Supporting Information

Reaction of arynes with sulfoxides

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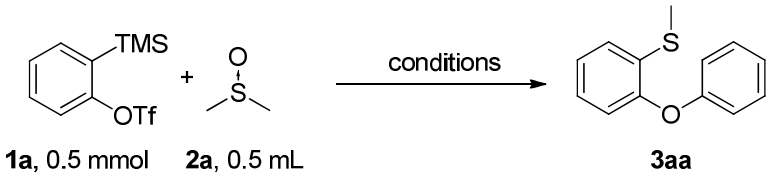
Contents

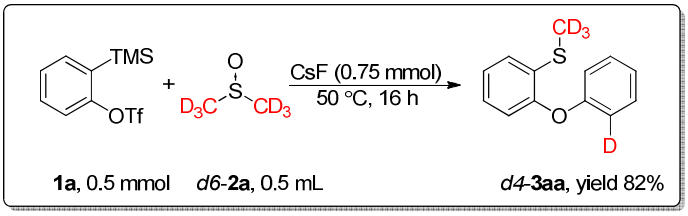
1. Table 1S. Optimization of the reaction conditions[a]



Entry	Fluoride	Temperature (°C)	Yield (%)
1	n-Bu_4NF	25	trace
2	KF	25	trace
3	AlF_3	25	0
4	CaF_2	25	0
5	NaF	25	0
6	MgF_2	25	0
7	CsF	25	23
8	CsF	40	35
9	CsF	50	39
10	CsF	60	38
11[b]	CsF	50	80

[a]Reaction Conditions: **1a** (0.5 mmol), **2a** (0.5 mL) and fluoride (0.75 mmol) under air for 3 h, isolated yield. [b]16 h.

2. The reaction of benzyne with *d6*-DMSO



To disclose the position of deuteration, we have performed 1D and 2D NMR experiments (Scheme 1S-5S). Based on our observation, we conclude that the site of deuteration is in the *ortho* position of **3aa**. Herein, we supply our analysis in this SI.

1) General remarks:

As described in the ref. 1 (Vanderheiden, S.; Bulat, B.; Zevaco, T.; Jung, N.; Brase, S., *Chem. Commun.* **2011**, *47*, 9063-9065.), when carbons are directly connected to deuterium, the ^{13}C NMR signals are often hard to detect owing to the lower sensitivity compared to ^{1}H NMR. Our observations are in agreement with this reported.[1]

2) Analysis of ^{1}H NMR and ^{13}C NMR

As shown in Scheme 1S and 2S, in the^{13}C NMR spectrum of *d4*-**3aa**, the carbon signals of -CD_3 (14.849 ppm) and -CD (two C_a at 117.891ppm *vs* one C_a at 117.915 ppm) are both disappeared.[1] Moreover, the symmetry of meta-position(C_b) is broken due to the deuteration. Compared with **3aa**, a new carbon signal (129.584 ppm) is appeared in the spectrumof *d4*-**3aa** (Scheme 1S). The ^{1}H NMR spectrum of *d4*-**3aa** clearly indicates that one proton signal (6.959-6.981 ppm) is disappeared (Scheme 2S).

3) Analysis of HSQC of 3aa and *d4*-3aa

The deuteration in *ortho* position was further verified with the aid of HSQC two-dimensional NMR experiments (Scheme 3S, 4S). Both HSQC spectrums of *d4*-**3aa** and **3aa** showed that H signals (6.96-6.98 ppm, Peak 1) were correlated to C signal (117.9 ppm), and H signals (7.30-7.34 ppm, Peak 2) were correlated to C signal (129.7). The chemical shifts of CaHa are less than that of CbHb because of the electron-donating effect of O-group effect. Thus the chemical shifts at 6.96-6.98 ppm (H signals, Peak 1) and 117.9 ppm (C signal) were assigned for *ortho* position. We also performed ^{1}H-^{1}H COSY spectrum of *d4*-**3aa** (Scheme 5S), and the result showed the correlations as follows:

Peak 1 with Peak 2; Peak 2 with Peak 1 and Peak 3.

From the correlations in the HSQC and COSY spectra, the following signals were assigned:

ortho position of **3aa**: Peak 1, H_a, 6.96-6.98 ppm; C_a, 117.9 ppm.

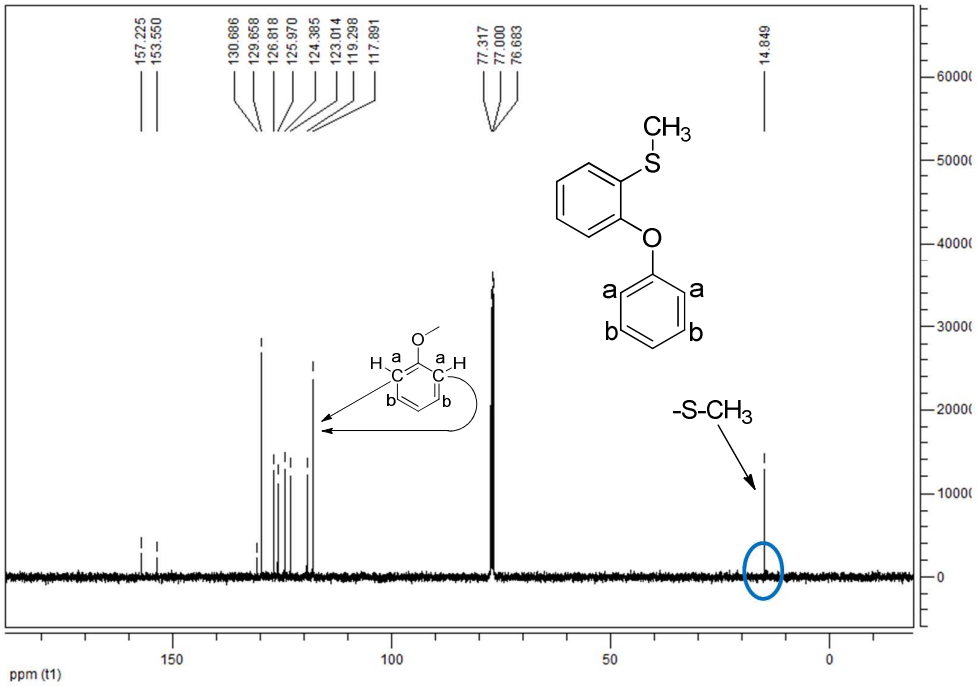
meta position of **3aa**: Peak 2, H_b, 7.30-7.34 ppm; C_b, 129.7 ppm.

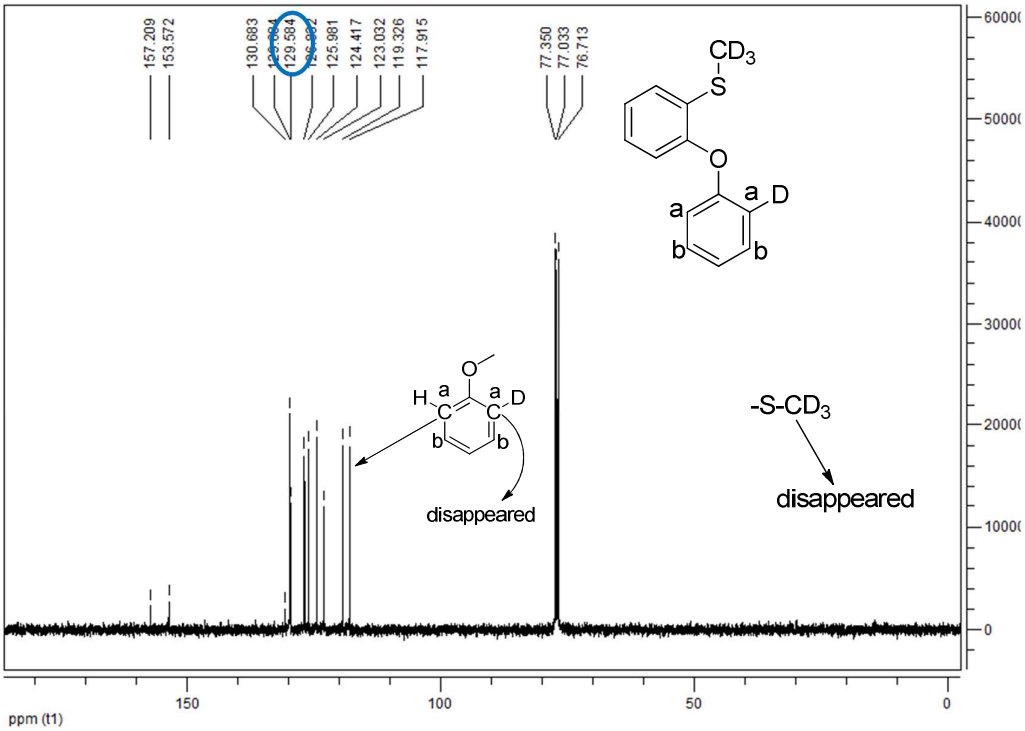
ortho position of *d4*-**3aa**: Peak 1, H_a, 6.96-6.98 ppm; C_a, 117.9 ppm.

meta position of *d4*-**3aa**: Peak 2, H_b, 7.30-7.34 ppm; C_b, 129.6, 129.7 ppm.

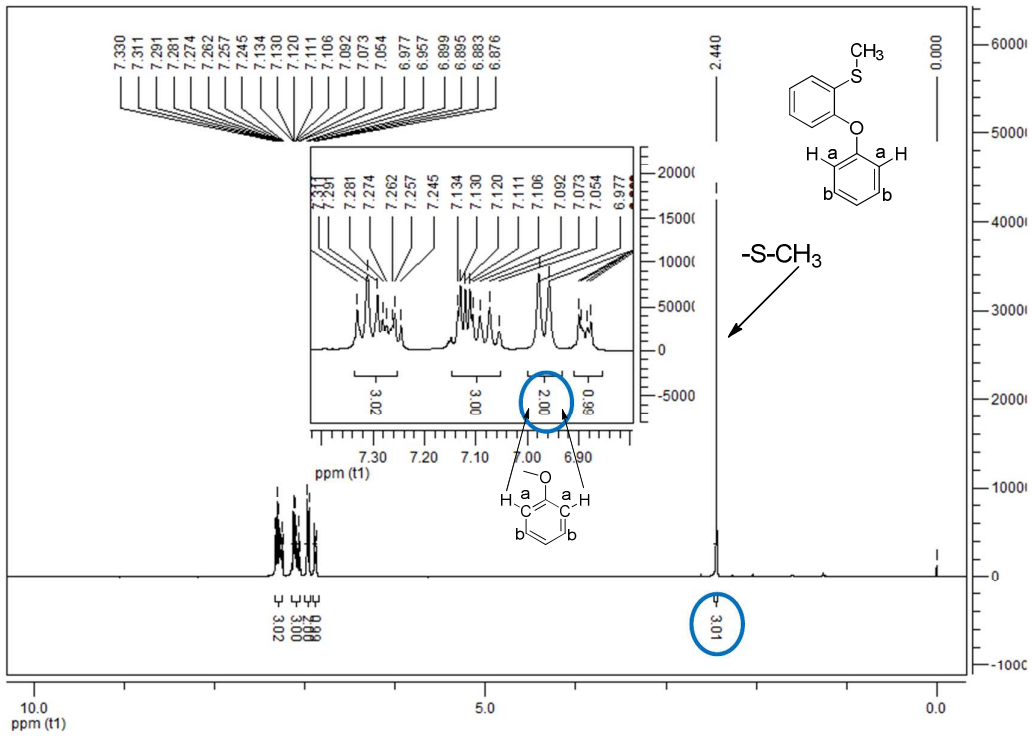
In summary, these results clearly indicate the deuteration is in *ortho* position.

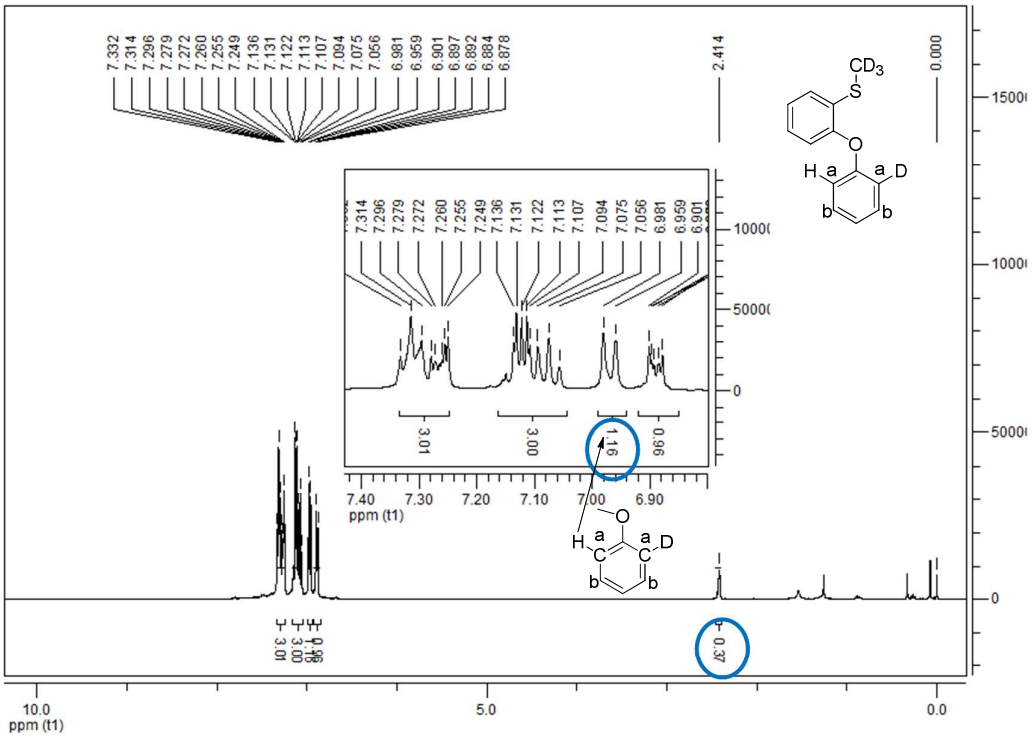
Scheme 1S. The ^{13}C NMR of 3aa and *d4*-3aa



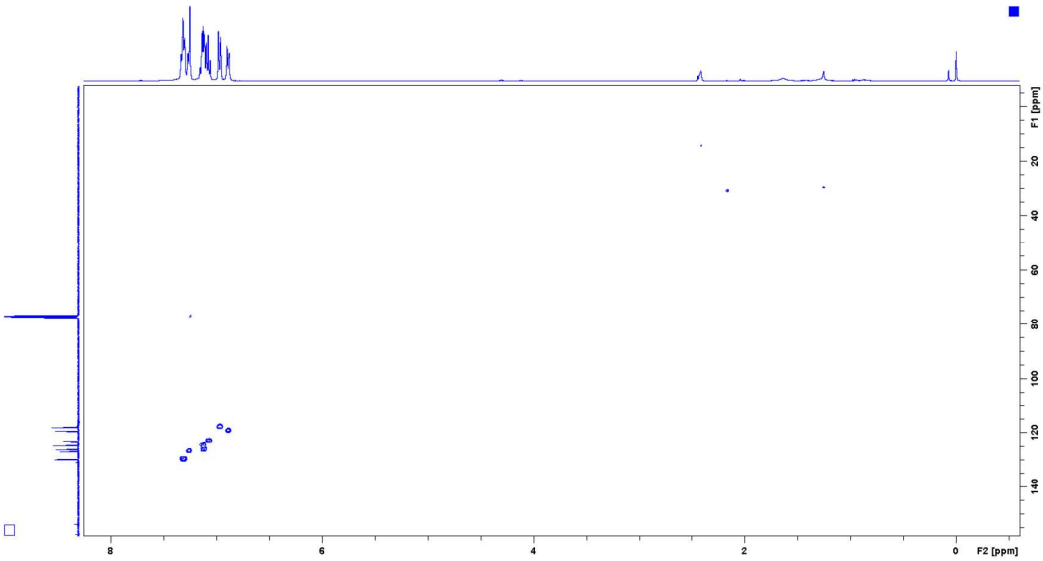


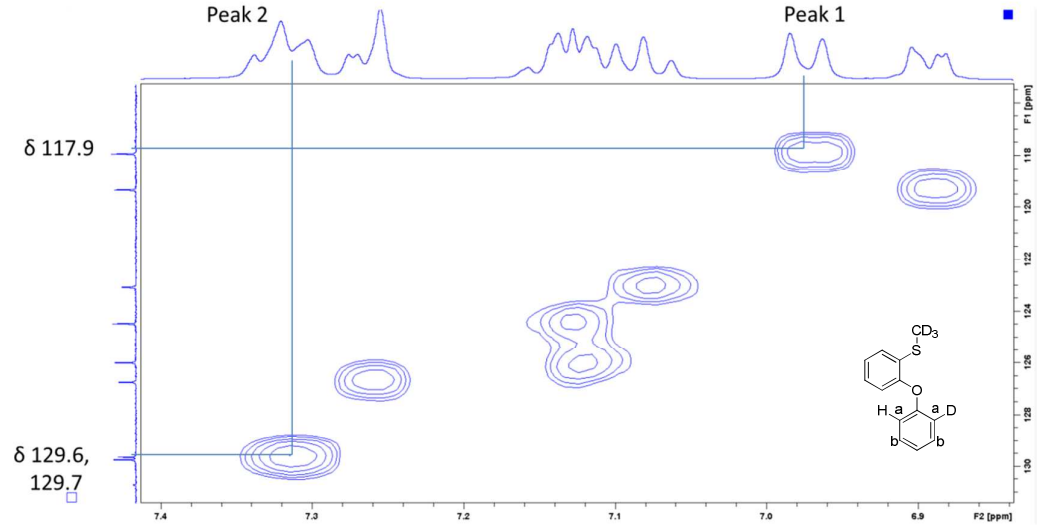
Scheme 2S. The ^{1}H NMR of 3aa and *d4*-3aa



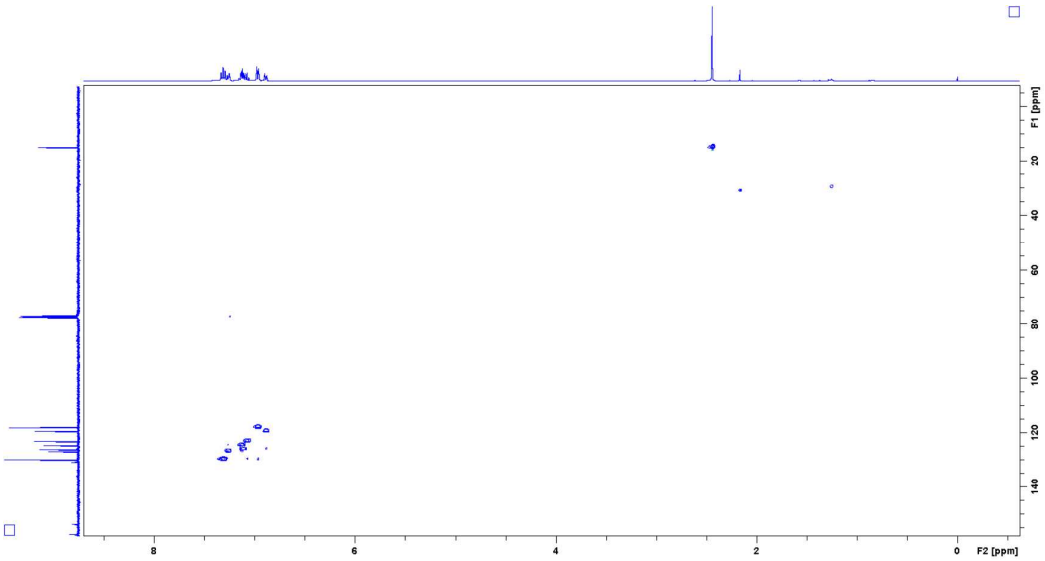


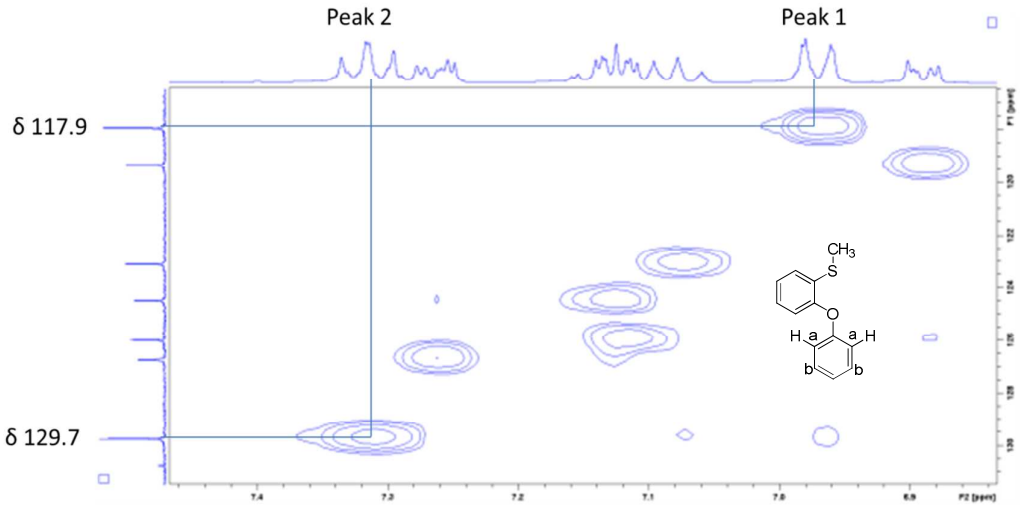
Scheme 3S. HSQC of *d4*-3aa



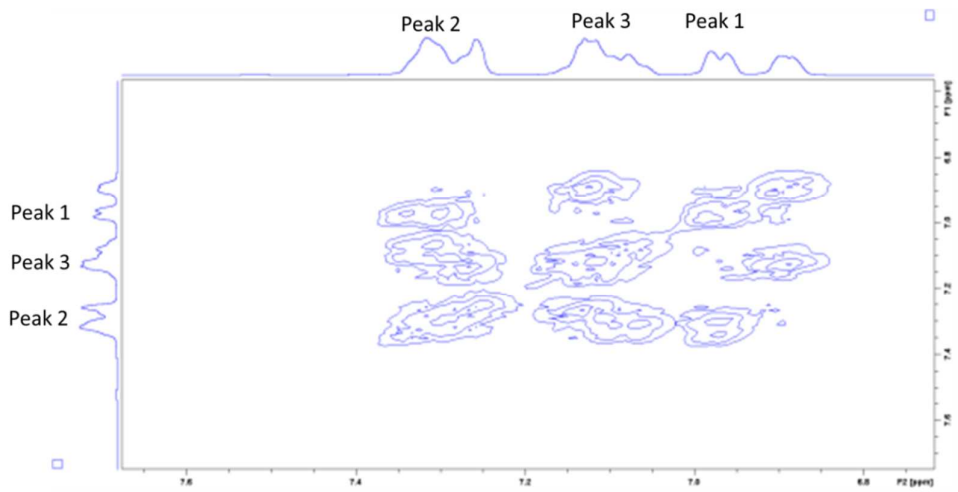


Scheme 4S. HSQC of 3aa



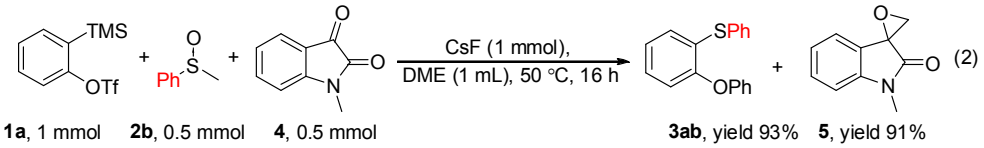


Scheme 5S. ^{1}H-^{1}H COSY of *d4*-3aa



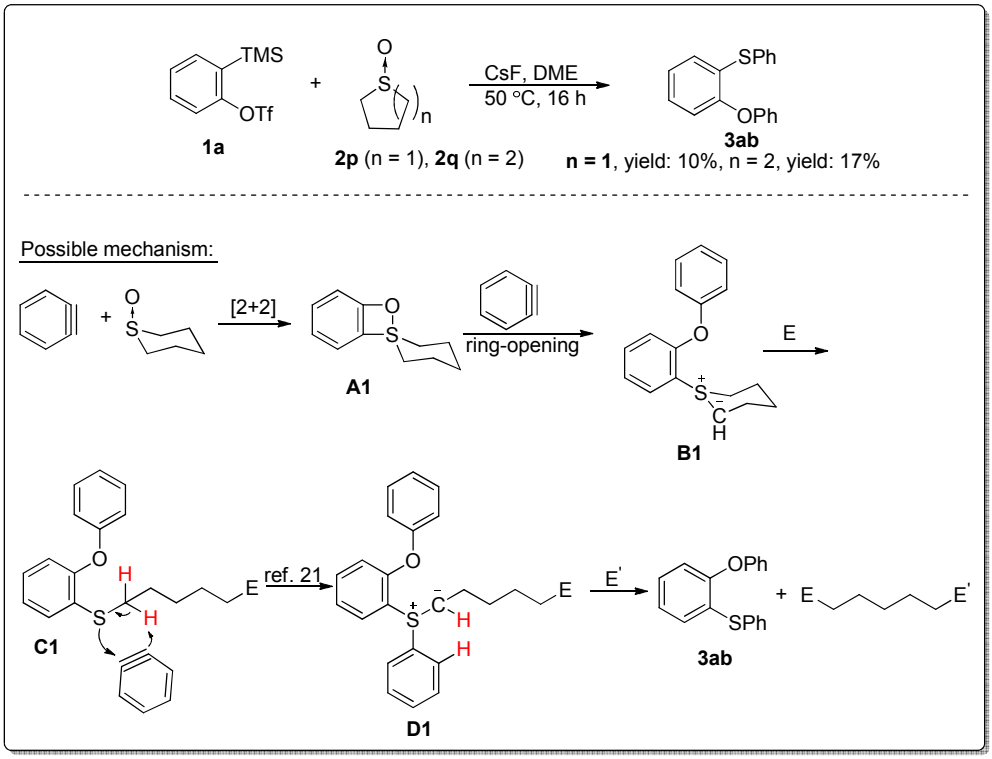
3. Ylide trapping experiment with 2b and isatin

Scheme 6S. Ylide trapping experiment with 2b and isatin



4. Reactions of cyclic sulfloxide and unsymmetrical 3-methoxybenzyne

Scheme 7S. The reaction of benzyne with cyclic sulfloxide 2p or 2q.



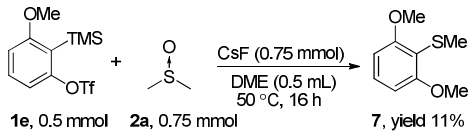
When the cyclic sulfloxide **2p** or **2q** was used as a substrate, the double de-alkylation of sulfoxide was occurred. Three molecules of benzyne participated in assembling the product **3ab**, accompanying the double de-alkylation of sulfoxide (Scheme 7S). The reactions gave low yields (10% and 17%). Based on our primary results and previous report (Ref. 21 in maintext), we herein present a possible mechanism to explain the formation of unexpected product **3ab** (Scheme 7S). The product thioether **C1** could be obtained *via* the formation of **A1** and subsequent ylide reaction of **B1** with **E**. This pathway has been described in the Scheme 4

in the maintext. However, we think that **C1** is not the final product. The reaction does not stop at the stage of formation of **C1**, and a subsequent reaction of **C1** with benzyne occurs to give another ylide **D1**, which undergoes ylide reaction with electrophile **E'** to provide product **3ab**. The similar ylide forming pathway of **D1** from benzyne and thioether has been recently disclosed by ref. 21. In the cases of cyclic sulfloxide **2p** and **2q**, we speculated that above side-reactions led to the unexpected product **3ab**.

Ref. 21 in maintext:

(21) Xu, H.-D.; Cai, M.-Q.; He, W.-J.; Hu, W.-H.; Shen, M.-H. *RSC Adv.* **2014**, *4*, 7623.

Scheme 8S. The reaction of unsymmetrical 3-methoxybenzyne with DMSO.



As shown in Scheme 8S, the reaction of unsymmetrical 3-methoxybenzyne **1e** produced a mixture of isomers, which could not be separated using column chromatography. Only one insertion product **7** was obtained by HPLC.

5. Experimental details and characterization data for compounds 3-7

5.1 General remarks

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE AV400 (400MHz for H and 100MHz for C). Signal positions were recorded in ppm with the abbreviations s, d, t, q, and m denoting singlet, doublet, triplet, quartet, and multiplet respectively. All NMR chemical shifts were referenced to residual solvent peaks or to $Si(CH_3)_4$ as an internal standard. NMR Spectra recorded in $CDCl_3$ were referenced to residual $CHCl_3$ at 7.26 ppm for ^{1}H or 77.0 ppm for ^{13}C. NMR spectra recorded in CD_3OD were referenced to residual CH_3OH at 3.34 ppm for ^{1}H or 49.86 ppm for ^{13}C. All coupling constants *J* were quoted in Hz. Data were reported as follows: chemical shift, multiplicity, coupling constant and integration. Reactions were monitored by thin-layer chromatography (TLC) on 0.25mm silica gel glass plates coated with 60 F254. Column chromatography was performed on silica gel (200-300 mesh) using a mixture of petroleum ether (60-90°C)/ethyl acetate as eluant. Commercially available reagents were used as received without further purification. Raw materials **1c**[2], **2b-2p**[3] were prepared relied on the related references.

5.2 Representative Procedure

Preparation of methyl(2-phenoxyphenyl)sulfane 3aa

2-(Trimethylsilyl)phenyl trifluoromethanesulfonate **1a** (0.5 mmol, 122 μL, 1 equiv) was added to a mixture of DMSO **2a** (7.0 mmol, 0.5 mL, 14 equiv) and CsF (0.75 mmol, 113 mg, 1.5 equiv) under air. The mixture was stirred at 50 °C for 16 h. Then 10 mL of water was added to the reaction mixture. The resulting mixture was extracted by ethyl acetate (10 mL) for 3 times. The combined organic phase was concentrated under reduced pressure and the residue was purified by silica gel column chromatography to give the product methyl(2-phenoxyphenyl)sulfane **3aa** (43 mg, 80%).

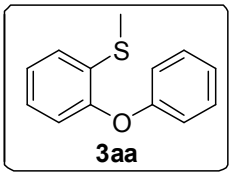
Preparation of (2-phenoxyphenyl)(phenyl)sulfane 3ab and

(2-methoxyphenyl)(phenyl)sulfane 6ab

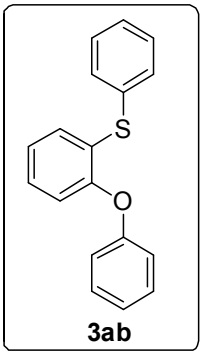
2-(Trimethylsilyl)phenyl trifluoromethanesulfonate **1a** (0.5 mmol, 122 μL, 1 equiv) was added to a mixture of methyl phenyl sulfoxide **2b** (0.75 mmol, 105 mg, 1.5 equiv), CsF (0.75 mmol, 113 mg, 1.5 equiv) and DME (0.5 mL) under air. The mixture was stirred at 50 °C for 16 h. Then 10 mL of water was added to the reaction mixture. The resulting mixture was extracted by ethyl acetate (10 mL) for 3 times. The combined organic phase was concentrated under reduced pressure and the residue was purified by silica gel column chromatography to give the product (2-phenoxyphenyl)(phenyl)sulfane **3ab** (46 mg, 72%) and (2-methoxyphenyl)(phenyl)sulfane **6ab** (20 mg, 8%).

5.3 The characterization of the products

Methyl(2-phenoxyphenyl)sulfane (3aa). White solid (43.2 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.25 (m, 3H), 7.13-7.05 (m, 3H), 6.97 (d, J = 8.0 Hz, 2H), 6.90-6.88 (m, 1H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 153.6, 130.7, 129.7, 126.8, 126.0, 124.4, 123.0, 119.3, 117.9, 14.8; HRMS (ESI) m/z calcd for $C_{13}H_{12}OS[M+Na]^+$: 239.0501, found 239.0505.



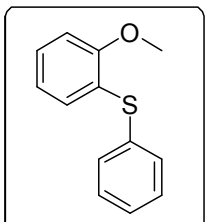
3aa



3ab

(2-Phenoxyphenyl)(phenyl)sulfane (3ab). Yellow oil (45.9 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42-7.40 (m, 2H), 7.33-7.24 (m, 5H), 7.20-7.16 (m, 2H), 7.08 (t, J = 7.6 Hz, 1H), 7.04-6.99 (m, 1H), 6.94-6.89 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 154.7, 134.0, 132.3, 131.7, 129.7, 129.2, 128.4, 128.1, 127.5, 124.2, 123.2, 119.4, 118.3; HRMS (ESI) m/z calcd for $C_{18}H_{14}OS[M+Na]^+$: 301.0658, found 301.0663.

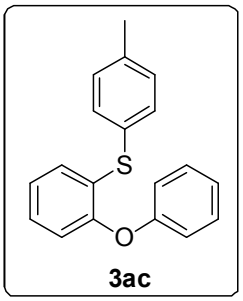
(2-Methoxyphenyl)(phenyl)sulfane (6ab). Yellow oil (19.5 mg, 8%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.29 (m, 4H), 7.27-7.25 (m, 1H), 7.24-7.22 (m, 1H), 7.09 (dd, J = 1.6 Hz, J = 7.6 Hz, 1H), 6.92-6.86 (m, 2H); 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.4, 134.5, 131.7, 131.5, 129.1, 128.3, 127.0, 124.1, 121.2, 110.9, 55.9; HRMS (ESI) m/z



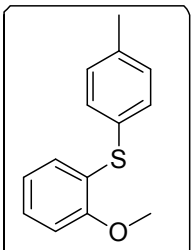
6ab

calcd for $C_{13}H_{12}OS[M+Na]^+$: 239.0501, found 239.0504.

(2-Phenoxyphenyl)(p-tolyl)sulfane (3ac). Yellow oil. (43.8 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.29 (m, 4H), 7.16-6.95 (m, 8H), 6.89 (d, *J* = 8.0 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 153.9, 138.1, 133.5, 130.3, 130.2, 129.9, 129.6, 129.4, 127.3, 124.2, 123.1, 119.4, 118.2, 21.2; HRMS (ESI) m/z calcd for $C_{19}H_{16}OS[M+Na]^+$: 315.0814, found 315.0817.



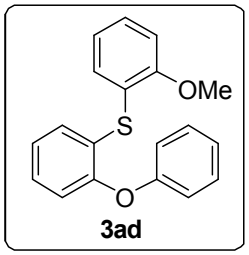
3ac



6ac

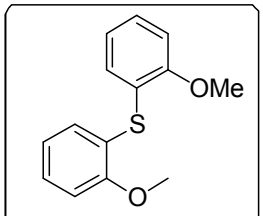
(2-Methoxyphenyl)(p-tolyl)sulfane (6ac). Yellow oil. (11.5 mg, 10%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (d, *J* = 8.0 Hz,2H), 7.19-7.14 (m, 3H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.83(t, *J* = 7.6 Hz, 1H), 3.89 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.6, 137.7, 132.9, 130.1, 129.9, 129.8, 127.4, 125.7, 121.2, 110.6, 55.9, 21.1; HRMS (ESI) m/z calcd for $C_{14}H_{14}OS[M+Na]^+$: 253.0658, found 253.0649.

(2-Methoxyphenyl)(2-phenoxyphenyl)sulfane (3ad). Yellow oil (42.4 mg, 55%). (?? mg, 55%).^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.23 (m, 4H), 7.18-7.11 (m, 2H), 7.07 (t, *J* = 7.6 Hz, 1H), 7.02-6.95 (m, 3H), 6.92-6.88 (m, 3H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.3, 157.1, 155.2, 133.2, 131.7, 129.6, 129.0, 127.9, 127.1, 124.0, 123.2, 122.0, 121.2, 119.1, 118.5, 111.1, 55.9; HRMS (ESI) m/z calcd for $C_{19}H_{16}O_2S[M+Na]^+$: 331.0763, found 331.0760.

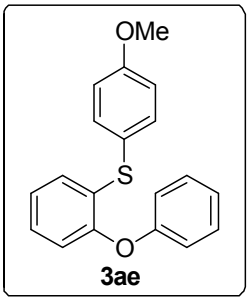


3ad

Bis(2-methoxyphenyl)sulfane (6ad). White solid (5 mg, 4%).^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26-7.22 (m, 2H), 7.06 (dd, *J* = 1.6 Hz, *J* = 7.6 Hz, 2H), 6.92-6.85 (m, 4H), 3.86 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.9, 132.0, 128.4, 122.7, 121.2, 110.8, 55.9; HRMS (ESI) m/z calcd for $C_{14}H_{14}O_2S[M+Na]^+$: 269.0607, found 269.0610.

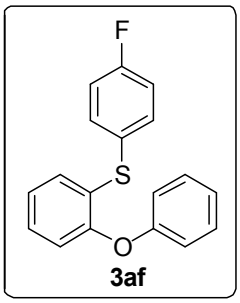


6ad



3ae

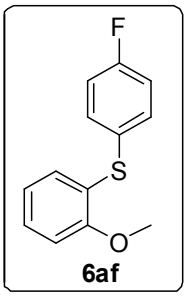
(4-Methoxyphenyl)(2-phenoxyphenyl)sulfane (3ae). Yellow oil (37.8 mg, 49%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.36 (m, 2H), 7.26-7.23 (m, 2H), 7.03-6.99 (m, 2H), 6.91-6.82 (m, 7H), 3.74(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.1, 157.2, 153.1, 136.3, 131.3, 129.7, 128.9, 126.7, 124.3, 123.1, 122.6, 119.3, 118.1, 115.1, 55.4; HRMS (ESI) m/z calcd for $C_{19}H_{16}O_2S[M+Na]^+$: 331.0763, found 331.0765.



3af

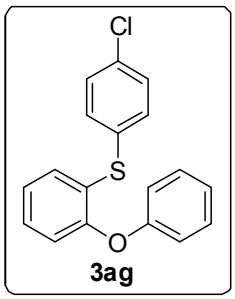
(4-Fluorophenyl)(2-phenoxyphenyl)sulfane (3af). White solid (40.0 mg, 54%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45-7.42 (m, 2H), 7.35-7.31 (m, 2H), 7.20-7.15 (m, 1H), 7.12-7.01 (m, 5H), 6.96-6.90 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.7 (d, J = 246.6 Hz), 157.0, 154.3, 135.1 (d, J = 8.4 Hz), 130.8, 129.7, 129.0, 128.6 (d, J = 3.3 Hz), 127.9, 124.3, 123.3, 119.5, 118.2, 116.4 (d, J = 21.8 Hz); HRMS (ESI) m/z calcd for $C_{18}H_{13}FOS[M+Na]^+$: 319.0563, found 319.0567.

(4-Fluorophenyl)(2-methoxyphenyl)sulfane (6af). Yellow oil (26.9 mg, 23%) ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.37 (m, 2H), 7.26-7.20 (m, 1H), 7.06-6.97 (m, 3H), 6.90-6.84 (m, 2H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4 (d, J = 245.9 Hz), 156.8, 134.4 (d, J = 8.0 Hz), 130.4, 129.0, 128.0, 125.0, 121.3, 116.3 (d, J = 21.9 Hz), 110.8, 55.9; HRMS (ESI) m/z calcd for $C_{13}H_{11}FOS[M+Na]^+$: 257.0407, found 257.0408.



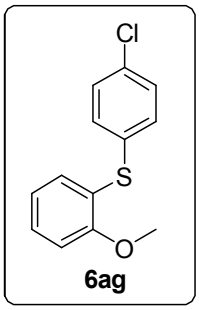
6af

(4-Chlorophenyl)(2-phenoxyphenyl)sulfane (3ag). White solid (39.8 mg, 51%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.19 (m, 8H), 7.10-7.02 (m, 2H), 6.92-6.90 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.9, 155.1, 133.4, 133.0, 132.3, 129.7, 129.6, 129.3, 128.7, 127.3, 124.3, 123.3, 119.5, 118.3; HRMS (ESI) m/z calcd for $C_{18}H_{13}ClOS[M+Na]^+$: 335.0268, found 335.0265.

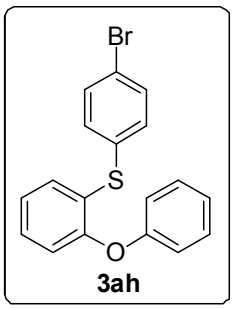


3ag

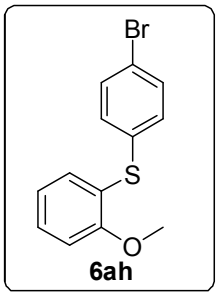
(4-Chlorophenyl)(2-methoxyphenyl)sulfane (6ag). White solid (20.0 mg, 16%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.24 (m, 5H), 7.15 (dd, *J* = 1.6 Hz, *J* = 7.6 Hz, 1H), 6.92-6.88 (m, 2H); 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.7, 133.7, 132.8, 132.4, 132.0, 129.2, 129.0, 123.0, 121.3, 111.1, 55.9; HRMS (ESI) m/z calcd for $C_{13}H_{11}ClOS[M+Na]^+$: 273.0111, found 273.0115.



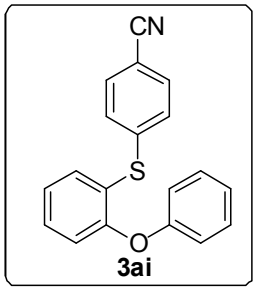
(4-Bromophenyl)(2-phenoxyphenyl)sulfane (3ah). White solid (40.9 mg, 46%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (d, *J* = 8.4 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.25-7.21 (m, 4H), 7.10-7.02 (m, 2H), 6.92-6.89 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.9, 155.3, 133.8, 133.0, 132.6, 132.2, 129.7, 128.8, 127.0, 124.3, 123.3, 121.3, 119.5, 118.3; HRMS (ESI) m/z calcd for $C_{18}H_{13}BrOS[M+Na]^+$: 378.9763, found 378.9765.



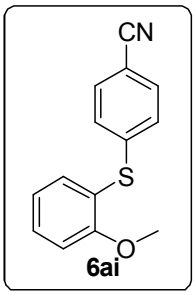
(4-Bromophenyl)(2-methoxyphenyl)sulfane (6ah). Yellow oil (23.5 mg, 16%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (d, *J* = 8.4 Hz, 2H), 7.30-7.25 (m, 1H), 7.18-7.14(m, 3H), 6.92-6.88 (m, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.8, 134.6, 132.7, 132.1, 132.0, 129.2, 122.6, 121.3, 120.6, 111.1, 55.9; HRMS (ESI) m/z calcd for $C_{13}H_{11}BrOS[M+Na]^+$: 316.9606, found 316.9605.



4-((2-Phenoxyphenyl)thio)benzonitrile (3ai). Yellow oil (21.2 mg, 28%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.17-7.08 (m, 2H), 6.97 (d, *J* = 8.4 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.6, 156.3, 144.4, 136.3, 132.2, 131.2, 129.8, 127.8, 124.3, 123.8, 122.0, 119.3, 118.8, 118.7, 108.9; HRMS (ESI) m/z calcd for $C_{19}H_{13}NOS[M+Na]^+$: 326.0610, found 326.0612.

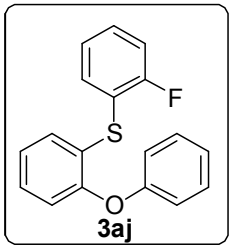


4-((2-Methoxyphenyl)thio)benzonitrile (6ai). White solid (15.7 mg, 13%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49-7.44 (m, 4H), 7.12 (d, J = 8.8 Hz, 2H), 7.03-6.99 (m, 2H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.6, 145.1, 136.6, 132.1, 131.6, 126.8, 121.6, 118.9, 118.1, 111.7, 108.3, 55.9; HRMS (ESI) m/z calcd for $C_{14}H_{11}NOS[M+Na]^+$: 264.0454, found 264.0456.



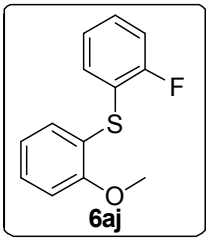
6ai

(2-Fluorophenyl)(2-phenoxyphenyl)sulfane (3aj). Yellow oil (34.0 mg, 46%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.26 (m, 4H), 7.22-7.16 (m, 2H), 7.12-7.08 (m, 3H), 7.05-7.01 (m, 1H), 6.96-6.90 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.9 (d, J = 246.2 Hz), 156.9, 155.0, 134.6, 131.4, 129.9, (d, J = 7.7 Hz) 129.7, 128.3, 126.6, 124.7, 124.2, 123.3, 119.3, 118.4, 116.1, 115.9; HRMS (ESI) m/z calcd for $C_{18}H_{13}FOS[M+Na]^+$: 319.0563, found 319.0564.



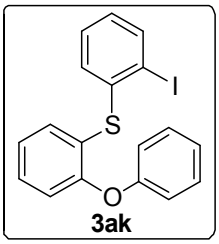
3aj

(2-Fluorophenyl)(2-methoxyphenyl)sulfane (6aj). Yellow oil (10.6 mg, 9%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.21 (m, 3H), 7.12-7.05 (m, 3H), 6.91-6.85 (m, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5 (d, J = 245.6 Hz), 157.5, 133.7, 131.4, 129.3 (d, J = 7.8 Hz), 128.6, 124.6, 122.3, 121.6 (d, J = 17.9 Hz), 121.3, 115.9 (d, J = 22.0 Hz), 111.0, 55.9; HRMS (ESI) m/z calcd for $C_{13}H_{11}FOS[M+Na]^+$: 257.0407, found 257.0406.



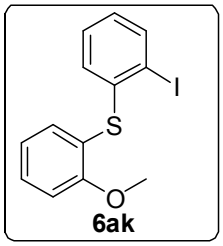
6aj

(2-Iodophenyl)(2-phenoxyphenyl)sulfane (3ak). White solid (24.3 mg, 24%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, J = 7.6 Hz, 1H), 7.32-7.23 (m, 5H), 7.17 (d, J = 7.6 Hz, 1H), 7.09-7.07 (m, 2H), 6.95-6.88 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.7, 156.1, 140.3, 139.8, 133.5, 130.9, 129.7, 129.4, 128.7, 128.0, 124.2, 123.5, 119.2, 118.8, 118.3, 101.3; HRMS (ESI) m/z calcd for $C_{18}H_{13}IOS[M+Na]^+$: 426.9624, found 426.9615.



3ak

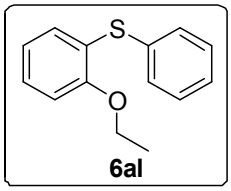
(2-Iodophenyl)(2-methoxyphenyl)sulfane (6ak). Yellow oil (25.7 mg, 15%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (dd, J = 1.2 Hz, J =8.0 Hz, 1H), 7.38-7.34 (m, 1H), 7.26-7.24 (m, 1H), 7.21-7.17 (m, 1H), 6.97-6.91 (m, 3H), 6.89-6.85 (m, 1H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ



6ak

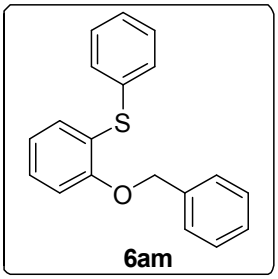
158.6, 141.1, 139.6, 134.2, 130.0, 129.4, 128.6, 127.3, 122.0, 121.5, 111.4, 99.6, 55.9.

(2-Ethoxyphenyl)(phenyl)sulfane (6al). Yellow oil (18.4 mg, 16%). ^{1}H NMR (400 MHz, $CDCl_3$):



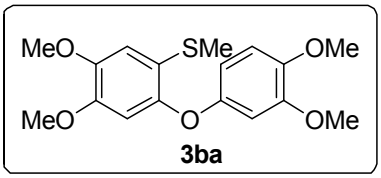
δ 7.30-7.28 (m, 2H), 7.24-7.09 (m, 4H), 7.01 (dd, J = 1.6 Hz, J = 7.6 Hz, 1H), 6.80-6.74 (m, 2H); 3.98 (q, J = 6.8 Hz, 2H), 1.26 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.6, 134.6, 131.7, 131.3, 129.0, 128.1, 127.0, 124.7, 121.0, 112.0, 64.3, 14.6; MS (EI) m/z calcd for $C_{14}H_{14}OS$: 230.0, found 230.0.

(2-(Benzyloxy)phenyl)(phenyl)sulfane (6am). Yellow oil (20.5 mg, 14%). ^{1}H NMR (400 MHz,



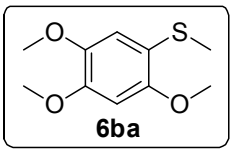
$CDCl_3$): δ 7.37-7.35 (m, 2H), 7.31-7.26 (m, 7H), 7.24-7.14 (m, 3H), 6.92 (d, J = 8 Hz, 1H), 6.89-6.85 (m, 1H); 5.11 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.5, 136.7, 134.8, 131.9, 131.4, 129.1, 128.4, 128.3, 127.7, 127.0, 125.5, 124.8, 121.5, 112.6, 70.4; MS (EI) m/z calcd for $C_{19}H_{16}OS$: 292.0, found 292.1.

(2-(3,4-Dimethoxyphenoxy)-4,5-dimethoxyphenyl)(methyl)sulfane (3ba). Yellow solid (42.0



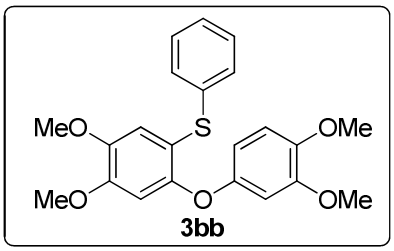
mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.92 (s, 1H), 6.77 (d, J = 8.8 Hz, 1H), 6.62 (d, J = 2.8 Hz, 1H), 6.54 (s, 1H), 6.37 (dd, J = 2.4 Hz, J = 8.4 Hz, 1H), 3.90 (s, 3H), 3.85 (s, 3H), 3.84 (s, 3H), 3.76 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.1, 149.9, 148.9, 148.7, 145.8, 144.7, 119.7, 113.5, 111.7, 107.7, 104.8, 102.5, 56.5, 56.3, 56.2, 55.9, 17.2; HRMS (ESI) m/z calcd for $C_{17}H_{20}O_5S[M+H]^+$: 337.1104, found 337.1110.

Methyl(2,4,5-trimethoxyphenyl)sulfane (6ba). Yellow solid (10.7 mg, 10%). ^{1}H NMR (400

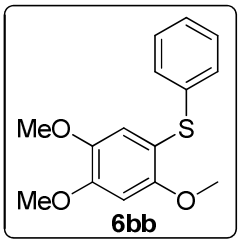


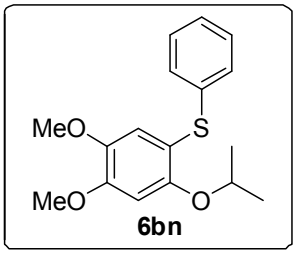
MHz, $CDCl_3$): δ 6.90 (s, 1H), 6.54 (s, 1H), 3.89 (s, 3H), 3.88 (s, 3H), 3.85 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 148.8, 143.3, 115.8, 115.0, 98.1, 56.8, 56.7, 56.3, 17.0; HRMS (ESI) m/z calcd for $C_{10}H_{14}O_3S[M+H]^+$: 237.0556, found 237.0558.

(2-(3,4-Dimethoxyphenoxy)-4,5-dimethoxyphenyl)(phenyl)sulfane (3bb). Yellow oil (58.7 mg, 59%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23-7.22 (m, 4H), 7.16-7.13 (m, 1H), 6.95 (s, 1H), 6.73 (d, J = 8.8 Hz, 1H), 6.56 (s, 1H), 6.47 (d, J = 2.4 Hz, 1H), 6.33 (dd, J = 2.8 Hz, J = 8.8 Hz, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.773-3.769 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.8, 151.0, 150.4, 149.8, 145.6, 144.8, 137.1, 128.8, 126.0, 117.4, 115.3, 111.6, 108.4, 104.4, 102.8, 56.3, 56.2, 56.1, 55.8; HRMS (ESI) m/z calcd for $C_{22}H_{22}O_5S[M+H]^+$: 399.1261, found 399.1267.



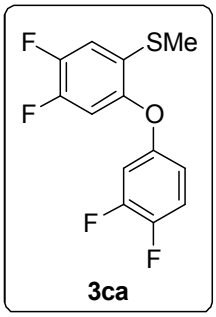
Phenyl(2,4,5-trimethoxyphenyl)sulfane (6bb). Yellow oil (22.1 mg, 16%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.20 (m, 2H), 7.15-7.12 (m, 3H), 6.95 (s, 1H), 6.60 (s, 1H), 3.93 (s, 3H), 3.82 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.5, 150.8, 143.5, 137.7, 128.8, 127.7, 125.5, 118.9, 110.8, 98.1, 57.0, 56.6, 56.2; HRMS (ESI) m/z calcd for $C_{15}H_{16}O_3S[M+H]^+$: 277.0893, found 277.0888.



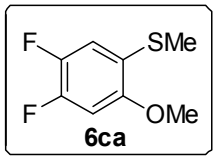


(2-Isopropoxy-4,5-dimethoxyphenyl)(phenyl)sulfane (6bn). Yellow oil (10.6 mg, 7%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25-7.18 (m, 4H), 7.15-7.11 (m, 1H), 6.90 (s, 1H), 6.58 (s, 1H), 4.47-4.38 (m, 1H), 3.89 (s, 3H), 3.77 (s, 3H), 1.23 (s, 3H), 1.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 150.2, 144.0, 137.8, 128.7, 128.5, 125.7, 117.9, 114.2, 102.4, 73.2, 56.4, 56.1, 22.1; HRMS (ESI) m/z calcd for $C_{17}H_{20}O_3S[M+H]^+$: 305.1206, found 305.1211.

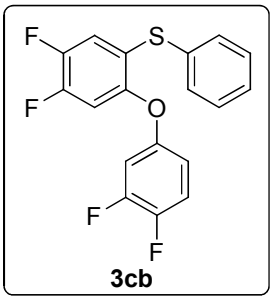
(2-(3,4-Difluorophenoxy)-4,5-difluorophenyl)(methyl)sulfane (3ca). Yellow oil (7.2 mg, 10%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.15-7.06 (m, 2H), 6.81-6.75 (m, 2H), 6.68-6.66 (m, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.8 (d, J = 7.9 Hz), 150.6 (dd, J = 248.8 Hz, 13.9 Hz), 148.0 (dd, J = 247.7 Hz, 13.9 Hz), 148.4 (d, J = 4.6 Hz), 147.7 (dd, J = 202.2 Hz, 12.9 Hz), 145.6 (d, J = 12.7 Hz), 127.4 (d, J = 4.0 Hz), 117.7 (d, J = 18.7 Hz), 115.4 (d, J = 20.7 Hz), 113.1, 109.3 (d, J = 20.0 Hz), 107.4 (d, J = 20.1 Hz), 15.2; MS (EI) m/z calcd for $C_{13}H_8F_4OS$: 288.0, found 288.1.



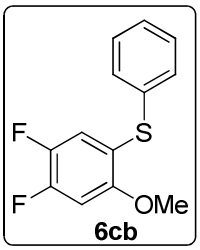
(4,5-Difluoro-2-methoxyphenyl)(methyl)sulfane (6ca). Yellow oil (6.7 mg, 7%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.98 (dd, *J* = 8.4 Hz, *J* =10.4 Hz, 1H), 6.67 (dd, *J* = 6.8 Hz, *J* =12.0 Hz, 1H), 3.85 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.5 (d, J = 7.3 Hz), 148.1 (dd, *J* = 244.5 Hz, 13.5 Hz), 144.7 (dd, *J* = 239.9 Hz, 12.8 Hz), 122.6 (d, *J* = 4.9 Hz), 115.2 (d, *J* = 20.6 Hz), 110.5 (d, *J* = 21.5 Hz), 56.5, 15.2; MS (EI) m/z calcd for $C_8H_8F_2OS$: 190.0, found 190.0.



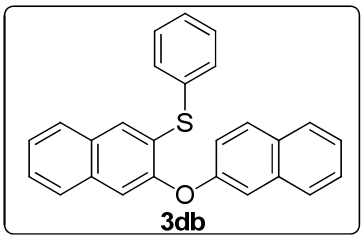
(2-(3,4-Difluorophenoxy)-4,5-difluorophenyl)(phenyl)sulfane (3cb). Yellow oil (25.4 mg, 29%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.35 (m, 5H), 7.11 (dd, *J* = 8.8 Hz, 18.4 Hz, 1H), 6.98-6.93 (m, 1H), 6.80-6.71 (m, 2H), 6.65-6.62 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.7 (d, J = 5.7 Hz), 151.2 (dd, *J* = 134.2 Hz, 14.1 Hz), 149.5-149.3 (m), 148.5 (d, *J* = 12.9 Hz), 148.1-147.9 (m), 145.8 (dd, *J* = 12.9 Hz, 39.0 Hz), 132.8 , 132.3, 129.6, 128.5, 125.5 (d, *J* = 4.6 Hz), 119.3 (d, *J* = 20.3 Hz), 117.7(d, *J* = 18.6 Hz), 113.4, 109.3 (d, *J* = 20.2 Hz), 107.7 (d, *J* = 20.0 Hz); MS (EI) m/z calcd for $C1_8H_{10}F_4OS$: 350.0, found 350.1.



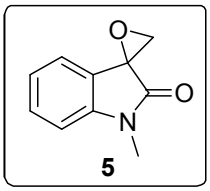
(4,5-Difluoro-2-methoxyphenyl)(phenyl)sulfane (6cb). Yellow oil (34.0 mg, 27%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.30 (m, 5H), 6.90-6.85 (m, 1H), 6.73 (dd, *J* = 12.0 Hz, 6.8 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4 (d, *J* = 7.1 Hz), 148.5 (dd, *J* = 13.9 Hz, 13.9 Hz), 143.6 (d, *J* = 12.9 Hz, 12.4 Hz), 132.4, 130.9, 128.7, 128.4, 126.8, 118.4 (d, *J* = 20.1 Hz), 99.9 (d, *J* = 21.6 Hz), 55.6; MS (EI) m/z calcd for $C_{13}H_{10}F_2OS$: 252.0, found 252.0.



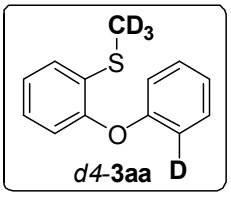
(3-(Naphthalen-2-yloxy)naphthalen-2-yl)(phenyl)sulfane (3db). White solid (10.4 mg, 11%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78-7.75 (m, 2H), 7.62-7.52 (m, 4H), 7.42-7.16 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.7, 153.1, 134.3, 133.7, 133.1, 132.6, 130.6, 130.5, 130.4, 129.9, 129.3, 129.1, 127.8, 127.7, 127.2, 127.0, 126.9, 126.5, 126.3, 125.3, 124.8, 119.9, 114.9, 114.4; HRMS (ESI) m/z calcd for $C_{26}H_{18}OS[M+Na]^+$: 401.0971, found 401.0969.



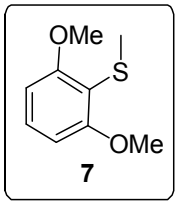
1-Methylspiro[indoline-3,2'-oxiran]-2-one (5)[4]**.** White solid. (80 mg, 91%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (t, *J* = 7.6 Hz, 1H), 7.12-7.06 (m, 2H), 6.92 (d, *J* = 8.0 H, 1H), 3.59 (d, *J* = 6.4 Hz, 1H), 3.43 (d, *J* = 6.8 Hz, 1H), 3.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.8, 145.1, 130.4, 122.9, 122.7, 122.1, 108.9, 56.4, 54.1, 26.7.



Methyl(2-phenoxyphenyl)sulfane-*d4* (*d4*-3aa)[5]**.** White solid. (45 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.25 (m, 3H), 7.14-7.06 (m, 3H), 6.97 (d, *J* = 8.0 H, 1H), 6.90-6.88 (m, 1H), 2.41 (s, 0.37H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 153.6, 129.7, 129.6, 126.8, 126.0, 124.4, 123.0, 119.3, 117.9; MS (EI) m/z calcd for $C_{13}H_8D_4OS$: 220.1, found 220.1.



(2,6-Dimethoxyphenyl)(methyl)sulfane (7)[6]**.** White solid (10.2 mg, 11%). ^{1}H NMR (400 MHz, CD_3OD-d_4): δ 7.32 (t, *J* = 8.4 Hz, 1H), 6.71 (d, *J* = 8.4 Hz, 2H), 3.92 (s, 6H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD-d_4): δ 160.6, 129.2, 119.5, 104.1, 55.2, 16.3.

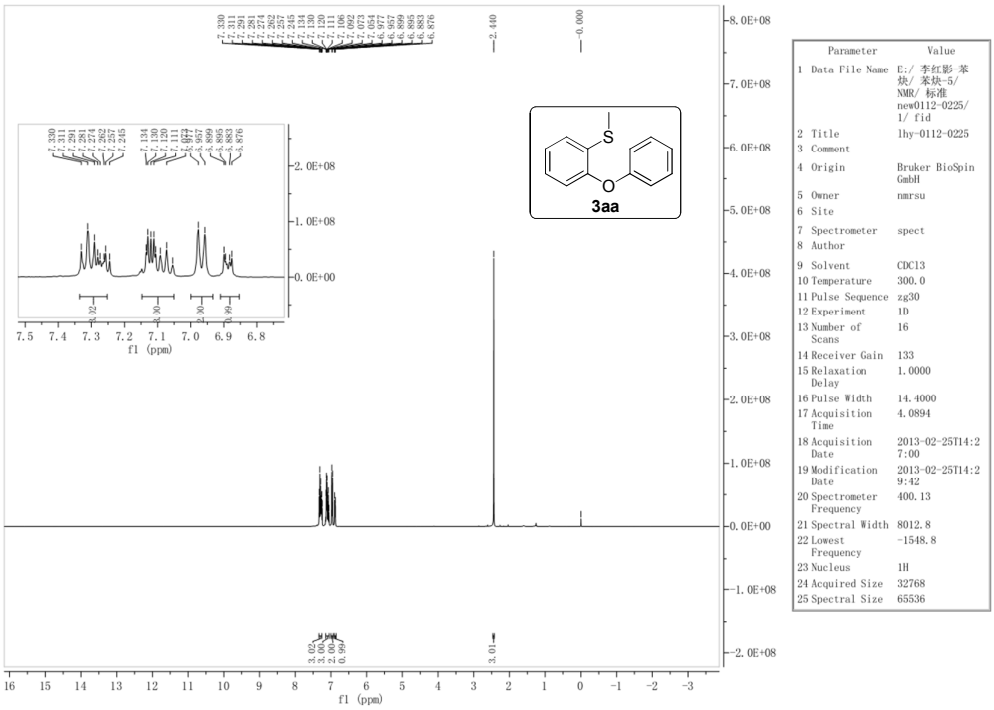


6. References

1. Vanderheiden, S.; Bulat, B.; Zevaco, T.; Jung, N.; Brase, S. *Chem. Commun.* **2011,** *47*, 9063-9065.
2. Pena, D.; Perez, D.; Guitian, E.; Castedo, L. *J. Am. Chem. Soc.* **1999**, *121*, 5827-5828.
3. Shi, F.; Tse, M. K.; Kaiser, H. M.; Beller, M. *Adv. Synth. Catal.* **2007**, *349*, 2425-2430.
4. Gorokhovik, I.; Neuville, L.; Zhu, J. *Org. Lett.* **2011,** *13*, 5536-5539.
5. Baciocchi, E.; Chiappe, C.; Del Giacco, T.; Fasciani, C.; Lanzalunga, O.; Lapi, A.; Melai, B. *Org. Lett.* **2009,** *11*, 1413-1416.
6. Joseph, P. J. A.; Priyadarshini, S.; Kantam, M. L.; Sreedhar, B. *Tetrahedron* **2013,** *69*, 8276-8283.

7. Copies of ^{1}H NMR, ^{13}C NMR and MS spectra for compounds 3-7

Methyl(2-phenoxyphenyl)sulfane (3aa)



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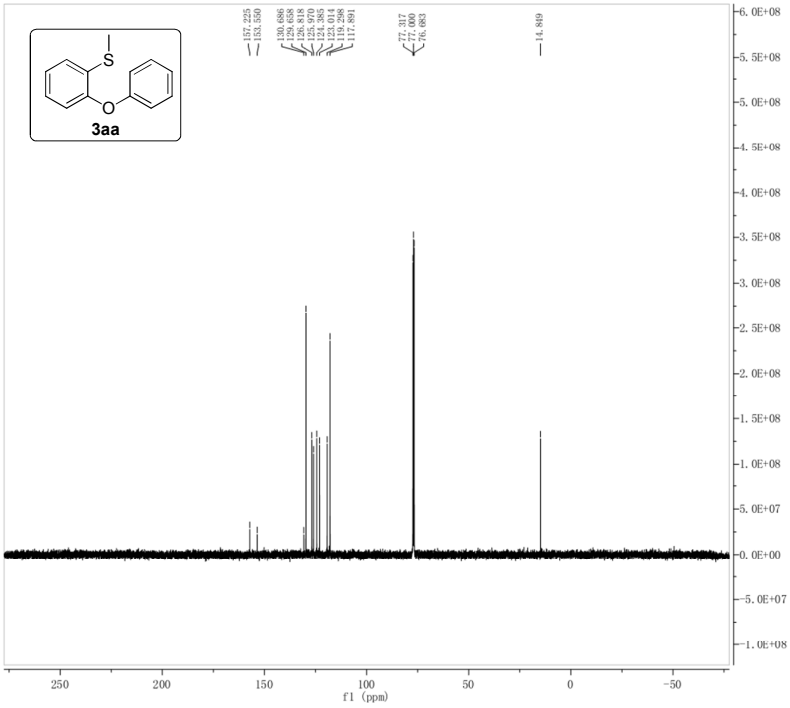

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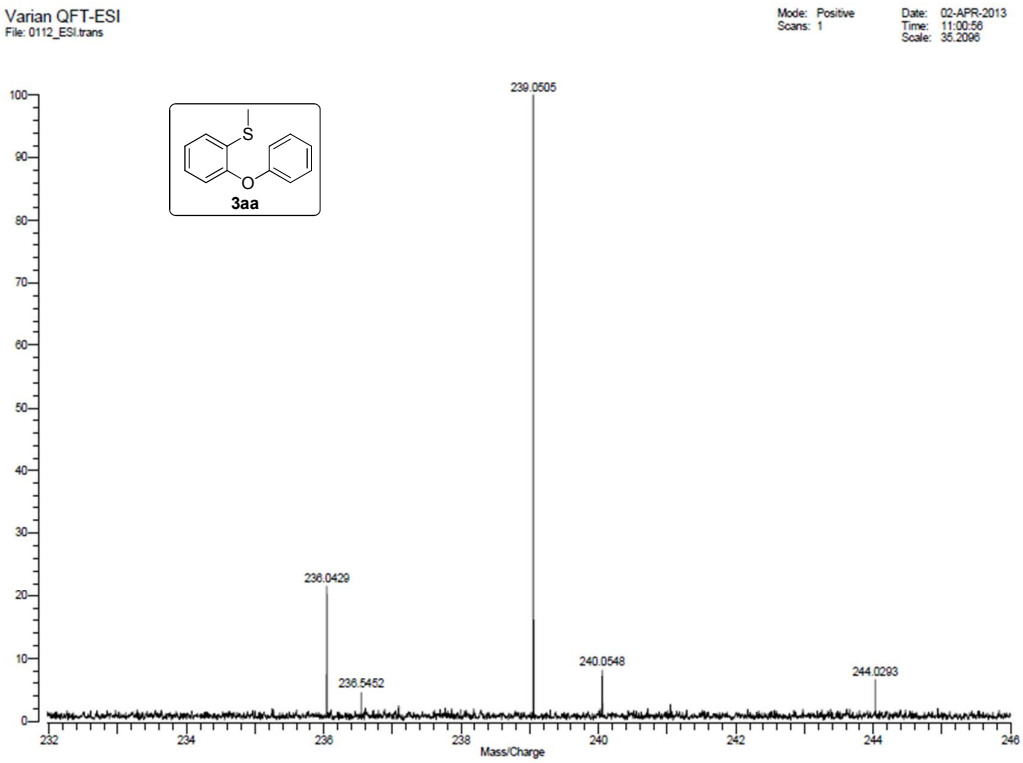
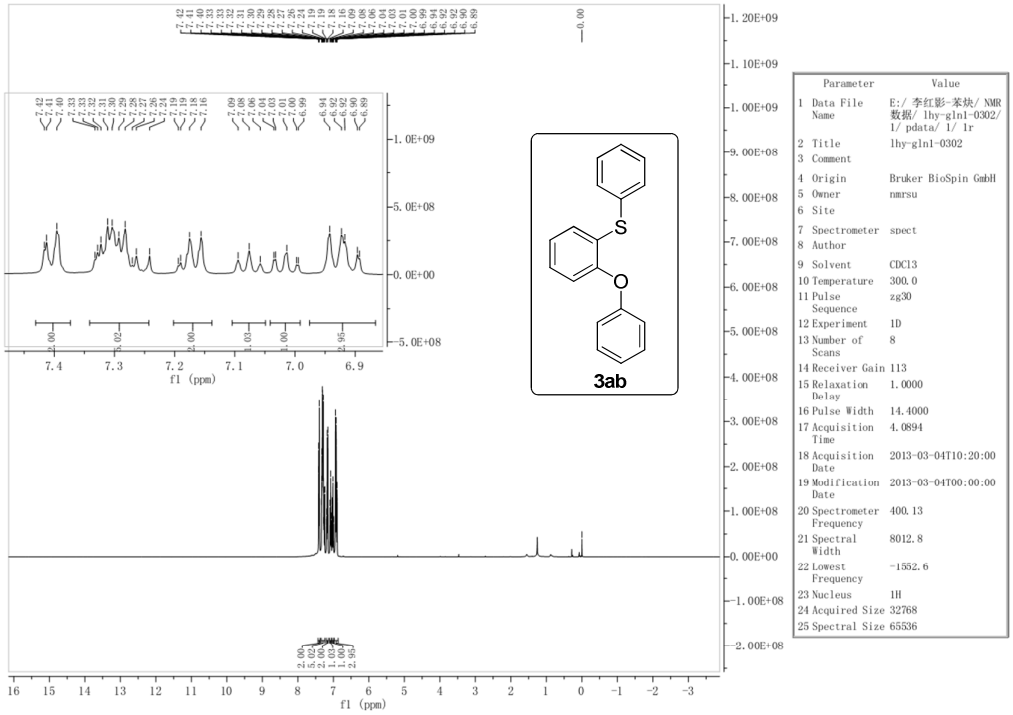
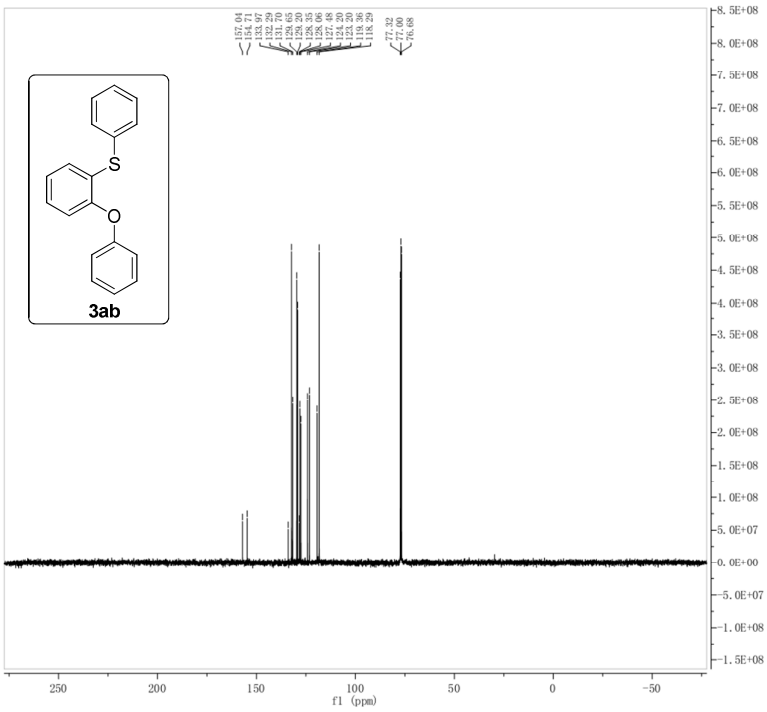


(2-Phenoxyphenyl)(phenyl)sulfane (3ab).





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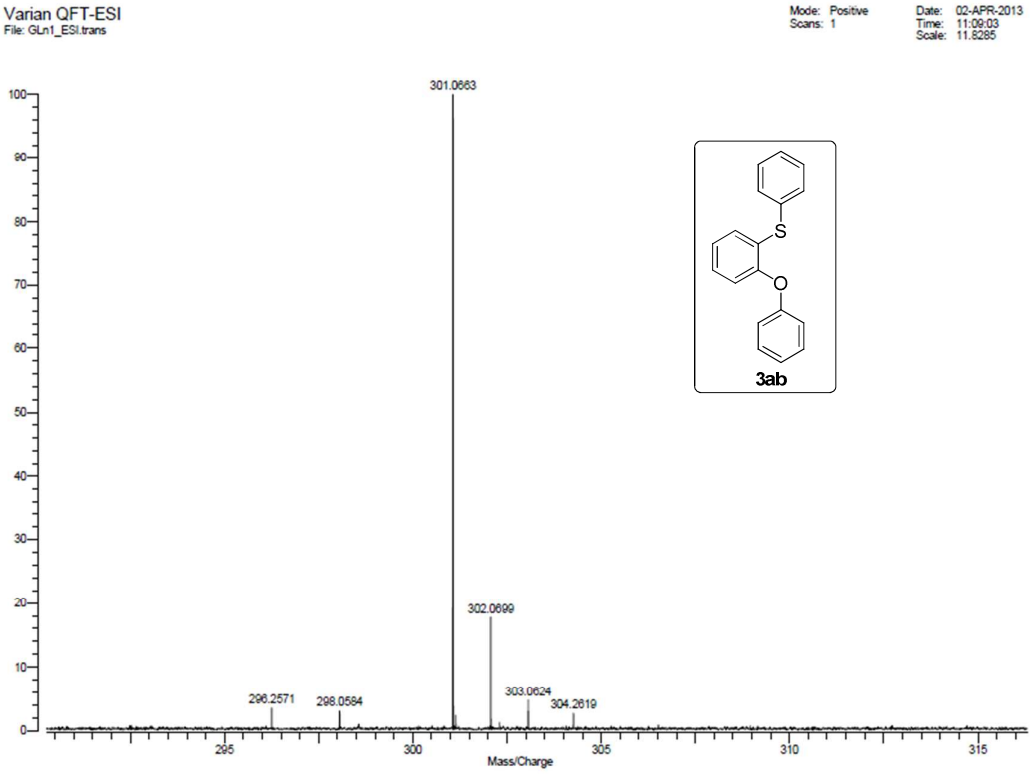
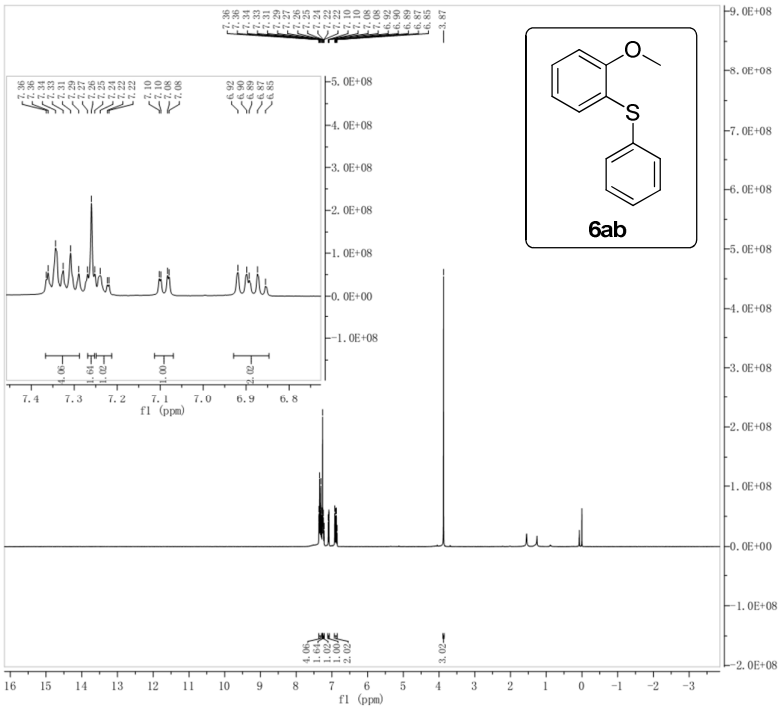


(2-Methoxyphenyl)(phenyl)sulfane (6ab).



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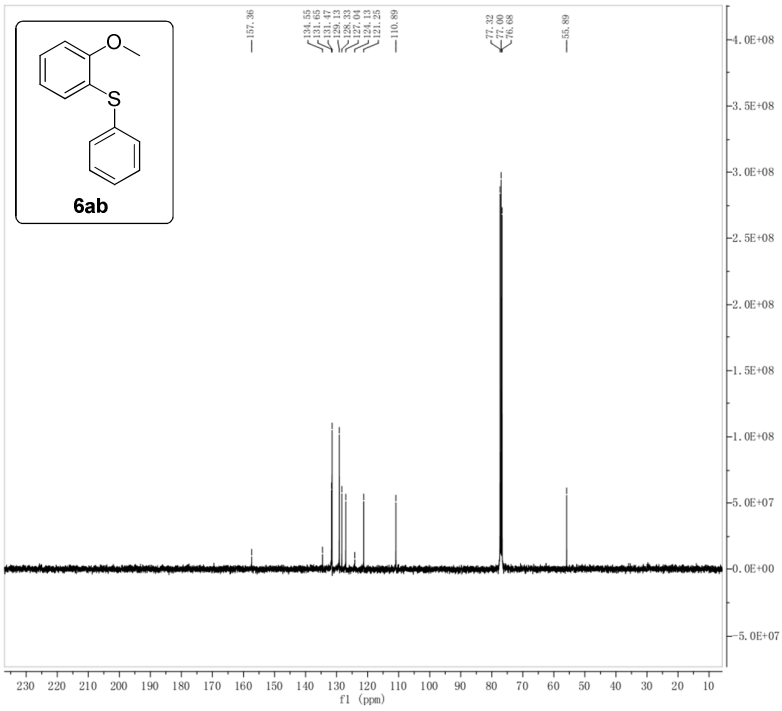

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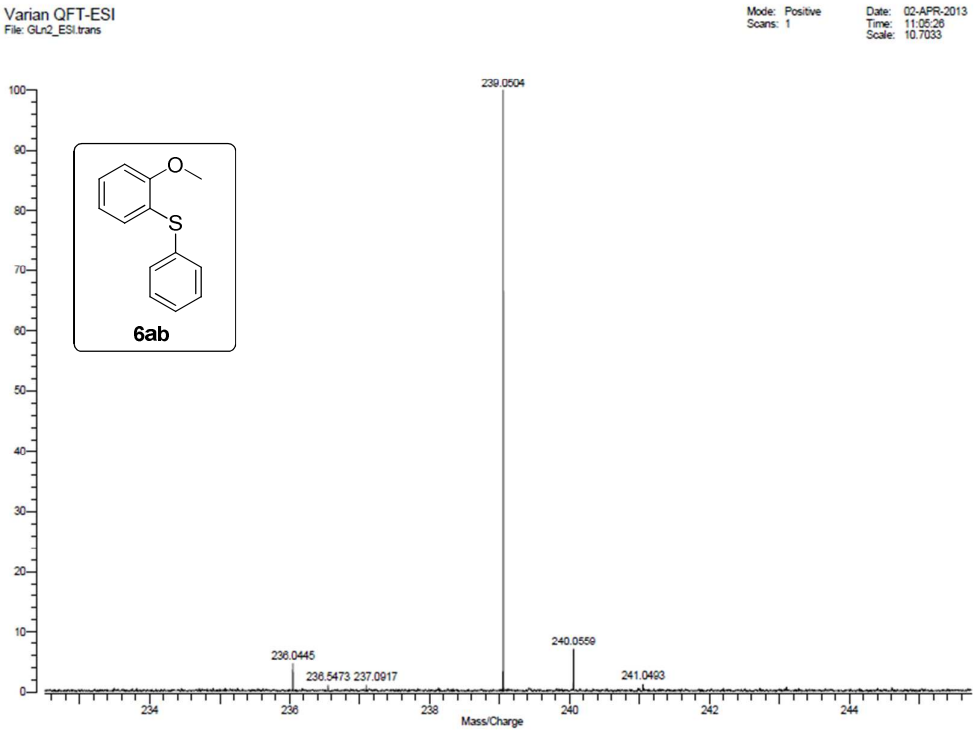
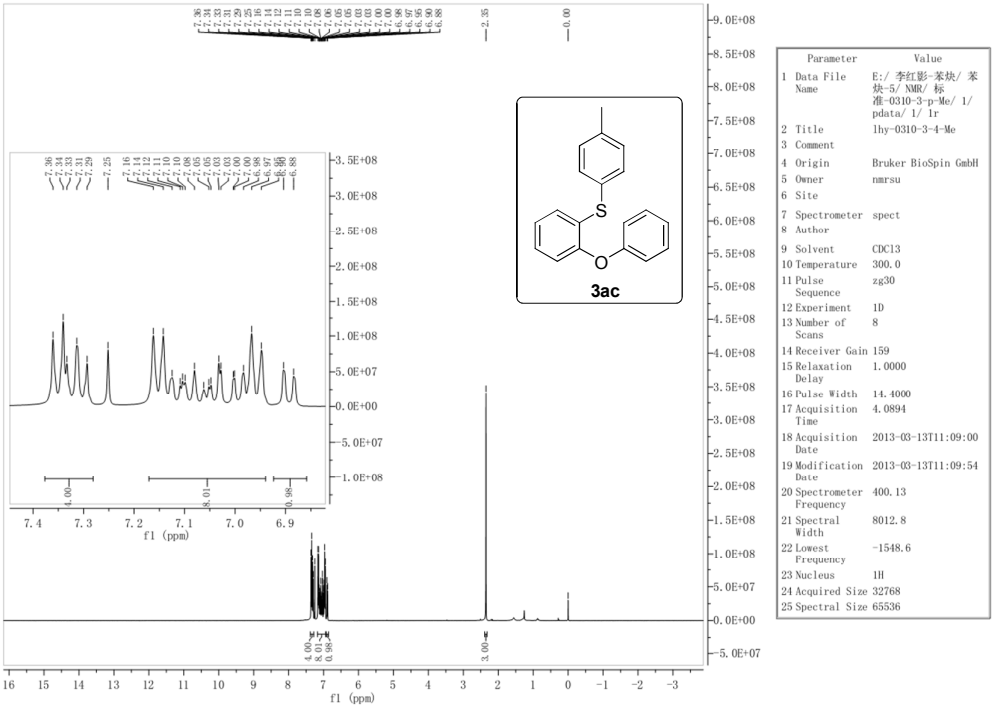
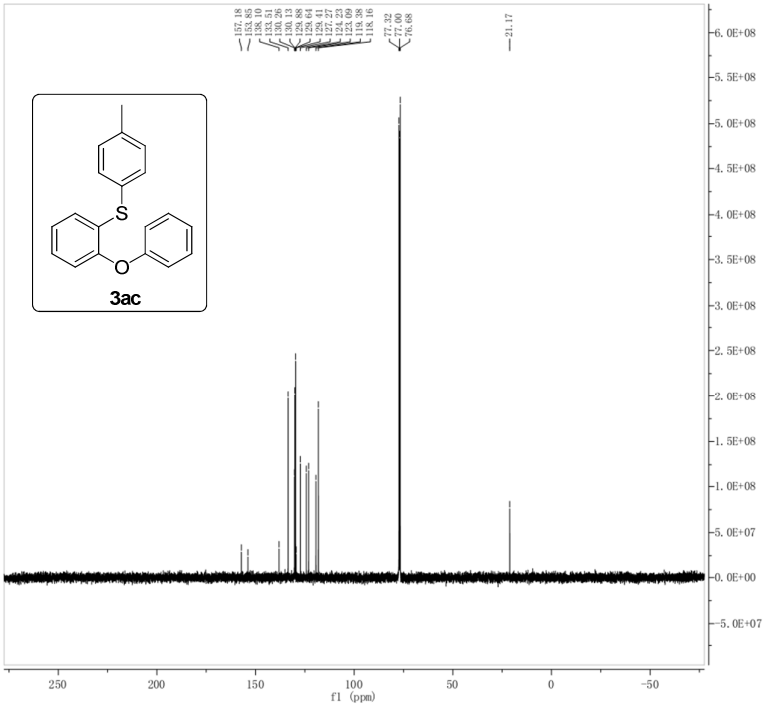


(2-Phenoxyphenyl)(p-tolyl)sulfane (3ac).





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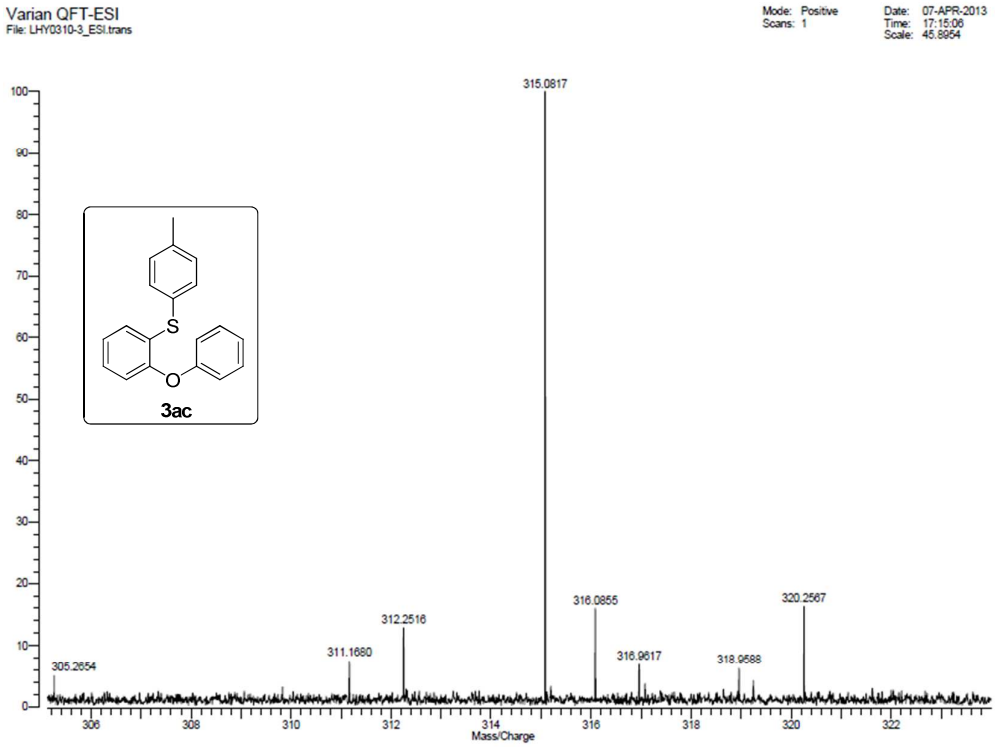
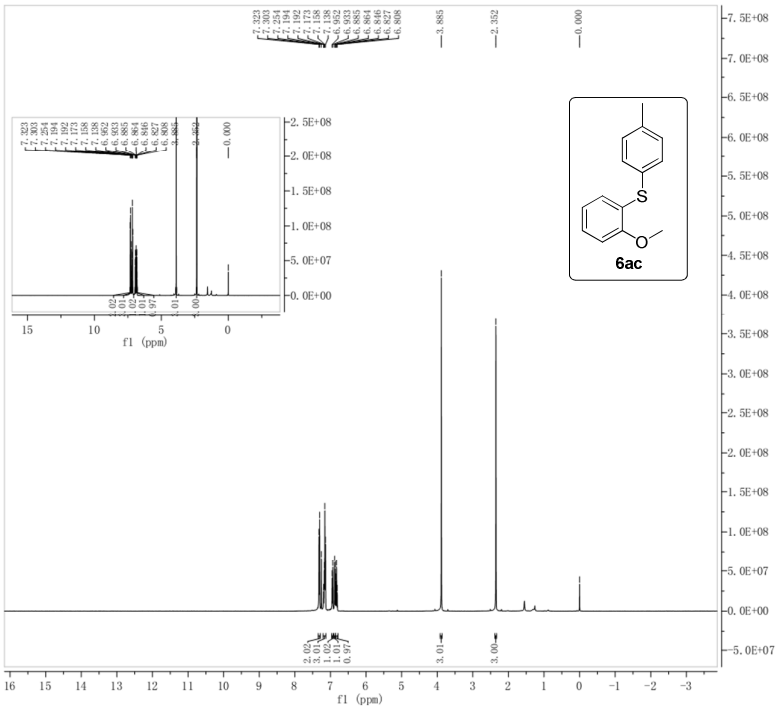


(2-Methoxyphenyl)(p-tolyl)sulfane (6ac).



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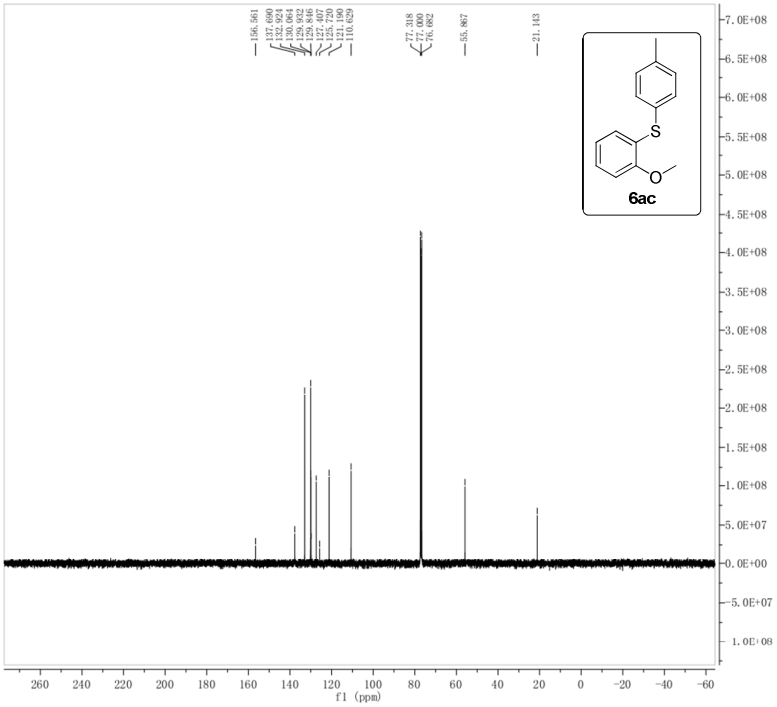

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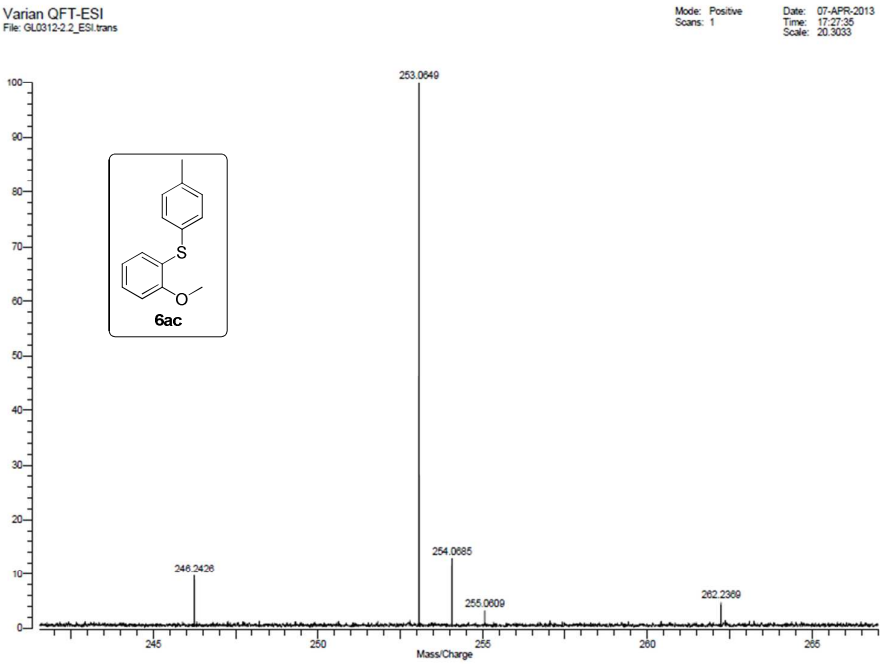
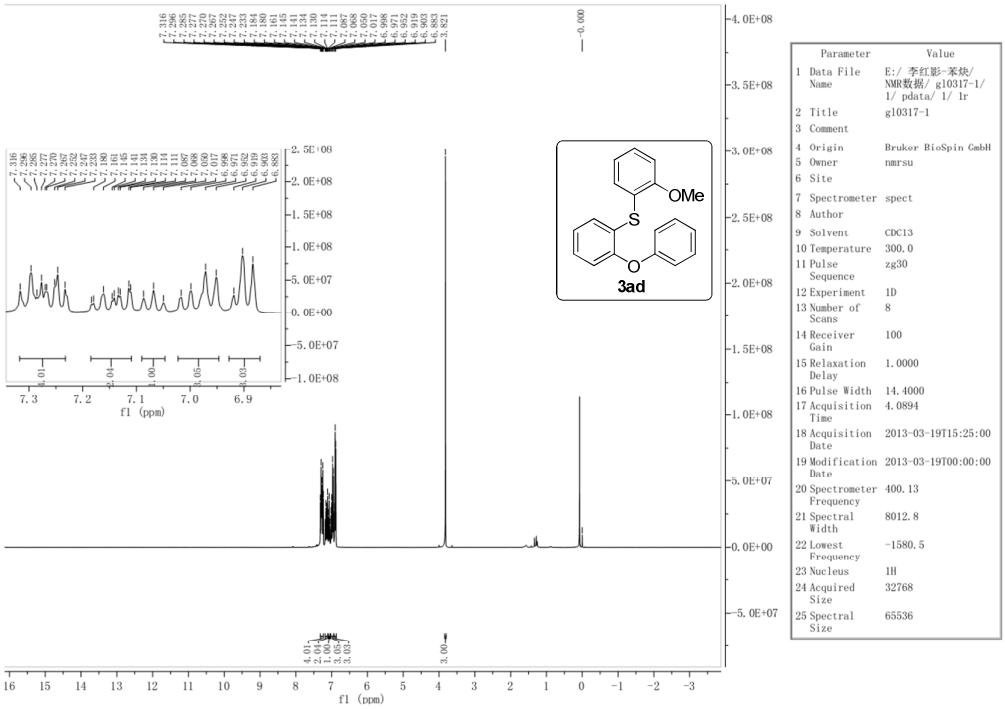
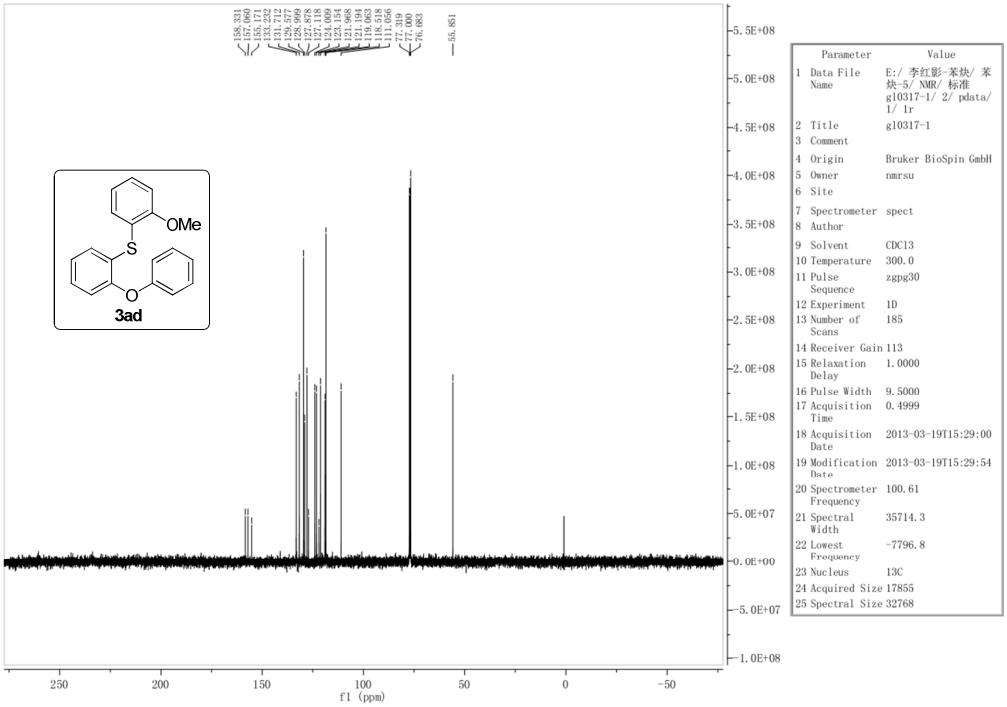
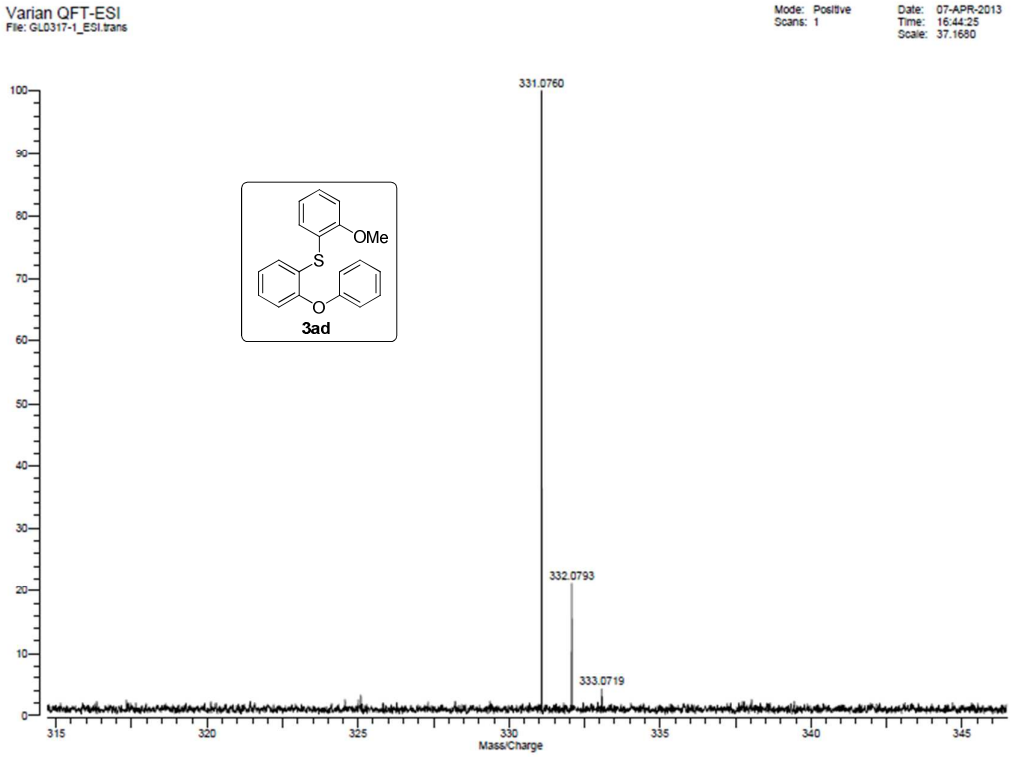


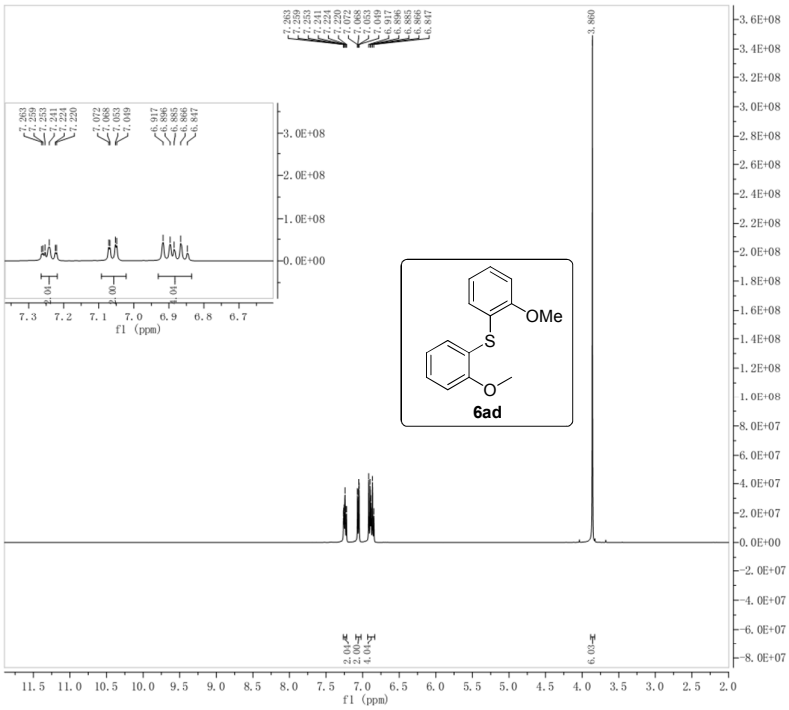
(2-Methoxyphenyl)(2-phenoxyphenyl)sulfane (3ad).







Bis(2-methoxyphenyl)sulfane (6ad).



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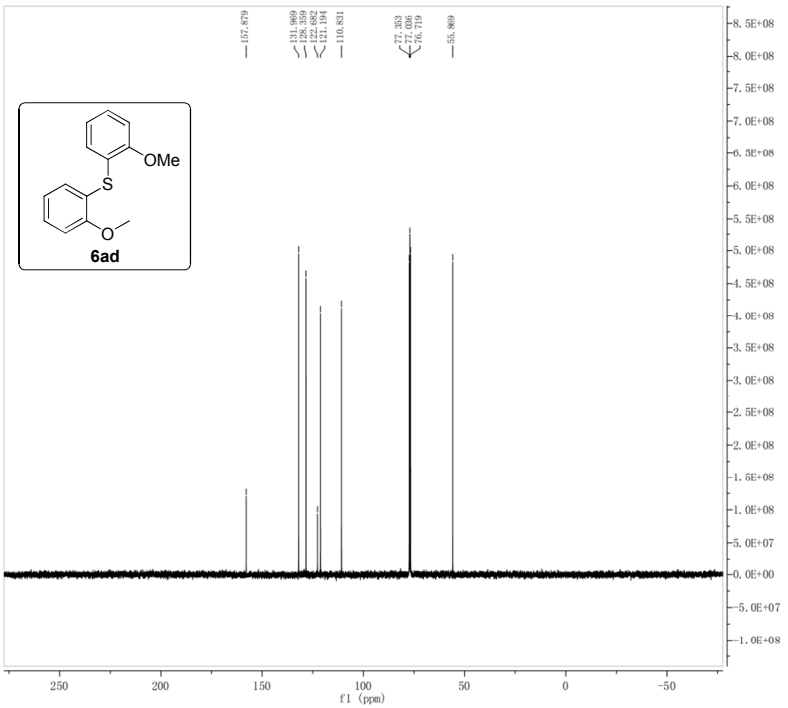

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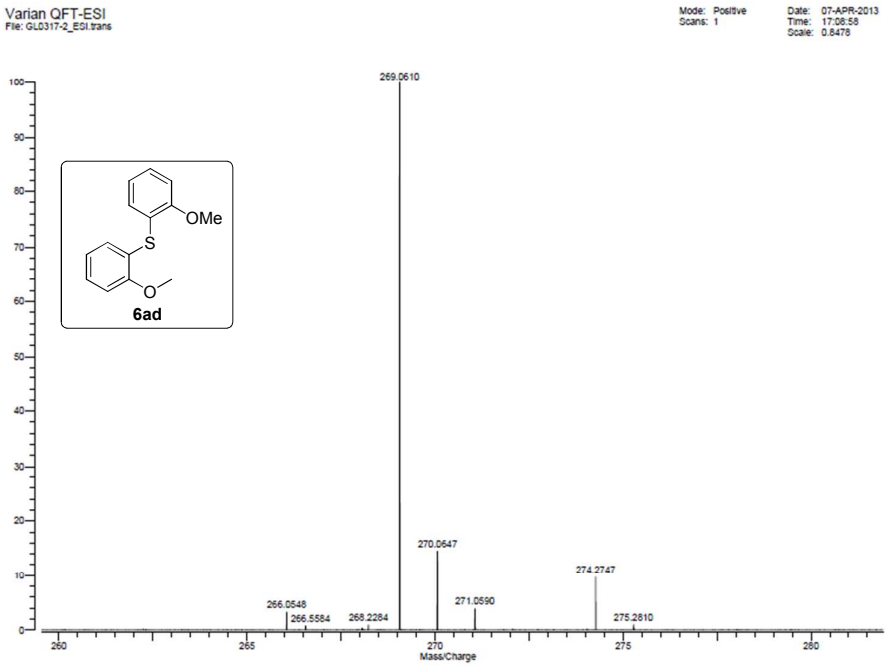
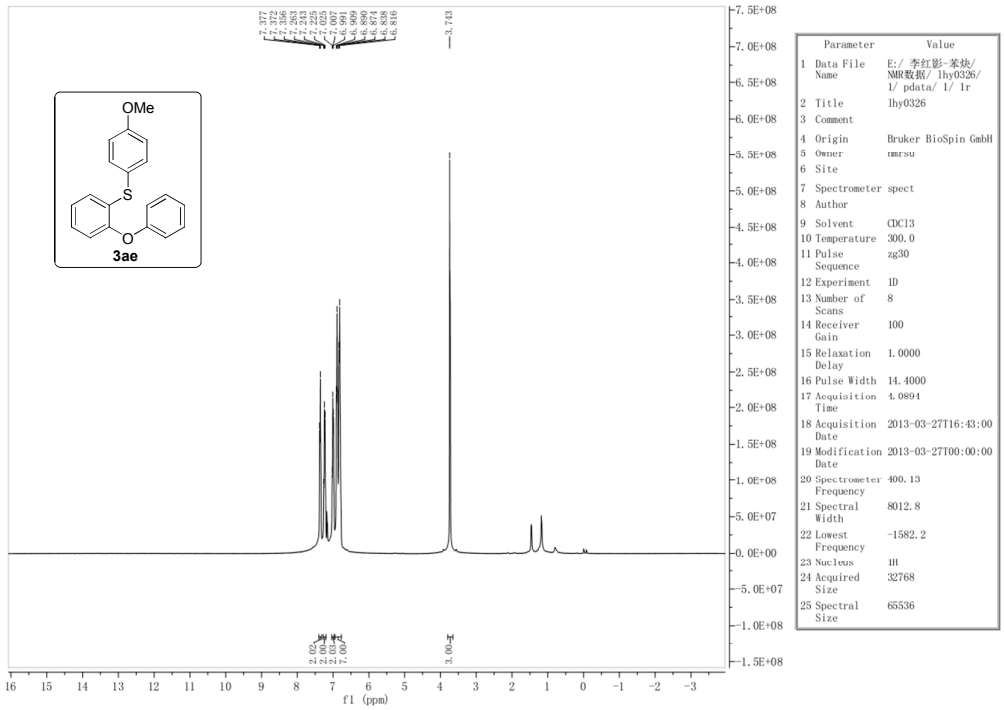
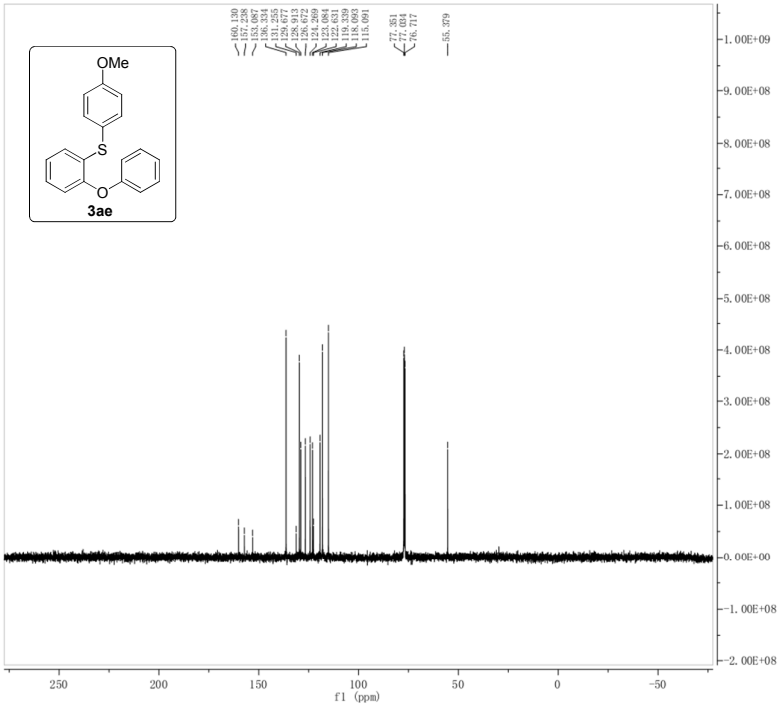
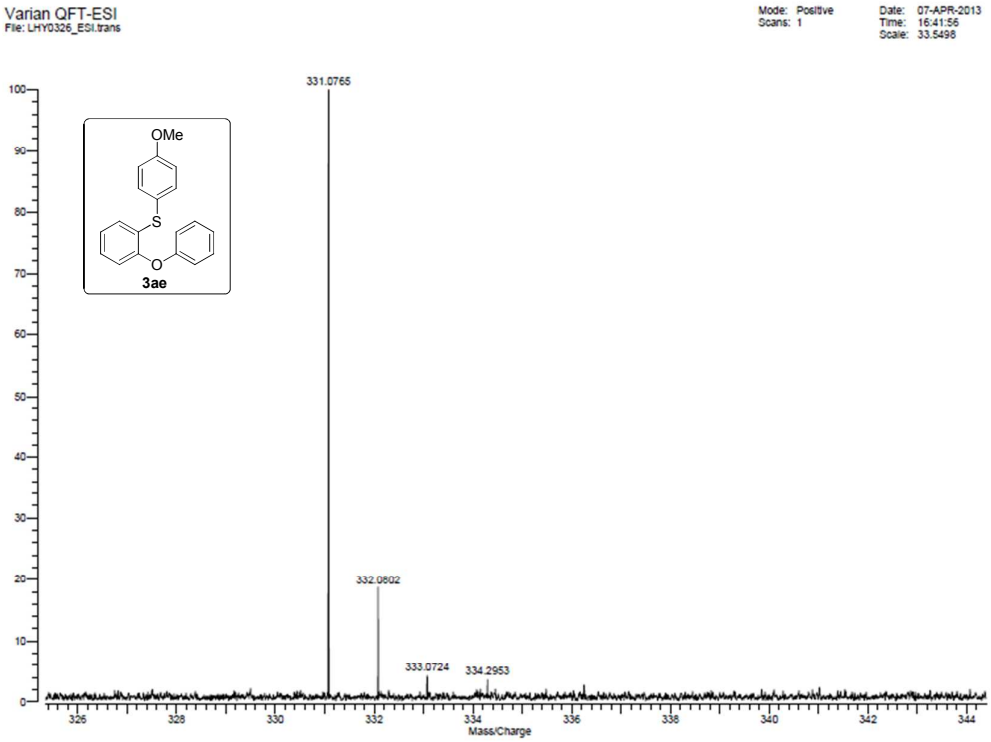


(4-Methoxyphenyl)(2-phenoxyphenyl)sulfane (3ae).

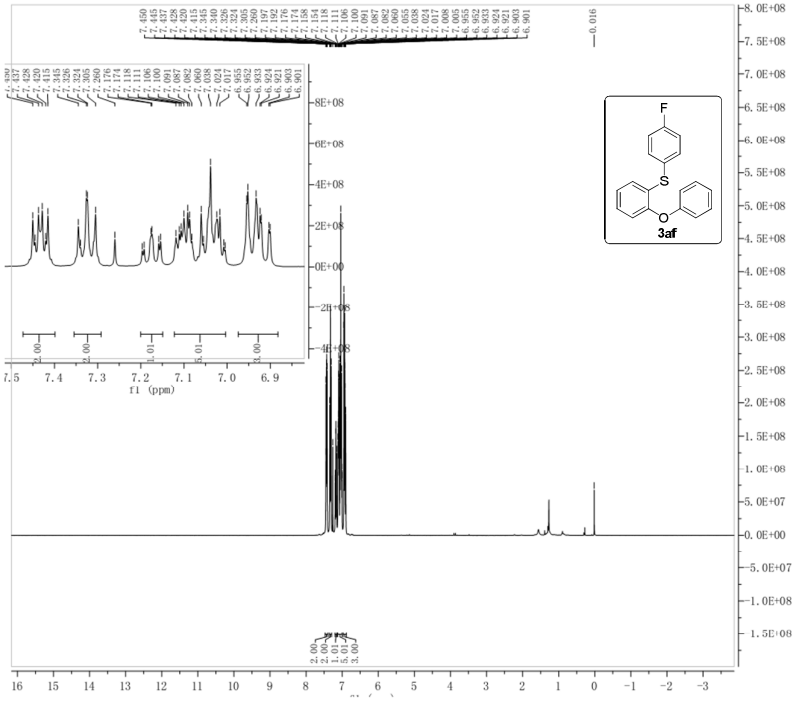




Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 lhy0326-4-OMe/ 2/ pdata/ 1/ 1r
2 Title	lhy0326
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	414
14 Receiver Gain	113
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-03-27T16:45:00
19 Modification Date	2013-03-27T16:53:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768



(4-Fluorophenyl)(2-phenoxyphenyl)sulfane (3af).



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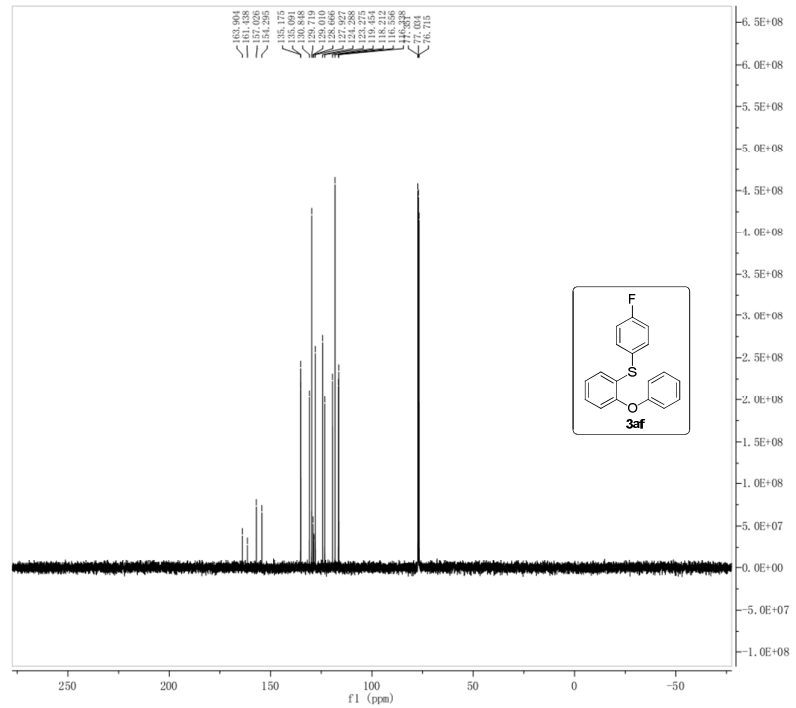
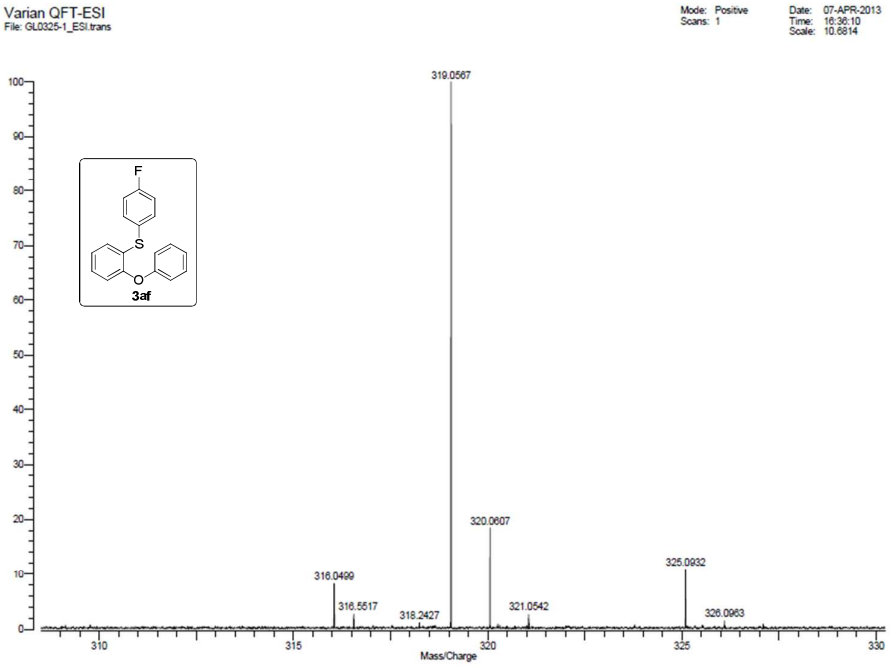
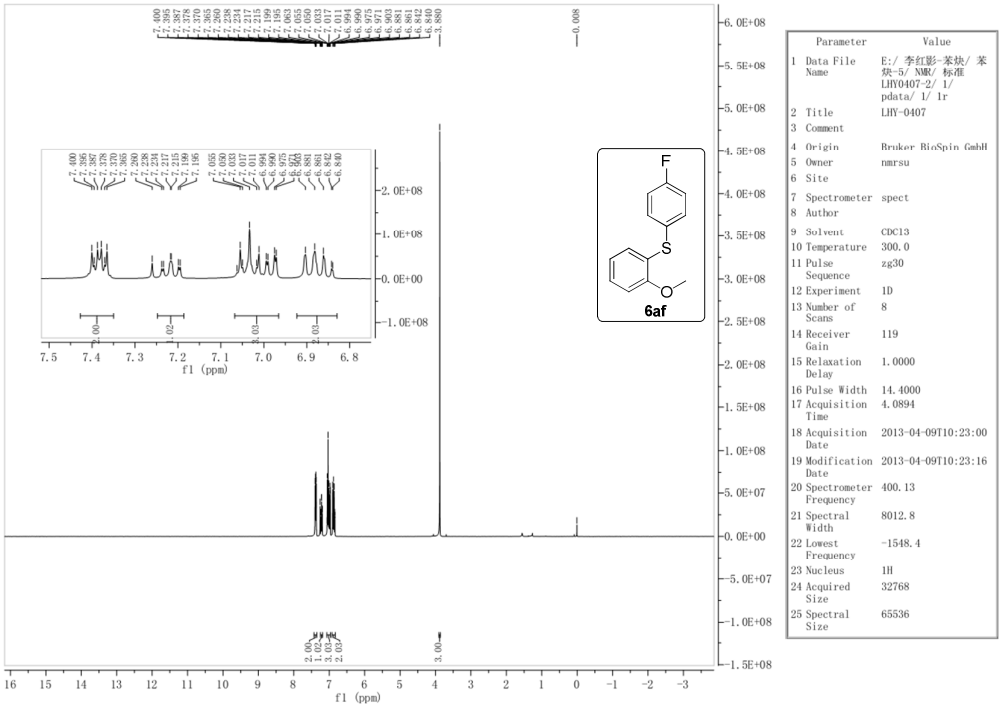
2	Title	GL0325-1
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	14.4000
17	Acquisition Time	4.0894
18	Acquisition Date	2013-03-26T10:53:00
19	Modification Date	2013-03-26T00:00:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1551.5
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	65536

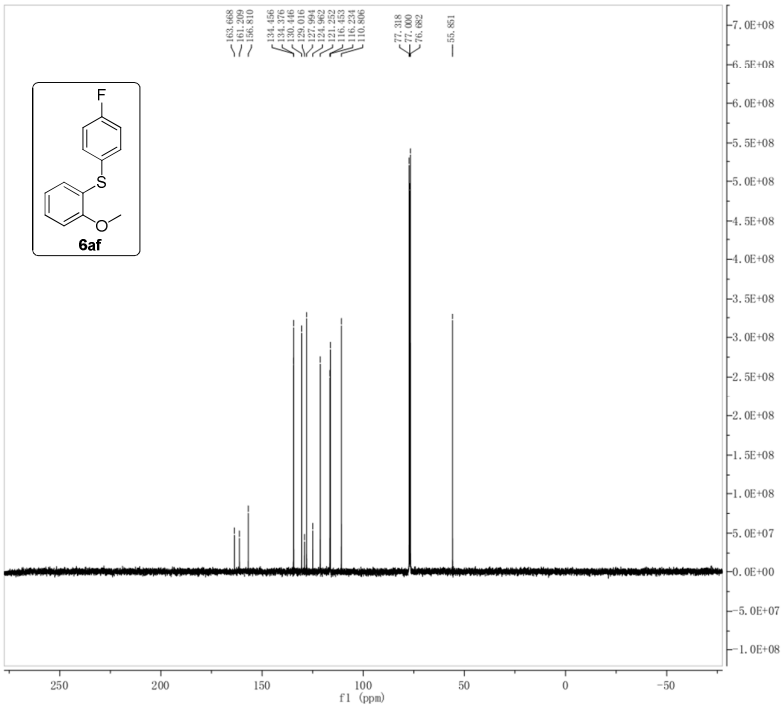


	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ NMR数据/ GL0325-1/ 2/ pdata/ 1/ 1r
2	Title	GL0325-1
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	200
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-03-26T10:55:00
19	Modification Date	2013-03-26T00:00:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768

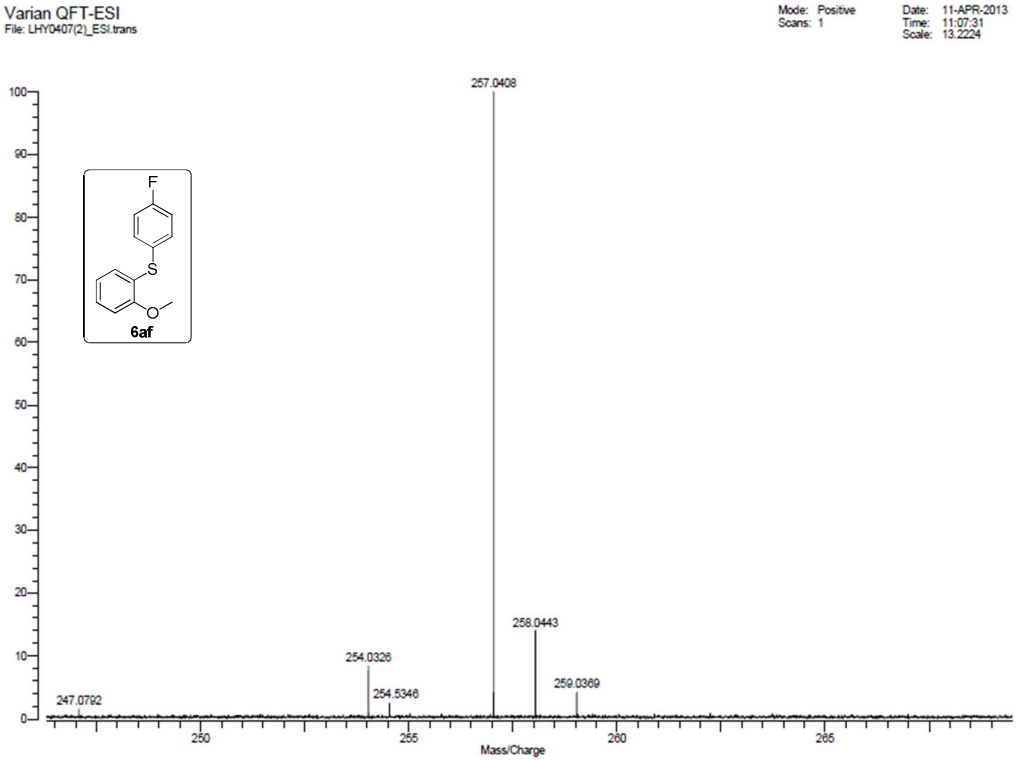


(4-Fluorophenyl)(2-methoxyphenyl)sulfane (6af).

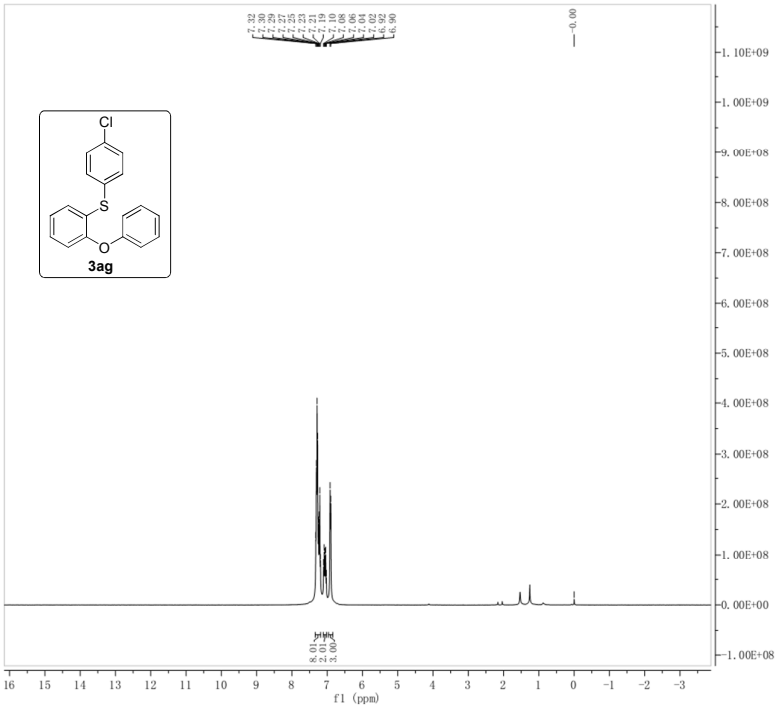




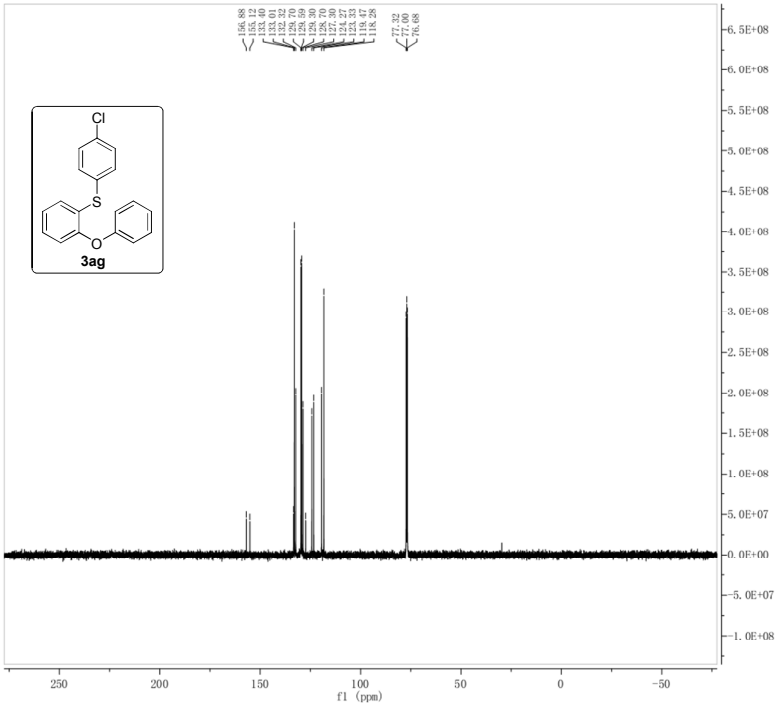
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ NMR数据/ LHY-0407/ 2/ pdata/ 1/ 1r
2 Title	LHY-0407
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	978
14 Receiver Gain	133
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-04-09T10:25:00
19 Modification Date	2013-04-09T00:00:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768



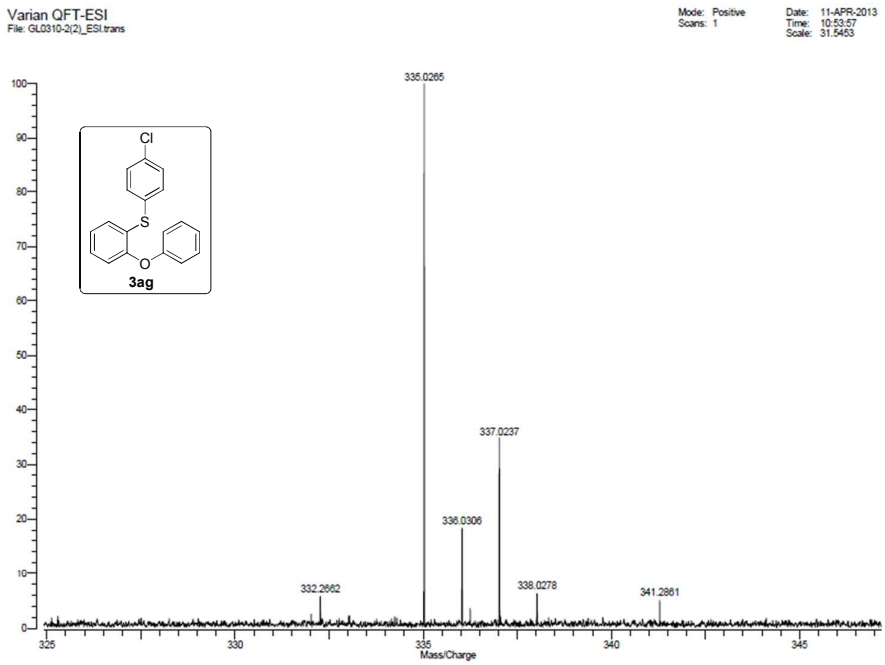
(4-Chlorophenyl)(2-phenoxyphenyl)sulfane (3ag).



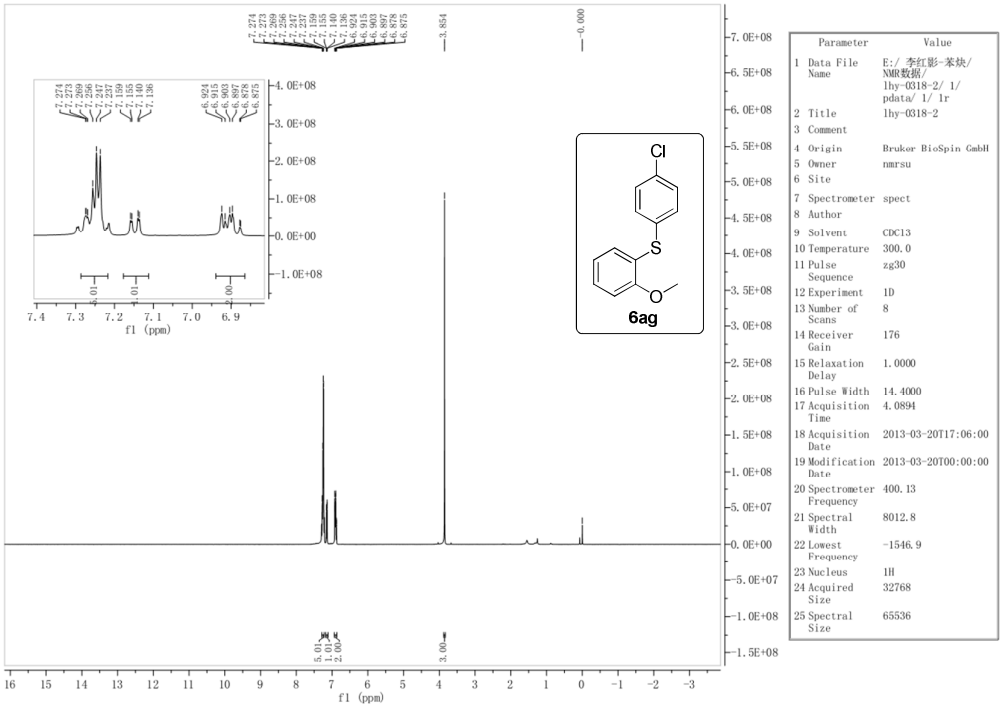
	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 gl0310-4-Cl/ 1/ pdata/ 1/ 1r
2	Title	1hy-gl-0310-4-Cl
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	14.4000
17	Acquisition Time	4.0894
18	Acquisition Date	2013-03-12T10:29:00
19	Modification Date	2013-03-12T10:28:42
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1551.1
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	65536

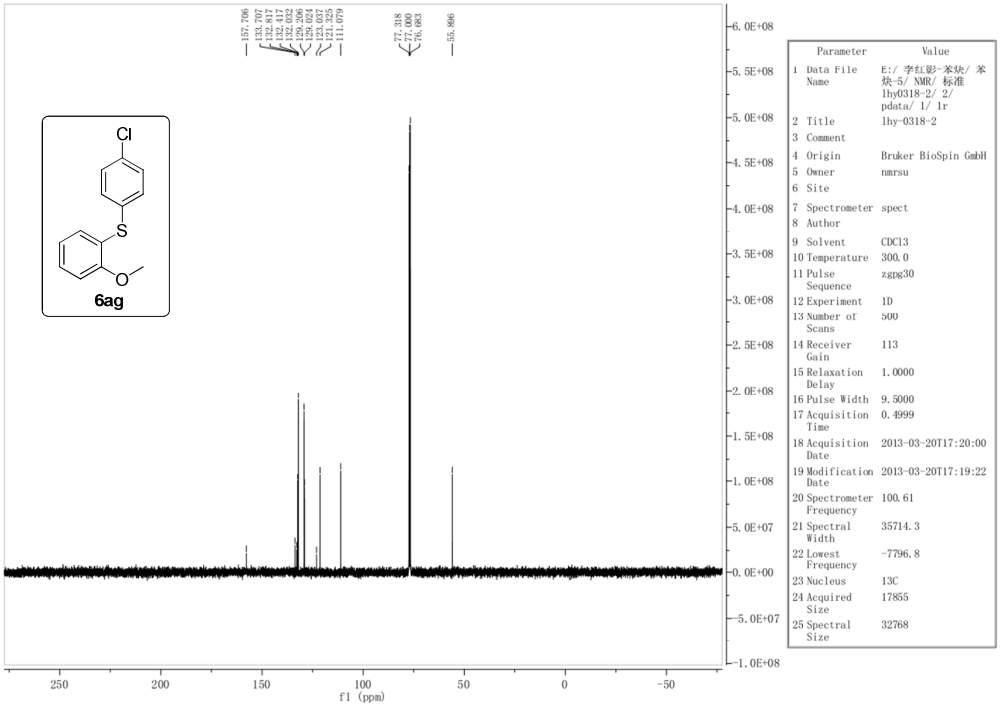


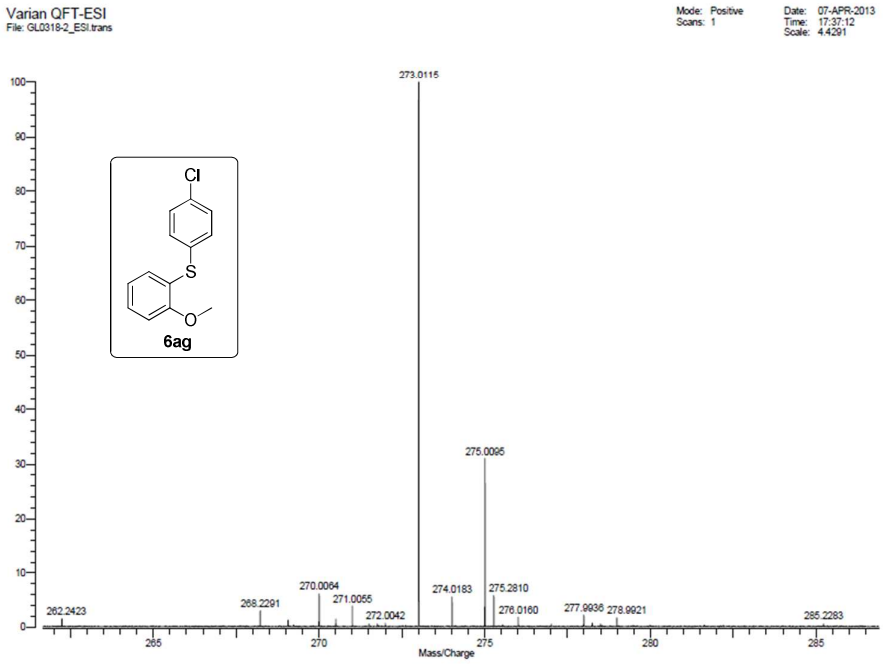
	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ NMR数据/ 1hy-gl-0310-4-Cl/ 2/ pdata/ 1/ 1r
2	Title	1hy-gl-0310-4-Cl
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	500
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-03-12T10:42:00
19	Modification Date	2013-03-12T00:00:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768



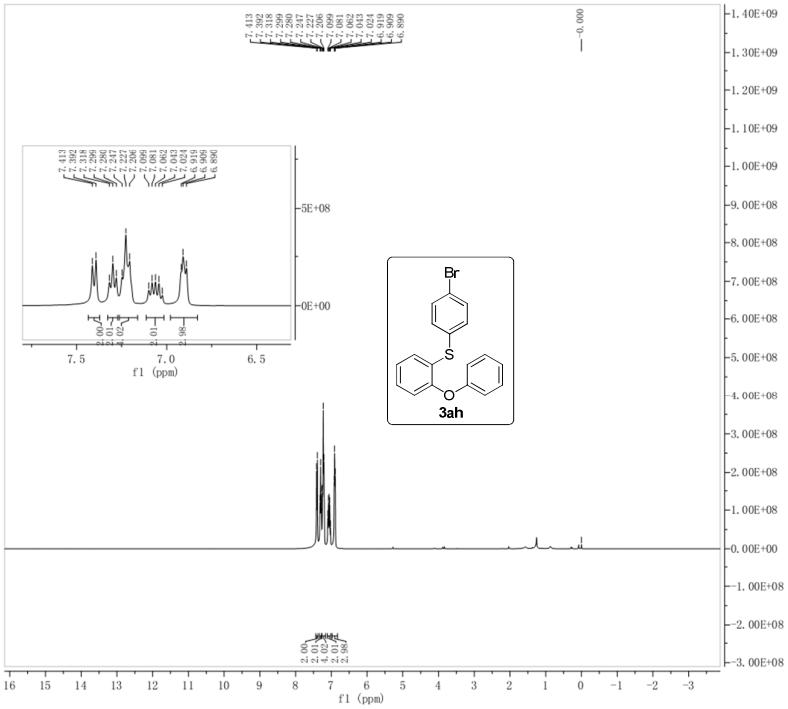
(4-Chlorophenyl)(2-methoxyphenyl)sulfane (6ag).



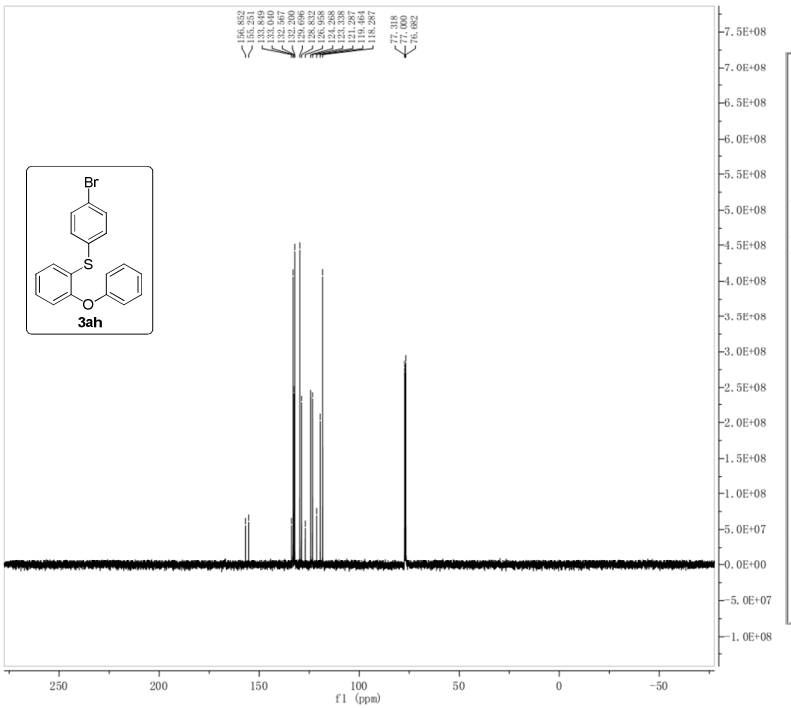




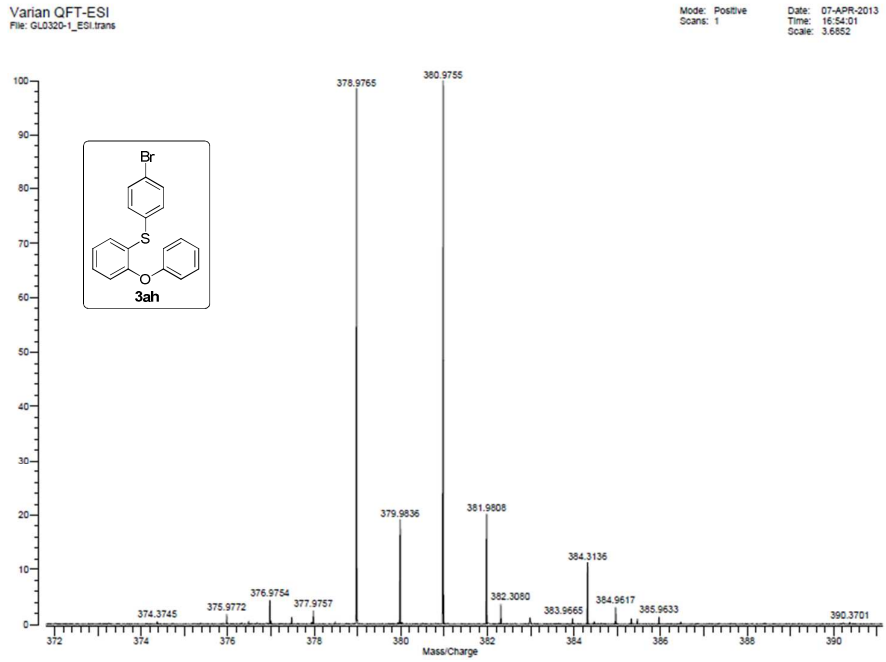
(4-Bromophenyl)(2-phenoxyphenyl)sulfane (3ah).



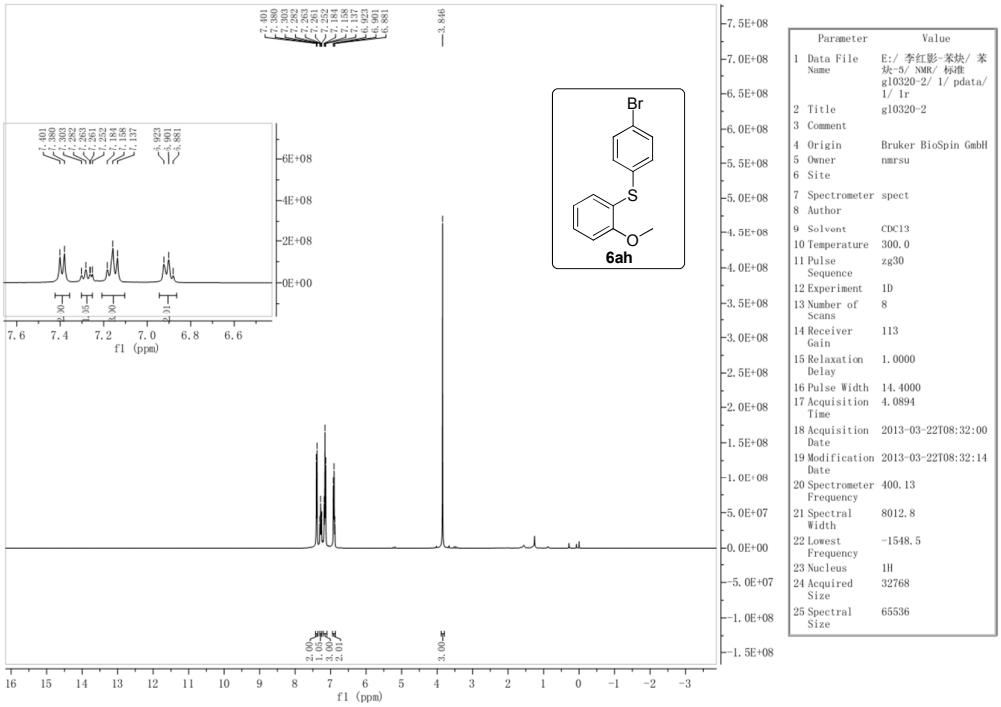
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 gl0320-1/ 1/ pdata/ 1/ 1r
2 Title	gl0320-1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	78
15 Relaxation Delay	1.0000
16 Pulse Width	14.4000
17 Acquisition Time	4.0894
18 Acquisition Date	2013-03-21T17:22:00
19 Modification Date	2013-03-21T17:21:12
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1553.4
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



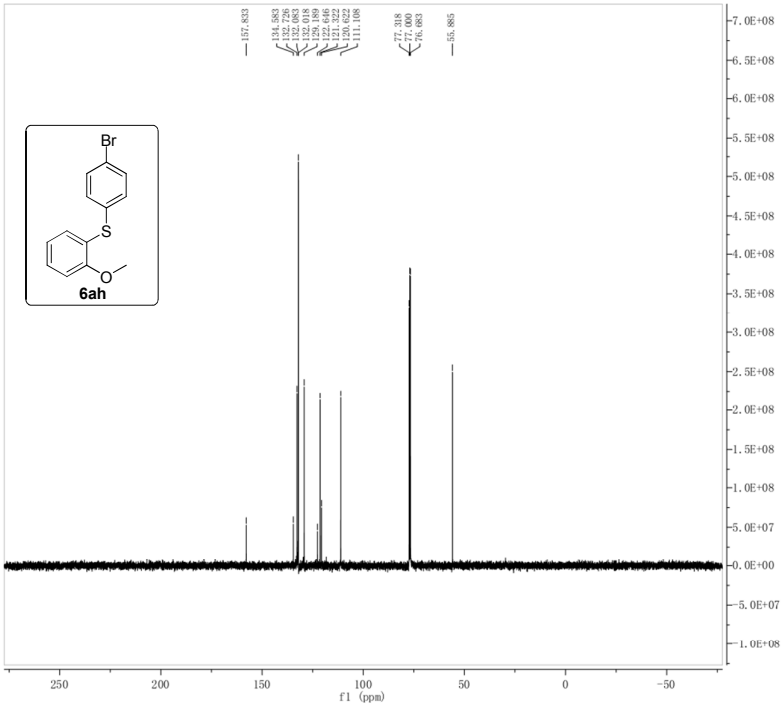
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 gl0320-1/ 2/ pdata/ 1/ 1r
2 Title	gl0320-1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	158
14 Receiver Gain	119
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-03-21T17:23:00
19 Modification Date	2013-03-21T17:26:08
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768



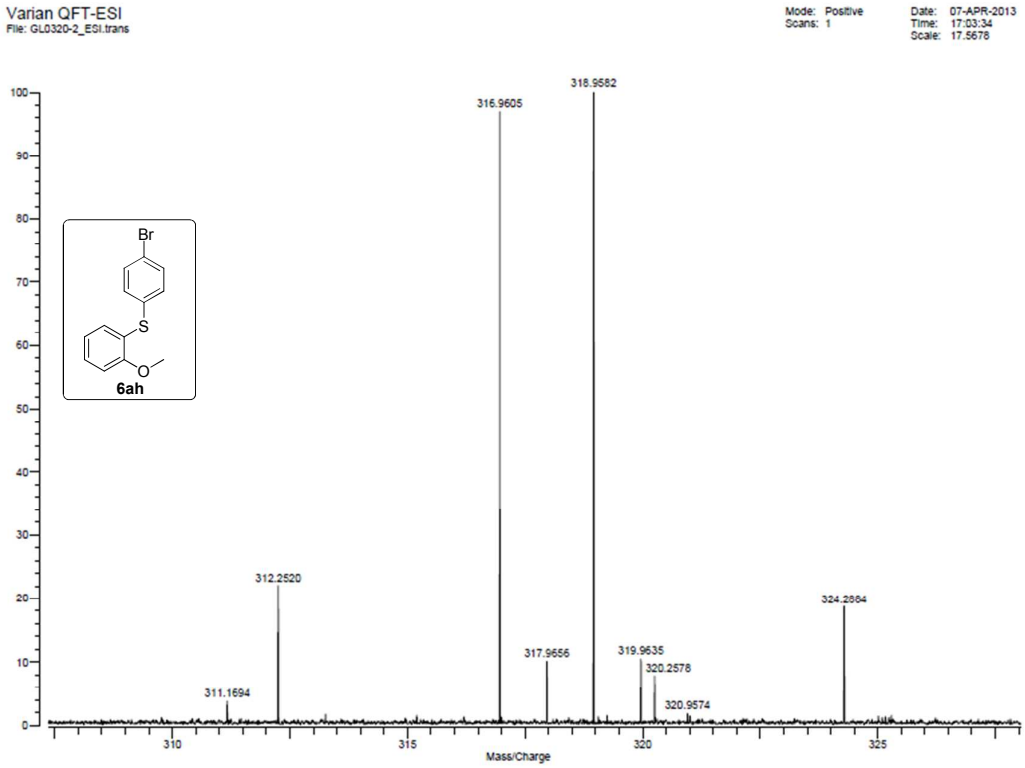
(4-Bromophenyl)(2-methoxyphenyl)sulfane (6ah).



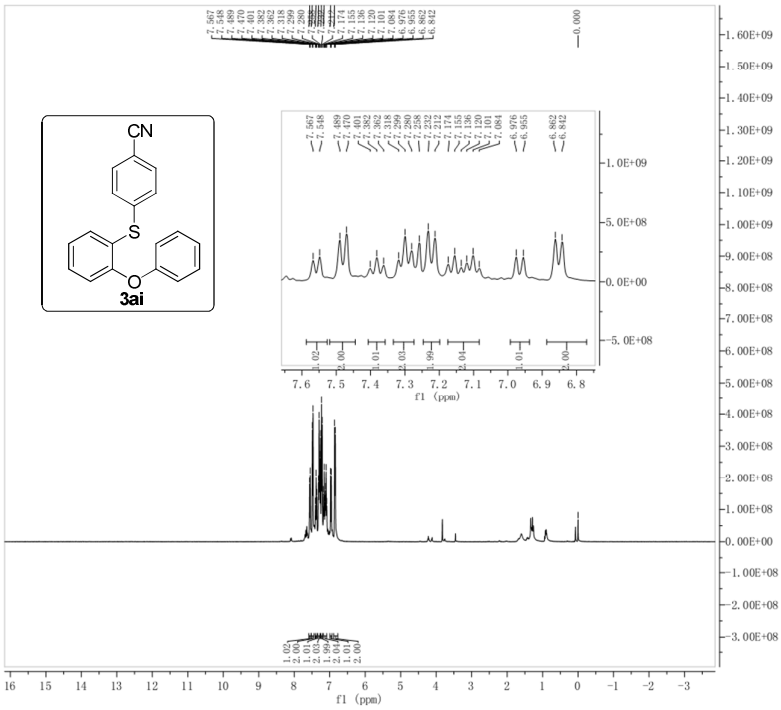
Parameter	Value
1 Data File Name	E:/ 李红影-苯块/ 苯块-5/ NMR/ 标准 gl0320-2/ 1/ pdata/ 1/ 1r
2 Title	gl0320-2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	113
15 Relaxation Delay	1.0000
16 Pulse Width	14.4000
17 Acquisition Time	4.0894
18 Acquisition Date	2013-03-22T08:32:00
19 Modification Date	2013-03-22T08:32:14
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1548.5
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



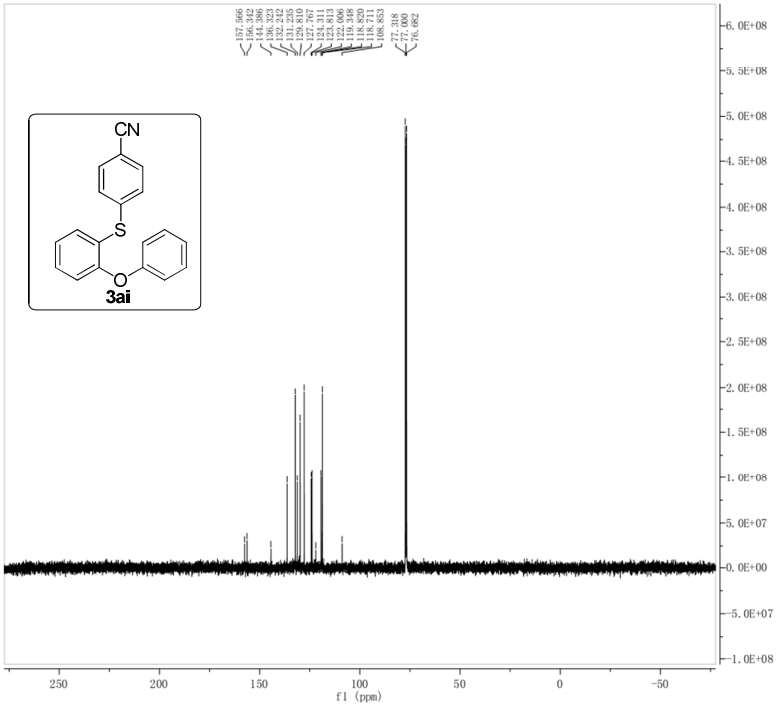
	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 gl0320-2/ 2/ pdata/ 1/ 1r
2	Title	gl0320-2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	445
14	Receiver Gain	119
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-03-24T14:43:00
19	Modification Date	2013-03-24T14:53:54
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768



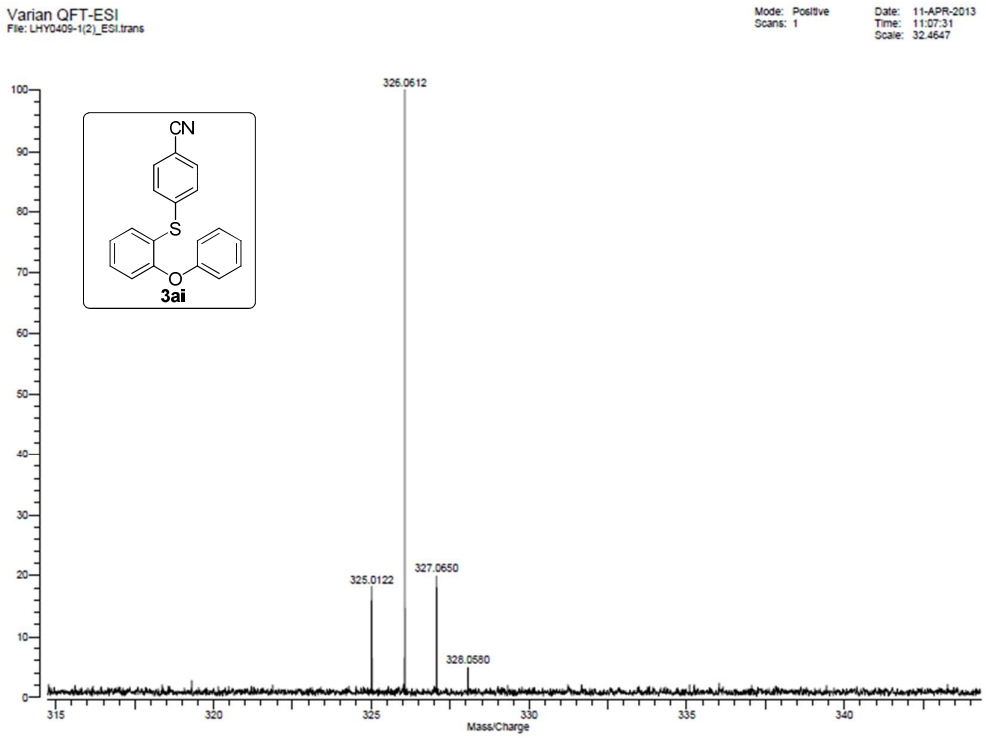
4-((2-Phenoxyphenyl)thio)benzonitrile (3ai).



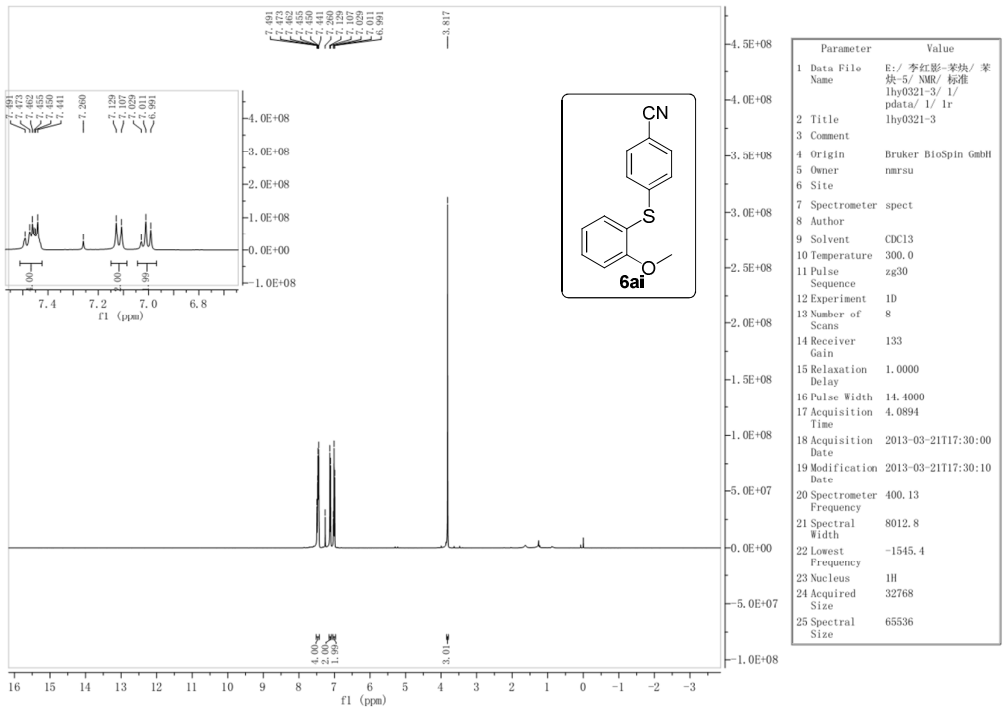
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ NMR数据/ lhy0409-1/ 1/ pdata/ 1/ 1r
2 Title	lhy0409-1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	159
15 Relaxation Delay	1.0000
16 Pulse Width	14.4000
17 Acquisition Time	4.0894
18 Acquisition Date	2013-04-10T09:37:00
19 Modification Date	2013-04-10T00:00:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1545.8
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

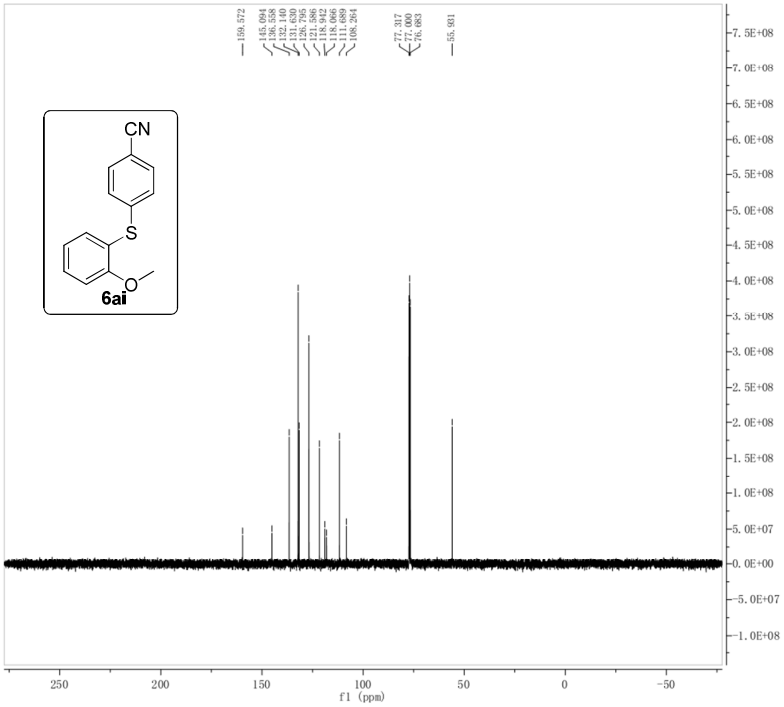


Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ NMR数据/ lhy0409-1/ 2/ pdata/ 1/ 1r
2 Title	lhy0409-1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	658
14 Receiver Gain	119
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-04-10T09:40:00
19 Modification Date	2013-04-10T00:00:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768

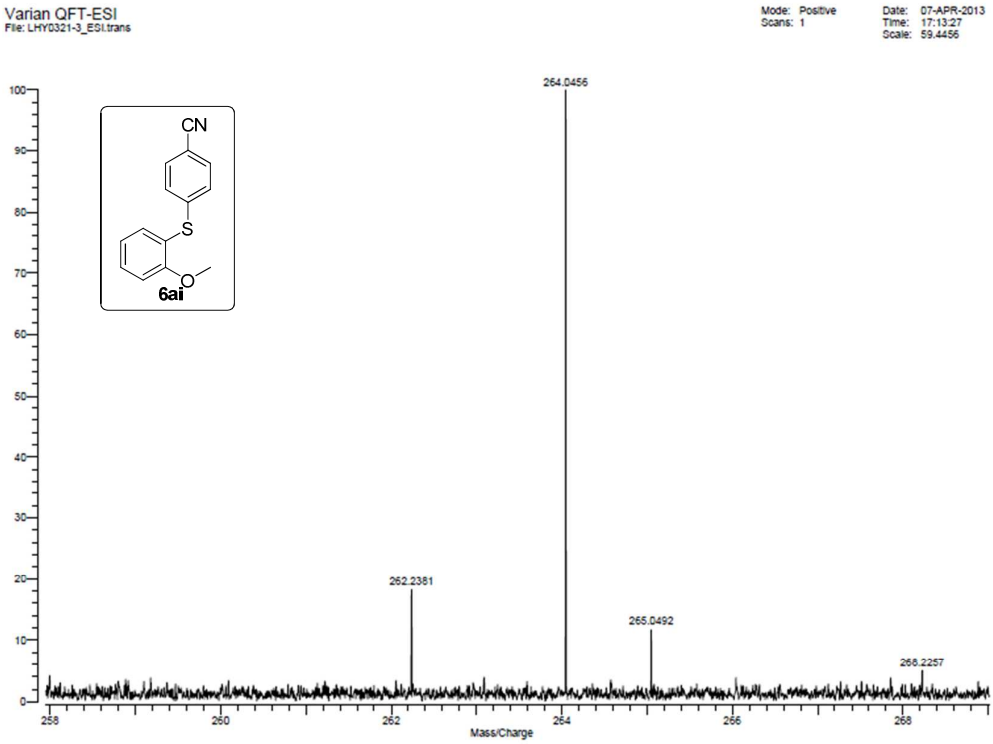


4-((2-Methoxyphenyl)thio)benzonitrile (6ai).

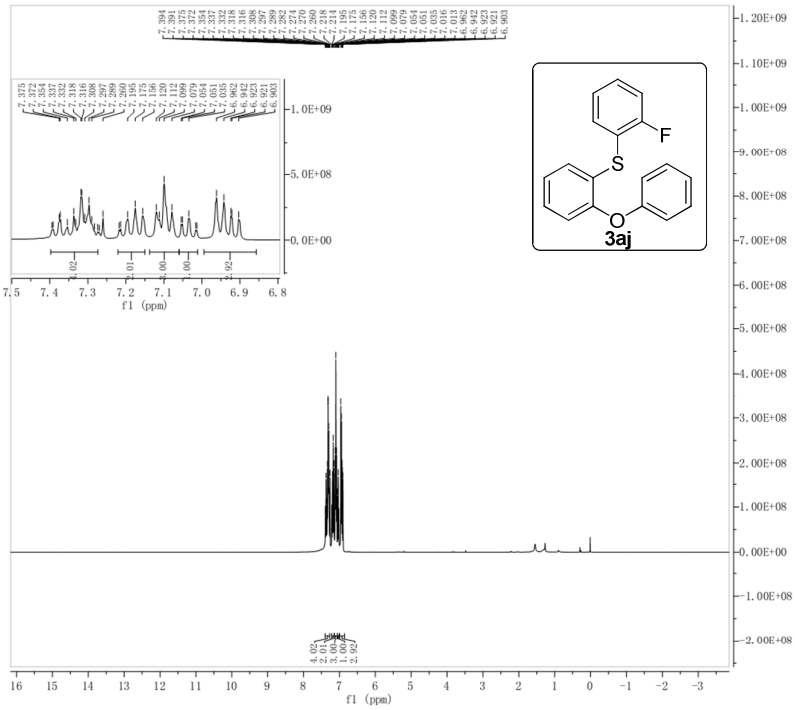




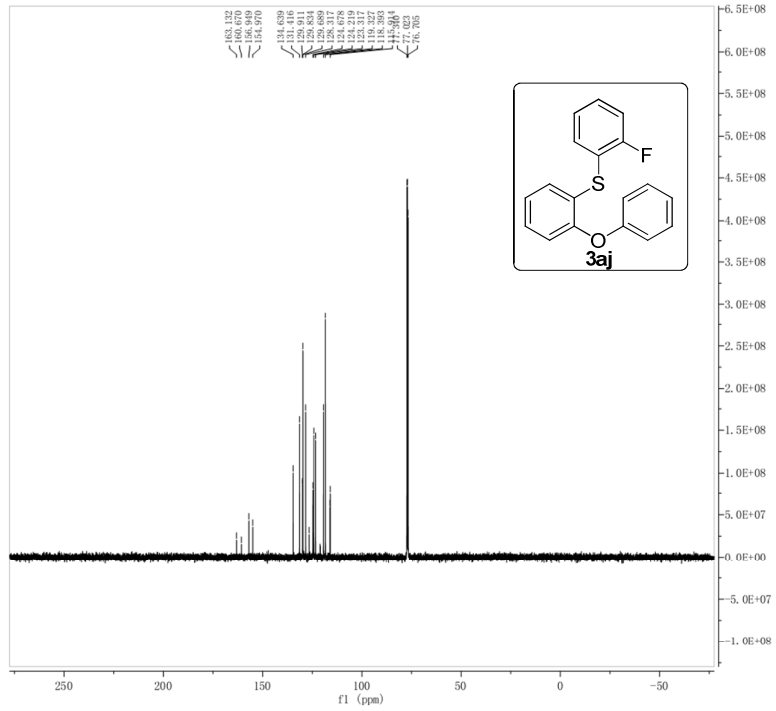
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0321-3/ 2/ pdata/ 1/ 1r
2 Title	1hy0321-3
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	214
14 Receiver Gain	113
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-03-21T17:32:00
19 Modification Date	2013-03-21T17:36:32
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768



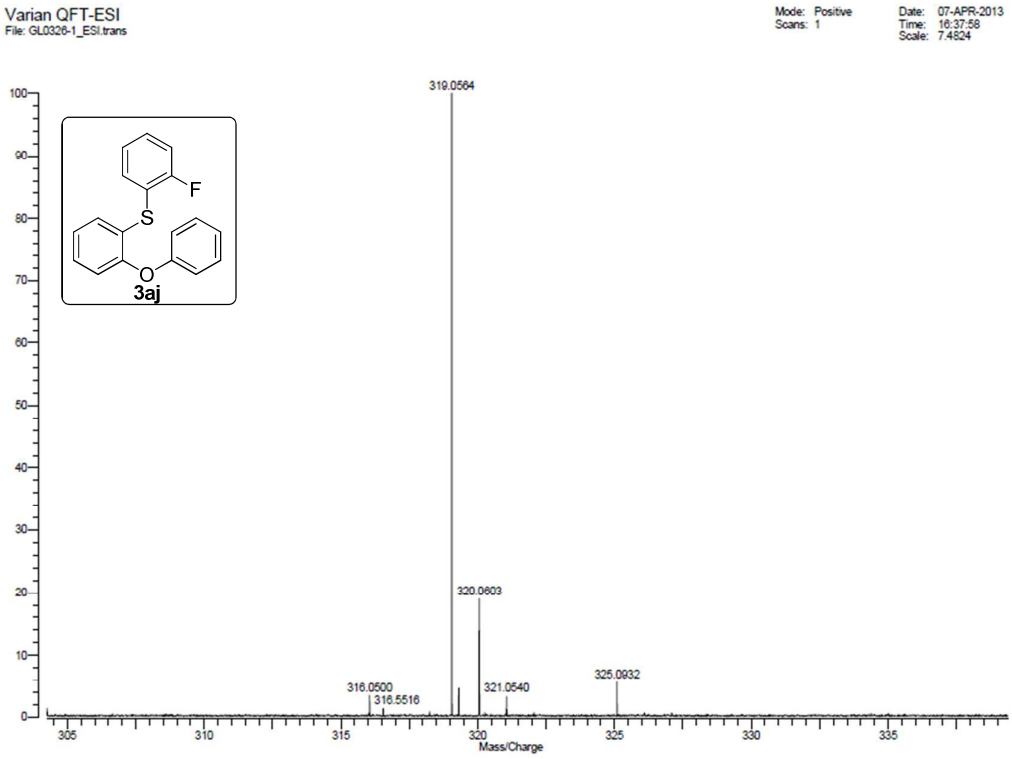
(2-Fluorophenyl)(2-phenoxyphenyl)sulfane (3aj).



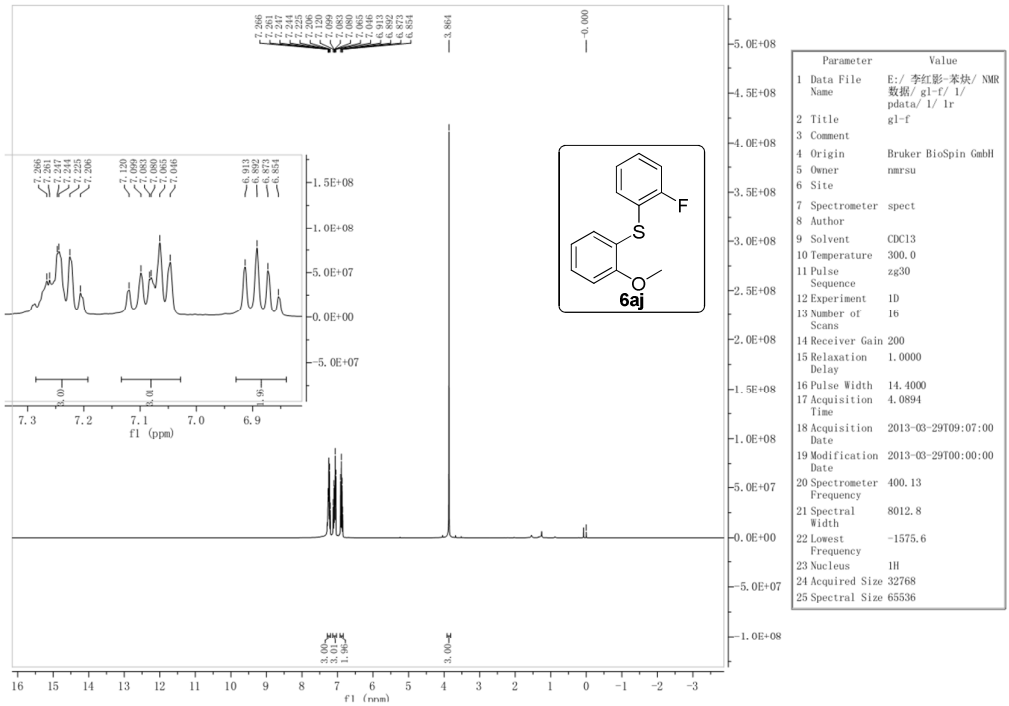
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 GL0326-1/ 1/ pdata/ 1/ 1r
2 Title	typ20130327-ii-1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	133
15 Relaxation Delay	1.0000
16 Pulse Width	14.4000
17 Acquisition Time	4.0894
18 Acquisition Date	2013-03-27T10:33:00
19 Modification Date	2013-03-27T10:32:10
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1550.1
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

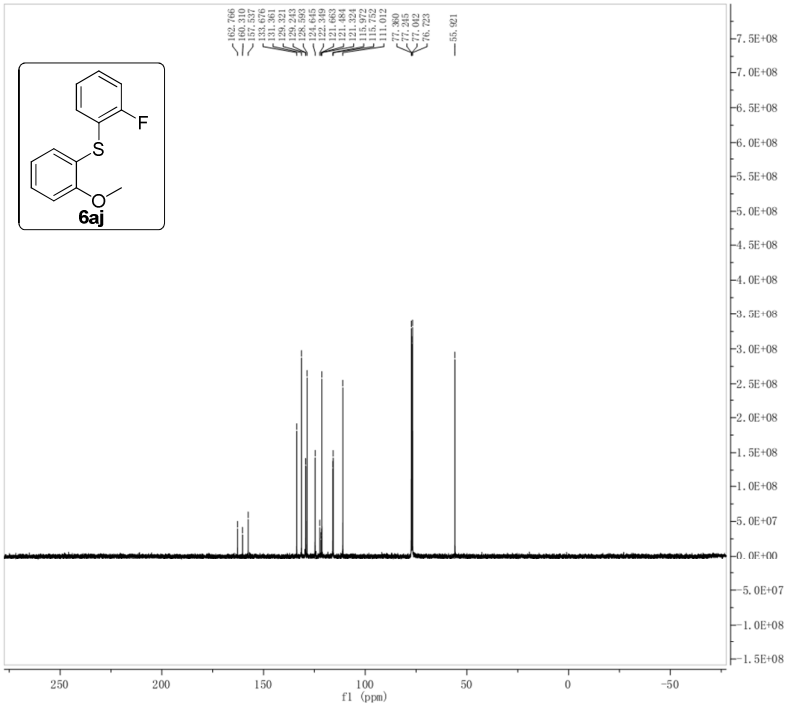


Parameter	Value
1 Data File Name	E:/ 李红影 苯炔/ NMR数据/ gl-f/ 2/ pdata/ 1/ 1r
2 Title	gl-f
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	76
14 Receiver Gain	88
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-03-29T09:09:00
19 Modification Date	2013-03-29T00:00:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768

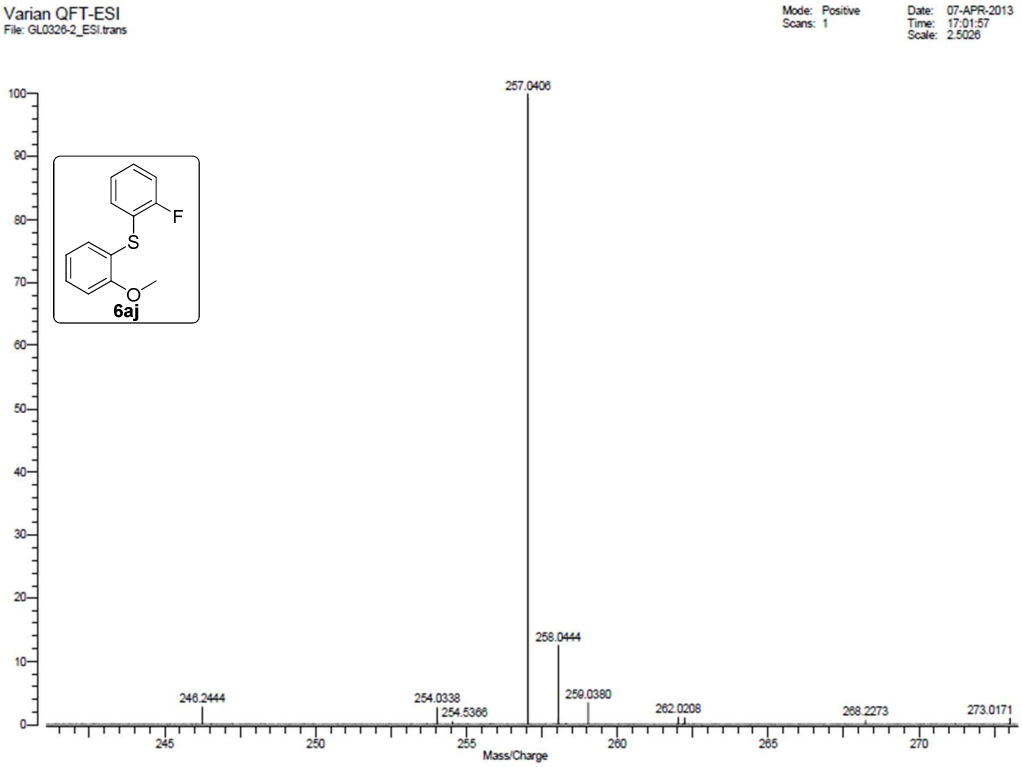


(2-Fluorophenyl)(2-methoxyphenyl)sulfane (6aj).

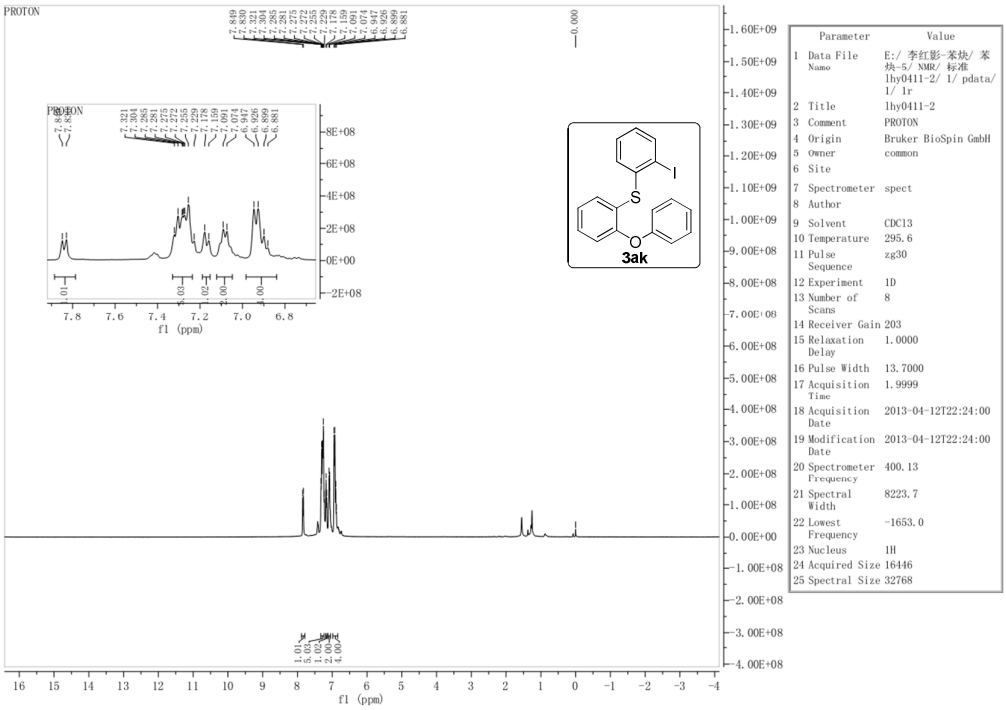




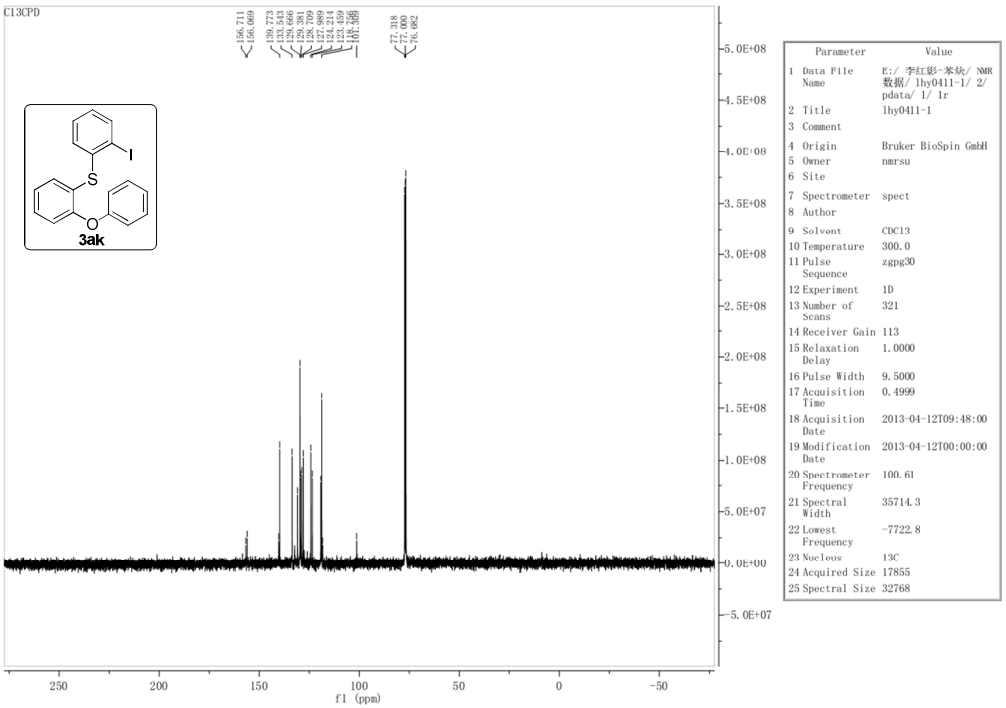
	Parameter	Value
1	Data File Name	F:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 GL0326-2/ 1/ pdata/ 1/ 1r
2	Title	GL3802-C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	841
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-03-29T14:23:00
19	Modification Date	2013-03-29T14:42:38
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768



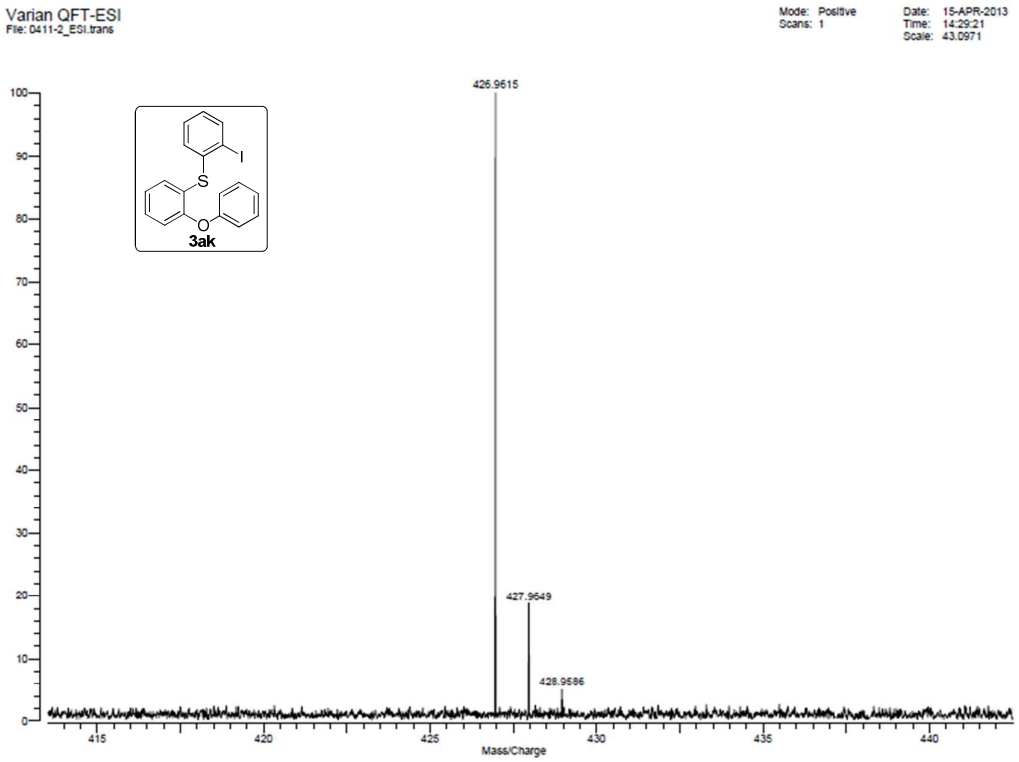
(2-Iodophenyl)(2-phenoxyphenyl)sulfane (3ak).



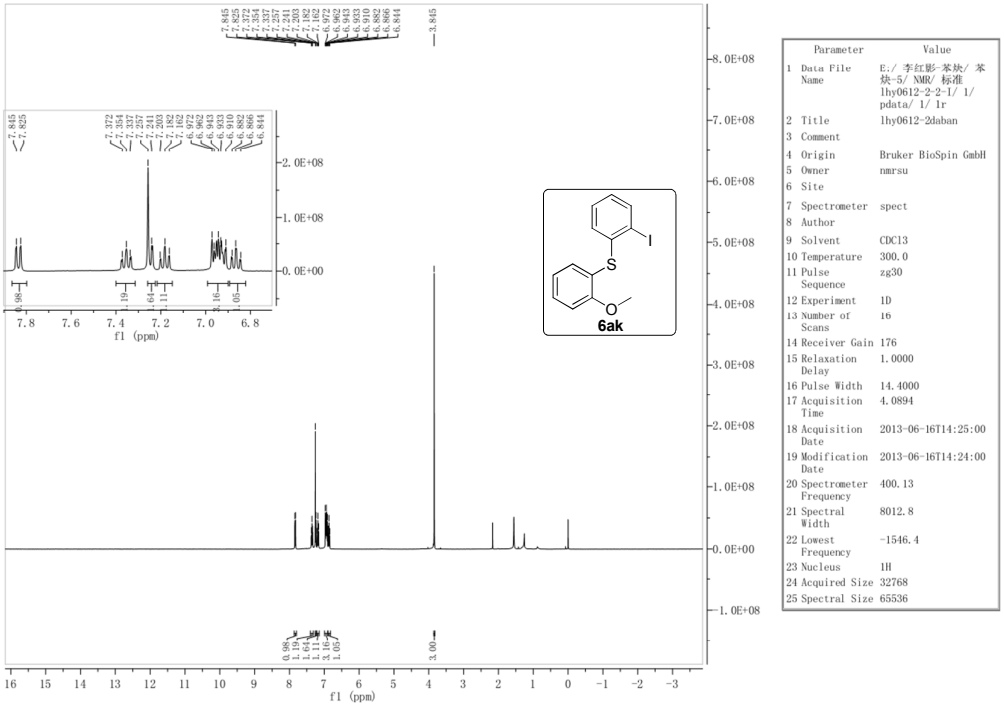
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0411-2/ 1/ pdata/ 1/ 1r
2 Title	1hy0411-2
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	13.7000
17 Acquisition Time	1.9999
18 Acquisition Date	2013-04-12T22:24:00
19 Modification Date	2013-04-12T22:24:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8223.7
22 Lowest Frequency	-1653.0
23 Nucleus	1H
24 Acquired Size	16446
25 Spectral Size	32768

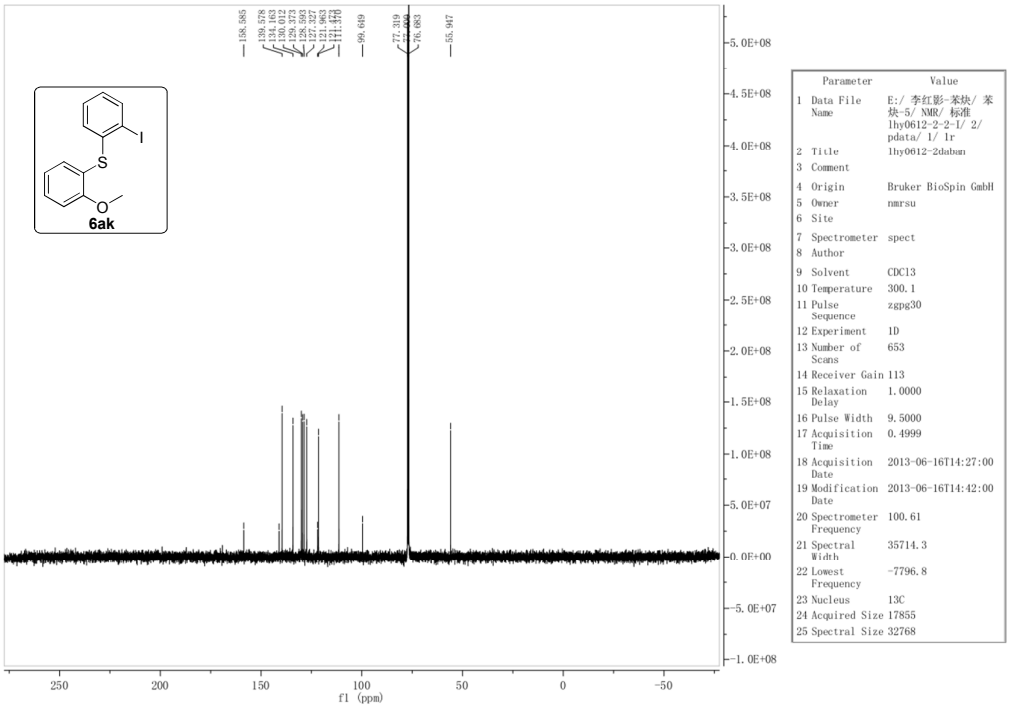


Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ NMR 数据/ 1hy0411-1/ 2/ pdata/ 1/ 1r
2 Title	1hy0411-1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	321
14 Receiver Gain	113
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-04-12T09:48:00
19 Modification Date	2013-04-12T00:00:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7722.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768

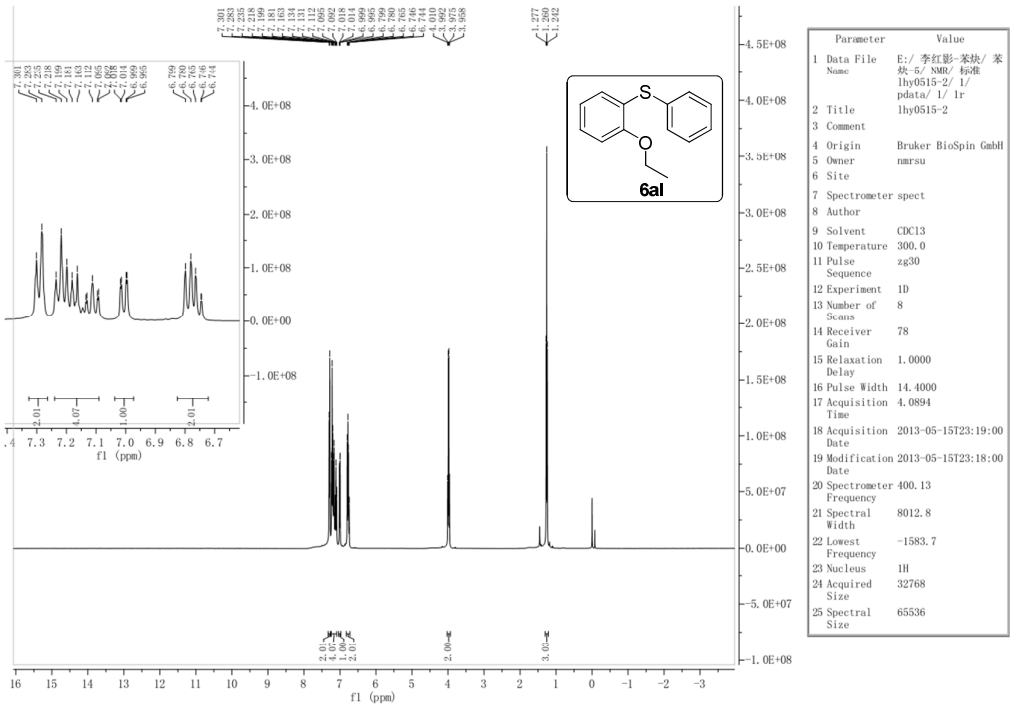


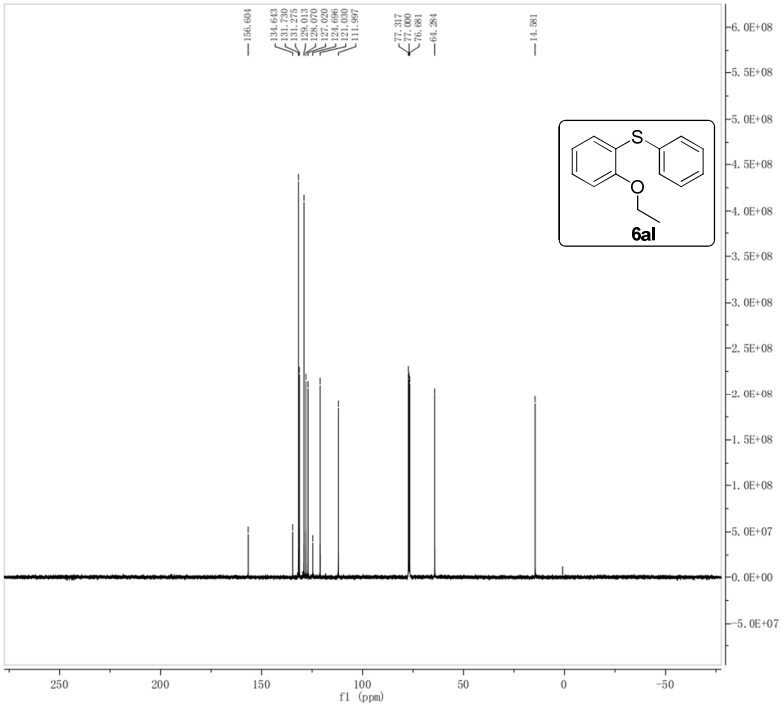
(2-Iodophenyl)(2-methoxyphenyl)sulfane (6ak).



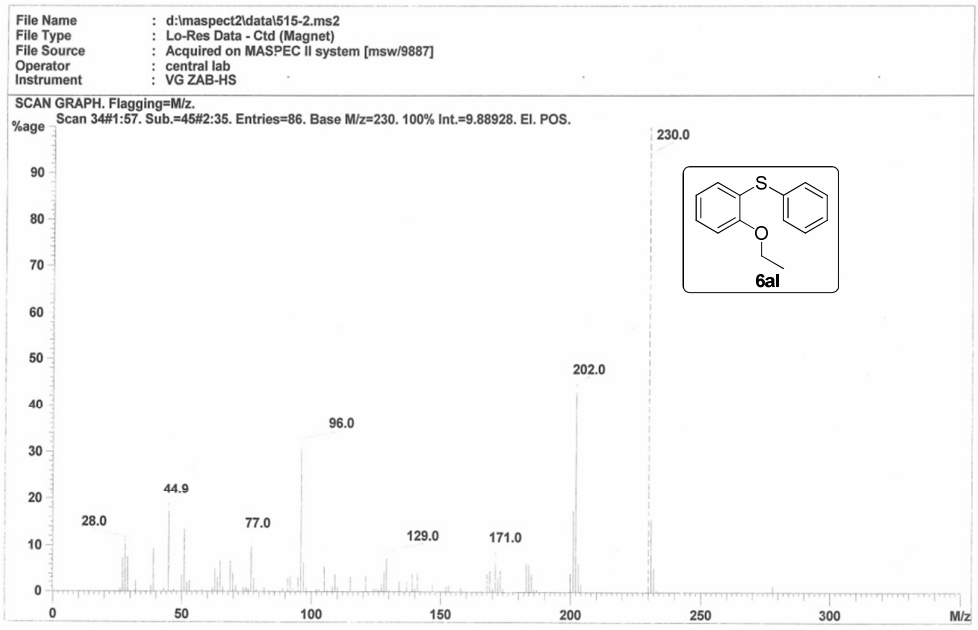


(2-Ethoxyphenyl)(phenyl)sulfane (6al).

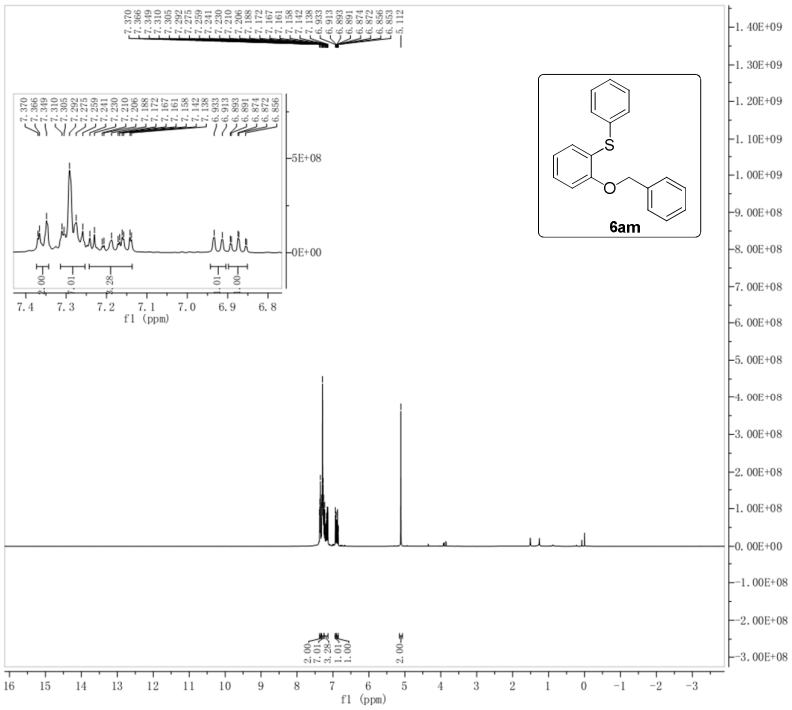




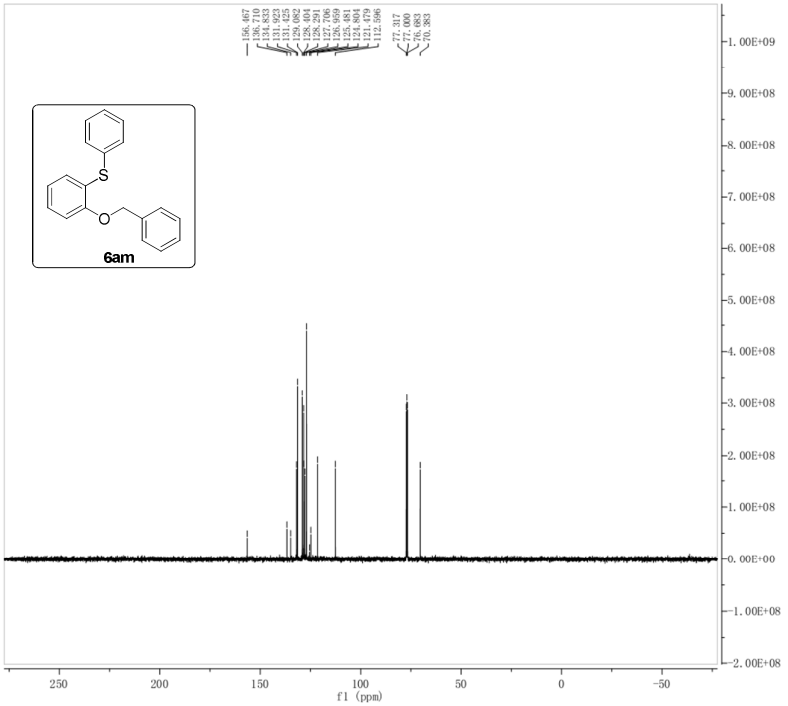
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0515-2/ 2/ pdata/ 1/ 1r
2 Title	1hy0515-2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1024
14 Receiver Gain	119
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-05-15T23:47:00
19 Modification Date	2013-05-15T23:45:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768



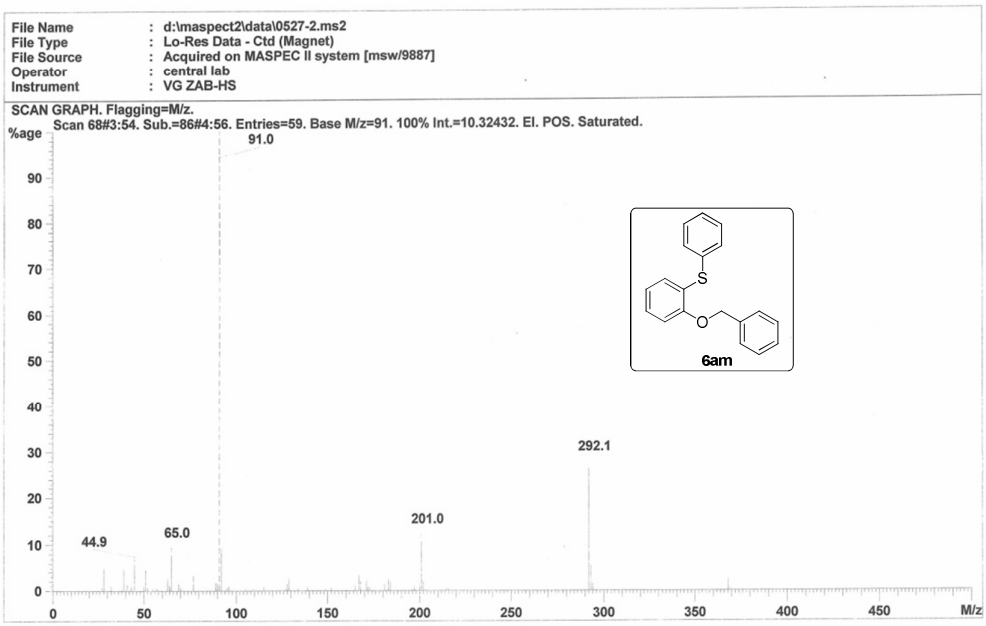
(2-(Benzyloxy)phenyl)(phenyl)sulfane (6am).



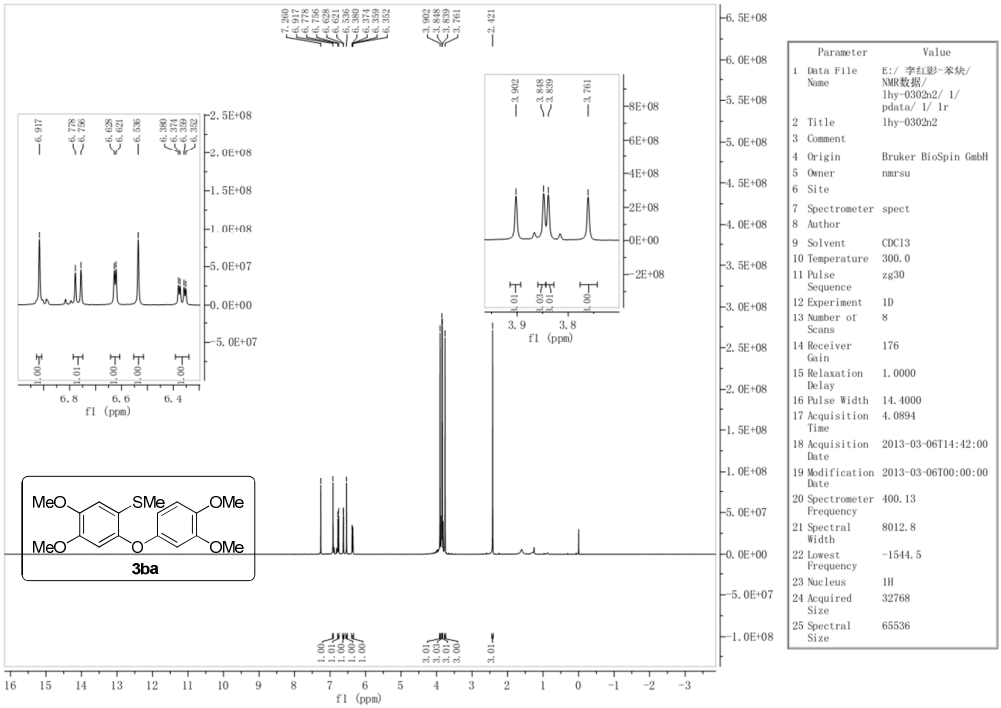
Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0527-2/ 3-H/ pdata/ 1/ 1r
2 Title	1hy0527-2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	78
15 Relaxation Delay	1.0000
16 Pulse Width	14.4000
17 Acquisition Time	4.0894
18 Acquisition Date	2013-05-28T19:34:00
19 Modification Date	2013-05-28T19:32:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1557.0
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

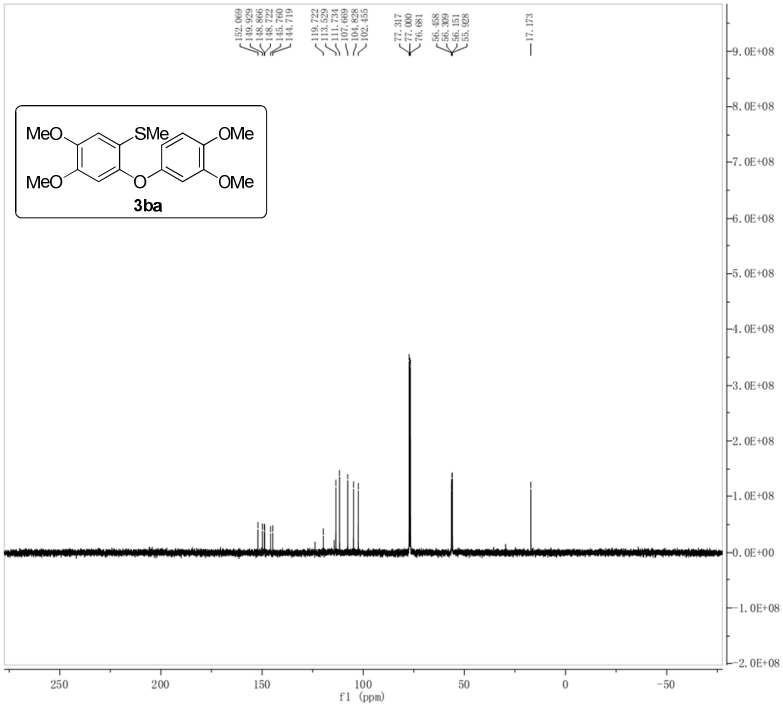


Parameter	Value
1 Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0527-2/ 4-C/ pdata/ 1/ 1r
2 Title	1hy0527-2
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	128
14 Receiver Gain	113
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-05-28T19:35:00
19 Modification Date	2013-05-28T19:37:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768



(2-(3,4-Dimethoxyphenoxy)-4,5-dimethoxyphenyl)(methyl)sulfane (3ba).

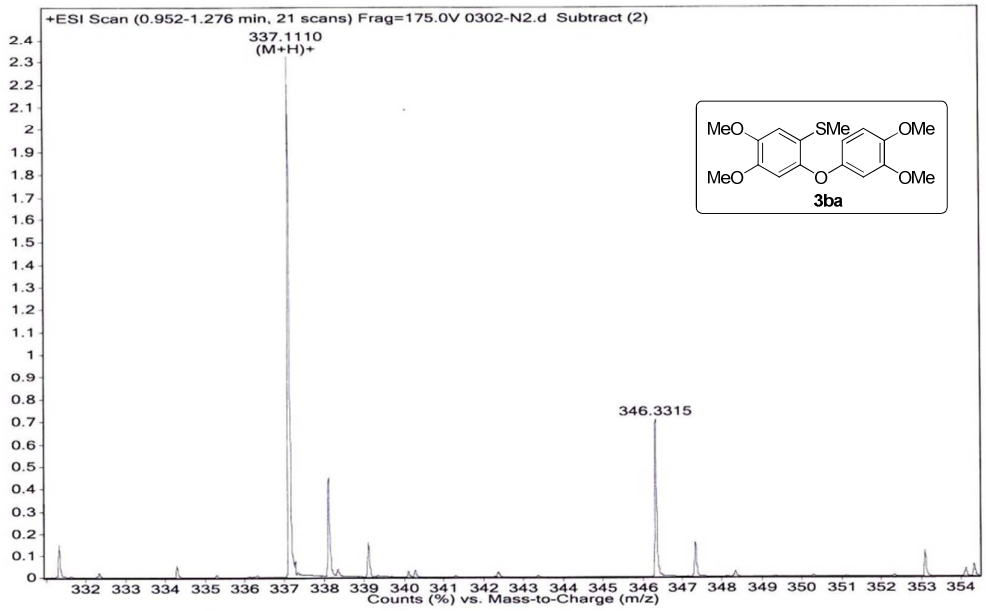




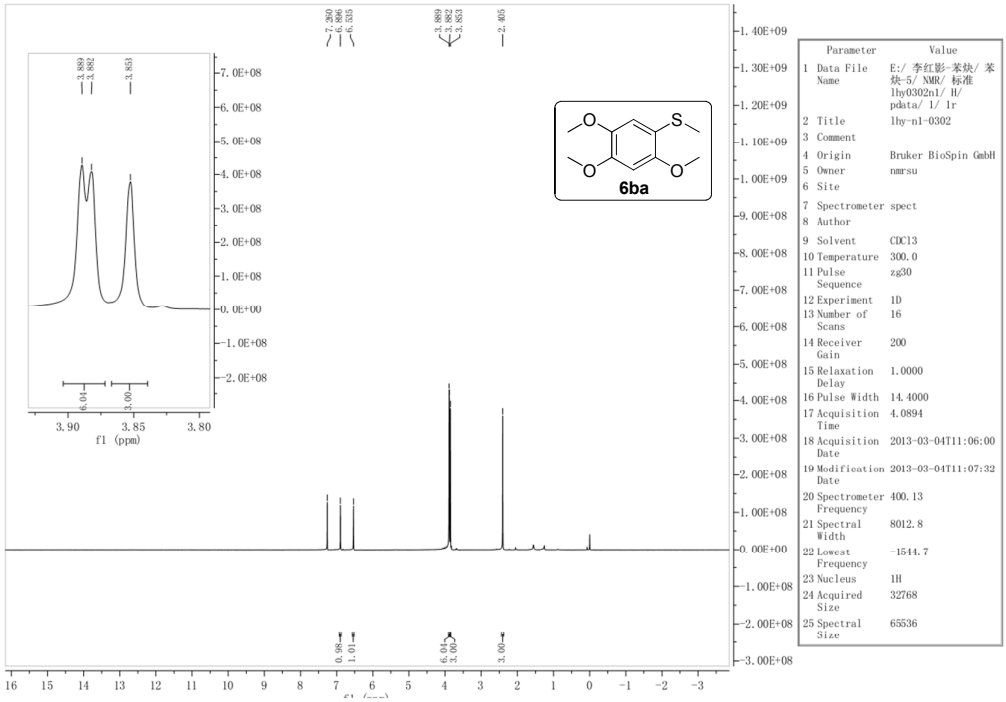
	Parameter	Value
1	Data File Name	F:/ 李红影-苯妙/ NMR数据/ lhy-0302n2/ 2/ pdata/ 1/ 1r
2	Title	lhy-0302n2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	489
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-03-06T14:44:00
19	Modification Date	2013-03-06T00:00:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768

337.1104

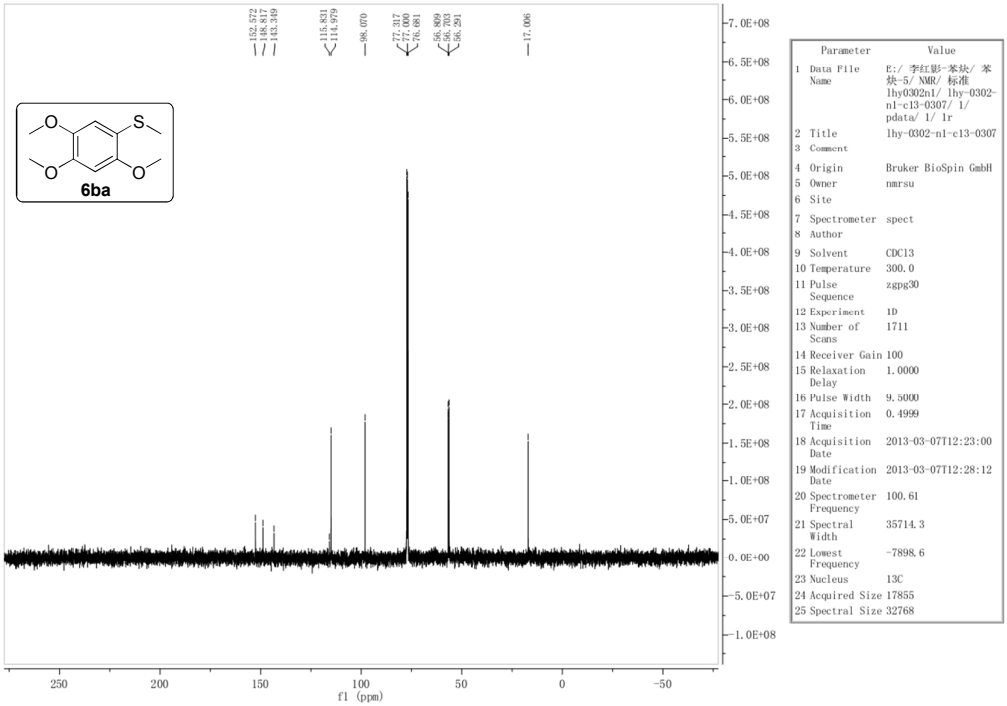
Sample Name	LC/MS	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	0302-N2.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/7/2013 12:11:44 PM



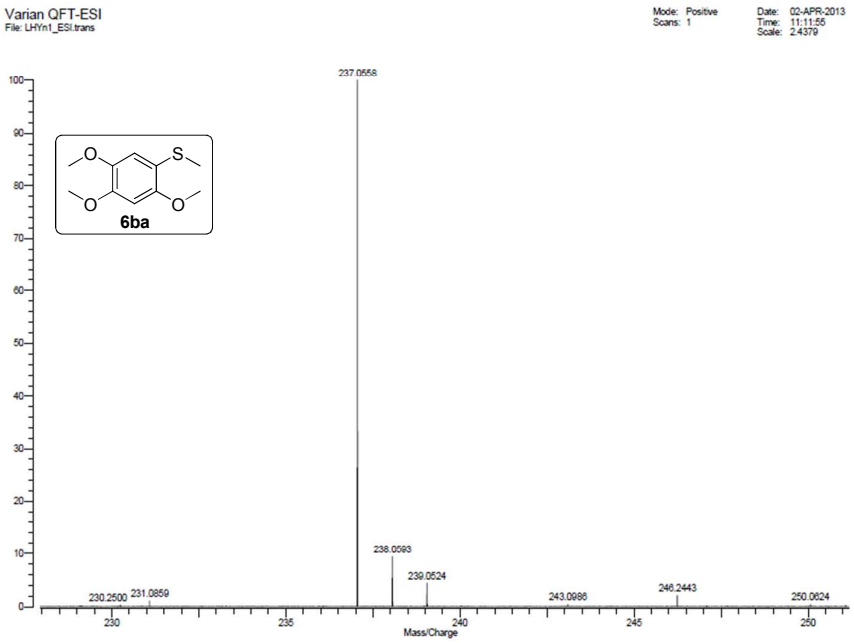
Methyl(2,4,5-trimethoxyphenyl)sulfane (6ba).



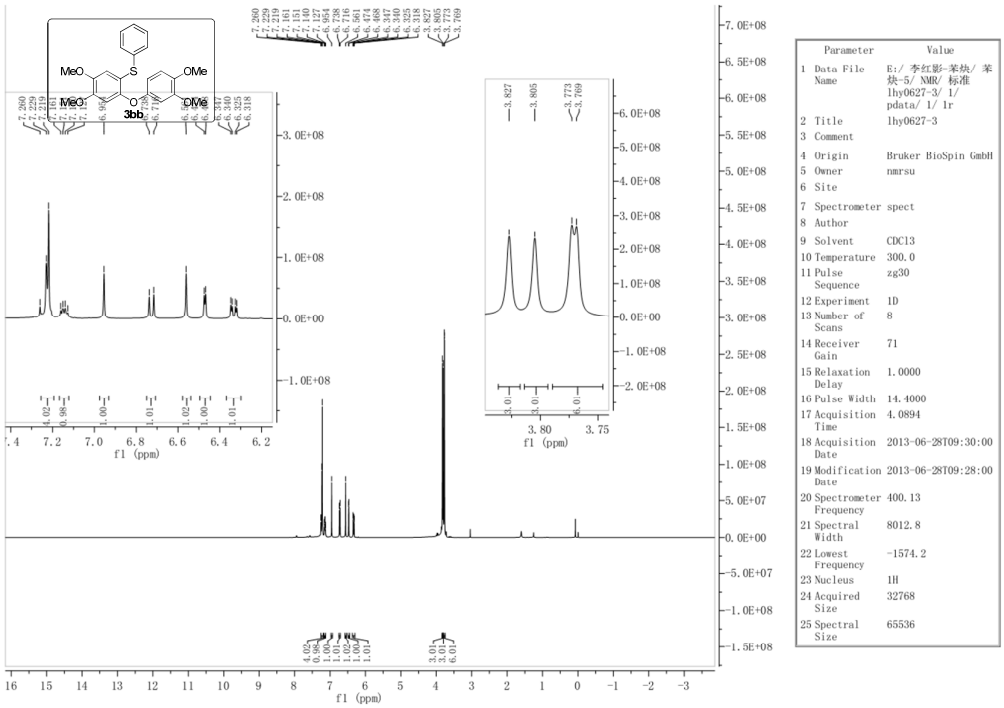
	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0302n1/ H/ pdata/ 1/ 1r
2	Title	1hy-n1-0302
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	200
15	Relaxation Delay	1.0000
16	Pulse Width	14.4000
17	Acquisition Time	4.0894
18	Acquisition Date	2013-03-04T11:06:00
19	Modification Date	2013-03-04T11:07:32
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1544.7
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	65536

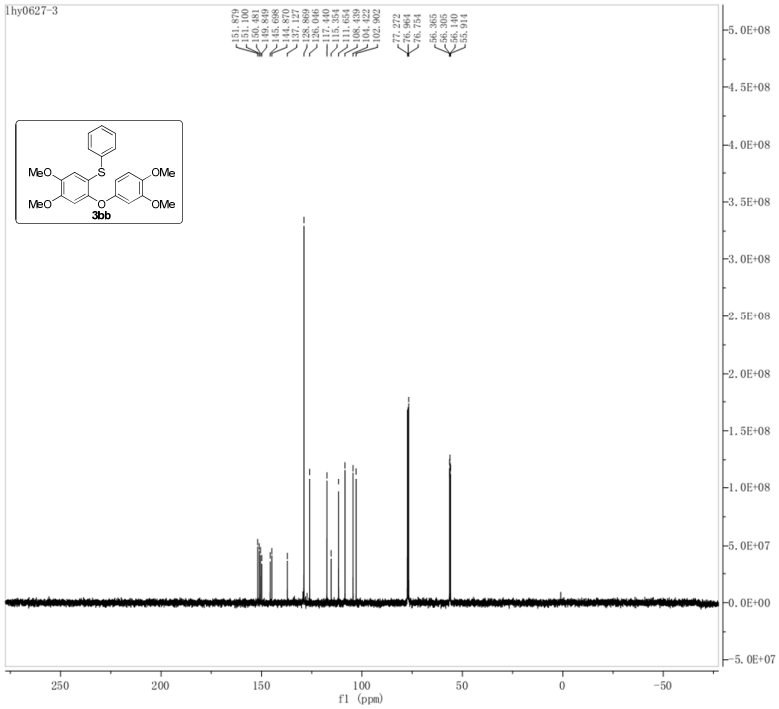


	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0302n1/ 1hy-0302-n1-c13-0307/ 1/ pdata/ 1/ 1r
2	Title	1hy-0302-n1-c13-0307
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1711
14	Receiver Gain	100
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-03-07T12:23:00
19	Modification Date	2013-03-07T12:28:12
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7898.6
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768



(2-(3,4-Dimethoxyphenoxy)-4,5-dimethoxyphenyl)(phenyl)sulfane (3bb).

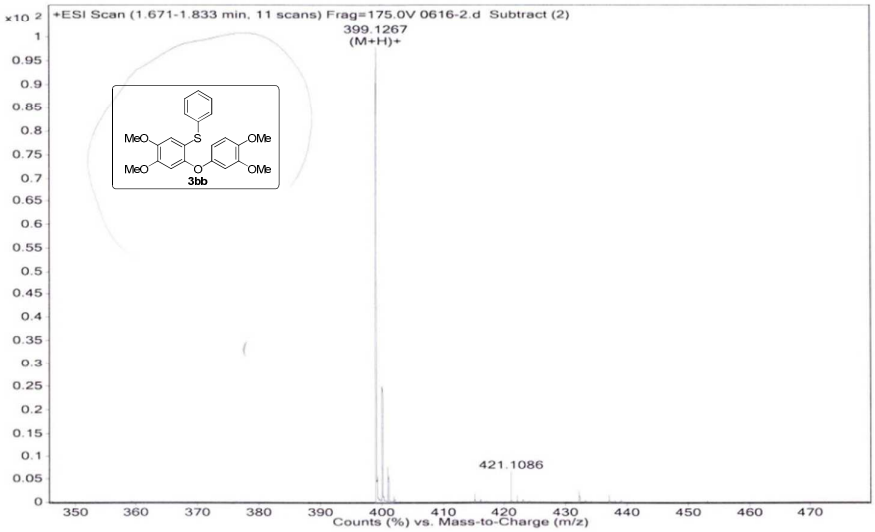




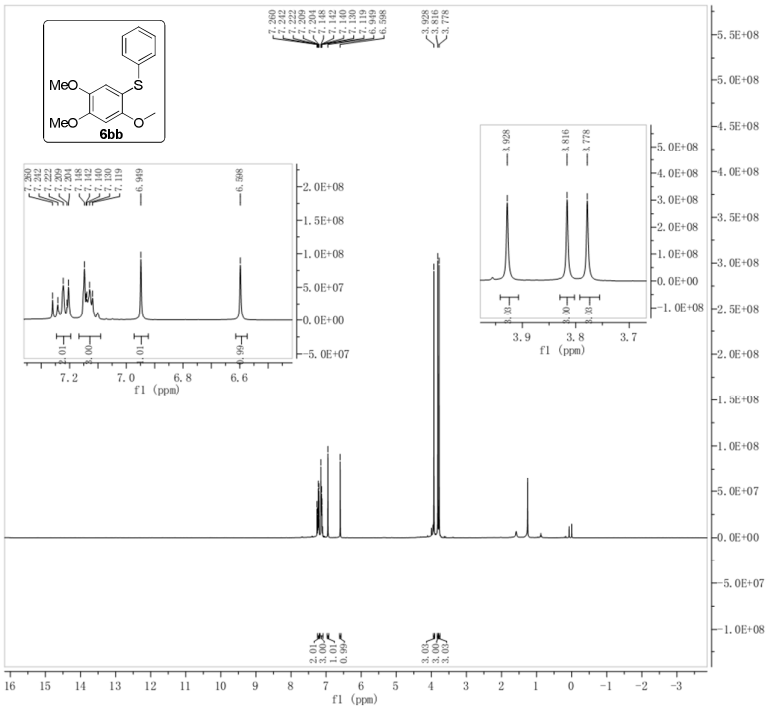
	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ NMR数据/ 1hy0627-3/ 2/ pdata/ 1/ 1r
2	Title	1hy0627-3
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	190
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-06-28T09:35:00
19	Modification Date	2013-06-28T00:00:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768

399.1261

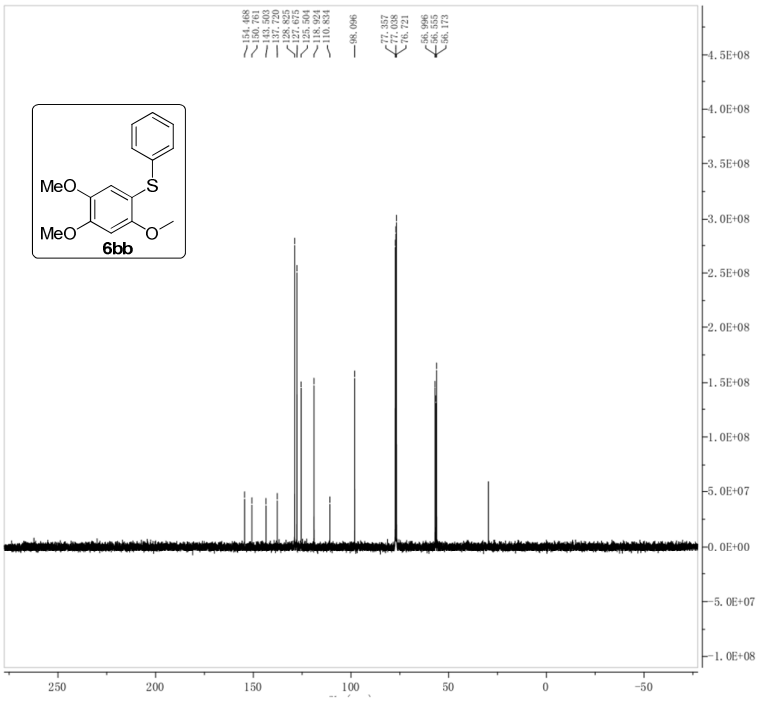
Sample Name	lc/ms	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	0616-2.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	6/25/2013 10:04:24 AM



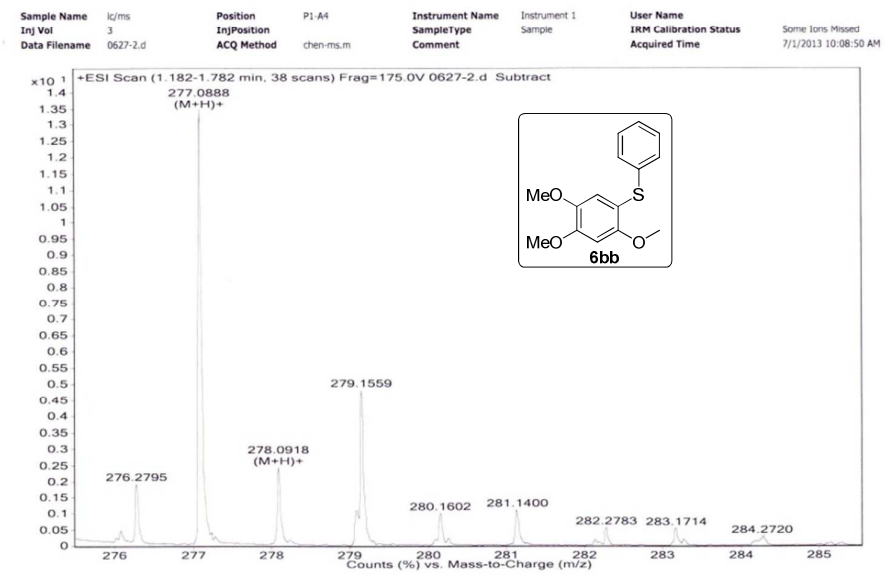
Phenyl(2,4,5-trimethoxyphenyl)sulfane (6bb).



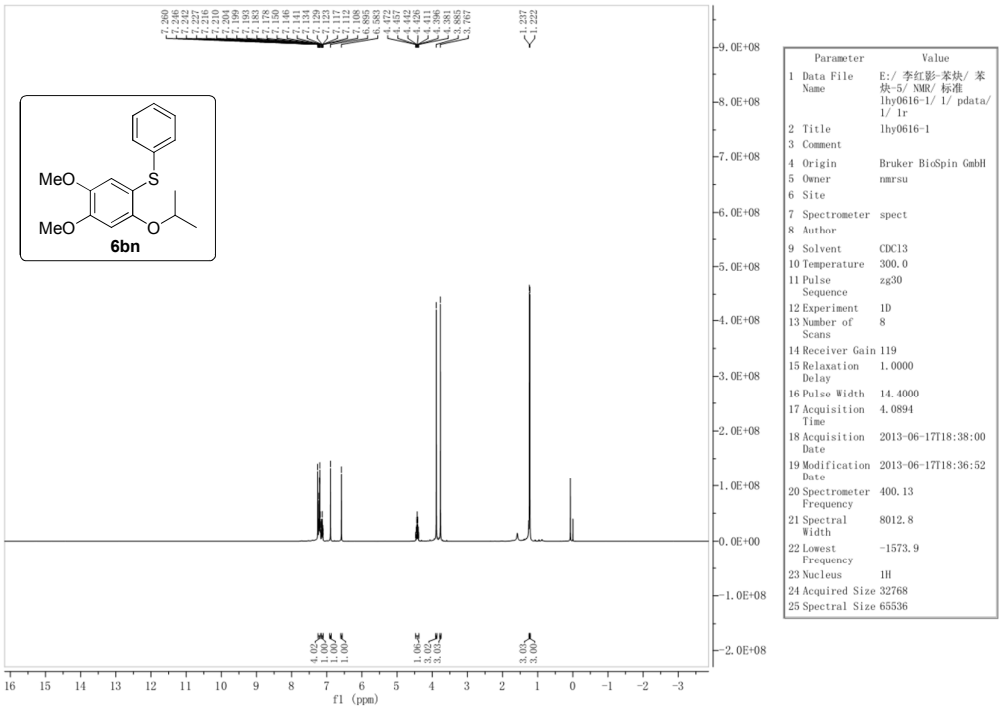
	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0627-2/ 1/ pdata/ 1/ 1r
2	Title	1hy0627-2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	14.4000
17	Acquisition Time	4.0894
18	Acquisition Date	2013-06-28T09:39:00
19	Modification Date	2013-06-28T09:38:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1545.1
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	65536

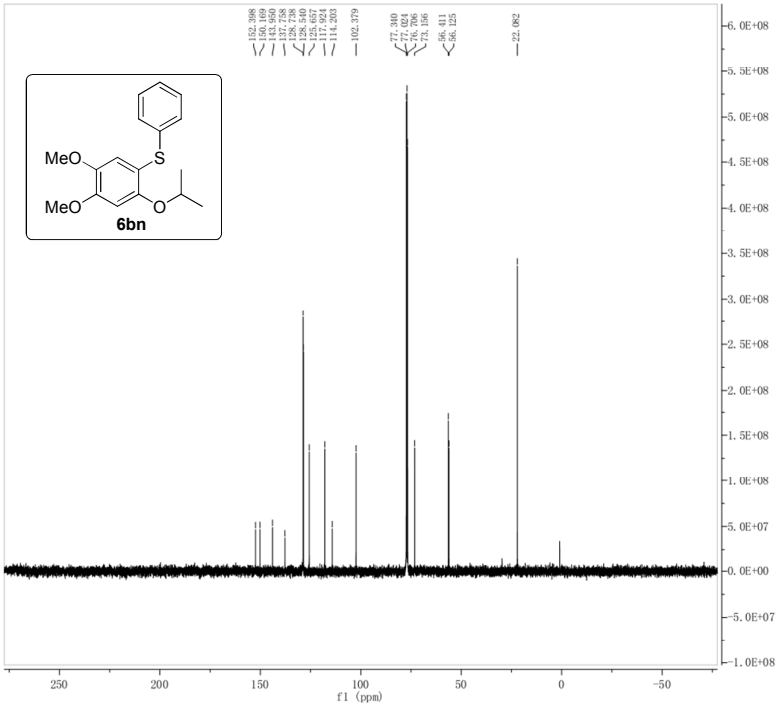


	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0627-2/ 2/ pdata/ 1/ 1r
2	Title	1hy0627-2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	377
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-06-28T09:41:00
19	Modification Date	2013-06-28T09:49:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768



(2-Isopropoxy-4,5-dimethoxyphenyl)(phenyl)sulfane (6bn).





	Parameter	Value
1	Data File Name	E:/ 李红影-苯炔/ 苯炔-5/ NMR/ 标准 1hy0616-1/ 2/ pdata/ 1/ 1r
2	Title	1hy0616-1
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	625
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-06-17T18:40:00
19	Modification Date	2013-06-17T18:53:56
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768

305.1206

Sample Name	lc/ms	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	3	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
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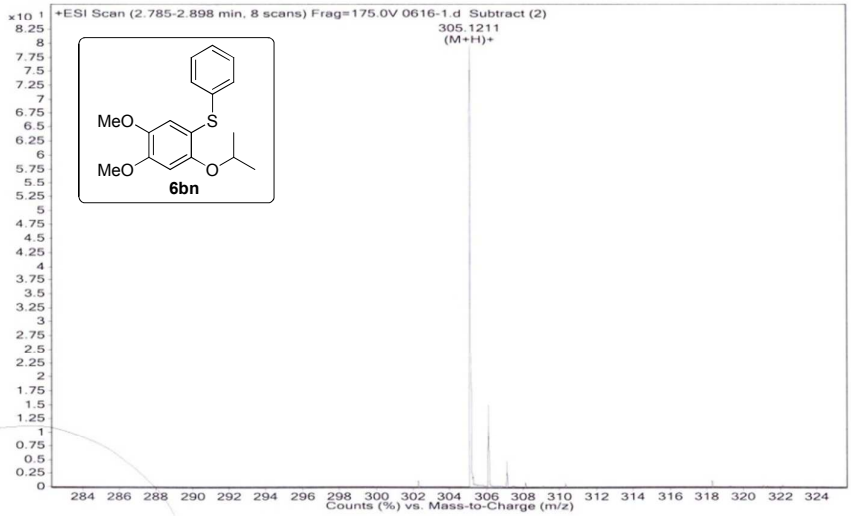
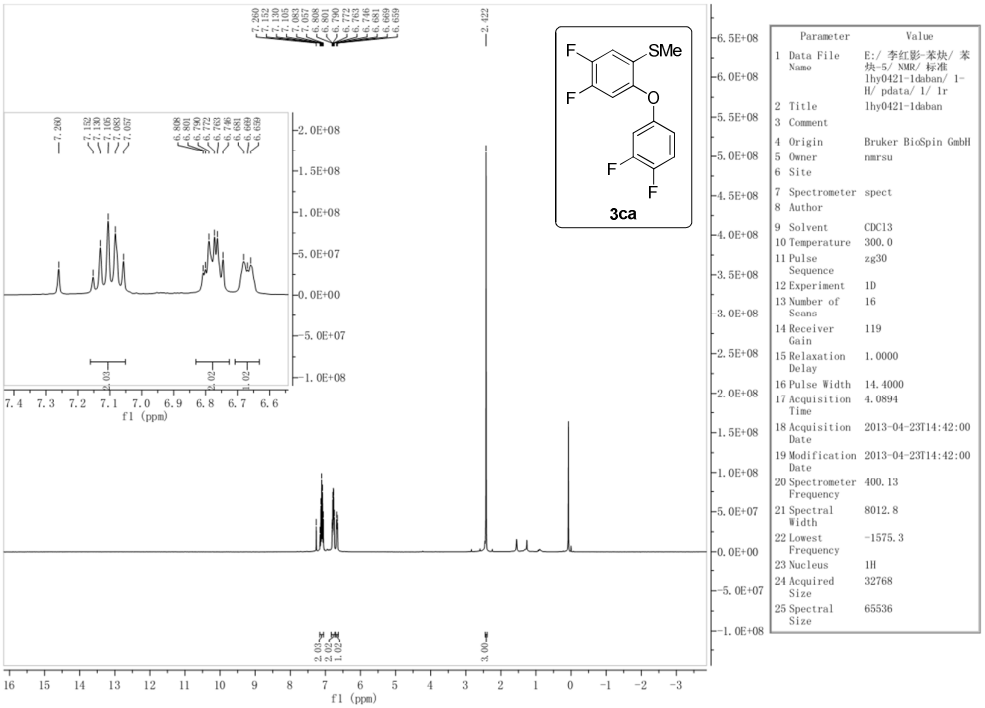


(2-(3,4-Difluorophenoxy)-4,5-difluorophenyl)(methyl)sulfane (3ca).



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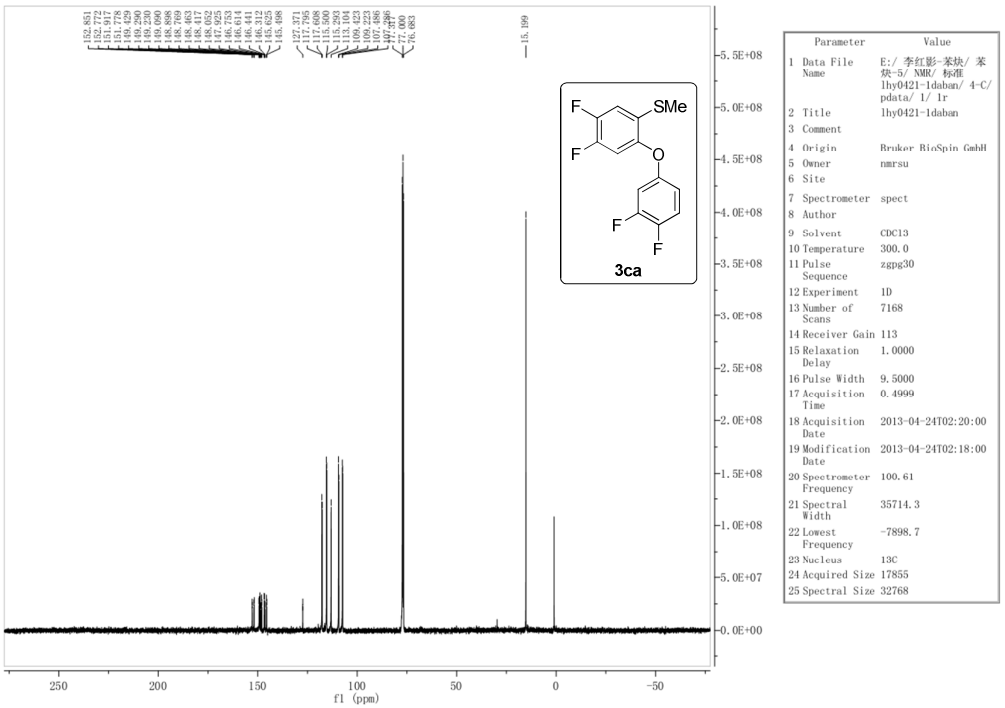
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	119
15	Relaxation Delay	1.0000
16	Pulse Width	14.4000
17	Acquisition Time	4.0894
18	Acquisition Date	2013-04-23T14:42:00
19	Modification Date	2013-04-23T14:42:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1575.3
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	65536



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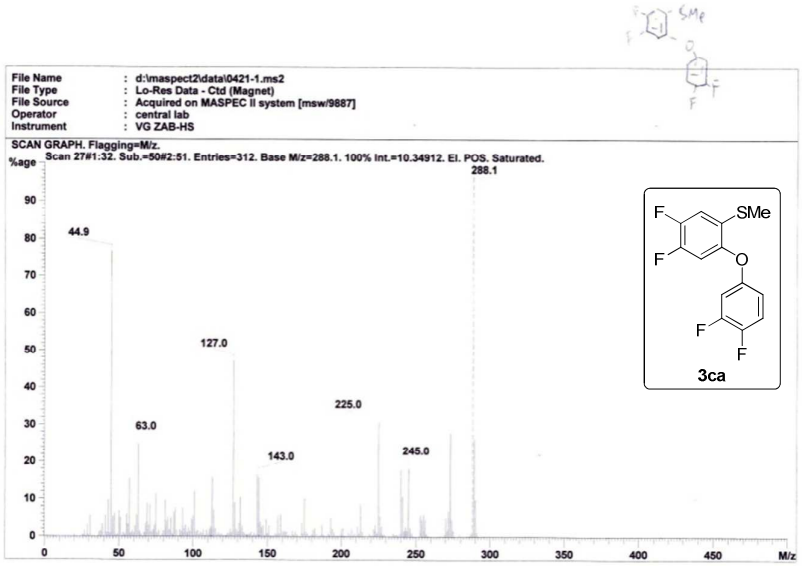
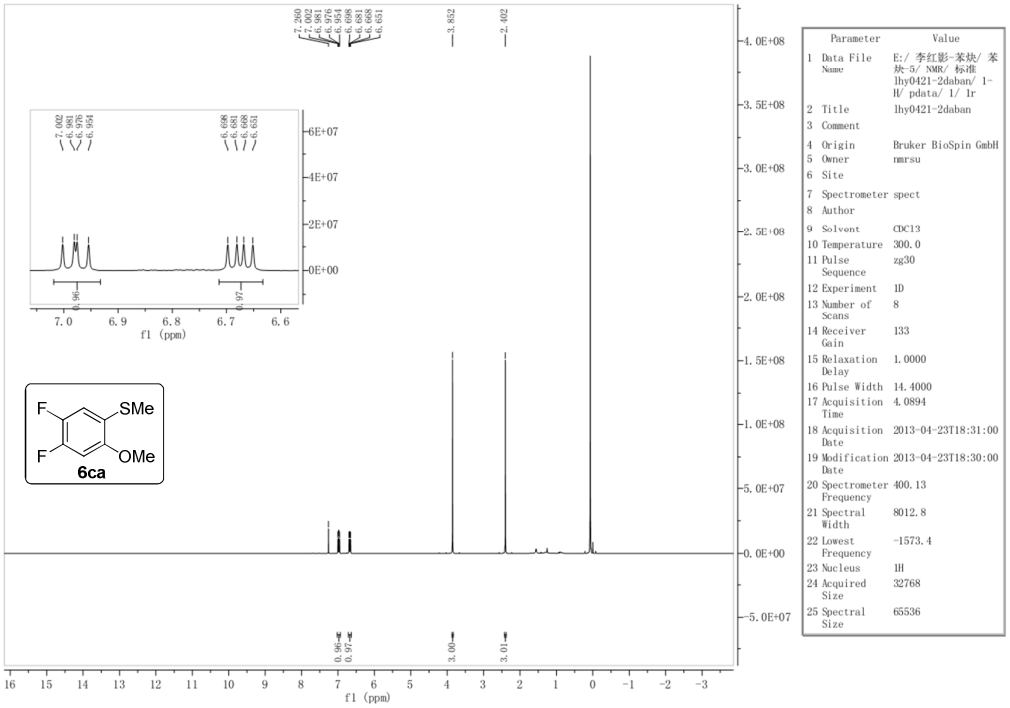
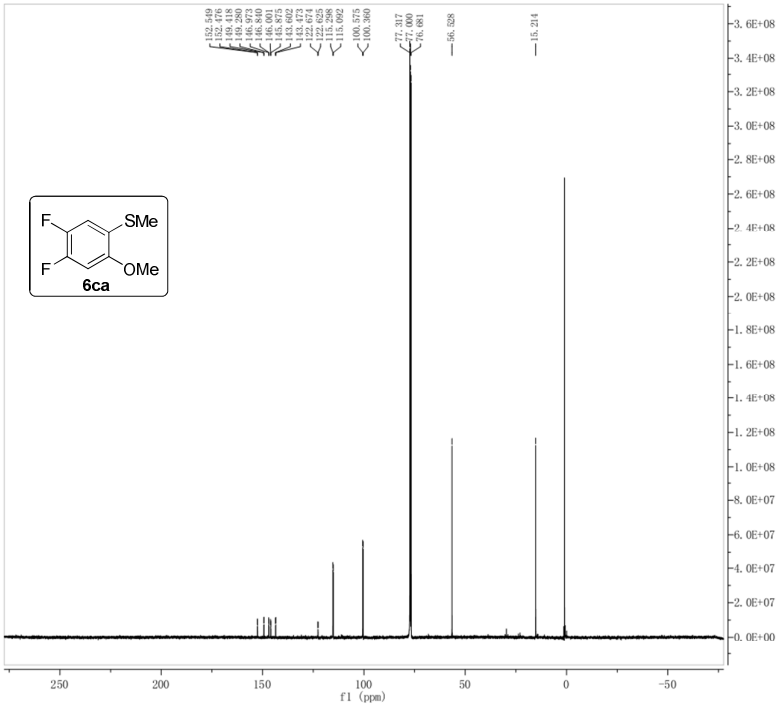
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	7168
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-04-24T02:20:00
19	Modification Date	2013-04-24T02:18:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7898.7
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768



(4,5-Difluoro-2-methoxyphenyl)(methyl)sulfane (6ca).





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2 Title	1hy0421-2daban
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	12928
14 Receiver Gain	113
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-04-24T08:00:00
19 Modification Date	2013-04-24T00:00:00
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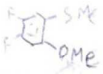
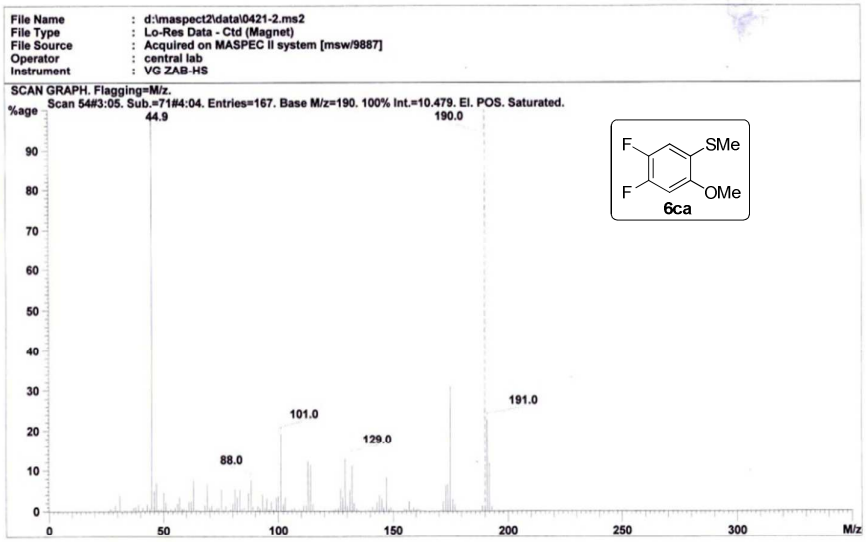
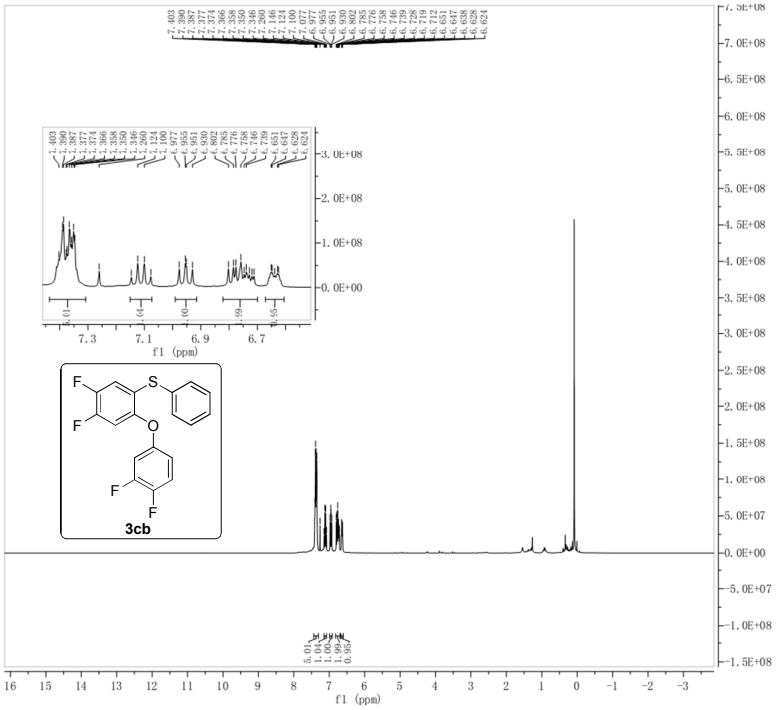
22 Lowest Frequency	-7898.6
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768





(2-(3,4-Difluorophenoxy)-4,5-difluorophenyl)(phenyl)sulfane (3cb).



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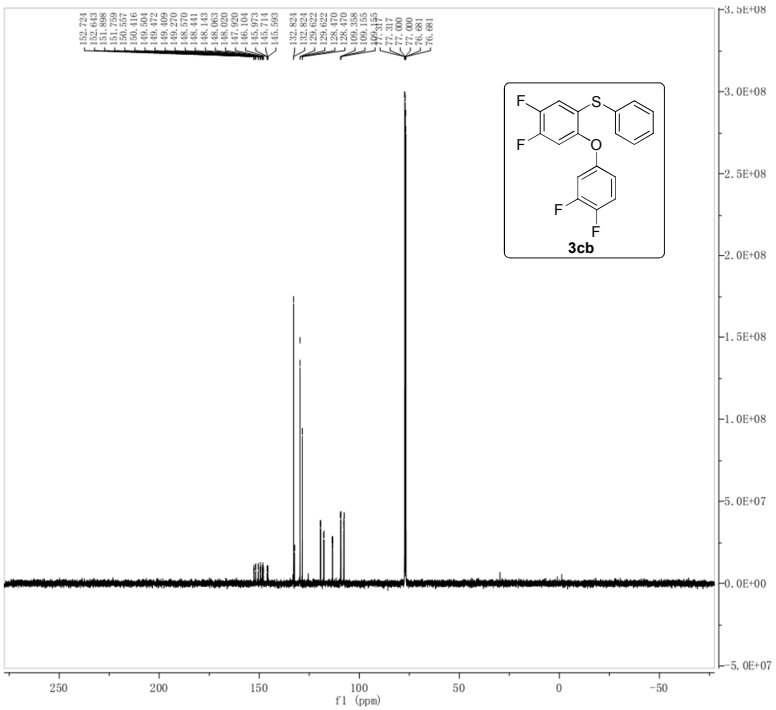
2 Title	lhy0424-1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	100
15 Relaxation Delay	1.0000
16 Pulse Width	14.4000
17 Acquisition Time	4.0894
18 Acquisition Date	2013-04-24T22:11:00
19 Modification Date	2013-04-24T22:10:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1578.8
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



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1 Data File Name	E:/ 李红影-苯炔/ NMR 数据/ lhy0417-1/ 2/ pdata/ 1/ 1r
2 Title	lhy0417-1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1345
14 Receiver Gain	113
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-04-17T20:39:00
19 Modification Date	2013-04-17T00:00:00
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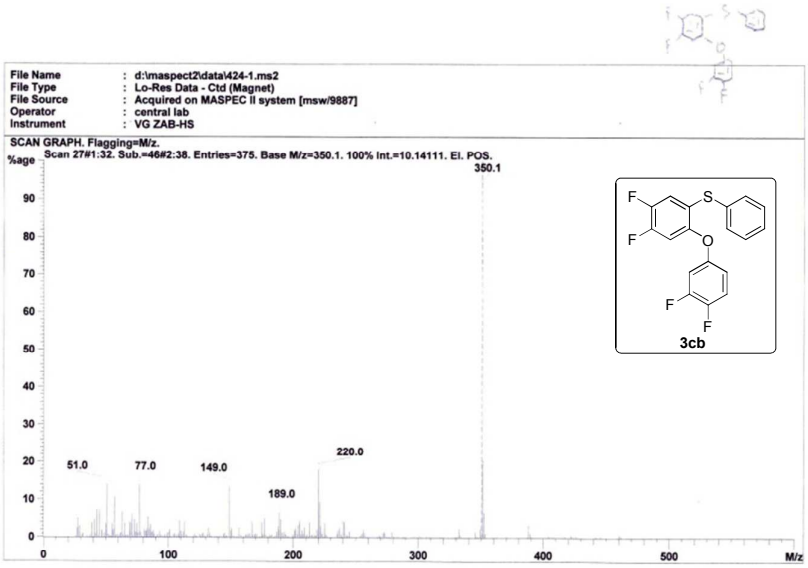
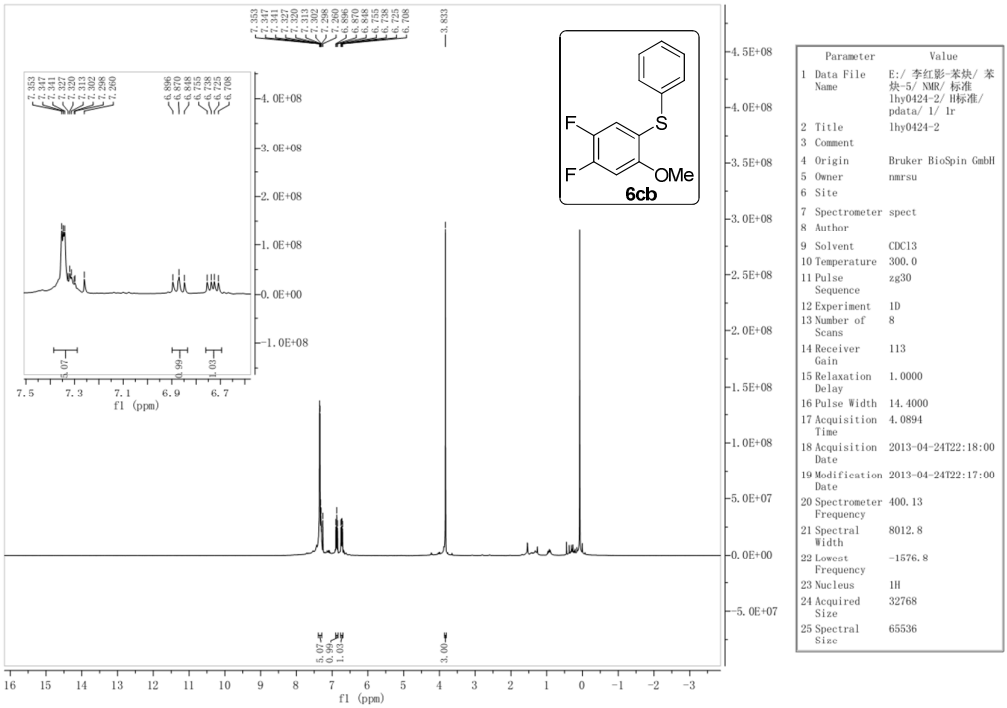
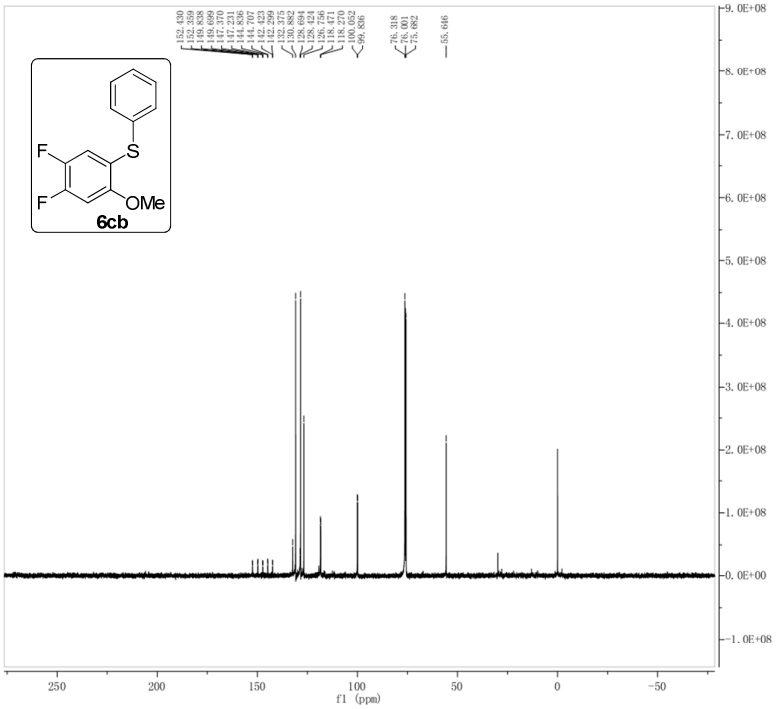
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	32768



(4,5-Difluoro-2-methoxyphenyl)(phenyl)sulfane (6cb).





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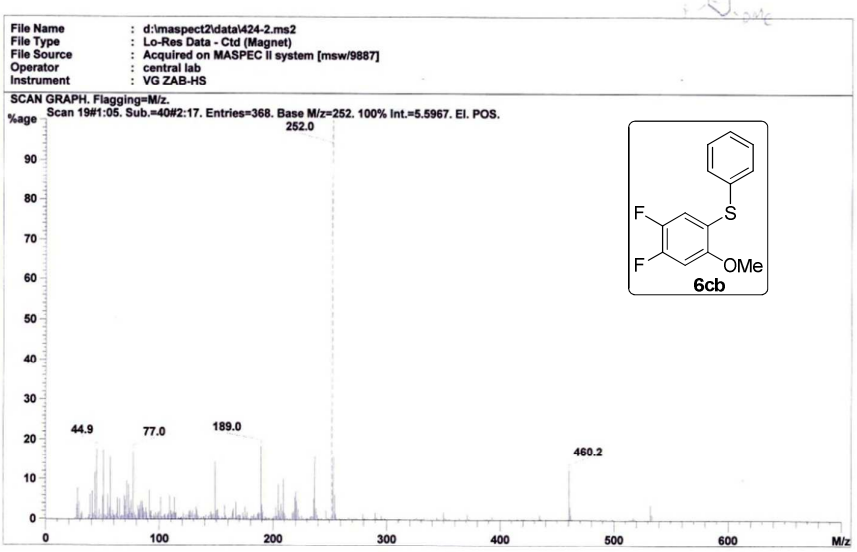
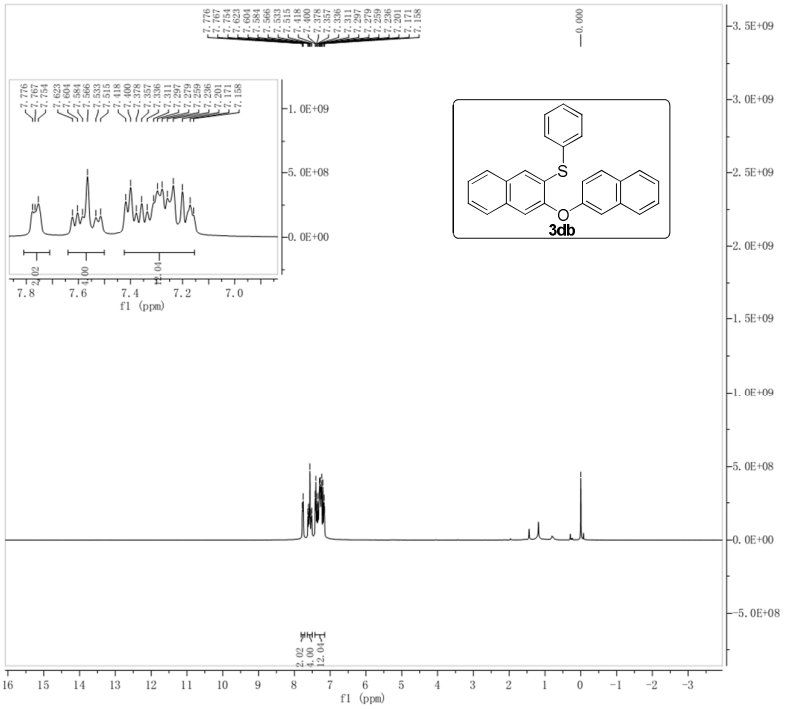
2	Title	lhy0424-2-c-2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	4184
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-04-26T11:14:00
19	Modification Date	2013-04-26T13:02:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7899.5
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768



(3-(Naphthalen-2-yloxy)naphthalen-2-yl)(phenyl)sulfane (3db).



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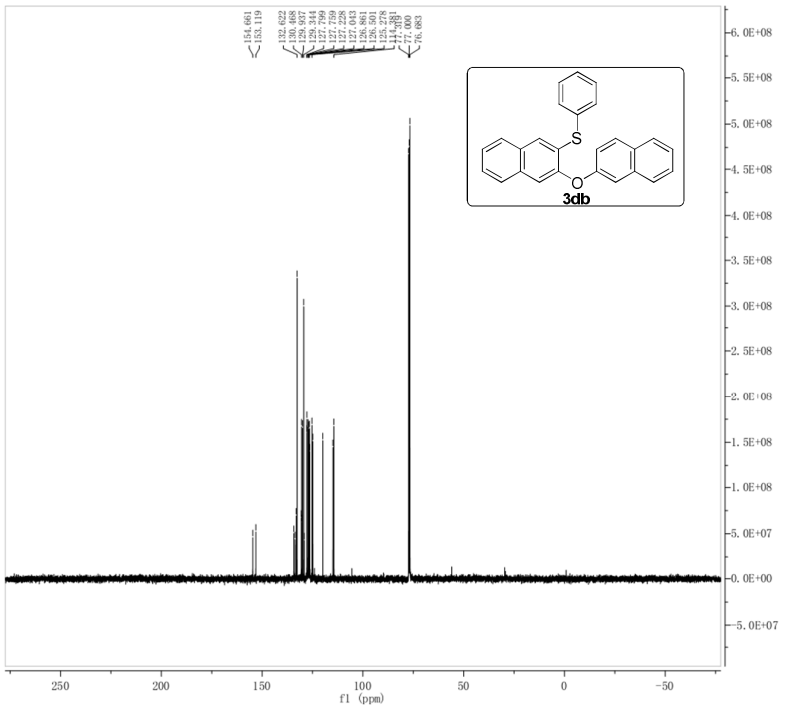
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	14.4000
17	Acquisition Time	4.0894
18	Acquisition Date	2013-04-08T08:59:00
19	Modification Date	2013-04-08T00:00:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1554.8
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	65536



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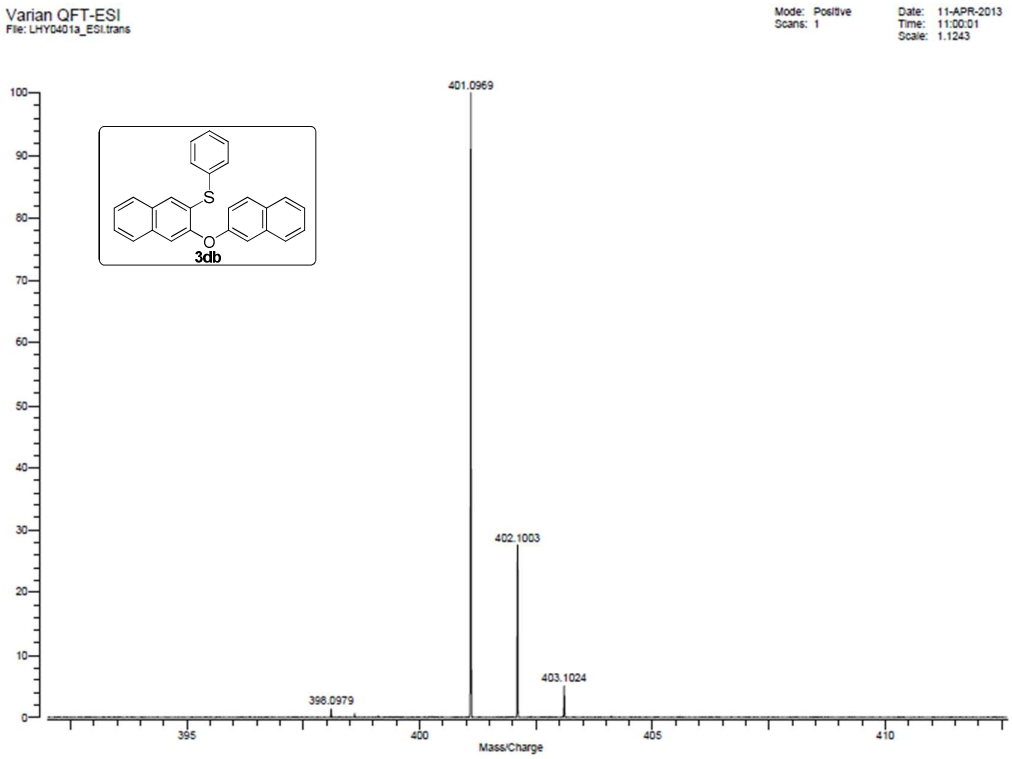
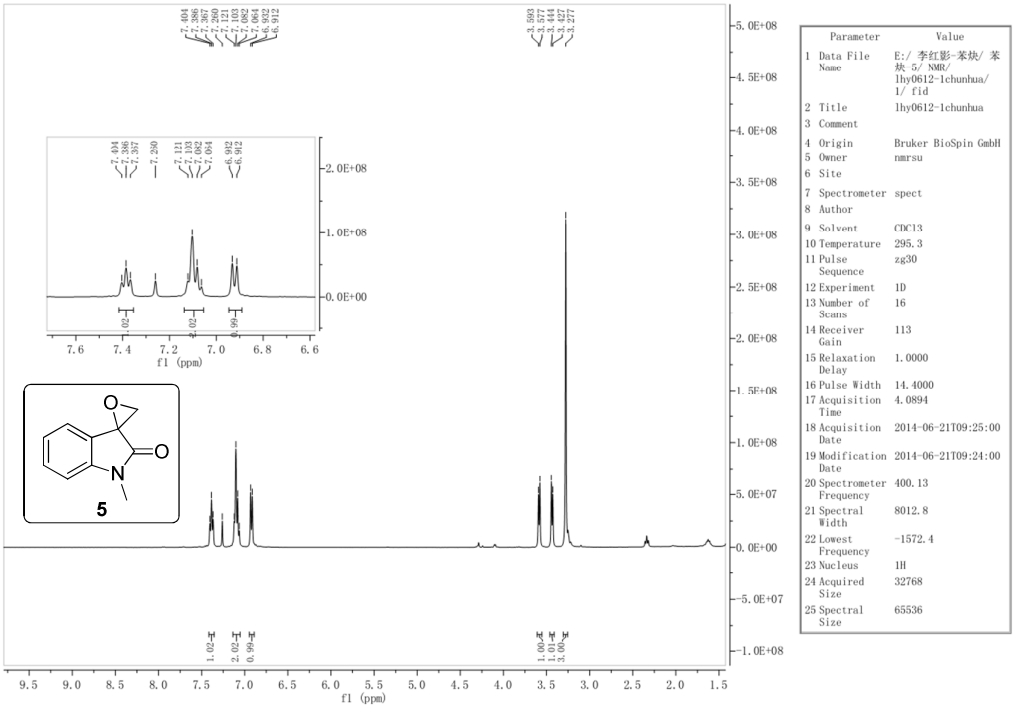
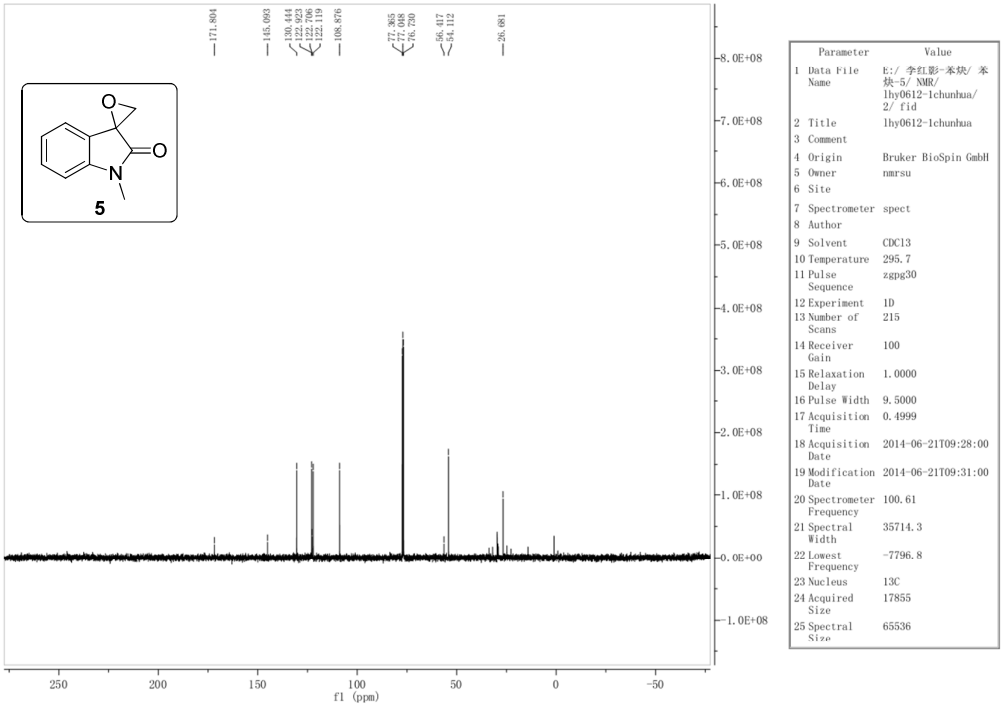
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	113
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2013-04-08T09:05:00
19	Modification Date	2013-04-08T00:00:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	32768

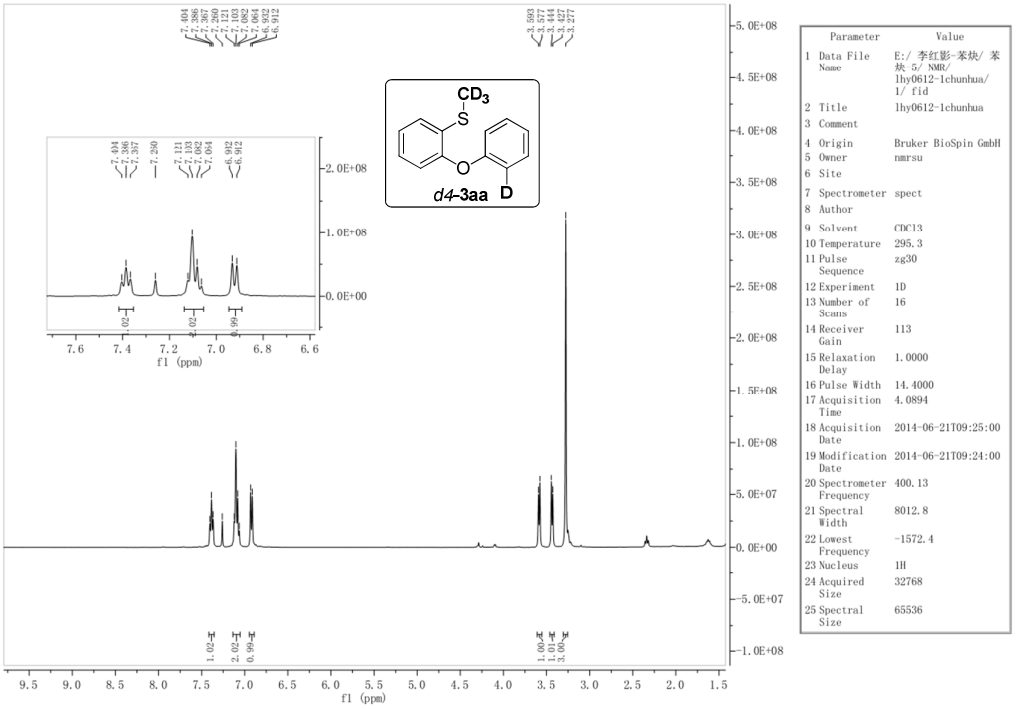


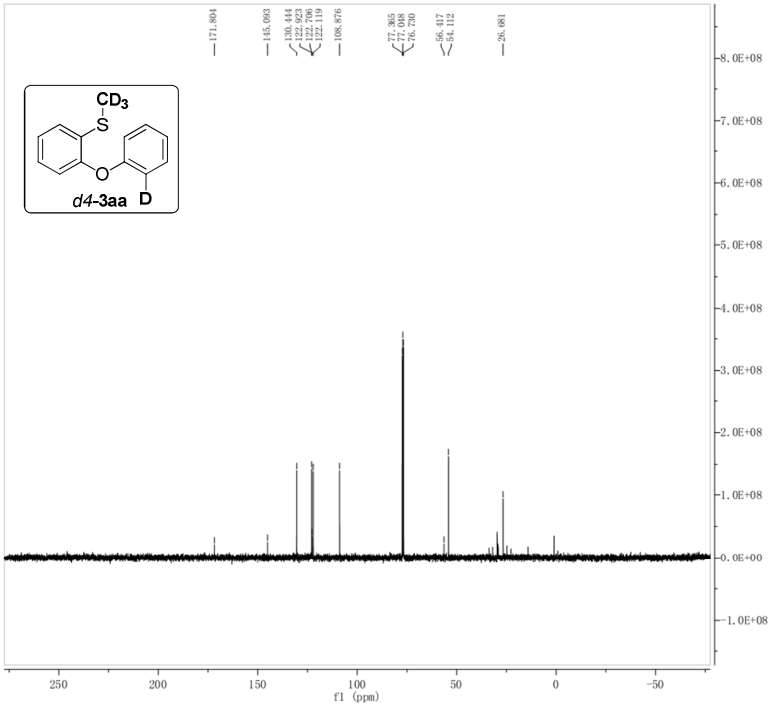
1-Methylspiro[indoline-3,2'-oxiran]-2-one (5).





Methyl(2-phenoxyphenyl)sulfane-*d4* (*d4*-3aa).





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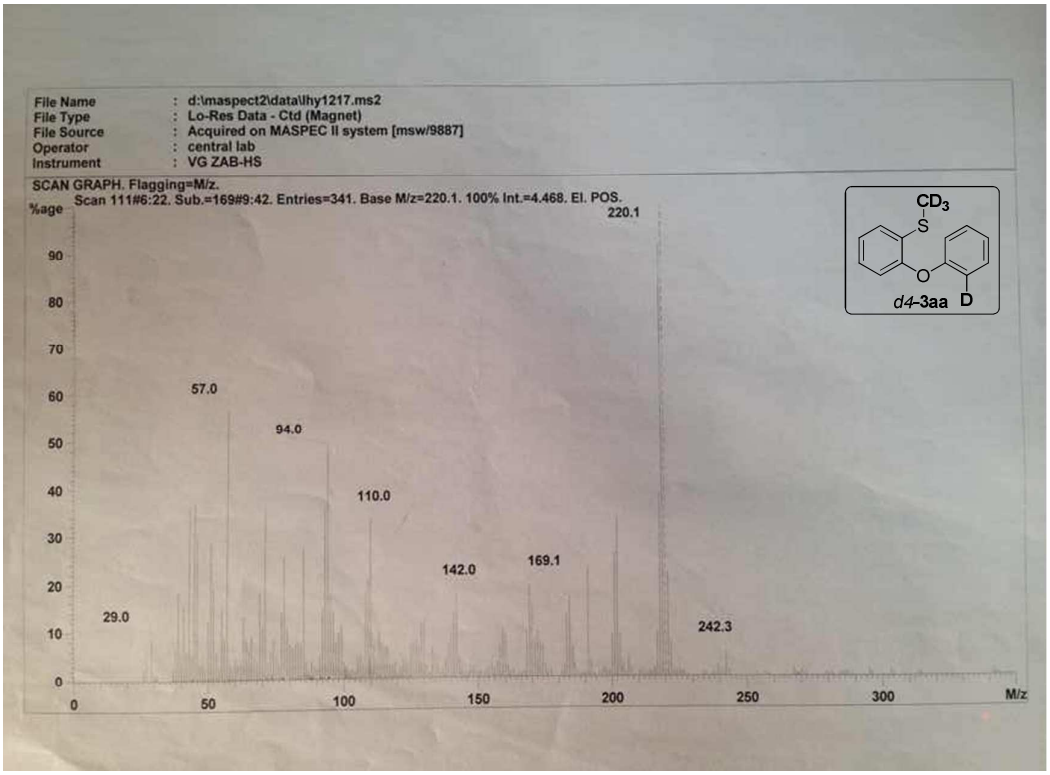
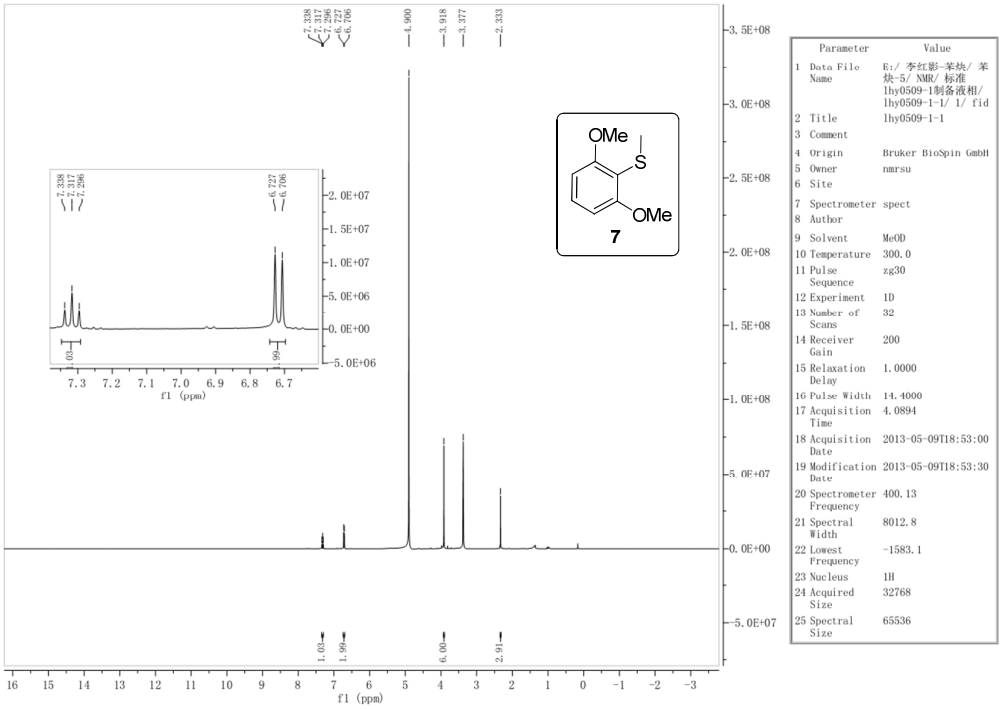
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	215
14	Receiver Gain	100
15	Relaxation Delay	1.0000
16	Pulse Width	9.5000
17	Acquisition Time	0.4999
18	Acquisition Date	2014-06-21T09:28:00
19	Modification Date	2014-06-21T09:31:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	17855
25	Spectral Size	65536



(2,6-Dimethoxyphenyl)(methyl)sulfane (7).



Parameter	Value
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3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	32
14 Receiver Gain	200
15 Relaxation Delay	1.0000
16 Pulse Width	14.4000
17 Acquisition Time	4.0894
18 Acquisition Date	2013-05-09T18:53:00
19 Modification Date	2013-05-09T18:53:30
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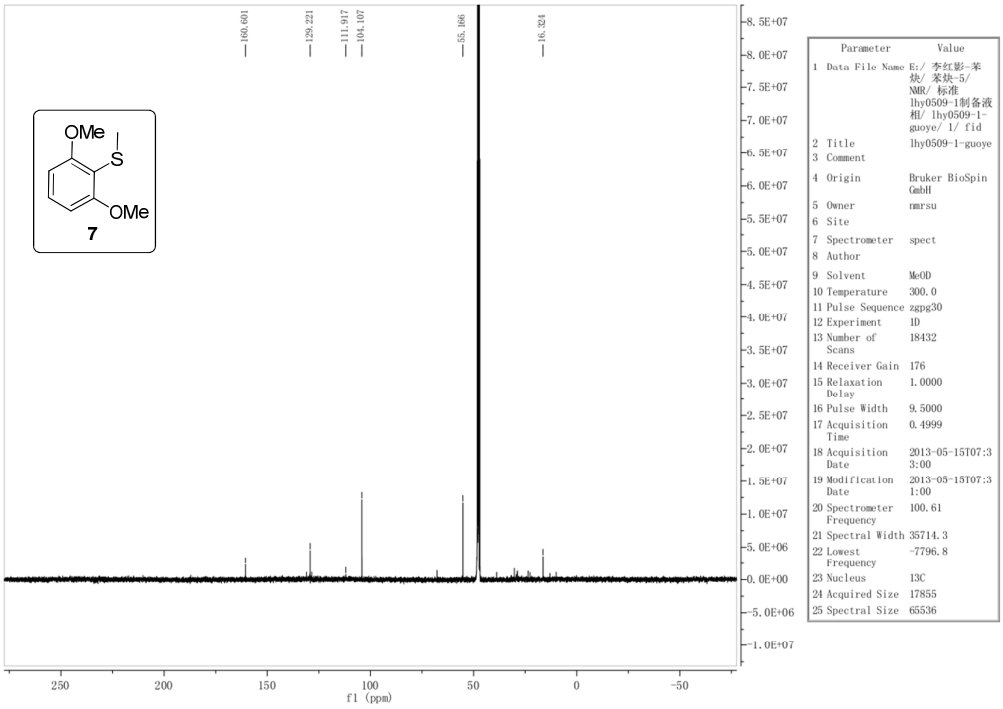
21 Spectral Width	8012.8
22 Lowest Frequency	-1583.1
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



Parameter	Value
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3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	18432
14 Receiver Gain	176
15 Relaxation Delay	1.0000
16 Pulse Width	9.5000
17 Acquisition Time	0.4999
18 Acquisition Date	2013-05-15T07:33:00
19 Modification Date	2013-05-15T07:31:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	17855
25 Spectral Size	65536