Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.
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Supplementary Information

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1. General information

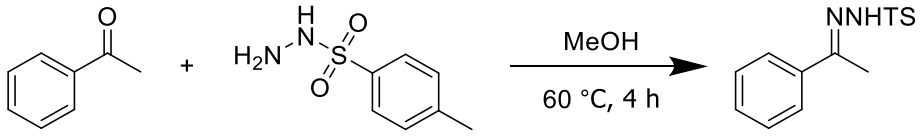
1.1 General reagent information

Dichloromethane (DCM) was distilled from CaH_2 before use. Other reagents and solvents were of commercial grade and were used without further purification.

1.2 General analytical information

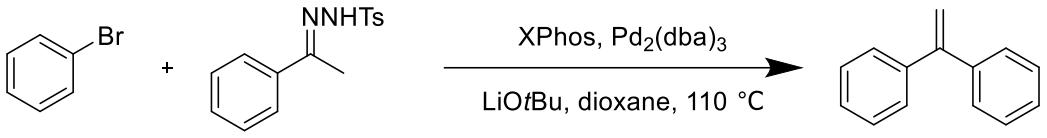
Nuclear magnetic resonance (NMR) was recorded on an Advance III 600 MHz Bruker spectrometer at 298 K. ^{1}H NMR signals were measured relative to the signal for residual chloroform (7.26 ppm) in $CDCl_3$, and are reported in δ units, parts per million (ppm). ^{13}C NMR signals were reported in ppm units relative to $CDCl_3$ (77.16 ppm), and obtained with 1H decoupling. Copies of ^{1}H NMR and ^{13}C NMR spectra of unknown compounds can be found at the end of the supplementary information. The melting points (m.p.) were measured by the XT-4A melting point apparatus without correction. Gas chromatography (GC) measurements were carried out on SHIMADZU GC-2014 instrument using achiral capillary columns. High-resolution mass spectrometry (HRMS) was performed by liquid chromatography/mass selective detector time-of-flight (LC/MSD TOF) using an Agilent instrument. The reactions were monitored by thin-layer chromatography (TLC) using silica gel GF254. Column chromatography was performed with 200–300 mesh silica gel. All yields refer to isolated products after purification.

2. Synthesis and characterization of substrate[1]



General procedure: A 100 mL round bottom flask equipped with a stir bar was charged with acetophenone (6.01 g, 50 mmol), *p*-toluenesulfonyl hydrazide (10.24 g, 55 mmol) and 100 mL MeOH. After stirring at 60 ºC for 4 h, a white powder is

precipitated and the target compound (12.40 g, 86%) is obtained by suction filtration.



General procedure: An oven-dried schlenk tube equipped with a stir bar was charged with acetophenone tosylhydrazone (4.76 g, 16.5 mmol), $Pd_2(dba)_3$ (138.3 mg, 0.15 mmol), XPhos (143.0 mg, 0.3 mmol,) and Li*O*t*B*u (2.64 g, 33 mmol) under N_2. A solution of bromobenzene (2.36 g, 15 mmol) in 100 mL dry dioxane was added via a syringe into the tube under N_2. Then, the reaction mixture was stirred at 110 ºC for 7 h. The obtained residue was purified by flash column chromatography over silica gel (eluting with petroleum ether) to give target compound (2.22 g, 82%).

3. Experimental procedures of flow synthesis

3.1 General material Information

All tubing, connectors, nuts, ferrules, fittings and back-pressure regulators were purchased from IDEX Health and Science. Syringe pumps were purchased from Longer company. The equipment configurations that were used for the flow reactions are depicted in Figure S1. The tubing reactors and all connecting tubing were made of PFA plastic tubing (ID = 1.0 mm, OD = 1.6 mm). Connections for all reactors were made using super flangeless ferrules and super flangeless nuts. The mixers and backpressure regulators used in this work were made of PEEK. Ice water bath were used for keeping the temperature at 0 ºC.

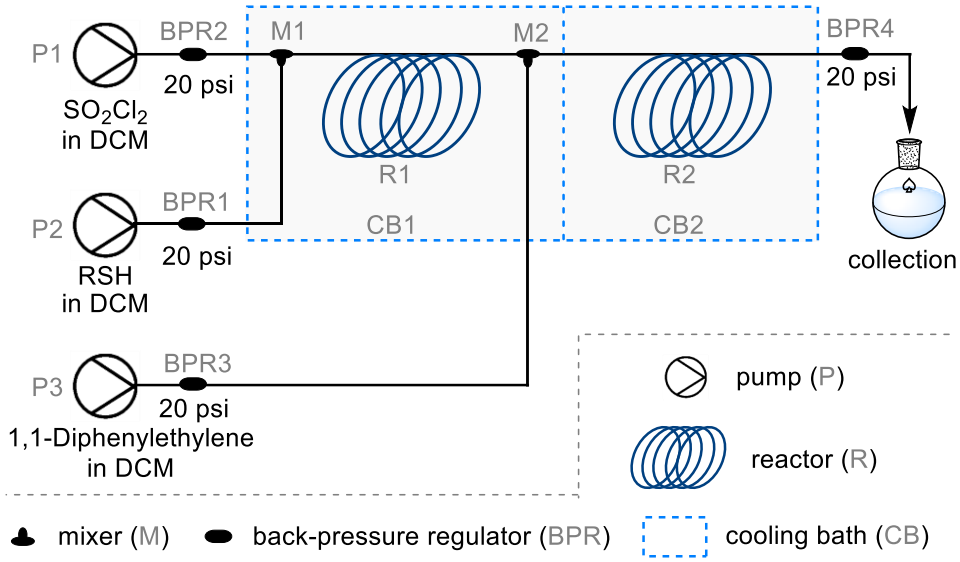


Figure S1. Flow setup for the synthesis

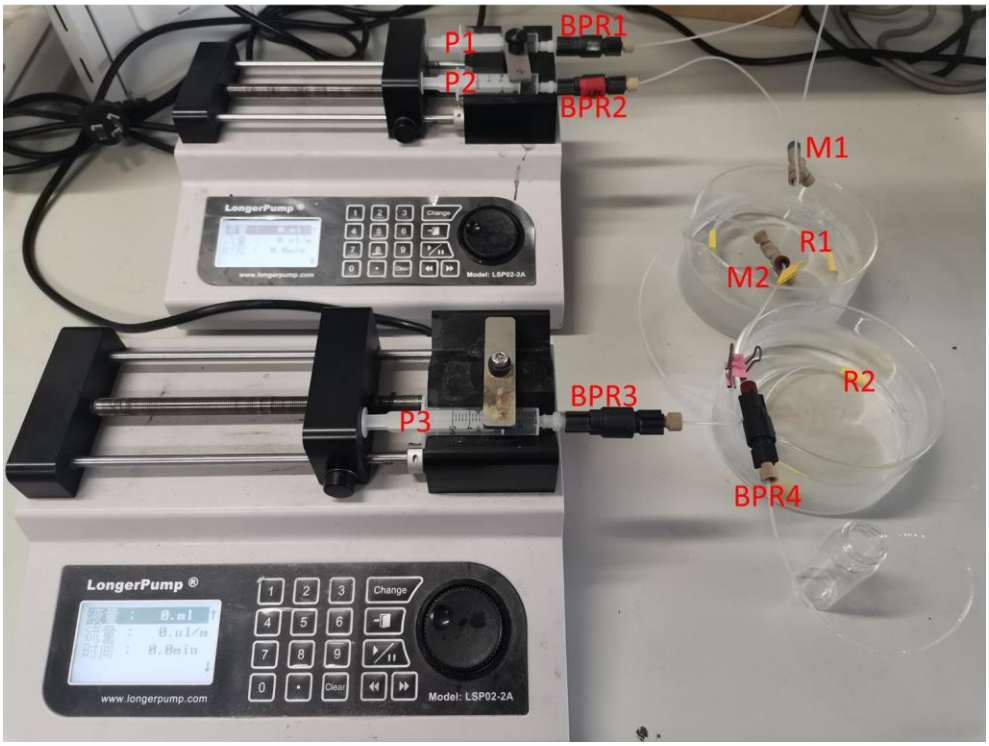


Figure S2. Flow system

3.2 General procedure of flow synthesis

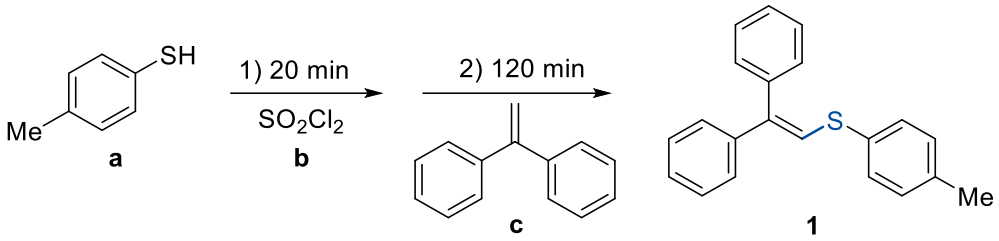
Syringe A was loaded with the solution of *p*-toluenethiol **a** (0.5-1.0 M) in anhydrous DCM, and fitted to a syringe pump 1 (P1). Syringe B was loaded with the solution of SO_2Cl_2 **b** (0.5-1.05 M) in anhydrous DCM, and fitted to a same syringe pump 2 (P2). Syringe C was loaded with the solution of 1,1-diphenylethylene **c** (0.5 M) in anhydrous DCM, and fitted to the second syringe pump 3 (P3). Following the setup as shown in Figure S1, solutions of *p*-toluenethiol and SO_2Cl_2 were mixed and reacted in tubing reactor R1 submerged in ice water bath. When the reaction was complete, the resulting solution was mixed with the solution of 1,1-diphenylethylene and reacted in tubing reactor R2 submerged in ice water bath. After reaction, the resulting mixture was passed through a back-pressure regulator (BPR4, 20 psi) before collection. After reaching the steady state in 10 min (monitored by GC), 0.5-2.0 mmol samples were collected. The separated organic phase was washed with brine and $NaHCO_3$, dried over Na_2SO_4 and concentrated under vacuum. The resulting residue was purified by column chromatography. A small aliquot of the resulting mixture was directly analyzed with TLC and GC.

Table S1 Optimization of the flow conditions

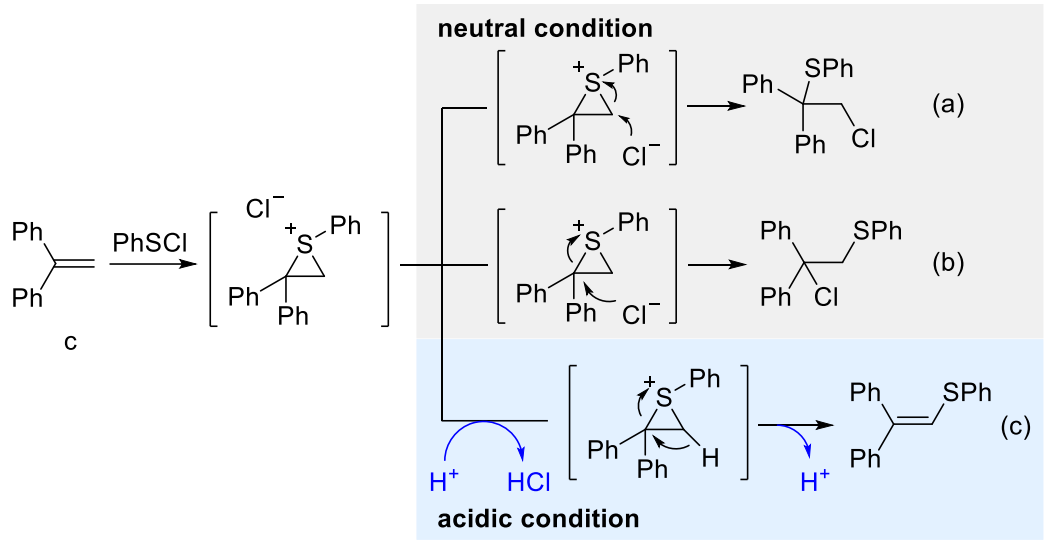
Entry	Concentration (mmol/mL)			Flow rate (μL/min)			Volume of reactor (mL)	
	a	**b**	**c**	**a**	**b**	**c**	R_1	R_2
1	1	1.05	1	10	10	10	2	3
2	1	1.05	1	10	10	10	4	5
3	1	1.05	1	10	10	20	4	6
4	2	2.1	1	10	10	20	4	6
5	1.5	1.5	1	10	10	20	4	6

4. Experimental procedures for the two-step synthesis under batch conditions

Taking the synthesis of compound 1 as an example (Table 1, entry 4)



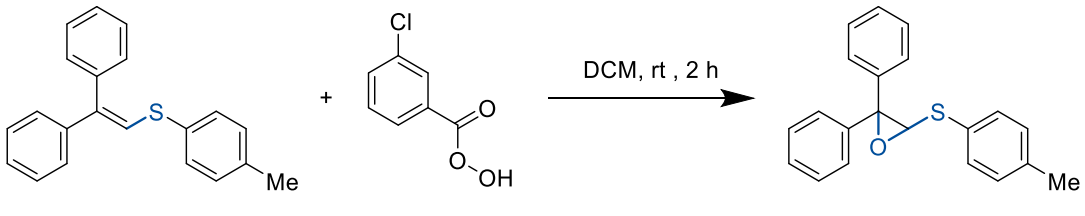
An oven-dried flask equipped with a stir bar was charged with *p*-toluenethiol **a** (248.4 mg, 2 mmol) and 2 mL anhydrous DCM at 0 ºC. 2 mL SO_2Cl_2 **b** (1.05 M) in DCM was dropwise added into the flask under nitrogen atmosphere at -20 ºC. The color of the solution changes to yellow. The mixture was stirred at -20 ºC for 20 min to afford the complete conversion of *p*-toluenethiol as monitored by TLC analysis before next step. Then, 1,1-diphenylethylene **c** (1 mmol) was dropwise added into the flask at -20 ºC. After stirring at -20 ºC for 120 min, the mixture was extracted with DCM. The obtained organic layer was dried over Na_2SO_4 and concentrated under vacuum. The obtained residue was purified by flash column chromatography over silica gel (eluting with petroleum ether) to give target compound **1** (101.2 mg, 50%) as a white solid.



Scheme S1. Proposed reaction mechanism. The reaction between alkene **c** and PhSCl would first generate a thiiranium ion intermediate.[2, 3] Under neutral conditions, the intermediate would be attacked by the chloride anion via pathway a or b from different directions, resulting in addition products. Under acidic conditions, the nucleophilicity of chloride anion was reduced. As driven by the ring strain and electron-withdrawing property of the thiiranium ion intermediate, a proton would be eliminated to regenerate a carbon-carbon double bond. The $pK_{a,DCE}$ value of HCl is 45.2 at 25 °C in 1,2-dichloroethane[4] (for other substances, $HClO_4$, $pK_{a,DCE}$ = 32.2; TfOH, $pK_{a,DCE}$ = 33.7, HBF_4 = 35.0, etc.), suggesting that chloride anion could act as a weak base in nonpolar solvent.

5. Synthesis of expansion of target compounds

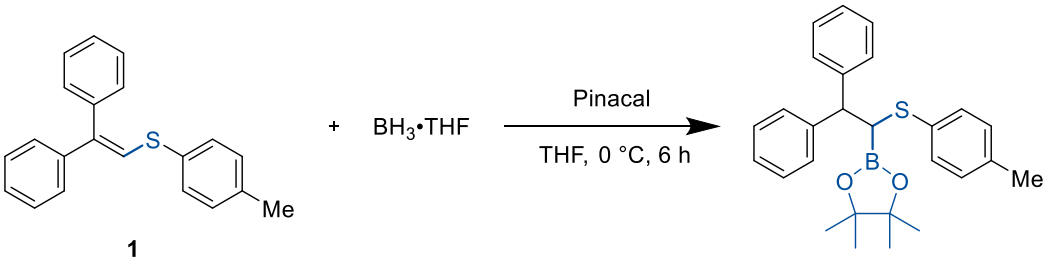
5.1 Synthesis and characterization of epoxidation product of 1[5]



1

An oven-dried flask equipped with a stir bar was charged with **1** (302.4 mg, 1.0 mmol) in DCM (10 mL) and *m*-CPBA (345.2 mg, 2.0 mmol) at room temperature (rt). The reaction mixture was stirred for 2 h. After reaction, the reaction was quenched by saturated aqueous Na_2SO_3 (5 mL) and treated with DCM. The separated organic phase was washed with brine, dried over Na_2SO_4 and concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel (eluting with 0-20% ethyl acetate in petroleum ether) to afford the desired epoxide product (280.2 mg, 88%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.50 – 7.44 (m, 2 H), 7.40 – 7.32 (m, 2 H), 7.29 (m, 4 H), 7.22 – 7.17 (m, 2 H), 7.14 (d, *J* = 7.8 Hz, 2 H), 7.12 – 7.06 (m, 2 H), 6.99 (s, 1 H), 2.37 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 154.70, 143.75, 139.28, 138.70, 135.61, 130.22, 129.79, 129.34, 129.02, 128.84, 128.58, 128.21, 127.81, 127.72, 21.55 ppm.

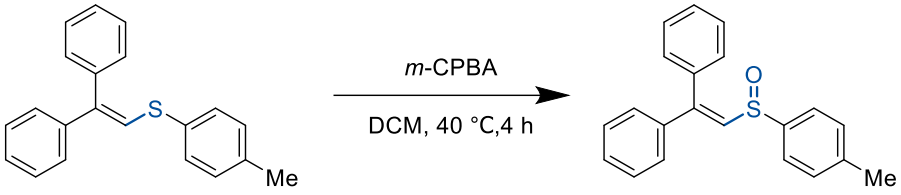
5.2 Synthesis and characterization of pinacolborane product of 1[6]



An oven-dried flask equipped with a stir bar was charged with **1** (302.4 mg, 1.0 mmol) in dry THF (10 mL) and added BH_3·THF (1.0 M, 3.0 mL) at 0 ºC. The reaction mixture was stirred for 4 h at rt. and then the reaction was added pinacal (236.2 mg, 2.0 mmol) at 0 ºC. The reaction mixture was stirred for 4 h at rt., After reaction, the reaction was treated with DCM. The separated organic phase was washed with brine, dried over Na_2SO_4 and concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel (eluting with 0-20% ethyl acetate in petroleum ether) to afford the target product (365.8 mg, 85%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.38 – 7.29 (m, 4 H), 7.27 – 7.15 (m, 6 H), 7.12 (m, 2 H), 7.01 – 6.86 (m, 2 H), 4.19 (s, 1 H), 3.49 (s, 1 H), 2.25 (s, 3

H), 0.87 (s, 6 H), 0.83 (s, 6 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 144.00, 143.05, 136.57, 132.60, 132.16, 129.26, 129.24, 128.44, 128.43, 128.40, 128.38, 128.09, 128.08, 128.05, 126.65, 126.53, 83.68, 83.66, 53.20, 24.37, 24.35, 24.32, 24.30, 21.07 ppm.

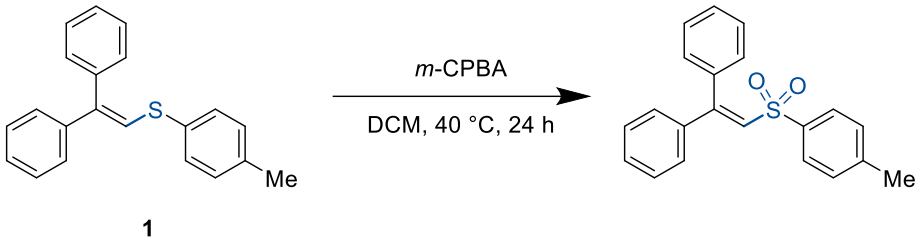
5.3 Synthesis and characterization of pinacolborane product of 1[7]



1

An oven-dried flask equipped with a stir bar was charged with **1** (302.4 mg, 1.0 mmol) and *m*-chloroperoxybenzoic acid (172.6 mg, 1.0 mmol). The reaction mixture was heated at reflux for 4 h. After the mixture was left to room temperature, the reaction was quenched with saturated sodium hydrogen carbonate solution (15 mL) and treated with DCM. The separated organic phase was washed with brine, dried over Na_2SO_4 and concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel (eluting with 0-10% ethyl acetate in petroleum ether) to afford the desired epoxide product (273.8 mg, 86%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.57 (d, J = 7.8 Hz, 2 H), 7.46 (dd, J = 3.0, 1.2 Hz, 3 H), 7.36 (m, 3 H), 7.34 – 7.28 (m, 4 H), 7.28 – 7.24 (m, 2 H), 6.84 (d, J = 1.2 Hz, 1 H), 2.41 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 152.41, 141.42, 139.07, 137.08, 133.58, 133.07, 130.20, 130.14, 129.76, 129.65, 129.19, 128.53, 128.45, 128.41, 128.15, 124.73, 21.43 ppm.

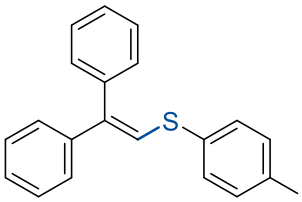
5.4 Synthesis and characterization of pinacolborane product of 1[8]



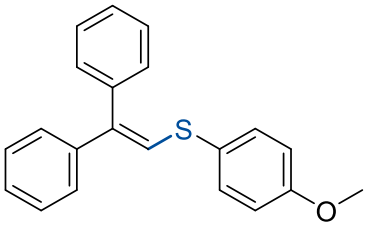
1

An oven-dried flask equipped with a stir bar was charged with **1** (302.4 mg, 1.0 mmol) and *m*-CPBA (862.8 mg, 5.0 mmol) in dry DCM (20 ml) and heated to reflux for 24 h under nitrogen atmosphere. After cooling, the reaction was treated with DCM. The separated organic phase was washed with brine, dried over Na_2SO_4 and concentrated under vacuum. The crude product was purified by flash column chromatography on silica gel (eluting with 0-10% ethyl acetate in petroleum ether) to afford the desired epoxide product (274.2 mg, 82%) . ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.47 (d, *J* = 8.4 Hz, 2 H), 7.36 (dd, *J* = 7.8, 6.0 Hz, 2 H), 7.32 – 7.27 (m, 4 H), 7.20 (dd, *J* = 7.8, 1.8 Hz, 2 H), 7.15 (d, *J* = 7.8 Hz, 2 H), 7.10 (dd, *J* = 8.4, 1.2 Hz, 2 H), 6.99 (s, 1 H), 2.37 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 154.70, 143.74, 139.28, 138.71, 135.61, 130.21, 129.79, 129.33, 129.02, 128.83, 128.57, 128.21, 127.81, 127.71, 21.54 ppm.

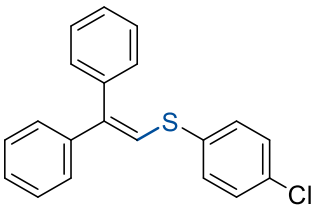
6. Characterization results for Table 2



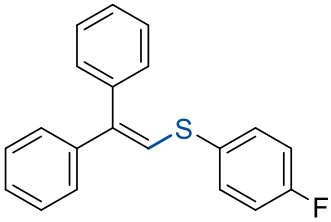
1[9] The target compound was isolated (244.7 mg, 81%) as a white solid by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.45 – 7.39 (m, 2 H), 7.37 – 7.32 (m, 5 H), 7.26 (d, *J* = 7.2 Hz, 3 H), 7.24 – 7.19 (m, 2 H), 7.14 (d, *J* = 7.8 Hz, 2 H), 6.82 (s, 1 H), 2.33 (s, 3 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ: 141.60, 140.24, 139.30, 137.04, 132.89, 130.13, 129.93, 129.82, 128.41, 128.31, 127.77, 127.25, 127.19, 125.28, 21.09. ppm.



2[9] The target compound was isolated (248.4 mg, 78%) as a white solid by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.44 – 7.40 (m, 4 H), 7.38 – 7.35 (m, 3 H), 7.29 – 7.25 (m, 2 H), 7.24 – 7.20 (m, 3 H), 6.88 (d, *J* = 9.0 Hz, 2 H), 6.77 (s, 1 H), 3.81 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 159.35, 141.60, 139.32, 139.30, 132.60, 129.83, 128.43, 128.31, 127.75, 127.17, 127.11 126.90, 126.61, 114.86, 55.42. ppm.

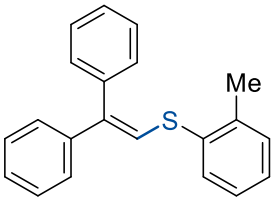


3[9] The target compound was isolated (242.1 mg, 75%) as a white solid by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.42 (t, *J* = 7.2 Hz, 2 H), 7.37 – 7.32 (m, 5 H), 7.31 – 7.27 (m, 4 H), 7.25 (t, *J* = 8.4 Hz, 3 H), 6.77 (s, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 142.01, 141.28, 139.03, 135.11, 132.85, 130.74, 129.74, 129.30, 128.47, 128.41, 128.00, 127.55, 127.27, 123.24 ppm.

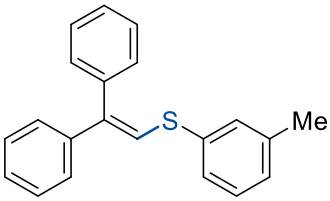


4 The target compound was isolated (223.7 mg, 73%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 76.5 – 77.1 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.42 (m, 4 H), 7.39 – 7.31 (m, 3 H), 7.30 – 7.26 (m, 2 H), 7.26 – 7.21 (m, 3 H), 7.08 – 6.99 (m, 2

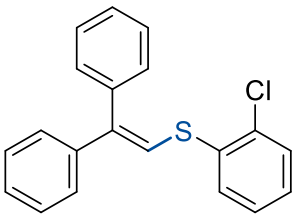
H), 6.76 (s, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 162.16 (d, *J* = 246.0 Hz), 141.36, 140.91, 139.09, 132.10 (d, *J* = 7.5 Hz), 132.07, 131.54, 129.75, 128.45, 128.36, 127.91, 127.38, 127.21, 124.66, 116.29 (d, *J* = 22.5 Hz) ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ: -114.60 ppm. HRMS (ESI): m/z calculated for $C_{20}H_{16}FS^+$ [M+H$^+$]: 307.0951, found: 307.0950.



5[9] The target compound was isolated (263.1 mg, 87%) as a white solid by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.50 – 7.45 (m, 1 H), 7.42 (t, *J* = 7.2 Hz, 2 H), 7.39 – 7.33 (m, 3 H), 7.30 – 7.21 (m, 5 H), 7.21 – 7.14 (m, 3 H), 6.75 (s, 1 H), 2.38 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 141.64, 141.39, 139.30, 138.35, 135.66, 130.39, 130.34, 129.84, 128.42, 128.34, 127.79, 127.31, 127.23, 127.12, 126.73, 124.32, 20.70 ppm.

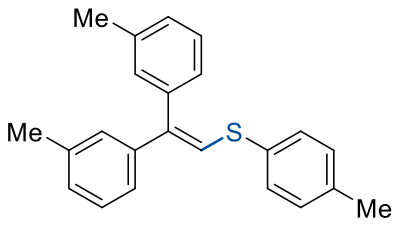


6[9] The target compound was isolated (235.9 mg, 78%) as a white solid by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.45 – 7.39 (m, 2 H), 7.39 – 7.32 (m, 3 H), 7.29 – 7.20 (m, 8 H), 7.09 – 7.01 (m, 1 H), 6.86 (s, 1 H), 2.34 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 141.58, 140.79, 139.29, 139.04, 136.22, 130.24, 129.83, 129.01, 128.45, 128.36, 127.82, 127.76, 127.30, 127.24, 126.69, 124.45, 21.42 ppm.

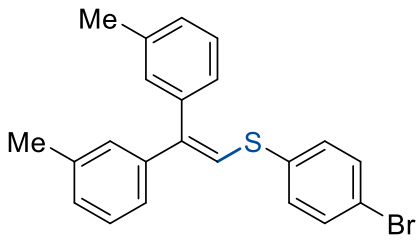


7 The target compound was isolated (248.6 mg, 77%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 54.6 – 55.7 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.49 (d, *J* = 7.8 Hz, 1 H), 7.42 (t, *J* = 8.4 Hz, 2 H), 7.36 (m, 4 H), 7.32 – 7.20 (m, 6 H), 7.16 (t, *J* = 7.8 Hz, 1 H), 6.76 (s, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 143.93, 141.45, 138.95, 136.00, 133.73, 129.92, 129.87, 129.78, 128.45, 128.39, 128.01, 127.70, 127.53,

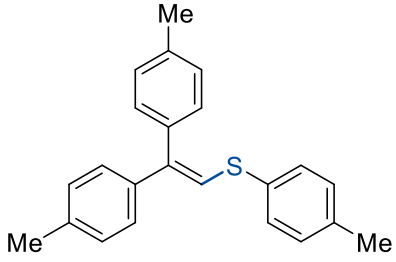
127.40, 127.37, 121.59 ppm. HRMS (ESI): m/z calculated for $C_{20}H_{16}ClS^+$ [M+H$^+$]: 323.0656, found: 323.0648.



8[9] The target compound was isolated (241.3 mg, 73%) as a white solid by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.37 (d, *J* = 6.6 Hz, 2 H), 7.30 – 7.26 (m, 1 H), 7.17 (dd, *J* = 10.2, 5.4 Hz, 2 H), 7.10 (d, *J* = 7.2 Hz, 5 H), 7.04 – 6.96 (m, 2 H), 6.55 (s, 1 H), 2.37 – 2.34 (s, 3 H), 2.32 – 2.29 (m, 6 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 144.15, 140.24, 138.07, 137.84, 137.64, 137.48, 133.96, 130.38, 129.83, 128.86, 128.73, 128.59, 128.37, 128.32, 128.09, 126.97, 124.96, 115.59, 21.49, 21.44, 21.10 ppm.

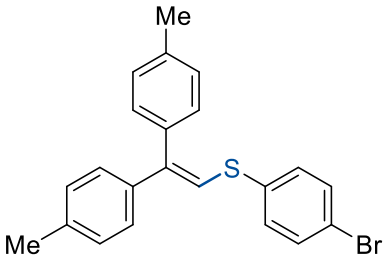


9 The target compound was isolated (320.2 mg, 81%) as yellow oil by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.42 (dd, *J* = 8.4, 2.4 Hz, 2 H), 7.32 – 7.24 (m, 3 H), 7.19 – 7.09 (m, 4 H), 7.08 – 7.01 (m, 3 H), 6.72 (s, 1 H), 2.36 (d, *J* = 3.0 Hz, 3 H), 2.30 (d, *J* = 3.0 Hz, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 142.58, 141.38, 139.08, 138.06, 137.97, 136.05, 132.18, 130.92, 130.25, 128.73, 128.34, 128.28, 128.19, 127.87, 126.81, 124.54, 122.55, 120.62, 21.53, 21.49 ppm. HRMS (ESI): m/z calculated for $C_{22}H_{20}BrS^+$ [M+H$^+$]: 395.0464, found: 395.0465.

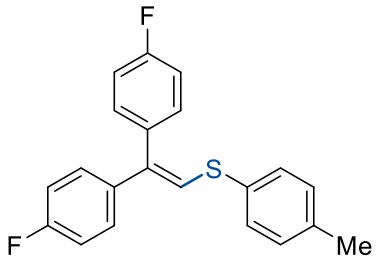


10[9] The target compound was isolated (280.6 mg, 85%) as a white solid by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.37 (d, *J* = 7.8 Hz, 2 H), 7.30 – 7.24 (m, 4 H), 7.17 (m, 4 H), 7.11 (d, *J* = 7.8 Hz, 2 H), 6.78 (s, 1 H), 2.43 (s, 3 H), 2.37 (m, 6 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 140.59,

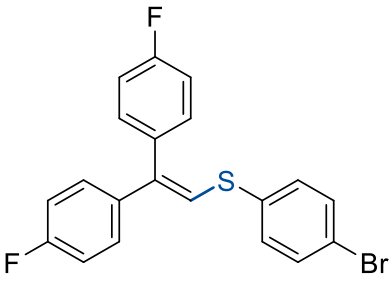
139.06, 137.45, 136.99, 136.80, 136.52, 133.25, 129.95, 129.88, 129.72, 129.08, 129.00, 127.18, 123.61, 21.38, 21.11, 21.07 ppm.



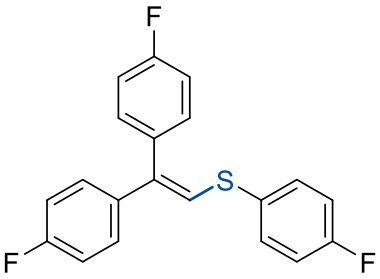
11 The target compound was isolated (355.8 mg, 90%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 147.0 – 148.5 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.45 – 7.38 (m, 2 H), 7.27 – 7.23 (m, 2 H), 7.21 (d, *J* = 12.0 Hz, 4 H), 7.16 – 7.12 (m, 2 H), 7.08 (d, *J* = 7.8 Hz, 2 H), 6.68 (s, 1 H), 2.38 (s, 3 H), 2.32 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 142.63, 138.72, 137.79, 137.47, 136.23, 136.18, 132.17, 130.71, 129.66, 129.15, 129.11, 127.29, 121.27, 120.48, 21.46, 21.22 ppm. HRMS (ESI): m/z calculated for $C_{22}H_{20}BrS^+$ [M+H$^+$]: 395.0464, found: 395.0465.



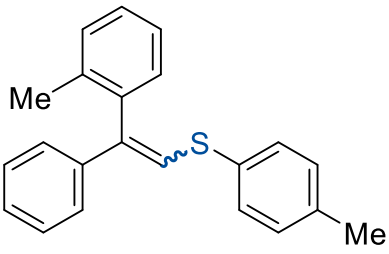
12 The target compound was isolated (280.9 mg, 83%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 114.7 – 116.0 °C ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.37 – 7.30 (m, 4 H), 7.17 (m, 4 H), 7.11 (d, *J* = 3.0 Hz, 2 H), 6.97 (d, *J* =3.0 Hz, 2 H), 6.74 (s, 1 H), 2.35 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 162.27 (d, *J* = 246.0 Hz), 162.23 (d, *J* = 246.0 Hz), 138.09, 137.68, 137.31, 134.99, 132.43, 131.54 (d, *J* = 7.55 Hz), 130.25, 130.01, 128.76 (d, *J* = 7.5 Hz), 125.49, 151.50 (d, *J* = 21.0 Hz), 151.26 (d, *J* = 21.0 Hz), 21.09 ppm. ^{19}F NMR (565 MHz, $CDCl_3$) δ: -113.58, -114.92 ppm. HRMS (ESI): m/z calculated for $C_{21}H_{17}F_2S^+$ [M+H$^+$]: 339.1014, found: 339.1010.



13 The target compound was isolated (306.5 mg, 76%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 121.3 – 122.6 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.48 – 7.39 (m, 2 H), 7.32 – 7.26 (m, 4 H), 7.21 – 7.15 (m, 2 H), 7.11 (d, *J* = 8.4 Hz, 2 H), 6.98 (d, *J* = 8.4 Hz, 2 H), 6.69 (s, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 162.42 (d, *J* = 246.0 Hz), 162.39 (d, *J* = 246.0 Hz), 140.04, 137.37 135.33, 134.71, 132.29, 131.47(d, *J* = 7.5 Hz), 131.04, 128.86 (d, *J* = 7.5 Hz), 123.20, 120.98, 115.57 (d, *J* = 21.0 Hz), 115.37 (d, *J* = 21.0 Hz) ppm. ^{19}F NMR (565 MHz, $CDCl_3$) δ: -113.18, -114.3 ppm HRMS (ESI): m/z calculated for $C_{20}H_{14}BrF_2S^+$ [M+H$^+$]: 402.9962, found: 402.9958.

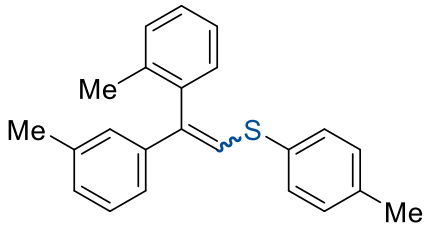


14 The target compound was isolated (232.8 mg, 68%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 79.5 – 80.6 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.42 (d, *J* = 9.0 Hz, 2 H), 7.31 (d, *J* = 8.4 Hz, 2 H), 7.18 (d, *J* = 8.4 Hz, 2 H), 7.11 (d, *J* = 8.4 Hz, 2 H), 7.05 (d, *J* = 8.4 Hz, 2 H), 6.97 (d, *J* = 8.4 Hz, 2 H), 6.67 (s, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 162.33 (d, *J* = 246.0 Hz), 162.31 (d, *J* = 246.0 Hz), 162.29 (d, *J* = 246.0 Hz), 138.74, 137.45, 134.79, 132.25 (d, *J* = 7.5 Hz), 131.48 (d, *J* = 7.5 Hz), 131.10, 128.78 (d, *J* = 7.5 Hz), 124.87, 116.39 (d, *J* = 21.0 Hz), 115.55 (d, *J* = 21.0Hz), 115.32 (d, *J* = 21.0 Hz) ppm. ^{19}F NMR (565 MHz, $CDCl_3$) δ: -113.35, -114.24, -114.61 ppm. HRMS (ESI): m/z calculated for $C_{20}H_{14}F_3S^+$ [M+H$^+$]: 343.0763, found: 343.0760.

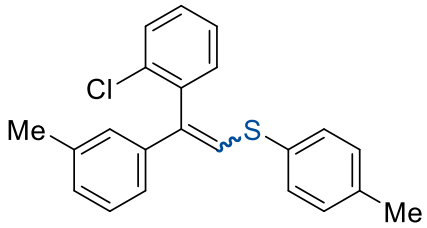


15 The target compound was isolated (256.3 mg, 81%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 85.6 – 86.2 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.37 – 7.32 (m, 2 H), 7.31 – 7.28 (m, 3 H), 7.25 – 7.22 (m, 2 H), 7.21 – 7.18 (m, 4 H), 7.12 (d, *J* = 7.8 Hz, 2 H), 6.99 (s, 1 H), 2.32 (s, 3 H), 2.19 (s, 3 H)

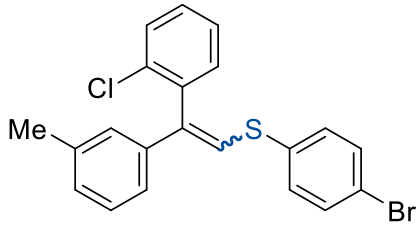
ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 139.77, 139.21, 138.58, 136.97, 136.54, 132.69, 130.48, 130.01, 129.97, 129.94, 128.53, 128.06, 127.09, 126.21, 125.70, 125.42, 21.13, 19.56 ppm. HRMS (ESI): m/z calculated for $C_{22}H_{21}S^+$ [M+H$^+$]: 317.1358, found: 317.1351.



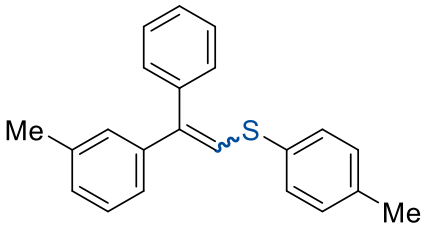
16 The target compound was isolated (257.8 mg, 78%) as yellow oil by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.40 – 7.34 (m, 2 H), 7.30 – 7.19 (m, 3 H), 7.18 – 7.11 (m, 2 H), 7.08 (t, *J* = 7.8 Hz, 3 H), 7.03 – 6.94 (m, 2 H), 6.71 (s, 1 H), 2.30 (s, 3 H), 2.28 (s, 3 H), 2.14 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 143.61, 138.62, 138.24, 137.48, 137.30, 136.36, 133.99, 130.27, 129.83, 129.58, 128.86, 128.62, 128.52, 128.02, 127.06, 125.87, 123.76, 116.73, 21.48, 21.09, 19.50 ppm. HRMS (ESI): m/z calculated for $C_{23}H_{23}S^+$ [M+H$^+$]: 331.1515, found: 331.1515.



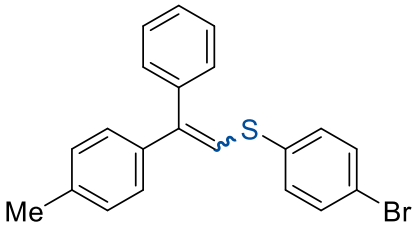
17 The target compound was isolated (291.3 mg, 83%) as yellow oil by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.48-7.46 (m, 1 H), 7.41 – 7.30 (m, 4 H), 7.25 (m, 1 H), 7.20 – 7.15 (m, 1 H), 7.13 – 7.07 (m, 3 H), 7.04 – 6.96 (m, 2 H), 6.75 (s, 1 H), 2.32 – 2.29 (m, 6 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 141.76, 138.29, 137.87, 137.48, 136.70, 133.94, 133.52, 131.31, 129.89, 129.84, 129.39, 129.06, 128.58, 128.55, 127.09, 126.90, 123.75, 118.16, 21.52, 21.11 ppm. HRMS (ESI): m/z calculated for $C_{22}H_{20}ClS^+$ [M+H$^+$]: 351.0969, found: 351.0965.



18 The target compound was isolated (320.1 mg, 77%) as yellow oil by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.50 – 7.46 (m, 1 H), 7.43 – 7.38 (m, 2 H), 7.34 – 7.25 (m, 5 H), 7.16 (t, *J* = 7.8 Hz, 1 H), 7.05 (t, *J* = 6.0 Hz, 2 H), 7.01 – 6.96 (m, 1 H), 6.96 (s, 1 H), 2.29 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 139.68, 138.91, 138.24, 137.81, 135.32, 133.68, 132.23, 131.61, 131.08, 130.09, 129.47, 128.60, 128.55, 127.19, 126.47, 124.57, 123.24, 120.86, 21.62 ppm. HRMS (ESI): m/z calculated for $C_{21}H_{17}ClBrS^+$ [M+H$^+$]: 414.9917, found: 414.9911.

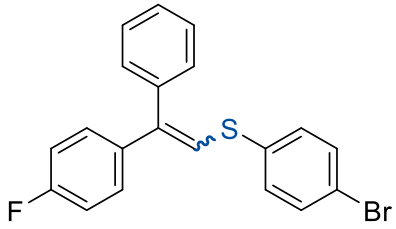


19 The target compound (ratio of Z/E isomers is 1.36: 1) was isolated (246.8 mg, 78%) as yellow oil by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.43 – 7.39 (m, 1 H), 7.37 – 7.30 (m, 4 H), 7.29 – 7.25 (m, 1 H), 7.24 – 7.20 (m, 1 H), 7.18 – 7.12 (m, 4 H), 7.05 (m, 2 H), 6.80 (s, 1 H), 2.34 (m, 6 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 141.65, 140.43, 139.40, 138.02, 136.96, 133.00, 130.31, 130.10, 129.86, 128.52, 128.30, 128.17, 127.79, 127.15, 126.87, 124.98, 21.49, 21.05 ppm. HRMS (ESI): m/z calculated for $C_{22}H_{21}S^+$ [M+H$^+$]: 317.1358, found: 317.1355.

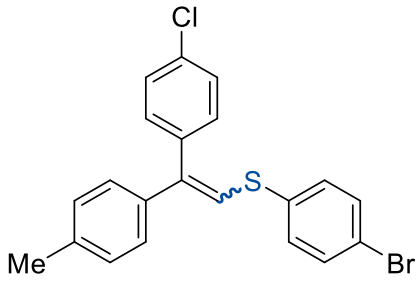


20 The target compound (ratio of Z/E isomers is 1.28: 1) was isolated (312.7 mg, 82%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 112.5 – 113.5 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.44 – 7.39 (m, 3 H), 7.39 – 7.31 (m, 2 H), 7.31 – 7.23 (m, 6 H), 7.14 (d, *J* = 8.4 Hz, 1 H), 7.10 (d, *J* = 8.0 Hz, 1 H), 6.73 (s, 1 H), 2.36 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 142.51, 141.46, 139.17, 137.83, 136.02, 132.26, 130.86, 129.71, 129.15, 128.40, 127.93, 127.33,

122.45, 120.62, 21.39 ppm. HRMS (ESI): m/z calculated for $C_{21}H_{18}BrS^+$ [M+H$^+$]: 381.0307, found: 381.0314.

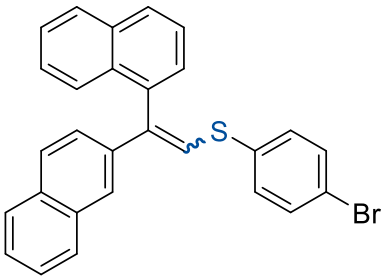


21 The target compound (ratio of Z/E isomers is 1.10: 1) was isolated (300.5 mg, 78%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 103.9 – 105.3 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.48 – 7.38 (m, 3 H), 7.37 – 7.25 (m, 6 H), 7.24 – 7.18 (m, 2 H), 7.11 (t, *J* = 8.4 Hz, 1 H), 6.98 (t, *J* = 8.4 Hz, 1 H), 6.73 (s, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 162.36 (d, *J* = 246.0 Hz), 141.14, 138.85, 137.49, 135.65, 134.88, 132.23, 131.54 (d, J=7.5 Hz), 130.99, 128.53, 127.21, 122.85, 120.85, 115.48 (d, *J* = 21.0 Hz), ppm. ^{19}F NMR (565 MHz, $CDCl_3$) δ: -113.46, -114.56 ppm. HRMS (ESI): m/z calculated for $C_{20}H_{15}BrFS^+$ [M+H$^+$]: 385.0056, found: 385.0049.

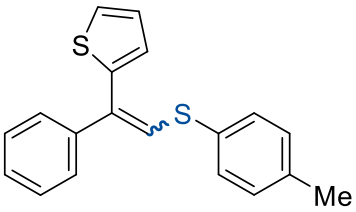


22 The target compound (ratio of Z/E isomers is 1.11: 1) was isolated (357.6 mg, 86%) as a white solid by column chromatography (eluting with petroleum ether). m.p. = 97.3 – 98.5 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.36 – 7.32 (m, 2 H), 7.24 (m, 3 H), 7.22 – 7.17 (m, 3 H), 7.14 – 7.09 (m, 3 H), 7.07 (d, *J* = 2.4 Hz, 1 H), 6.54 (s, 1 H), 2.36 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 142.80, 138.91, 138.29, 136.93, 136.15, 134.19, 134.04, 133.74, 131.32, 129.49, 129.04, 128.61, 128.48, 115.98, 21.34 ppm. HRMS (ESI): m/z calculated for $C_{21}H_{17}BrClS^+$ [M+H$^+$]: 414.9917, found: 414.9915.

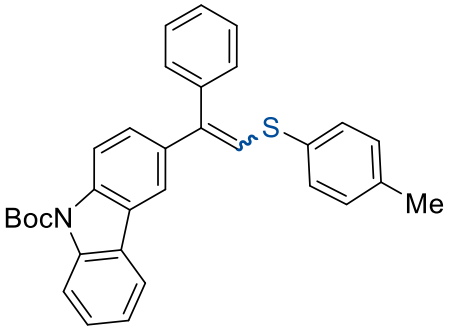
7. Characterization results for Table 3



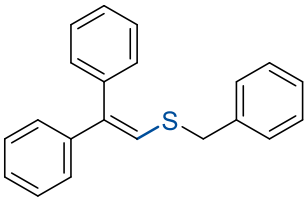
23 The target compound was isolated (317.8 mg, 68%) as white soild by column chromatography (eluting with petroleum ether). m.p. = 111.0 – 112.5 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.41 (d, *J* = 8.4 Hz, 1 H), 8.04 (d, *J* = 7.2 Hz, 1 H), 7.88 – 7.86 (m, 2 H), 7.79 – 7.71 (m, 2 H), 7.62 – 7.59 (m, 1 H), 7.56 (t, *J* = 7.8 Hz, 2 H), 7.52 – 7.50 (m, 2 H), 7.45 (m, 2 H), 7.42 (d, *J* = 8.4 Hz, 2 H), 7.32 – 7.29 (m, 2 H), 7.23 (d, *J* = 7.2 Hz, 1 H), 7.14 (d, *J* = 1.8 Hz, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 137.51, 136.92, 136.84, 135.30, 133.96, 133.52, 132.15, 131.61, 131.55, 131.04, 129.02, 128.81, 128.58, 128.15, 128.01, 127.49, 127.42, 126.81, 126.73, 126.67, 126.51, 126.02, 125.86, 125.39, 125.33, 120.79 ppm. HRMS (ESI): m/z calculated for $C_{28}H_{20}BrS^{+}$ [M+H^{+}]: 467.0464, found: 467.0464.



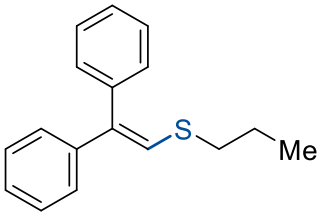
24 The target compound (ratio of Z/E isomers is 1.16: 1) was isolated (215.9 mg, 70%) as yellow oil by column chromatography (eluting with 0-5% ethyl acetate in petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.39 (m, 5 H), 7.35 – 7.32 (m, 1 H), 7.29 – 7.25 (m, 2 H), 7.23 – 7.21 (m, 1 H), 7.17 (d, *J* = 7.8 Hz, 1 H), 7.13 (s, 1 H), 6.75 – 6.69 (m, 1 H), 6.55 – 6.40 (m, 1 H), 2.33 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 140.15, 139.91, 138.41, 138.12, 133.13, 131.64, 130.96, 130.26, 130.05, 129.60, 129.21, 128.53, 128.19, 125.41, 21.22 ppm. HRMS (ESI): m/z calculated for $C_{19}H_{17}S_2^{+}$ [M+H^{+}]: 309.0766, found: 309.0765.



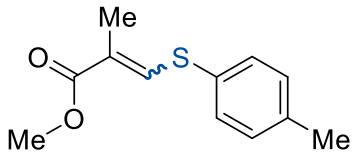
25 The target compound (ratio of Z/E isomers is 1.08: 1) was isolated (295.0 mg, 60%) as yellow oil by column chromatography (eluting with 0-10% ethyl acetate in petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 8.36 (d, *J* = 17.4 Hz, 1 H), 8.18 (d, *J* = 21.6 Hz, 1 H), 7.81 (d, *J* = 15.6 Hz, 1 H), 7.43 – 7.40 (m, 4 H), 7.35 (m, 3 H), 7.27 – 7.26 (m, 2 H), 7.13 (m, 3 H), 6.89 (d, *J* = 9.6 Hz, 1 H), 6.85 (s, 1 H), 2.32 (s, 3 H), 1.74 (m, 9 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 150.96, 141.76, 140.49, 140.10, 139.58, 138.13, 137.10, 137.00, 132.95, 130.16, 129.96, 129.90, 128.47, 127.84, 127.20, 127.05, 125.81, 125.45, 124.75, 121.00, 118.31, 116.03, 84.11, 28.40, 21.10 ppm. HRMS (ESI): m/z calculated for $C_{32}H_{30}NO_2S^+$ [M+H$^+$]: 492.1992, found: 492.1988.



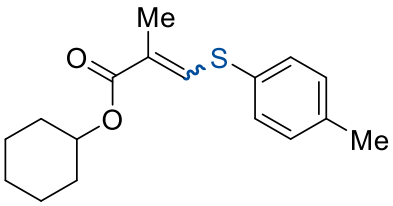
26[10] The target compound was isolated (229.8 mg, 76 %) by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.36– 7.32 (m, 5 H), 7.32 – 7.28 (m, 3 H), 7.27 – 7.23 (m, 4 H), 7.22 (d, *J* = 2.4 Hz, 1 H), 7.13 – 7.11 (m, 2 H), 6.57 (s, 1 H), 3.94 (s, 2 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 141.85, 139.53, 139.25, 137.76, 129.75, 128.99, 128.71, 128.32, 128.27, 127.60, 127.35, 127.12, 127.12, 126.97, 124.75, 38.92 ppm.



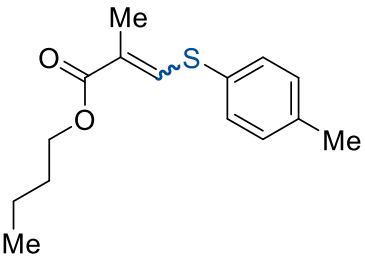
27 The target compound was isolated (208.6 mg, 82%) as yellow oil by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.38 (dd, *J* = 8.4, 6.0 Hz, 2 H), 7.31 (d, *J* = 7.8 Hz, 3 H), 7.26 (dd, *J* = 8.4, 6.0 Hz, 2 H), 7.21 (m, 3 H), 6.58 (s, 1 H), 2.73 (t, *J* = 7.2 Hz, 2 H), 1.71 (m, *J* = 7.2 Hz, 2 H), 1.01 (t, *J* = 7.2 Hz, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 142.05, 139.68, 138.38, 129.77, 128.32, 128.27, 127.46, 127.04, 126.82, 126.42, 36.95, 23.74, 13.32 ppm. HRMS (ESI): m/z calculated for $C_{17}H_{19}S^+$ [M+H$^+$]: 255.1202, found: 255.1196.



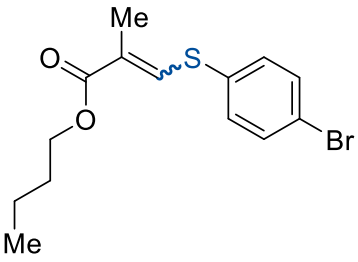
28 The target compound (ratio of Z/E isomers is 1.20: 1) was isolated (146.7 mg, 66%) as white oil by column chromatography (eluting with petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.50 (d, *J* = 7.8 Hz, 1 H), 7.44 (d, *J* = 7.8 Hz, 1 H), 7.20 (dd, *J* = 7.8, 3.6 Hz, 2 H), 5.60 (s, 1 H), 3.83 (s, 3 H), 2.37 (s, 3 H), 1.95 (s, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 168.84, 139.67, 133.97, 133.54, 130.23, 128.66, 78.32, 53.61, 23.36, 21.22. ppm. HRMS (ESI): m/z calculated for $C_{12}H_{15}O_2S^+$ [M+H$^+$]: 223.0787, found: 223.0790.



29 The target compound (ratio of Z/E isomers is 1.23: 1) was isolated (174.1 mg, 60%) as white oil by column chromatography (eluting with 0-20% DCM in petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.51 (d, *J* = 7.8 Hz, 1 H), 7.45 (d, *J* = 7.8 Hz, 1 H), 7.20 (t, *J* = 7.2 Hz, 2 H), 5.62 (s, 1 H), 4.90 (m, 1 H), 2.37 (s, 3 H), 1.94 (s, 3 H), 1.88 – 1.83 (m, 2 H), 1.75 – 1.69 (m, 2 H), 1.51 (m, 2 H), 1.42 – 1.27 (m, 4 H). ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 167.59, 133.81, 130.20, 128.69, 75.47, 70.77, 31.11, 25.27, 23.44, 23.38, 21.24. ppm. HRMS (ESI): m/z calculated for $C_{17}H_{23}O_2S^+$ [M+H$^+$]: 291.1413, found: 291.1410.

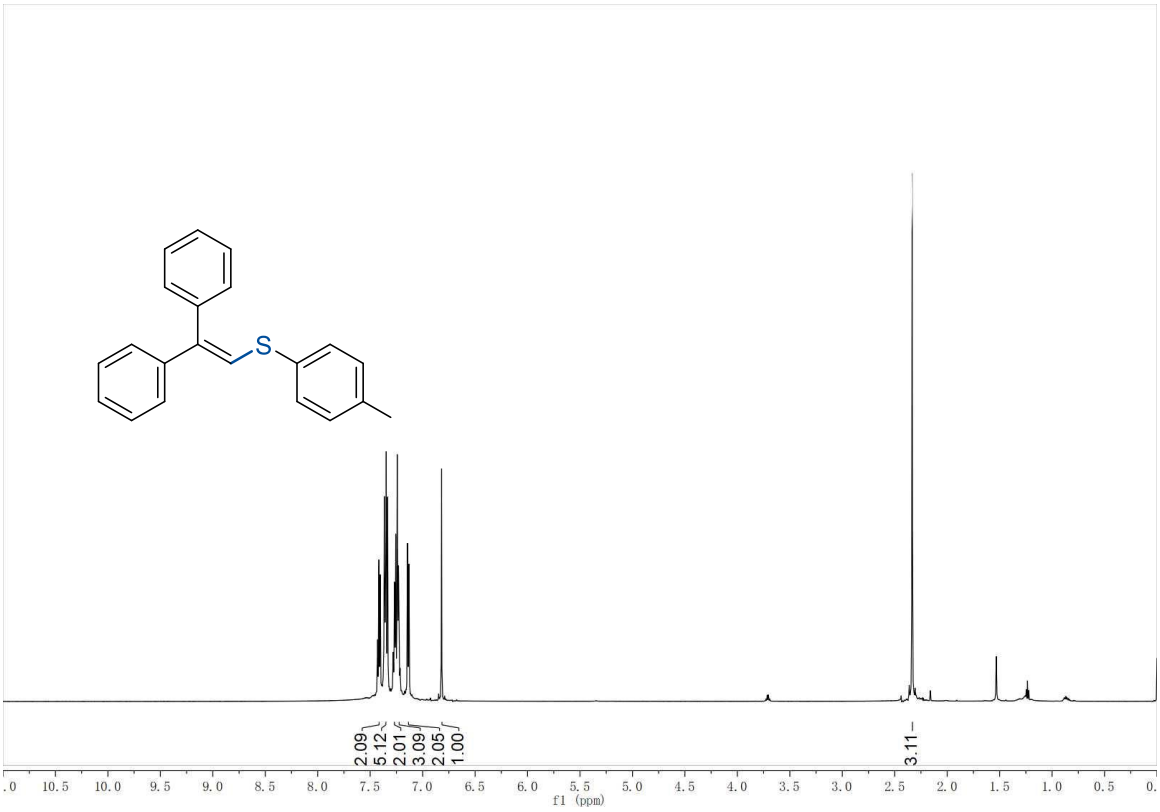


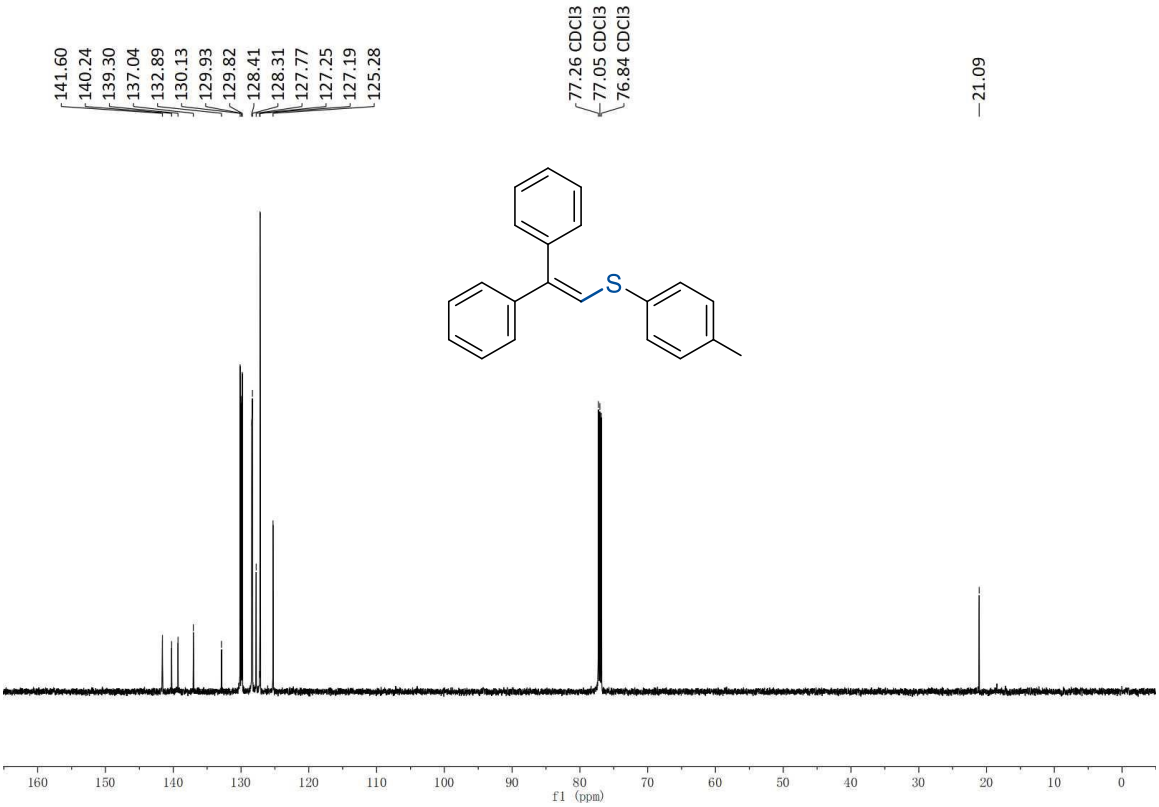
30 The target compound (ratio of Z/E isomers is 1.09: 1) was isolated (153.1 mg, 58%) as white oil by column chromatography (eluting with 0-20% DCM in petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.50 (d, *J* = 7.8 Hz, 1 H), 7.44 (d, *J* = 7.8 Hz, 1 H), 7.20 (t, *J* = 7.2 Hz, 2 H), 5.61 (s, 1 H), 4.23 (m, 2 H), 2.37 (s, 3 H), 1.94 (s, 3 H), 1.67 – 1.63 (m, 2 H), 1.41 – 1.37 (m, 2 H), 0.93 (t, *J* = 7.2 Hz, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 168.35, 139.55, 133.83, 130.21, 128.70, 78.26, 70.66, 66.73, 30.35, 26.93, 21.25, 19.02, 13.62. ppm. HRMS (ESI): m/z calculated for $C_{15}H_{21}O_2S^+$ [M+H$^+$]: 265.1257, found: 265.1257.

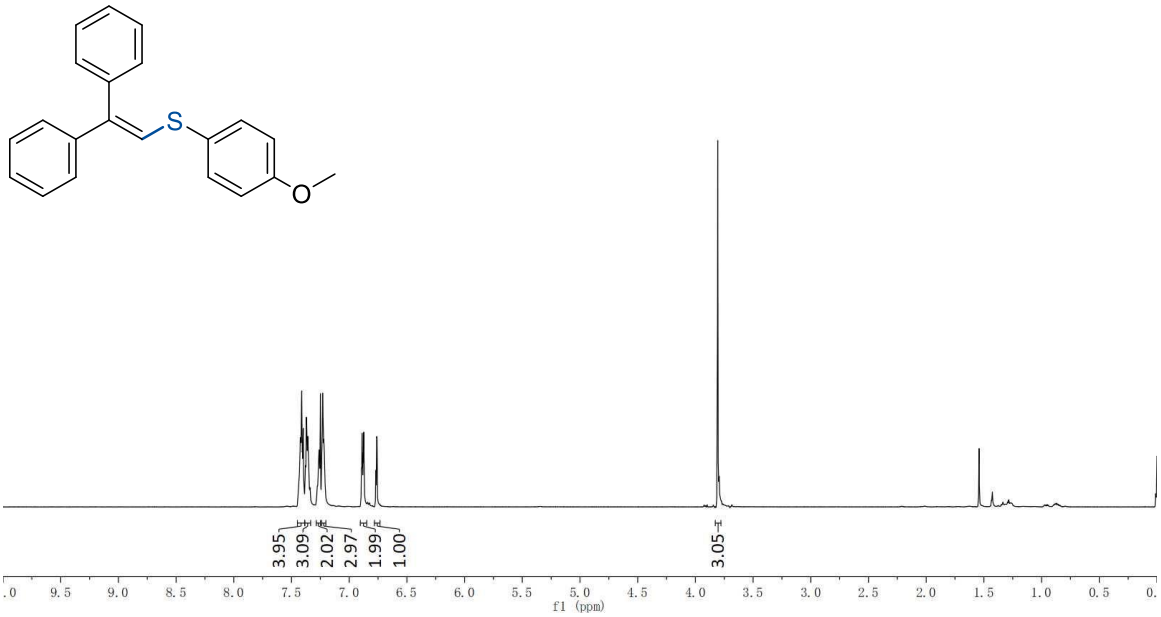


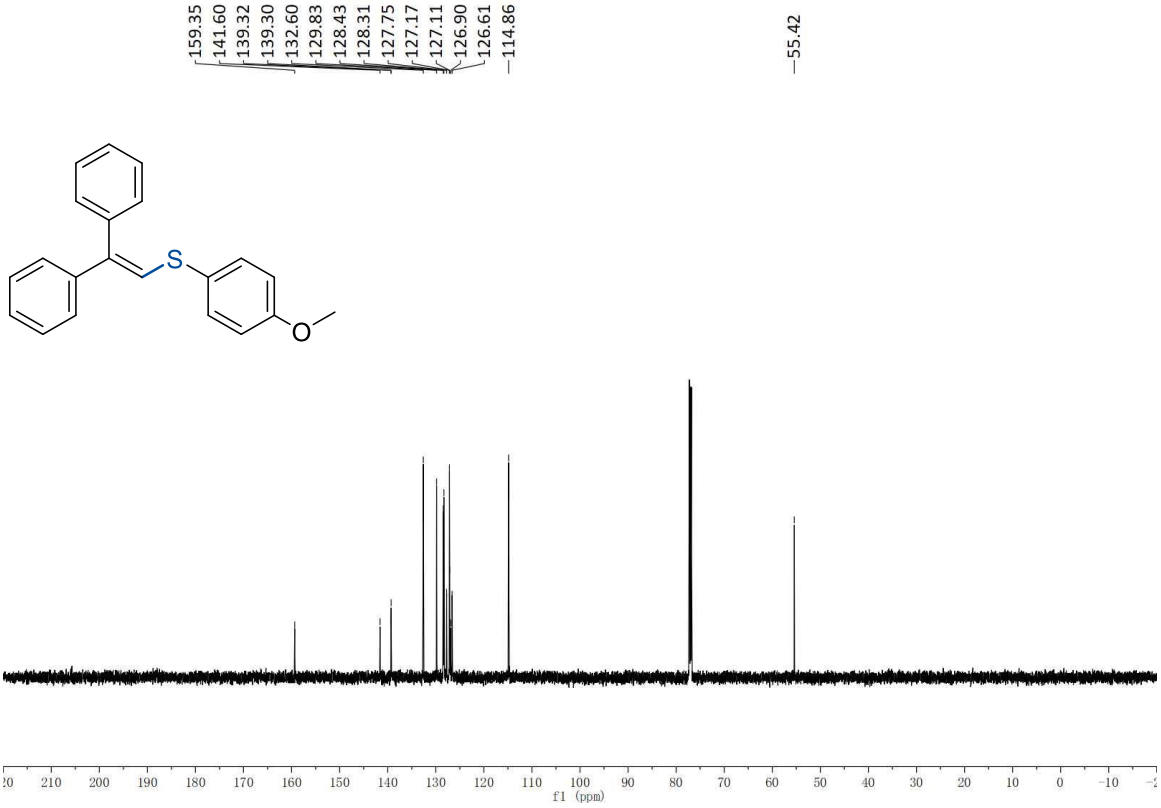
31 The target compound (ratio of Z/E isomers is 1.34: 1) was isolated (217.2 mg, 66%) as white oil by column chromatography (eluting with 0-20% DCM in petroleum ether). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.52 (t, *J* = 5.4, 4.2 Hz, 2 H), 7.47 (d, *J* = 8.4 Hz, 1 H), 7.42 (d, *J* = 8.4 Hz, 1 H), 5.61 (s, 1 H), 4.28 – 4.18 (m, 2 H), 1.94 (s, 3 H), 1.69 – 1.62 (m, 2 H), 1.39 (m, 2 H), 0.93 (t, *J* = 6.0 Hz, 3 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$) δ: 168.15, 134.97, 134.41, 132.63, 131.38, 123.72, 70.55, 66.86, 30.35, 23.51, 19.04, 13.64 ppm. HRMS (ESI): m/z calculated for $C_{14}H_{18}O_2BrS^+$ [M+H$^+$]: 329.0205, found: 329.0204.

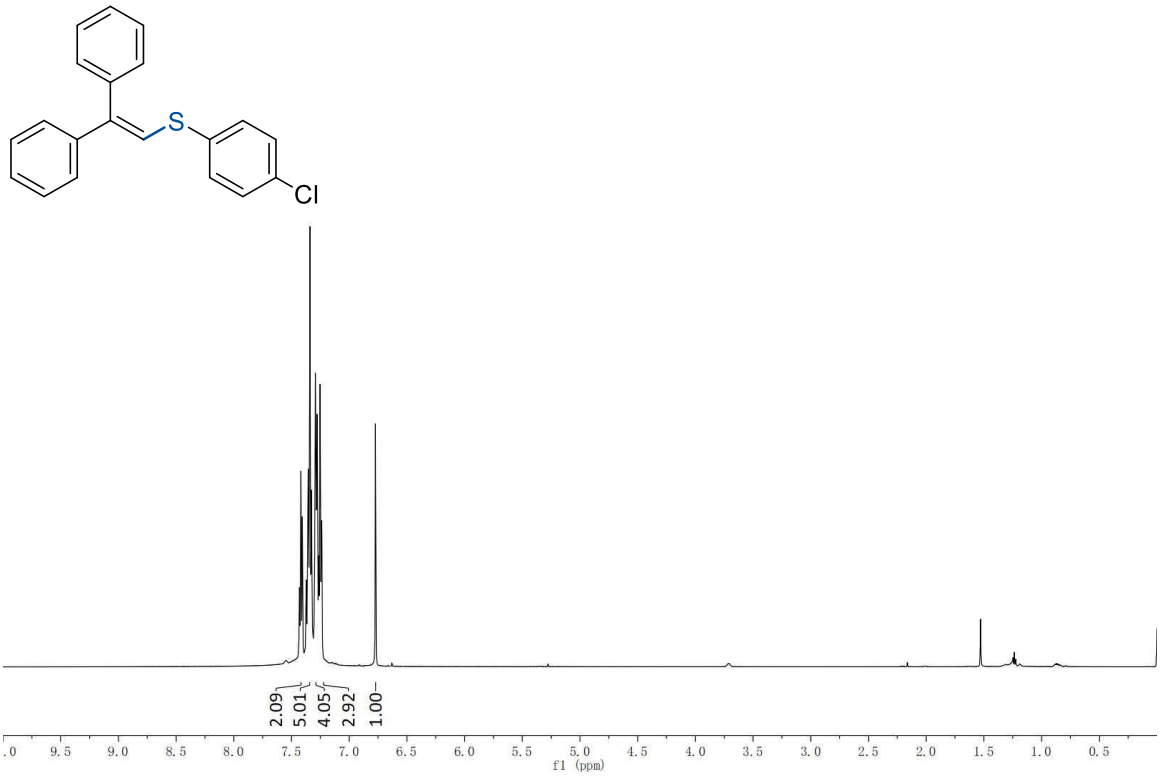
8. NMR Spectra

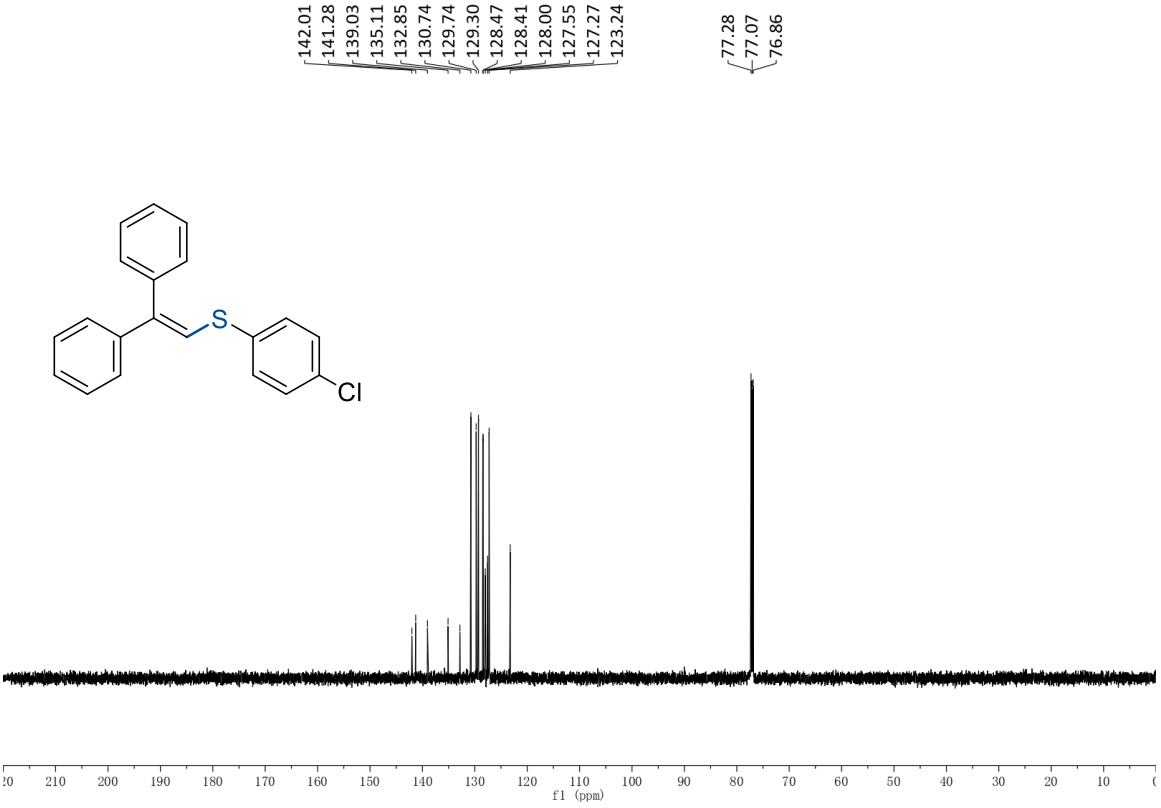


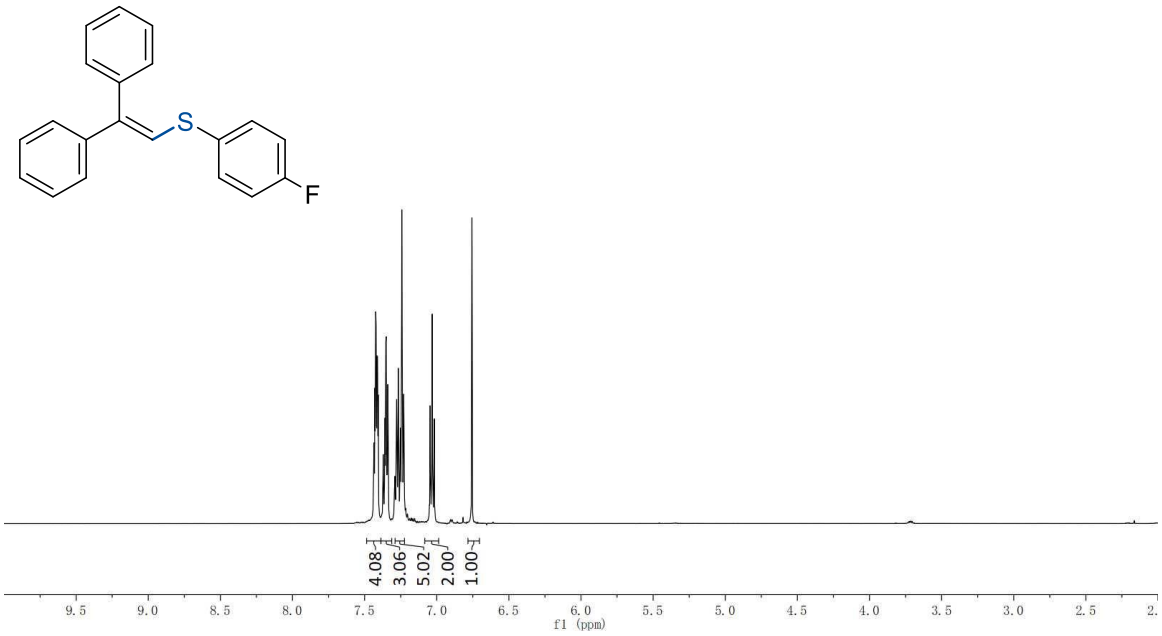


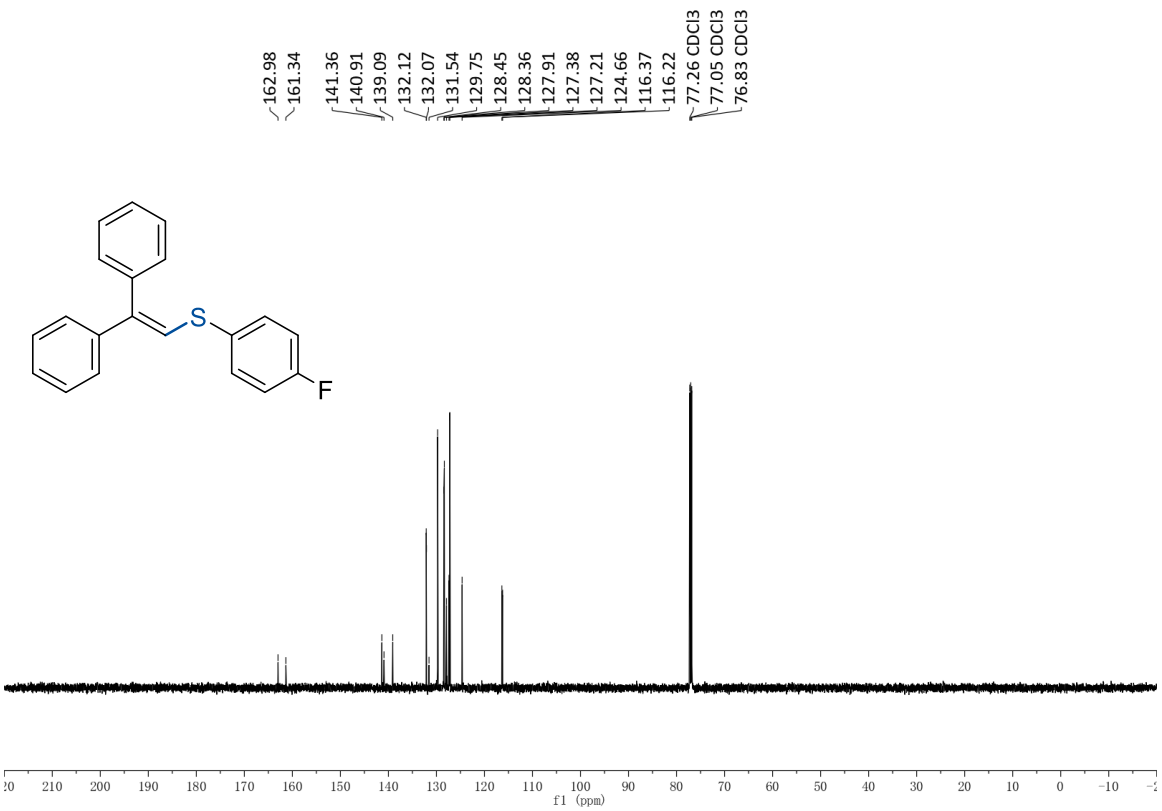

S
O
3.95
3.09
2.02
2.97
1.99
1.00
3.05
f1 (ppm)

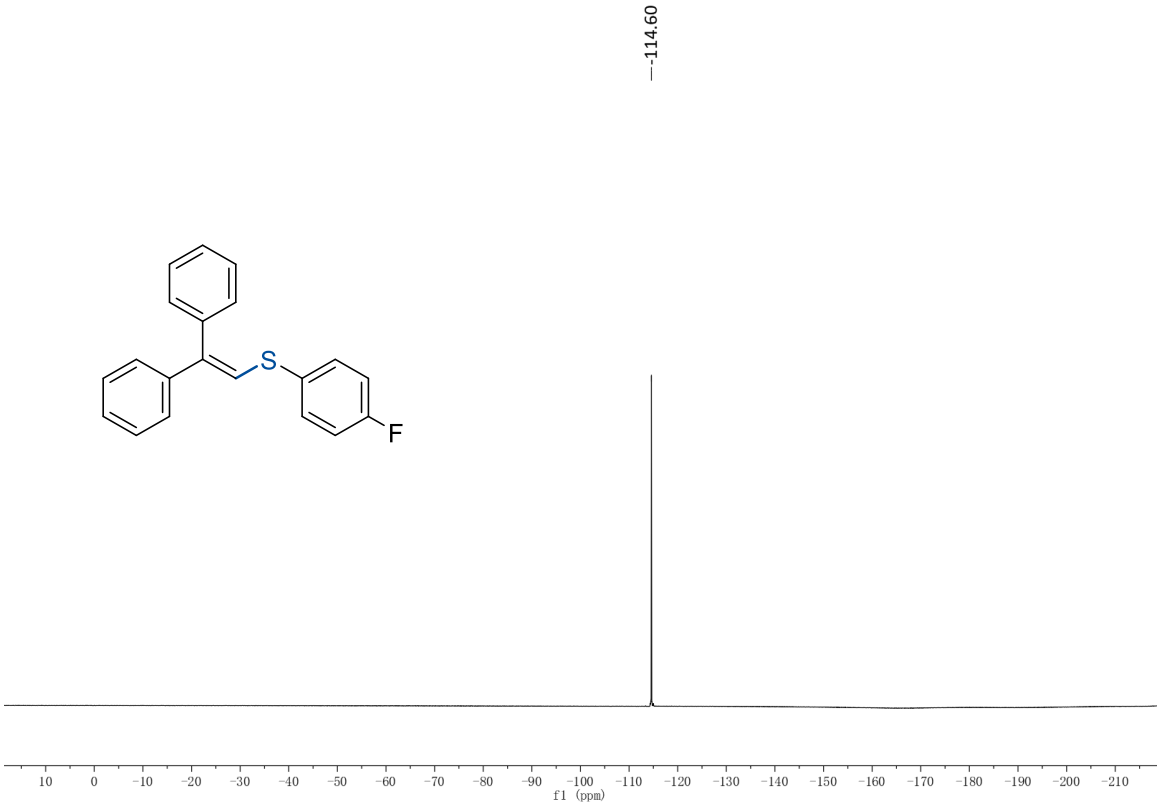

159.35
141.60
139.32
139.30
132.60
129.83
128.43
128.31
127.75
127.17
127.11
126.90
126.61
114.86
55.42
S
O
f1 (ppm)

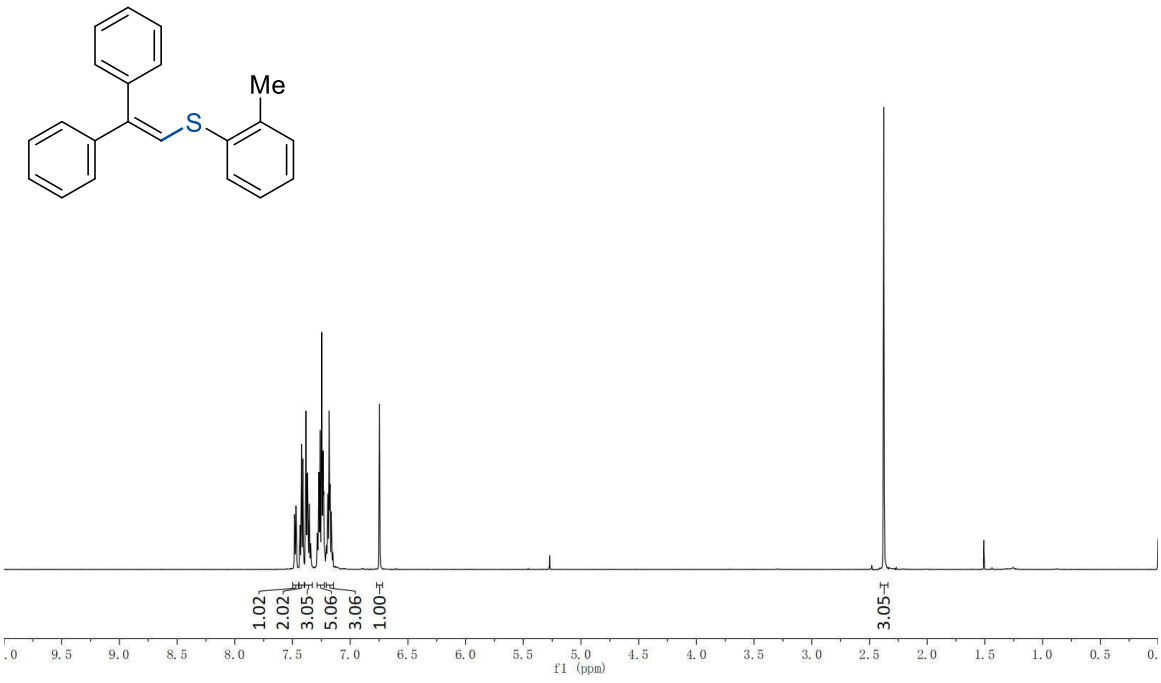

S
Cl
2.09
5.01
4.05
2.92
1.00
f1 (ppm)

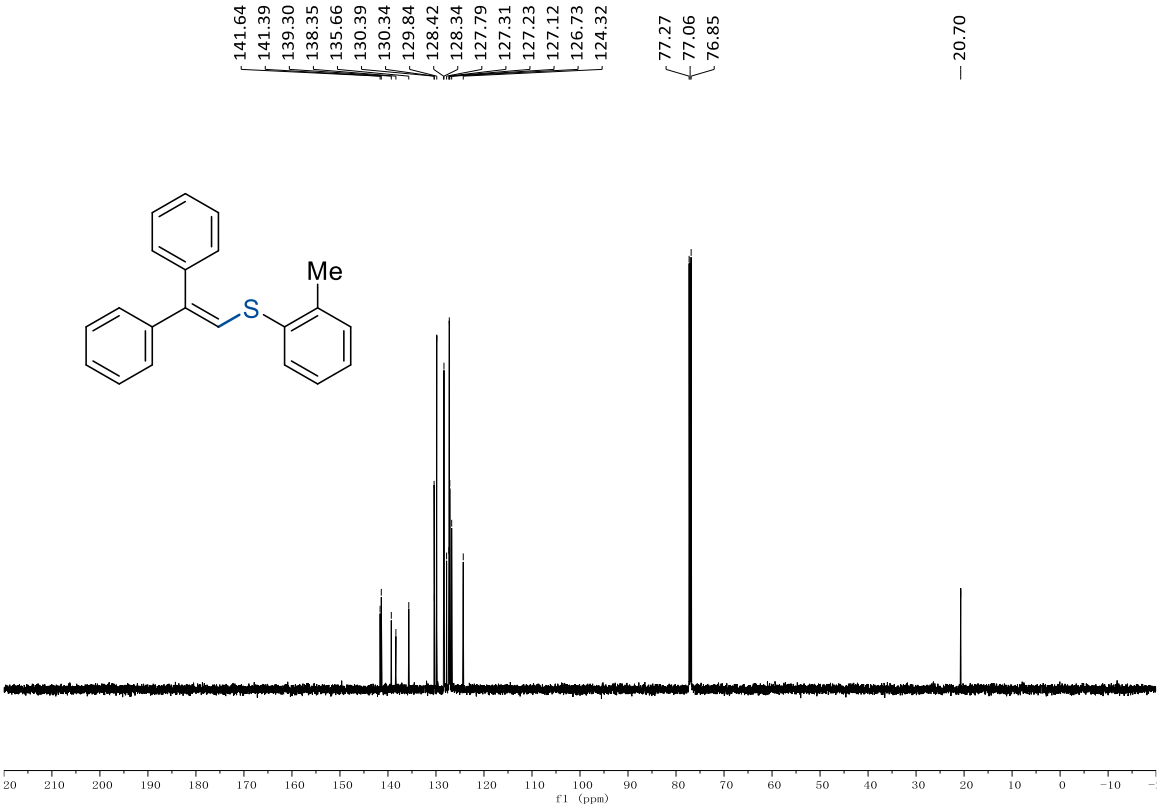

142.01
141.28
139.03
135.11
132.85
130.74
129.74
129.30
128.47
128.41
128.00
127.55
127.27
123.24
77.28
77.07
76.86
S
Cl
f1 (ppm)

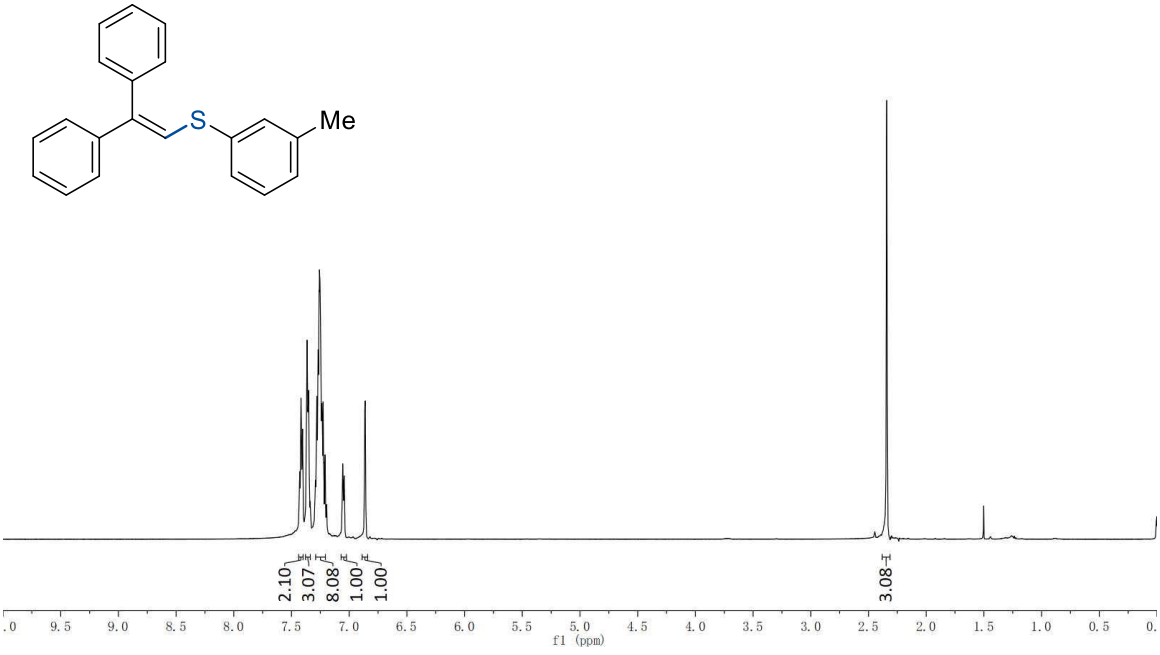

S
F
4.08
3.06
5.02
2.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5
f1 (ppm)

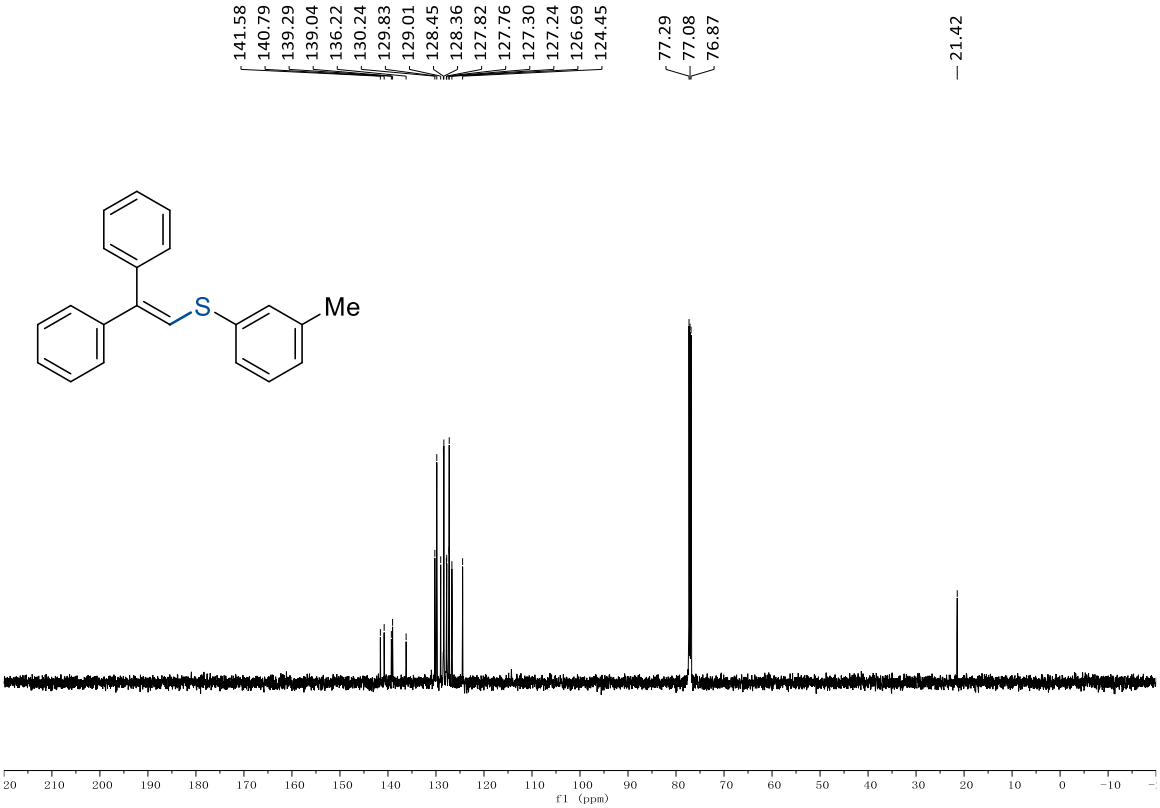

162.98
161.34
141.36
140.91
139.09
132.12
132.07
131.54
129.75
128.45
128.36
127.91
127.38
127.21
124.66
116.37
116.22
77.26 CDCl3
77.05 CDCl3
76.83 CDCl3
S
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

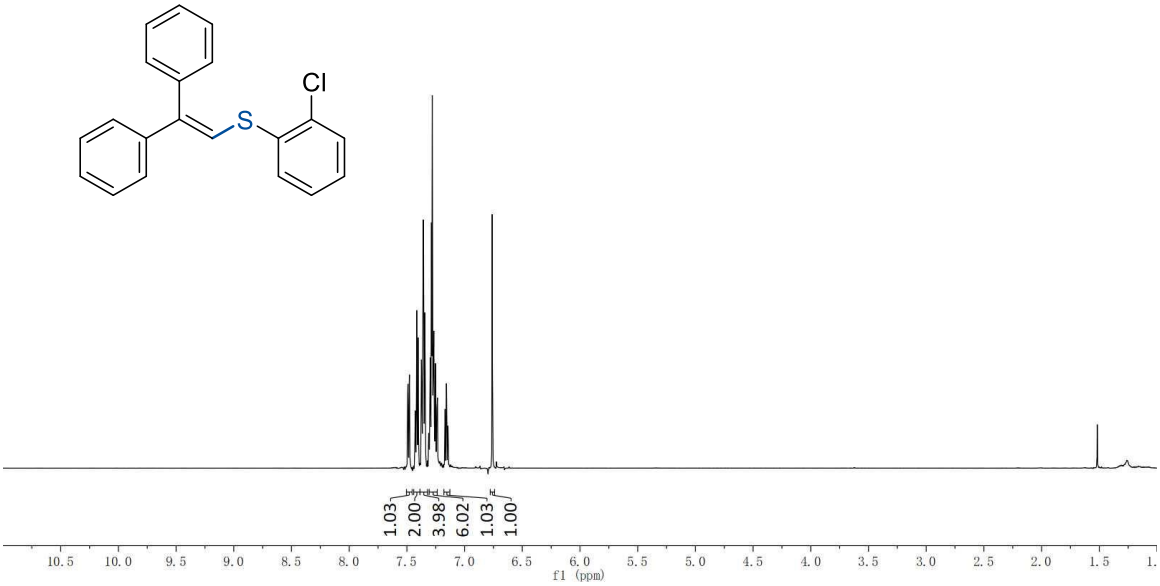

-114.60
S
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

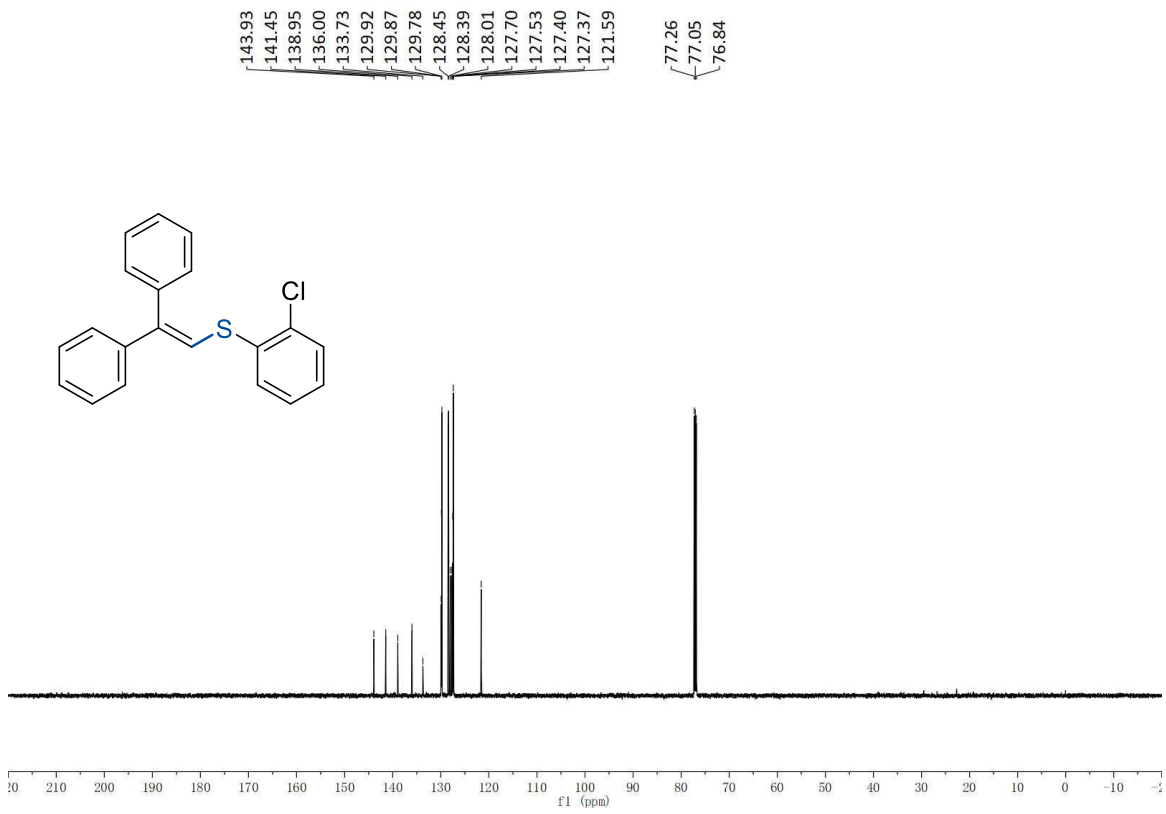

Me
S
1.02
2.02
3.05
5.06
3.06
1.00
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


141.64
141.39
139.30
138.35
135.66
130.39
130.34
129.84
128.42
128.34
127.79
127.31
127.23
127.12
126.73
124.32
77.27
77.06
76.85
20.70
Me
S
f1 (ppm)


S
Me
2.10
3.07
8.08
1.00
1.00
3.08
f1 (ppm)


141.58
140.79
139.29
139.04
136.22
130.24
129.83
129.01
128.45
128.36
127.82
127.76
127.30
127.24
126.69
124.45
77.29
77.08
76.87
21.42
S
Me
f1 (ppm)


Cl
S
1.03
2.00
3.98
6.02
1.03
1.00
f1 (ppm)


143.93
141.45
138.95
136.00
133.73
129.92
129.87
129.78
128.45
128.39
128.01
127.70
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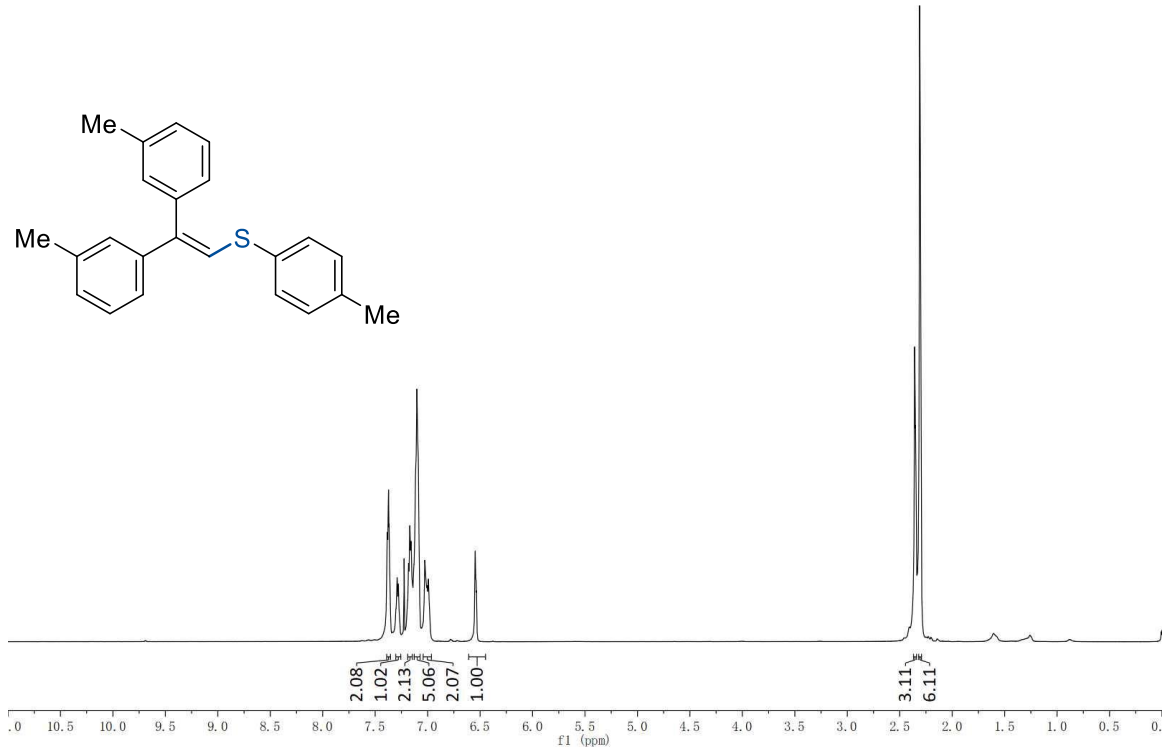
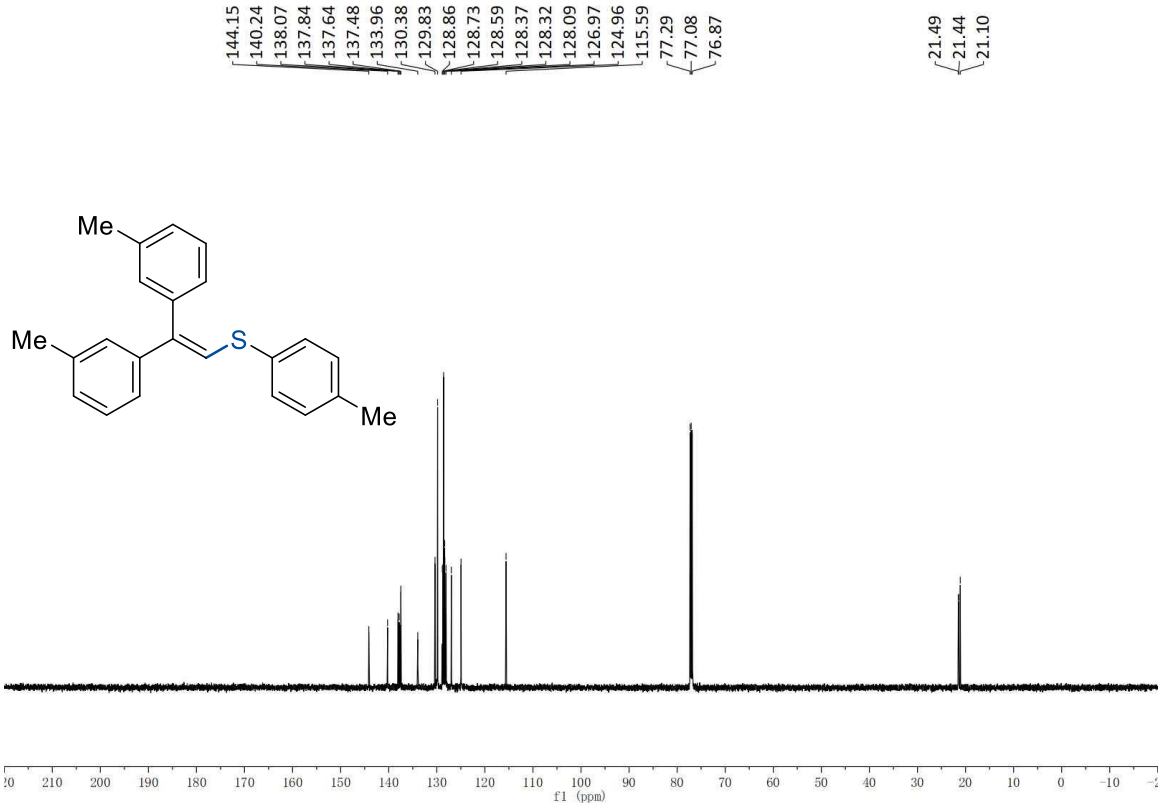
127.37
121.59
77.26
77.05
76.84
Cl
S
f1 (ppm)


Me
Me
S
Me
2.08
1.02
2.13
5.06
2.07
1.00
3.11
6.11
f1 (ppm)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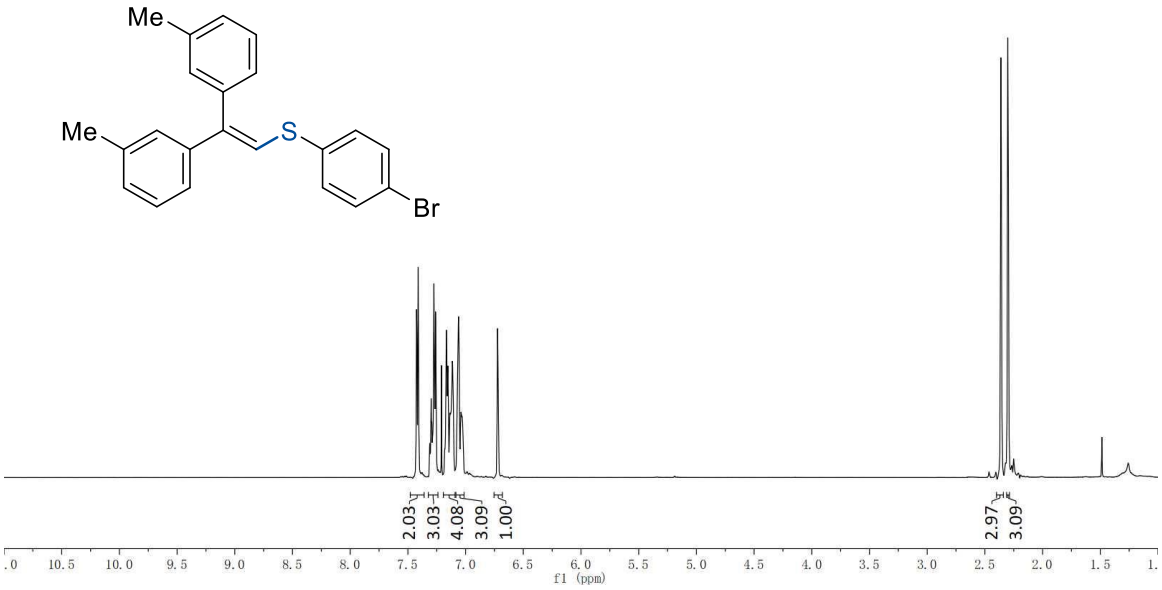
138.07
137.84
137.64
137.48
133.96
130.38
129.83
128.86
128.73
128.59
128.37
128.32
128.09
126.97
124.96
115.59
77.29
77.08
76.87
21.49
21.44
21.10
Me
Me
S
Me
f1 (ppm)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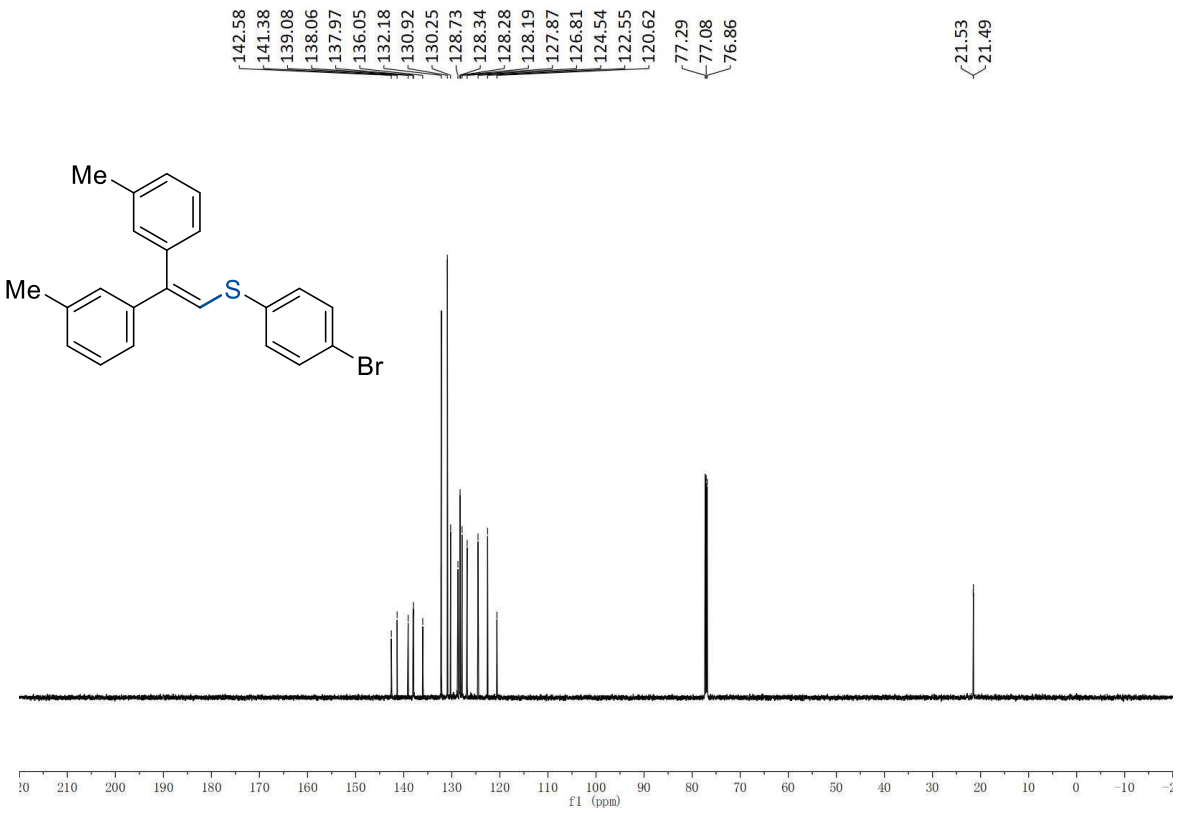
Me
S
Br
2.03
3.03
4.08
3.09
1.00
2.97
3.09
f1 (ppm)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139.08
138.06
137.97
136.05
132.18
130.92
130.25
128.73
128.34
128.28
128.19
127.87
126.81
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122.55
120.62
77.29
77.08
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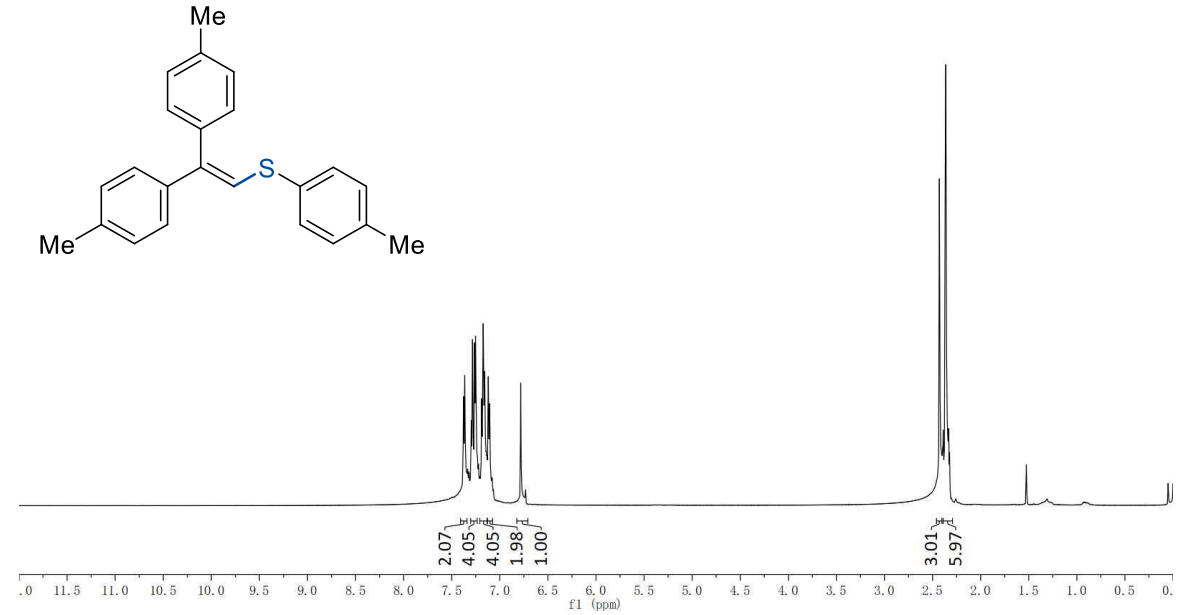
21.53
21.49
Me
Me
S
Br
f1 (ppm)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S
Me
Me
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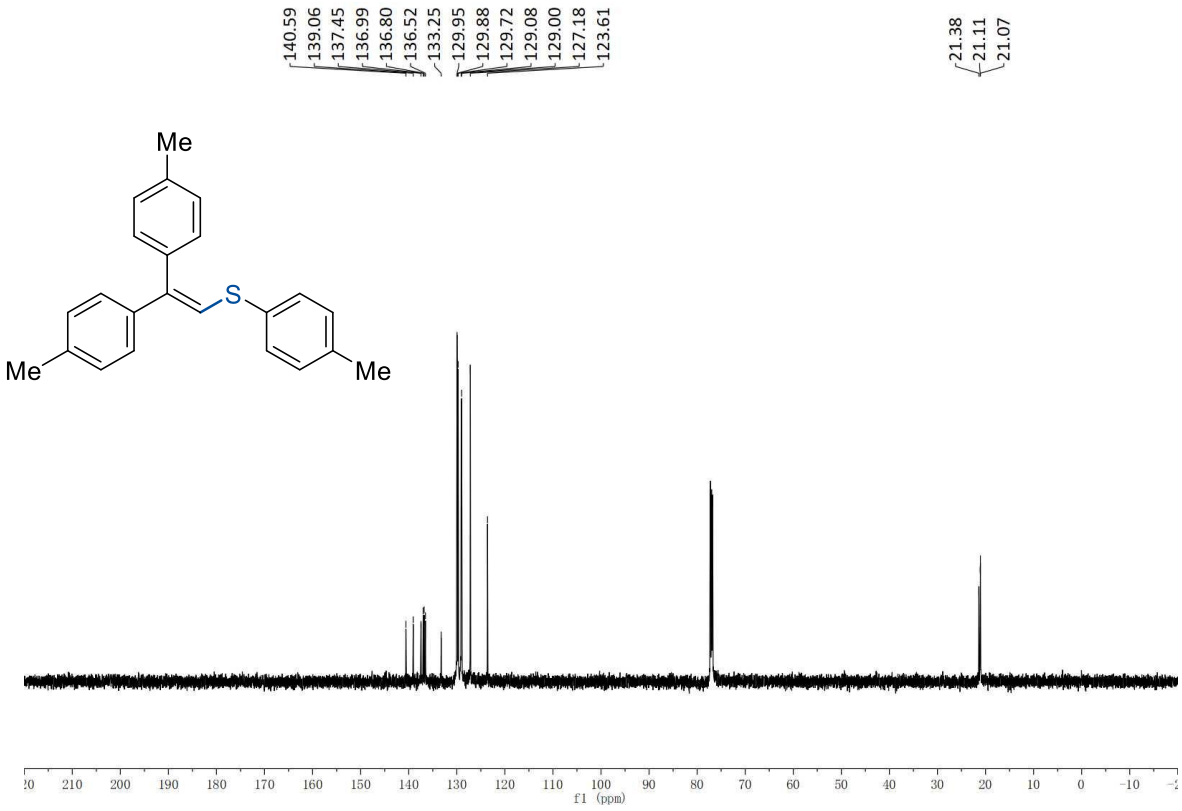
4.05
4.05
1.98
1.00
3.01
5.97
f1 (ppm)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137.45
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133.25
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129.72
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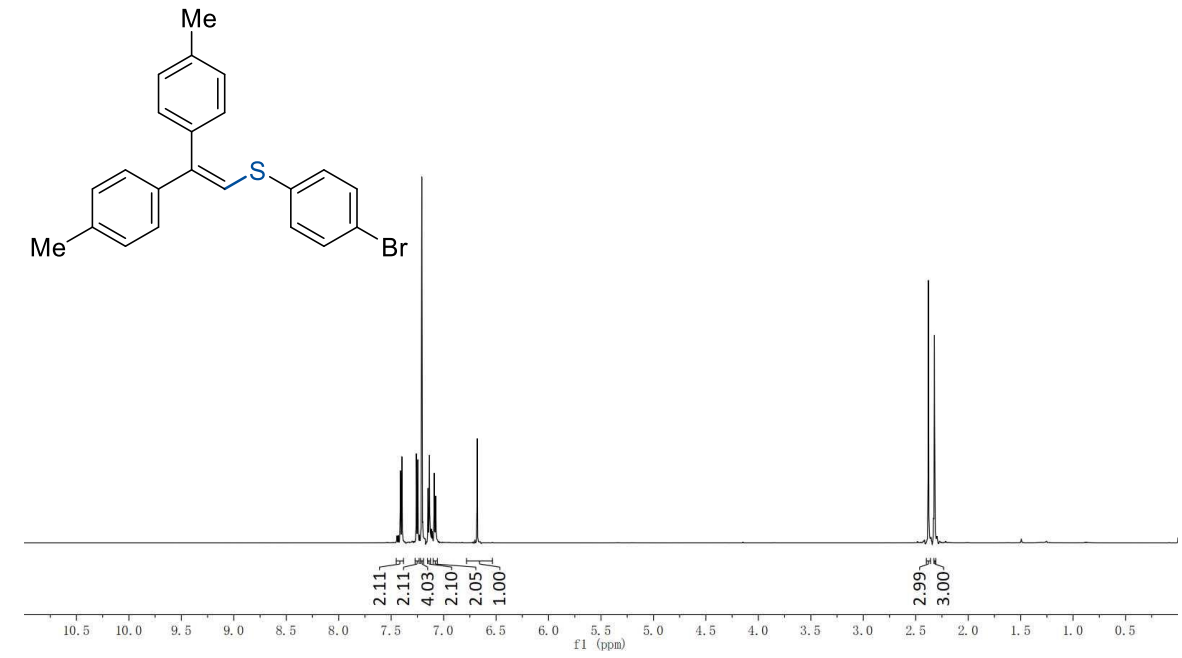
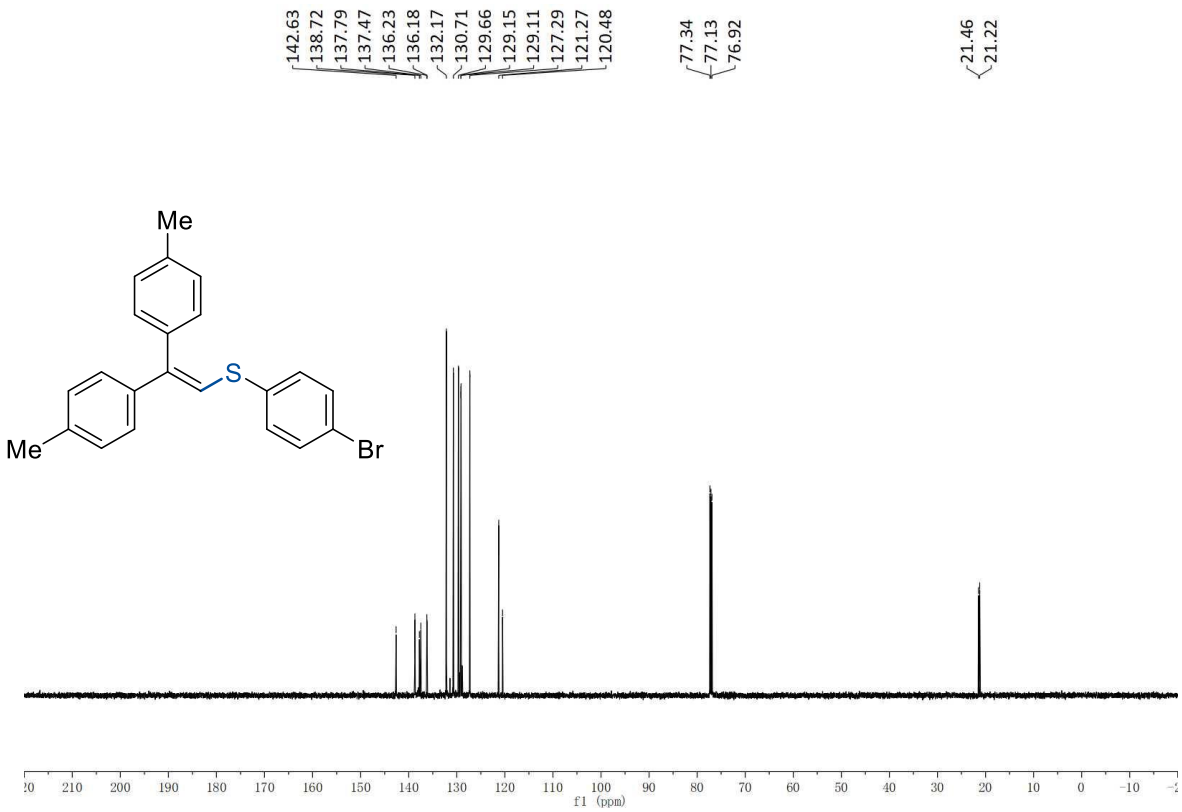
129.00
127.18
123.61
21.38
21.11
21.07
Me
S
Me
Me
f1 (ppm)


Me
S
Me
Br
2.11
2.11
4.03
2.10
2.05
1.00
2.99
3.00
f1 (ppm)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130.71
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129.15
129.11
127.29
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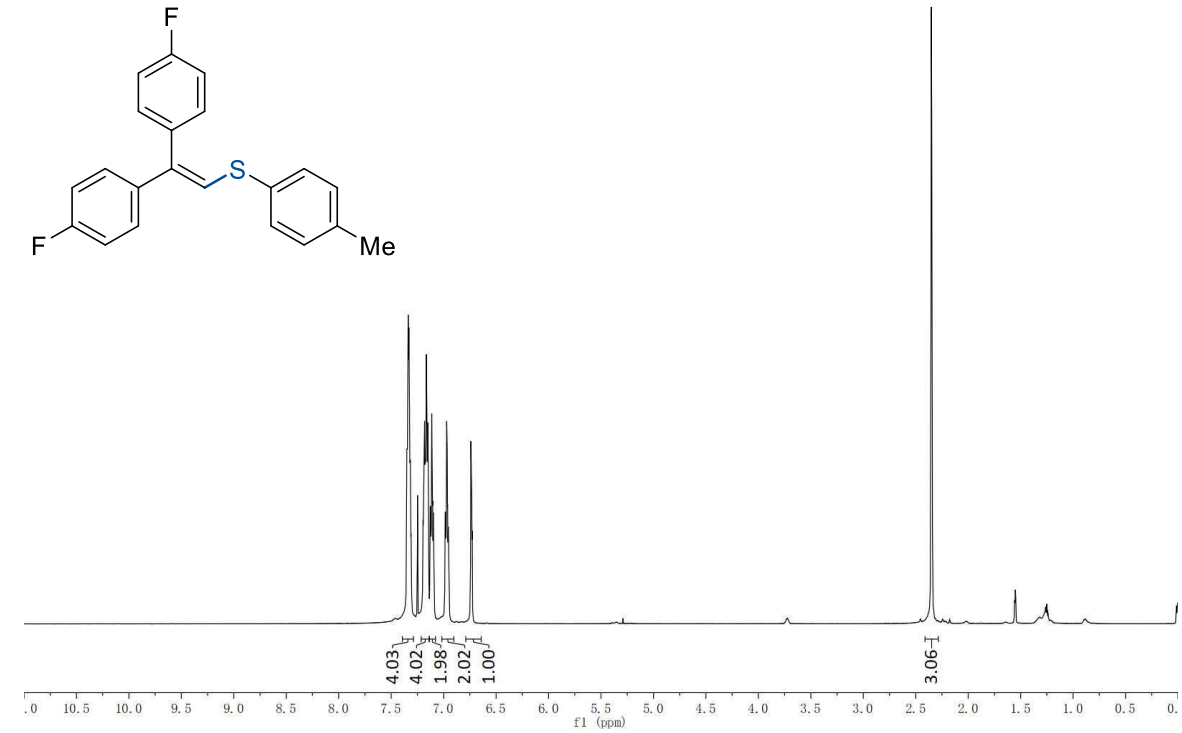
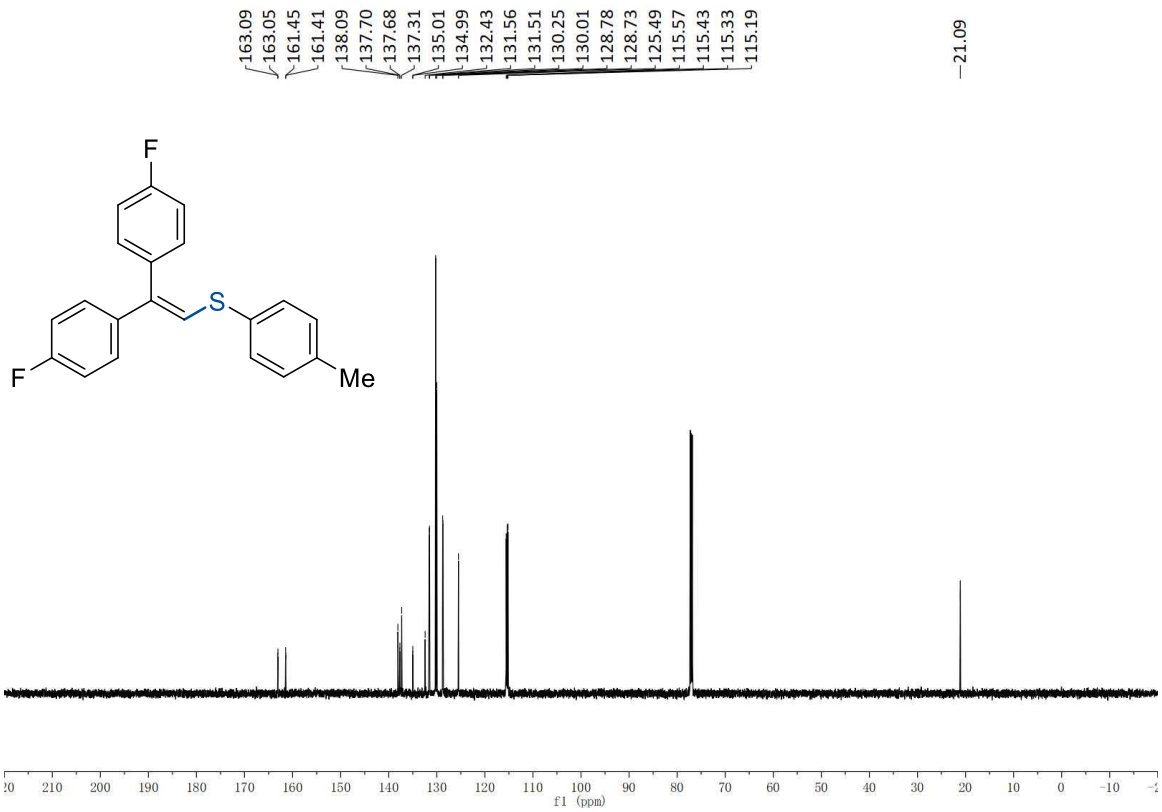
120.48
77.34
77.13
76.92
21.46
21.22
Me
S
Me
Br
f1 (ppm)


F
S
F
Me
4.03
4.02
1.98
2.02
1.00
3.06
f1 (ppm)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163.05
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161.41
138.09
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132.43
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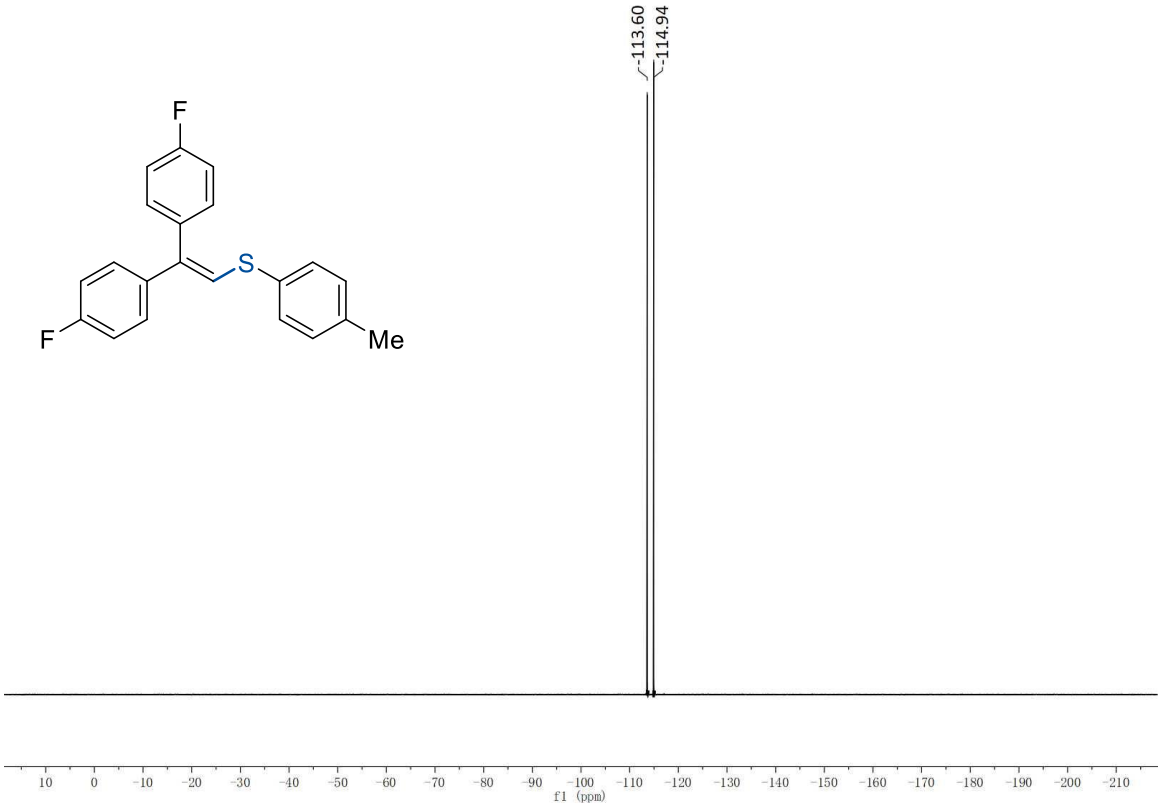
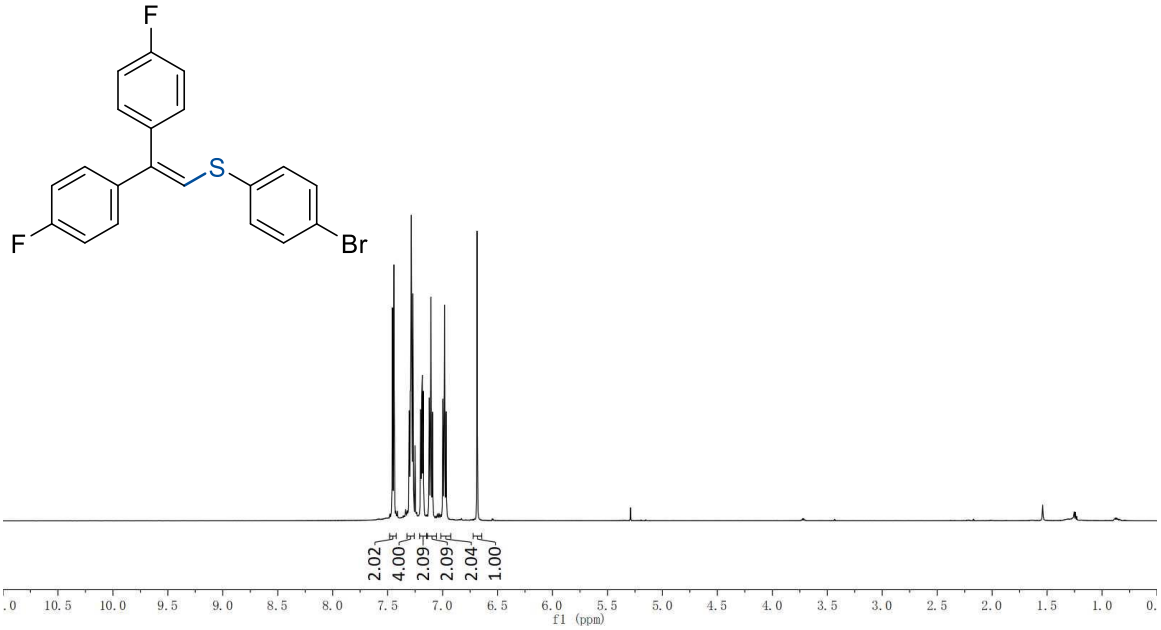
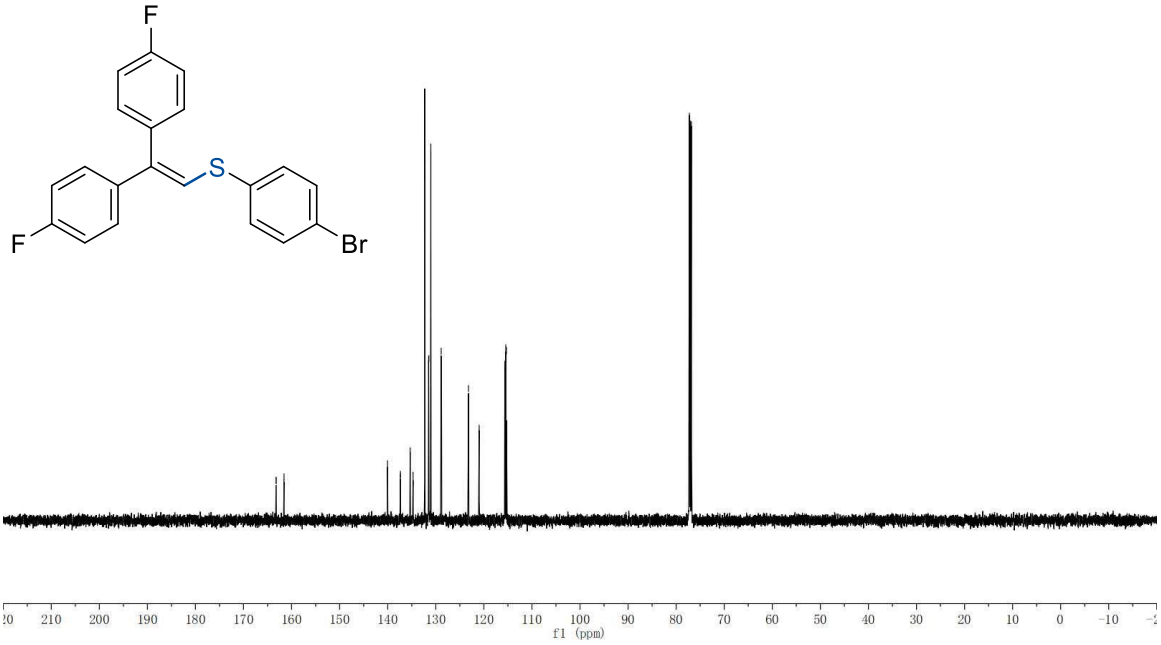
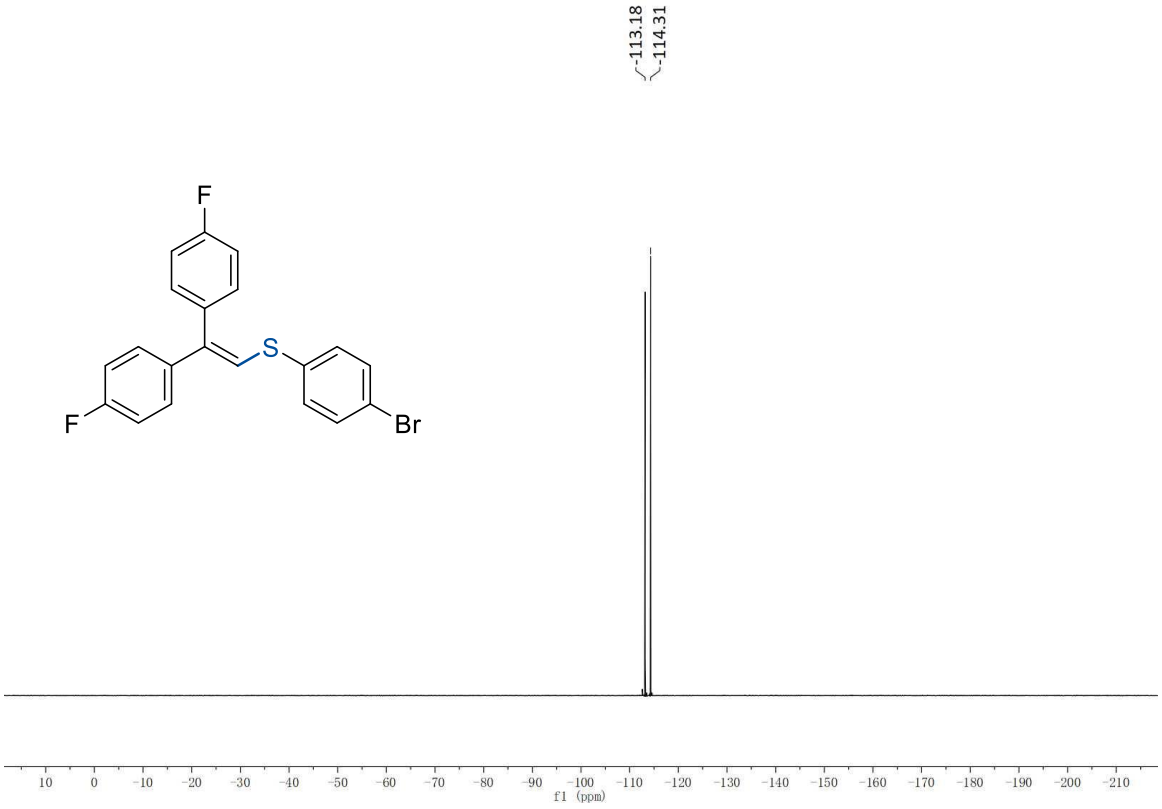
131.51
130.25
130.01
128.78
128.73
125.49
115.57
115.43
115.33
115.19
21.09
F
S
F
Me
f1 (ppm)

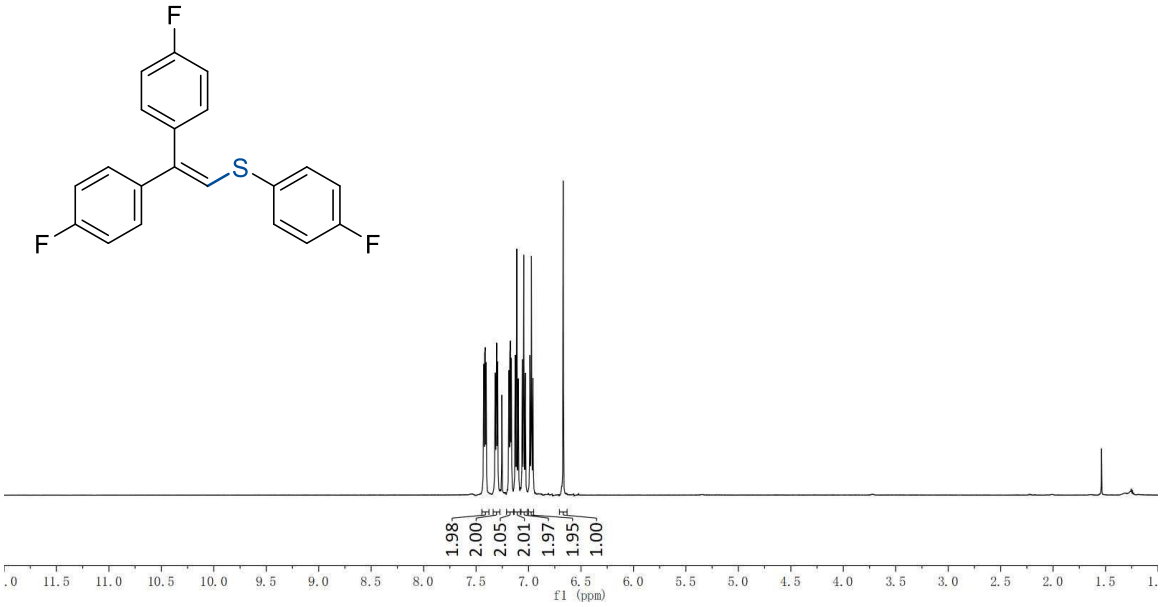

-113.60
-114.94
F
S
F
Me
f1 (ppm)

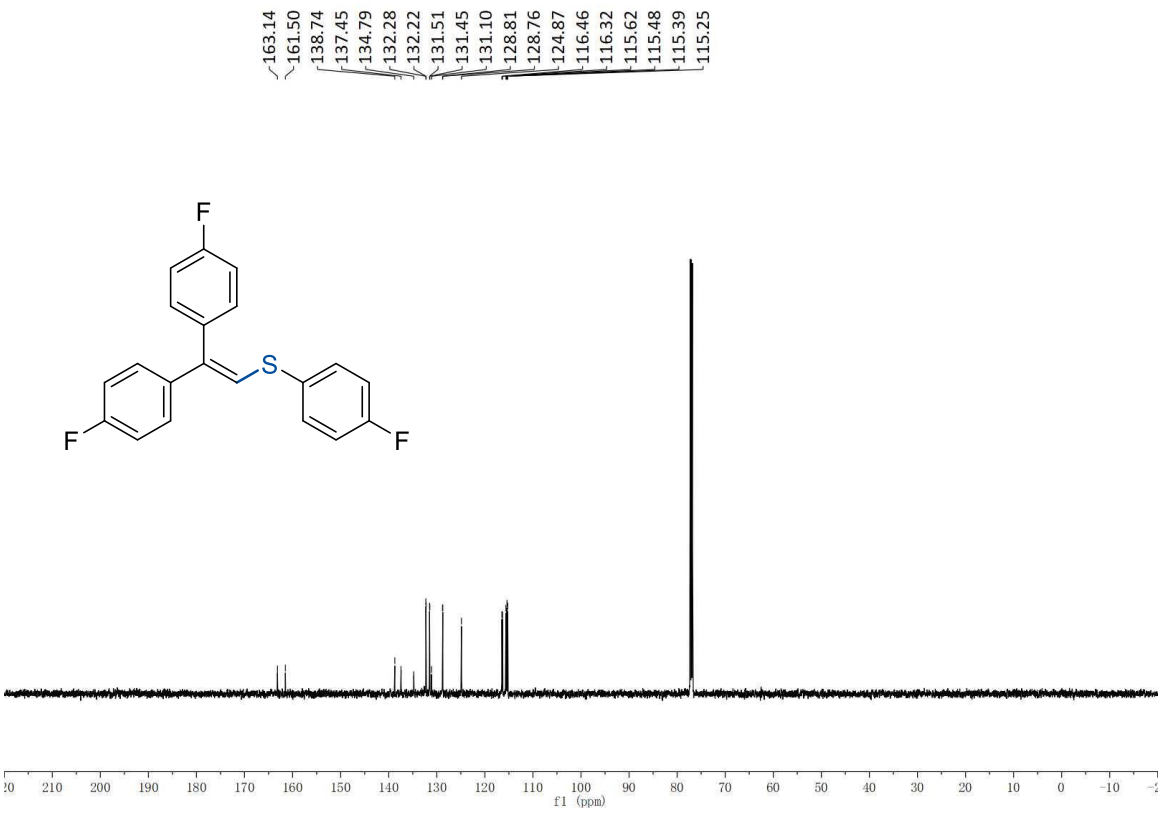

F
S
F
Br
2.02
4.00
2.09
2.09
2.04
1.00
f1 (ppm)

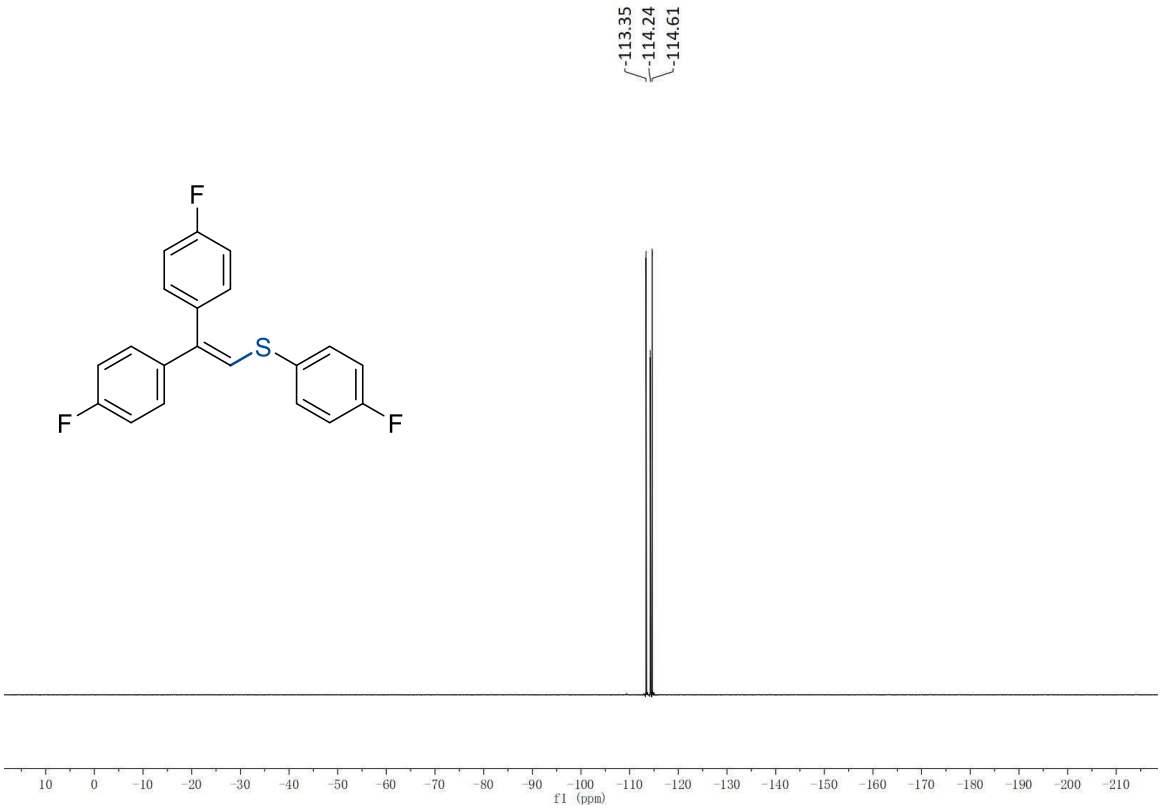

163.24
163.21
161.60
161.57
140.04
137.37
137.35
135.33
134.73
134.71
132.29
131.50
131.45
131.04
128.88
128.83
123.20
120.98
115.64
115.50
115.44
115.30
77.25
77.04
76.82

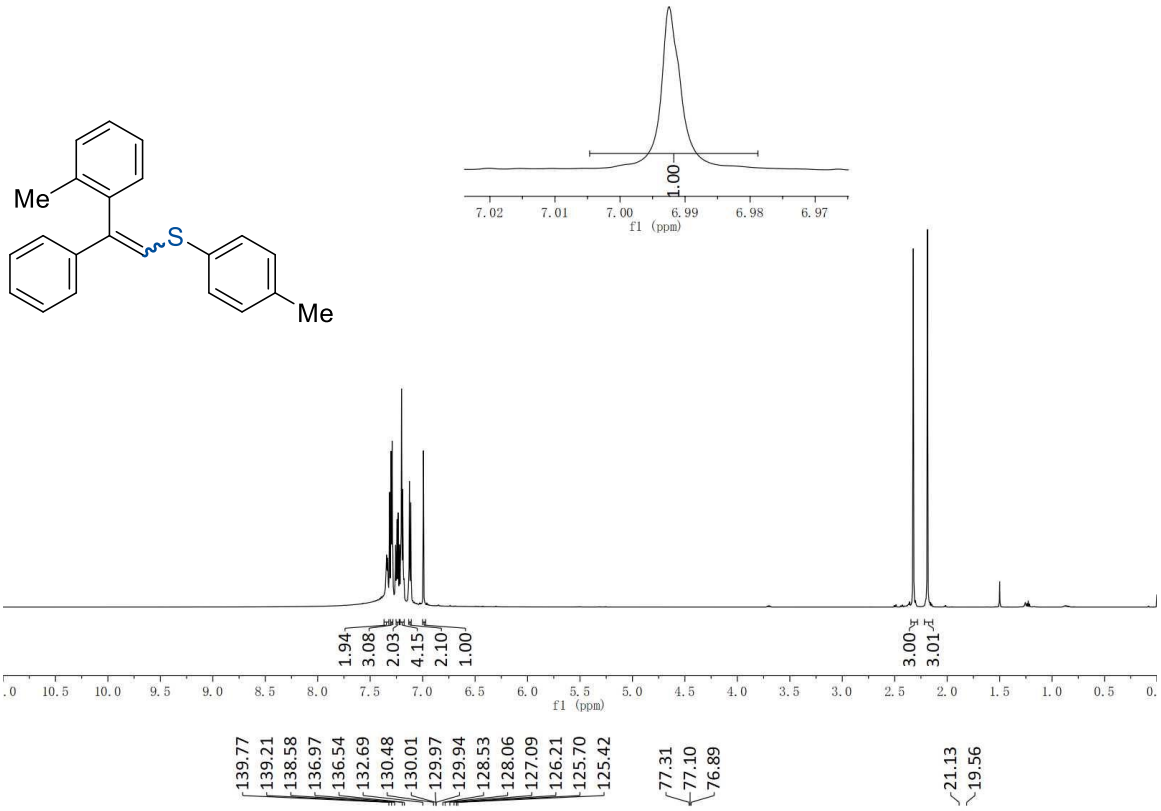

F
S
F
Br
f1 (ppm)


-113.18
-114.31
F
S
F
Br
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

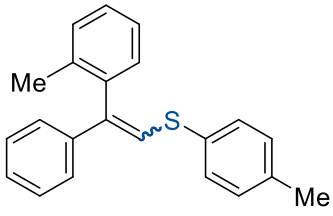

F
S
F
F
1.98
2.00
2.05
2.01
1.97
1.95
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)

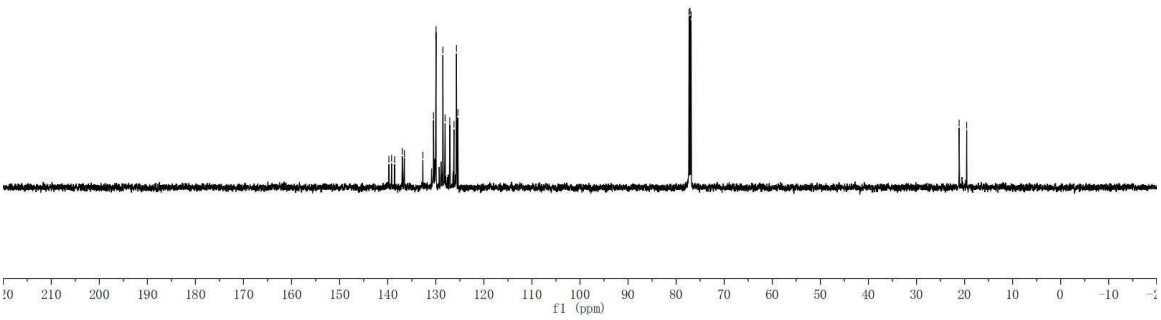

163.14
161.50
138.74
137.45
134.79
132.28
132.22
131.51
131.45
131.10
128.81
128.76
124.87
116.46
116.32
115.62
115.48
115.39
115.25
F
S
F
F
f1 (ppm)

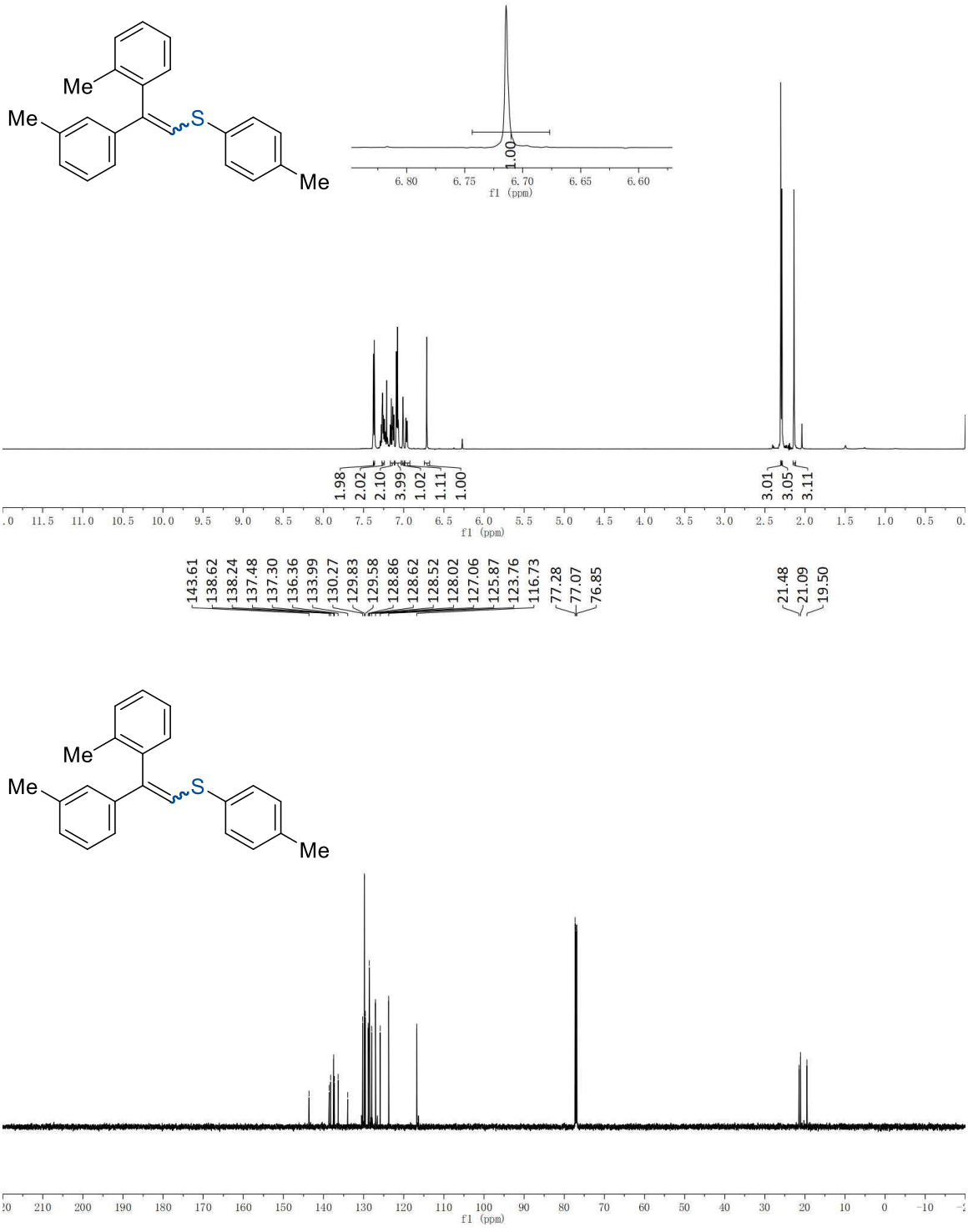

-113.35
-114.24
-114.61
F
S
F
F
f1 (ppm)

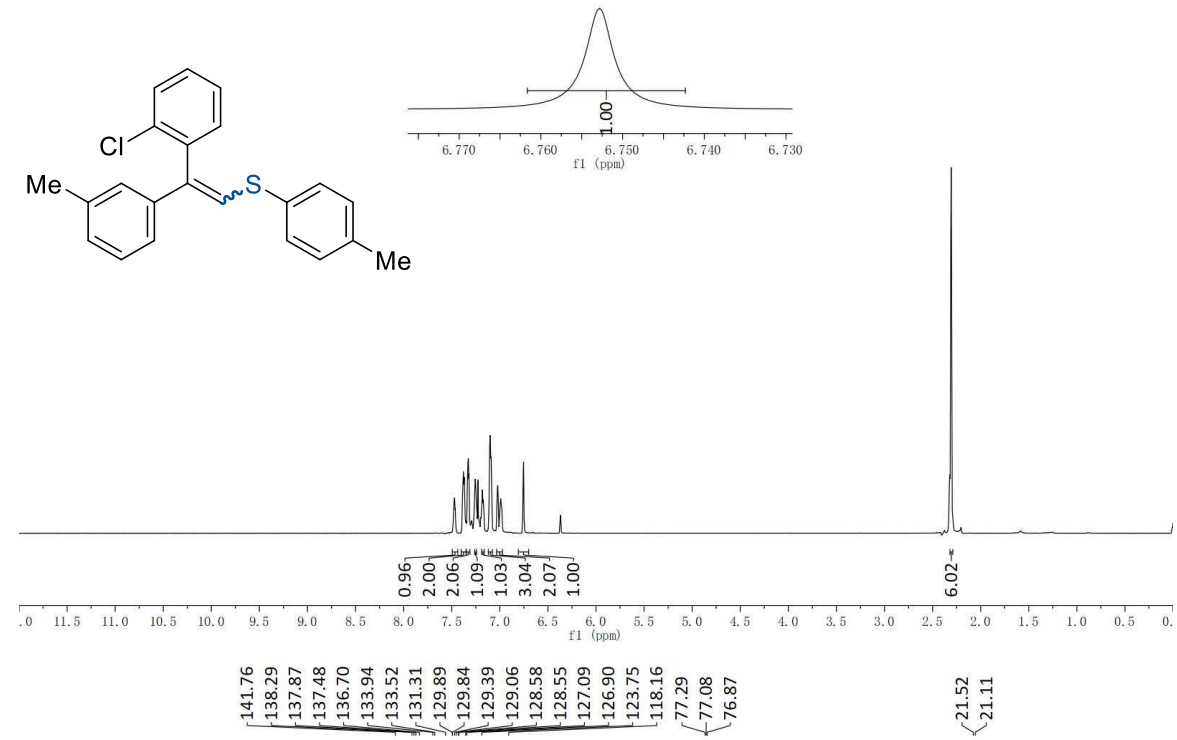

Me
S
Me
1.00
7.02
7.01
7.00
6.99
6.98
6.97
f1 (ppm)
1.94
3.08
2.03
4.15
2.10
1.00
3.00
3.01
f1 (ppm)

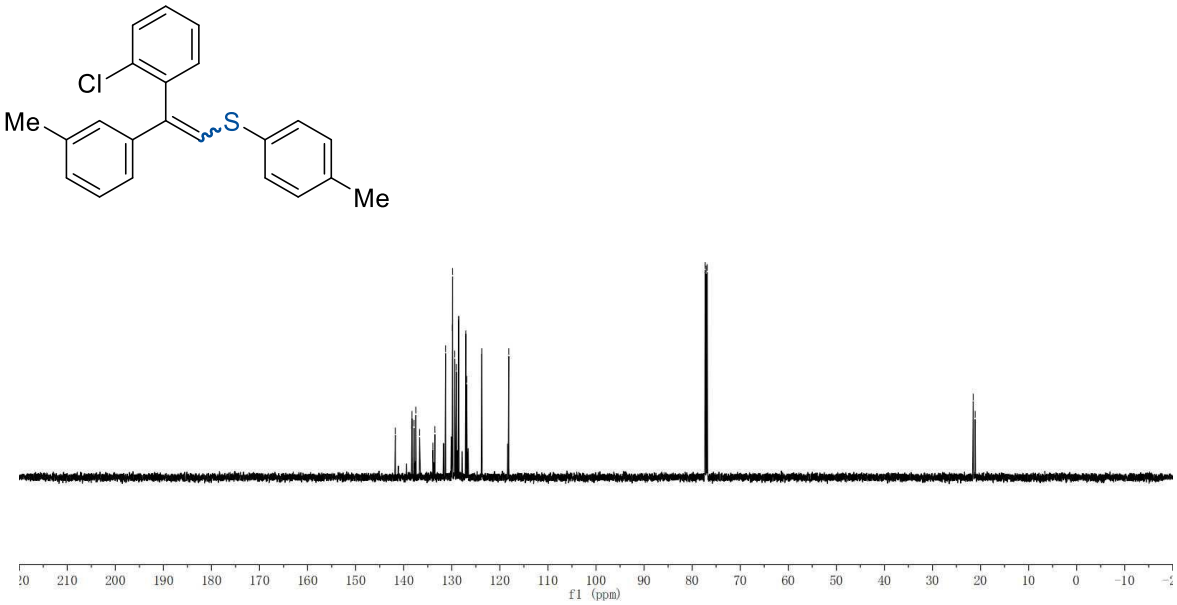
139.77
139.21
138.58
136.97
136.54
132.69
130.48
130.01
129.97
129.94
128.53
128.06
127.09
126.21
125.70
125.42
77.31
77.10
76.89
21.13
19.56

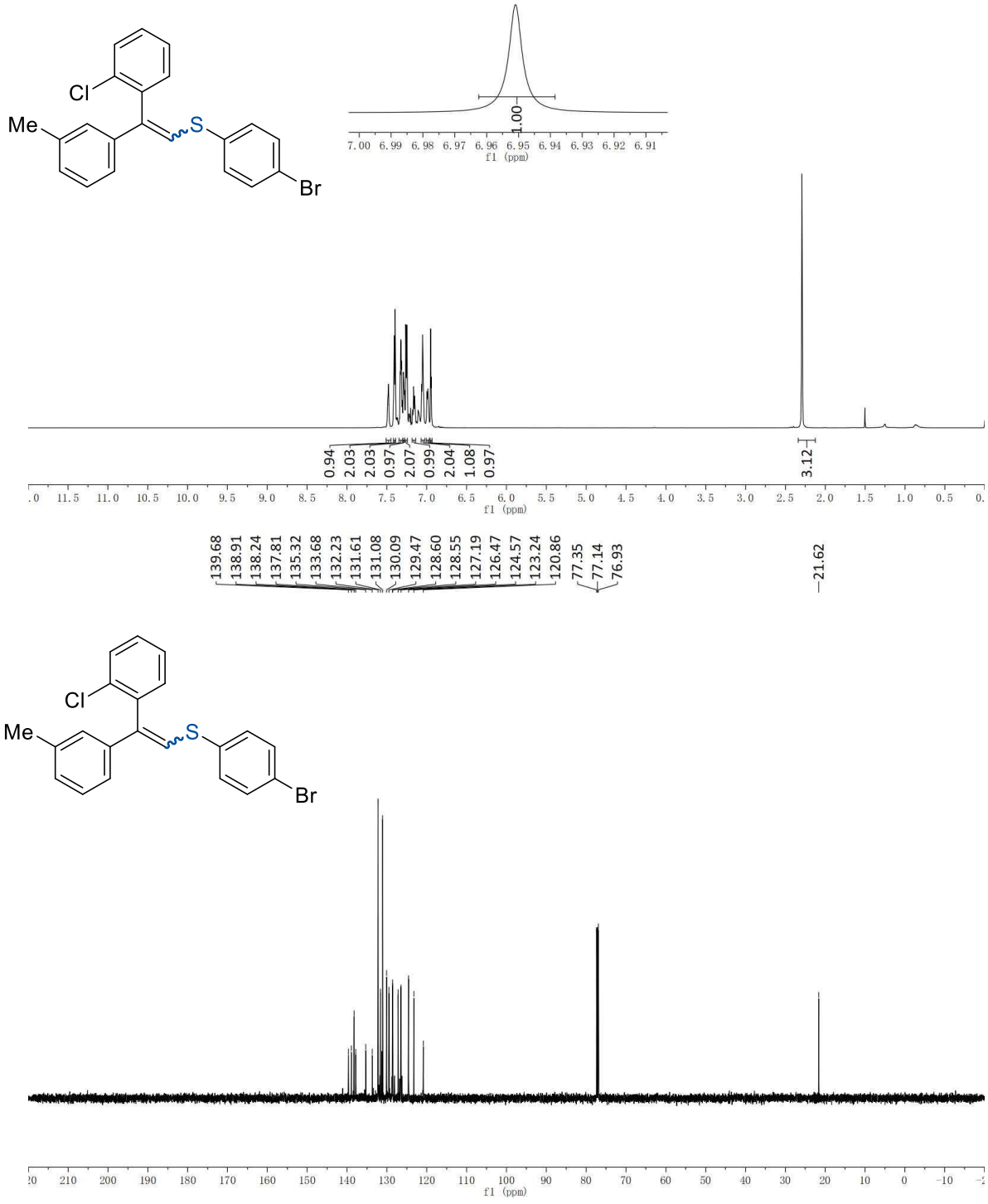

Me
S
Me

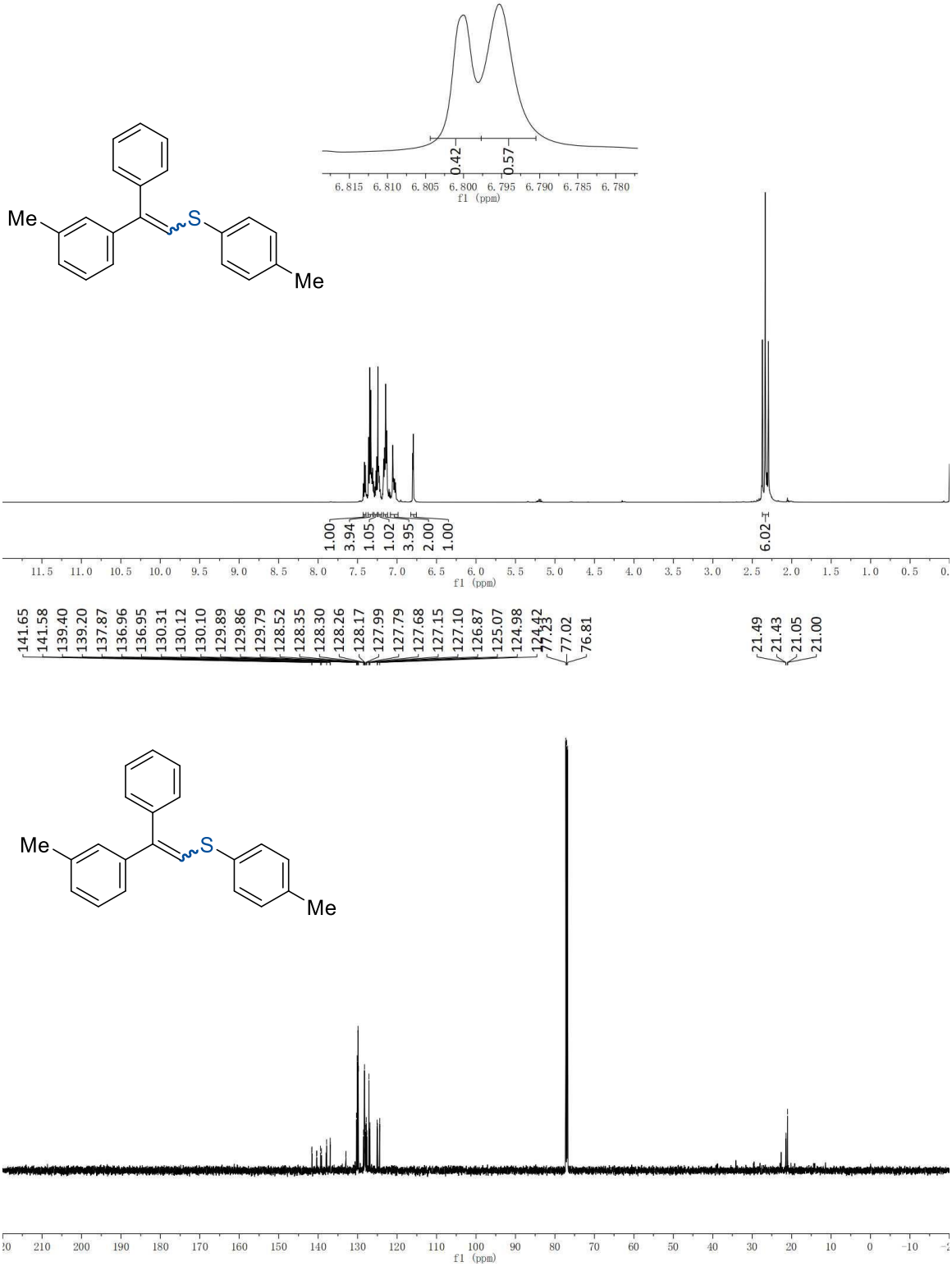

f1 (ppm)

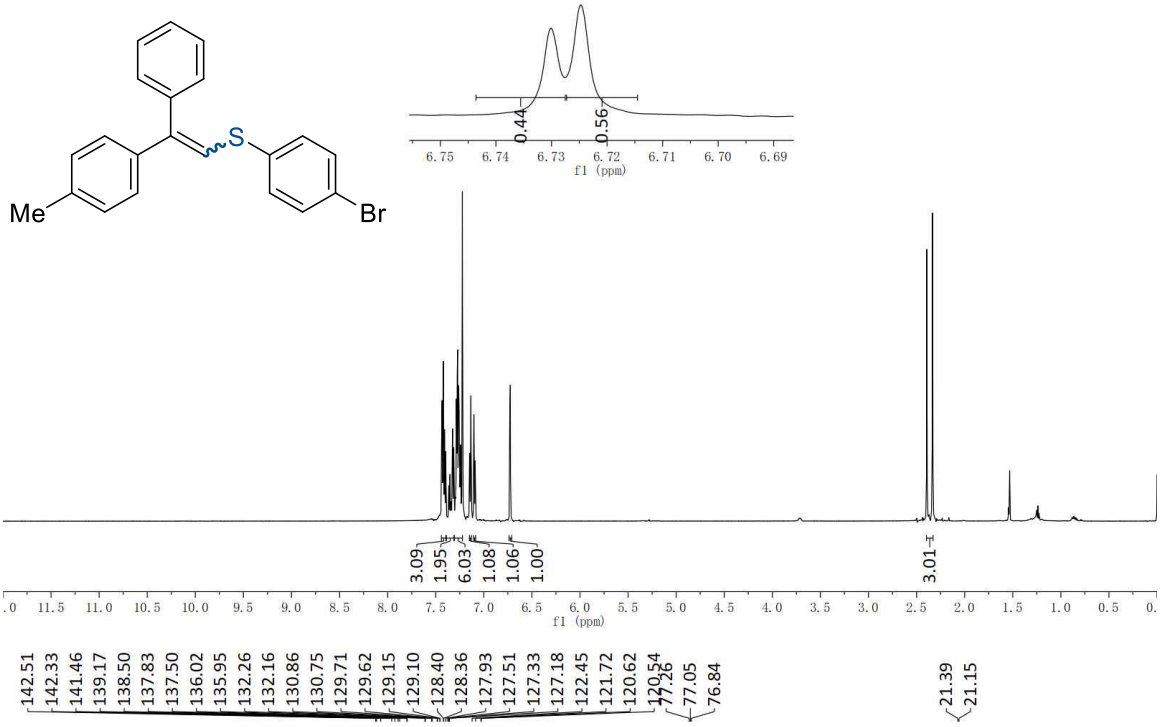

Me
Me
S
Me
1.00
6.80
6.75
6.70
6.65
6.60
f1 (ppm)
1.98
2.02
2.10
3.99
1.02
1.11
1.00
3.01
3.05
3.11
f1 (ppm)
143.61
138.62
138.24
137.48
137.30
136.36
133.99
130.27
129.83
129.58
128.86
128.62
128.52
128.02
127.06
125.87
123.76
116.73
77.28
77.07
76.85
21.48
21.09
19.50
Me
Me
S
Me
f1 (ppm)


Cl
Me
S
Me
1.00
6.770
6.760
6.750
6.740
6.730
f1 (ppm)
0.96
2.00
2.06
1.09
1.03
3.04
2.07
1.00
6.02
f1 (ppm)
141.76
138.29
137.87
137.48
136.70
133.94
133.52
131.31
129.89
129.84
129.39
129.06
128.58
128.55
127.09
126.90
123.75
118.16
77.29
77.08
76.87
21.52
21.11

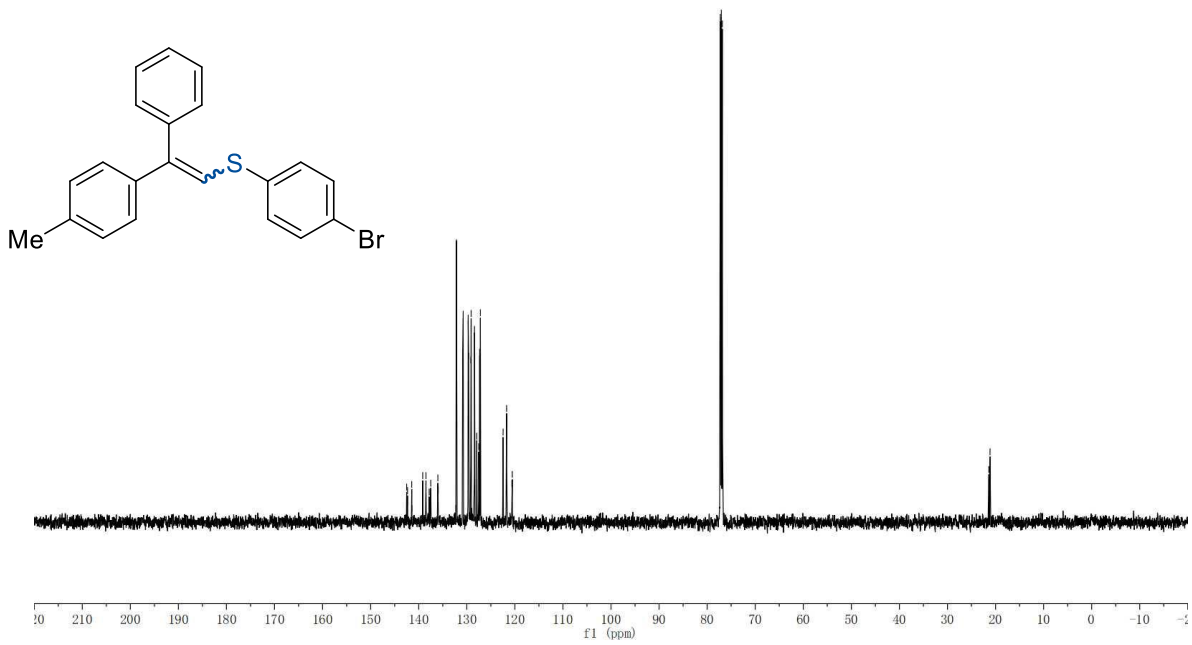

Cl
Me
S
Me
f1 (ppm)

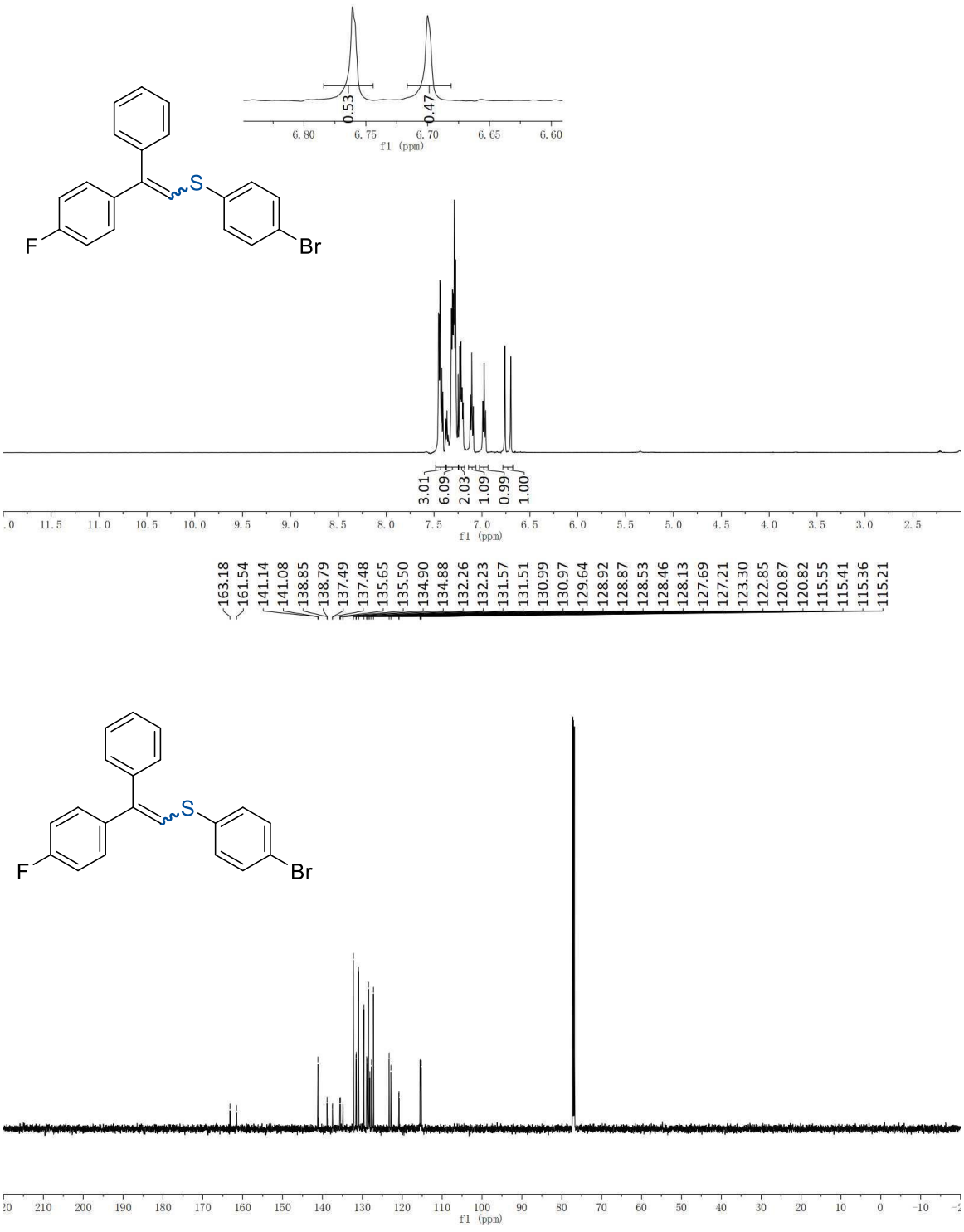

Cl
Me
S
Br
1.00
7.00 6.99 6.98 6.97 6.96 6.95 6.94 6.93 6.92 6.91
f1 (ppm)
0.94 2.03 2.03 0.97 2.07 0.99 2.04 1.08 0.97
3.12
f1 (ppm)
139.68 138.91 138.24 137.81 135.32 133.68 132.23 131.61 131.08 130.09 129.47 128.60 128.55 127.19 126.47 124.57 123.24 120.86
77.35 77.14 76.93
21.62
Cl
Me
S
Br
f1 (ppm)

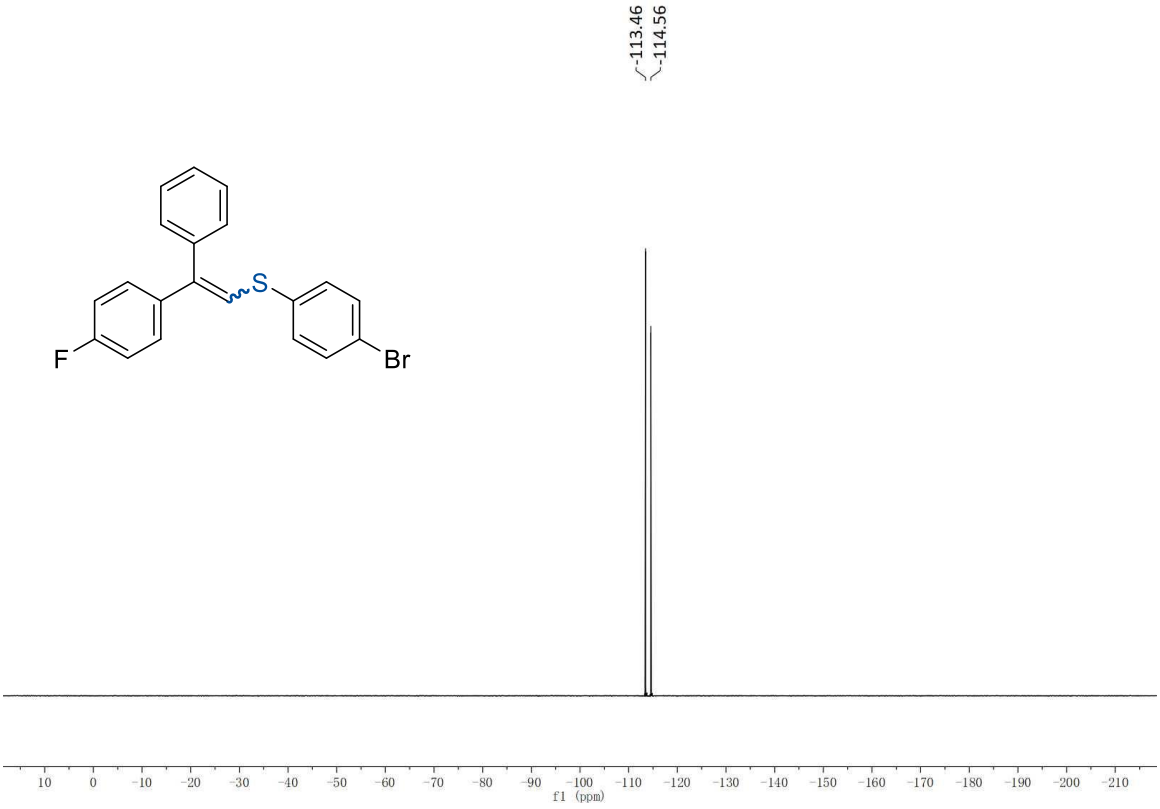

Me
S
Me
0.42
0.57
6.815 6.810 6.805 6.800 6.795 6.790 6.785 6.780
f1 (ppm)
1.00
3.94
1.05
1.02
3.95
2.00
1.00
6.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)
141.65
141.58
139.40
139.20
137.87
136.96
136.95
130.31
130.12
130.10
129.89
129.86
129.79
128.52
128.35
128.30
128.26
128.17
127.99
127.79
127.68
127.15
127.10
126.87
125.07
124.98
124.42
77.23
77.02
76.81
21.49
21.43
21.05
21.00
Me
S
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

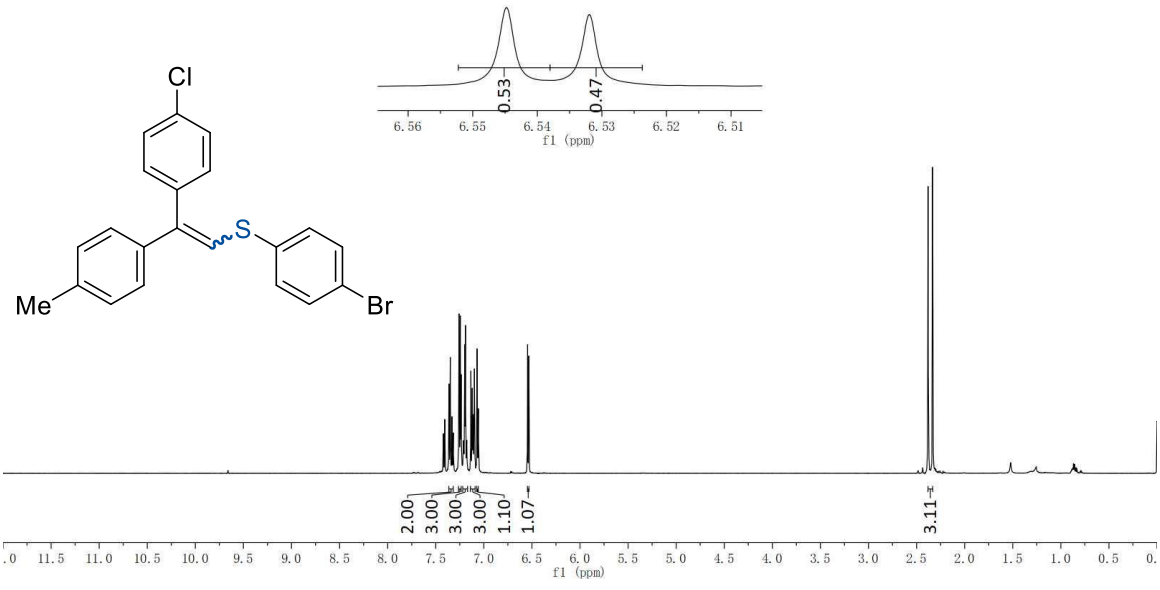


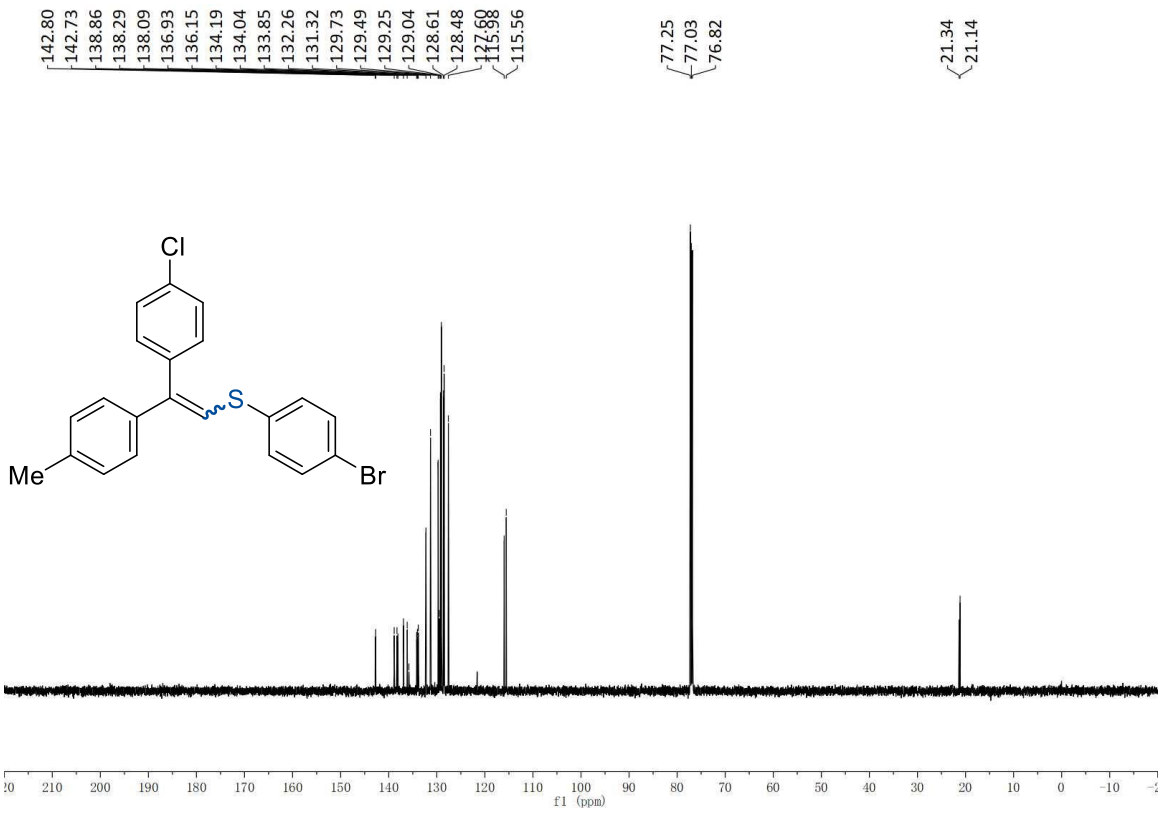
142.51 142.33 141.46 139.17 138.50 137.83 137.50 136.02 135.95 132.26 132.16 130.86 130.75 129.71 129.62 129.15 129.10 128.40 128.36 127.93 127.51 127.33 127.18 122.45 121.72 120.62 120.54 77.26 77.05 76.84 21.39 21.15

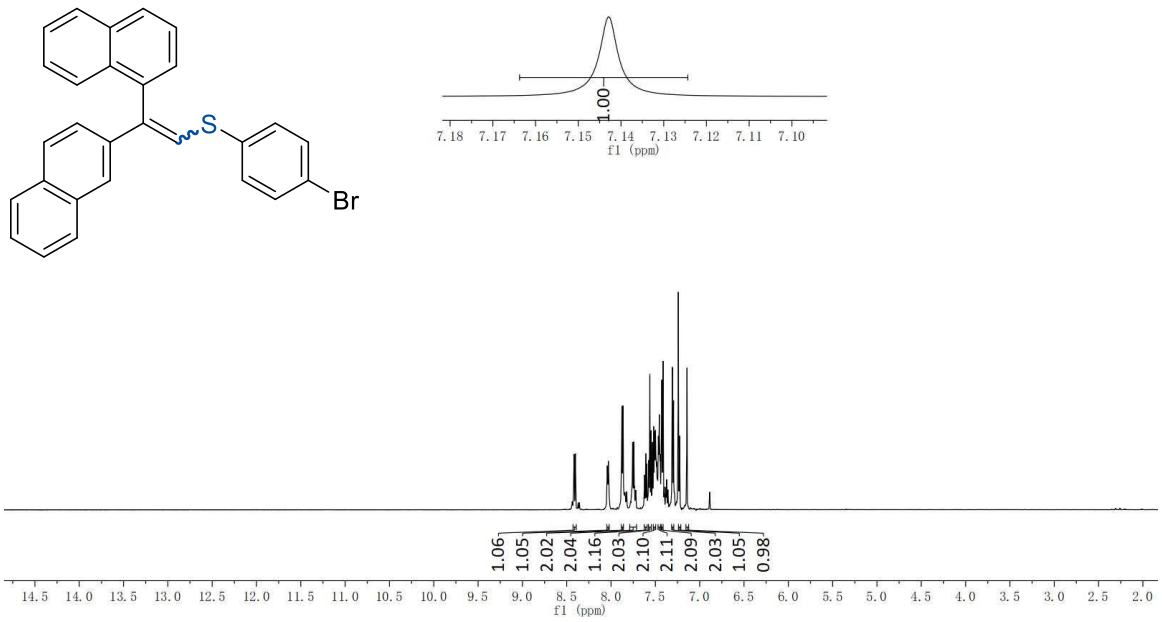


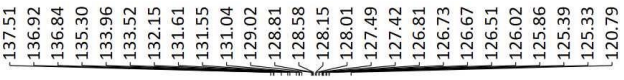

F
S
Br
0.53
0.47
6.80
6.75
6.70
6.65
6.60
f1 (ppm)
3.01
6.09
2.03
1.09
0.99
1.00
f1 (ppm)
163.18
161.54
141.14
141.08
138.85
138.79
137.49
137.48
135.65
135.50
134.90
134.88
132.26
132.23
131.57
131.51
130.99
130.97
129.64
128.92
128.87
128.53
128.46
128.13
127.69
127.21
123.30
122.85
120.87
120.82
115.55
115.41
115.36
115.21
F
S
Br
f1 (ppm)


-113.46
-114.56
F
S
Br
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


Cl
S
Me
Br
0.53
0.47
6.56 6.55 6.54 6.53 6.52 6.51
f1 (ppm)
2.00
3.00
3.00
3.00
1.10
1.07
3.11
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


142.80
142.73
138.86
138.29
138.09
136.93
136.15
134.19
134.04
133.85
132.26
131.32
129.73
129.49
129.25
129.04
128.61
128.48
77.25
77.03
76.82
21.34
21.14
Cl
S
Me
Br
f1 (ppm)


S
Br
1.00
7.18 7.17 7.16 7.15 7.14 7.13 7.12 7.11 7.10
f1 (ppm)
1.06
1.05
2.02
2.04
1.16
2.03
2.10
2.11
2.09
2.03
1.05
0.98
f1 (ppm)


137.51
136.92
136.84
135.30
133.96
133.52
132.15
131.61
131.55
131.04
129.02
128.81
128.58
128.15
128.01
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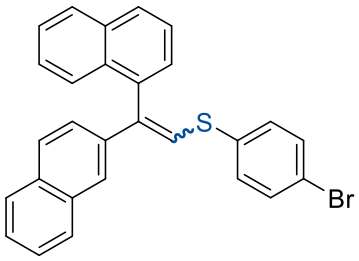
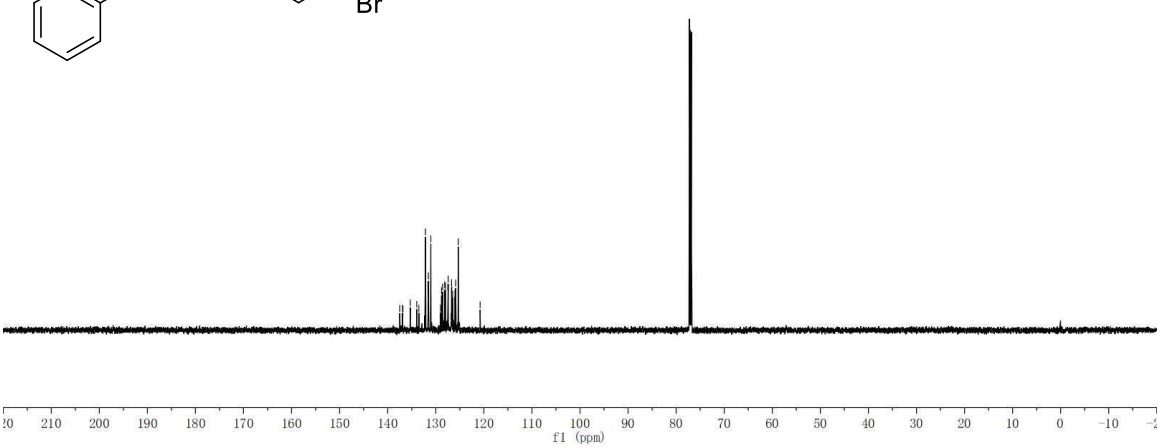
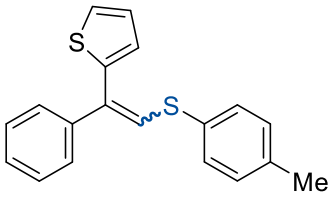
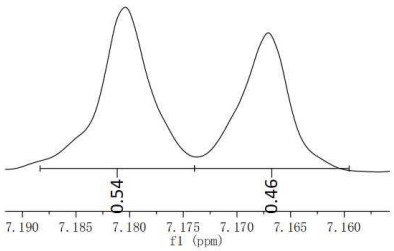
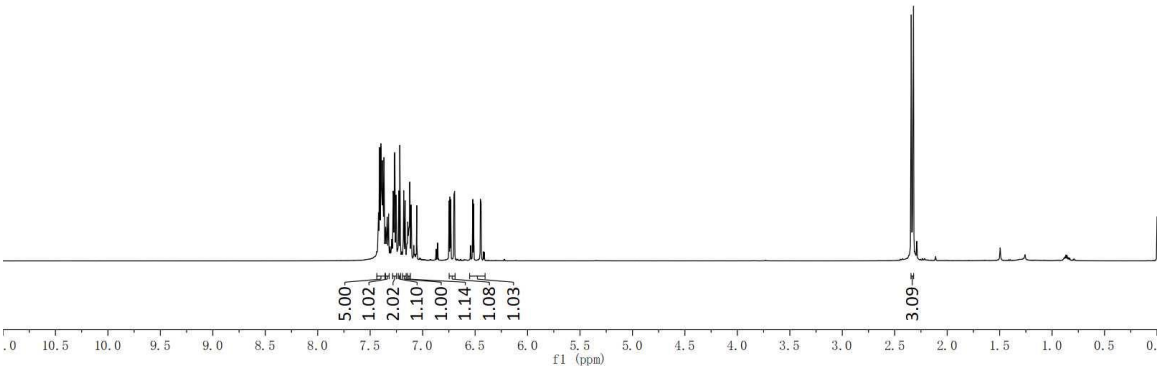
126.81
126.73
126.67
126.51
126.02
125.86
125.39
125.33
120.79

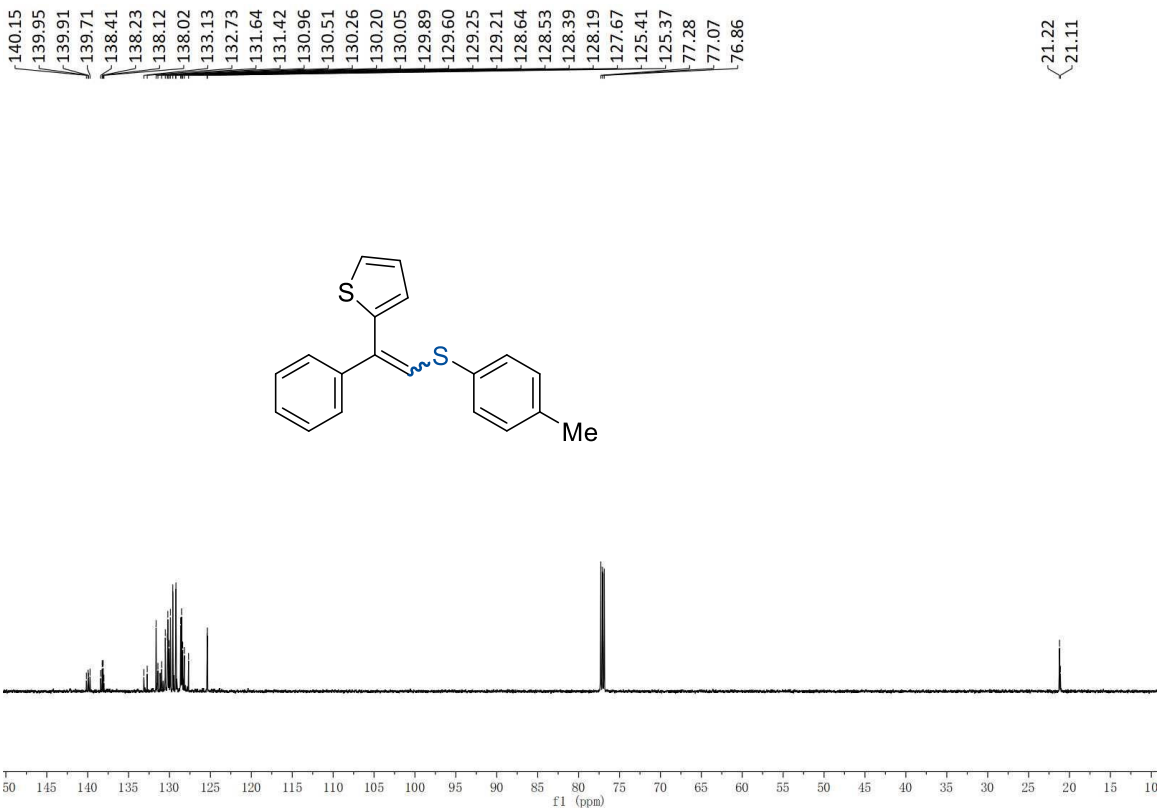

S
Br

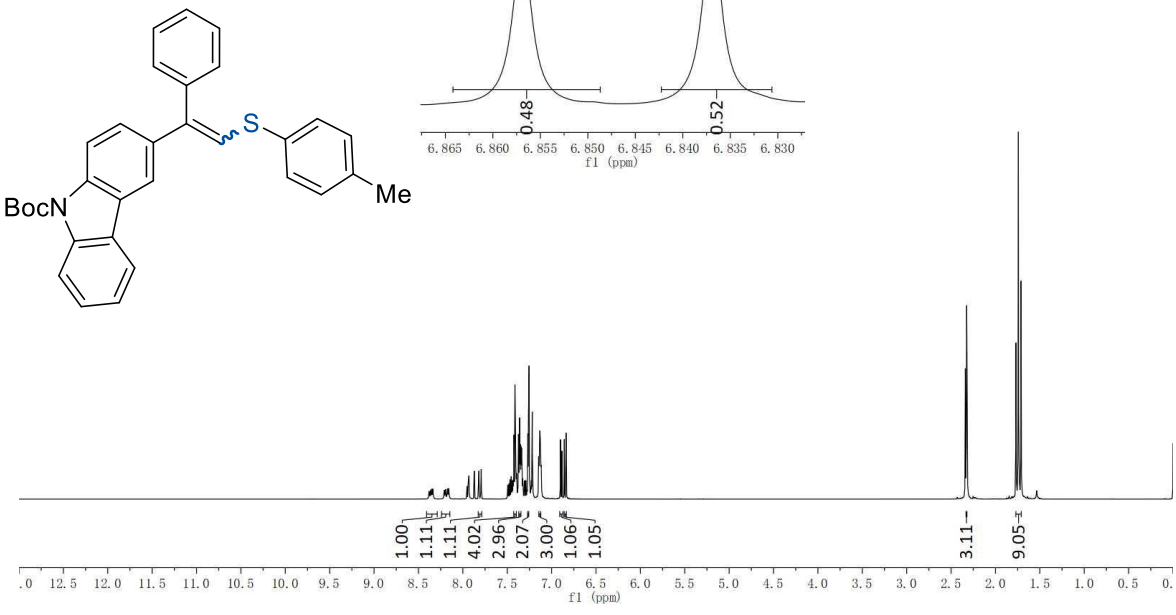

f1 (ppm)

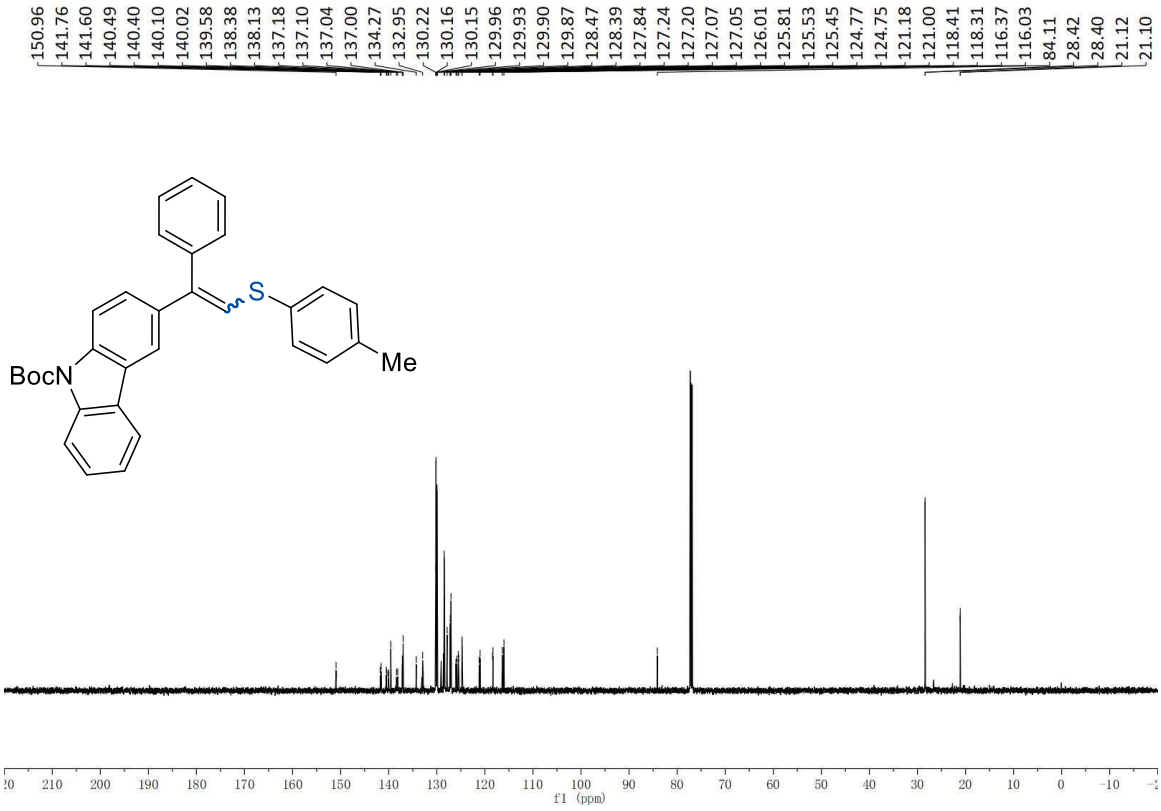

S
S
Me

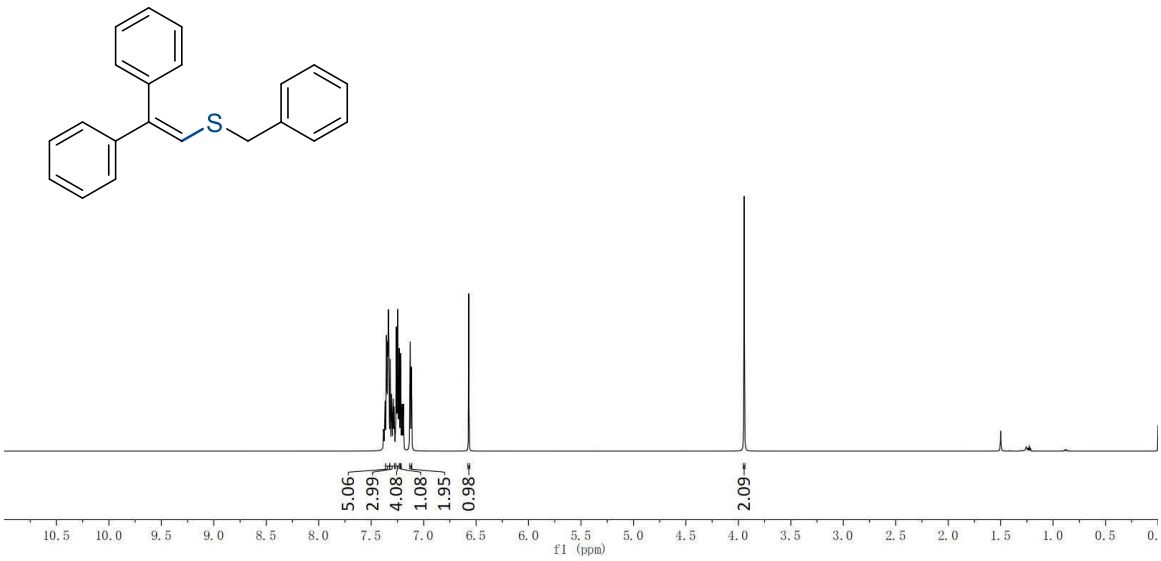

0.54
0.46
7.190
7.185
7.180
7.175
7.170
7.165
7.160
f1 (ppm)

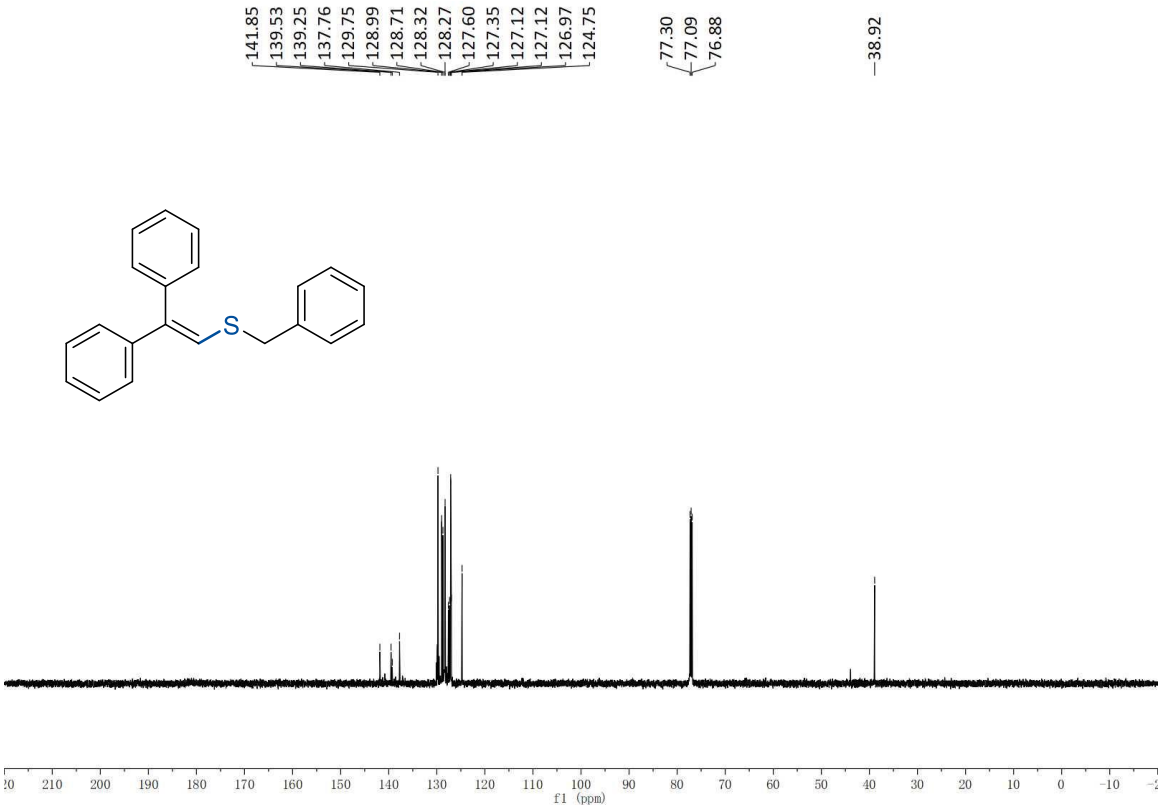

5.00
1.02
2.02
1.10
1.00
1.14
1.08
1.03
3.09
f1 (ppm)

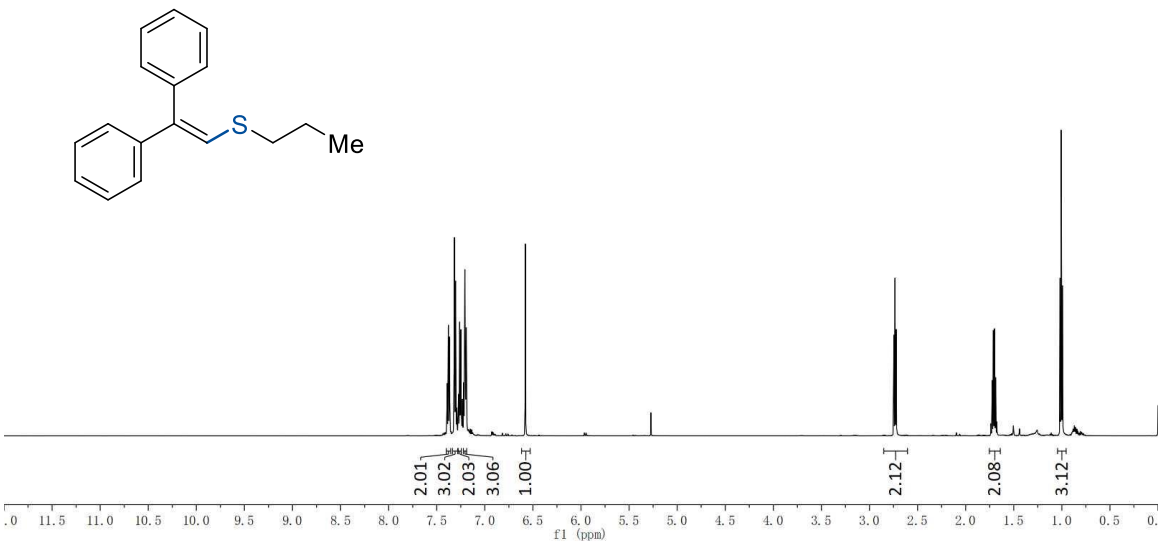

140.15
139.95
139.91
139.71
138.41
138.23
138.12
138.02
133.13
132.73
131.64
131.42
130.96
130.51
130.26
130.20
130.05
129.89
129.60
129.25
129.21
128.64
128.53
128.39
128.19
127.67
125.41
125.37
77.28
77.07
76.86
21.22
21.11
S
S
Me
f1 (ppm)

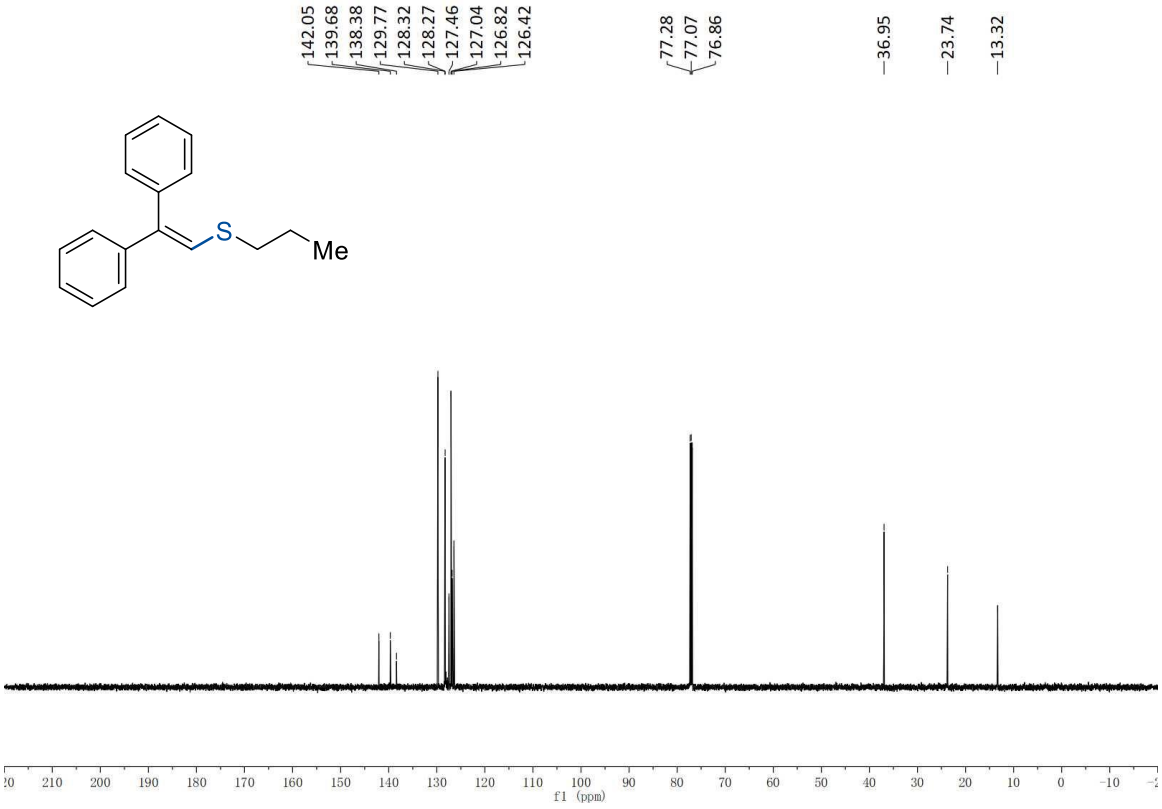

BocN
S
Me
0.48
0.52
f1 (ppm)
1.00
1.11
1.11
4.02
2.96
2.07
3.00
1.06
1.05
3.11
9.05
f1 (ppm)

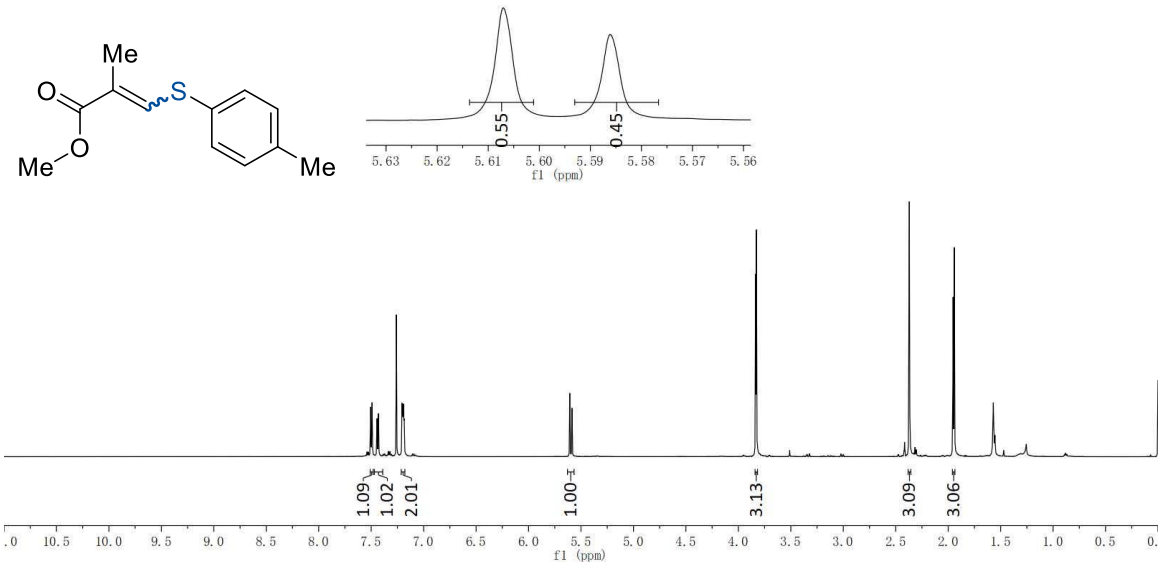

150.96
141.76
141.60
140.49
140.40
140.10
140.02
139.58
138.38
138.13
137.18
137.10
137.04
137.00
134.27
132.95
130.22
130.16
130.15
129.96
129.93
129.90
129.87
128.47
128.39
127.84
127.24
127.20
127.07
127.05
126.01
125.81
125.53
125.45
124.77
124.75
121.18
121.00
118.41
118.31
116.37
116.03
84.11
28.42
28.40
21.12
21.10
BocN
S
Me
f1 (ppm)

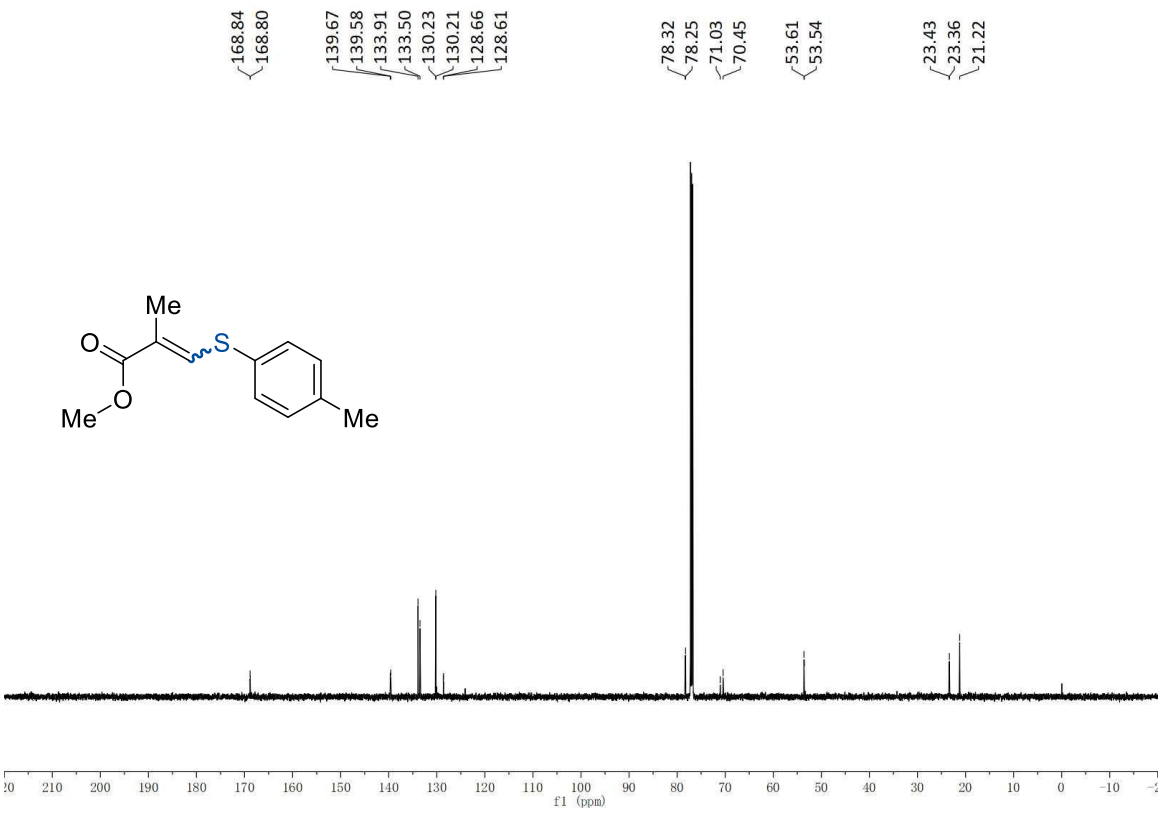

S
5.06
2.99
4.08
1.08
1.95
0.98
2.09
f1 (ppm)


141.85
139.53
139.25
137.76
129.75
128.99
128.71
128.32
128.27
127.60
127.35
127.12
127.12
126.97
124.75
77.30
77.09
76.88
38.92
S
f1 (ppm)


S
Me
2.01
3.02
2.03
3.06
1.00
2.12
2.08
3.12
f1 (ppm)


142.05
139.68
138.38
129.77
128.32
128.27
127.46
127.04
126.82
126.42
77.28
77.07
76.86
36.95
23.74
13.32
S
Me
f1 (ppm)


Me
O
S
O
Me
Me
0.55
0.45
5.63
5.62
5.61
5.60
5.59
5.58
5.57
5.56
f1 (ppm)
1.09
1.02
2.01
1.00
3.13
3.09
3.06
f1 (ppm)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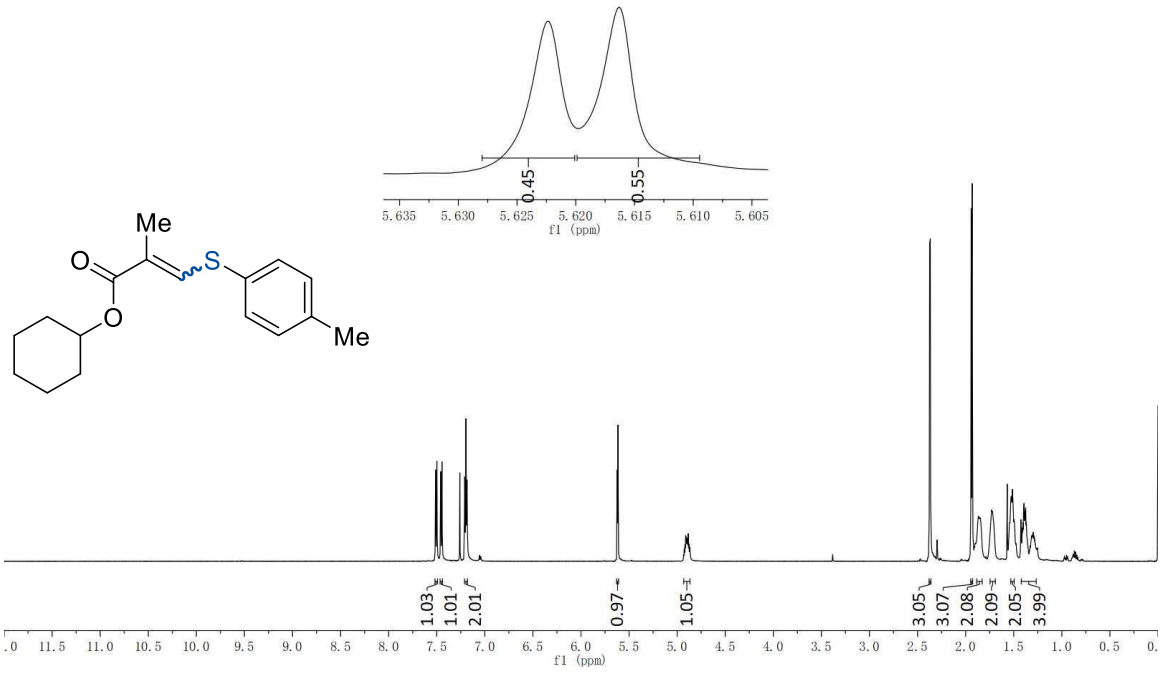
168.80
139.67
139.58
133.91
133.50
130.23
130.21
128.66
128.61
78.32
78.25
71.03
70.45
53.61
53.54
23.43
23.36
21.22
Me
O
S
Me
O
Me
f1 (ppm)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0.55
5.635
5.630
5.625
5.620
5.615
5.610
5.605
f1 (ppm)
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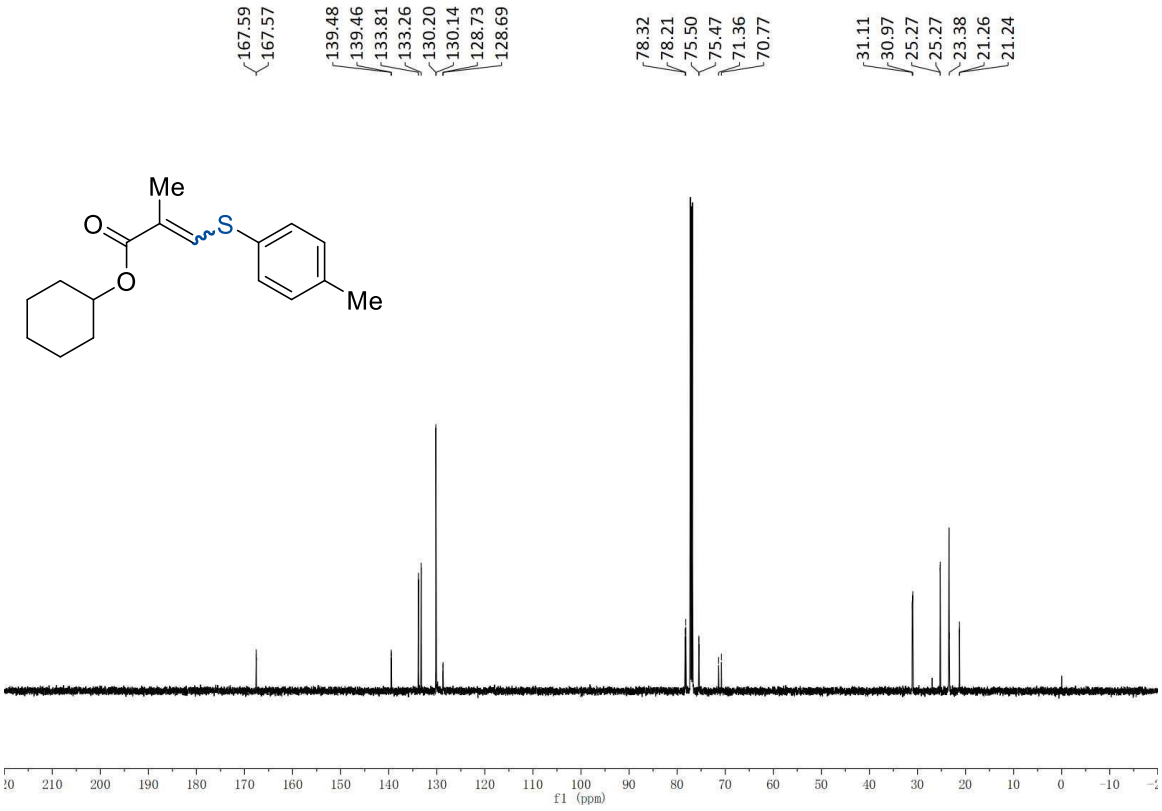
O
S
O
Me
1.03
1.01
2.01
0.97
1.05
3.05
3.07
2.08
2.09
2.05
3.99
f1 (ppm)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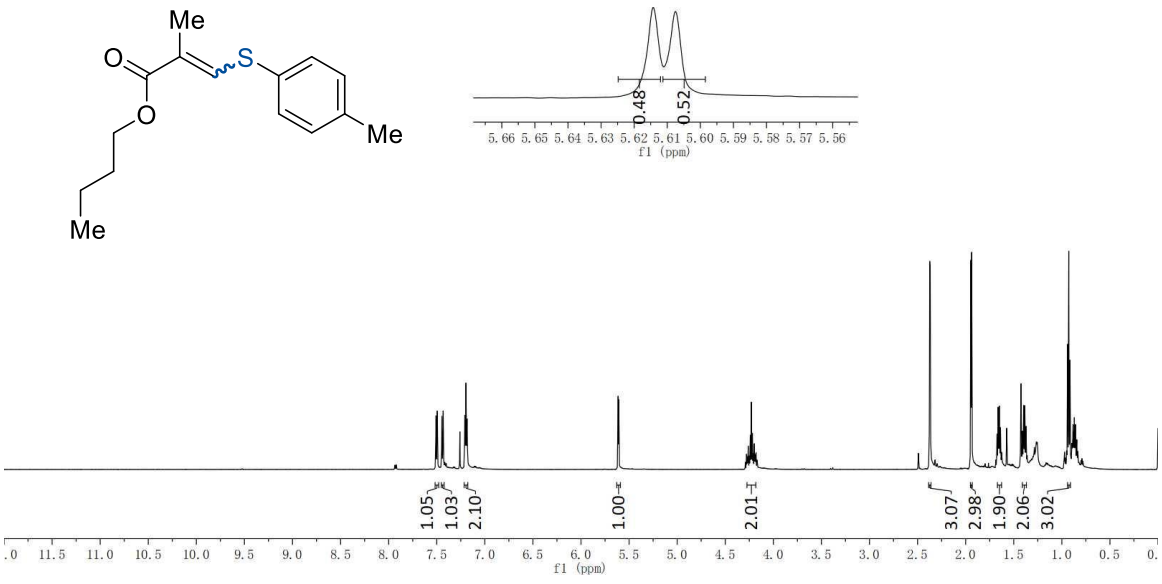
167.57
139.48
139.46
133.81
133.26
130.20
130.14
128.73
128.69
78.32
78.21
75.50
75.47
71.36
70.77
31.11
30.97
25.27
25.27
23.38
21.26
21.24
Me
O
S
O
Me
f1 (ppm)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S
O
Me
Me
0.48
0.52
f1 (ppm)
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1.03
2.10
1.00
2.01
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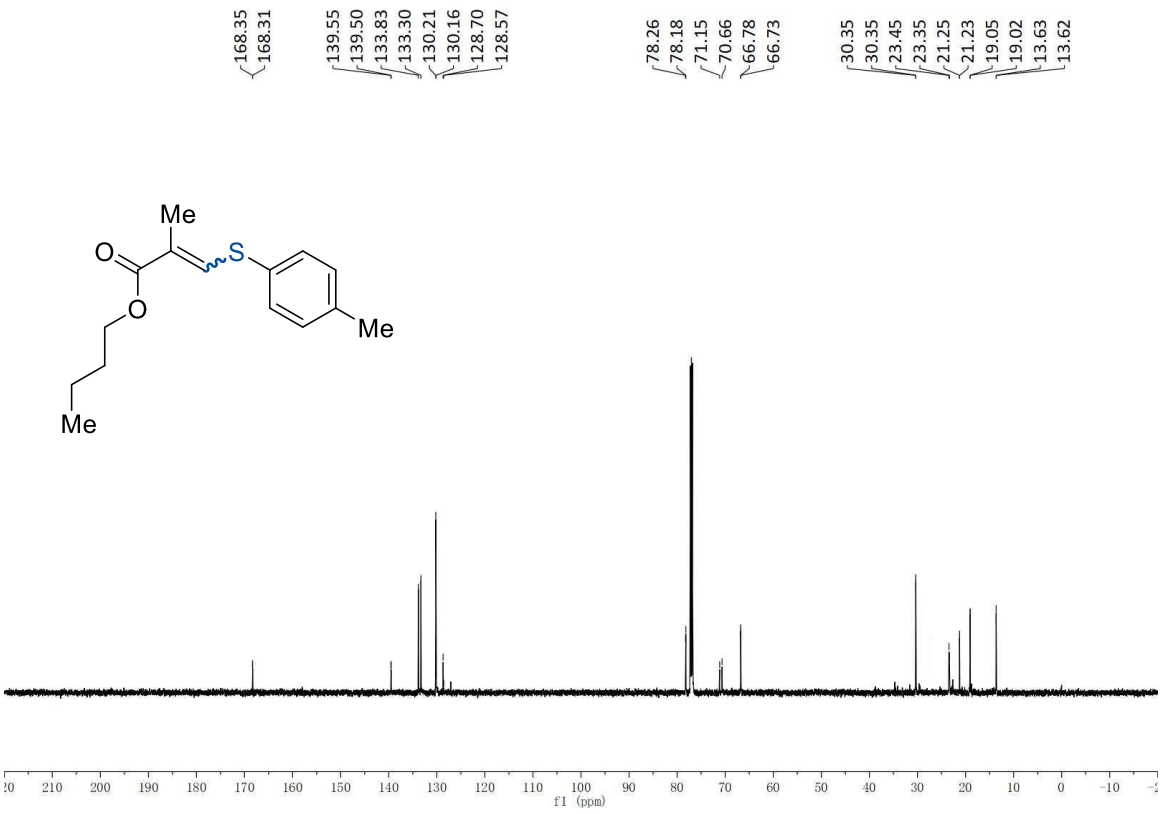
2.98
1.90
2.06
3.02
f1 (ppm)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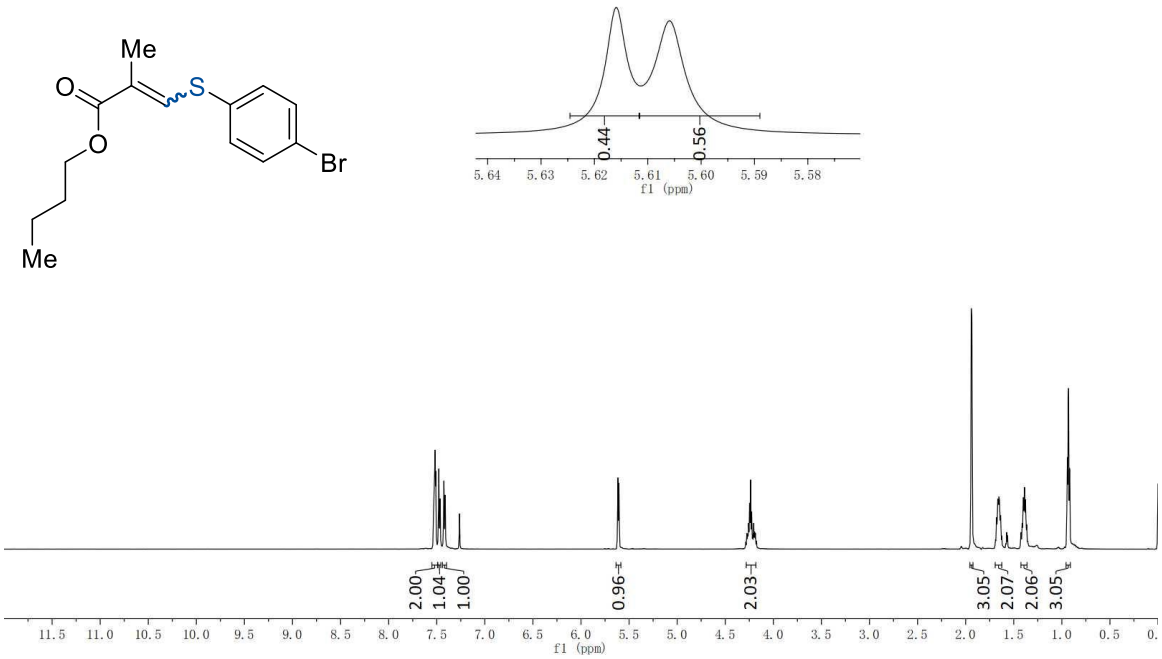
139.50
133.83
133.30
130.21
130.16
128.70
128.57
78.26
78.18
71.15
70.66
66.78
66.73
30.35
30.35
23.45
23.35
21.25
21.23
19.05
19.02
13.63
13.62
Me
O
S
O
Me
Me
f1 (ppm)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O
S
O
Br
Me
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0.56
f1 (ppm)
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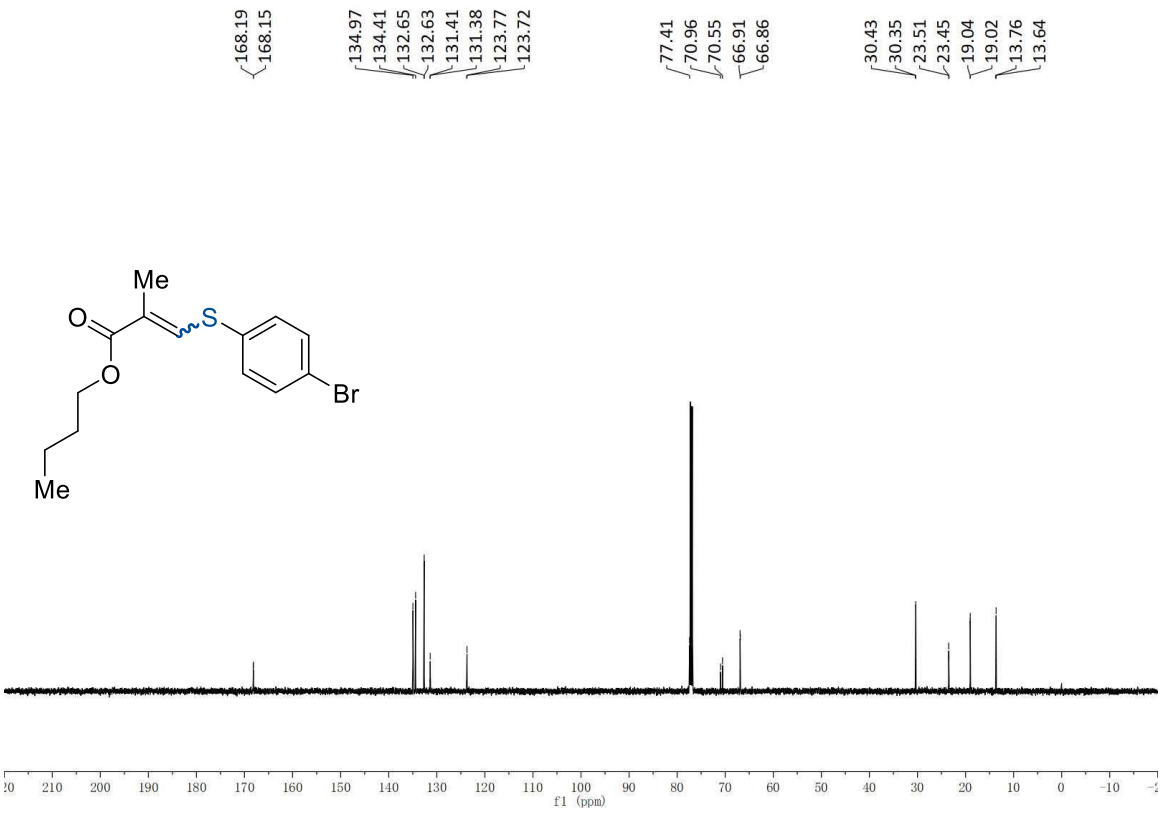
1.04
1.00
0.96
2.03
3.05
2.07
2.06
3.05
f1 (ppm)



9. X-ray Characterization of 15 and 23

9.1 X-ray Characterization of 15

Crystals of compound **15** suitable for X-ray analysis were obtained by slow evaporation from n-hexane. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC # 1974710). Copies of the data can be obtained free of charge through application to the CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)-1223-336-033, e-mail: deposit@ccdc.cam.ac.uk).

```
Bond precision:  C-C = 0.0100 A          Wavelength=0.71073

Cell:              a=5.87(3)     b=9.46(4)            c=16.79(8)
                   alpha=90      beta=92.493(5)       gamma=90
Temperature:       296 K

                 Calculated                Reported
Volume           932(8)                    931(7)
Space group      P 21                      P 21
Hall group       P 2yb                     P 2yb
Moiety formula   C22 H20 S                 ?
Sum formula      C22 H20 S                 C22 H20 S
Mr               316.44                    316.44
Dx,g cm-3        1.128                     1.129
Z                2                         2
Mu (mm-1)        0.171                     0.171
F000             336.0                     336.0
F000'            336.36
h,k,lmax         7,12,21                   7,12,21
Nref             4271[ 2266]               4119
Tmin,Tmax        0.976,0.981
Tmin'            0.975

Correction method= Not given

Data completeness= 1.82/0.96       Theta(max)= 27.442

R(reflections)= 0.0544( 2396)      wR2(reflections)= 0.1322( 4119)

S = 0.988                  Npar= 210
```

Figure S3. Crystal data and structure refinement for **15**.

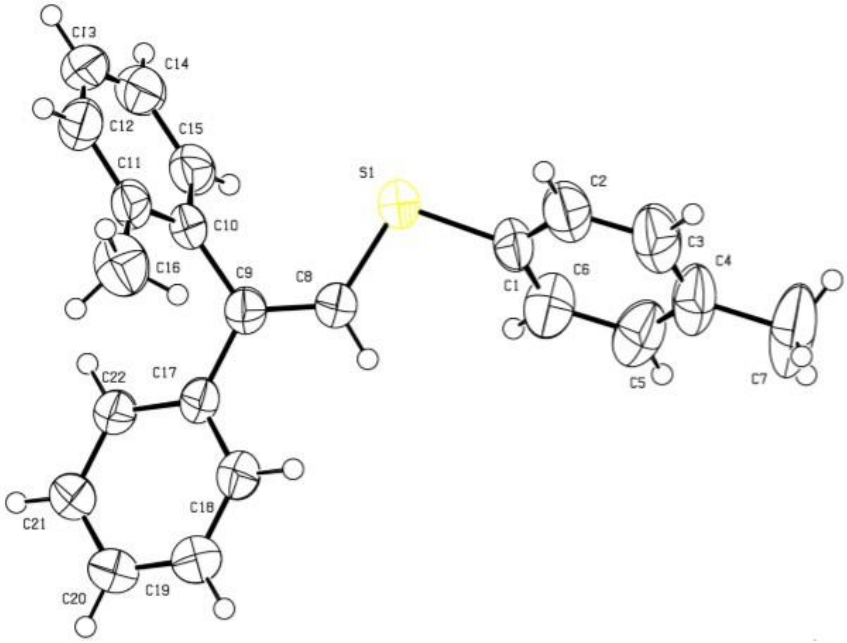


Figure S4. ORTEP diagram of **15**.

Table S2 Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for (**15**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	X	Y	Z	U(eq)
S1	0.4319(2)	0.20154(13)	0.68490(7)	0.0732(4)
C1	0.5987(8)	0.2027(6)	0.5967(2)	0.0621(10)
C2	0.7904(10)	0.1172(6)	0.5956(3)	0.0795(13)
C3	0.9158(10)	0.1105(7)	0.5271(3)	0.0894(15)
C4	0.8599(8)	0.1900(8)	0.4598(3)	0.0817(12)
C5	0.6672(9)	0.2768(7)	0.4616(3)	0.0841(14)
C6	0.5381(9)	0.2823(6)	0.5299(3)	0.0807(14)
C7	1.0080(10)	0.1846(10)	0.3856(3)	0.1300(2)
C8	0.4238(8)	0.3831(4)	0.7106(2)	0.0581(11)
C9	0.3352(7)	0.4362(5)	0.7771(2)	0.0502(8)
C10	0.2199(7)	0.3409(4)	0.8357(2)	0.0487(7)

C11	0.3055(8)	0.3275(5)	0.9153(3)	0.0562(8)
C12	0.1918(10)	0.2352(5)	0.9664(3)	0.0795(11)
C13	-0.0016(10)	0.1587(5)	0.9405(4)	0.0895(13)
C14	-0.0845(9)	0.1735(5)	0.8630(4)	0.0840(12)
C15	0.0241(8)	0.2643(5)	0.8099(3)	0.0627(9)
C16	0.5125(9)	0.4119(6)	0.9474(3)	0.0765(12)
C17	0.3423(7)	0.5927(5)	0.7933(2)	0.0477(8)
C18	0.5215(7)	0.6788(5)	0.7684(2)	0.0607(10)
C19	0.5180(9)	0.8255(5)	0.7805(3)	0.0710(12)
C20	0.3406(9)	0.8897(5)	0.8198(3)	0.0670(11)
C21	0.1666(8)	0.8051(5)	0.8471(3)	0.0625(11)
C22	0.1639(7)	0.6584(4)	0.8334(2)	0.0524(9)

Table S3. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **15**

	X	Y	Z	U(eq)
H2	0.8351	0.0645	0.6403	0.0950
H3	1.0415	0.0506	0.5266	0.1070
H5	0.6244	0.3311	0.4173	0.1010
H6	0.4100	0.3402	0.5303	0.0970
H7A	1.0060	0.0905	0.3642	0.1950
H7B	1.1620	0.2107	0.4007	0.1950
H7C	0.9476	0.2493	0.3460	0.1950
H8	0.4858	0.4470	0.6754	0.0700
H12	0.2472	0.2249	1.0189	0.0950
H13	-0.0735	0.0985	0.9753	0.1070

H14	-0.2133	0.1231	0.8455	0.1010
H15	-0.0336	0.2738	0.7577	0.0750
H16A	0.6160	0.4264	0.9054	0.1150
H16B	0.5884	0.3606	0.9901	0.1150
H16C	0.4628	0.5018	0.9667	0.1150
H18	0.6439	0.6379	0.7435	0.0730
H19	0.6358	0.8808	0.7621	0.0850
H20	0.3387	0.9871	0.8276	0.0800
H21	0.0499	0.8462	0.8749	0.0750
H22	0.0436	0.6042	0.8508	0.0630

Table S4. Anisotropic displacement parameters ($Å^2$) for 7f. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
S1	0.1029(9)	0.0533(7)	0.0665(7)	-0.0088(7)	0.0395(7)	-0.0030(7)
C1	0.075(2)	0.062(3)	0.0506(17)	-0.0174(18)	0.0174(18)	-0.0037(19)
C2	0.095(3)	0.076(3)	0.069(2)	-0.010(2)	0.017(2)	0.016(2)
C3	0.082(3)	0.100(4)	0.088(2)	-0.022(2)	0.026(2)	0.014(2)
C4	0.068(2)	0.122(4)	0.0552(18)	-0.0349(19)	0.0145(17)	-0.023(2)
C5	0.083(3)	0.116(4)	0.054(2)	0.001(2)	0.0095(18)	-0.013(2)
C6	0.078(3)	0.101(4)	0.064(2)	0.001(2)	0.0141(18)	0.010(2)
C7	0.100(4)	0.219(8)	0.074(2)	-0.053(3)	0.039(2)	-0.042(4)
C8	0.079(3)	0.0467(19)	0.050(2)	0.0004(15)	0.0212(18)	0.002(2)
C9	0.054(2)	0.0502(9)	0.0465(13)	-0.0011(10)	0.0098(14)	0.0050(13)
C10	0.0563(18)	0.0424(14)	0.0485(11)	-0.0063(13)	0.0163(10)	0.0073(13)
C11	0.071(2)	0.050(2)	0.0485(13)	0.0009(14)	0.0168(12)	0.0188(14)

C12	0.116(3)	0.061(3)	0.0650(17)	0.0125(18)	0.0412(17)	0.0230(18)
C13	0.121(3)	0.049(3)	0.103(2)	0.008(2)	0.067(2)	0.0063(19)
C14	0.088(3)	0.056(3)	0.112(2)	-0.014(2)	0.0507(19)	-0.011(2)
C15	0.059(2)	0.056(3)	0.0742(17)	-0.0123(17)	0.0204(14)	-0.0018(14)
C16	0.082(3)	0.084(3)	0.062(2)	-0.005(2)	-0.0096(18)	0.0157(18)
C17	0.0558(19)	0.0498(9)	0.038(2)	0.0009(14)	0.0107(16)	0.0025(10)
C18	0.065(2)	0.0569(12)	0.062(2)	-0.005(2)	0.0240(19)	-0.0041(14)
C19	0.087(3)	0.0558(12)	0.073(3)	-0.003(2)	0.025(2)	-0.0108(17)
C20	0.091(3)	0.0435(16)	0.068(3)	0.000(2)	0.017(2)	-0.0008(15)
C21	0.079(2)	0.0470(13)	0.063(3)	0.001(2)	0.019(2)	0.0078(17)
C22	0.059(2)	0.0464(13)	0.053(2)	0.0038(17)	0.0168(17)	0.0049(14)

Table S5. Bond lengths [Å] and angles [°] for **15**.

S1-C8	1.772(9)
S1-C1	1.810(7)
C1-C6	1.385(8)
C1-C2	1.386(8)
C2-C3	1.393(8)
C2-H2	0.930
C3-C4	1.385(9)
C3-H3	0.930
C4-C5	1.398(9)
C4-C7	1.550(8)
C5-C6	1.403(8)
C5-H5	0.930
C6-H6	0.930
C7-H7A	0.960
C7-H7B	0.960
C7-H7C	0.960
C8-C9	1.349(7)

C8-H8	0.930
C9-C17	1.505(9)
C9-C10	1.516(7)
C10-C15	1.410(7)
C10-C11	1.414(8)
C11-C12	1.412(7)
C11-C16	1.531(8)
C12-C13	1.399(9)
C12-H12	0.930
C13-C14	1.377(10)
C13-H13	0.930
C14-C15	1.410(7)
C14-H14	0.930
C15-H15	0.930
C16-H16A	0.960
C16-H16B	0.960
C16-H16C	0.960
C17-C18	1.408(7)
C17-C22	1.413(7)
C18-C19	1.403(9)
C18-H18	0.930
C19-C20	1.395(7)
C19-H19	0.930
C20-C21	1.390(8)
C20-H20	0.930
C21-C22	1.407(9)
C21-H21	0.930
C22-H22	0.930
C8-S1-C1	102.4(2)
C6-C1-C2	119.1(4)
C6-C1-S1	122.5(4)

C2-C1-S1	118.4(4)
C1-C2-C3	119.7(5)
C1-C2-H2	120.10
C3-C2-H2	120.10
C4-C3-C2	122.3(6)
C4-C3-H3	118.90
C2-C3-H3	118.90
C3-C4-C5	117.6(5)
C3-C4-C7	121.1(6)
C5-C4-C7	121.3(6)
C4-C5-C6	120.4(5)
C4-C5-H5	119.80
C6-C5-H5	119.80
C1-C6-C5	120.9(6)
C1-C6-H6	119.50
C5-C6-H6	119.50
C4-C7-H7A	109.50
C4-C7-H7B	109.50
H7A-C7-H7B	109.50
C4-C7-H7C	109.50
H7A-C7-H7C	109.50
H7B-C7-H7C	109.50
C9-C8-S1	125.3(3)
C9-C8-H8	117.30
S1-C8-H8	117.30
C8-C9-C17	120.5(4)
C8-C9-C10	121.0(5)
C17-C9-C10	118.6(4)
C15-C10-C11	119.7(4)
C15-C10-C9	119.2(5)
C11-C10-C9	121.1(4)

C12-C11-C10	118.2(5)
C12-C11-C16	119.8(5)
C10-C11-C16	122.0(4)
C13-C12-C11	122.0(6)
C13-C12-H12	119.00
C11-C12-H12	119.00
C14-C13-C12	119.3(5)
C14-C13-H13	120.30
C12-C13-H13	120.30
C13-C14-C15	120.6(6)
C13-C14-H14	119.70
C15-C14-H14	119.70
C14-C15-C10	120.2(5)
C14-C15-H15	119.90
C10-C15-H15	119.90
C11-C16-H16A	109.50
C11-C16-H16B	109.50
H16A-C16-H16B	109.50
C11-C16-H16C	109.50
H16A-C16-H16C	109.50
H16B-C16-H16C	109.50
C18-C17-C22	117.7(5)
C18-C17-C9	122.1(4)
C22-C17-C9	120.2(4)
C19-C18-C17	120.9(4)
C19-C18-H18	119.60
C17-C18-H18	119.60
C20-C19-C18	121.0(4)
C20-C19-H19	119.50
C18-C19-H19	119.50
C21-C20-C19	118.6(5)

C21-C20-H20	120.70
C19-C20-H20	120.70
C20-C21-C22	121.1(5)
C20-C21-H21	119.40
C22-C21-H21	119.40
C21-C22-H17	120.6(4)
C21-C22-H22	119.70
C17-C22-H22	119.70

9.2 X-ray Characterization of 23

Crystals of compound **23** suitable for X-ray analysis were obtained by slow evaporation from n-hexane. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC # 1974711). Copies of the data can be obtained free of charge through application to the CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)-1223-336-033, e-mail: deposit@ccdc.cam.ac.uk).

```
Bond precision:  C-C = 0.0121 A          Wavelength=0.71073

Cell:             a=12.91(3)     b=6.391(14)         c=25.90(5)
                  alpha=90       beta=96.40(3)       gamma=90
Temperature:      296 K

                Calculated                Reported
Volume          2124(8)                   2124(8)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C28 H19 Br S              ?
Sum formula     C28 H19 Br S              C28 H19 Br S
Mr              467.39                    467.40
Dx,g cm-3       1.462                     1.462
Z               4                         4
Mu (mm-1)       2.046                     2.047
F000            952.0                     952.0
F000'           951.64
h,k,lmax        15,7,31                   15,7,31
Nref            3849                      3844
Tmin,Tmax       0.863,0.921
Tmin'           0.815

Correction method= Not given

Data completeness= 0.999          Theta(max)= 25.247

R(reflections)= 0.0644( 1663)     wR2(reflections)= 0.2052( 3844)

S = 1.017                 Npar= 271
```

Figure S5 Crystal data and structure refinement for **23.**

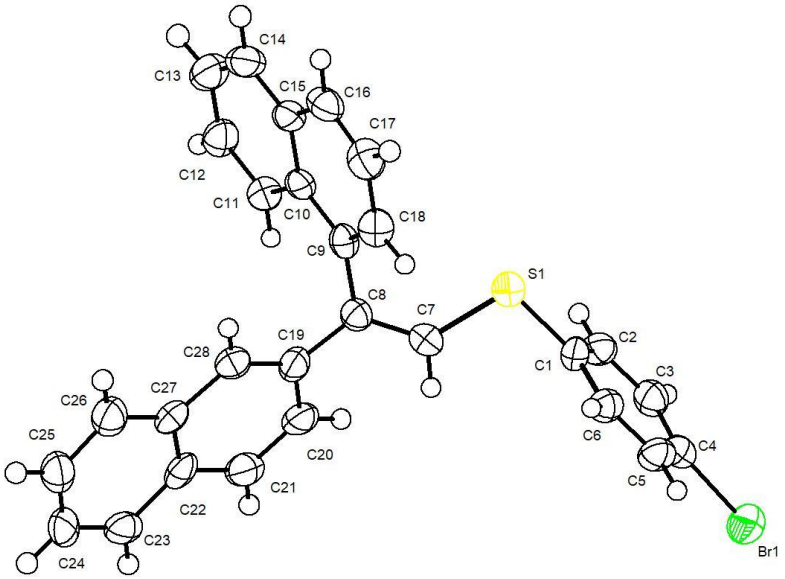


Figure S6. ORTEP diagram of **23**.

Table S6 Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for (**23**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	X	Y	Z	U(eq)
Br1	0.04355(7)	0.86082(14)	0.43167(3)	0.0915(4)
S1	0.40077(16)	0.2545(4)	0.54085(7)	0.0811(7)
C1	0.3012(6)	0.4211(12)	0.5101(2)	0.0614(19)
C2	0.3261(6)	0.6226(14)	0.4957(3)	0.076(2)
C3	0.2507(7)	0.7527(13)	0.4710(3)	0.072(2)
C4	0.1512(6)	0.6836(12)	0.4611(3)	0.068(2)
C5	0.1277(6)	0.4794(13)	0.4745(3)	0.072(2)
C6	0.2024(6)	0.3501(12)	0.4984(3)	0.0678(19)
C7	0.3862(6)	0.3084(12)	0.6065(3)	0.072(2)
C8	0.4470(5)	0.2297(11)	0.6479(3)	0.0606(18)
C9	0.5295(6)	0.0709(11)	0.6408(3)	0.0592(18)
C10	0.6360(6)	0.1009(11)	0.6603(2)	0.0591(19)

C11	0.6723(6)	0.2849(12)	0.6883(3)	0.066(2)
C12	0.7758(6)	0.3044(13)	0.7077(3)	0.077(2)
C13	0.8463(7)	0.1456(18)	0.7012(4)	0.097(3)
C14	0.8129(7)	-0.0292(16)	0.6728(3)	0.088(3)
C15	0.7104(6)	-0.0561(13)	0.6533(3)	0.066(2)
C16	0.6770(7)	-0.2393(13)	0.6244(3)	0.077(2)
C17	0.5762(8)	-0.2593(14)	0.6065(3)	0.087(2)
C18	0.5013(6)	-0.1088(12)	0.6144(3)	0.073(2)
C19	0.4242(5)	0.2929(13)	0.7002(3)	0.067(2)
C20	0.3792(5)	0.5001(14)	0.7089(3)	0.079(2)
C21	0.3488(5)	0.5448(13)	0.7563(3)	0.079(2)
C22	0.3605(5)	0.4039(13)	0.7977(3)	0.068(2)
C23	0.3228(5)	0.4531(15)	0.8479(4)	0.081(2)
C24	0.3349(6)	0.3131(18)	0.8862(3)	0.085(3)
C25	0.3834(7)	0.1234(16)	0.8779(3)	0.086(2)
C26	0.4213(6)	0.0689(14)	0.8320(3)	0.084(2)
C27	0.4080(5)	0.2105(12)	0.7918(3)	0.0635(19)
C28	0.4390(5)	0.1568(14)	0.7399(3)	0.074(2)

Table S7. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **23**

	X	Y	Z	U(eq)
H2	0.3942	0.6706	0.5028	0.0910
H3	0.2681	0.8870	0.4612	0.0860
H5	0.0599	0.4302	0.4670	0.0860
H6	0.1856	0.2136	0.5067	0.0810
H7	0.3325	0.3980	0.6132	0.0860
H11	0.6258	0.3919	0.6935	0.0790
H12	0.7986	0.4256	0.7253	0.0920
H13	0.9152	0.1567	0.7158	0.1170

H14	0.8612	-0.1318	0.6667	0.1060
H16	0.7246	-0.3430	0.6182	0.0930
H17	0.5551	-0.3793	0.5879	0.1040
H18	0.4320	-0.1310	0.6016	0.0870
H20	0.3718	0.5988	0.6823	0.0950
H21	0.3189	0.6746	0.7613	0.0950
H23	0.2909	0.5808	0.8528	0.0970
H24	0.3112	0.3417	0.9180	0.1020
H25	0.3907	0.0273	0.9051	0.1030
H26	0.4544	-0.0585	0.8283	0.1010
H28	0.4690	0.0273	0.7348	0.0890

Table S8. Anisotropic displacement parameters ($Å^2$) for 7f. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br1	0.0877(7)	0.0982(7)	0.0874(7)	0.0176(5)	0.0041(5)	0.0155(5)
S1	0.0772(14)	0.1041(16)	0.0618(13)	0.0030(11)	0.0069(11)	0.0188(12)
C1	0.061(5)	0.072(5)	0.048(4)	0.000(4)	-0.004(4)	0.005(4)
C2	0.052(5)	0.102(7)	0.073(5)	-0.010(5)	0.008(4)	-0.006(5)
C3	0.076(6)	0.075(5)	0.066(5)	0.011(4)	0.014(4)	-0.006(5)
C4	0.072(6)	0.077(6)	0.057(5)	-0.003(4)	0.015(4)	0.009(5)
C5	0.051(5)	0.081(6)	0.083(6)	0.002(5)	0.008(4)	-0.008(4)
C6	0.060(5)	0.070(5)	0.073(5)	-0.005(4)	0.006(4)	-0.002(4)
C7	0.069(5)	0.087(6)	0.060(5)	-0.003(4)	0.015(4)	0.005(4)
C8	0.060(4)	0.066(5)	0.056(5)	0.007(4)	0.008(4)	-0.003(4)
C9	0.068(5)	0.060(5)	0.050(4)	0.008(4)	0.009(4)	-0.005(4)
C10	0.060(5)	0.071(5)	0.049(4)	0.016(4)	0.018(4)	0.006(4)
C11	0.063(5)	0.069(5)	0.067(5)	0.000(4)	0.007(4)	0.000(4)
C12	0.064(5)	0.088(6)	0.077(5)	0.008(4)	0.003(4)	-0.013(5)

C13	0.065(6)	0.130(9)	0.097(7)	0.029(7)	0.009(5)	0.007(7)
C14	0.075(7)	0.106(7)	0.089(7)	0.027(6)	0.033(5)	0.026(6)
C15	0.061(5)	0.079(6)	0.061(5)	0.014(4)	0.017(4)	0.011(5)
C16	0.093(7)	0.072(6)	0.072(5)	0.004(5)	0.029(5)	0.020(5)
C17	0.104(8)	0.076(6)	0.080(6)	0.002(5)	0.011(6)	0.005(6)
C18	0.075(5)	0.070(5)	0.072(5)	0.003(4)	0.006(4)	-0.010(5)
C19	0.054(4)	0.084(6)	0.061(5)	0.010(4)	-0.004(4)	-0.002(4)
C20	0.048(4)	0.105(7)	0.081(5)	-0.017(5)	-0.005(4)	0.008(5)
C21	0.061(5)	0.085(5)	0.088(5)	-0.021(5)	0.001(4)	0.009(4)
C22	0.040(4)	0.082(6)	0.077(6)	0.021(5)	-0.013(4)	-0.015(4)
C23	0.051(5)	0.107(7)	0.083(6)	-0.034(6)	-0.001(5)	0.001(5)
C24	0.067(5)	0.131(8)	0.054(5)	-0.014(6)	-0.008(4)	-0.019(6)
C25	0.080(6)	0.110(8)	0.066(6)	0.012(5)	0.003(5)	-0.016(6)
C26	0.074(6)	0.100(6)	0.076(6)	0.009(5)	0.000(5)	-0.009(5)
C27	0.044(4)	0.069(5)	0.074(6)	0.000(5)	-0.010(4)	-0.002(4)
C28	0.044(4)	0.104(6)	0.073(5)	-0.003(5)	0.003(4)	-0.009(4)

Table S9. Bond lengths [Å] and angles [°] for **23**.

Br1-C4	1.886(8)
S1-C7	1.765(8)
S1-C1	1.787(8)
C1-C6	1.355(10)
C1-C2	1.388(10)
C2-C3	1.383(10)
C2-H2	0.9300
C3-C4	1.356(10)
C3-H3	0.9300
C4-C5	1.392(10)
C5-C6	1.366(10)
C5-H5	0.9300
C6-H6	0.9300

C7-C8	1.353(9)
C7-H7	0.9300
C8-C19	1.476(10)
C8-C9	1.497(10)
C9-C18	1.366(9)
C9-C10	1.423(10)
C10-C15	1.415(9)
C10-C11	1.433(10)
C11-C12	1.380(10)
C11-H11	0.9300
C12-C13	1.385(11)
C12-H12	0.9300
C13-C14	1.380(12)
C13-H13	0.9300
C14-C15	1.373(11)
C14-H14	0.9300
C15-C16	1.430(11)
C16-C17	1.338(11)
C16-H16	0.9300
C17-C18	1.395(11)
C17-H17	0.9300
C18-H18	0.9300
C19-C28	1.343(10)
C19-C20	1.473(11)
C20-C21	1.360(10)
C20-H20	0.9300
C21-C22	1.397(10)
C21-H21	0.9300
C22-C27	1.396(10)
C22-C23	1.472(11)
C23-C24	1.332(11)

C23-H23	0.9300
C24-C25	1.392(11)
C24-H24	0.9300
C25-C26	1.381(11)
C25-H25	0.9300
C26-C27	1.375(10)
C26-H26	0.9300
C27-C28	1.485(10)
C28-H28	0.9300
C7-S1-C1	99.5(4)
C6-C1-C2	119.4(7)
C6-C1-S1	120.8(6)
C2-C1-S1	119.7(6)
C3-C2-C1	120.6(7)
C3-C2-H2	119.70
C1-C2-H2	119.70
C4-C3-C2	119.7(7)
C4-C3-H3	120.20
C2-C3-H3	120.20
C3-C4-C5	119.1(7)
C3-C4-Br1	121.4(6)
C5-C4-Br1	119.5(6)
C6-C5-C4	121.2(7)
C6-C5-H5	119.40
C4-C5-H5	119.40
C1-C6-C5	119.9(7)
C1-C6-H6	120.10
C5-C6-H6	120.10
C8-C7-S1	125.2(6)
C8-C7-H7	117.40
S1-C7-H7	117.40

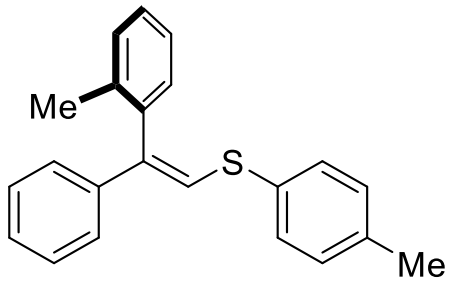
C7-C8-C19	117.9(7)
C7-C8-C9	120.9(7)
C19-C8-C9	121.0(6)
C18-C9-C10	118.9(7)
C18-C9-C8	118.6(7)
C10-C9-C8	122.5(7)
C15-C10-C9	120.1(7)
C15-C10-C11	117.2(7)
C9-C10-C11	122.6(7)
C12-C11-C10	120.5(7)
C12-C11-H11	119.80
C10-C11-H11	119.80
C11-C12-C13	120.8(8)
C11-C12-H12	119.60
C13-C12-H12	119.60
C14-C13-C12	119.2(8)
C14-C13-H13	120.40
C12-C13-H13	120.40
C15-C14-C13	121.9(8)
C15-C14-H14	119.10
C13-C14-H14	119.10
C14-C15-C10	120.3(8)
C14-C15-C16	121.1(8)
C10-C15-C16	118.5(7)
C17-C16-C15	119.0(8)
C17-C16-H16	120.50
C15-C16-H16	120.50
C16-C17-C18	123.1(9)
C16-C17-H17	118.40
C18-C17-H17	118.40

C9-C18-C17	120.2(8)
C9-C18-H18	119.90
C17-C18-H18	119.90
C28-C19-C20	119.4(7)
C28-C19-C8	120.0(7)
C20-C19-C8	120.5(7)
C21-C20-C19	118.9(8)
C21-C20-H20	120.50
C19-C20-H20	120.50
C20-C21-C22	122.7(8)
C20-C21-H21	118.60
C22-C21-H21	118.60
C27-C22-C21	119.9(8)
C27-C22-C23	118.6(7)
C21-C22-C23	121.5(8)
C24-C23-C22	119.4(8)
C24-C23-H23	120.30
C22-C23-H23	120.30
C23-C24-C25	119.2(9)
C23-C24-H24	120.40
C25-C24-H24	120.40
C26-C25-C24	124.1(8)
C26-C25-H25	118.00
C24-C25-H25	118.00
C27-C26-C25	117.4(9)
C27-C26-H26	121.30
C25-C26-H26	121.30
C26-C27-C22	121.3(8)
C26-C27-C28	120.6(8)
C22-C27-C28	118.0(7)

C19-C28-C27	120.9(8)
C19-C28-H28	119.60
C27-C28-H28	119.60

10. DFT calculations for different stereoisomers of compound 15

All of the density functional theory (DFT) calculations conducted in this study were carried out using the GAUSSIAN 09 series of programs[11]. DFT method B3LYP with a standard 6-311G basis set was applied for the calculation of energy. Standard orientation of molecular structure and electronic energy are shown below.



Standard orientation:

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3	1	0	-0.458909	1.451730	0.097240
4	6	0	2.227142	1.489991	-0.105210
5	6	0	3.603897	1.295702	-0.220404
6	6	0	1.711755	2.781592	0.002911
7	6	0	4.465047	2.392789	-0.226787
8	1	0	4.009961	0.277261	-0.304854
9	6	0	2.572958	3.879174	-0.004449
10	1	0	0.626670	2.934913	0.093531
11	6	0	3.949430	3.684983	-0.119135
12	1	0	5.550280	2.239694	-0.316949
13	1	0	2.166282	4.897451	0.080403
14	1	0	4.628607	4.549846	-0.124249
15	6	0	1.848521	-1.146439	-0.217221

16	6	0	2.015967	-1.727537	-1.474503
17	6	0	2.199255	-1.855983	0.931291
18	6	0	2.533407	-3.018149	-1.583119
19	1	0	1.738640	-1.168176	-2.379736
20	6	0	2.717788	-3.146624	0.822764
21	6	0	2.884779	-3.727828	-0.434158
22	1	0	2.664832	-3.476481	-2.574056
23	1	0	2.994623	-3.705674	1.728469
24	1	0	3.292797	-4.745393	-0.520050
25	6	0	2.014750	-1.214675	2.319197
26	1	0	2.859657	-0.597066	2.541890
27	1	0	1.126472	-0.618137	2.321222
28	1	0	1.929928	-1.983238	3.058802
29	16	0	-1.160227	-0.938666	0.022940
30	6	0	-2.846963	-0.370722	-0.004621
31	6	0	-3.893677	-1.293140	-0.002432
32	6	0	-3.122303	0.996456	-0.028296
33	6	0	-5.215395	-0.848401	-0.024596
34	1	0	-3.676264	-2.370940	0.015458
35	6	0	-4.444380	1.441510	-0.049472
36	1	0	-2.297452	1.723606	-0.029845
37	6	0	-5.490889	0.519365	-0.047764
38	1	0	-6.040472	-1.575411	-0.023505
39	1	0	-4.661176	2.519537	-0.067721
40	6	0	-6.950404	1.010102	-0.072150
41	1	0	-7.287279	1.077103	-1.085523
42	1	0	-7.567745	0.319964	0.464040
43	1	0	-7.010265	1.974205	0.388090

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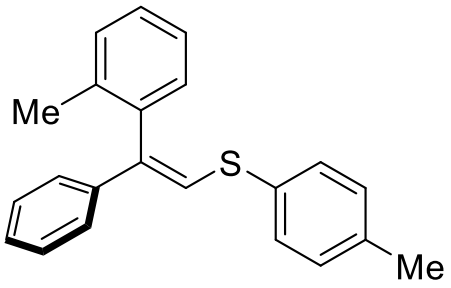

Standard orientation:

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3	1	0	0.511160	-1.426958	0.169940
4	6	0	-2.177927	-1.341343	0.032830
5	6	0	-2.693007	-1.844590	1.227781
6	6	0	-2.571715	-1.896181	-1.184804
7	6	0	-3.601148	-2.902884	1.205042
8	1	0	-2.381764	-1.407454	2.187615
9	6	0	-3.480878	-2.954153	-1.207774
10	1	0	-2.165986	-1.499548	-2.126715
11	6	0	-3.995514	-3.457643	-0.013126
12	1	0	-4.006702	-3.300015	2.146907
13	1	0	-3.791495	-3.391148	-2.167997
14	1	0	-4.711607	-4.292025	-0.030808
15	6	0	-1.685647	1.278454	0.001481
16	6	0	-0.778832	2.338473	0.024283
17	6	0	-3.054931	1.533565	-0.072865
18	6	0	-1.241322	3.653288	-0.026573
19	1	0	0.300582	2.137032	0.083677
20	6	0	-3.517675	2.848703	-0.124739

21	6	0	-2.611161	3.908528	-0.101468
22	1	0	-0.526653	4.488872	-0.007972
23	1	0	-4.597330	3.049535	-0.183769
24	1	0	-2.975578	4.945294	-0.141615
25	6	0	-4.056069	0.363661	-0.098299
26	1	0	-4.152862	-0.001239	-1.099488
27	1	0	-3.702007	-0.422595	0.535216
28	1	0	-5.008934	0.701963	0.251703
29	16	0	1.315715	0.931845	0.159890
30	6	0	2.974555	0.292476	0.071242
31	6	0	3.188338	-1.084037	-0.006097
32	6	0	4.060704	1.167558	0.078980
33	6	0	4.488034	-1.585300	-0.074997
34	1	0	2.331854	-1.773710	-0.011401
35	6	0	5.360826	0.666354	0.009071
36	1	0	3.892384	2.252502	0.139751
37	6	0	5.574651	-0.709841	-0.067773
38	1	0	4.656641	-2.670302	-0.135325
39	1	0	6.216999	1.356578	0.014777
40	6	0	7.009608	-1.263643	-0.143945
41	1	0	7.363705	-1.473790	0.843654
42	1	0	7.014493	-2.163077	-0.723509
43	1	0	7.647640	-0.538846	-0.604906

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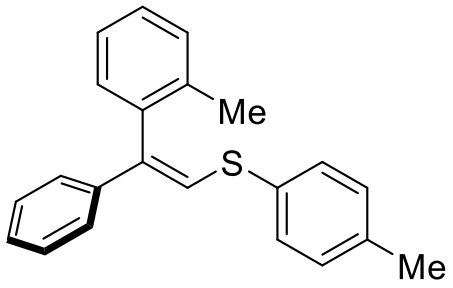

Standard orientation:

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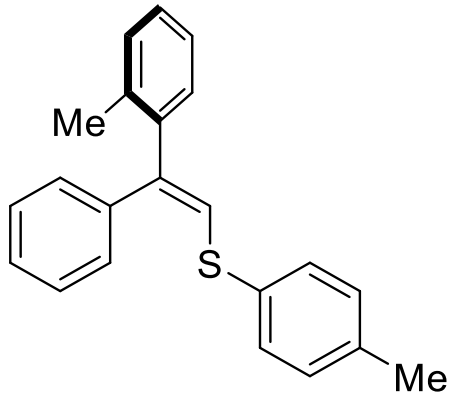
4	6	0	-2.443729	-1.387039	0.022693
5	6	0	-2.968924	-1.878171	1.218281
6	6	0	-2.844656	-1.938957	-1.193938
7	6	0	-3.894325	-2.921441	1.197186
8	1	0	-2.652057	-1.443350	2.177327
9	6	0	-3.771074	-2.981889	-1.215268
10	1	0	-2.430955	-1.551870	-2.136351
11	6	0	-4.295828	-3.473272	-0.019980
12	1	0	-4.307860	-3.309029	2.139555
13	1	0	-4.087312	-3.416581	-2.174700
14	1	0	-5.025530	-4.295807	-0.036367
15	6	0	-1.908344	1.224197	-0.015604
16	6	0	-3.273482	1.501479	-0.092969
17	6	0	-0.984602	2.269086	0.005755
18	6	0	-3.714652	2.823364	-0.149638
19	1	0	-4.001448	0.677466	-0.110565
20	6	0	-1.425794	3.591454	-0.049931

21	6	0	-2.790564	3.868733	-0.127756
22	1	0	-4.790620	3.041982	-0.211252
23	1	0	-0.697255	4.415109	-0.032658
24	1	0	-3.138651	4.910914	-0.172389
25	6	0	0.522297	1.963276	0.091400
26	1	0	0.797240	1.808301	1.113793
27	1	0	0.739965	1.081378	-0.474089
28	1	0	1.076688	2.787669	-0.306000
29	16	0	1.086650	0.828721	0.148756
30	6	0	2.734880	0.161880	0.064724
31	6	0	2.926100	-1.218189	-0.008188
32	6	0	3.835272	1.018990	0.071654
33	6	0	4.217477	-1.740975	-0.073471
34	1	0	2.058389	-1.893688	-0.012856
35	6	0	5.127078	0.496253	0.005363
36	1	0	3.684736	2.106734	0.128936
37	6	0	5.318344	-0.883497	-0.067055
38	1	0	4.368298	-2.828779	-0.130309
39	1	0	5.994485	1.172310	0.010430
40	6	0	6.744110	-1.461061	-0.139232
41	1	0	7.093127	-1.674055	0.849565
42	1	0	6.735113	-2.362181	-0.716122
43	1	0	7.394719	-0.748242	-0.601289

E(RB3LYP) = -1246.96286357 A.U.

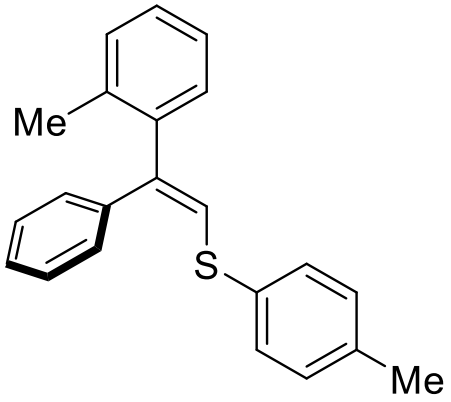


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.275768	-0.064758	-0.199725
2	6	0	-1.757631	1.395187	-0.110470
3	6	0	-3.123386	1.678125	-0.076835
4	6	0	-0.828731	2.434636	-0.063144
5	6	0	-3.560061	3.000280	0.003428
6	1	0	-3.855469	0.858464	-0.114938
7	6	0	-1.265361	3.757193	0.018139
8	1	0	0.247737	2.211806	-0.089465
9	6	0	-2.630779	4.040165	0.051292
10	1	0	-4.636555	3.223409	0.029311
11	1	0	-0.532729	4.576523	0.055854
12	1	0	-2.975317	5.082556	0.114634
13	6	0	0.049751	-0.344901	-0.232685
14	1	0	0.384553	-1.359279	-0.294700
15	16	0	1.237885	0.979156	-0.172605
16	6	0	2.881330	0.299729	-0.096001
17	6	0	3.985881	1.150274	-0.041132
18	6	0	3.064921	-1.082955	-0.090714

19	6	0	5.273729	0.618170	0.018327
20	1	0	3.840843	2.240311	-0.046092
21	6	0	4.353048	-1.615384	-0.030246
22	1	0	2.194465	-1.753463	-0.133775
23	6	0	5.457404	-0.765104	0.024133
24	1	0	6.144426	1.288517	0.060944
25	1	0	4.497476	-2.705611	-0.025678
26	6	0	6.879537	-1.352314	0.089875
27	1	0	7.561271	-0.691953	-0.404150
28	1	0	7.171446	-1.466196	1.112969
29	1	0	6.894000	-2.306791	-0.393514
30	6	0	-2.303704	-1.210291	-0.251705
31	6	0	-2.772994	-1.671061	-1.482123
32	6	0	-2.765500	-1.787272	0.931252
33	6	0	-3.704377	-2.708127	-1.529456
34	1	0	-2.409305	-1.215452	-2.414536
35	6	0	-3.696426	-2.825327	0.884043
36	6	0	-4.166005	-3.285719	-0.346027
37	1	0	-4.074795	-3.070941	-2.499226
38	1	0	-4.060044	-3.280337	1.816900
39	1	0	-4.900324	-4.103435	-0.383600
40	6	0	-2.247451	-1.279006	2.289519
41	1	0	-1.187389	-1.415249	2.340576
42	1	0	-2.478851	-0.239483	2.393172
43	1	0	-2.716169	-1.829142	3.078540

E(RB3LYP) = -1248.47824699 A.U.



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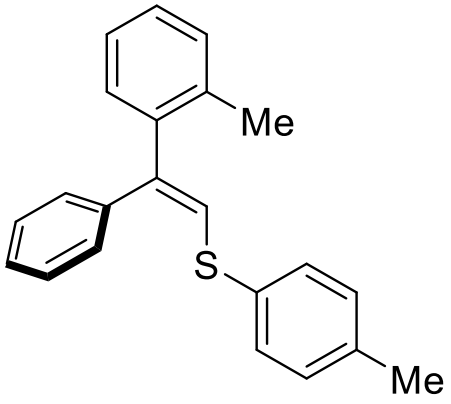
3	6	0	1.953903	-1.830156	1.219045
4	6	0	2.044165	-1.856891	-1.195303
5	6	0	2.472114	-3.124576	1.253040
6	1	0	1.714873	-1.308595	2.157171
7	6	0	2.561616	-3.152079	-1.161502
8	1	0	1.875619	-1.357325	-2.160266
9	6	0	2.775751	-3.785926	0.062394
10	1	0	2.641182	-3.624221	2.217958
11	1	0	2.800809	-3.673038	-2.100044
12	1	0	3.184277	-4.806549	0.089446
13	6	0	-0.171082	0.431387	-0.094602
14	1	0	-0.568247	1.424610	-0.120456
15	16	0	-1.273740	-0.965712	-0.120278
16	6	0	-2.958254	-0.394466	-0.053289
17	6	0	-4.007474	-1.313998	-0.061630
18	6	0	-3.229344	0.972408	0.007654

19	6	0	-5.327474	-0.866640	-0.009719
20	1	0	-3.793440	-2.391517	-0.110459
21	6	0	-4.549665	1.420027	0.060581
22	1	0	-2.402511	1.697273	0.014417
23	6	0	-5.598697	0.500793	0.051767
24	1	0	-6.154549	-1.591341	-0.016923
25	1	0	-4.763094	2.497790	0.109041
26	6	0	-7.056312	0.994417	0.109159
27	1	0	-7.684235	0.315538	-0.429112
28	1	0	-7.376238	1.043860	1.129013
29	1	0	-7.121220	1.966827	-0.332549
30	6	0	2.122552	1.442184	-0.020163
31	6	0	1.607192	2.738237	-0.053680
32	6	0	3.501794	1.241304	0.033574
33	6	0	2.470978	3.833095	-0.034142
34	1	0	0.519806	2.896263	-0.096820
35	6	0	4.365943	2.336400	0.054119
36	6	0	3.850796	3.632164	0.020134
37	1	0	2.064863	4.854679	-0.061191
38	1	0	5.453353	2.177713	0.096905
39	1	0	4.531662	4.495575	0.035589
40	6	0	4.070886	-0.189202	0.070830
41	1	0	3.709227	-0.694357	0.941991
42	1	0	3.759197	-0.719961	-0.804410
43	1	0	5.139641	-0.147210	0.100795

E(RB3LYP) = -1248.50489288 A.U.



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	6	0	-2.221424	2.041594	-1.189431
5	6	0	-2.629139	3.322890	1.255277
6	1	0	-1.894266	1.500212	2.164375
7	6	0	-2.721905	3.343522	-1.159210
8	1	0	-2.060853	1.536665	-2.152962
9	6	0	-2.925923	3.984176	0.062869
10	1	0	-2.790232	3.827905	2.218763
11	1	0	-2.955700	3.864429	-2.099141
12	1	0	-3.321075	5.010122	0.087100
13	6	0	-0.034529	-0.271689	-0.084312
14	1	0	0.349621	-1.270085	-0.107421
15	16	0	1.086199	1.110826	-0.116273
16	6	0	2.763226	0.517897	-0.049831
17	6	0	3.824324	1.423642	-0.062781
18	6	0	3.016575	-0.852184	0.015291

19	6	0	5.138459	0.959292	-0.011299
20	1	0	3.624275	2.503691	-0.114904
21	6	0	4.331029	-1.316796	0.067789
22	1	0	2.180378	-1.566183	0.025686
23	6	0	5.391934	-0.411348	0.054367
24	1	0	5.974895	1.673122	-0.022136
25	1	0	4.530469	-2.397082	0.119544
26	6	0	6.843078	-0.923736	0.111283
27	1	0	7.478984	-0.254894	-0.430173
28	1	0	7.163866	-0.973951	1.130829
29	1	0	6.894647	-1.898374	-0.327262
30	6	0	-2.341025	-1.252250	-0.003143
31	6	0	-3.717749	-1.033008	0.051948
32	6	0	-1.842934	-2.554765	-0.033283
33	6	0	-4.596084	-2.116103	0.077571
34	1	0	-4.110087	-0.006017	0.076475
35	6	0	-2.721441	-3.638291	-0.008653
36	6	0	-4.097829	-3.419183	0.046903
37	1	0	-5.681221	-1.943378	0.121627
38	1	0	-2.328447	-4.665153	-0.032843
39	1	0	-4.790560	-4.273005	0.067055
40	6	0	-0.323334	-2.797019	-0.094345
41	1	0	0.072655	-2.355863	-0.985117
42	1	0	0.143085	-2.354142	0.760765
43	1	0	-0.129916	-3.849371	-0.101110

E(RB3LYP) = -1248.49357665 A.U.

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