

Supporting Information

Benzyl Thioethers Formation Merging Copper Catalysis

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I. Experimental Section

Part 1. General Information

1. Chemicals and Reagents

All operations were carried out under an atmosphere of air in a sealed flask. DCE (1,2-dichloroethane) and DCM (methylene dichloride) was purchased (Sinopharm Group Co., China) and used directly. Deuterated solvents were used as received (CDCl_3 from Maclin Co., China). $\text{Zn}(\text{OTf})_2$ (Energy Chemical, China), $\text{Cu}(\text{OTf})_2$ (Energy Chemical, China), $\text{Sc}(\text{OTf})_2$ (Energy Chemical, China), $\text{Ni}(\text{OTf})_2$ (Energy Chemical, China) was purchased and used as received. Unless otherwise noted, all other reagents and starting materials were purchased from commercial sources and used without further purification.

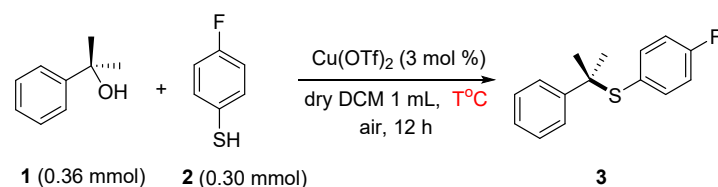
2. Physical Method

Column chromatography was performed using silica gel 300-400 mesh (purchased from Qingdao-Haiyang Co., China) as the solid support. All NMR spectra were recorded on Bruker Avance 500 MHz spectrometer at STP unless otherwise indicated. ^1H NMR and ^{13}C NMR chemical shifts are reported in δ units, parts per million (ppm) relative to the chemical shift of residual solvent. Reference peaks for chloroform in ^1H NMR and ^{13}C NMR spectra were set at 7.26 ppm and 77.16 ppm, respectively. High resolution mass spectra were measured on Bruker MicroTOF II ESI-TOF mass spectrometer. Low resolution mass spectra were measured on Agilent 1260 Infinity II/6125 mass spectrometer. Melting point was recorded on a micro melting point apparatus (X-4, YUHUA Co., Ltd, Gongyi, China).

Part 2. Details of Optimization and Control Experiments

Typical procedure for optimization reaction conditions: 2-Phenyl-2-Propanol (0.36 mmol), the catalyst were added to a dried test tube equipped with a stir bar under air. The tube was capped with a rubber septum. 4-Fluorothiophenol and a solvent were then added via syringes. After the reaction mixture was allowed to stir overnight under the air atmosphere at 25 °C, it was directly loaded onto a silica column without work-up. The residue in the reaction vessel was rinsed with small amount of CH₂Cl₂ or eluent. A quick flash column offered a mixture of the product with other impurities.

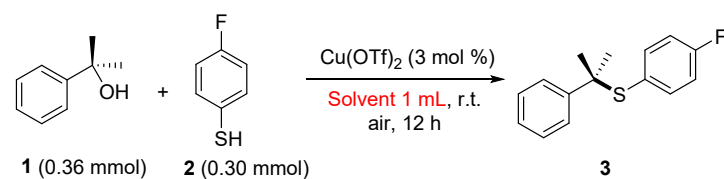
Table S1. Screening of temperature for the reaction of **1** and **2**



Entry	T ^o C	yield% ^a
1	0 ^o C	34
2	r.t.(25 ^o C)	96
3	50 ^o C	98
4	80 ^o C	75

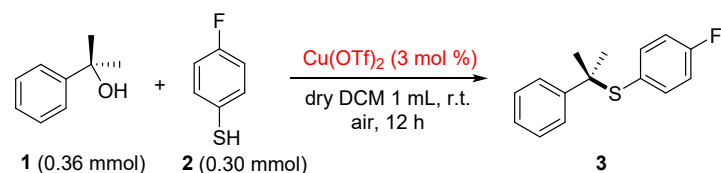
^aIsolated yield.

Table S2. Screening of solvent for the reaction of **1** and **2**



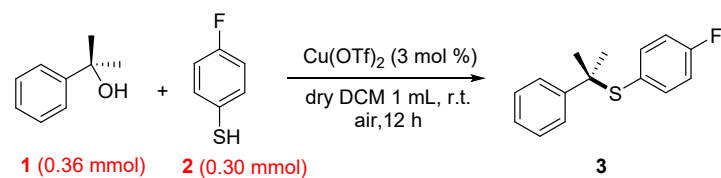
entry	Solvent	yield% ^a
1	dry DCM	96
2	DCE instead of DCM	91

^aIsolated yield.

Table S3. Change of Cu(OTf)₂ loading for the reaction of **1** and **2**

Entry	Catalyst	yield% ^a
1	w/o Cu(OTf) ₂	ND ^b
2	1 mmol % Cu(OTf) ₂	65
3	3 mmol % Cu(OTf) ₂	96
4	5 mmol % Cu(OTf) ₂	99
5	8 mmol % Cu(OTf) ₂	99
6	3 mmol % Ni(OTf) ₂	61
7	3 mmol % Zn(OTf) ₂	15
8	3 mmol % Sc(OTf) ₂	44

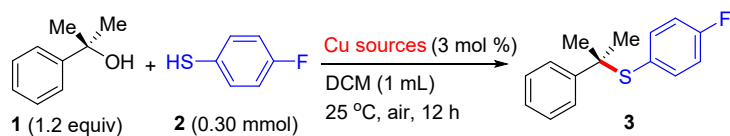
^aIsolated yield.; ^bNot detected.

Table S4. Variation of the molar ratios of **1** and **2**

Entry	Variation	yield% ^a
1	none	96
2	1 (0.30 mmol)	84
3	2 (1.5 equiv)	99

^aIsolated yield.

Table S5. Screening of Cu sources for the reaction of **1** and **2**



entry	Cu sources	yield% ^a	entry	Cu sources	yield% ^a
1	Cu	ND ^b	16	Copper(II) pyrophosphate	5
2	CuO	ND ^b	17	Copper(II) oxalate	1
3	Cu ₂ O	ND ^b	18	Copper(II) phthalocyanine	ND ^b
4	CuS	39	19	Copper(I) thiophene-2-carboxylate	ND ^b
5	Cu ₂ S	87	20	Copper(II) D-gluconate	ND ^b
6	CuF ₂	5	21	Copper(I) diphenylphosphinate	ND ^b
7	CuCl	11	22	Cu(OTs) ₂	36
8	CuBr ₂	24	23	CuOTf	84
9	CuBr	35	24	CuSO ₄	20
10	CuBr•DMS	36	25	CuSO ₄ •5H ₂ O	27
11	CuI	5	26	Cu(acac) ₂	ND ^b
12	Cu(OAc) ₂	ND ^b	27	Cu(PPh ₃) ₃ Cl	ND ^b
13	CuOAc	ND ^b	28	Cu(Py) ₄ (OTf) ₂	ND ^b
14	CuSCN	ND ^b	29	Cu(CH ₃ CN) ₄ BF ₄	45
15	Cu(BF ₄) ₂	77	30	Cu(CH ₃ CN) ₄ OTf	66

^aisolated yield; ^bNot detected.

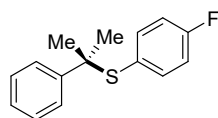
Part 3. Coupling of Benzyl Alcohols with Thiols

1. General Procedure

General procedure for the reaction of benzyl alcohols with thiols (method A): To a dried test tube was charged with benzyl alcohols (49.0 mg, 0.36 mmol, 120 mol %), Cu(OTf)₂ (3.3 mg, 0.009 mmol, 3 mol %) at r.t. The tube was capped with a rubber septum. Thiols (0.30 mmol, 100 mol %) was added followed by addition of DCM (1 mL) via syringes. The reaction mixture was allowed to maintain r.t. and stirred overnight. The reaction mixture was purified by column chromatograph to afford the product as a solid or oil.

2. Experimental Details

(4-Fluorophenyl)(2-phenylpropan-2-yl)sulfane (3).



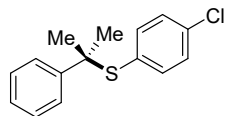
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 96% yield (70.9 mg, 0.288 mmol) as a pale yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.41–7.32 (m, 2H), 7.29–7.25 (m, 2H), 7.22–7.17 (m, 1H), 7.12–7.02 (m, 2H), 6.92–6.78 (m, 2H), 1.67 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 146.04, 138.58, 138.51, 127.92, 126.62, 126.55, 115.41, 115.24, 51.03, 29.46.

¹⁹F NMR (471 MHz, CDCl₃): δ -112.66 (s).

(4-Chlorophenyl)(2-phenylpropan-2-yl)sulfane (4).

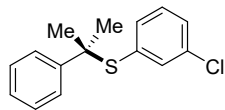


This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 99% yield (77.9 mg, 0.296 mmol) as a colorless oil.

¹H NMR (500 MHz, CDCl₃): δ 7.42–7.34 (m, 2H), 7.30–7.24 (m, 2H), 7.23–7.18 (m, 1H), 7.17–7.09 (m, 2H), 7.06–6.96 (m, 2H), 1.68 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 146.00, 137.62, 134.97, 128.44, 127.98, 126.69, 126.57, 51.28, 29.59.

(3-Chlorophenyl)(2-phenylpropan-2-yl)sulfane (5).

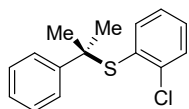


This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 76% yield (59.9 mg, 0.228 mmol) as a colorless oil.

¹H NMR (500 MHz, CDCl₃): δ 7.43–7.36 (m, 2H), 7.32–7.27 (m, 2H), 7.25–7.20 (m, 2H), 7.13–7.03 (m, 2H), 6.97 (dt, J = 7.8, 1.3 Hz, 1H), 1.70 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 148.07, 146.55, 129.70, 127.86, 126.80, 126.38, 123.89, 119.08, 110.52, 55.77, 55.54, 29.38.

(2-Chlorophenyl)(2-phenylpropan-2-yl)sulfane (6).

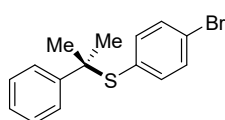


This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 83% yield (65.4 mg, 0.249 mmol) as a pale yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.46 (dd, J = 8.4, 1.3 Hz, 2H), 7.40 (dd, J = 8.0, 1.4 Hz, 1H), 7.31–7.25 (m, 2H), 7.25–7.21 (m, 1H), 7.17 (ddd, J = 8.0, 7.2, 1.8 Hz, 1H), 7.00–6.91 (m, 2H), 1.74 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 145.97, 137.50, 129.82, 129.42, 128.08, 126.76, 126.52, 126.37, 52.88, 29.77.

(4-Bromophenyl)(2-phenylpropan-2-yl)sulfane (7).

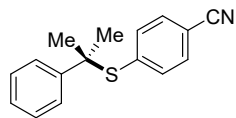


This compound was prepared according to the method A. After purification by column chromatography (SiO₂: 2% ethyl acetate in petroleum ether), the title compound was isolated in 93% yield (85.7 mg, 0.279 mmol) as a colorless oil.

¹H NMR (500 MHz, CDCl₃): δ 7.39 (d, J = 8.1 Hz, 2H), 7.30–7.24 (m, 4H), 7.20 (td, J = 6.7, 6.1, 1.5 Hz, 1H), 6.94 (dd, J = 8.4, 2.5 Hz, 2H), 1.68 (d, J = 2.6 Hz, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 145.99, 137.83, 132.01, 131.40, 127.99, 126.70, 126.57, 123.25, 51.27, 29.62.

4-((2-Phenylpropan-2-yl)thio)benzonitrile (8).



This compound was prepared according to the method A. After purification by column chromatography (SiO₂: 5% ethyl acetate in petroleum ether), the title compound was isolated in 49% yield (37.3 mg, 0.147 mmol) as a yellow oil.

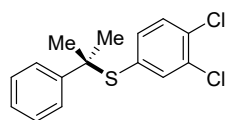
¹H NMR (500 MHz, CDCl₃): δ 7.41 (dd, *J* = 16.8, 8.0 Hz, 4H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 8.2 Hz, 2H), 1.73 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 145.67, 134.81, 131.66, 128.27, 127.01, 126.51, 118.58, 111.30, 52.31, 30.03.

HRMS (ESI) *m/z* ([*M*+*H*]⁺) calcd for C₁₆H₁₆NS: 254.0998. Found: 254.0959.

M.p.: 124-126 °C.

(3,4-Dichlorophenyl)(2-phenylpropan-2-yl)sulfane (9).

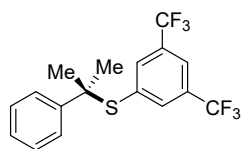


This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 95% yield (84.7 mg, 0.285 mmol) as a pale yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.43–7.36 (m, 2H), 7.30 (dd, *J* = 8.4, 6.7 Hz, 2H), 7.25–7.20 (m, 2H), 7.12 (s, 1H), 6.87 (dd, *J* = 8.3, 2.1 Hz, 1H), 1.70 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 145.61, 137.50, 135.19, 131.97, 129.90, 128.07, 126.91, 126.56, 51.79, 29.56.

(3,5-Bis(trifluoromethyl)phenyl)(2-phenylpropan-2-yl)sulfane (10).



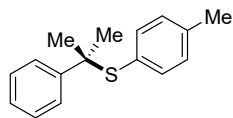
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 60% yield (65.6 mg, 0.180 mmol) as a pale yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.70 (s, 1H), 7.38 (s, 2H), 7.34 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.31–7.26 (m, 2H), 7.26–7.21 (m, 1H), 1.74 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 144.92, 136.35, 135.49, 131.45, 131.19, 128.24, 127.21, 126.49, 123.94, 121.98, 121.95, 121.92, 121.76, 52.48, 29.47.

¹⁹F NMR (471 MHz, CDCl₃): δ -63.12 (s).

(2-Phenylpropan-2-yl)(p-tolyl)sulfane (11).



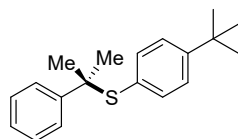
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 80% yield (57.9 mg, 0.239 mmol) as a colorless oil.

¹H NMR (500 MHz, CDCl₃): δ 7.41 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.27 (t, *J* = 7.7 Hz, 2H), 7.22–7.17 (m, 1H), 7.05–6.93 (m, 4H), 2.29 (s, 3H), 1.67 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 146.48, 138.66, 136.62, 129.29, 129.07, 127.87, 126.58, 126.47, 50.76, 29.63, 21.22.

HRMS (ESI) *m/z* ([*M*+*H*]⁺) calcd for C₁₆H₁₉S: 243.1202. Found: 243.1198.

(4-(Tert-butyl)phenyl)(2-phenylpropan-2-yl)sulfane (12).



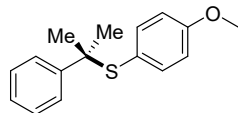
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 99% yield (84.5 mg, 0.297 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.45–7.41 (m, 2H), 7.28 (dd, *J* = 8.4, 6.8 Hz, 2H), 7.22–7.17 (m, 3H), 7.11–7.06 (m, 2H), 1.68 (s, 6H), 1.27 (s, 9H).

¹³C NMR (126 MHz, CDCl₃): δ 151.73, 136.19, 127.88, 126.54, 126.48, 125.30, 50.82, 34.59, 31.25, 29.73.

HRMS (ESI) *m/z* ([*M*+*H*]⁺) calcd for C₁₉H₂₅S: 285.1671. Found: 285.1686.

(4-Methoxyphenyl)(2-phenylpropan-2-yl)sulfane (13).



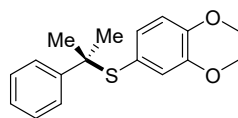
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 94% yield (73.2 mg, 0.283 mmol) as a yellow solid.

¹H NMR (500 MHz, CDCl₃): δ 7.42–7.33 (m, 2H), 7.28–7.24 (m, 2H), 7.23–7.16 (m, 1H), 7.11–7.00 (m, 2H), 6.77–6.64 (m, 2H), 3.76 (s, 3H), 1.66 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 160.19, 146.39, 138.31, 127.84, 126.55, 126.44, 123.66, 113.76, 55.23, 50.73, 29.42.

M.p.: 49-51 °C.

(3,4-Dimethoxyphenyl)(2-phenylpropan-2-yl)sulfane (14).



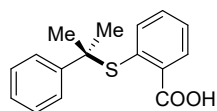
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: 10% ethyl acetate in petroleum ether), the title compound was isolated in 73% yield (63.2 mg, 0.219 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.41–7.35 (m, 2H), 7.27 (dd, *J* = 8.4, 6.8 Hz, 2H), 7.22–7.15 (m, 1H), 6.86 (dd, *J* = 8.2, 2.0 Hz, 1H), 6.71 (d, *J* = 8.3 Hz, 1H), 6.34 (d, *J* = 2.0 Hz, 1H), 3.84 (s, 3H), 3.55 (s, 3H), 1.68 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 149.64, 146.55, 129.70, 127.86, 126.80, 126.37, 123.88, 119.08, 110.52, 55.77, 55.54, 50.91, 29.37.

HRMS (ESI) *m/z* ([*M*+*H*]⁺) calcd for C₁₇H₂₁O₂S: 289.1257. Found: 289.1256.

2-((2-Phenylpropan-2-yl)thio)benzoic acid (15).



This compound was prepared according to the method A. After purification by column chromatography (SiO₂: 20% ethyl acetate in petroleum ether), the title compound was isolated in 96% yield (78.5 mg, 0.288 mmol) as a white solid.

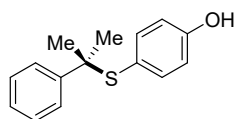
¹H NMR (500 MHz, CDCl₃): δ 8.28 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.7 Hz, 2H), 7.30 (dddd, *J* = 17.5, 9.0, 4.5, 2.0 Hz, 4H), 7.04 (dd, *J* = 7.8, 1.3 Hz, 1H), 1.76 (s, 6H).

¹³C NMR (126 MHz, MeOD): δ 146.48, 136.93, 134.45, 133.56, 129.81, 128.75, 127.84, 126.87, 126.32, 126.29, 51.39, 29.37.

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₆H₁₆KO₂S: 311.0503. Found: 311.0494.

M.p.: 112-114 °C.

4-((2-Phenylpropan-2-yl)thio)phenol (16).



This compound was prepared according to the method A. After purification by column chromatography (SiO₂: 10% ethyl acetate in petroleum ether),

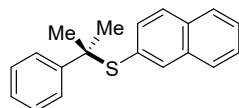
the title compound was isolated in 99% yield (72.6 mg, 0.297 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.40–7.35 (m, 2H), 7.26 (dd, *J* = 8.4, 6.8 Hz, 2H), 7.23–7.15 (m, 1H), 7.08–6.95 (m, 2H), 6.69–6.57 (m, 2H), 5.24 (s, 1H), 1.66 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 156.38, 138.56, 127.85, 126.55, 126.47, 115.32, 50.77, 29.38.

HRMS (ESI) *m/z* ([*M*+Na]⁺) calcd for C₁₅H₁₆NaOS: 267.0814. Found: 267.0818.

Naphthalen-2-yl(2-phenylpropan-2-yl)sulfane (17).



This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 89% yield (74.4 mg, 0.267 mmol) as a white solid.

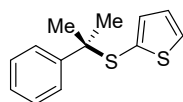
¹H NMR (500 MHz, CDCl₃): δ 7.80–7.72 (m, 1H), 7.70–7.56 (m, 3H), 7.49–7.36 (m, 4H), 7.28 (t, *J* = 7.4 Hz, 2H), 7.24–7.20 (m, 1H), 7.13 (dd, *J* = 8.5, 1.7 Hz, 1H), 1.73 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 146.41, 136.18, 133.18, 130.37, 127.96, 127.87, 127.52, 126.65, 126.60, 126.55, 126.11, 51.38, 29.76.

HRMS (ESI) *m/z* ([*M*+H]⁺) calcd for C₁₉H₁₉S: 279.1202. Found: 279.0928.

M.p.: 53–55 °C.

2-((2-Phenylpropan-2-yl)thio)thiophene (18).

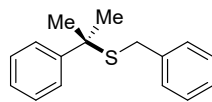


This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 71% yield (49.9 mg, 0.213 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.46–7.40 (m, 2H), 7.33–7.26 (m, 3H), 7.24–7.19 (m, 1H), 6.91 (dd, *J* = 5.4, 3.6 Hz, 1H), 6.85 (dd, *J* = 3.5, 1.3 Hz, 1H), 1.71 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 145.63, 136.61, 130.80, 127.99, 127.16, 126.76, 126.62, 52.27, 29.29.

Benzyl(2-phenylpropan-2-yl)sulfane (19).



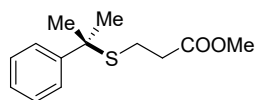
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 87% yield (63.3 mg, 0.261 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.58 (d, *J* = 7.8 Hz, 2H), 7.35 (t, *J* = 7.7 Hz, 2H), 7.25 (s, 1H), 7.24–7.19 (m, 2H), 7.17 (d, *J* = 7.0 Hz, 1H), 7.12 (d, *J* = 7.1 Hz, 2H), 3.39 (s, 2H), 1.72 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 146.35, 138.21, 128.98, 128.39, 128.20, 126.76, 126.68, 126.59, 48.60, 34.58, 30.29.

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₆H₁₈KS: 281.0761. Found: 281.0952.

Methyl 3-((2-phenylpropan-2-yl)thio)propanoate (20).



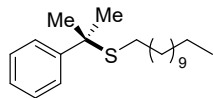
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: 5% ethyl acetate in petroleum ether), the title compound was isolated in 64% yield (46.0 mg, 0.193 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.60–7.47 (m, 2H), 7.32 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.21 (td, *J* = 7.1, 1.2 Hz, 1H), 3.62 (s, 3H), 2.49 (t, *J* = 7.6 Hz, 2H), 2.32 (t, *J* = 7.5 Hz, 2H), 1.71 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 146.29, 128.14, 126.57, 126.47, 51.68, 47.85, 34.14, 30.16, 24.47.

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₃H₁₈O₂KS: 277.0659. Found: 277.0840.

Dodecyl(2-phenylpropan-2-yl)sulfane (21).



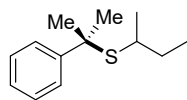
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 97% yield (93.1 mg, 0.290 mmol) as a pale yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.61–7.46 (m, 2H), 7.31 (t, *J* = 7.8 Hz, 2H), 7.19 (t, *J* = 7.3 Hz, 1H), 2.20 (t, *J* = 7.4 Hz, 2H), 1.70 (s, 6H), 1.40–1.33 (m, 2H), 1.31–1.14 (m, 18H), 0.88 (t, *J* = 6.9 Hz, 3H).

¹³C NMR (126 MHz, CDCl₃): δ 127.99, 126.46, 126.29, 47.34, 31.93, 30.29, 29.65, 29.64, 29.58, 29.46, 29.43, 29.36, 29.18, 29.07, 22.70, 14.13.

HRMS (ESI) *m/z* ([*M*+*H*]⁺) calcd for C₂₁H₃₇S: 321.2610. Found: 321.3147.

sec-Butyl(2-phenylpropan-2-yl)sulfane (22).



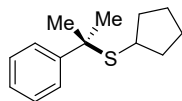
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was

isolated in 83% yield (51.7 mg, 0.248 mmol) as a pale yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.60–7.48 (m, 2H), 7.33–7.27 (m, 2H), 7.22–7.15 (m, 1H), 2.31 (h, *J* = 6.8 Hz, 1H), 1.72 (d, *J* = 3.1 Hz, 6H), 1.34 (ddt, *J* = 14.4, 9.7, 7.2 Hz, 2H), 1.01 (d, *J* = 6.9 Hz, 3H), 0.78 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (126 MHz, CDCl₃): δ 147.14, 127.88, 126.60, 126.29, 47.97, 40.64, 31.09, 30.90, 30.81, 22.81, 11.19.

Cyclopentyl(2-phenylpropan-2-yl)sulfane (23).



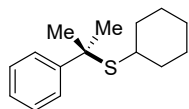
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 52% yield (34.4 mg, 0.156 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.58–7.52 (m, 2H), 7.31 (t, *J* = 7.8 Hz, 2H), 7.20 (t, *J* = 7.3 Hz, 1H), 2.66 (p, *J* = 7.8 Hz, 1H), 1.73 (s, 6H), 1.62–1.52 (m, 3H), 1.44–1.26 (m, 5H).

¹³C NMR (126 MHz, DMSO-*d*₆): δ 123.20, 121.76, 121.54, 43.23, 37.65, 30.31, 26.15, 20.06.

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₄H₂₀KS: 259.0917. Found: 259.1111.

Cyclohexyl(2-phenylpropan-2-yl)sulfane (24).



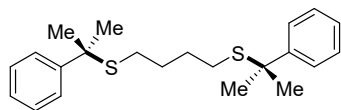
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 74% yield (52.2 mg, 0.222 mmol) as a pale yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.55 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.34–7.26 (m, 2H), 7.22–7.15 (m, 1H), 2.30 (ddd, *J* = 10.2, 6.5, 3.5 Hz, 1H), 1.71 (s, 6H), 1.60 (tq, *J* = 13.7, 4.5, 4.0 Hz, 4H), 1.43 (s, 1H), 1.27–1.13 (m, 5H).

¹³C NMR (126 MHz, CDCl₃): δ 127.88, 126.53, 126.27, 48.17, 42.49, 35.32, 30.95, 26.12, 25.55.

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₅H₂₂KS: 273.1074. Found: 273.1258.

1,4-Bis((2-phenylpropan-2-yl)thio)butane (25).



This compound was prepared according to the method A except using 2-phenyl-2-propanol (98.0 mg, 0.72 mmol, 240 mol %).

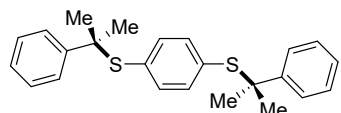
After purification by column chromatography (SiO₂: 5% ethyl acetate in petroleum ether), the title compound was isolated in 99% yield (55.8 mg, 0.156 mmol) as a colorless oil.

¹H NMR (500 MHz, CDCl₃): δ 7.49 (d, J = 8.0 Hz, 4H), 7.32–7.24 (m, 4H), 7.18 (t, J = 7.3 Hz, 2H), 2.08 (t, J = 6.6 Hz, 4H), 1.66 (s, 12H), 1.32 (dd, J = 9.9, 3.5 Hz, 4H).

¹³C NMR (126 MHz, CDCl₃): δ 146.69, 128.00, 126.44, 126.33, 47.39, 30.26, 28.83, 28.35.

HRMS (ESI) m/z ([M+Na]⁺) calcd for C₂₂H₃₀NaS₂: 381.1681. Found: 381.1636.

1,4-Bis((2-phenylpropan-2-yl)thio)benzene (26).



This compound was prepared according to the method A except using 2-phenyl-2-propanol (98.0 mg, 0.72 mmol, 240 mol %).

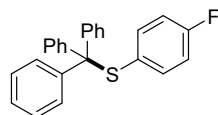
After purification by column chromatography (SiO₂: 5% ethyl acetate in petroleum ether), the title compound was isolated in 85% yield (48.4 mg, 0.128 mmol) as a pale yellow solid.

¹H NMR (500 MHz, CDCl₃): δ 7.39–7.32 (m, 4H), 7.25 (t, J = 7.6 Hz, 4H), 7.19 (t, J = 7.2 Hz, 2H), 6.89 (s, 4H), 1.65 (s, 12H).

¹³C NMR (126 MHz, CDCl₃): δ 146.13, 135.95, 133.60, 127.92, 126.51, 51.26, 29.69.

M.p.: 137-139 °C.

(4-Fluorophenyl)(trityl)sulfane (27).



This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was

isolated in 67% yield (74.5 mg, 0.201 mmol) as a colorless oil.

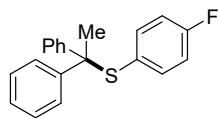
¹H NMR (500 MHz, CDCl₃): δ 7.41–7.38 (m, 6H), 7.22 (dd, J = 8.4, 6.4 Hz, 6H), 7.20–7.15 (m, 3H), 6.95–6.89 (m, 2H), 6.71–6.66 (m, 2H).

¹³C NMR (126 MHz, CDCl₃): δ 144.39, 137.55, 137.48, 129.93, 127.71, 126.71, 115.28, 115.11, 71.05.

¹⁹F NMR (471 MHz, CDCl₃): δ -112.63 (s).

HRMS (ESI) m/z ([M+Na]⁺) calcd for C₂₅H₁₉FNaS: 393.1084. Found: 393.1099.

(1,1-Diphenylethyl)(4-fluorophenyl)sulfane (28).



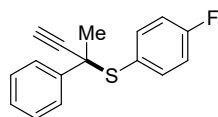
This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 69% yield (63.8 mg, 0.207 mmol) as a colorless oil.

¹H NMR (500 MHz, CDCl₃): δ 7.41–7.33 (m, 4H), 7.27 (t, J = 7.4 Hz, 4H), 7.24–7.19 (m, 2H), 7.02–6.95 (m, 2H), 6.84–6.75 (m, 2H), 1.90 (s, 3H).

¹³C NMR (126 MHz, DMSO-*d*₆): δ 141.31, 134.07, 134.00, 123.57, 123.12, 121.96, 110.63, 110.46, 55.02, 25.54.

¹⁹F NMR (471 MHz, CDCl₃): δ -112.22 (s).

(4-Fluorophenyl)(2-phenylbut-3-yn-2-yl)sulfane (29).



This compound was prepared according to the method A. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 83% yield (63.8 mg, 0.249 mmol) as a yellow oil.

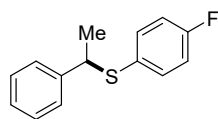
¹H NMR (500 MHz, CDCl₃): δ 7.57–7.49 (m, 2H), 7.31–7.28 (m, 2H), 7.27 (s, 1H), 7.27–7.21 (m, 2H), 6.95–6.87 (m, 2H), 2.71 (s, 1H), 1.94 (s, 3H).

¹³C NMR (126 MHz, CDCl₃): δ 141.64, 138.69, 138.62, 128.07, 127.53, 126.70, 115.49, 115.32, 85.94, 74.90, 29.68.

¹⁹F NMR (471 MHz, CDCl₃): δ -111.65 (s).

HRMS (ESI) m/z ([$M+H$]⁺) calcd for C₁₆H₁₄FS: 257.0795. Found: 257.0776.

(4-Fluorophenyl)(1-phenylethyl)sulfane (30).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 40°C. After purification by column chromatography (SiO₂: 5% ethyl acetate in petroleum ether), the title compound was isolated in 64% yield (44.6 mg, 0.192 mmol, 0% *ee*) as a colorless oil.

¹H NMR (500 MHz, CDCl₃): δ 7.28–7.19 (m, 7H), 6.97–6.82 (m, 2H), 4.22 (q, J = 7.0 Hz, 1H), 1.61 (d, J = 7.0 Hz, 3H).

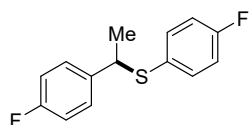
¹³C NMR (126 MHz, CDCl₃): δ 143.01, 135.74, 135.67, 128.36, 127.30, 127.18, 115.80, 115.63, 48.90, 21.92.

¹⁹F NMR (471 MHz, CDCl₃): δ -113.92 (s).

HRMS (ESI) m/z ([M+H]⁺) calcd for C₁₄H₁₄FS: 271.0354. Found: 271.0561.

HPLC analysis: CHIRALCEL OD-H column, 0.5% *i*PrOH in hexane, 0.5 mL/min, 254 nm UV detector, *t*_R (minor) = 9.0 min, *t*_R (major) = 8.7 min.

(4-Fluorophenyl)(1-(4-fluorophenyl)ethyl)sulfane (31).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 40°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 60% yield (45.1 mg, 0.180 mmol) as a pale yellow oil.

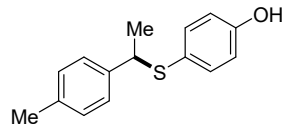
¹H NMR (500 MHz, CDCl₃): δ 7.25–7.19 (m, 2H), 7.19–7.13 (m, 2H), 6.97–6.87 (m, 4H), 4.20 (q, *J* = 7.0 Hz, 1H), 1.59 (d, *J* = 7.0 Hz, 3H).

¹³C NMR (126 MHz, CDCl₃): δ 135.92, 135.86, 128.83, 128.77, 115.88, 115.71, 115.23, 115.06, 48.21, 29.71, 21.97.

¹⁹F NMR (471 MHz, CDCl₃): δ -113.59 (s), -115.31 (s).

HRMS (ESI) m/z ([M+K]⁺) calcd for C₁₄H₁₂F₂KS: 289.0259. Found: 289.0455.

4-((1-(*p*-tolyl)ethyl)thio)phenol (32).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 40°C. After purification by column chromatography (SiO₂: 5% ethyl acetate in petroleum ether), the title compound was isolated in 96% yield (70.4 mg, 0.288 mmol) as a white solid.

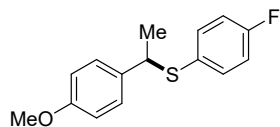
¹H NMR (500 MHz, CDCl₃): δ 7.20–7.16 (m, 2H), 7.13–7.10 (m, 2H), 7.06 (d, *J* = 7.9 Hz, 2H), 6.71–6.64 (m, 2H), 5.01 (s, OH), 4.14 (q, *J* = 7.0 Hz, 1H), 2.31 (s, 3H), 1.56 (d, *J* = 7.0 Hz, 3H).

¹³C NMR (126 MHz, DMSO-*d*₆): δ 150.84, 135.49, 131.90, 131.39, 124.23, 122.45, 120.73, 110.96, 44.12, 17.15, 16.35.

HRMS (ESI) m/z ([M+Na]⁺) calcd for C₁₅H₁₆NaOS: 267.0814. Found: 267.0330.

M.p.: 94-96 °C.

(4-Fluorophenyl)(1-(4-methoxyphenyl)ethyl)sulfane (33).



This compound was prepared according to the method A except using $\text{Cu}(\text{OTf})_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 40°C . After purification by column chromatography (SiO_2 : petroleum ether), the title compound was isolated in 88% yield (69.3 mg, 0.264 mmol) as a yellow oil.

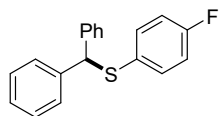
$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.25–7.20 (m, 2H), 7.19–7.12 (m, 2H), 6.93–6.87 (m, 2H), 6.84–6.76 (m, 2H), 4.2–4.16 (m, 1H), 3.78 (s, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3): δ 158.65, 135.72, 135.65, 135.03, 128.35, 115.78, 115.61, 113.70, 55.26, 48.31, 22.05.

$^{19}\text{F NMR}$ (471 MHz, CDCl_3): δ -114.07 (s).

HRMS (ESI) m/z ($[\text{M}+\text{NH}_4]^+$) calcd for $\text{C}_{15}\text{H}_{19}\text{FNOS}$: 280.1166. Found: 280.0336.

Benzhydryl(4-fluorophenyl)sulfane (34).



This compound was prepared according to the method A except using $\text{Cu}(\text{OTf})_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 40°C . After purification by column chromatography (SiO_2 : petroleum ether), the title compound was isolated in 53% yield (46.8 mg, 0.159 mmol) as a pale yellow oil.

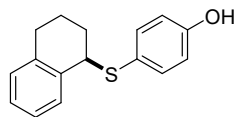
$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.38 (dd, $J = 8.5, 1.1$ Hz, 4H), 7.28 (dd, $J = 8.3, 6.7$ Hz, 4H), 7.25–7.17 (m, 4H), 6.91–6.81 (m, 2H), 5.41 (s, 1H).

$^{13}\text{C NMR}$ (126 MHz, $\text{DMSO}-d_6$): δ 136.08, 129.39, 129.33, 123.79, 123.64, 122.57, 111.16, 110.98, 53.97.

$^{19}\text{F NMR}$ (471 MHz, CDCl_3): δ -114.34 (s).

HRMS (ESI) m/z ($[\text{M}+\text{K}]^+$) calcd for $\text{C}_{19}\text{H}_{15}\text{FKS}$: 333.0510. Found: 333.0745.

(4-Fluorophenyl)(1,2,3,4-tetrahydronaphthalen-1-yl)sulfane (35).



This compound was prepared according to the method A except using $\text{Cu}(\text{OTf})_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 40°C . After purification by column chromatography (SiO_2 : 5% ethyl acetate in petroleum ether), the title compound was isolated in 90% yield (69.2 mg, 0.270 mmol) as a yellow oil.

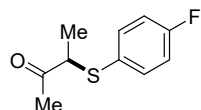
$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.46–7.42 (m, 2H), 7.35 (dd, $J = 7.0, 2.1$ Hz, 1H), 7.13 (ddd, $J =$

7.2, 4.7, 1.9 Hz, 2H), 7.10–7.06 (m, 1H), 7.03–6.98 (m, 2H), 4.44 (t, $J = 4.1$ Hz, 1H), 2.86–2.69 (m, 2H), 2.27–2.15 (m, 1H), 1.96 (dtd, $J = 10.6, 9.3, 8.8, 5.5$ Hz, 2H), 1.75 (tdd, $J = 9.6, 5.1, 2.4$ Hz, 1H).

^{13}C NMR (126 MHz CDCl_3): δ 137.58, 135.39, 135.23, 135.17, 130.45, 129.31, 127.15, 125.70, 116.11, 115.94, 48.75, 29.10, 28.40, 18.57.

HRMS (ESI) m/z ($[\text{M}+\text{K}]^+$) calcd for $\text{C}_{16}\text{H}_{16}\text{KOS}$: 295.0553. Found: 295.0573.

3-((4-Fluorophenyl)thio)butan-2-one (36).



This compound was prepared according to the method A except using $\text{Cu}(\text{OTf})_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 40°C .

After purification by column chromatography (SiO_2 : 5% ethyl acetate in petroleum ether), the title compound was isolated in 64% yield (35.0 mg, 0.136 mmol) as a pale yellow oil.

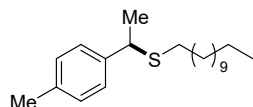
^1H NMR (500 MHz, CDCl_3): δ 7.40–7.34 (m, 2H), 7.03–6.98 (m, 2H), 3.67 (q, $J = 7.0$ Hz, 1H), 2.29 (s, 3H), 1.37 (d, $J = 7.0$ Hz, 3H).

^{13}C NMR (126 MHz, CDCl_3): δ 205.08, 135.96, 135.89, 116.34, 116.17, 52.42, 29.71, 15.87.

^{19}F NMR (471 MHz, CDCl_3): δ -112.45 (s).

HRMS (ESI) m/z ($[\text{M}+\text{H}]^+$) calcd for $\text{C}_{10}\text{H}_{12}\text{FOS}$: 199.0587. Found: 199.0577.

Cyclohexyl(1-(*p*-tolyl)ethyl)sulfane (37).



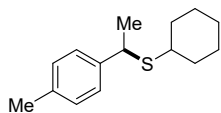
This compound was prepared according to the method A except using $\text{Cu}(\text{OTf})_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at

40°C . After purification by column chromatography (SiO_2 : petroleum ether), the title compound was isolated in 63% yield (60.6 mg, 0.189 mmol) as a colorless oil.

^1H NMR (500 MHz, CDCl_3): δ 7.22 (d, $J = 8.0$ Hz, 2H), 7.11 (d, $J = 7.9$ Hz, 2H), 3.91 (q, $J = 7.0$ Hz, 1H), 2.33 (s, 3H), 2.32–2.23 (m, 2H), 1.54 (d, $J = 7.0$ Hz, 3H), 1.48 (dq, $J = 14.8, 7.3, 6.6$ Hz, 2H), 1.25 (d, $J = 2.4$ Hz, 18H), 0.88 (t, $J = 6.9$ Hz, 3H).

^{13}C NMR (126 MHz, CDCl_3): δ 141.21, 136.52, 129.10, 127.11, 43.73, 31.94, 31.31, 29.67, 29.65, 29.61, 29.50, 29.40, 29.37, 29.22, 28.96, 22.71, 21.08, 14.14.

Cyclohexyl(1-(*p*-tolyl)ethyl)sulfane (38).

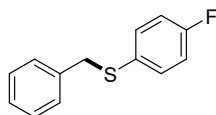


This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 40°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 59% yield (41.5 mg, 0.177 mmol) as a colorless oil.

¹H NMR (500 MHz, CDCl₃): δ 7.23 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 4.01 (q, *J* = 7.0 Hz, 1H), 2.39 (tt, *J* = 10.5, 3.6 Hz, 1H), 2.33 (s, 3H), 1.96 (d, *J* = 12.9 Hz, 1H), 1.73 (t, *J* = 11.2 Hz, 2H), 1.66 (dd, *J* = 10.0, 3.9 Hz, 1H), 1.53 (d, *J* = 7.0 Hz, 3H), 1.35–1.12 (m, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 141.67, 136.42, 129.12, 127.00, 42.70, 42.12, 33.88, 33.30, 26.01, 25.89, 25.85, 23.20, 21.10.

Benzyl(4-fluorophenyl)sulfane (39).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 76% yield (49.7 mg, 0.228 mmol) as a colorless oil.

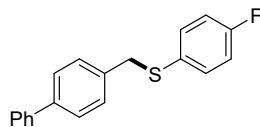
¹H NMR (500 MHz, CDCl₃): δ 7.29–7.19 (m, 7H), 6.98–6.89 (m, 2H), 4.03 (s, 2H).

¹³C NMR (126 MHz, CDCl₃): δ 137.52, 133.46, 133.40, 128.85, 128.46, 127.20, 115.99, 115.82, 40.46.

¹⁹F NMR (471 MHz, CDCl₃): δ -114.84 (s).

HRMS (ESI) *m/z* ([M+NH₄]⁺) calcd for C₁₃H₁₅FNS: 236.0904. Found: 236.0833.

([1,1'-Biphenyl]-4-ylmethyl)(4-fluorophenyl)sulfane (40).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 74% yield (65.4 mg, 0.222 mmol) as a white solid.

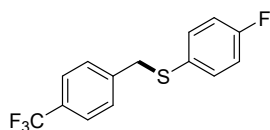
¹H NMR (500 MHz, CDCl₃): δ 7.57 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.52–7.48 (m, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.35 (t, *J* = 1.3 Hz, 0H), 7.33–7.24 (m, 5H), 7.00–6.89 (m, 2H), 4.07 (s, 2H).

¹³C NMR (126 MHz, CDCl₃): δ 140.67, 140.10, 136.60, 133.50, 133.44, 129.27, 128.79, 127.33, 127.18, 127.02, 116.05, 115.88, 40.20.

¹⁹F NMR (471 MHz, CDCl₃): δ -114.75 (s).

M.p.: 157-159 °C.

(4-Fluorophenyl)(4-(trifluoromethyl)benzyl)sulfane (41).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 57% yield (48.9 mg, 0.171 mmol) as a colorless oil.

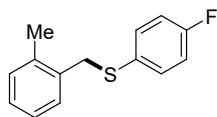
¹H NMR (500 MHz, CDCl₃): δ 7.52 (d, *J* = 8.1 Hz, 2H), 7.27 (dd, *J* = 16.8, 7.6 Hz, 4H), 7.00–6.91 (m, 2H), 4.04 (s, 2H).

¹³C NMR (126 MHz, CDCl₃): δ 163.36, 161.39, 141.87, 133.98, 133.92, 129.11, 125.45, 125.42, 125.39, 125.36, 116.20, 116.02, 40.15.

¹⁹F NMR (471 MHz, CDCl₃): δ -62.47 (s), -113.97 (s).

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₄H₁₀F₄KS: 325.0071. Found: 325.0271.

(4-Fluorophenyl)(2-methylbenzyl)sulfane (42).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 65% yield (45.3 mg, 0.195 mmol) as a yellow oil.

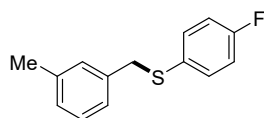
¹H NMR (500 MHz, CDCl₃): δ 7.30–7.26 (m, 2H), 7.15 (d, *J* = 4.0 Hz, 2H), 7.06 (dd, *J* = 8.3, 3.3 Hz, 1H), 7.01 (d, *J* = 7.4 Hz, 1H), 6.98–6.92 (m, 2H), 4.02 (s, 2H), 2.36 (s, 3H).

¹³C NMR (126 MHz, CDCl₃): δ 163.25, 136.72, 133.97, 133.91, 131.06, 130.58, 129.90, 127.61, 126.00, 116.03, 115.86, 38.78, 19.22.

¹⁹F NMR (471 MHz, CDCl₃): δ -114.60 (s).

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₄H₁₃FKS: 271.0354. Found: 271.0641.

(4-Fluorophenyl)(3-methylbenzyl)sulfane (43).



This compound was prepared according to the method A except using

Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 99% yield (69.0 mg, 0.297 mmol) as a yellow oil.

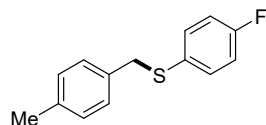
¹H NMR (500 MHz, CDCl₃): δ 7.28–7.24 (m, 2H), 7.15 (t, *J* = 7.8 Hz, 1H), 7.06–7.02 (m, 2H), 7.02–6.99 (m, 1H), 6.96–6.92 (m, 2H), 4.00 (s, 2H), 2.30 (s, 3H).

¹³C NMR (126 MHz, CDCl₃): δ 138.14, 137.32, 133.27, 133.20, 129.60, 128.35, 127.98, 125.88, 115.96, 115.79, 40.40, 21.34.

¹⁹F NMR (471 MHz, CDCl₃): δ -115.00 (s).

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₄H₁₃FKS: 271.0354. Found: 271.0570.

(4-Fluorophenyl)(4-methylbenzyl)sulfane (44).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 67% yield (23.0 mg, 0.105 mmol) as a white solid.

¹H NMR (500 MHz, CDCl₃): δ 7.29–7.24 (m, 2H), 7.09 (q, *J* = 8.0 Hz, 4H), 6.94 (t, *J* = 8.7 Hz, 2H), 4.00 (s, 2H), 2.31 (s, 3H).

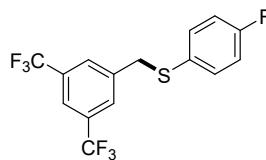
¹³C NMR (126 MHz, CDCl₃): δ 136.87, 134.38, 133.21, 133.15, 129.17, 128.72, 115.97, 115.79, 40.11, 21.12.

¹⁹F NMR (471 MHz, CDCl₃): δ -115.07 (s).

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₄H₁₃FKS: 271.0354. Found: 271.0556.

M.p.: 52-54 °C.

(3,5-Bis(trifluoromethyl)benzyl)(4-fluorophenyl)sulfane (45).



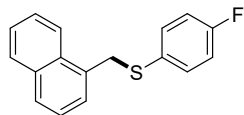
This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 59% yield (62.7 mg, 0.177 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.73 (s, 1H), 7.56 (s, 2H), 7.25 (dd, *J* = 7.5, 4.6 Hz, 2H), 6.97 (t, *J* = 8.4 Hz, 2H), 4.07 (s, 2H).

¹³C NMR (126 MHz, CDCl₃): δ 163.77, 161.79, 140.47, 134.97, 131.83, 131.57, 128.91, 124.24, 121.13, 121.10, 121.07, 121.04, 121.01, 116.41, 116.23.

¹⁹F NMR (471 MHz, CDCl₃): δ -63.02 (s), -112.90 (s).

(4-Fluorophenyl)(naphthalen-1-ylmethyl)sulfane (46).



This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 66% yield (53.1 mg, 0.198 mmol) as a white solid.

¹H NMR (500 MHz, CDCl₃): δ 8.11 (d, *J* = 8.3 Hz, 1H), 7.86 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.52 (dddd, *J* = 23.4, 8.0, 6.8, 1.4 Hz, 2H), 7.32–7.28 (m, 1H), 7.27–7.25 (m, 1H), 7.24 (s, 1H), 7.17 (dd, *J* = 6.9, 1.1 Hz, 1H), 6.97–6.87 (m, 2H), 4.47 (s, 2H).

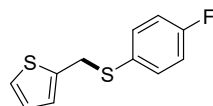
¹³C NMR (126 MHz, CDCl₃): δ 133.99, 133.93, 132.85, 131.34, 128.84, 128.31, 127.39, 126.23, 125.86, 125.15, 123.88, 116.00, 115.82, 38.59.

¹⁹F NMR (471 MHz, CDCl₃): δ -114.57 (s).

HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₇H₁₃FKS: 307.0354. Found: 307.0556.

M.p.: 72-74 °C.

2-(((4-Fluorophenyl)thio)methyl)thiophene (47).



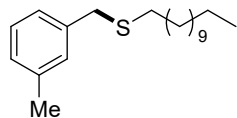
This compound was prepared according to the method A except using Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C. After purification by column chromatography (SiO₂: petroleum ether), the title compound was isolated in 40% yield (26.9 mg, 0.120 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.34–7.30 (m, 2H), 7.17 (d, *J* = 5.1 Hz, 1H), 6.99–6.94 (m, 2H), 6.88–6.84 (m, 1H), 6.78 (d, *J* = 3.0 Hz, 1H), 4.23 (s, 2H).

¹³C NMR (126 MHz CDCl₃): δ 163.33, 140.82, 133.92, 133.86, 130.23, 126.69, 126.35, 125.05, 116.09, 115.92, 35.07.

¹⁹F NMR (471 MHz, CDCl₃): δ -114.26 (s).

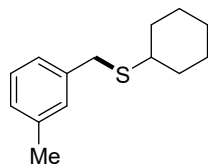
HRMS (ESI) *m/z* ([*M*+*K*]⁺) calcd for C₁₁H₉FKS₂: 262.9761. Found: 262.9978.

Butyl(3-methylbenzyl)sulfane (48).

This compound was prepared according to the method A except using $\text{Cu}(\text{OTf})_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C . After purification by column chromatography (SiO_2 : petroleum ether), the title compound was isolated in 48% yield (44.1 mg, 0.144 mmol) as a colorless oil.

$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.19 (t, $J = 7.5$ Hz, 1H), 7.13 (s, 1H), 7.09 (d, $J = 7.5$ Hz, 1H), 7.04 (d, $J = 7.5$ Hz, 1H), 3.66 (s, 2H), 2.43–2.39 (m, 2H), 2.34 (s, 3H), 1.58–1.52 (m, 3H), 1.37 (s, 2H), 1.25 (s, 16H), 0.88 (t, $J = 6.9$ Hz, 4H).

$^{13}\text{C NMR}$ (126 MHz CDCl_3): δ 138.57, 138.10, 129.56, 128.30, 127.64, 125.88, 36.28, 31.94, 31.48, 29.68, 29.66, 29.62, 29.54, 29.37, 29.27, 29.26, 28.92, 22.71, 21.39, 14.14.

Cyclohexyl(3-methylbenzyl)sulfane (49).

This compound was prepared according to the method A except using $\text{Cu}(\text{OTf})_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at 80°C . After purification by column chromatography (SiO_2 : petroleum ether), the title compound was isolated in 42% yield (27.8 mg, 0.126 mmol) as a colorless oil.

$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.18 (t, $J = 7.5$ Hz, 1H), 7.14 (s, 1H), 7.11 (d, $J = 7.5$ Hz, 1H), 7.04 (d, $J = 7.5$ Hz, 1H), 3.71 (s, 2H), 2.58 (tt, $J = 10.6, 3.7$ Hz, 1H), 2.33 (s, 3H), 1.98–1.93 (m, 2H), 1.78–1.71 (m, 2H), 1.62–1.56 (m, 1H), 1.36 (d, $J = 9.0$ Hz, 1H), 1.35–1.32 (m, 1H), 1.29 (d, $J = 6.7$ Hz, 1H), 1.27 (d, $J = 3.0$ Hz, 1H), 1.25–1.22 (m, 1H).

$^{13}\text{C NMR}$ (126 MHz CDCl_3): δ 138.80, 138.10, 129.51, 128.31, 127.57, 125.80, 43.01, 34.56, 33.40, 26.01, 25.90, 21.40.

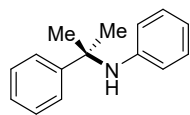
Part 4. The Amination of Benzyl Alcohols with Benzenamine

1. General procedure

General procedure for the reaction of benzenamine with benzyl alcohol (method B): To a dried test tube was charged with benzyl alcohol (0.18 mmol, 100 mol %), Cu(OTf)₂ (8.7 mg, 0.024 mmol, 8 mol %) at r.t. The tube was capped with a rubber septum. Benzenamine (0.30 mmol, 167 mol %) was added followed by addition of DCE (1 mL) via syringes. The reaction mixture was allowed to warm to 70 °C and stirred overnight. The reaction mixture was purified by column chromatography to afford the product as a solid or oil.

2. Experimental details

N-(2-phenylpropan-2-yl)aniline (50).



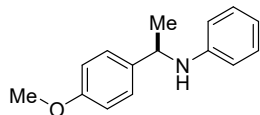
This compound was prepared according to the method B. After purification by column chromatography (SiO₂: 5% ethyl acetate in petroleum ether), the title compound was isolated in 33% yield (12.55 mg, 0.0594 mmol) as a yellow oil.

¹H NMR (500 MHz, CDCl₃): δ 7.45 (d, *J* = 8.2 Hz, 2H), 7.30 (t, *J* = 7.7 Hz, 2H), 7.19 (t, *J* = 7.3 Hz, 1H), 6.90–6.85 (m, 2H), 6.41 (t, *J* = 7.3 Hz, 1H), 6.29 (d, *J* = 7.7 Hz, 2H), 5.88 (s, 1H), 1.56 (s, 6H).

¹³C NMR (126 MHz, CDCl₃): δ 148.47, 147.29, 126.45, 125.82, 115.85, 115.03, 55.42, 30.60.

HRMS (ESI) *m/z* ([M+H]⁺) calcd for C₁₅H₁₈N: 212.1434. Found: 212.1452.

4-fluoro-N-(1-phenylethyl)aniline (51).



This compound was prepared according to the method B. After purification by column chromatography (SiO₂: 5% ethyl acetate in petroleum ether), the title compound was isolated in 47% yield (30.4 mg, 0.141 mmol) as a yellow oil.

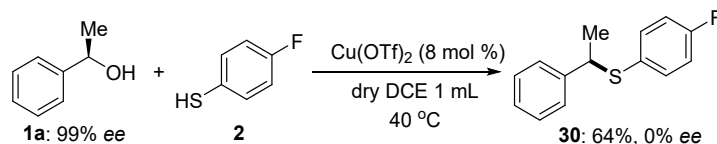
¹H NMR (500 MHz, CDCl₃): δ 7.27 (d, *J* = 8.6 Hz, 2H), 7.14–7.03 (m, 2H), 6.85 (d, *J* = 8.7 Hz, 2H), 6.63 (t, *J* = 7.3 Hz, 1H), 6.51 (d, *J* = 7.7 Hz, 2H), 4.44 (q, *J* = 6.7 Hz, 1H), 1.48 (d, *J* = 6.7 Hz, 3H).

¹³C NMR (126 MHz CDCl₃): δ 158.30, 148.47, 138.42, 129.07, 127.38, 115.91, 114.15, 113.26, 55.41, 51.86, 25.27.

HRMS (ESI) m/z ($[M+H]^+$) calcd for $C_{15}H_{17}NO$: 228.1383. Found: 228.1361.

Part 5. Mechanism Verification

(4-Fluorophenyl)(1-phenylethyl)sulfane (30).



This compound was prepared according to the method A except using $Cu(OTf)_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at $40\text{ }^\circ\text{C}$. After purification by column chromatography (SiO_2 : 5% ethyl acetate in petroleum ether), the title compound was isolated in 64% yield (44.6 mg, 0.192 mmol, 0% ee) as a colorless oil.

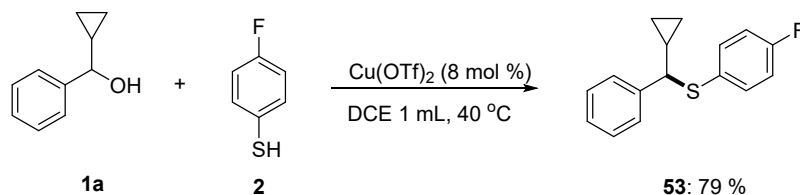
1H NMR (500 MHz, $CDCl_3$): δ 7.28–7.19 (m, 7H), 6.97–6.82 (m, 2H), 4.22 (q, $J = 7.0$ Hz, 1H), 1.61 (d, $J = 7.0$ Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 143.01, 135.74, 135.67, 128.36, 127.30, 127.18, 115.80, 115.63, 48.90, 21.92.

HRMS (ESI) m/z ($[M+H]^+$) calcd for $C_{14}H_{14}FS$: 271.0354. Found: 271.0561.

HPLC analysis: CHIRALCEL OD-H column, 0.5% *i*PrOH in hexane, 0.5 mL/min, 254 nm UV detector, t_R (minor) = 9.0 min, t_R (major) = 8.7 min.

(Cyclopropyl(phenyl)methyl)(4-fluorophenyl)sulfane (53).



The title compound was prepared according the method A except using $Cu(OTf)_2$ (8.7 mg, 0.024 mmol, 8 mol %), DCE (1 mL) and running at $40\text{ }^\circ\text{C}$. After purification by a flash column chromatography (SiO_2 : petroleum ether), the title compound was isolated in 79% yield (61.2 mg, 0.237 mmol) as a pale yellow oil.

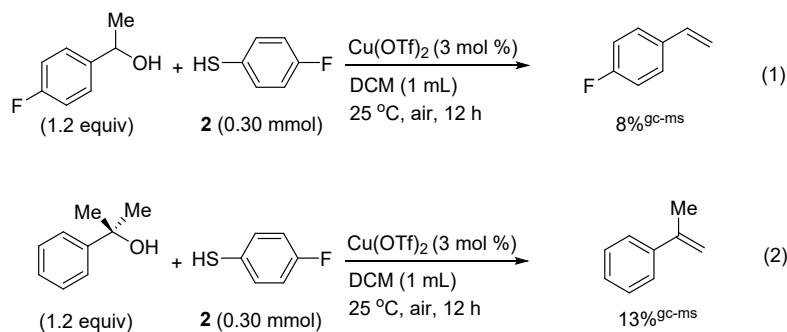
¹H NMR (500 MHz, CDCl₃): δ 7.28–7.17 (m, 7H), 6.86 (td, *J* = 8.7, 2.0 Hz, 2H), 3.38 (d, *J* = 9.7 Hz, 1H), 1.36–1.28 (m, 1H), 0.69 (dd, *J* = 7.7, 3.2 Hz, 1H), 0.54 (dd, *J* = 9.1, 4.4 Hz, 1H), 0.33 (dd, *J* = 9.3, 4.6 Hz, 1H), 0.23 (dd, *J* = 9.8, 5.1 Hz, 1H).

¹³C NMR (126 MHz, CDCl₃): δ 163.55, 161.58, 141.99, 136.18, 136.11, 128.24, 127.88, 127.12, 115.66, 115.49, 59.97, 16.78, 6.61, 5.18.

¹⁹F NMR (471 MHz, CDCl₃): δ -113.97 (s).

HRMS (ESI) *m/z* ([*M*+*H*]⁺) calcd for C₁₆H₁₆FS: 297.0510. Found: 297.0720.

Control experiments.

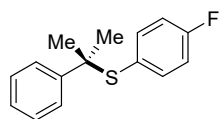


During the reaction of 1-(4-fluorophenyl)ethanol with thiol **2**, we observed the formation of 4-fluorostyrene in ~8 % yield detected by GC-MS (eq 1). Similar elimination product can also be found in reaction of tertiary benzyl alcohol (2-phenyl-2-propanol) with thiol **2** (eq 2). These findings may suggest the occurrence of an E1 reaction, which would compete with an S_N1 reaction. The formation of styrene supported a possible elimination of carbocation intermediate, which can be promoted by Cu(OTf)₂ in DCM (or DCE) at 25°C or elevated temperatures. Moreover, 2-phenyl-3-butyne-2-ol, 1-phenylethanol, 1-(4-methylphenyl)ethanol, 1-(4-methoxyphenyl)ethanol, 1,2,3,4-tetrahydro-1-naphthol and so on were subjected to the reaction conditions in the presence of thiol **2** to check for a possible E1 reaction. As the result, no elimination was observed. Moreover, in the presence of radical inhibitors such as BHT, the reactions were not inhibited, which exhibited that long-lived radical intermediates might not be involved in the reaction processes. All these above suggested that the S_N1 reaction was the most possible mechanism taking place under these conditions.

II. Spectral Data for New Compounds

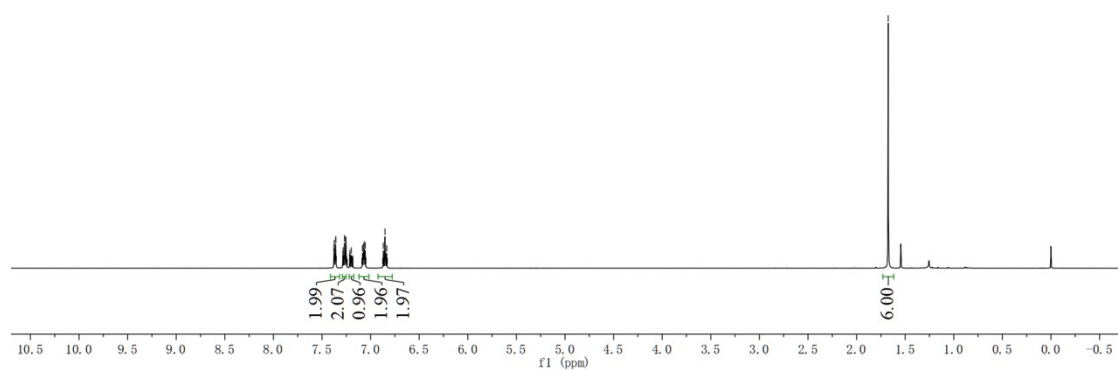
1. NMR Data for New Compounds

A021-155-2-10-61
PROTON CDCl3

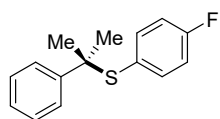


3

¹H NMR(500 MHz, CDCl₃)

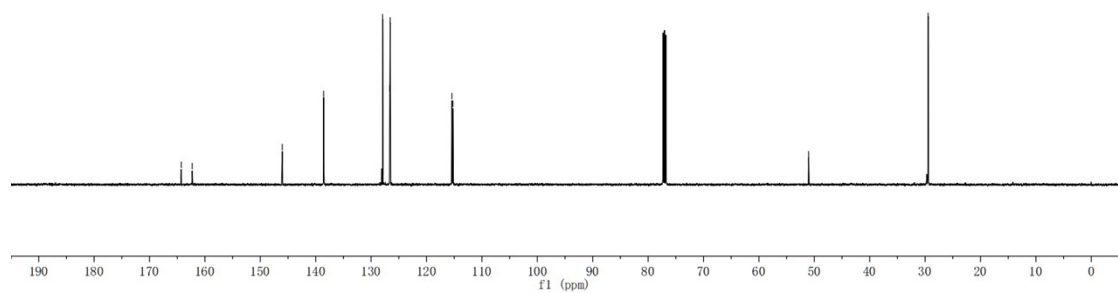


A021-155-3-C-11.fid
C13CPD CDCl3 E:\ \ CCY 30

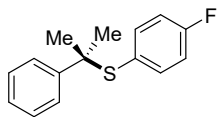


3

¹³C NMR(126 MHz, CDCl₃)

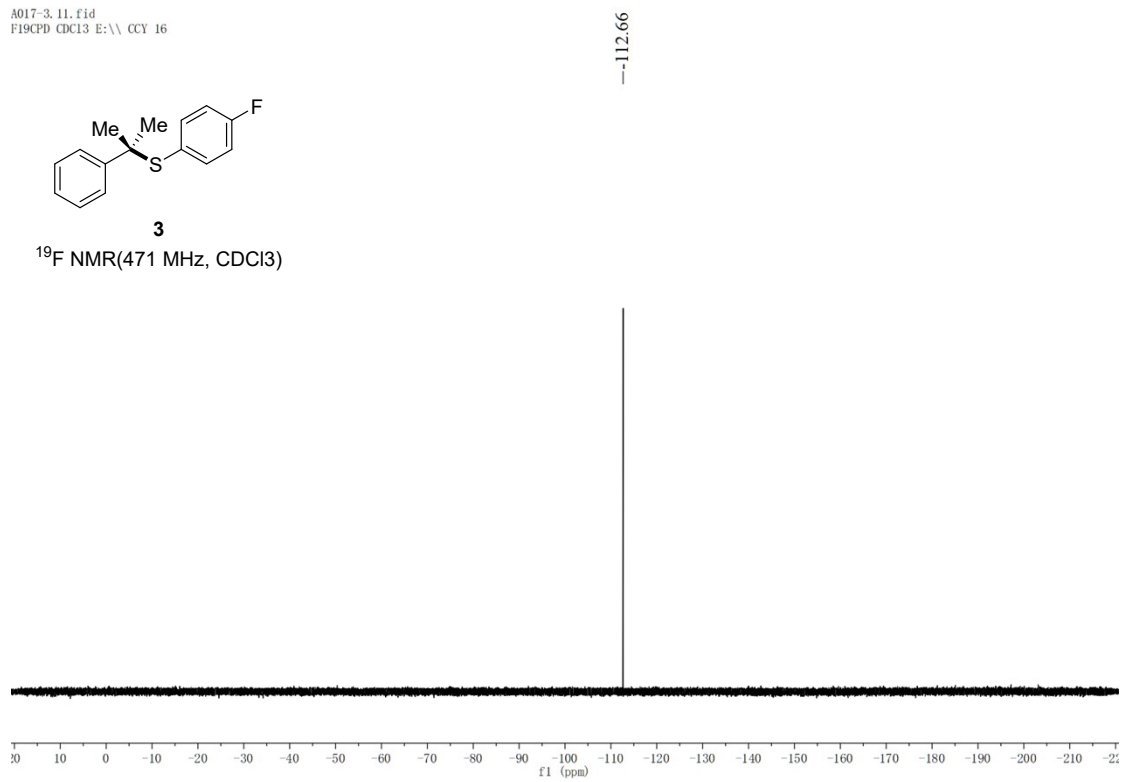


A017-3.11.fid
F19CPD CDCl3 E:\\ CCY 16



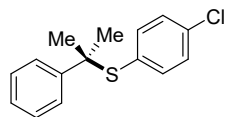
3

¹⁹F NMR(471 MHz, CDCl₃)



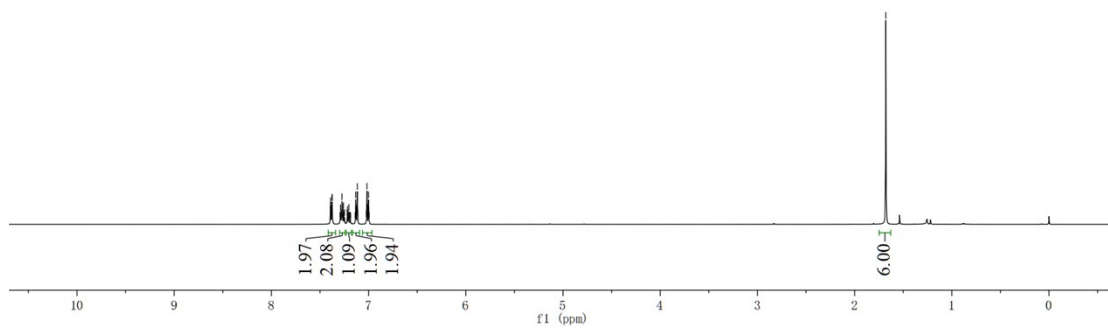
7.62
7.61
7.56
7.55
7.53
7.52
7.51
7.49
7.48
7.29
7.27
7.26
7.26
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7.12
7.11
7.11
7.02
7.02
7.01
7.00
7.00
7.00

-1.68



4

¹H NMR(500 MHz, CDCl₃)

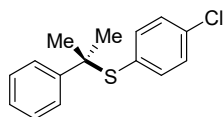


A021-162-3-C.11.fid
C13CPD CDCl3 E:\ \ CCY 2

-146.00
137.62
134.97
131.37
128.44
127.98
126.69
126.57

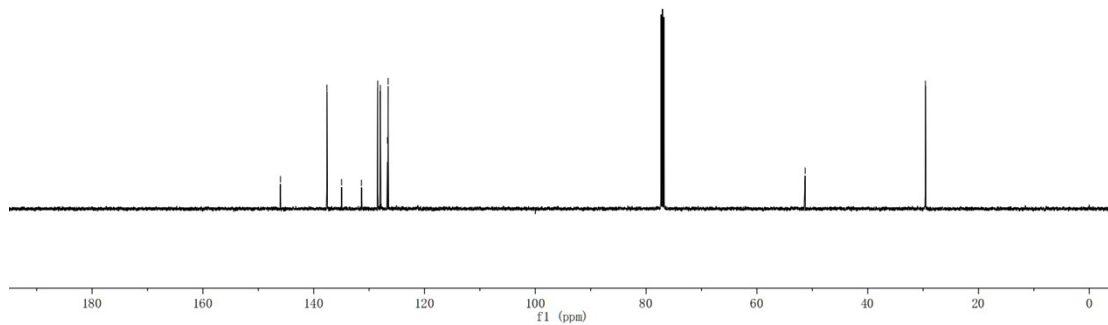
-51.28

-29.59



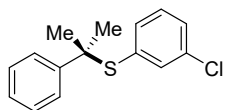
4

¹³C NMR(126 MHz, CDCl₃)



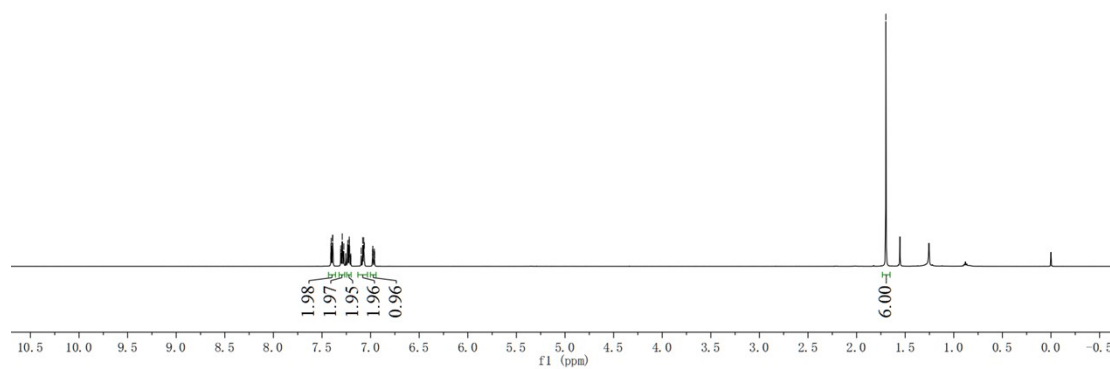
7.17
7.16
7.15
7.14
7.13
7.12
7.11
7.10
7.09
7.08
7.07
7.06
7.05
7.04
7.03
7.02
7.01
7.00
6.99
6.98
6.97
6.96
6.95

-1.70



5

¹H NMR(500 MHz, CDCl₃)



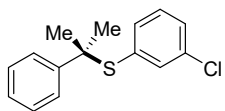
A017-101-2.11.fid
C13CPD CDCl3 E:\ \ CCY 7

149.64
148.07
146.55

129.70
127.86
126.80
126.38
123.89
119.08
110.52

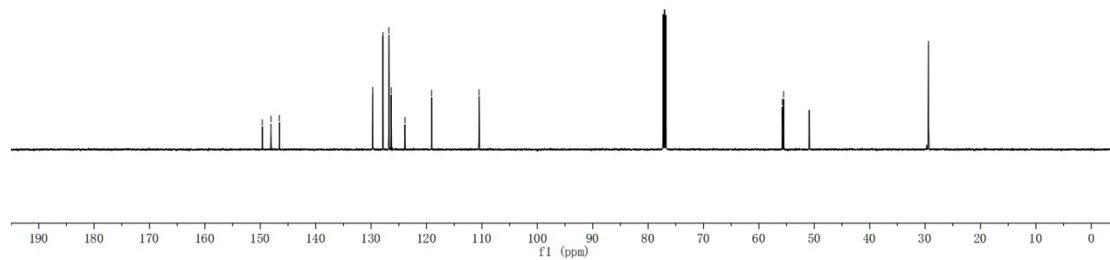
55.77
55.54

29.38

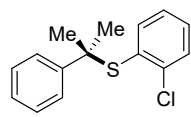


5

¹³C NMR(126 MHz, CDCl₃)

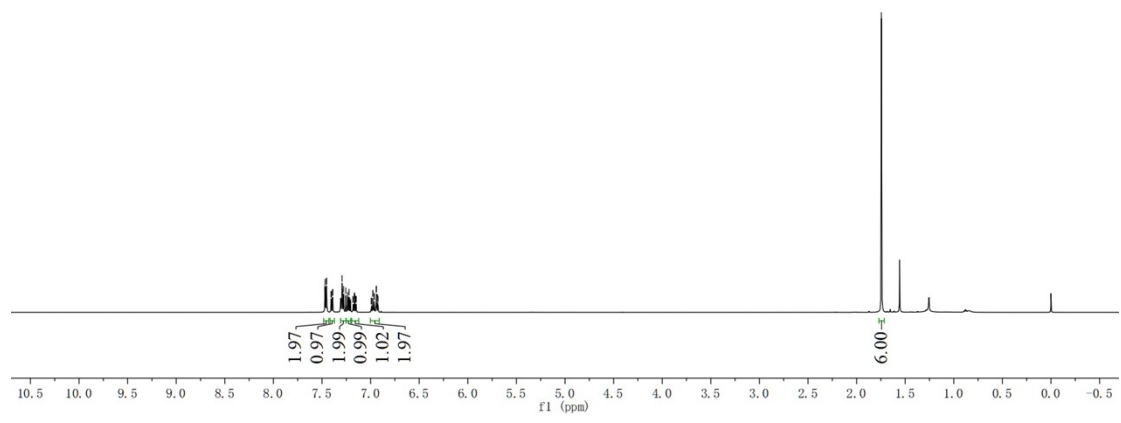


A017-101-1.10.fid
 PROTON CDCl3 E:\ \ CCY 14

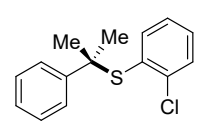


6

¹H NMR(500 MHz, CDCl₃)

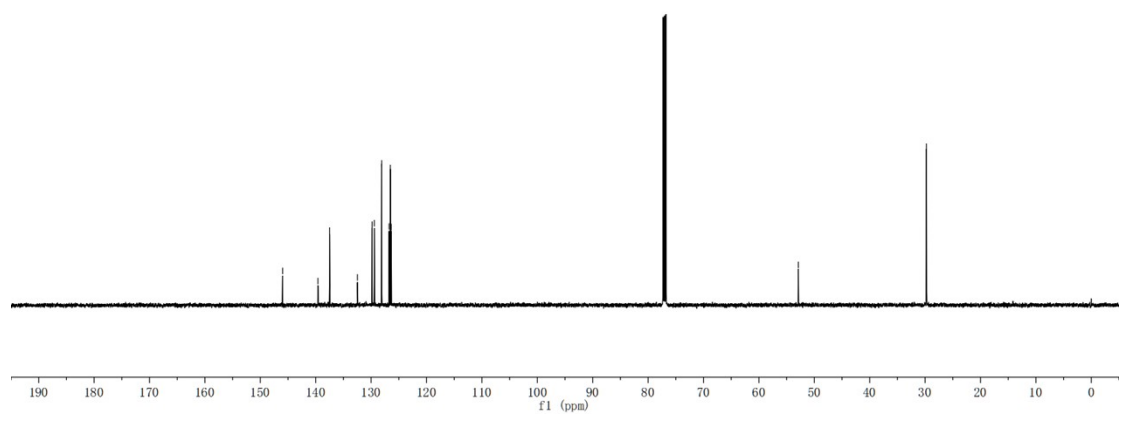


A017-101-1.11.fid
 C13CPD CDCl3 E:\ \ CCY 14

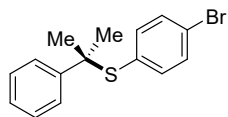


6

¹³C NMR(126 MHz, CDCl₃)

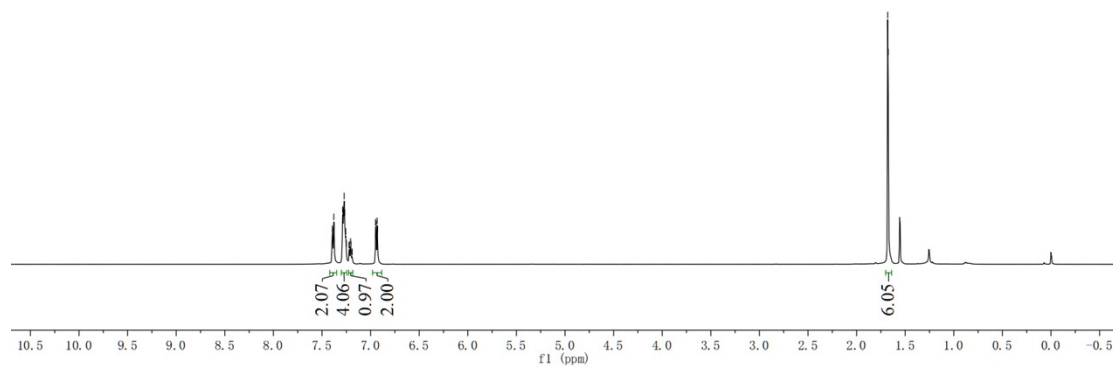


A017-102-3.10.fid
PROTON CDCl3 E:\

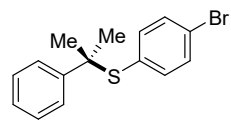


7

¹H NMR(500 MHz, CDCl₃)

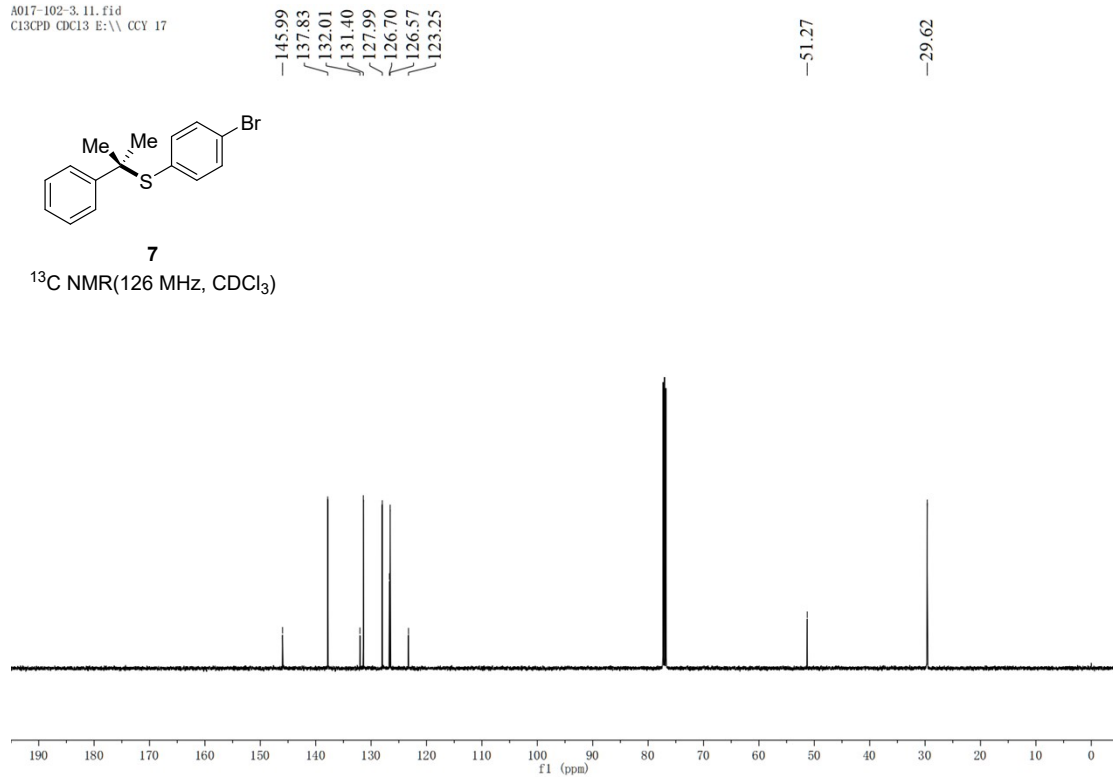


A017-102-3.11.fid
C13CPD CDCl3 E:\



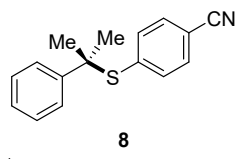
7

¹³C NMR(126 MHz, CDCl₃)

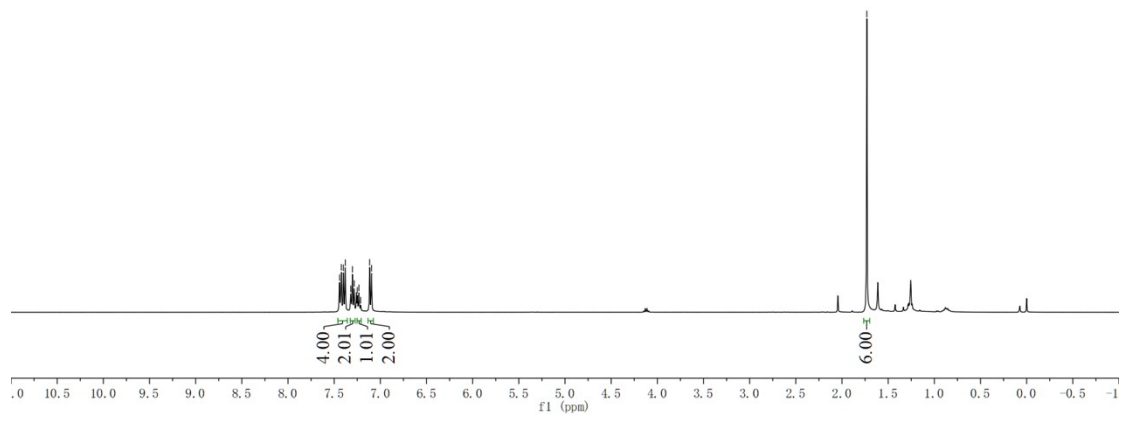


A017-131-7.1.fid
 PROTON CDCl3 (D:\20210804) root 38
 7.44
 7.42
 7.40
 7.38
 7.32
 7.30
 7.28
 7.25
 7.23
 7.21
 7.12
 7.10

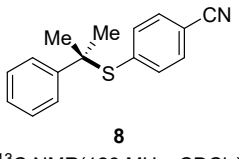
-1.73



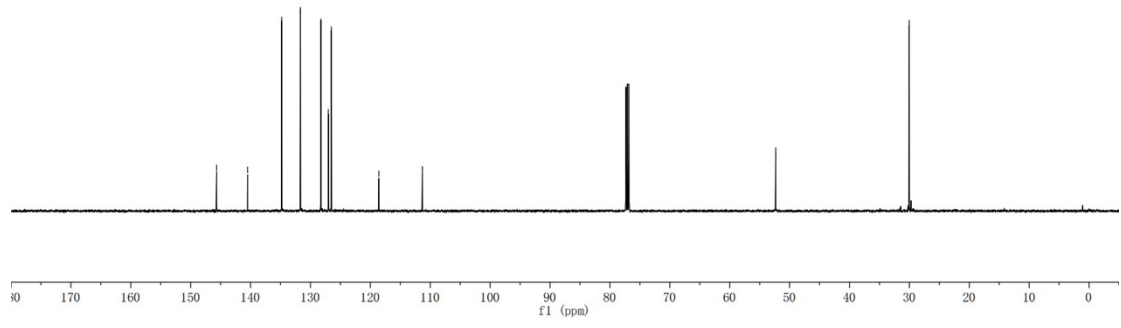
¹H NMR(500 MHz, CDCl₃)

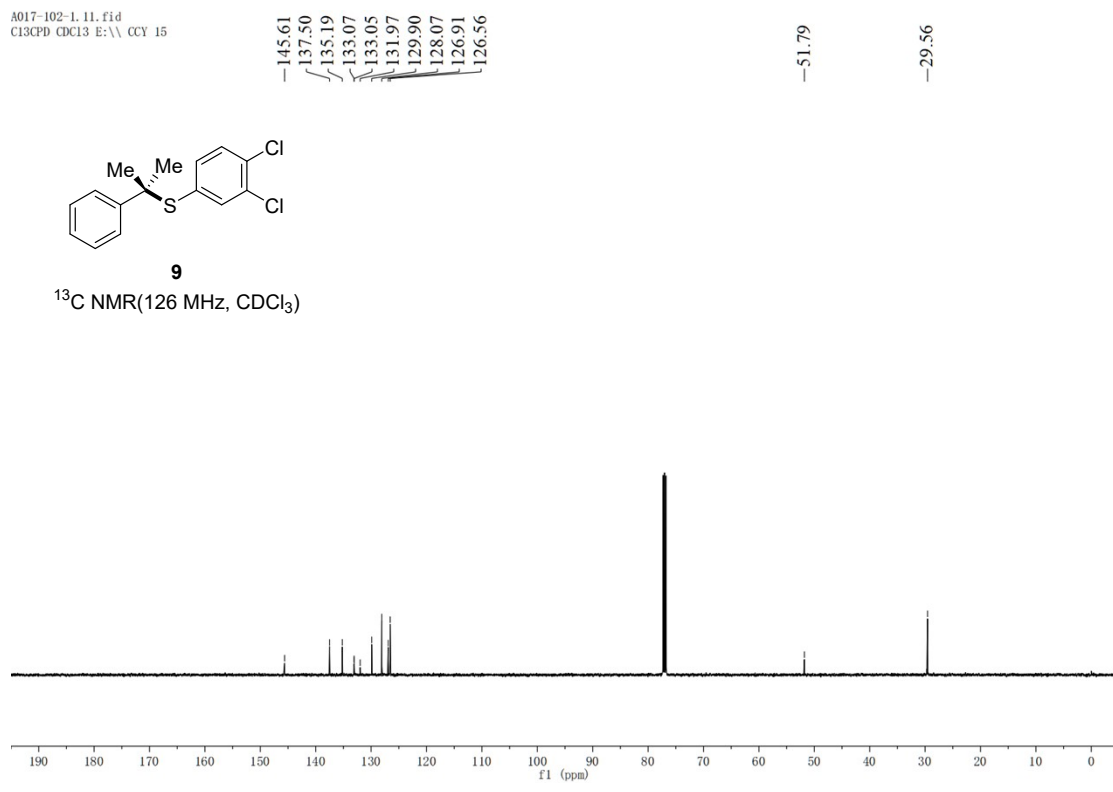
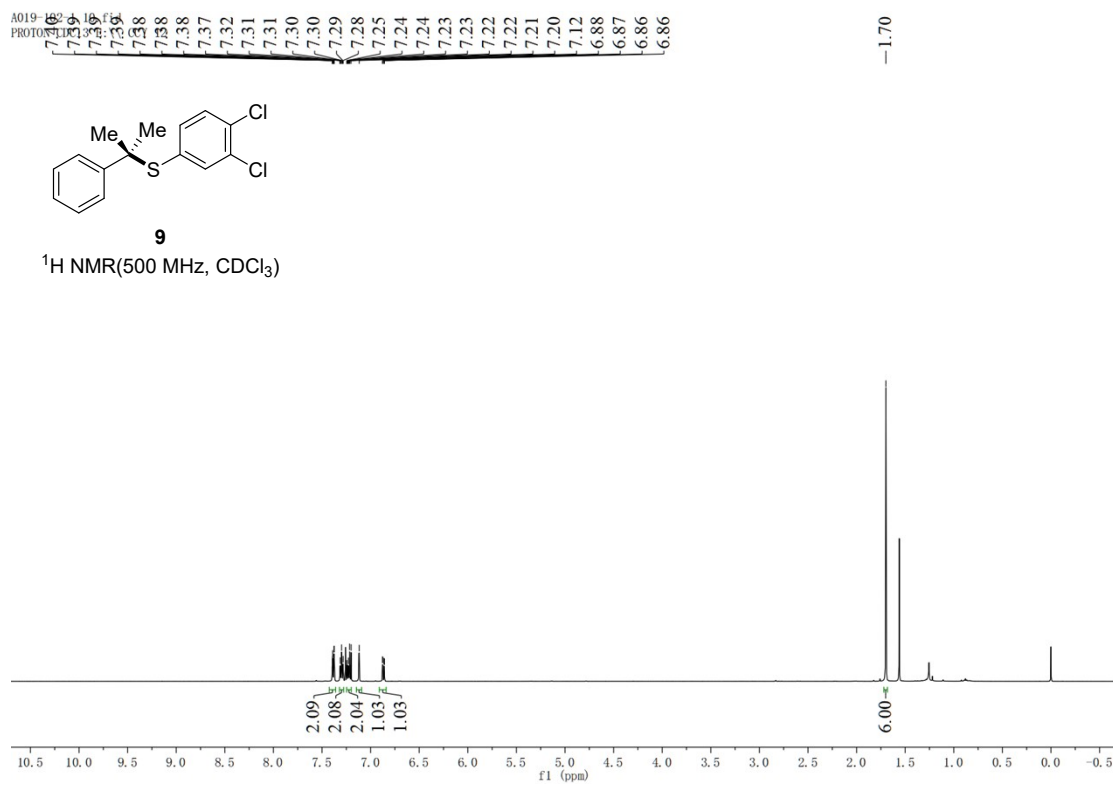


A017-8B.10.fid
 C13CPD CDCl3 E:\ \ CCY 38
 145.67
 140.50
 134.81
 131.66
 128.27
 127.01
 126.51
 -118.58
 -111.30
 -52.31
 -30.03



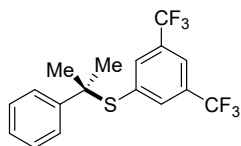
¹³C NMR(126 MHz, CDCl₃)





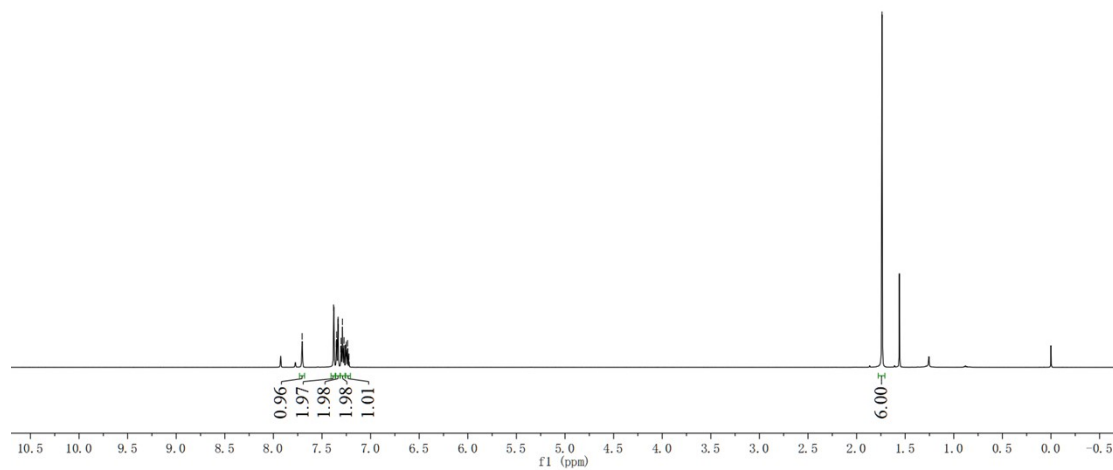
A017-103-4.10.fid
 PROTON CDCl3 E:\ \ 7.30
 7.28
 7.35
 7.34
 7.34
 7.33
 7.31
 7.30
 7.30
 7.29
 7.28
 7.27
 7.25
 7.24
 7.24
 7.23
 7.22

-1.74



10

¹H NMR(500 MHz, CDCl₃)

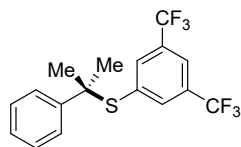


A017-103-4.11.fid
 C13CPD CDCl3 E:\ \ CCY 8

144.92
 136.35
 135.49
 131.45
 131.19
 128.24
 127.21
 126.49
 123.94
 121.98
 121.95
 121.92
 121.76

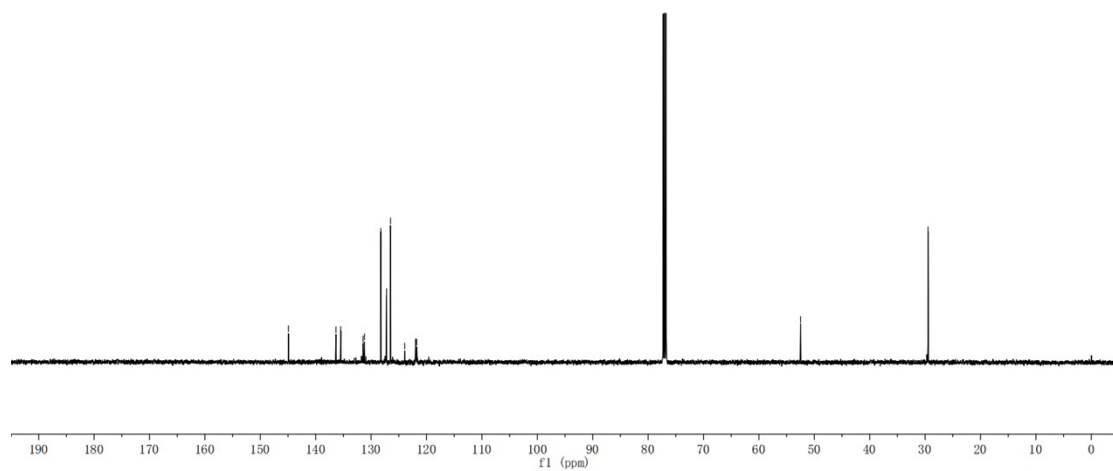
-52.48

-29.47

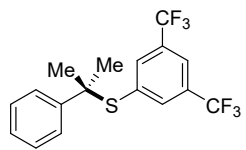


10

¹³C NMR(126 MHz, CDCl₃)



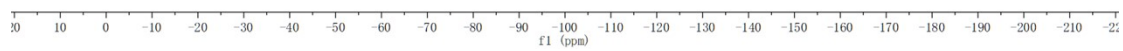
A017-10.11.fid
F19CPD CDCl3 E:\\ CCY 6



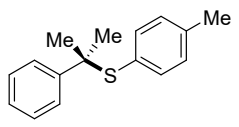
10

¹⁹F NMR(471 MHz, CDCl₃)

-63.12

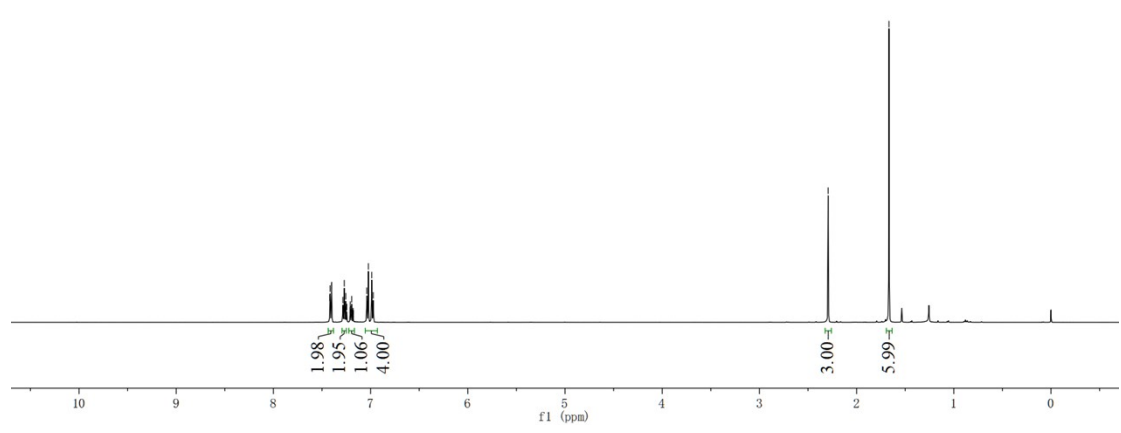


A021-162-2.10.F1d
 PROTON CDCl3 E:\CCY 7

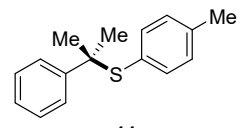


11

¹H NMR(500 MHz, CDCl₃)

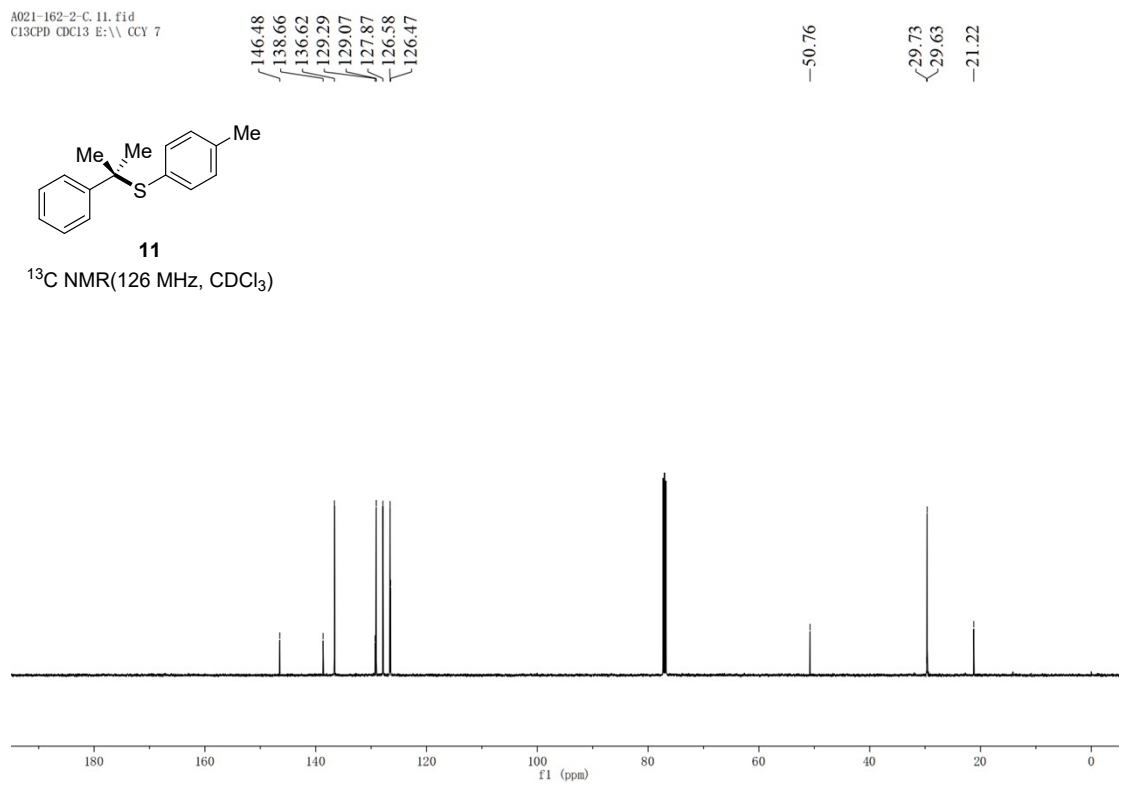


A021-162-2-C.11.f1d
 C13CPD CDCl3 E:\CCY 7



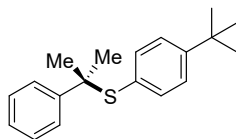
11

¹³C NMR(126 MHz, CDCl₃)



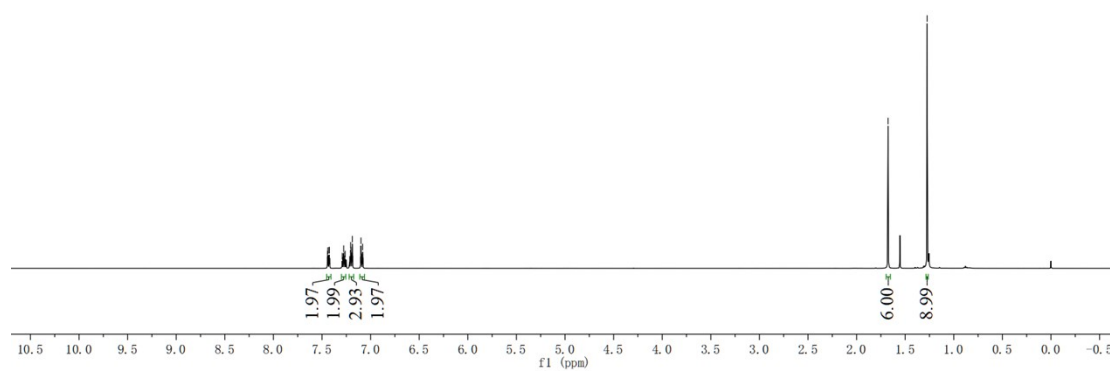
A017-103-5.11.fid
 PROTON
 7.54
 7.53
 7.44
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 7.29
 7.28
 7.27
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 7.19
 7.19
 7.18
 7.10
 7.10
 7.09
 7.08
 7.08

-1.68
 -1.27



12

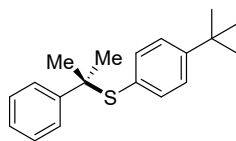
¹H NMR(500 MHz, CDCl₃)



A017-103-5.11.fid
 C13CPD CDCl3 E:\CCY 8

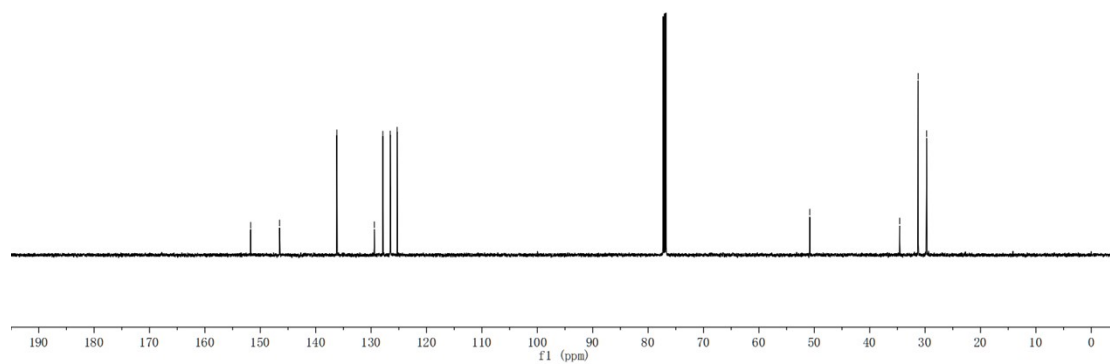
-151.73
 -146.52
 136.19
 129.42
 127.88
 126.54
 126.48
 125.30

-50.82
 34.59
 31.25
 29.73

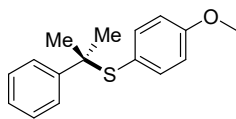


12

¹³C NMR(126 MHz, CDCl₃)

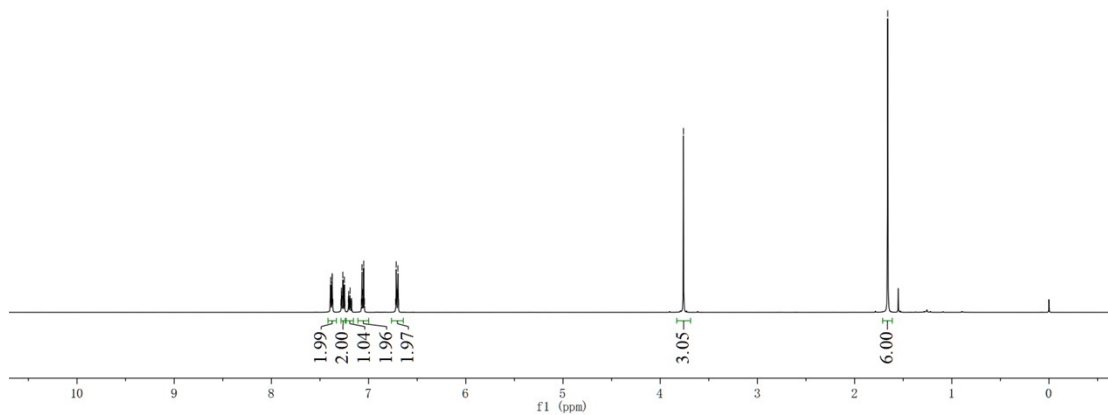


A017-162-1-C-11.fid
 PROTON CDCl3
 7.36
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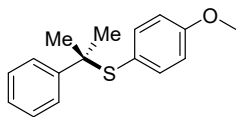
13

¹H NMR(500 MHz, CDCl₃)



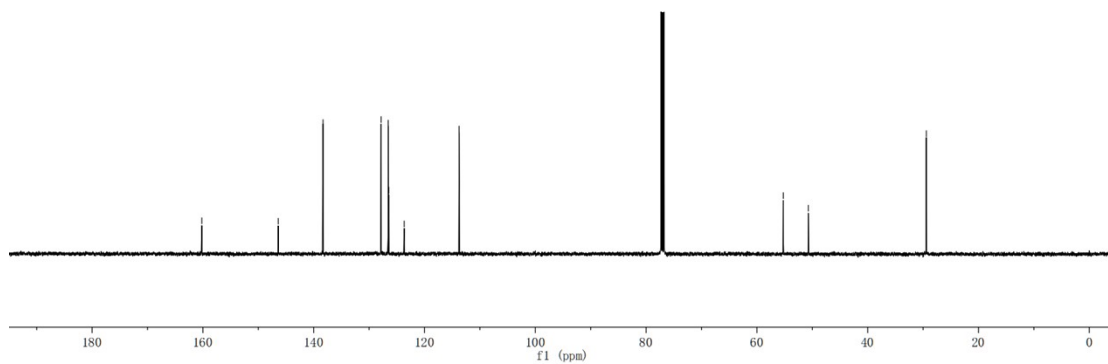
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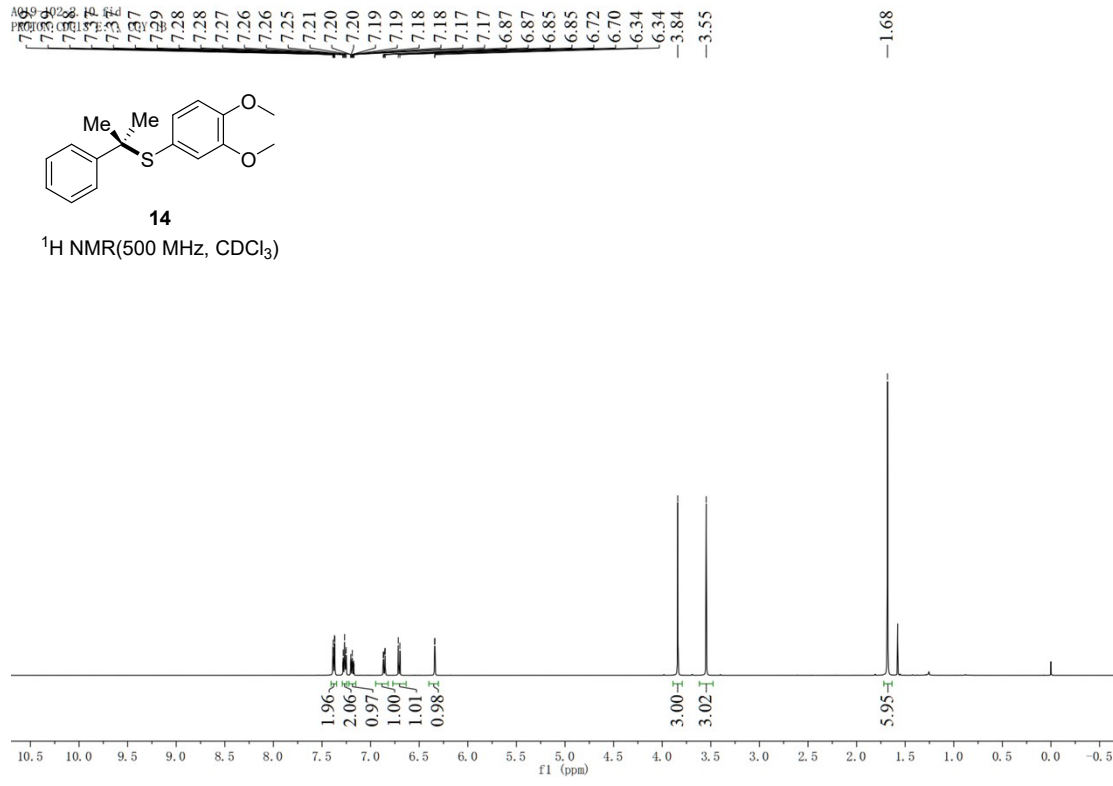
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 146.39
 138.31
 127.84
 126.55
 126.44
 123.66
 113.76
 55.23
 50.73
 29.42



13

¹³C NMR(126 MHz, CDCl₃)





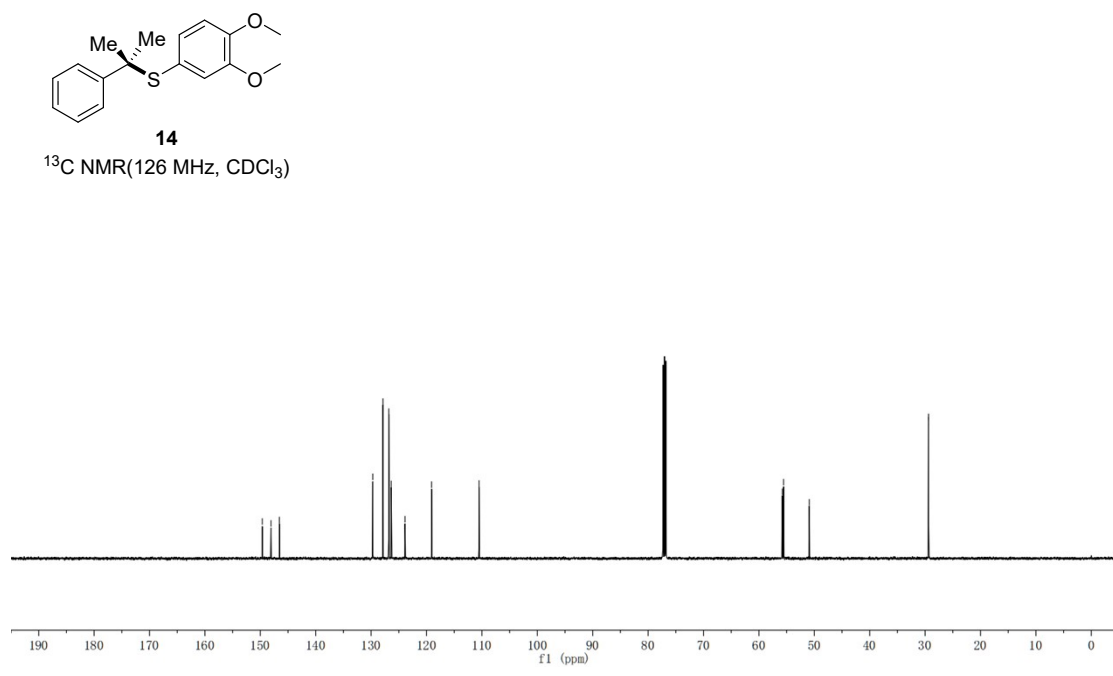
A017-102-2.11.fid
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149.64
 148.07
 146.55

129.70
 127.86
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 126.37
 123.88
 119.08
 110.52

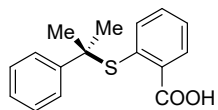
55.77
 55.54
 50.91

29.37



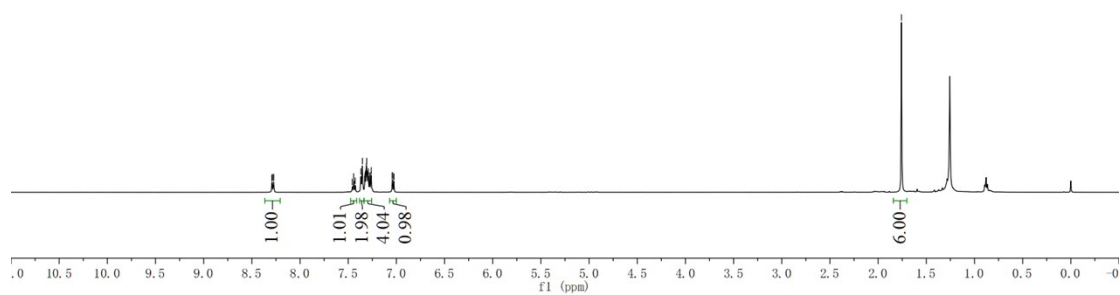
A017-103-2.10.fid
PROTON CDCl3 E:\ \ CCY 11

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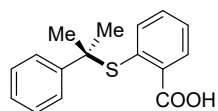
15

¹H NMR(500 MHz, CDCl₃)



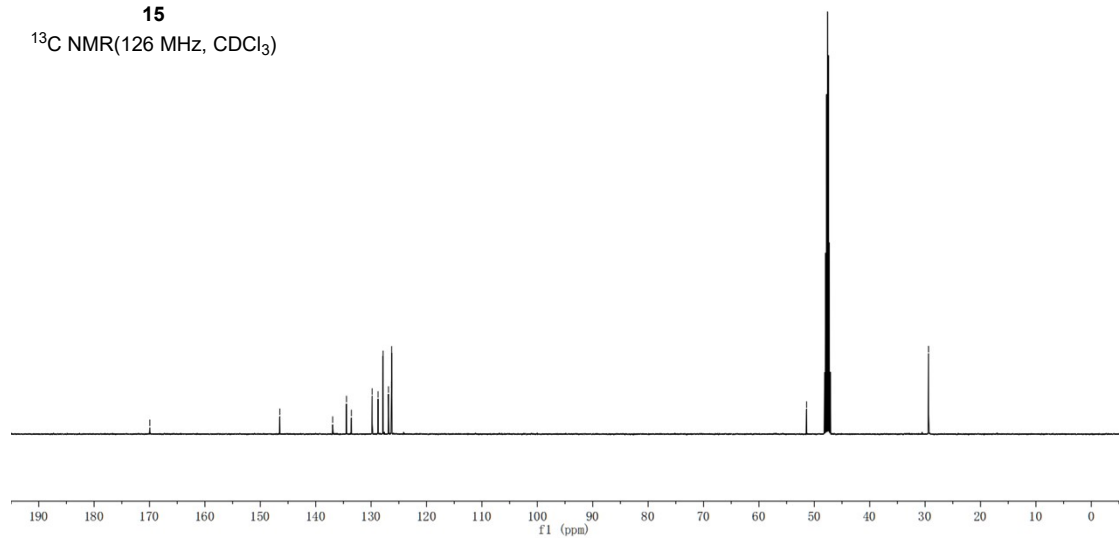
A017-103-2.11.fid
C13CPD Me00 E:\ \ CCY 11

169.94
146.48
136.93
134.45
133.56
129.81
128.75
127.84
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126.32
126.29
-51.39
-29.37

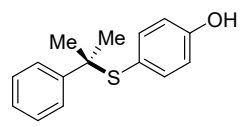


15

¹³C NMR(126 MHz, CDCl₃)

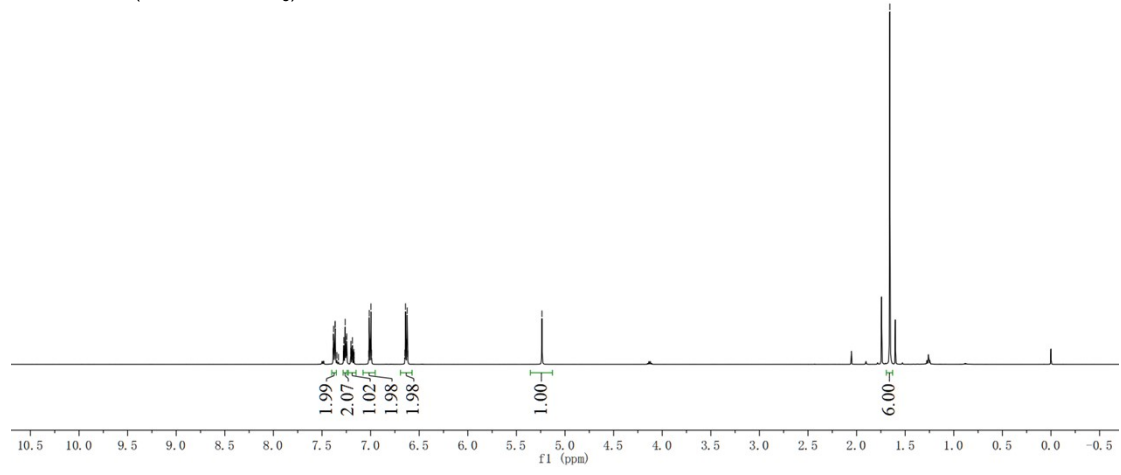


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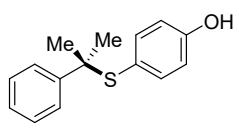
16

¹H NMR(500 MHz, CDCl₃)



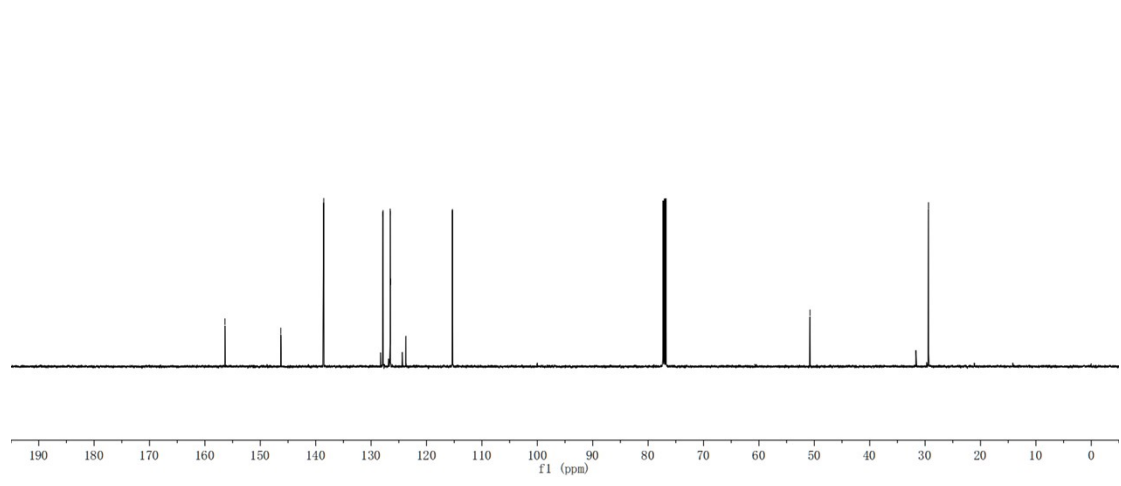
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146.30
138.56
127.85
126.55
126.47
115.32
50.77
29.38



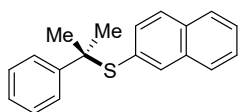
16

¹³C NMR(126 MHz, CDCl₃)



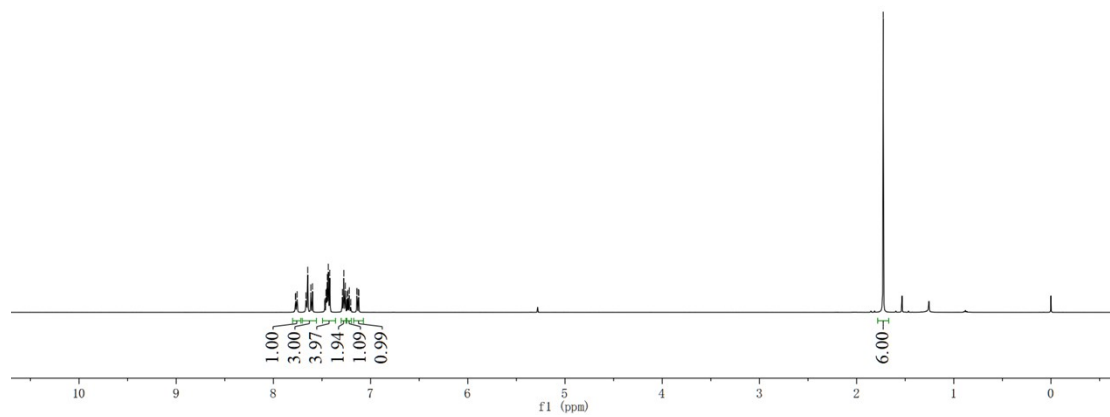
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 7.14
 7.12
 7.12

-1.73



17

¹H NMR(500 MHz, CDCl₃)

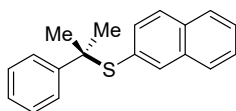


A021-165-1-C.11.fid
 C13CPD CDCl₃ E:\ \ CCY 9

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 -146.41
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 -133.24
 -133.18
 -132.97
 -130.37
 -127.96
 -127.87
 -127.52
 -126.65
 -126.60
 -126.55
 -126.11

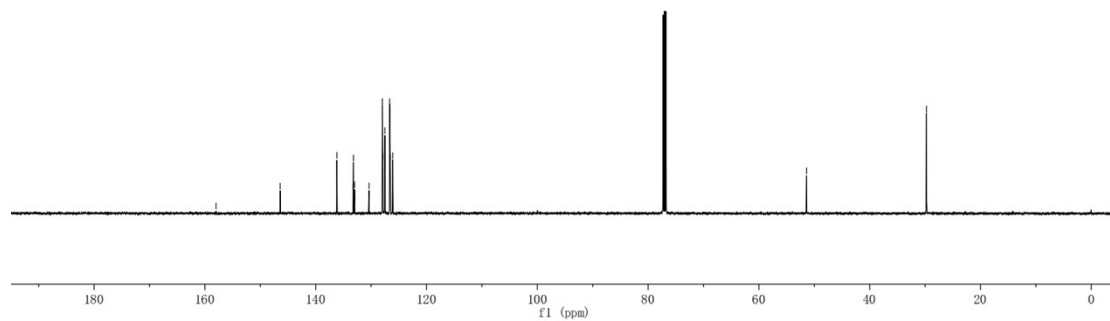
-51.38

-29.76

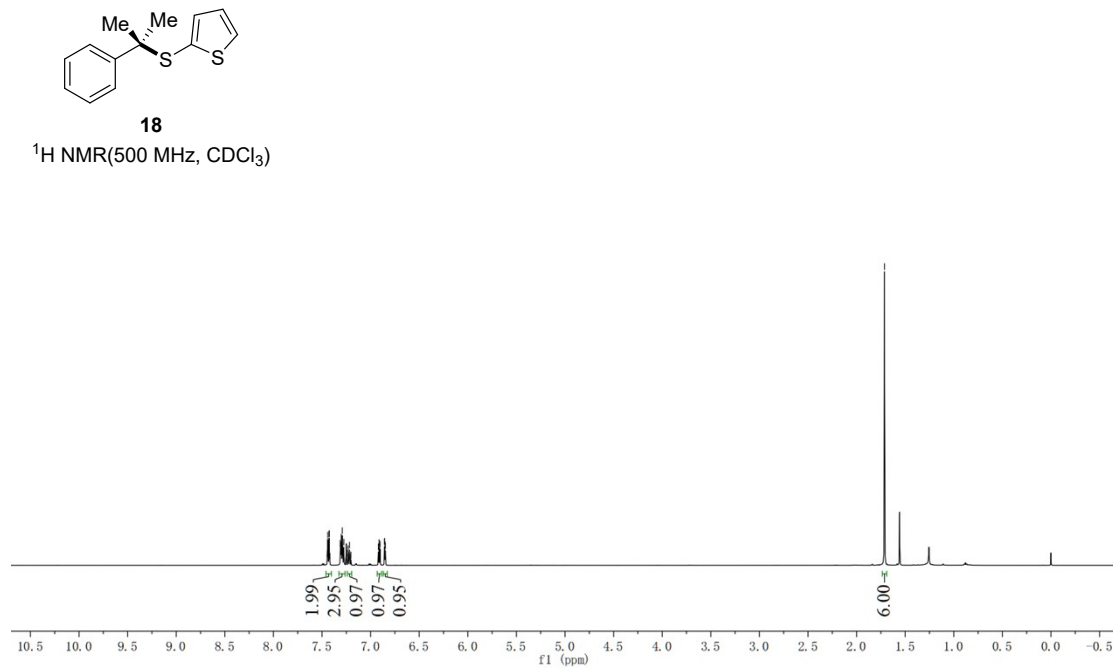


17

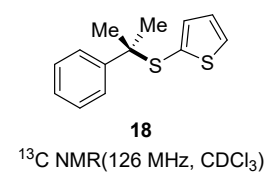
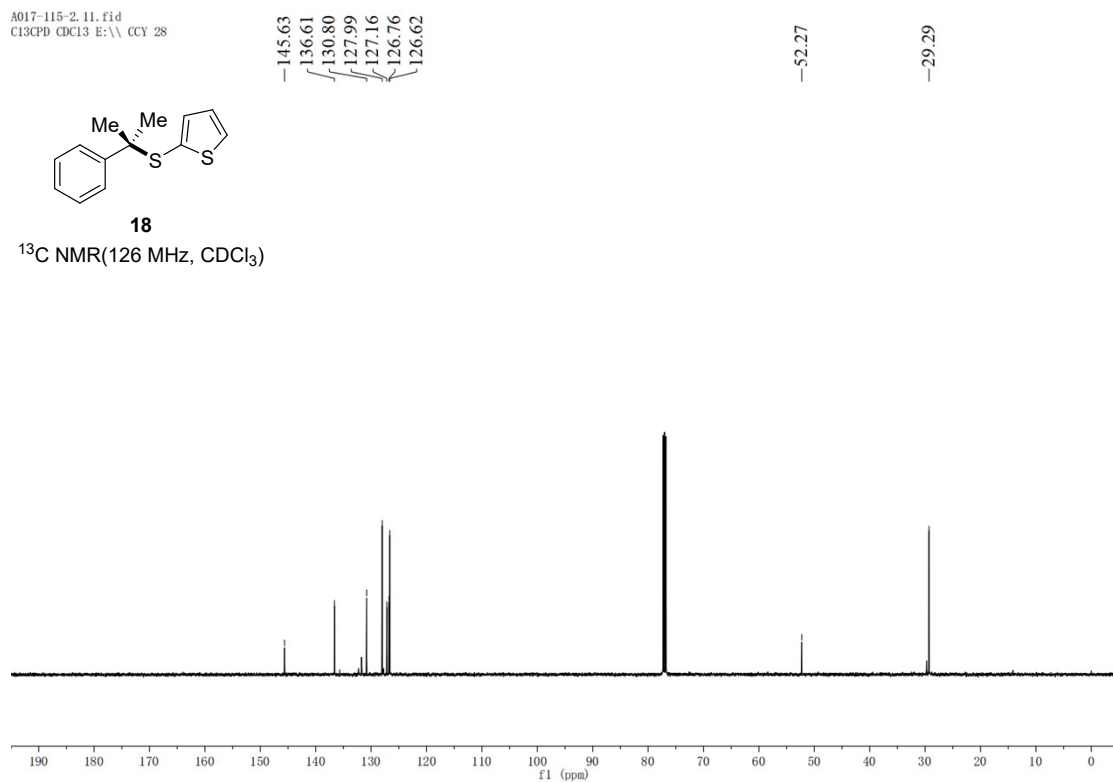
¹³C NMR(126 MHz, CDCl₃)



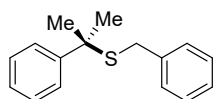
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 PROTONS CDCl3



A017-115-2.11.fid
 C13CPD CDCl3 E:\ \ CCY 28

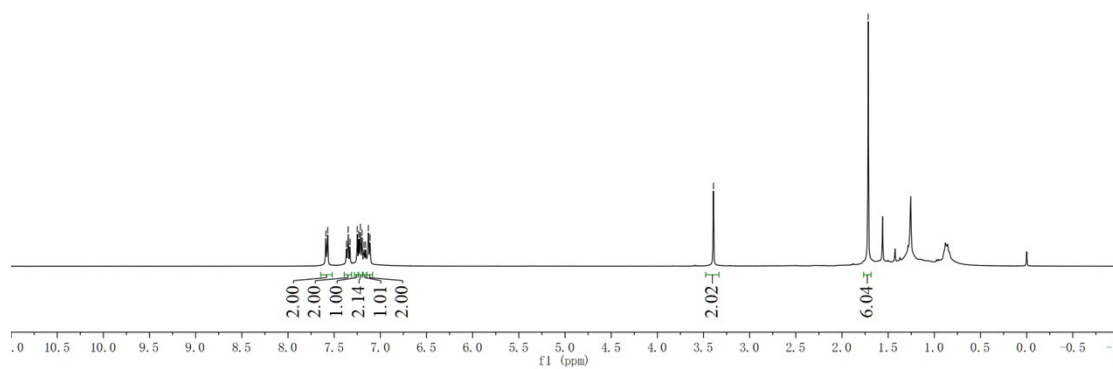


A017-131-8.1.fid
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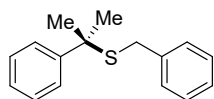


19

¹H NMR(500 MHz, CDCl₃)

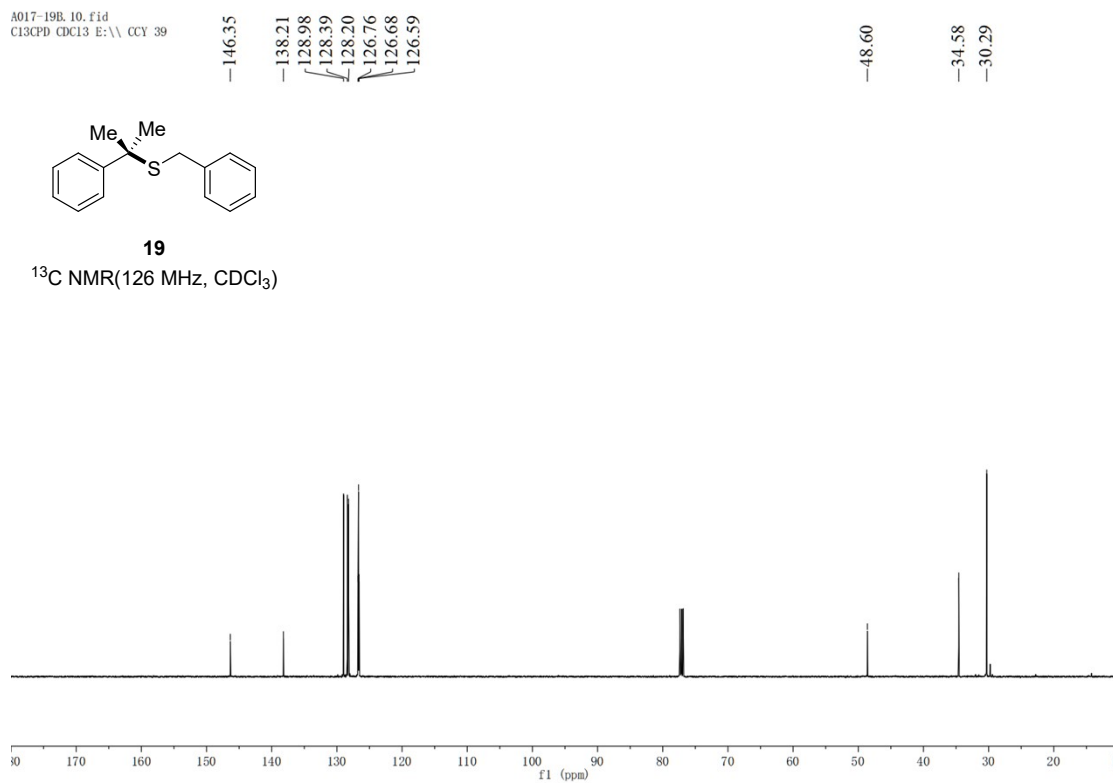


A017-19B.10.fid
C13CPD CDCl3 E:\ \ CCY 39

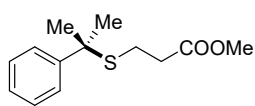


19

¹³C NMR(126 MHz, CDCl₃)

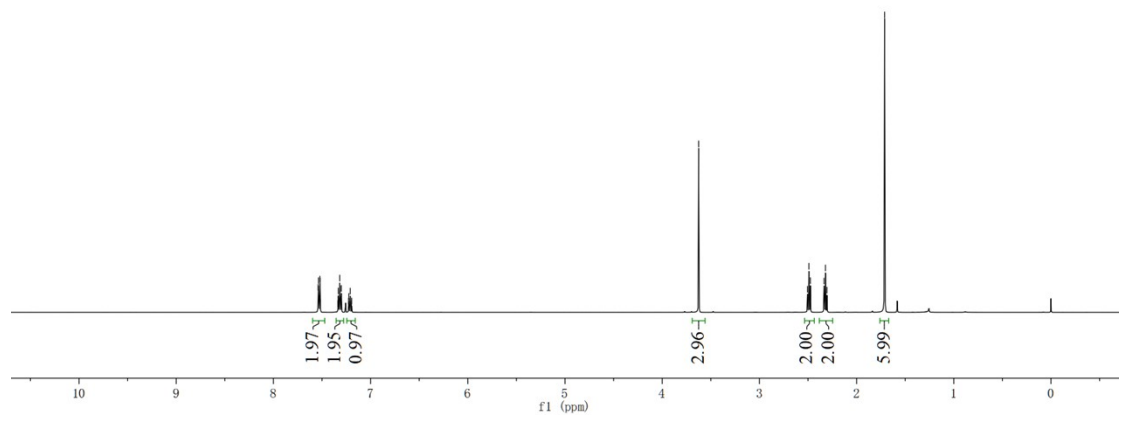


A021-160-3-10.fid
 PROTON CDCl3 E:\ \

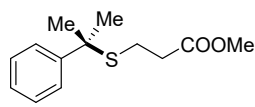


20

¹H NMR(500 MHz, CDCl₃)

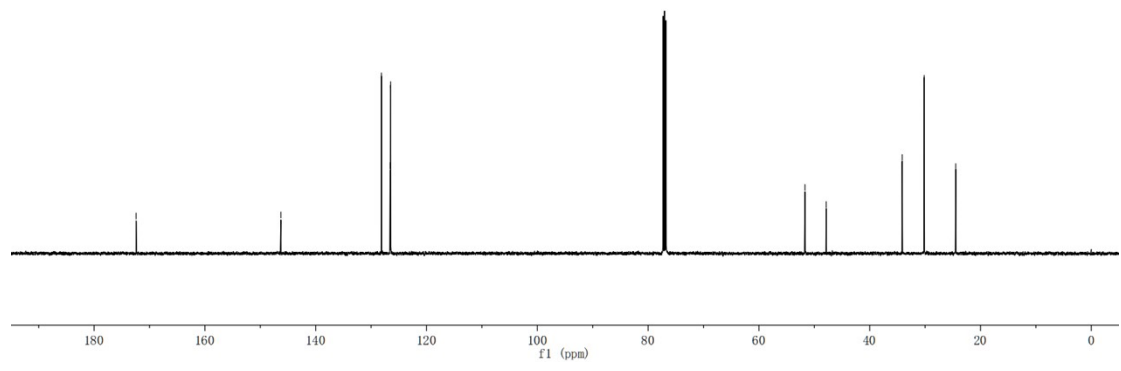


A021-160-3-C-11.fid
 C13CPD CDCl3 E:\ \



20

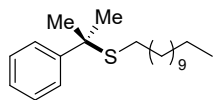
¹³C NMR(126 MHz, CDCl₃)



A021-160-2.10.fid
PROTON CDCl3 E:\ \ CCY 11

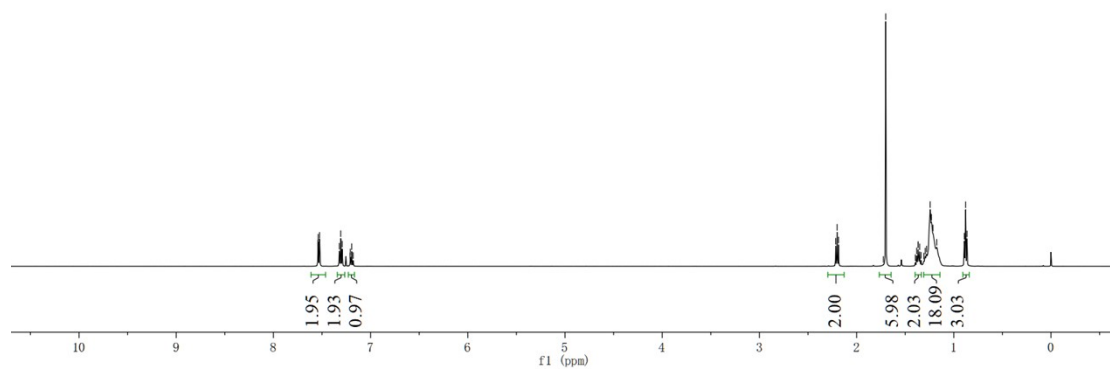
7.54
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0.86



21

¹H NMR(500 MHz, CDCl₃)

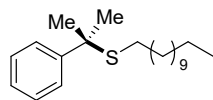


A021-160-2-C.11.fid
C13CPD CDCl3 E:\ \ CCY 46

146.83

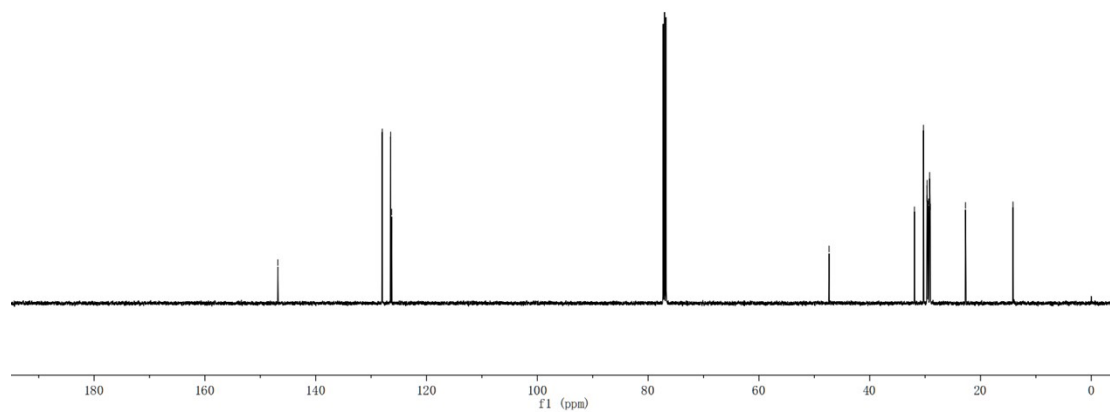
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47.34
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29.07
22.70
14.13

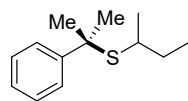


21

¹³C NMR(126 MHz, CDCl₃)

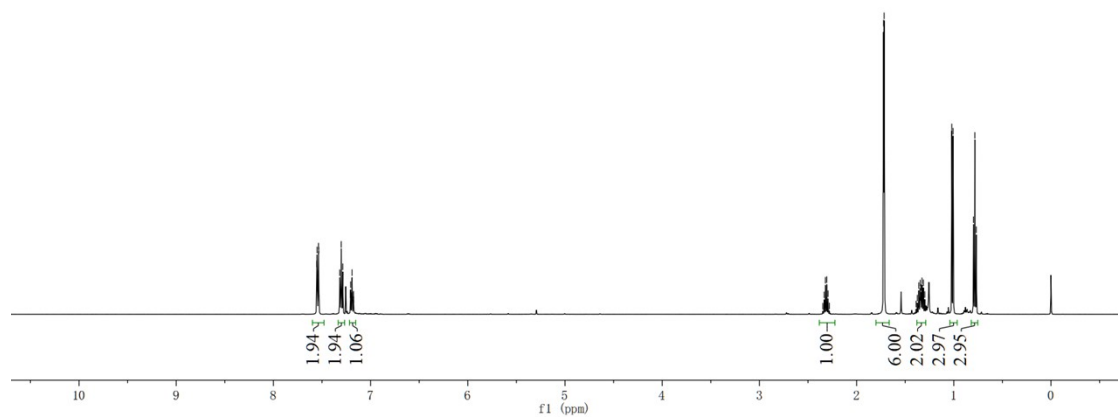


A021-160-1.10.f44
 PROTON CDCl3 E:\ \ CCY 45

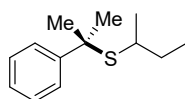


22

¹H NMR(500 MHz, CDCl₃)

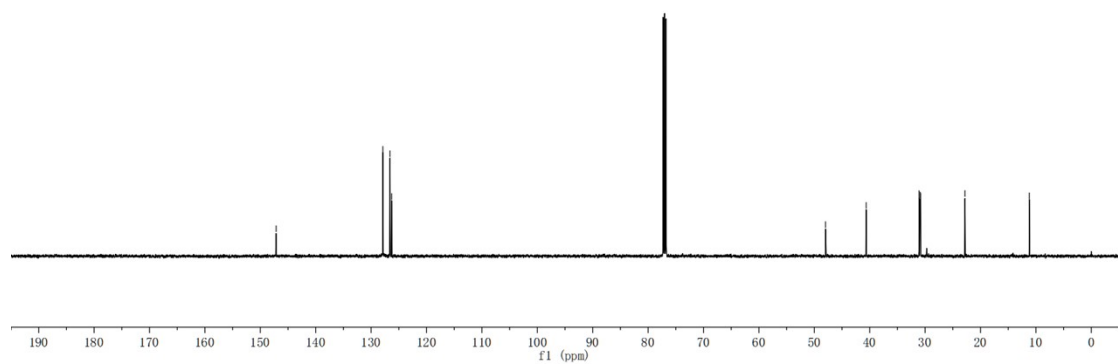


A021-160-1-C.11.fid
 C13CPD CDCl3 E:\ \ CCY 45



22

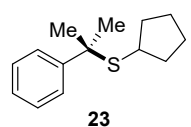
¹³C NMR(126 MHz, CDCl₃)



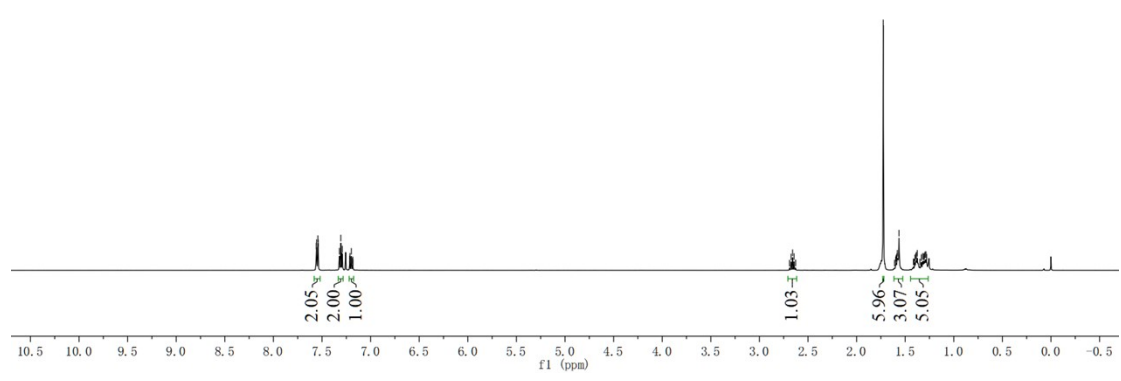
A017-115-3.10.fid
PROTON CDCl3 E:\ \ CCY

7.56
7.56
7.55
7.54
7.54
7.32
7.32
7.31
7.29
7.29
7.22
7.21
7.21
7.20
7.19
7.18
7.18

2.69
2.67
2.66
2.64
2.63
1.73
1.61
1.60
1.59
1.59
1.58
1.56
1.42
1.41
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1.33
1.32
1.31
1.30
1.30
1.28
1.28

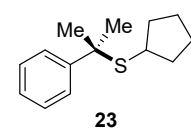


¹H NMR(500 MHz, CDCl₃)

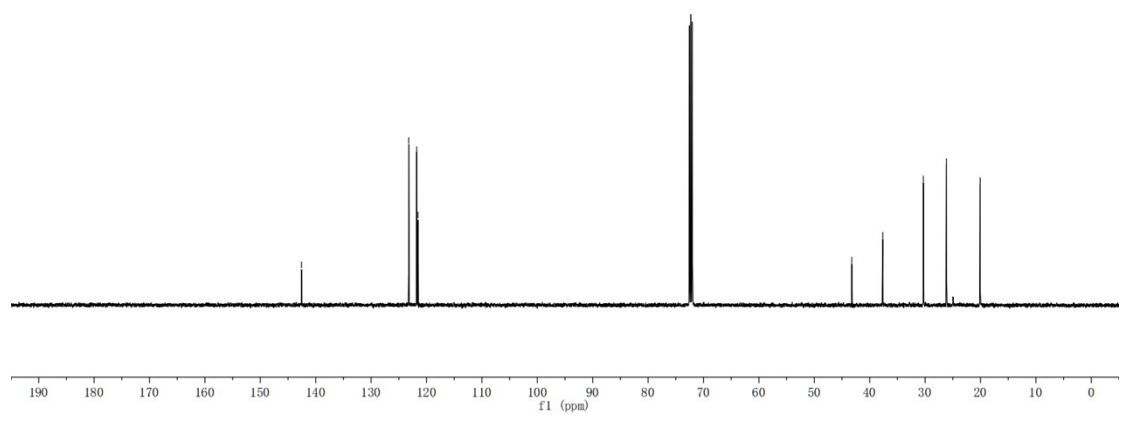


A017-115-3.11.fid
C13CPD CDCl3 E:\ \ CCY 40

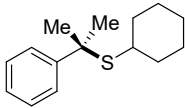
142.56
123.20
121.76
121.54
43.23
37.65
30.31
26.15
20.06



¹³C NMR(126 MHz, CDCl₃)

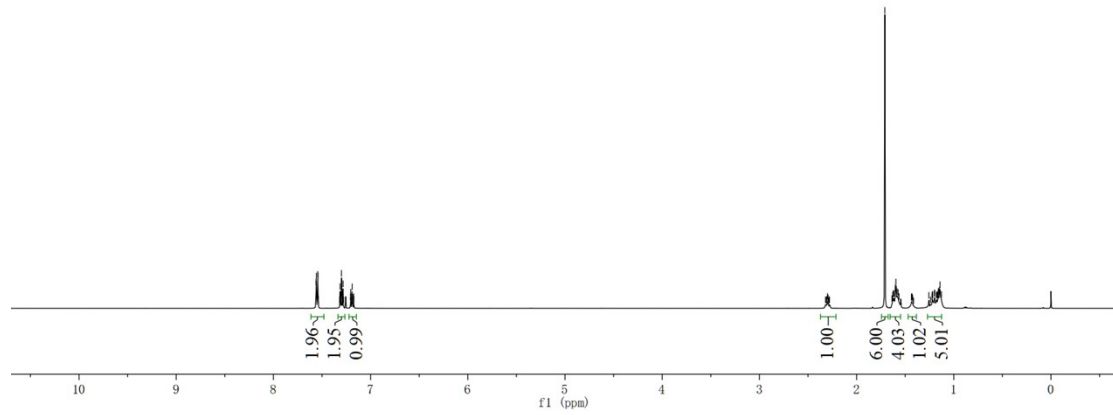


A021-160-5-C.11.fid
 1H NMR (500 MHz, CDCl₃)
 7.16, 7.15, 7.14, 7.13, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13



24

¹H NMR(500 MHz, CDCl₃)



A021-160-5-C.11.fid
 C13CPD CDCl₃ E:\ \ CCY 48

147.25

127.88

126.53

126.27

48.17

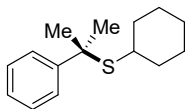
42.49

35.32

30.95

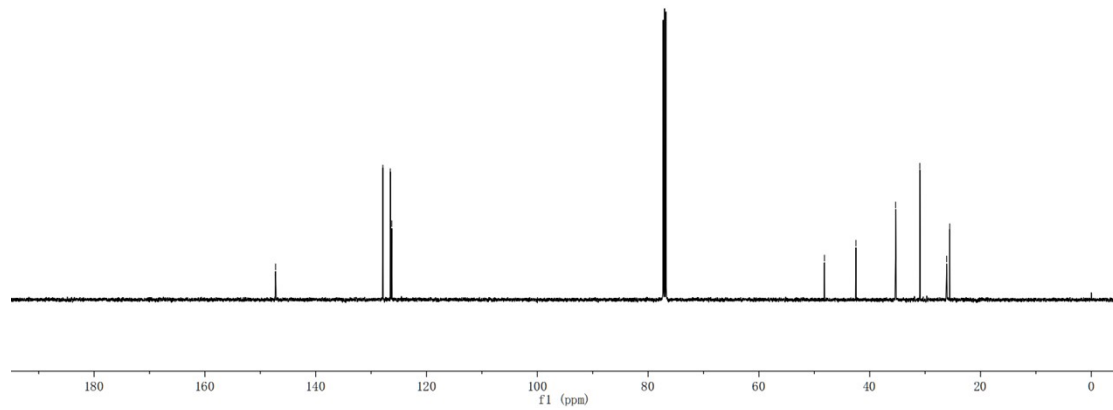
26.12

25.55



24

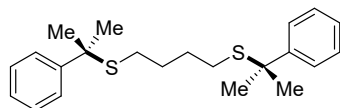
¹³C NMR(126 MHz, CDCl₃)



A021-165-2.10.fid
PROTON CDCl3 E:\ \ CCY 20

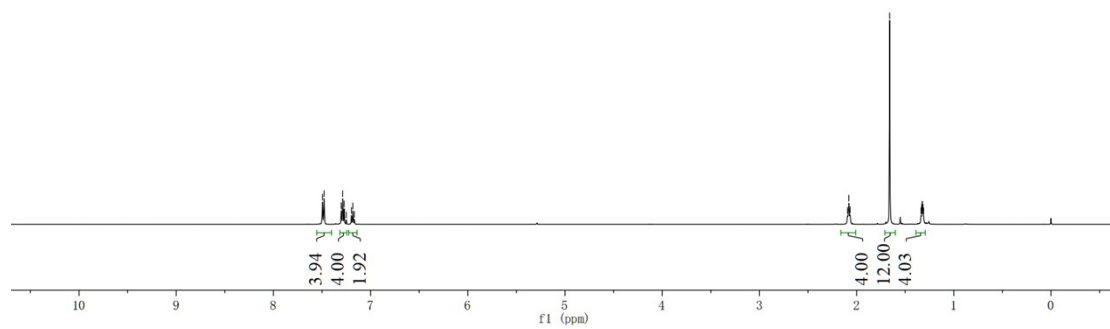
7.49
7.48
7.30
7.29
7.27
7.25
7.20
7.18
7.17

2.09
2.08
2.07
1.66
1.34
1.33
1.32
1.31



25

¹H NMR(500 MHz, CDCl₃)



A021-165-2-C.11.fid
C13CPD CDCl3 E:\ \ CCY 10

146.69

128.00

126.44

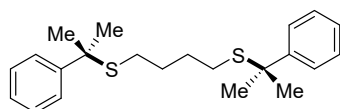
126.33

47.39

30.26

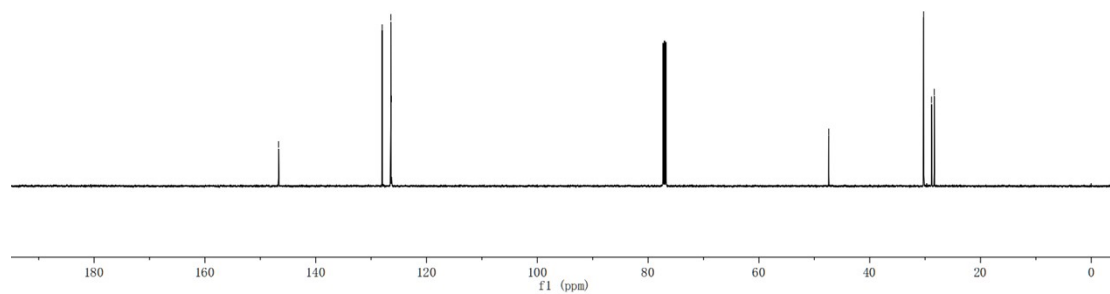
28.83

28.35



25

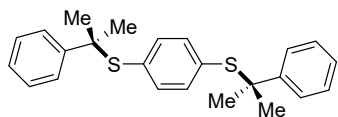
¹³C NMR(126 MHz, CDCl₃)



A021-162-4.10.fid
PROTON CDCl3 E:\ \ CCY 46

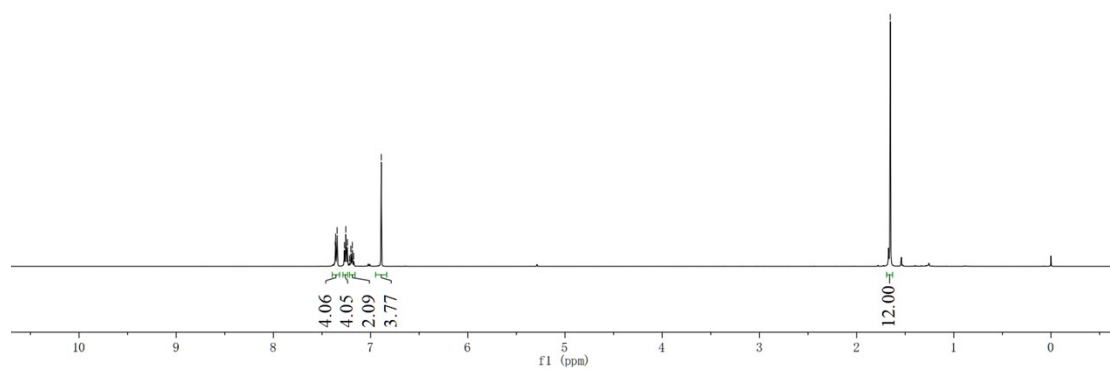
7.36
7.36
7.34
7.27
7.27
7.25
7.24
7.22
7.20
7.19
7.17
6.89

1.65



26

¹H NMR(500 MHz, CDCl₃)

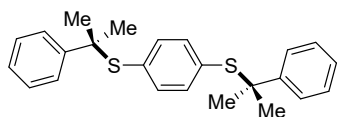


A021-162-4-C.11.fid
C13CPD CDCl3 E:\ \ CCY 22

146.13
135.95
133.60
127.92
126.51

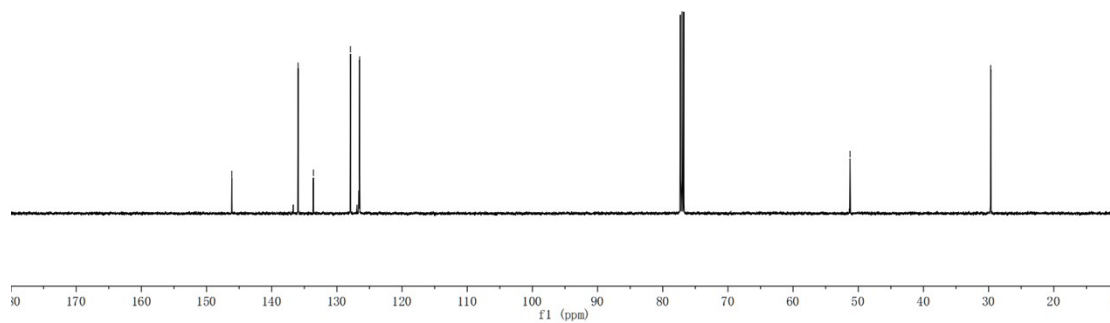
51.26

29.69

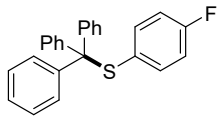


26

¹³C NMR(126 MHz, CDCl₃)

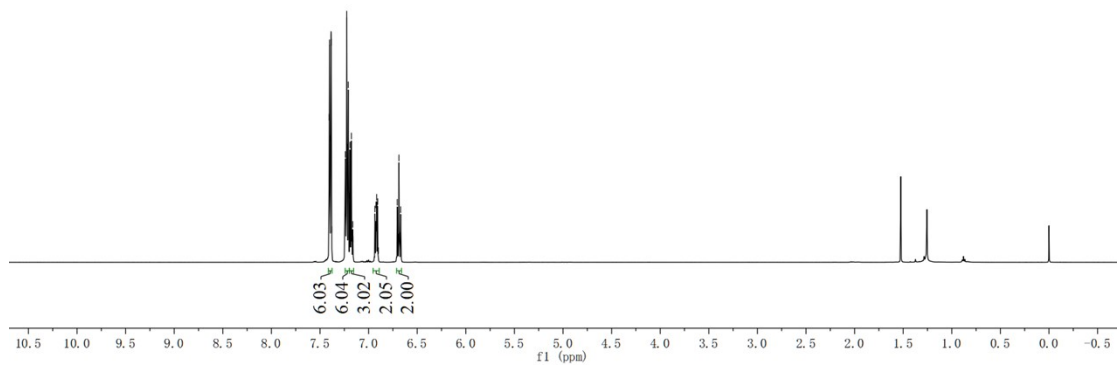


7.17
7.16
7.15
7.14
7.13
7.12
7.11
7.10
7.09
7.08
7.07
7.06
7.05
7.04
7.03
7.02
7.01
7.00
6.99
6.98
6.97
6.96
6.95
6.94
6.93
6.92
6.91
6.90
6.89
6.88
6.87
6.86
6.85
6.84
6.83
6.82
6.81
6.80
6.79
6.78
6.77
6.76
6.75
6.74
6.73
6.72
6.71
6.70
6.69
6.68
6.67



27

¹H NMR(500 MHz, CDCl₃)



A017-119-1.11.fid

C13CPD CDCl3 E:\CCY 32

163.91

161.93

144.39

137.55

137.48

129.93

129.09

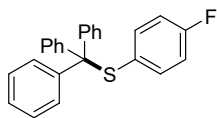
127.71

126.71

115.28

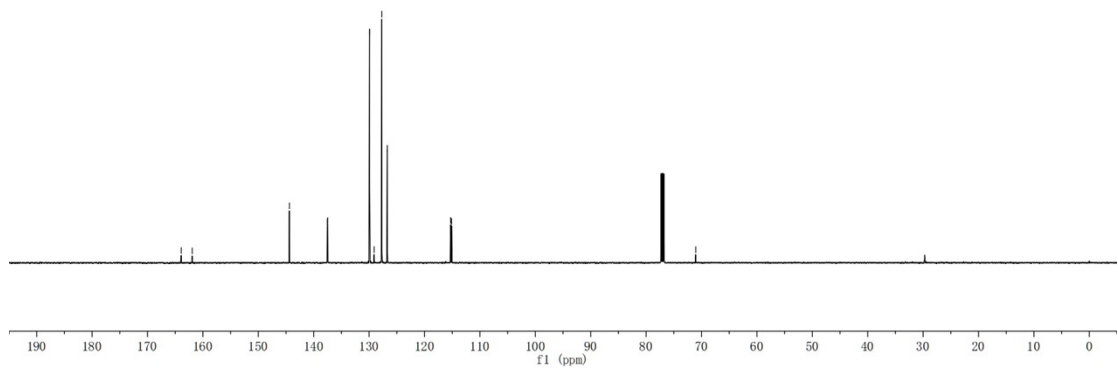
115.11

-71.05

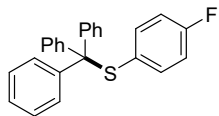


27

¹³C NMR(126 MHz, CDCl₃)

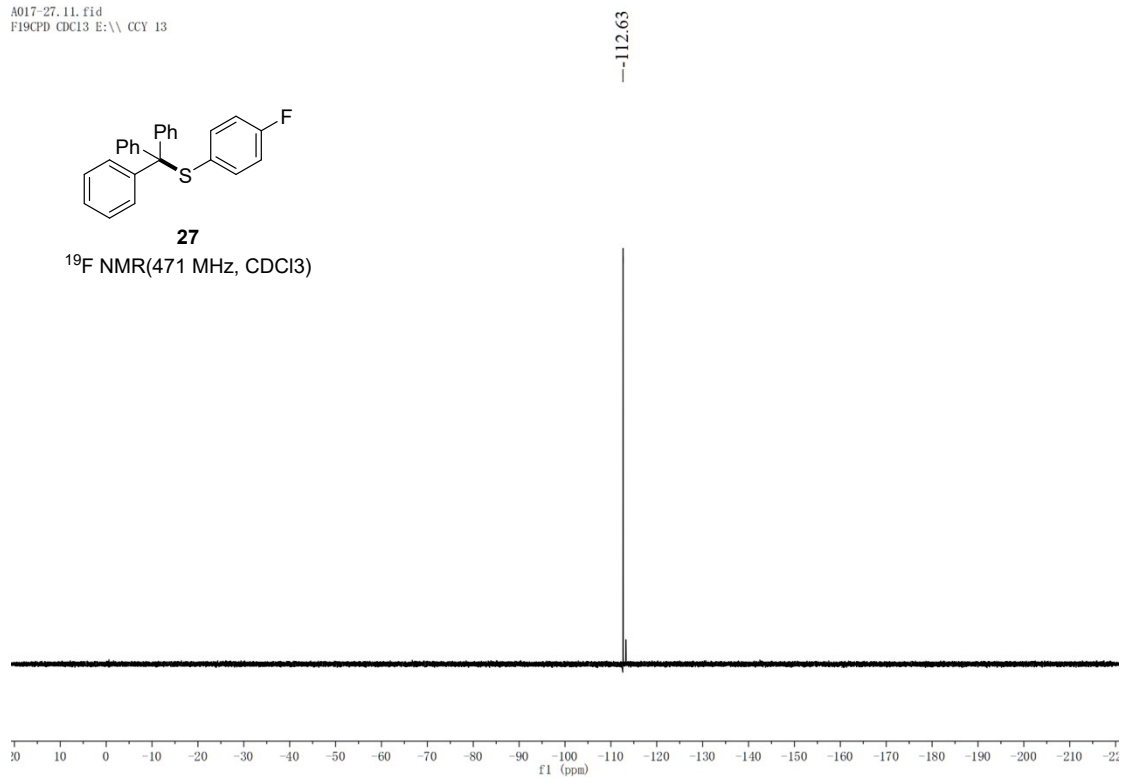


A017-27.11.fid
F19CPD CDCl3 E:\\ CCY 13

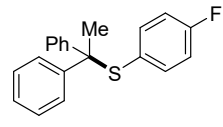


27

¹⁹F NMR(471 MHz, CDCl₃)

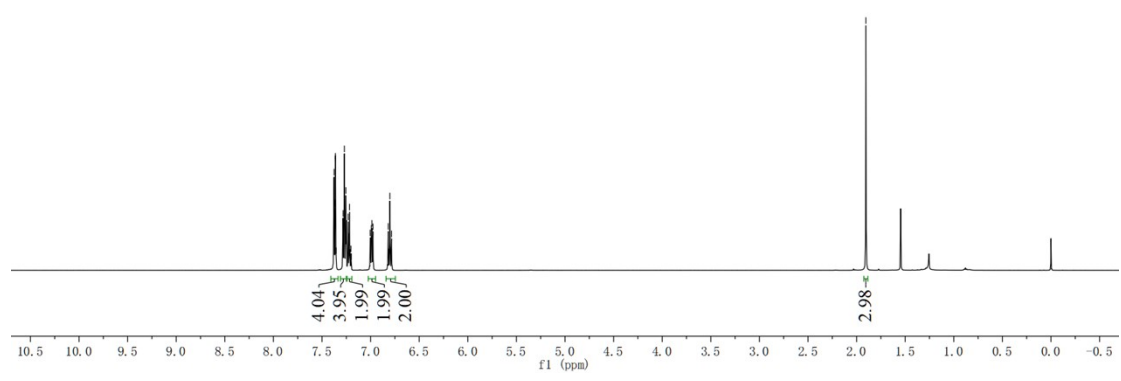


7.36
7.35
7.34
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.20
7.19
7.18
7.17
7.16
7.15
7.14
7.13
7.12
7.11
7.10
7.09
7.08
7.07
7.06
7.05
7.04
7.03
7.02
7.01
7.00
6.99
6.98
6.97
6.96
6.95
6.94
6.93
6.92
6.91
6.90
6.89
6.88
6.87
6.86
6.85
6.84
6.83
6.82
6.81
6.80
6.79
6.78



28

¹H NMR(500 MHz, CDCl₃)

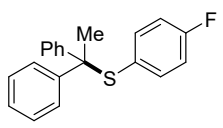


A017-112-6.11.fid
C13CPD CDCl3 E:\ \ CCY 39

159.58
157.60
141.31
134.07
134.00
123.57
123.12
121.96
110.63
110.46

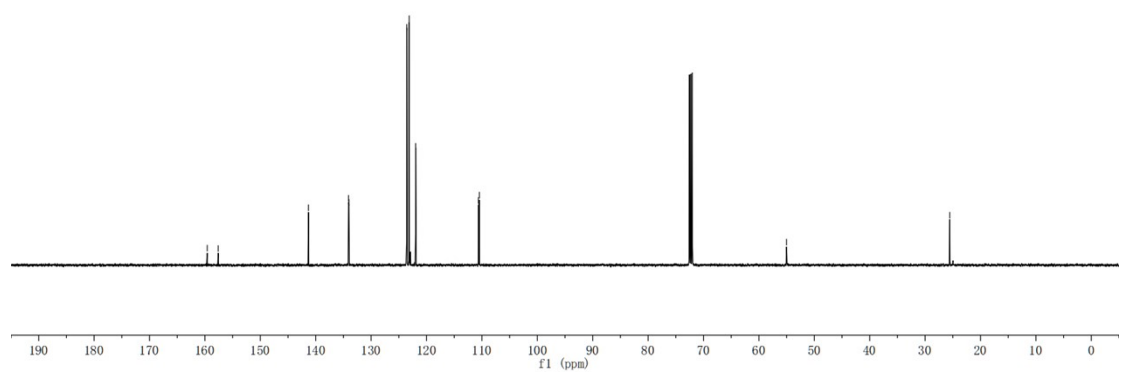
-55.02

-25.54

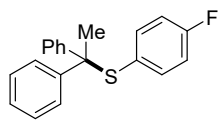


28

¹³C NMR(126 MHz, CDCl₃)

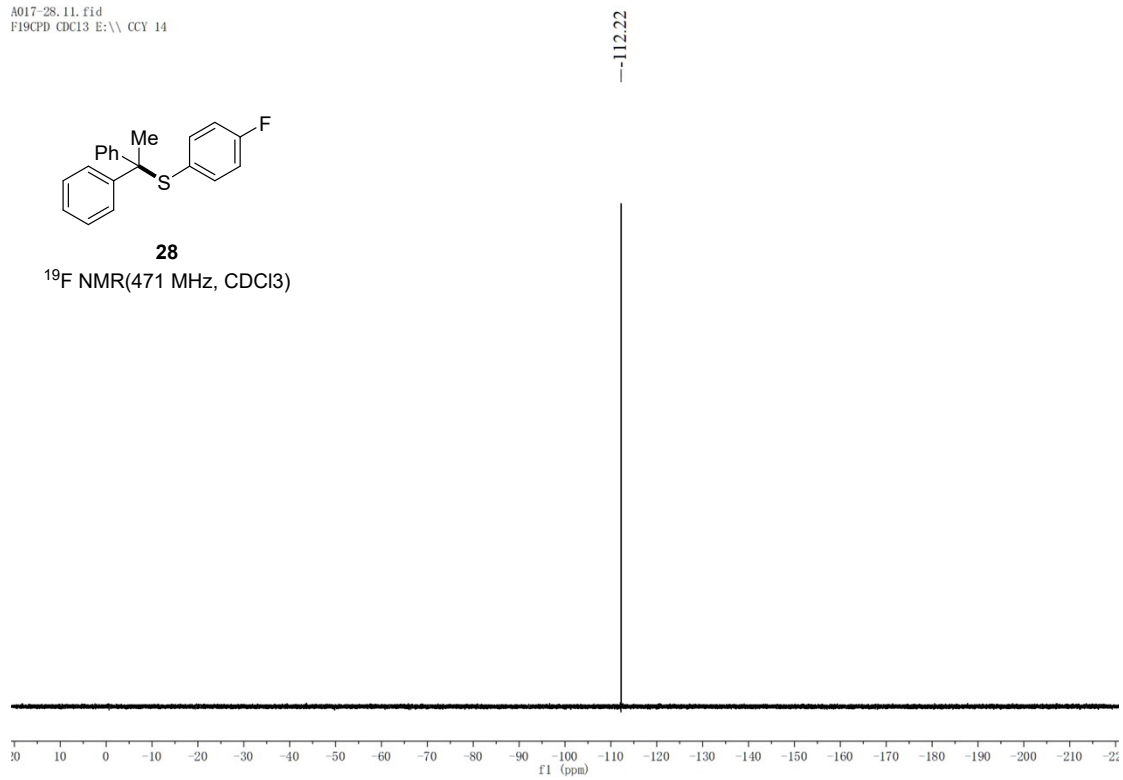


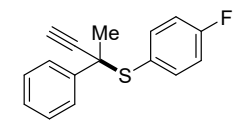
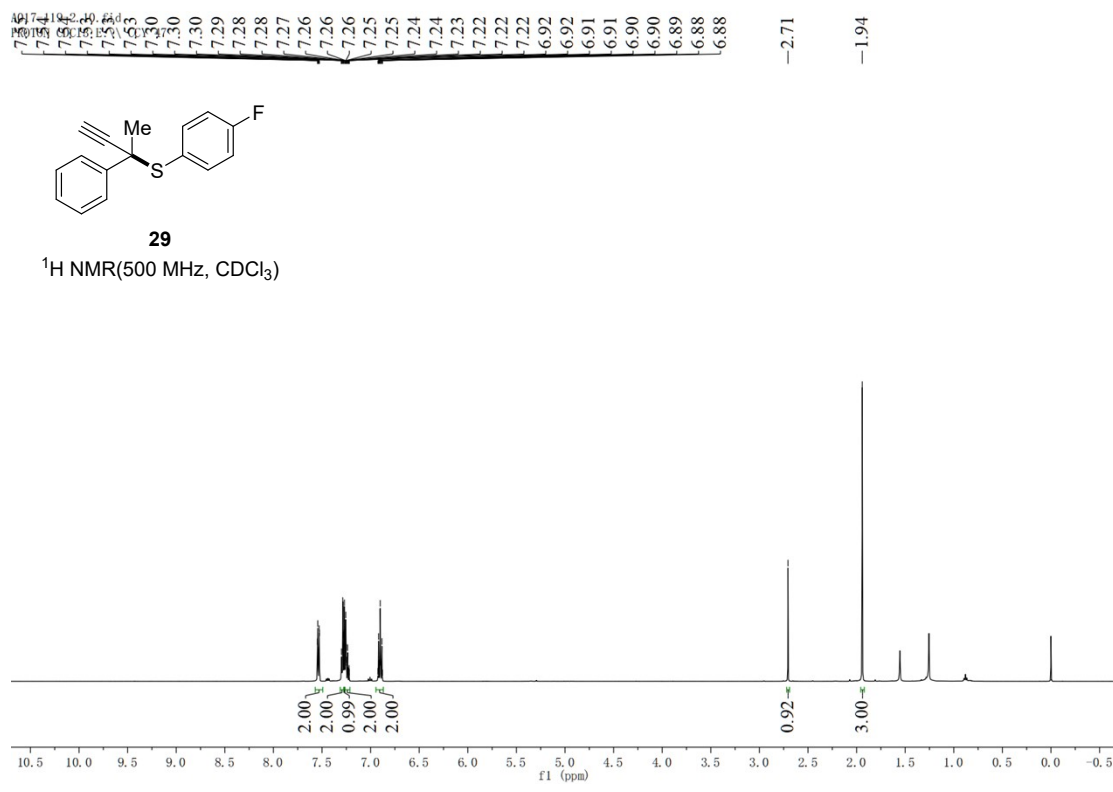
A017-28.11.fid
F19CPD CDCl3 E:\ CCY 14



28

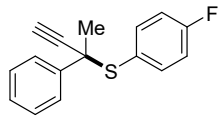
¹⁹F NMR(471 MHz, CDCl₃)





29

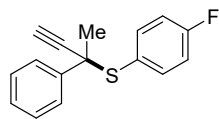
¹H NMR(500 MHz, CDCl₃)



29

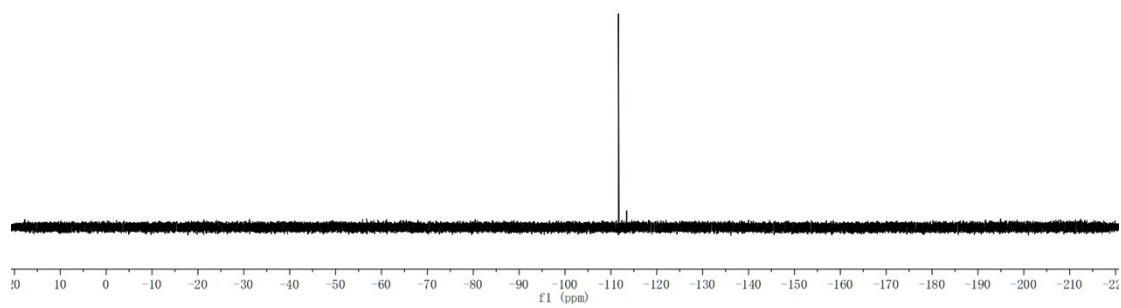
¹³C NMR(126 MHz, CDCl₃)

-111.65

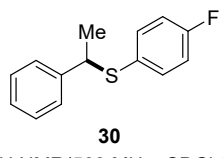


29

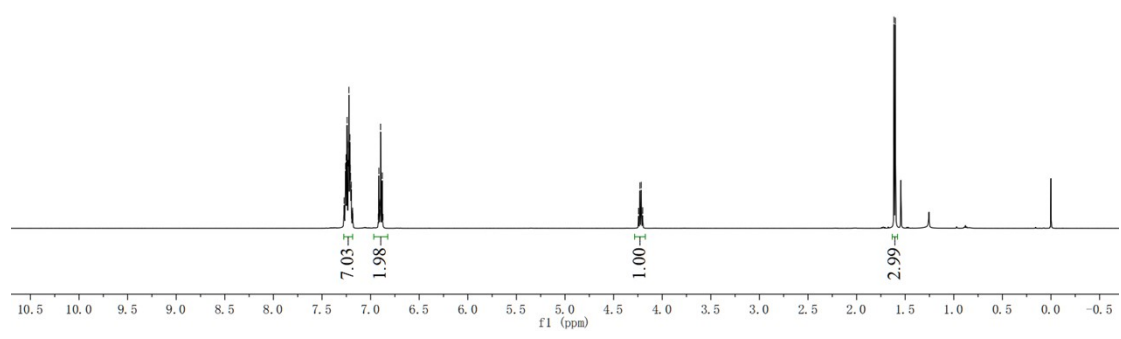
¹⁹F NMR(471 MHz, CDCl₃)



A021-155-1-C.11.fid
 PRB01
 7.24
7.23
7.22
7.22
7.22
7.21
7.21
7.20
7.19
7.19
7.18
6.92
6.91
6.91
6.90
6.90
6.89
6.89
6.88
6.88
6.87
4.23
4.24
4.21
4.20
1.61
1.60



¹H NMR(500 MHz, CDCl₃)

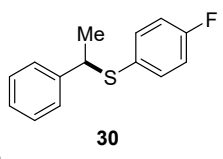


A021-155-1-C.11.fid
C13CPD CDCl3 E:\ \ CCY 29

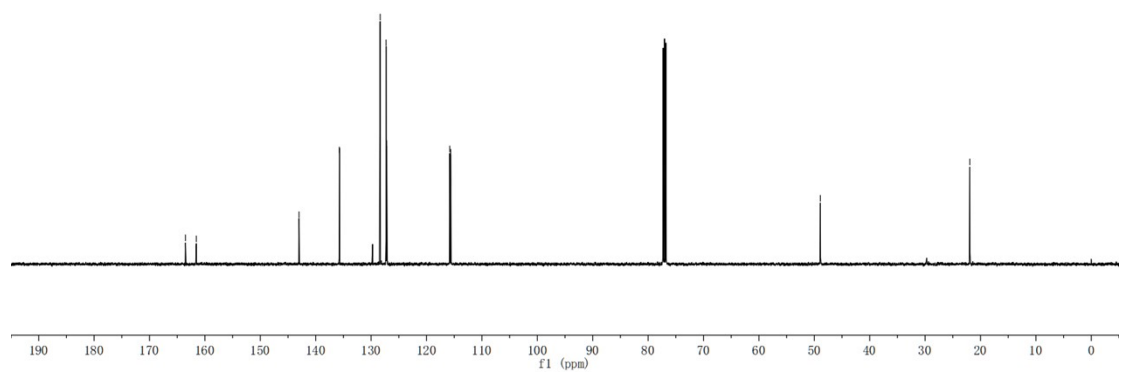
163.51
 161.55
 143.01
 135.74
 135.67
 128.36
 127.30
 127.18
 115.80
 115.63

-48.90

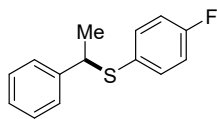
-21.92



¹³C NMR(126 MHz, CDCl₃)

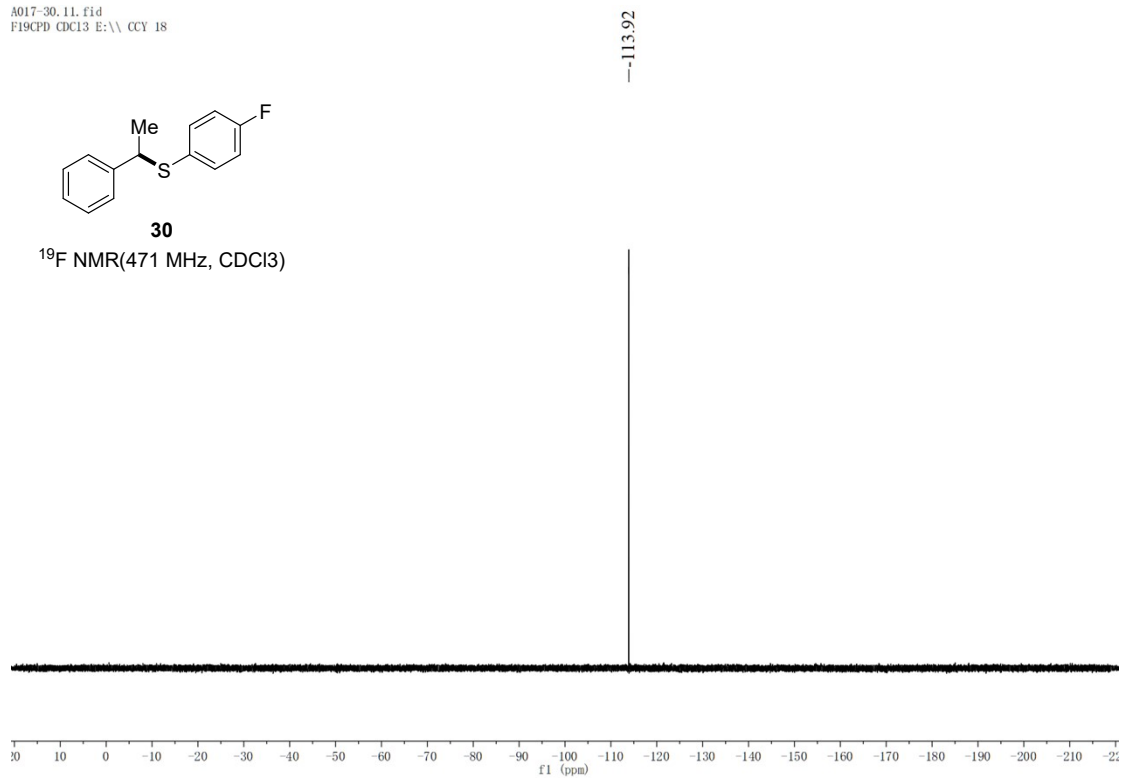


A017-30.11.fid
F19CPD CDCl3 E:\\ CCY 18

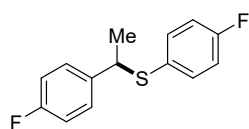


30

¹⁹F NMR(471 MHz, CDCl₃)

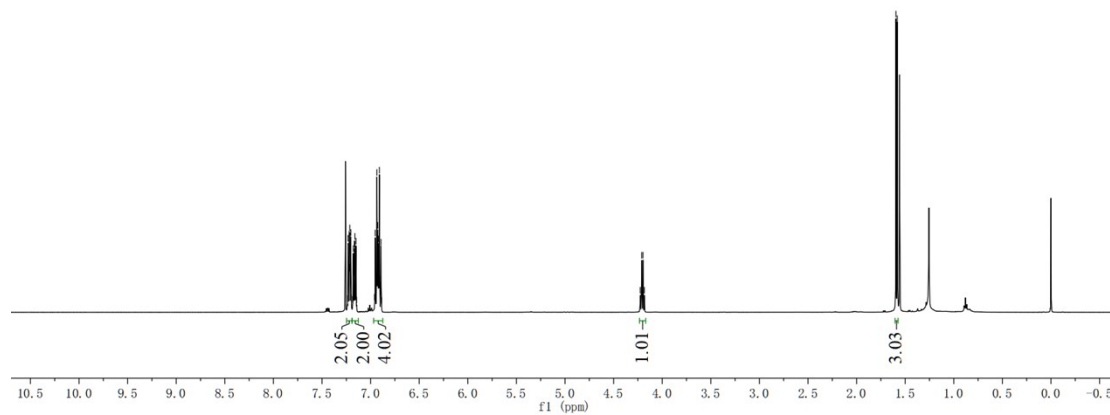


A017-123-2-1.11.fid
PROTON CDCl3
7.93, 7.91, 7.89, 7.87, 7.85, 7.82, 7.82, 7.72, 7.21, 7.20, 7.20, 7.19, 7.18, 7.17, 7.17, 7.16, 7.16, 7.15, 7.14, 7.14, 6.96, 6.95, 6.94, 6.94, 6.93, 6.93, 6.92, 6.92, 6.91, 6.91, 6.91, 6.91, 6.89, 6.89, 4.23, 4.21, 4.20, 4.18, 1.60, 1.58



31

$^1\text{H NMR}$ (500 MHz, CDCl_3)



A017-123-2-1.11.fid
C13CPD CDCl3 E:\ \ CCY

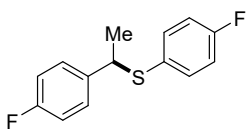
163.60
162.77
161.63
160.82

135.92
135.86
128.83
128.77
115.88
115.71
115.23
115.06

-48.21

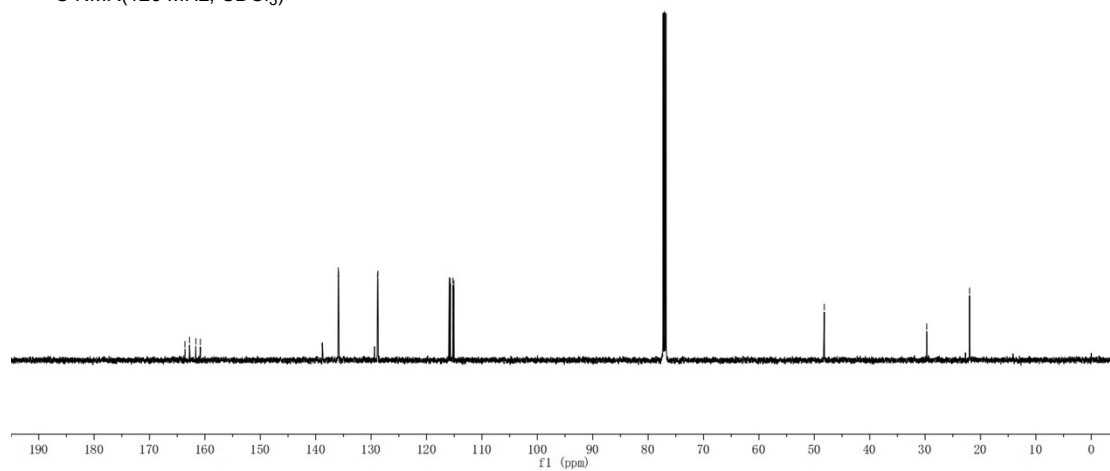
-29.71

-21.97

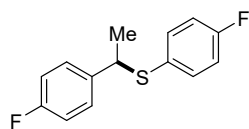


31

$^{13}\text{C NMR}$ (126 MHz, CDCl_3)



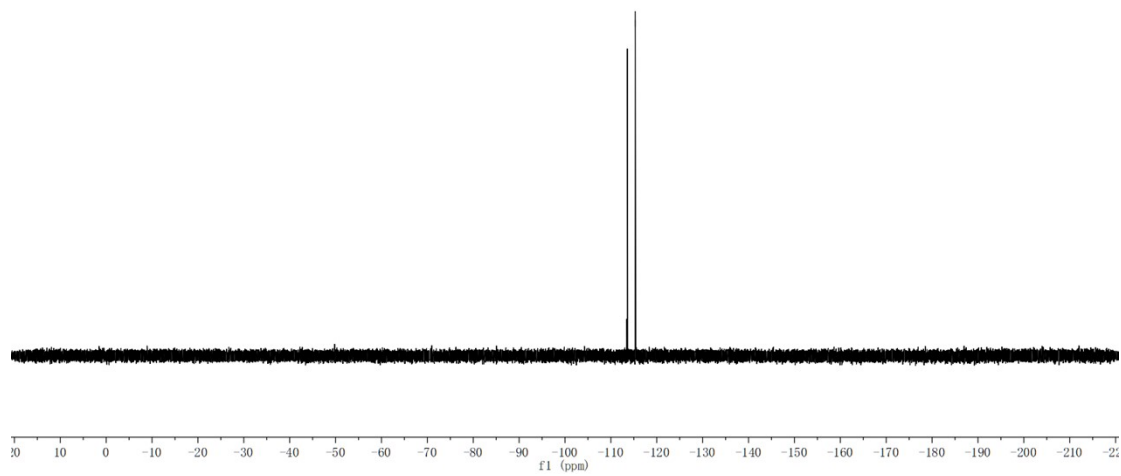
A017-31.11.fid
F19CPD CDCl3 E:\\ CCY 19



31

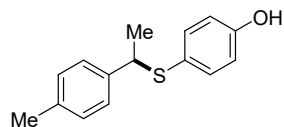
¹⁹F NMR(471 MHz, CDCl₃)

~113.59
~115.31



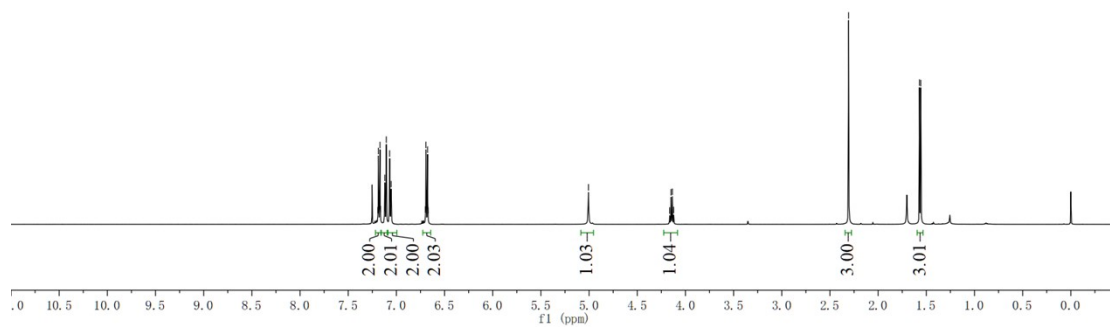
A017-116-3.10.fid
PROTON CDCl3 E:\ \ CCY 18

7.19
7.19
7.18
7.17
7.17
7.16
7.12
7.10
7.10
7.07
7.05
6.70
6.69
6.69
6.68
6.68
6.67
5.01
4.16
4.15
4.14
4.12
-2.31
1.57
1.56



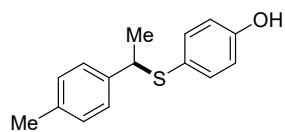
32

¹H NMR(500 MHz, CDCl₃)



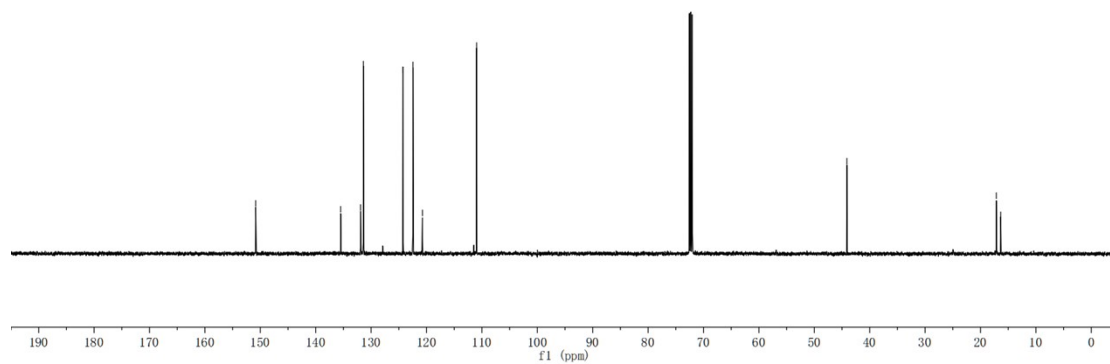
A017-116-3.11.fid
C13CPD CDCl3 E:\ \ CCY 41

150.84
135.49
131.90
131.39
124.23
122.45
120.73
110.96
-44.12
17.15
16.35

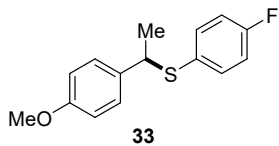


32

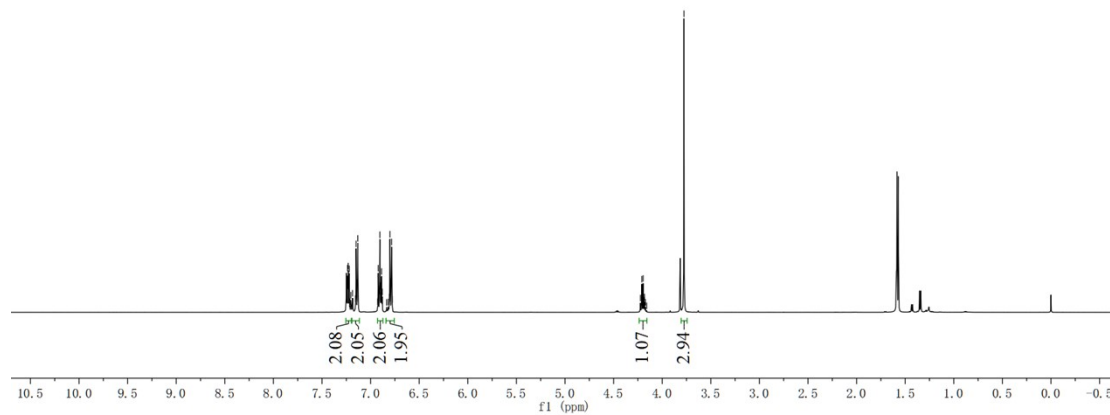
¹³C NMR(126 MHz, CDCl₃)



A017-122-2
 PROTON
 7.34
 7.33
 7.22
 7.21
 7.20
 7.19
 7.18
 7.16
 7.15
 7.14
 7.13
 7.13
 6.93
 6.92
 6.91
 6.91
 6.90
 6.90
 6.89
 6.89
 6.89
 6.88
 6.83
 6.82
 6.81
 6.80
 6.80
 6.79
 6.78
 6.78
 4.22
 4.21
 4.20
 4.19
 4.18
 4.17
 4.16
 3.78

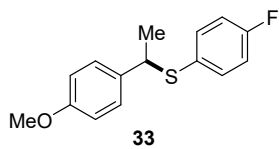


¹H NMR(500 MHz, CDCl₃)

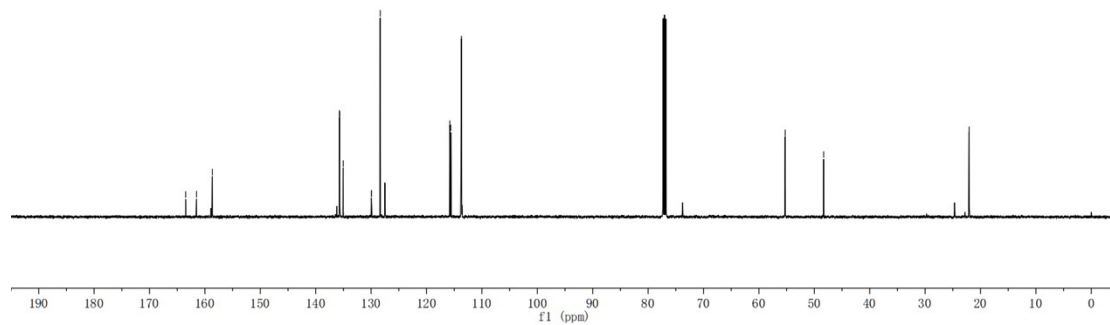


A017-112-2.11.fid
 C13CPD CDCl3 E:\ \ CCY 5

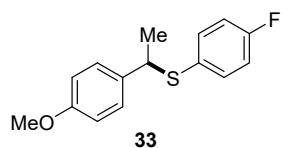
163.47
 161.51
 158.65
 135.72
 135.65
 135.03
 129.95
 129.92
 128.35
 115.78
 115.61
 113.70
 -55.26
 -48.31
 -22.05



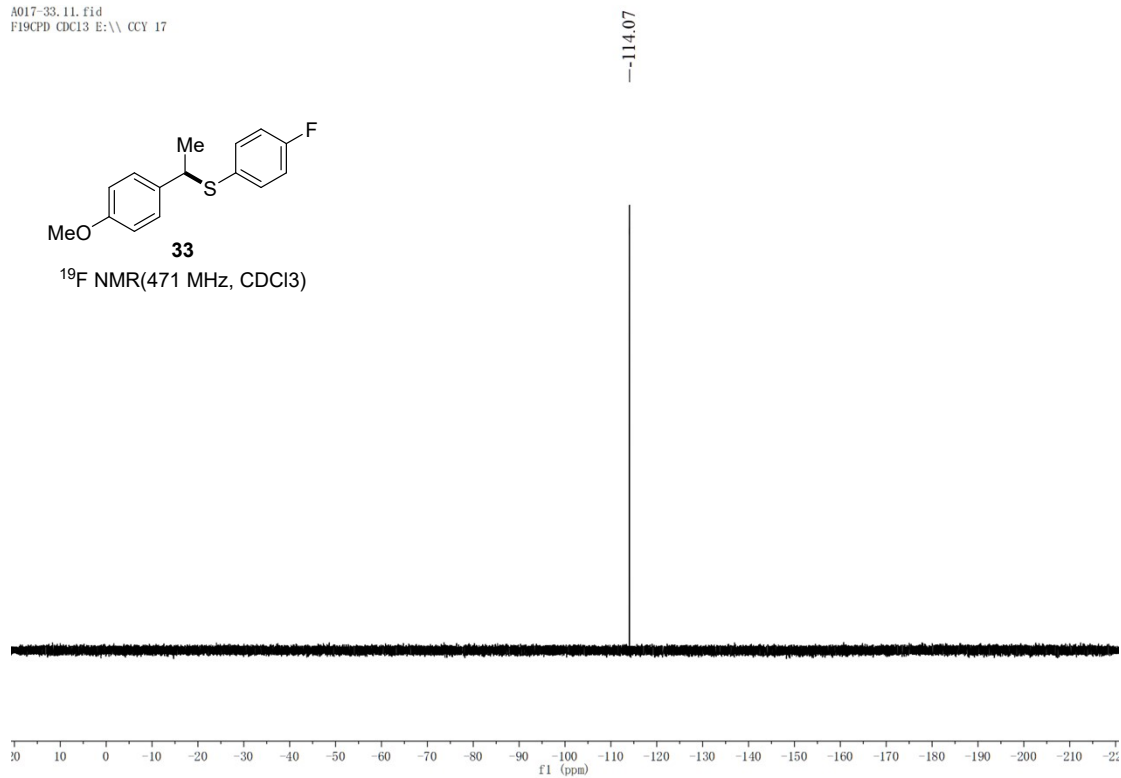
¹³C NMR(126 MHz, CDCl₃)



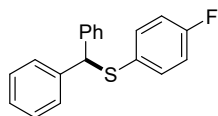
A017-33.11.fid
F19CPD CDCl3 E:\\ CCY 17



33
¹⁹F NMR(471 MHz, CDCl₃)

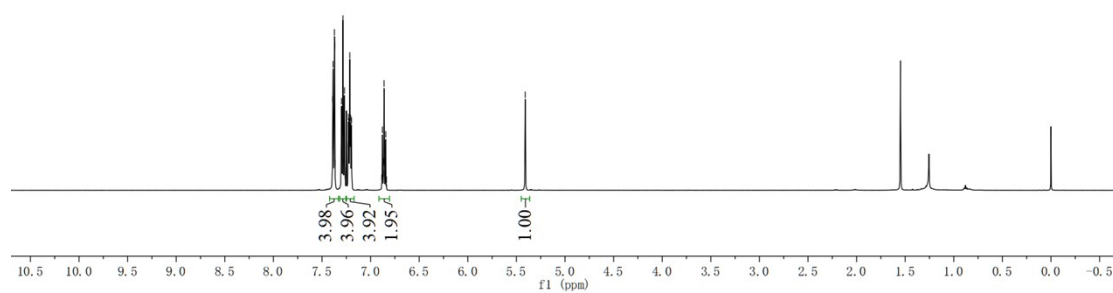


A017-112-3.11.fid
 PROTON
 7.30, 7.28, 7.27, 7.27, 7.23, 7.23, 7.23, 7.23, 7.22, 7.21, 7.20, 7.20, 7.20, 6.89, 6.88, 6.87, 6.87, 6.86, 6.86, 6.85, 6.85, 6.84, 6.84, 5.41



34

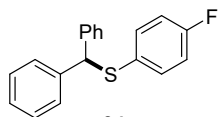
¹H NMR(500 MHz, CDCl₃)



A017-112-3.11.fid
 C13CPD CDCl3 E:\ \ CCY 38

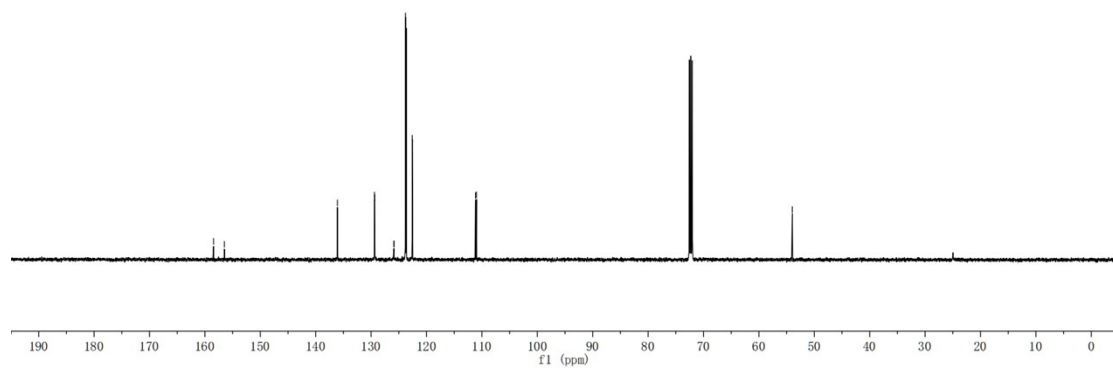
158.44
 156.48
 136.08
 129.39
 129.33
 125.88
 125.85
 123.79
 123.64
 122.57
 111.16
 110.98

-53.97

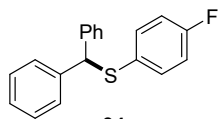


34

¹³C NMR(126 MHz, CDCl₃)

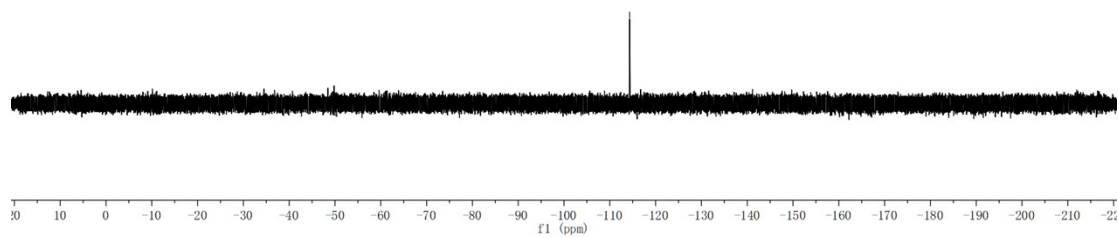


A017-34.11.fid
F19CPD CDCl3 E:\\ CCY 13



¹⁹F NMR(471 MHz, CDCl₃)

-114.34



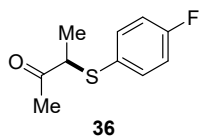
A021-153-3-2.10.fid
PROTON CDCl3 E:\ \ CCY 13

7.39
7.38
7.37
7.36
7.35
7.03
7.02
7.01
7.00
6.99
6.99
6.98

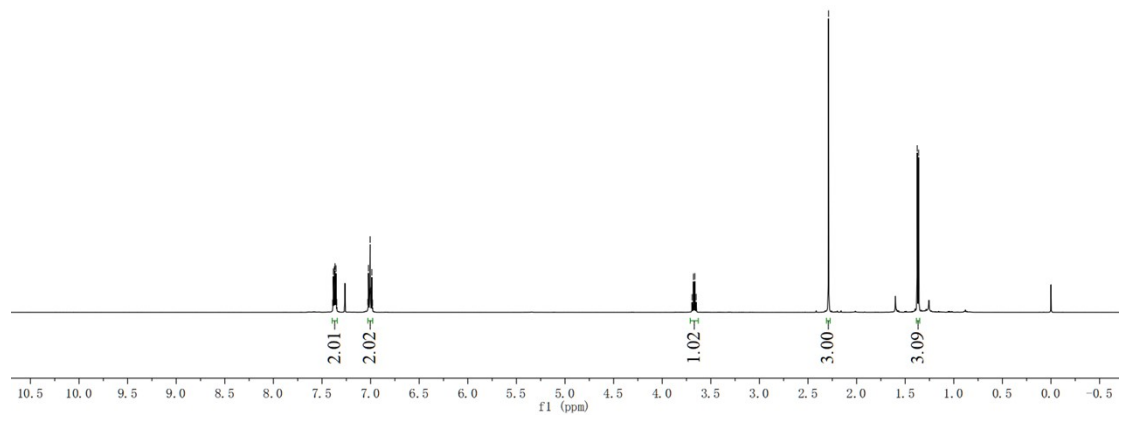
3.69
3.68
3.66
3.65

2.29

1.38
1.36



¹H NMR(500 MHz, CDCl₃)



A017-C...fid
C13CPD...E:\ \ CCY 5

205.08

164.04
162.05

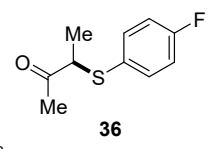
135.96
135.89

116.34
116.17

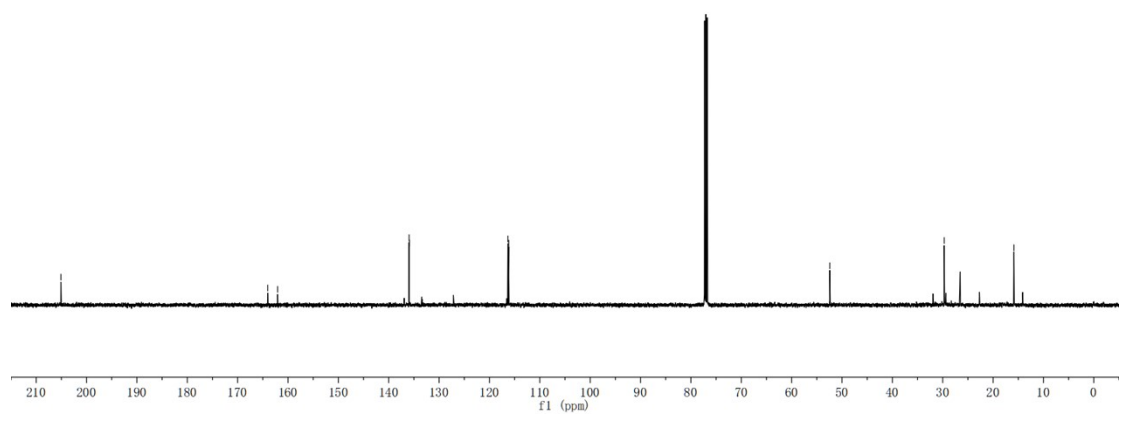
52.42

29.71

15.87

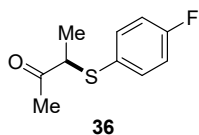


¹³C NMR(126 MHz, CDCl₃)

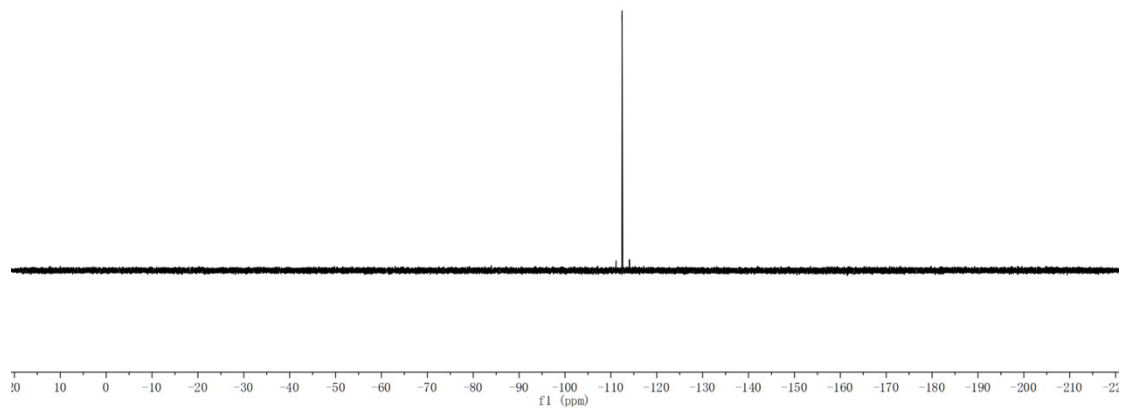


A017-36.11.fid
F19CPD CDCl3 E:\ \ CCY 14

--112.45

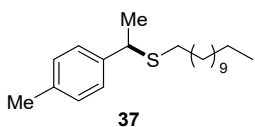


¹⁹F NMR(471 MHz, CDCl₃)

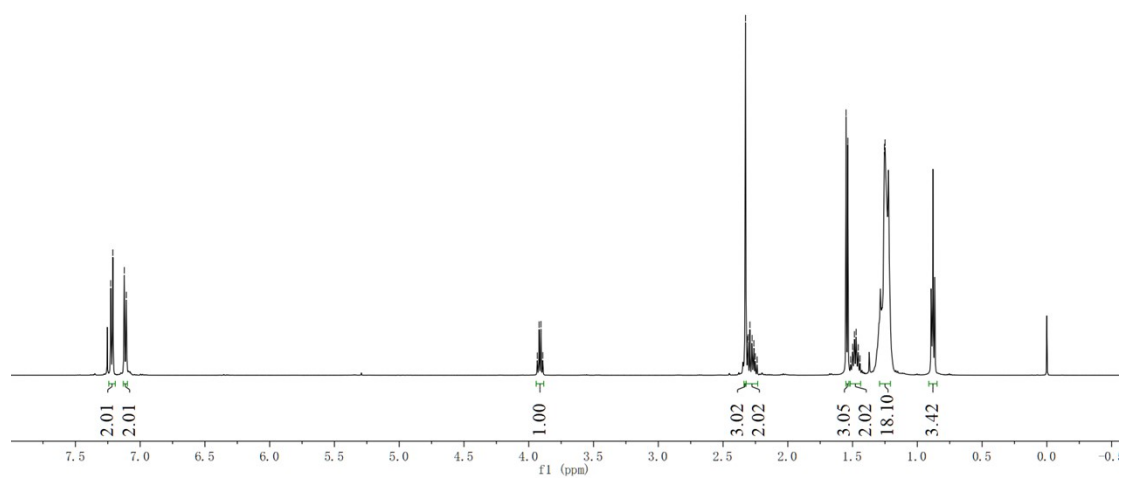


A017-145-1.11.fid
 PROTON CDCl₃

3.93
 3.92
 3.91
 3.89
 2.33
 2.31
 2.31
 2.29
 2.28
 2.26
 2.25
 2.24
 1.55
 1.54
 1.52
 1.50
 1.49
 1.47
 1.46
 1.44
 1.25
 1.25

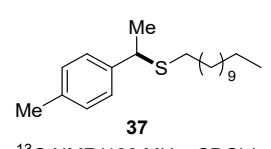


¹H NMR(500 MHz, CDCl₃)

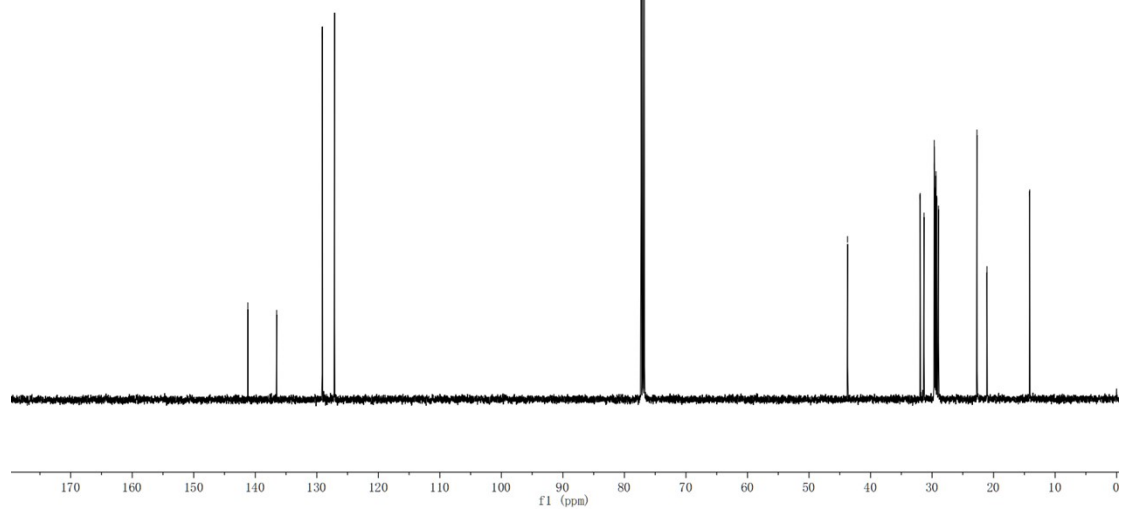


A017-145-1.11.fid
 C13CPD CDCl₃ E:\ \ CCY 2

141.21
 136.52
 129.10
 127.11
 43.73
 31.94
 29.67
 29.65
 29.61
 29.50
 29.40
 29.37
 29.22
 28.96
 22.71
 14.14

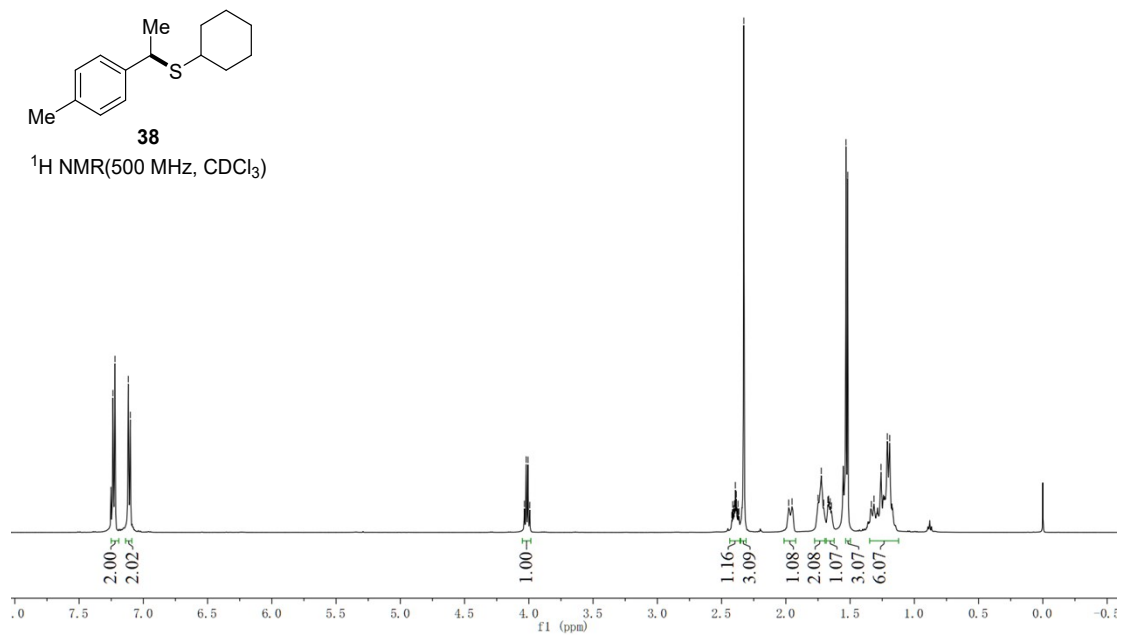
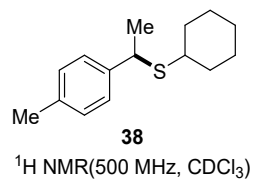


¹³C NMR(126 MHz, CDCl₃)



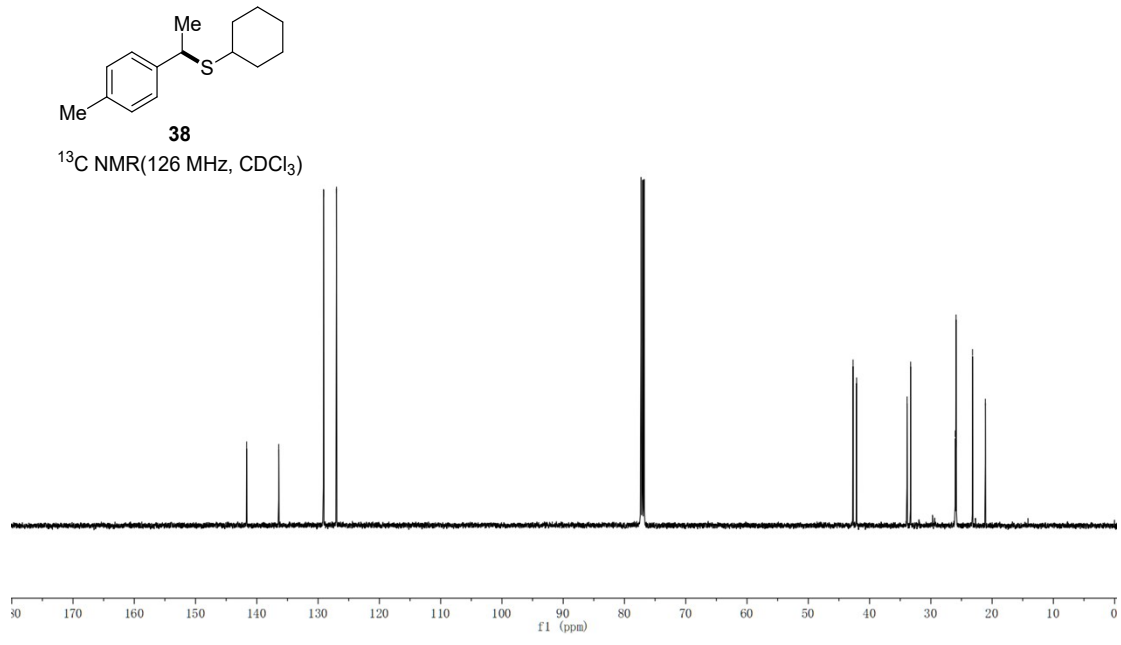
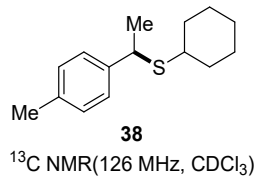
A017-145-2.11.fid
 PROTON CDCl3

4.03
 4.02
 4.01
 3.99
 2.42
 2.41
 2.41
 2.40
 2.39
 2.39
 2.38
 2.37
 2.36
 2.33
 1.98
 1.95
 1.75
 1.72
 1.71
 1.67
 1.67
 1.65
 1.65
 1.53
 1.52
 1.33
 1.31
 1.26
 1.21
 1.19

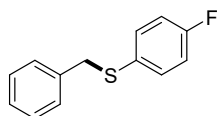


A017-145-2.11.fid
 C13CPD CDCl3 E:\ \ CCY 3

141.67
 136.42
 129.12
 127.00
 42.70
 42.12
 33.88
 33.30
 26.01
 25.89
 25.85
 23.20
 21.10

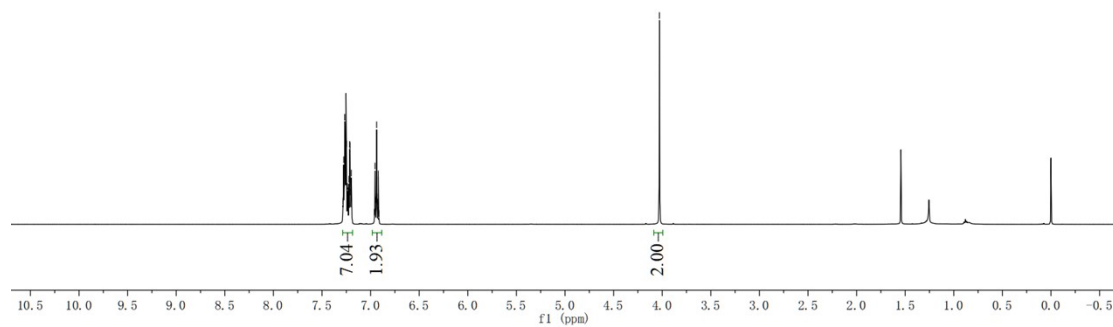


A021-153-5.09.fid
 PROTON CDCl3 E:\ \ CCY 28
 7.288
 7.288
 7.277
 7.27
 7.26
 7.26
 7.25
 7.24
 7.24
 7.23
 7.23
 7.22
 7.22
 7.21
 7.21
 7.20
 7.20
 6.96
 6.96
 6.95
 6.94
 6.94
 6.93
 6.93
 6.92
 6.92
 6.91
 6.91
 -4.03



39

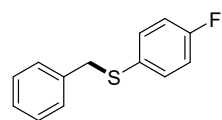
¹H NMR(500 MHz, CDCl₃)



A021-161-7-C.11.fid
 C13CPD CDCl3 E:\ \ CCY 28

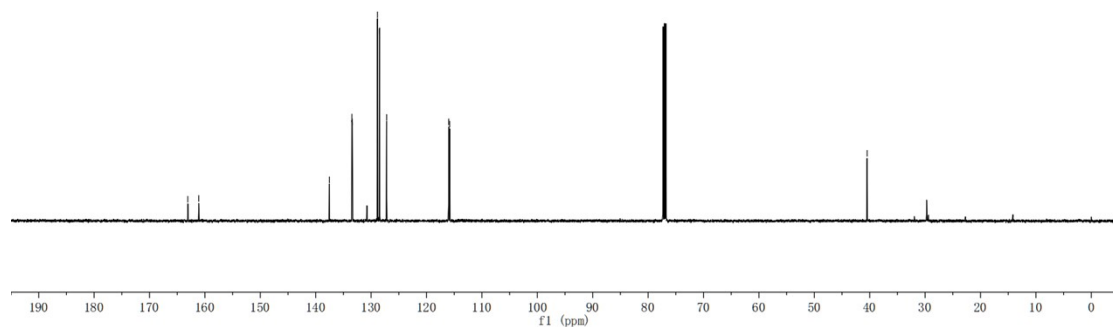
163.08
 161.12
 137.52
 133.46
 133.40
 128.85
 128.46
 127.20
 115.99
 115.82

-40.46

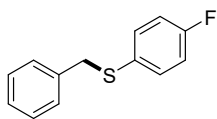


39

¹³C NMR(126 MHz, CDCl₃)

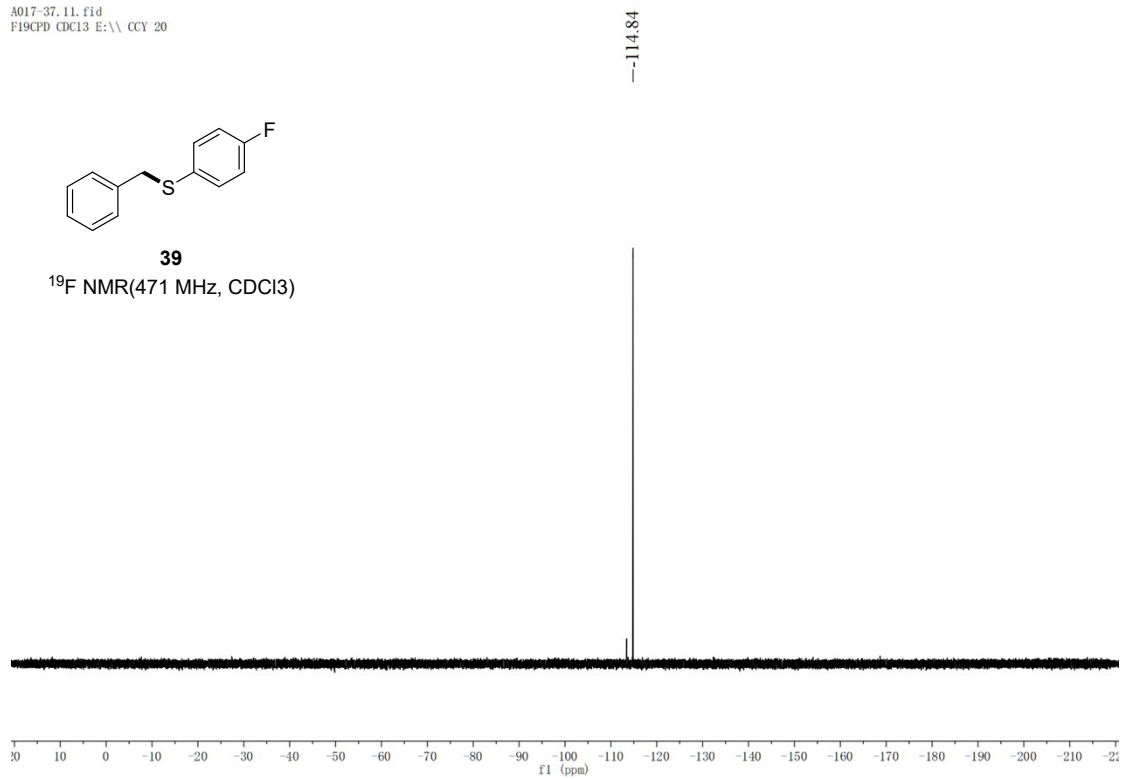


A017-37.11.fid
F19CPD CDCl3 E:\\ CCY 20

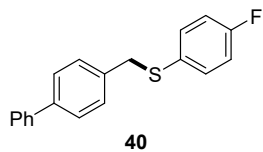


39

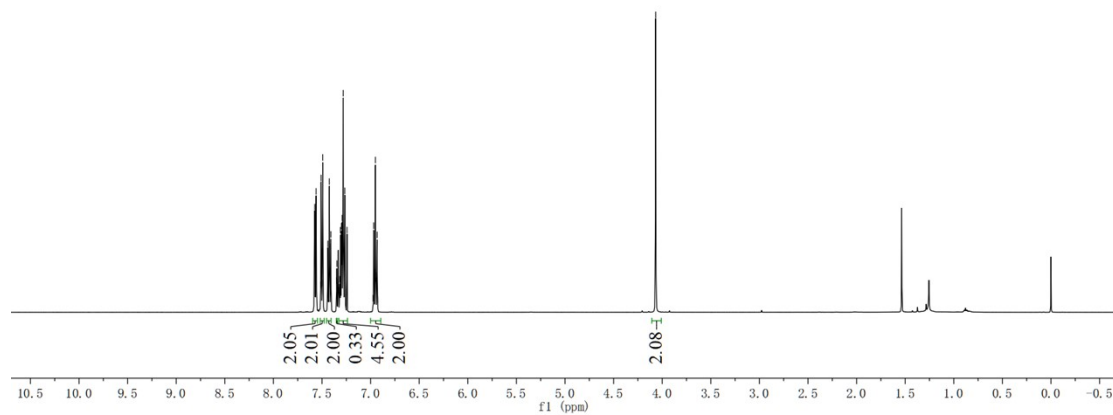
¹⁹F NMR(471 MHz, CDCl₃)



A017-120-3.11.fid
 PROTON CDCl3
 7.38 7.37 7.36 7.35 7.34 7.33 7.32 7.31 7.30 7.29 7.28 7.27 7.24 6.97 6.96 6.95 6.95 6.94 6.93 6.93 4.07



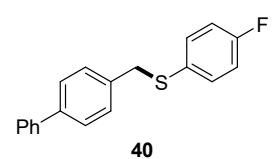
¹H NMR(500 MHz, CDCl₃)



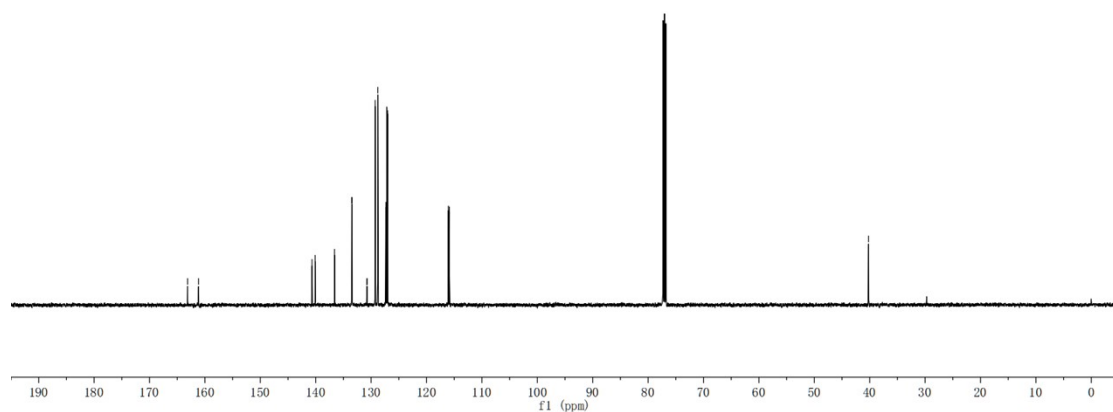
A017-120-3.11.fid
 C13CPD CDCl3 E: \\

163.42
 161.16
 140.67
 140.10
 136.60
 133.50
 133.44
 130.76
 129.27
 128.79
 127.33
 127.18
 127.02
 116.05
 115.88

-40.20

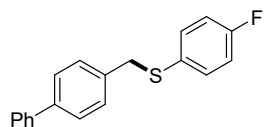


¹³C NMR(126 MHz, CDCl₃)



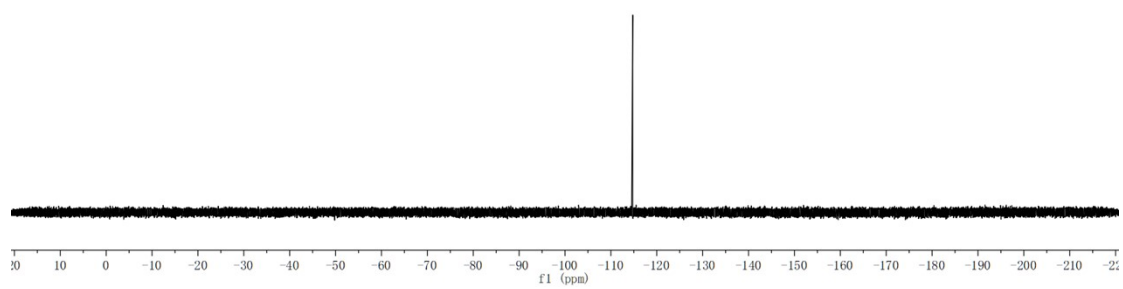
A017-38.11.fid
F19CPD CDCl3 E:\ \ CCY 11

-114.75



40

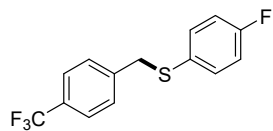
¹⁹F NMR(471 MHz, CDCl₃)



A017-122-2.1.fid
PROTON CDCl3 [D:\20210804] root 51

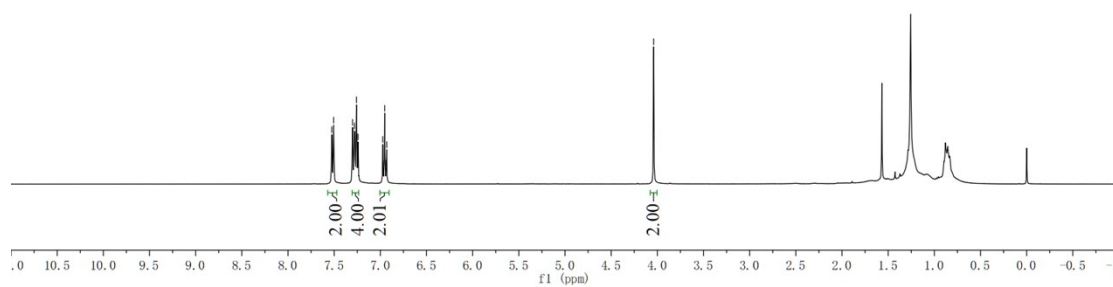
7.53
7.51
7.30
7.28
7.26
7.24
6.97
6.95
6.94
6.93

-4.04



41

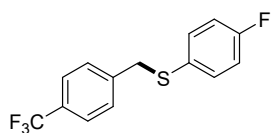
¹H NMR(500 MHz, CDCl₃)



A017-39B.10.fid
C13CPD CDCl3 root 40

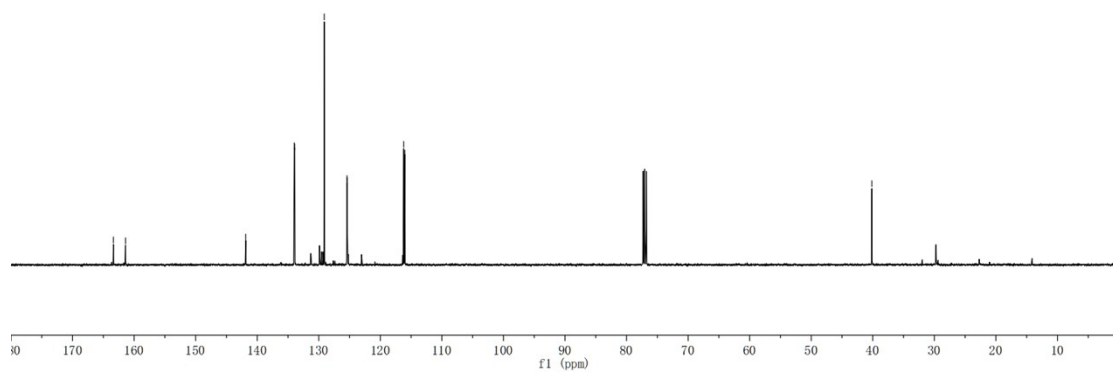
163.36
161.39
141.87
133.98
133.92
129.11
125.45
125.42
125.39
125.36
116.20
116.02

-40.15

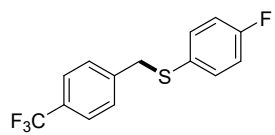


41

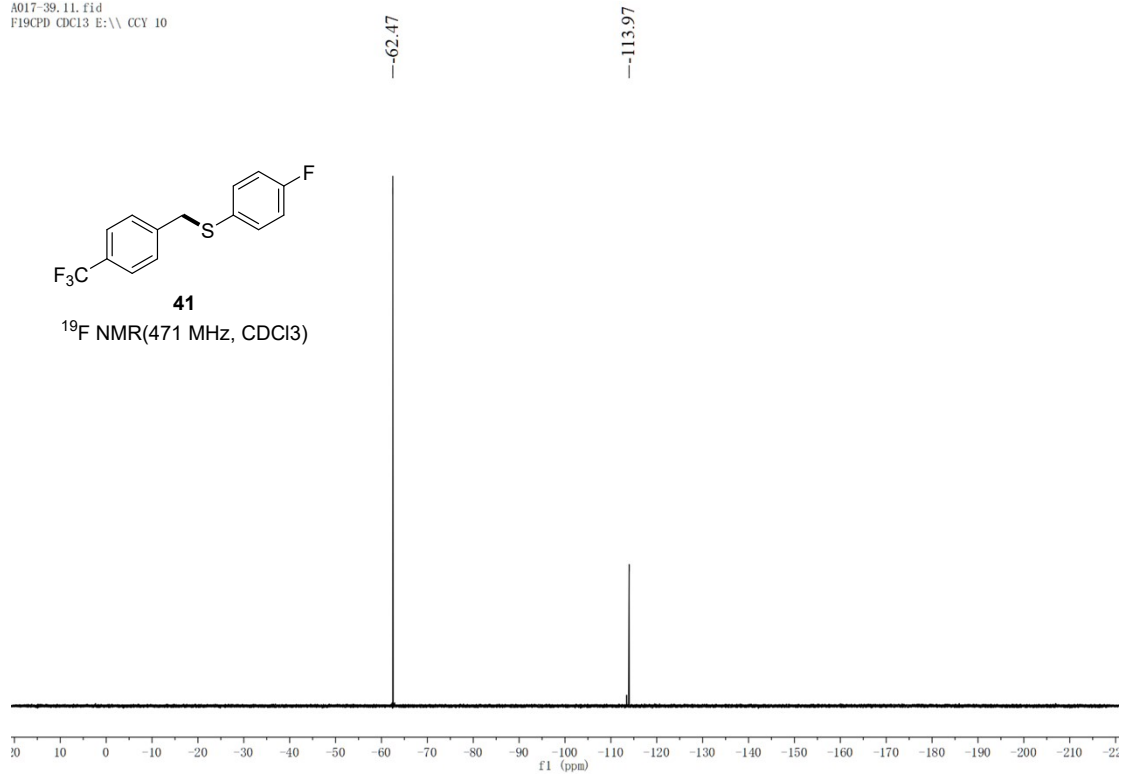
¹³C NMR(126 MHz, CDCl₃)



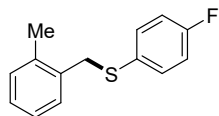
A017-39.11.fid
F19CPD CDCl3 E:\ \ CCY 10



¹⁹F NMR(471 MHz, CDCl₃)

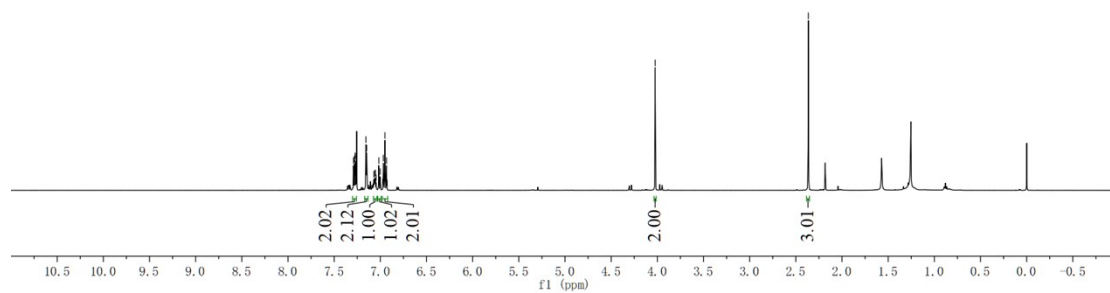


A017-122-1-1.10. fid
 PROTON CDCl3 E:\ \ CD
 7.29 7.28 7.27 7.26 7.16 7.15 7.07 7.06 7.05 7.05 7.02 7.00 6.97 6.96 6.95 6.94 6.93
 -4.02 -2.36

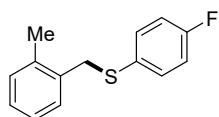


42

¹H NMR(500 MHz, CDCl₃)

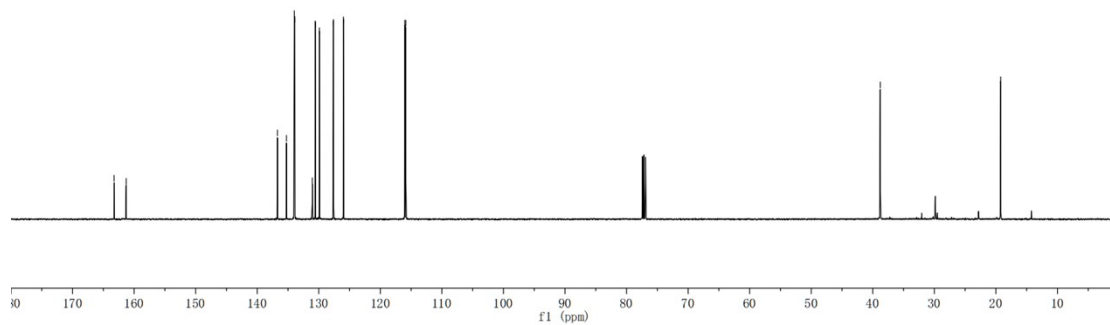


A017-40B.10. fid
 C13CPD CDCl3 E:\ \ CD
 163.25 161.29 136.72 135.25 133.97 133.91 131.06 130.58 129.90 127.61 126.00 116.03 115.86
 -38.78 -19.22

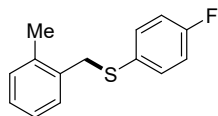


42

¹³C NMR(126 MHz, CDCl₃)



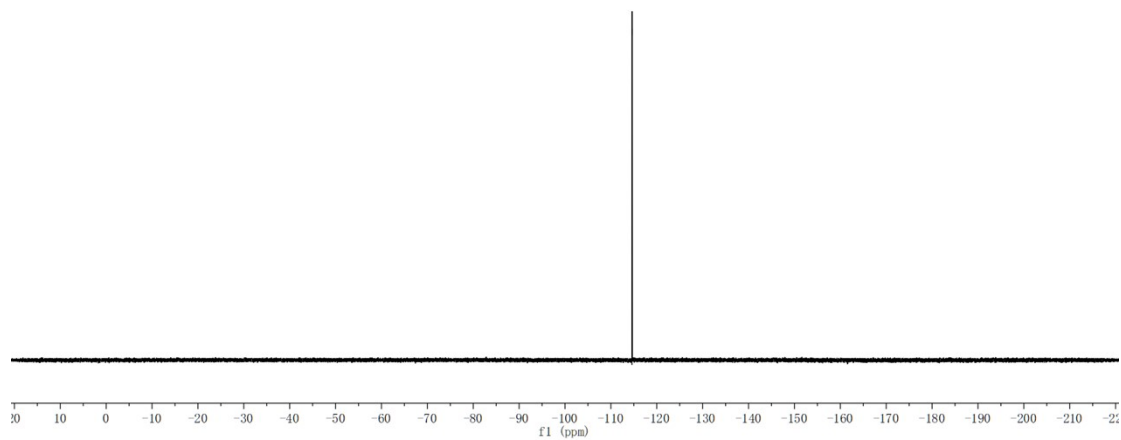
A017-406.11.fid
F19CPD CDCl3 E:\\ CCY 1



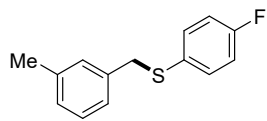
42

¹⁹F NMR(471 MHz, CDCl₃)

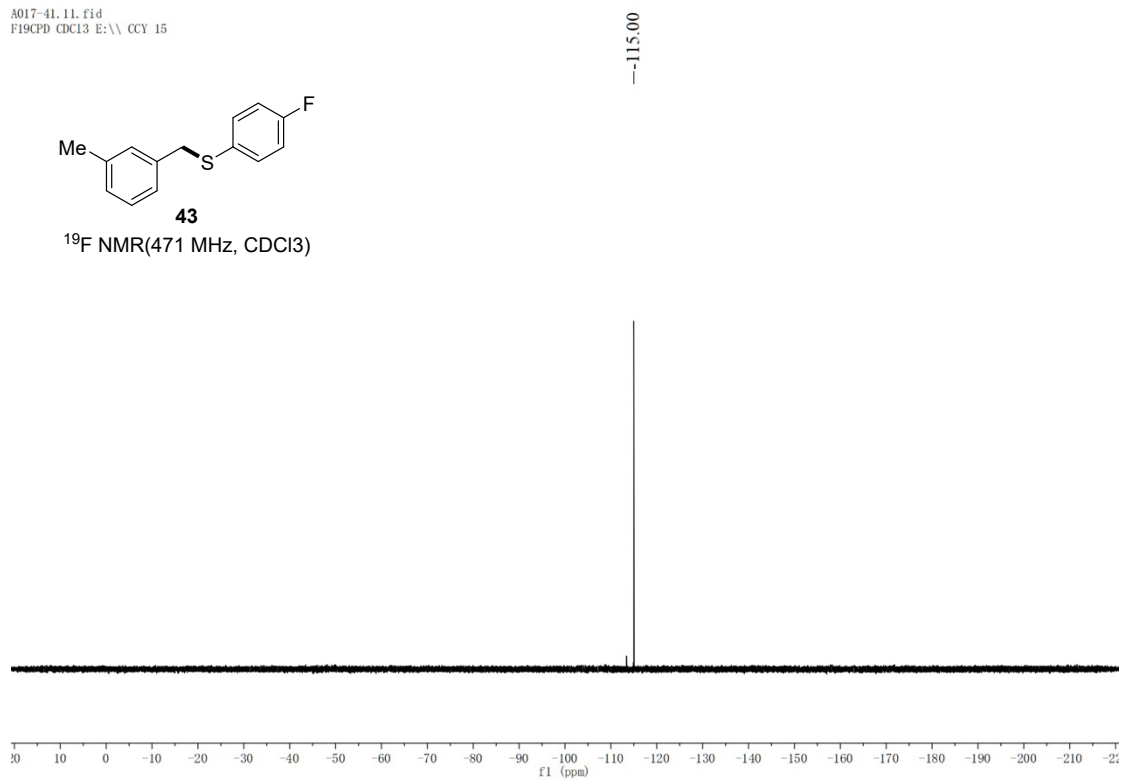
-114.60



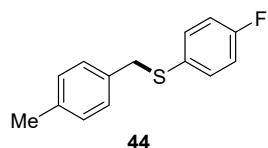
A017-41.11.fid
F19CPD CDCl3 E:\\ CCY 15



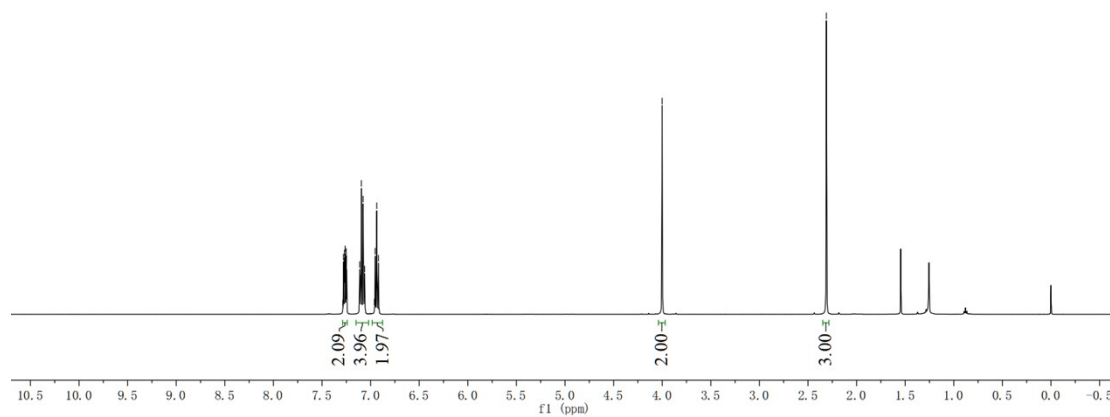
¹⁹F NMR(471 MHz, CDCl₃)



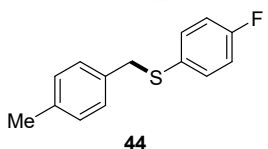
A017-120-2.10.fid
 PROTON CDCl3 E: 7.28 7.28 7.27 7.27 7.26 7.26 7.11 7.11 7.10 7.10 7.08 7.06 6.96 6.95 6.95 6.94 6.94 6.94 6.93 6.92 6.92



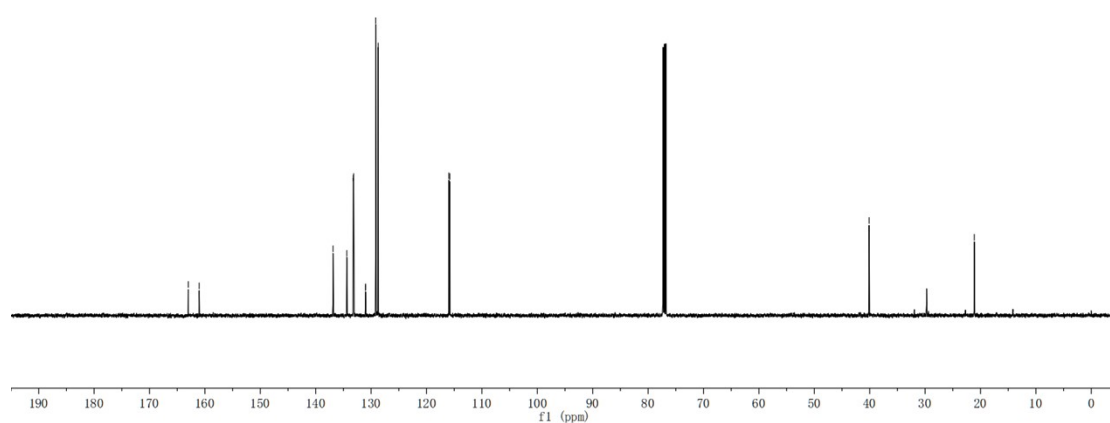
¹H NMR(500 MHz, CDCl₃)



A017-120-2.10.fid
 C13CPD CDCl3 E:\ \ CCY 14
 162.99 161.03 136.87 134.38 133.21 133.15 131.03 131.01 129.17 128.72 115.97 115.79

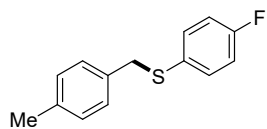


¹³C NMR(126 MHz, CDCl₃)

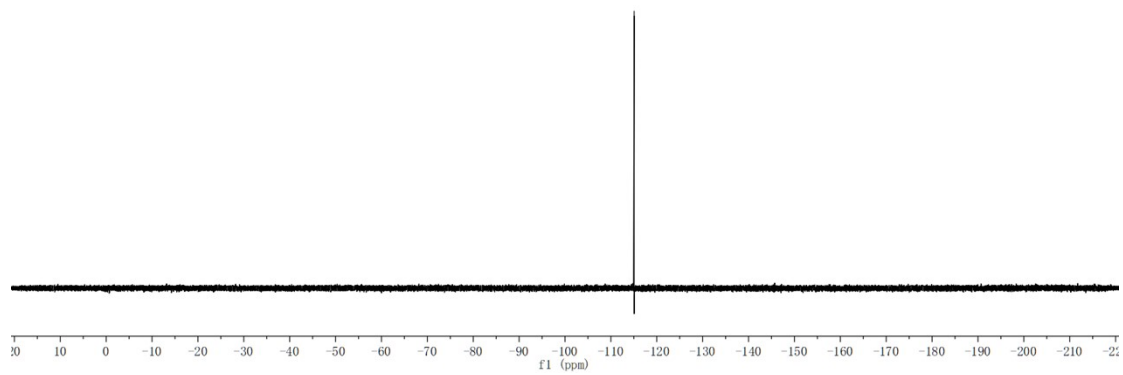


A017-426.11.fid
F19CPD CDCl3 E:\ \ CCY 2

--115.07



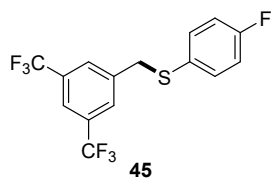
44
¹⁹F NMR(471 MHz, CDCl₃)



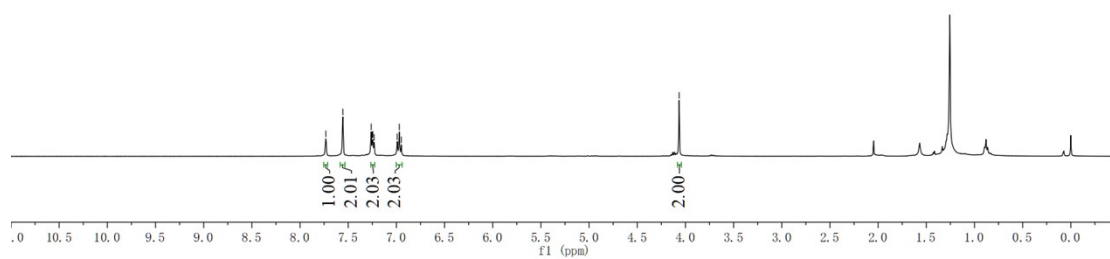
A017-126-3.1.fid
PROTON CDCl3 (D:\20210808) root 14

7.73
7.56
7.26
7.25
7.24
7.23
6.99
6.95

-4.07



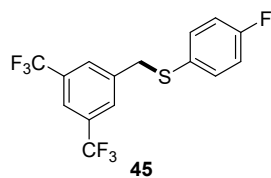
¹H NMR(500 MHz, CDCl₃)



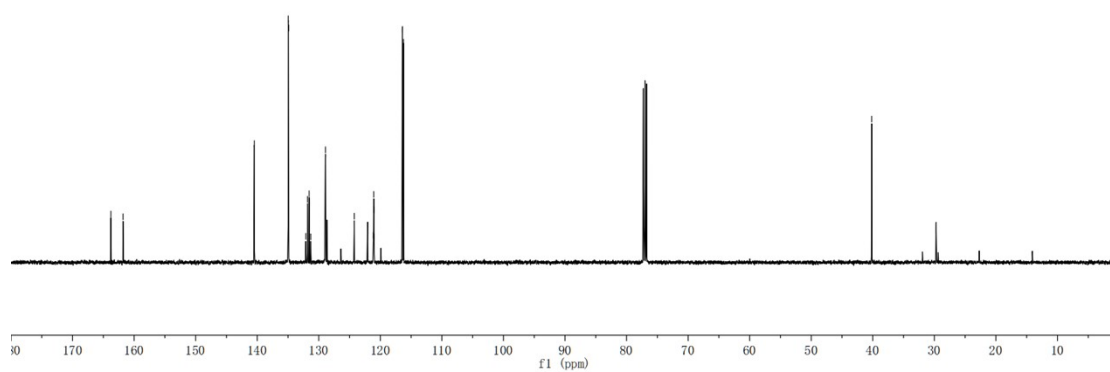
A017-43B.10.f
C13CPD CDCl3

163.77
161.79
140.37
134.97
134.90
132.10
131.83
131.57
131.30
128.91
124.24
121.13
121.10
121.07
121.04
121.01
116.41
116.23

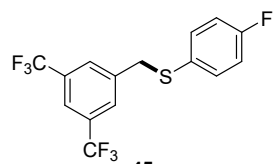
-40.18



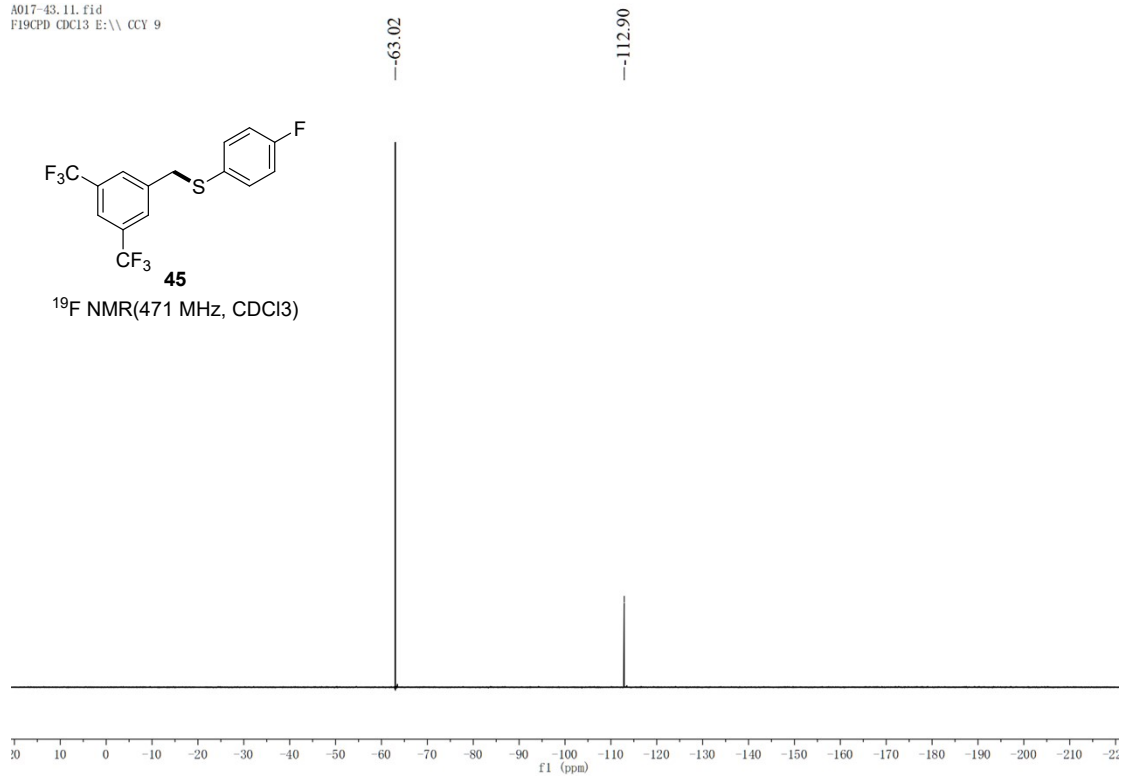
¹³C NMR(126 MHz, CDCl₃)



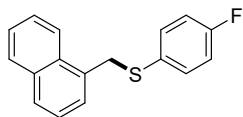
A017-43.11.fid
F19CPD CDCl3 E:\ \ CCY 9



¹⁹F NMR(471 MHz, CDCl₃)

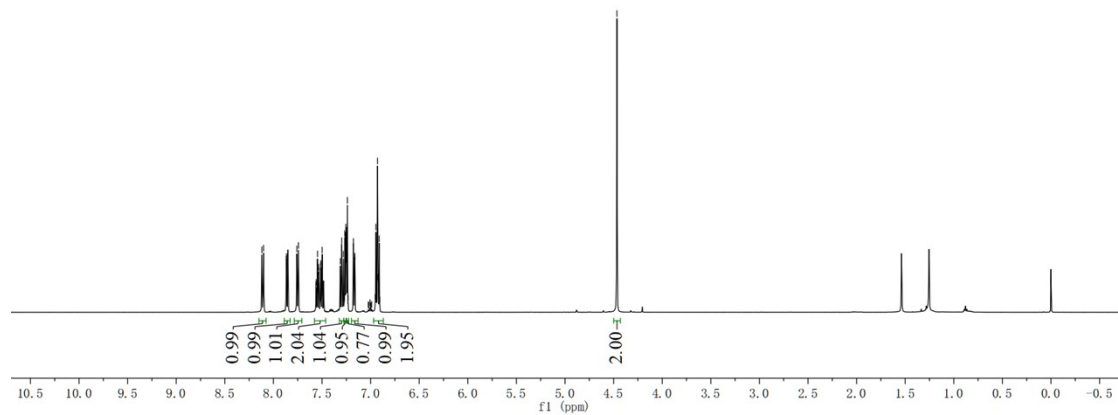


8.17
8.16
7.97
7.97
7.87
7.85
7.85
7.76
7.74
7.56
7.56
7.55
7.55
7.54
7.53
7.53
7.51
7.51
7.50
7.50
7.50
7.49
7.48
7.48
7.31
7.30
7.28
7.27
7.27
7.26
7.26
7.24
7.23
7.18
7.17
7.16
7.16
7.02
7.02
7.01
7.00
7.00
6.99
6.95
6.95
6.94
6.93
6.93
6.92
6.92
6.91
6.90
4.47

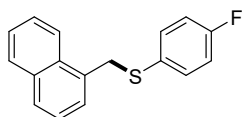


46

¹H NMR(500 MHz, CDCl₃)

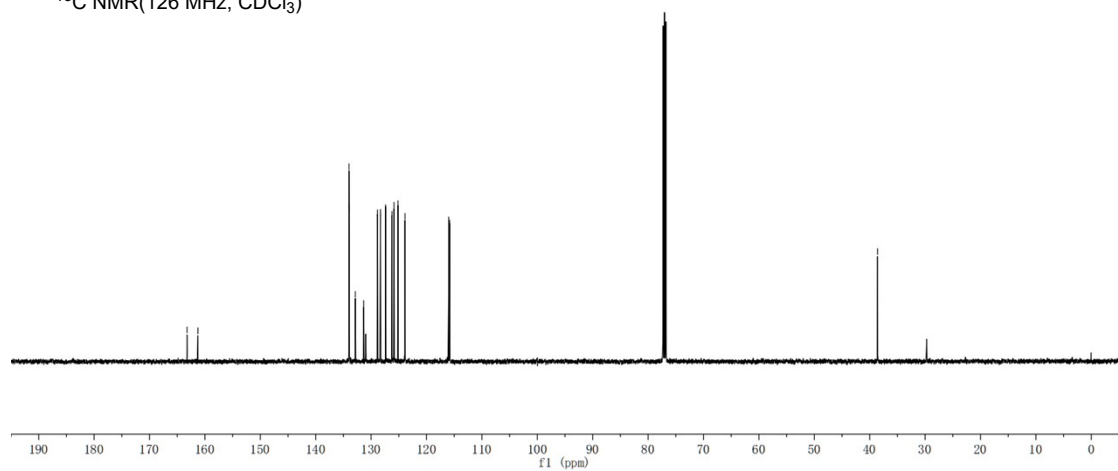


A017-120-1.10.fid
C13CPD CDCl3 E:\ \ CCY
163.22
161.26
133.99
133.93
132.85
131.34
128.84
128.31
127.39
126.23
125.86
125.15
123.88
116.00
115.82
-38.59

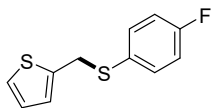


46

¹³C NMR(126 MHz, CDCl₃)

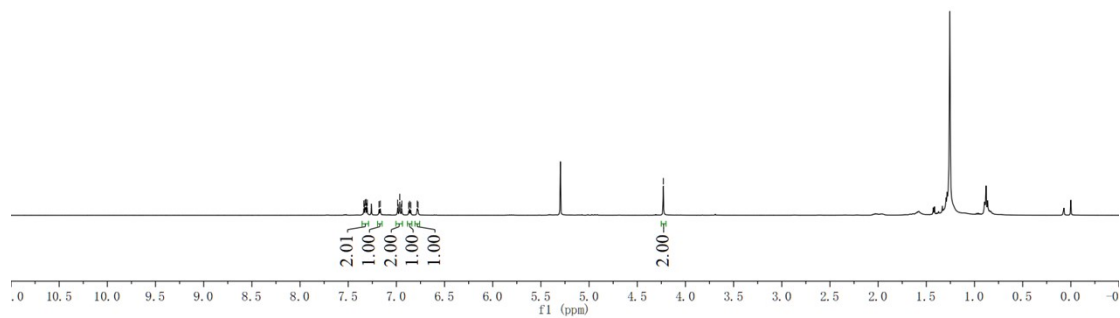


A017-126-1.1.fid
 PROTON CDCl3 (D:\20210808) f1
 7.34 7.33 7.32 7.32 7.31 7.30 7.18 7.17 6.99 6.98 6.97 6.95 6.94 6.87 6.86 6.85 6.78 6.78
 -4.23

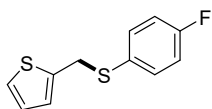


47

¹H NMR(500 MHz, CDCl₃)

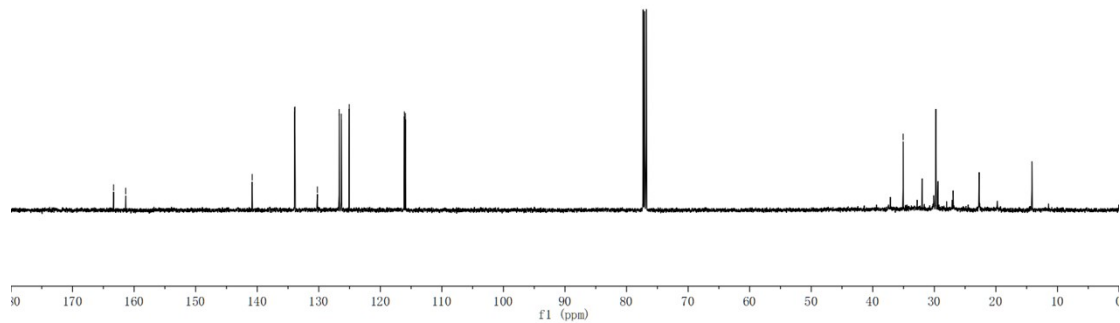


A017-45B.10.fid
 C13CPD CDCl3 f1
 163.33 161.36 140.82 133.92 133.86 130.23 126.69 126.35 125.05 116.09 115.92
 -35.07



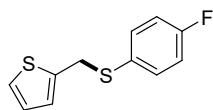
47

¹³C NMR(126 MHz, CDCl₃)



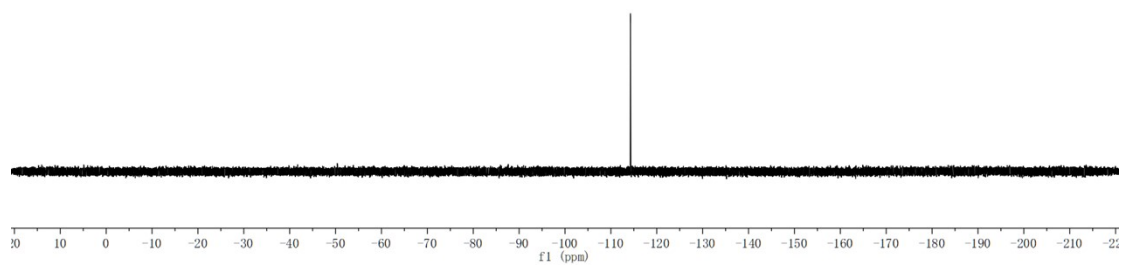
A017-45.11.fid
F19CPD CDCl3 E:\\ CCY 7

-114.26



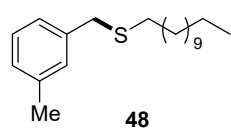
47

¹⁹F NMR(471 MHz, CDCl₃)

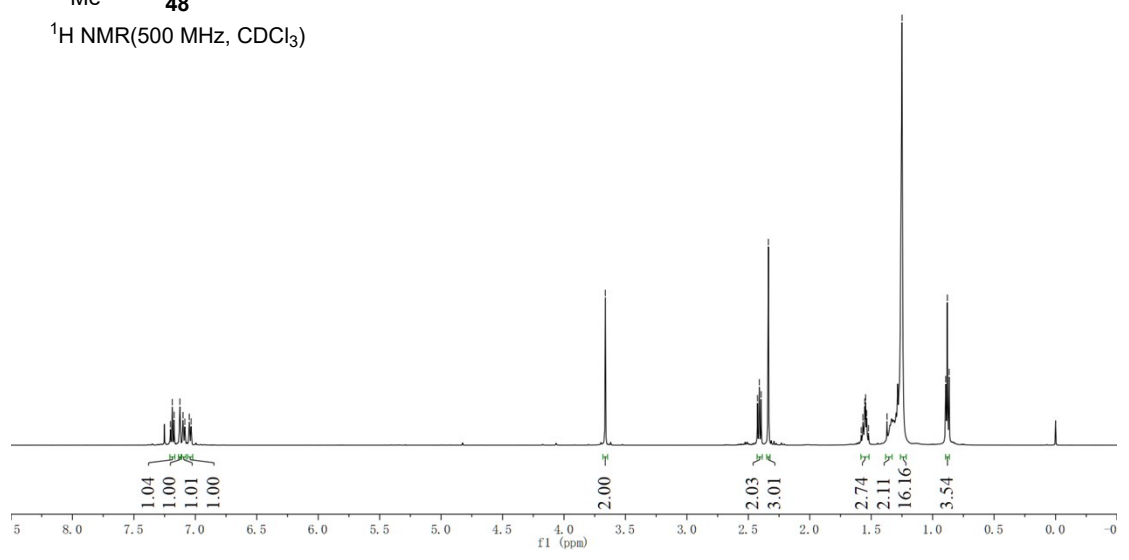


A017-148-1.10
 PROTON CDCl3
 7.26
 7.19
 7.17
 7.13
 7.10
 7.09
 7.03

-3.66
 2.43
 2.41
 2.40
 2.34
 1.58
 1.57
 1.55
 1.55
 1.54
 1.52
 1.37
 1.25
 0.89
 0.88
 0.87



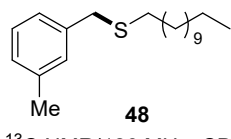
¹H NMR(500 MHz, CDCl₃)



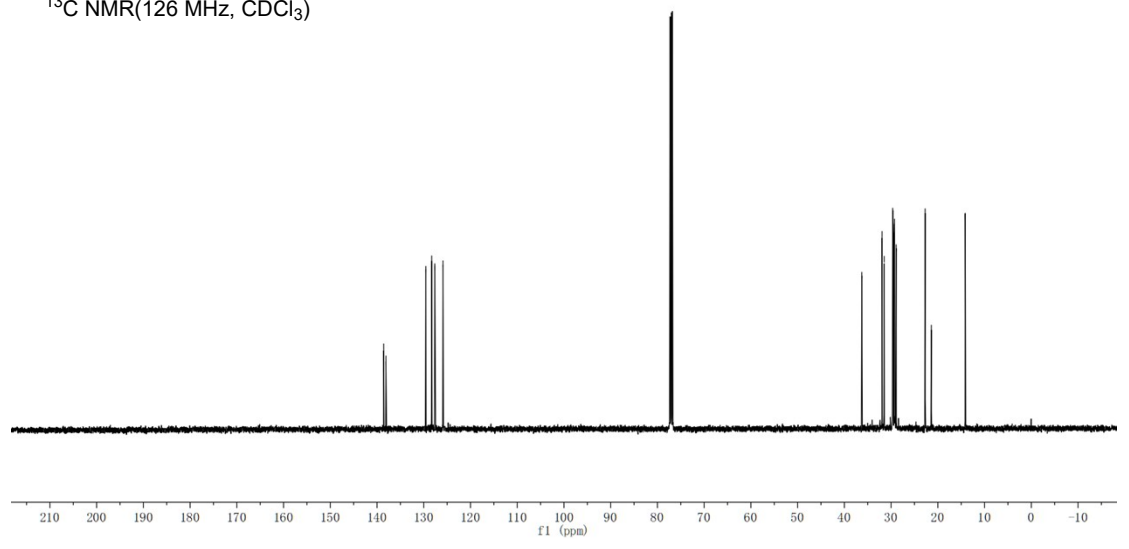
A017-148-1.11.fid
 C13CPD CDCl3 E:\ \ CCY 11

138.57
 138.10
 129.56
 128.30
 127.64
 125.88

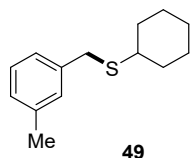
36.28
 31.94
 31.48
 29.68
 29.66
 29.62
 29.54
 29.37
 29.27
 29.26
 28.92
 22.71
 21.39
 14.14



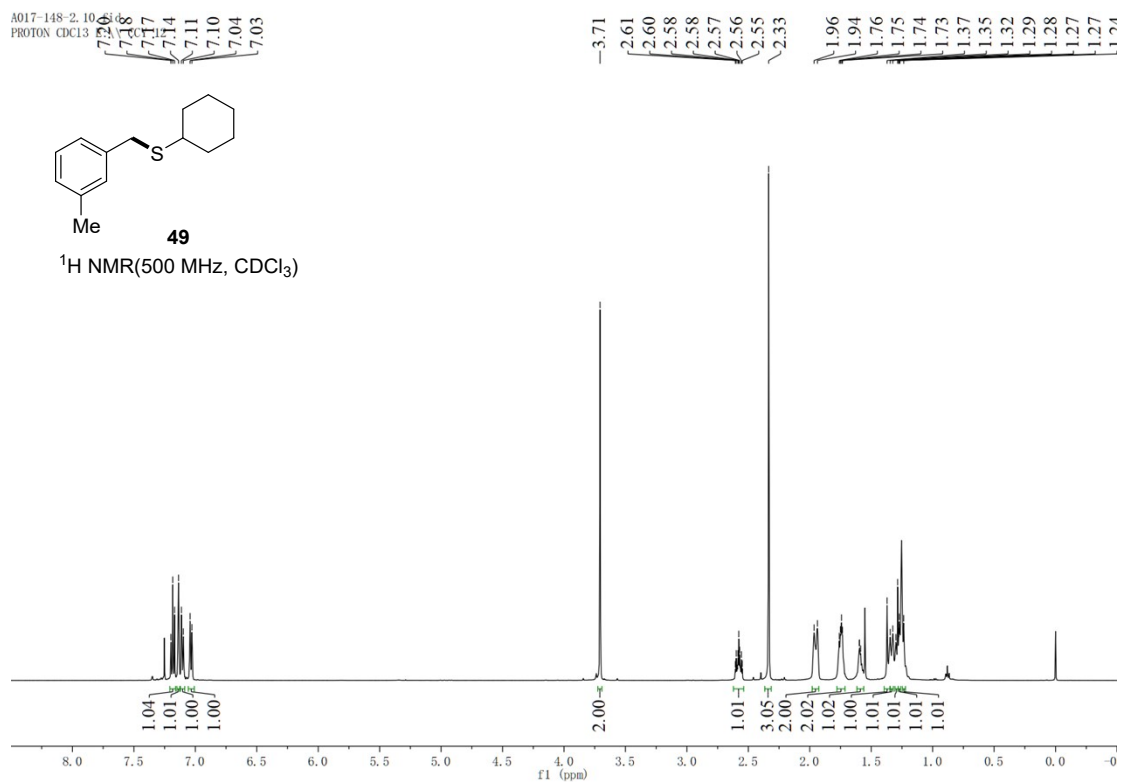
¹³C NMR(126 MHz, CDCl₃)



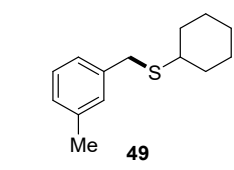
A017-148-2.10
PROTON CDCl₃



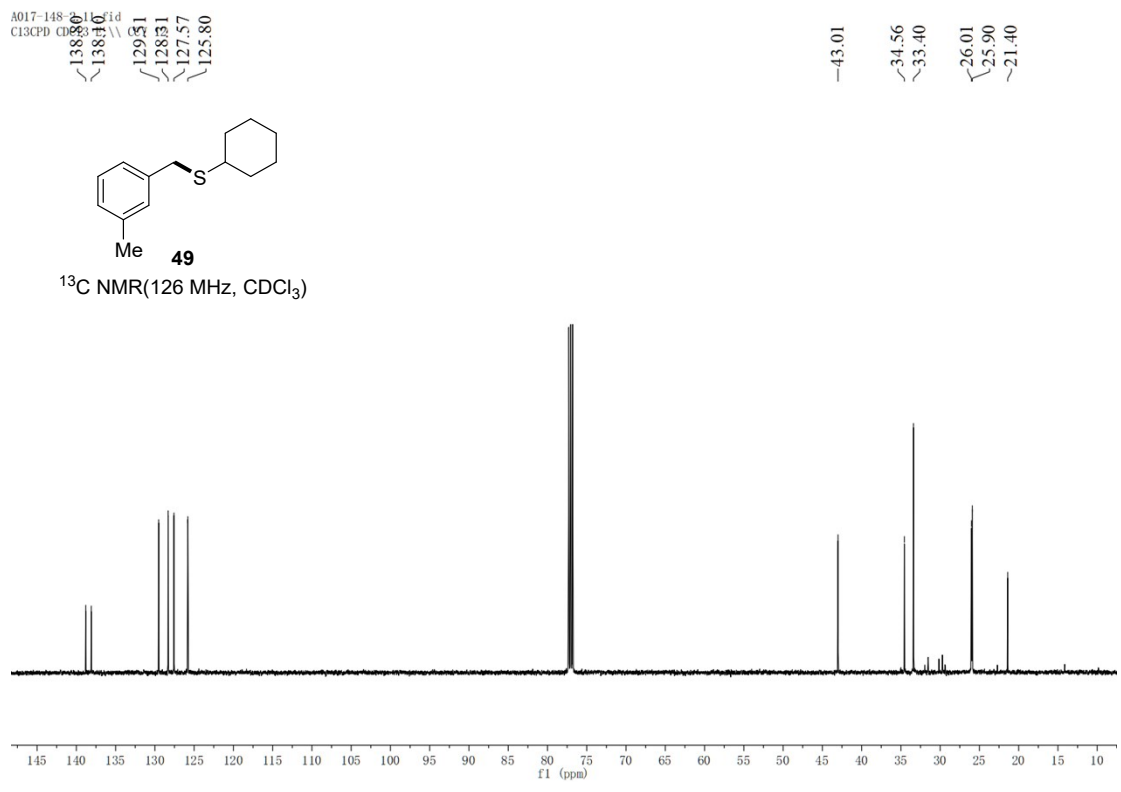
¹H NMR(500 MHz, CDCl₃)



A017-148-2.10
C13CPD CDCl₃



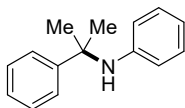
¹³C NMR(126 MHz, CDCl₃)



A017-48b.10.fid
PROTON DMSO E:\ \ CCY 22

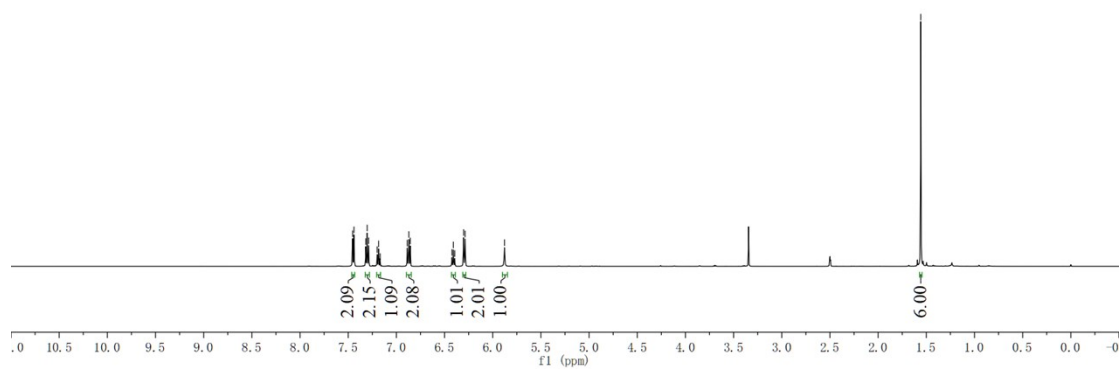
7.45
7.44
7.32
7.30
7.29
7.20
7.18
7.17
6.89
6.87
6.86
6.42
6.41
6.39
6.30
6.29
5.88

-1.56



50

¹H NMR(500 MHz, CDCl₃)

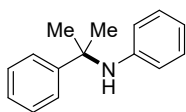


A017-48b.11.fid
C13CPD DMSO E:\ \ CCY

148.87
147.29
128.82
128.68
126.45
125.82
115.85
115.03

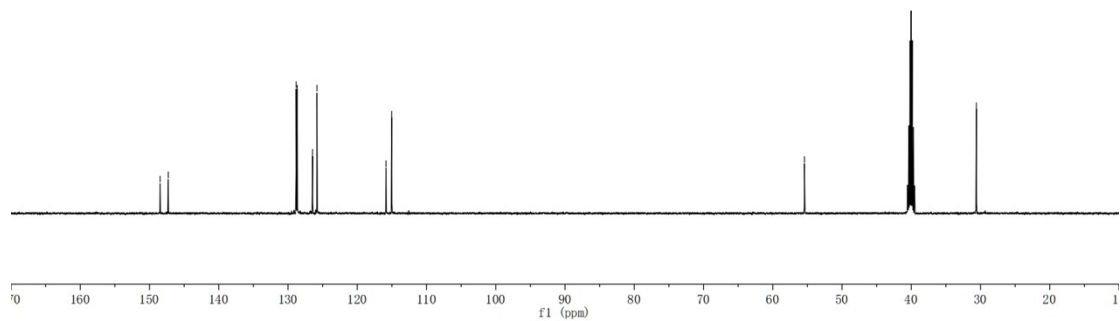
-55.42

-30.60

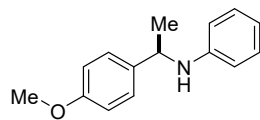


50

¹³C NMR(126 MHz, CDCl₃)

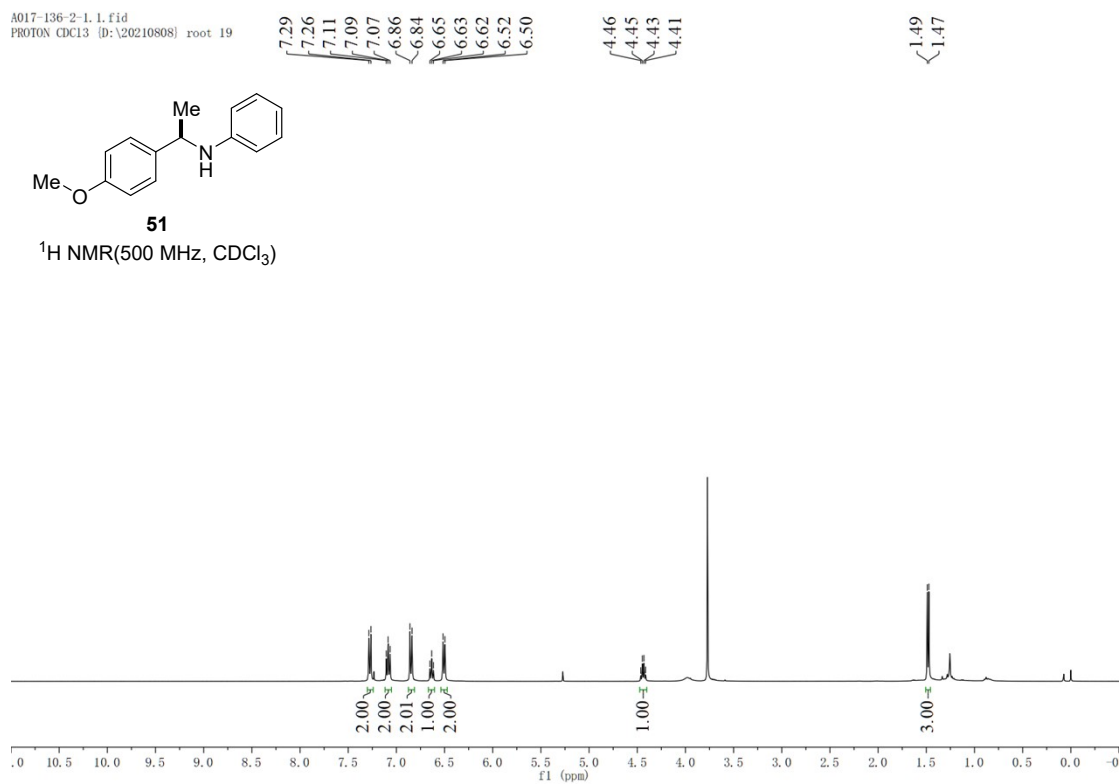


A017-136-2-1.1.fid
PROTON CDCl3 (D:\20210808) root 19

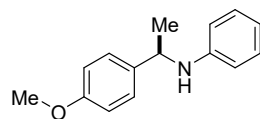


51

¹H NMR(500 MHz, CDCl₃)

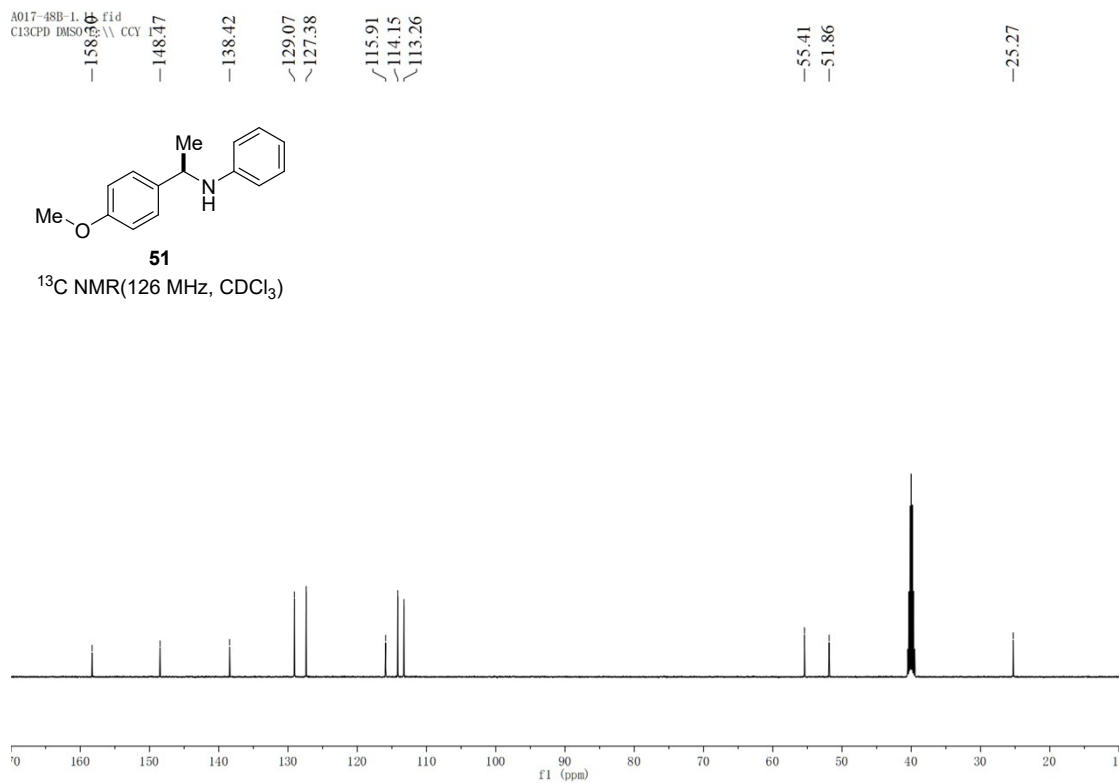


A017-48B-1.fid
C13CPD DMSO



51

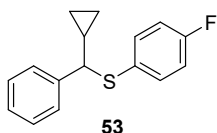
¹³C NMR(126 MHz, CDCl₃)



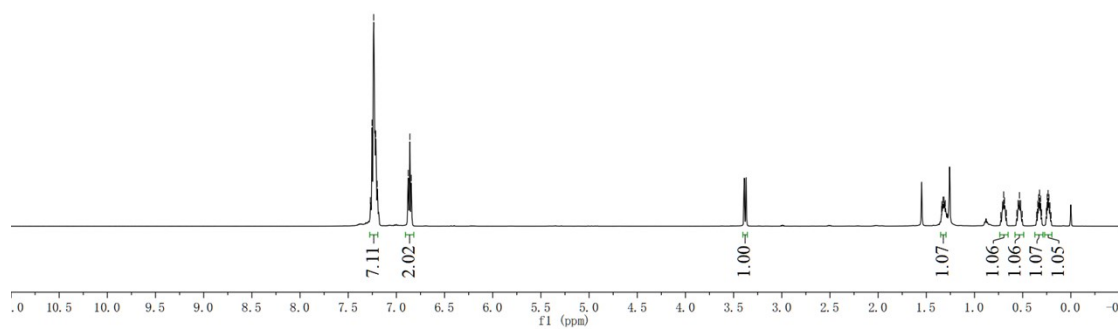
A029-41.10.fid
PROTON CDCl3 E:\\\\ CCY 18

7.27
7.25
7.24
7.21
7.20
6.88
6.86
6.85

1.34
1.34
1.33
1.32
1.30
0.73
0.71
0.70
0.69
0.67
0.56
0.55
0.53
0.52
0.50
0.36
0.34
0.33
0.32
0.31
0.30
0.25
0.25
0.24
0.23
0.22
0.21



¹H NMR(500 MHz, CDCl₃)



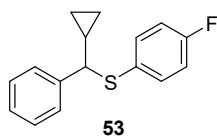
A029-41.10.fid
C13 CDCl3 E:\\\\ CCY 18

166.17
166.16
141.99
136.18
136.11
128.24
127.88
127.12
115.66
115.49

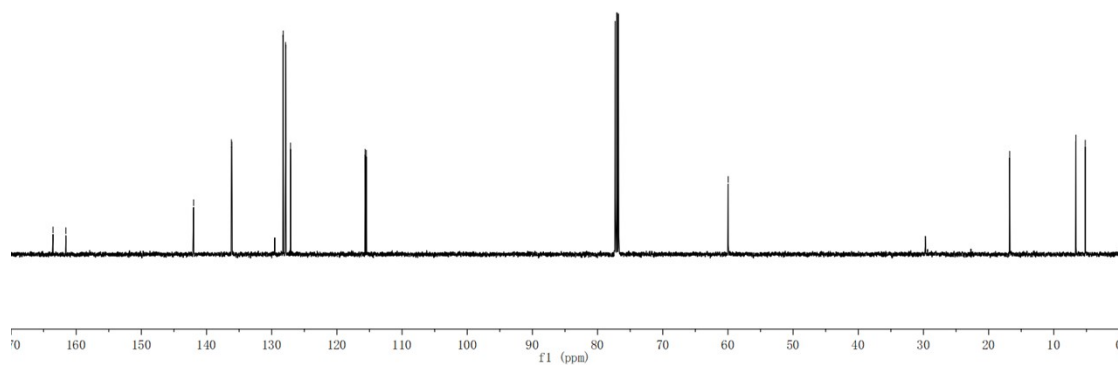
59.97

16.78

6.61
5.18

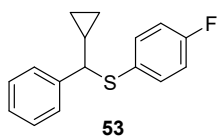


¹³C NMR(126 MHz, CDCl₃)

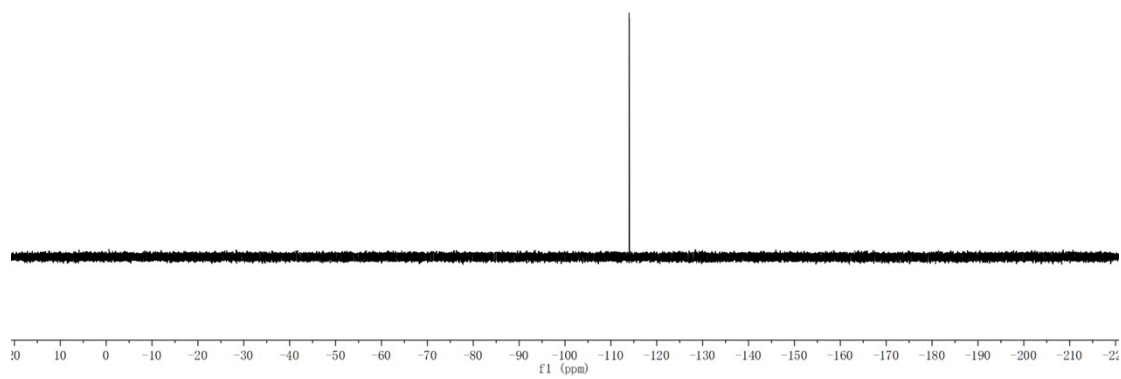


A017-49.11.fid
F19CPD CDCl3 E:\\ CCY 12

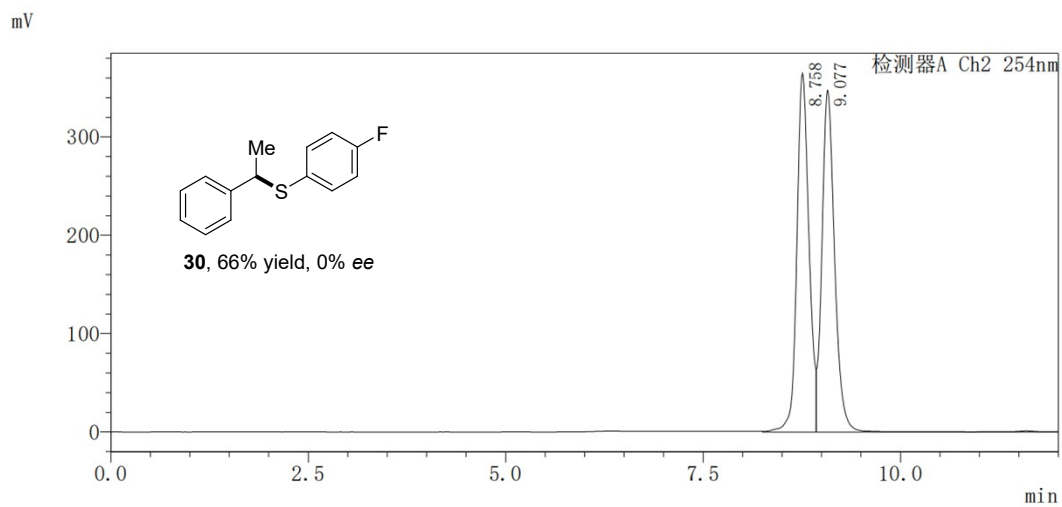
--113.97



¹⁹F NMR(471 MHz, CDCl₃)



2. Spectroscopic Data (HPLC Trace)



PDA Ch2 254nm

Peak#	Resolution Time	Area	Height	Area %	Height %
1	8.758	3910792	364791	49.622	51.219
2	9.077	3970440	347423	50.378	48.781
Total		7881232	712214	100.000	100.000

III. References

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