	0.83454700	-4.60676100	2.06846600
C	3.91417300	-3.16729700	-2.65119200
H	4.91882300	-3.57337900	-2.52655800

H	3.20866000	-3.98365200	-2.83957100
H	3.88645800	-2.49666500	-3.51564800
H	1.55650600	-5.41506500	2.20071900
H	0.37367800	-4.39335400	3.03986600
H	0.04701500	-4.89988700	1.37096500
H	1.85414700	0.47178900	5.04785100
H	2.10272900	1.92676600	4.07123000
H	0.48824700	1.18311400	4.10301200
H	4.19752700	3.13992500	0.14328100
H	5.65338700	2.25131400	-0.38369800
H	4.29704600	2.56568800	-1.52056900
C	-0.37759200	-1.22980300	-2.03302600
O	-0.79004200	-2.37668000	-2.04546500
O	0.22945700	-0.64748700	-3.09562600
C	0.54641600	-1.53841200	-4.17274300
H	-0.36117200	-1.99767200	-4.57362000
H	1.02919100	-0.91678500	-4.92789700
H	1.22701600	-2.31498000	-3.82111000
C	-0.20494600	1.01696600	-0.93018600
C	-0.04608900	2.27269800	-0.96368100
C	0.73990100	3.23461700	-0.19687500
C	1.54890000	4.19191400	-0.82675600
C	0.62348200	3.24260700	1.20580800
C	2.26199300	5.12303000	-0.07125200
H	1.64388700	4.18221800	-1.90930900
C	1.33293400	4.18275800	1.95014600
H	-0.03161100	2.52552000	1.68967600
C	2.15862000	5.12032800	1.32120800
H	2.89887100	5.84818700	-0.57102600
H	1.23292400	4.18454900	3.03213200
H	2.70789500	5.84916100	1.91063400
C	-4.87533500	-1.47029000	-2.29537200
C	-5.31385600	0.61467500	-1.17872400
C	-4.13500000	0.47930900	-0.44922200
C	-3.32387500	-0.63251100	-0.66186000
C	-3.69521400	-1.62625100	-1.56760300
H	-5.16788800	-2.24123000	-3.00388700
H	-5.95404200	1.47701200	-1.00607000
H	-3.82940300	1.20909400	0.29222500
H	-3.06802800	-2.49784500	-1.70650100
C	-6.95796800	-0.17568400	-2.93082500
H	-6.78391600	0.48174300	-3.79347400
H	-7.75758400	0.27833000	-2.33574900
H	-7.32221600	-1.13263200	-3.31733100
C	-5.69802600	-0.35052400	-2.11916900
S	-1.80738900	-0.81144800	0.32446500
N	-1.82076100	0.53872700	1.25904000
C	-1.91402200	0.45006500	2.62269700
C	-2.36002200	-0.85137400	3.38024500
O	-1.67507100	1.46103600	3.28972100
C	-2.77321400	-0.46383700	4.81490700
C	-1.14724900	-1.79533700	3.48465600
C	-3.55911500	-1.48789500	2.67491700
C	-4.72748500	-0.72947200	2.50074300
C	-3.55052600	-2.79722900	2.17667300
C	-5.83946400	-1.25139800	1.84518400
H	-4.75219000	0.29481400	2.86223500
C	-4.66062300	-3.32285200	1.51208600
H	-2.66075500	-3.40788800	2.27846300

C	-5.80974800	-2.55252400	1.34089300
H	-6.72302300	-0.63399100	1.70946200
H	-4.61991700	-4.33622800	1.12180500
H	-6.66912400	-2.95669600	0.81371300
H	-1.93206200	-0.00605700	5.33971700
H	-3.59431000	0.25663600	4.82017300
H	-3.09320000	-1.36062400	5.35755600
H	-1.40685400	-2.67686000	4.08338400
H	-0.77929400	-2.12475900	2.51337900
H	-0.32840100	-1.27726100	3.99046400
H	-0.87047200	2.80199000	-1.98758600
N	-1.61828000	3.19526000	-2.95155700
C	-2.37123100	1.93133400	-3.21120100
H	-1.64747700	1.20182700	-3.57437400
H	-2.69205800	1.56690700	-2.23584700
C	-2.46282900	4.30582400	-2.38275500
H	-3.18289300	4.60478800	-3.15399600
C	-0.65583300	3.62647800	-4.02762300
H	-0.00307600	4.34121900	-3.52071400
C	-3.57804400	2.00512800	-4.14202500
H	-4.32174400	2.72924200	-3.79571400
H	-3.30504600	2.25731600	-5.16953300
H	-4.05866600	1.02192400	-4.14784200
C	0.23096800	2.46613800	-4.48955800
H	1.07519200	2.88011400	-5.05081400
H	0.62514300	1.88782100	-3.65048200
H	-0.30323800	1.78410000	-5.15900000
C	-1.30449900	4.33804200	-5.21911800
H	-1.89185300	3.64996100	-5.83266500
H	-1.95140300	5.16537000	-4.91591400
H	-0.51379400	4.75198900	-5.85396900
C	-3.23574000	3.81088600	-1.15454200
H	-3.99388700	3.07066100	-1.41404700
H	-2.56665700	3.37036400	-0.40827100
H	-3.74678500	4.66143900	-0.69378700
C	-1.61268300	5.52474600	-2.00681400
H	-0.83118200	5.25955900	-1.28898800
H	-1.14506900	6.00526700	-2.87001500
H	-2.26351400	6.26752700	-1.53627000

TS3”

C	3.50374900	-2.81239000	-0.13628700
C	1.50279500	-1.43711500	2.68063000
C	2.06516100	2.03236100	1.35369400
C	4.06280600	0.66523500	-1.40945100
O	0.84192300	-1.30721700	1.60136000
O	2.71601700	-1.12529700	2.87871500
O	1.26563400	1.40330700	0.58999400
O	3.15550100	1.59397200	1.83958300
O	2.84683400	0.35200200	-1.60757600
O	4.73450700	0.50307500	-0.34411700
O	2.41734800	-2.36886700	-0.62699000
O	4.28100000	-2.21886600	0.67074400
Rh	1.75264300	-0.48361200	-0.06567100
Rh	3.79851900	-0.30405300	1.31383100
C	0.01588100	-0.59242500	-1.26298200
C	4.76676000	1.33268400	-2.57399600
C	1.67798200	3.45724800	1.68777200
C	0.73828000	-1.99629300	3.86425100
C	3.89478200	-4.20984200	-0.57731500

H	3.10488800	-4.91307600	-0.29329200
H	3.98223300	-4.23628200	-1.66854000
H	4.84038100	-4.50859200	-0.12148400
H	1.38573900	-2.64731800	4.45738200
H	0.41819600	-1.16440800	4.50223800
H	-0.14688300	-2.53739000	3.52409700
H	2.30641700	4.13455600	1.09679400
H	0.63024300	3.63886800	1.44051300
H	1.87642800	3.66038200	2.74446100
H	4.48438200	0.84555700	-3.51099400
H	4.44054800	2.37759600	-2.63136100
H	5.84947900	1.30468900	-2.43566900
C	-0.23656500	-1.98702800	-1.67188600
O	-0.71631200	-2.87043100	-0.98365700
O	0.24957800	-2.22352200	-2.92149200
C	0.30933700	-3.60539600	-3.27868300
H	0.71807500	-3.62872800	-4.29074600
H	0.96561300	-4.14323100	-2.58839000
H	-0.68529500	-4.06081100	-3.25668100
C	-0.33142400	0.51629600	-1.95468200
C	-0.95863000	1.61055200	-1.95257400
C	-1.50518400	2.70023200	-2.70233700
C	-1.40797200	2.63686100	-4.11277800
C	-2.14857300	3.80952700	-2.12391400
C	-1.92924200	3.65089100	-4.90792800
H	-0.91886600	1.77741400	-4.56049200
C	-2.67691400	4.81331800	-2.93390400
H	-2.19254600	3.87208000	-1.04272500
C	-2.57455700	4.74588600	-4.32457400
H	-1.84067700	3.58114000	-5.98978300
H	-3.16980500	5.66337300	-2.46734300
H	-2.99082300	5.53393800	-4.94750100
C	-4.74611600	-2.74621500	-0.99009100
C	-5.13972600	-0.60155000	-2.00086600
C	-4.00561700	-0.08663300	-1.37489800
C	-3.24385200	-0.91305500	-0.54737000
C	-3.60791300	-2.25105000	-0.36238100
H	-5.02883700	-3.78607400	-0.83824500
H	-5.73027000	0.04534700	-2.64653900
H	-3.70977900	0.94727300	-1.50660200
H	-2.99569200	-2.89398000	0.25923000
C	-6.78480900	-2.47272500	-2.46470000
H	-7.12363300	-1.82368200	-3.27936800
H	-7.61093500	-2.55352700	-1.74450000
H	-6.62127200	-3.47520000	-2.87832300
C	-5.53451400	-1.93083700	-1.81418800
S	-1.82011700	-0.29501000	0.32976400
N	-1.95087800	1.32210400	0.02005800
C	-1.93001800	2.22555800	1.04106000
C	-2.32992100	1.80198800	2.50522700
O	-1.65570600	3.41645800	0.85322700
C	-2.74727900	3.07464500	3.27203200
C	-1.07287300	1.22645800	3.18598600
C	-3.51954100	0.84141000	2.50429200
C	-4.65651000	1.16461600	1.74870500
C	-3.54026000	-0.34960900	3.23952400
C	-5.76084200	0.31758500	1.70292800
H	-4.65375200	2.07123900	1.15031700
C	-4.64602700	-1.20051800	3.20023000

H	-2.67100800	-0.64204000	3.81804700
C	-5.76076600	-0.87434200	2.42818600
H	-6.61043500	0.57613700	1.07687800
H	-4.62630900	-2.13018900	3.76390000
H	-6.61223600	-1.54776400	2.37896900
H	-3.61059100	3.55572800	2.80392800
H	-3.01594000	2.80901900	4.30143200
H	-1.92839400	3.79679500	3.28339200
H	-0.26565000	1.96105200	3.13222000
H	-1.26932000	1.02382800	4.24597200
H	-0.72290400	0.31031000	2.70855300

TS4

C	1.79633200	0.36551300	-2.28340500
C	2.41266600	3.30658000	-0.19303800
C	5.09424500	1.44625300	1.68883300
C	4.38697100	-1.56542200	-0.48729700
O	1.98672200	2.45072400	0.65061500
O	3.37347400	3.12610400	-1.00859900
O	3.99528200	0.89508300	2.01263400
O	5.48151200	1.73438600	0.51223800
O	3.38750300	-1.39931400	0.28267900
O	5.00464700	-0.65605100	-1.12683000
O	1.39875300	0.15844700	-1.08858400
O	2.96025800	0.78060200	-2.59892700
Rh	2.63037100	0.50569500	0.50438400
Rh	4.25986600	1.26694600	-1.09014400
C	-1.03578400	-0.39912300	0.53971700
C	4.86978700	-2.98334500	-0.68263700
C	6.01928700	1.82610700	2.82526800
C	1.67197300	4.61736100	-0.23937000
C	0.80344100	0.08241900	-3.37105600
H	-0.15153300	0.55217400	-3.11504300
H	0.64062700	-1.00375300	-3.38819400
H	1.17046400	0.44481900	-4.33304300
H	1.50858700	4.98823100	0.77697900
H	0.68592200	4.43169900	-0.68505300
H	2.21949400	5.35272700	-0.83171400
H	5.70511600	2.79709500	3.22587400
H	7.04795700	1.91169900	2.46933100
H	5.94913400	1.09039300	3.63001500
H	4.56474600	-3.61030100	0.15668600
H	5.95508200	-2.99966000	-0.80804000
H	4.41304300	-3.37942700	-1.59668000
C	0.01223300	-0.89969000	1.41469900
O	0.91668400	-0.19102900	1.88843000
O	-0.07077000	-2.20564600	1.65225800
C	1.04725400	-2.79605300	2.34865000
H	0.80958600	-3.85666600	2.40467700
H	1.14281300	-2.35672500	3.34492100
H	1.96136700	-2.63121800	1.77680200
C	-1.94544300	-1.14594300	-0.06640200
C	-3.03803800	-1.63705400	-0.59749400
C	-4.38182800	-1.46001300	-0.03421200
C	-4.61115200	-0.76001600	1.16294000
C	-5.48146900	-1.99985700	-0.71962800
C	-5.90119200	-0.59946500	1.65314700
H	-3.76924800	-0.33762600	1.70015600
C	-6.77601500	-1.83743700	-0.22648700
H	-5.30827700	-2.55200000	-1.63905500

C	-6.99183800	-1.13821800	0.96230000
H	-6.05748700	-0.04565800	2.57509300
H	-7.61586900	-2.26289000	-0.76972900
H	-8.00036300	-1.01126800	1.34725500
C	-1.50029200	3.11953100	3.69464500
C	-3.65531000	2.86036400	2.64508000
C	-3.05555600	2.27352400	1.53524600
C	-1.67091400	2.11212700	1.52426600
C	-0.87806600	2.54004000	2.58773900
H	-0.89384000	3.45108300	4.53444100
H	-4.73432600	2.99359300	2.65064000
H	-3.64425100	1.95119100	0.68483000
H	0.19899300	2.41840200	2.54179900
C	-3.55207200	3.95070300	4.92405500
H	-2.90930400	3.92210500	5.81011500
H	-3.77734100	5.00516700	4.71471600
H	-4.50049900	3.46260800	5.17584200
C	-2.88975600	3.28901400	3.73952000
S	-0.84828300	1.35966900	0.09874900
N	-1.98318700	1.41281500	-1.11794300
C	-2.05547500	2.64422100	-1.66770800
C	-3.22642200	2.73980400	-2.69022400
O	-1.39415800	3.65349900	-1.36284700
C	-3.02953800	3.97073200	-3.59113700
C	-3.28499000	1.47959400	-3.56740400
C	-4.46822400	2.89961500	-1.79929100
C	-4.61635700	4.06164500	-1.02461300
C	-5.41724900	1.88133200	-1.64184400
C	-5.68160200	4.20656800	-0.13758700
H	-3.85950000	4.83627700	-1.08172800
C	-6.48340900	2.02108400	-0.75155900
H	-5.31655600	0.95332700	-2.19089600
C	-6.62340200	3.18519000	0.00390600
H	-5.76391000	5.11276300	0.45767200
H	-7.18786000	1.20366500	-0.63619300
H	-7.45057500	3.29122100	0.70158100
H	-2.87432900	4.87931100	-3.00824600
H	-3.90174600	4.10540600	-4.24130000
H	-2.14364000	3.83381500	-4.22055400
H	-4.15129200	1.51526500	-4.23955700
H	-3.32951600	0.57129800	-2.96525100
H	-2.38129200	1.41924800	-4.18292500
C	0.24834900	-4.60614900	-0.50979900
C	-0.43957800	-5.42444000	0.40259000
C	0.26788000	-6.37088400	1.15552500
C	1.64830300	-6.50716400	1.01620300
C	2.33091600	-5.69596100	0.11065600
C	1.62958900	-4.75163700	-0.63757500
H	-0.26982200	-7.00048700	1.85492300
H	2.18106800	-7.24403000	1.61146900
H	3.40636000	-5.79942700	-0.01331000
H	2.12363800	-4.10027000	-1.35062300
C	-1.93629000	-5.36011300	0.59815900
S	-0.49823600	-3.19682500	-1.50934000
O	0.65454100	-2.89546400	-2.45567400
O	-1.71325800	-3.83047600	-2.16412000
F	-2.38451800	-4.10150200	0.76012400
F	-2.62002400	-5.91943000	-0.41572200
F	-2.31088000	-6.03869100	1.72442800

H	-2.93444300	-2.28454800	-1.47697100
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TS5

C	-4.14236400	2.16962400	-1.28537200
C	-1.89518000	1.15594400	-4.07540300
C	-2.57173000	-2.42022700	-3.33001500
C	-4.81820900	-1.45984700	-0.56436400
O	-1.34613600	0.89399900	-2.96058000
O	-3.08718800	0.86231400	-4.41719800
O	-1.81497400	-1.89851600	-2.45107600
O	-3.65573600	-1.93103900	-3.77931300
O	-3.60605400	-1.23393400	-0.25117600
O	-5.40170100	-1.09011100	-1.63101900
O	-3.14217400	1.60611500	-0.73713600
O	-4.81801500	1.71419700	-2.26199200
Rh	-2.41108300	-0.13831500	-1.54042800
Rh	-4.28854900	-0.10742400	-3.06157100
C	1.47127100	0.29557700	0.87714700
C	-5.62490600	-2.26308000	0.43162800
C	-2.12563400	-3.74925700	-3.89908200
C	-1.05737800	1.91041800	-5.08044000
C	-4.53633900	3.51658800	-0.72829300
H	-4.54272100	3.47928300	0.36457700
H	-5.51298200	3.82171200	-1.10759100
H	-3.77734900	4.24734700	-1.02634700
H	-1.48507200	1.81925800	-6.08052500
H	-0.02981400	1.53904400	-5.06347600
H	-1.03427900	2.96568100	-4.78963100
H	-1.22933900	-3.59918400	-4.51122400
H	-2.91292800	-4.18528600	-4.51597100
H	-1.86257800	-4.42825200	-3.08274800
H	-5.47282800	-1.86488800	1.43895400
H	-5.26643800	-3.29847100	0.43025400
H	-6.68460300	-2.24769200	0.17199700
C	-0.01653500	0.18621700	0.74800400
O	-0.58329100	-0.03609500	-0.32081400
O	-0.61669100	0.36490200	1.91641000
C	-2.00841600	0.02575100	2.02326300
H	-2.61194400	0.71837100	1.43466700
H	-2.23662200	0.10823300	3.08610000
H	-2.16308900	-0.99461500	1.68019600
C	2.14685800	0.68624700	-0.38234500
C	1.83848900	1.69340000	-1.23050200
C	0.81803000	2.73753800	-1.19242700
C	0.07517200	3.11745700	-0.06125000
C	0.63757800	3.47920200	-2.37640500
C	-0.82703600	4.17605600	-0.12941600
H	0.24361700	2.64763900	0.89772500
C	-0.26329000	4.53547600	-2.44484800
H	1.22671200	3.21448300	-3.25005700
C	-1.00624100	4.88881500	-1.31532400
H	-1.36755000	4.46381900	0.76653200
H	-0.37317000	5.09611900	-3.37027800
H	-1.69565000	5.72864600	-1.35288600
C	3.17889800	-0.04906700	5.28390900
C	0.98373500	-1.01300900	5.53990500
C	0.93062400	-1.27979700	4.17425400
C	2.02182100	-0.93331700	3.38418700
C	3.15544600	-0.32838300	3.92067700
H	4.04102700	0.46598900	5.69798000

H	0.13719000	-1.28534500	6.16625000
H	0.06629400	-1.74924700	3.72361000
H	3.97535300	-0.02049600	3.28299700
C	2.15745100	-0.11070700	7.59406900
H	2.58407100	0.87876000	7.79419400
H	1.16005400	-0.14788800	8.04507400
H	2.78421100	-0.84507500	8.11831700
C	2.10263600	-0.39345300	6.11191300
S	2.02108200	-1.28676100	1.62264300
N	0.64026000	-2.21357500	1.37804600
C	0.87004000	-3.53123000	1.57490000
C	-0.43733500	-4.37539300	1.42859000
O	1.93371100	-4.07051100	1.91695700
C	-1.18051200	-4.01196600	0.13538000
C	-0.06700000	-5.86902600	1.39004400
C	-1.26903600	-4.07442200	2.68099700
C	-2.56102600	-3.53790800	2.62297400
C	-0.70797400	-4.30558500	3.94770800
C	-3.27106800	-3.24426900	3.78989900
H	-3.01101900	-3.31522400	1.66284700
C	-1.41302200	-4.01304500	5.11318700
H	0.31155300	-4.67315200	4.01155800
C	-2.70290500	-3.48047400	5.04115900
H	-4.27061700	-2.82134000	3.71597900
H	-0.94703900	-4.18679200	6.07982100
H	-3.25308900	-3.24628900	5.94888700
H	-2.11339300	-4.58517900	0.05049000
H	-0.55479300	-4.26152200	-0.72333200
H	-1.40755700	-2.94843400	0.07252000
H	0.56302600	-6.07401500	0.51804800
H	0.49697700	-6.16763500	2.27504800
H	-0.97562200	-6.47936000	1.32228100
C	3.10404200	-1.82865000	-1.19991000
C	3.81542300	-3.00926000	-0.92212600
C	3.24201100	-4.23189700	-1.27571000
C	2.00120900	-4.28862900	-1.90761300
C	1.30892500	-3.11467500	-2.18571100
C	1.85930100	-1.88715000	-1.82862000
H	3.77424100	-5.14437900	-1.04103400
H	1.57251900	-5.25424000	-2.15997200
H	0.32309000	-3.12571200	-2.63256600
H	1.29073900	-0.98079900	-2.00211900
C	5.16477100	-3.03582700	-0.23780200
S	3.68793000	-0.14626300	-0.83767000
O	4.19923300	0.40333000	-2.10908800
O	4.56259700	-0.12371800	0.34599000
F	5.72870400	-4.27008200	-0.33490700
F	5.09510800	-2.74925300	1.06912500
F	6.03386400	-2.17993600	-0.81698700
H	2.48138300	1.75845800	-2.10298400
H	1.73741400	1.32674600	1.84657100
C	3.24295500	3.86677300	1.30504000
C	2.60061200	5.01277700	0.81324900
C	2.88731000	5.46624800	-0.47638100
C	3.79941200	4.77644800	-1.27452600
C	4.44764500	3.64573900	-0.77824400
C	4.17541500	3.20135000	0.51587200
H	2.37695600	6.34226000	-0.85916100
H	3.99832800	5.12401800	-2.28451500

H	5.13962100	3.08725300	-1.40136000
H	4.66791000	2.32656300	0.92914700
C	1.66901300	5.81834100	1.67656000
S	2.93751800	3.16561400	2.99625800
O	4.19829400	2.37957900	3.24264300
O	1.69549300	2.21451300	2.67391600
F	2.35165400	6.53173400	2.60930100
F	0.77865100	5.06133400	2.35319800
F	0.95163200	6.71620700	0.95695900

TS6

C	-1.01618200	1.27055100	1.63222000
C	2.31277400	1.99096300	0.17095300
C	2.33579100	5.33778200	1.81484900
C	-1.01637900	4.65202100	3.27255000
O	2.45172000	1.82299200	1.42722900
O	1.44192600	2.72526100	-0.39233000
O	2.47703400	4.44143500	2.70685900
O	1.47136100	5.33770300	0.87971300
O	-0.15342200	3.90759900	3.84535600
O	-1.14161800	4.81794700	2.01940900
O	-0.14387700	1.27542700	2.56629700
O	-1.17001200	2.18346600	0.76424300
Rh	1.19341900	2.84288100	2.70059100
Rh	0.12383800	3.79289900	0.76827700
C	0.47005300	0.70200700	5.43579100
C	-1.99283800	5.36771600	4.17364900
C	3.26075700	6.52894100	1.88945400
C	3.29475600	1.27237900	-0.72278800
C	-1.92690100	0.06994400	1.58339700
H	-1.32534200	-0.83628800	1.46133900
H	-2.45406100	-0.02649600	2.53677500
H	-2.64114300	0.16034300	0.76379700
H	3.53231500	0.28869800	-0.31060700
H	2.89383600	1.17917500	-1.73341700
H	4.22327000	1.85346300	-0.76508800
H	3.57766900	6.82180100	0.88552200
H	2.71495200	7.37346600	2.32596900
H	4.12527500	6.30214300	2.51530600
H	-1.46954800	5.79051000	5.03550200
H	-2.51931600	6.15044600	3.62576100
H	-2.71906100	4.64077600	4.55425100
C	1.82487400	0.73700500	4.79988600
O	2.33851400	1.77896700	4.39777200
O	2.37894800	-0.44929800	4.62125900
C	3.65986300	-0.44184500	3.94242800
H	4.38640100	0.08355100	4.56305300
H	3.92414000	-1.49279900	3.83278100
H	3.55967300	0.05412800	2.97537200
C	0.12882300	1.57410100	6.49744100
C	-1.13346600	1.46478500	7.08167900
C	-2.40400800	1.40009300	6.32900600
C	-3.55549000	0.90274100	6.96348600
C	-2.49560800	1.85077000	5.00457200
C	-4.75890200	0.82132700	6.26841300
H	-3.46967000	0.54726700	7.98610100
C	-3.70571400	1.77184300	4.31307200
H	-1.62421900	2.27855800	4.52670200
C	-4.83797400	1.24702200	4.93770600
H	-5.63971700	0.42313600	6.76436400

H	-3.76141800	2.12887600	3.28779600
H	-5.77885100	1.18231300	4.39848100
C	-0.83051600	-3.41941400	3.19851300
C	-2.86481200	-2.48233200	4.07965200
C	-2.15194100	-1.85963300	5.09845500
C	-0.76840800	-2.02503600	5.15793300
C	-0.09935400	-2.80407900	4.21538300
H	-0.31286600	-4.03302000	2.46575000
H	-3.94310500	-2.35101900	4.03207600
H	-2.65335000	-1.25577800	5.84467100
H	0.97573600	-2.93814900	4.27931800
C	-3.00551600	-3.90876600	1.99546600
H	-2.40542400	-4.64714800	1.45512700
H	-3.34073600	-3.15795700	1.26821800
H	-3.90202800	-4.41163100	2.37508400
C	-2.21912600	-3.26768400	3.11214000
S	0.21914200	-1.25427300	6.44168500
N	-0.88614000	-0.64241000	7.46530400
C	-1.06366500	-0.98885100	8.79024900
C	-0.30775800	-2.20712000	9.39308200
O	-1.82629100	-0.32145700	9.48046700
C	-0.97139200	-2.57695900	10.73400800
C	1.13352400	-1.72621500	9.67359200
C	-0.39061000	-3.40739200	8.44942600
C	-1.64310400	-3.78627500	7.94179600
C	0.72989000	-4.14906700	8.05869400
C	-1.77127000	-4.85187500	7.05501500
H	-2.52410200	-3.21482100	8.22258900
C	0.60601400	-5.21988200	7.17046200
H	1.71320500	-3.87708800	8.42598600
C	-0.64297600	-5.57304500	6.66062000
H	-2.74920200	-5.10633200	6.65665200
H	1.49241000	-5.77425500	6.87375700
H	-0.73660200	-6.39730100	5.95947300
H	-0.43443400	-3.41802300	11.18515700
H	-0.95032000	-1.72524900	11.41746900
H	-2.01547900	-2.86939700	10.59353800
H	1.68458000	-2.48804200	10.23554900
H	1.69520900	-1.49194300	8.76603800
H	1.10074000	-0.81622800	10.27982000
C	2.19052200	3.45497100	6.92541900
C	3.56410900	3.72654100	6.79814600
C	3.95082700	4.94218100	6.22769500
C	3.00624100	5.87370000	5.80232400
C	1.65115900	5.60440700	5.95494900
C	1.24776100	4.39744900	6.51853200
H	5.00640500	5.15712900	6.12170400
H	3.33582700	6.80527800	5.35305200
H	0.90498800	6.31931100	5.62353300
H	0.19356700	4.16580500	6.60070700
C	4.66484200	2.78200600	7.23215800
S	1.48208000	1.93436400	7.62046700
O	2.44319900	0.82297000	7.46434900
O	0.93838700	2.26258300	8.94803300
F	4.47527700	2.32049000	8.48049500
F	4.79511300	1.72497200	6.40168200
F	5.86678600	3.40971200	7.23082800
H	-1.21637500	1.75604300	8.12565400
H	-0.29395000	0.52509800	4.68440200

TS7

C	2.36412500	2.87833000	-0.59476200
C	3.35956800	1.40141600	2.65511100
C	3.70815000	-1.94085900	1.06071300
C	2.72545900	-0.56162200	-2.18917700
O	2.19689700	0.96849600	2.36644600
O	4.36552200	1.43537200	1.88212700
O	2.47471800	-1.63780800	1.12585100
O	4.64861900	-1.19378300	0.64632100
O	1.69846100	-0.54344000	-1.43795300
O	3.87302400	-0.09547000	-1.90961600
O	1.41119900	2.13676500	-0.17972400
O	3.58564800	2.55778900	-0.67773700
Rh	1.84365900	0.21165200	0.47778900
Rh	4.18130800	0.69026300	-0.02984500
C	-0.36247100	-0.38747800	0.93665400
C	2.54562500	-1.22447500	-3.53601100
C	4.07173800	-3.33206200	1.52755800
C	3.55759000	1.89351100	4.07115800
C	1.97800700	4.27350400	-1.03335400
H	2.86164100	4.84159800	-1.32665500
H	1.46046400	4.78213000	-0.21411100
H	1.27971300	4.21443200	-1.87424500
H	3.80482600	1.03816400	4.71125500
H	2.63657900	2.34625100	4.44560900
H	4.38375200	2.60574300	4.11477100
H	3.82007000	-3.43587400	2.58819800
H	5.13564400	-3.52288500	1.37979000
H	3.47554000	-4.06552400	0.97576900
H	3.41909300	-1.05881200	-4.16844900
H	1.64329000	-0.83544700	-4.01532400
H	2.40246100	-2.30009000	-3.38346800
C	-0.41983400	-0.11718400	2.38427900
O	-0.78153200	0.94643300	2.86765000
O	-0.00823700	-1.16818000	3.12142300
C	0.20739200	-0.88143600	4.51022200
H	0.96430600	-0.10076000	4.61026400
H	0.55738700	-1.81749900	4.94646300
H	-0.71999900	-0.55596500	4.98876300
C	-0.38434500	-1.69448000	0.40812800
C	-0.32763500	-2.78019900	-0.13685900
C	-0.24308000	-4.00306300	-0.84867800
C	-0.29573400	-5.24582400	-0.18622800
C	-0.10828100	-3.98493100	-2.25346800
C	-0.21815500	-6.43268900	-0.91046900
H	-0.38775700	-5.26187600	0.89557300
C	-0.04202000	-5.17750700	-2.96749200
H	-0.05623900	-3.02644700	-2.75813200
C	-0.09587300	-6.40568400	-2.30205700
H	-0.25490500	-7.38408400	-0.38689300
H	0.06017900	-5.15014500	-4.04921400
H	-0.03846300	-7.33404400	-2.86289900
C	-1.90462600	-1.00567500	-3.47056500
C	-0.50620500	0.92114500	-3.81750000
C	-0.56600900	1.21836900	-2.45933300
C	-1.30139200	0.39305000	-1.61127600
C	-1.96716600	-0.72397300	-2.10942500
H	-2.42808900	-1.87611800	-3.85732300
H	0.05651000	1.57476600	-4.47866400
H	-0.05048200	2.07710900	-2.05484200

H	-2.52868400	-1.36694700	-1.45188700
C	-1.07065200	-0.52897000	-5.81175800
H	-0.19822000	-1.16661500	-6.00781100
H	-1.95546000	-1.07097600	-6.16056700
H	-0.95710800	0.37249900	-6.42247600
C	-1.16981300	-0.19259000	-4.34484300
S	-1.34809400	0.88705200	0.10646700
N	-2.96554400	0.73334500	0.62108800
H	-3.63013500	-0.30132800	1.00366600
C	-3.60740600	1.88864400	1.04598800
C	-3.10430300	3.32082200	0.70326500
O	-4.64928600	1.76338400	1.68811700
C	-4.27043900	4.29395200	1.00015000
C	-1.93180200	3.69942100	1.63956800
C	-2.77827900	3.46121600	-0.78466300
C	-1.74347700	4.28635400	-1.24020200
C	-3.60712500	2.85378900	-1.74079500
C	-1.54783800	4.50414500	-2.60564700
H	-1.08247600	4.76495800	-0.52724600
C	-3.40639500	3.05635200	-3.10382600
H	-4.41821700	2.20989500	-1.41217500
C	-2.37616600	3.88864700	-3.54375500
H	-0.74460100	5.15828800	-2.93459200
H	-4.05192200	2.55971800	-3.82257500
H	-2.21805000	4.05098600	-4.60600700
H	-3.95788100	5.31117100	0.74300100
H	-4.54373300	4.25637400	2.05707500
H	-5.15618800	4.04325900	0.41094800
H	-2.17663500	3.41995800	2.66728800
H	-1.78072500	4.78412700	1.61426600
H	-0.99425000	3.20801900	1.37921400
N	-4.36642800	-1.35235000	1.43100000
C	-3.37274800	-2.45689800	1.27479400
H	-2.61576700	-2.31796000	2.04567900
H	-2.84983400	-2.27719800	0.33820900
C	-5.56132300	-1.53215800	0.52587300
H	-6.00598700	-2.50580100	0.76308500
C	-4.75998800	-1.05350900	2.85937300
H	-5.34190500	-0.13847700	2.77523900
C	-3.86237700	-3.90528100	1.27941800
H	-4.55940800	-4.11419600	0.46240800
H	-4.33979400	-4.19603000	2.21735600
H	-2.98918500	-4.54871300	1.12844900
C	-3.55097900	-0.70143700	3.72464200
H	-2.91041000	-1.56515500	3.93177000
H	-3.91851600	-0.33294400	4.68835800
H	-2.94588000	0.08822000	3.28001100
C	-5.60903100	-2.13931700	3.53121200
H	-6.03022400	-1.73057400	4.45612800
H	-5.01054200	-3.01304200	3.80553200
H	-6.44475000	-2.47708600	2.91164800
C	-5.13371500	-1.55397300	-0.94443500
H	-4.43967600	-2.36729800	-1.17189000
H	-4.66895400	-0.60667100	-1.23183100
H	-6.01965300	-1.70119400	-1.56972800
C	-6.63927000	-0.46119600	0.72693700
H	-7.40594400	-0.59739200	-0.04283300
H	-6.22432700	0.54462900	0.64436300
H	-7.13670600	-0.54168700	1.69643800

(R)-TS

C	0.60671100	-2.66240700	1.21052200
C	0.16371800	-4.01494600	1.72261500
C	1.22436400	-5.08447000	1.43823800
H	0.87903100	-6.07493000	1.16850700
H	2.08456900	-4.73857500	0.88296100
C	1.08510600	-4.63665400	2.84828800
C	2.17719600	-3.81969000	3.49286000
C	1.87526900	-2.70980800	4.28685000
H	0.84659600	-2.39125600	4.40349200
C	2.89428000	-1.97493600	4.88914200
H	2.63606300	-1.10451800	5.48380400
C	4.22788500	-2.35024000	4.71682400
H	5.02399300	-1.77418300	5.18173100
C	4.53308600	-3.47485900	3.94522900
H	5.56801300	-3.78113800	3.81325200
C	3.51201900	-4.20796100	3.34075700
H	3.74707900	-5.07983400	2.73818600
C	0.45338700	-5.59204400	3.82739200
C	-0.54032200	-5.16630300	4.71382300
H	-0.89005600	-4.14363400	4.66135000
C	-1.09433800	-6.05088700	5.63553900
H	-1.87702400	-5.70841800	6.30747700
C	-0.65522800	-7.37581600	5.68804000
H	-1.09104500	-8.06832200	6.40316300
C	0.34489100	-7.80530800	4.81447200
H	0.69614600	-8.83328400	4.85029100
C	0.89620200	-6.91773100	3.88901400
H	1.67412600	-7.25189800	3.20882100
C	-1.29287100	-4.38423000	1.73144400
C	-1.69091600	-5.73368300	1.74462500
H	-0.95290700	-6.52347100	1.70700600
C	-3.02663300	-6.10209700	1.83245600
H	-3.29958100	-7.15249800	1.83607400
C	-4.01583300	-5.12132000	1.90487300
C	-3.64678600	-3.77919300	1.88953200
H	-4.40222500	-3.00924500	1.95544300
C	-2.30581700	-3.41443200	1.79724600
H	-2.05263300	-2.36580300	1.75011000
C	0.99356800	1.01728600	2.34988100
C	0.83221000	2.09904800	3.39272100
C	0.31854900	1.75608000	4.82194000
C	-0.51796200	2.55216900	3.84296800
H	-1.38573400	2.07884000	3.40156500
H	-0.65566400	3.60894000	4.03309900
C	1.91859400	3.13231800	3.21597700
C	1.59087000	4.44658100	2.86349200
H	0.55335900	4.71767000	2.70722000
C	2.58459200	5.41118200	2.70310300
H	2.31675500	6.42839400	2.43828600
C	3.92289400	5.06922000	2.89697100
C	4.26475300	3.75259800	3.22123500
H	5.30655800	3.48315400	3.36152000
C	3.27131400	2.79206700	3.36705700
H	3.53640800	1.76625400	3.58897100
C	0.99965800	2.50570900	5.93311500
C	2.29136300	2.13898600	6.33685500
H	2.78436800	1.31395300	5.83177200
C	2.93919900	2.81934300	7.36493600
H	3.94318100	2.52523800	7.65885200
C	2.30189900	3.88287400	8.00917500
H	2.80739800	4.42029500	8.80690800

C	1.01439600	4.25150900	7.62050100
H	0.50957200	5.07562400	8.11739500
C	0.36824100	3.56455400	6.59049300
H	-0.63549600	3.85311900	6.29334500
C	-0.19325100	0.37992900	5.17676100
C	-1.01228000	-0.35377200	4.29929700
H	-1.19213100	-0.00765900	3.28863600
C	-1.64931500	-1.52059800	4.71831700
H	-2.31085500	-2.03827400	4.03353500
C	-1.45856200	-2.00817000	6.01214000
H	-1.97115800	-2.90703500	6.34189400
C	-0.60183600	-1.32673500	6.87307200
H	-0.42592000	-1.69803800	7.87902400
C	0.01476200	-0.14452600	6.46262800
H	0.63865600	0.39286300	7.16592400
C	2.66465300	1.79039500	-0.70200400
C	3.25911000	3.07105000	-1.22706400
C	4.33179500	3.68947600	-0.35930500
H	4.33784500	4.76747100	-0.26943200
H	4.56074900	3.15867200	0.55547600
C	4.77203500	3.04825800	-1.64126100
C	5.51590700	1.74320100	-1.54315300
C	5.11608200	0.62307100	-2.27692400
H	4.22084300	0.67101900	-2.88745100
C	5.84507600	-0.56246400	-2.21099900
H	5.51028100	-1.41804500	-2.78558800
C	6.97954900	-0.64747300	-1.40426500
H	7.54393000	-1.57504400	-1.34787800
C	7.38483600	0.46763400	-0.66578600
H	8.26707000	0.41219000	-0.03316900
C	6.65904700	1.65612000	-0.74220600
H	6.97201600	2.52525600	-0.16982700
C	5.18008000	3.91242400	-2.81243000
C	5.71605100	3.32487100	-3.96882300
H	5.87264400	2.25433900	-4.00019600
C	6.03799000	4.09368300	-5.08675400
H	6.44458800	3.60617200	-5.96936800
C	5.84234400	5.47440800	-5.07465700
H	6.08912200	6.07469400	-5.94607900
C	5.32719000	6.07495600	-3.92570100
H	5.16850500	7.14942100	-3.89457000
C	5.00362400	5.30425800	-2.81090800
H	4.58438000	5.80033700	-1.94405700
C	2.30329500	3.96696700	-1.95592200
C	1.51033200	4.86048500	-1.23404400
H	1.60186500	4.89976300	-0.15424600
C	0.57029200	5.65685000	-1.88284500
H	-0.07612700	6.31397100	-1.31231100
C	0.43119500	5.57609800	-3.26845100
C	1.23917900	4.70522200	-4.00562700
H	1.12883800	4.64194900	-5.08227000
C	2.16396000	3.90469400	-3.34657300
H	2.79193200	3.22780000	-3.90885100
C	2.20319700	-1.93810900	-1.79338400
C	2.43960100	-3.09816100	-2.74025500
C	2.86600500	-2.77821400	-4.21454900
C	1.48279000	-3.27285600	-3.88398100
H	0.64566200	-2.58927500	-3.94172200
H	1.24666300	-4.28451400	-4.19292600
C	2.95887800	-4.31122200	-2.00952800
C	4.11174100	-4.24068400	-1.20728000
H	4.66069400	-3.31058200	-1.14901800

C	4.51867600	-5.32939400	-0.44667400
H	5.39589900	-5.24883100	0.18687000
C	3.78687000	-6.52065800	-0.47761700
C	2.65929700	-6.61830400	-1.28990900
H	2.08671600	-7.53906300	-1.31589800
C	2.25187800	-5.51961300	-2.04473500
H	1.35066900	-5.60257900	-2.64096700
C	3.78751600	-3.77764400	-4.86317100
C	3.37141900	-4.46124800	-6.01077600
H	2.37612600	-4.27530900	-6.40457800
C	4.21896000	-5.36622400	-6.65001100
H	3.87797300	-5.88881700	-7.53959100
C	5.50031800	-5.59926400	-6.14798300
H	6.16053200	-6.30718900	-6.64141000
C	5.92813100	-4.91801600	-5.00725500
H	6.92324300	-5.09253700	-4.60746300
C	5.07753600	-4.01354100	-4.37258000
H	5.41295700	-3.49025300	-3.48444200
C	3.04154800	-1.34815500	-4.67484900
C	2.01454800	-0.39540700	-4.55350200
H	1.08049700	-0.63884900	-4.06485500
C	2.17172800	0.89656600	-5.05227900
H	1.35061500	1.59766800	-4.95663000
C	3.36092000	1.27666900	-5.67543900
H	3.48710100	2.28593000	-6.05598200
C	4.39253400	0.34588900	-5.79268000
H	5.32816600	0.62386800	-6.27045600
C	4.23199100	-0.95044000	-5.30498400
H	5.03903100	-1.66285600	-5.42773000
O	0.16177800	1.01386700	1.39478400
O	2.01045300	0.26059300	2.46956200
O	1.53698900	1.42561900	-1.16202600
O	3.34106300	1.16476300	0.17796100
O	1.04090000	-1.42951600	-1.79125900
O	3.15869600	-1.60587600	-1.02876500
O	-0.23217700	-1.82902200	0.73799800
O	1.86370800	-2.47404200	1.25489900
Rh	0.54767300	-0.15385400	-0.25600900
Rh	2.66862400	-0.67625600	0.76036400
C	-0.66181700	6.34278800	-3.94816400
C	4.14913900	-7.63178000	0.45711800
C	5.00339200	6.08761600	2.69632700
C	-5.45327800	-5.51882900	2.04070500
F	5.48547400	-7.77379900	0.59554000
F	3.64921300	-8.82402400	0.06819700
F	3.66106300	-7.39897400	1.71153800
F	-0.37819200	6.59947500	-5.25043600
F	-1.83385500	5.65878500	-3.93869500
F	-0.90589600	7.53200100	-3.35073800
F	-5.75747800	-6.58187700	1.25805100
F	-6.29889600	-4.51784300	1.71370200
F	-5.75742000	-5.88619200	3.31339600
F	4.55959100	7.35149000	2.87702500
F	6.04172200	5.89824000	3.54353500
F	5.52694500	6.04029100	1.44083800
C	-3.44865700	1.00696500	-0.84126200
C	-2.20055900	1.05277300	-1.61280200
O	-1.28898000	0.22749200	-1.43938300
O	-2.11555500	2.05471000	-2.46288400
C	-0.87652600	2.21640300	-3.17859800
H	-0.06191100	2.35510200	-2.47479200
H	-1.03402600	3.09245500	-3.79804900

H	-0.71710100	1.33640500	-3.80304900
C	-4.07066500	-0.32723900	-0.75018900
C	-4.76834300	-0.92865500	0.23324900
C	-4.97116600	-0.57722600	1.63924400
C	-4.05012400	0.14921600	2.40769300
C	-6.13539200	-1.06453200	2.26382900
C	-4.31817000	0.43674200	3.74315800
H	-3.12866600	0.49548500	1.96419500
C	-6.39295600	-0.79045800	3.60390000
H	-6.83455700	-1.66058600	1.68486700
C	-5.49057900	-0.02443000	4.34528400
H	-3.59842400	1.01125000	4.31694500
H	-7.29452200	-1.17907400	4.06965700
H	-5.68897100	0.19410700	5.39112700
S	-4.59550100	2.34009000	-1.41331100
C	-3.35948200	-2.88007200	-1.94357700
C	-3.97762700	-4.12732900	-1.72137100
C	-3.16093700	-5.24081300	-1.49070600
C	-1.77321800	-5.12971300	-1.46883000
C	-1.17514900	-3.89244700	-1.67249400
C	-1.96790700	-2.77432800	-1.91354800
H	-3.62619900	-6.19941300	-1.30568300
H	-1.16818100	-6.00730600	-1.26276200
H	-0.10030000	-3.77549600	-1.62690500
H	-1.50541800	-1.80766800	-2.06234200
C	-5.47192900	-4.38483300	-1.75485500
S	-4.19042600	-1.29315900	-2.33249400
O	-5.60295200	-1.55858300	-2.64375400
O	-3.32124100	-0.66130800	-3.33930700
F	-6.16807700	-3.60186500	-0.90056900
F	-5.75103200	-5.66134100	-1.38160800
F	-5.99114000	-4.23061600	-2.98410700
H	-5.30517000	-1.82811100	-0.05054700
H	-2.97092100	1.72842100	0.33698800
C	-2.70471200	4.89551800	0.44656800
C	-3.43065000	5.65693400	1.37774900
C	-4.34693200	6.60687100	0.91892600
C	-4.54038500	6.79070400	-0.45181100
C	-3.81092800	6.04094300	-1.37243500
C	-2.88363200	5.10229900	-0.91603100
H	-4.90872300	7.19618200	1.63457200
H	-5.26725700	7.52119800	-0.79522000
H	-3.97372400	6.14024100	-2.43837100
H	-2.31332100	4.50279100	-1.61402800
C	-3.24241100	5.47020800	2.85756100
S	-1.52381600	3.57108200	0.95575000
O	-0.75828300	3.30620400	-0.30807000
O	-2.58909300	2.40750300	1.25645800
F	-3.58322000	4.23039200	3.28009400
F	-3.97662300	6.34329100	3.58438200
F	-1.94442500	5.65641700	3.23721500
N	-5.11653400	1.85805000	-2.91170500
C	-4.93859100	2.84191700	-3.83559100
C	-5.00215900	2.32375100	-5.30370400
O	-4.70560700	4.04340500	-3.63031300
C	-5.68197300	0.95139300	-5.40676800
C	-5.81547200	3.33774200	-6.13626300
C	-3.54270100	2.29286500	-5.79635000
H	-6.71766600	1.02803700	-5.06133600
H	-5.19342200	0.20081300	-4.78870100
H	-5.69383700	0.61401500	-6.45144600
H	-5.44814000	4.35513500	-5.99717800

H	-5.76966600	3.08018500	-7.20076100
H	-6.86575000	3.31779700	-5.82171500
C	-2.84242600	3.49469500	-5.99449900
C	-2.86334200	1.09347400	-6.04956300
C	-1.53312000	3.50106900	-6.47353800
H	-3.31547900	4.43137000	-5.72975800
C	-1.54898400	1.09579200	-6.52480000
H	-3.34811500	0.14633200	-5.85322300
C	-0.88031700	2.29848900	-6.75433900
H	-1.02480400	4.45122700	-6.61328200
H	-1.04509500	0.14958500	-6.70774100
H	0.13977500	2.29608200	-7.13101100
C	-5.97622200	2.01611300	-0.32342100
C	-5.94133400	2.56017100	0.96359600
C	-7.04383700	1.23090100	-0.75102600
C	-7.00049000	2.30911900	1.82831000
H	-5.08558000	3.13804000	1.29433600
C	-8.09548200	0.99103400	0.13346600
H	-7.02423800	0.81038300	-1.75092800
C	-8.08947000	1.52183300	1.42860100
H	-6.96852000	2.70889600	2.83835800
H	-8.92795000	0.36804700	-0.18471000
C	-9.21635800	1.24248300	2.39136500
H	-9.73307800	2.16535100	2.68408900
H	-9.95835800	0.56701400	1.95370400
H	-8.83527700	0.77858200	3.30904500

(R)-TS'

C	0.93008900	-2.76259500	0.91794700
C	0.48889200	-4.11086900	1.43818700
C	1.59628800	-5.15646000	1.30169600
H	1.30286200	-6.17309700	1.06850900
H	2.48525700	-4.81450600	0.79157000
C	1.33589800	-4.63809300	2.67080700
C	2.32695300	-3.73497800	3.35753700
C	1.88177900	-2.65264800	4.12090500
H	0.82388800	-2.42102300	4.17283200
C	2.79315000	-1.83403500	4.78332200
H	2.42451600	-0.98860000	5.35552300
C	4.16231100	-2.08828400	4.69369600
H	4.87480100	-1.44410500	5.20279400
C	4.61175800	-3.18086700	3.94566700
H	5.67601000	-3.39261100	3.87641700
C	3.69768700	-4.00414600	3.28843900
H	4.04339400	-4.85339600	2.70728500
C	0.64700900	-5.55149800	3.65116300
C	-0.42921200	-5.10512900	4.42590600
H	-0.80869300	-4.10073000	4.28330400
C	-1.03858900	-5.95467900	5.34522400
H	-1.88666900	-5.59929700	5.92454400
C	-0.57302700	-7.26173700	5.51004700
H	-1.05268200	-7.92701900	6.22295300
C	0.50930500	-7.70899300	4.75116500
H	0.88118700	-8.72274300	4.87550300
C	1.11600500	-6.85734900	3.82622100
H	1.95774800	-7.20402100	3.23268300
C	-0.95438200	-4.51891500	1.39903500
C	-1.32052700	-5.87602300	1.44365900
H	-0.56450700	-6.64897400	1.40683600
C	-2.64391200	-6.27122100	1.58200100
H	-2.89240300	-7.32611800	1.63054100

C	-3.65233800	-5.31008500	1.66170400
C	-3.31531800	-3.96174500	1.57477400
H	-4.08801200	-3.20665800	1.62624100
C	-1.98511500	-3.57052700	1.44234100
H	-1.74688200	-2.52030700	1.38037400
C	1.05910800	0.89771800	2.21020700
C	0.86831200	1.95822200	3.26772400
C	-0.07341900	1.64039800	4.47316300
C	-0.46748000	2.61786300	3.39741700
H	-1.23343900	2.34848400	2.68399800
H	-0.48290600	3.66235700	3.67679500
C	2.12534100	2.77018900	3.45450400
C	2.10742000	4.15592700	3.25314200
H	1.18209700	4.64921900	2.97948700
C	3.27271500	4.91278800	3.36723500
H	3.24402200	5.98350600	3.19506400
C	4.47956600	4.28921100	3.68176600
C	4.51199600	2.90748800	3.89260900
H	5.45075600	2.41846500	4.13122200
C	3.34748800	2.15863400	3.78057500
H	3.38306600	1.08514600	3.91156900
C	0.31709200	2.23218900	5.80077600
C	1.48946700	1.84804300	6.46316500
H	2.15313400	1.13207300	5.99171700
C	1.81809500	2.38821200	7.70595200
H	2.73644900	2.08288900	8.20018900
C	0.97411700	3.32326100	8.30769000
H	1.23073900	3.74903800	9.27395900
C	-0.19875600	3.71127500	7.65794800
H	-0.86182800	4.43927200	8.11769700
C	-0.52229800	3.16877800	6.41420700
H	-1.43391600	3.47173600	5.90692700
C	-0.79681900	0.31608100	4.54445100
C	-1.72328000	-0.06257000	3.55853800
H	-1.89396300	0.55334600	2.68478500
C	-2.47469100	-1.22738200	3.69578200
H	-3.22092400	-1.45913000	2.94713800
C	-2.30008200	-2.06215300	4.79851700
H	-2.89537700	-2.96583400	4.89611900
C	-1.36132500	-1.71443500	5.77087900
H	-1.20348600	-2.35494700	6.63457700
C	-0.62701800	-0.53424500	5.64883200
H	0.06554800	-0.26056500	6.43627800
C	2.86803200	1.91369800	-0.46653100
C	3.36624100	3.30658200	-0.72563500
C	4.33089800	3.88556900	0.27832900
H	4.23716400	4.94124900	0.50068100
H	4.56809700	3.26364000	1.12967800
C	4.90250700	3.45913900	-1.03970000
C	5.77683000	2.23205000	-0.99083300
C	5.57568200	1.13437800	-1.83116000
H	4.74172000	1.12972000	-2.52375000
C	6.42196900	0.02818600	-1.76218100
H	6.23777200	-0.81679900	-2.41495700
C	7.48015000	0.00563200	-0.85458400
H	8.13695200	-0.85918800	-0.80037900
C	7.68932000	1.10091100	-0.01190300
H	8.50953600	1.09324500	0.70140400
C	6.84217100	2.20572600	-0.08206200

H	6.98934000	3.05082200	0.58493100
C	5.28365500	4.47653100	-2.08474300
C	5.98456800	4.07407100	-3.23192100
H	6.28269500	3.03856100	-3.33698300
C	6.29940000	4.98325700	-4.24156500
H	6.84194600	4.63926200	-5.11877800
C	5.92619100	6.32219400	-4.12742400
H	6.16766500	7.03150300	-4.91433100
C	5.24000300	6.73952400	-2.98660100
H	4.94014300	7.77823500	-2.87831600
C	4.92668500	5.82973900	-1.97885900
H	4.37527600	6.18260500	-1.11597000
C	2.37124300	4.23811900	-1.34738600
C	1.65355300	5.11341900	-0.52889400
H	1.81488500	5.09093300	0.54393800
C	0.71891200	5.99374500	-1.06838700
H	0.14850100	6.64812000	-0.42052900
C	0.49689200	5.99780200	-2.44351500
C	1.20569400	5.12319200	-3.27240500
H	1.02717900	5.13282100	-4.34338300
C	2.13758300	4.25149500	-2.72458600
H	2.70768000	3.58586100	-3.36082300
C	2.83011800	-1.78214400	-1.88902000
C	3.27227900	-2.86418100	-2.85311100
C	3.91341200	-2.42582700	-4.20941200
C	2.52465300	-3.01557000	-4.14350500
H	1.66956300	-2.37010000	-4.30292100
H	2.40319700	-4.01652300	-4.54237300
C	3.73549300	-4.08798700	-2.10035700
C	4.74304200	-4.00058300	-1.12341900
H	5.23124400	-3.05103600	-0.95021400
C	5.07099800	-5.09792700	-0.33811800
H	5.83204200	-5.00513700	0.42985000
C	4.40067500	-6.31296100	-0.51360700
C	3.42234900	-6.42662400	-1.49892300
H	2.89998400	-7.36633700	-1.64051400
C	3.09721900	-5.32031800	-2.28311400
H	2.30902900	-5.41700500	-3.02037000
C	4.99672900	-3.32439300	-4.74118200
C	4.82173600	-3.98987800	-5.95889100
H	3.88846500	-3.86473100	-6.50071400
C	5.82961500	-4.80185500	-6.48017700
H	5.67537600	-5.31314400	-7.42649800
C	7.03138100	-4.95625500	-5.78783400
H	7.81590400	-5.59161300	-6.18945300
C	7.21958500	-4.29031900	-4.57515000
H	8.15141800	-4.40423400	-4.02819600
C	6.20974800	-3.47971400	-4.05864800
H	6.35801700	-2.96509200	-3.11569600
C	4.06188500	-0.95769300	-4.54201900
C	2.98568300	-0.06014000	-4.42863800
H	2.02918200	-0.38554300	-4.04283700
C	3.12483800	1.27736100	-4.79348900
H	2.27073300	1.93860800	-4.69721500
C	4.34090800	1.76225700	-5.27500500
H	4.44992300	2.80851000	-5.54235000
C	5.41872500	0.88490600	-5.38600500
H	6.37775000	1.24113700	-5.75224300
C	5.27897600	-0.45694200	-5.03082800

H	6.12727000	-1.12173600	-5.14142500
O	0.34737100	0.96723100	1.16348500
O	1.98902900	0.05213100	2.42048600
O	1.87740500	1.49272100	-1.14583300
O	3.48670600	1.25177600	0.42910900
O	1.62093600	-1.40433600	-1.95844600
O	3.68610800	-1.38937400	-1.04031900
O	0.09931300	-1.92939700	0.43540300
O	2.18670900	-2.56232300	0.98981000
Rh	0.88888700	-0.19825100	-0.44752400
Rh	2.91678300	-0.67852300	0.74527000
C	-0.47640600	6.95032500	-3.06777400
C	4.66749400	-7.43853100	0.43701200
C	5.75969800	5.06481100	3.66291400
C	-5.06388600	-5.73373800	1.92907000
F	5.98596000	-7.59069400	0.69268100
F	4.19945300	-8.62232700	-0.01173200
F	4.07156800	-7.21680200	1.64457100
F	0.15637700	7.87459400	-3.84050700
F	-1.34926700	6.31613500	-3.88691400
F	-1.19695100	7.63406200	-2.15452400
F	-5.37209900	-6.90296700	1.32365800
F	-5.97344300	-4.81771900	1.52631600
F	-5.27820800	-5.92545600	3.25879800
F	5.57590900	6.37523400	3.93889600
F	6.66400100	4.58663100	4.54810300
F	6.35890100	5.01122600	2.43976100
C	-3.15253100	0.75850400	-1.58099500
C	-1.83125600	0.73201000	-2.23515600
O	-0.91319500	0.03146500	-1.79090000
O	-1.67298700	1.53915800	-3.27694100
C	-0.33303900	1.66490000	-3.78172600
H	0.34792000	1.91838100	-2.97129200
H	-0.38276600	2.47273000	-4.51256100
H	-0.04126100	0.72843900	-4.26575600
C	-3.72966100	-0.57776400	-1.29730900
C	-4.54583400	-1.05360500	-0.33293500
C	-5.00809200	-0.56283200	0.96638200
C	-4.61291200	0.63556100	1.58284900
C	-5.87524000	-1.42127800	1.67529600
C	-5.03089500	0.93177100	2.87701500
H	-3.98737000	1.34159900	1.06430600
C	-6.30336600	-1.11444600	2.96436700
H	-6.20091600	-2.34648700	1.20968000
C	-5.87234800	0.06351600	3.57666800
H	-4.68946100	1.85355100	3.33901900
H	-6.96097000	-1.80116800	3.49008300
H	-6.18646100	0.30187600	4.58914500
C	-6.02689200	-0.18449200	-5.40810100
C	-7.46857500	-0.39206000	-3.48941500
C	-6.60210400	0.39568500	-2.73980900
C	-5.44746700	0.88793800	-3.34297100
C	-5.15337500	0.61531000	-4.67746600
H	-5.79841000	-0.41701100	-6.44537800
H	-8.37053900	-0.77694700	-3.02064100
H	-6.81384900	0.63727500	-1.70602300
H	-4.24474300	1.00199800	-5.12609900
C	-8.09270200	-1.62809300	-5.60217500
H	-7.77837900	-2.67218700	-5.47271900

H	-9.13116800	-1.55420900	-5.26101600
H	-8.06808100	-1.40815300	-6.67528900
C	-7.18756000	-0.70639100	-4.82358900
S	-4.31494700	1.91911400	-2.39837000
N	-5.20182500	2.38189100	-1.05408100
C	-6.05901600	3.37374900	-1.38774000
C	-6.97593600	3.79293000	-0.20247300
O	-6.21533000	3.87561100	-2.51635200
C	-6.14153100	3.99621600	1.07061100
C	-7.68529000	5.11450600	-0.54587200
C	-7.99274600	2.65006100	-0.07956300
C	-8.85689300	2.38399100	-1.15437800
C	-8.04395200	1.79779700	1.02949300
C	-9.74564000	1.31106100	-1.11707000
H	-8.79040300	2.99401200	-2.04923800
C	-8.92815200	0.71769100	1.06767400
H	-7.37100700	1.94944400	1.86304400
C	-9.78591300	0.46892900	-0.00346300
H	-10.39365200	1.12187200	-1.96940000
H	-8.92671600	0.06231400	1.93404600
H	-10.46910200	-0.37622300	0.02307300
H	-5.44278600	4.82322600	0.92090000
H	-5.55489100	3.11083500	1.30748300
H	-6.78643800	4.24268400	1.92375300
H	-8.22871400	5.05035400	-1.48944400
H	-8.38673000	5.38020900	0.25393400
H	-6.94665500	5.91604600	-0.64684700
C	-2.56447600	-3.22510300	-2.18536300
C	-3.03739600	-4.52736800	-1.90708100
C	-2.09723200	-5.54681300	-1.72678900
C	-0.72849200	-5.29371500	-1.78277700
C	-0.27618400	-4.00334200	-2.01619500
C	-1.19412000	-2.97759500	-2.22852200
H	-2.44834800	-6.54628400	-1.51162400
H	-0.02348700	-6.10221600	-1.61201900
H	0.77952600	-3.77094400	-2.02367000
H	-0.84129600	-1.97532000	-2.42440700
C	-4.49252000	-4.95104500	-1.82579900
S	-3.59403300	-1.80405600	-2.70643900
O	-4.92473800	-2.34073600	-3.02385600
O	-2.80068700	-1.14573200	-3.76378400
F	-5.23992000	-4.14941700	-1.03797700
F	-4.59895800	-6.19243600	-1.27732600
F	-5.07972000	-5.02910000	-3.03163100
H	-4.94613600	-2.04090800	-0.54018700
H	-2.74695600	1.57948300	-0.45762600
C	-2.41040200	4.78717600	-0.29555700
C	-2.75342700	5.79607900	0.61456800
C	-3.63794200	6.80900200	0.22787700
C	-4.19266300	6.80093900	-1.05039000
C	-3.84055600	5.80271000	-1.95854800
C	-2.92810300	4.81862900	-1.58468500
H	-3.89555300	7.59161900	0.93217600
H	-4.89400700	7.57842400	-1.33762800
H	-4.28105900	5.77866900	-2.94801400
H	-2.59355900	4.06862900	-2.29179500
C	-2.18335800	5.81382100	2.00112800
S	-1.25363700	3.38876200	0.10798200
O	-0.66842200	3.08860200	-1.24204800

O	-2.31842700	2.25643500	0.48516900
F	-2.53022500	4.71744300	2.71768500
F	-2.58257000	6.88730200	2.71793400
F	-0.81598600	5.84987800	1.99469300

(S)-TS

C	2.76175800	0.40439700	1.20868000
C	3.80819000	1.39545100	1.66299800
C	3.92228900	1.53269400	3.17134800
H	4.04478300	2.52868600	3.58044800
H	3.27660500	0.88607100	3.75300500
C	5.06537600	0.87603500	2.45485600
C	5.27323100	-0.60392500	2.64634700
C	5.41876900	-1.46463600	1.55326800
H	5.32544700	-1.07722600	0.54638400
C	5.62529400	-2.82833200	1.74613300
H	5.71256200	-3.48000500	0.88198800
C	5.70973700	-3.34827000	3.04112500
H	5.86304500	-4.41324100	3.19342900
C	5.60706300	-2.48889300	4.13656200
H	5.69054800	-2.88028800	5.14738700
C	5.39735100	-1.12200200	3.93720200
H	5.31770500	-0.45270600	4.78996700
C	6.36625300	1.63960900	2.30173600
C	7.52719700	0.96934500	1.88337100
H	7.50282900	-0.09856500	1.71280700
C	8.72550100	1.65335500	1.67774000
H	9.59514200	1.09812200	1.33656900
C	8.79943800	3.02751400	1.90231200
H	9.72997900	3.56451000	1.74042900
C	7.66130000	3.70376200	2.34373500
H	7.69844300	4.77389400	2.52836200
C	6.46387500	3.01891000	2.54084900
H	5.59387000	3.58402000	2.85381000
C	3.95527800	2.57482500	0.74422900
C	3.02044100	3.61363000	0.73741900
H	2.20344800	3.59591000	1.44241000
C	3.11071900	4.65055100	-0.18935200
H	2.35794700	5.43150600	-0.19958700
C	4.15616900	4.65923600	-1.11637500
C	5.11336200	3.64291600	-1.10186800
H	5.92864000	3.65234400	-1.81584300
C	5.00232100	2.60756700	-0.18202300
H	5.74086900	1.81949000	-0.16731900
C	3.05256100	-1.06176900	-1.93374700
C	4.09300400	-0.76799800	-2.99091600
C	3.89000900	0.38108900	-4.03319100
C	3.65826600	-1.05147600	-4.41936100
H	2.62322900	-1.35407500	-4.54047400
H	4.36437900	-1.55260700	-5.07355300
C	5.47688700	-1.08230500	-2.49614600
C	5.93102700	-2.40148000	-2.39659800
H	5.31315300	-3.20888900	-2.77832600
C	7.13745800	-2.69062400	-1.76211800
H	7.47212500	-3.71810300	-1.66448500
C	7.90903800	-1.65391300	-1.22848200
C	7.48932500	-0.32989200	-1.36401100
H	8.08858000	0.47736200	-0.95991500
C	6.28124700	-0.05513600	-1.99378000
H	5.94944000	0.96749800	-2.09876700

C	5.13768400	1.08408900	-4.53472800
C	5.25145900	2.47539500	-4.38061500
H	4.42994900	3.03676400	-3.95715800
C	6.40782500	3.15393400	-4.76343600
H	6.46071800	4.22821300	-4.60827600
C	7.47634300	2.45920700	-5.33042700
H	8.37977800	2.98387300	-5.62902500
C	7.36776800	1.08026200	-5.51495100
H	8.18758900	0.52252300	-5.95984700
C	6.21408500	0.40322100	-5.12159600
H	6.17836700	-0.67280000	-5.25066200
C	2.71536600	1.31581100	-3.92416800
C	1.98897200	1.64245200	-5.07460900
H	2.22724300	1.14737900	-6.01332500
C	0.97657800	2.60373600	-5.02124700
H	0.41161200	2.84488000	-5.91846800
C	0.67547300	3.23779900	-3.81489000
H	-0.13369900	3.95546500	-3.75031100
C	1.40226600	2.91571600	-2.66823800
H	1.14895900	3.37966300	-1.72650700
C	2.42199500	1.97221900	-2.72686600
H	2.96913000	1.72825800	-1.82602400
C	0.26845400	-3.38846600	-1.34341300
C	-0.29817800	-4.51873900	-2.16462700
C	0.74981700	-5.38950300	-2.83509500
H	0.53253300	-5.73683000	-3.83941400
H	1.78299900	-5.11690000	-2.65257000
C	-0.00373600	-5.98505000	-1.68044000
C	0.75316600	-6.17523800	-0.38990300
C	0.28388300	-5.64995300	0.81721400
H	-0.63215000	-5.07023200	0.83491800
C	1.01381700	-5.81675500	1.99243400
H	0.64735200	-5.36523600	2.90745500
C	2.21522100	-6.52739800	1.97827200
H	2.79040800	-6.64695300	2.89282000
C	2.67643100	-7.08068100	0.78098700
H	3.60713500	-7.64216800	0.76102700
C	1.94529200	-6.90573900	-0.39413400
H	2.30919200	-7.32304600	-1.32962700
C	-1.04655100	-7.04631200	-1.95078000
C	-1.55625300	-7.29481200	-3.23511400
H	-1.21657600	-6.71063800	-4.08191000
C	-2.53699300	-8.26049100	-3.44959700
H	-2.91771100	-8.41858800	-4.45491400
C	-3.03454500	-9.01125500	-2.38406400
H	-3.80256900	-9.76148100	-2.55073300
C	-2.53225900	-8.78384300	-1.10367000
H	-2.90271300	-9.36039100	-0.25990000
C	-1.54968600	-7.81660600	-0.89143800
H	-1.17358500	-7.65283600	0.11031700
C	-1.57387800	-4.21847900	-2.89431700
C	-1.54025700	-3.58164800	-4.13973500
H	-0.58239200	-3.30257600	-4.57098400
C	-2.71917000	-3.27761500	-4.81154300
H	-2.68930500	-2.74856200	-5.75845800
C	-3.94865900	-3.62165200	-4.24564600
C	-3.99479000	-4.27955500	-3.01839100
H	-4.95002200	-4.51910000	-2.56526100
C	-2.80964500	-4.56617500	-2.34789500

H	-2.83838400	-5.06688400	-1.38994400
C	-0.20924000	-1.68124700	2.10587400
C	-0.92664300	-1.53220600	3.43263700
C	-2.08000100	-2.49095600	3.83010700
C	-2.35992000	-1.09349500	3.33819200
H	-2.74789000	-0.93159100	2.33810700
H	-2.74588800	-0.38718400	4.06216100
C	0.00680200	-0.99320700	4.48170400
C	1.32694200	-1.46401400	4.55766900
H	1.65619400	-2.24676200	3.88783600
C	2.23925900	-0.89490200	5.43813900
H	3.26032100	-1.25266800	5.44762400
C	1.84740200	0.15651400	6.26711000
C	0.52034000	0.59399700	6.25062800
H	0.20702100	1.40279200	6.90280000
C	-0.38822300	0.01906900	5.36870000
H	-1.40363100	0.39444300	5.34340700
C	-2.29272000	-2.70526500	5.30751400
C	-3.53137900	-2.37002400	5.86759300
H	-4.29759100	-1.93854700	5.22898300
C	-3.78002100	-2.58004500	7.22371000
H	-4.74665100	-2.31322900	7.64290600
C	-2.78929000	-3.12867400	8.04057500
H	-2.97902300	-3.28768300	9.09871700
C	-1.55170700	-3.46709400	7.49107800
H	-0.77185600	-3.88797200	8.12009400
C	-1.30649900	-3.25696600	6.13403600
H	-0.33621600	-3.50335200	5.71486100
C	-2.42636600	-3.69111100	2.98656500
C	-3.13710000	-3.55334700	1.79004800
H	-3.39727300	-2.57202100	1.41831100
C	-3.56920800	-4.67765900	1.08596200
H	-4.17029900	-4.53366500	0.19824100
C	-3.27180400	-5.95994900	1.54412400
H	-3.61082100	-6.83008300	0.99066600
C	-2.53172100	-6.10866300	2.71882700
H	-2.28008000	-7.10003600	3.08612800
C	-2.12378400	-4.98651400	3.43662800
H	-1.58953100	-5.11907600	4.37095700
O	1.84517700	-0.74287300	-2.15160000
O	3.48021000	-1.65091900	-0.88435300
O	-0.40345400	-2.31328900	-1.23878400
O	1.41597900	-3.59756500	-0.82937100
O	-0.43357200	-0.74373100	1.27908900
O	0.62304800	-2.63078500	1.94769500
O	1.95993600	0.76502200	0.28847500
O	2.73266400	-0.73001600	1.78429300
Rh	0.62724300	-0.67270300	-0.46299000
Rh	2.11308100	-2.26196900	0.53627300
C	-5.21418500	-3.26834700	-4.96674300
C	2.86760200	0.90800800	7.06060300
C	9.13254400	-1.96274400	-0.42116100
C	4.21104700	5.70035100	-2.19292100
F	2.39563100	1.32454100	8.25632400
F	3.27046700	2.03297200	6.39723300
F	3.98680000	0.18550800	7.29175000
F	-6.29368800	-3.28949800	-4.15572700
F	-5.15068900	-2.03751400	-5.52474800
F	-5.47402100	-4.13374200	-5.98474900

F	3.56474100	5.29880300	-3.31670900
F	5.48832100	5.97174100	-2.57184800
F	3.64776500	6.86695500	-1.81510500
F	10.04129200	-0.95716300	-0.45977000
F	8.83094200	-2.15235600	0.88958600
F	9.75724500	-3.08704900	-0.83921900
C	-2.97567900	1.88353400	-0.99235200
C	-1.75737600	1.32861900	-1.60098600
O	-0.78267200	0.99654100	-0.91321600
O	-1.85238800	1.11981700	-2.90615000
C	-0.91072200	0.21153300	-3.51944600
H	-1.11199000	-0.79186400	-3.14813600
H	-1.11852200	0.27990700	-4.58686300
H	0.10782800	0.52450200	-3.31324500
C	-2.84071300	2.74928600	0.19627500
C	-3.49657800	2.74505100	1.37621500
C	-4.50577100	1.86987700	1.97417900
C	-5.52177600	1.19948200	1.27702800
C	-4.45951000	1.74622500	3.37640200
C	-6.43384900	0.40271300	1.96351500
H	-5.61986400	1.35598200	0.21384900
C	-5.35799200	0.93228400	4.05910300
H	-3.69911300	2.29490900	3.92744300
C	-6.34984200	0.25167500	3.34772900
H	-7.21778800	-0.10177400	1.40919500
H	-5.29451300	0.83984000	5.14039500
H	-7.06313100	-0.37904700	3.87203300
C	-2.36232100	4.60224100	-5.13956200
C	-2.83541700	6.11162300	-3.32407200
C	-3.42683600	5.07716400	-2.60523800
C	-3.45343800	3.79916000	-3.15456500
C	-2.93784800	3.55349700	-4.42618500
H	-1.95703300	4.41602400	-6.13159400
H	-2.78834900	7.10416000	-2.88378300
H	-3.83705800	5.25022100	-1.61848400
H	-2.98138100	2.55506900	-4.84659800
C	-1.59444300	7.00300000	-5.34179900
H	-1.99026900	7.98375900	-5.05809800
H	-1.70614800	6.88892000	-6.42570000
H	-0.51842800	7.00815300	-5.12270200
C	-2.28664000	5.89049600	-4.59364000
S	-4.19020800	2.41586700	-2.25976500
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C	-8.03634600	5.36456700	-1.48834700
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H	-8.33097100	2.06365700	-0.44098100
H	-9.52231800	3.38021100	-0.31576800
H	-7.25673000	6.13266700	-1.51276800
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C	-5.85690000	-0.32170200	-2.72949000
H	-9.00263700	-1.55582000	-0.85419300
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(S)-TS'

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C	8.71198300	1.50598500	1.48888800
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H	9.78774300	3.37822200	1.44421400
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C	3.04212500	3.63906800	0.46124500
H	2.22793700	3.67662700	1.16804400
C	3.15502900	4.62674800	-0.51468300
H	2.42275800	5.42581500	-0.55942200
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H	5.93508500	3.47558200	-2.10350600
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H	5.70172700	1.72347100	-0.37515100
C	2.98072300	-1.10199000	-1.97906300
C	4.01476300	-0.88288500	-3.05888600
C	3.81756500	0.21558300	-4.15438500
C	3.55946400	-1.23055900	-4.46666800
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H	4.25155700	-1.77670100	-5.09958100
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H	8.09708200	0.19075800	-6.12518000
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H	6.07543200	-0.93494100	-5.34031400
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H	0.36250800	2.58962400	-6.18550200
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C	-3.73334200	-2.16926600	5.75751500
H	-4.48809900	-1.75671800	5.09498600
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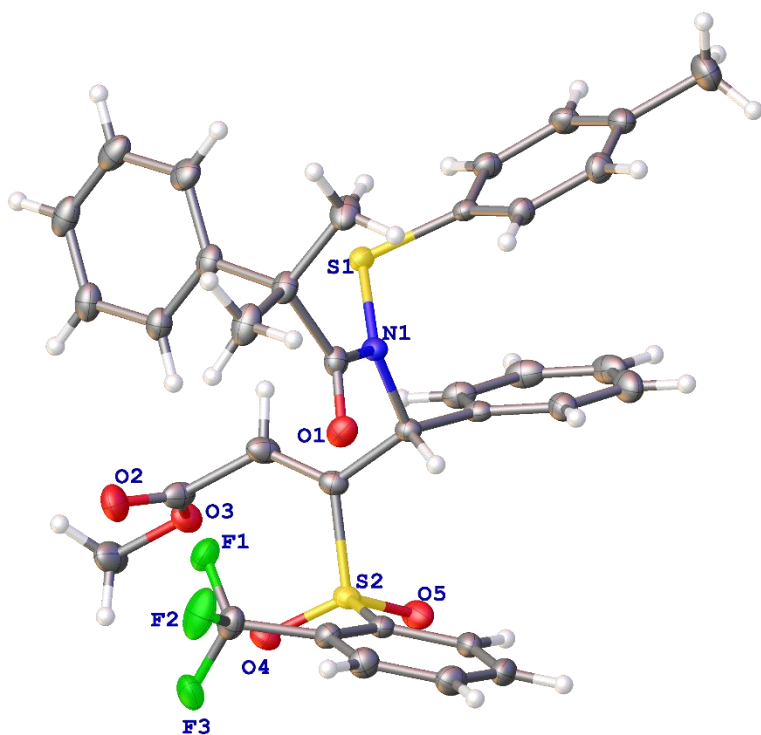
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H	-8.46394600	2.78549400	2.95489000

7. References

- (1) (a) Lai, Y.; Wang, X.; Liang, L.; Xia, X. Novel asymmetric synthesis method of (1S,2S)-2-fluorocyclopropanecarboxylic acid catalyzed by chiral rhodium. CN110483272, 2019. (b) Liao, K. B.; Liu, W. B.; Niemeyer, Z. L.; Ren, Z.; Bacsa, J.; Musaev, D. G.; Sigman, M. S.; Davies, H. M. L. Site-Selective Carbene-Induced C-H Functionalization Catalyzed by Dirhodium Tetrakis(triarylcyclopropanecarboxylate) Complexes. *ACS Catal.* **2018**, *8*, 678-682. (c) Löffler, L. E.; Buchsteiner, M.; Collins, L. R.; Caló, F. P.; Singha, S.; Fürstner, A. [Rh₂(MEPY)₄] and [BiRh(MEPY)₄]: Convenient Syntheses and Computational Analysis of Strikingly Dissimilar Siblings. *Helv. Chim. Acta* **2021**, *104*, e2100042. (d) Wertz, B.; Ren, Z.; Bacsa, J.; Musaev, D. G.; Davies, H. M. L. Comparison of 1,2-Diarylcyclopropanecarboxylates with 1,2,2-Triarylcyclopropanecarboxylates as Chiral Ligands for Dirhodium-Catalyzed Cyclopropanation and C-H Functionalization. *J. Org. Chem.* **2020**, *85*, 12199-12211. (e) Liu, W.; Ren, Z.; Bosse, A. T.; Liao, K.; Goldstein, E. L.; Bacsa, J.; Musaev, D. G.; Stoltz, B. M.; Davies, H. M. L. Catalyst-Controlled Selective Functionalization of Unactivated C-H Bonds in the Presence of Electronically Activated C-H Bonds. *J. Am. Chem. Soc.* **2018**, *140*, 12247-12255. (f) Qin, C.; Boyarskikh, V.; Hansen, J. H.; Hardcastle, K. I.; Musaev, D. G.; Davies, H. M. L. D₂-Symmetric Dirhodium Catalyst Derived from a 1,2,2-Triarylcyclopropanecarboxylate Ligand: Design, Synthesis and Application. *J. Am. Chem. Soc.* **2011**, *133*, 19198-19204. (g) Liao, K.; Yang, Y.-F.; Li, Y.; Sanders, J. N.; Houk, K. N.; Musaev, D. G.; Davies, H. M. L. Design of catalysts for site-selective and enantioselective functionalization of non-activated primary C-H bonds. *Nat. Chem.* **2018**, *10*, 1048-1055. (h) Liao, K.; Negretti, S.; Musaev, D. G.; Bacsa, J.; Davies, H. M. L. Site-selective and stereoselective functionalization of unactivated C-H bonds. *Nature (London, U. K.)* **2016**, *533*, 230-234. (i) Fu, L.; Hoang, K.; Tortoreto, C.; Liu, W.; Davies, H. M. L. Formation of Tertiary Alcohols from the Rhodium-Catalyzed Reactions of Donor/Acceptor Carbenes with Esters. *Org. Lett.* **2018**, *20*, 2399-2402.
- (2) Li, L.; Sivaguru, P.; Han, X.; Karmakar, S.; Bi, X. Ligand-enabled silver-catalyzed carbene insertion into the N-H bond of aliphatic and electron-rich aromatic amines. *Org. Chem. Front.* **2023**, *10*, 1746-1753.
- (3) (a) Klose, I.; Di Mauro, G.; Kaldre, D.; Maulide, N. Inverse hydride shuttle catalysis enables the stereoselective one-step synthesis of complex frameworks. *Nat. Chem.* **2022**, *14*, 1306-1310. (b) Sharma, A.; Jamwal, P.; Vaid, H.; Gurubrahmam, R. Synthesis of Alkynyl Hydrazones from Unprotected Hydrazine and Their Reactivity as Diazo Precursors. *Org. Lett.* **2023**, *25*, 1889-1894. (c) Whittaker, R. E.; Dong, G. Controlled Rh-Catalyzed Mono- and Double-decarbonylation of Alkynyl α -Diones To Form Conjugated Ynones and Disubstituted Alkynes. *Org. Lett.* **2015**, *17*, 5504-5507.
- (4) (a) Greenwood, N. S.; Cerny, N. P.; Deziel, A. P.; Ellman, J. A. Synthesis of N - Acylsulfenamides from (Hetero)Aryl Iodides and Boronic Acids by One - Pot Sulfur - Arylation and Dealkylation. *Angew. Chem. Int. Ed.* **2023**, *63*. (b) Liu, J. T.; Brandes, D. S.; Greenwood, N. S.; Ellman, J. A. Synthesis of N-Acylsulfenamides from Amides and N-Thiosuccinimides. *Synthesis* **2022**, *55*, 2353-2360. (c) Tang, J.-J.; Yan, N.; Zhang, Y.; Wang, Y.; Bao, M.; Yu, X. Visible-light-induced iron-catalyzed S-N cross-coupling of thiols with dioxazolones. *Green Chem.* **2023**, *25*, 7529-7533. (d) Zhou, Q.; Li, J.; Wang, T.; Yang, X. Base-Promoted S-Arylation of Sulfenamides for the Synthesis of Sulfilimines. *Org. Lett.* **2023**, *25*, 4335-4339. (e) Chen, Y.; Fang, D.-m.; Huang, H.-s.; Nie, X.-k.; Zhang, S.-q.; Cui, X.; Tang, Z.; Li, G.-x. Synthesis of Sulfilimines via Selective S - C Bond Formation in Water. *Org. Lett.* **2023**. (f) Lu, X.; Huang, G.; Ye, J.; Bashir, M. A.; Su, J.; Yang, K.; Liang, F.; Xu, X. Hypervalent Iodine-Mediated Synthesis of Sulfinimidate Esters from Sulfenamides. *Org. Lett.* **2023**.
- (5) (a) Barraza, S. J.; Denmark, S. E. Synthesis, Reactivity, Functionalization, and ADMET Properties of Silicon-Containing Nitrogen Heterocycles. *J. Am. Chem. Soc.* **2018**, *140*, 6668-6684. (b) Kort, M. E.; Carroll, W. A.; Perez, M. A.; Dinges, J.; Gregg, R. J.; Basha, F. Z. Preparation of amination diones as potassium channel openers. WO2002062761, 2002. (c) Greenwood, N. S.; Cerny, N. P.; Deziel, A. P.; Ellman, J. A. Synthesis of N - Acylsulfenamides from (Hetero)Aryl Iodides and Boronic Acids by One - Pot Sulfur - Arylation and Dealkylation. *Angew. Chem. Int. Ed.* **2023**, *63*.
- (6) Han, Y.; Yuan, Y.; Qi, S.; Zhang, Z.-K.; Kong, X.; Yang, J.; Zhang, J. Copper-Catalyzed Sulfur Alkylation of Sulfenamides with N-Sulfonylhydrazones. *Org. Lett.* **2024**, *26*, 3906-3910.
- (7) Xiao, Z.; Pu, M.; Li, Y.; Yang, W.; Wang, F.; Feng, X.; Liu, X. Asymmetric Catalytic Synthesis of Allylic Sulfenamides from Vinyl α -Diazo Compounds by a Rearrangement Route. *Angew. Chem. Int. Ed.* **2024**, *n/a*, e202414712.
- (8) Xu, W.-B., Sun, M., Shu, M. & Li, C. Rhodium-Catalyzed Regio- and Enantioselective Allylic Amination of Racemic 1,2-Disubstituted Allylic Phosphates. *J. Am. Chem. Soc.* **2021**, *143*, 8255-8260.

8. X-Ray Crystallographic Data

Crystallographic Data and structure of 3



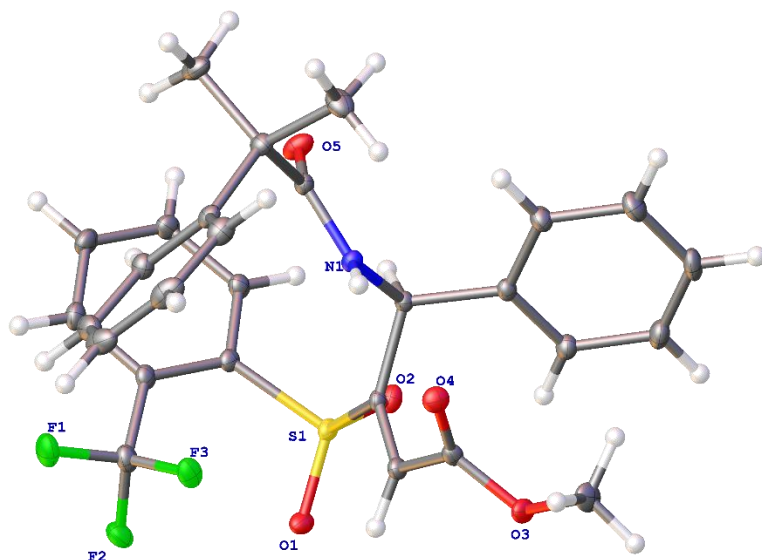
3 (CCDC 2406862)

Table 1 Crystal data and structure refinement for WB-5-7.

Identification code	WB-5-7
Empirical formula	C ₃₅ H ₃₂ F ₃ NO ₅ S ₂
Formula weight	667.73
Temperature/K	150.00(10)
Crystal system	trigonal
Space group	P3 ₂
a/Å	14.7946(2)
b/Å	14.7946(2)
c/Å	13.0738(2)
α /°	90
β /°	90
γ /°	120
Volume/Å ³	2478.21(8)
Z	3
ρ _{calc} /cm ³	1.342
μ /mm ⁻¹	1.973
F(000)	1044.0
Crystal size/mm ³	0.15 × 0.12 × 0.1
Radiation	Cu K α (λ = 1.54184)
2 θ range for data collection/°	6.9 to 146.646
Index ranges	-17 ≤ h ≤ 18, -18 ≤ k ≤ 12, -16 ≤ l ≤ 16
Reflections collected	20784
Independent reflections	6438 [R _{int} = 0.0349, R _{sigma} = 0.0282]
Data/restraints/parameters	6438/9/458
Goodness-of-fit on F ²	1.038
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0291, wR ₂ = 0.0768
Final R indexes [all data]	R ₁ = 0.0295, wR ₂ = 0.0771

Largest diff. peak/hole / e Å⁻³ 0.22/-0.17
 Flack parameter 0.008(10)

Crystallographic Data and structure of *rac*-(*E*)-52

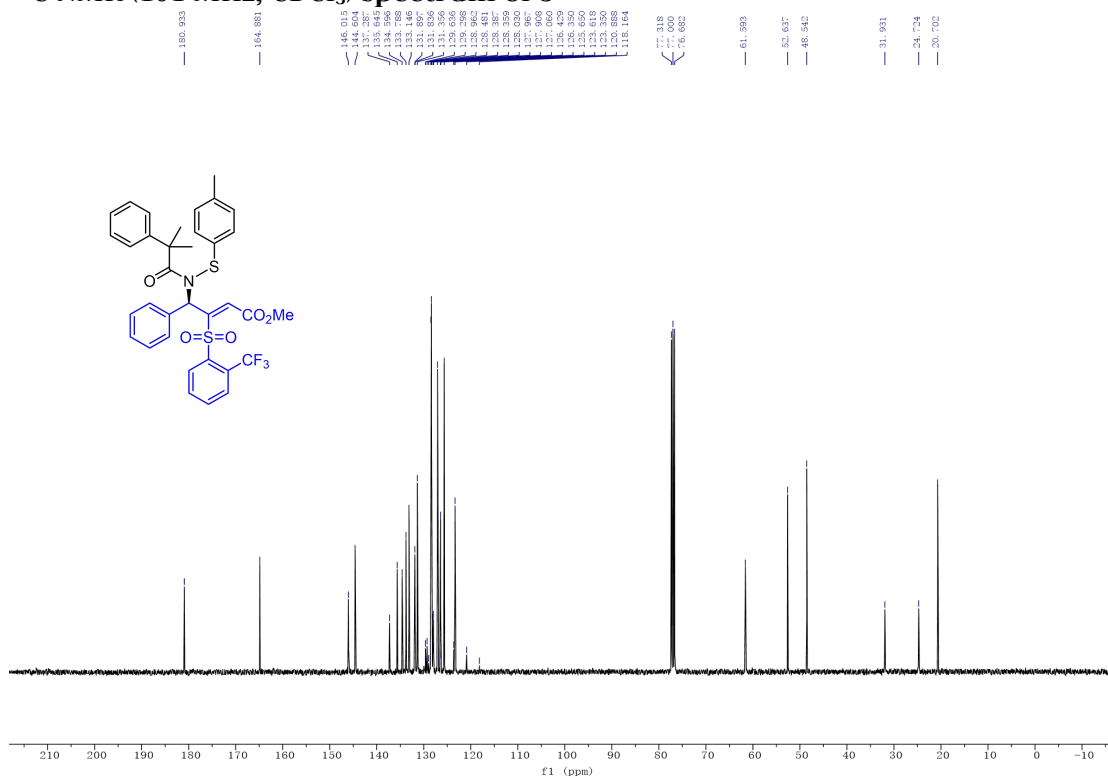


rac-(*E*)-52 (CCDC 2406864)

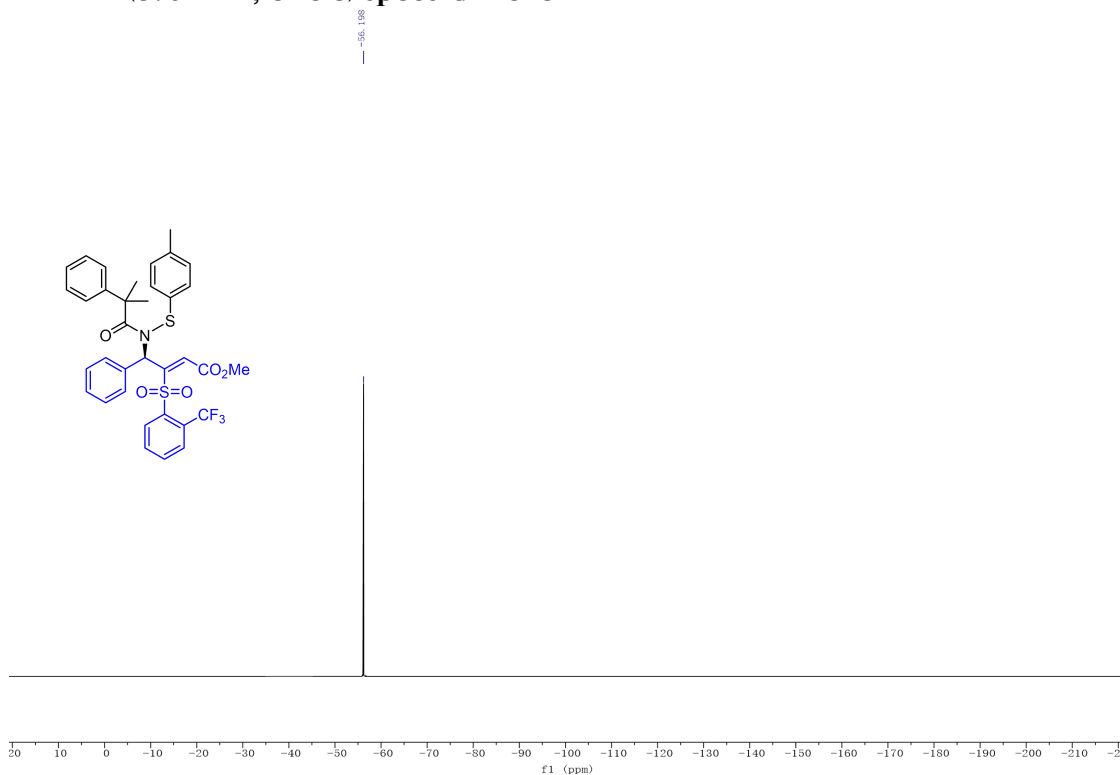
Table 1 Crystal data and structure refinement for 2505.

Identification code	2505
Empirical formula	C ₂₈ H ₂₆ F ₃ NO ₅ S
Formula weight	545.56
Temperature/K	150.00
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	17.1590(19)
b/Å	10.5048(11)
c/Å	14.7965(17)
α /°	90
β /°	100.496(5)
γ /°	90
Volume/Å ³	2622.5(5)
Z	4
ρ _{calc} /cm ³	1.382
μ /mm ⁻¹	1.631
F(000)	1136.0
Crystal size/mm ³	0.15 × 0.12 × 0.1
Radiation	CuK α (λ = 1.54178)
2 Θ range for data collection/°	5.238 to 136.762
Index ranges	-20 ≤ h ≤ 20, -12 ≤ k ≤ 12, -17 ≤ l ≤ 17
Reflections collected	44165
Independent reflections	4777 [R _{int} = 0.0502, R _{sigma} = 0.0281]
Data/restraints/parameters	4777/0/350
Goodness-of-fit on F ²	1.106
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0397, wR ₂ = 0.1014
Final R indexes [all data]	R ₁ = 0.0413, wR ₂ = 0.1023
Largest diff. peak/hole / e Å ⁻³	0.25/-0.46

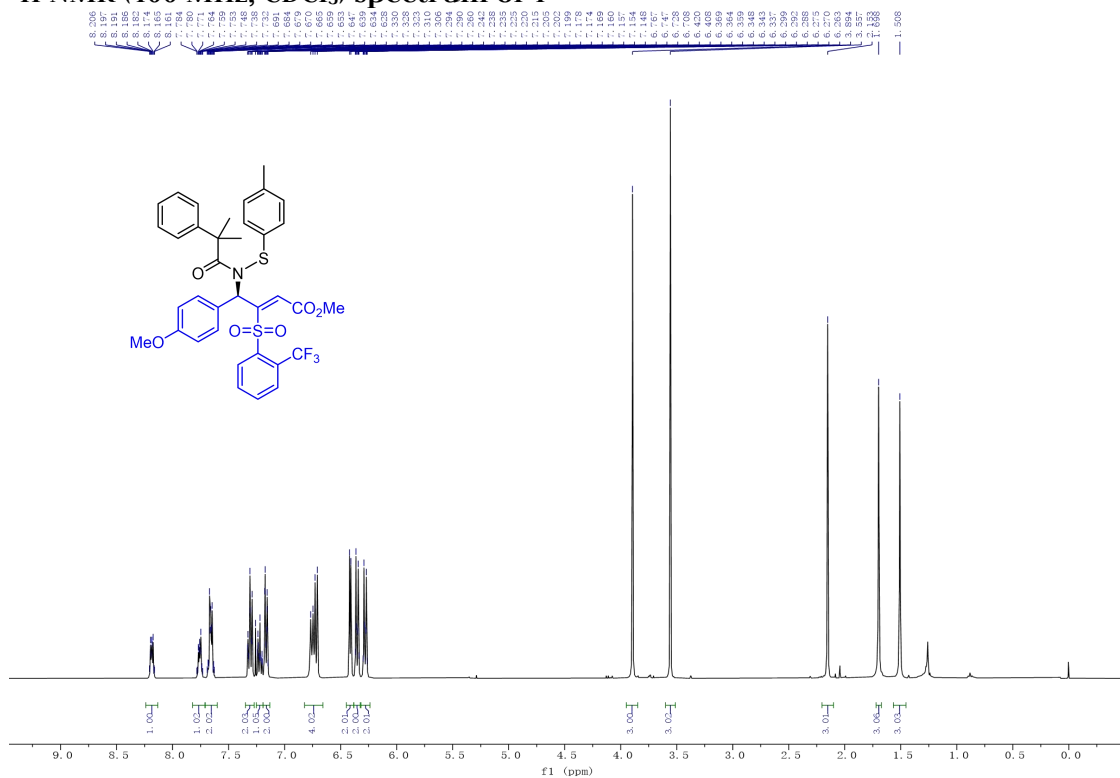
¹H NMR (400 MHz, CDCl₃) spectrum of 3



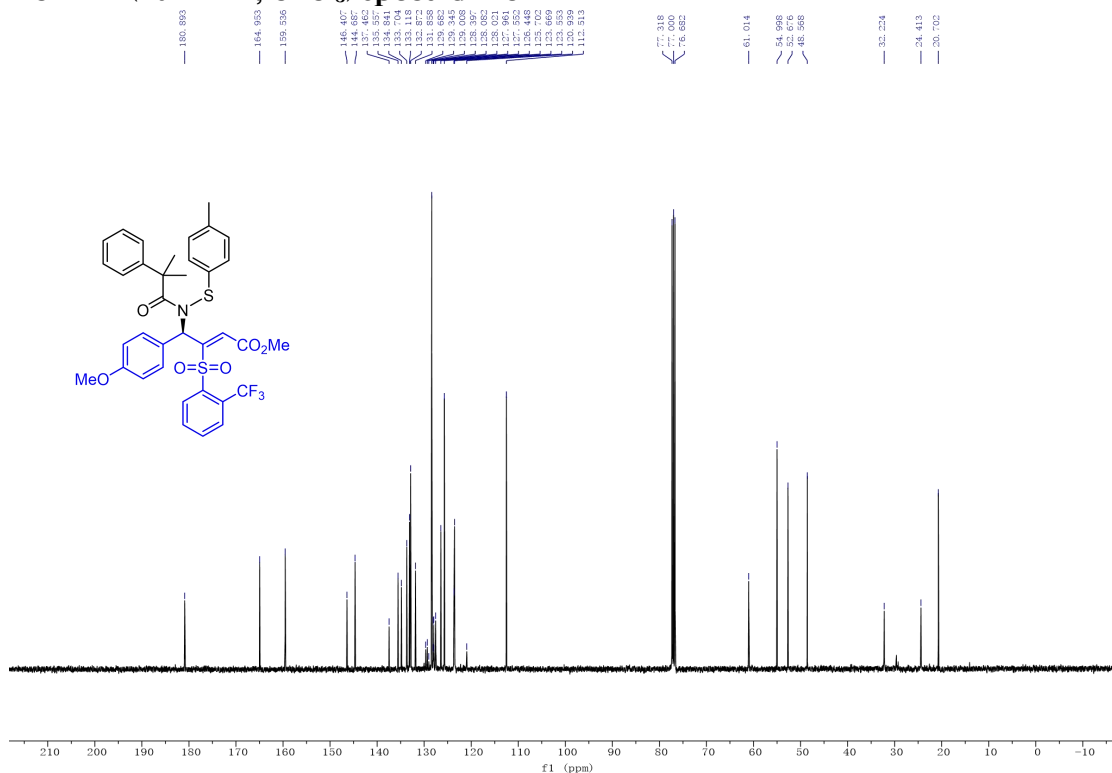
^{19}F NMR (376 MHz, CDCl_3) spectrum of 3



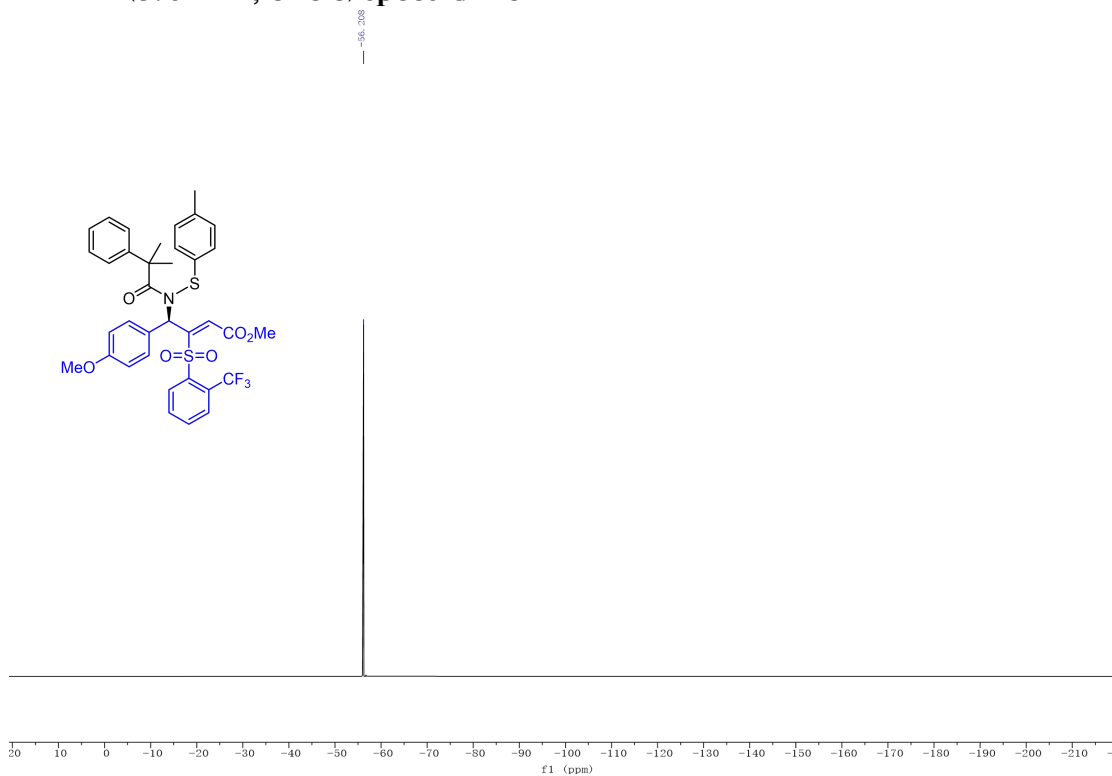
^1H NMR (400 MHz, CDCl_3) spectrum of 4



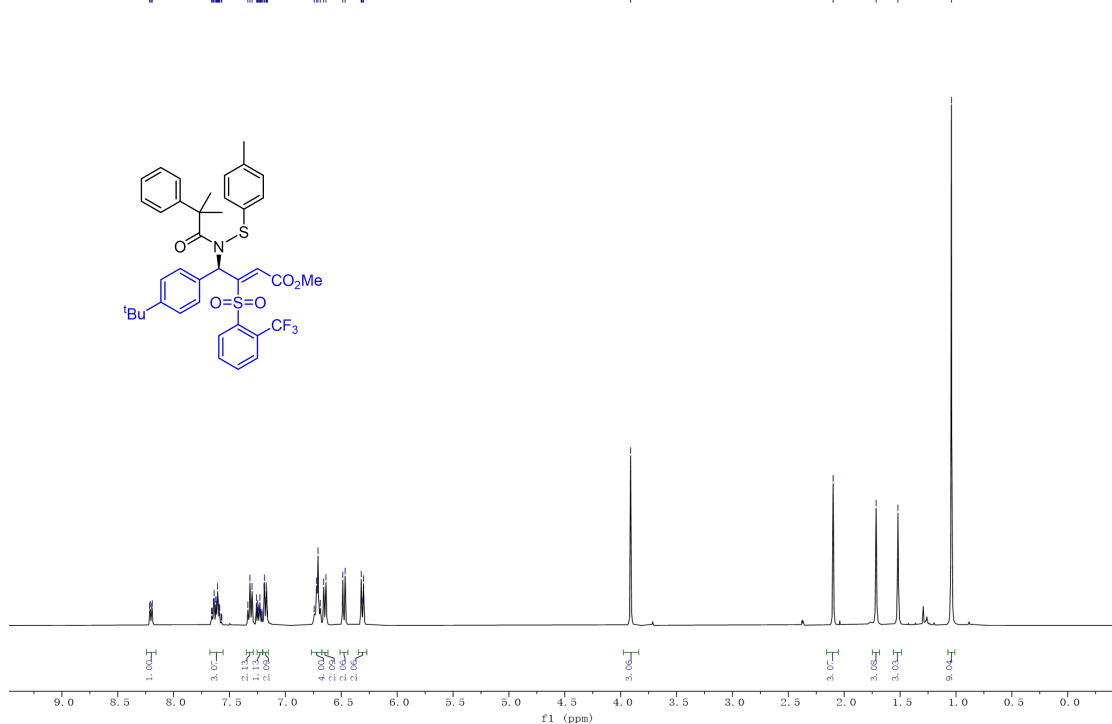
¹³C NMR (101 MHz, CDCl₃) spectrum of 4



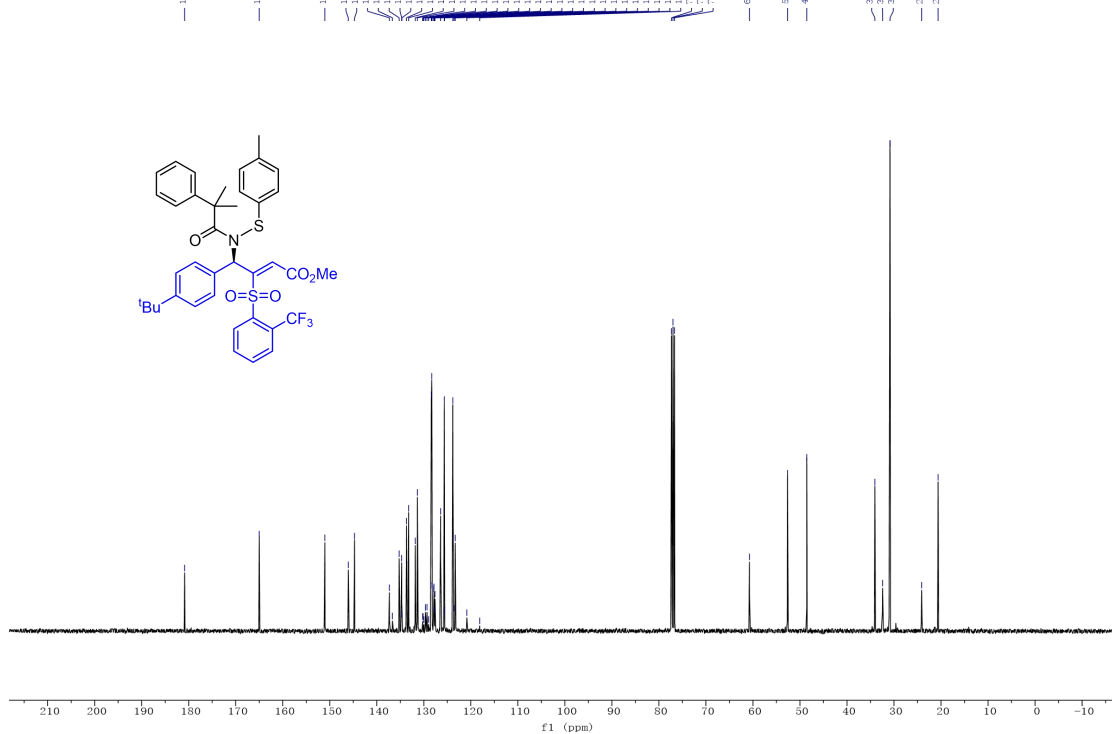
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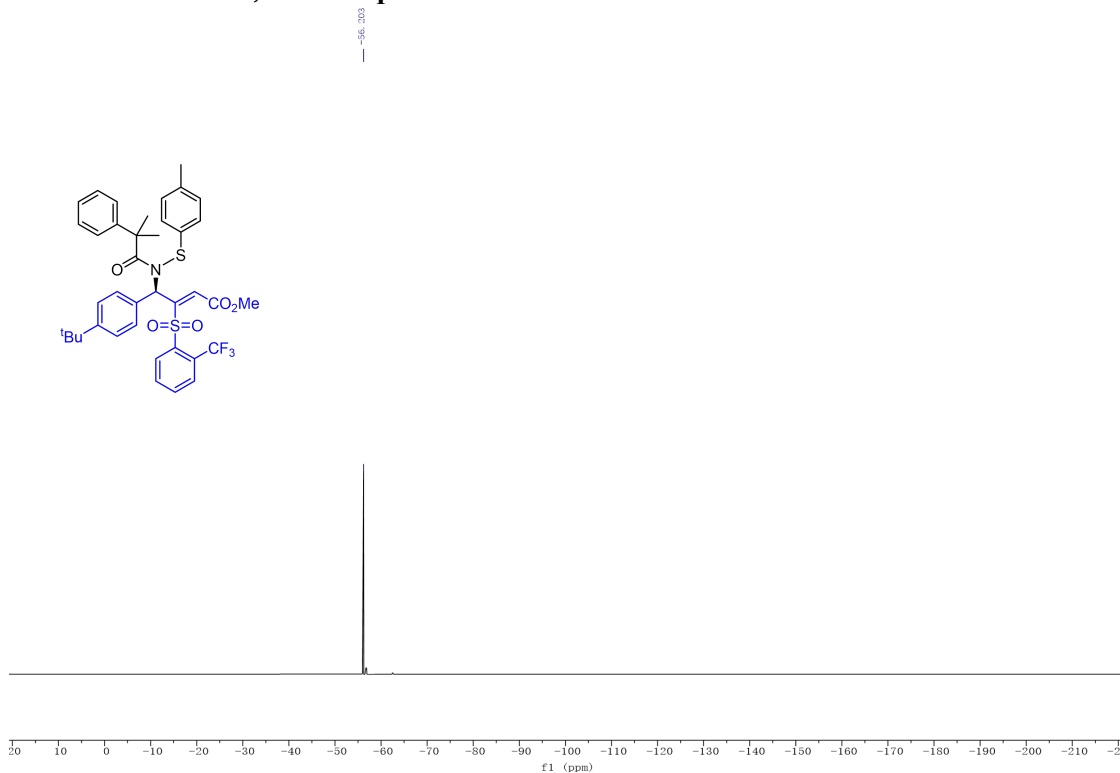
8.215	8.210	8.205	8.200	8.195	8.190	8.185	8.180	8.175	8.170	8.165	8.160	8.155	8.150	8.145	8.140	8.135	8.130	8.125	8.120	8.115	8.110	8.105	8.100	8.095	8.090	8.085	8.080	8.075	8.070	8.065	8.060	8.055	8.050	8.045	8.040	8.035	8.030	8.025	8.020	8.015	8.010	8.005	8.000	7.995	7.990	7.985	7.980	7.975	7.970	7.965	7.960	7.955	7.950	7.945	7.940	7.935	7.930	7.925	7.920	7.915	7.910	7.905	7.900	7.895	7.890	7.885	7.880	7.875	7.870	7.865	7.860	7.855	7.850	7.845	7.840	7.835	7.830	7.825	7.820	7.815	7.810	7.805	7.800	7.795	7.790	7.785	7.780	7.775	7.770	7.765	7.760	7.755	7.750	7.745	7.740	7.735	7.730	7.725	7.720	7.715	7.710	7.705	7.700	7.695	7.690	7.685	7.680	7.675	7.670	7.665	7.660	7.655	7.650	7.645	7.640	7.635	7.630	7.625	7.620	7.615	7.610	7.605	7.600	7.595	7.590	7.585	7.580	7.575	7.570	7.565	7.560	7.555	7.550	7.545	7.540	7.535	7.530	7.525	7.520	7.515	7.510	7.505	7.500	7.495	7.490	7.485	7.480	7.475	7.470	7.465	7.460	7.455	7.450	7.445	7.440	7.435	7.430	7.425	7.420	7.415	7.410	7.405	7.400	7.395	7.390	7.385	7.380	7.375	7.370	7.365	7.360	7.355	7.350	7.345	7.340	7.335	7.330	7.325	7.320	7.315	7.310	7.305	7.300	7.295	7.290	7.285	7.280	7.275	7.270	7.265	7.260	7.255	7.250	7.245	7.240	7.235	7.230	7.225	7.220	7.215	7.210	7.205	7.200	7.195	7.190	7.185	7.180	7.175	7.170	7.165	7.160	7.155	7.150	7.145	7.140	7.135	7.130	7.125	7.120	7.115	7.110	7.105	7.100	7.095	7.090	7.085	7.080	7.075	7.070	7.065	7.060	7.055	7.050	7.045	7.040	7.035	7.030	7.025	7.020	7.015	7.010	7.005	7.000	6.995	6.990	6.985	6.980	6.975	6.970	6.965	6.960	6.955	6.950	6.945	6.940	6.935	6.930	6.925	6.920	6.915	6.910	6.905	6.900	6.895	6.890	6.885	6.880	6.875	6.870	6.865	6.860	6.855	6.850	6.845	6.840	6.835	6.830	6.825	6.820	6.815	6.810	6.805	6.800	6.795	6.790	6.785	6.780	6.775	6.770	6.765	6.760	6.755	6.750	6.745	6.740	6.735	6.730	6.725	6.720	6.715	6.710	6.705	6.700	6.695	6.690	6.685	6.680	6.675	6.670	6.665	6.660	6.655	6.650	6.645	6.640	6.635	6.630	6.625	6.620	6.615	6.610	6.605	6.600	6.595	6.590	6.585	6.580	6.575	6.570	6.565	6.560	6.555	6.550	6.545	6.540	6.535	6.530	6.525	6.520	6.515	6.510	6.505	6.500	6.495	6.490	6.485	6.480	6.475	6.470	6.465	6.460	6.455	6.450	6.445	6.440	6.435	6.430	6.425	6.420	6.415	6.410	6.405	6.400	6.395	6.390	6.385	6.380	6.375	6.370	6.365	6.36
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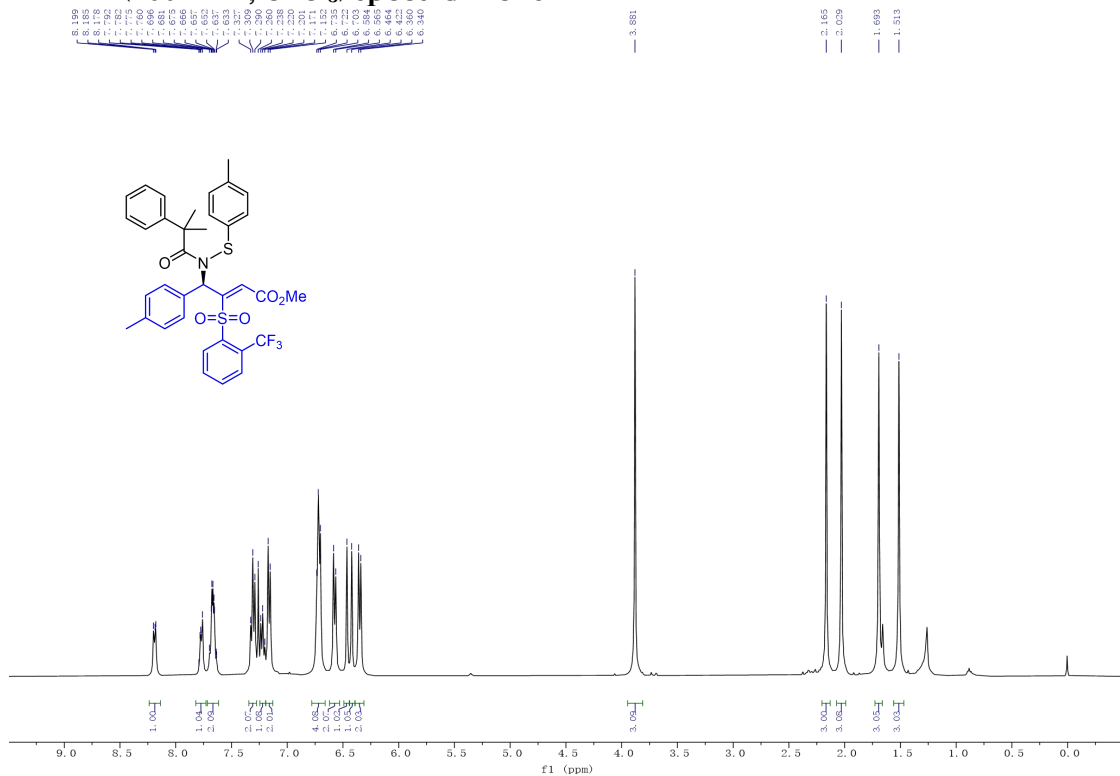
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34. 657	29. 987
33. 668	29. 649
33. 222	29. 315
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31. 366	28. 399
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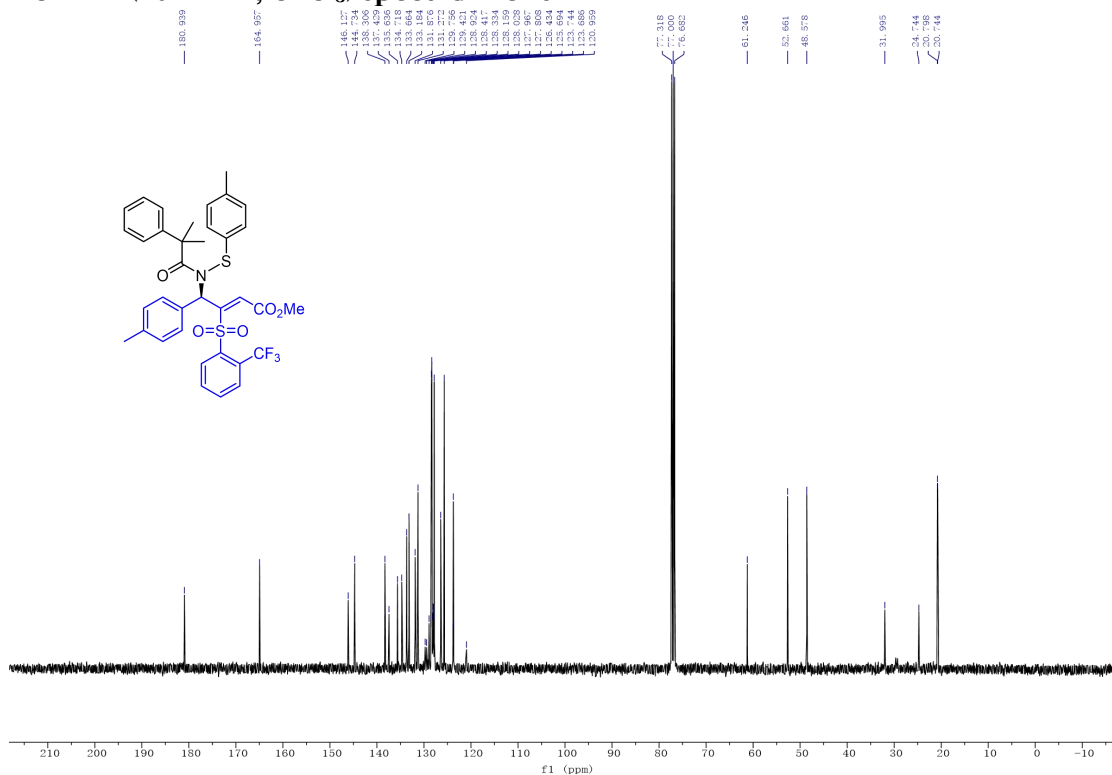
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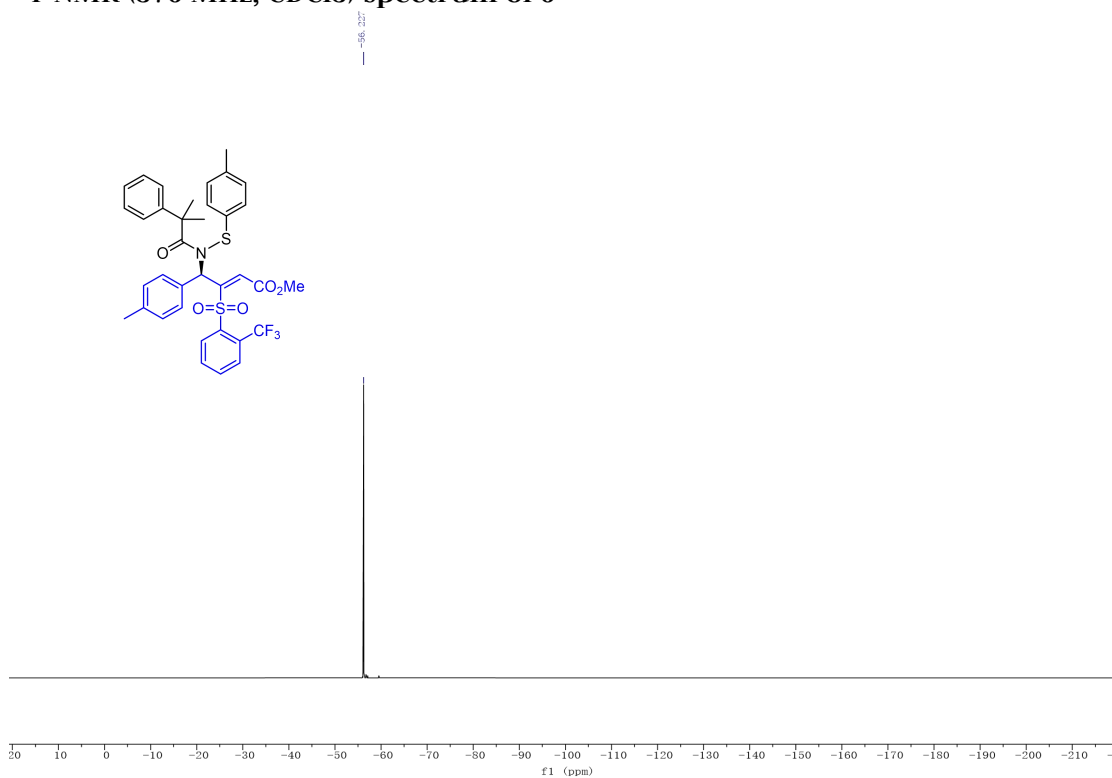
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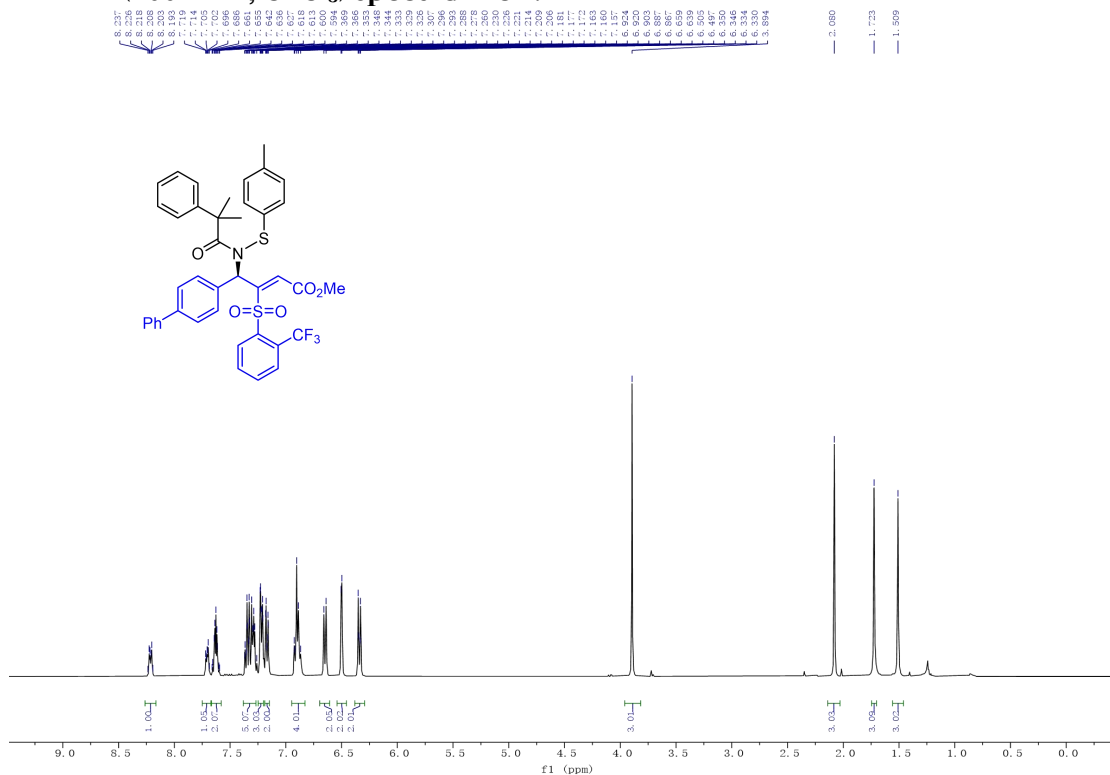
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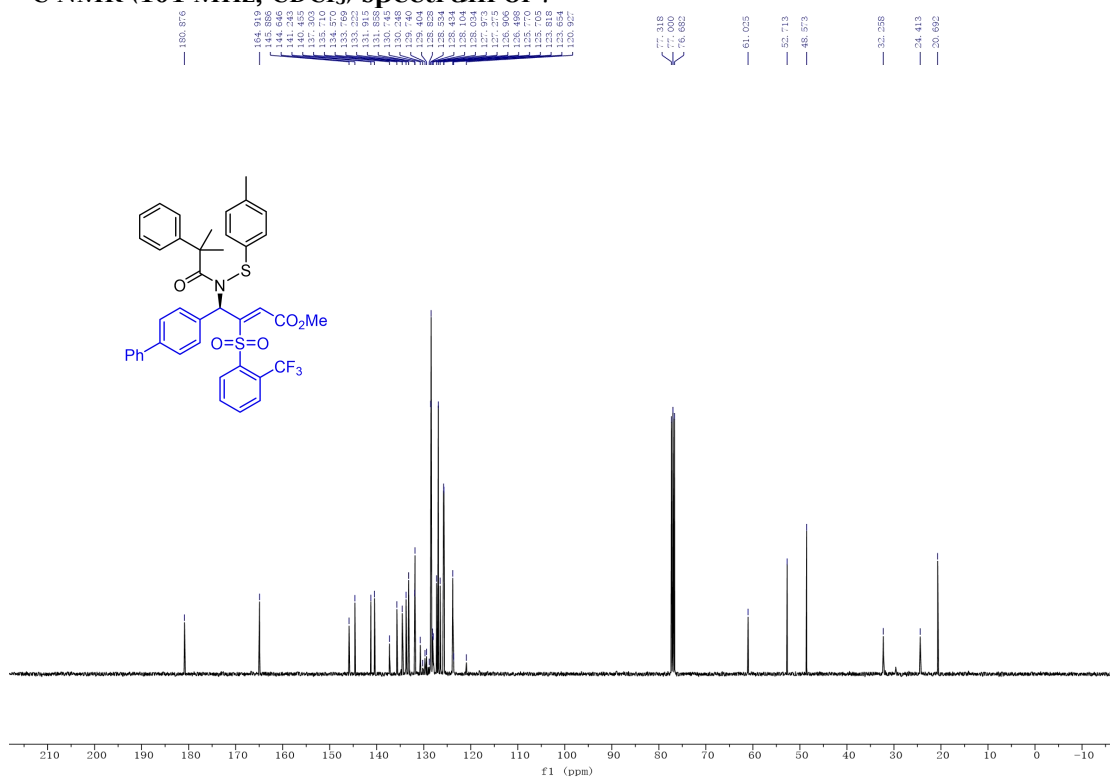
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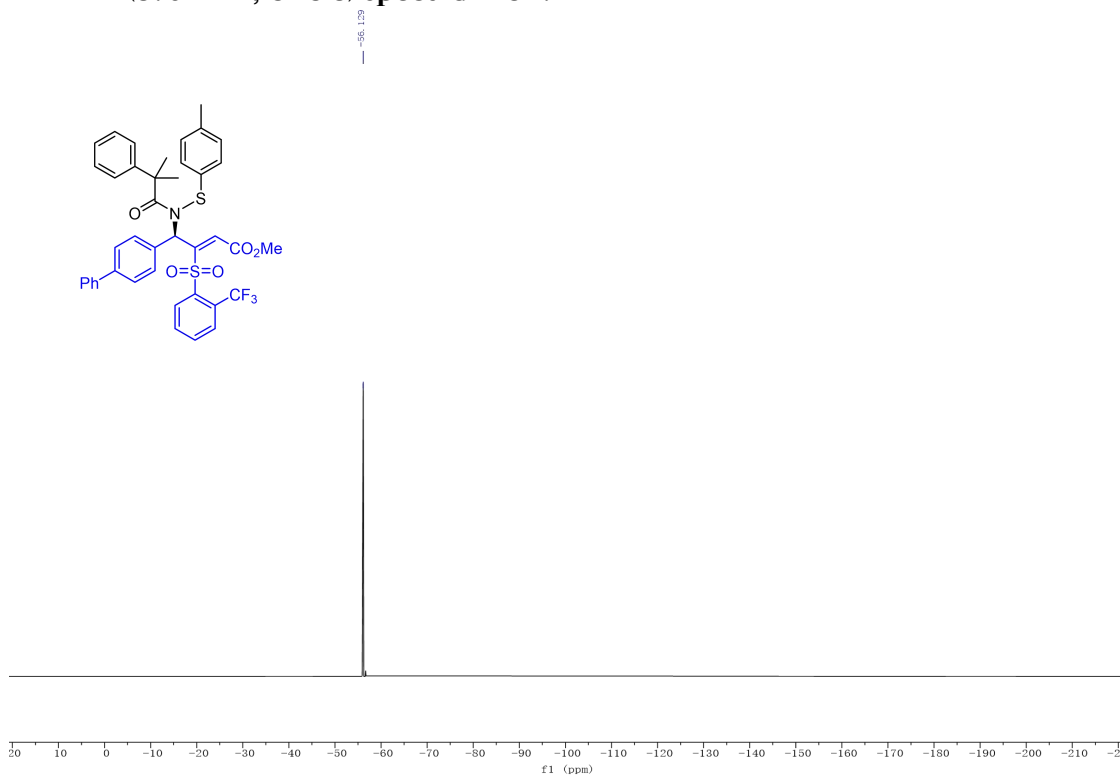
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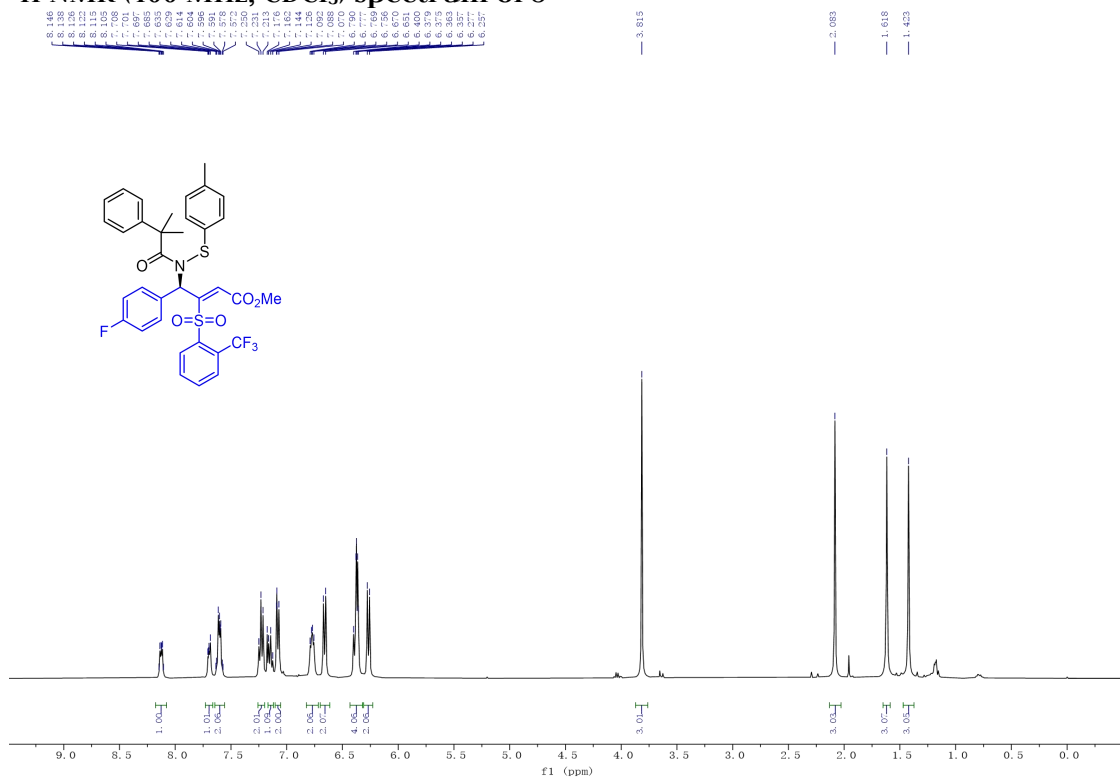
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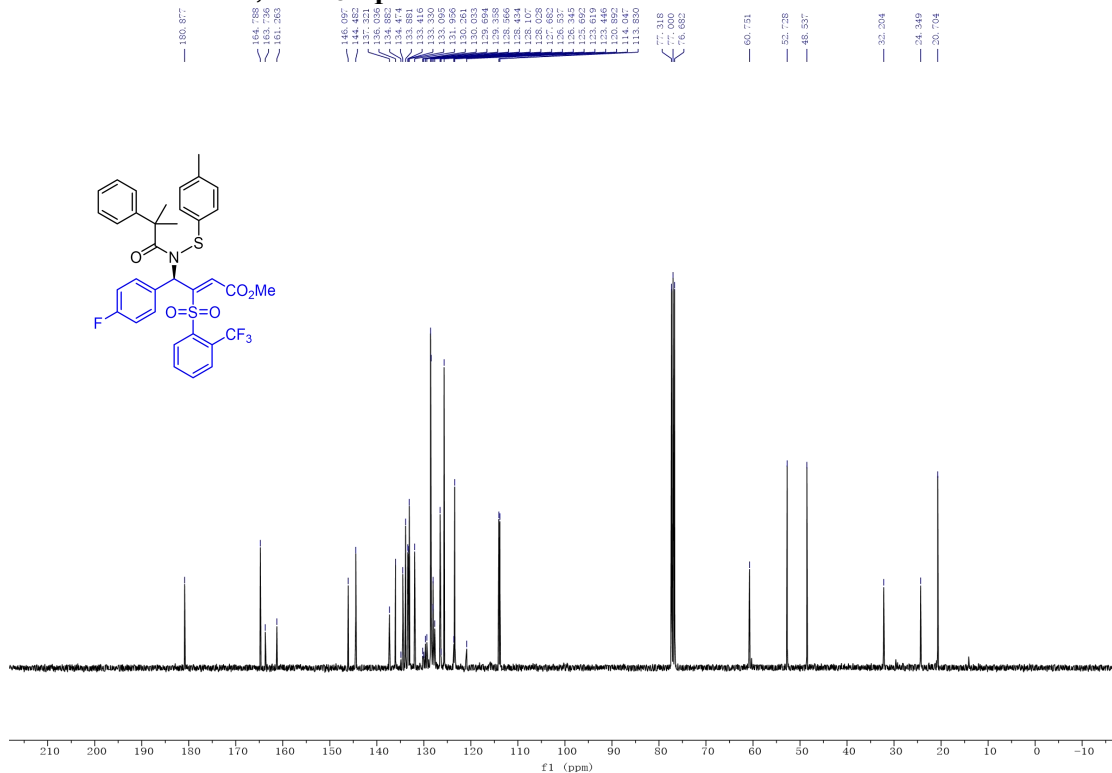
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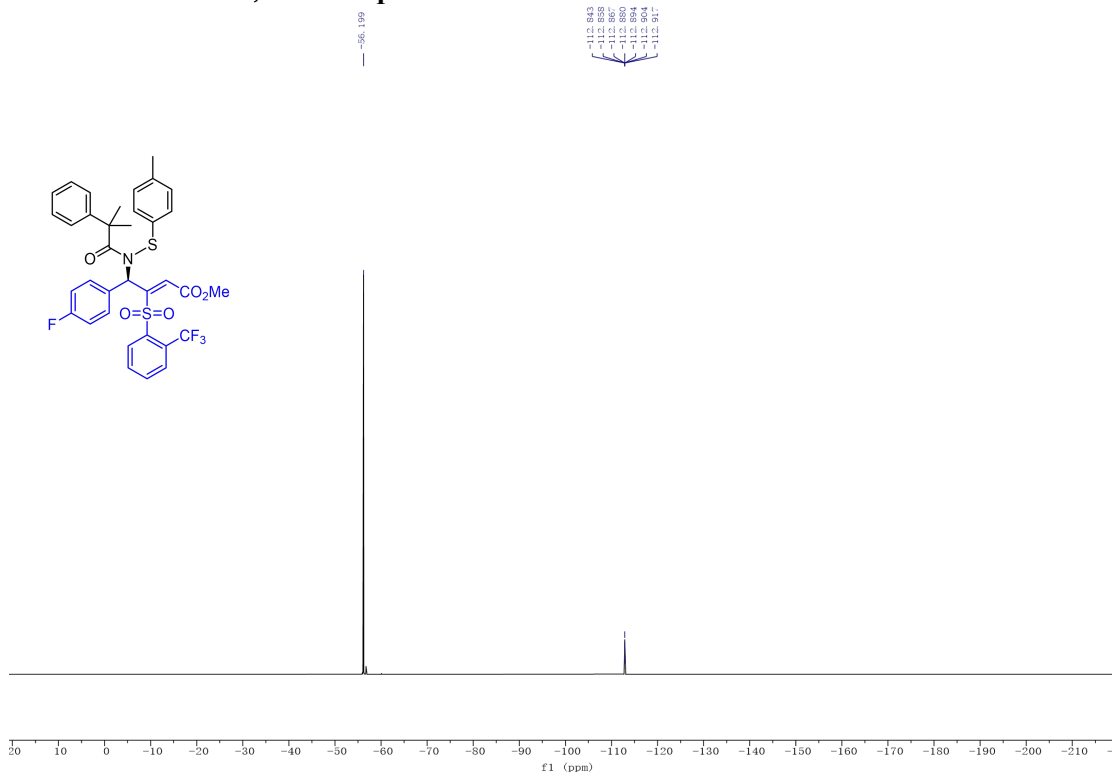
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¹³C NMR (101 MHz, CDCl₃) spectrum of 8



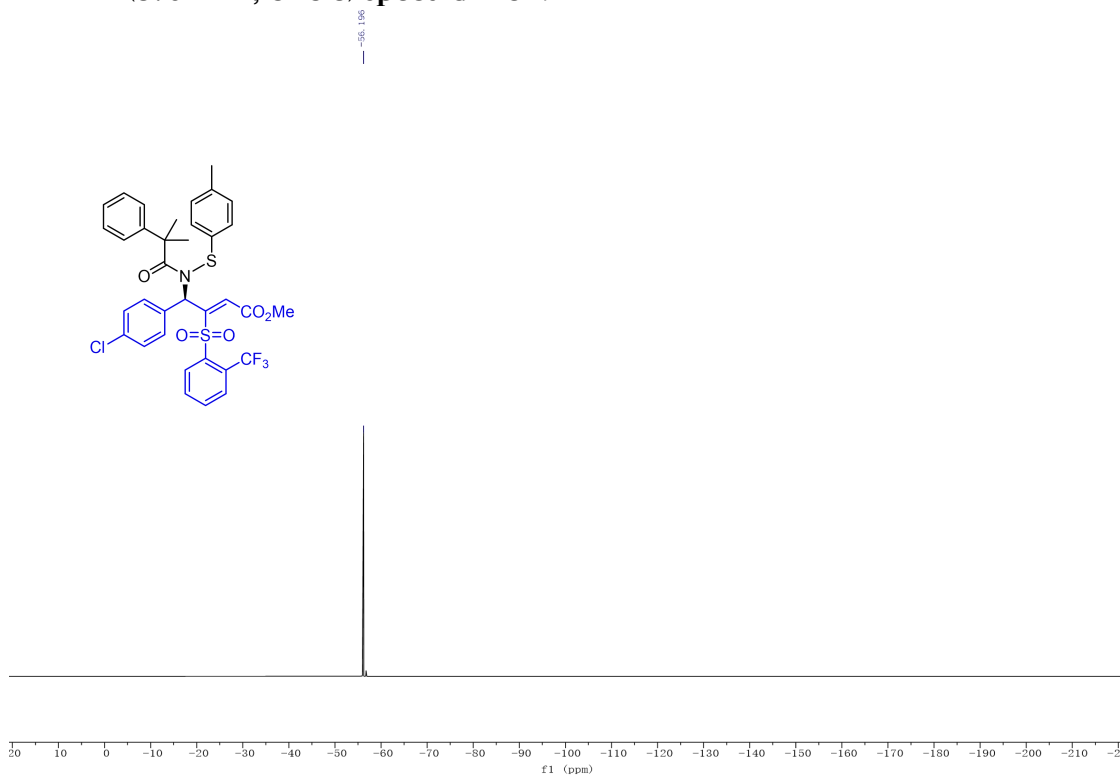
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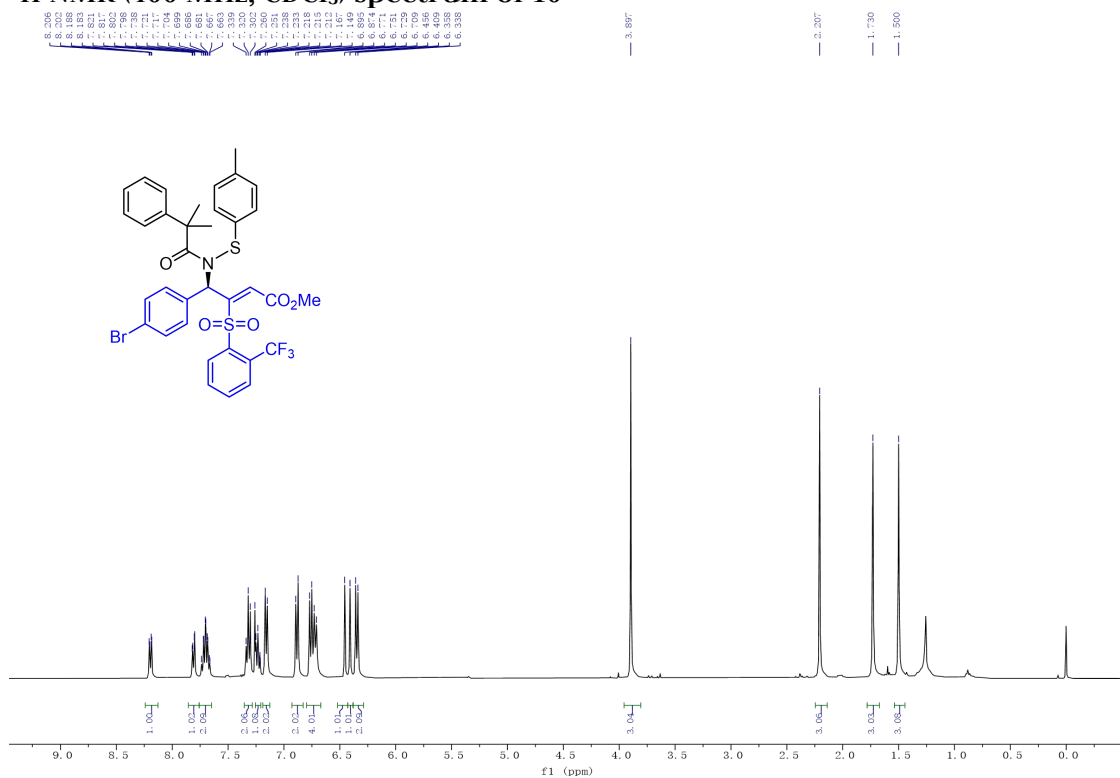
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180.851
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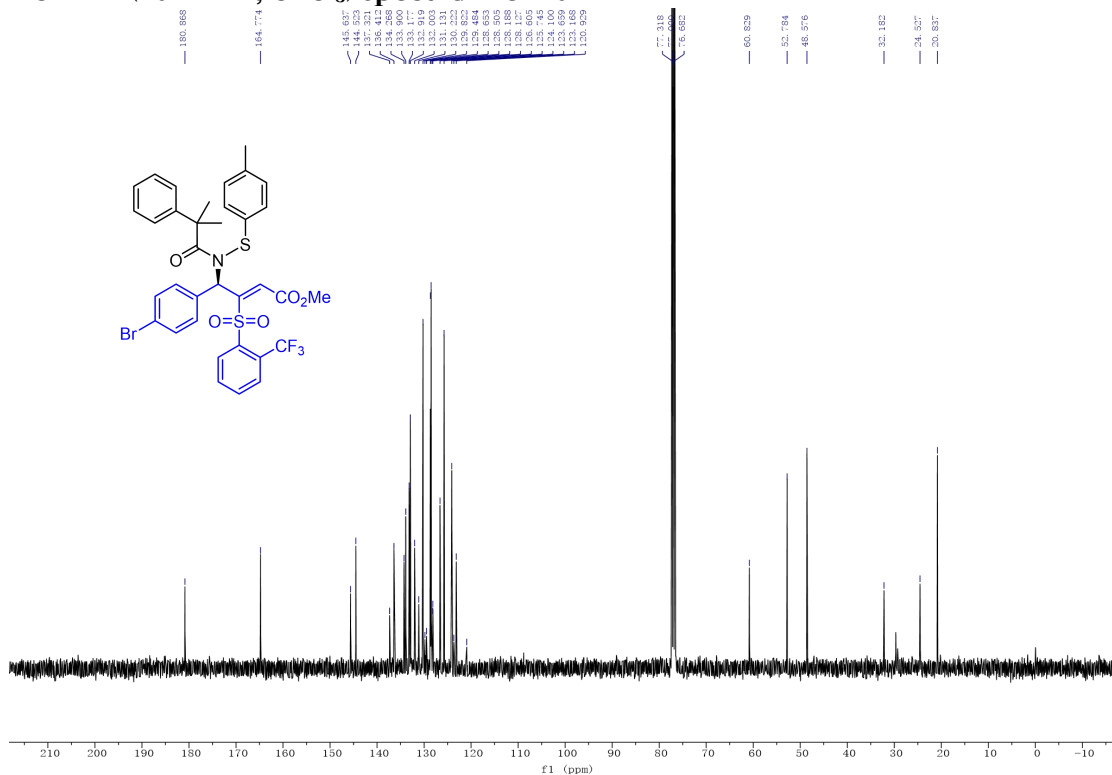
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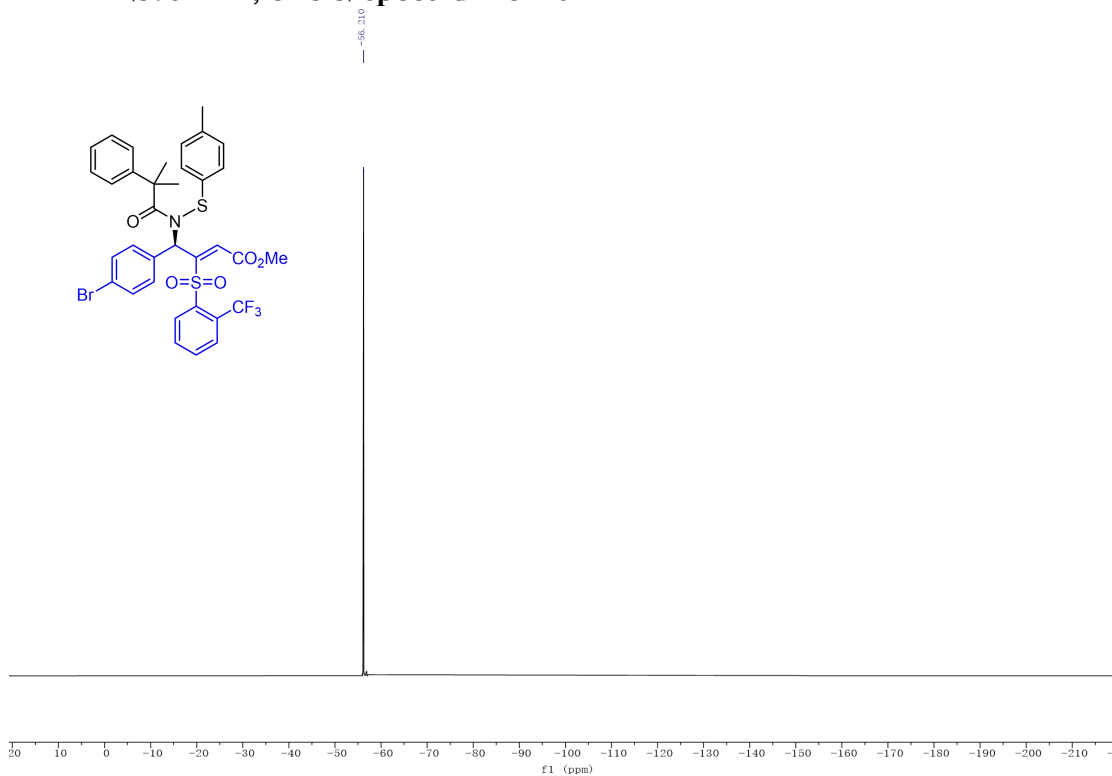
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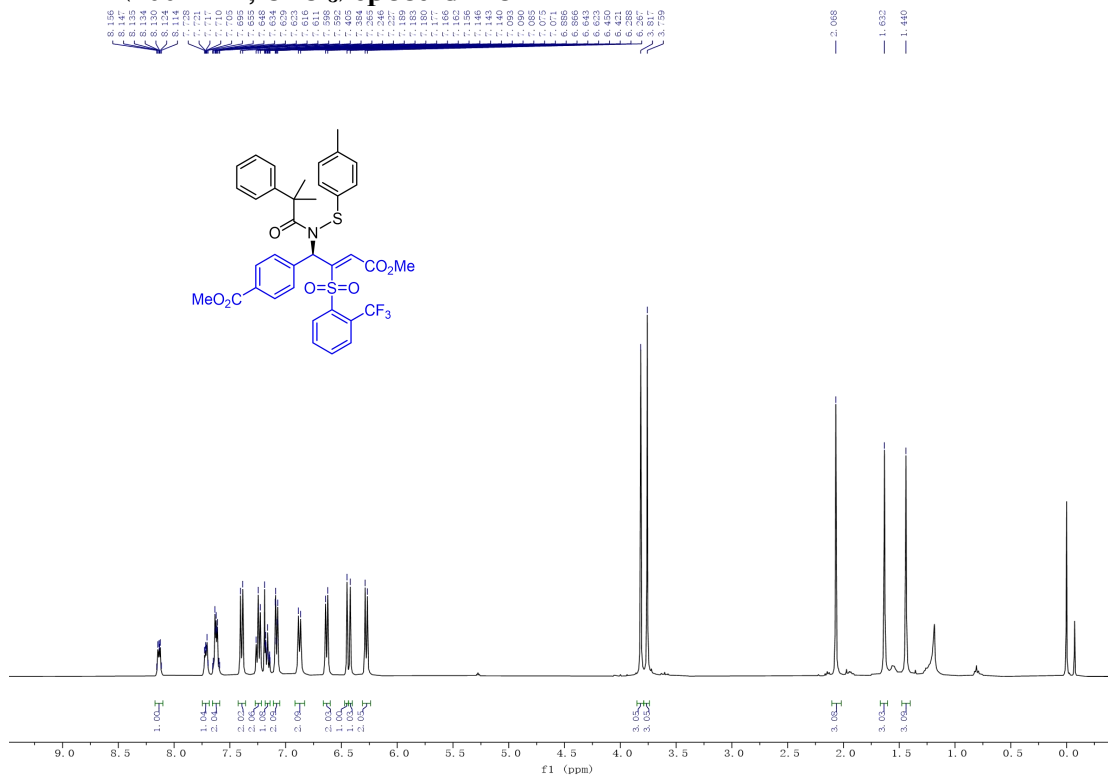
¹³C NMR (101 MHz, CDCl₃) spectrum of 10



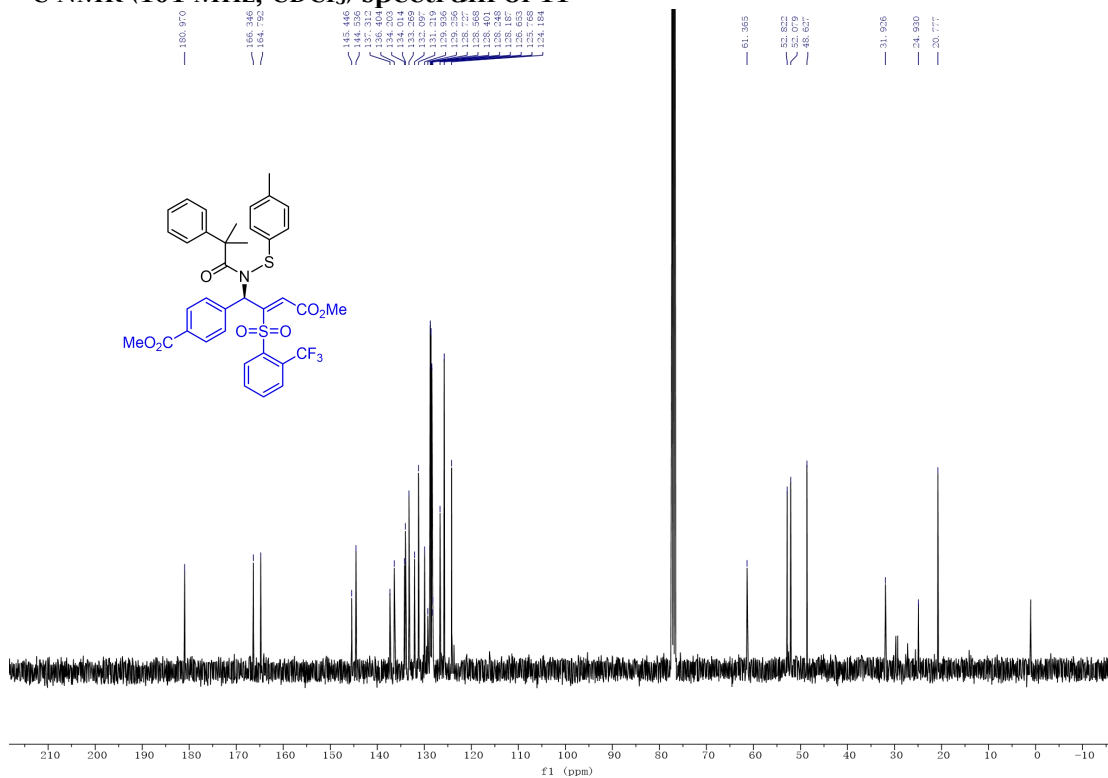
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 10



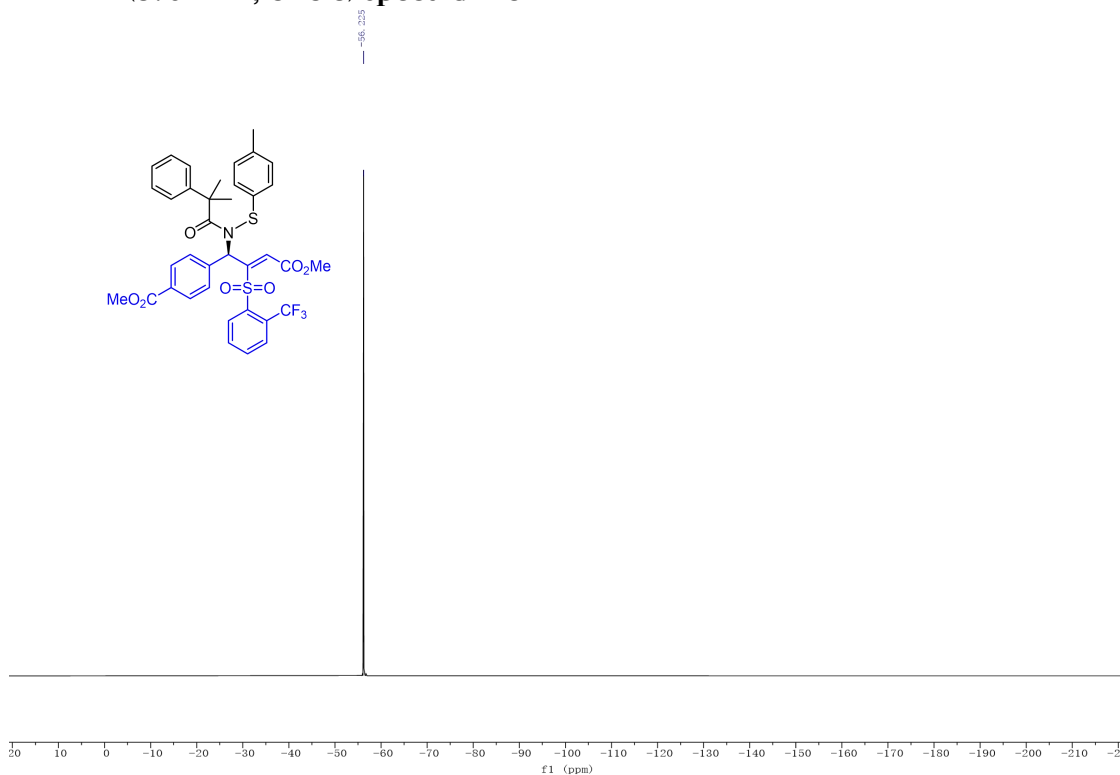
¹H NMR (400 MHz, CDCl₃) spectrum of 11



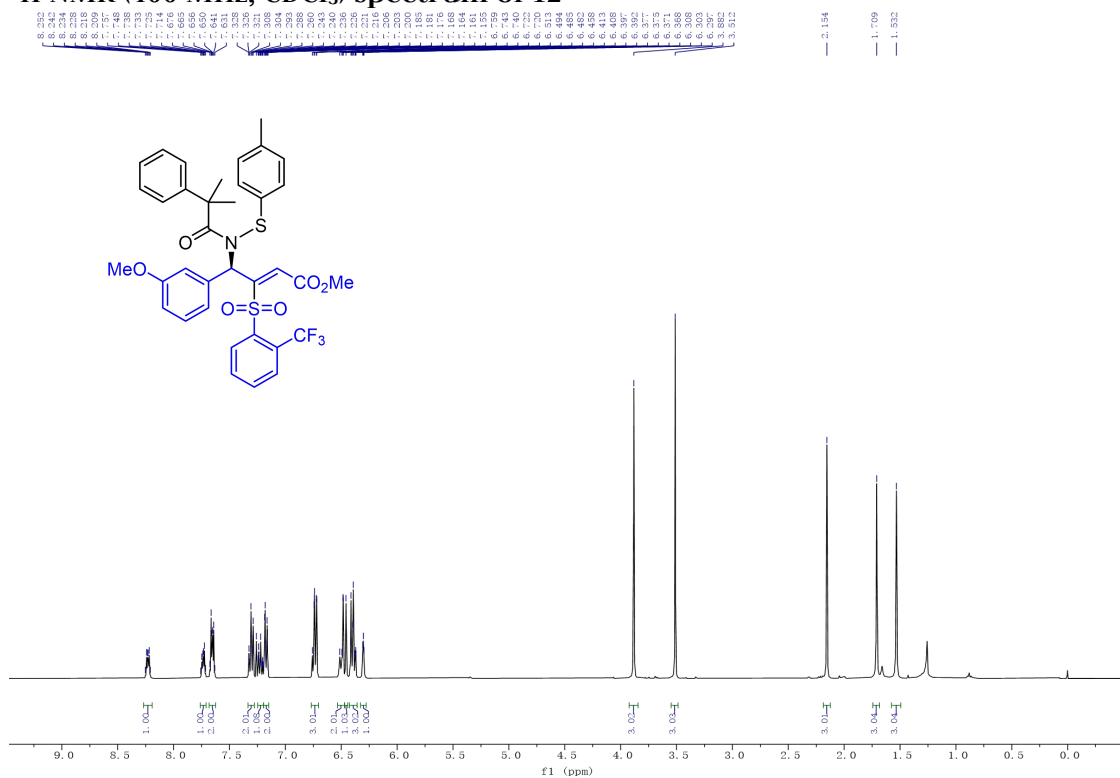
¹³C NMR (101 MHz, CDCl₃) spectrum of 11



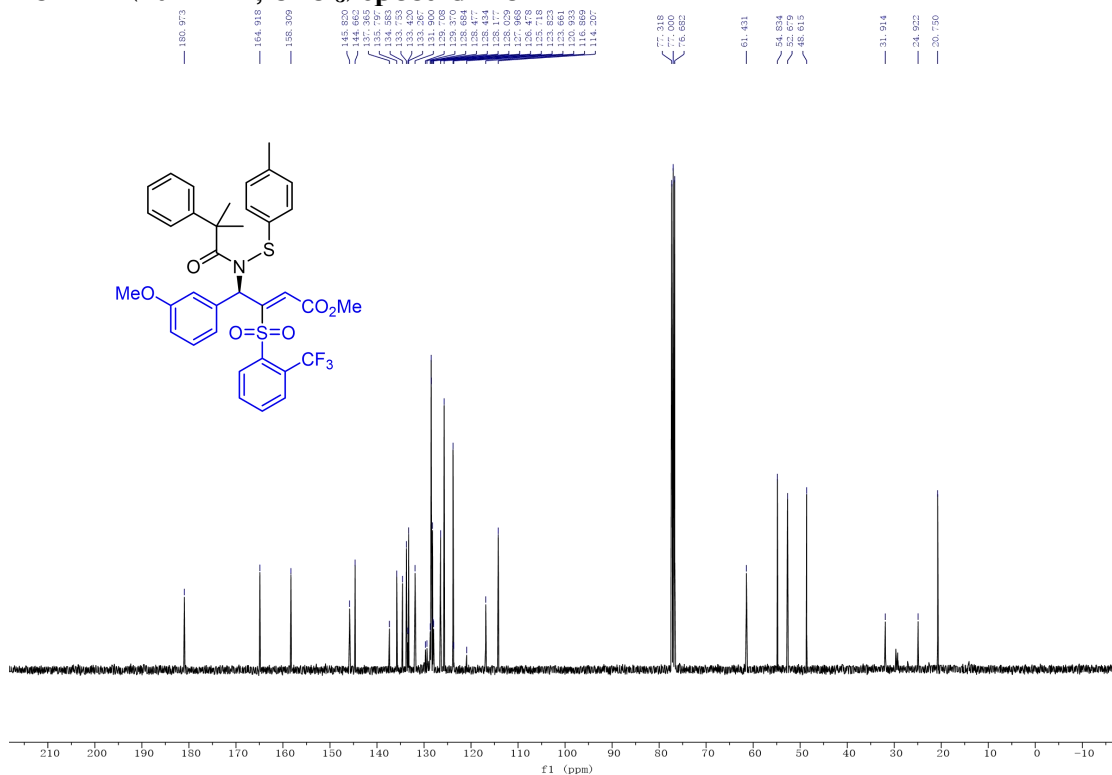
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 11



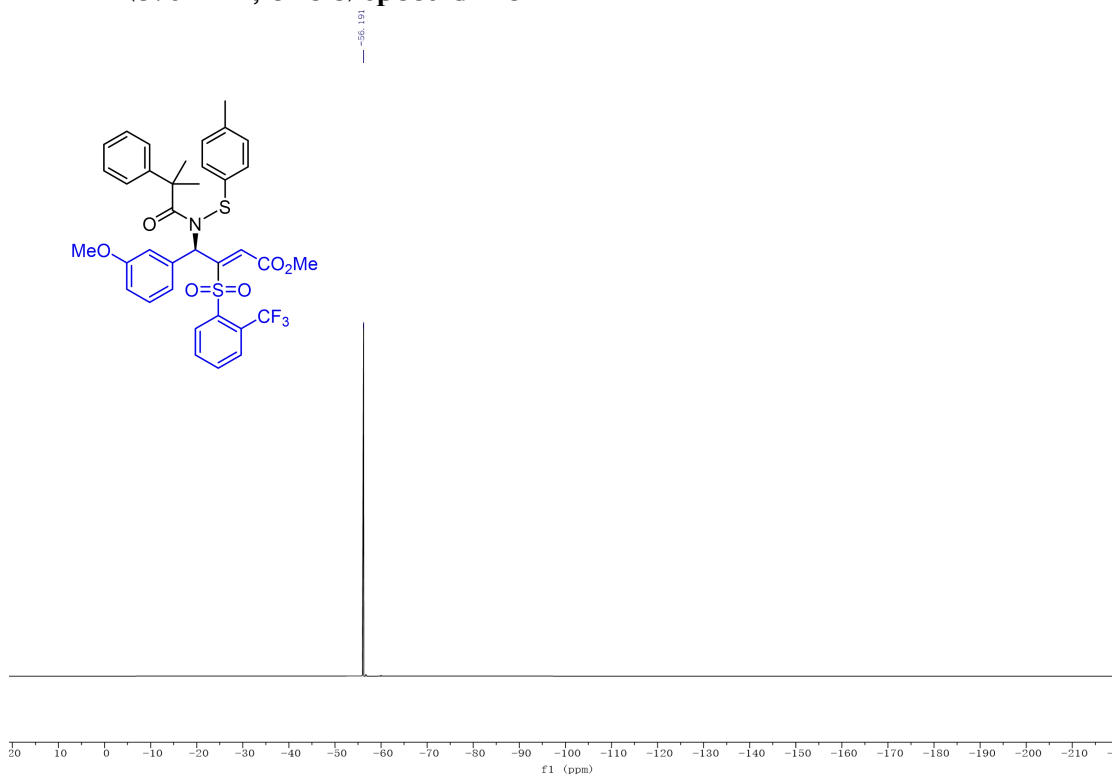
¹H NMR (400 MHz, CDCl₃) spectrum of 12



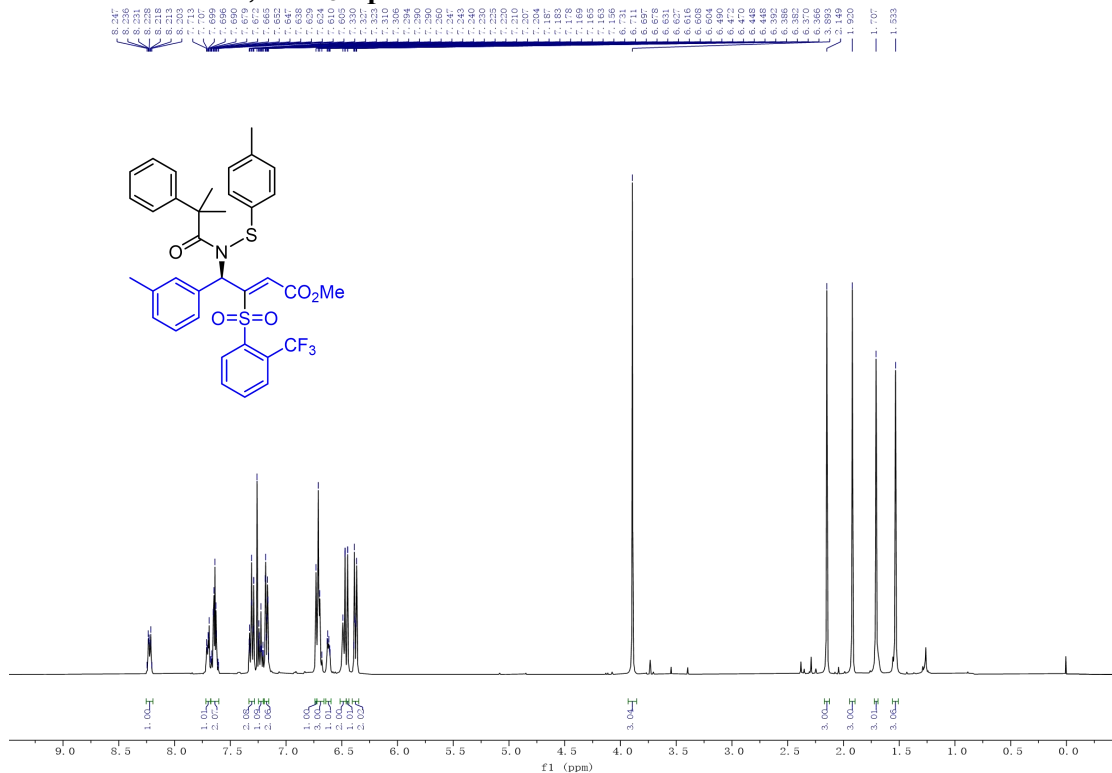
¹³C NMR (101 MHz, CDCl₃) spectrum of 12



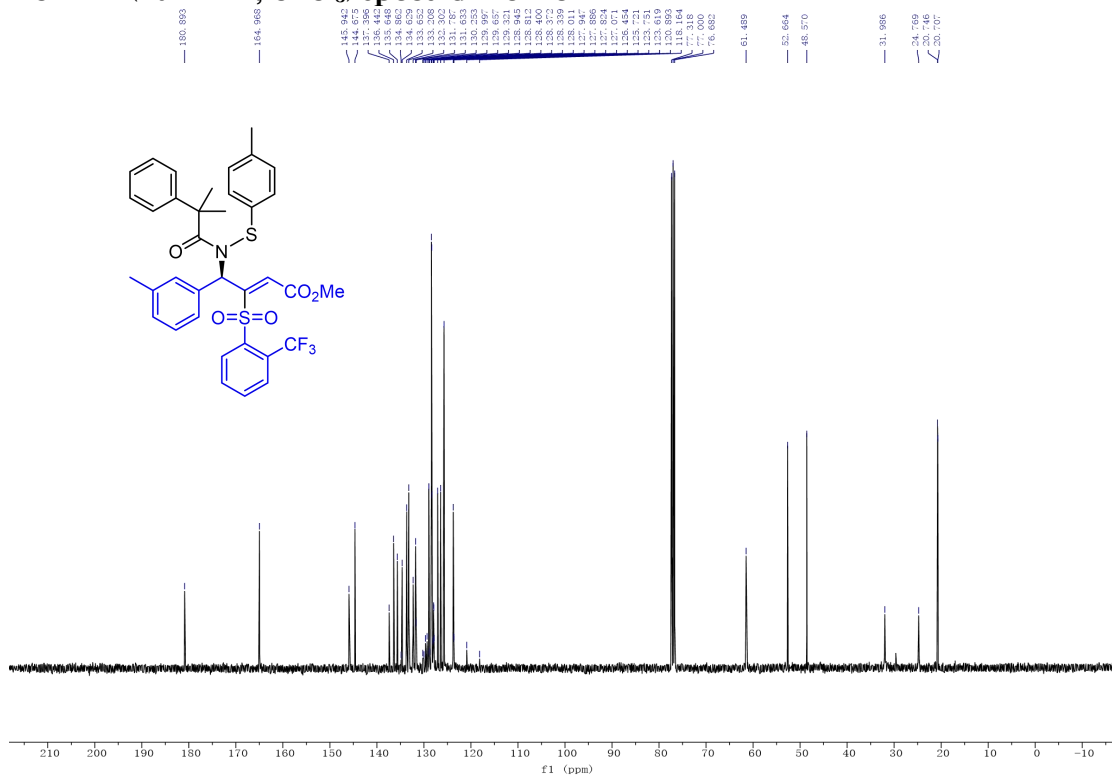
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 12



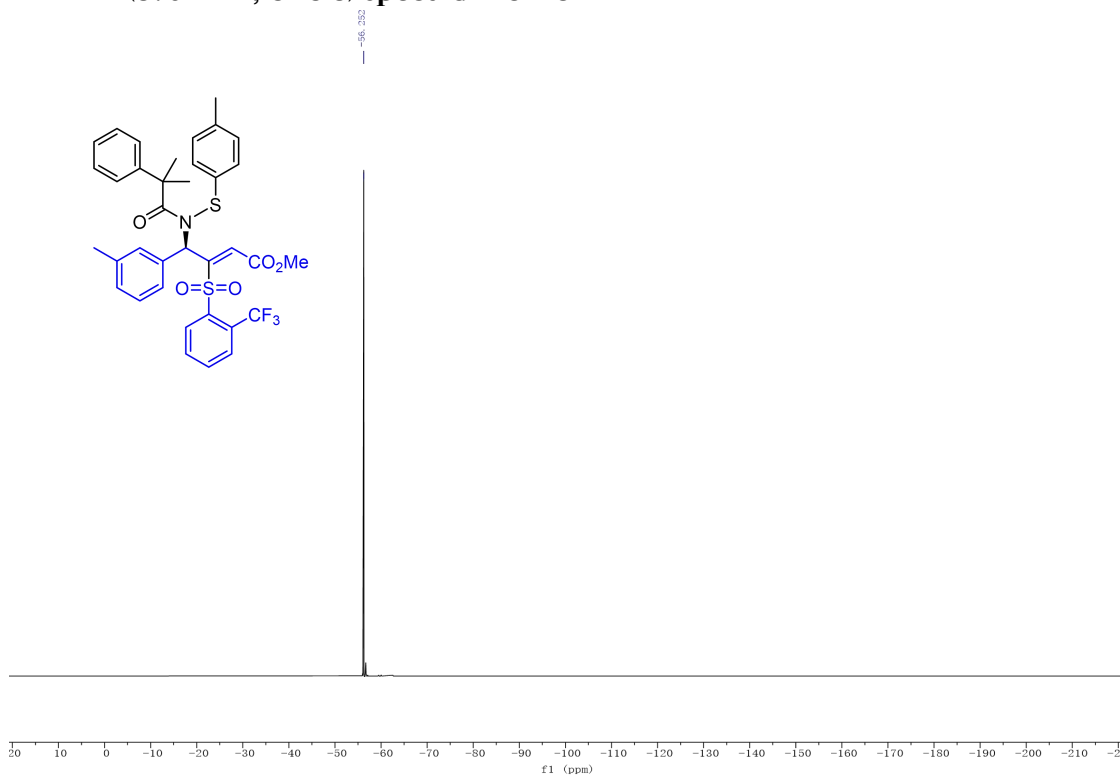
¹H NMR (400 MHz, CDCl₃) spectrum of 13



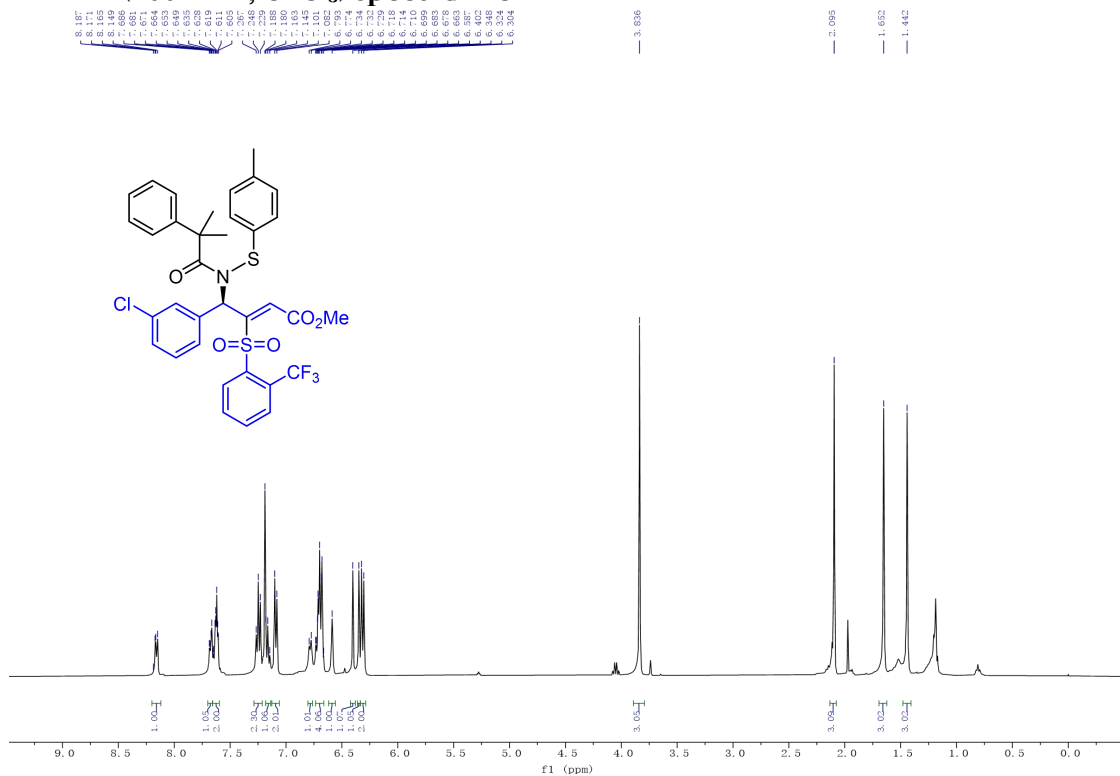
¹³C NMR (101 MHz, CDCl₃) spectrum of 13



^{19}F NMR (376 MHz, CDCl_3) spectrum of 13



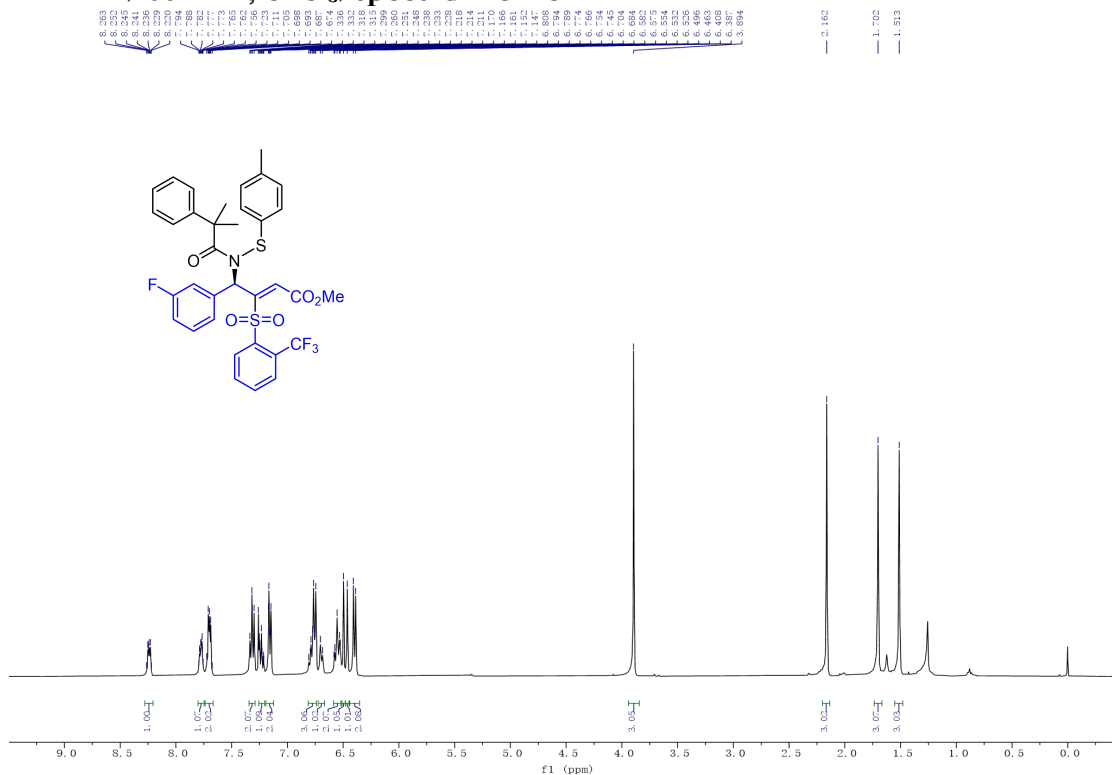
^1H NMR (400 MHz, CDCl_3) spectrum of 14



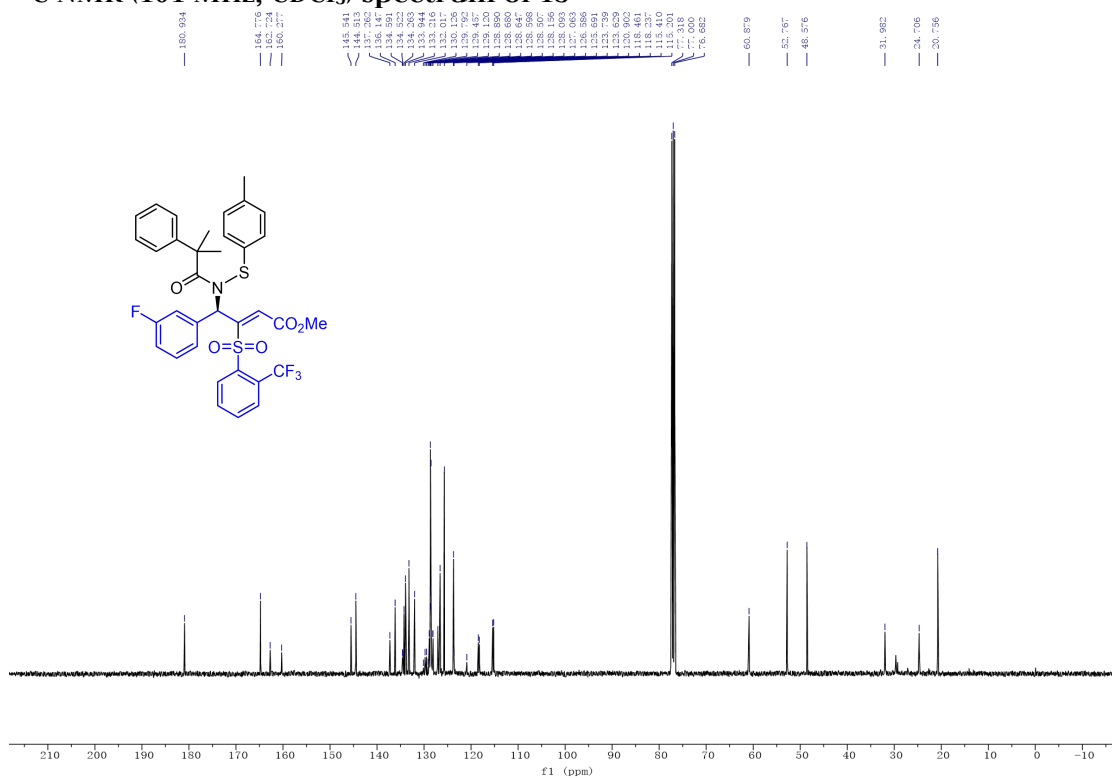
Chemical structure of compound 10b is shown above the spectrum. The structure is a substituted benzothiazine derivative. The spectrum shows peaks corresponding to the following chemical shifts (ppm): 180.845, 164.796, 145.418, 144.510, 142.510, 138.6319, 138.4142, 137.8642, 135.753, 133.976, 133.9596, 131.626, 128.794, 128.678, 128.659, 128.522, 128.340, 128.121, 128.111, 127.955, 127.955, 127.955, 126.610, 126.887, 77.317, 76.484, 60.927, 52.804, 48.588, 32.155, 24.559, 20.786.

¹H NMR spectrum of compound 10 in CDCl₃. The x-axis represents the chemical shift in ppm, ranging from 20 to -5. A single sharp peak is visible at approximately 2.9 ppm, corresponding to the methyl group of the ester. The solvent peak for CDCl₃ is present at 7.26 ppm.

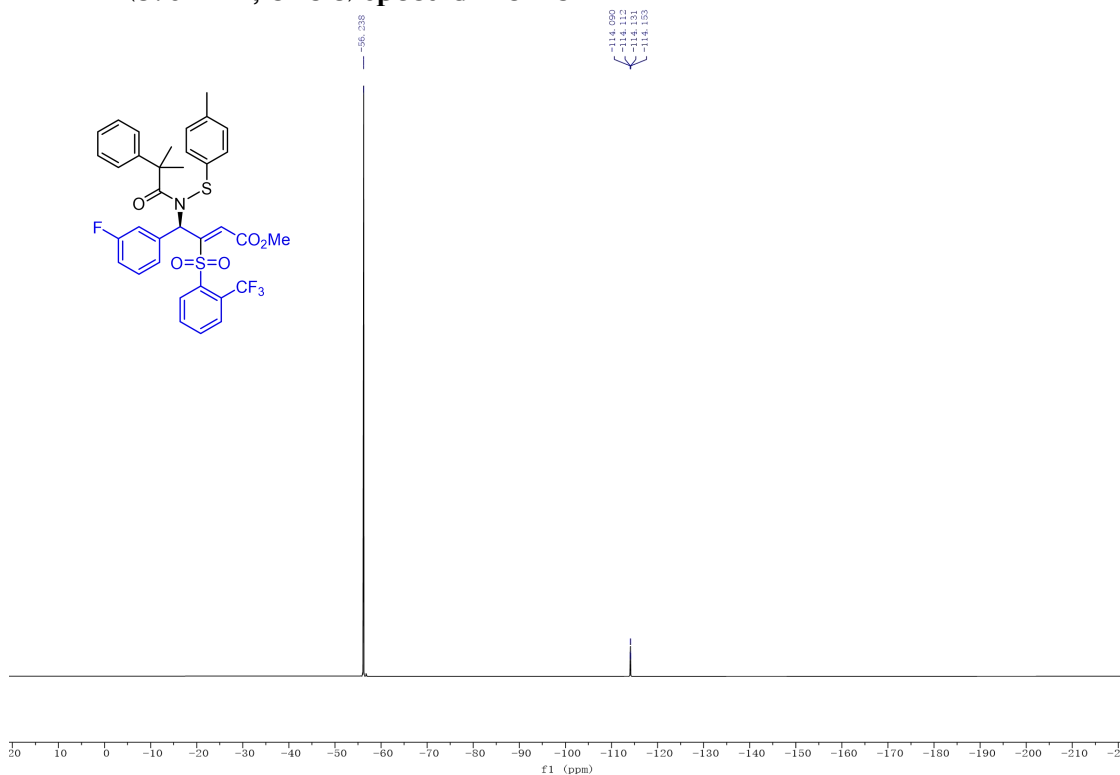
¹H NMR (400 MHz, CDCl₃) spectrum of 15



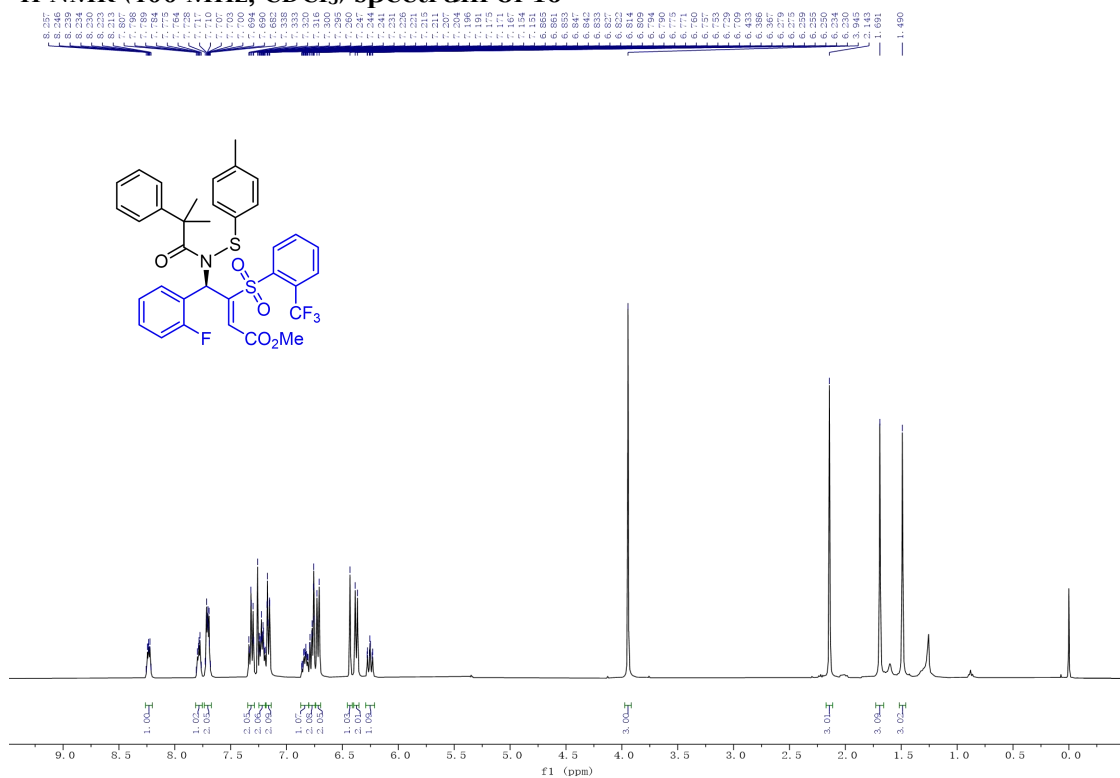
¹³C NMR (101 MHz, CDCl₃) spectrum of 15



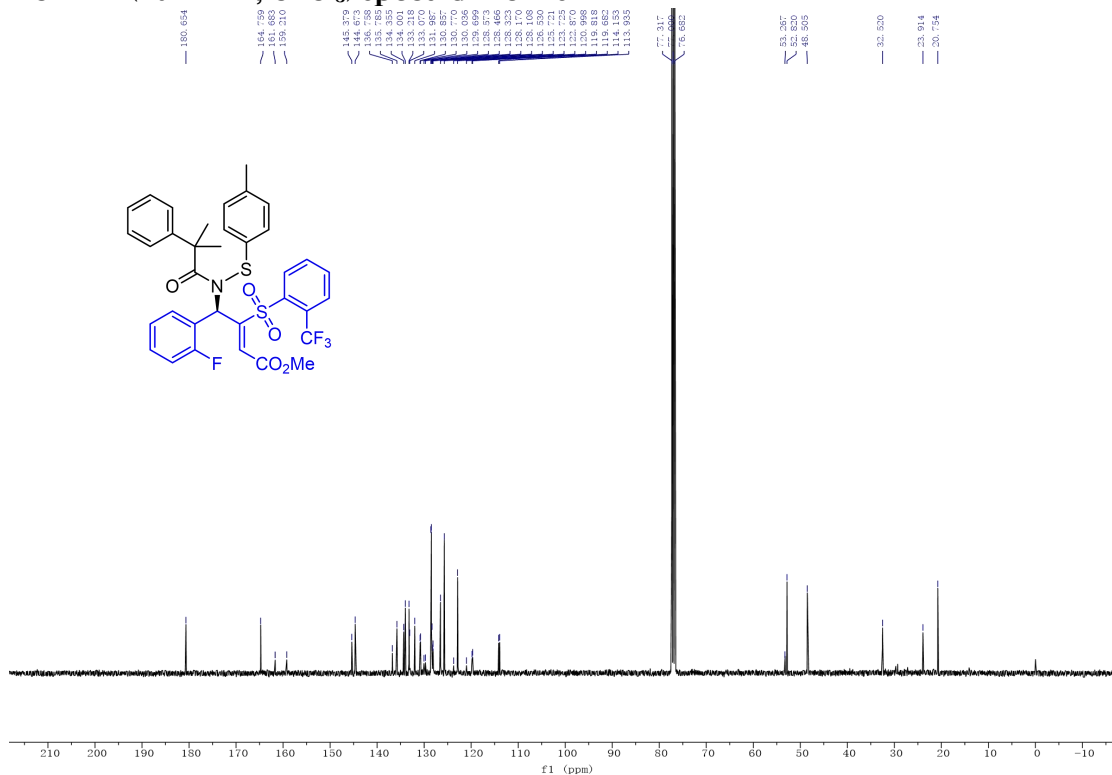
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 15



¹H NMR (400 MHz, CDCl₃) spectrum of 16



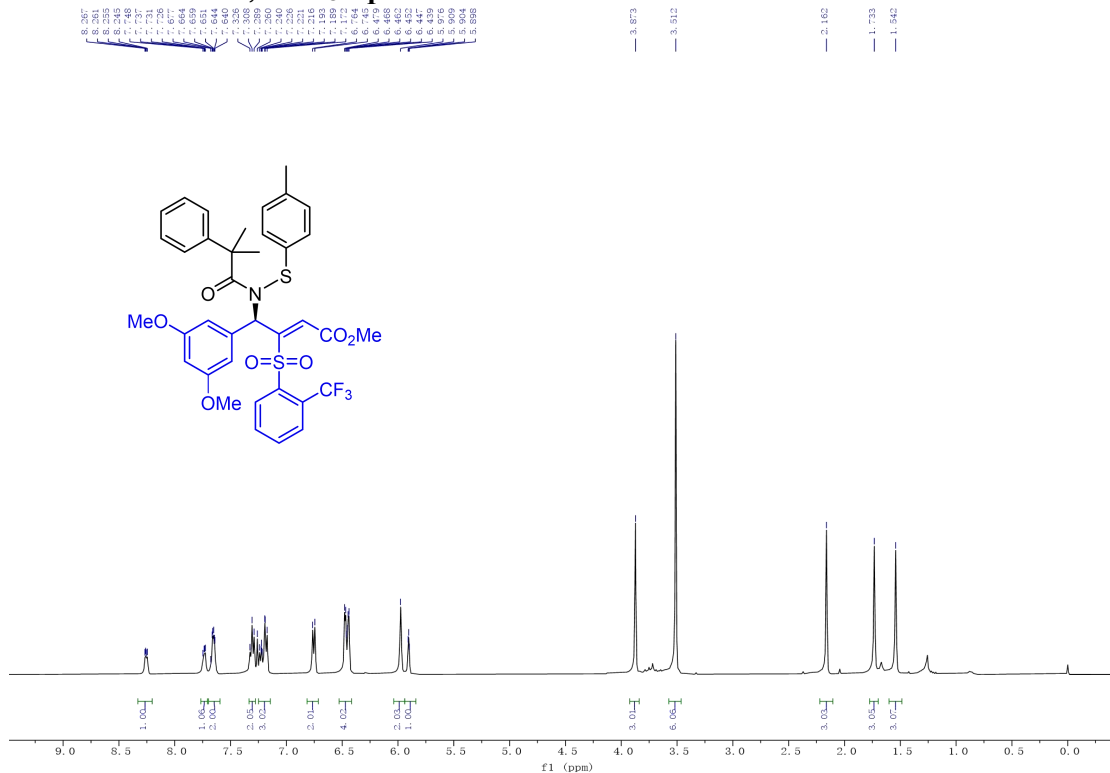
^{13}C NMR (101 MHz, CDCl_3) spectrum of 16



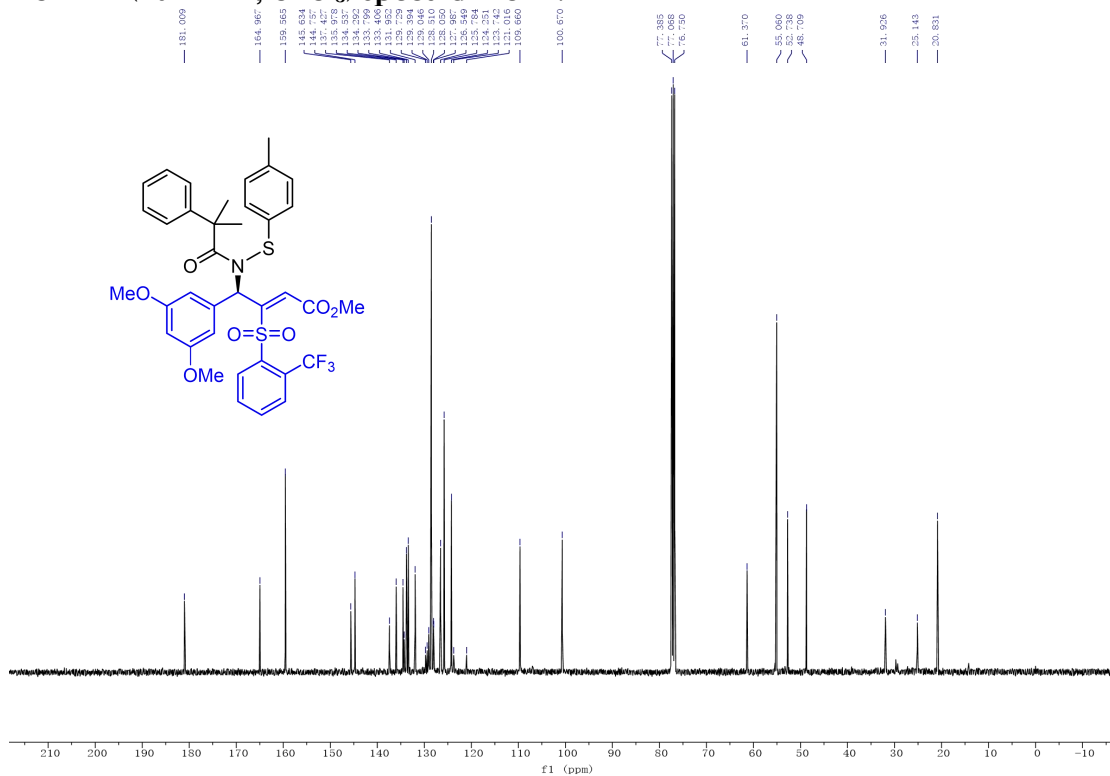
^{19}F NMR (376 MHz, CDCl_3) spectrum of 16



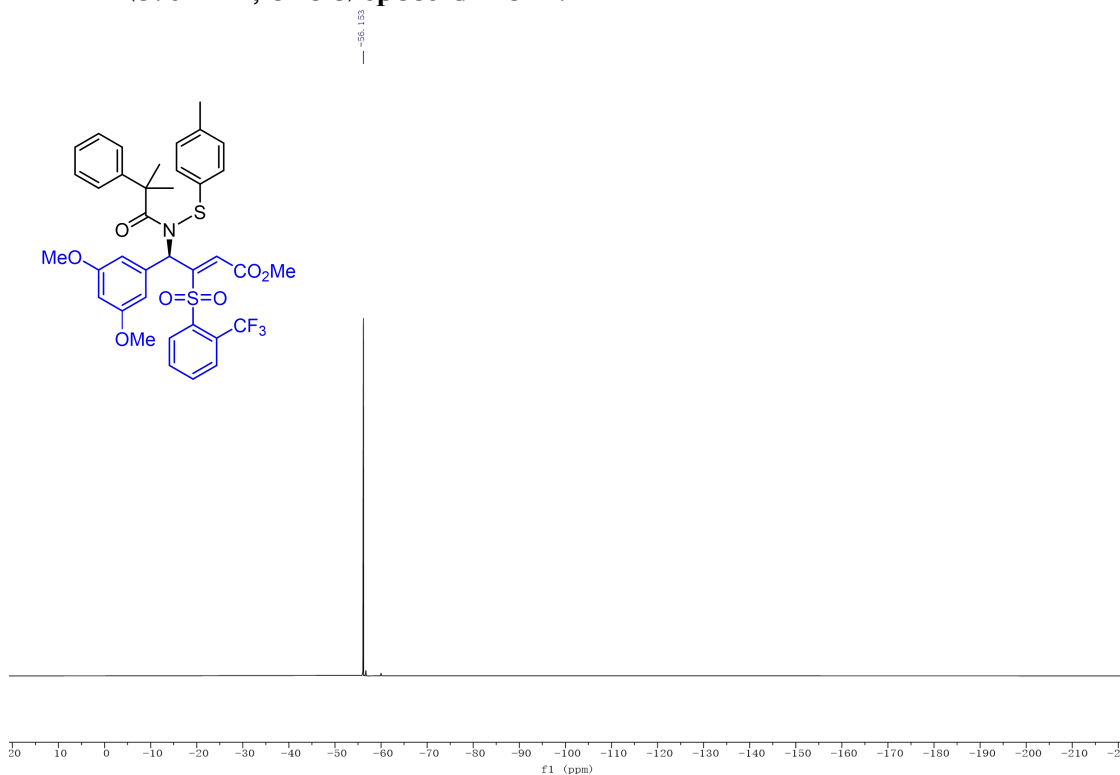
¹H NMR (400 MHz, CDCl₃) spectrum of 17



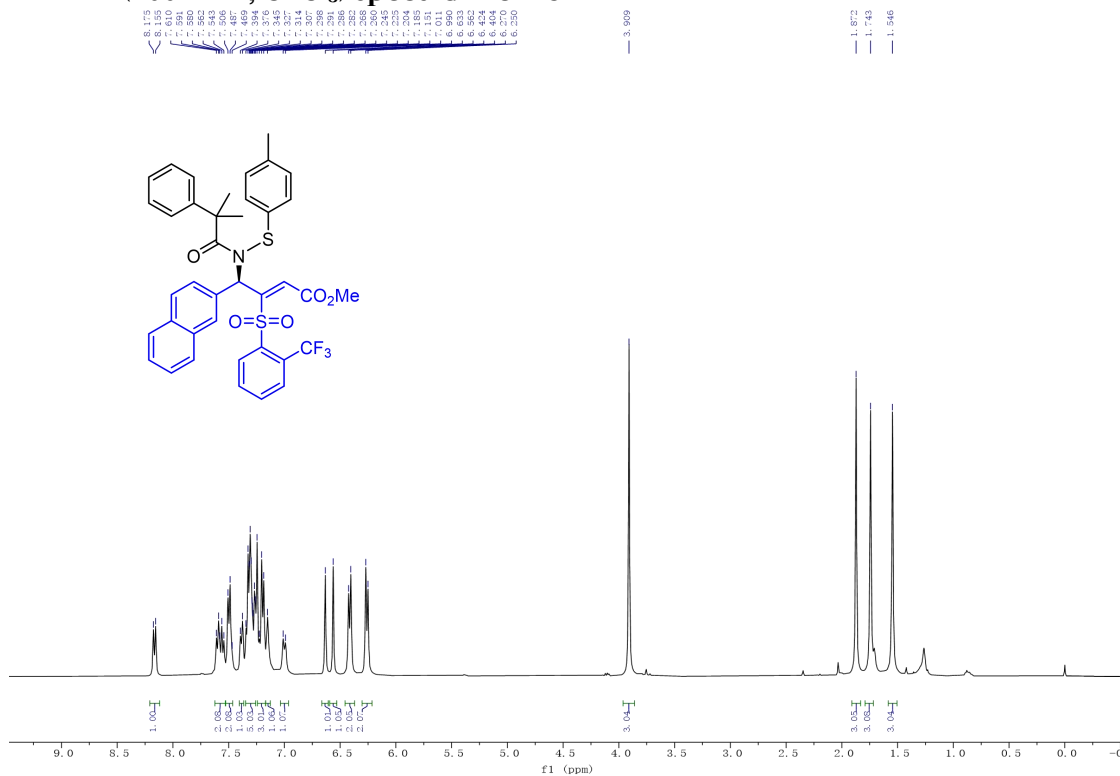
^{13}C NMR (101 MHz, CDCl_3) spectrum of 17



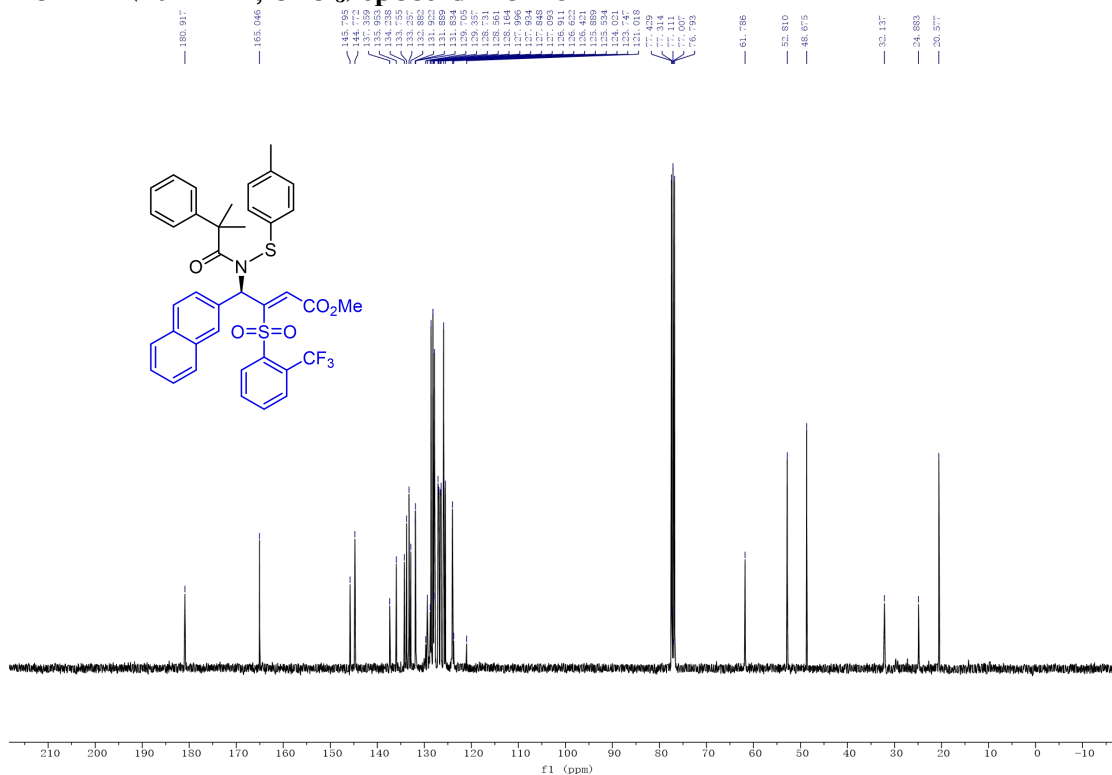
^{19}F NMR (376 MHz, CDCl_3) spectrum of 17



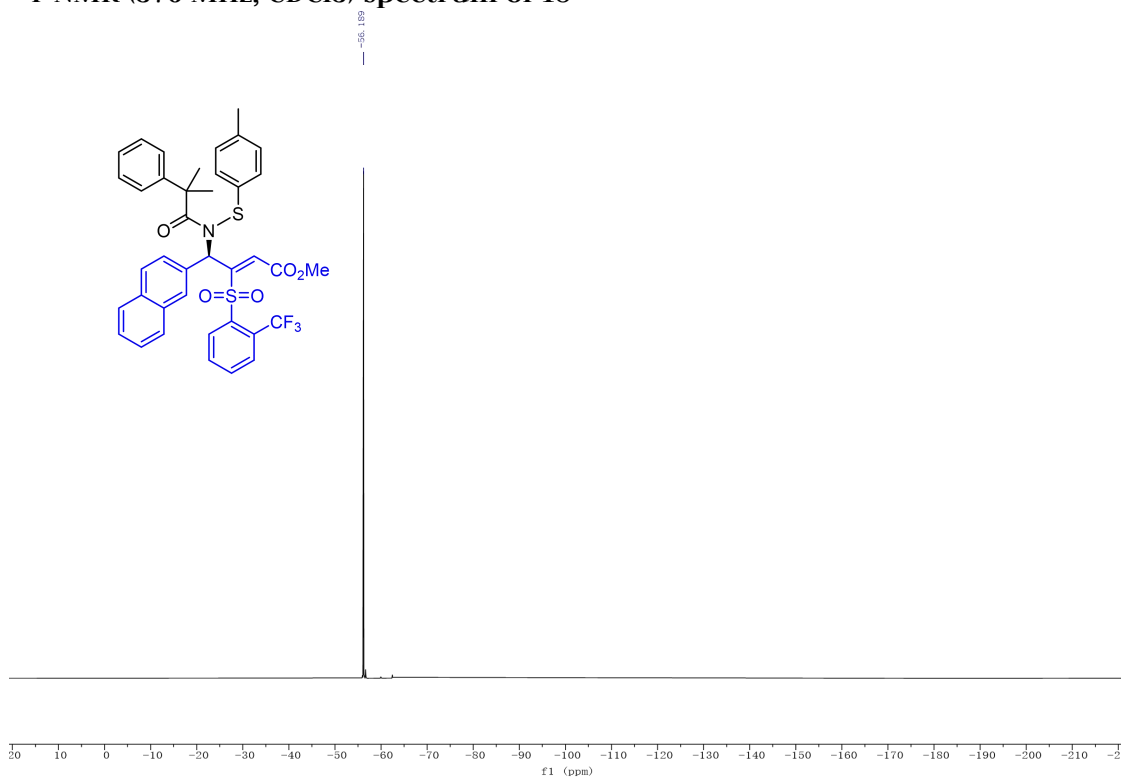
^1H NMR (400 MHz, CDCl_3) spectrum of 18



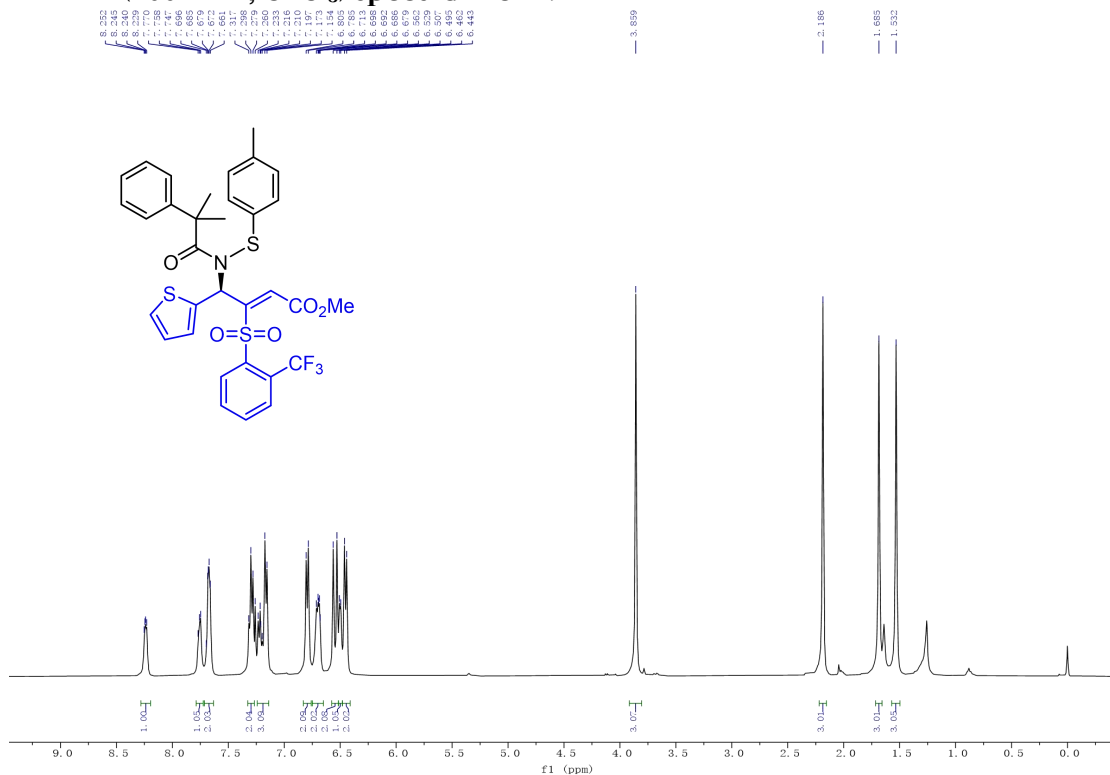
^{13}C NMR (101 MHz, CDCl_3) spectrum of 18



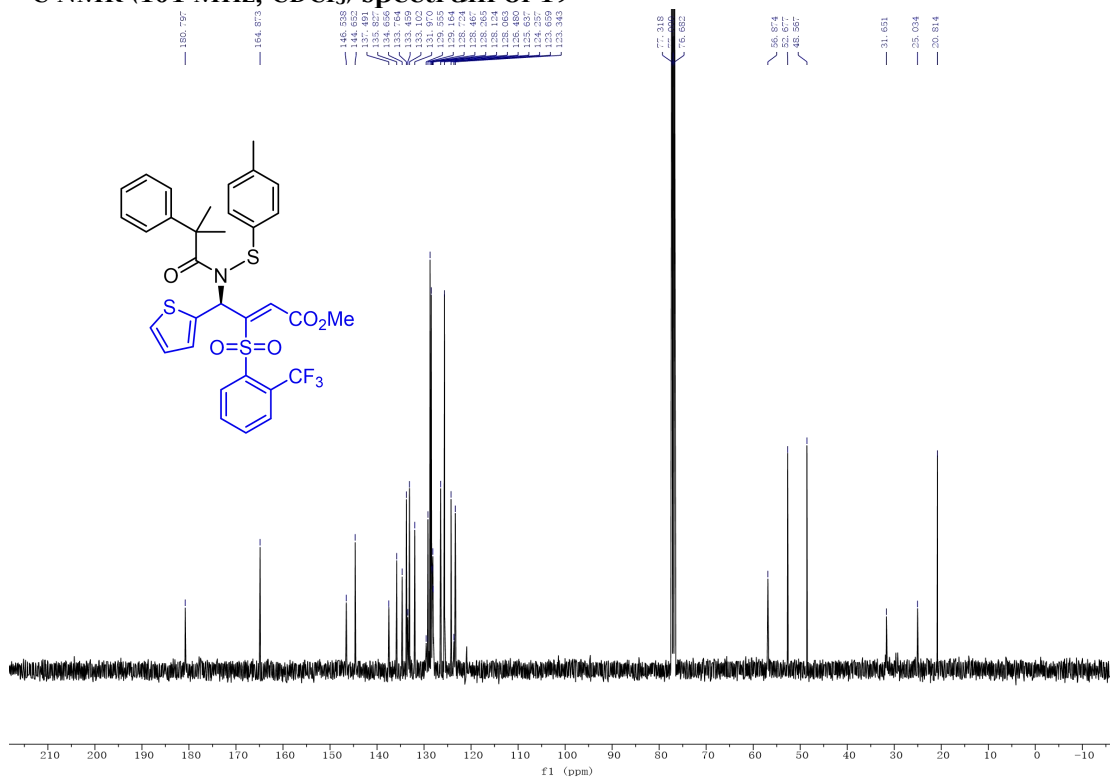
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 18



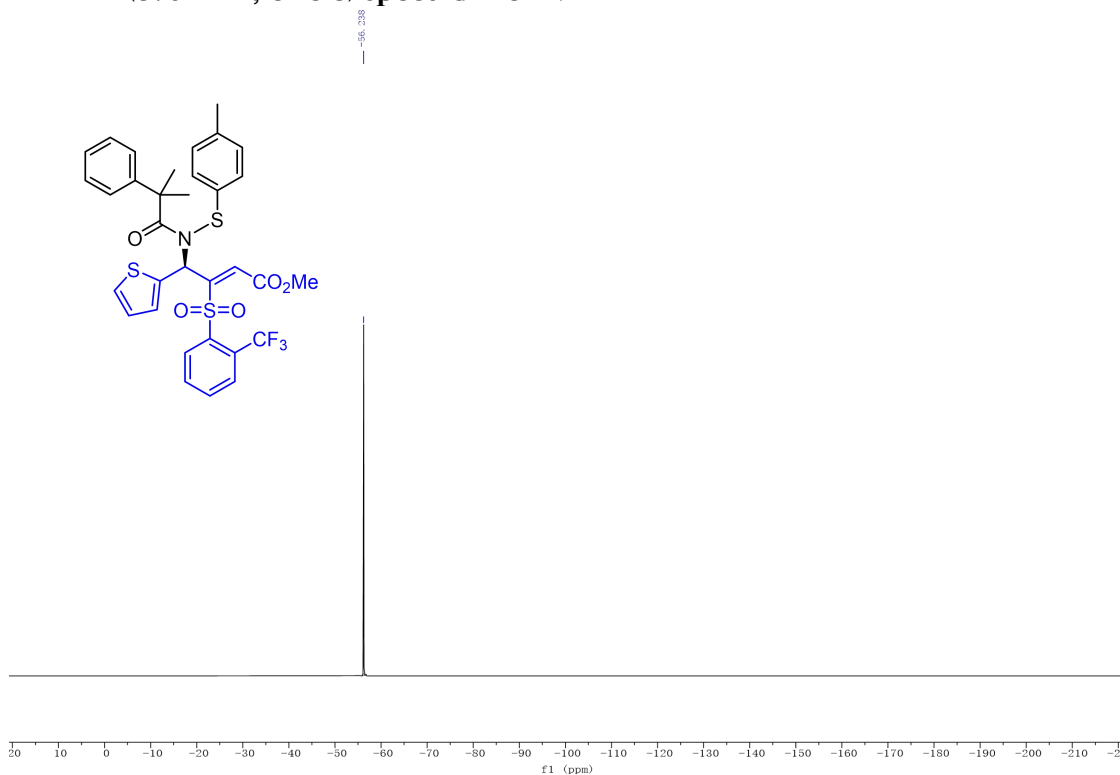
¹H NMR (400 MHz, CDCl₃) spectrum of 19



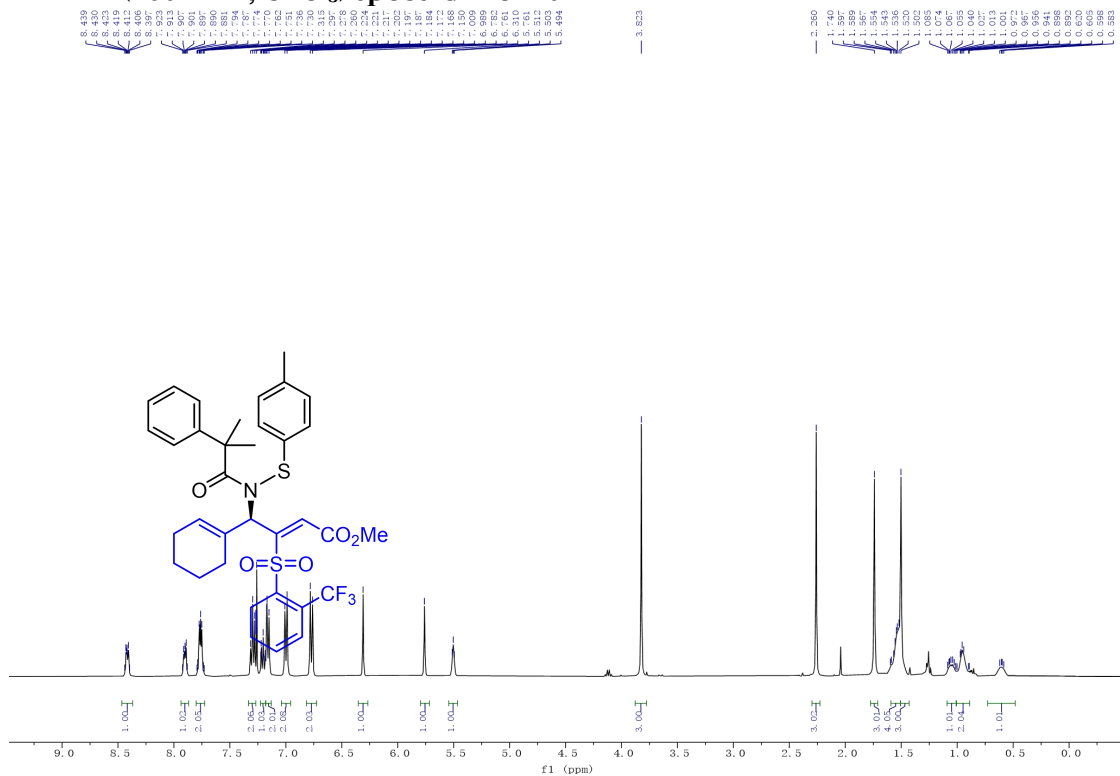
¹³C NMR (101 MHz, CDCl₃) spectrum of 19



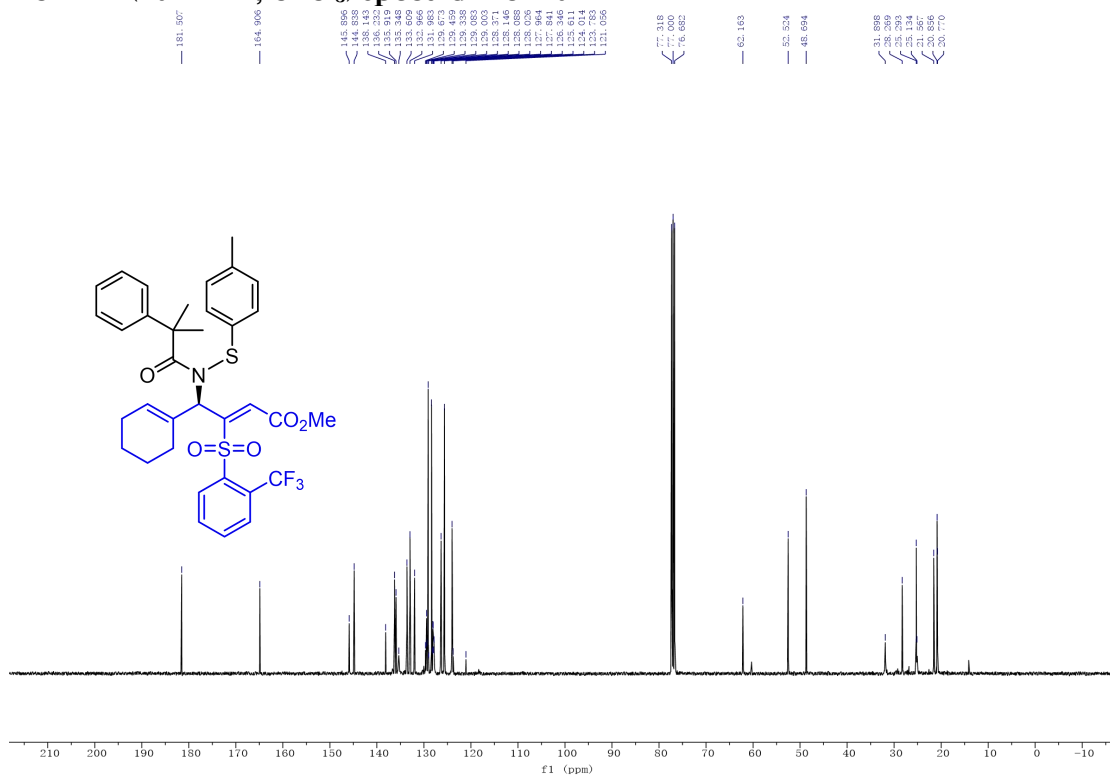
^{19}F NMR (376 MHz, CDCl_3) spectrum of 19



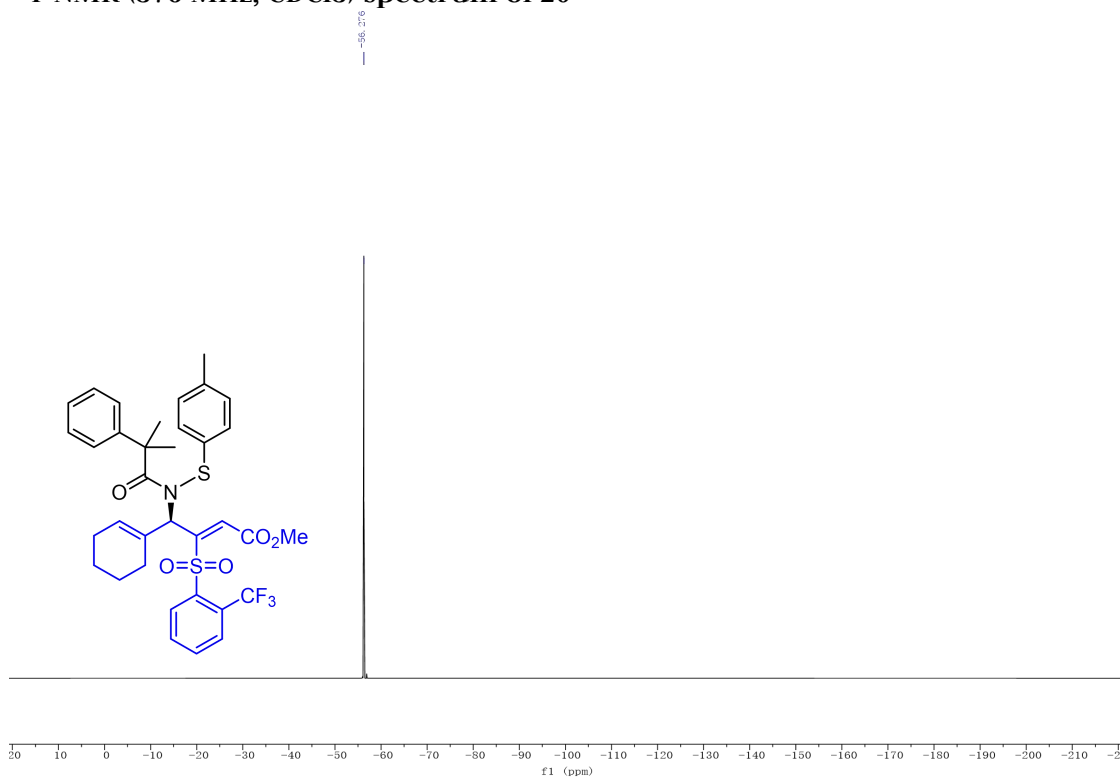
^1H NMR (400 MHz, CDCl_3) spectrum of 20



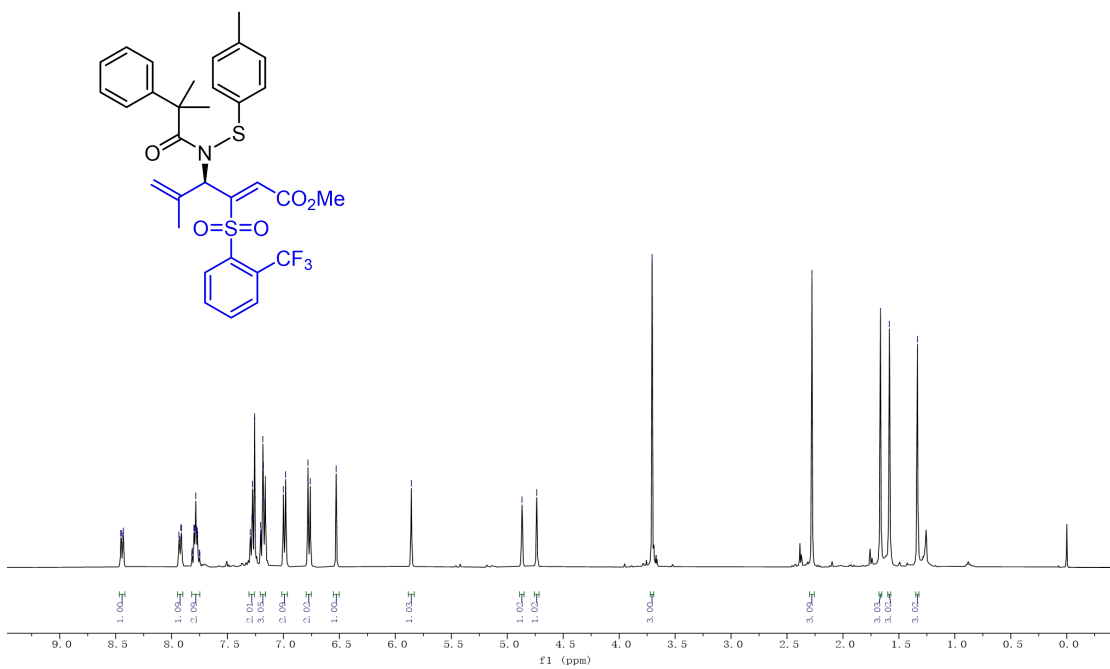
^{13}C NMR (101 MHz, CDCl_3) spectrum of 20



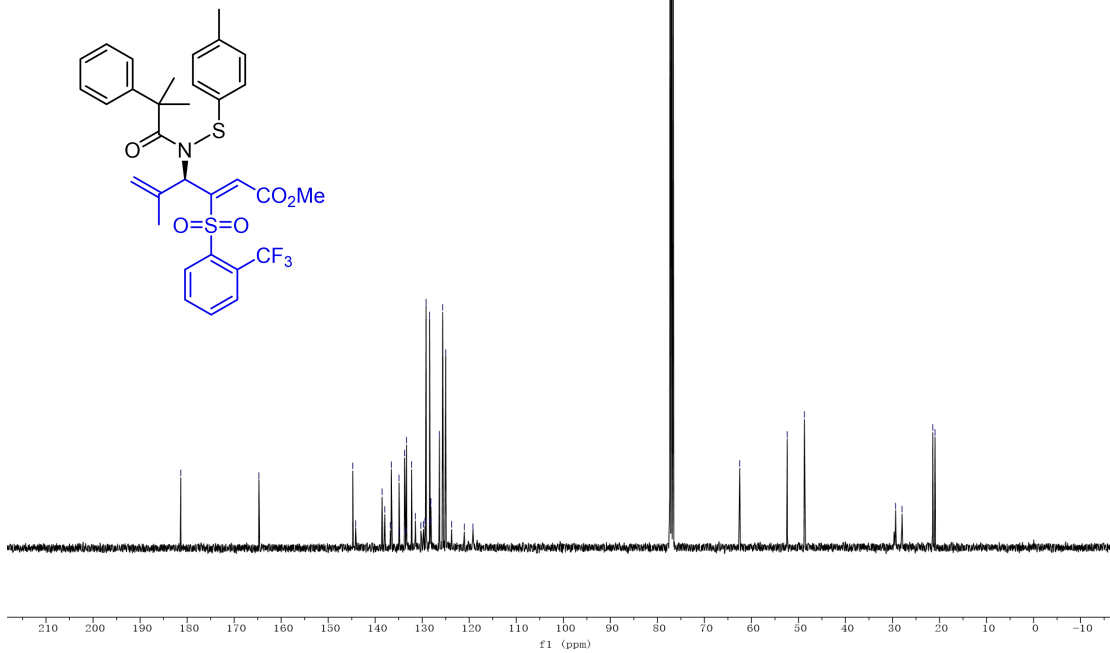
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 20



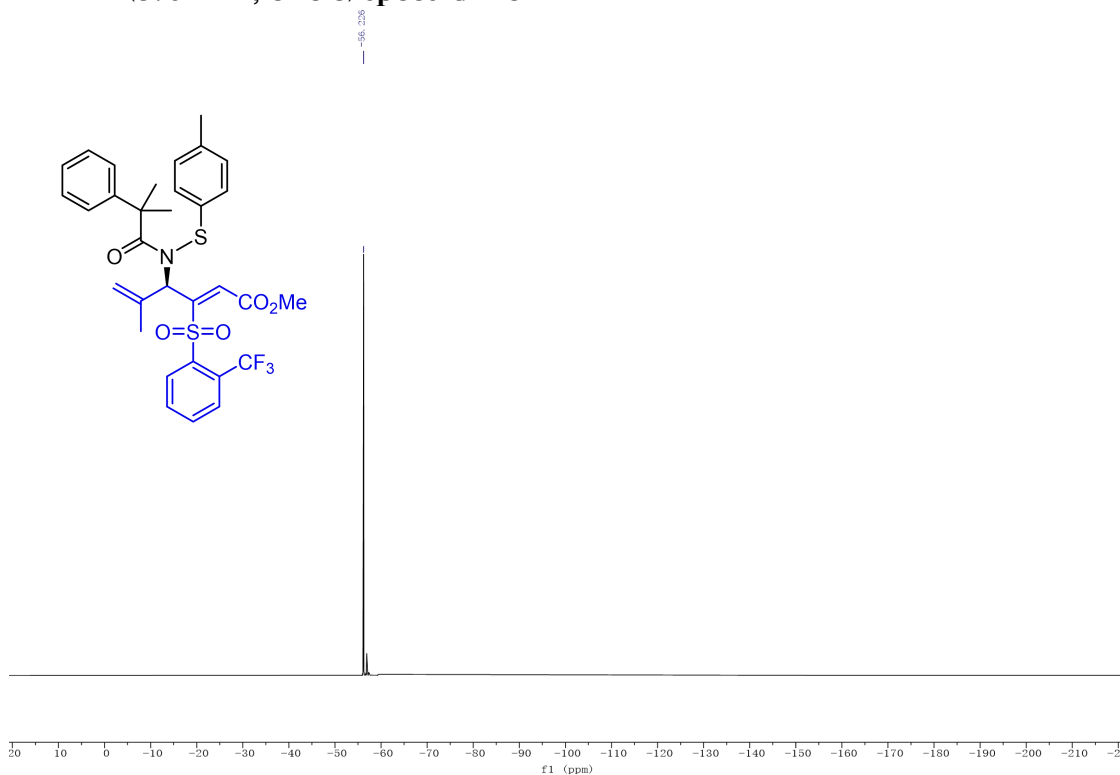
8.444
8.449
8.436
8.431
7.935
7.930
7.917
7.912
7.820
7.815
7.801
7.796
7.789
7.784
7.777
7.771
7.766
7.752
7.747
7.296
7.291
7.281
7.276
7.259
7.207
7.203
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7.180
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7.163
7.001
6.981
6.782
6.761
6.529
5.858



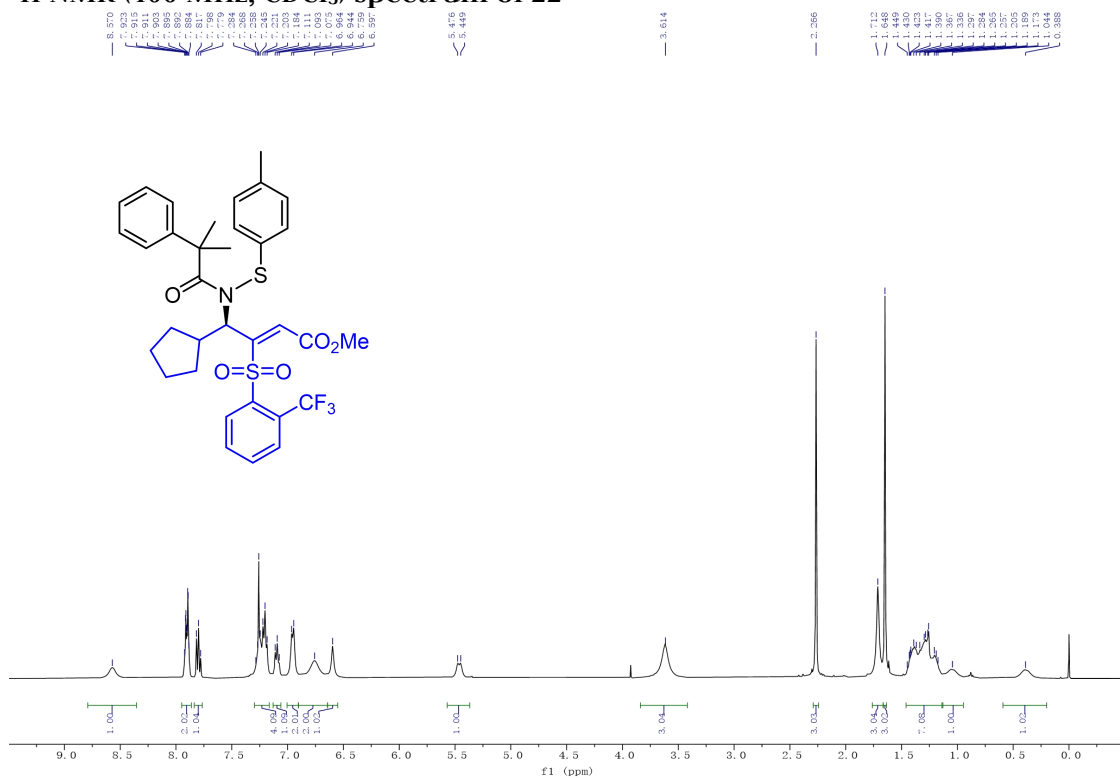
— 181.351 — 164.23 —



¹⁹F NMR (376 MHz, CDCl₃) spectrum of 21



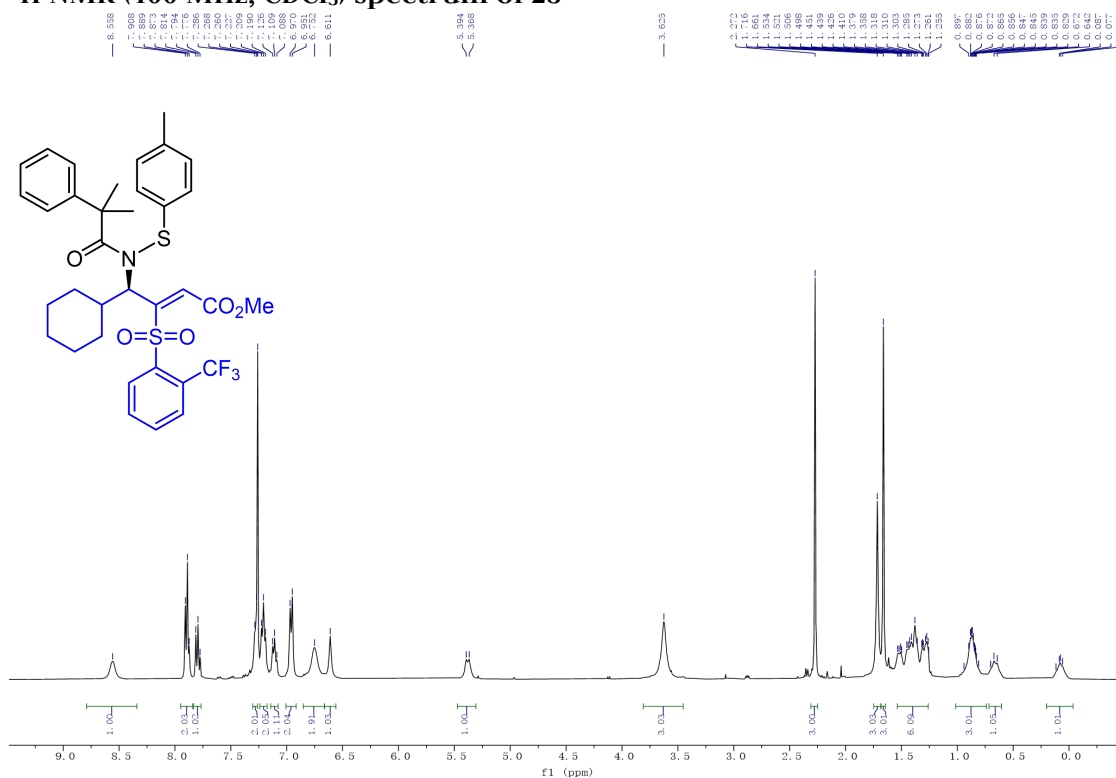
¹H NMR (400 MHz, CDCl₃) spectrum of 22



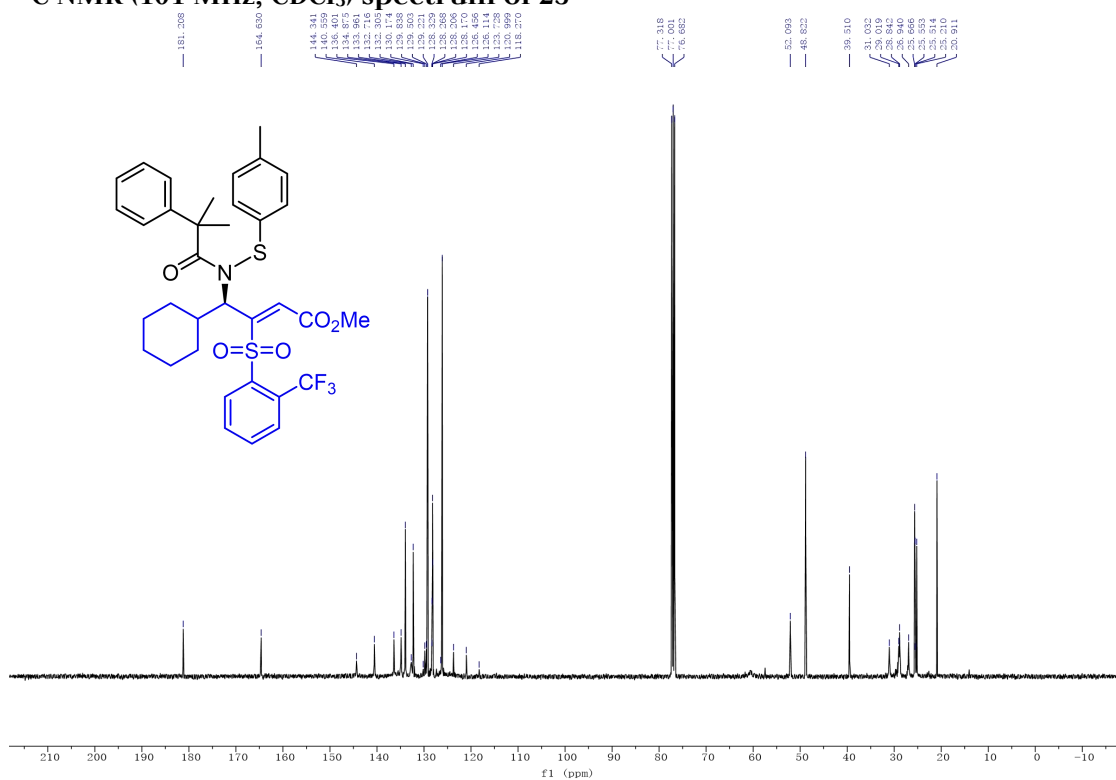
The figure displays the ¹³C NMR spectrum of compound 10. The chemical structure of compound 10 is shown as an overlay on the spectrum. The structure consists of a central chiral carbon atom bonded to a cyclopentyl group, a methoxycarbonyl group (CO₂Me), a trifluoromethylphenylsulfonyl group (SO₂CF₃), and a 4-methyl-2-((2-oxo-2-phenylpropan-2-ylthio)methyl)phenyl group. The spectrum shows peaks corresponding to these various carbon environments. Key peaks are labeled with their chemical shifts in ppm: 181.235, 164.969, 144.567, 136.509, 134.982, 134.882, 133.340, 132.340, 130.191, 129.518, 129.209, 128.909, 128.180, 127.614, 125.935, 121.022, 77.318, 76.053, 52.109, 48.852, 42.767, 30.089, 29.727, 29.522, 28.259, 24.739, 24.533, and 20.922. The x-axis is labeled 'f1 (ppm)' and ranges from -10 to 210.

Chemical structure of compound 10 is shown in the top left corner. The structure features a central carbon atom bonded to a phenyl group, a p-tolyl group, a tert-butyl group, and a nitrogen atom. The nitrogen atom is part of a sulfonamide group, with a sulfonyl group (SO₂) attached to a phenyl ring. The sulfonyl group is also bonded to a cyclopentyl ring and a methoxycarbonyl group (CO₂Me).

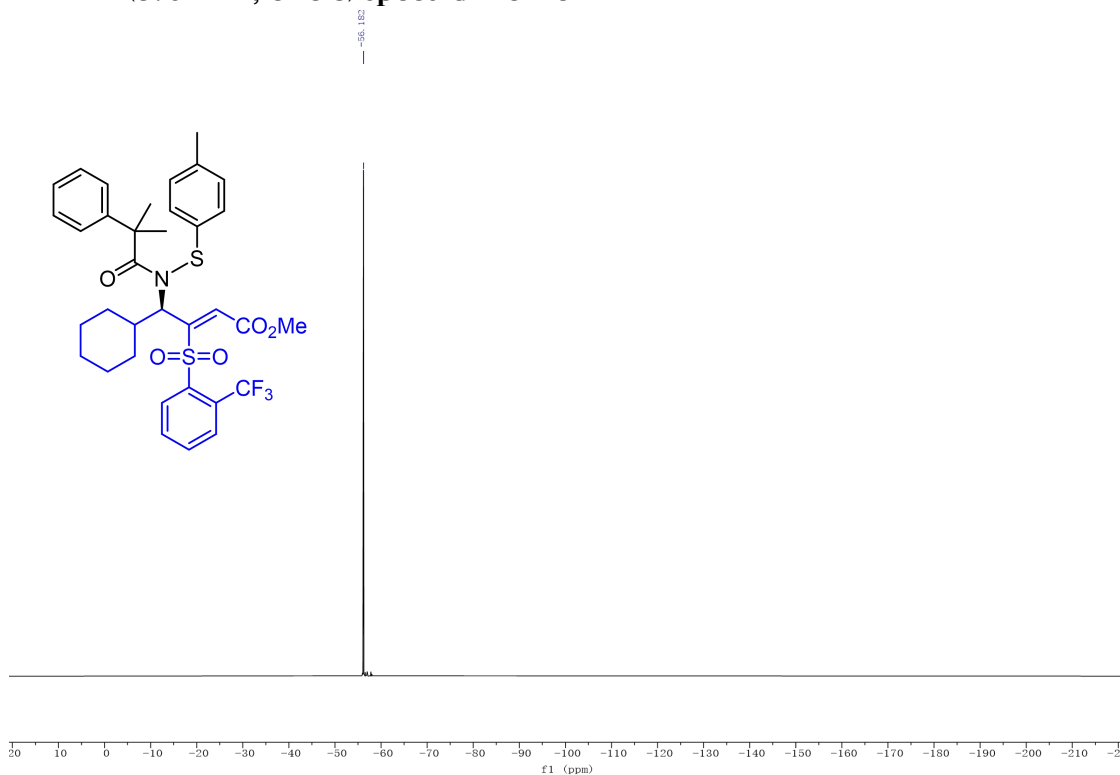
¹H NMR (400 MHz, CDCl₃) spectrum of 23



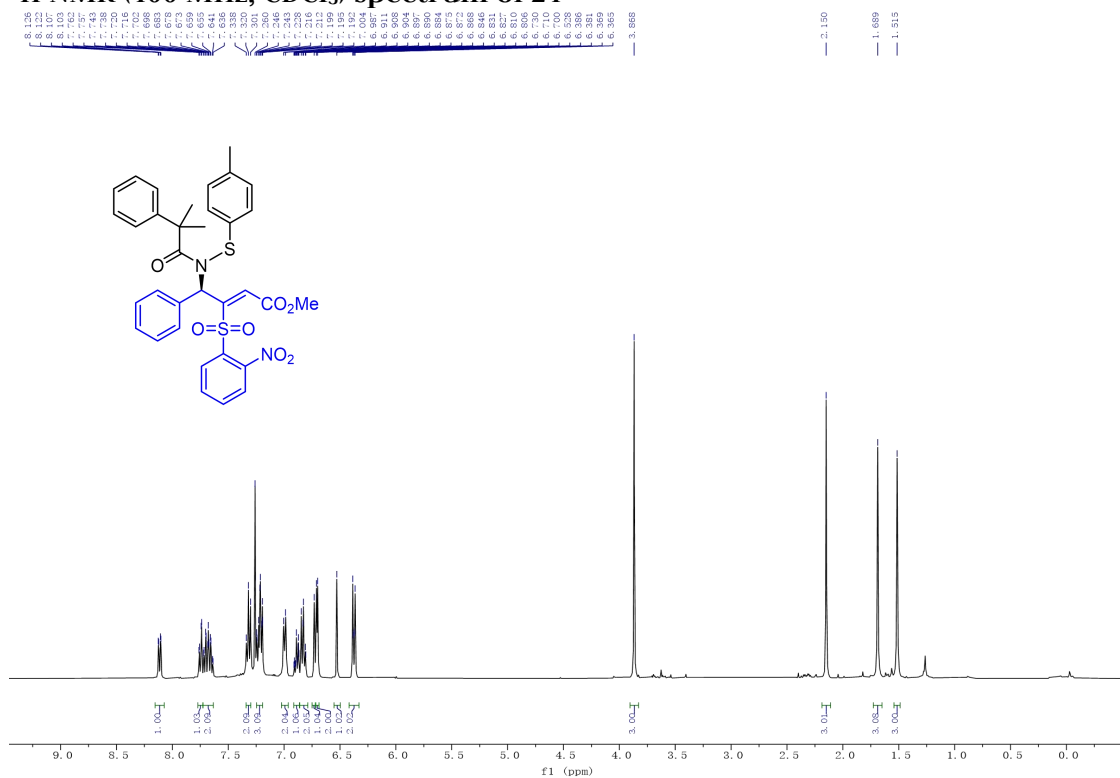
¹³C NMR (101 MHz, CDCl₃) spectrum of 23



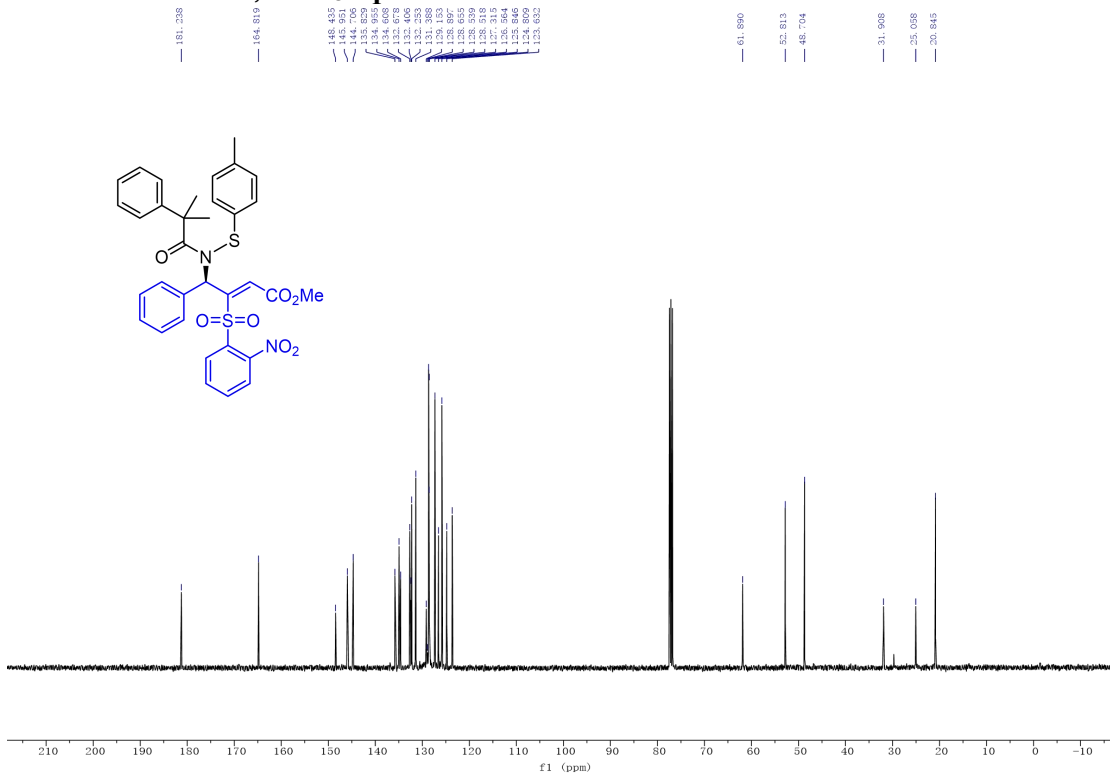
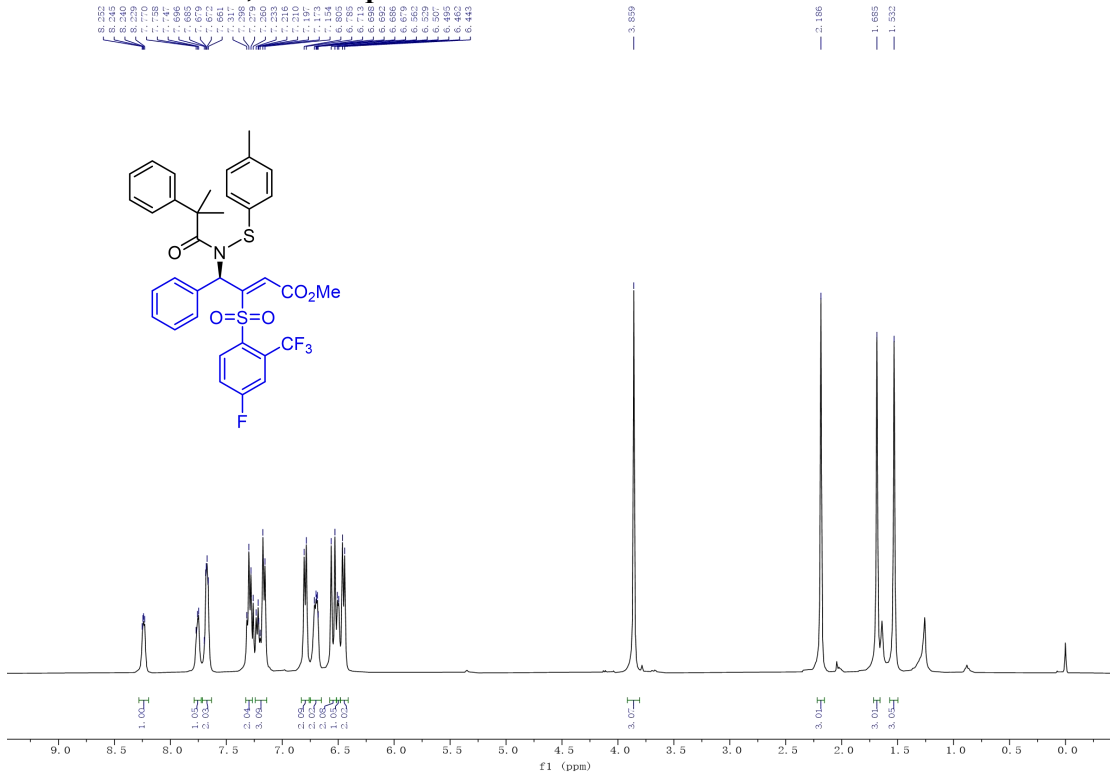
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 23



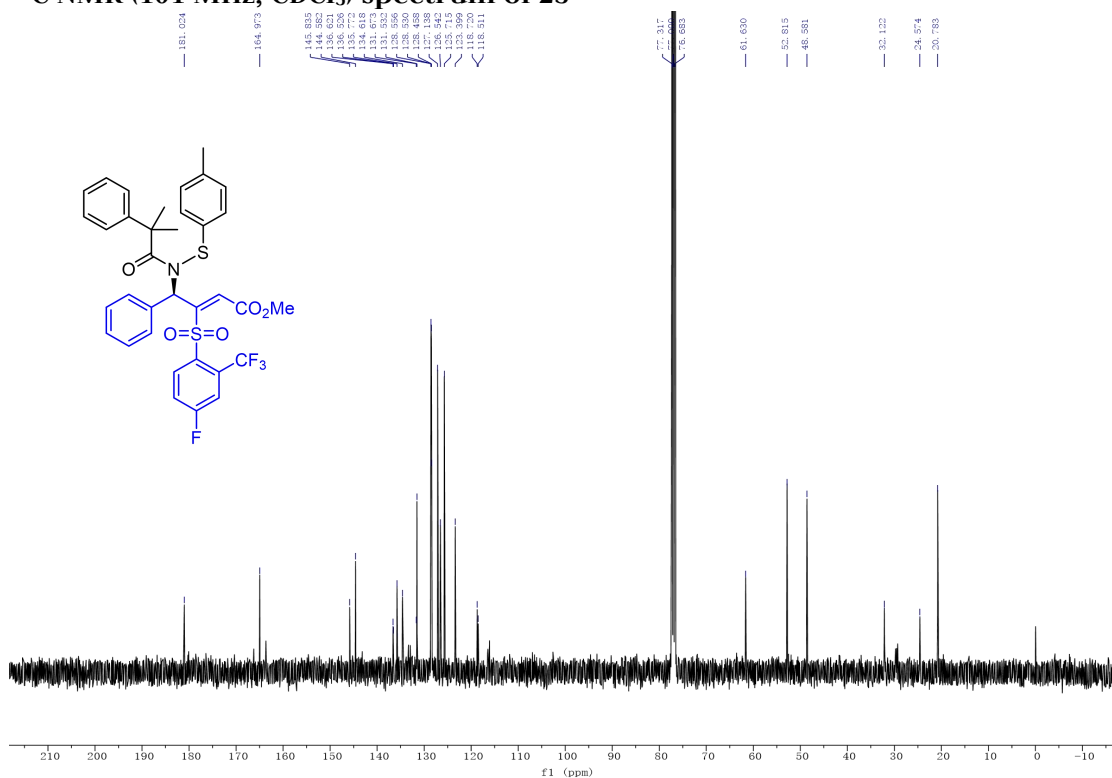
¹H NMR (400 MHz, CDCl₃) spectrum of 24



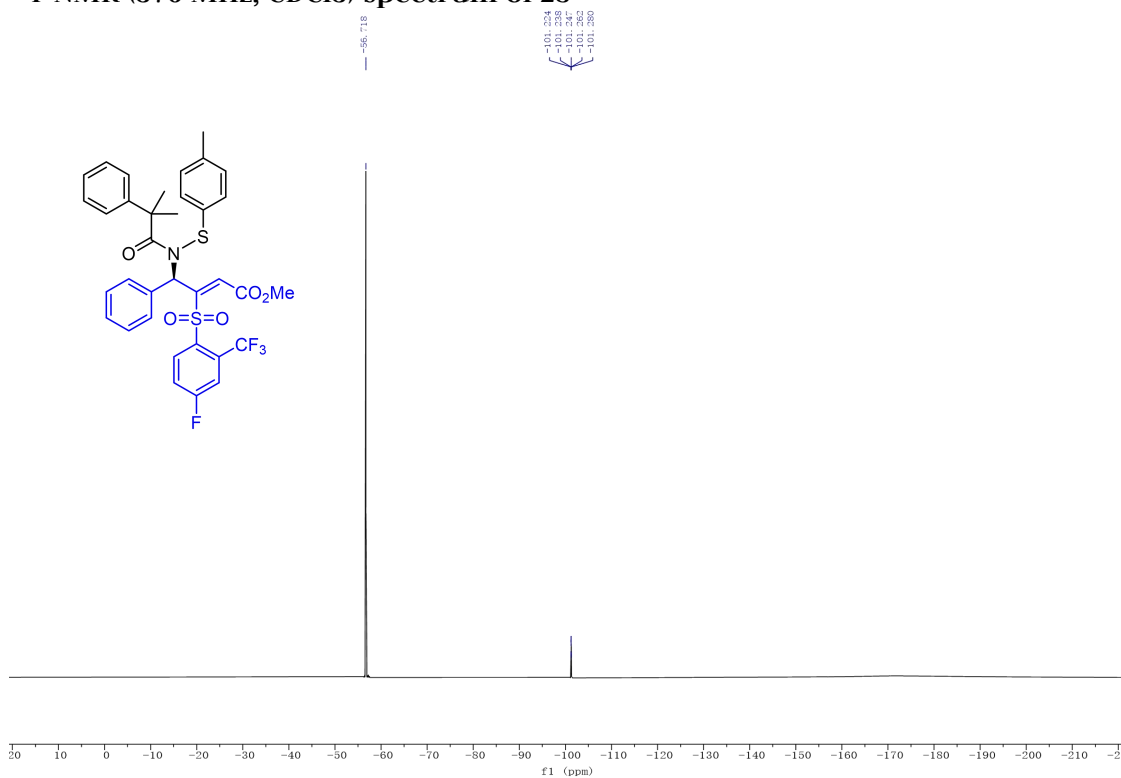
¹³C NMR (101 MHz, CDCl₃) spectrum of 24

¹H NMR (400 MHz, CDCl₃) spectrum of 25

¹³C NMR (101 MHz, CDCl₃) spectrum of 25



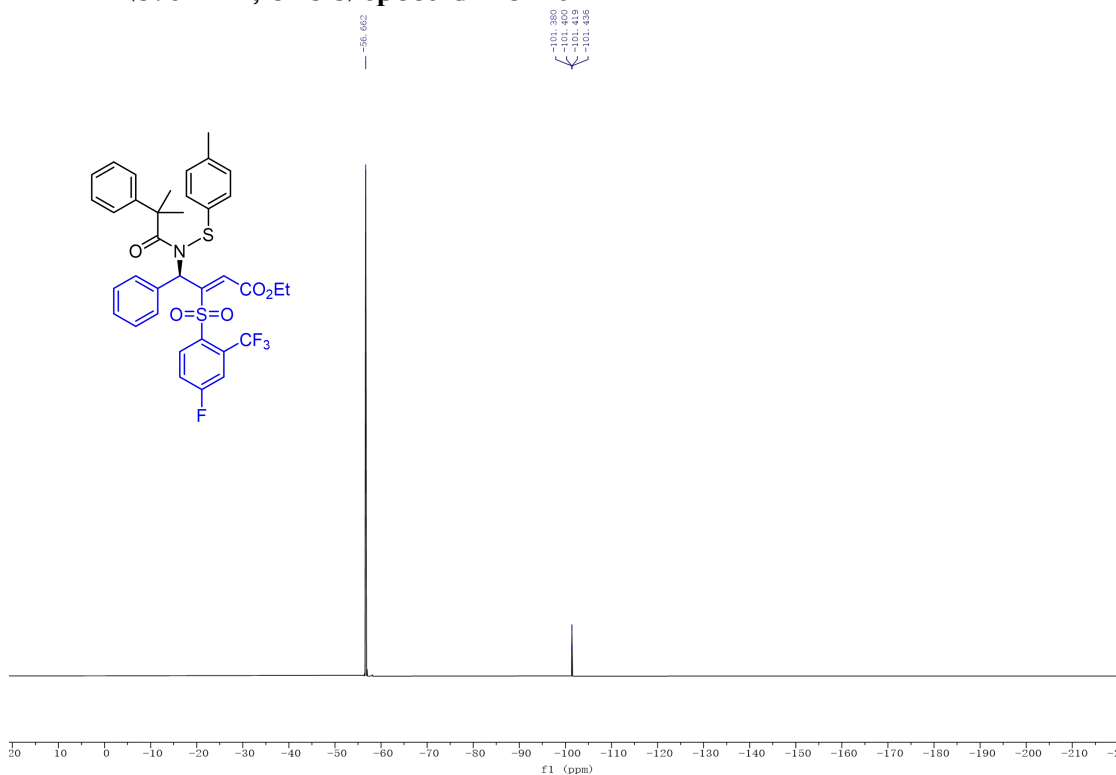
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 25



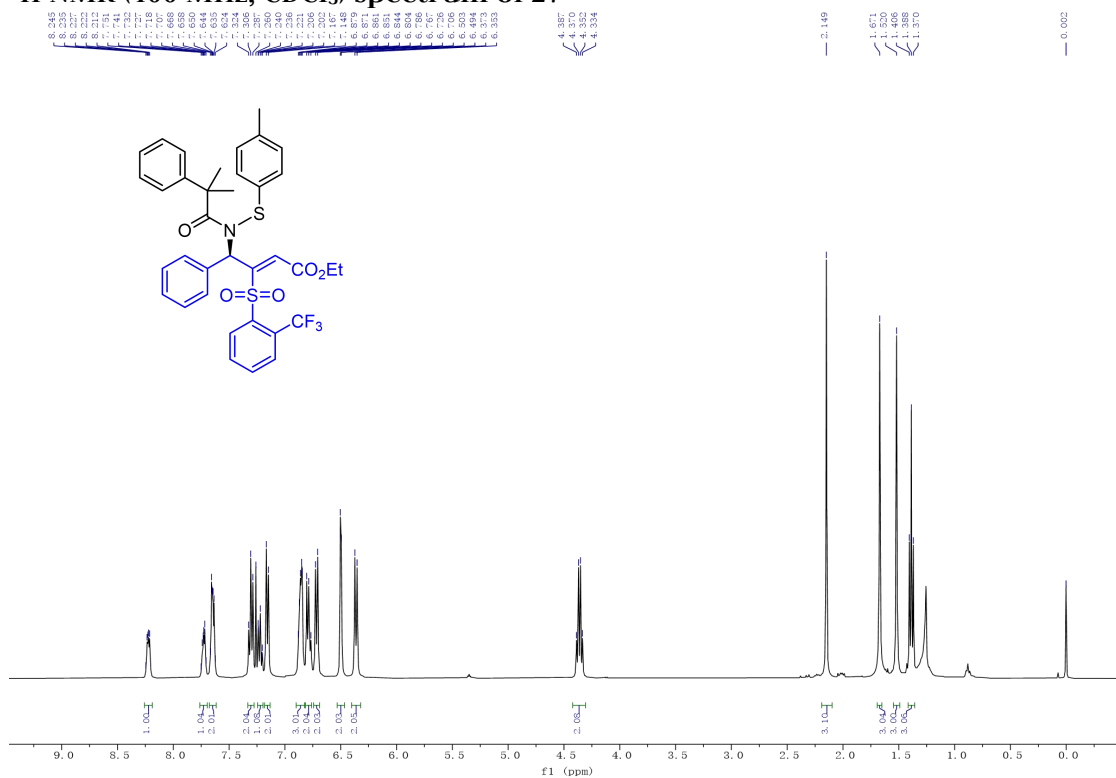
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6	2.62	4	3.99
6	2.53	4	3.62
8	2.39	4	3.54
1	4.11		
1	4.04		
1	3.98		
1	3.82		
1	3.76		
1	3.71		
1	3.68		
1	3.64		
1	3.57		
1	3.50		
1	3.43		
1	3.40		
1	3.35		
1	3.25		
1	3.20		
1	3.07		
1	3.03		
1	2.99		
1	2.95		
1	2.92		
1	2.86		
1	2.83		
1	2.80		
1	2.75		
1	2.70		
1	2.65		
1	2.63		
1	2.60		
1	2.55		
1	2.50		
1	2.40		
1	2.35		
1	2.30		
1	2.20		
1	2.07		
1	2.03		
1	1.99		
1	1.95		
1	1.92		
1	1.89		
1	1.86		
1	1.84		
1	1.80		
1	1.72		
1	1.67		
1	1.65		
1	1.63		
1	1.61		
1	1.59		
1	1.58		
1	1.56		
1	1.54		
1	1.52		
1	1.50		
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1	1.34		
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1	1.28		
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1	1.24		
1	1.22		
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1	1.18		
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1	1.14		
1	1.12		
1	1.10		
1	1.08		
1	1.06		
1	1.04		
1	1.02		
1	1.00		
1	0.98		
1	0.96		
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1	0.92		
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1	0.68		
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1	0.64		
1	0.62		
1	0.60		
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1	0.56		
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1	0.52		
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1	0.42		
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1	0.36		
1	0.34		
1	0.32		
1	0.30		
1	0.28		
1	0.26		
1	0.24		
1	0.22		
1	0.20		
1	0.18		
1	0.16		
1	0.14		
1	0.12		
1	0.10		
1	0.08		
1	0.06		
1	0.04		
1	0.02		
1	0.00		

151.060	145.340
	144.702
	136.646
	136.555
	135.778
	134.706
	133.581
	131.833
	131.540
	129.023
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	128.529
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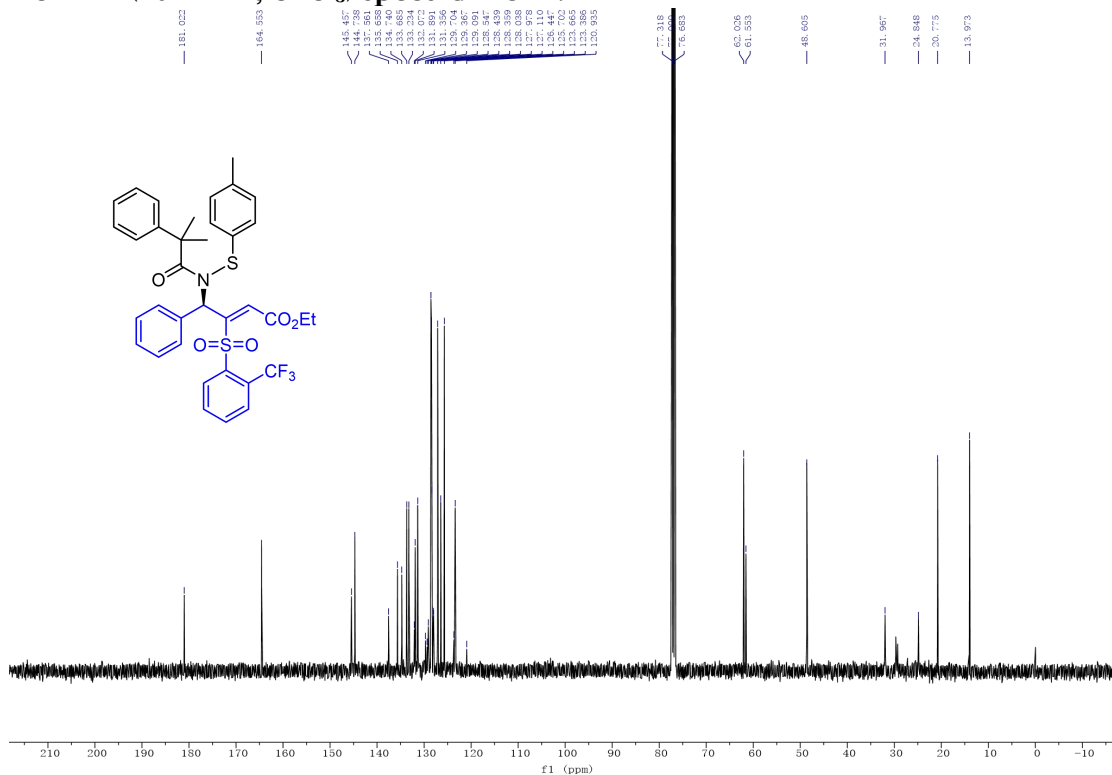
^{19}F NMR (376 MHz, CDCl_3) spectrum of 26



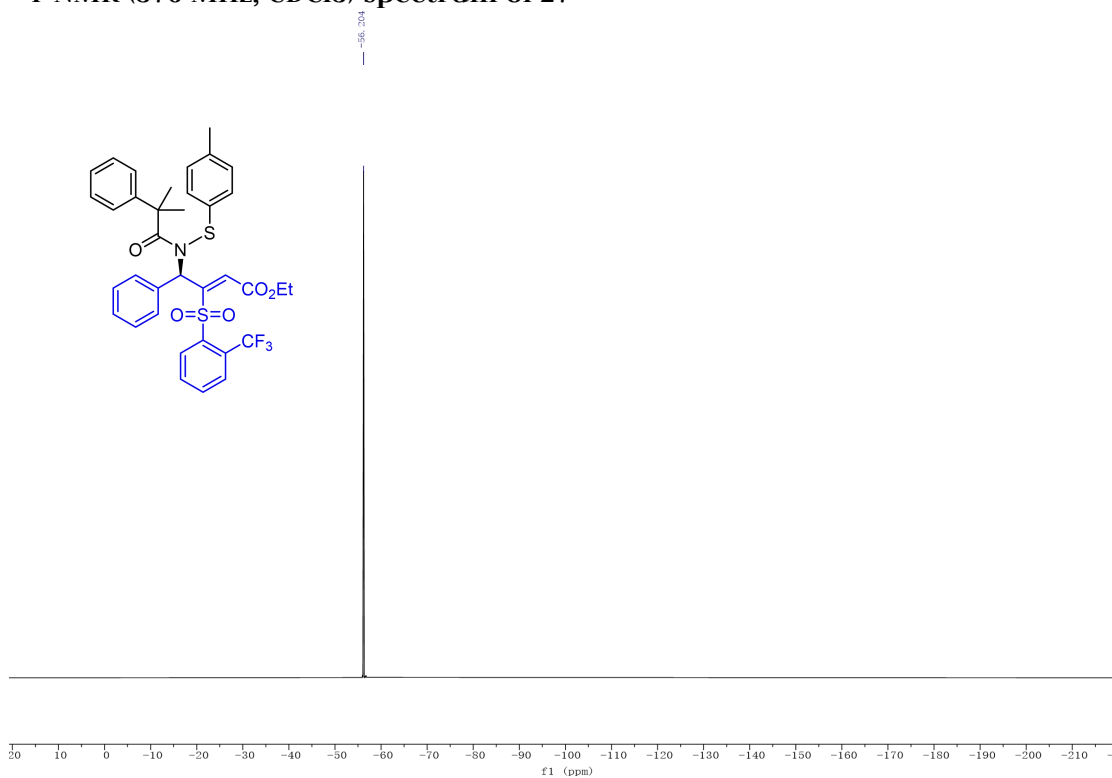
^1H NMR (400 MHz, CDCl_3) spectrum of 27



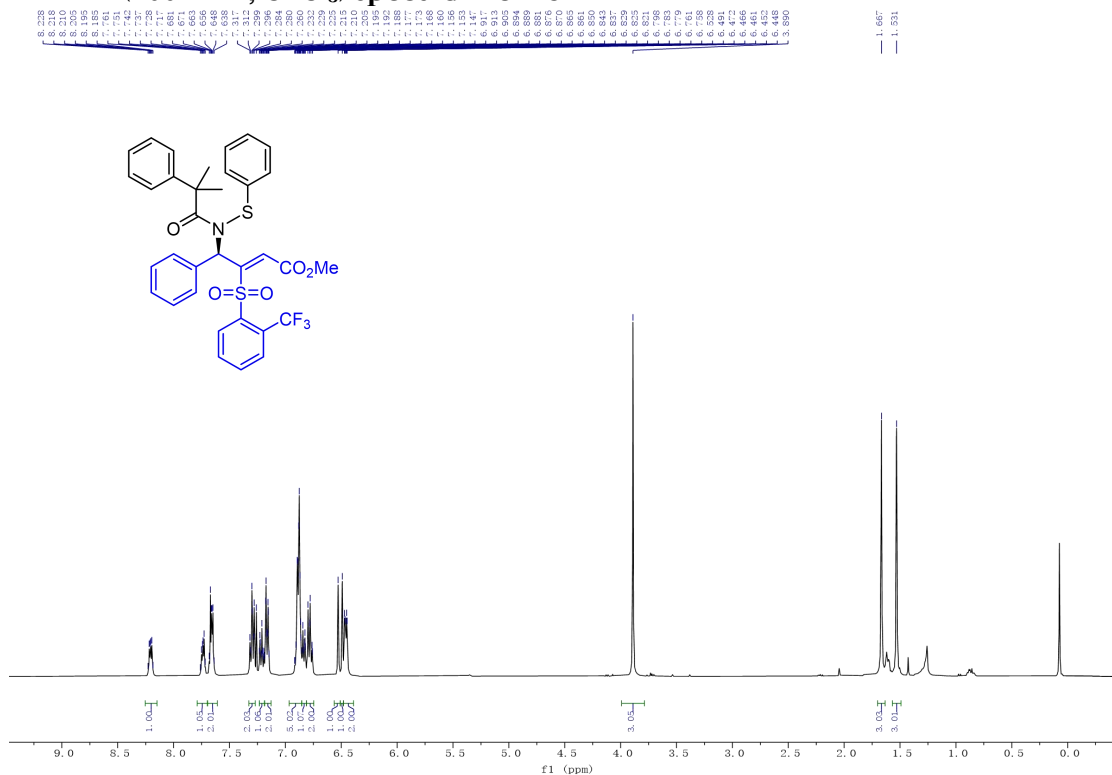
¹³C NMR (101 MHz, CDCl₃) spectrum of 27



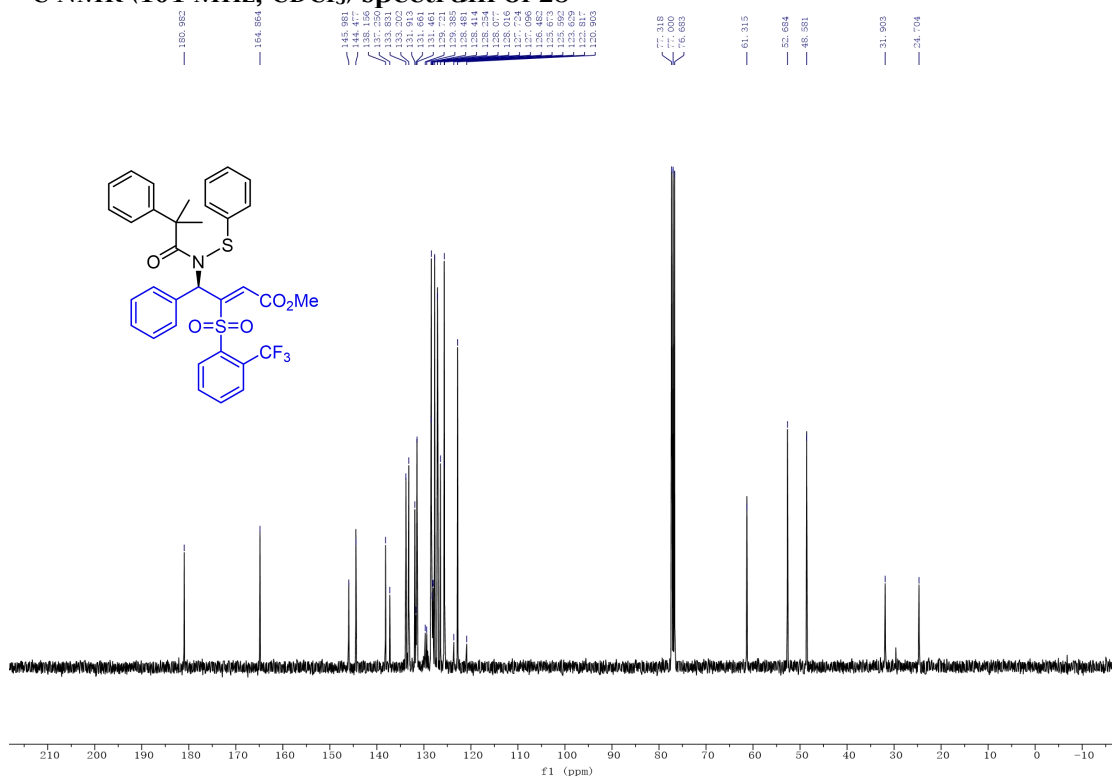
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 27



¹H NMR (400 MHz, CDCl₃) spectrum of 28



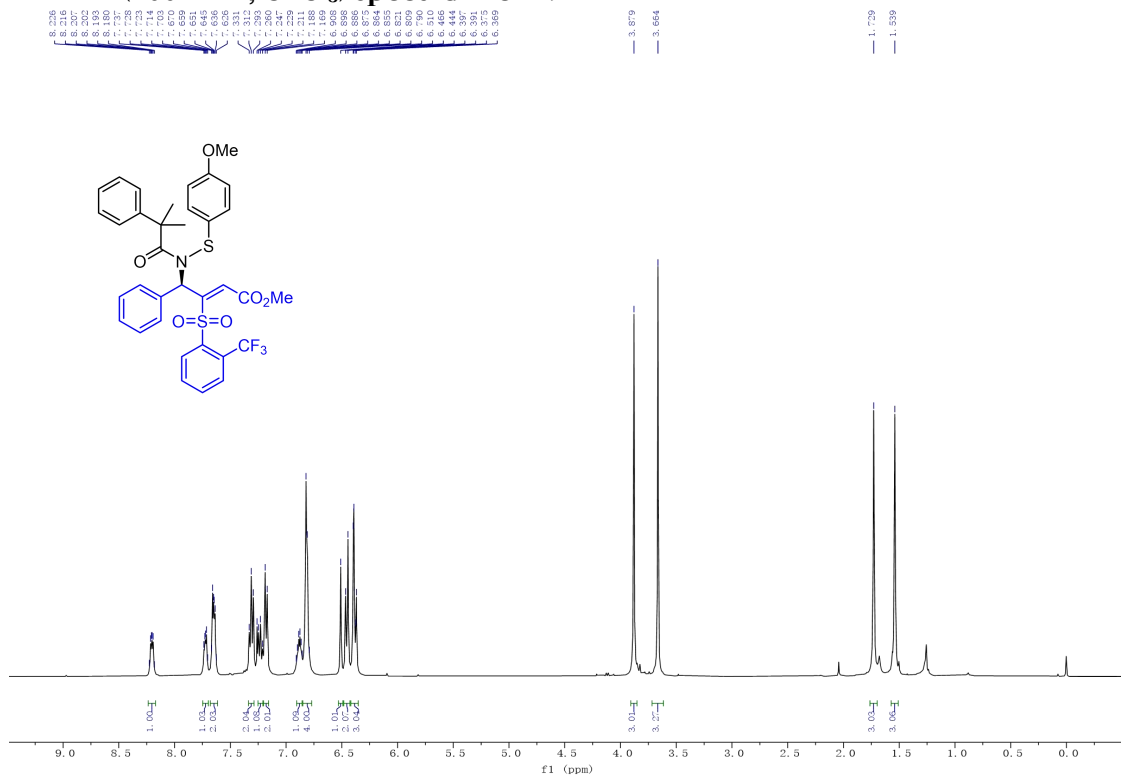
¹³C NMR (101 MHz, CDCl₃) spectrum of 28



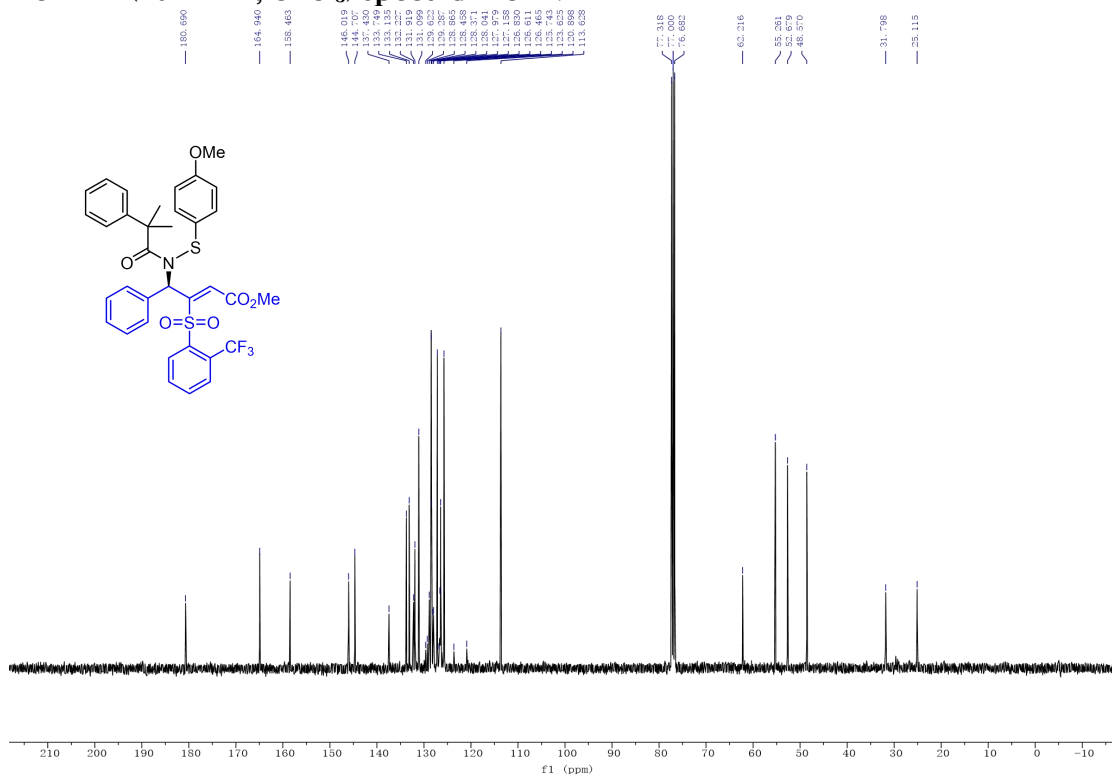
^{19}F NMR (376 MHz, CDCl_3) spectrum of 28



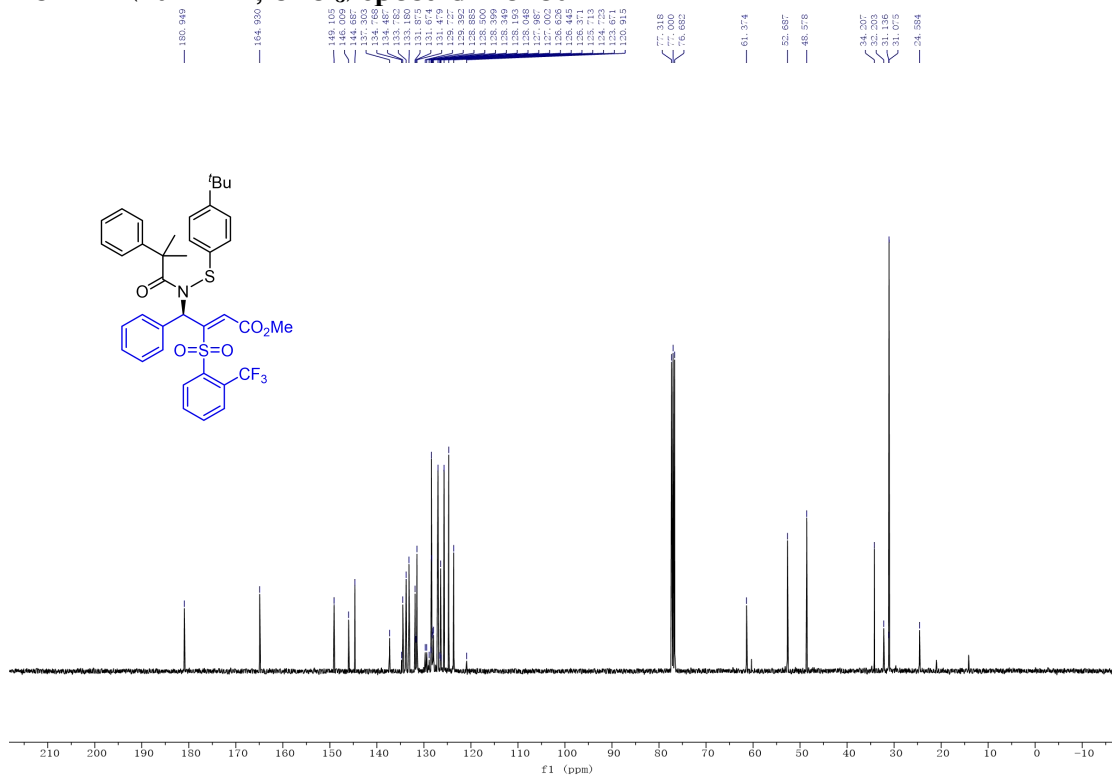
^1H NMR (400 MHz, CDCl_3) spectrum of 29



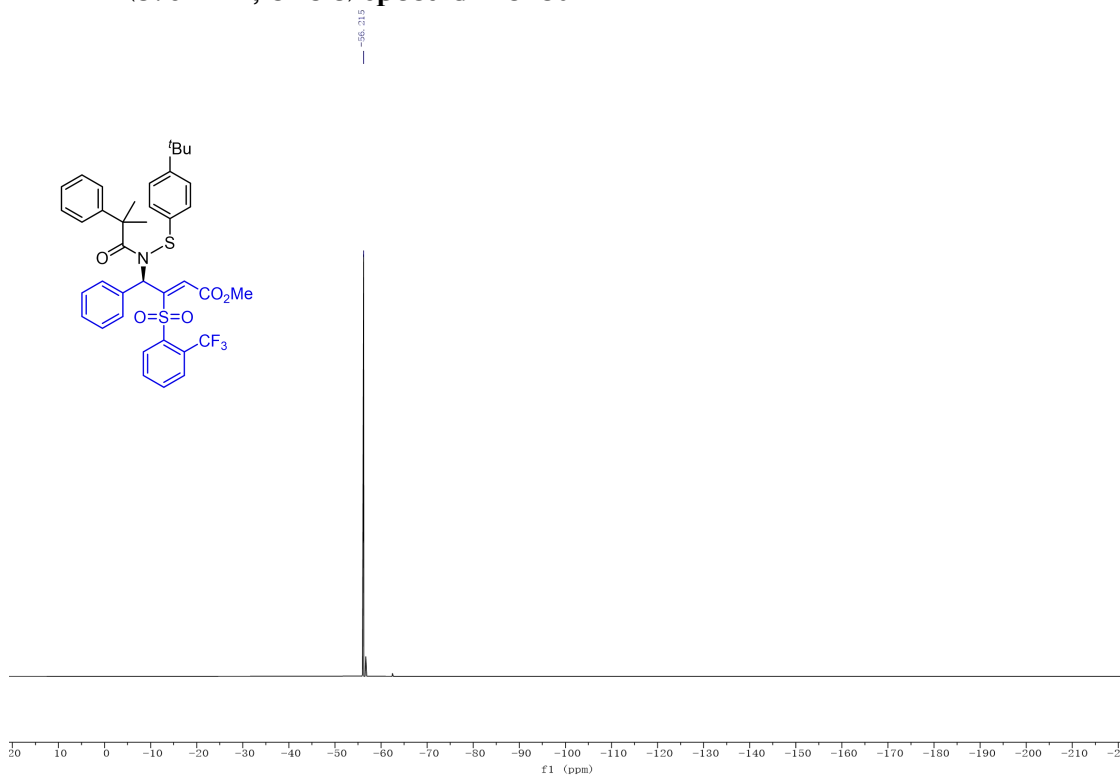
¹³C NMR (101 MHz, CDCl₃) spectrum of 29



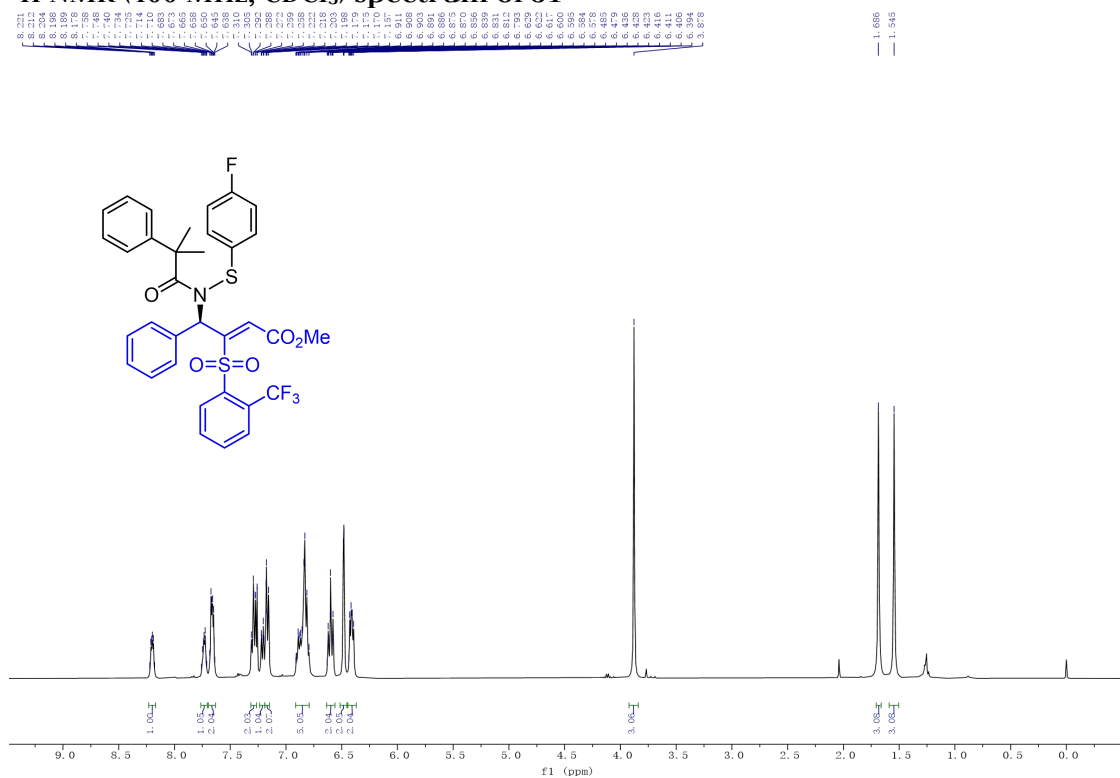
8.215	8.216	8.217	8.218	8.219	8.220	8.221	8.222	8.223	8.224	8.225	8.226	8.227	8.228	8.229	8.230	8.231	8.232	8.233	8.234	8.235	8.236	8.237	8.238	8.239	8.240	8.241	8.242	8.243	8.244	8.245	8.246	8.247	8.248	8.249	8.250	8.251	8.252	8.253	8.254	8.255	8.256	8.257	8.258	8.259	8.260	8.261	8.262	8.263	8.264	8.265	8.266	8.267	8.268	8.269	8.270	8.271	8.272	8.273	8.274	8.275	8.276	8.277	8.278	8.279	8.280	8.281	8.282	8.283	8.284	8.285	8.286	8.287	8.288	8.289	8.290	8.291	8.292	8.293	8.294	8.295	8.296	8.297	8.298	8.299	8.300	8.301	8.302	8.303	8.304	8.305	8.306	8.307	8.308	8.309	8.310	8.311	8.312	8.313	8.314	8.315	8.316	8.317	8.318	8.319	8.320	8.321	8.322	8.323	8.324	8.325	8.326	8.327	8.328	8.329	8.330	8.331	8.332	8.333	8.334	8.335	8.336	8.337	8.338	8.339	8.340	8.341	8.342	8.343	8.344	8.345	8.346	8.347	8.348	8.349	8.350	8.351	8.352	8.353	8.354	8.355	8.356	8.357	8.358	8.359	8.360	8.361	8.362	8.363	8.364	8.365	8.366	8.367	8.368	8.369	8.370	8.371	8.372	8.373	8.374	8.375	8.376	8.377	8.378	8.379	8.380	8.381	8.382	8.383	8.384	8.385	8.386	8.387	8.388	8.389	8.390	8.391	8.392	8.393	8.394	8.395	8.396	8.397	8.398	8.399	8.400	8.401	8.402	8.403	8.404	8.405	8.406	8.407	8.408	8.409	8.410	8.411	8.412	8.413	8.414	8.415	8.416	8.417	8.418	8.419	8.420	8.421	8.422	8.423	8.424	8.425	8.426	8.427	8.428	8.429	8.430	8.431	8.432	8.433	8.434	8.435	8.436	8.437	8.438	8.439	8.440	8.441	8.442	8.443	8.444	8.445	8.446	8.447	8.448	8.449	8.450	8.451	8.452	8.453	8.454	8.455	8.456	8.457	8.458	8.459	8.460	8.461	8.462	8.463	8.464	8.465	8.466	8.467	8.468	8.469	8.470	8.471	8.472	8.473	8.474	8.475	8.476	8.477	8.478	8.479	8.480	8.481	8.482	8.483	8.484	8.485	8.486	8.487	8.488	8.489	8.490	8.491	8.492	8.493	8.494	8.495	8.496	8.497	8.498	8.499	8.500	8.501	8.502	8.503	8.504	8.505	8.506	8.507	8.508	8.509	8.510	8.511	8.512	8.513	8.514	8.515	8.516	8.517	8.518	8.519	8.520	8.521	8.522	8.523	8.524	8.525	8.526	8.527	8.528	8.529	8.530	8.531	8.532	8.533	8.534	8.535	8.536	8.537	8.538	8.539	8.540	8.541	8.542	8.543	8.544	8.545	8.546	8.547	8.548	8.549	8.550	8.551	8.552	8.553	8.554	8.555	8.556	8.557	8.558	8.559	8.560	8.561	8.562	8.563	8.564	8.565	8.566	8.567	8.568	8.569	8.570	8.571	8.572	8.573	8.574	8.575	8.576	8.577	8.578	8.579	8.580	8.581	8.582	8.583	8.584	8.585	8.586	8.587	8.588	8.589	8.590	8.591	8.592	8.593	8.594	8.595	8.596	8.597	8.598	8.599	8.600	8.601	8.602	8.603	8.604	8.605	8.606	8.607	8.608	8.609	8.610	8.611	8.612	8.613	8.614	8.615	8.616	8.617	8.618	8.619	8.620	8.621	8.622	8.623
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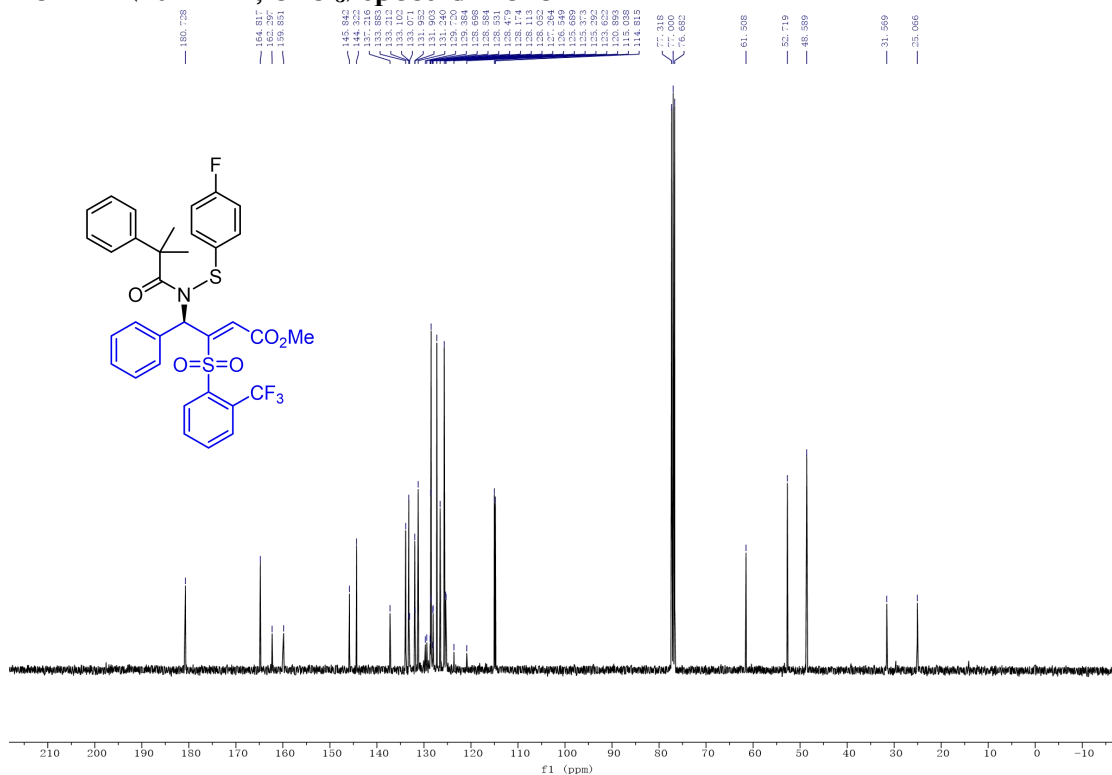
^{19}F NMR (376 MHz, CDCl_3) spectrum of 30



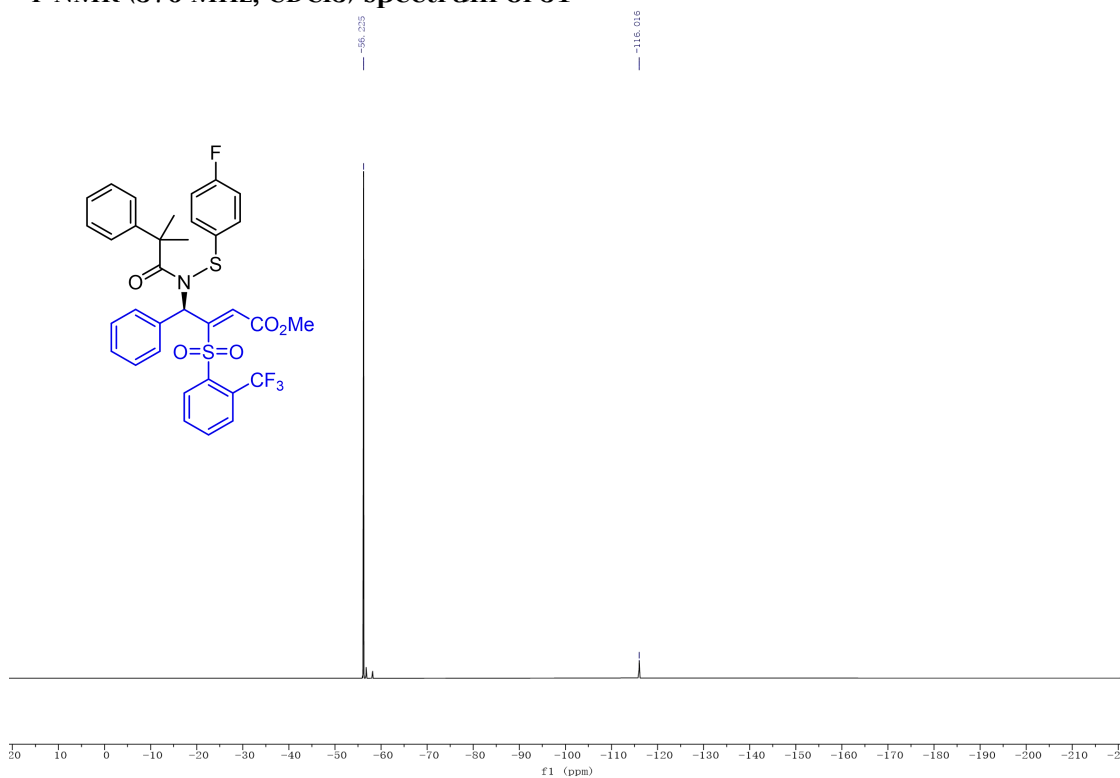
^1H NMR (400 MHz, CDCl_3) spectrum of 31



^{13}C NMR (101 MHz, CDCl_3) spectrum of 31



^{19}F NMR (376 MHz, CDCl_3) spectrum of 31



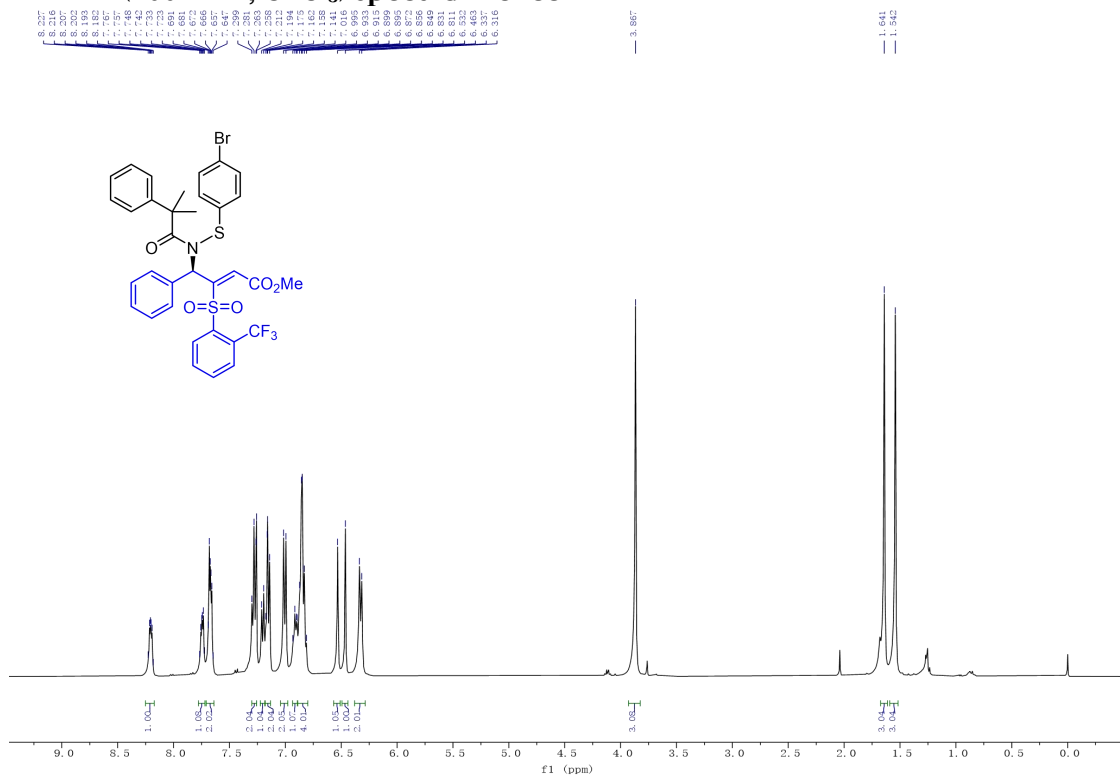
Chemical structure of compound 10 is shown in the top left. The structure is a complex molecule with a central carbon atom bonded to a phenyl ring, a (4-chlorophenyl)thio group, a (4-(trifluoromethyl)phenyl)sulfonyl group, and a (4-methoxycarbonylphenyl) group.

¹H NMR spectrum (CDCl₃) of compound 10. The spectrum shows peaks from 0.0 to 8.5 ppm. The x-axis is labeled f1 (ppm). The y-axis represents intensity. The spectrum shows a broad peak at 7.8 ppm (1H), a multiplet at 7.4 ppm (1H), a multiplet at 7.2 ppm (1H), a multiplet at 7.0 ppm (1H), a multiplet at 6.8 ppm (1H), a multiplet at 6.6 ppm (1H), a multiplet at 6.4 ppm (1H), a multiplet at 6.2 ppm (1H), a multiplet at 6.0 ppm (1H), a multiplet at 5.8 ppm (1H), a multiplet at 5.6 ppm (1H), a multiplet at 5.4 ppm (1H), a multiplet at 5.2 ppm (1H), a multiplet at 5.0 ppm (1H), a multiplet at 4.8 ppm (1H), a multiplet at 4.6 ppm (1H), a multiplet at 4.4 ppm (1H), a multiplet at 4.2 ppm (1H), a multiplet at 4.0 ppm (1H), a multiplet at 3.8 ppm (1H), a multiplet at 3.6 ppm (1H), a multiplet at 3.4 ppm (1H), a multiplet at 3.2 ppm (1H), a multiplet at 3.0 ppm (1H), a multiplet at 2.8 ppm (1H), a multiplet at 2.6 ppm (1H), a multiplet at 2.4 ppm (1H), a multiplet at 2.2 ppm (1H), a multiplet at 2.0 ppm (1H), a multiplet at 1.8 ppm (1H), a multiplet at 1.6 ppm (1H), a multiplet at 1.4 ppm (1H), a multiplet at 1.2 ppm (1H), a multiplet at 1.0 ppm (1H), a multiplet at 0.8 ppm (1H), a multiplet at 0.6 ppm (1H), a multiplet at 0.4 ppm (1H), a multiplet at 0.2 ppm (1H).

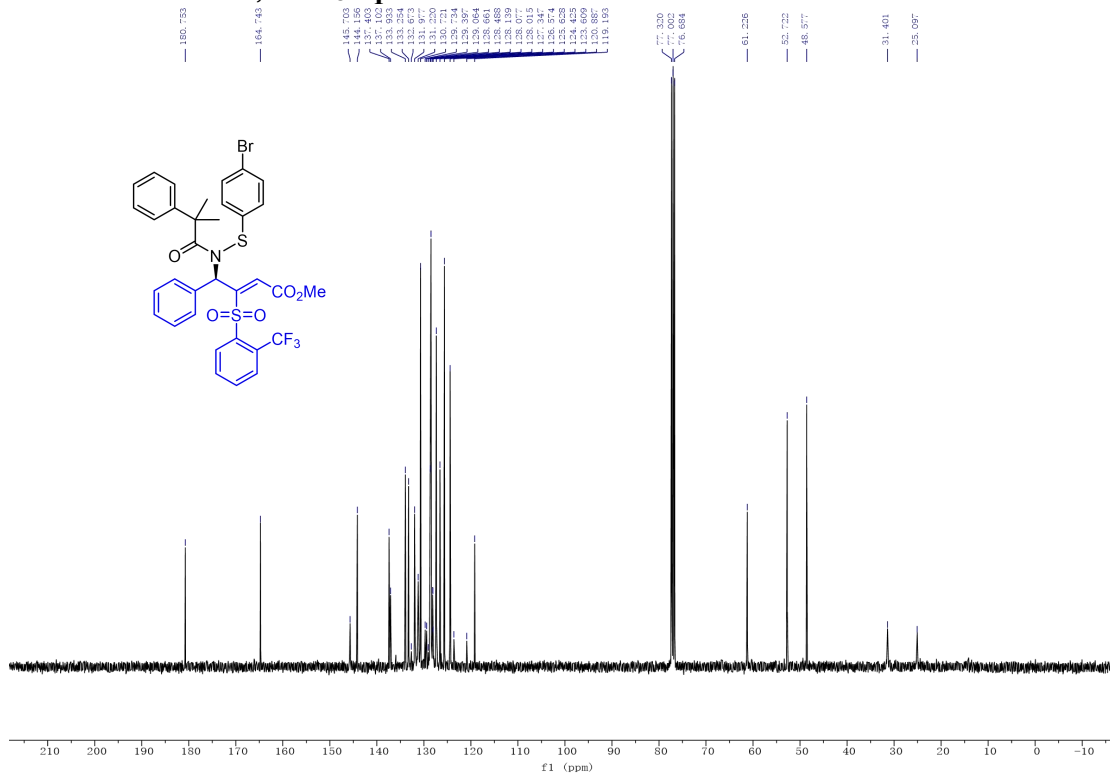
^{19}F NMR (376 MHz, CDCl_3) spectrum of 32



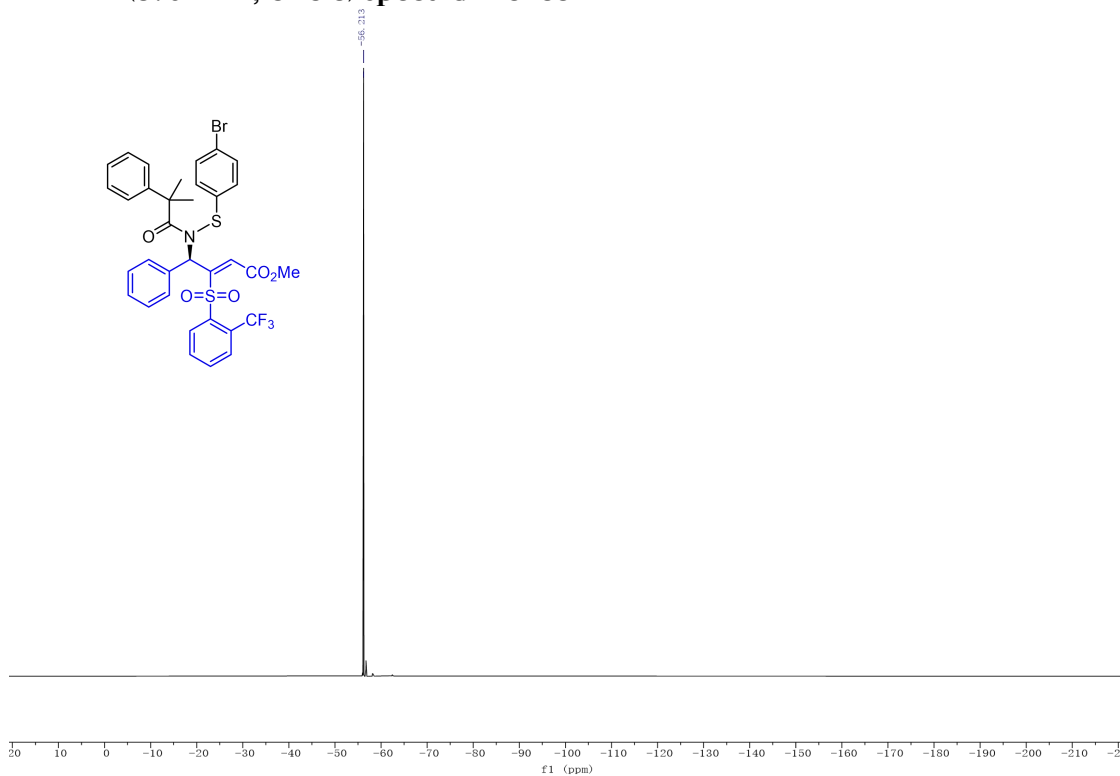
^1H NMR (400 MHz, CDCl_3) spectrum of 33



^{13}C NMR (101 MHz, CDCl_3) spectrum of 33



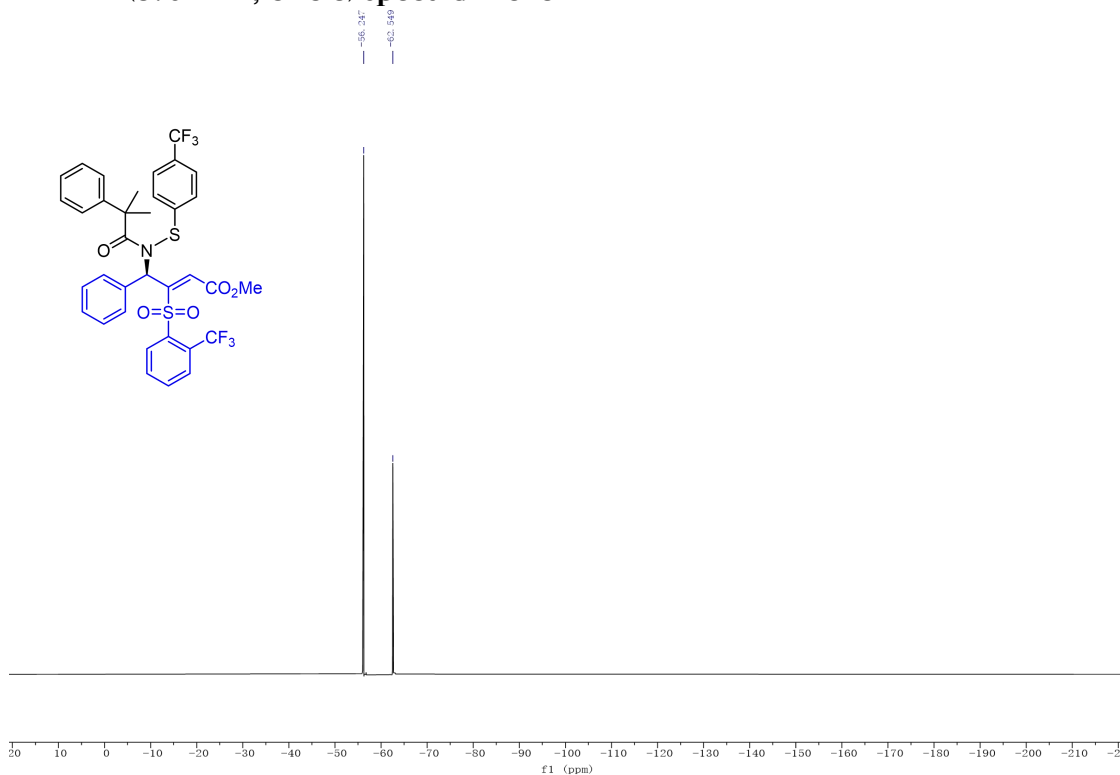
^{19}F NMR (376 MHz, CDCl_3) spectrum of 33



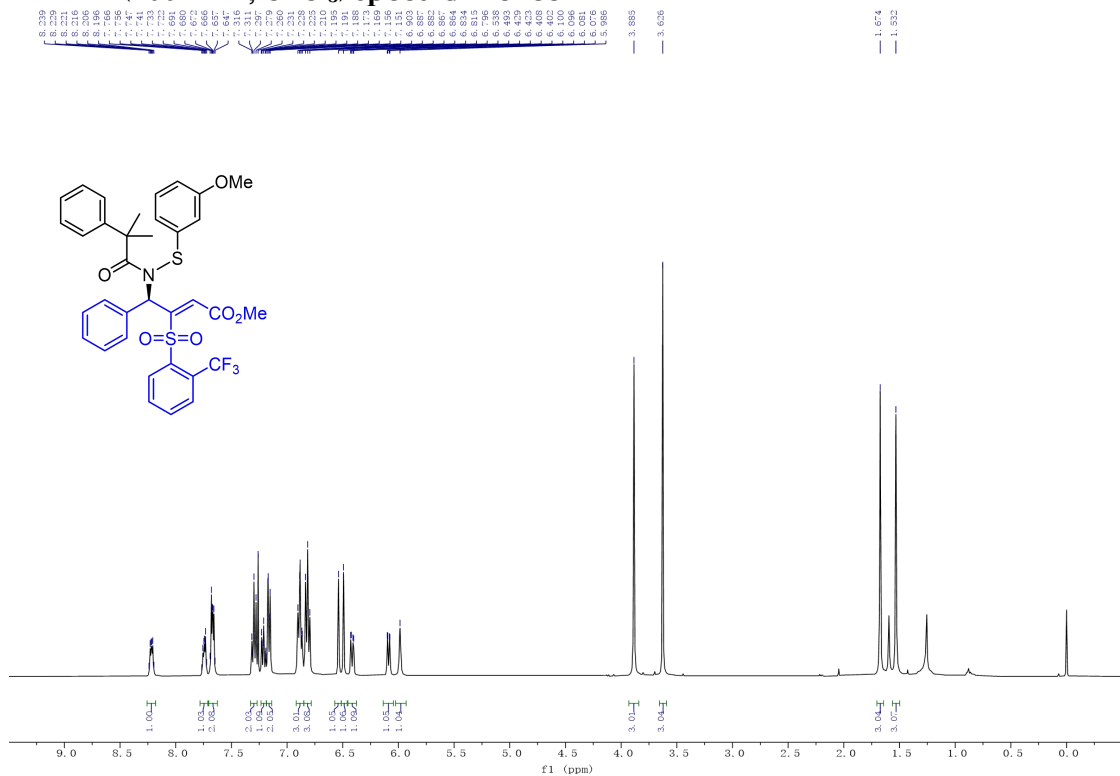
[illegible]

Chemical structure of compound 10 is shown above the spectrum. The spectrum displays peaks corresponding to the chemical shifts of the compound, with the following labeled values (ppm): 180.750, 164.697, 143.740, 143.740, 137.076, 134.086, 133.024, 132.896, 132.896, 132.872, 132.872, 132.818, 132.818, 132.747, 132.747, 132.747, 132.747, 132.638, 132.638, 132.661, 132.661, 132.590, 132.590, 132.540, 132.540, 132.488, 132.488, 132.425, 132.425, 77.319, 76.681, 61.072, 52.720, and 48.653.

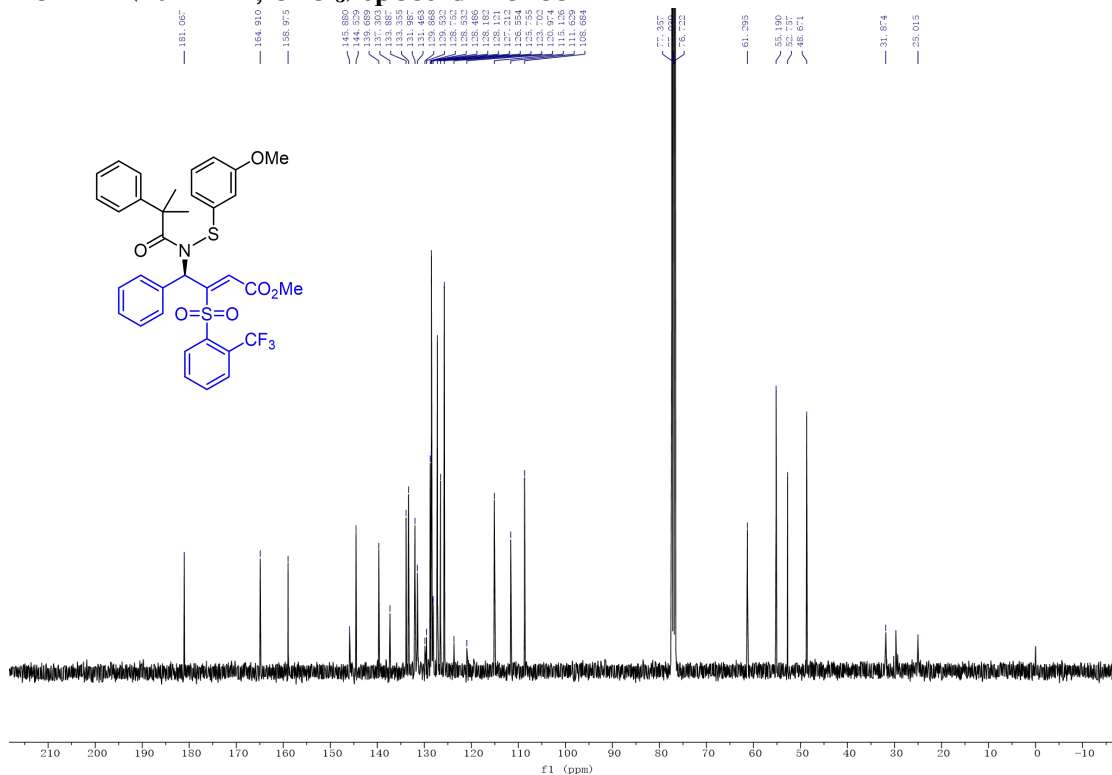
^{19}F NMR (376 MHz, CDCl_3) spectrum of 34



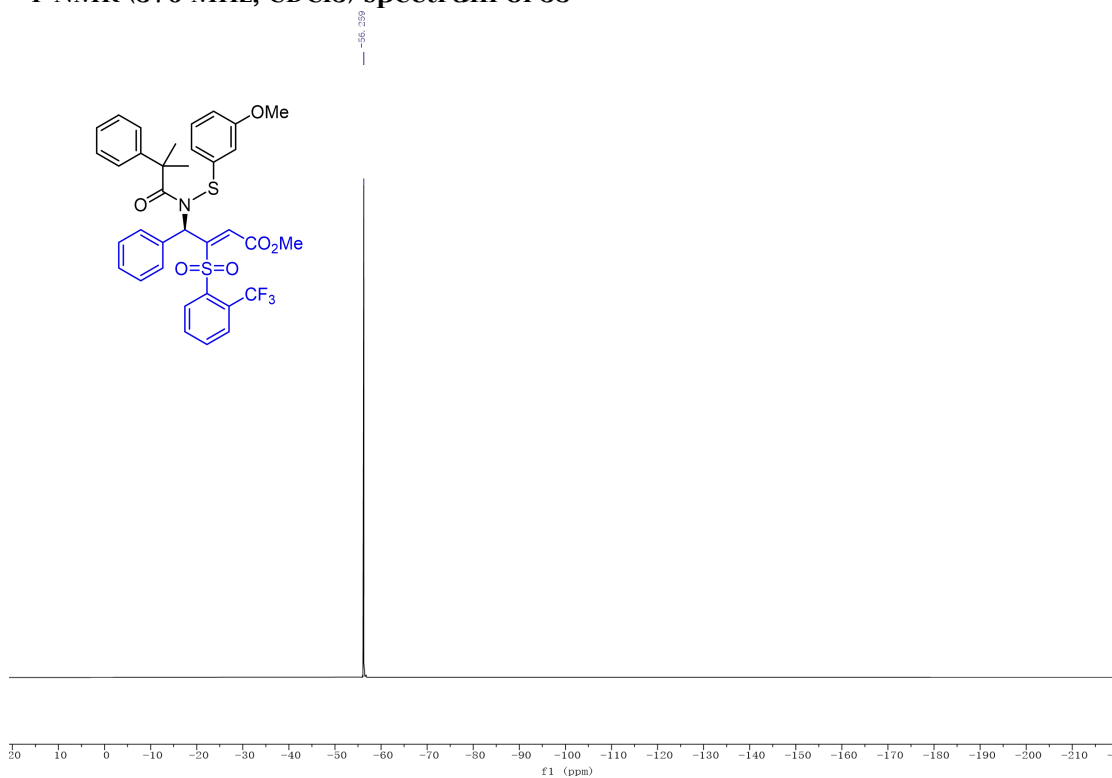
^1H NMR (400 MHz, CDCl_3) spectrum of 35



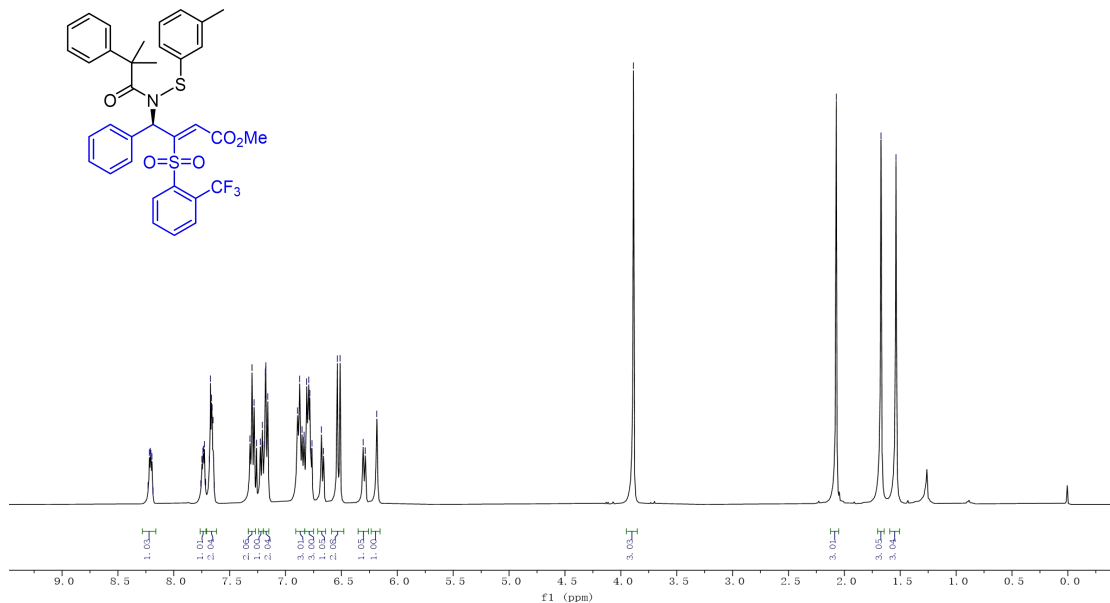
¹³C NMR (101 MHz, CDCl₃) spectrum of 35



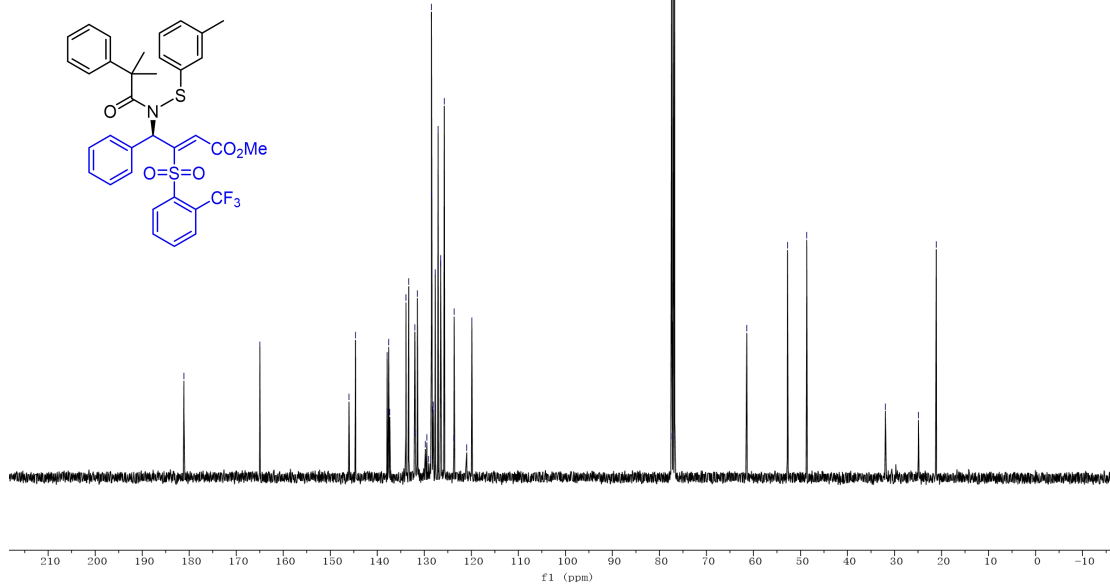
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 35



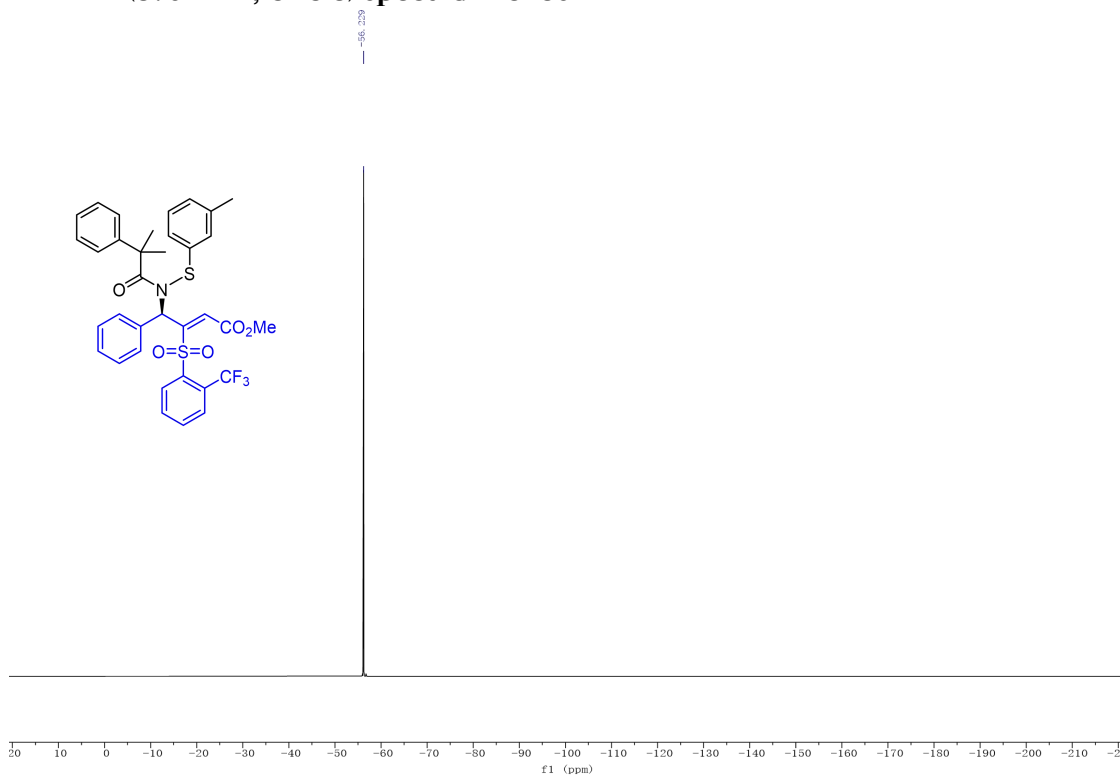
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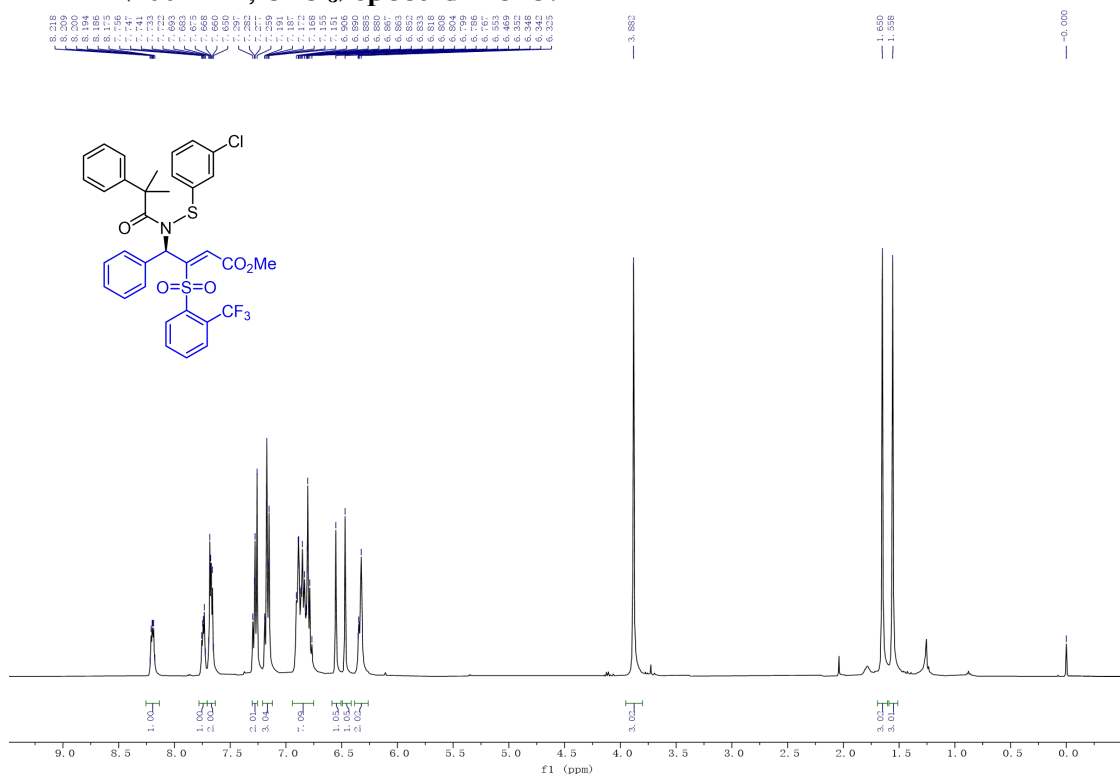
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144. 615
137. 911
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133. 909
133. 309
132. 007
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129. 796
129. 460
129. 121
128. 474
128. 450
128. 160
128. 100
127. 670
127. 076
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126. 499
125. 755



^{19}F NMR (376 MHz, CDCl_3) spectrum of 36



^1H NMR (400 MHz, CDCl_3) spectrum of 37



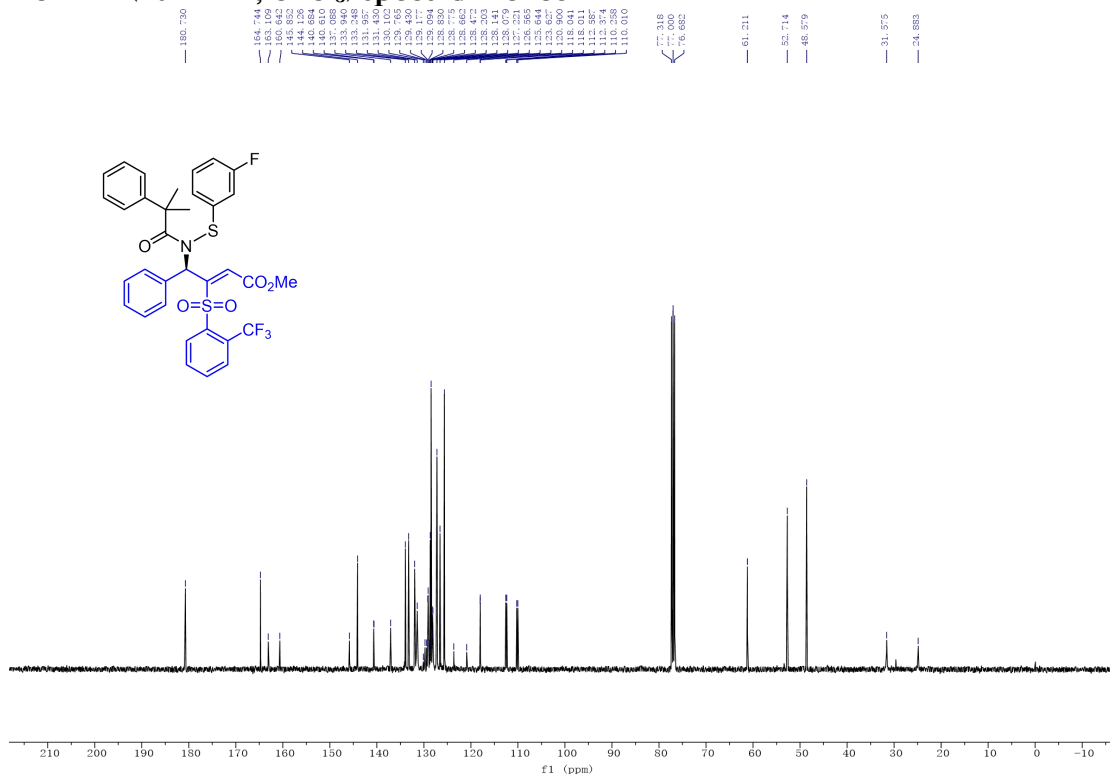
Chemical structure of compound 10 is shown above the ^{13}C NMR spectrum. The structure is a complex molecule featuring a central carbon atom bonded to a phenyl ring, a 4-chlorophenyl ring, a 2-methyl-2-phenylpropan-1-yl group, and a 2-(2-(trifluoromethyl)phenyl)-2-oxo-1-phenylethan-1-yl group.

The ^{13}C NMR spectrum (f1 (ppm)) shows the following chemical shifts (ppm):

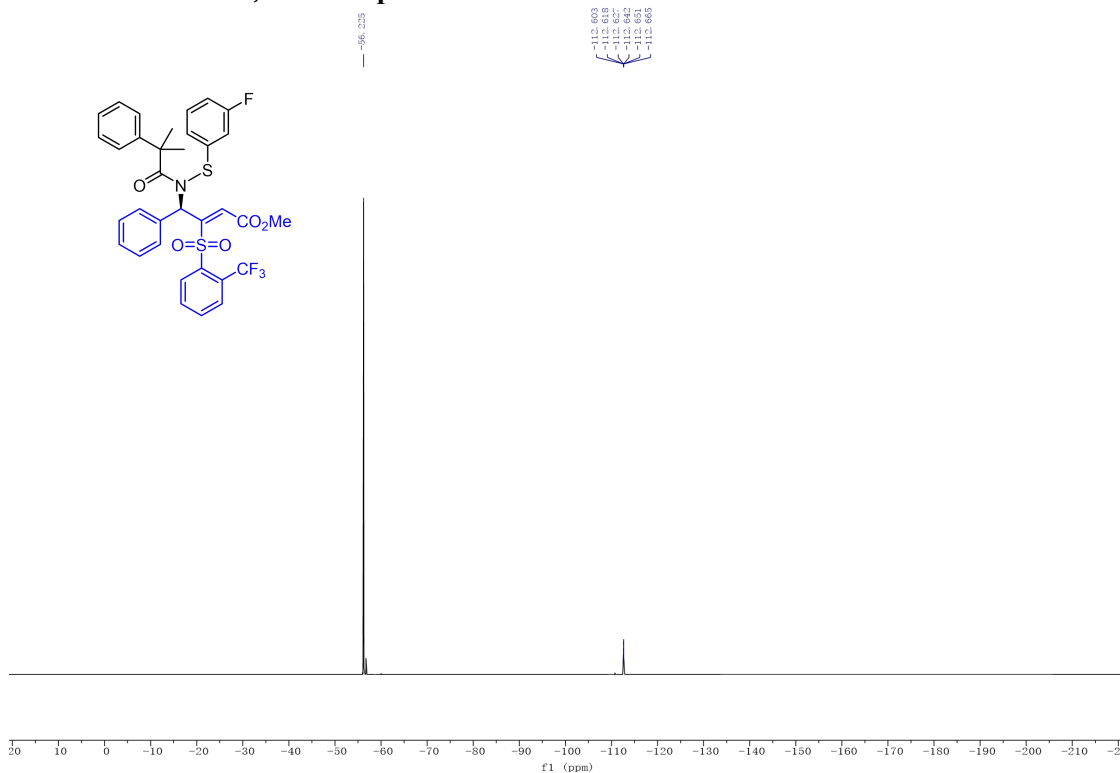
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- 145.653
- 140.044
- 137.093
- 136.421
- 135.749
- 133.269
- 131.865
- 131.583
- 129.781
- 128.746
- 128.695
- 128.446
- 128.159
- 128.088
- 127.990
- 127.950
- 127.528
- 127.528
- 125.631
- 122.812
- 120.318
- 77.318
- 76.682
- 61.209
- 52.736
- 48.600
- 31.401
- 25.046

Chemical structure of the compound is shown above the spectrum. The structure is a complex molecule featuring a central carbon atom bonded to a phenyl group, a sulfonamide group, a sulfonamide group, and a sulfonamide group. The sulfonamide group is further substituted with a phenyl ring and a trifluoromethyl group. The sulfonamide group is also substituted with a phenyl ring and a trifluoromethyl group. The sulfonamide group is also substituted with a phenyl ring and a trifluoromethyl group.

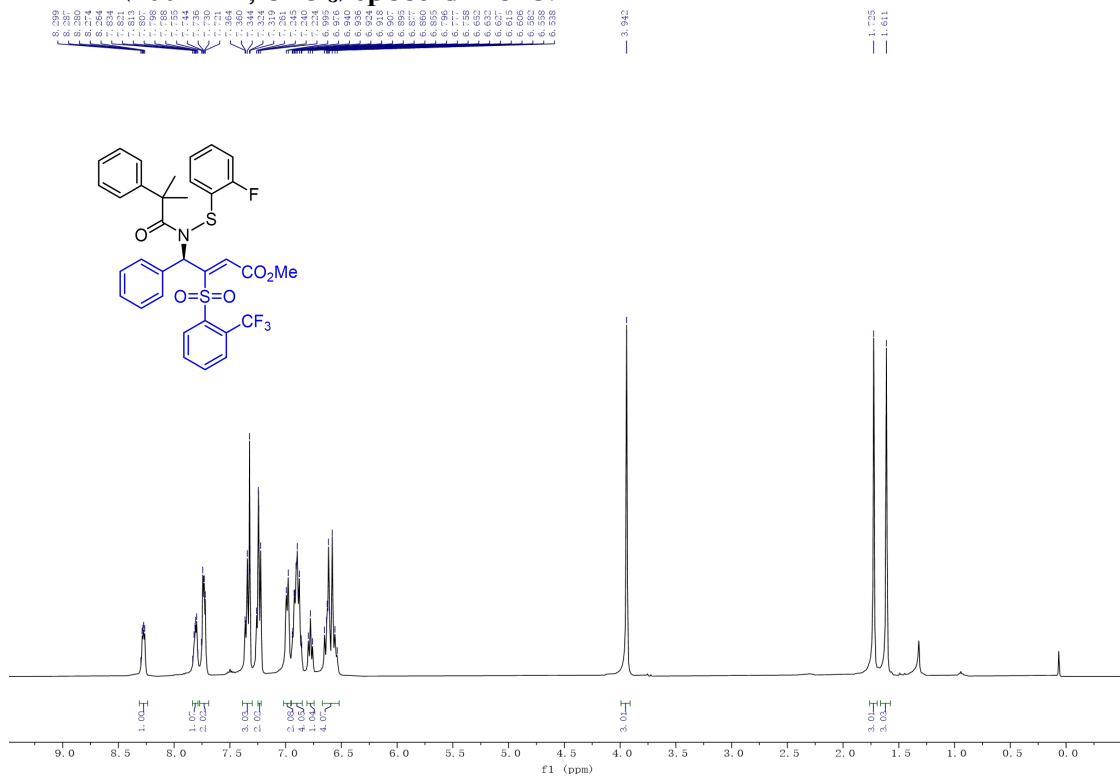
(continued)



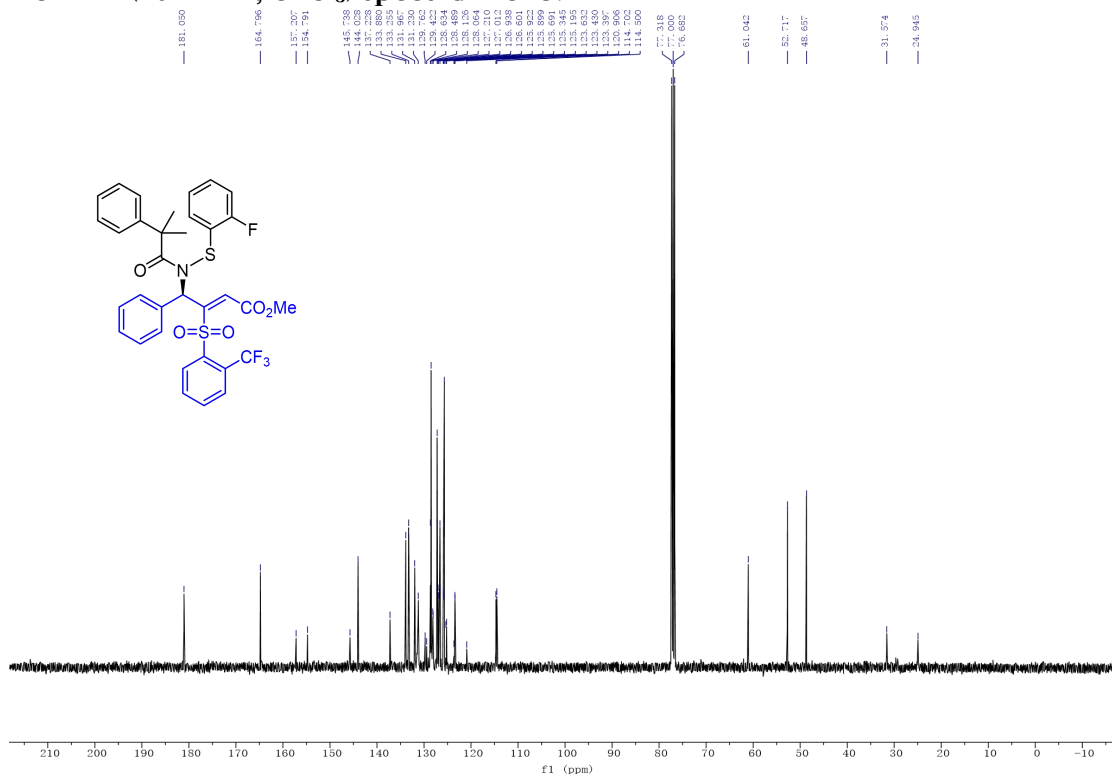
^{19}F NMR (376 MHz, CDCl_3) spectrum of 38



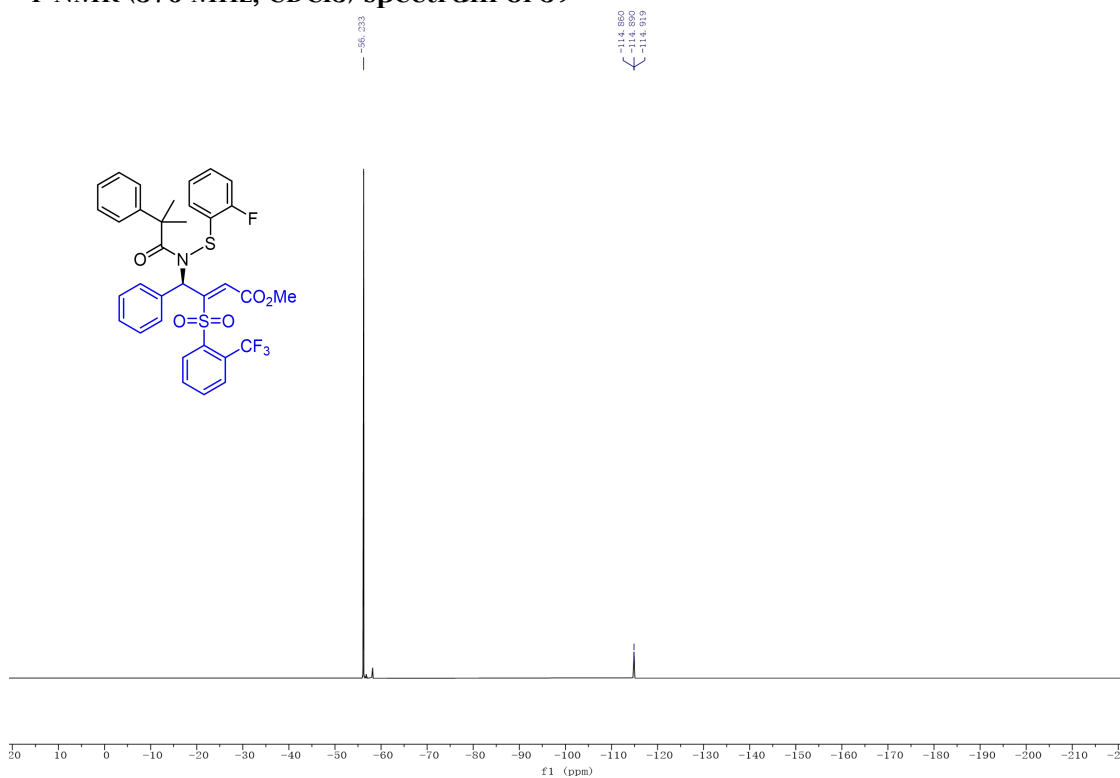
^1H NMR (400 MHz, CDCl_3) spectrum of 39



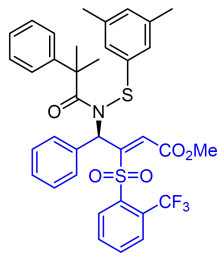
¹³C NMR (101 MHz, CDCl₃) spectrum of 39



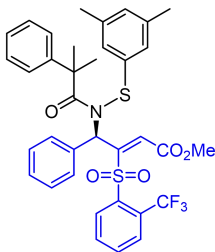
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 39



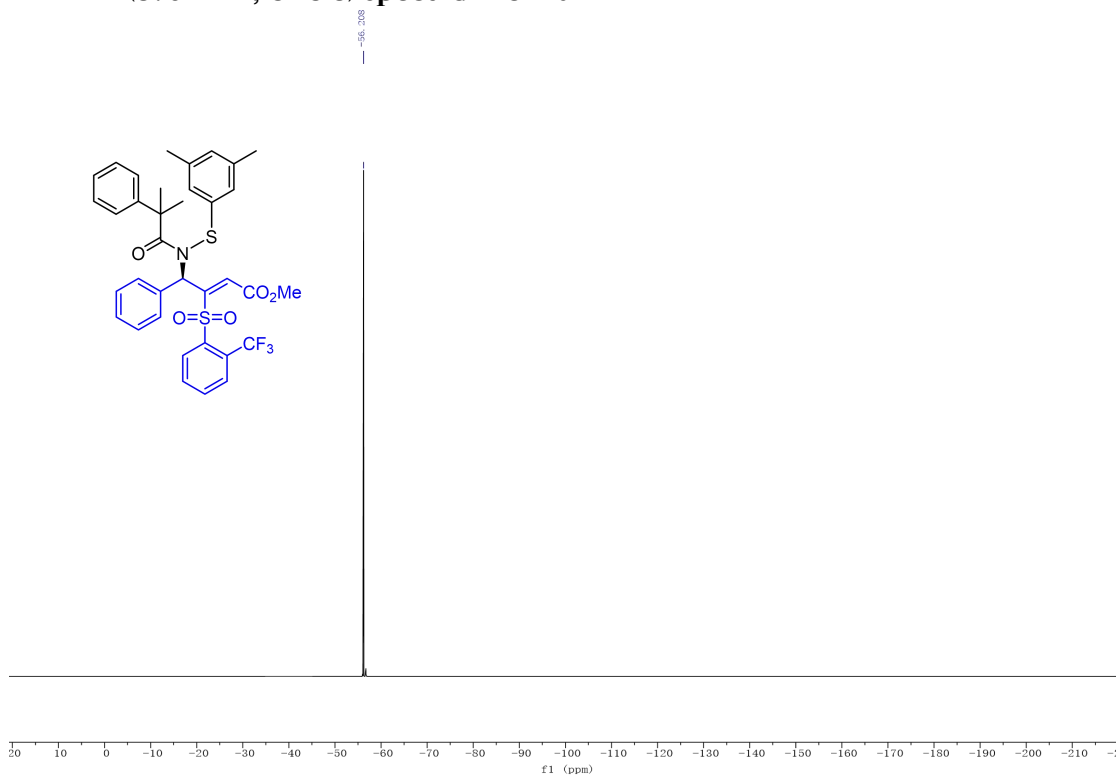
8. 236
8. 216
8. 202
8. 193
8. 183
7. 795
7. 736
7. 731
7. 722
7. 712
7. 680
7. 669
7. 661
7. 654
7. 646
7. 636
7. 321
7. 302
7. 293
7. 260
7. 268
7. 258
7. 224
7. 209
7. 191
7. 183
7. 179
7. 166
7. 161
6. 897
6. 878
6. 854
6. 850
6. 846
6. 825
6. 810
6. 806
6. 790
6. 785
6. 541
6. 533
6. 429



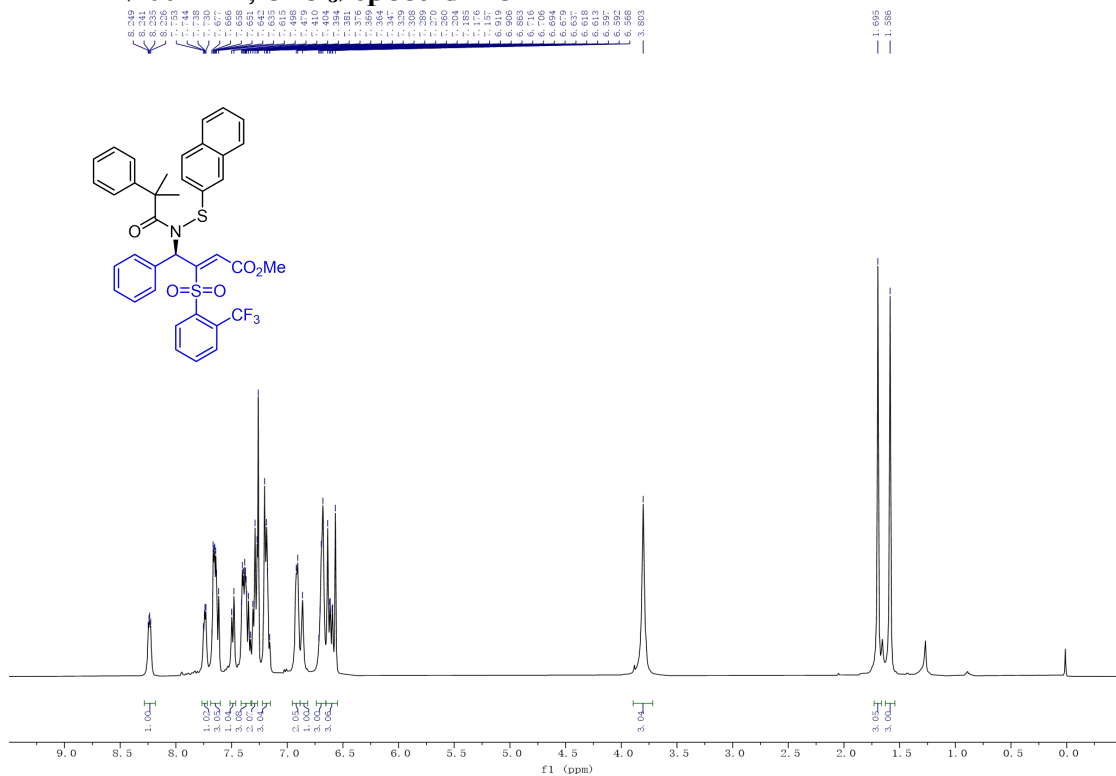
— 181.064 — 184.883 — 185.934 — 186.985 — 188.036 — 189.087 — 190.138 — 191.189 — 192.240 — 193.291 — 194.342 — 195.393 — 196.444 — 197.495 — 198.546 — 199.597 — 200.648 — 201.699 — 202.750 — 203.801 — 204.852 — 205.903 — 206.954 — 208.005 — 209.056 — 210.107 — 211.158 — 212.209 — 213.260 — 214.311 — 215.362 — 216.413 — 217.464 — 218.515 — 219.566 — 220.617 — 221.668 — 222.719 — 223.770 — 224.821 — 225.872 — 226.923 — 227.974 — 229.025 — 230.076 — 231.127 — 232.178 — 233.229 — 234.280 — 235.331 — 236.382 — 237.433 — 238.484 — 239.535 — 240.586 — 241.637 — 242.688 — 243.739 — 244.790 — 245.841 — 246.892 — 247.943 — 248.994 — 250.045 — 251.096 — 252.147 — 253.198 — 254.249 — 255.300 — 256.351 — 257.402 — 258.453 — 259.504 — 260.555 — 261.606 — 262.657 — 263.708 — 264.759 — 265.810 — 266.861 — 267.912 — 268.963 — 270.014 — 271.065 — 272.116 — 273.167 — 274.218 — 275.269 — 276.320 — 277.371 — 278.422 — 279.473 — 280.524 — 281.575 — 282.626 — 283.677 — 284.728 — 285.779 — 286.830 — 287.881 — 288.932 — 289.983 — 291.034 — 292.085 — 293.136 — 294.187 — 295.238 — 296.289 — 297.340 — 298.391 — 299.442 — 300.493 — 301.544 — 302.595 — 303.646 — 304.697 — 305.748 — 306.799 — 307.850 — 308.901 — 309.952 — 311.003 — 312.054 — 313.105 — 314.156 — 315.207 — 316.258 — 317.309 — 318.360 — 319.411 — 320.462 — 321.513 — 322.564 — 323.615 — 324.666 — 325.717 — 326.768 — 327.819 — 328.870 — 329.921 — 330.972 — 332.023 — 333.074 — 334.125 — 335.176 — 336.227 — 337.278 — 338.329 — 339.380 — 340.431 — 341.482 — 342.533 — 343.584 — 344.635 — 345.686 — 346.737 — 347.788 — 348.839 — 349.890 — 350.941 — 351.992 — 353.043 — 354.094 — 355.145 — 356.196 — 357.247 — 358.298 — 359.349 — 360.400 — 361.451 — 362.502 — 363.553 — 364.604 — 365.655 — 366.706 — 367.757 — 368.808 — 369.859 — 370.910 — 371.961 — 373.012 — 374.063 — 375.114 — 376.165 — 377.216 — 378.267 — 379.318 — 380.369 — 381.420 — 382.471 — 383.522 — 384.573 — 385.624 — 386.675 — 387.726 — 388.777 — 389.828 — 390.879 — 391.930 — 392.981 — 394.032 — 395.083 — 396.134 — 397.185 — 398.236 — 399.287 — 400.338 — 401.389 — 402.440 — 403.491 — 404.542 — 405.593 — 406.644 — 407.695 — 408.746 — 409.797 — 410.848 — 411.899 — 412.950 — 414.001 — 415.052 — 416.103 — 417.154 — 418.205 — 419.256 — 420.307 — 421.358 — 422.409 — 423.460 — 424.511 — 425.562 — 426.613 — 427.664 — 428.715 — 429.766 — 430.817 — 431.868 — 432.919 — 433.970 — 435.021 — 436.072 — 437.123 — 438.174 — 439.225 — 440.276 — 441.327 — 442.378 — 443.429 — 444.480 — 445.531 — 446.582 — 447.633 — 448.684 — 449.735 — 450.786 — 451.837 — 452.888 — 453.939 — 454.990 — 456.041 — 457.092 — 458.143 — 459.194 — 460.245 — 461.296 — 462.347 — 463.398 — 464.449 — 465.500 — 466.551 — 467.602 — 468.653 — 469.704 — 470.755 — 471.806 — 472.857 — 473.908 — 474.959 — 476.010 — 477.061 — 478.112 — 479.163 — 480.214 — 481.265 — 482.316 — 483.367 — 484.418 — 485.469 — 486.520 — 487.571 — 488.622 — 489.673 — 490.724 — 491.775 — 492.826 — 493.877 — 494.928 — 495.979 — 497.030 — 498.081 — 499.132 — 500.183 — 501.234 — 502.285 — 503.336 — 504.387 — 505.438 — 506.489 — 507.540 — 508.591 — 509.642 — 510.693 — 511.744 — 512.795 — 513.846 — 514.897 — 515.948 — 516.999 — 518.050 — 519.101 — 520.152 — 521.203 — 522.254 — 523.305 — 524.356 — 525.407 — 526.458 — 527.509 — 528.560 — 529.611 — 530.662 — 531.713 — 532.764 — 533.815 — 534.866 — 535.917 — 536.968 — 538.019 — 539.070 — 540.121 — 541.172 — 542.223 — 543.274 — 544.325 — 545.376 — 546.427 — 547.478 — 548.529 — 549.580 — 550.631 — 551.682 — 552.733 — 553.784 — 554.835 — 555.886 — 556.937 — 557.988 — 559.039 — 560.090 — 561.141 — 562.192 — 563.243 — 564.294 — 565.345 — 566.396 — 567.447 — 568.498 — 569.549 — 570.600 — 571.651 — 572.702 — 573.753 — 574.804 — 575.855 — 576.906 — 577.957 — 579.008 — 580.059 — 581.110 — 582.161 — 583.212 — 584.263 — 585.314 — 586.365 — 587.416 — 588.467 — 589.518 — 590.569 — 591.620 — 592.671 — 593.722 — 594.773 — 595.824 — 596.875 — 597.926 — 598.977 — 599.999



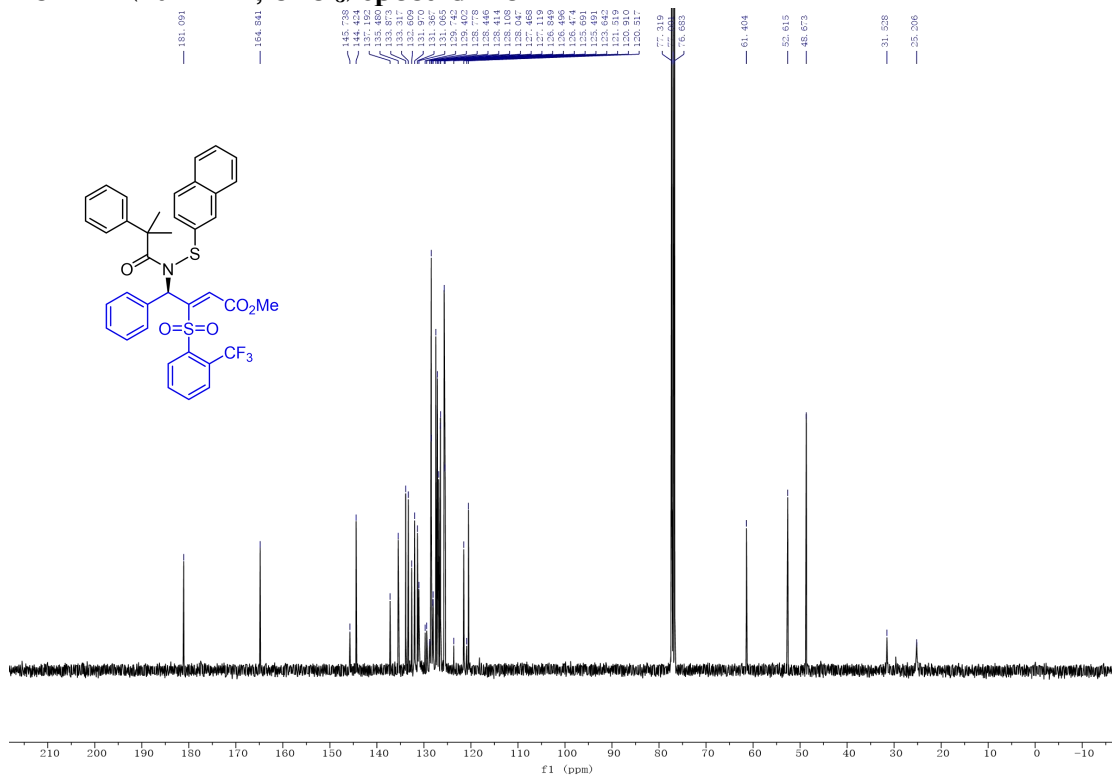
^{19}F NMR (376 MHz, CDCl_3) spectrum of 40



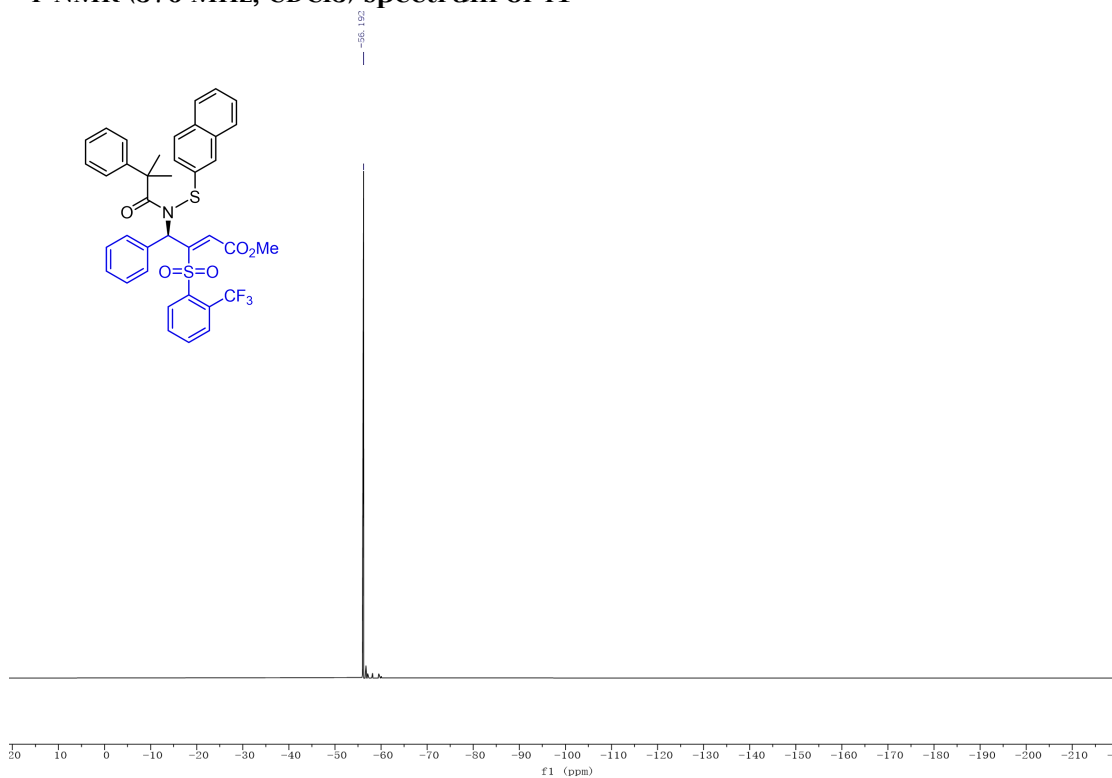
^1H NMR (400 MHz, CDCl_3) spectrum of 41



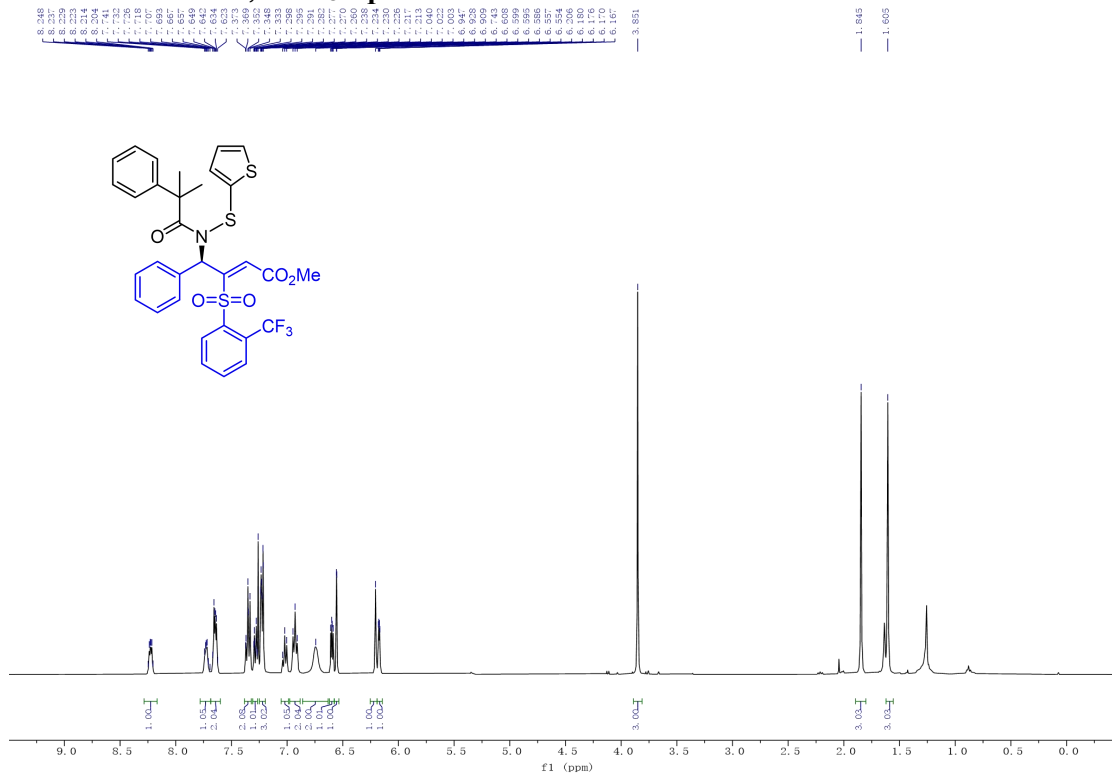
¹³C NMR (101 MHz, CDCl₃) spectrum of 41



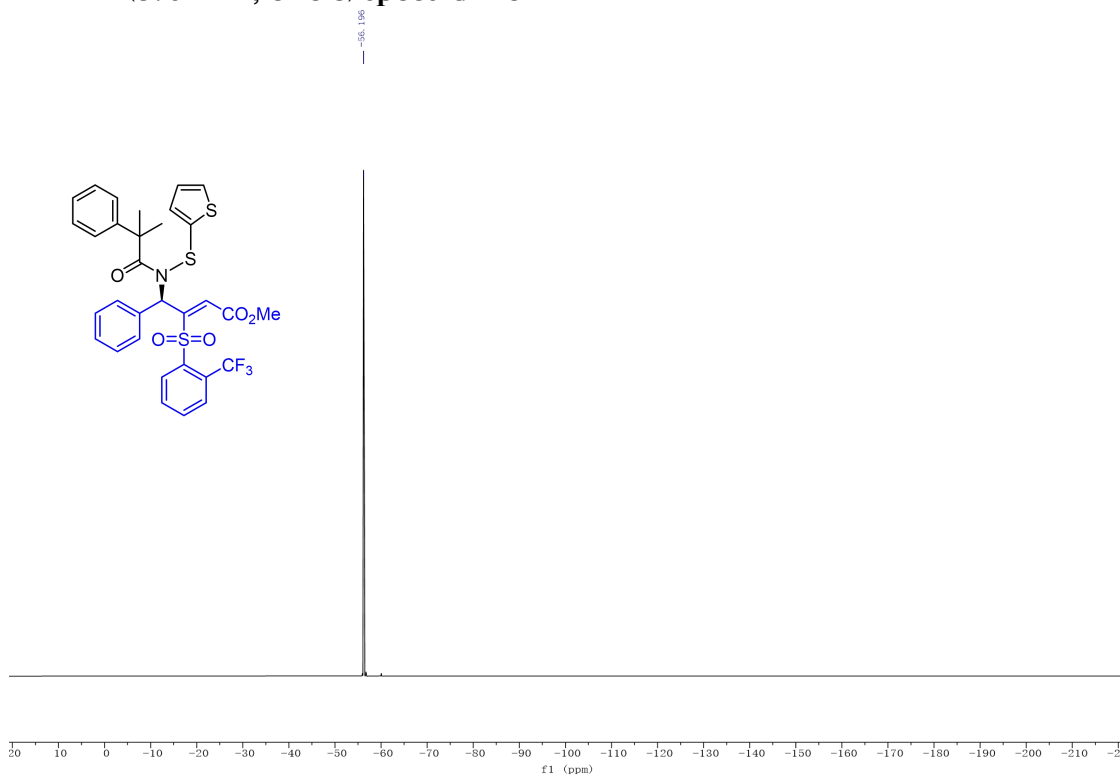
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 41



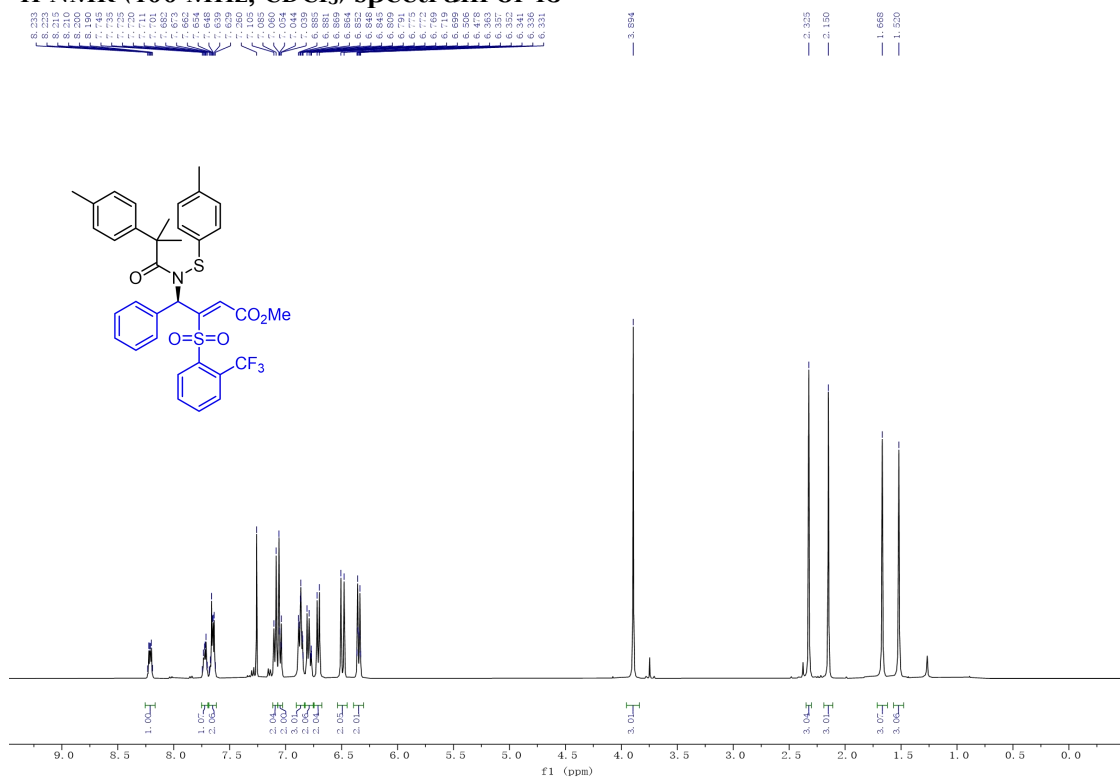
¹H NMR (400 MHz, CDCl₃) spectrum of 42



¹⁹F NMR (376 MHz, CDCl₃) spectrum of 42

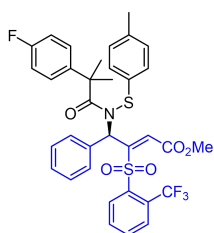
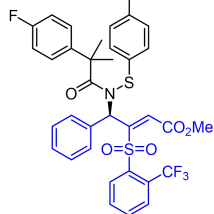


¹H NMR (400 MHz, CDCl₃) spectrum of 43



Chemical structure of compound 10 is shown above the spectrum. The structure is a 1,3-bis(4-methylphenyl)propan-2-one derivative. The spectrum shows peaks for the compound and solvent. The x-axis is labeled 'f1 (ppm)' and ranges from 10 to 210. The y-axis is labeled 'Intensity' and ranges from 0 to 100. The spectrum shows a broad peak at ~7.2 ppm (CDCl₃), a sharp peak at ~7.1 ppm (H₂O), and several peaks in the aromatic region between 7.0 and 8.0 ppm. A large peak is at ~7.2 ppm (CDCl₃). Other peaks are at ~6.1 ppm, ~5.2 ppm, ~4.8 ppm, ~3.1 ppm, ~2.4 ppm, ~2.0 ppm, and ~1.8 ppm.

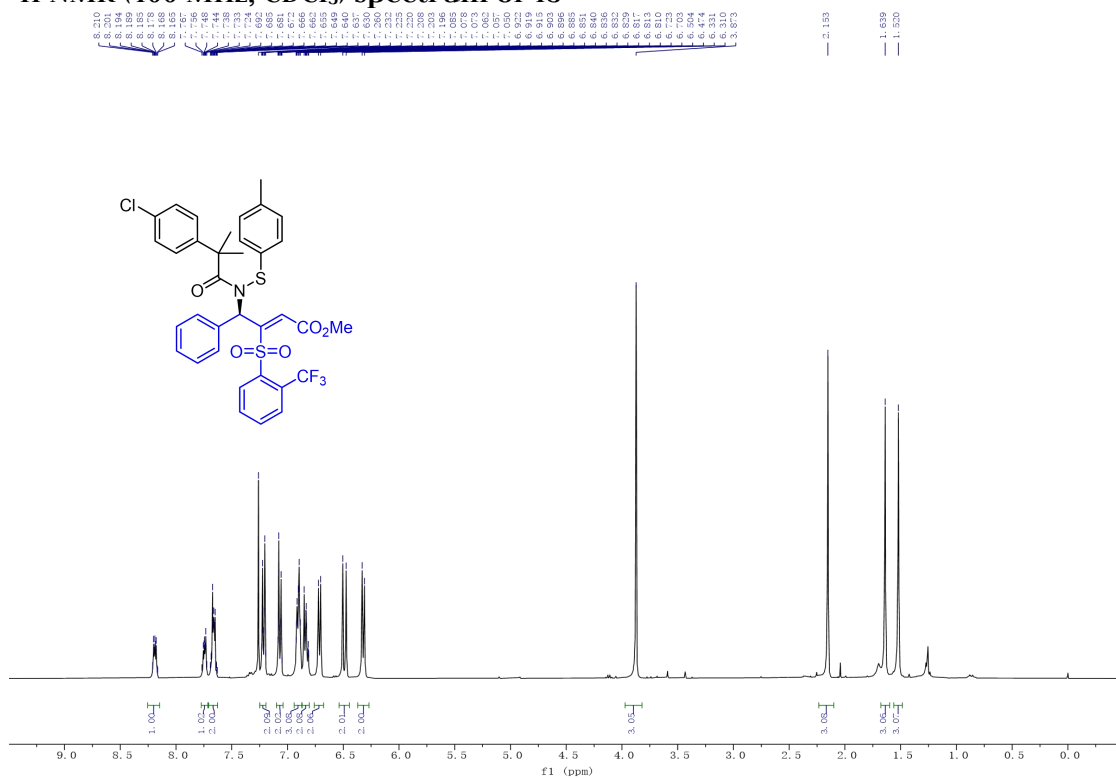
Chemical structure of the compound and its ^{13}C NMR spectrum (CDCl₃) are shown below. The spectrum displays a single sharp peak at $\delta = 56.21$ ppm, corresponding to the methoxy carbon of the ester group.

[illegible][illegible]

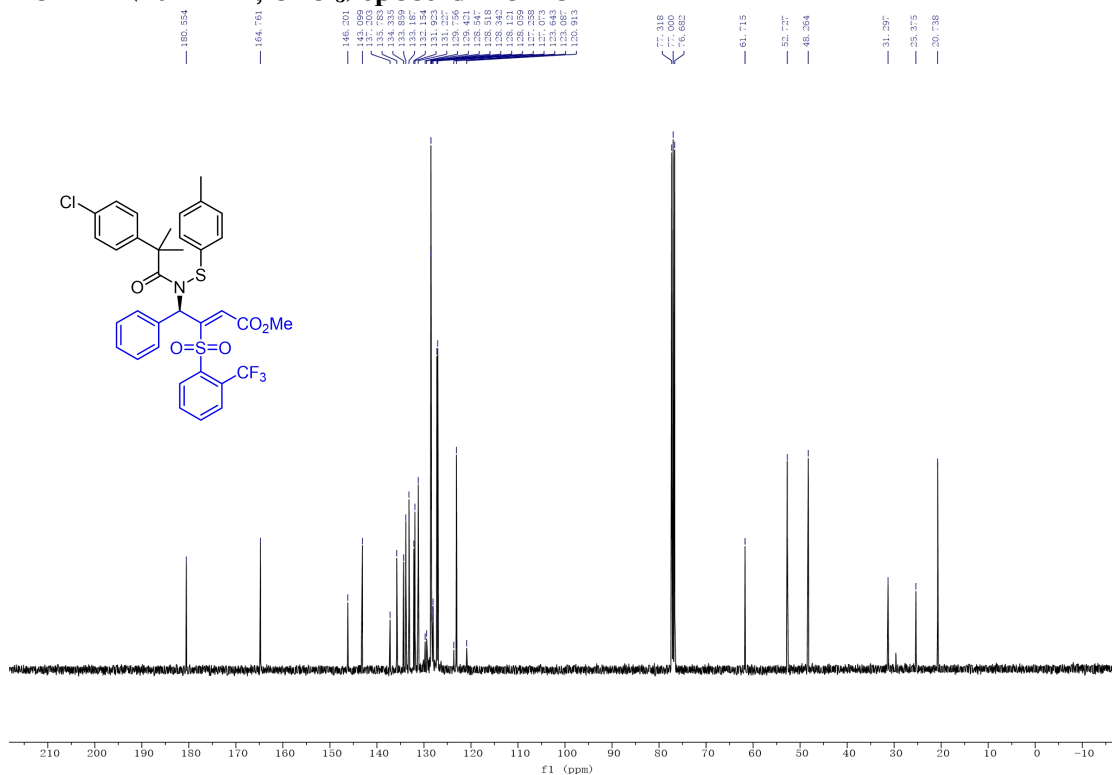
^{19}F NMR (376 MHz, CDCl_3) spectrum of 44



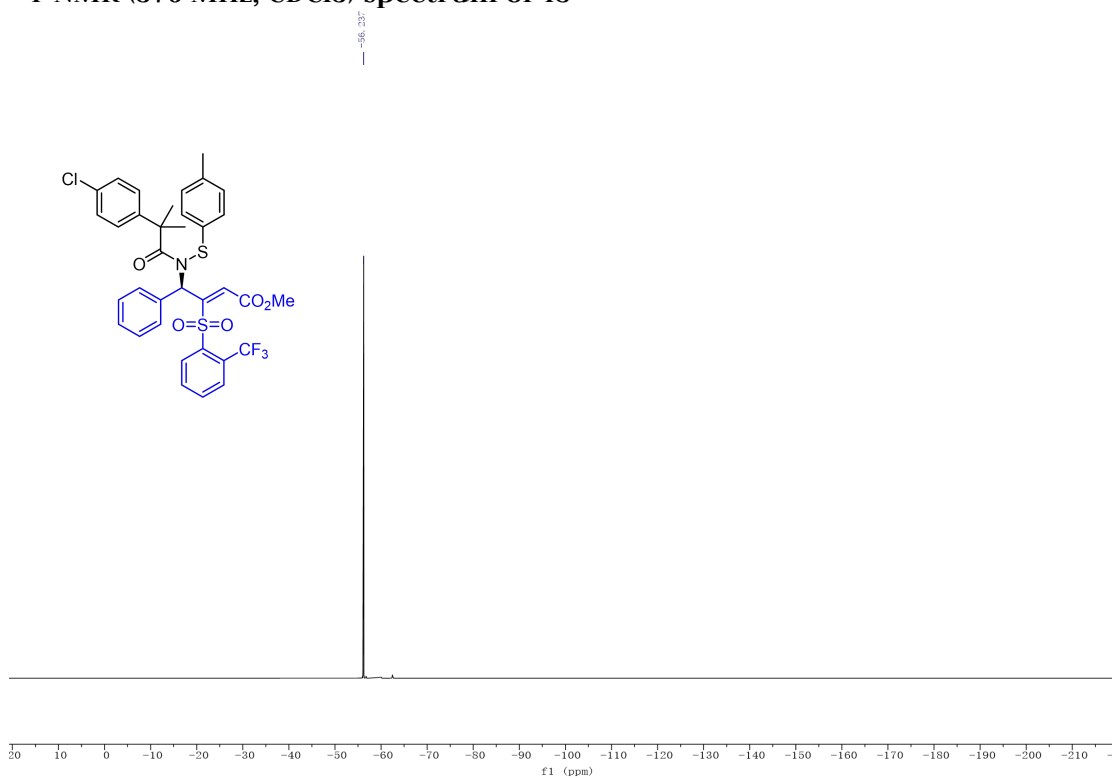
^1H NMR (400 MHz, CDCl_3) spectrum of 45



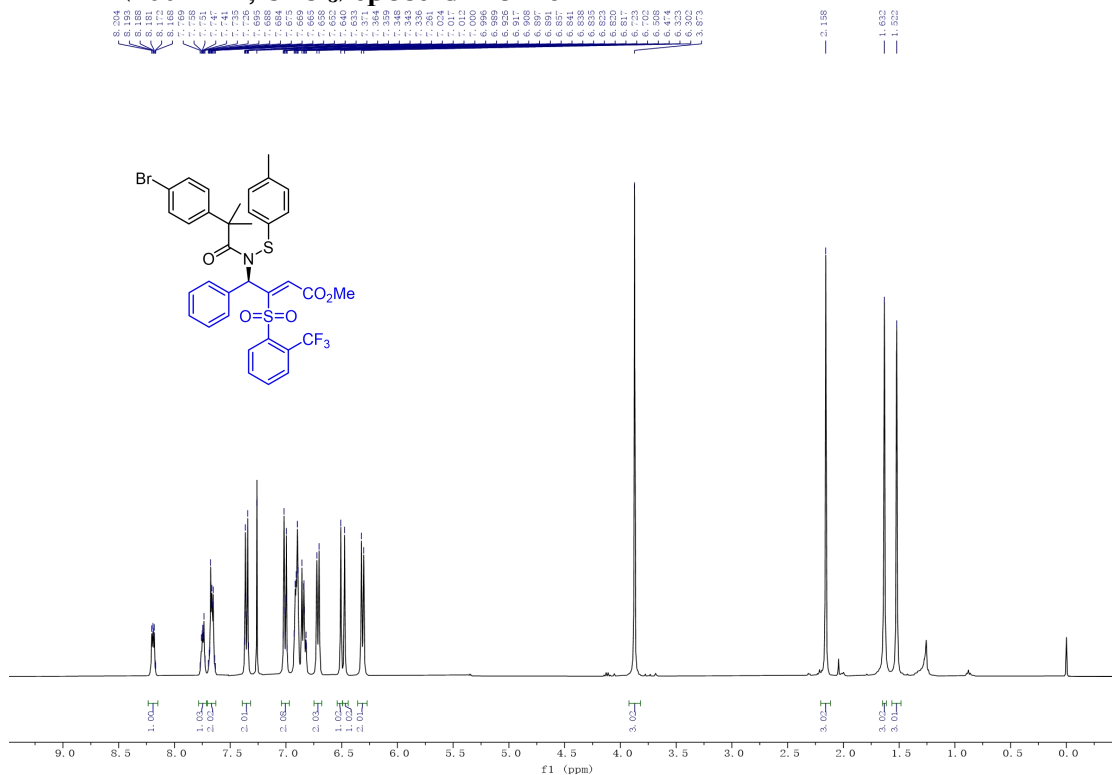
¹³C NMR (101 MHz, CDCl₃) spectrum of 45



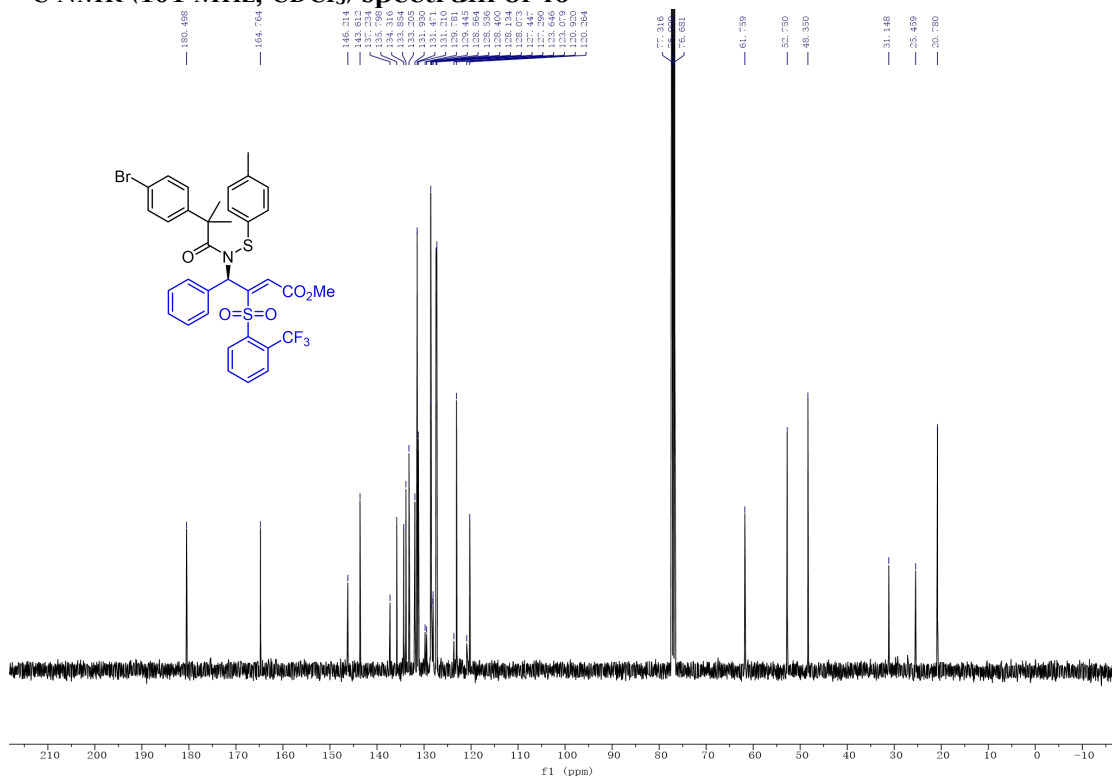
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 45



¹H NMR (400 MHz, CDCl₃) spectrum of 46



¹³C NMR (101 MHz, CDCl₃) spectrum of 46



Chemical structure of the compound is shown above the spectrum. The structure is a complex molecule featuring a central carbon atom bonded to a bromophenyl group, a 4-methylphenyl group, a methyl group, and a nitrogen atom. The nitrogen atom is part of a sulfonamide group, which is further substituted with a phenyl ring and a trifluoromethyl group. The spectrum shows a single sharp peak at approximately 195 ppm, indicating a highly symmetric or a single environment for the carbon atoms in the molecule.

¹³C NMR

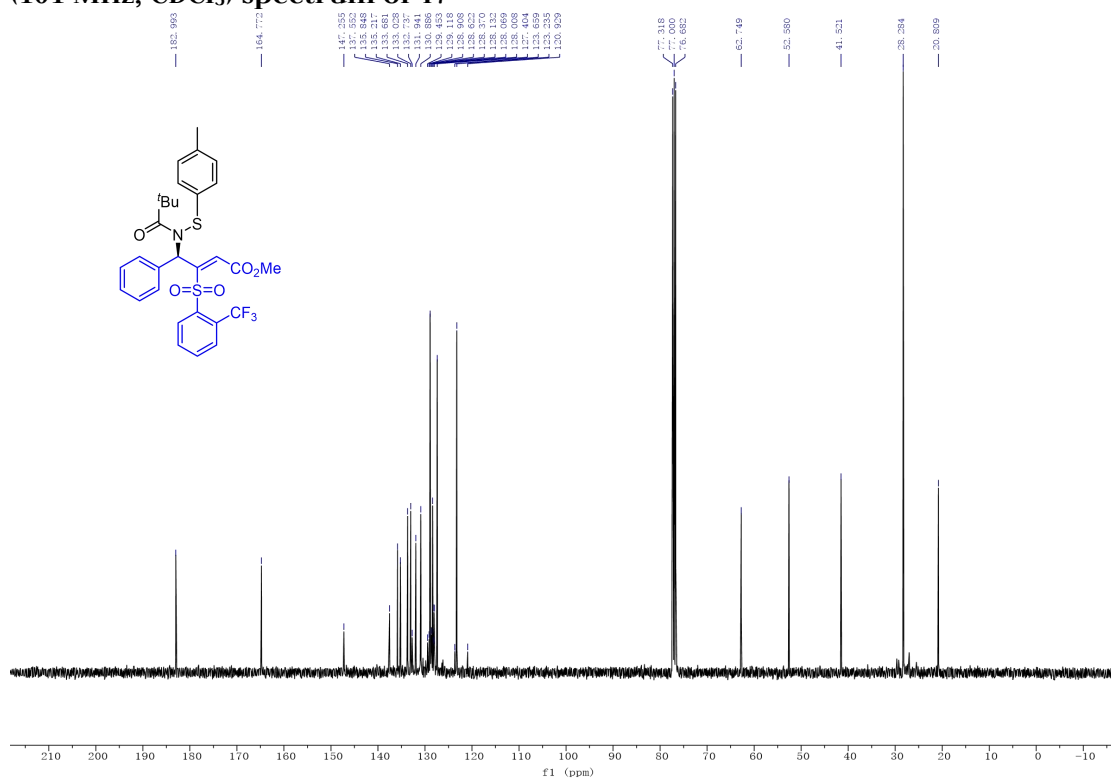
Chemical structure of the compound is shown above the spectrum. The structure is a complex molecule featuring a central carbon atom bonded to a phenyl ring, a sulfonamide group (SO₂CF₃), a methoxycarbonyl group (CO₂Me), and a chiral auxiliary group (a benzyl group with a tert-butyl sulfonamide). The spectrum displays peaks corresponding to the various carbon environments in the molecule, with chemical shifts ranging from approximately 1.2 to 8.2 ppm. The x-axis is labeled f1 (ppm) and the y-axis represents intensity.

Chemical structure: CC(C)(C)S(=O)(=O)c1ccc(cc1)[C@H](c2ccccc2)C(=O)OC(=O)c3ccccc3S(=O)(=O)C(F)(F)F

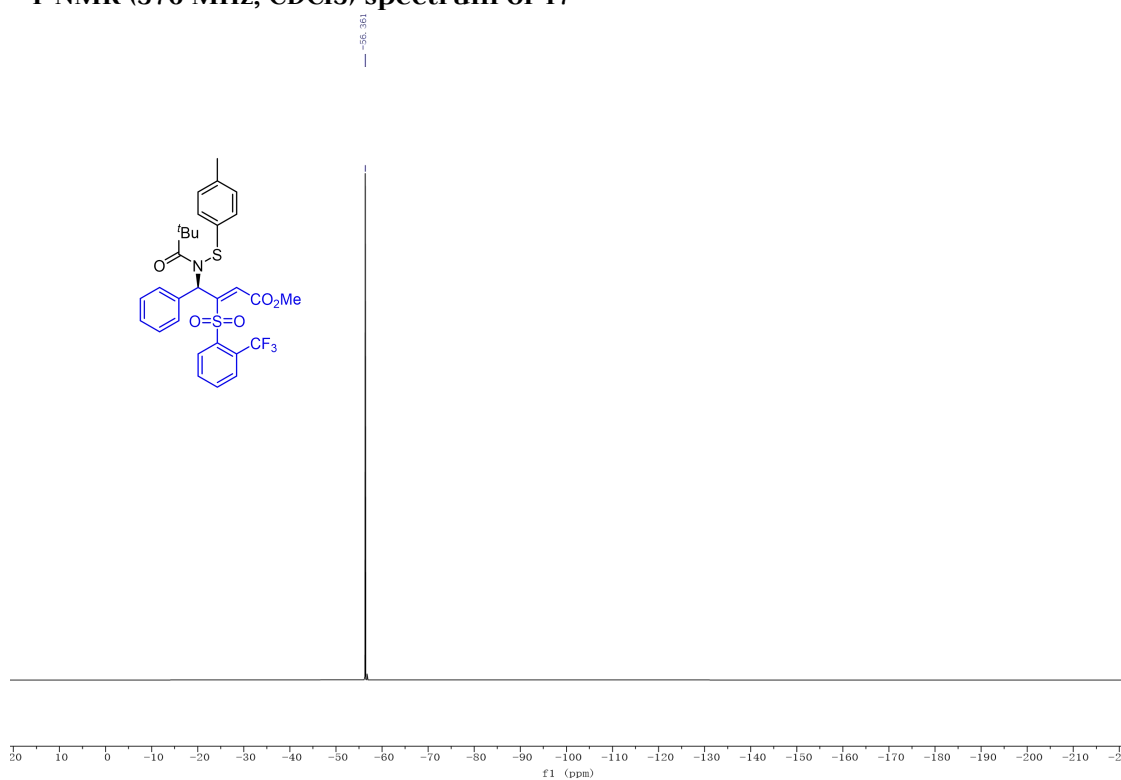
¹³C NMR spectrum (ppm):

- 8.215, 8.198, 8.182, 8.165, 8.148, 8.132, 8.116, 7.765, 7.749, 7.733, 7.717, 7.701, 7.685, 7.669, 7.653, 7.637, 7.621, 7.605, 7.589, 7.573, 7.557, 7.541, 7.525, 7.509, 7.493, 7.477, 7.461, 7.445, 7.429, 7.413, 7.397, 7.381, 7.365, 7.349, 7.333, 7.317, 7.301, 7.285, 7.269, 7.253, 7.237, 7.221, 7.205, 7.189, 7.173, 7.157, 7.141, 7.125, 7.109, 7.093, 7.077, 7.061, 7.045, 7.029, 7.013, 6.997, 6.981, 6.965, 6.949, 6.933, 6.917, 6.901, 6.885, 6.869, 6.853, 6.837, 6.821, 6.805, 6.789, 6.773, 6.757, 6.741, 6.725, 6.709, 6.693, 6.677, 6.661, 6.645, 6.629, 6.613, 6.597, 6.581, 6.565, 6.549, 6.533, 6.517, 6.501, 6.485, 6.469, 6.453, 6.437, 6.421, 6.405, 6.389, 6.373, 6.357, 6.341, 6.325, 6.309, 6.293, 6.277, 6.261, 6.245, 6.229, 6.213, 6.197, 6.181, 6.165, 6.149, 6.133, 6.117, 6.101, 6.085, 6.069, 6.053, 6.037, 6.021, 6.005, 5.989, 5.973, 5.957, 5.941, 5.925, 5.909, 5.893, 5.877, 5.861, 5.845, 5.829, 5.813, 5.797, 5.781, 5.765, 5.749, 5.733, 5.717, 5.701, 5.685, 5.669, 5.653, 5.637, 5.621, 5.605, 5.589, 5.573, 5.557, 5.541, 5.525, 5.509, 5.493, 5.477, 5.461, 5.445, 5.429, 5.413, 5.397, 5.381, 5.365, 5.349, 5.333, 5.317, 5.301, 5.285, 5.269, 5.253, 5.237, 5.221, 5.205, 5.189, 5.173, 5.157, 5.141, 5.125, 5.109, 5.093, 5.077, 5.061, 5.045, 5.029, 5.013, 4.997, 4.981, 4.965, 4.949, 4.933, 4.917, 4.901, 4.885, 4.869, 4.853, 4.837, 4.821, 4.805, 4.789, 4.773, 4.757, 4.741, 4.725, 4.709, 4.693, 4.677, 4.661, 4.645, 4.629, 4.613, 4.597, 4.581, 4.565, 4.549, 4.533, 4.517, 4.501, 4.485, 4.469, 4.453, 4.437, 4.421, 4.405, 4.389, 4.373, 4.357, 4.341, 4.325, 4.309, 4.293, 4.277, 4.261, 4.245, 4.229, 4.213, 4.197, 4.181, 4.165, 4.149, 4.133, 4.117, 4.101, 4.085, 4.069, 4.053, 4.037, 4.021, 4.005, 3.989, 3.973, 3.957, 3.941, 3.925, 3.909, 3.893, 3.877, 3.861, 3.845, 3.829, 3.813, 3.797, 3.781, 3.765, 3.749, 3.733, 3.717, 3.701, 3.685, 3.669, 3.653, 3.637, 3.621, 3.605, 3.589, 3.573, 3.557, 3.541, 3.525, 3.509, 3.493, 3.477, 3.461, 3.445, 3.429, 3.413, 3.397, 3.381, 3.365, 3.349, 3.333, 3.317, 3.301, 3.285, 3.269, 3.253, 3.237, 3.221, 3.205, 3.189, 3.173, 3.157, 3.141, 3.125, 3.109, 3.093, 3.077, 3.061, 3.045, 3.029, 3.013, 2.997, 2.981, 2.965, 2.949, 2.933, 2.917, 2.901, 2.885, 2.869, 2.853, 2.837, 2.821, 2.805, 2.789, 2.773, 2.757, 2.741, 2.725, 2.709, 2.693, 2.677, 2.661, 2.645, 2.629, 2.613, 2.597, 2.581, 2.565, 2.549, 2.533, 2.517, 2.501, 2.485, 2.469, 2.453, 2.437, 2.421, 2.405, 2.389, 2.373, 2.357, 2.341, 2.325, 2.309, 2.293, 2.277, 2.261, 2.245, 2.229, 2.213, 2.197, 2.181, 2.165, 2.149, 2.133, 2.117, 2.101, 2.085, 2.069, 2.053, 2.037, 2.021, 2.005, 1.989, 1.973, 1.957, 1.941, 1.925, 1.909, 1.893, 1.877, 1.861, 1.845, 1.829, 1.813, 1.797, 1.781, 1.765, 1.749, 1.733, 1.717, 1.701, 1.685, 1.669, 1.653, 1.637, 1.621, 1.605, 1.589, 1.573, 1.557, 1.541, 1.525, 1.509, 1.493, 1.477, 1.461, 1.445, 1.429, 1.413, 1.397, 1.381, 1.365, 1.349, 1.333, 1.317, 1.301, 1.285, 1.269, 1.253, 1.237, 1.221, 1.205, 1.189, 1.173, 1.157, 1.141, 1.125, 1.109, 1.093, 1.077, 1.061, 1.045, 1.029, 1.013, 0.997, 0.981, 0.965, 0.949, 0.933, 0.917, 0.901, 0.885, 0.869, 0.853, 0.837, 0.821, 0.805, 0.789, 0.773, 0.757, 0.741, 0.725, 0.709, 0.693, 0.677, 0.661, 0.645, 0.629, 0.613, 0.597, 0.581, 0.565, 0.549, 0.533, 0.517, 0.501, 0.485, 0.469, 0.453, 0.437, 0.421, 0.405, 0.389, 0.373, 0.357, 0.341, 0.325, 0.309, 0.293, 0.277, 0.261, 0.245, 0.229, 0.213, 0.197, 0.181, 0.165, 0.149, 0.133, 0.117, 0.101, 0.085, 0.069, 0.053, 0.037, 0.021, 0.005.

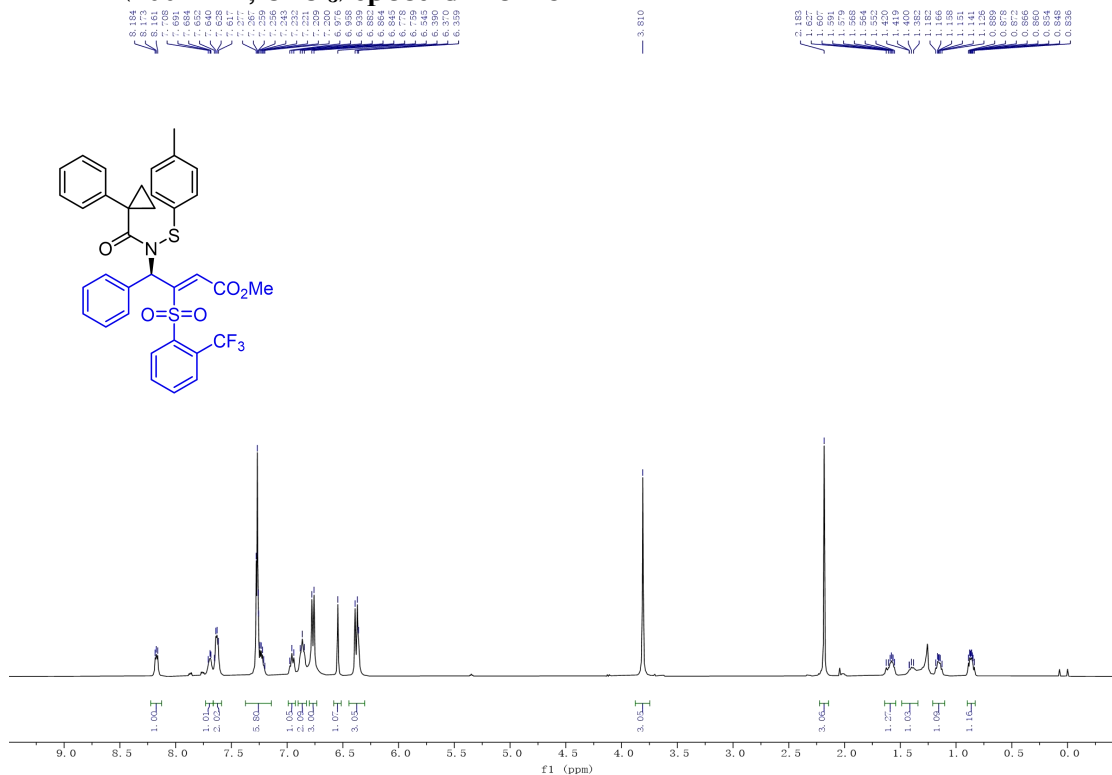
(101 MHz, CDCl₃) spectrum of 47



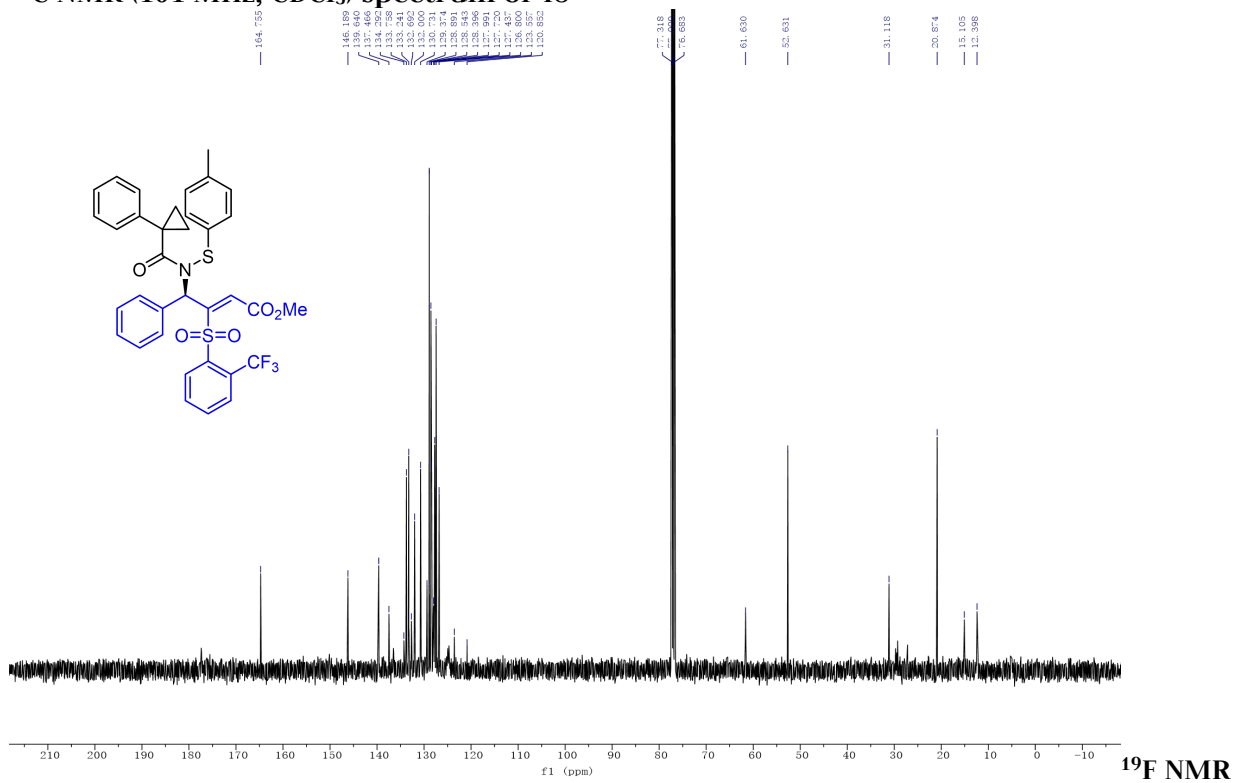
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 47



¹H NMR (400 MHz, CDCl₃) spectrum of 48



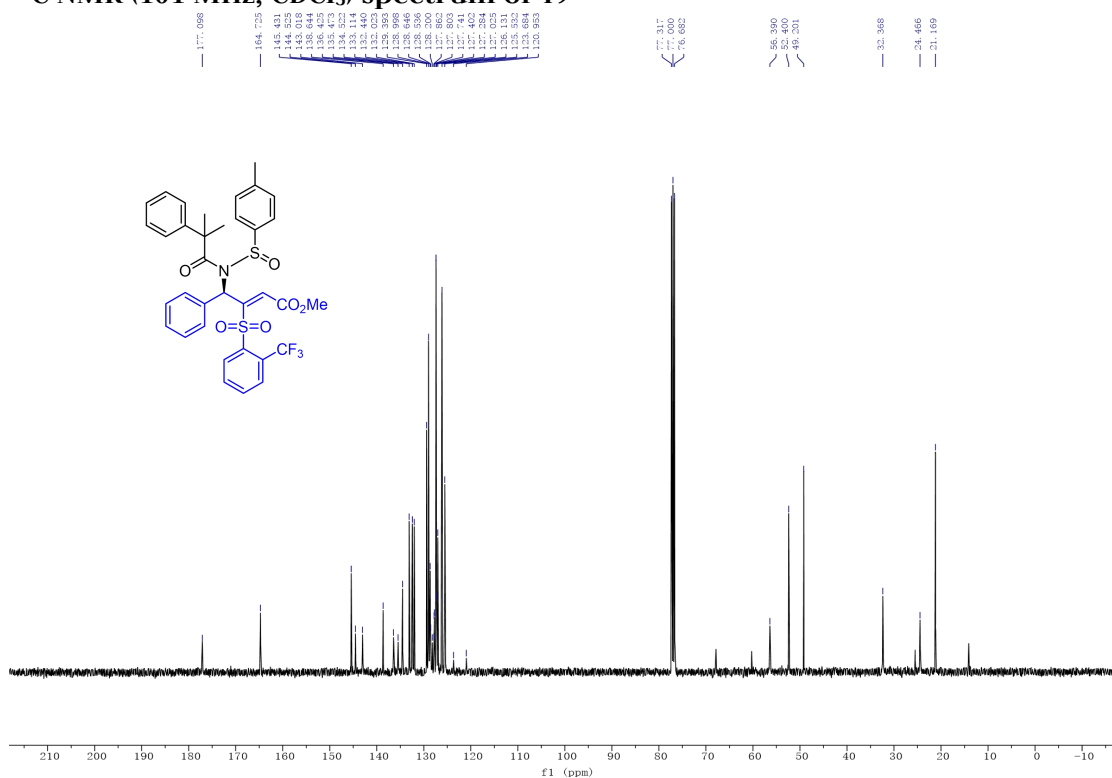
^{13}C NMR (101 MHz, CDCl_3) spectrum of 48



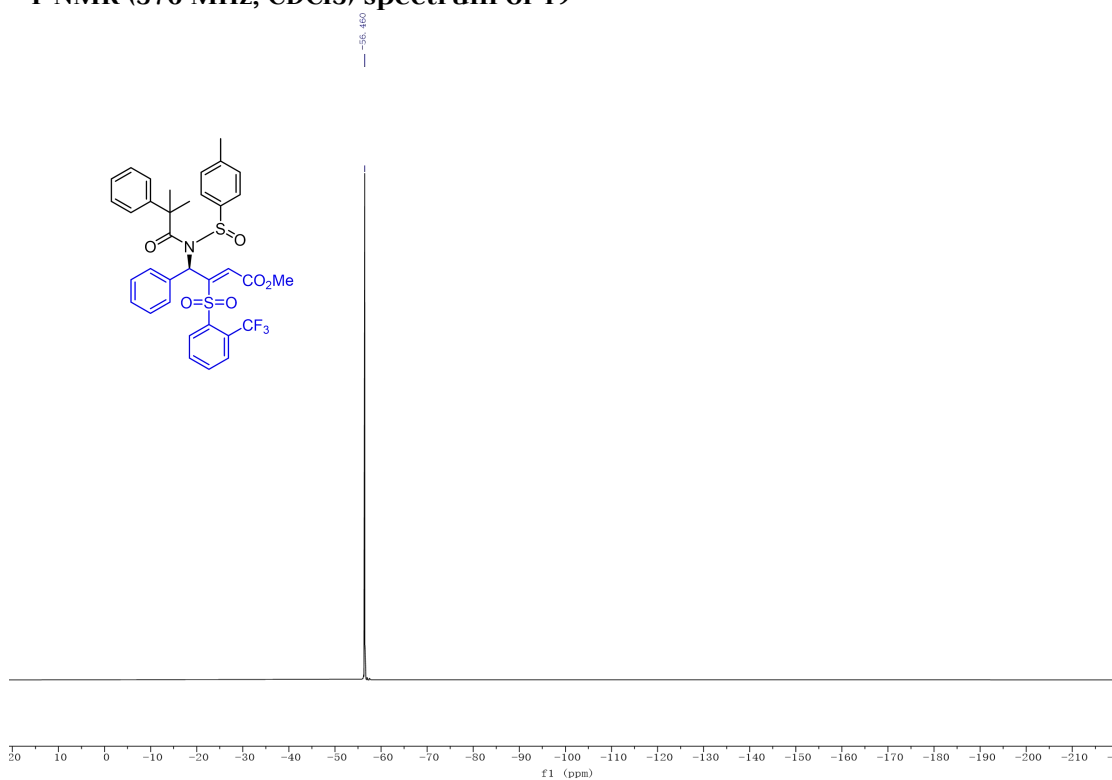
Chemical structure of the compound is shown above the spectrum. The structure is a complex molecule featuring a central carbon atom bonded to a phenyl group, a sulfonamide group (SO₂CF₃), a methoxycarbonyl group (CO₂Me), and a chiral auxiliary group (a cyclopropane ring substituted with a phenyl group and a 4-methylphenyl group).

[illegible]

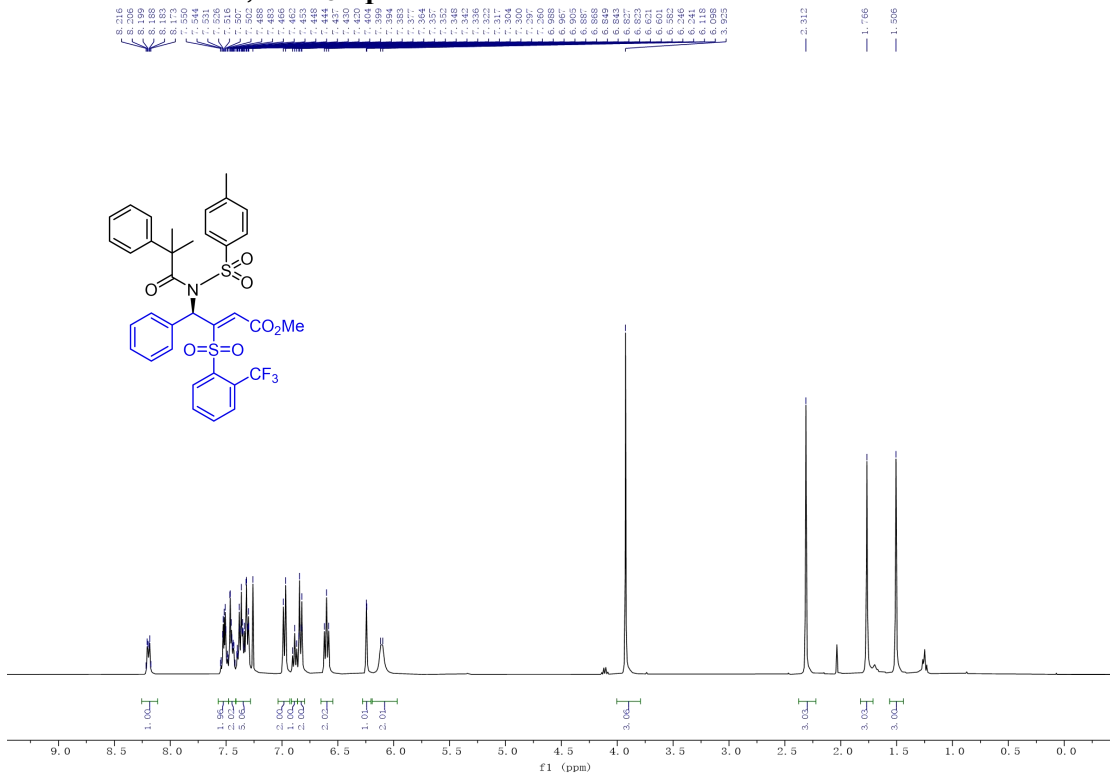
¹³C NMR (101 MHz, CDCl₃) spectrum of 49



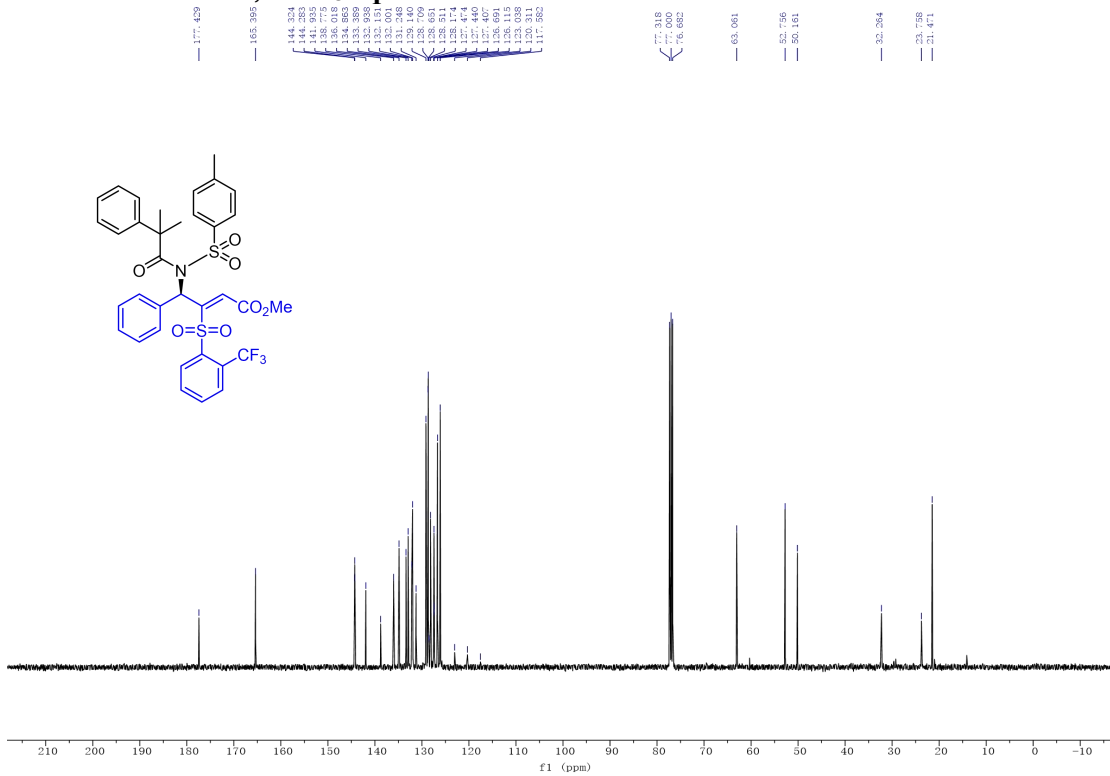
¹⁹F NMR (376 MHz, CDCl₃) spectrum of 49



¹H NMR (400 MHz, CDCl₃) spectrum of 50



¹³C NMR (101 MHz, CDCl₃) spectrum of 50



Chemical structure of the compound is shown above the spectrum. The structure is a complex molecule featuring a central carbon atom bonded to a phenyl ring, a sulfonamide group, a sulfonamide group, and a sulfonamide group. The sulfonamide groups are further substituted with a phenyl ring and a trifluoromethyl group. The spectrum shows a single sharp peak at approximately 195 ppm, indicating a highly symmetric molecule or a specific functional group.

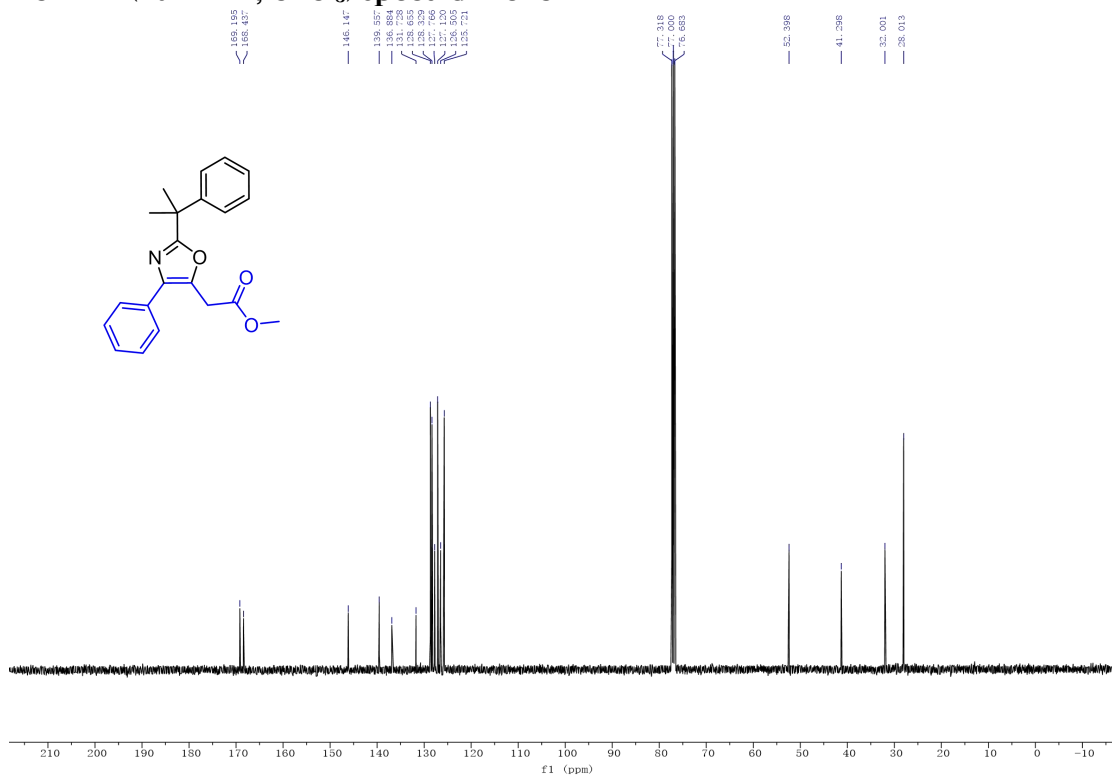
Chemical structure of compound 10: CC(C)C(c1ccccc1)c2nc(c3ccccc3)c(COC(=O)C)o2

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm (f1), ranging from 0.0 to 9.0. The spectrum shows several peaks corresponding to the structure, with integration values provided below the baseline.

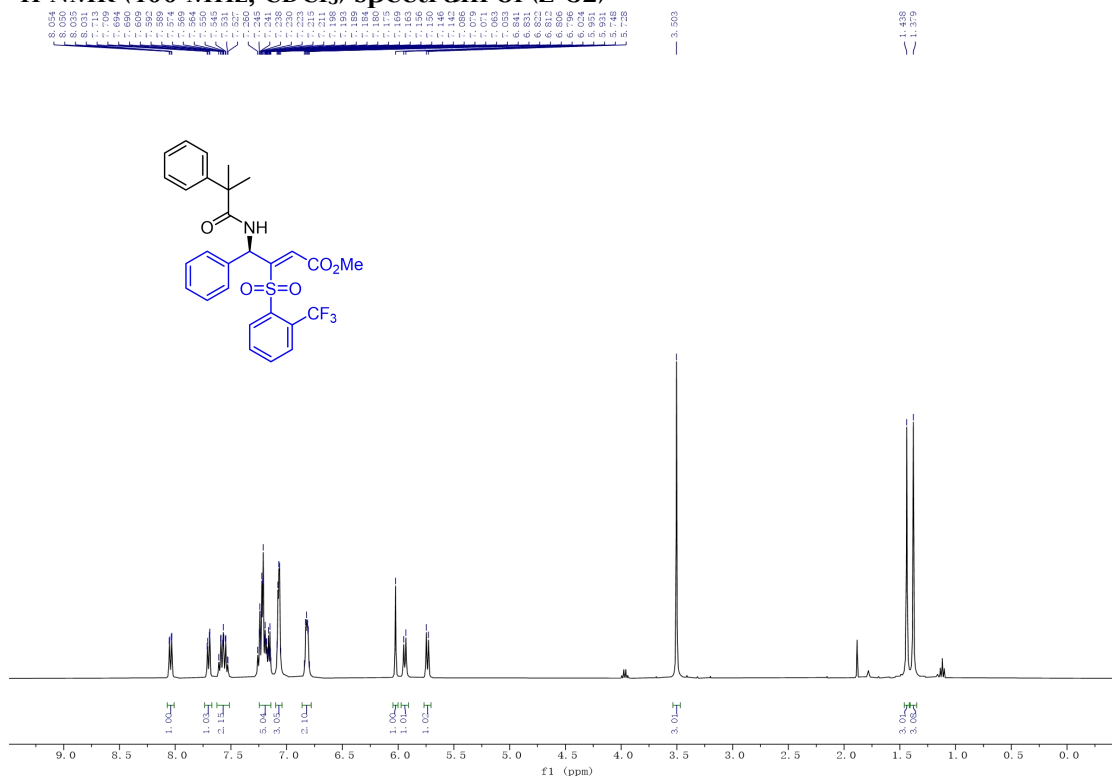
Integration values (from left to right):

- 7.69, 7.67, 7.65, 7.63, 7.61, 7.59, 7.57, 7.55, 7.53, 7.51, 7.49, 7.47, 7.45, 7.43, 7.41, 7.39, 7.37, 7.35, 7.33, 7.31, 7.29, 7.27, 7.25, 7.23, 7.21, 7.19, 7.17, 7.15, 7.13, 7.11, 7.09, 7.07, 7.05, 7.03, 7.01, 6.99, 6.97, 6.95, 6.93, 6.91, 6.89, 6.87, 6.85, 6.83, 6.81, 6.79, 6.77, 6.75, 6.73, 6.71, 6.69, 6.67, 6.65, 6.63, 6.61, 6.59, 6.57, 6.55, 6.53, 6.51, 6.49, 6.47, 6.45, 6.43, 6.41, 6.39, 6.37, 6.35, 6.33, 6.31, 6.29, 6.27, 6.25, 6.23, 6.21, 6.19, 6.17, 6.15, 6.13, 6.11, 6.09, 6.07, 6.05, 6.03, 6.01, 5.99, 5.97, 5.95, 5.93, 5.91, 5.89, 5.87, 5.85, 5.83, 5.81, 5.79, 5.77, 5.75, 5.73, 5.71, 5.69, 5.67, 5.65, 5.63, 5.61, 5.59, 5.57, 5.55, 5.53, 5.51, 5.49, 5.47, 5.45, 5.43, 5.41, 5.39, 5.37, 5.35, 5.33, 5.31, 5.29, 5.27, 5.25, 5.23, 5.21, 5.19, 5.17, 5.15, 5.13, 5.11, 5.09, 5.07, 5.05, 5.03, 5.01, 4.99, 4.97, 4.95, 4.93, 4.91, 4.89, 4.87, 4.85, 4.83, 4.81, 4.79, 4.77, 4.75, 4.73, 4.71, 4.69, 4.67, 4.65, 4.63, 4.61, 4.59, 4.57, 4.55, 4.53, 4.51, 4.49, 4.47, 4.45, 4.43, 4.41, 4.39, 4.37, 4.35, 4.33, 4.31, 4.29, 4.27, 4.25, 4.23, 4.21, 4.19, 4.17, 4.15, 4.13, 4.11, 4.09, 4.07, 4.05, 4.03, 4.01, 3.99, 3.97, 3.95, 3.93, 3.91, 3.89, 3.87, 3.85, 3.83, 3.81, 3.79, 3.77, 3.75, 3.73, 3.71, 3.69, 3.67, 3.65, 3.63, 3.61, 3.59, 3.57, 3.55, 3.53, 3.51, 3.49, 3.47, 3.45, 3.43, 3.41, 3.39, 3.37, 3.35, 3.33, 3.31, 3.29, 3.27, 3.25, 3.23, 3.21, 3.19, 3.17, 3.15, 3.13, 3.11, 3.09, 3.07, 3.05, 3.03, 3.01, 2.99, 2.97, 2.95, 2.93, 2.91, 2.89, 2.87, 2.85, 2.83, 2.81, 2.79, 2.77, 2.75, 2.73, 2.71, 2.69, 2.67, 2.65, 2.63, 2.61, 2.59, 2.57, 2.55, 2.53, 2.51, 2.49, 2.47, 2.45, 2.43, 2.41, 2.39, 2.37, 2.35, 2.33, 2.31, 2.29, 2.27, 2.25, 2.23, 2.21, 2.19, 2.17, 2.15, 2.13, 2.11, 2.09, 2.07, 2.05, 2.03, 2.01, 1.99, 1.97, 1.95, 1.93, 1.91, 1.89, 1.87, 1.85, 1.83, 1.81, 1.79, 1.77, 1.75, 1.73, 1.71, 1.69, 1.67, 1.65, 1.63, 1.61, 1.59, 1.57, 1.55, 1.53, 1.51, 1.49, 1.47, 1.45, 1.43, 1.41, 1.39, 1.37, 1.35, 1.33, 1.31, 1.29, 1.27, 1.25, 1.23, 1.21, 1.19, 1.17, 1.15, 1.13, 1.11, 1.09, 1.07, 1.05, 1.03, 1.01, 0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87, 0.85, 0.83, 0.81, 0.79, 0.77, 0.75, 0.73, 0.71, 0.69, 0.67, 0.65, 0.63, 0.61, 0.59, 0.57, 0.55, 0.53, 0.51, 0.49, 0.47, 0.45, 0.43, 0.41, 0.39, 0.37, 0.35, 0.33, 0.31, 0.29, 0.27, 0.25, 0.23, 0.21, 0.19, 0.17, 0.15, 0.13, 0.11, 0.09, 0.07, 0.05, 0.03, 0.01, 0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87, 0.85, 0.83, 0.81, 0.79, 0.77, 0.75, 0.73, 0.71, 0.69, 0.67, 0.65, 0.63, 0.61, 0.59, 0.57, 0.55, 0.53, 0.51, 0.49, 0.47, 0.45, 0.43, 0.41, 0.39, 0.37, 0.35, 0.33, 0.31, 0.29, 0.27, 0.25, 0.23, 0.21, 0.19, 0.17, 0.15, 0.13, 0.11, 0.09, 0.07, 0.05, 0.03, 0.01

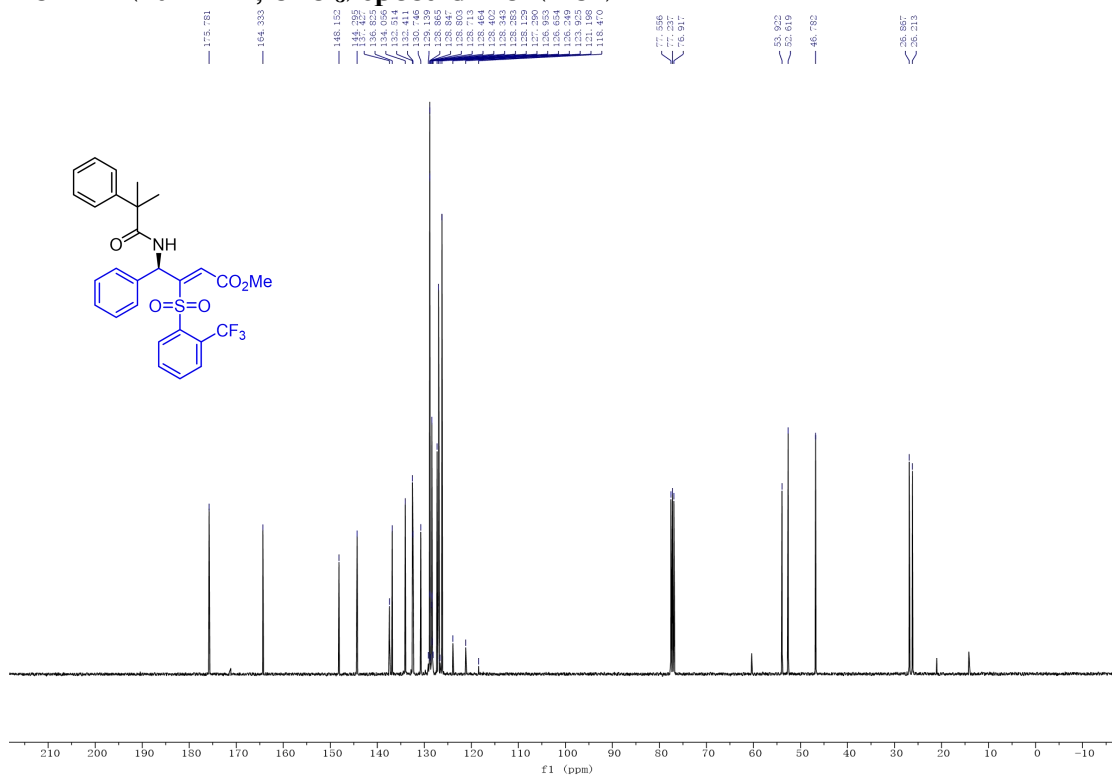
¹³C NMR (101 MHz, CDCl₃) spectrum of 51



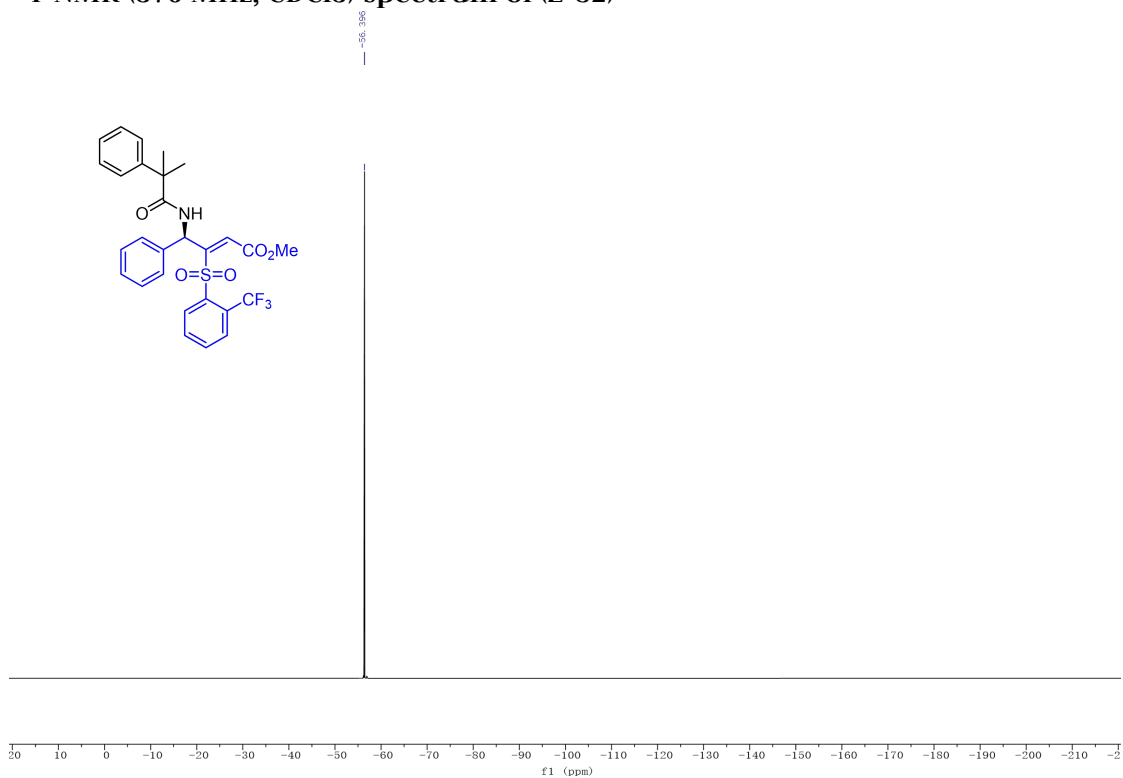
¹H NMR (400 MHz, CDCl₃) spectrum of (Z)-52



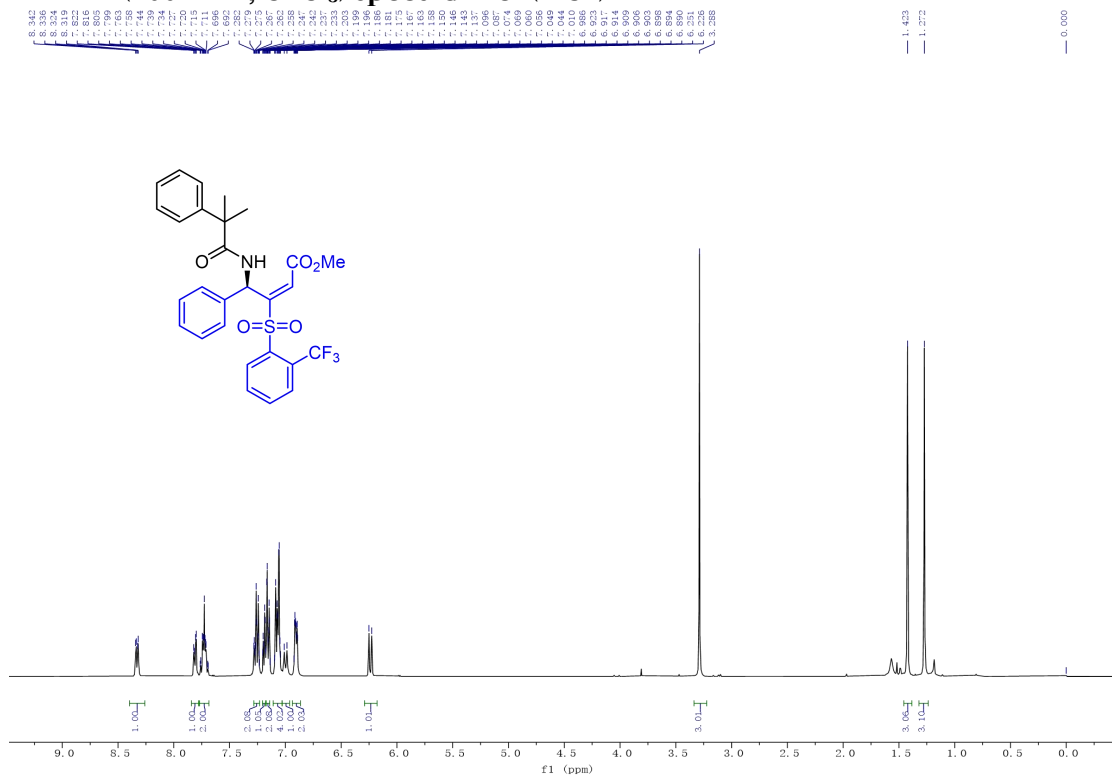
^{13}C NMR (101 MHz, CDCl_3) spectrum of (Z-52)



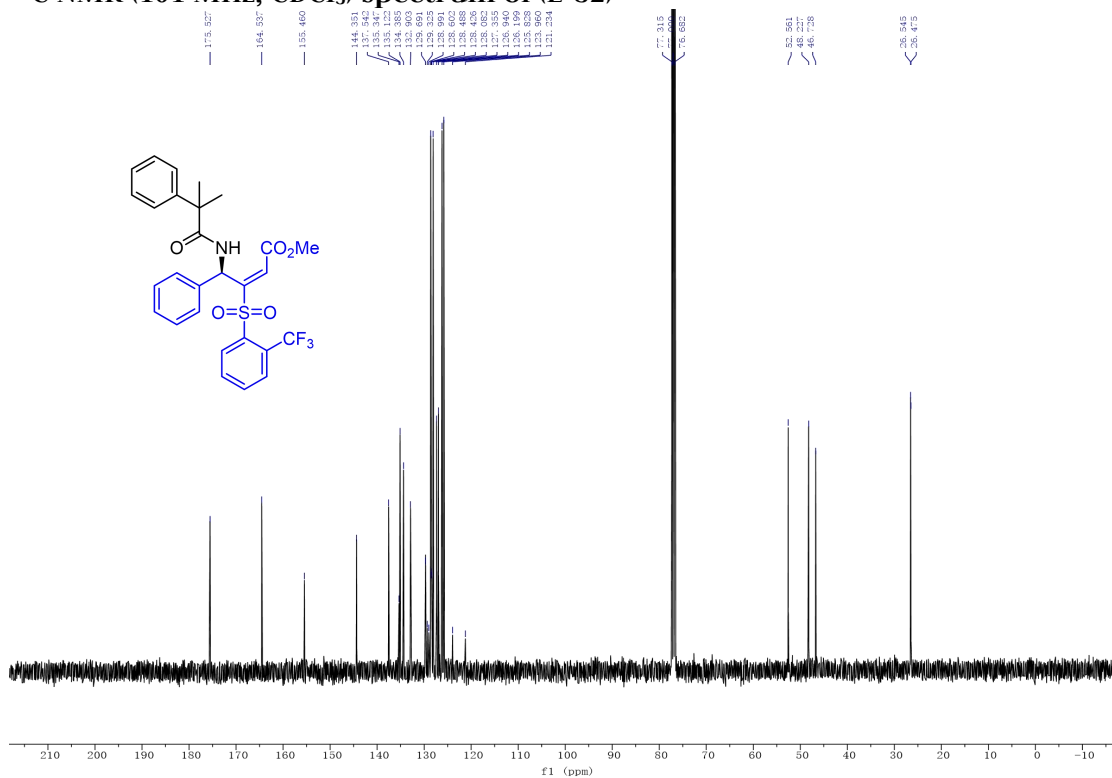
¹⁹F NMR (376 MHz, CDCl₃) spectrum of (Z-52)



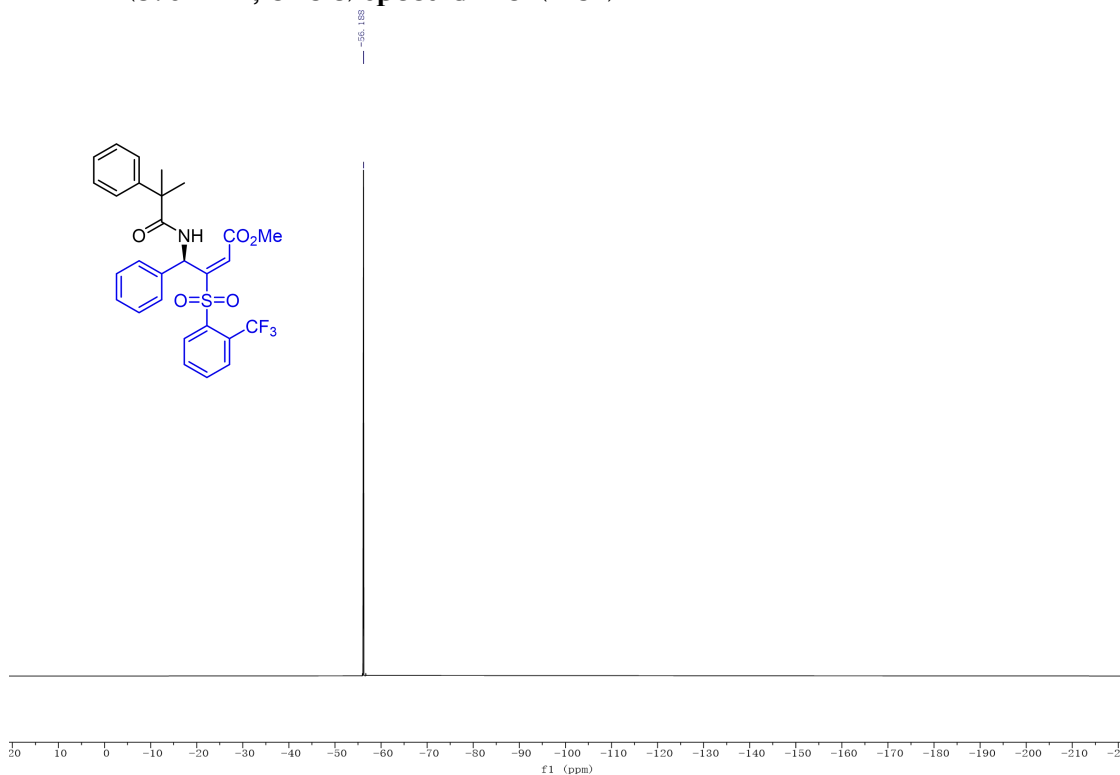
¹H NMR (400 MHz, CDCl₃) spectrum of (E-52)



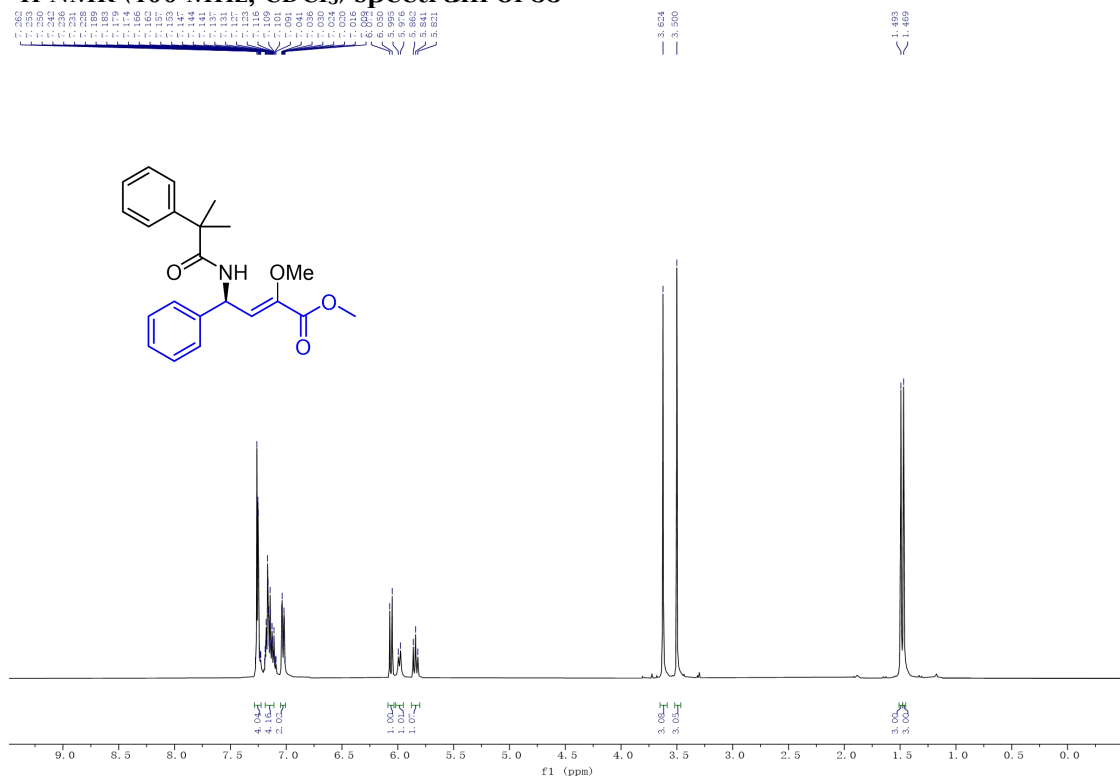
¹³C NMR (101 MHz, CDCl₃) spectrum of (E-52)



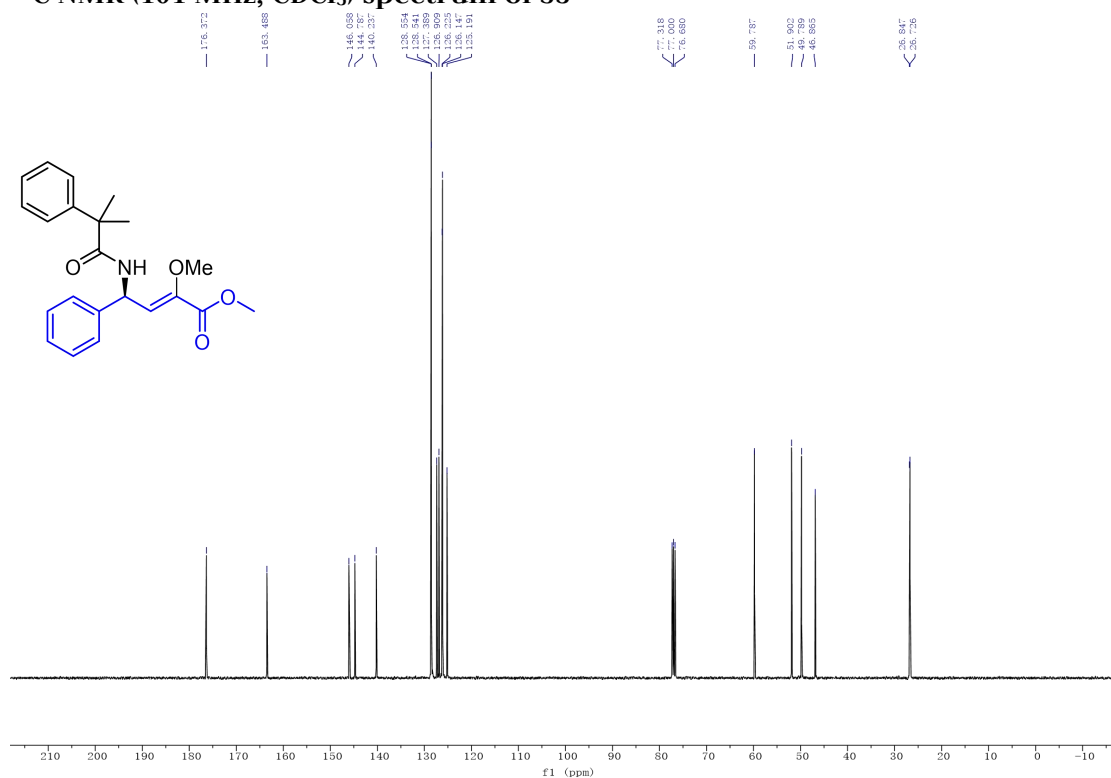
¹⁹F NMR (376 MHz, CDCl₃) spectrum of (E-52)



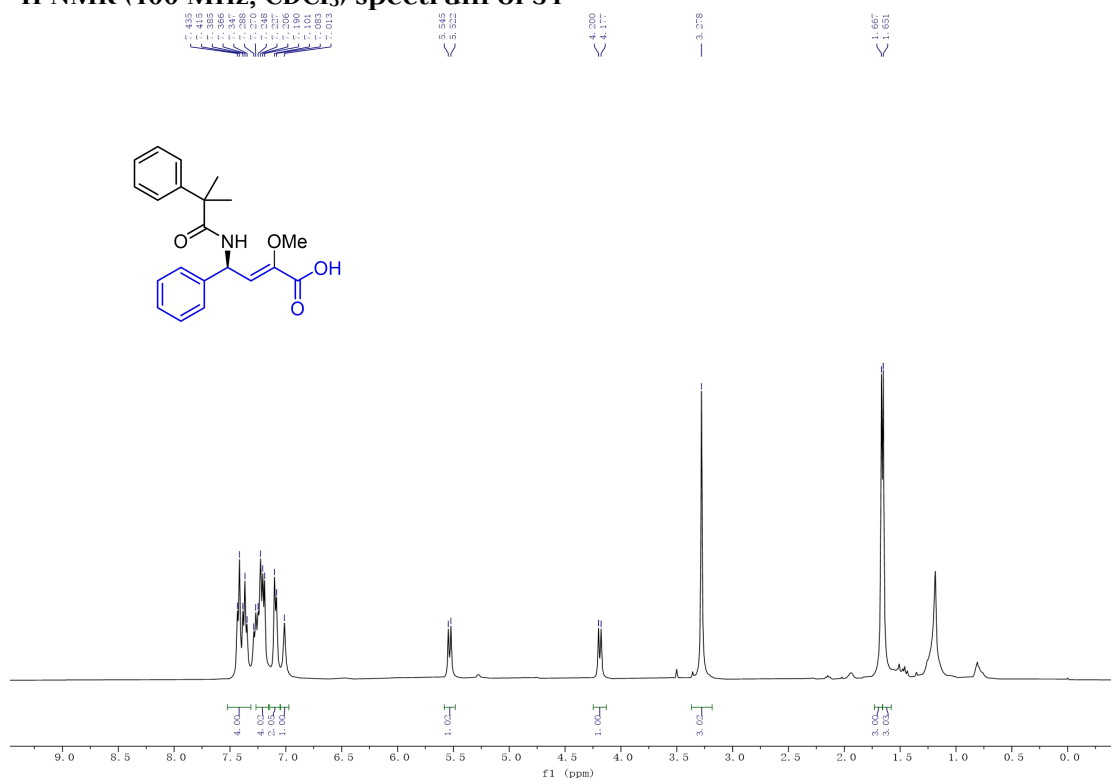
¹H NMR (400 MHz, CDCl₃) spectrum of 53



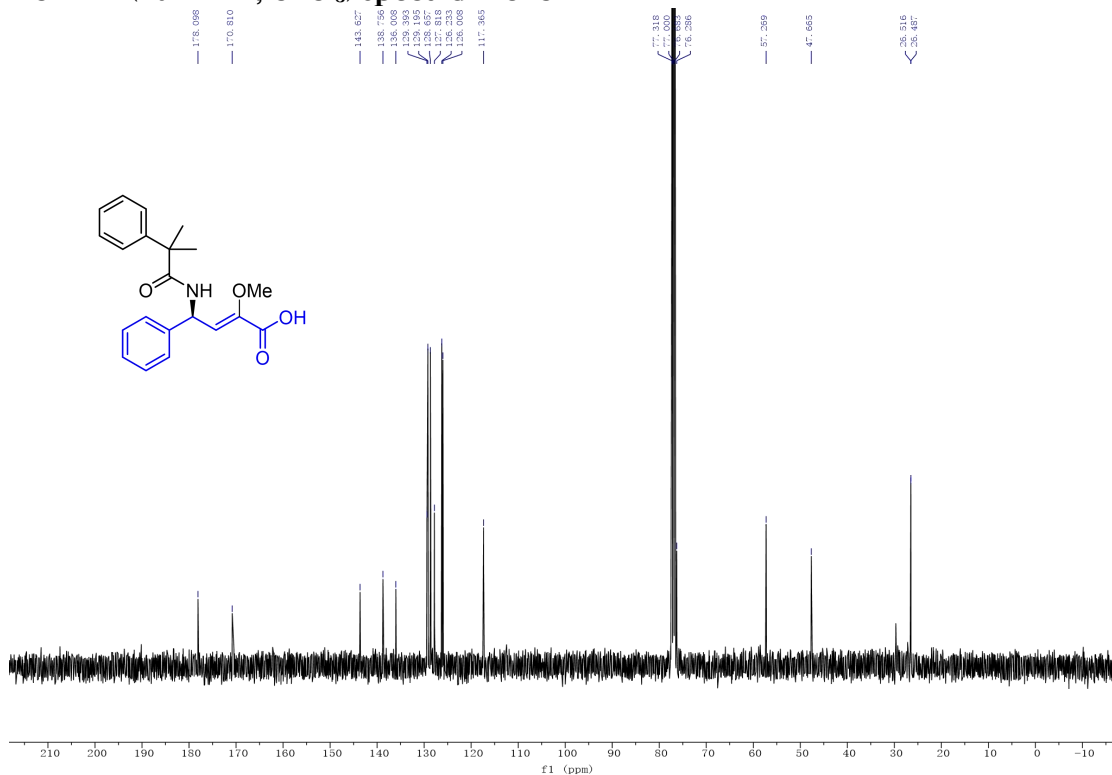
^{13}C NMR (101 MHz, CDCl_3) spectrum of 53



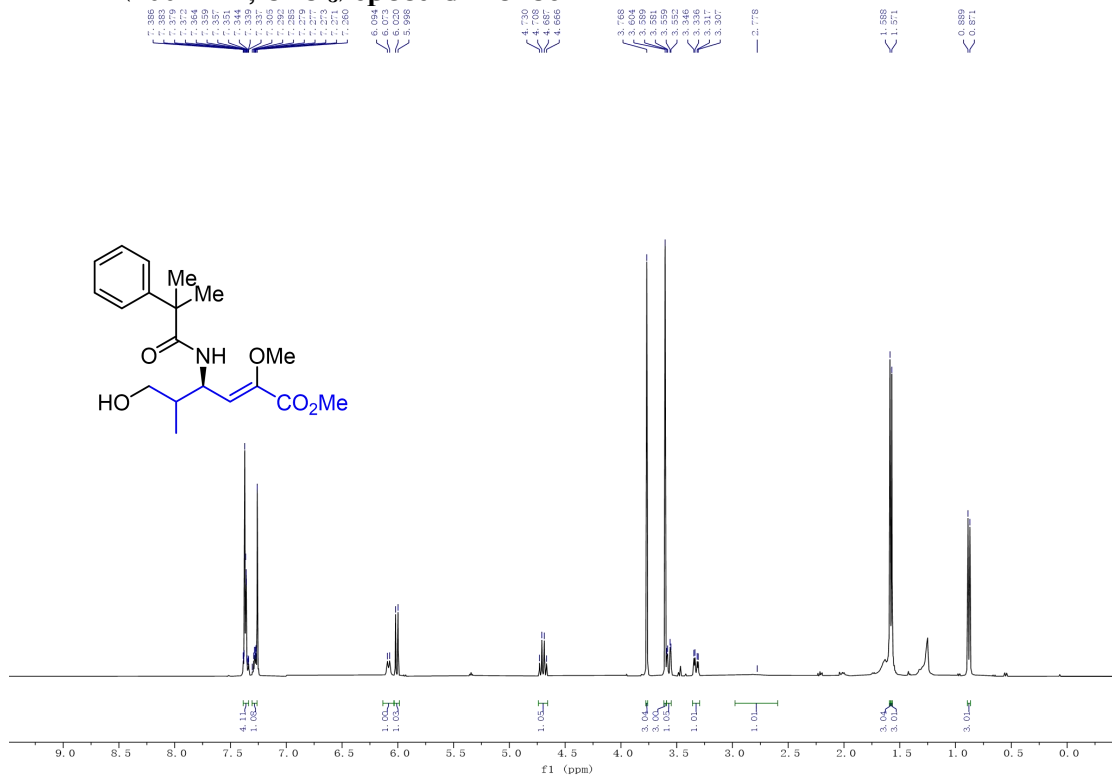
^1H NMR (400 MHz, CDCl_3) spectrum of 54



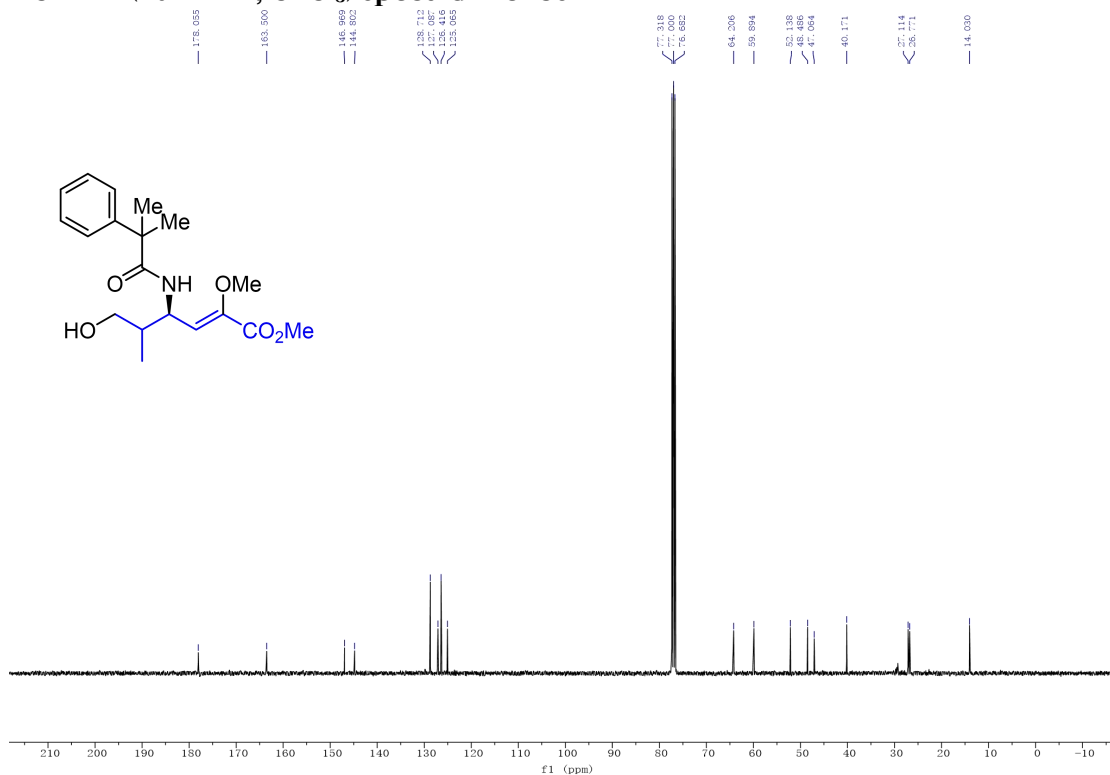
^{13}C NMR (101 MHz, CDCl_3) spectrum of 54



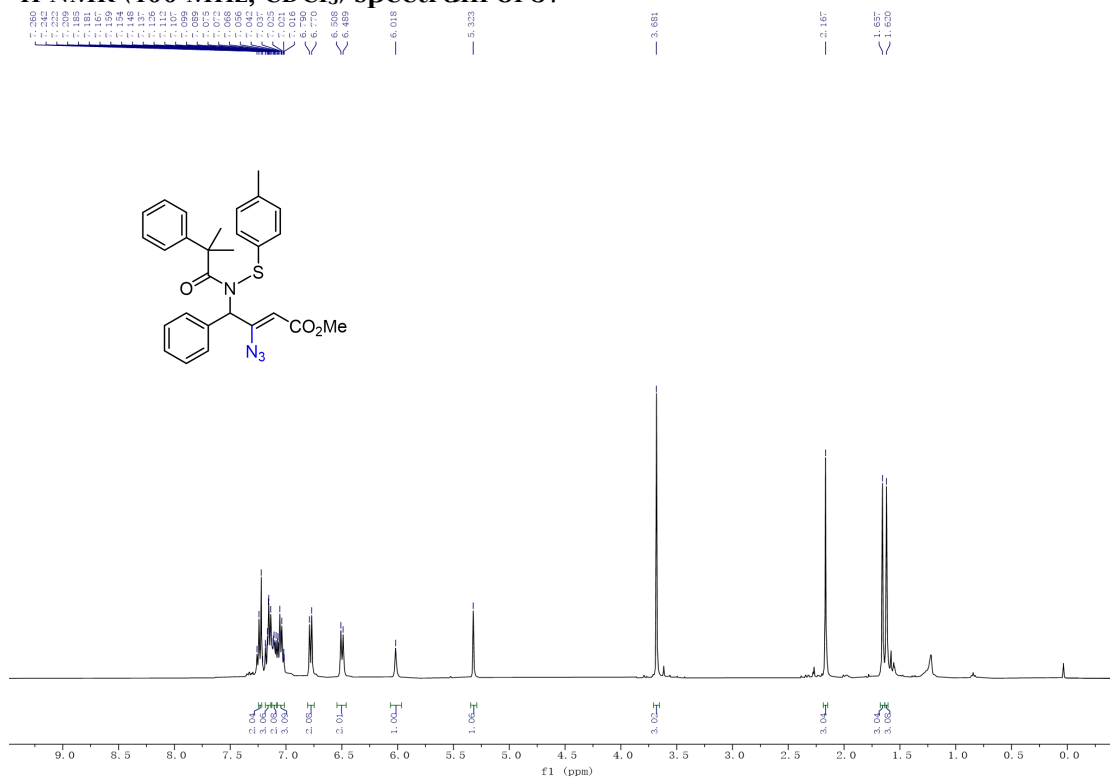
^1H NMR (400 MHz, CDCl_3) spectrum of 56



¹³C NMR (101 MHz, CDCl₃) spectrum of 56



¹H NMR (400 MHz, CDCl₃) spectrum of 57



¹³C NMR (101 MHz, CDCl₃) spectrum of 57

