Electronic Supplementary Information

Diverse Patterns of Rhodium-Catalyzed Enantioselective C-H Alkynylation of Sulfoxides: Desymmetrization, Kinetic Resolution, and Parallel Kinetic Resolution

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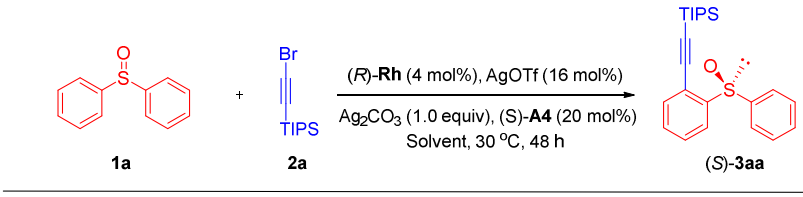
Contents

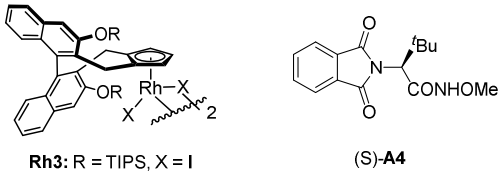
1. General Information.

All chemicals were obtained from commercial sources and were used as received unless otherwise noted. All reactions were carried out using test tube or pressure tube at air atmosphere. NMR spectra were recorded on a 600 or 400 MHz NMR spectrometer in the deuterated solvent indicated. The chemical shift is given in dimensionless δ values and is frequency referenced relative to TMS in ^{1}H and ^{13}C NMR spectroscopy. HRMS data were obtained on a Thermo Scientific LTQ Orbitrap Discovery spectrometer (Bremen, Germany). Column chromatography was performed on silica gel (200-300 mesh) using ethyl acetate/petroleum ether. The enantiomeric excess (ee) of the products were determined by high-performance liquid chromatography (HPLC) with a chiral stationary phase in comparison with the authenticated racemate. All the chiral stationary phases including Chiralcel IC, IG, IE, IA, OX-H and OD-H used were purchased from Daicel Chiral Technologies. Optical rotations were reported as follows: $[\alpha]_D^T$ = (*c*: g/100 mL in $CDCl_3$). Chiral rhodium catayst[1], diaryl sulfoxides,[2] aryl alkyl sulfoxide,[3] and alkynyl bromide[4] were prepared according to the published procedures.

2. Optimization Studies

Table S1. Optimization Studies of the Solvent.[a]



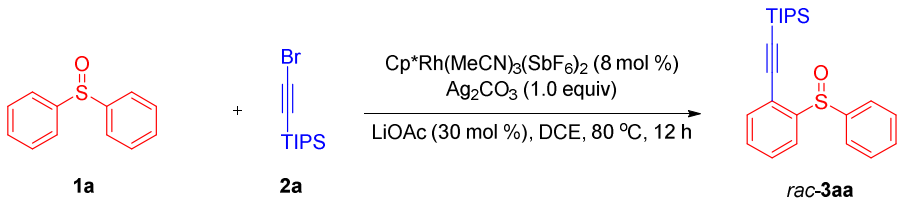


Entry	Solvent	Yield (%)	ee (%)[b]
1	Ph-CF_3	25	79%
2	1, 4-dioxane	-	-
3	MeCN	-	-
4	MeOH	-	-
5	THF	-	-
6	PhOMe	30	84
7	TFE	-	-
8	HFIP	-	-
9	TCE	20	49
10	$CHCl_3$	-	-

[a]Reaction conditions: **1** (0.05 mmol), **2** (0.06 mmol), (*R*)-**Rh** (4 mol %), AgOTf (16 mol %), (S)-**A4** (20 mol %), Ag_2CO_3 (1.0 equiv) in solvent (1.0 mL) at 30 °C for 48 h under N_2 in a sealed reaction tube, isolated yield. [b]The ee value was determined by chiral HPLC.

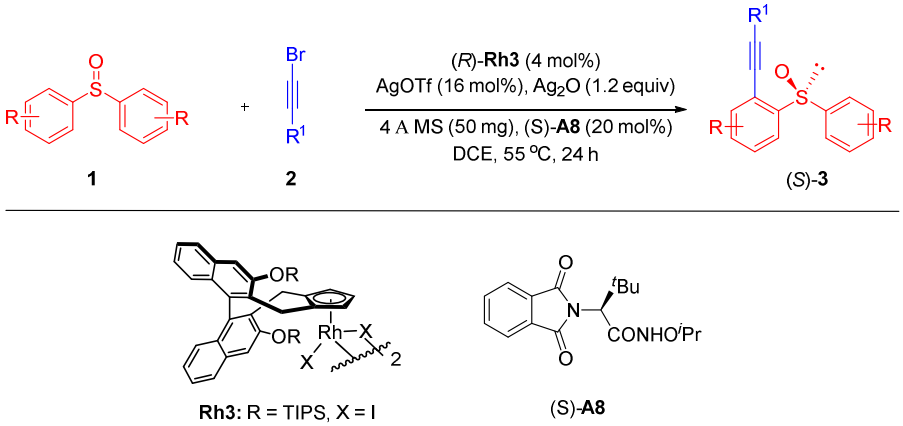
3. Experimental Section.

3.1 General Synthetic Procedure of 3.



Racemic Synthesis:

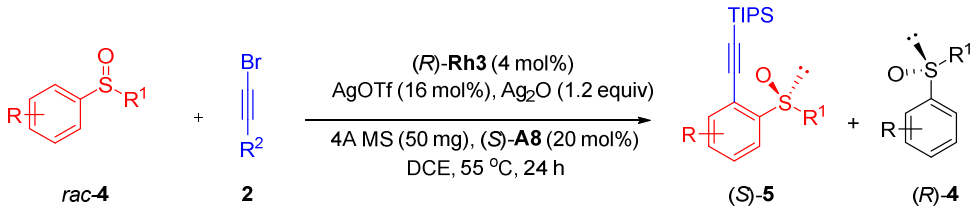
Representative Synthesis of the Product (*rac*)-3aa. A pressure tube was charged with **1a** (10.1 mg, 0.05 mmol), **2a** (15.9 mg, 0.06 mmol), [Cp*Rh(MeCN)$_3$(SbF$_6$)$_2$] (3.3 mg, 8 mol%), Ag_2CO_3 (13.8 mg, 1.0 equiv), LiOAc (1.0 mg, 30 mol %) and DCE (1.0 mL). The reaction mixture was stirred under N_2 at 80 °C for 12 h. After the reaction was completed as indicated by TLC analysis, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate 8:1 (v/v) to give the racemic product **3aa**.



Asymmetric Synthesis:

Representative Synthesis of Product (*S*)-3. A pressure tube was charged with **1** (0.1 mmol), **2** (0.12 mmol), (*R*)-**Rh3** (8.0 mg, 4 mol%), AgOTf (4.2 mg, 16 mol %), Ag_2O (23.2 mg, 1.2 equiv), (*S*)-**A8** (6.4 mg, 20 mol %), 4Å MS (50 mg), and DCE (2.0 mL). The reaction mixture was stirred under N_2 at 55 °C for 48 h. After the reaction was completed as indicated by TLC analysis, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate 8:1 (v/v) to give the product (*S*)-**3**.

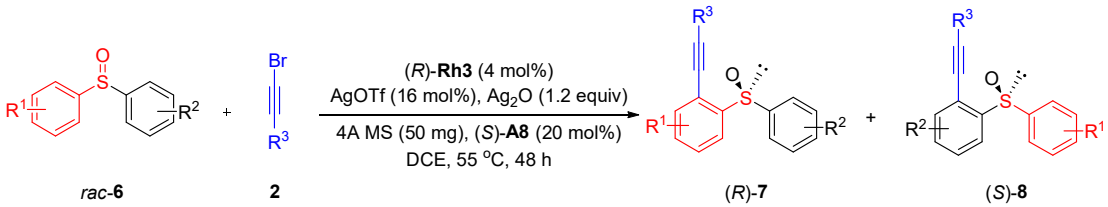
3.2 General Synthetic Procedure of 5.



Representative Synthesis of Product (*S*)-5. A pressure tube was charged with *rac*-**4** (0.2 mmol), **2** (0.15 mmol), (*R*)-**Rh3** (8.0 mg, 4 mol%), AgOTf (4.2 mg, 16 mol %), Ag_2O (23.2 mg, 1.2 equiv), (*S*)-**A8** (6.4 mg, 20 mol %), 4Å MS (50 mg), and DCE (2.0 mL). The reaction mixture was stirred under N_2 at 55 °C for 24 h. After the reaction was completed as indicated by TLC analysis, the solvent was removed under reduced pressure and the residue was purified by silica gel

chromatography using petroleum ether/ethyl acetate 8:1-3:1 (v/v) to give the product **5** and the recovered sulfoxide **4**.

3.3 General Synthetic Procedure of 7 and 8.

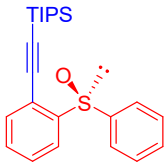


rac-**6** **2** (*R*)-**7** (*S*)-**8**

Representative Synthesis of Product (*R*)-7 and (*S*)-8. A pressure tube was charged with *rac*-**6** (0.1 mmol), **2** (0.15 mmol), (*R*)-**Rh3** (8.0 mg, 4 mol%), AgOTf (4.2 mg, 16 mol %), Ag_2O (23.2 mg, 1.2 equiv), (*S*)-**A8** (6.4 mg, 20 mol %), 4Å MS (50 mg), and DCE (2.0 mL). The reaction mixture was stirred under N_2 at 55 °C for 48 h. After the reaction was completed as indicated by TLC analysis, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate 8:1-3:1 (v/v) to give the coupled products **7** and **8**.

4. NMR and HPLC Data.

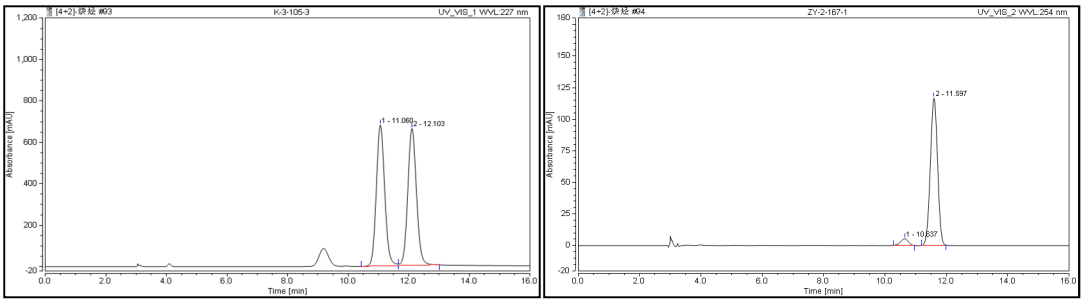
(*S*)-Triisopropyl((2-(phenylsulfinyl)phenyl)ethynyl)silane (**3aa**)



(*S*)-**3aa**

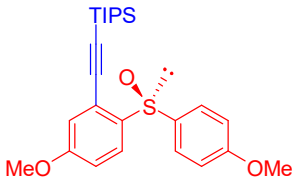
Product (*S*)-**3aa** was isolated in 70% yield (26.7 mg, in 0.1 mmol scale) as a light yellow oil. Eluent: PE/EA = 6/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (dd, J = 8.3, 1.3 Hz, 1H), 7.81 – 7.77 (m, 2H), 7.51 – 7.49 (m, 2H), 7.42 – 7.36 (m, 4H), 1.18 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 147.4, 145.8, 133.8, 131.0, 130.6, 129.7, 129.3, 125.0, 123.8, 121.1, 102.5, 100.4, 18.8, 11.4. **HRMS** (ESI) calculated for $C_{23}H_{31}NaOSSi^+$ $[M+Na]^+$: 405.1679, found: 405.1682. $[\alpha]_D^{20}$ = -185 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IG column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 11.6 min, t_R (minor) = 10.6 min, 91% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.060	218.862	49.97	1	10.637	1.516	4.57
2	12.103	219.153	50.03	2	11.597	31.684	95.43

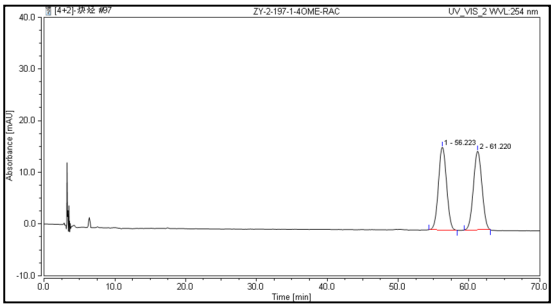
(*S*)-triisopropyl((5-methoxy-2-((4-methoxyphenyl)sulfinyl)phenyl)ethynyl)silane (**3ba**)

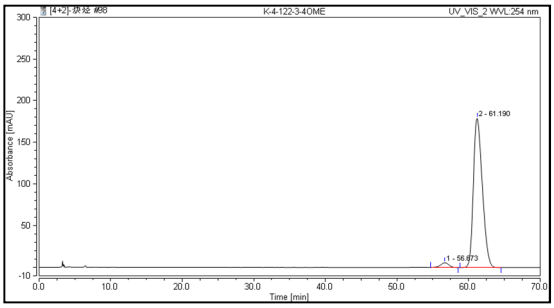


(*S*)-**3ba**

Product (*S*)-**3ba** was isolated in 50% yield (22.2 mg, in 0.1 mmol scale) as a light yellow solid. Eluent: PE/EA = 6/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, J = 8.8 Hz, 1H), 7.63 (d, J = 8.8 Hz, 2H), 7.03 (dd, J = 8.8, 2.6 Hz, 1H), 6.97 (d, J = 2.6 Hz, 1H), 6.90 (d, J = 8.8 Hz, 2H), 3.82 (s, 3H), 3.79 (s, 3H), 1.16 – 1.10 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.8, 161.3, 138.9, 137.5, 127.2, 125.7, 122.4, 118.6, 116.1, 114.7, 102.3, 99.9, 55.8, 55.6, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{25}H_{34}NaO_3SSi^+$ $[M+Na]^+$: 465.1890, found: 465.1889. $[\alpha]_D^{20}$ = -123 (c = 0.05, $CHCl_3$).

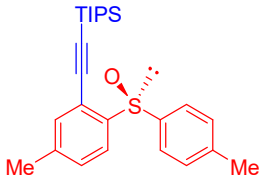
HPLC conditions: Daicel Chiralpak IE column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 61.2 min, t_R (minor) = 56.7 min, 94% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	56.223	22.899	49.72	1	56.673	7.530	2.84
2	61.207	23.158	50.28	2	61.190	257.970	97.16

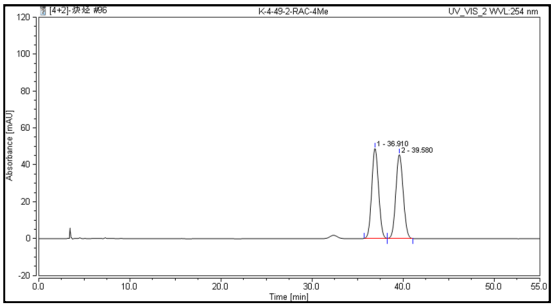
(*S*)-Triisopropyl((5-methyl-2-(p-tolylsulfinyl)phenyl)ethynyl)silane (**3ca**)

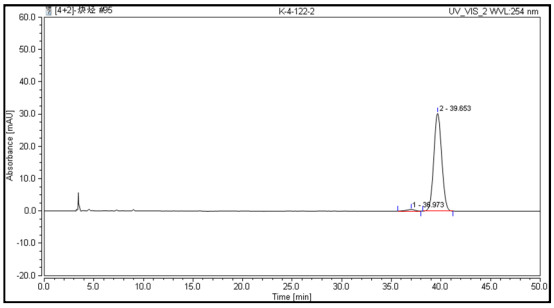


(*S*)-**3ca**

Product (*S*)-**3ca** was isolated in 48% yield (29.5 mg, in 0.1 mmol scale) as a light yellow oil. Eluent: PE/EA = 6/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (d, J = 8.5 Hz, 1H), 7.64 (d, J = 8.0 Hz, 2H), 7.30 – 7.28 (m, 2H), 7.19 (d, J = 8.0 Hz, 2H), 2.35 – 2.32 (m, 6H), 1.16 – 1.12 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.6, 143.1, 141.4, 141.0, 134.2, 130.7, 129.9, 125.1, 123.8, 120.9, 102.7, 99.6, 21.5, 21.2, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{25}H_{34}NaOSSi^+$ $[M+Na]^+$: 433.1992, found: 433.1988. $[\alpha]_D^{20}$ = -73 (c = 0.05, $CHCl_3$).

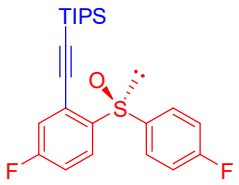
HPLC conditions: Daicel Chiralpak IE column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 39.6 min, t_R (minor) = 37.0 min, 96% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	36.910	42.534	50.00	1	36.973	0.533	1.87
2	39.580	42.538	50.00	2	39.653	28.033	98.13

(*S*)-((5-Fluoro-2-((4-fluorophenyl)sulfinyl)phenyl)ethynyl)triisopropylsilane (**3da**)

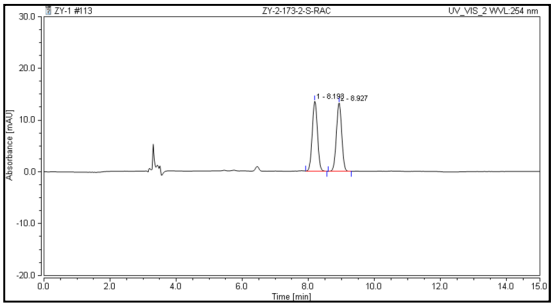


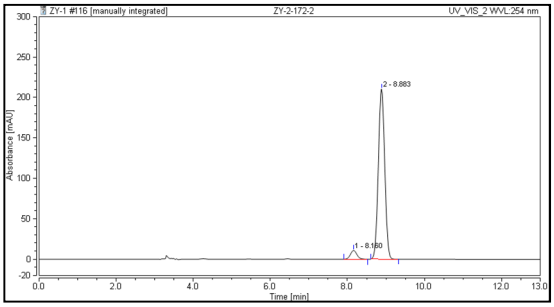
(*S*)-**3da**

Product (*S*)-**3da** was isolated in 60% yield (25.2 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 7/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (dd, J = 8.7, 5.5 Hz, 1H), 7.78 – 7.73 (m, 2H), 7.24 – 7.17 (m, 2H), 7.13 – 7.08 (m, 2H), 1.18 – 1.10 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 164.4 (d, $J_{C\text{-}F}$ = 250.6 Hz), 163.8 (d, $J_{C\text{-}F}$ = 250.8 Hz), 142.9 (d, $J_{C\text{-}F}$ = 2.1 Hz), 141.3 (d, $J_{C\text{-}F}$ = 2.2 Hz), 127.3 (d, $J_{C\text{-}F}$ = 8.8 Hz), 126.2 (d, $J_{C\text{-}F}$ = 9.6 Hz), 122.9 (d, $J_{C\text{-}F}$ = 9.9 Hz), 120.7 (d, $J_{C\text{-}F}$ = 23.7 Hz), 117.6 (d, $J_{C\text{-}F}$ = 22.2 Hz), 116.6 (d, $J_{C\text{-}F}$ = 22.4 Hz), 102.2, 101.1 (d, $J_{C\text{-}F}$ = 1.9 Hz), 18.8, 11.4. **HRMS** (ESI) calculated for $C_{23}H_{28}F_2NaOSSi^+$ $[M+Na]^+$: 441.1490, found: 441.1489. $[\alpha]_D^{20}$ = -175 (c = 0.05, $CHCl_3$).

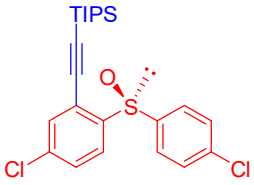
HPLC conditions: Daicel Chiralpak IE column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 8.9 min, t_R (minor) = 8.2 min, 90% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.193	2.474	50.10	1	8.160	2.104	4.95
2	8.927	2.464	49.90	2	8.883	40.439	95.05

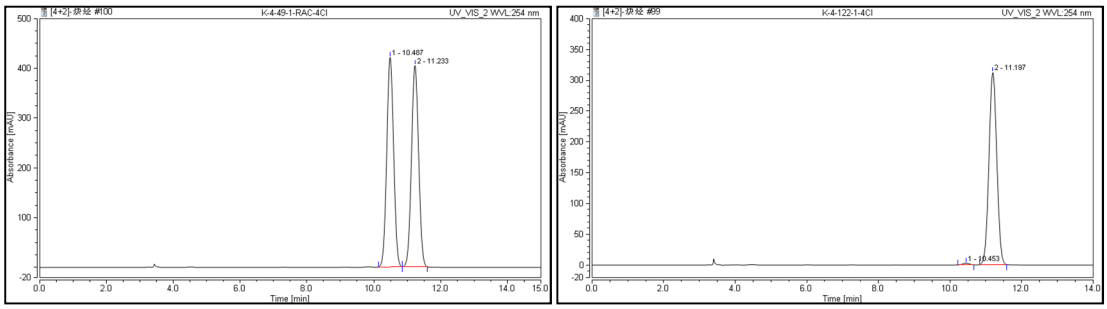
(*S*)-((5-Chloro-2-((4-chlorophenyl)sulfinyl)phenyl)ethynyl)triisopropylsilane (**3ea**)



(*S*)-**3ea**

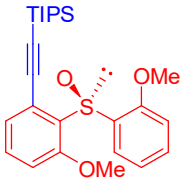
Product (*S*)-**3ea** was isolated in 67% yield (30.2 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 7/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 9.2 Hz, 1H), 7.72 (d, J = 8.6 Hz, 2H), 7.47 (d, J = 7.7 Hz, 2H), 7.39 (d, J = 8.6 Hz, 2H), 1.18 – 1.13 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.8, 144.1, 137.6, 137.1, 133.5, 130.2, 129.7, 126.2, 125.2, 122.4, 102.6, 101.1, 18.8, 11.4. **HRMS** (ESI) calculated for $C_{23}H_{28}Cl_2NaOSSi^+$ $[M+Na]^+$: 473.0899, found: 473.0899. $[\alpha]_D^{20}$ = -279 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IE column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 11.2 min, t_R (minor) = 10.5 min, 99% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.487	100.633	50.08	1	10.453	0.592	0.74
2	11.233	100.294	49.92	2	11.197	79.069	99.26

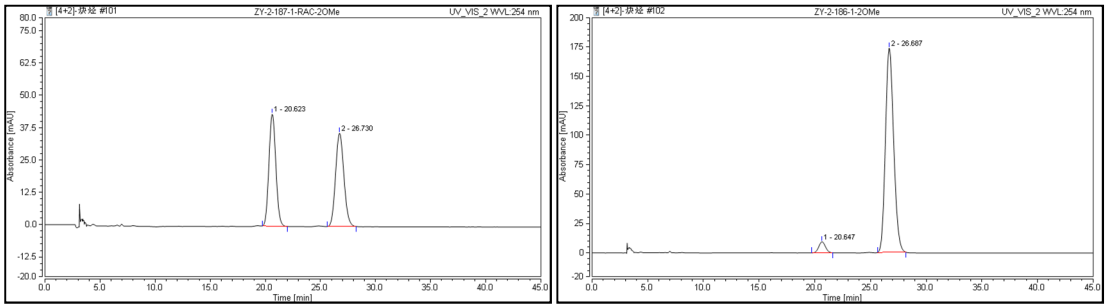
(*S*)-Triisopropyl((3-methoxy-2-((2-methoxyphenyl)sulfinyl)phenyl)ethynyl)silane (**3fa**)



(*S*)-**3fa**

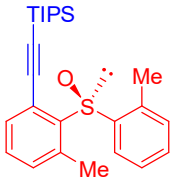
Product (*S*)-**3fa** was isolated in 97% yield (42.9 mg, in 0.2 mmol scale) as a light yellow solid. Eluent: PE/EA = 7/1, R_f = 0.3. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.05 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.37 – 7.34 (m, 1H), 7.29 – 7.27 (m, 1H), 7.17 – 7.12 (m, 2H), 6.77 (dd, *J* = 8.1, 2.3 Hz, 2H), 3.63 (s, 3H), 3.55 (s, 3H), 1.19 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.0, 155.3, 132.6, 132.4, 131.4, 131.0, 127.4, 126.7, 125.9, 120.3, 113.2, 110.6, 103.1, 97.8, 55.9, 55.5, 18.8, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{25}H_{34}NaO_3SSi^+$ $[M+Na]^+$: 465.1890, found: 465.1885. $[\alpha]_D^{20}$ = -205 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 26.7 min, t_R (minor) = 20.6 min, 92% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	20.623	31.578	49.97	1	20.647	6.519	4.19
2	26.730	31.620	50.03	2	26.687	148.921	95.81

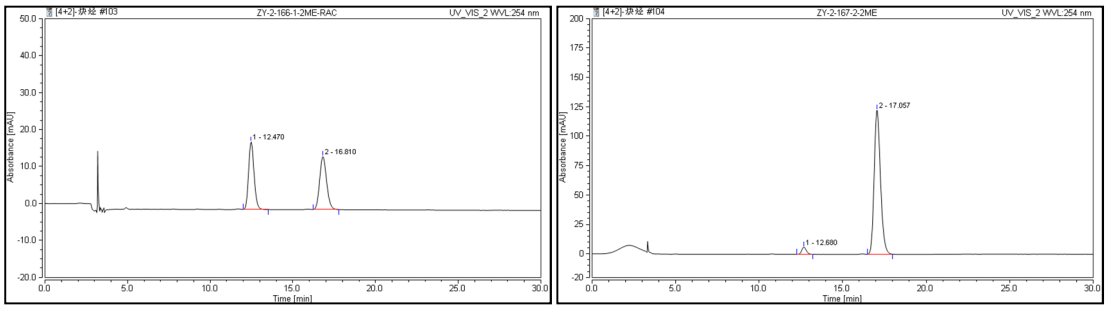
(*S*)-triisopropyl((3-methyl-2-(o-tolylsulfinyl)phenyl)ethynyl)silane (**3ga**)



(*S*)-**3ga**

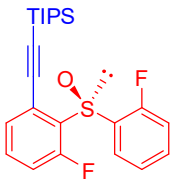
Product (*S*)-**3ga** was isolated in 76% yield (31.2 mg, in 0.1 mmol scale) as a light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 7.9 Hz, 1H), 7.44 (d, *J* = 7.7 Hz, 1H), 7.42 – 7.40 (m, 1H), 7.36 – 7.33 (m, 1H), 7.30 – 7.27 (m, 1H), 7.14 (d, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 2.26 (s, 3H), 2.18 (s, 3H), 1.18 – 1.10 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.2, 141.1, 140.2, 135.7, 133.5, 131.9, 131.4, 131.2, 130.2, 126.4, 126.3, 125.8, 103.4, 99.7, 19.3, 18.8, 18.4, 11.5. **HRMS** (ESI) calculated for $C_{25}H_{34}NaOSSi^+$ $[M+Na]^+$: 433.1992, found: 433.1994. $[\alpha]_D^{20}$ = -288 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 17.1 min, t_R (minor) = 12.7 min, 93% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.470	7.032	50.19	1	12.680	1.972	3.53
2	16.810	6.979	49.81	2	17.057	53.863	96.47

(S)-((3-Fluoro-2-((2-fluorophenyl)sulfinyl)phenyl)ethynyl)triisopropylsilane (**3ha**)

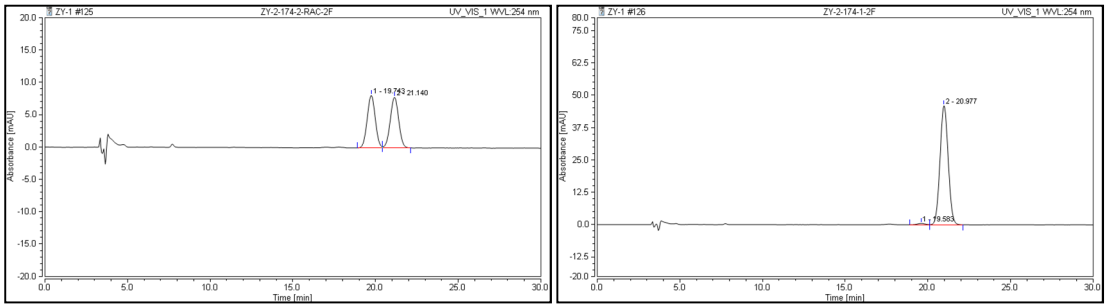


(*S*)-**3ha**

Product (*S*)-**3ha** was isolated in 49% yield (20.4 mg, in 0.1 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

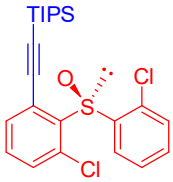
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 – 8.11 (m, 1H), 7.48 – 7.44 (m, 1H), 7.42 – 7.36 (m, 3H), 7.04 – 6.97 (m, 2H), 1.19 – 1.13 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.5 (d, J_{C-F} = 256.5 Hz), 158.0 (d, J_{C-F} = 247.9 Hz) , 133.5 (d, J_{C-F} = 9.7 Hz), 132.8 (d, J_{C-F} = 14.4 Hz), 132.6 (d, J_{C-F} = 7.5 Hz), 130.6 (d, J_{C-F} = 16.4 Hz), 129.8 (d, J_{C-F} = 3.4 Hz), 127.0 (d, J_{C-F} = 1.1 Hz), 126.0 (d, J_{C-F} = 3.3 Hz), 124.7 (d, J_{C-F} = 3.5 Hz), 117.63 (d, J_{C-F} = 21.3 Hz), 115.8 (d, J_{C-F} = 19.7 Hz), 101.0 (d, J_{C-F} = 3.7 Hz), 100.7, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{23}H_{28}F_2NaOSSi^+$ $[M+Na]^+$: 441.1490, found: 441.1487. $[\alpha]_D^{20}$ = -150 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IG column (98:2 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 21.0 min, t_R (minor) = 19.6 min, 98% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	19.743	4.611	49.88	1	19.583	0.297	1.11
2	21.140	4.632	50.12	2	20.977	26.421	98.89

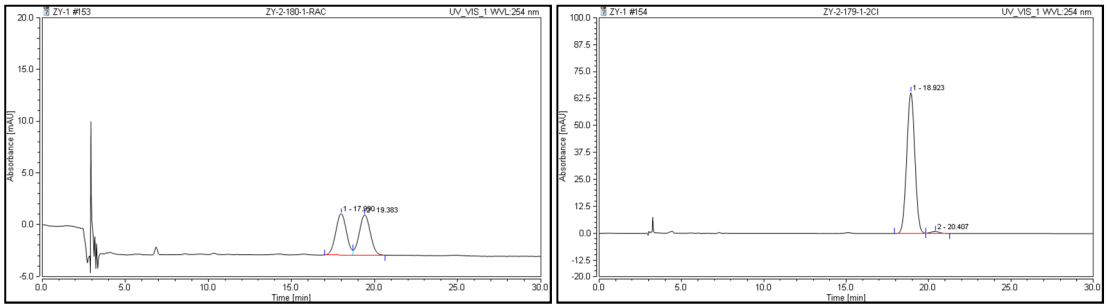
(*S*)-((3-Chloro-2-((2-chlorophenyl)sulfinyl)phenyl)ethynyl)triisopropylsilane (**3ia**)



(*S*)-**3ia**

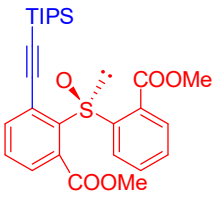
Product (*S*)-**3ia** was isolated in 55% yield (24.9 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (dd, J = 7.9, 1.6 Hz, 1H), 7.53 – 7.50 (m, 2H), 7.43 – 7.40 (m, 1H), 7.35 – 7.30 (m, 2H), 7.28 (dd, J = 8.0, 1.3 Hz, 1H), 1.16 – 1.13 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.0, 139.7, 135.8, 133.1, 132.4, 132.3, 131.8, 130.9, 130.2, 129.9, 128.9, 126.5, 102.0, 101.6, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{23}H_{28}Cl_2NaOSSi^+$ $[M+Na]^+$: 473.0899, found: 473.0898. $[\alpha]_D^{20}$ = -153 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IG column (98:2 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 18.9 min, t_R (minor) = 20.4 min, 97% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	17.990	2.980	49.77	1	18.923	37.427	98.44
2	19.383	3.008	50.23	2	20.407	0.592	1.56

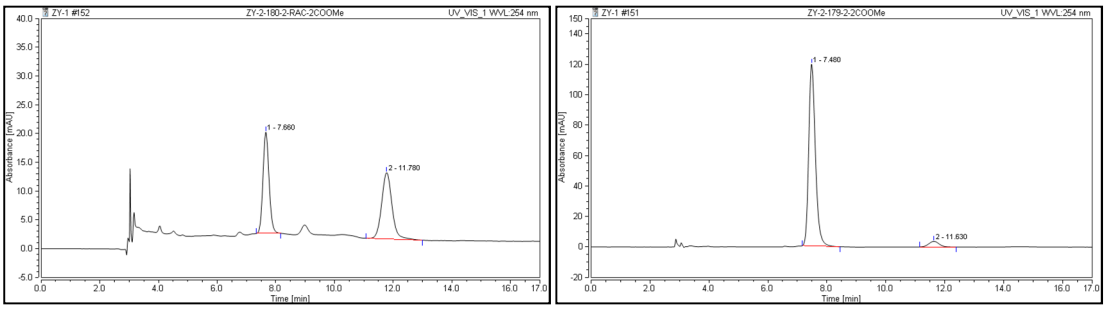
(*S*)-Methyl 2-((2-(methoxycarbonyl)phenyl)sulfinyl)-3-((triisopropylsilyl)ethynyl)benzoate (**3ja**)



(*S*)-**3ja**

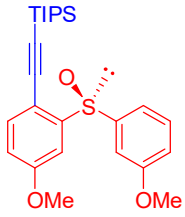
Product (*S*)-**3ja** was isolated in 55% yield (27.2 mg, in 0.1 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (dd, J = 7.7, 1.4 Hz, 1H), 7.93 (dd, J = 7.9, 1.2 Hz, 1H), 7.64 – 7.62 (m, 2H), 7.55 – 7.53 (m, 2H), 7.47 – 7.44 (m, 1H), 3.83 (s, 3H), 3.68 (s, 3H), 1.08 – 1.02 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.5, 165.6, 144.7, 143.3, 136.5, 134.2, 132.4, 131.4, 130.7, 130.6, 129.6, 129.5, 129.2, 125.2, 102.7, 101.7, 52.6, 52.6, 18.7, 18.7, 11.3. **HRMS** (ESI) calculated for $C_{27}H_{34}NaO_5SSi^+$ $[M+Na]^+$: 521.1788, found: 521.1770. $[\alpha]_D^{20}$ = -57 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IA column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 7.5 min, t_R (minor) = 11.6 min, 91% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.660	4.429	49.40	1	7.480	31.314	95.35
2	11.780	4.538	50.60	2	11.630	1.528	4.65

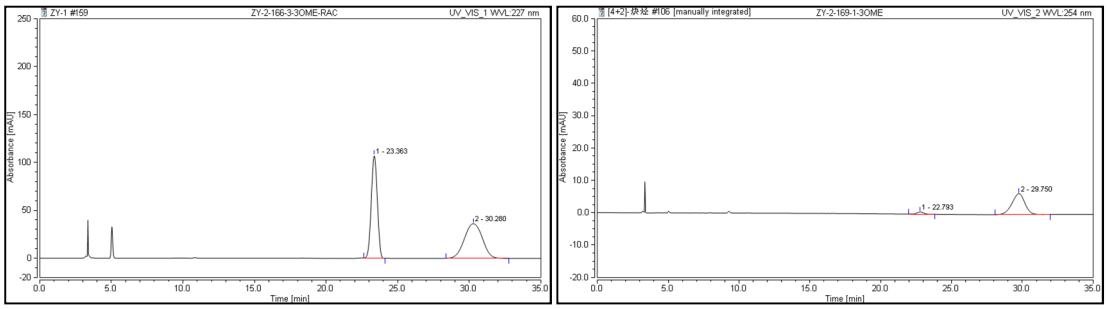
(*S*)-Triisopropyl((4-methoxy-2-((3-methoxyphenyl)sulfinyl)phenyl)ethynyl)silane (**3ka**)



(*S*)-**3ka**

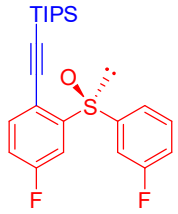
Product (*S*)-**3ka** was isolated in 45% yield (19.9 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, J = 2.6 Hz, 1H), 7.43 (d, J = 8.5 Hz, 1H), 7.39 (d, J = 7.7 Hz, 1H), 7.35 – 7.33 (m, 1H), 7.31 – 7.28 (m, 1H), 6.92 (dd, J = 8.2, 2.6 Hz, 1H), 6.89 (dd, J = 8.5, 2.7 Hz, 1H), 3.85 (s, 3H), 3.80 (s, 3H), 1.16 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.9, 160.4, 149.1, 147.1, 135.3, 130.2, 117.9, 117.3, 117.1, 113.2, 109.5, 107.6, 102.6, 98.2, 55.9, 55.6, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{25}H_{34}NaO_3SSi^+$ $[M+Na]^+$: 465.1890, found: 465.1879. $[\alpha]_D^{20}$ = -163 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 29.8 min, t_R (minor) = 22.8 min, 90% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	23.363	52.303	49.70	1	22.793	0.366	5.10
2	30.280	52.935	50.30	2	29.750	6.812	94.90

(*S*)-((4-Fluoro-2-((3-fluorophenyl)sulfinyl)phenyl)ethynyl)triisopropylsilane (**3la**)



(*S*)-**3la**

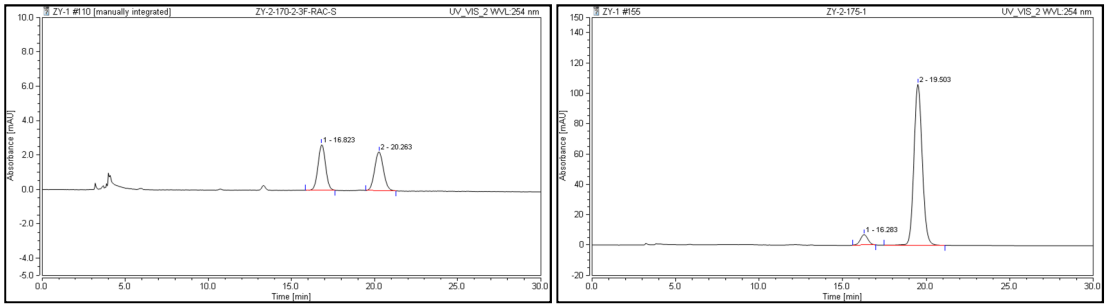
Product (*S*)-**3la** was isolated in 80% yield (33.4 mg, in 0.1 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, J = 1.0 Hz, 1H), 7.63 (d, J = 7.9 Hz, 1H), 7.56 – 7.54 (m, 1H), 7.51 – 7.47 (m, 1H), 7.42 – 7.49 (m, 1H), 7.18 – 7.15 (m, 1H), 7.13 – 7.10 (m, 1H), 1.21 – 1.12 (m, 21H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 163.5 (d, $J_{C\text{-}F}$ = 255.7 Hz), 163.0 (d, $J_{C\text{-}F}$ = 250.4 Hz), 149.2, 147.9 (d, $J_{C\text{-}F}$ = 5.7 Hz), 131.0 (d, $J_{C\text{-}F}$ = 7.6 Hz), 130.8 (d, $J_{C\text{-}F}$ = 8.1 Hz), 120.6 (d, $J_{C\text{-}F}$ = 3.3 Hz), 119.1 (d, $J_{C\text{-}F}$ = 3.5 Hz), 118.5 (d, $J_{C\text{-}F}$ = 21.5 Hz), 118.0 (d, $J_{C\text{-}F}$ = 21.5 Hz), 112.1 (d, $J_{C\text{-}F}$ = 24.1 Hz), 110.0 (d, $J_{C\text{-}F}$ = 18.4 Hz), 107.2 (d, $J_{C\text{-}F}$ = 3.8 Hz), 95.3, 18.7, 11.4.

HRMS (ESI) calculated for $C_{23}H_{28}F_2NaOSSi^+$ $[M+Na]^+$: 441.1490, found: 441.1480. $[\alpha]_D^{20}$ = -340 (c = 0.05, $CHCl_3$).

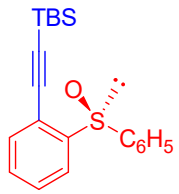
HPLC conditions: Daicel Chiralpak IC column (99:1 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 19.5 min, t_R (minor) = 16.3 min, 89% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)

1	16.053	1.491	49.79	1	16.283	3.578	5.54
2	19.613	1.503	50.21	2	19.503	61.055	94.46

(*S*)-*tert*-Butyldimethyl((2-(phenylsulfinyl)phenyl)ethynyl)silane (**3ab**)



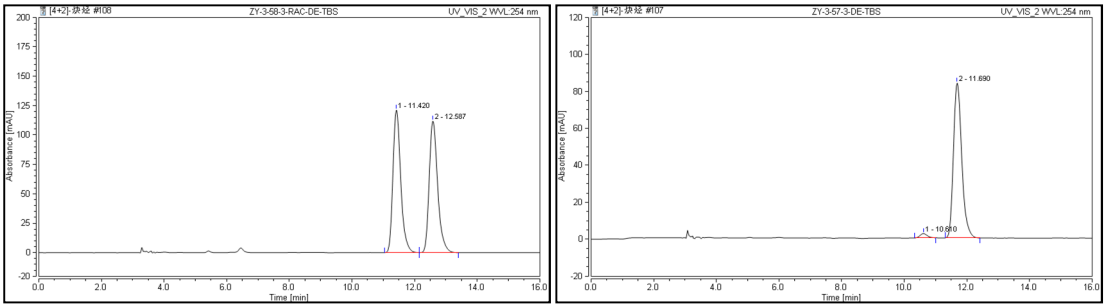
(*S*)-**3ab**

Product (*S*)-**3ab** was isolated in 46% yield (15.6 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 7/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (d, J = 7.9 Hz, 1H), 7.78 – 7.76 (m, 2H), 7.53 – 7.50 (m, 1H), 7.48 (d, J = 7.5 Hz, 1H), 7.44 – 7.40 (m, 3H), 7.38 – 7.36 (m, 1H), 1.00 (s, 9H), 0.22 (s, 3H), 0.21 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 147.6, 145.8, 133.5, 131.2, 130.6, 129.8, 129.2, 125.4, 123.8, 120.9, 102.3, 101.3, 26.3, 16.9, -4.61, -4.63.

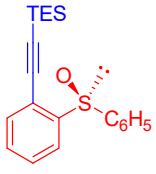
HRMS (ESI) calculated for $C_{20}H_{24}NaOSSi^+$ $[M+Na]^+$: 363.1209, found: 363.1209. $[\alpha]_D^{20}$ = -253 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 11.7 min, t_R (minor) = 10.6 min, 95% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.420	35.028	49.98	1	10.610	0.626	2.37
2	12.587	35.054	50.02	2	11.690	25.786	97.63

(*S*)-Triethyl((2-(phenylsulfinyl)phenyl)ethynyl)silane (**3ac**)



(*S*)-**3ac**

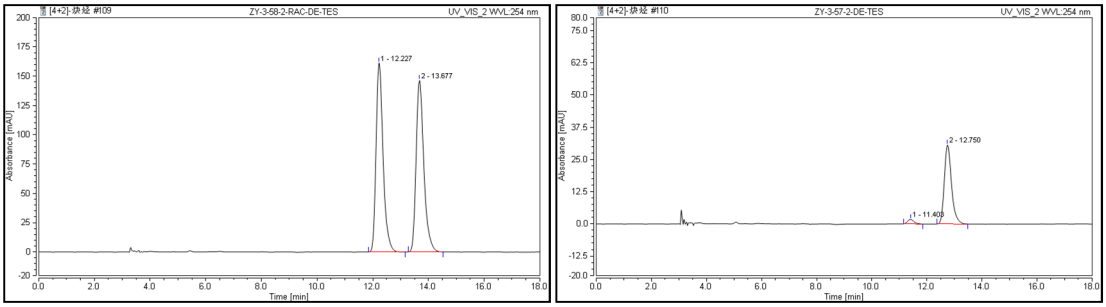
Product (*S*)-**3ac** was isolated in 54% yield (18.2 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (dd, J = 8.0, 1.2 Hz, 1H), 7.82 – 7.75 (m, 2H), 7.53 – 7.50 (m, 1H), 7.48 (dd, J = 7.6, 1.3 Hz, 1H), 7.43 – 7.39 (m, 3H), 7.39 – 7.36 (m, 1H), 1.05 (t, J = 7.9 Hz, 9H), 0.71

(q, J = 7.7 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 147.5, 145.8, 133.6, 131.1, 130.5, 129.8, 129.2, 125.4, 123.7, 120.9, 101.7, 101.6, 7.6, 4.4.

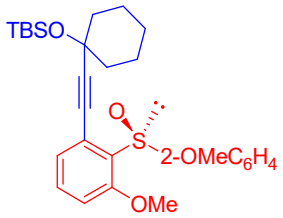
HRMS (ESI) calculated for $C_{20}H_{24}NaOSSi^+$ $[M+Na]^+$: 363.1209, found: 363.1210. $[\alpha]_D^{20}$ = -96 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 12.7 min, t_R (minor) = 11.4 min, 90% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.227	47.111	50.02	1	11.403	0.469	4.83
2	13.677	47.077	49.98	2	12.750	9.247	95.17

(S)-*tert*-Butyl((1-((3-methoxy-2-((2-methoxyphenyl)sulfinyl)phenyl)ethynyl)cyclohexyl)oxy)dimethylsilane (**3fd**)



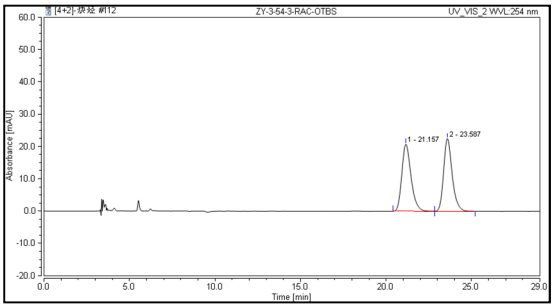
(*S*)-**3fd**

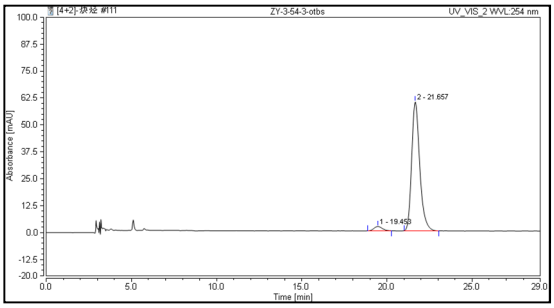
Product (*S*)-**3fd** was isolated in 70% yield (34.9 mg, in 0.2 mmol scale) as light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (dd, J = 7.8, 1.7 Hz, 1H), 7.38 – 7.35 (m, 1H), 7.32 – 7.29 (m, 1H), 7.18 – 7.16 (m, 1H), 7.08 (dd, J = 7.7, 1.0 Hz, 1H), 6.81 – 6.76 (m, 2H), 3.64 (s, 3H), 3.56 (s, 3H), 1.99 – 1.95 (m, 2H), 1.73 – 1.65 (m, 6H), 1.47 – 1.45 (m, 1H), 1.26 – 1.25 (m, 1H), 0.92 (s, 9H), 0.26 (d, J = 2.9 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 155.4, 132.5, 131.54, 131.5, 131.0, 127.5, 126.7, 124.7, 120.4, 112.9, 110.7, 81.8, 70.3, 55.9, 55.5, 41.5, 41.3, 31.7, 30.3, 26.0, 25.5, 23.1, 23.0, 18.3, -2.6.

HRMS (ESI) calculated for $C_{28}H_{38}NaO_4SSi^+$ $[M+Na]^+$: 521.2151, found: 521.2150. $[\alpha]_D^{20}$ = -107 (c = 0.05, $CHCl_3$).

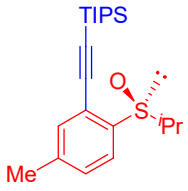
HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 21.6 min, t_R (minor) = 19.5 min, 93% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	21.157	13.030	49.87	1	19.453	1.126	3.30
2	23.587	13.099	50.13	2	21.657	32.947	96.70

(*S*)-Triisopropyl((2-(isopropylsulfinyl)-5-methylphenyl)ethynyl)silane (**5aa**)

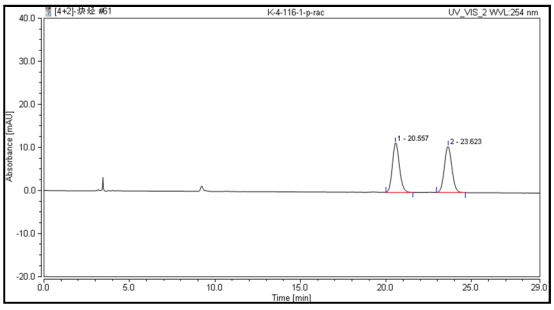


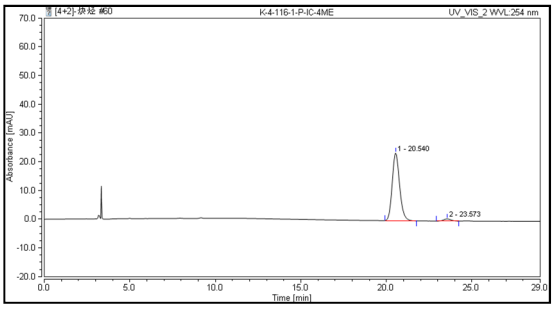
(*S*)-**5aa**

Product (*S*)-**5aa** was isolated in 38% yield (27.5 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 – 7.69 (m, 1H), 7.35 – 7.33 (m, 2H), 3.18 (hept, J = 6.9 Hz, 1H), 2.38 (s, 3H), 1.41 (d, J = 7.1 Hz, 3H), 1.17 – 1.11 (m, 21H), 0.99 (d, J = 6.7 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.3, 140.6, 134.0, 130.0, 125.20, 120.12, 102.12, 99.55, 52.05, 21.18, 18.78, 17.72, 12.24, 11.39. **HRMS** (ESI) calculated for $C_{21}H_{34}NaOSSi^+$ $[M+Na]^+$: 385.1992, found: 385.1997. $[\alpha]_D^{20}$ = -138 (c = 0.05, $CHCl_3$).

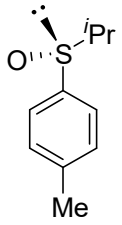
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 20.5 min, t_R (minor) = 23.6 min, 94% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	20.557	5.450	49.93	1	20.540	11.795	96.94
2	23.623	5.465	50.07	2	23.573	0.372	3.06

(*R*)-1-(Isopropylsulfinyl)-4-methylbenzene (**4a**)

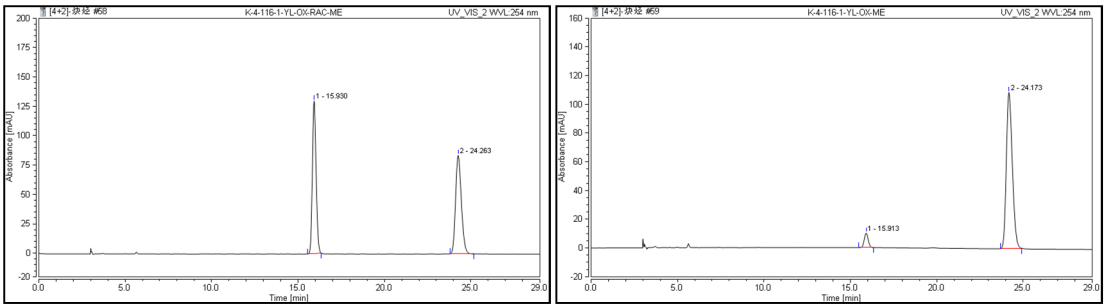


(*R*)-**4a**

Recovered sulfoxide (*R*)-**4a** was isolated in 41% yield (14.9 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.4.

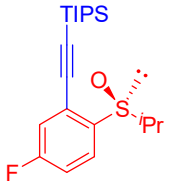
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 7.8 Hz, 2H), 2.81 (hept, J = 6.8 Hz, 1H), 2.41 (s, 3H), 1.20 (d, J = 6.9 Hz, 3H), 1.15 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5, 138.6, 129.7, 125.2, 54.7, 21.5, 15.9, 14.3. $[\alpha]_D^{20}$ = +96 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 24.2 min, t_R (minor) = 15.9 min, 89% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	15.930	32.246	49.83	1	15.913	2.655	5.74
2	24.263	32.461	50.17	2	24.173	43.640	94.26

(*S*)-((5-Fluoro-2-(isopropylsulfinyl)phenyl)ethynyl)triisopropylsilane (**5ba**)

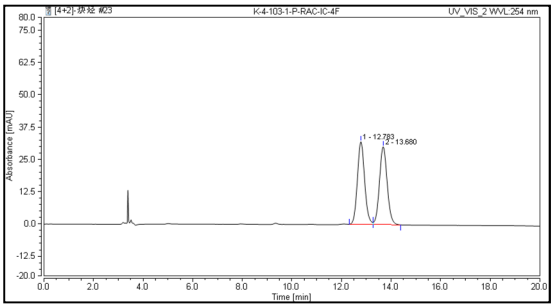


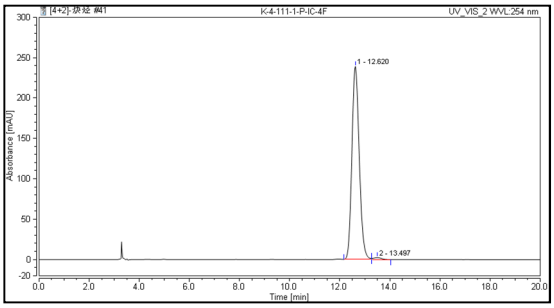
(*S*)-**5ba**

Product (*S*)-**5ba** was isolated in 43% yield (31.6 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (dd, J = 8.6, 5.6 Hz, 1H), 7.26 – 7.21 (m, 2H), 3.18 (hept, J = 6.9 Hz, 1H), 1.42 (d, J = 7.1 Hz, 3H), 1.16 – 1.12 (m, 21H), 0.99 (d, J = 6.7 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.6 (d, $J_{C\text{-}F}$ = 249.5 Hz), 140.1 (d, $J_{C\text{-}F}$ = 3.5 Hz), 127.6 (d, $J_{C\text{-}F}$ = 9.2 Hz), 122.2 (d, $J_{C\text{-}F}$ = 9.9 Hz), 120.4 (d, $J_{C\text{-}F}$ = 23.6 Hz), 116.7 (d, $J_{C\text{-}F}$ = 21.9 Hz), 101.8, 100.6, 18.8, 17.7, 12.2, 11.4. **HRMS** (ESI) calculated for $C_{20}H_{31}FNaOSSi^+$ $[M+Na]^+$: 389.1741, found: 389.1744. $[\alpha]_D^{20}$ = -176 (c = 0.05, $CHCl_3$).

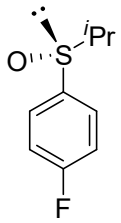
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 12.6 min, t_R (minor) = 13.5 min, 98% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.783	10.845	49.89	1	12.620	81.007	98.97
2	13.680	10.893	50.11	2	13.497	0.845	1.03

(*R*)-1-Fluoro-4-(isopropylsulfinyl)benzene (**4b**)

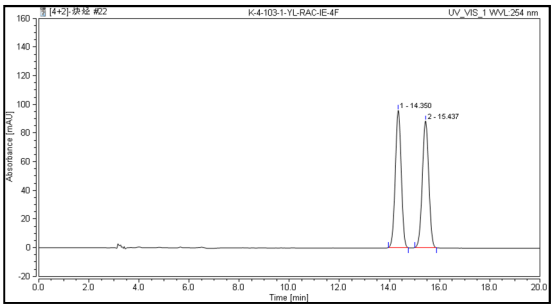


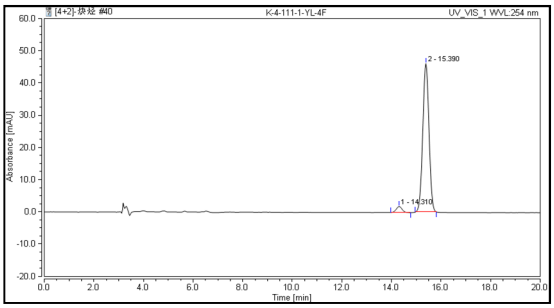
(*R*)-**4b**

Recovered sulfoxide (*R*)-**4b** was isolated in 40% yield (14.9 mg, in 0.2 mmol scale) as a light yellow liquid. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 – 7.59 (m, 2H), 7.23 – 7.20 (m, 2H), 2.82 (hept, J = 6.9 Hz, 1H), 1.21 (d, J = 7.0 Hz, 3H), 1.15 (d, J = 6.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.4 (d, $J_{C\text{-}F}$ = 251.0 Hz), 137.2, 127.3 (d, $J_{C\text{-}F}$ = 8.8 Hz), 116.3 (d, $J_{C\text{-}F}$ = 22.5 Hz), 54.7, 15.7, 14.0. $[\alpha]_D^{20}$ = +70 (c = 0.05, $CHCl_3$).

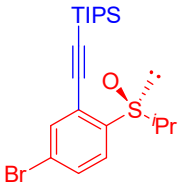
HPLC conditions: Daicel Chiralpak IE column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 15.4 min, t_R (minor) = 14.3 min, 93% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	14.350	26.378	50.04	1	14.310	0.512	3.69
2	15.437	26.340	49.96	2	15.390	13.353	96.31

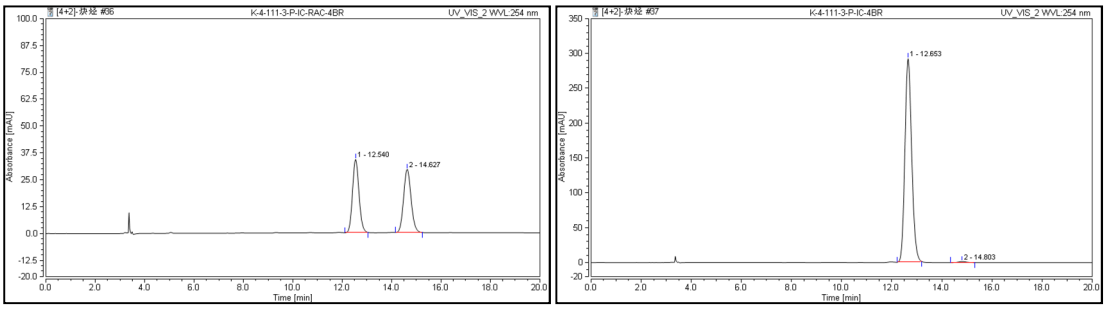
(*S*)-((5-Bromo-2-(isopropylsulfinyl)phenyl)ethynyl)triisopropylsilane (**5ca**)



(*S*)-**5ca**

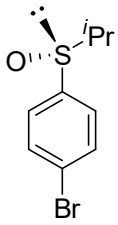
Product (*S*)-**5ca** was isolated in 42% yield (35.9 mg, in 0.2 mmol scale) as a light yellow liquid. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 – 7.62 (m, 3H), 3.20 (hept, J = 6.9 Hz, 1H), 1.43 (d, J = 7.1 Hz, 3H), 1.17 – 1.12 (m, 21H), 0.98 (d, J = 6.7 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.7, 136.0, 132.3, 126.9, 124.4, 121.9, 102.1, 100.4, 52.0, 18.8, 17.8, 12.1, 11.3. **HRMS** (ESI) calculated for $C_{20}H_{31}BrNaOSSi^+$ $[M+Na]^+$: 449.0940, found: 449.0946. $[\alpha]_D^{20}$ = -79 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 12.7 min, t_R (minor) = 14.8 min, 99% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.540	10.340	50.02	1	12.653	91.253	99.45
2	14.627	10.330	49.98	2	14.803	0.501	0.55

(*R*)-1-Bromo-4-(isopropylsulfinyl)benzene (**4c**)

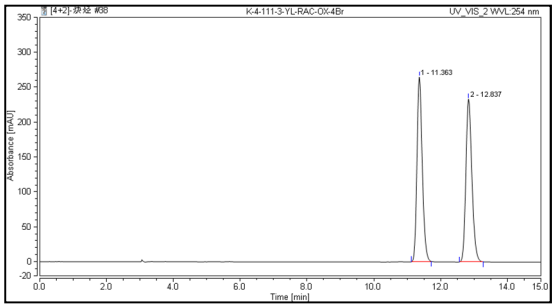


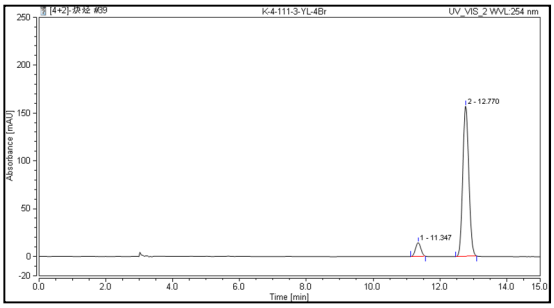
(*R*)-**4c**

Recovered sulfoxide (*R*)-**4c** was isolated in 45% yield (22.2 mg, in 0.2 mmol scale) as a light yellow liquid. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.67 – 7.63 (m, 2H), 7.48 – 7.44 (m, 2H), 2.81 (hept, J = 6.9 Hz, 1H), 1.24 (d, J = 6.9 Hz, 3H), 1.13 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.1, 132.2, 126.7, 125.5, 54.7, 15.9, 13.9. $[\alpha]_D^{20}$ = +67 (c = 0.05, $CHCl_3$).

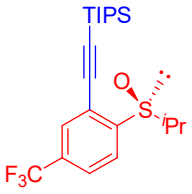
HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 12.8 min, t_R (minor) = 11.3 min, 85% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.363	48.583	49.97	1	11.347	2.677	7.53
2	12.837	48.650	50.03	2	12.770	32.898	92.47

(*S*)-Triisopropyl((2-(isopropylsulfinyl)-5-(trifluoromethyl)phenyl)ethynyl)silane (**5da**)



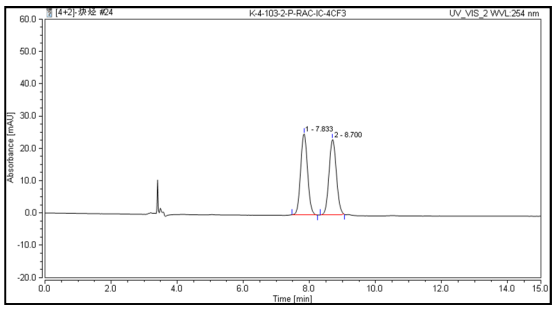
(*S*)-**5da**

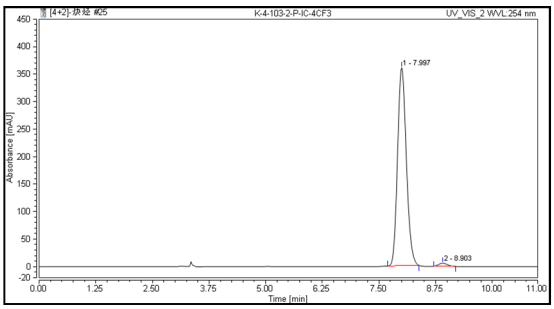
Product (*S*)-**5da** was isolated in 43% yield (35.8 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, J = 8.2 Hz, 1H), 7.78 (dd, J = 8.2, 1.8 Hz, 1H), 7.74 (s, 1H), 3.29 (hept, J = 6.9 Hz, 1H), 1.47 (d, J = 7.1 Hz, 3H), 1.19 – 1.13 (m, 21H), 0.98 (d, J = 6.7 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 148.9, 132.7 (q, $J_{C\text{-}F}$ = 32.9 Hz), 130.3 (q, $J_{C\text{-}F}$ = 3.7 Hz), 126.1, 125.5 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.4 (q, $J_{C\text{-}F}$ = 271.3 Hz), 121.0, 102.8, 100.4, 51.9, 18.8, 18.0, 12.0, 11.3. **HRMS** (ESI) calculated for $C_{21}H_{31}F_3NaOSSi^+$ $[M+Na]^+$: 439.1709, found: 439.1710. $[\alpha]_D^{20}$ = -90 (c = 0.05, $CHCl_3$).

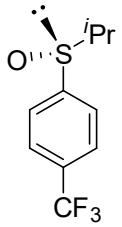
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 8.0 min, t_R (minor) = 8.9 min, 97% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.833	6.101	50.45	1	7.997	81.025	98.43
2	8.700	5.992	49.55	2	8.903	1.291	1.57

(*R*)-1-(Isopropylsulfinyl)-4-(trifluoromethyl)benzene (**4d**)

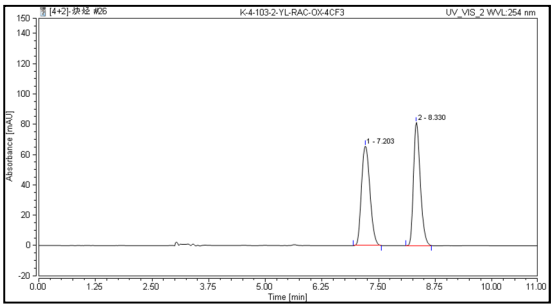


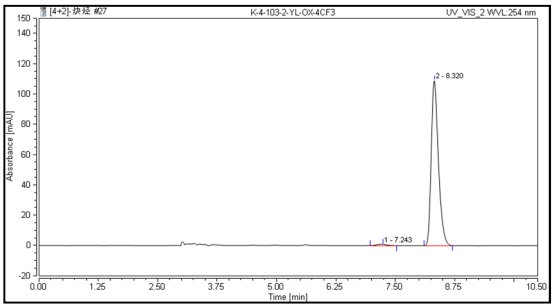
(*R*)-**4d**

Recovered sulfoxide (*R*)-**4d** was isolated in 42% yield (19.8 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, J = 8.1 Hz, 2H), 7.73 (d, J = 8.1 Hz, 2H), 2.87 (hept, J = 6.9 Hz, 1H), 1.30 (d, J = 7.0 Hz, 3H), 1.13 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.5, 133.1 (q, $J_{C\text{-}F}$ = 32.9 Hz), 126.0 (q, $J_{C\text{-}F}$ = 3.7 Hz), 125.5, 123.7 (q, $J_{C\text{-}F}$ = 272.7 Hz), 54.8, 16.1, 13.6. $[\alpha]_D^{20}$ = +67 (c = 0.05, $CHCl_3$).

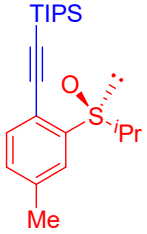
HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 8.3 min, t_R (minor) = 7.2 min, 98% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.203	14.198	50.15	1	7.243	0.213	1.11
2	8.330	14.112	49.85	2	8.320	19.043	98.89

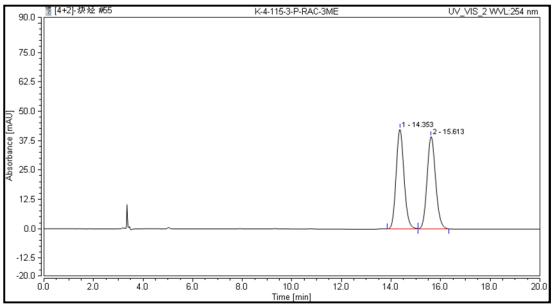
(*S*)-Triisopropyl((2-(isopropylsulfinyl)-4-methylphenyl)ethynyl)silane (**5ea**)

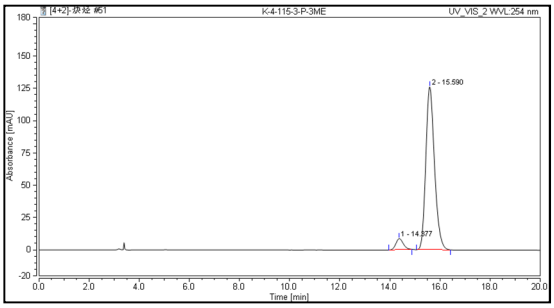


(*S*)-**5ea**

Product (*S*)-**5ea** was isolated in 50% yield (36.3 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.40 (d, J = 7.8 Hz, 1H), 7.19 (d, J = 7.7 Hz, 1H), 3.22 (hept, J = 6.9 Hz, 1H), 2.43 (s, 3H), 1.41 (d, J = 7.1 Hz, 3H), 1.15 – 1.10 (m, 21H), 0.98 (d, J = 6.7 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.1, 139.8, 133.5, 131.0, 125.4, 117.3, 102.1, 99.2, 51.9, 21.8, 18.8, 17.9, 12.3, 11.4. **HRMS** (ESI) calculated for $C_{21}H_{34}NaOSSi^+$ $[M+Na]^+$: 385.1992, found: 385.1995. $[\alpha]_D^{20}$ = -126 (c = 0.05, $CHCl_3$).

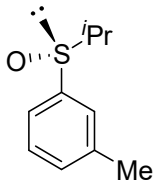
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 15.6 min, t_R (minor) = 14.4 min, 89% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	14.353	15.685	50.13	1	14.377	2.949	5.49
2	15.613	15.606	49.87	2	15.590	50.798	94.51

(*R*)-1-(Isopropylsulfinyl)-3-methylbenzene (**4e**)

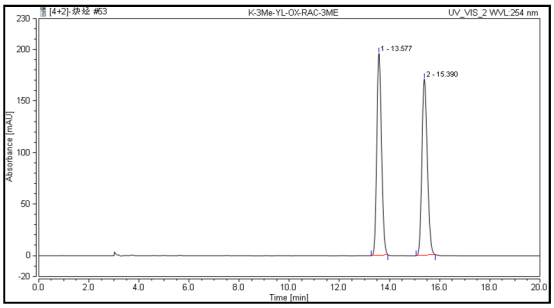


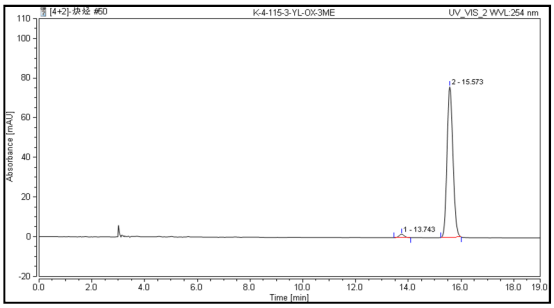
(*R*)-**4e**

Recovered sulfoxide (*R*)-**4e** was isolated in 42% yield (15.3 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (s, 1H), 7.40 – 7.33 (m, 2H), 7.30 – 7.28 (m, 1H), 2.83 (hept, J = 6.9 Hz, 1H), 2.42 (s, 3H), 1.23 (d, J = 6.9 Hz, 3H), 1.15 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.8, 139.2, 131.9, 128.8, 125.4, 122.3, 54.7, 21.6, 16.1, 14.1. $[\alpha]_D^{20}$ = +78 (c = 0.05, $CHCl_3$).

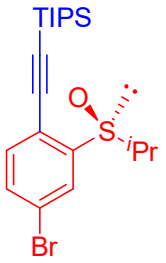
HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 15.6 min, t_R (minor) = 13.7 min, 96% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	13.577	42.923	50.04	1	13.743	0.376	1.87
2	15.390	42.856	49.96	2	15.573	19.706	98.13

(*S*)-((4-Bromo-2-(isopropylsulfinyl)phenyl)ethynyl)triisopropylsilane (**5fa**)

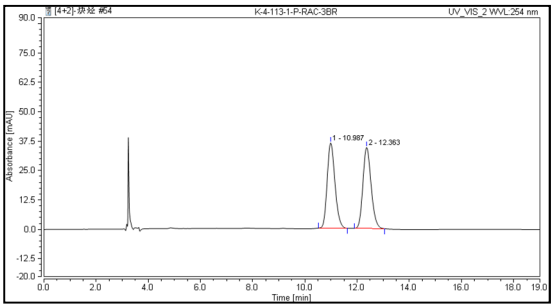


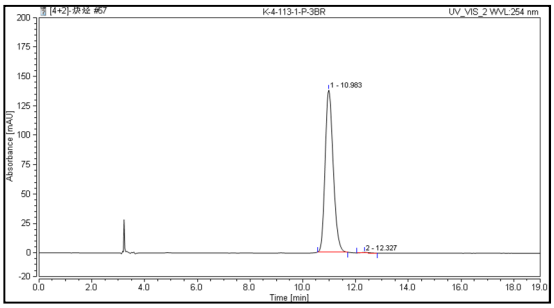
(*S*)-**5fa**

Product (*S*)-**5fa** was isolated in 30% yield (25.7 mg, in 0.2 mmol scale) as a light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, J = 2.0 Hz, 1H), 7.53 (dd, J = 8.1, 2.1 Hz, 1H), 7.36 (d, J = 8.1 Hz, 1H), 3.23 (hept, J = 6.9 Hz, 1H), 1.43 (d, J = 7.1 Hz, 3H), 1.16 – 1.09 (m, 21H), 0.99 (d, J = 6.7 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 146.6, 134.8, 133.5, 128.3, 123.9, 119.0, 101.8, 100.9, 52.0, 18.8, 17.9, 12.2, 11.3. **HRMS** (ESI) calculated for $C_{20}H_{31}BrNaOSSi^+$ $[M+Na]^+$: 449.0940, found: 449.0944. $[\alpha]_D^{20}$ = -93 (c = 0.05, $CHCl_3$).

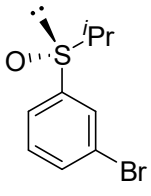
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 11.0 min, t_R (minor) = 12.3 min, 99% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.987	12.567	50.01	1	10.983	48.901	99.63
2	12.363	12.561	49.99	2	12.327	0.180	0.37

(*R*)-1-Bromo-3-(isopropylsulfinyl)benzene (**4f**)

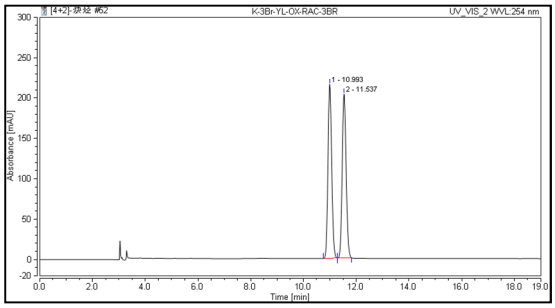


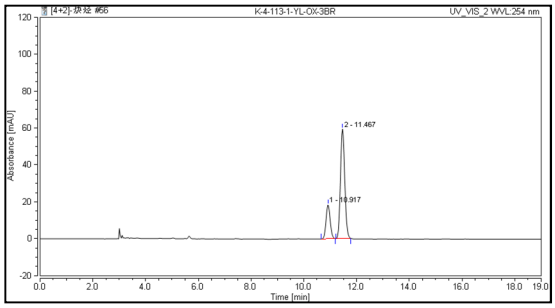
(*R*)-**4f**

Recovered sulfoxide (*R*)-**4f** was isolated in 61% yield (30.1 mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 – 7.74 (m, 1H), 7.63 – 7.61 (m, 1H), 7.50 – 7.48 (m, 1H), 7.40 – 7.37 (m, 1H), 2.84 (hept, J = 6.8 Hz, 1H), 1.27 (d, J = 6.9 Hz, 3H), 1.14 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.5, 134.2, 130.5, 127.9, 123.7, 123.4, 54.9, 16.1, 13.9. **$[\alpha]_D^{20}$** = +51 (c = 0.05, $CHCl_3$).

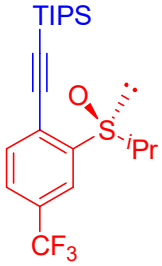
HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 11.5 min, t_R (minor) = 10.9 min, 54% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.993	35.122	50.18	1	10.917	3.338	22.93
2	11.537	34.867	49.82	2	11.467	11.220	77.07

(*S*)-Triisopropyl((2-(isopropylsulfinyl)-4-(trifluoromethyl)phenyl)ethynyl)silane (**5ga**)

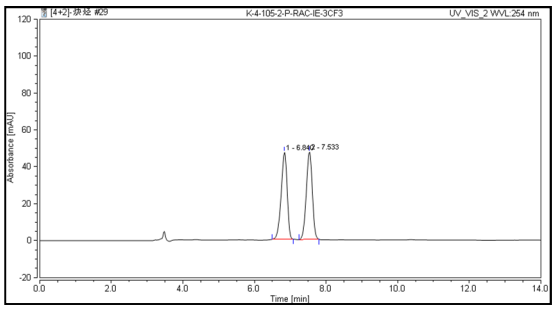


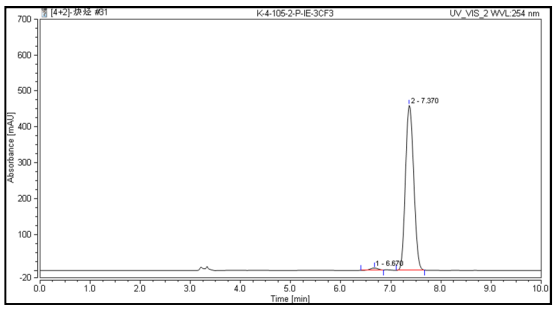
(*S*)-**5ga**

Product (*S*)-**5ga** was isolated in 47% yield (39.2 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.68 – 7.60 (m, 2H), 3.25 (hept, J = 6.9 Hz, 1H), 1.45 (d, J = 7.1 Hz, 3H), 1.18 – 1.09 (m, 21H), 0.97 (d, J = 6.8 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 146.2, 133.9, 131.2 (q, $J_{C\text{-}F}$ = 33.3 Hz), 127.0 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.8, 123.5 (q, $J_{C\text{-}F}$ = 271.2 Hz), 122.6 (q, $J_{C\text{-}F}$ = 3.9 Hz), 103.8, 100.6, 52.1, 18.7, 17.9, 12.1, 11.4, 11.3. **HRMS** (ESI) calculated for $C_{21}H_{31}F_3NaOSSi^+$ $[M+Na]^+$: 439.1709, found: 439.1709. $[\alpha]_D^{20}$ = -196 (c = 0.05, $CHCl_3$).

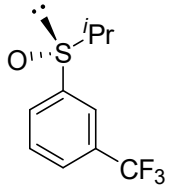
HPLC conditions: Daicel Chiralpak IE column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 7.4 min, t_R (minor) = 6.7 min, 98% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	6.840	9.119	49.72	1	6.670	1.046	1.18
2	7.533	9.222	50.28	2	7.370	87.425	98.82

(*R*)-1-(Isopropylsulfinyl)-3-(trifluoromethyl)benzene (**4g**)

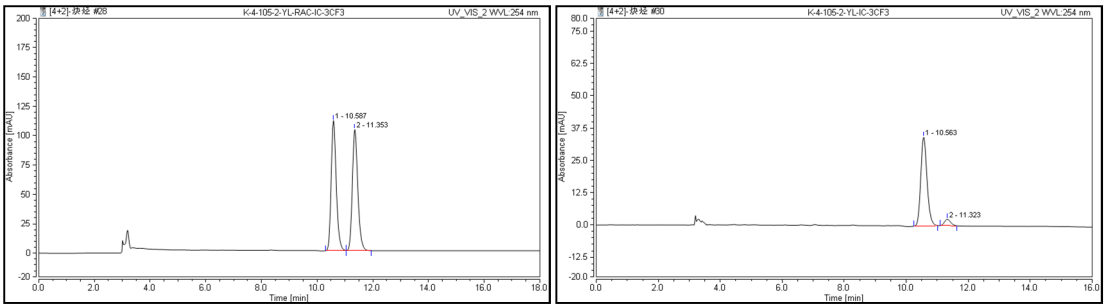


(*R*)-**4g**

Recovered sulfoxide (*R*)-**4g** was isolated in 43% yield (20.3 mg, in 0.2 mmol scale) as light yellow liquid. Eluent: PE/EA = 3/1, R_f = 0.4.

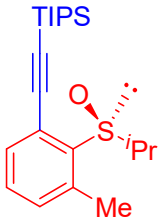
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.80 – 7.74 (m, 2H), 7.68 – 7.65 (m, 1H), 2.87 (hept, J = 6.9 Hz, 1H), 1.28 (d, J = 6.9 Hz, 3H), 1.13 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.7, 131.8 (q, $J_{C\text{-}F}$ = 33.1 Hz), 129.6, 128.4, 127.8 (q, $J_{C\text{-}F}$ = 3.7 Hz), 123.6 (q, $J_{C\text{-}F}$ = 272.9 Hz), 122.1 (q, $J_{C\text{-}F}$ = 3.9 Hz), 54.9, 16.1, 13.7. **[α]$_D^{20}$** = +21 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 11.3 min, t_R (minor) = 10.6 min, 87% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.587	23.535	49.97	1	10.563	8.062	93.31
2	11.353	23.565	50.03	2	11.323	0.578	6.69

(*S*)-Triisopropyl((2-(isopropylsulfinyl)-3-methylphenyl)ethynyl)silane (**5ha**)

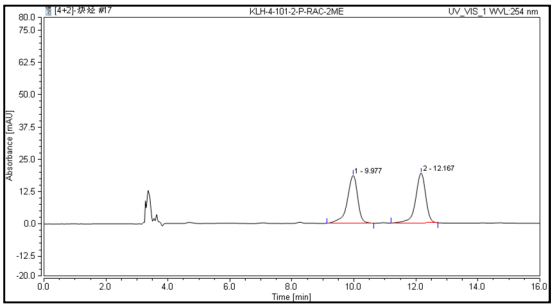


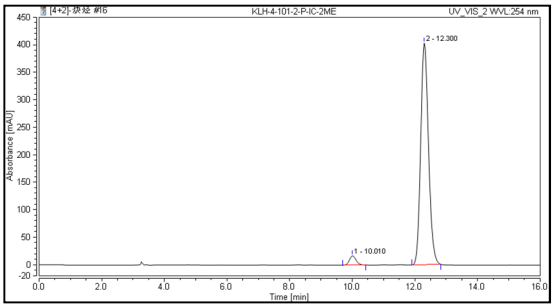
(*S*)-**5ha**

Product (*S*)-**5ha** was isolated in 49% yield (35.6 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 7/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (d, J = 7.6 Hz, 1H), 7.27 – 7.25 (m, 1H), 7.16 (d, J = 7.6 Hz, 1H), 3.52 (hept, J = 6.9 Hz, 1H), 2.69 (s, 3H), 1.43 (d, J = 6.8 Hz, 3H), 1.18 (d, J = 7.0 Hz, 3H), 1.15 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.4, 140.1, 133.2, 132.4, 130.2, 123.6, 103.0, 100.2, 52.7, 18.8, 18.8, 17.1, 16.3, 11.5. **HRMS** (ESI) calculated for $C_{21}H_{34}NaOSSi^+$ $[M+Na]^+$: 385.1992, found: 385.1991. $[\alpha]_D^{20}$ = -153 (c = 0.05, $CHCl_3$).

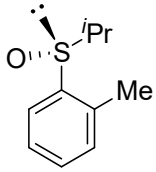
HPLC conditions: Daicel Chiralpak IC column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 12.3 min, t_R (minor) = 10.0 min, 93% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	9.977	7.173	49.91	1	10.010	4.175	3.46
2	12.167	7.200	50.09	2	12.300	116.335	96.54

(*R*)-1-(Isopropylsulfinyl)-2-methylbenzene (**4h**)

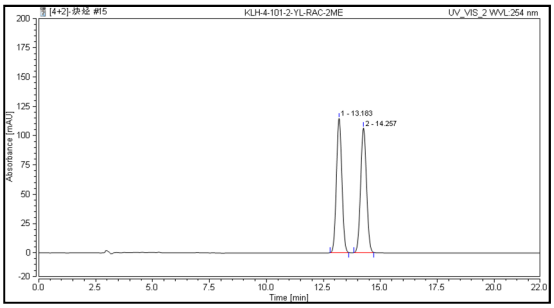


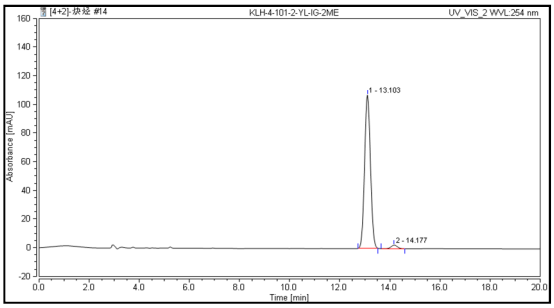
(*R*)-**4h**

Recovered sulfoxide (*R*)-**4h** was isolated in 41% yield (14.9 mg, in 0.2 mmol scale) as light yellow liquid. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, J = 7.4 Hz, 1H), 7.43 – 7.33 (m, 2H), 7.20 (d, J = 7.3 Hz, 1H), 2.85 (hept, J = 6.9 Hz, 1H), 2.39 (s, 3H), 1.30 (d, J = 7.0 Hz, 3H), 1.15 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.8, 135.4, 130.7, 130.6, 126.8, 125.0, 53.0, 18.6, 17.0, 13.5. $[\alpha]_D^{20}$ = +45 (c = 0.05, $CHCl_3$).

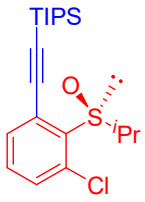
HPLC conditions: Daicel Chiralpak IG column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 13.1 min, t_R (minor) = 14.2 min, 95% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	13.183	31.934	50.05	1	13.103	29.042	97.56
2	14.257	31.865	49.95	2	14.177	0.725	2.44

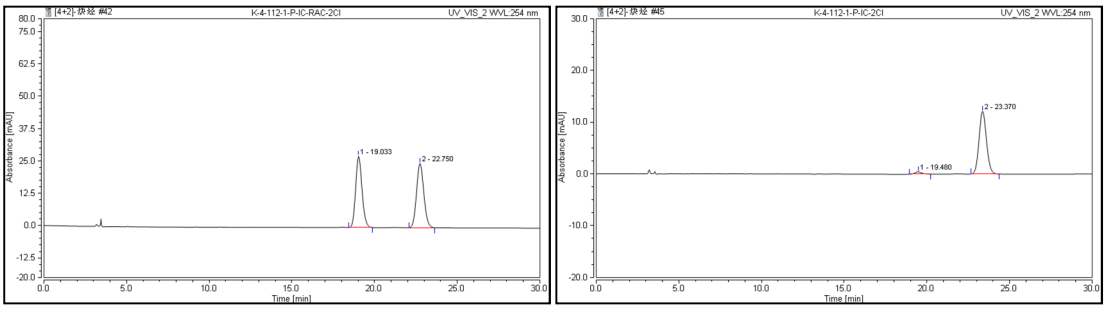
(*S*)-((3-Chloro-2-(isopropylsulfinyl)phenyl)ethynyl)triisopropylsilane (**5ia**)



(*S*)-**5ia**

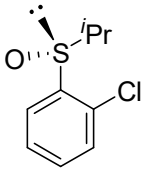
Product (*S*)-**5ia** was isolated in 47% yield (36.0 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.47 (dd, J = 7.6, 1.4 Hz, 1H), 7.37 (dd, J = 8.1, 1.3 Hz, 1H), 7.32 – 7.29 (m, 1H), 3.92 (hept, J = 6.8 Hz, 1H), 1.49 (d, J = 6.9 Hz, 3H), 1.14 – 1.09 (m, 24H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.2, 135.0 133.7, 131.8, 131.5, 126.3, 102.4, 101.5, 51.9, 18.8, 17.1, 16.6, 11.4. **HRMS** (ESI) calculated for $C_{20}H_{31}ClNaOSSi^+$ $[M+Na]^+$: 405.1446, found: 405.1447. $[\alpha]_D^{20}$ = -84 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 23.4 min, t_R (minor) = 19.5 min, 94% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	19.033	12.366	49.35	1	19.480	0.210	3.23
2	22.750	12.690	50.65	2	23.370	6.294	96.77

(*R*)-1-Chloro-2-(isopropylsulfinyl)benzene (**4i**)

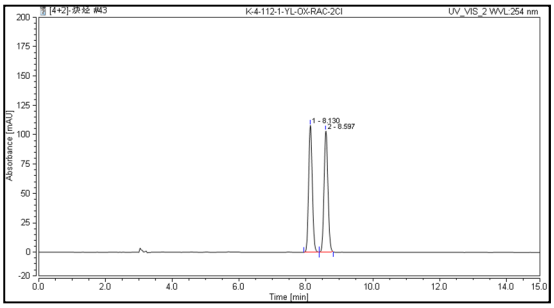


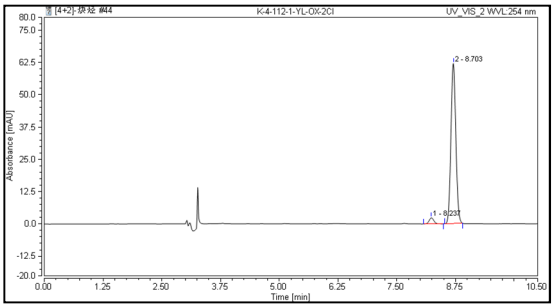
(*R*)-**4i**

Recovered sulfoxide (*R*)-**4i** was isolated in 42% yield (17.1 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (dd, J = 7.8, 1.6 Hz, 1H), 7.51 – 7.49 (m, 1H), 7.44 – 7.42 (m, 1H), 7.39 (dd, J = 7.9, 1.3 Hz, 1H), 3.18 (hept, J = 6.9 Hz, 1H), 1.46 (d, J = 7.1 Hz, 3H), 1.03 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.6, 131.9, 130.7, 129.9, 127.6, 127.3, 51.6, 17.7, 12.3. $[\alpha]_D^{20}$ = +32 (c = 0.05, $CHCl_3$).

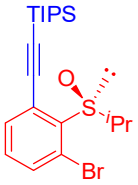
HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 8.7 min, t_R (minor) = 8.2 min, 93% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.130	13.710	49.87	1	8.237	0.270	3.48
2	8.597	13.781	50.13	2	8.703	7.474	96.52

(*S*)-((3-Bromo-2-(isopropylsulfinyl)phenyl)ethynyl)triisopropylsilane (**5ja**)

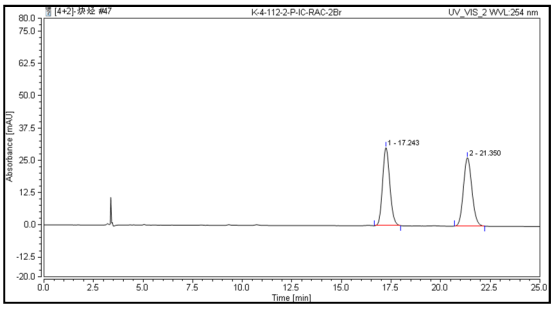


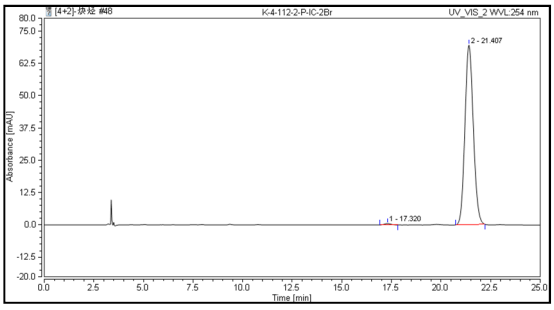
(*S*)-**5ja**

Product (*S*)-**5ja** was isolated in 40% yield (33.9 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 (dd, J = 8.0, 1.2 Hz, 1H), 7.53 (dd, J = 7.7, 1.2 Hz, 1H), 7.23 – 7.21 (m, 1H), 3.95 (hept, J = 6.9 Hz, 1H), 1.49 (d, J = 6.9 Hz, 3H), 1.15 – 1.09 (m, 24H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.6, 135.0, 134.8, 131.5, 126.3, 123.0, 102.8, 101.4, 52.1, 18.8, 17.0, 16.7, 11.5. **HRMS** (ESI) calculated for $C_{20}H_{31}BrNaOSSi^+$ $[M+Na]^+$: 449.0940, found: 449.0944. $[\alpha]_D^{20}$ = -78 (c = 0.05, $CHCl_3$).

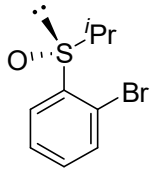
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 21.4 min, t_R (minor) = 17.3 min, 99% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	17.243	12.760	49.30	1	17.320	0.214	0.62
2	21.350	13.123	50.70	2	21.407	34.048	99.38

(*R*)-1-Bromo-2-(isopropylsulfinyl)benzene (**4j**)

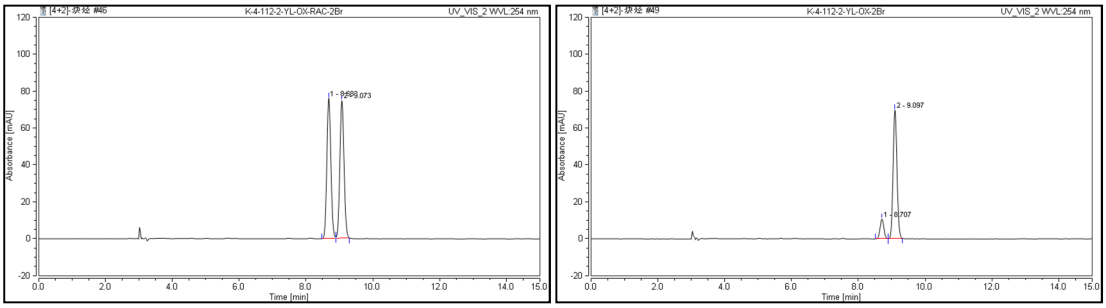


(*R*)-**4j**

Recovered sulfoxide (*R*)-**4j** was isolated in 51% yield (25.2mg, in 0.2 mmol scale) as a light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.4.

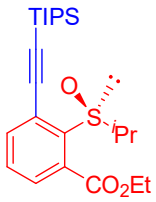
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, J = 7.8 Hz, 1H), 7.57 – 7.53 (m, 2H), 7.39 – 7.33 (m, 1H), 3.21 (hept, J = 7.0 Hz, 1H), 1.47 (d, J = 7.0 Hz, 3H), 1.01 (d, J = 6.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.3, 133.0, 132.2, 128.1, 127.7, 119.4, 51.5, 17.9, 12.0. **$[\alpha]_D^{20}$** = +65 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 9.1 min, t_R (minor) = 8.7 min, 74% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.683	10.646	49.86	1	8.707	1.408	13.07
2	9.073	10.707	50.14	2	9.097	9.368	86.93

(*S*)-Ethyl 2-(isopropylsulfinyl)-3-((triisopropylsilyl)ethynyl)benzoate (**5ka**)

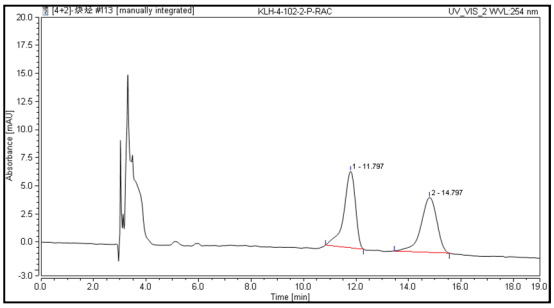


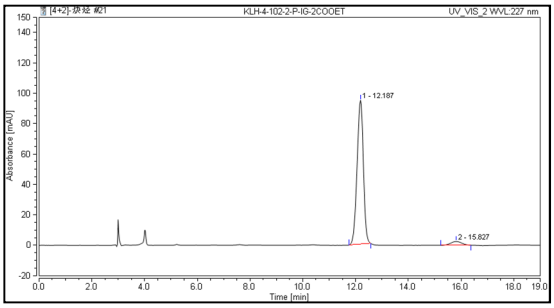
(*S*)-**5ka**

Product (*S*)-**5ka** was isolated in 45% yield (37.9 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (dd, J = 7.2, 1.7 Hz, 1H), 7.47 – 7.38 (m, 2H), 4.39 (q, J = 7.1 Hz, 2H), 3.80 (hept, J = 6.9 Hz, 1H), 1.38 (t, J = 7.2 Hz, 3H), 1.34 (d, J = 6.8 Hz, 3H), 1.31 (d, J = 7.0 Hz, 3H), 1.17 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.1, 142.9, 135.3, 134.0, 130.1, 129.2, 122.7, 102.0, 101.6, 62.1, 54.3, 18.8, 17.5, 15.8, 14.2, 11.4. **HRMS** (ESI) calculated for $C_{23}H_{36}NaOSSi^+$ $[M+Na]^+$: 443.2047, found: 443.2050. $[\alpha]_D^{20}$ = -43 (c = 0.05, $CHCl_3$).

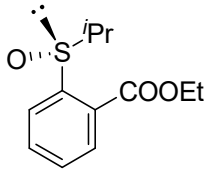
HPLC conditions: Daicel Chiralpak IG column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 12.2 min, t_R (minor) = 15.8 min, 91% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.797	3.486	50.44	1	12.187	26.169	95.62
2	14.797	3.426	49.56	2	15.827	1.198	4.38

(*R*)-ethyl 2-(isopropylsulfinyl)benzoate (**4k**)

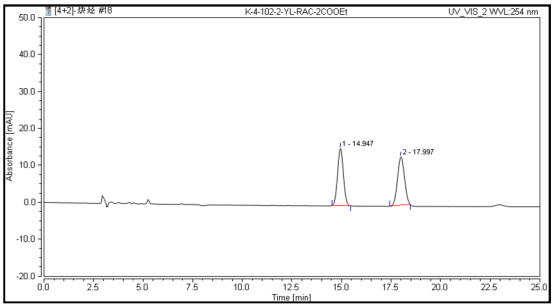


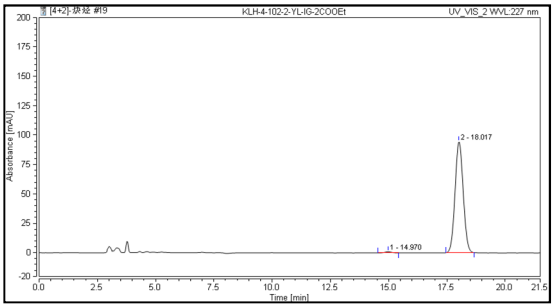
(*R*)-**4k**

Recovered sulfoxide (*R*)-**4k** was isolated in 46% yield (22.1 mg, in 0.2 mmol scale) as light yellow iquid. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (dd, J = 7.9, 1.3 Hz, 1H), 8.12 (dd, J = 7.7, 1.4 Hz, 1H), 7.79 - 7.76 (m, 1H), 7.56 – 7.53 (m, 1H), 4.40 (q, J = 7.1 Hz, 2H), 3.18 (hept, J = 6.9 Hz, 1H), 1.54 (d, J = 7.1 Hz, 3H), 1.42 (t, J = 7.2 Hz, 3H), 0.91 (d, J = 6.8 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.4, 147.2, 133.2, 131.1, 130.0, 127.3, 126.1, 61.9, 52.6, 18.9, 14.4, 11.8. $[\alpha]_D^{20}$ = +89 (c = 0.05, $CHCl_3$).

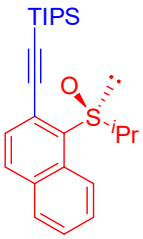
HPLC conditions: Daicel Chiralpak IG column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 18.0 min, t_R (minor) = 15.0 min, 98% ee.





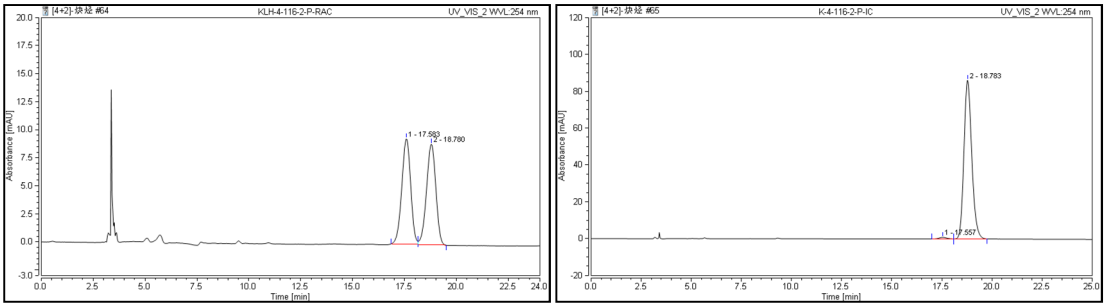
No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	14.947	5.260	49.74	1	14.970	0.311	0.81
2	17.997	5.316	50.26	2	18.017	38.108	99.19

(*S*)-triisopropyl((1-(isopropylsulfinyl)naphthalen-2-yl)ethynyl)silane (**5la**)



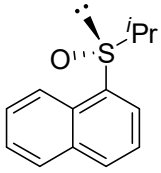
Product (*S*)-**5la** was isolated in 37% yield (29.3 mg, in 0.2 mmol scale) as light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.29 (d, J = 8.4 Hz, 1H), 7.89 – 7.82 (m, 2H), 7.59 – 7.53 (m, 2H), 7.51 (d, J = 8.4 Hz, 1H), 3.79 – 3.73 (m, 1H), 1.52 (d, J = 6.8 Hz, 3H), 1.20 – 1.14 (m, 21H), 1.13 (d, J = 6.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.7, 134.0, 131.6, 131.3, 129.4, 129.0, 127.7, 127.5, 124.4, 122.8, 103.3, 102.0, 53.6, 18.9, 18.8, 17.2, 17.0, 11.5. **HRMS** (ESI) calculated for $C_{24}H_{34}NaOSSi^+$ $[M+Na]^+$: 421.1992, found: 421.1996. $[\alpha]_D^{20}$ = -91 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 18.8 min, t_R (minor) = 17.6 min, 98% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	17.583	4.779	50.37	1	17.557	0.392	1.00
2	18.780	4.708	49.63	2	18.783	39.041	99.00

(*R*)-1-(isopropylsulfinyl)naphthalene (**4l**)

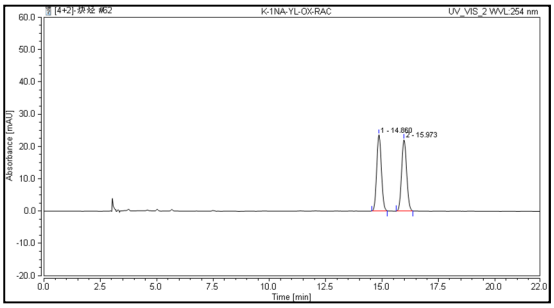


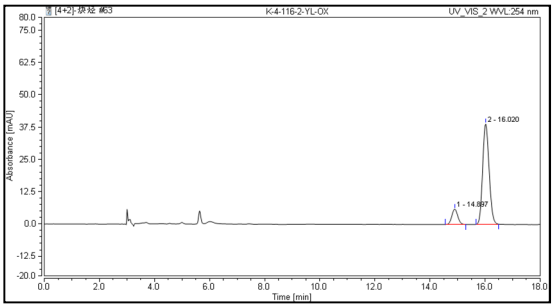
(*R*)-**4l**

Recovered sulfoxide (*R*)-**4l** was isolated in 54% yield (23.5 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (dd, J = 7.2, 1.2 Hz, 1H), 8.03 – 7.99 (m, 1H), 7.97 (d, J = 8.2 Hz, 1H), 7.96 – 7.92 (m, 1H), 7.67 – 7.64 (m, 1H), 7.60 – 7.54 (m, 2H), 3.10 – 3.03 (m, 1H), 1.39 (d, J = 7.0 Hz, 3H), 1.07 (d, J = 6.7 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) ^{13}C NMR (151 MHz, $CDCl_3$) δ 133.6, 131.3, 129.7, 129.2, 127.2, 126.7, 125.5, 124.4, 122.2, 53.3, 17.6, 13.3. $\mathbf{[\alpha]_D^{20}}$ = +85 (c = 0.05, $CHCl_3$).

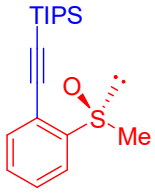
HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 16.0 min, t_R (minor) = 14.9 min, 75% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	14.860	5.669	49.83	1	14.897	1.489	12.39
2	15.973	5.708	50.17	2	16.020	10.531	87.61

(*S*)-Triisopropyl((2-(methylsulfinyl)phenyl)ethynyl)silane (**5ma**)

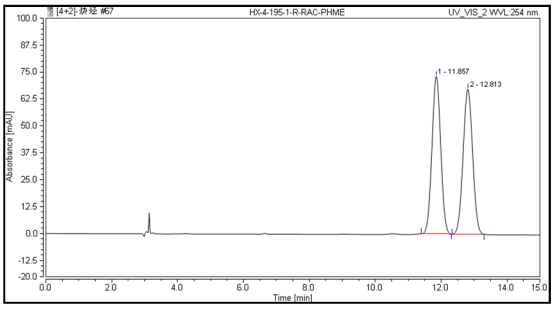


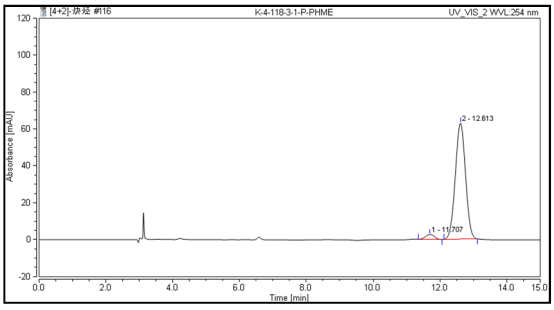
(*S*)-**5ma**

Product (*S*)-**5ma** was isolated in 25% yield (16.0 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 5/1, R_f = 0.4.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, J = 7.9 Hz, 1H), 7.59 – 7.56 (m, 1H), 7.52 (d, J = 7.2 Hz, 1H), 7.44 – 7.42 (m, 1H), 2.84 (s, 3H), 1.16 – 1.12 (m, 21H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 147.7, 133.3, 130.4, 129.8, 123.3, 119.6, 101.4, 101.2, 42.3, 18.8, 18.76, 11.4. **HRMS** (ESI) calculated for $C_{18}H_{28}NaOSSi^+$ $[M+Na]^+$: 343.1522, found: 343.1522. $[\alpha]_D^{20}$ = -75 (c = 0.05, $CHCl_3$).

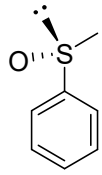
HPLC conditions: Daicel Chiralpak IG column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 12.6 min, t_R (minor) = 11.7 min, 93% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.857	22.482	49.95	1	11.707	0.833	3.61
2	12.813	22.523	50.05	2	12.613	22.229	96.39

(*R*)-(Methylsulfinyl)benzene (**4m**)

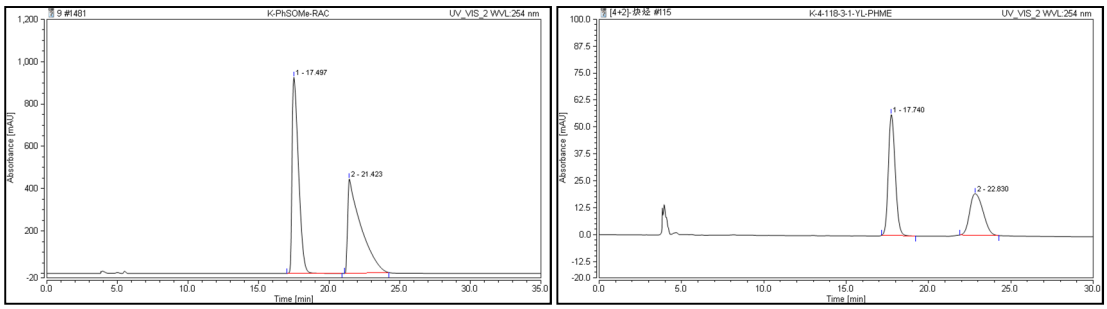


(*R*)-**4m**

Recovered sulfoxide (*R*)-**4m** was isolated in 62% yield (17.4 mg, in 0.2 mmol scale) as light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.4.

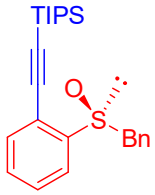
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.62 (m, 2H), 7.55 – 7.47 (m, 3H), 2.72 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 131.2, 129.5, 123.7, 123.6, 44.1. **$[\alpha]_D^{20}$** = +24 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OD-H column (95:5 hexane: 2-propanol, 0.8 mL/min, 40 °C, 254 nm); t_R (major) = 17.7 min, t_R (minor) = 22.8 min, 20% ee.



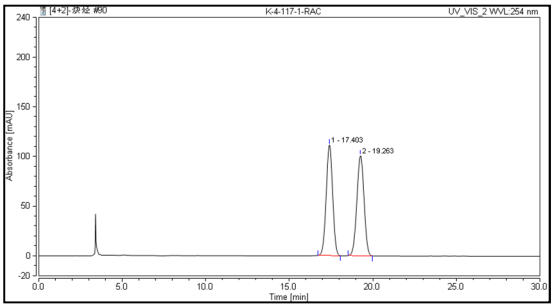
No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	17.497	488.670	50.23	1	17.740	27.200	60.07
2	21.423	484.117	49.77	2	22.830	18.079	39.93

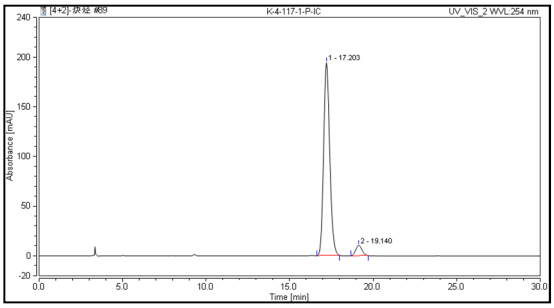
(*S*)-((2-(Benzylsulfinyl)phenyl)ethynyl)triisopropylsilane (**5na**)



Product (*S*)-**5na** was isolated in 25% yield (19.9 mg, in 0.2 mmol scale) as pale yellow oil. Eluent: PE/EA = 4/1, R_f = 0.4. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.7 Hz, 2H), 7.30 (t, *J* = 7.7 Hz, 1H), 7.24 – 7.19 (m, 3H), 7.17 – 7.14 (m, 2H), 4.71 – 4.61 (m, 2H), 1.16 – 1.13 (m, 42H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.7, 135.1, 130.7, 130.4, 130.3, 128.7, 128.1, 123.6, 101.6, 101.5, 58.8, 18.9, 11.5. **HRMS** (ESI) calculated for $C_{24}H_{32}NaOSSi^+$ $[M+Na]^+$: 419.1835, found: 419.1841. $[\alpha]_D^{20}$ = -78 (c = 0.05, $CHCl_3$).

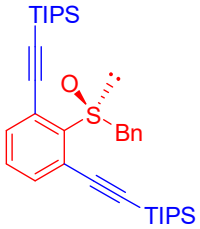
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 17.2 min, t_R (minor) = 19.1 min, 90% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	17.403	49.976	49.91	1	17.203	82.449	94.81
2	19.263	50.160	50.09	2	19.140	4.517	5.19

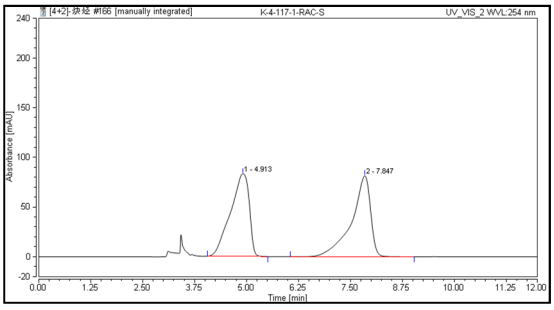
(*S*)-((2-(Benzylsulfinyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) (**5na'**)

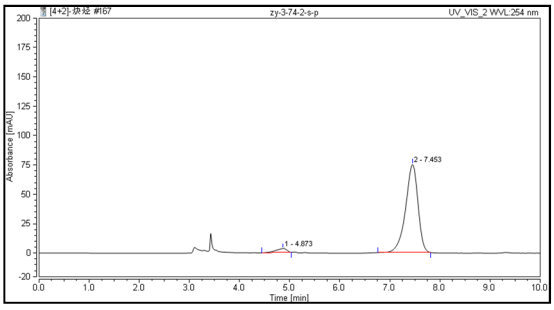


Product (*S*)-**5na'** was isolated in 16% yield (18.5 mg, in 0.2 mmol scale) as light yellow solid. Eluent: PE/EA = 10/1, R_f = 0.4. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, J = 7.5 Hz, 1H), 7.38 – 7.36 (m, 1H), 7.33 – 7.32 (m, 2H), 7.24 (t, J = 7.4 Hz, 1H), 7.21 – 7.18 (m, 2H), 6.95 (d, J = 7.2 Hz, 2H), 4.29 – 4.12 (m, 2H), 1.22 – 1.15 (m, 21H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.4, 133.2, 130.6, 130.3, 129.2, 129.1, 128.2, 128.1, 125.0, 119.8, 101.7, 100.9, 59.0, 18.8, 11.4.

HRMS (ESI) calculated for $C_{35}H_{52}NaOSSi_2^+$ $[M+Na]^+$: 599.3170, found: 599.3168. $[\alpha]_D^{20}$ = -87 (c = 0.05, $CHCl_3$).

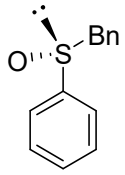
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 7.5 min, t_R (minor) = 4.9 min, 92% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	4.913	43.440	50.26	1	4.873	0.845	3.79
2	7.847	42.997	49.74	2	7.453	21.468	96.21

(*R*)-(benzylsulfinyl)benzene (**4n**)

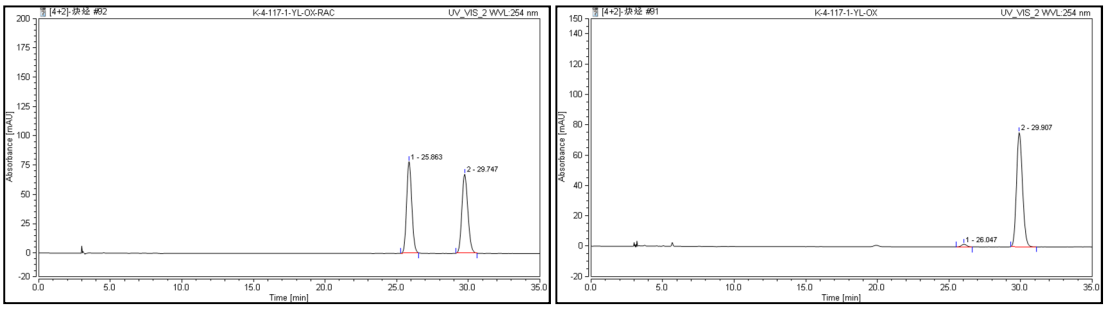


(*R*)-**4n**

Recovered sulfoxide (*R*)-**4n** was isolated in 40% yield (17.3 mg, in 0.2 mmol scale) as white solid. Eluent: PE/EA = 3/1, R_f = 0.4.

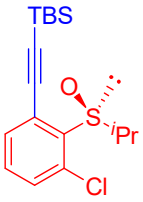
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.41 (m, 5H), 7.29 – 7.20 (m, 3H), 6.98 – 6.94 (m, 2H), 4.12 – 3.94 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.8, 131.3, 130.5, 129.0, 128.6, 128.4, 124.6, 63.7. **[α]$_D^{20}$** = +35 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 29.9 min, t_R (minor) = 26.0 min, 96% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	25.863	32.494	49.91	1	26.047	0.745	1.99
2	29.747	32.605	50.09	2	29.907	36.655	98.01

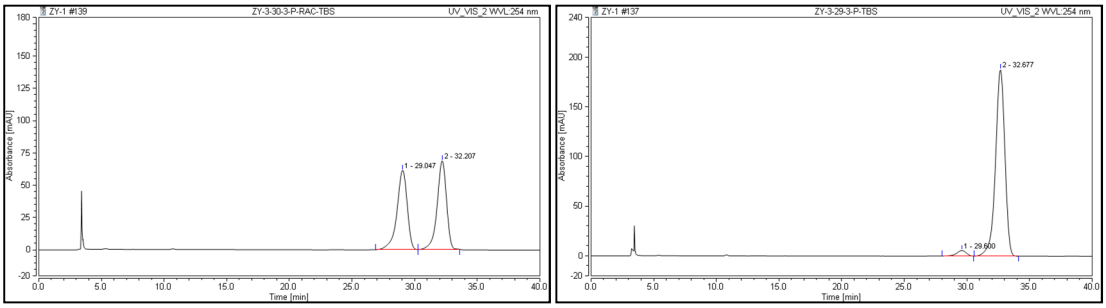
(*S*)-*tert*-Butyl((3-chloro-2-(isopropylsulfinyl)phenyl)ethynyl)dimethylsilane (**5ia**)



(*S*)-**5ib**

Product (*S*)-**5ib** was isolated in 48% yield (32.7 mg, in 0.2 mmol scale) as pale yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.47 – 7.45 (m, 1H), 7.37 – 7.35 (m, 1H), 7.32 – 7.29 (m, 1H), 3.90 (p, *J* = 6.9 Hz, 1H), 1.49 (d, *J* = 6.9 Hz, 3H), 1.10 (d, *J* = 7.0 Hz, 3H), 0.99 (s, 9H), 0.18 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.4, 133.5, 131.8, 131.5, 125.9, 104.0, 100.3, 51.9, 26.3, 17.0, 16.9, 16.6, -4.7. **HRMS** (ESI) calculated for $C_{17}H_{25}ClNaO_2SSi^+$ $[M+Na]^+$: 363.0976, found: 363.0981. $[\alpha]_D^{20}$ = -116 (c = 0.05, $CHCl_3$).

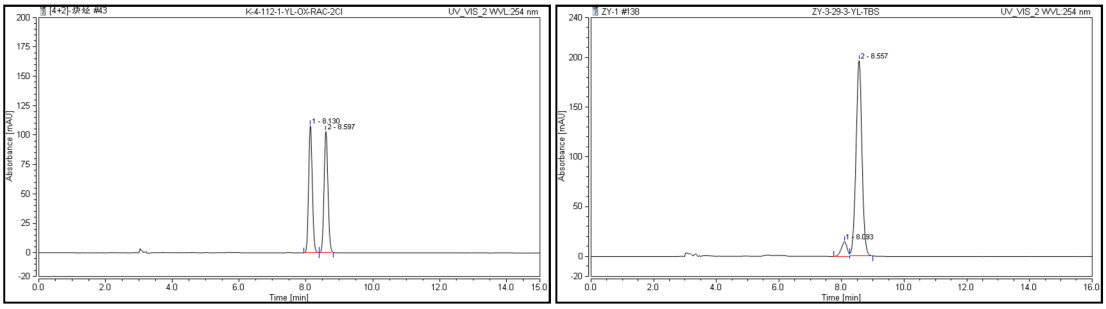
HPLC conditions: Daicel Chiralpak IC column (98:2 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 29.6 min, t_R (minor) = 32.7 min, 94% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	29.047	58.354	49.55	1	29.600	4.963	2.95
2	32.207	59.416	50.45	2	32.677	163.184	97.05

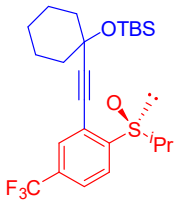
Recovered sulfoxide (*R*)-**4i** was isolated in 49% yield (21.2 mg, in 0.2 mmol scale) as pale yellow liquid. Eluent: PE/EA = 3/1, R_f = 0.4.

HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 8.6 min, t_R (minor) = 8.1 min, 87% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.130	13.710	49.87	1	8.093	3.085	6.65
2	8.597	13.781	50.13	2	8.557	43.333	93.35

(S)-*tert*-butyl((1-((2-(isopropylsulfinyl)-5-(trifluoromethyl)phenyl)ethynyl)cyclohexyl)oxy)dimethylsilane (**5dd**)

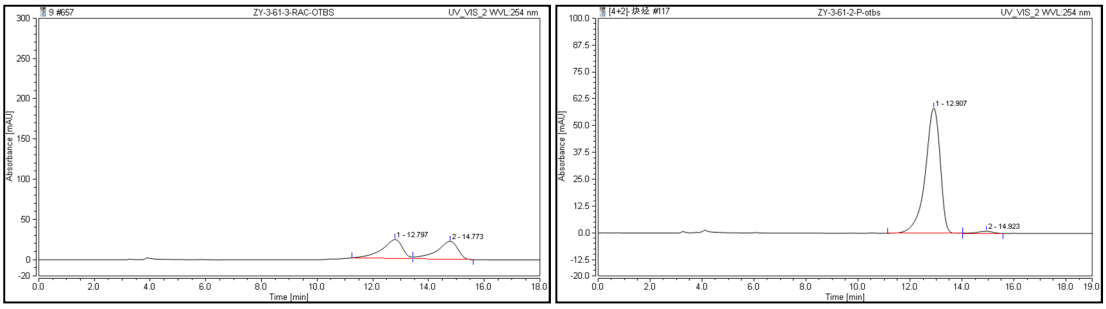


(*S*)-**5dd**

Product (*S*)-**5dd** was isolated in 47% yield (44.5 mg, in 0.2 mmol scale) as pale yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, J = 8.2 Hz, 1H), 7.78 – 7.75 (m, 1H), 7.67 (s, 1H), 3.26 – 3.19 (m, 1H), 1.94 – 1.86 (m, 2H), 1.75 – 1.70 (m, 4H), 1.59 – 1.52 (m, 3H), 1.47 (d, J = 7.1 Hz, 3H), 1.37 – 1.35 (m, 1H), 0.98 (d, J = 6.7 Hz, 3H), 0.90 (s, 9H), 0.20 (s, 3H), 0.17 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.7, 132.9 (q, $J_{C\text{-}F}$ = 32.9 Hz), 129.4 (q, $J_{C\text{-}F}$ = 3.7 Hz), 126.2, 125.4 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.4 (q, $J_{C\text{-}F}$ = 271.0 Hz), 120.8, 104.3, 79.0, 70.1, 52.2, 41.2, 41.0, 25.9, 25.3, 23.3, 22.9, 18.3,

17.9, 12.0, -2.5, -2.6. **HRMS** (ESI) calculated for $C_{24}H_{35}F_3NaO_2SSi^+$ $[M+Na]^+$: 495.1971, found: 495.1970. $[\alpha]_D^{20}$ = -165 (c = 0.05, $CHCl_3$).

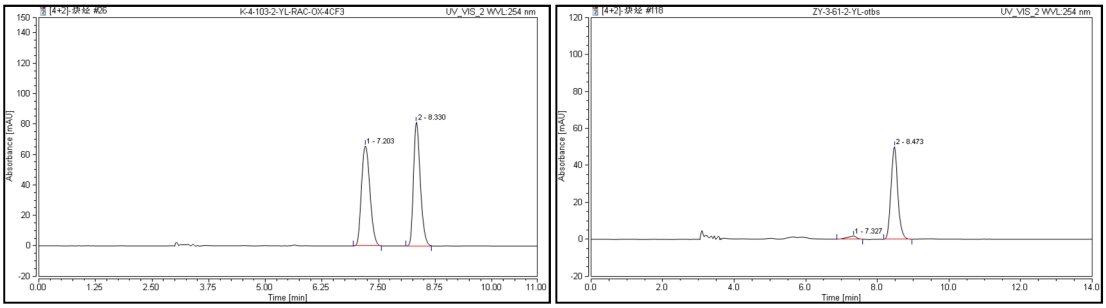
HPLC conditions: Daicel Chiralpak IC column (99:1 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 12.9 min, t_R (minor) = 14.9 min, 97% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.797	20.063	50.61	1	12.907	38.642	98.33
2	14.773	19.580	49.39	2	14.923	0.657	1.67

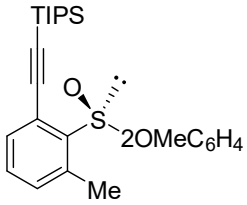
Recovered sulfoxide (*R*)-**4d** was isolated in 46% yield (21.2 mg, in 0.2 mmol scale) as light yellow liquid. Eluent: PE/EA = 3/1, R_f = 0.4.

HPLC conditions: Daicel Chiralpak OX-H column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 8.5 min, t_R (minor) = 7.3 min, 91% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.203	14.198	50.15	1	7.327	0.512	4.45
2	8.330	14.112	49.85	2	8.473	10.985	95.55

(*R*)-Triisopropyl((2-((2-methoxyphenyl)sulfinyl)-3-methylphenyl)ethynyl)silane (**7aa**)

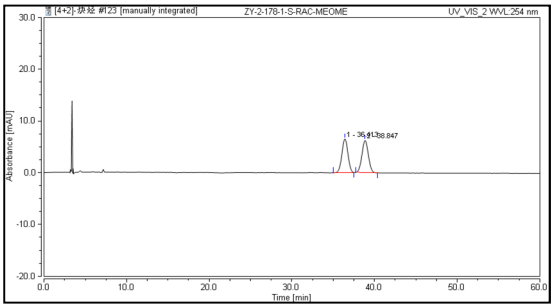


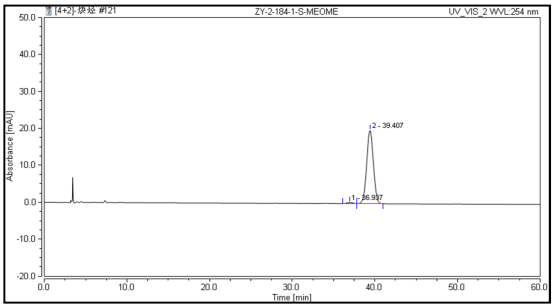
(*R*)-**7aa**

Product (*R*)-**7aa** was isolated in 47% yield (20.0 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (dd, J = 7.8, 1.7 Hz, 1H), 7.43 – 7.37 (m, 2H), 7.24 – 7.21 (m, 1H), 7.17 – 7.13 (m, 1H), 7.03 (d, J = 7.6 Hz, 1H), 6.81 (d, J = 8.1 Hz, 1H), 3.62 (s, 3H),

2.34 (s, 3H), 1.16 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.7, 141.6, 140.2, 132.8, 131.8, 131.7, 130.7, 130.6, 127.4, 125.8, 120.5, 111.0, 103.7, 97.9, 55.4, 18.8, 18.8, 18.0, 11.6. **HRMS** (ESI) calculated for $C_{25}H_{34}NaO_2SSi^+$ $[M+Na]^+$: 449.1941, found: 449.1938. $[\alpha]_D^{20}$ = -118 (c = 0.05, $CHCl_3$).

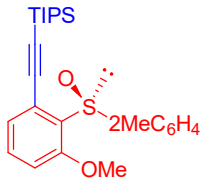
HPLC conditions: Daicel Chiralpak IE column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 39.4 min, t_R (minor) = 36.9 min, 97% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	36.413	5.576	50.07	1	36.937	0.279	1.47
2	38.847	5.560	49.93	2	39.407	18.686	98.53

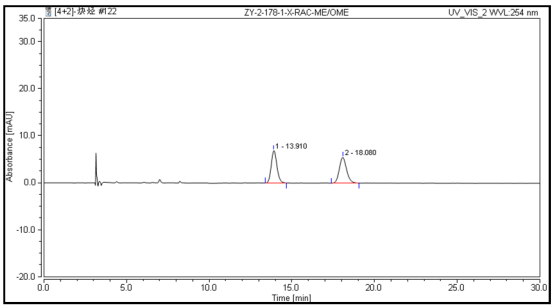
(*S*)-Triisopropyl((3-methoxy-2-(o-tolylsulfinyl)phenyl)ethynyl)silane (**8aa**)

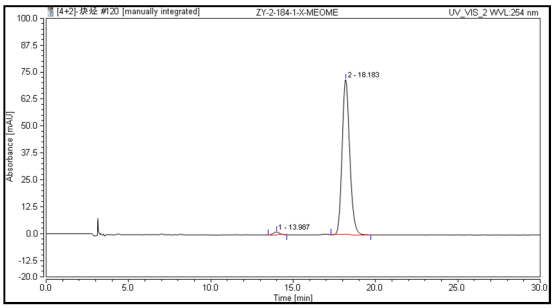


(*S*)-**8aa**

Product (*S*)-**8aa** was isolated in 47% yield (19.9 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (dd, J = 8.0, 1.3 Hz, 1H), 7.43 – 7.41 (m, 1H), 7.35 – 7.32 (m, 1H), 7.32 – 7.29 (m, 1H), 7.17 (dd, J = 7.7, 1.1 Hz, 1H), 7.08 (d, J = 7.4 Hz, 1H), 6.80 (d, J = 8.3 Hz, 1H), 3.54 (s, 3H), 2.17 (s, 3H), 1.20 – 1.14 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 141.8, 134.7, 133.1, 131.1, 130.3, 129.6, 127.0, 126.6, 126.1, 125.4, 113.5, 102.8, 99.4, 55.7, 19.0, 18.9, 11.5. **HRMS** (ESI) calculated for $C_{25}H_{34}NaO_2SSi^+$ $[M+Na]^+$: 449.1941, found: 449.1940. $[\alpha]_D^{20}$ = -128 (c = 0.05, $CHCl_3$).

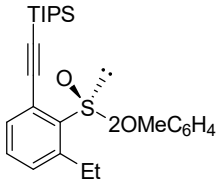
HPLC conditions: Daicel Chiralpak IC column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 18.2 min, t_R (minor) = 14.0 min, 97% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	13.910	2.732	49.37	1	13.987	0.573	1.46
2	18.080	2.803	50.63	2	18.183	38.688	98.54

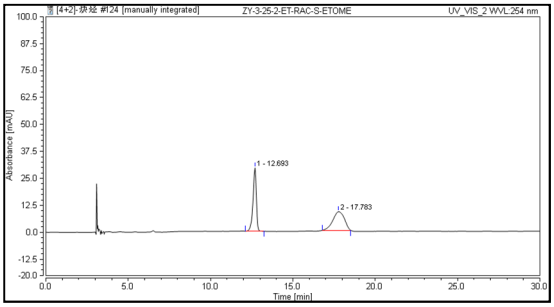
(*R*)-((3-Ethyl-2-((2-methoxyphenyl)sulfinyl)phenyl)ethynyl)triisopropylsilane (**7ba**)

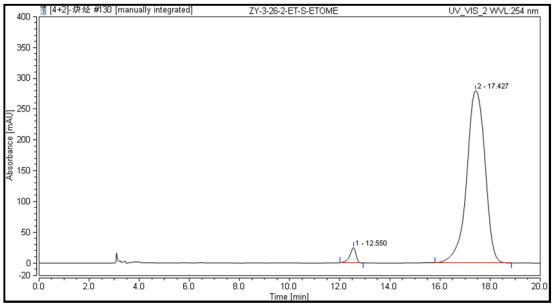


(*R*)-**7ba**

Product (*R*)-**7ba** was isolated in 47% yield (20.6 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.98 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.42 – 7.36 (m, 2H), 7.30 – 7.27 (m, 1H), 7.18 – 7.13 (m, 2H), 6.80 (d, *J* = 8.3 Hz, 1H), 3.61 (s, 3H), 2.93 – 2.82 (m, 2H), 1.16 – 1.10 (m, 21H), 0.79 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) *δ* 155.8, 146.4, 141.7, 131.82, 131.80, 131.6, 131.1, 130.8, 126.8, 125.8, 120.9, 111.0, 103.8, 98.0, 55.4, 23.4, 18.8, 15.1, 11.6. **HRMS** (ESI) calculated for $C_{26}H_{36}NaO_2SSi^+$ $[M+Na]^+$: 463.2097, found: 463.2097. $[\alpha]_D^{20}$ = -76 (c = 0.05, $CHCl_3$).

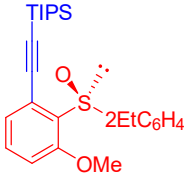
HPLC conditions: Daicel Chiralpak OX-H column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 17.4 min, t_R (minor) = 12.6 min, 94% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.693	6.917	49.77	1	12.550	6.962	2.87
2	17.783	6.981	50.23	2	17.427	235.318	97.13

(*S*)-((2-((2-Ethylphenyl)sulfinyl)-3-methoxyphenyl)ethynyl)triisopropylsilane (**8ba**)

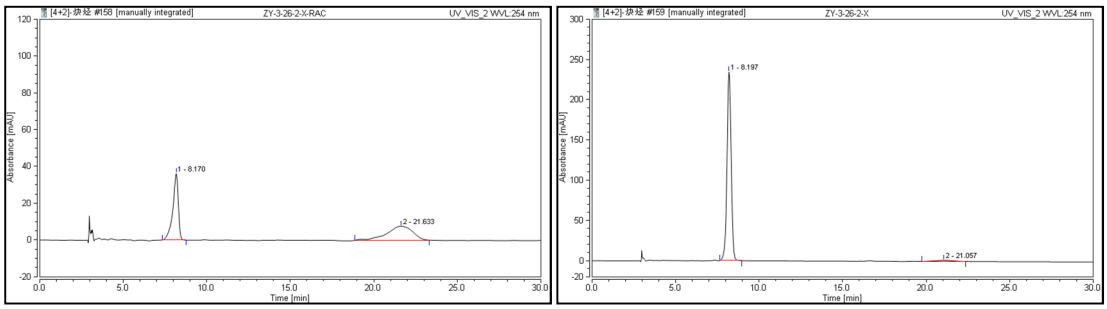


(*S*)-**8ba**

Product (*S*)-**8ba** was isolated in 42% yield (18.6 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 3/1, R_f = 0.3.

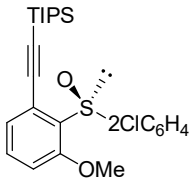
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (dd, J = 7.9, 1.4 Hz, 1H), 7.44 – 7.41 (m, 1H), 7.37 – 7.35 (m, 1H), 7.34 – 7.32 (m, 1H), 7.19 – 7.16 (m, 2H), 6.79 (dd, J = 8.4, 1.1 Hz, 1H), 3.53 (s, 3H), 2.72 – 2.65 (m, 1H), 2.53 – 2.47 (m, 1H), 1.20 – 1.14 (m, 21H), 0.84 (t, J = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 141.1, 140.7, 133.1, 132.0, 129.9, 128.3, 126.6, 126.6, 126.3, 125.3, 113.4, 102.7, 99.4, 55.7, 24.7, 18.8, 14.2. **HRMS** (ESI) calculated for $C_{26}H_{36}NaO_2SSi^+$ $[M+Na]^+$: 463.2097, found: 463.2096. $[\alpha]_D^{20}$ = -89 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IA column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 8.2 min, t_R (minor) = 21.1 min, 94% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	8.170	13.758	50.38	1	8.197	67.766	97.19
2	21.633	13.552	49.62	2	21.057	1.961	2.81

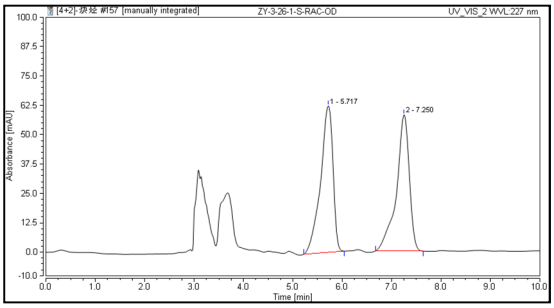
(*R*)-((2-((2-Chlorophenyl)sulfinyl)-3-methoxyphenyl)ethynyl)triisopropylsilane (**7ca**)

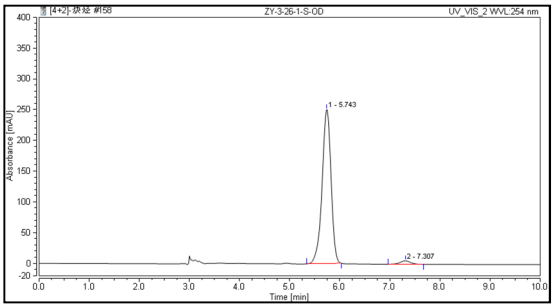


(*R*)-**7ca**

Product (*R*)-**7ca** was isolated in 31% yield (14.0 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.08 (dd, J = 7.8, 1.7 Hz, 1H), 7.47 (dd, J = 6.4, 2.6 Hz, 1H), 7.43 – 7.40 (m, 1H), 7.28 – 7.24 (m, 2H), 7.19 – 7.16 (m, 1H), 6.83 – 6.79 (m, 1H), 3.64 (s, 3H), 1.16 – 1.13 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.4, 141.3, 135.5, 132.9, 132.0, 131.9, 131.5, 129.7, 128.6, 127.5, 120.5, 110.7, 102.3, 100.3, 55.4, 18.8, 11.6. **HRMS** (ESI) calculated for $C_{24}H_{31}ClNaO_2SSi^+$ $[M+Na]^+$: 469.1395, found: 469.1389. $[\alpha]_D^{20}$ = -115 (c = 0.05, $CHCl_3$).

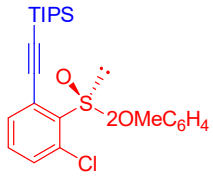
HPLC conditions: Daicel Chiralpak OD column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 5.7 min, t_R (minor) = 7.3 min, 95% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	5.717	18.167	50.85	1	5.743	51.905	97.51
2	7.250	17.561	49.15	2	7.307	1.328	2.49

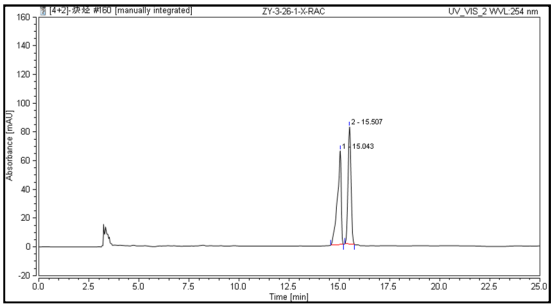
(*S*)-((3-Chloro-2-((2-methoxyphenyl)sulfinyl)phenyl)ethynyl)triisopropylsilane (**8ca**)

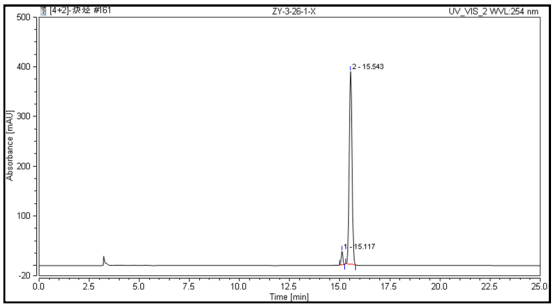


(*S*)-**8ca**

Product (*S*)-**8ca** was isolated in 30% yield (13.4 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (dd, J = 8.0, 1.6 Hz, 1H), 7.52 – 7.49 (m, 1H), 7.37 – 7.34 (m, 2H), 7.28 – 7.25 (m, 1H), 7.18 (dd, J = 7.7, 1.1 Hz, 1H), 6.80 (d, J = 8.3 Hz, 1H), 3.53 (s, 3H), 1.18 – 1.14 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.9, 141.7, 133.3, 131.0, 130.9, 130.5, 129.5, 128.92, 128.9, 127.9, 126.1, 113.2, 102.7, 99.3, 55.7, 18.9, 11.6. **HRMS** (ESI) calculated for $C_{24}H_{31}ClNaO_2SSi^+$ $[M+Na]^+$: 469.1395, found: 469.1400. $[\alpha]_D^{20}$ = -115 (c = 0.05, $CHCl_3$).

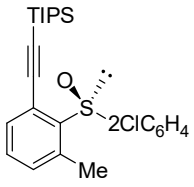
HPLC conditions: Daicel Chiralpak IC column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 15.5 min, t_R (minor) = 15.1 min, 92% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	15.043	14.323	50.24	1	15.117	2.580	3.96
2	15.507	14.186	49.76	2	15.543	62.484	96.04

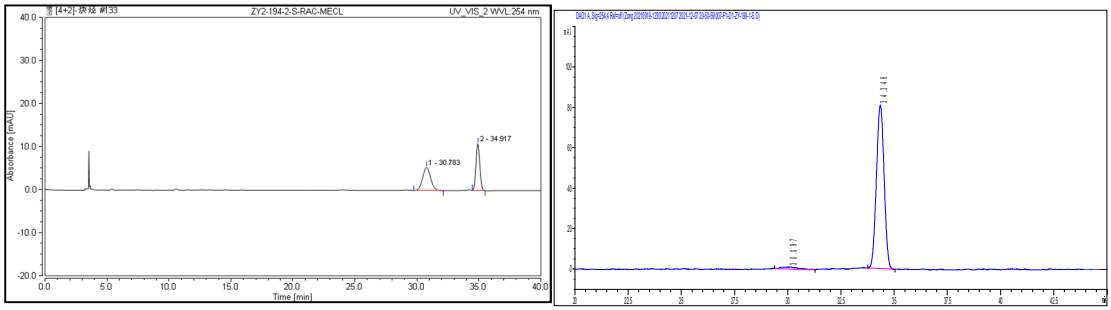
(*R*)-((2-((2-Chlorophenyl)sulfinyl)-3-methylphenyl)ethynyl)triisopropylsilane (**7da**)



(*R*)-**7da**

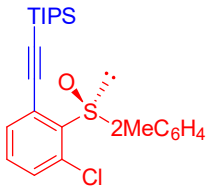
Product (*R*)-**7da** was isolated in 33% yield (14.2 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (dd, J = 7.9, 1.4 Hz, 1H), 7.52 (dd, J = 7.6, 1.5 Hz, 1H), 7.44 – 7.41 (m, 1H), 7.38 – 7.35 (m, 1H), 7.34 – 7.31 (m, 1H), 7.29 – 7.27 (m, 1H), 7.14 (d, J = 7.4 Hz, 1H), 2.20 (s, 3H), 1.19 – 1.11 (m, 21H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.2, 139.8, 136.1, 135.2, 133.1, 132.6, 132.2, 130.9, 130.5, 128.0, 127.8, 125.8, 102.1, 101.9, 19.3, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{24}H_{31}ClNaOSSi^+$ $[M+Na]^+$: 453.1446, found: 453.1443. $[\alpha]_D^{20}$ = -86 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (98:2 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 34.3 min, t_R (minor) = 30.1 min, 95% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	30.783	3.980	50.53	1	30.097	51.9	2.48
2	34.917	3.896	49.47	2	34.346	2037.5	97.52

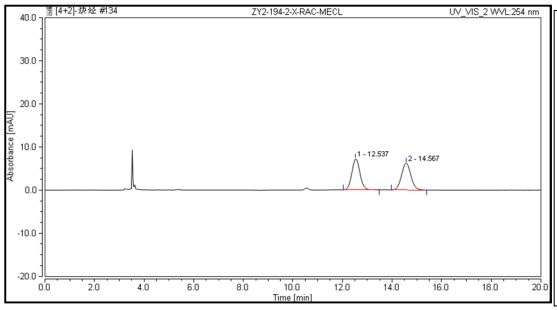
(*S*)-((3-chloro-2-(o-tolylsulfinyl)phenyl)ethynyl)triisopropylsilane (**8da**)

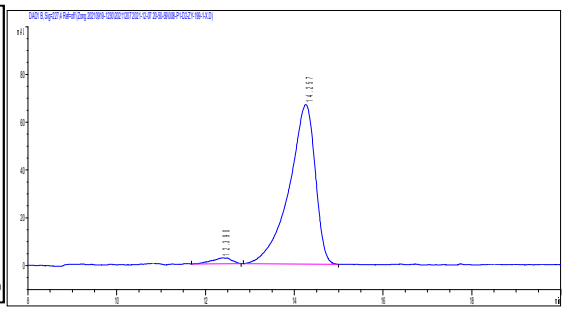


(*S*)-**8da**

Product (*S*)-**8da** was isolated in 38% yield (16.2 mg, in 0.1 mmol scale) light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (d, J = 7.9 Hz, 1H), 7.52 – 7.49 (m, 1H), 7.44 (d, J = 7.7 Hz, 1H), 7.41 – 7.38 (m, 1H), 7.32 (d, J = 7.9 Hz, 1H), 7.30 – 7.28 (m, 1H), 7.07 (d, J = 7.6 Hz, 1H), 2.26 (s, 3H), 1.20 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.9, 140.5, 140.0, 133.1, 132.1, 131.6, 131.5, 131.4, 130.3, 128.8, 127.3, 126.6, 103.3, 99.5, 18.9, 18.4, 11.5. **HRMS** (ESI) calculated for $C_{24}H_{31}ClNaOSSi^+$ $[M+Na]^+$: 453.1446, found: 453.1443. $[\alpha]_D^{20}$ = -105 (c = 0.05, $CHCl_3$).

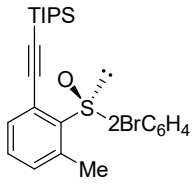
HPLC conditions: Daicel Chiralpak IC column (98:2 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 14.3 min, t_R (minor) = 12.4 min, 95% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.537	2.736	50.29	1	12.390	74.9	2.68
2	14.567	2.705	49.71	2	14.257	2725.1	97.32

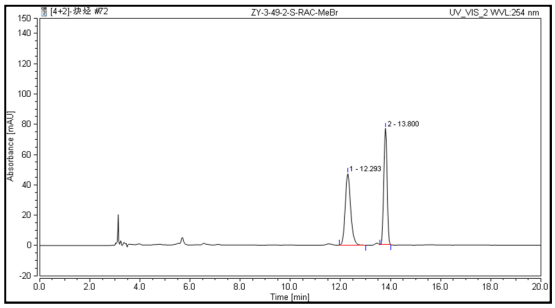
(*R*)-((2-((2-bromophenyl)sulfinyl)-3-methylphenyl)ethynyl)triisopropylsilane (**7ea**)

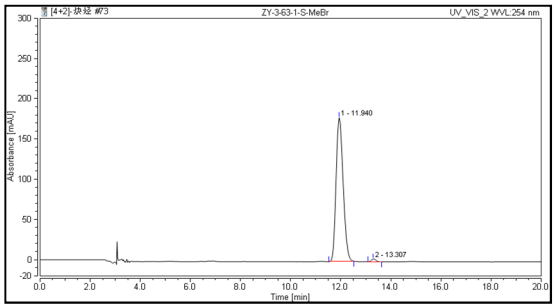


(*R*)-**7ea**

Product (*R*)-**7ea** was isolated in 43% yield (20.5 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.56 – 7.54 (m, 1H), 7.52 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.44 (d, *J* = 7.1 Hz, 1H), 7.34 – 7.31 (m, 1H), 7.30 – 7.28 (m, 1H), 7.07 (d, *J* = 7.6 Hz, 1H), 2.23 (s, 3H), 1.17 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) *δ* 142.8, 140.4, 140.2, 133.6, 133.2, 132.2, 131.8, 131.6, 129.5, 127.9, 127.1, 120.0, 103.5, 99.7, 18.9, 18.7, 11.6. **HRMS** (ESI) calculated for $C_{24}H_{31}BrNaOSSi^+$ $[M+Na]^+$: 497.0940, found: 497.0940. $[\alpha]_D^{20}$ = -127 (c = 0.05, $CHCl_3$).

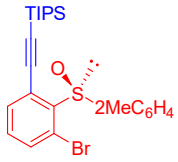
HPLC conditions: Daicel Chiralpak OX-H column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 11.9 min, t_R (minor) = 13.3 min, 98% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	12.293	11.828	50.22	1	11.940	58.430	98.78
2	13.800	11.724	49.78	2	13.307	0.722	1.22

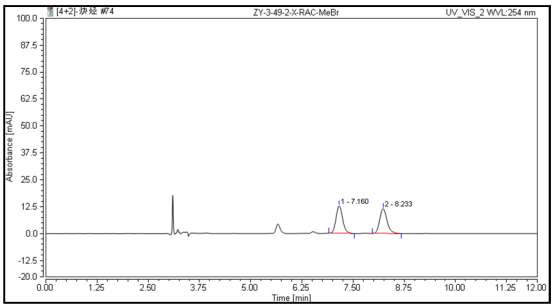
(*S*)-((3-bromo-2-(o-tolylsulfinyl)phenyl)ethynyl)triisopropylsilane (**8ea**)

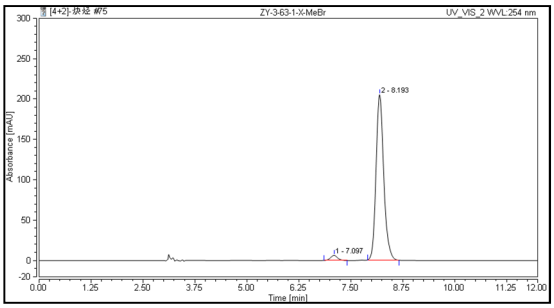


(*S*)-**8ea**

Product (*S*)-**8ea** was isolated in 45% yield (21.4 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.20 (dd, J = 7.7, 1.6 Hz, 1H), 7.56 (dd, J = 7.8, 1.3 Hz, 1H), 7.51 (dd, J = 8.0, 1.3 Hz, 1H), 7.40 – 7.34 (m, 2H), 7.24 – 7.22 (m, 1H), 7.14 (d, J = 7.2 Hz, 1H), 2.21 (s, 3H), 1.16 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 142.8, 140.4, 140.2, 133.6, 133.2, 132.2, 131.8, 131.6, 129.5, 128.0, 127.1, 120.0, 103.5, 99.7, 18.9, 18.7, 11.6. **HRMS** (ESI) calculated for $C_{24}H_{31}BrNaOSSi^+$ $[M+Na]^+$: 497.0940, found: 497.0939. $[\alpha]_D^{20}$ = -84 (c = 0.05, $CHCl_3$).

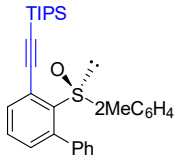
HPLC conditions: Daicel Chiralpak OX-H column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 8.2 min, t_R (minor) = 7.1 min, 94% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.160	2.364	49.68	1	7.097	1.211	2.95
2	8.233	2.395	50.32	2	8.193	43.955	97.05

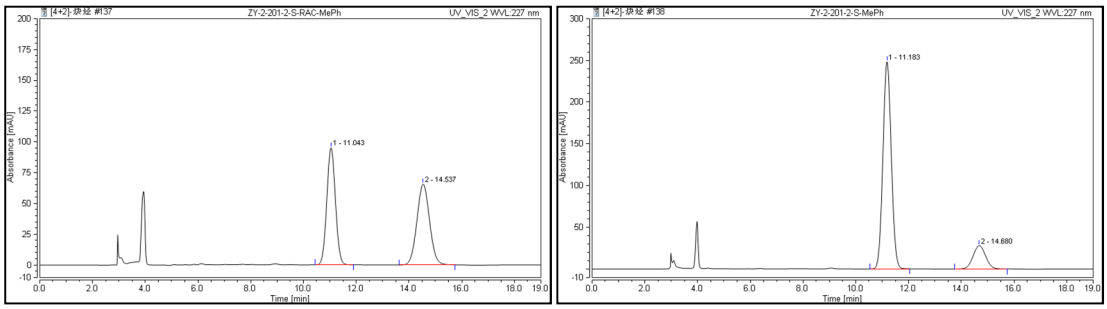
(*R*)-Triisopropyl((2-(o-tolylsulfinyl)-[1,1'-biphenyl]-3-yl)ethynyl)silane (**7fa**)



(*R*)-**7fa**

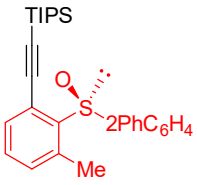
Product (*R*)-**7fa** was isolated in 55% yield (26.2 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.62 (d, J = 7.7 Hz, 1H), 7.42 (t, J = 7.7 Hz, 1H), 7.24 – 7.21 (m, 1H), 7.20 – 6.84 (m, 8H), 6.82 – 6.80 (m, 1H), 1.87 (s, 3H), 1.20 – 1.15 (m, 21H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.7, 141.7, 141.7, 140.6, 137.9, 133.6, 133.5, 133.1, 131.1, 129.9, 129.1, 127.6, 127.3, 127.2, 125.6, 125.6, 103.1, 100.4, 18.9, 18.85, 18.7, 11.5. **HRMS** (ESI) calculated for $C_{30}H_{36}NaOSSi^+$ $[M+Na]^+$: 495.2148, found: 495.2146. $[\alpha]_D^{20}$ = -78 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IG column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 11.2 min, t_R (minor) = 14.7 min, 71% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.043	35.735	49.78	1	11.183	90.509	85.55
2	14.537	36.055	50.22	2	14.680	15.282	14.45

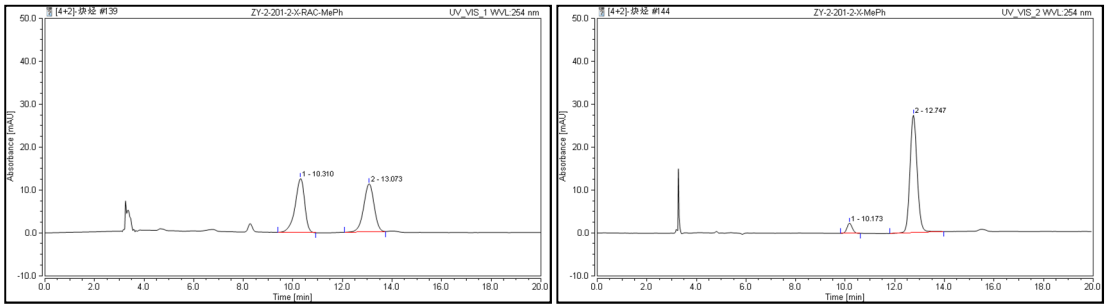
(*S*)-((2-([1,1'-biphenyl]-2-ylsulfinyl)-3-methylphenyl)ethynyl)triisopropylsilane (**8fa**)



(*S*)-**8fa**

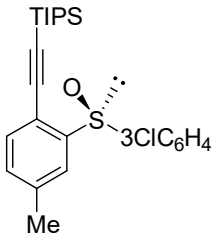
Product (*S*)-**8fa** was isolated in 32% yield (15.3 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.60 (m, 1H), 7.51 – 7.48 (m, 1H), 7.18 – 7.14 (m, 2H), 7.11 – 7.09 (m, 2H), 7.03 – 7.00 (m, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 7.4 Hz, 2H), 6.86 (d, *J* = 7.4 Hz, 1H), 1.87 (s, 3H), 1.20 – 1.14 (m, 21H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.4, 141.2, 140.3, 139.7, 138.9, 132.3, 132.0, 130.8, 130.0, 128.7, 128.1, 127.7, 127.6, 127.4, 127.0, 126.6, 103.7, 98.6, 18.9, 18.5, 11.6. **HRMS** (ESI) calculated for $C_{30}H_{36}NaOSSi^+$ $[M+Na]^+$: 495.2148, found: 495.2144. $[\alpha]_D^{20}$ = -84 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 13.2 min, t_R (minor) = 10.4 min, 89% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.310	5.614	50.89	1	10.173	0.538	5.72
2	13.073	5.418	49.11	2	12.747	8.872	94.28

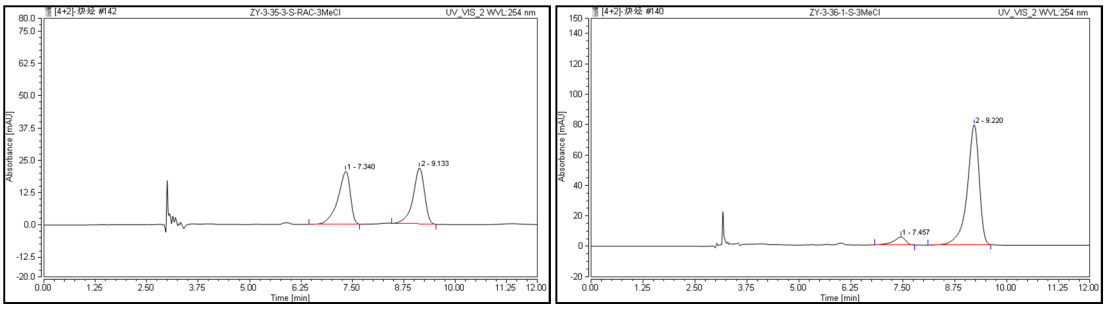
(*R*)-((2-((3-chlorophenyl)sulfinyl)-4-methylphenyl)ethynyl)triisopropylsilane (**7ga**)



(*R*)-**7ga**

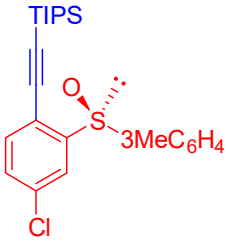
Product (*R*)-**7ga** was isolated in 29% yield (12.6 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, J = 2.2 Hz, 1H), 7.60 – 7.58 (m, 2H), 7.42 (d, J = 8.2 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.23 (d, J = 7.6 Hz, 1H), 2.36 (s, 3H), 1.18 – 1.12 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.5, 145.2, 139.7, 136.3, 135.0, 132.3, 130.9, 129.3, 125.2, 124.1, 122.1, 119.4, 109.3, 101.5, 21.6, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{24}H_{31}ClNaOSSi^+$ $[M+Na]^+$: 453.1446, found: 453.1444. $[\alpha]_D^{20}$ = -114 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IG column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 9.2 min, t_R (minor) = 7.5 min, 87% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.340	7.138	50.52	1	7.457	1.769	6.34
2	9.133	6.990	49.48	2	9.220	26.148	93.66

(*S*)-((4-chloro-2-(m-tolylsulfinyl)phenyl)ethynyl)triisopropylsilane (**8ga**)

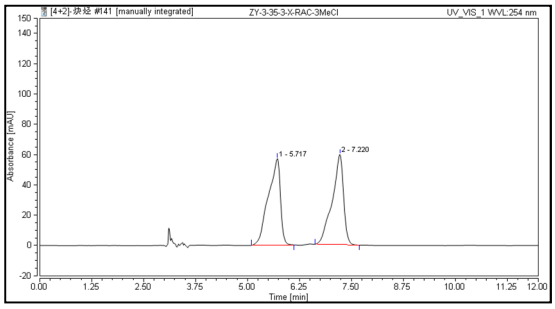


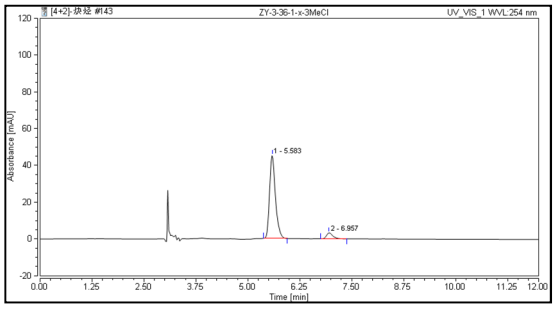
(*S*)-**8ga**

Product (*S*)-**8ga** was isolated in 28% yield (11.9 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 – 7.80 (d, J = 1.9 Hz, 1H), 7.73 – 7.69 (m, 2H), 7.42 (d, J = 7.8 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.20 (dd, J = 7.8, 1.7 Hz, 1H), 2.40 (s, 3H), 1.17 – 1.12 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.1, 146.6, 140.8, 135.5, 133.9, 131.9, 131.1, 130.5,

124.8, 123.9, 122.8, 118.1, 102.5, 99.8, 21.8, 18.82, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{24}H_{31}ClNaOSSi^+$ $[M+Na]^+$: 453.1446, found: 453.1442. $[\alpha]_D^{20}$ = -105 (c = 0.05, $CHCl_3$).

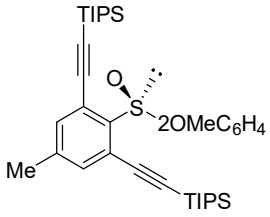
HPLC conditions: Daicel Chiralpak OX-H column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 5.7 min, t_R (minor) = 7.0 min, 86% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	5.717	19.213	50.53	1	5.583	7.372	92.76
2	7.220	18.811	49.47	2	6.957	0.576	7.24

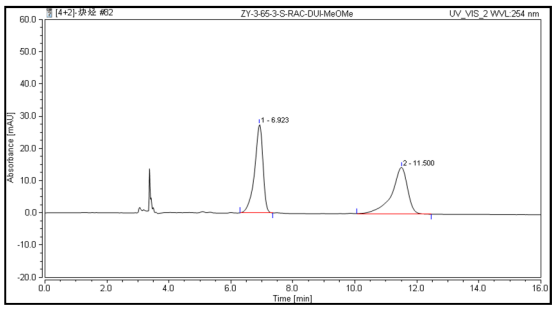
(*R*)-((2-((2-methoxyphenyl)sulfinyl)-5-methyl-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) (**7ha**)

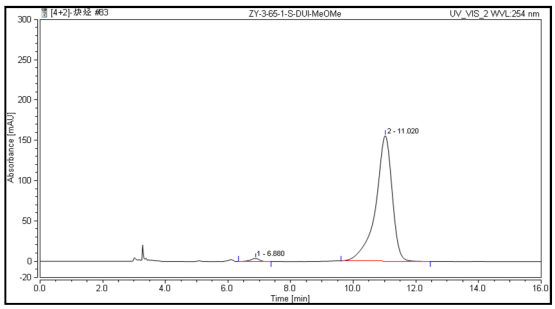


(*R*)-**7ha**

Product (*R*)-**7ha** was isolated in 23% yield (14.0 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (dd, J = 7.7, 1.7 Hz, 1H), 7.36 – 7.33 (m, 1H), 7.25 (s, 2H), 7.10 – 7.07 (m, 1H), 6.76 (d, J = 8.0 Hz, 1H), 3.63 (s, 3H), 2.28 (s, 3H), 1.17 – 1.09 (m, 42H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.3, 141.6, 140.5, 135.7, 131.3, 130.6, 128.4, 124.3, 120.2, 110.3, 102.4, 99.4, 55.1, 20.8, 18.7, 18.7, 11.4. **HRMS** (ESI) calculated for $C_{36}H_{54}NaO_2SSi^+$ $[M+Na]^+$: 629.3275, found: 629.3274. $[\alpha]_D^{20}$ = -154 (c = 0.05, $CHCl_3$).

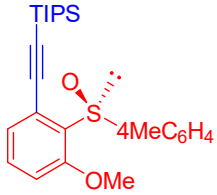
HPLC conditions: Daicel Chiralpak IC column (97:3 hexane: 2-propanol, 1.0 mL/min, 40 ºC, 254 nm); t_R (major) = 11.0 min, t_R (minor) = 6.9 min, 97% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	6.923	8.548	49.95	1	6.880	1.210	1.27
2	11.500	8.566	50.05	2	11.020	94.356	98.73

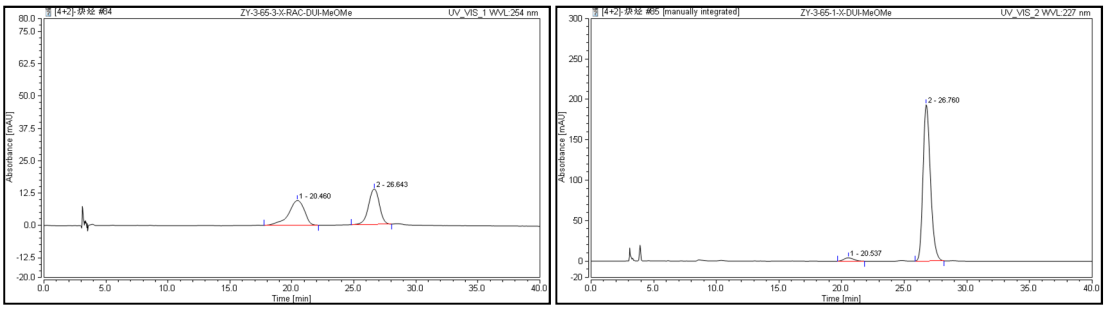
(*S*)-triisopropyl((3-methoxy-2-(p-tolylsulfinyl)phenyl)ethynyl)silane (**8ha**)



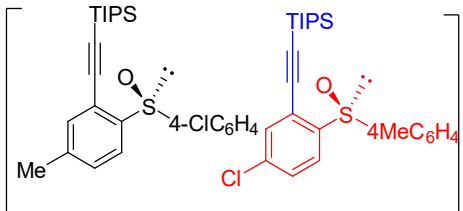
(*S*)-**8ha**

Product (*S*)-**8ha** was isolated in 48% yield (20.5 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, J = 8.2 Hz, 2H), 7.33 – 7.30 (m, 1H), 7.22 (d, J = 8.0 Hz, 2H), 7.15 (dd, J = 7.7, 1.1 Hz, 1H), 6.82 (dd, J = 8.4, 1.1 Hz, 1H), 3.67 (s, 3H), 2.37 (s, 3H), 1.19 – 1.11 (m, 21H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.0, 141.4, 139.9, 134.0, 132.7, 129.2, 126.2, 125.6, 124.4, 113.3, 102.7, 99.8, 56.1, 21.5, 18.8, 11.5. **HRMS** (ESI) calculated for $C_{25}H_{34}NaO_2SSi^+$ $[M+Na]^+$: 449.1941, found: 449.1944. $[\alpha]_D^{20}$ = -115 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OX-H column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 26.8 min, t_R (minor) = 20.5 min, 95% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	20.460	14.122	50.48	1	20.537	3.685	2.68
2	26.643	13.854	49.52	2	26.760	133.588	97.32



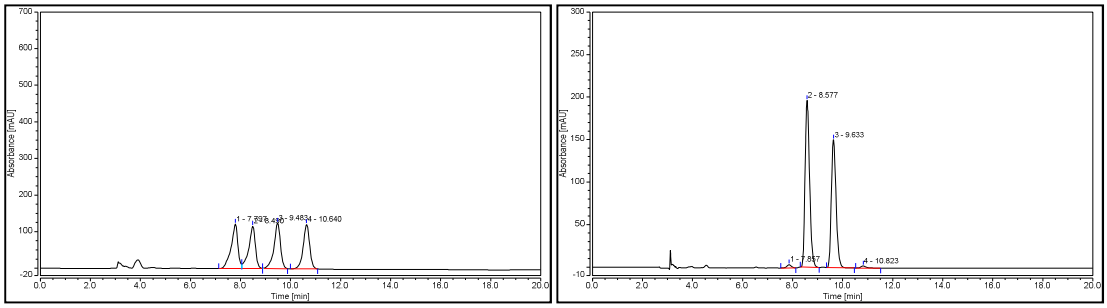
(*R*)-**7ia** + (*S*)-**8ia** = 1.3:1

Product (*R*)-**7ia** and (*S*)-**8ia** was isolated in 60% yield (25.9 mg, in 0.1 mmol scale) as light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 8.4 Hz, 1H), 7.78 (d, J = 8.0 Hz, 0.76H), 7.73 – 7.71 (m, 1.58H), 7.63 – 7.61 (m, 2H), 7.48 – 7.43 (m, 2H), 7.38 – 7.34 (m, 1.55H), 7.31 – 7.28 (d, J = 9.8 Hz, 1.58H), 7.20 (d, J = 8.1 Hz, 2H), 2.33 (s, 5.54H), 1.14 – 1.09 (m, 37.2H). ^{13}C NMR (151 MHz, $CDCl_3$)

δ 146.2, 144.8, 144.1, 142.3, 141.9, 141.4, 137.1, 136.7, 134.4, 133.4, 130.9, 130.1, 130.0, 129.5, 126.2, 125.3, 125.1, 123.7, 122.3, 120.8, 102.6, 102.1, 101.1, 100.1, 21.5, 21.2, 18.8, 18.7, 11.5, 11.4.

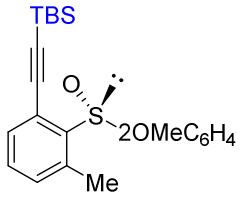
HRMS (ESI) calculated for $C_{24}H_{31}NaClOSSi^+$ $[M+Na]^+$: 453.1446, found: 453.1449.

HPLC conditions: Daicel Chiralpak OX-H column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 9.6 min, t_R (minor) = 7.9 min, 96% ee; t_R (major) = 8.6 min, t_R (minor) = 10.8 min, 97% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.797	38.441	25.92	1	7.857	0.787	1.04
2	8.490	36.057	24.31	2	8.577	41.305	54.79
3	9.483	37.737	25.44	3	9.633	32.692	43.36
4	10.640	36.092	24.33	4	10.823	0.605	0.80

(*R*)-*tert*-Butyl((2-((2-methoxyphenyl)sulfinyl)-3-methylphenyl)ethynyl)dimethylsilane (**7ab**)

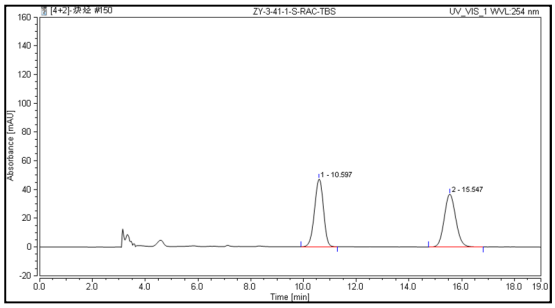


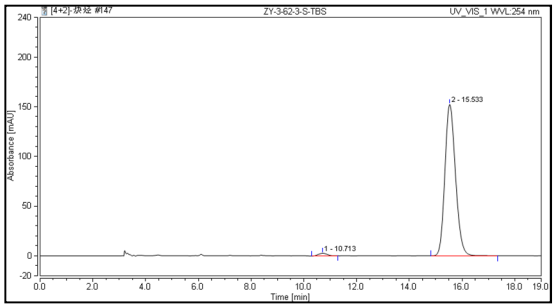
(*R*)-**7ab**

Product (*R*)-**7ab** was isolated in 48% yield (18.6 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (dd, J = 7.7, 1.7 Hz, 1H), 7.42 – 7.36 (m, 2H), 7.23 – 7.20 (m, 1H), 7.17 – 7.14 (m, 1H), 7.04 (d, J = 7.6 Hz, 1H), 6.81 (d, J = 8.1 Hz, 1H), 3.64 (s, 3H), 2.38 (s, 3H), 0.99 (s, 9H), 0.20 (s, 3H), 0.18 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 155.7, 141.7, 140.2, 132.8, 131.9, 131.7, 130.7, 130.6, 127.6, 125.4, 120.5, 111.1, 102.5, 99.8, 55.4, 26.3, 18.1, 17.0, -4.5.

HRMS (ESI) calculated for $C_{22}H_{28}NaO_2SSi^+$ $[M+Na]^+$: 407.1471 found: 407.1472. $[\alpha]_D^{20}$ = -106 (c = 0.05, $CHCl_3$).

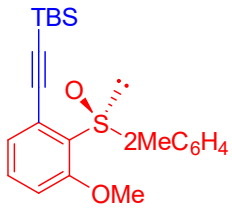
HPLC conditions: Daicel Chiralpak IC column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 15.5 min, t_R (minor) = 10.7 min, 97% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.597	18.534	49.98	1	10.713	1.066	1.48
2	15.547	18.546	50.02	2	15.533	70.913	98.52

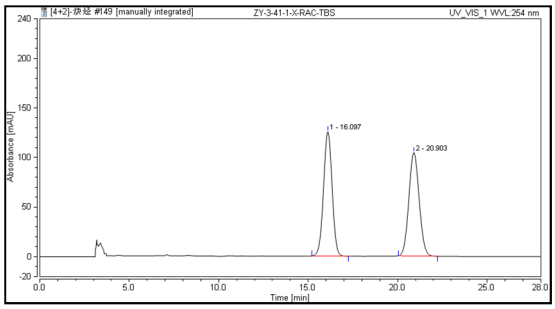
(*S*)-*tert*-Butyl((3-methoxy-2-(o-tolylsulfinyl)phenyl)ethynyl)dimethylsilane **(8ab)**

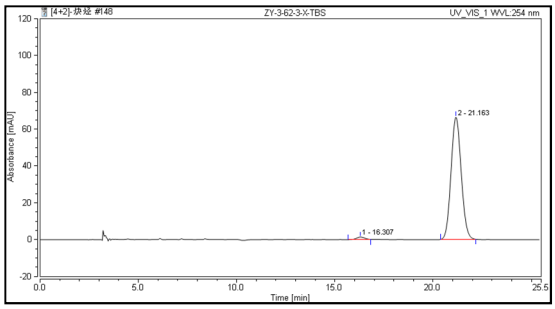


(*S*)-**8ab**

Product (*S*)-**8ab** was isolated in 48% yield (18.5 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.40 (m, 1H), 7.35 – 7.29 (m, 2H), 7.15 (d, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 8.3 Hz, 1H), 3.56 (s, 3H), 2.17 (s, 3H), 1.02 (s, 9H), 0.22 (s, 3H), 0.22 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.3, 141.8, 134.8, 133.1, 131.3, 130.3, 129.7, 126.7, 126.6, 126.0, 125.4, 113.6, 101.7, 101.1, 55.8, 26.3, 18.9, 17.0, -4.6. **HRMS** (ESI) calculated for $C_{22}H_{28}NaO_2SSi^+$ $[M+Na]^+$: 407.1471 found: 407.1467. $[\alpha]_D^{20}$ = -96 (c = 0.05, $CHCl_3$).

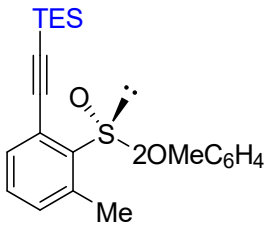
HPLC conditions: Daicel Chiralpak IC column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 21.2 min, t_R (minor) = 16.3 min, 97% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	16.097	69.880	50.13	1	16.307	0.628	1.55
2	20.903	69.529	49.87	2	21.163	39.854	98.45

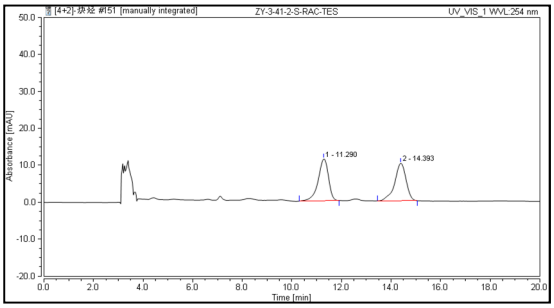
(*R*)-Triethyl((2-((2-methoxyphenyl)sulfinyl)-3-methylphenyl)ethynyl)silane (**7ac**)

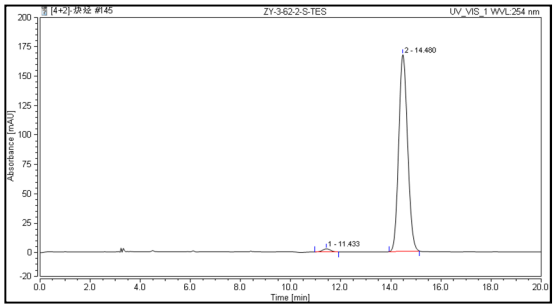


(*R*)-**7ac**

Product (*R*)-**7ac** was isolated in 43% yield (16.5 mg, in 0.1 mmol scale) as light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.99 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.41 – 7.37 (m, 2H), 7.23 – 7.20 (m, 1H), 7.17 – 7.14 (m, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.81 (d, *J* = 8.2 Hz, 1H), 3.64 (s, 3H), 2.38 (s, 3H), 1.04 (t, *J* = 7.9 Hz, 9H), 0.69 (q, *J* = 7.9 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.7, 141.7, 140.2, 132.8, 132.0, 131.7, 130.7, 130.6, 127.5, 125.5, 120.5, 111.1, 103.0, 99.1, 55.4, 18.1, 7.6, 4.6. **HRMS** (ESI) calculated for $C_{22}H_{28}NaO_2SSi^+$ $[M+Na]^+$: 407.1471 found: 407.1468. $[\alpha]_D^{20}$ = -87 (c = 0.05, $CHCl_3$).

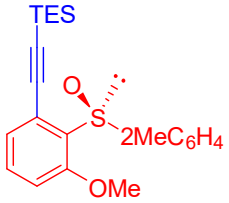
HPLC conditions: Daicel Chiralpak IC column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 14.5 min, t_R (minor) = 11.4 min, 97% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	11.290	5.436	50.17	1	11.433	0.973	1.39
2	14.393	5.400	49.83	2	14.480	68.782	98.61

(*S*)-Triethyl((3-methoxy-2-(o-tolylsulfinyl)phenyl)ethynyl)silane (**8ac**)

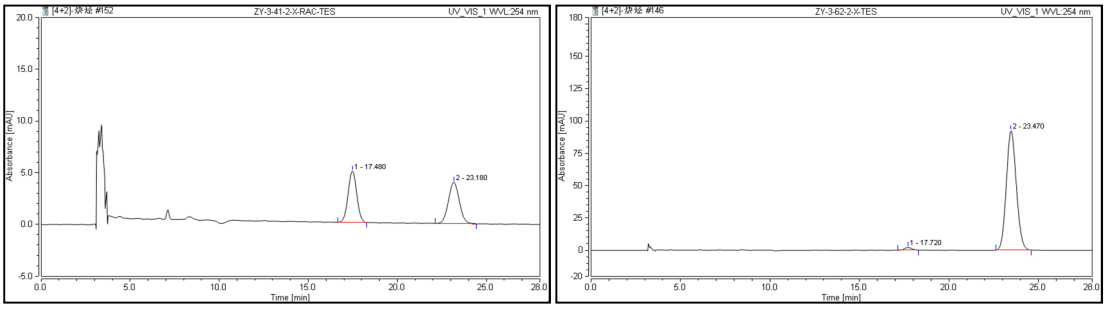


(*S*)-**8ac**

Product (*S*)-**8ac** was isolated in 45% yield (17.3 mg, in 0.1 mmol scale) as a light yellow oil. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.43 – 7.40 (m, 1H), 7.35 – 7.28 (m, 2H), 7.16 (d, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.80 (d, *J* = 8.3 Hz, 1H), 3.56 (s, 3H), 2.17 (s, 3H), 1.07 (t, *J* = 7.9 Hz, 9H), 0.72 (q, *J* = 7.9 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3,

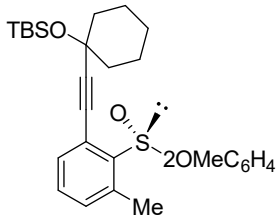
141.8, 134.8, 133.1, 131.2, 130.3, 129.7, 126.7, 126.7, 126.0, 125.4, 113.5, 102.1, 100.4, 55.8, 18.9, 7.7, 4.5. **HRMS** (ESI) calculated for $C_{22}H_{28}NaO_2SSi^+$ $[M+Na]^+$: 407.1471 found: 407.1467. $[\alpha]_D^{20}$ = -98 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IC column (90:10 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 23.5 min, t_R (minor) = 17.7 min, 97% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	17.480	2.818	50.57	1	17.720	0.980	1.62
2	23.180	2.755	49.43	2	23.470	59.658	98.38

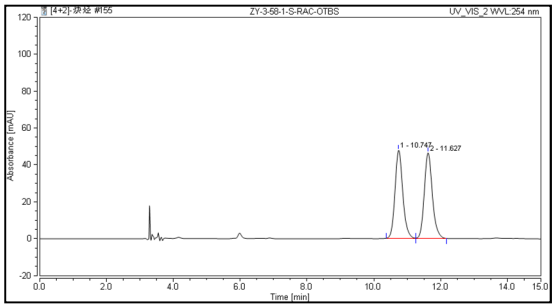
(*R*)-*tert*-Butyl((1-((2-((2-methoxyphenyl)sulfinyl)-3-methylphenyl)ethynyl)cyclohexyl)oxy)dimethylsilane (**7ad**)

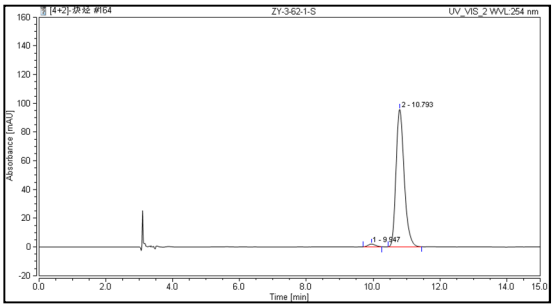


(*R*)-**7ad**

Product (*R*)-**7ad** was isolated in 42% yield (20.3 mg, in 0.1 mmol scale) as a light yellow oil. Eluent: PE/EA = 8/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (dd, J = 7.7, 1.7 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.33 (d, J = 7.7 Hz, 1H), 7.25 – 7.22 (m, 1H), 7.18 – 7.15 (m, 1H), 7.03 (d, J = 7.6 Hz, 1H), 6.82 (d, J = 8.1 Hz, 1H), 3.61 (s, 3H), 2.33 (s, 3H), 1.97 – 1.92 (m, 2H), 1.71 – 1.59 (m, 7H), 1.47 – 1.42 (m, 1H), 0.91 (s, 9H), 0.24 (s, 3H), 0.22 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.73, 141.56, 140.32, 132.54, 131.72, 130.77, 130.74, 130.56, 127.45, 125.74, 120.63, 111.19, 82.28, 70.19, 55.41, 41.47, 41.24, 26.00, 25.54, 22.96, 22.93, 18.30, 18.04, -2.61, -2.63. **HRMS** (ESI) calculated for $C_{28}H_{38}NaO_3SSi^+$ $[M+Na]^+$: 505.2203, found: 505.2200. $[\alpha]_D^{20}$ = -134 (c = 0.05, $CHCl_3$).

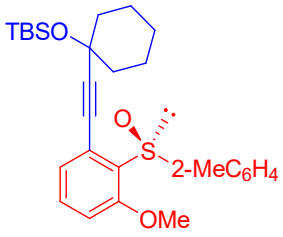
HPLC conditions: Daicel Chiralpak OX-H column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 10.8 min, t_R (minor) = 10.0 min, 97% ee.





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.747	12.890	49.81	1	9.947	0.473	1.71
2	11.627	12.988	50.19	2	10.793	27.125	98.29

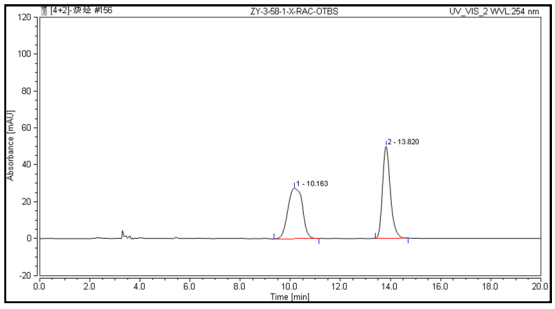
(*S*)-*tert*-Butyl((1-((3-methoxy-2-(o-tolylsulfinyl)phenyl)ethynyl)cyclohexyl)oxy)dimethylsilane (**8ad**)

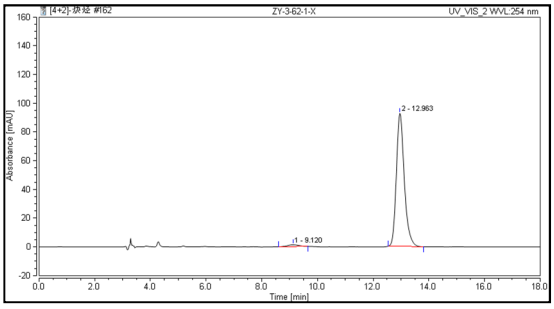


(*S*)-**8ad**

Product (*S*)-**8ad** was isolated in 43% yield (20.8 mg, in 0.1 mmol scale) as light yellow solid. Eluent: PE/EA = 3/1, R_f = 0.3. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.21 (dd, J = 8.0, 1.4 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.37 – 7.34 (m, 1H), 7.32 – 7.30 (m, 1H), 7.11 (dd, J = 7.7, 1.1 Hz, 1H), 7.09 (d, J = 7.5 Hz, 1H), 6.79 (dd, J = 8.4, 1.1 Hz, 1H), 3.54 (s, 3H), 2.15 (s, 3H), 1.97 – 1.94 (m, 2H), 1.74 – 1.68 (m, 4H), 1.66 – 1.62 (m, 3H), 1.51 – 1.44 (m, 1H), 0.92 (s, 9H), 0.25 (s, 3H), 0.23 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 141.8, 134.5, 133.3, 130.3, 129.7, 126.9, 126.6, 125.5, 125.0, 113.2, 101.4, 81.3, 70.1, 55.7, 41.2, 41.1, 26.0, 25.4, 23.0, 19.0, 18.3, -2.5, -2.6. **HRMS** (ESI) calculated for $C_{28}H_{38}NaO_3SSi^+$ $[M+Na]^+$: 505.2203, found: 505.2203. $[\alpha]_D^{20}$ = -107 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak OX-H column (95:5 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 13.0 min, t_R (minor) = 9.1 min, 96% ee.

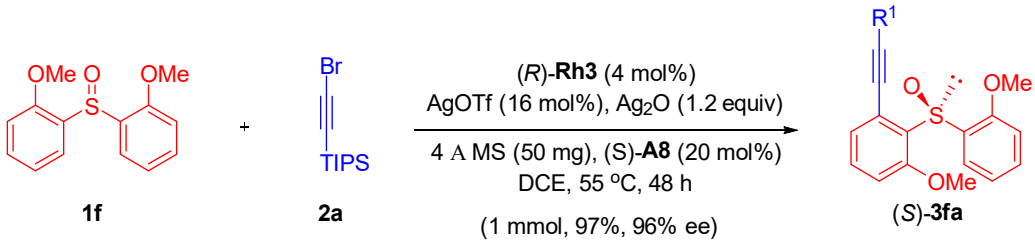




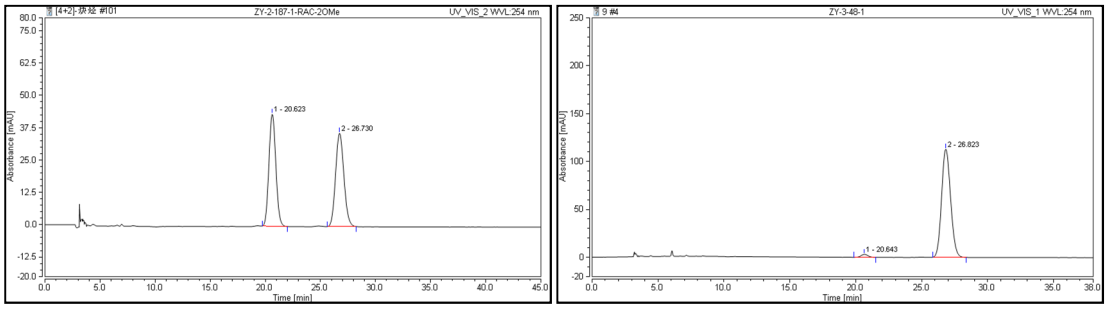
No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	10.163	18.474	50.53	1	9.120	0.572	1.84
2	13.820	18.085	49.47	2	12.963	30.587	98.16

5. Transformations and applications

5.1 Scale-up Synthesis of Product (*S*)-3fa

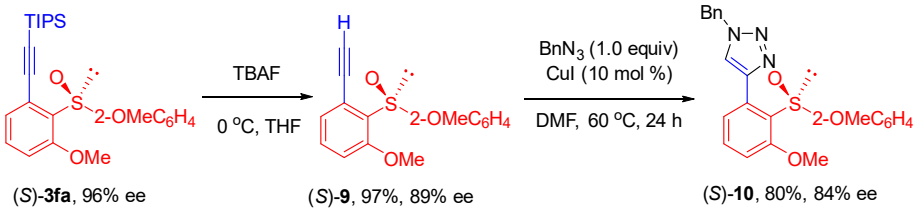


Sulfoxide **1f** (1.0 mmol, 262 mg), **2a** (1.2 mmol, 313 mg), (*R*)-**Rh3** (4 mol%, 80 mg), AgOTf (42 mg, 16 mol %), Ag_2O (232 mg, 1.2 equiv), (*S*)-**A8** (64.0 mg, 20 mol %), and 4Å MS (500 mg) were weighted in a pressure tube equipped with a stir bar. DCE (20 mL) were added and the mixture was stirred at 55 °C for 48 h under N_2 atmosphere. Afterwards, it was evaporated under reduced pressure, and the residue was purified by silica gel chromatography (petroleum ether:ethyl acetate = 8:1) to afford (*S*)-**3fa** (432.2 mg, 97% yield, 96% ee).



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	20.623	31.578	49.97	1	20.643	1.922	2.10
2	26.730	31.620	50.03	2	26.823	89.406	97.90

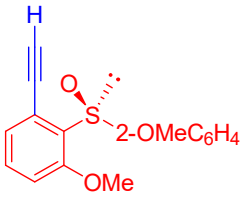
5.2 Derivatization of Product (*S*)-45



The compound (*S*)-**3fa** (88.6 mg, 0.2 mmol) was dissolved in THF and 1.0 M TBAF (0.3 mL, 1.5 equiv) was then added at 0 °C with constant stirring. The reaction progress was monitored by TLC. The mixture was diluted with water extracted with EtOAc, dried over anhydrous Na_2SO_4, filtered and evaporated in vacuo. The obtained crude product was purified by flash chromatography in petroleum ether: ethyl acetate= 2:1 to give (*S*)-**9** as white solid (55.5 mg, 97%, 89% ee).

Under nitrogen atm (*S*)-**9** (28.6 mg, 0.1 mmol), CuI (10 mol %) and benzyl azide (12.5 µl, 0.1 mmol) were dissolved in DMF (1 mL) and stirred at 60 °C (aluminum heat transfer block) for 16 h. After completion of the reaction saturated aq. NH_4Cl solution (5 mL) was added and the mixture was

extracted with dichloromethane (3 x 5 mL) and dried over anhydrous Na_2SO_4. After complete evaporation of the solvent, the obtained crude product was purified by column chromatography to afford (*S*)-**10** (33.5 mg, 80%, 84% ee).



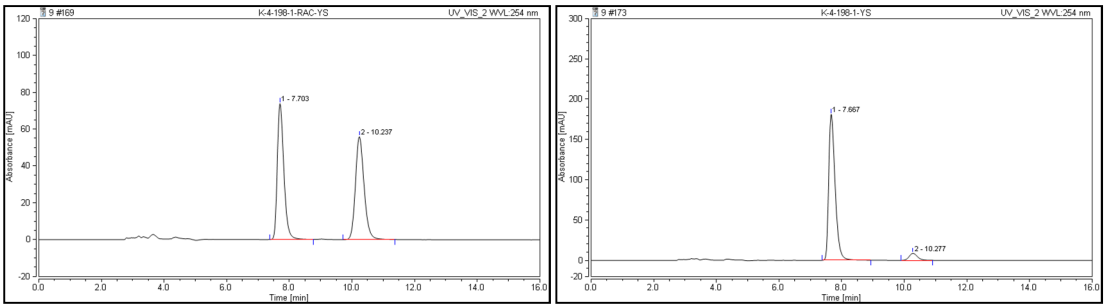
(*S*)-**9**

(*S*)-1-Ethynyl-3-methoxy-2-((2-methoxyphenyl)sulfinyl)benzene (**9**)

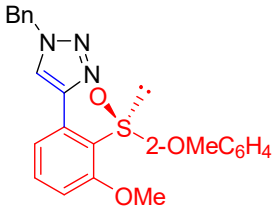
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (dd, J = 7.7, 1.8 Hz, 1H), 7.38 – 7.35 (m, 1H), 7.33 – 7.31 (m, 1H), 7.17 – 7.14 (m, 2H), 6.85 (d, J = 8.3 Hz, 1H), 6.79 (d, J = 8.1 Hz, 1H), 3.66 (s, 3H), 3.62 (s, 3H), 3.41 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.0, 155.3, 132.7, 132.5, 131.3, 130.9, 127.5, 126.1, 124.9, 120.3, 113.5, 110.7, 83.6, 80.0, 55.9, 55.6.

HRMS (ESI) calculated for $C_{16}H_{14}NaO_3S^+$ $[M+Na]^+$: 309.0556, found: 309.0553. $[\alpha]_D^{20}$ = -39 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IA column (80:20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 7.7 min, t_R (minor) = 10.3 min, 93% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	7.703	17.896	49.97	1	7.667	43.052	94.27
2	10.237	17.920	50.03	2	10.277	2.619	5.73



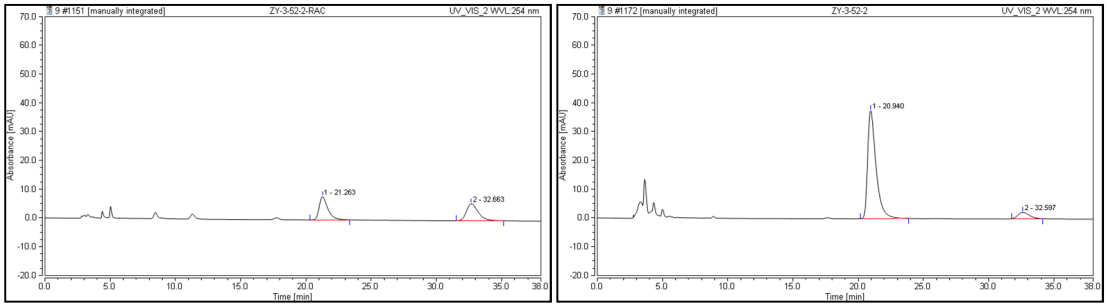
(*S*)-**10**

(*S*)-1-Benzyl-4-(3-methoxy-2-((2-methoxyphenyl)sulfinyl)phenyl)-1H-1,2,3-triazole (**10**)

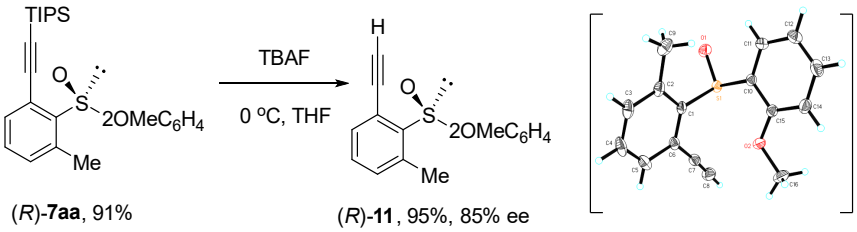
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.88 (dd, J = 7.8, 1.7 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.47 – 7.44 (m, 1H), 7.39 – 7.29 (m, 6H), 7.07 – 7.05 (m, 1H), 6.85 (d, J = 8.2 Hz, 1H), 6.70 (d, J = 8.1 Hz, 1H), 5.63 – 5.56 (m, 2H), 3.62 (s, 3H), 3.33 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.6, 154.9, 144.3, 134.9, 134.1, 133.1, 131.2, 130.8, 129.3, 128.9, 128.3, 127.5, 125.1, 122.7, 120.5, 112.7, 110.8, 56.0, 55.4, 54.4.

HRMS (ESI) calculated for $C_{23}H_{21}N_3NaO_3S^+$ [M+Na]$^+$: 442.1196, found: 442.1206. $[\alpha]_D^{20}$ = -107 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IA column (80:20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 20.9 min, t_R (minor) = 32.6 min, 93% ee.



No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	21.263	6.262	50.27	1	20.940	28.092	92.61
2	32.663	6.195	49.73	2	32.597	2.241	7.39



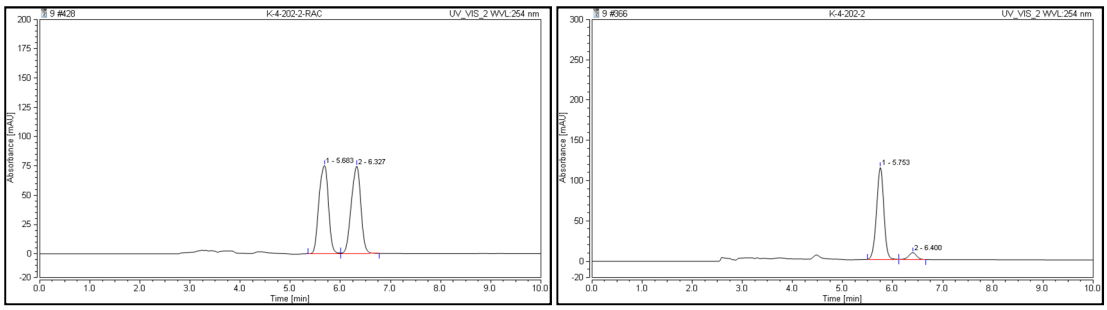
(*R*)-**7aa**, 91%

(*R*)-**11**, 95%, 85% ee

The compound (*R*)-**7aa** (42.7 mg, 0.1 mmol) was dissolved in THF and 1.0 M TBAF (0.15 mL, 1.5 equiv) was then added at 0 °C with constant stirring. The reaction progress was monitored by TLC. The mixture was diluted with water extracted with EtOAc, dried over anhydrous Na_2SO_4, filtered and evaporated in vacuo. The obtained crude product was purified by flash chromatography in petroleum ether: ethyl acetate= 2:1 to give (*S*)-**9** as white solid (25.7 mg, 95%, 85% ee).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.41 – 7.38 (m, 2H), 7.26 – 7.24 (m, 1H), 7.18 – 7.15 (m, 1H), 7.12 – 7.10 (m, 1H), 6.81 (dd, *J* = 8.2, 1.0 Hz, 1H), 3.63 (s, 3H), 3.38 (s, 1H), 2.44 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) *δ* 155.4, 142.0, 140.2, 132.9, 132.4, 131.8, 130.7, 130.1, 127.7, 123.8, 120.4, 111.1, 84.0, 80.5, 55.5, 18.3. **HRMS** (ESI) calculated for $C_{16}H_{14}NaO_2S^+$ [M+Na]$^+$: 293.0607, found: 293.0608. $[\alpha]_D^{20}$ = -98 (c = 0.05, $CHCl_3$).

HPLC conditions: Daicel Chiralpak IA column (80:20 hexane: 2-propanol, 1.0 mL/min, 40 °C, 254 nm); t_R (major) = 5.8 min, t_R (minor) = 6.4 min, 85% ee.

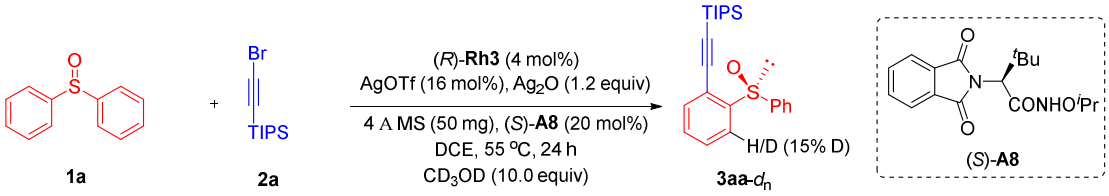


No.	Time	Area	Area (%)	No.	Time	Area	Area (%)

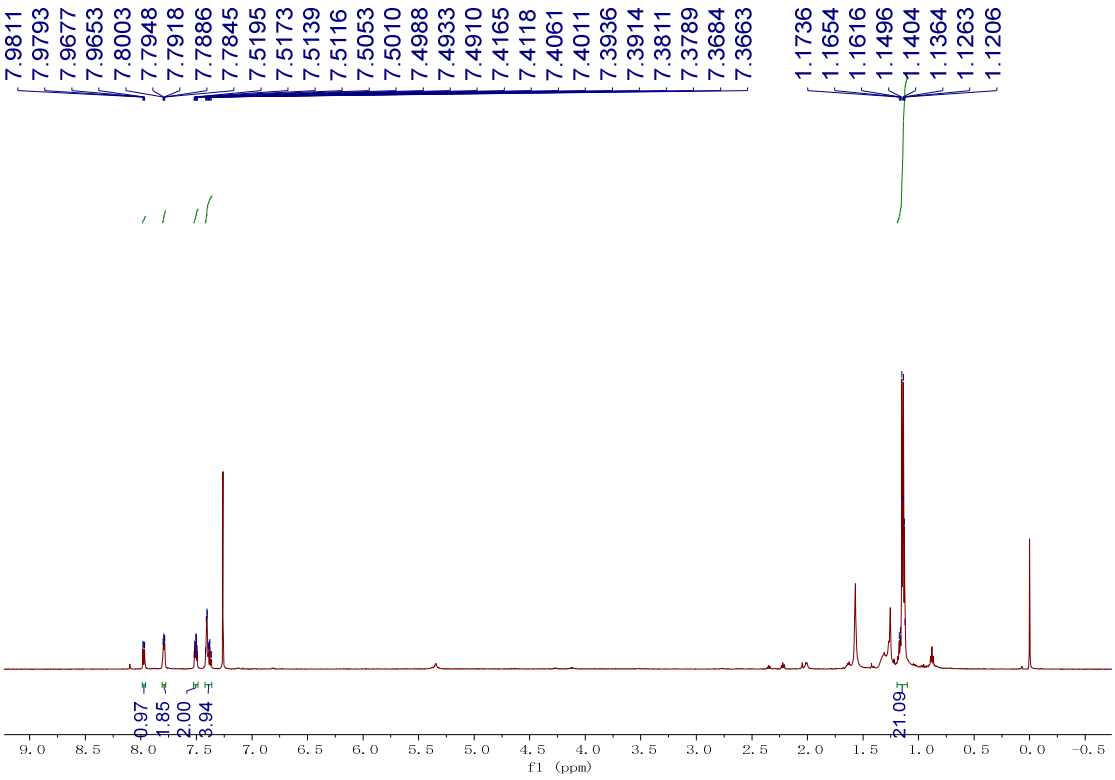
1	5.683	16.478	50.02	1	5.753	19.208	92.66
2	6.327	16.468	49.98	2	6.400	1.522	7.34

6. Mechanistic Studies

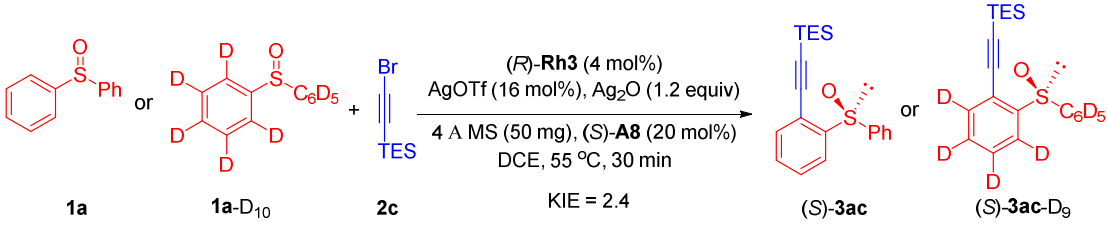
6.1 H/D Exchange Experiments



A pressure tube was charged with **1a** (20.2 mg, 0.1 mmol), **2a** (31.3 mg, 0.12 mmol), (*R*)-**Rh3** (8.0 mg, 4 mol%), AgOTf (4.2 mg, 16 mol %), Ag_2O (23.2 mg, 1.2 equiv), (*R*)-**A8** (6.4 mg, 20 mol %), 4Å MS (50 mg), CD_3OD (10.0 equiv), and DCE (2.0 mL). The reaction mixture was stirred under N_2 at 55 °C for 24 h. After the reaction was completed as indicated by TLC analysis, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate 8:1 (v/v) to give the product **3aa**-d_n (13.4 mg, 35%).

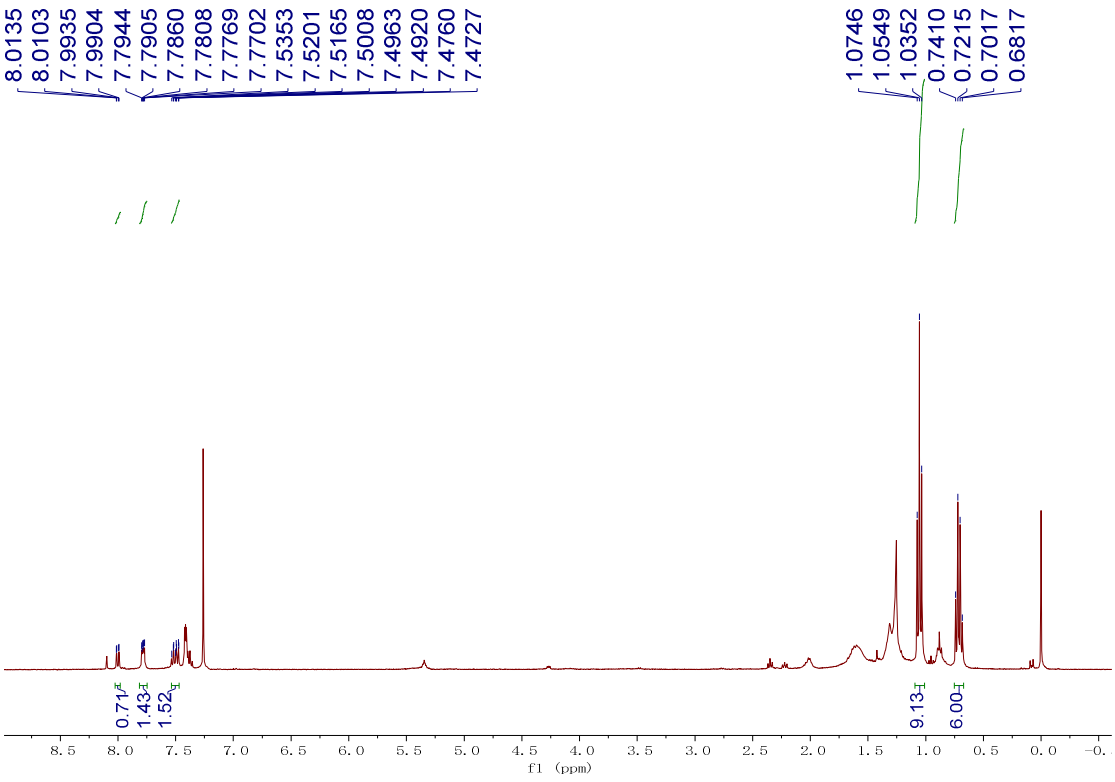


6.2 Parallel Kinetic Isotope Effect

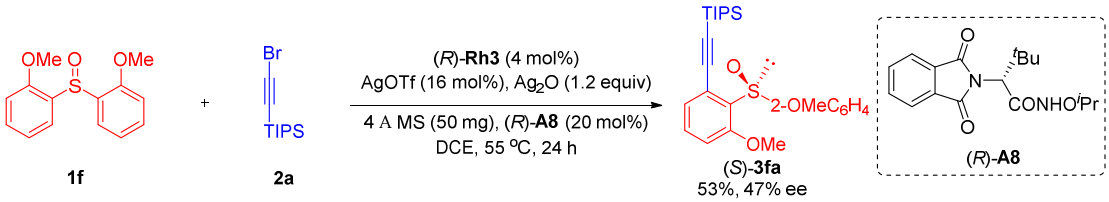


A Schlenk tube equipped with a stir bar was charged with **1a** (0.05 mmol)**, 2c** (0.06 mmol), (*R*)-**Rh3** (4 mg, 4 mol%), AgOTf (2.1 mg, 16 mol %), Ag_2O (11.6 mg, 1.2 equiv), (*R*)-**A8** (3.2 mg, 20 mol %), 4Å MS (25.0 mg), and DCE (1.0 mL), while the other Schlenk tube was charged with **1a**-D_{10} (0.05

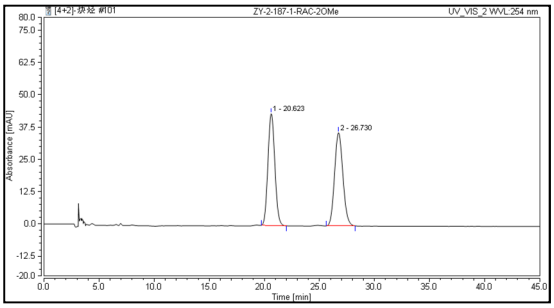
mmol)**, 2c** (0.06 mmol), (*R*)-**Rh3** (4 mg, 4 mol%), AgOTf (2.1 mg, 16 mol %), Ag_2O (11.6 mg, 1.2 equiv), (*R*)-**A8** (3.2 mg, 20 mol %), 4Å MS (25.0 mg), and DCE (1.0 mL). The two reaction mixtures were stirred side by side at 55 °C for 0.5 h under N_2. After that, the two reaction tubes were quenched with *n*-hexane and the resulting mixtures in the two tubes were rapidly combined. The solvent was rapidly removed under reduced pressure. The resulting residue was purified by silica gel chromatography using EA/PE to afford the rude products (*S*)-**3ac** and (*S*)-**3ac**-D_9. The KIE value was determined on the basis of ^{1}H NMR analysis.

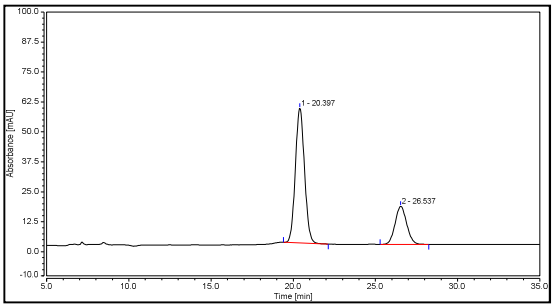


6.3 Significance of the Chirality of the Amide Additive



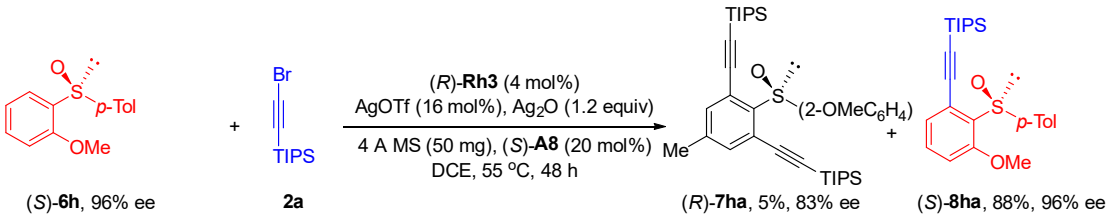
A pressure tube was charged with **1f** (26.2 mg, 0.1 mmol), **2a** (31.3 mg, 0.12 mmol), (*R*)-**Rh3** (8.0 mg, 4 mol%), AgOTf (4.2 mg, 16 mol %), Ag_2O (23.2 mg, 1.2 equiv), (*R*)-**A8** (6.4 mg, 20 mol %), 4Å MS (50 mg), and DCE (2.0 mL). The reaction mixture was stirred under N_2 at 55 °C for 48 h. After the reaction was completed as indicated by TLC analysis, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate 8:1 (v/v) to give the product **3fd** (23.5 mg, 53%, 47% ee).





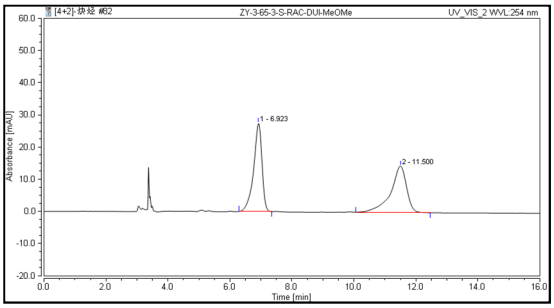
No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	20.623	31.578	49.97	1	20.397	36.457	73.62
2	26.730	31.620	50.03	2	26.537	13.061	26.38

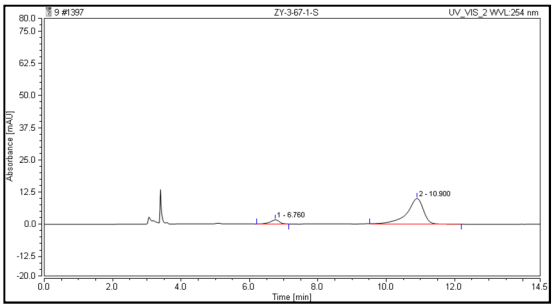
6.4 Alkynylation of an Enantio-Enriched Substrate



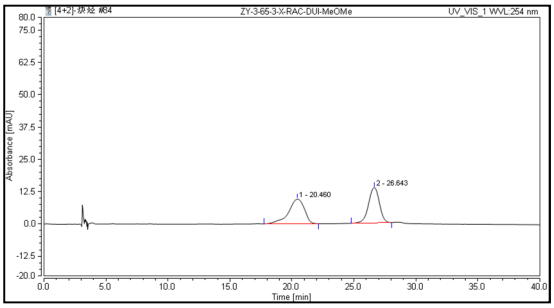
(*S*)-**6h**, 96% ee **2a** (*R*)-**7ha**, 5%, 83% ee (*S*)-**8ha**, 88%, 96% ee

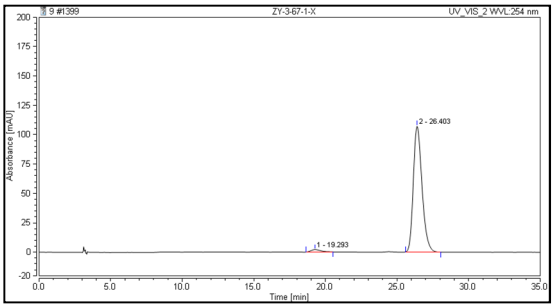
A pressure tube was charged with (*S*)-**6h** (24.6 mg, 0.1 mmol), **2a** (39.2 mg, 0.15 mmol), (*R*)-**Rh3** (8.0 mg, 4 mol%), AgOTf (4.2 mg, 16 mol %), Ag_2O (23.2 mg, 1.2 equiv), (*S*)-**A8** (6.4 mg, 20 mol %), 4Å MS (50 mg), and DCE (2.0 mL). The reaction mixture was stirred under N_2 at 55 °C for 48 h. After the reaction was completed as indicated by TLC analysis, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using petroleum ether/ethyl acetate 8:1-2:1 (v/v) to give the products (*R*)-**7ha** (8.9 mg, 5%, 83% ee) and (*S*)-**8ha** (37.4 mg, 88%, 96% ee).





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	6.923	8.548	49.95	1	6.760	0.496	8.29
2	11.500	8.566	50.05	2	10.900	5.489	91.71





No.	Time	Area	Area (%)	No.	Time	Area	Area (%)
1	20.460	14.122	50.48	1	19.293	1.627	2.12
2	26.643	13.854	49.52	2	26.403	75.297	97.88

7. Theoretical Calculations

Computational details

Density functional theory (DFT)[1] calculations were conducted using the Gaussian 16 program package[2]. For geometry optimization and harmonic frequency calculations, the popular hybrid functional B3LYP[3] augmented with empirical Grimme's dispersion of D3BJ[4] were utilized in combination with a Def2SVP basis set[5]. The stationary points were ascertained by vibrational frequency analysis with no imaginary frequencies. Only the transition states (**TS**) had one imaginary frequency, whereas the ground states had all positive frequencies. The continuity on the potential energy surface was confirmed by intrinsic reaction coordinate (IRC) calculations on the **TS**s. The single-point energies were refined at the B3LYP-D3/Def2TZVPP level[5]. All thermodynamic data were reported in 303.15 K and 1 atm, which are the same with the experimental conditions.

Reference

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3. (a) A. D. Becke, J. Chem. Phys., 1993, **98**, 1372-1377. (b) A. D. Becke, J. Chem. Phys., 1993, **98**, 5648-5652; (c) C. Lee, W. Yang, R. G. Parr, Phys. Rev. B, 1988, **37**, 785-789. (d) A. D. Becke, Phys. Rev. A, 1988, **38**, 3098-3100.
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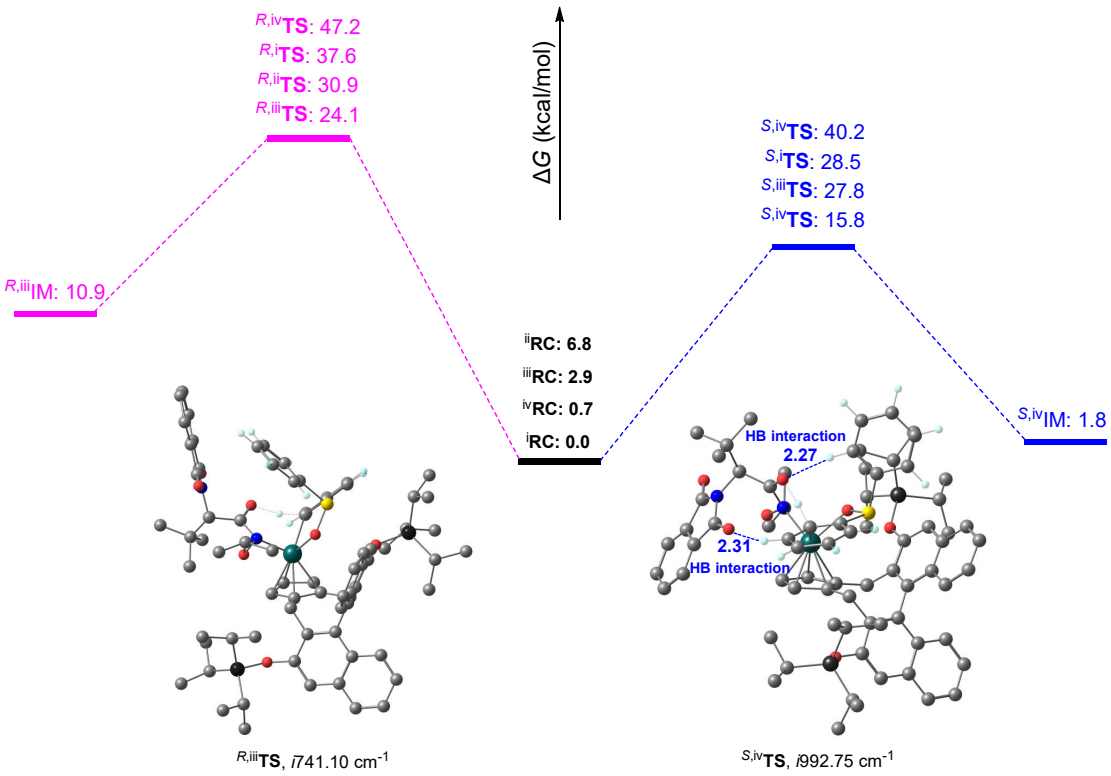

Scheme S1. Free Energy Profiles (in kcal mol^{-1}) of Eight Possible Pathways for C-H Activation to Give (S)- and (R)- Product. The Optimized Geometries of Two Lowest Transition States (^{R,iii}**TS** (left) and ^{S,iv}**TS** (right)) are Given. All Hydrogen Atoms except for Those on the Substrate are Omitted for Clarify.

Charge, Multiplicity, and Coordinates of Key Reaction Species

^{R,i}RC

Charge = 1 Multiplicity = 1

Rh 0.436264 -0.833506 -2.284392
O -0.516701 2.861741 -1.170732
C 1.713809 -0.898152 -3.998695
H 1.456111 -1.393561 -4.932514
C 4.131759 0.170277 -0.030688
C 0.566899 2.208141 2.288620
C 2.434636 1.836053 0.723998
C 6.524138 0.595334 0.139273
H 7.553570 0.256155 0.019452
O 5.720564 -1.550392 -0.541430
C -0.238195 2.600352 1.191936
H -1.272211 2.883898 1.371353
C 0.255429 2.580304 -0.096796
C 2.388628 -1.484018 -2.879118
H 2.690018 -2.525152 -2.790804
C 3.014398 -0.754189 -0.449224
H 2.163268 -0.639275 0.233262
H 3.345190 -1.795094 -0.397959
C 2.512633 -0.500373 -1.846203
C 1.509185 0.491560 -3.683642
H 1.002560 1.218085 -4.317259
C 0.045220 2.152763 3.611590
H -0.990866 2.455709 3.775244
C 6.269382 1.909181 0.609717
C 1.927226 1.818356 2.063821
C 0.823375 1.718113 4.662912
H 0.407375 1.676261 5.672142
C 5.721073 4.497875 1.586679
H 5.520122 5.502937 1.963956
C 4.914357 2.336056 0.804348
C 1.610025 2.186633 -0.333078
C 3.852530 1.432114 0.477878
C 2.706940 1.383719 3.172102
H 3.741570 1.085121 3.005720
C 2.104733 2.119728 -1.754670
H 1.545821 2.824427 -2.375221
H 3.166143 2.413871 -1.790367
C 2.167543 1.328603 4.440613
H 2.780265 0.989662 5.278920
C 4.674028 3.648559 1.298317
H 3.644692 3.978326 1.444792
C 5.487496 -0.266658 -0.155809
C 7.326436 2.810386 0.916359
H 8.357203 2.480325 0.765993
C 7.059798 4.074993 1.394642
H 7.881176 4.756756 1.626337
C 2.015875 0.760759 -2.388022
Si 6.137320 -2.846425 0.512948
C 6.012959 -4.313556 -0.677348
C 4.579942 -4.494783 -1.197092
C 6.598676 -5.632604 -0.151588
H 6.632945 -3.988863 -1.533736
H 4.206151 -3.565672 -1.651984
H 4.532357 -5.287121 -1.963425
H 3.885357 -4.778784 -0.389620
H 7.663558 -5.536703 0.105892
H 6.073057 -5.992724 0.746470
H 6.518517 -6.425025 -0.914782
C 7.893936 -2.530179 1.144812
C 8.901331 -2.500987 -0.015816
C 8.350045 -3.477824 2.266390
H 7.842865 -1.513211 1.576103
H 8.582757 -1.823730 -0.823923
H 9.894854 -2.169732 0.329721
H 9.030942 -3.501644 -0.459856
H 7.685888 -3.438988 3.142774
H 8.391534 -4.525327 1.930182
H 9.362465 -3.209894 2.612277
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H 3.915959 -4.158340 3.405006
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H 0.091859 7.303159 -3.535306
H -1.577976 6.717200 -3.623497
H 0.610197 3.593494 -3.907485
H -0.520263 4.633540 -4.783405
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^{S,ir}TS

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H 6.880046 -0.657499 -0.894256
O 4.616494 -2.022856 -0.835060
C 0.388712 3.654307 1.680478
H -0.436561 4.278839 2.012025
C 0.462327 3.268798 0.357404
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H 1.341451 -2.658205 -1.974974
C 2.297576 -0.685395 0.011769
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C 1.269311 0.721229 -1.963202
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H 7.167610 -5.404482 1.227223
H 8.246666 -4.218096 1.980924
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H -0.777734 -5.373079 0.092499
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H -0.407782 -2.581980 2.608659

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^{R,ir}TS

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H -1.061551 3.073335 1.735657
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H 2.320106 -3.104881 -1.756509
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H -0.614663 2.694372 4.131644
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C 1.267100 1.993001 4.903821
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H 8.428312 -2.938088 3.126771
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C -5.003213 -4.309180 -4.022167
H -5.742039 -4.577200 -3.250356
H -5.219252 -3.292098 -4.376470
H -5.142081 -4.994723 -4.872013
C -3.275320 -5.912474 -3.176025
H -4.003326 -6.325590 -2.460796
H -3.326088 -6.507772 -4.100215
H -2.273280 -6.039678 -2.744496
C -2.560769 -3.952528 -4.548318
H -2.674896 -2.882965 -4.755313
H -1.525609 -4.140171 -4.219449
H -2.714675 -4.516346 -5.481518
C -2.027630 -3.306133 -1.731758
O -1.570849 -2.182856 -2.145131
N -1.307932 -4.032209 -0.913410
O -1.950503 -5.108574 -0.323273
C -1.004950 -6.028235 0.255708
H -0.366705 -5.452093 0.951457
C -0.130377 -6.684499 -0.804121
H 0.392417 -5.926334 -1.405801
H 0.625108 -7.327246 -0.326584
H -0.735701 -7.308590 -1.479350
C -1.849784 -7.015375 1.040853
H -1.204811 -7.734944 1.566428
H -2.471488 -6.491189 1.780928

H -2.513640 -7.574185 0.363297

[ii]RC

Charge = 1 Multiplicity = 1

Rh -0.468798 -0.806894 -1.324254
O -0.502910 3.512927 -0.498589
C 0.290958 -1.229718 -3.288576
H -0.276072 -1.811572 -4.013344
C 3.829488 0.013985 -0.469633
C 1.628239 3.063730 2.475527
C 2.668924 2.007973 0.506537
C 6.108983 0.139339 -1.311681
H 6.975994 -0.340008 -1.766936
O 4.931133 -1.943655 -1.291338
C 0.556268 3.479459 1.647280
H -0.245914 4.070956 2.083619
C 0.509788 3.142922 0.307254
C 1.164964 -1.756091 -2.296403
H 1.396002 -2.806251 -2.131440
C 2.566933 -0.791669 -0.298211
H 2.021056 -0.452890 0.591412
H 2.793777 -1.851900 -0.157405
C 1.676187 -0.653238 -1.504094
C 0.238189 0.192121 -3.117010
H -0.333188 0.896584 -3.717892
C 1.654321 3.358119 3.866561
H 0.828367 3.929186 4.297669
C 6.158050 1.522734 -1.000508
C 2.707852 2.315578 1.905590
C 2.693438 2.925003 4.661858
H 2.698106 3.155793 5.729509
C 6.228464 4.267739 -0.357415
H 6.264908 5.331832 -0.113935
C 5.023630 2.149332 -0.386463
C 1.567413 2.357802 -0.262241
C 3.855181 1.358075 -0.130674
C 3.766610 1.883837 2.752037
H 4.586373 1.307789 2.321763
C 1.478879 1.981806 -1.720005
H 0.734421 2.620080 -2.202683
H 2.449883 2.176710 -2.208174
C 3.757947 2.176830 4.100404
H 4.575875 1.834445 4.737923
C 5.092886 3.536916 -0.078804
H 4.232332 4.022151 0.382786
C 4.982675 -0.610101 -1.039995
C 7.313835 2.305547 -1.274263
H 8.175548 1.821860 -1.740649
C 7.350520 3.646488 -0.958953
H 8.245153 4.235181 -1.173893
C 1.141654 0.556039 -2.054930
Si 5.685646 -3.180025 -0.355813
C 4.891938 -4.726185 -1.108850
C 3.387775 -4.799133 -0.803373
C 5.600425 -6.047323 -0.772580
H 5.000235 -4.554451 -2.196378
H 2.876785 -3.869373 -1.092665
H 2.909334 -5.628641 -1.351123
H 3.192431 -4.963598 0.268715
H 6.648165 -6.051003 -1.107075
H 5.597748 -6.255608 0.308753
H 5.096882 -6.894979 -1.267237
C 7.551361 -3.048817 -0.658045
C 7.884912 -3.262064 -2.143291
C 8.415096 -3.935843 0.253180
H 7.786933 -1.998472 -0.405207
H 7.275529 -2.620479 -2.799370
H 8.946292 -3.042345 -2.347395
H 7.706350 -4.305949 -2.449217
H 8.260651 -3.711467 1.319191
H 8.206521 -5.006852 0.107266
H 9.486416 -3.783189 0.039524
C 5.211334 -2.868460 1.462106
C 5.958300 -1.670721 2.075804
C 5.347578 -4.115658 2.352175
H 4.136920 -2.609099 1.426965
H 5.850793 -0.754555 1.477412
H 5.579797 -1.454152 3.089504
H 7.036511 -1.876102 2.170335
H 4.720937 -4.949037 2.001657
H 6.386162 -4.479202 2.394976
H 5.042455 -3.888293 3.387764
Si-1.329824 4.943853 -0.945127
C -0.297255 5.777730 -2.306970
C -0.742011 7.220443 -2.608601
C -0.227577 4.967661 -3.611377
H 0.723356 5.822979 -1.879791
H -0.719365 7.866019 -1.719563
H -0.080437 7.679591 -3.362266
H -1.764605 7.252930 -3.015442
H 0.098218 3.929743 -3.451202
H -1.208064 4.930383 -4.111382
H 0.480740 5.427037 -4.321128
C -3.007924 4.275013 -1.519839
C -2.908938 2.910583 -2.218310
C -3.817102 5.270180 -2.367373
H -3.557453 4.115761 -0.576513
H -2.366376 2.178944 -1.606437
H -3.917760 2.511355 -2.419089
H -2.397020 2.990555 -3.191500
H -3.924846 6.254626 -1.888821
H -3.351738 5.431730 -3.352531
H -4.833362 4.882593 -2.552881
C -1.492433 6.052709 0.593578
C -2.683161 7.023432 0.550097
C -0.187023 6.780964 0.955264
H -1.709148 5.327866 1.397627
H -3.640764 6.495816 0.424011
H -2.745468 7.601543 1.487973
H -2.594301 7.752605 -0.270236
H 0.677637 6.101605 0.997898
H 0.049880 7.569025 0.224424
H -0.270667 7.270769 1.940223
S -2.509531 0.186934 0.933014
O -1.428123 0.635348 -0.120206
C -3.495690 1.646057 1.225625
C -4.761119 1.657262 0.630569
C -3.043007 2.705042 2.017132
C -5.589581 2.763516 0.829263
C -3.886116 3.797696 2.217879
H -2.054711 2.661614 2.474415
C -5.154050 3.827373 1.625173
H -6.580219 2.790239 0.371180
H -3.556632 4.630908 2.841255
H -5.807962 4.686622 1.788644
C -1.598285 0.028126 2.474278
C -2.279226 -0.431126 3.606463
C -0.226827 0.272341 2.476276
C -1.549741 -0.630857 4.780042
H -3.349719 -0.637553 3.562545
C 0.487826 0.065489 3.658542
H -5.091102 0.806434 0.031381
C -0.171793 -0.385115 4.805156
H -2.060489 -0.986037 5.677620
H 1.560016 0.266489 3.681010
H 0.391902 -0.546055 5.726594
C -6.374359 -2.797648 0.475658
C -6.138902 -3.826441 -0.439867
C -7.160013 -4.347666 -1.222746
C -8.439522 -3.793271 -1.067291
C -8.673858 -2.754871 -0.153665
C -7.636416 -2.239927 0.637976
C -5.088175 -2.478626 1.148486
C -4.690900 -4.180099 -0.386653
H -6.967551 -5.155278 -1.931360
H -9.269346 -4.176326 -1.665194
H -9.681962 -2.346285 -0.055712
H -7.807225 -1.437205 1.357843
O -4.858071 -1.615599 1.970548
O -4.088584 -4.973754 -1.068213
N -4.139326 -3.372820 0.627584
C -2.739872 -3.259998 0.999834
H -2.765991 -2.574225 1.859025
C -2.043004 -4.571294 1.538102
C -3.108243 -5.468253 2.187423
H -3.707520 -4.914299 2.927385
H -3.787854 -5.909182 1.445335
H -2.611925 -6.297495 2.713737
C -1.032392 -4.146503 2.621941
H -1.538413 -3.645932 3.463074
H -0.514984 -5.033932 3.017648
H -0.281137 -3.454884 2.219280
C -1.306830 -5.340612 0.429003
H -1.983925 -5.598235 -0.394659
H -0.468471 -4.749871 0.029787
H -0.887569 -6.270767 0.842874
C -1.909352 -2.516148 -0.025205
O -0.707493 -2.170172 0.300861
N -2.221765 -2.037770 -1.212318
O -3.530029 -1.966601 -1.628843
C -3.618750 -1.882400 -3.072842
H -2.763232 -2.449277 -3.474859
C -3.544199 -0.423512 -3.499898
H -2.650104 0.065699 -3.091042
H -3.518844 -0.340839 -4.597521
H -4.425342 0.126133 -3.135062
C -4.915110 -2.562410 -3.474769
H -5.062845 -2.471344 -4.561378
H -4.895043 -3.627617 -3.209254
H -5.771592 -2.087318 -2.971929
H 0.261501 0.623423 1.569973

S,ir-**TS**

Charge = 1 Multiplicity = 1

Rh -0.556182 -0.346659 -0.993888
O 0.770838 3.625140 -0.488482
C 0.028809 -1.308610 -2.812069
H -0.664572 -1.796399 -3.493671
C 3.796754 -0.919962 -0.199820
C 3.122225 3.050795 2.299334
C 3.564361 1.466551 0.466450
C 5.822001 -1.804302 -1.216998
H 6.376768 -2.633521 -1.656130
O 3.924987 -3.218785 -0.821281
C 2.096300 3.623894 1.507294
H 1.538925 4.469360 1.904003
C 1.778634 3.119741 0.262136
C 0.718945 -1.927036 -1.720010
H 0.577481 -2.949134 -1.375389
C 2.351069 -1.144467 0.172522
H 2.031131 -0.435362 0.946459
H 2.191022 -2.158427 0.551538
C 1.513123 -0.944330 -1.055287
C 0.473594 0.059130 -2.868920
H 0.148981 0.807511 -3.589286
C 3.423907 3.539633 3.600223
H 2.856827 4.390210 3.987407
C 6.428662 -0.523336 -1.140559
C 3.867483 1.943342 1.782476
C 4.410604 2.952780 4.362904
H 4.632092 3.336736 5.361283
C 7.596861 2.041145 -0.996768
H 8.057450 3.030267 -0.948303
C 5.698048 0.573689 -0.574763
C 2.529086 2.024650 -0.272247
C 4.363435 0.343082 -0.108340
C 4.874688 1.355920 2.597336
H 5.438004 0.505207 2.212489
C 2.219843 1.545948 -1.669837
H 1.724755 2.346312 -2.226229
H 3.170433 1.328807 -2.187542
C 5.139780 1.847939 3.857952
H 5.915633 1.385361 4.471707
C 6.315508 1.854491 -0.523069
H 5.760970 2.692871 -0.099861
C 4.538237 -2.009180 -0.753617
C 7.749095 -0.296315 -1.618595
H 8.303135 -1.135435 -2.046406
C 8.321740 0.955205 -1.546910
H 9.337014 1.114228 -1.917191
C 1.400669 0.296608 -1.817594
Si 4.258731 -4.635718 0.099378
C 2.792720 -5.728334 -0.403253
C 1.475607 -5.246323 0.224869
C 2.994414 -7.233702 -0.171373
H 2.725721 -5.560110 -1.494755
H 1.333326 -4.160989 0.117839
H 0.604526 -5.742781 -0.235479
H 1.435690 -5.465224 1.303430
H 3.859993 -7.626230 -0.724438
H 3.147528 -7.469187 0.893889
H 2.108752 -7.801166 -0.504007
C 5.944867 -5.282867 -0.473906
C 5.927516 -5.616530 -1.974523
C 6.511642 -6.441143 0.362743
H 6.619796 -4.419309 -0.327518
H 5.533260 -4.783837 -2.578244
H 6.941593 -5.848501 -2.341000
H 5.299303 -6.497763 -2.183457
H 6.646097 -6.162020 1.418406
H 5.862786 -7.329982 0.335067
H 7.498795 -6.748870 -0.021349
C 4.234861 -4.132540 1.932080
C 5.446473 -3.271039 2.328456
C 4.068929 -5.325410 2.889370
H 3.329476 -3.504123 2.031017
H 5.549702 -2.375431 1.698506
H 5.358801 -2.933724 3.375185
H 6.386964 -3.840071 2.249472
H 3.156450 -5.904617 2.683946
H 4.920287 -6.020798 2.829309
H 4.009128 -4.978265 3.934689
Si 0.348322 5.247137 -0.873722
C 1.979132 6.212434 -0.932512
C 1.809904 7.714808 -1.215980
C 2.997273 5.573618 -1.890984
H 2.383581 6.113967 0.091814
H 1.062375 8.188221 -0.561347
H 2.763062 8.247727 -1.062812
H 1.500408 7.899483 -2.254922
H 3.194284 4.518680 -1.646390
H 2.650750 5.618134 -2.936424
H 3.962765 6.104994 -1.847964
C -0.571736 5.068858 -2.530241
C -0.104132 3.888879 -3.389408
C -0.601999 6.369681 -3.348771
H -1.607089 4.843770 -2.225410
H -0.210253 2.944154 -2.841639
H -0.706661 3.816490 -4.311589
H 0.948673 3.994519 -3.697138
H -0.932185 7.237936 -2.759280
H 0.391788 6.607565 -3.759102
H -1.290130 6.274176 -4.205713
C -0.865120 5.884497 0.460743
C -2.017221 6.738406 -0.095950
C -0.215023 6.620994 1.642240
H -1.303123 4.944862 0.846971
H -2.569037 6.234874 -0.902327
H -2.741330 6.976904 0.701469
H -1.654089 7.699678 -0.494437
H 0.624247 6.072653 2.091752
H 0.174336 7.603975 1.335765
H -0.952498 6.798516 2.442480
S -2.054800 0.814868 1.322876
O -0.541516 0.692240 0.877293
C -2.704760 1.648021 -0.155143
C -2.407320 0.949579 -1.346336
C -3.344028 2.879621 -0.138297
C -2.753628 1.582390 -2.554809
C -3.715105 3.455501 -1.360915
H -3.543875 3.397028 0.800776
C -3.407891 2.816033 -2.564287
H -2.551442 1.075184 -3.499762
H -4.230571 4.417985 -1.367013
H -3.682598 3.279960 -3.513835
C -2.086062 2.106421 2.550592
C -3.247741 2.215748 3.324325
C -0.965787 2.909152 2.756676
C -3.292039 3.205528 4.308867
H -4.087666 1.537590 3.154876
C -1.021144 3.874330 3.763622
H -2.668830 -0.287795 -1.426220
C -2.182058 4.029645 4.528348
H -4.189365 3.320356 4.920464
H -0.151904 4.506028 3.953593
H -2.218224 4.789497 5.312083
C -6.927561 -1.274893 1.214969
C -7.269154 -2.420402 0.494690
C -8.569947 -2.649361 0.067280
C -9.531417 -1.676618 0.380422
C -9.187403 -0.523175 1.100723
C -7.870439 -0.305073 1.531645
C -5.472841 -1.339187 1.504331
C -6.043953 -3.250067 0.313182
H -8.826698 -3.551762 -0.490516
H 10.566092 -1.818348 0.060723
H -9.959776 0.214250 1.329770
H -7.593093 0.587924 2.094708
O -4.770044 -0.510422 2.046922
O -5.952043 -4.294751 -0.284514
N -5.011410 -2.567965 0.992960
C -3.571327 -2.811643 0.986083
H -3.227258 -2.287002 1.887671
C -3.057968 -4.288931 1.129726
C -3.992970 -5.069676 2.068181
H -4.160874 -4.520497 3.008367
H -4.962628 -5.283587 1.603928
H -3.526744 -6.032873 2.325610
C -1.665135 -4.232349 1.790682
H -1.717001 -3.771189 2.789747
H -1.273881 -5.253817 1.909014
H -0.951335 -3.654784 1.190774
C -2.927195 -4.993211 -0.230457
H -3.887409 -5.028504 -0.757870
H -2.186844 -4.483313 -0.868298
H -2.575271 -6.025791 -0.081034
C -2.863420 -2.032755 -0.125889
O -1.664108 -1.677497 0.181574
N -3.337549 -1.615482 -1.271545
O -4.668275 -1.849493 -1.576592
C -4.817799 -2.347701 -2.925221
H -4.270506 -3.306432 -2.983154
C -4.249870 -1.372438 -3.948123
H -3.170438 -1.227642 -3.801670
H -4.406856 -1.761812 -4.965211
H -4.751363 -0.395474 -3.866360
C -6.306026 -2.590100 -3.109972
H -6.503624 -2.928542 -4.137760
H -6.666331 -3.359818 -2.416219
H -6.867420 -1.658571 -2.936921
H -0.073805 2.758878 2.150491

^{R,ii}TS

Charge = 1 Multiplicity = 1

Rh 0.011761 -1.358285 -1.407765
O -0.193179 3.103020 -1.284301
C 1.467405 -1.961069 -2.877930
H 1.208281 -2.701329 -3.635436
C 3.914713 -0.052846 0.568322
C 1.042787 3.413309 2.178314
C 2.581637 2.042740 0.820780
C 6.336222 -0.040267 0.354704
H 7.279086 -0.572007 0.226504
O 5.116956 -2.106673 0.347511
C 0.229330 3.584099 1.028659
H -0.654201 4.219074 1.094442
C 0.541342 2.962232 -0.165126
C 1.937825 -2.247027 -1.566574
H 2.149736 -3.238883 -1.176363
C 2.632959 -0.841673 0.555720
H 1.875211 -0.340376 1.169438
H 2.797771 -1.834954 0.976492
C 2.122212 -0.993708 -0.850902
C 1.304350 -0.543718 -2.970381
H 0.958958 0.005525 -3.843595
C 0.707110 4.005826 3.427155
H -0.196190 4.618282 3.492960
C 6.341972 1.377353 0.437700
C 2.239177 2.629983 2.083269
C 1.505566 3.821222 4.535960
H 1.234732 4.282988 5.488191
C 6.322600 4.194348 0.585152
H 6.325336 5.285264 0.636985
C 5.104365 2.083933 0.600810
C 1.723268 2.158006 -0.263191
C 3.886663 1.329939 0.665526
C 3.040553 2.459044 3.245314
H 3.948666 1.858913 3.176429
C 2.039264 1.530177 -1.596971
H 1.491211 2.060119 -2.382934
H 3.116730 1.655292 -1.807318
C 2.681219 3.036526 4.445373
H 3.306778 2.893471 5.329003
C 5.131117 3.504896 0.665581
H 4.192870 4.048824 0.779876
C 5.154755 -0.748914 0.424157
C 7.552966 2.119367 0.359745
H 8.493318 1.576330 0.237562
C 7.545441 3.495527 0.434135
H 8.483327 4.052051 0.373037
C 1.793157 0.058276 -1.751519
Si 5.593146 -3.255763 1.535718
C 5.053733 -4.875262 0.707203
C 3.523641 -5.008950 0.679292
C 5.710100 -6.147855 1.263056
H 5.393525 -4.746896 -0.337674
H 3.056035 -4.091025 0.298990
H 3.202194 -5.841149 0.033476
H 3.112645 -5.197739 1.684025
H 6.805715 -6.124367 1.171516
H 5.470405 -6.305440 2.326591
H 5.353235 -7.037208 0.716298
C 7.464709 -3.086300 1.766937
C 8.212699 -3.396526 0.459886
C 8.039882 -3.876207 2.953650
H 7.606923 -2.013023 1.991754
H 7.805822 -2.833362 -0.394809
H 9.283599 -3.148258 0.547833
H 8.149560 -4.466936 0.204891
H 7.598226 -3.564385 3.911834
H 7.875491 -4.959946 2.849883
H 9.128977 -3.720243 3.030944
C 4.606036 -2.858005 3.114768
C 5.074901 -1.557353 3.789774
C 4.552611 -4.018202 4.122690
H 3.573892 -2.691734 2.753394
H 5.065542 -0.700100 3.100778
H 4.425472 -1.303776 4.645048
H 6.100498 -1.655261 4.180400
H 4.126165 -4.933972 3.686513
H 5.551390 -4.273551 4.508558
H 3.932025 -3.748195 4.994544
Si-1.090704 4.425434 -1.914814
C -1.048510 4.111706 -3.786643
C -2.123321 4.900362 -4.554677
C -1.101389 2.622789 -4.158230
H -0.059428 4.498015 -4.098554
H -2.096016 5.978250 -4.339729
H -1.992866 4.779255 -5.643098
H -3.134844 4.539864 -4.309197
H -0.361955 2.032845 -3.599719
H -2.088298 2.193483 -3.932815
H -0.918370 2.480289 -5.236571
C -2.809841 4.297061 -1.123263
C -3.547312 3.029599 -1.586178
C -3.694312 5.545619 -1.250100
H -2.584711 4.164392 -0.050106
H -2.908784 2.136561 -1.524536
H -4.441002 2.850733 -0.965958
H -3.891263 3.128714 -2.628212
H -3.224916 6.433855 -0.800574
H -3.921767 5.784858 -2.300843
H -4.659185 5.390228 -0.737694
C -0.154607 6.017435 -1.461642
C -0.638247 7.241648 -2.259943
C 1.366227 5.847816 -1.623980
H -0.364913 6.206948 -0.392870
H -1.723689 7.402591 -2.185880
H -0.143398 8.158158 -1.898117
H -0.388004 7.143747 -3.328444
H 1.777052 5.063850 -0.972191
H 1.633252 5.594350 -2.663795
H 1.888444 6.787832 -1.379346
S -2.554338 -0.593716 0.067347
O -1.486749 0.082099 -0.880196
C -3.285207 0.736820 0.994815
C -4.676320 0.731798 1.130027
C -2.487566 1.742505 1.547142
C -5.283831 1.761520 1.852960
C -3.107823 2.761042 2.267398
H -1.406825 1.732603 1.406549
C -4.500323 2.771690 2.418857
H -6.369177 1.776475 1.969592
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H -4.978237 3.575514 2.982969
C -1.461547 -1.365957 1.278087
C -1.498122 -1.133393 2.648920
C -0.525597 -2.221337 0.667571
C -0.549219 -1.773998 3.456663
H -2.236162 -0.464405 3.091405
C 0.392336 -2.867811 1.514460
H -5.274418 -0.059690 0.673119
C 0.390501 -2.640701 2.891592
H -0.554389 -1.596357 4.534143
H 1.090490 -3.589580 1.089917
H 1.113804 -3.152855 3.530031
H -0.871501 -3.017057 -0.237661
C 1.528736 -6.533206 -2.760655
C 0.790353 -7.281075 -1.842904
C 1.389106 -8.250287 -1.048098
C 2.770498 -8.444201 -1.200225
C 3.512913 -7.690219 -2.122383
C 2.897268 -6.716650 -2.922444
C 0.598343 -5.581691 -3.422212
C -0.638695 -6.846593 -1.911913
H 0.800502 -8.831602 -0.335953
H 3.279761 -9.194900 -0.591867
H 4.586513 -7.867246 -2.216620
H 3.461927 -6.126175 -3.646423
O 0.867938 -4.696268 -4.208027
O -1.559771 -7.279684 -1.269477
N -0.687095 -5.845053 -2.917621
C -1.738202 -4.852114 -3.182593
H -1.448847 -4.414818 -4.144305
C -3.206833 -5.371640 -3.333821
C -3.187692 -6.741209 -4.031068
H -2.587974 -6.711906 -4.954764
H -2.790405 -7.527049 -3.376378
H -4.214497 -7.024885 -4.308236
C -3.944927 -4.370582 -4.240254
H -3.473712 -4.296215 -5.232739
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H -4.068138 -4.453181 -1.543441
H -4.971162 -5.848006 -2.169932
C -1.531351 -3.765738 -2.118693
O -1.288945 -4.148784 -0.940837
N -1.471325 -2.467044 -2.415848
O -1.620387 -2.173886 -3.767481
C -2.176196 -0.859194 -3.984917
H -1.543244 -0.145739 -3.434488
C -3.603795 -0.725540 -3.473605
H -3.688209 -1.106846 -2.447211
H -3.892852 0.336408 -3.465353
H -4.315452 -1.271130 -4.110287
C -2.046279 -0.629207 -5.479400
H -2.440820 0.361494 -5.745434
H -0.994536 -0.684135 -5.797403
H -2.614602 -1.390558 -6.035400

[iii]RC

Charge = 1 Multiplicity = 1

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H 1.526123 -2.319639 -3.531846
C 3.892287 0.316634 0.715720
C 1.207137 3.891975 2.213881
C 2.746209 2.508796 0.876725
C 6.305468 0.099042 0.499226
H 7.193435 -0.524826 0.393877
O 4.900655 -1.843036 0.600452
C 0.325581 3.938091 1.104392
H -0.611949 4.480887 1.201269
C 0.614986 3.254538 -0.062504
C 1.973499 -1.810526 -1.377098
H 2.043957 -2.783504 -0.897477
C 2.538639 -0.353357 0.712539
H 1.817508 0.272126 1.240070
H 2.576878 -1.320879 1.217534
C 2.110186 -0.557643 -0.710333
C 1.701622 -0.142483 -2.949203
H 1.489016 0.374510 -3.883878
C 0.878895 4.516666 3.450133
H -0.042766 5.100726 3.514625
C 6.443888 1.511585 0.526129
C 2.422080 3.137185 2.121815
C 1.696735 4.379072 4.551822
H 1.429099 4.860924 5.494971
C 6.681260 4.322990 0.576206
H 6.784519 5.410125 0.591152
C 5.276773 2.334558 0.663379
C 1.867113 2.571576 -0.195246
C 3.996235 1.701307 0.752327
C 3.241256 3.011253 3.277518
H 4.157782 2.423933 3.213910
C 2.213813 1.961290 -1.532268
H 1.683307 2.501318 -2.325513
H 3.293523 2.100170 -1.710803
C 2.886563 3.613642 4.466743
H 3.526582 3.506865 5.345217
C 5.432188 3.748602 0.679588
H 4.546019 4.377310 0.775445
C 5.063221 -0.492719 0.604036
C 7.717217 2.136940 0.421575
H 8.604074 1.506948 0.318464
C 7.834622 3.509851 0.448406
H 8.819053 3.976219 0.367833
C 1.958888 0.491941 -1.705407
Si 5.278655 -2.928867 1.880356
C 4.426046 -4.507394 1.261367
C 2.895017 -4.428983 1.382116
C 4.956964 -5.814039 1.870319
H 4.676265 -4.508780 0.183797
H 2.493478 -3.472385 1.016962
H 2.408163 -5.239092 0.812049
H 2.570295 -4.533747 2.429505
H 6.029759 -5.955106 1.675675
H 4.811308 -5.848296 2.961965
H 4.430444 -6.685578 1.445814
C 7.165895 -3.042490 1.975120
C 7.760584 -3.547666 0.650679
C 7.705190 -3.825469 3.183005
H 7.480559 -1.990390 2.106110
H 7.386532 -2.976143 -0.213346
H 8.860697 -3.470760 0.655501
H 7.512048 -4.607047 0.475034
H 7.376297 -3.390701 4.138889
H 7.386765 -4.879147 3.170891
H 8.808082 -3.821094 3.185837
C 4.494062 -2.223028 3.462049
C 5.214305 -0.971907 3.992387
C 4.315135 -3.266359 4.577090
H 3.485333 -1.910836 3.137746
H 5.308246 -0.185430 3.230240
H 4.665388 -0.541631 4.847891
H 6.229497 -1.211652 4.347486
H 3.711927 -4.128658 4.256259
H 5.280769 -3.657172 4.933056
H 3.812745 -2.819372 5.452880
Si-1.595263 3.985082 -1.722720
C -0.927490 5.679737 -2.255243
C -1.933887 6.446275 -3.129869
C 0.456314 5.607955 -2.918571
H -0.807380 6.242864 -1.312017
H -2.944602 6.471801 -2.690962
H -1.613837 7.491035 -3.278215
H -2.022908 5.988834 -4.127571
H 1.200357 5.125193 -2.266488
H 0.425802 5.044689 -3.864366
H 0.829349 6.619002 -3.154007
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C -4.304283 3.680232 -0.643617
C -2.930343 5.545520 0.343295
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H -4.319640 2.672625 -1.079385
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H -4.797340 4.365873 -1.351409
H -1.943665 5.916243 0.660442
H -3.344111 6.294492 -0.350002
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O -1.415814 0.071905 -0.380387
C -0.478612 0.029015 2.137692
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C 1.028154 -1.293981 4.046156
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H 0.549522 -3.099036 2.951770
H 1.619265 -1.818583 4.798847
C -3.086745 0.502673 1.592834
C -3.567249 -0.807111 1.505366
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C -4.754554 -1.121794 2.163920
H -3.026098 -1.561903 0.932901
C -4.977229 1.172973 2.917576
H 0.009881 1.850891 3.204723
C -5.456600 -0.137840 2.869819
H -5.139084 -2.141564 2.120343
H -5.532750 1.943332 3.456271
H -6.388339 -0.395565 3.376226
H -3.385782 2.520480 2.320059
C -6.409271 -1.758773 -0.508335
C -6.070148 -0.424690 -0.753538
C -6.821690 0.621654 -0.237862
C -7.943416 0.288562 0.536410
C -8.286460 -1.049161 0.779008
C -7.515615 -2.099666 0.258163
C -5.398060 -2.624759 -1.176269
C -4.845762 -0.398959 -1.606359
H -6.543772 1.659222 -0.426921
H -8.562948 1.083790 0.956670
H -9.169712 -1.274798 1.380614
H -7.770771 -3.145193 0.441222
O -5.289800 -3.827989 -1.160102
O -4.229393 0.559698 -2.006356
N -4.529502 -1.743255 -1.859080
C -3.509780 -2.265229 -2.758801
H -3.470629 -3.328795 -2.487079
C -3.884403 -2.216786 -4.274007
C -5.212850 -2.971209 -4.454188
H -5.157769 -3.998552 -4.063729
H -6.040603 -2.457303 -3.942140
H -5.470630 -3.021439 -5.522726
C -2.777416 -2.962710 -5.041706
H -2.636454 -3.984027 -4.651329
H -3.049918 -3.047940 -6.104218
H -1.816617 -2.430401 -4.985637
C -4.033057 -0.790938 -4.827963
H -4.872840 -0.258658 -4.361080
H -3.126042 -0.197298 -4.663952
H -4.234173 -0.842401 -5.909601
C -2.122489 -1.743628 -2.435594
O -1.539609 -0.775046 -3.022244
N -1.327537 -2.325786 -1.547247
O -1.936735 -3.022608 -0.526062
C -1.300813 -4.295102 -0.265619
H -0.224824 -4.092202 -0.101589
C -1.476674 -5.239542 -1.444071
H -1.068603 -4.795555 -2.363773
H -0.947149 -6.185922 -1.256588
H -2.544005 -5.462488 -1.597961
C -1.946177 -4.798151 1.013681
H -1.518896 -5.770666 1.298634
H -1.790958 -4.093227 1.844048
H -3.029028 -4.924778 0.860309

S,iii**TS**

Charge = 1 Multiplicity = 1

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O 0.243327 3.085951 -1.583485
C 1.769456 -2.014970 -3.005221
H 1.425941 -2.761073 -3.719496
C 4.407263 -0.041705 0.343153
C 1.413333 3.335030 1.901347
C 2.989901 2.010156 0.549833
C 6.832847 0.068574 0.242490
H 7.800909 -0.427933 0.175946
O 5.709864 -2.047242 0.257763
C 0.651647 3.568792 0.730345
H -0.217643 4.215678 0.796377
C 0.971277 2.957262 -0.469401
C 2.298834 -2.268534 -1.711656
H 2.458449 -3.246808 -1.264362
C 3.147652 -0.863819 0.325911
H 2.410888 -0.383554 0.975987
H 3.329507 -1.865293 0.722870
C 2.574957 -1.008130 -1.056810
C 1.709356 -0.591852 -3.174246
H 1.336821 -0.063386 -4.048793
C 1.017130 3.856509 3.165046
H 0.117829 4.476016 3.218153
C 6.778031 1.486294 0.288456
C 2.602291 2.541522 1.823813
C 1.751648 3.590765 4.302209
H 1.433608 3.995233 5.265912
C 6.636862 4.301484 0.394024
H 6.593200 5.392100 0.431328
C 5.506942 2.143234 0.388024
C 2.158895 2.150470 -0.552365
C 4.320586 1.339791 0.417383
C 3.346107 2.298609 3.010911
H 4.255377 1.699393 2.951089
C 2.502385 1.509119 -1.875379
H 1.963396 2.021365 -2.678966
H 3.582575 1.632896 -2.070296
C 2.926322 2.802258 4.225237
H 3.504691 2.600930 5.129444
C 5.472187 3.564658 0.436381
H 4.508542 4.070534 0.505151
C 5.679781 -0.688415 0.279189
C 7.959908 2.276605 0.246913
H 8.925936 1.771535 0.171359
C 7.892384 3.652051 0.300121
H 8.808152 4.246500 0.267449
C 2.255855 0.031973 -1.997843
Si 6.125689 -3.125510 1.532037
C 5.926537 -4.793976 0.661140
C 4.465876 -5.035782 0.251183
C 6.513176 -5.995679 1.417066
H 6.511465 -4.663103 -0.268271
H 4.080436 -4.190013 -0.337556
H 4.368240 -5.947158 -0.362423
H 3.811193 -5.162332 1.129499
H 7.586901 -5.870940 1.620825
H 6.012248 -6.163570 2.383223
H 6.398460 -6.920639 0.827292
C 7.900570 -2.739509 2.064998
C 8.897915 -3.042671 0.934560
C 8.325676 -3.403923 3.384853
H 7.899503 -1.646610 2.234152
H 8.596874 -2.587463 -0.022240
H 9.904327 -2.666794 1.183352
H 8.991491 -4.127207 0.762724
H 7.693749 -3.092015 4.229687
H 8.284071 -4.502976 3.327569
H 9.364421 -3.132918 3.637584
C 4.850479 -2.844183 2.919321
C 5.042105 -1.492792 3.627617
C 4.743604 -3.995521 3.931202
H 3.886578 -2.802988 2.382642
H 5.082666 -0.651056 2.920936
H 4.213843 -1.294183 4.330012
H 5.974182 -1.474548 4.214461
H 4.471345 -4.947360 3.451029
H 5.686035 -4.160454 4.475302
H 3.971777 -3.776467 4.690120
Si-1.347614 3.595017 -2.028170
C -1.105549 5.372871 -2.642656
C -2.396201 5.998886 -3.196680
C 0.059332 5.525540 -3.631900
H -0.831144 5.927571 -1.725299
H -3.257359 5.866950 -2.522741
H -2.270136 7.082189 -3.360338
H -2.669800 5.555026 -4.166024
H 0.987726 5.080036 -3.243333
H -0.166111 5.040585 -4.594916
H 0.258310 6.589478 -3.844430
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C -0.698245 2.042496 -4.348275
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H -1.669251 5.423305 0.414198
H -3.272360 5.570860 -0.305302
H -3.081193 4.736216 1.246732
S -0.474697 0.513074 0.944714
O -0.751394 0.289654 -0.588033
C 0.041678 -1.130797 1.485307
C 0.615771 -1.281670 2.745025
C -0.005760 -2.160527 0.529156
C 1.156193 -2.525878 3.084118
C 0.545411 -3.402103 0.907845
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C 1.125050 -3.582339 2.164102
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H 0.489017 -4.241752 0.210214
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C -4.594003 0.977324 2.822468
H -5.257162 -0.556940 1.441531
H -3.669075 2.493267 4.060824
H -5.580072 1.105157 3.274564
H -1.412729 2.215505 3.011256
C -6.689210 -2.053438 -1.477723
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C -7.920422 -2.298125 -0.884032
C -5.734018 -2.987748 -2.140407
C -4.800600 -0.859484 -2.167323
H -6.331963 1.310960 -0.949118
H -8.571287 0.908880 0.126194
H -9.557888 -1.357509 0.169487
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O -5.798219 -4.186788 -2.261605
O -3.954797 -0.001488 -2.291206
N -4.664336 -2.183516 -2.591239
C -3.415314 -2.774089 -3.053976
H -3.540430 -3.844376 -2.827450
C -3.193835 -2.673219 -4.589488
C -4.433378 -3.277011 -5.275144
H -4.623938 -4.307634 -4.939239
H -5.335842 -2.683000 -5.068496
H -4.286749 -3.290774 -6.365670
C -1.967882 -3.525335 -4.964339
H -2.080311 -4.562554 -4.607269
H -1.859032 -3.563194 -6.058891
H -1.045441 -3.107735 -4.540466
C -3.007855 -1.226771 -5.070004
H -3.906303 -0.624215 -4.876502
H -2.163427 -0.742823 -4.565971
H -2.829331 -1.217628 -6.156878
C -2.270085 -2.315558 -2.135374
O -1.234428 -1.746161 -2.626684
N -2.324011 -2.545419 -0.849997
O -3.508042 -3.085845 -0.354067
C -3.277185 -4.233452 0.486222
H -2.509326 -3.951217 1.230423
C -2.790506 -5.417203 -0.337526
H -1.872980 -5.160504 -0.889261
H -2.566585 -6.275397 0.314434
H -3.563547 -5.719204 -1.060794
C -4.603993 -4.485596 1.180714
H -4.515243 -5.331184 1.878665
H -4.918588 -3.596015 1.746403
H -5.379764 -4.725142 0.437758

R,iii**TS**

Charge = 1 Multiplicity = 1

Rh -0.585258 0.315102 -1.297724
O 1.394374 3.681135 -0.172362
C -0.057193 -0.443083 -3.242977
H -0.775484 -0.601452 -4.045027
C 3.381396 -1.460184 -0.203294
C 2.566179 1.976380 2.881415
C 3.358757 0.775745 0.878501
C 5.438500 -2.593365 -0.828473
H 5.952620 -3.455123 -1.253682
O 3.313966 -3.645189 -1.172075
C 1.951149 2.925647 2.026401
H 1.390314 3.751389 2.461977
C 2.012261 2.794926 0.655993
C 0.328817 -1.396445 -2.260676
H -0.095321 -2.388709 -2.128165
C 1.875907 -1.437365 -0.162182
H 1.551028 -0.876573 0.719197
H 1.464459 -2.445015 -0.079515
C 1.281430 -0.791661 -1.377940
C 0.747044 0.742056 -3.030226
H 0.707279 1.653432 -3.622145
C 2.469177 2.069863 4.297203
H 1.914412 2.905503 4.731857
C 6.197811 -1.481402 -0.378444
C 3.298483 0.888466 2.305591
C 3.062891 1.127161 5.109502
H 2.980141 1.210193 6.195613
C 7.674020 0.747046 0.530114
H 8.255591 1.603895 0.877247
C 5.525682 -0.348156 0.187918
C 2.692828 1.683618 0.068524
C 4.097881 -0.370350 0.267811
C 3.902519 -0.064861 3.171405
H 4.460811 -0.894847 2.736997
C 2.638572 1.493631 -1.429644
H 2.474754 2.454581 -1.924107
H 3.604863 1.097486 -1.783509
C 3.785348 0.049368 4.540992
H 4.252866 -0.692552 5.191900
C 6.299152 0.759058 0.634367
H 5.787812 1.622459 1.062796
C 4.060111 -2.595626 -0.743165
C 7.617273 -1.460867 -0.470337
H 8.127464 -2.325724 -0.901452
C 8.339062 -0.373813 -0.026175
H 9.428678 -0.372796 -0.103181
C 1.589935 0.532032 -1.916068
Si 3.027082 -5.173359 -0.437469
C 2.086757 -6.068060 -1.814271
C 0.734651 -5.393315 -2.090001
C 1.935813 -7.583681 -1.612909
H 2.725344 -5.908563 -2.702958
H 0.864486 -4.319889 -2.293819
H 0.234076 -5.841775 -2.964718
H 0.045985 -5.493356 -1.235326
H 2.907739 -8.085919 -1.496589
H 1.332509 -7.825206 -0.724196
H 1.432380 -8.043100 -2.480224
C 4.717872 -5.933346 -0.043272
C 5.475990 -6.295178 -1.331737
C 4.678321 -7.121247 0.931722
H 5.269862 -5.115502 0.456729
H 5.486027 -5.469545 -2.060586
H 6.523454 -6.561851 -1.112653
H 5.019486 -7.163261 -1.833658
H 4.262506 -6.841582 1.910909
H 4.075671 -7.956861 0.541587
H 5.694934 -7.511151 1.108199
C 1.957573 -4.858183 1.107334
C 2.722637 -4.102787 2.206955
C 1.271860 -6.115410 1.666721
H 1.151723 -4.195112 0.741343
H 3.170597 -3.165609 1.844383
H 2.053629 -3.845482 3.046069
H 3.538910 -4.715400 2.622160
H 0.601596 -6.582589 0.930228
H 1.997546 -6.878794 1.984985
H 0.661668 -5.862351 2.550732
Si 1.682416 5.369641 -0.354082
C 3.534784 5.640782 -0.058611
C 3.959287 7.119154 -0.116592
C 4.424985 4.774986 -0.964114
H 3.682292 5.293281 0.981229
H 3.312472 7.773782 0.486613
H 4.988405 7.239748 0.260246
H 3.946054 7.503368 -1.146839
H 4.239438 3.700870 -0.823521
H 4.273099 5.009450 -2.030418
H 5.491350 4.950398 -0.744021
C 1.048027 5.723509 -2.115295
C 1.114568 4.516011 -3.057700
C 1.695962 6.963016 -2.753208
H -0.020831 5.953776 -1.973130
H 0.578022 3.656044 -2.635957
H 0.659334 4.757906 -4.033097
H 2.155367 4.209985 -3.252503
H 1.637276 7.852006 -2.107397
H 2.759007 6.788294 -2.980883
H 1.198347 7.215053 -3.704686
C 0.598781 6.292387 0.924722
C -0.023581 7.594280 0.391203
C 1.287461 6.561509 2.273693
H -0.224969 5.574724 1.107274
H -0.609827 7.444031 -0.528097
H -0.696999 8.040233 1.142156
H 0.748072 8.348524 0.167074
H 1.777789 5.673583 2.696767
H 2.061753 7.337669 2.176555
H 0.559432 6.925095 3.017835
S -1.309611 2.641871 0.749822
O -0.402163 1.390917 0.497825
C -2.801030 1.996306 1.532549
C -2.606932 1.507679 2.832082
C -4.060932 1.986446 0.930895
C -3.691049 0.975255 3.526014
H -1.615075 1.530738 3.288368
C -5.142516 1.464503 1.645952
H -4.207583 2.368012 -0.077889
C -4.958267 0.956020 2.932996
H -3.549504 0.576570 4.532350
H -6.132364 1.446741 1.186718
H -5.806761 0.540244 3.477558
C -1.890473 3.043836 -0.893151
C -2.093234 4.374970 -1.239771
C -2.021447 1.976618 -1.808141
C -2.444582 4.678814 -2.560122
H -1.967379 5.168885 -0.501556
C -2.368970 2.323159 -3.126583
H -2.639843 0.904296 -1.506051
C -2.569371 3.654682 -3.502087
H -2.608010 5.718101 -2.851929
H -2.529655 1.525931 -3.855977
H -2.840866 3.894065 -4.532463
C -7.487906 -0.951251 0.186650
C -7.081024 -1.369120 1.455337
C -7.907453 -1.239739 2.564727
C -9.168762 -0.659125 2.364436
C -9.575356 -0.233836 1.090781
C -8.736036 -0.379676 -0.024353
C -6.393642 -1.243376 -0.788583
C -5.698513 -1.905138 1.340165
H -7.583250 -1.582331 3.549424
H -9.848728 -0.539301 3.210659
H 10.564384 0.212694 0.967060
H -9.043732 -0.061182 -1.022147
O -6.407453 -1.064536 -1.980172
O -4.972599 -2.323714 2.214475
N -5.351490 -1.815080 -0.022999
C -4.019707 -2.229637 -0.443184
H -3.624773 -2.743794 0.435636
C -3.945053 -3.266346 -1.631377
C -5.181770 -4.177335 -1.570956
H -5.320827 -4.600330 -0.563454
H -6.098208 -3.646611 -1.860530
H -5.050831 -5.017099 -2.270236
C -2.691216 -4.134585 -1.418610
H -2.743718 -4.699271 -0.475210
H -2.593724 -4.856828 -2.242972
H -1.777157 -3.529829 -1.380267
C -3.847331 -2.596202 -3.012052
H -4.674441 -1.897891 -3.180754
H -2.899801 -2.043199 -3.115608
H -3.863678 -3.370831 -3.794308
C -3.163457 -0.993912 -0.700913
O -3.666090 -0.033793 -1.343714
N -1.900253 -0.919536 -0.290438
O -1.390889 -2.001325 0.413885
C -1.533582 -1.889350 1.866833
H -2.467302 -1.336834 2.052395
C -0.359007 -1.160604 2.500344
H -0.178778 -0.193525 2.016204
H -0.572782 -0.981229 3.565608
H 0.556617 -1.767205 2.446925
C -1.672371 -3.316790 2.368769
H -1.699605 -3.322084 3.468390
H -2.598206 -3.784884 2.009283
H -0.811740 -3.921053 2.044100

^{R,iii}IM

Charge = 1 Multiplicity = 1

Rh -0.485438 0.332979 -1.267950
O 1.450860 3.586961 -0.147054
C 0.023179 -0.592209 -3.142388
H -0.683340 -0.812479 -3.940138
C 3.546968 -1.485672 -0.165192
C 2.935829 2.033577 2.849581
C 3.599599 0.788128 0.826004
C 5.558268 -2.681105 -0.825898
H 6.041131 -3.574266 -1.222667
O 3.409528 -3.726021 -0.993604
C 2.212202 2.926154 2.019392
H 1.657354 3.744738 2.475096
C 2.170593 2.754056 0.652838
C 0.467039 -1.508237 -2.120359
H 0.049148 -2.492268 -1.923888
C 2.044406 -1.443906 -0.068703
H 1.749780 -0.831103 0.790977
H 1.636268 -2.445326 0.077889
C 1.424240 -0.873298 -1.308862
C 0.815461 0.597377 -3.004923
H 0.764435 1.479688 -3.638955
C 2.961604 2.182238 4.263747
H 2.419091 3.017732 4.713870
C 6.349976 -1.552567 -0.485015
C 3.651346 0.947580 2.250226
C 3.657133 1.292909 5.054816
H 3.669882 1.418770 6.139916
C 7.892411 0.706185 0.214377
H 8.499036 1.574749 0.479981
C 5.719002 -0.380939 0.049886
C 2.851889 1.655273 0.042272
C 4.297319 -0.380664 0.208778
C 4.356511 0.046039 3.095409
H 4.900315 -0.785532 2.646608
C 2.718208 1.442611 -1.447790
H 2.514828 2.396175 -1.943006
H 3.672945 1.060152 -1.845584
C 4.358991 0.213406 4.464554
H 4.906325 -0.488024 5.097970
C 6.525255 0.740019 0.390908
H 6.044887 1.632248 0.795656
C 4.186733 -2.659770 -0.669809
C 7.762498 -1.554035 -0.653216
H 8.241160 -2.448008 -1.060523
C 8.516766 -0.452050 -0.311347
H 9.600622 -0.468235 -0.446379
C 1.662128 0.457706 -1.869855
Si 3.121635 -5.189617 -0.141503
C 2.069381 -6.140667 -1.395576
C 0.726822 -5.436214 -1.645740
C 1.882677 -7.632703 -1.081026
H 2.659314 -6.065739 -2.327976
H 0.884723 -4.389213 -1.942330
H 0.159500 -5.931334 -2.451962
H 0.085517 -5.439704 -0.748363
H 2.843830 -8.159476 -0.985386
H 1.325882 -7.792749 -0.144836
H 1.315174 -8.131971 -1.884487
C 4.810044 -5.977798 0.201861
C 5.481063 -6.438714 -1.102942
C 4.795625 -7.101332 1.250697
H 5.411505 -5.147152 0.616780
H 5.474256 -5.655818 -1.877548
H 6.530789 -6.727788 -0.927377
H 4.969997 -7.318137 -1.526871
H 4.441370 -6.749815 2.230998
H 4.151799 -7.942242 0.947320
H 5.810403 -7.508157 1.397050
C 2.159274 -4.740963 1.440985
C 3.011875 -3.940843 2.439744
C 1.463387 -5.928954 2.124468
H 1.355141 -4.075415 1.077055
H 3.472997 -3.051337 1.985731
H 2.401627 -3.595683 3.292014
H 3.826630 -4.556189 2.853980
H 0.741852 -6.424923 1.458459
H 2.179604 -6.692908 2.462878
H 0.907022 -5.589411 3.015046
Si 1.585337 5.293704 -0.340525
C 3.419110 5.718576 -0.116190
C 3.718690 7.225024 -0.210584
C 4.340818 4.913364 -1.045618
H 3.634779 5.400551 0.921015
H 3.042951 7.834722 0.407916
H 4.747938 7.436373 0.123715
H 3.634077 7.588856 -1.244880
H 4.227387 3.828590 -0.906143
H 4.146463 5.140964 -2.106368
H 5.398857 5.157204 -0.851758
C 0.860131 5.584511 -2.074705
C 1.094703 4.423523 -3.048879
C 1.295239 6.921722 -2.695873
H -0.227892 5.635980 -1.903749
H 0.702702 3.485158 -2.639125
H 0.586012 4.613715 -4.009278
H 2.165643 4.284734 -3.269086
H 1.146621 7.776677 -2.019471
H 2.359560 6.904018 -2.977857
H 0.721393 7.126807 -3.615180
C 0.477932 6.119260 0.986530
C -0.328802 7.323484 0.472341
C 1.202190 6.498911 2.289198
H -0.240743 5.313047 1.228102
H -0.924172 7.087928 -0.422238
H -1.024171 7.686044 1.248288
H 0.329210 8.169258 0.215284
H 1.815613 5.684635 2.700104
H 1.873580 7.357354 2.135622
H 0.477684 6.792632 3.067082
S -1.104808 2.487440 0.982694
O -0.257288 1.216655 0.636196
C -2.614328 1.823609 1.736473
C -2.432341 1.240921 2.997078
C -3.873602 1.861933 1.133600
C -3.520922 0.653106 3.640517
H -1.444471 1.232351 3.462565
C -4.960151 1.284762 1.796285
H -4.016728 2.332757 0.162549
C -4.783897 0.672312 3.039075
H -3.384752 0.182503 4.616264
H -5.948796 1.312654 1.334758
H -5.634778 0.211332 3.542852
C -1.714049 2.990918 -0.619452
C -2.293294 4.248523 -0.784969
C -1.556049 2.048711 -1.655629
C -2.766570 4.605004 -2.050063
H -2.377255 4.942164 0.054462
C -2.039145 2.452403 -2.915805
H -3.100019 0.866842 -1.665611
C -2.637040 3.703995 -3.110196
H -3.225693 5.582933 -2.206112
H -1.960475 1.772976 -3.767920
H -3.002024 3.976973 -4.102955
C -7.621293 -0.695965 0.038398
C -7.209949 -1.290763 1.233552
C -8.005033 -1.263571 2.372751
C -9.239720 -0.603946 2.280121
C -9.651209 -0.002997 1.081037
C -8.843356 -0.044026 -0.065656
C -6.560936 -0.903634 -0.992044
C -5.862881 -1.877596 1.015647
H -7.678076 -1.742475 3.297772
H -9.894963 -0.559836 3.152693
H 10.619261 0.500985 1.040768
H -9.155514 0.413883 -1.006125
O -6.578856 -0.560985 -2.146855
O -5.149866 -2.457925 1.802259
N -5.528149 -1.612451 -0.331571
C -4.233514 -2.055279 -0.835325
H -3.853391 -2.687490 -0.030794
C -4.235908 -2.962409 -2.127563
C -5.482831 -3.858640 -2.075485
H -5.562144 -4.383734 -1.110358
H -6.406198 -3.287318 -2.241976
H -5.418654 -4.620572 -2.866694
C -2.979554 -3.851797 -2.070749
H -2.962553 -4.482899 -1.169745
H -2.955233 -4.511034 -2.951201
H -2.059272 -3.252998 -2.071576
C -4.206209 -2.165460 -3.441836
H -5.040010 -1.458340 -3.509534
H -3.265015 -1.601557 -3.544007
H -4.260581 -2.865974 -4.289239
C -3.293358 -0.876022 -0.952985
O -3.792232 0.170281 -1.566842
N -2.068453 -0.850350 -0.517916
O -1.640746 -2.037564 0.081045
C -1.786048 -2.092820 1.539137
H -2.690203 -1.519454 1.795418
C -0.571741 -1.522983 2.250939
H -0.332867 -0.513415 1.899468
H -0.774519 -1.479592 3.332246
H 0.303475 -2.170992 2.102284
C -1.997804 -3.564585 1.854210
H -2.035143 -3.705399 2.944385
H -2.940617 -3.941094 1.437151
H -1.159887 -4.161557 1.461717

[iv]RC

Charge = 1 Multiplicity = 1

Rh 0.641034 -1.667411 -1.865416
O 0.359523 2.644111 -2.100870
C 2.177723 -2.541770 -3.034473
H 1.960575 -3.367834 -3.709767
C 4.343823 -0.282363 0.383160
C 1.375669 3.282430 1.385301
C 3.007521 1.819630 0.254981
C 6.774728 -0.277393 0.398122
H 7.721105 -0.816715 0.449871
O 5.554690 -2.322923 0.658876
C 0.668743 3.386473 0.161919
H -0.214768 4.021702 0.120786
C 1.051365 2.653631 -0.946424
C 2.538556 -2.654113 -1.650447
H 2.609139 -3.587519 -1.094332
C 3.053684 -1.057326 0.341832
H 2.271465 -0.466915 0.823137
H 3.132536 -2.000522 0.889132
C 2.669411 -1.354560 -1.079611
C 2.125939 -1.137604 -3.329237
H 1.862439 -0.694956 -4.289071
C 0.924674 3.929866 2.570231
H 0.031352 4.558081 2.519416
C 6.781063 1.135605 0.261722
C 2.561411 2.481643 1.445313
C 1.598602 3.773298 3.763666
H 1.235909 4.271346 4.665634
C 6.756690 3.947016 0.019705
H 6.758900 5.035005 -0.075652
C 5.536415 1.847770 0.217555
C 2.238855 1.851226 -0.899296
C 4.317013 1.099124 0.278222
C 3.242484 2.353050 2.687015
H 4.142175 1.739789 2.734313
C 2.651855 1.095361 -2.139121
H 2.141682 1.521930 -3.010258
H 3.736773 1.230445 -2.293993
C 2.767274 2.974432 3.823572
H 3.296794 2.857619 4.771462
C 5.560720 3.264765 0.093627
H 4.616897 3.810366 0.055261
C 5.587795 -0.977355 0.477501
C 7.996278 1.870672 0.182462
H 8.942199 1.324733 0.216870
C 7.985815 3.243884 0.065601
H 8.927012 3.795006 0.006516
C 2.433203 -0.393665 -2.147527
Si 5.837905 -3.144674 2.146739
C 5.241066 -4.888481 1.710906
C 3.718611 -4.933580 1.507412
C 5.713475 -5.993114 2.668499
H 5.711908 -5.072421 0.726943
H 3.383670 -4.167129 0.793700
H 3.397084 -5.914739 1.119199
H 3.173438 -4.761171 2.449069
H 6.810371 -6.053055 2.721011
H 5.341615 -5.839938 3.693865
H 5.348074 -6.979039 2.335204
C 7.694382 -3.022846 2.500802
C 8.513388 -3.687692 1.382748
C 8.118512 -3.519516 3.892377
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H 8.219821 -3.324483 0.385160
H 9.591202 -3.491482 1.509942
H 8.381803 -4.782142 1.384469
H 7.617174 -2.966976 4.701199
H 7.898098 -4.588538 4.035794
H 9.204716 -3.391572 4.035016
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H 4.006603 -4.104595 4.450305
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H 3.876209 -2.631661 5.434885
Si-0.840069 3.711990 -2.724923
C -0.171321 5.485856 -2.591236
C -0.861919 6.438387 -3.584341
C 1.358376 5.571088 -2.725985
H -0.437454 5.820857 -1.570930
H -1.959617 6.407938 -3.512729
H -0.549182 7.480201 -3.404043
H -0.590701 6.196170 -4.624003
H 1.879255 4.978123 -1.960323
H 1.698050 5.217037 -3.711712
H 1.696202 6.615832 -2.621920
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H 0.454089 4.238064 -5.572791
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H -2.201236 4.607628 -5.436370
H -2.317822 3.028835 -6.231256
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C -3.000949 2.060573 -1.886148
C -3.466231 4.558390 -1.840428
H -2.051193 3.505097 -0.632965
H -2.252020 1.264776 -1.760887
H -3.811721 1.865534 -1.165905
H -3.430816 1.961383 -2.894210
H -3.074431 5.555457 -1.587174
H -3.856160 4.606829 -2.869665
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C -4.424620 0.178127 1.320171
H -2.969599 -1.128309 0.368104
C -3.544553 2.248882 2.234238
H 0.862447 0.677344 3.113372
C -4.623209 1.397572 1.980567
H -5.272324 -0.481715 1.123687
H -3.703649 3.199174 2.747970
H -5.627853 1.685008 2.298005
H -1.404297 2.542891 2.010345
C -2.314149 -4.690497 -6.491117
C -0.965862 -4.920062 -6.197864
C -0.039198 -5.176638 -7.199452
C -0.508182 -5.199456 -8.522022
C -1.859564 -4.967520 -8.815583
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C -3.026348 -4.429456 -5.210542
C -0.784773 -4.809814 -4.722551
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H 0.189046 -5.401567 -9.338052
H -2.192917 -4.992072 -9.855322
H -3.842078 -4.523030 -8.012621
O -4.171858 -4.095245 -5.024568
O 0.243378 -4.837348 -4.079289
N -2.065244 -4.611043 -4.191539
C -2.362345 -4.258290 -2.807462
H -3.318313 -3.716034 -2.876236
C -2.614818 -5.478476 -1.874612
C -3.704402 -6.348214 -2.525926
H -4.615613 -5.769270 -2.739303
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H -3.971111 -7.176726 -1.852679
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H -4.054478 -4.343568 -0.672641
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H -0.969589 -6.725190 -2.609197
H -0.552077 -5.746689 -1.185689
H -1.595714 -7.186663 -1.012560
C -1.336846 -3.237467 -2.336679
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C -2.374497 -0.704688 -4.310124
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C -3.702020 -0.916065 -3.598685
H -3.540731 -1.124773 -2.530671
H -4.318862 -0.008721 -3.669272
H -4.254966 -1.750430 -4.055451
C -2.516321 -0.401441 -5.789628
H -3.096084 0.522313 -5.931008
H -1.529872 -0.269072 -6.258044
H -3.041825 -1.221780 -6.302639

S,iv**TS**

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H 1.389238 -3.025600 -3.716314
C 4.377018 -0.153877 0.247115
C 1.425389 3.349030 1.555684
C 3.018028 1.942679 0.304102
C 6.807184 -0.121708 0.193460
H 7.760432 -0.650087 0.180516
O 5.618500 -2.197462 0.306144
C 0.639831 3.454890 0.380178
H -0.258483 4.070482 0.408714
C 0.992286 2.787764 -0.780659
C 2.243445 -2.443457 -1.721940
H 2.339894 -3.399368 -1.213243
C 3.096325 -0.944229 0.248327
H 2.359411 -0.406323 0.851780
H 3.240327 -1.922741 0.712233
C 2.554328 -1.162151 -1.138933
C 1.764337 -0.837666 -3.299663
H 1.463824 -0.345710 -4.221195
C 1.041265 3.984805 2.769290
H 0.136223 4.598016 2.777211
C 6.795616 1.297012 0.147464
C 2.627766 2.572188 1.532802
C 1.795670 3.838545 3.915082
H 1.487479 4.332017 4.839690
C 6.739708 4.116316 0.065148
H 6.728939 5.207844 0.029707
C 5.543881 1.996387 0.177247
C 2.197549 2.008578 -0.812140
C 4.332911 1.232534 0.235106
C 3.385830 2.445663 2.728964
H 4.301700 1.853844 2.713603
C 2.566687 1.306768 -2.097045
H 2.047442 1.784598 -2.935180
H 3.651380 1.414779 -2.270271
C 2.976374 3.056729 3.896431
H 3.568053 2.945826 4.807499
C 5.552408 3.418283 0.131147
H 4.603476 3.955680 0.146526
C 5.630375 -0.840307 0.250336
C 8.001870 2.047868 0.079998
H 8.953113 1.510528 0.058573
C 7.976151 3.425250 0.041391
H 8.910406 3.988807 -0.010216
C 2.294028 -0.169377 -2.150063
Si 5.947646 -3.231407 1.640657
C 5.788933 -4.929259 0.820017
C 4.351007 -5.180322 0.340584
C 6.327521 -6.103818 1.650585
H 6.425084 -4.833902 -0.079599
H 4.003425 -4.359558 -0.304334
H 4.280370 -6.116839 -0.238032
H 3.647131 -5.265566 1.185070
H 7.385995 -5.969745 1.918656
H 5.765942 -6.241557 2.587565
H 6.250845 -7.048099 1.085643
C 7.694002 -2.827523 2.251978
C 8.748656 -3.198798 1.196059
C 8.045289 -3.417735 3.627357
H 7.692436 -1.726540 2.358223
H 8.499896 -2.804176 0.198278
H 9.741623 -2.807680 1.473923
H 8.848032 -4.291775 1.096663
H 7.375912 -3.051676 4.419939
H 7.993820 -4.518050 3.631180
H 9.073412 -3.141718 3.915911
C 4.596816 -2.905995 2.943752
C 4.722603 -1.516480 3.589967
C 4.465847 -4.007558 4.007482
H 3.658622 -2.917919 2.361207
H 4.763340 -0.708249 2.844981
H 3.863311 -1.311248 4.251965
H 5.631554 -1.439665 4.207961
H 4.225069 -4.985325 3.564387
H 5.387016 -4.130856 4.596745
H 3.660547 -3.762939 4.722241
Si-1.113111 3.773082 -2.332060
C -0.644637 5.601454 -2.088370
C -1.525405 6.551170 -2.919034
C 0.846280 5.874599 -2.348948
H -0.842224 5.817842 -1.021926
H -2.601630 6.373614 -2.773841
H -1.325164 7.601435 -2.649529
H -1.313778 6.449448 -3.995038
H 1.500534 5.286953 -1.688930
H 1.124531 5.640456 -3.388660
H 1.077763 6.940125 -2.182756
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C 0.507037 -1.617824 2.611564
C -0.107525 -2.280277 0.316285
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H -3.221941 2.873269 3.906202
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C -1.223583 -4.983889 -5.692072
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C -2.398867 -4.207764 -5.207391
C -1.140862 -4.834338 -3.357711
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H 2.042186 -6.984402 -6.160139
H 0.704543 -6.315752 -8.127821
H -1.427136 -5.008333 -7.845127
O -3.237905 -3.617804 -5.842967
O -0.733913 -4.842077 -2.214167
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C -3.189138 -3.381409 -2.985934
H -3.649869 -2.705694 -3.719002
C -4.355081 -4.140979 -2.289068
C -5.153469 -4.865302 -3.388993
H -5.501311 -4.169791 -4.167451
H -4.550753 -5.645020 -3.877892
H -6.033173 -5.355937 -2.946300
C -5.278324 -3.109609 -1.615764
H -5.614896 -2.347169 -2.337965
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H -4.781229 -2.603339 -0.778498
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H -3.285980 -4.711238 -0.461017
H -4.728665 -5.696779 -0.826919
C -2.293737 -2.515933 -2.090855
O -2.413975 -2.540524 -0.828535
N -1.337434 -1.773002 -2.632335
O -1.219045 -1.863372 -4.017154
C -1.466403 -0.596908 -4.673118
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C -2.948731 -0.256098 -4.678861
H -3.349490 -0.220454 -3.656695
H -3.105466 0.735643 -5.128272
H -3.508449 -0.997972 -5.267236
C -0.891661 -0.750005 -6.070341
H -0.994354 0.194287 -6.625104
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H -1.431959 -1.535373 -6.620199

^{S,iv}IM

Charge = 1 Multiplicity = 1

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C 2.373137 3.970708 1.263430
C 2.797469 2.256473 -0.455255
C 5.388849 -0.671175 -2.283633
H 6.033577 -1.423375 -2.739542
O 4.154888 -2.370474 -1.125703
C 1.055515 4.111758 0.756661
H 0.381541 4.822421 1.231489
C 0.615207 3.350925 -0.309886
C 0.487072 -2.019684 -1.165485
H 0.744040 -2.963032 -0.690175
C 2.330329 -0.549203 -0.035199
H 2.110092 0.201194 0.730708
H 2.552080 -1.489307 0.477838
C 1.127513 -0.763707 -0.917663
C -0.518483 -0.424720 -2.522732
H -1.166506 0.042145 -3.261059
C 2.833153 4.738779 2.369845
H 2.160742 5.480881 2.808202
C 5.608729 0.702774 -2.565881
C 3.260083 3.017103 0.667921
C 4.100952 4.555165 2.881424
H 4.440658 5.153269 3.730214
C 6.019183 3.443279 -3.102350
H 6.185418 4.500796 -3.318879
C 4.766908 1.693793 -1.959319
C 1.500879 2.406559 -0.924965
C 3.708308 1.261042 -1.098208
C 4.558726 2.847594 1.222600
H 5.230850 2.112635 0.778521
C 1.002349 1.609392 -2.105642
H 0.196734 2.157907 -2.604218
H 1.824543 1.506626 -2.834359
C 4.969864 3.595413 2.306526
H 5.970337 3.452756 2.720270
C 4.999083 3.065799 -2.254923
H 4.356543 3.821073 -1.800211
C 4.373136 -1.066017 -1.436765
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H 7.292239 0.369946 -3.893980
C 6.854671 2.465144 -3.696215
H 7.660344 2.775741 -4.365235
C 0.532994 0.208288 -1.838080
Si 5.080422 -3.338220 -0.044558
C 3.916082 -4.816072 0.199548
C 2.698286 -4.463357 1.069355
C 4.599316 -6.097528 0.701368
H 3.549035 -5.008569 -0.826284
H 2.196098 -3.544169 0.734795
H 1.949869 -5.274081 1.052564
H 2.980489 -4.309214 2.122973
H 5.388748 -6.440990 0.017310
H 5.058261 -5.958674 1.693161
H 3.867987 -6.918209 0.795157
C 6.694778 -3.754431 -0.944770
C 6.416396 -4.510161 -2.254174
C 7.756811 -4.462861 -0.089125
H 7.102796 -2.761252 -1.210305
H 5.668249 -3.993503 -2.875746
H 7.336441 -4.618485 -2.852716
H 6.036268 -5.526467 -2.059795
H 8.048172 -3.866006 0.788061
H 7.409803 -5.441474 0.276694
H 8.671444 -4.643672 -0.678598
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C 6.352547 -1.165665 1.353053
C 5.754029 -3.192290 2.750309
H 4.368135 -1.883784 1.766092
H 6.065272 -0.493946 0.531661
H 6.422151 -0.558801 2.272031
H 7.366164 -1.538649 1.134570
H 5.007450 -3.968954 2.972636
H 6.718415 -3.699290 2.591762
H 5.862155 -2.571115 3.655670
Si-1.712127 4.712046 -1.173491
C -0.830266 5.869614 -2.397828
C -1.818634 6.642797 -3.288546
C 0.233405 5.157386 -3.249222
H -0.306653 6.605760 -1.758568
H -2.590368 7.171897 -2.709017
H -1.290114 7.395635 -3.896708
H -2.336827 5.967852 -3.988333
H 1.018867 4.694553 -2.633903
H -0.210706 4.367606 -3.876490
H 0.726415 5.871419 -3.930155
C -3.166879 3.706097 -1.855175
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C -4.470817 4.488346 -2.068530
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H -1.882929 2.299871 -2.938533
H -3.602096 2.206239 -3.385760
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H -4.830885 4.956029 -1.140870
H -4.358976 5.283927 -2.820924
H -5.270549 3.816488 -2.423264
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C -3.010083 6.883493 0.245389
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H -2.817754 5.203637 2.469504
H -3.686992 4.300299 1.213351
H -2.561679 7.604263 -0.455280
H -4.012325 6.632178 -0.133070
H -3.149622 7.406569 1.206531
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H -1.295736 -4.361466 3.404300
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C -4.284912 -3.405174 4.639099
C -4.782546 -4.691366 4.898199
C -5.785659 -5.255606 4.096363
C -6.326849 -4.551706 3.009535
C -6.166218 -2.300944 1.692868
C -4.503127 -1.370028 3.018455
H -3.499707 -2.957341 5.249637
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R,iv**TS**

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8. X-Ray Crystallographic Data

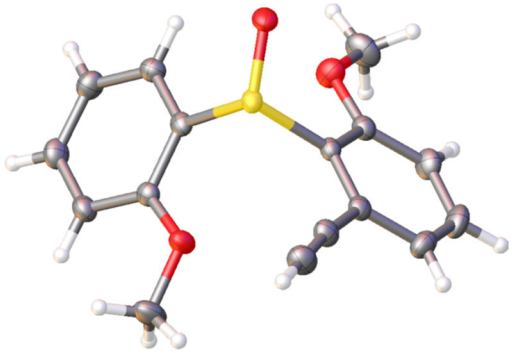


Table S2 Crystal data and structure refinement for **9**.

dentification code	s
Empirical formula	$C_{16}H_{14}O_3S$
Formula weight	286.33
Temperature/K	219.00
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.6531(5)
b/Å	10.1518(7)
c/Å	18.1461(13)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1409.82(17)
Z	4
ρ_{calc}g/cm^3	1.349
μ/mm^{-1}	2.080
F(000)	600.0
Crystal size/mm^3	0.5 × 0.4 × 0.3
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	9.748 to 137.014
Index ranges	-9 ⩽ h ⩽ 9, -12 ⩽ k ⩽ 12, -21 ⩽ l ⩽ 21
Reflections collected	26001

Independent reflections	2592 [R_{int} = 0.0487, R_{sigma} = 0.0218]
Data/restraints/parameters	2592/0/183
Goodness-of-fit on F^2	1.091
Final R indexes [I>=2σ (I)]	R_1 = 0.0233, wR_2 = 0.0611
Final R indexes [all data]	R_1 = 0.0242, wR_2 = 0.0617
Largest diff. peak/hole / e $Å^{-3}$	0.20/-0.18
Flack parameter	0.049(6)

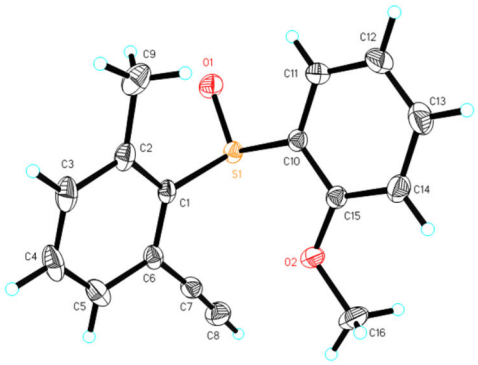


Table S3 Crystal data and structure refinement for **11**.

Identification code	mo_d8v22234_0m	
Empirical formula	C16 H14 O2 S	
Formula weight	270.33	
Temperature	213(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 7.6856(3) Å	α= 90°.
	b = 10.0965(4) Å	β= 90°.
	c = 18.0404(8) Å	γ = 90°.
Volume	1399.89(10) $Å^3$	
Z	4	
Density (calculated)	1.283 Mg/m^3	
Absorption coefficient	0.226 mm^{-1}	
F(000)	568	
Crystal size	0.200 x 0.150 x 0.110 mm^3	
Theta range for data collection	2.881 to 25.995°.	
Index ranges	-9<=h<=9, -12<=k<=10, -21<=l<=22	
Reflections collected	6756	

Independent reflections	2740 [R(int) = 0.0391]
Completeness to theta = 25.242°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6376
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2740 / 0 / 175
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0342, wR2 = 0.0863
R indices (all data)	R1 = 0.0358, wR2 = 0.0877
Absolute structure parameter	0.05(5)
Extinction coefficient	0.025(6)
Largest diff. peak and hole	0.274 and -0.178 e.$Å^{-3}$

9. References

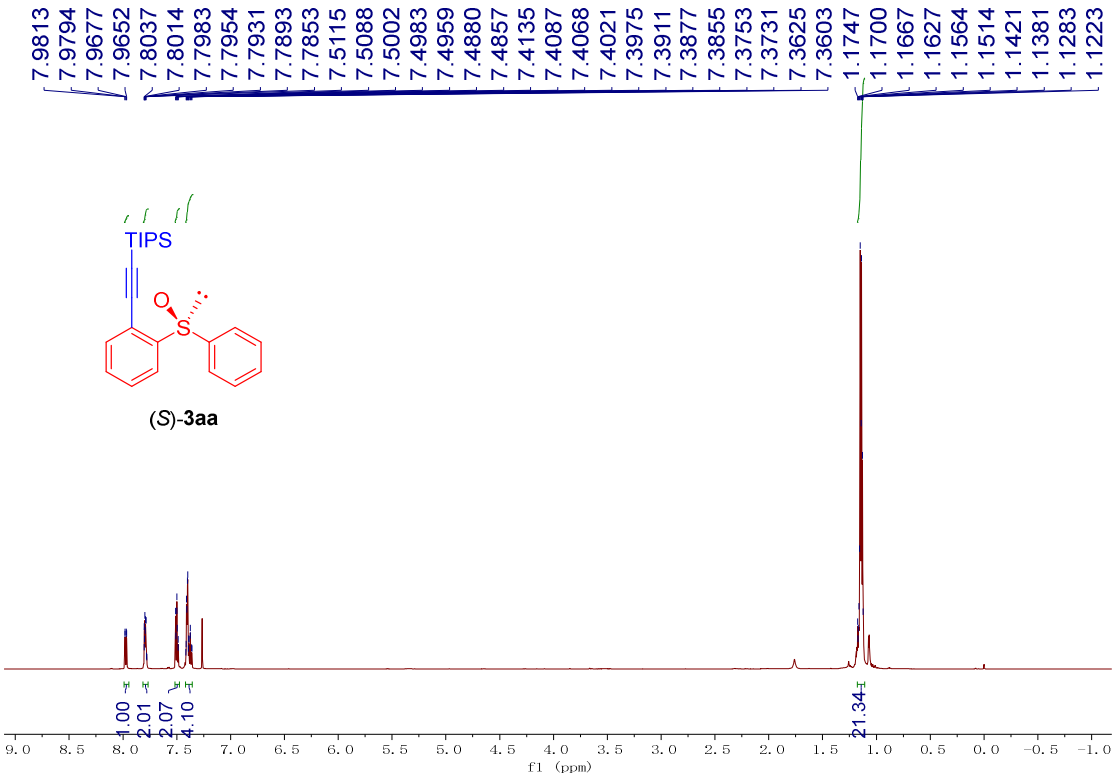
1. (a) B. Ye and N. Cramer, J. Am. Chem. Soc. 2013, **135**, 636-639; (b) B. Ye and N. Cramer, Angew. Chem., Int. Ed., 2014, **53**, 7896-7899.

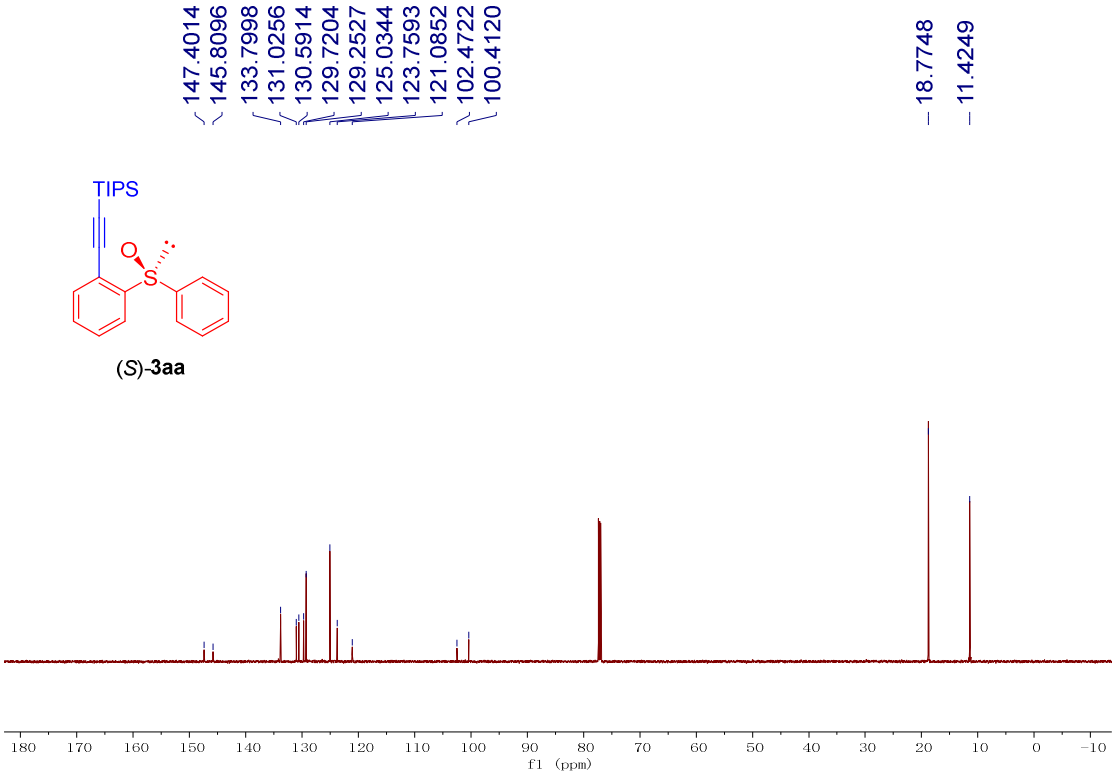
2. Y.-C. Zhu, Y. Li, B.-C. Zhang, F.-X. Zhang, Y.-N. Yang and X.-S. Wang, Angew. Chem., Int. Ed., 2018, **57**, 5129-5133.

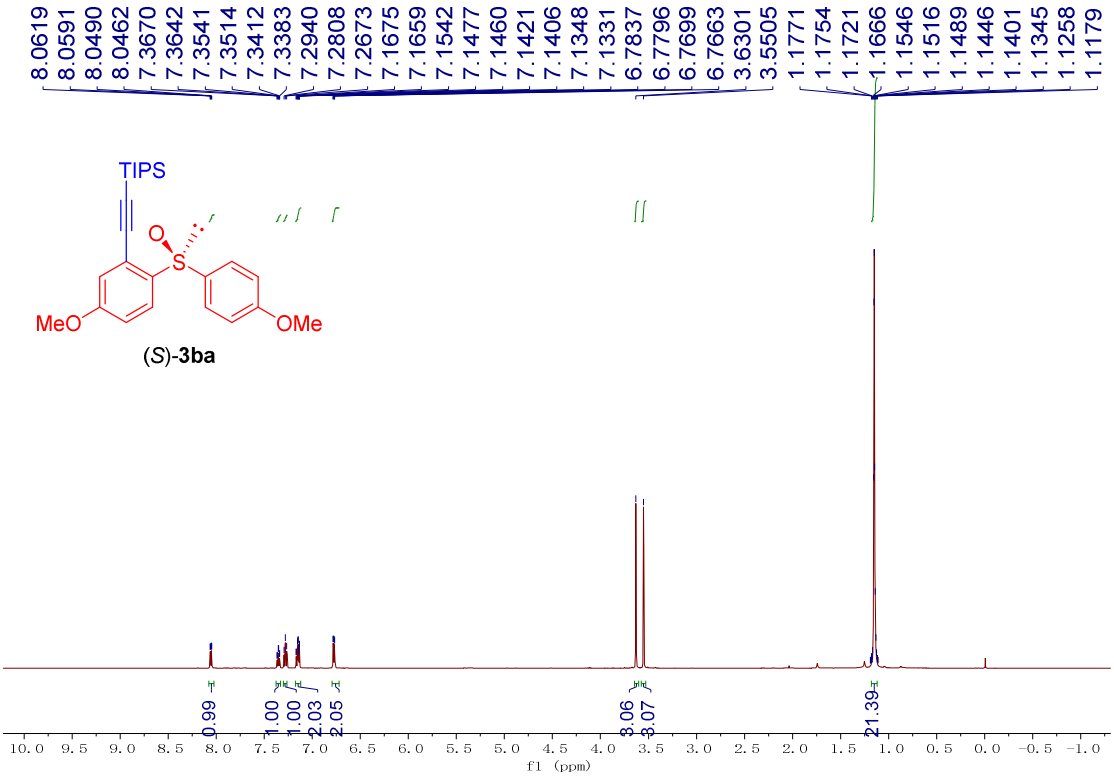
3. C. M. M. Hendriks, P. Lamers, J. Engel and C. Bolm, Adv. Synth. Catal. 2013, **355**, 3363-3368.

4. A. S. Dillon and B. L. Flynn, Org. Lett. 2020, **22**, 2987-2990.

10. ^{1}H and ^{13}C NMR Spectra



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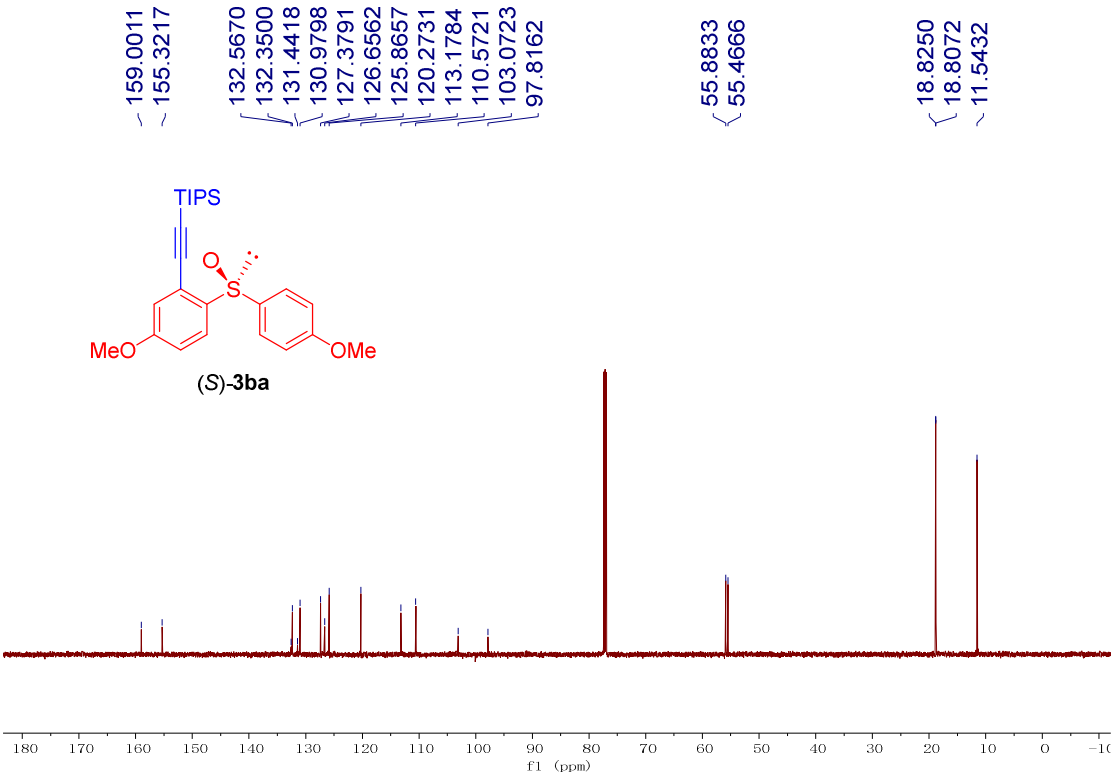
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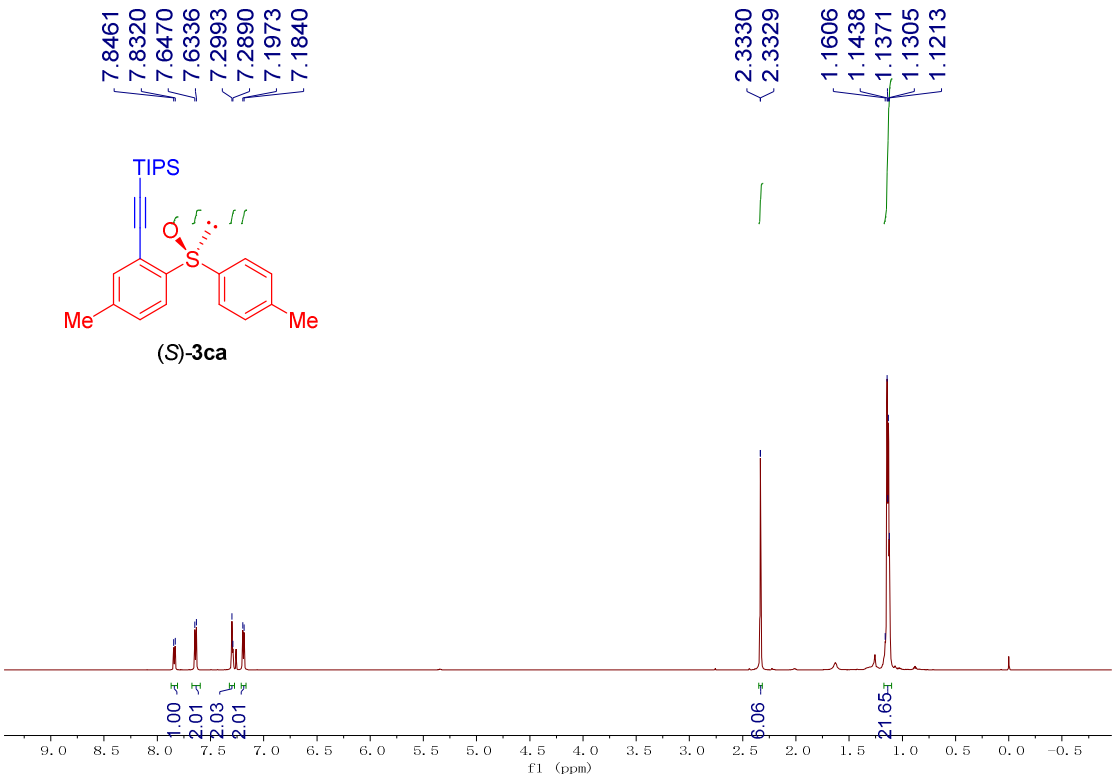
f1 (ppm)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2.01
6.06
21.65
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f1 (ppm)

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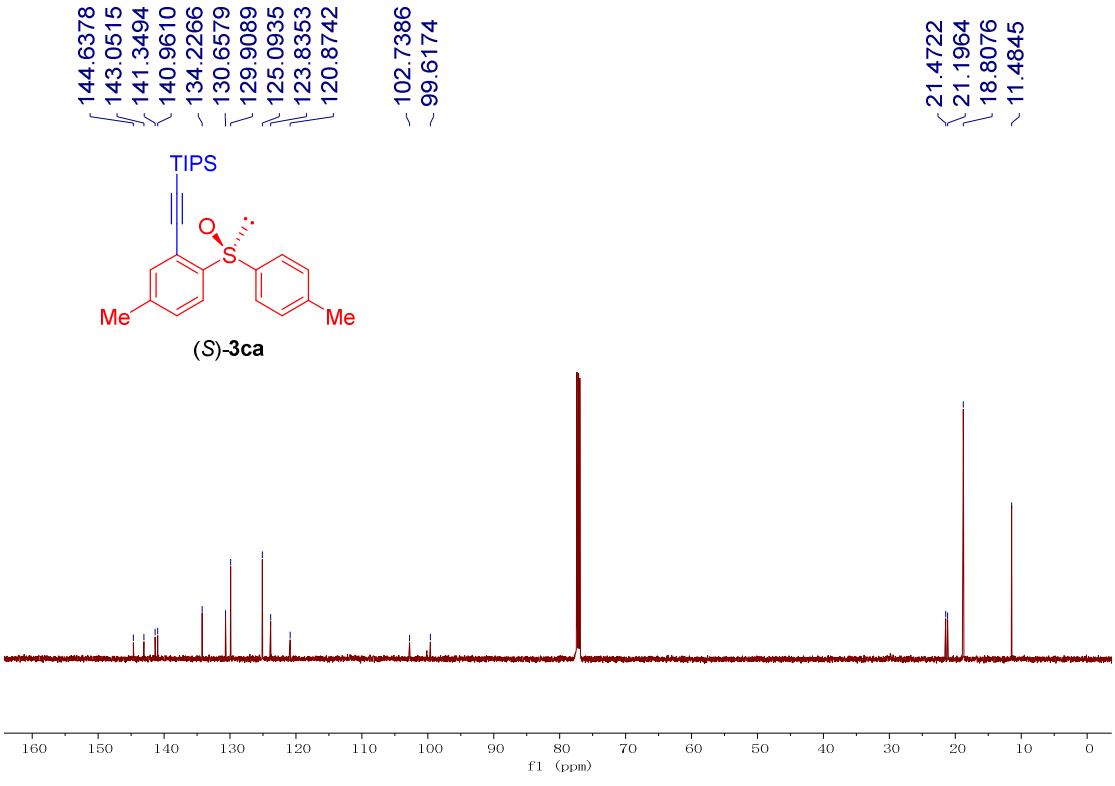
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f1 (ppm)

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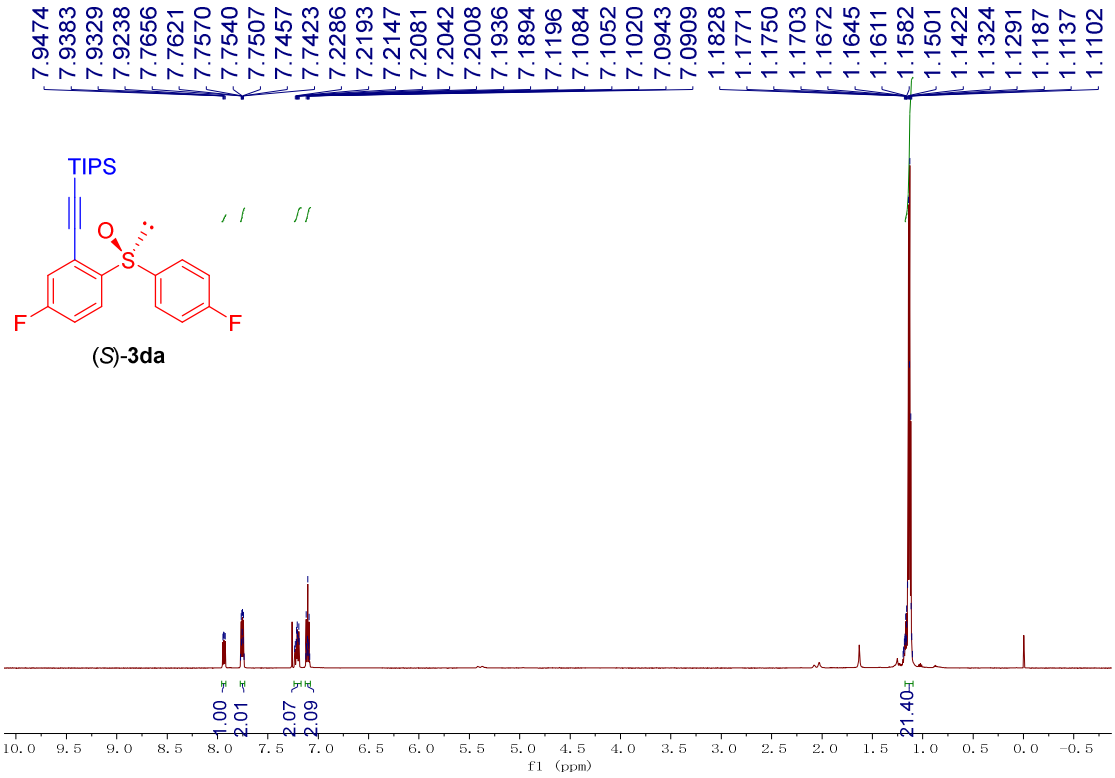
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F
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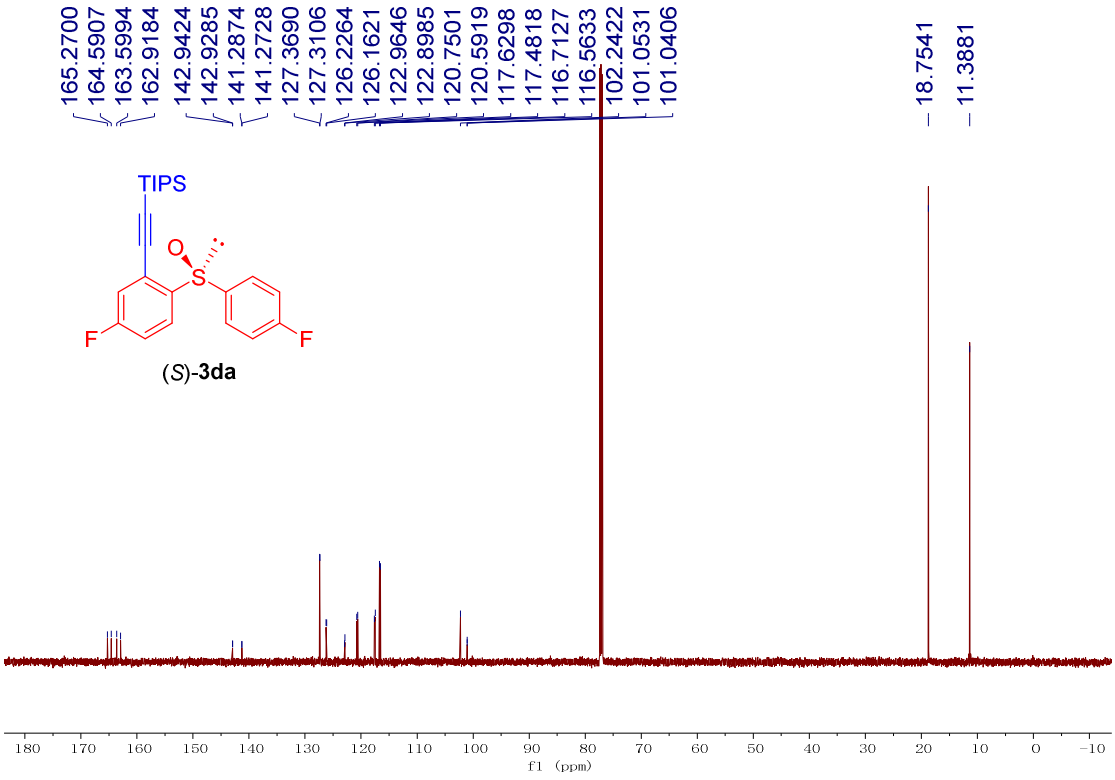
f1 (ppm)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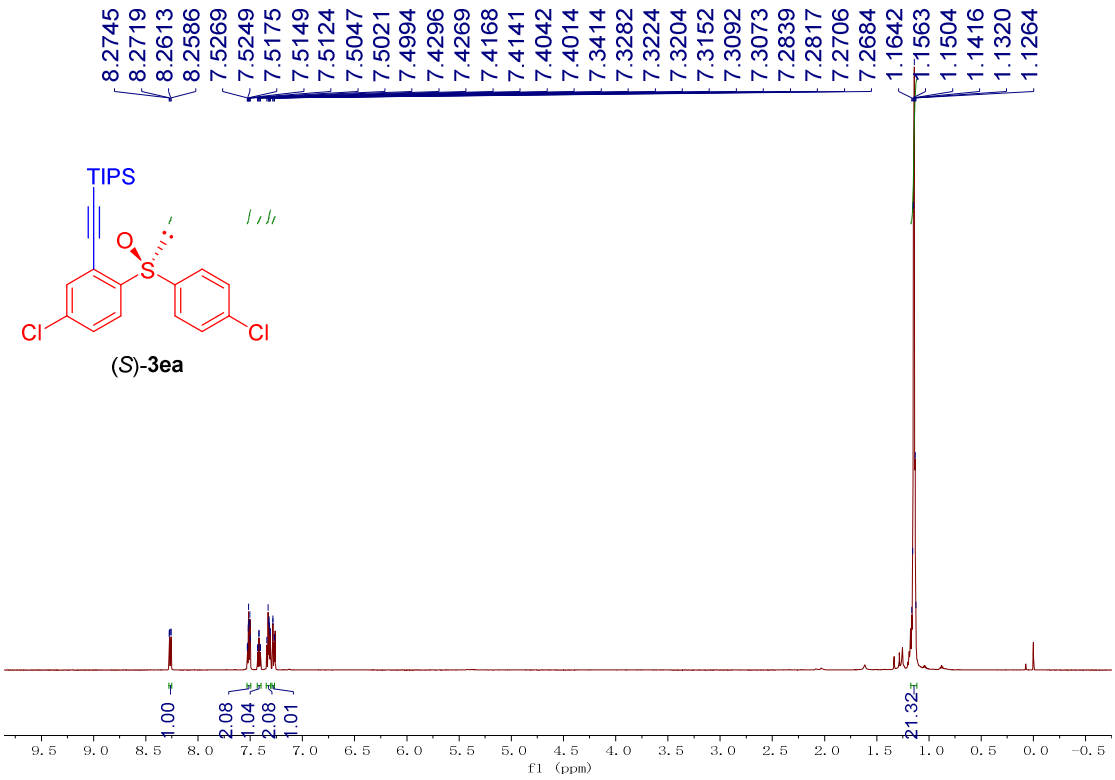
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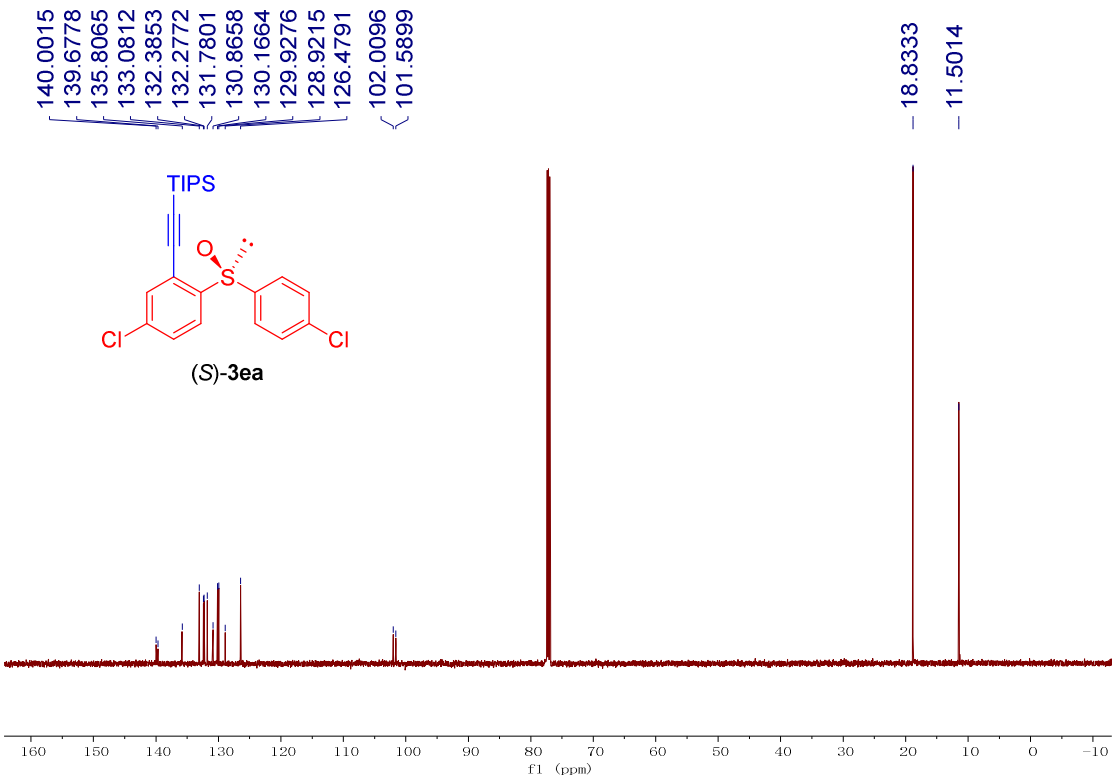
21.32
f1 (ppm)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132.3853
132.2772
131.7801
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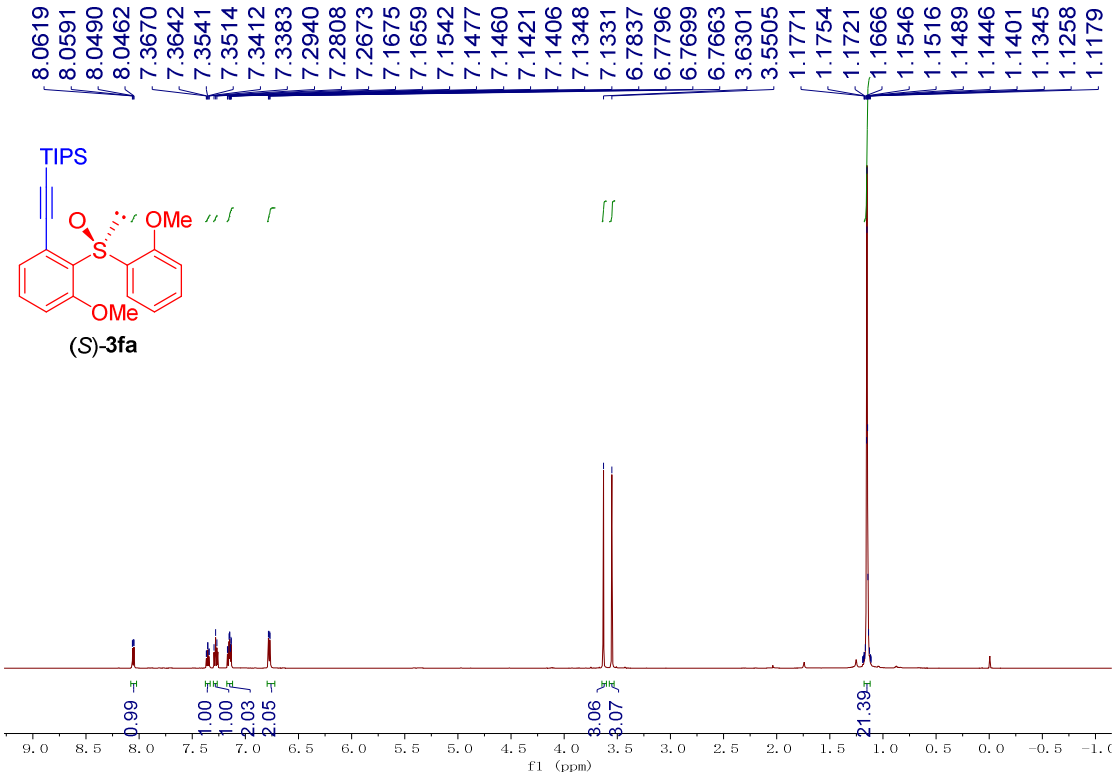
129.9276
128.9215
126.4791
102.0096
101.5899
18.8333
11.5014
TIPS
O
S
Cl
Cl
(S)-3ea
f1 (ppm)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8.0490
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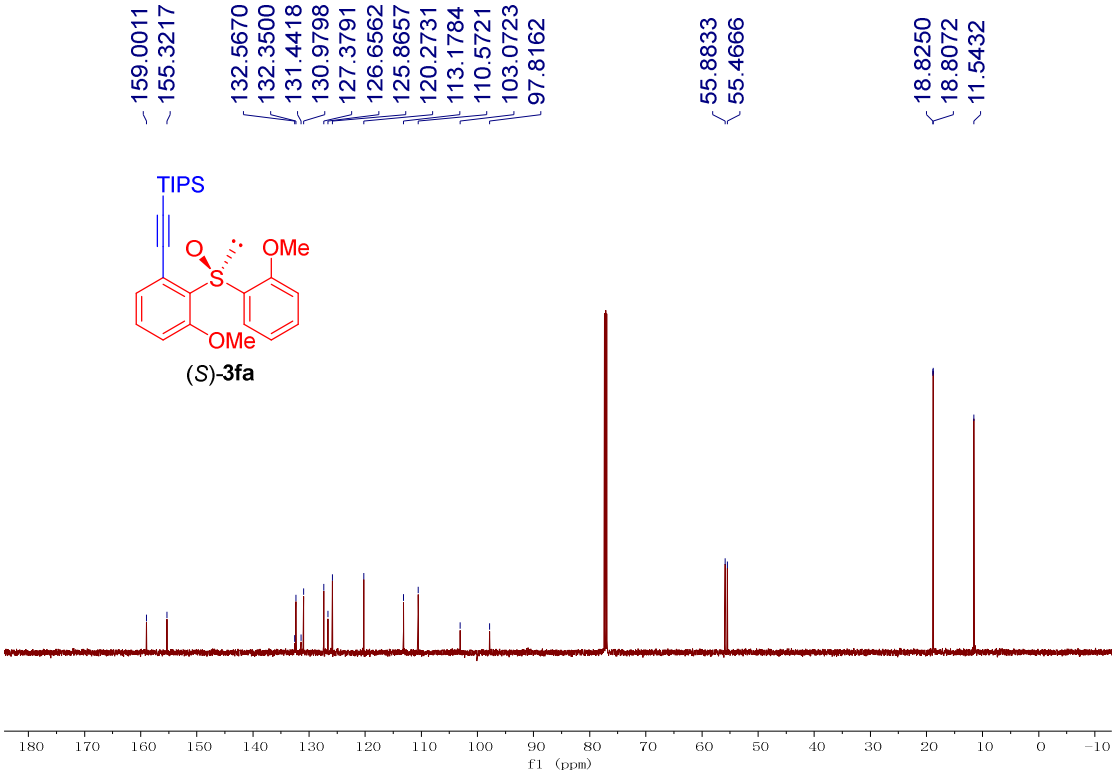
7.3642
7.3541
7.3514
7.3412
7.3383
7.2940
7.2808
7.2673
7.1675
7.1659
7.1542
7.1477
7.1460
7.1421
7.1406
7.1348
7.1331
6.7837
6.7796
6.7699
6.7663
3.6301
3.5505
1.1771
1.1754
1.1721
1.1666
1.1546
1.1516
1.1489
1.1446
1.1401
1.1345
1.1258
1.1179
TIPS
O
S
OMe
OMe
(S)-3fa
0.99
1.00
1.00
2.03
2.05
3.06
3.07
21.39
f1 (ppm)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113.1784
110.5721
103.0723
97.8162
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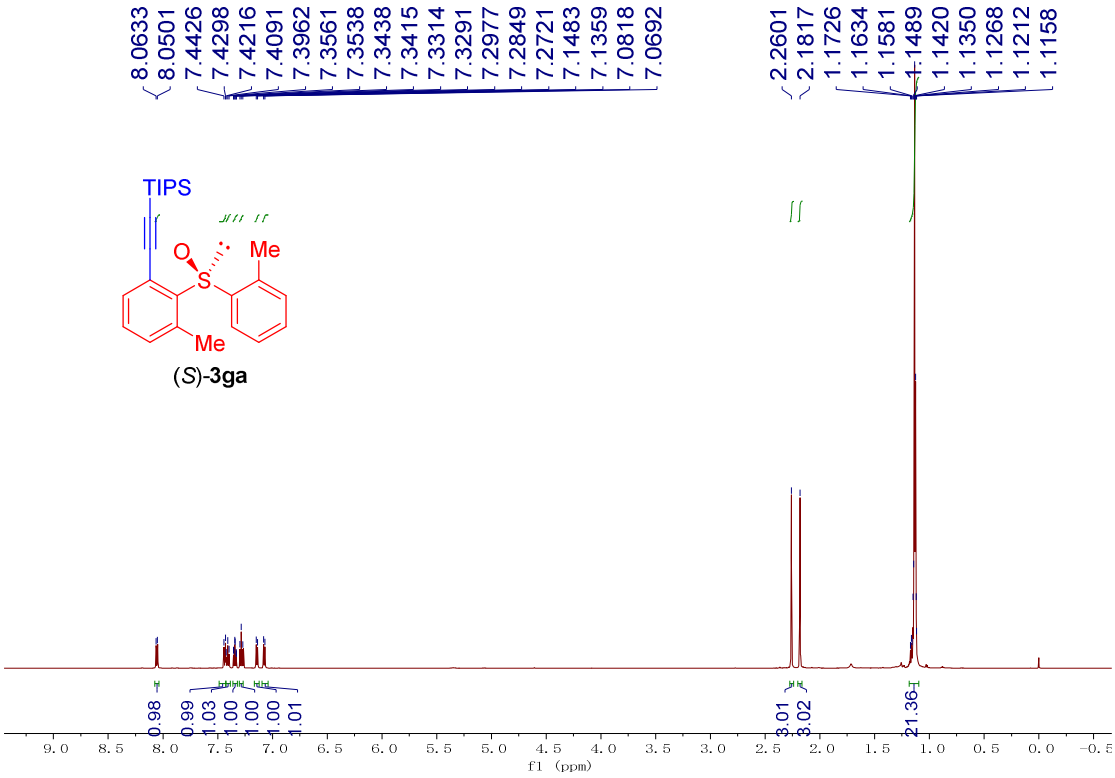
55.4666
18.8250
18.8072
11.5432
TIPS
O
S
OMe
OMe
(S)-3fa
f1 (ppm)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7.3962
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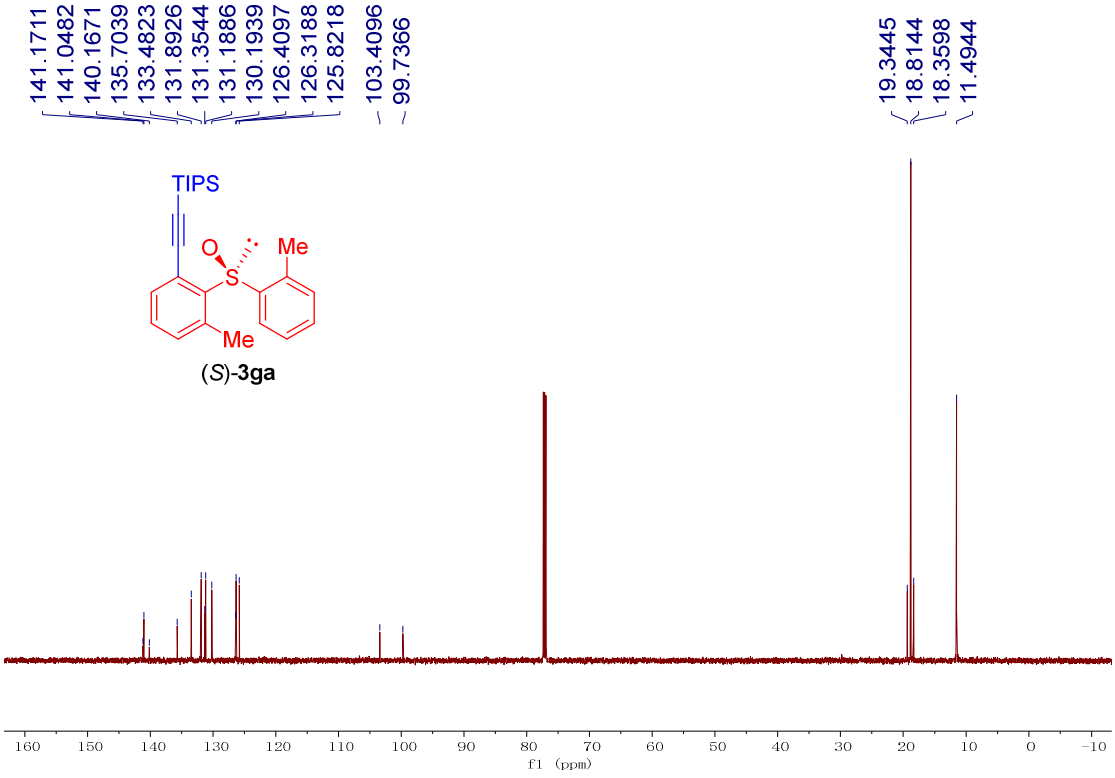
7.3538
7.3438
7.3415
7.3314
7.3291
7.2977
7.2849
7.2721
7.1483
7.1359
7.0818
7.0692
2.2601
2.1817
1.1726
1.1634
1.1581
1.1489
1.1420
1.1350
1.1268
1.1212
1.1158
TIPS
O
S
Me
Me
(S)-3ga
0.98
0.99
1.03
1.00
1.00
1.00
1.01
3.01
3.02
21.36
f1 (ppm)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126.3188
125.8218
103.4096
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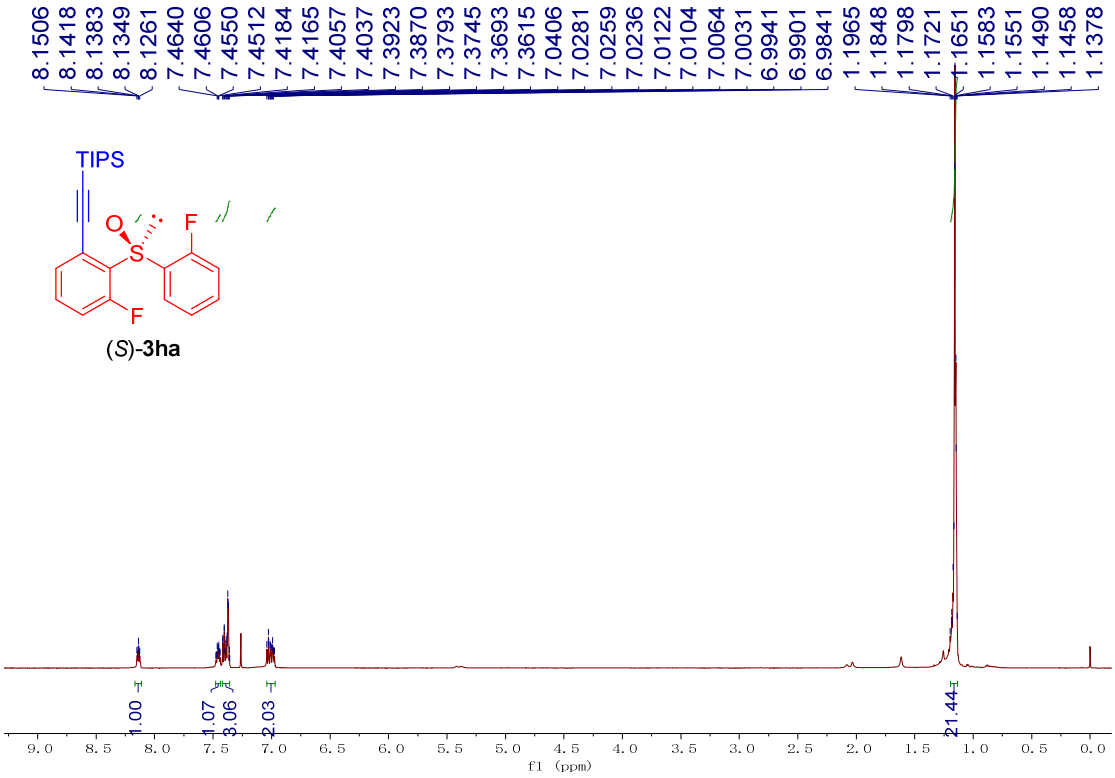
11.4944
TIPS
O
S
Me
Me
(S)-3ga
f1 (ppm)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8.1261
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7.4606
7.4550
7.4512
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7.4165
7.4057
7.4037
7.3923
7.3870
7.3793
7.3745
7.3693
7.3615
7.0406
7.0281
7.0259
7.0236
7.0122
7.0104
7.0064
7.0031
6.9941
6.9901
6.9841
1.1965
1.1848
1.1798
1.1721
1.1651
1.1583
1.1551
1.1490
1.1458
1.1378
TIPS
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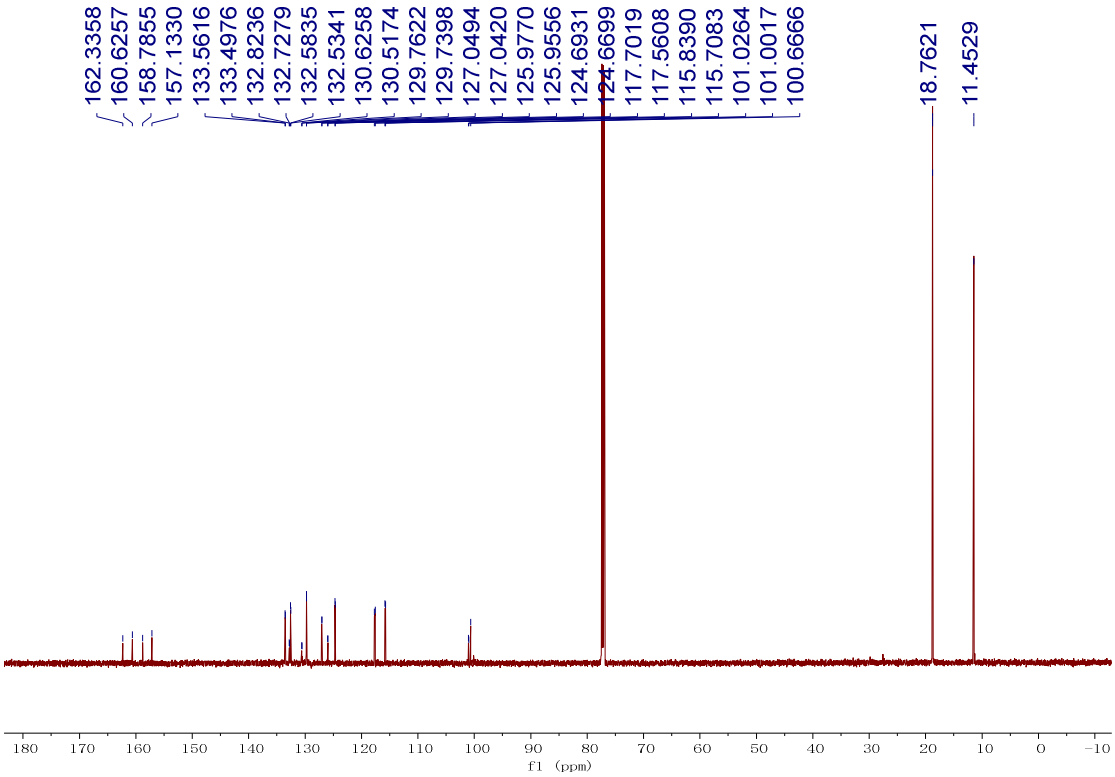
S
F
F
(S)-3ha
1.00
1.07
3.06
2.03
21.44
f1 (ppm)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133.4976
132.8236
132.7279
132.5835
132.5341
130.6258
130.5174
129.7622
129.7398
127.0494
127.0420
125.9770
125.9556
124.6931
124.6699
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115.8390
115.7083
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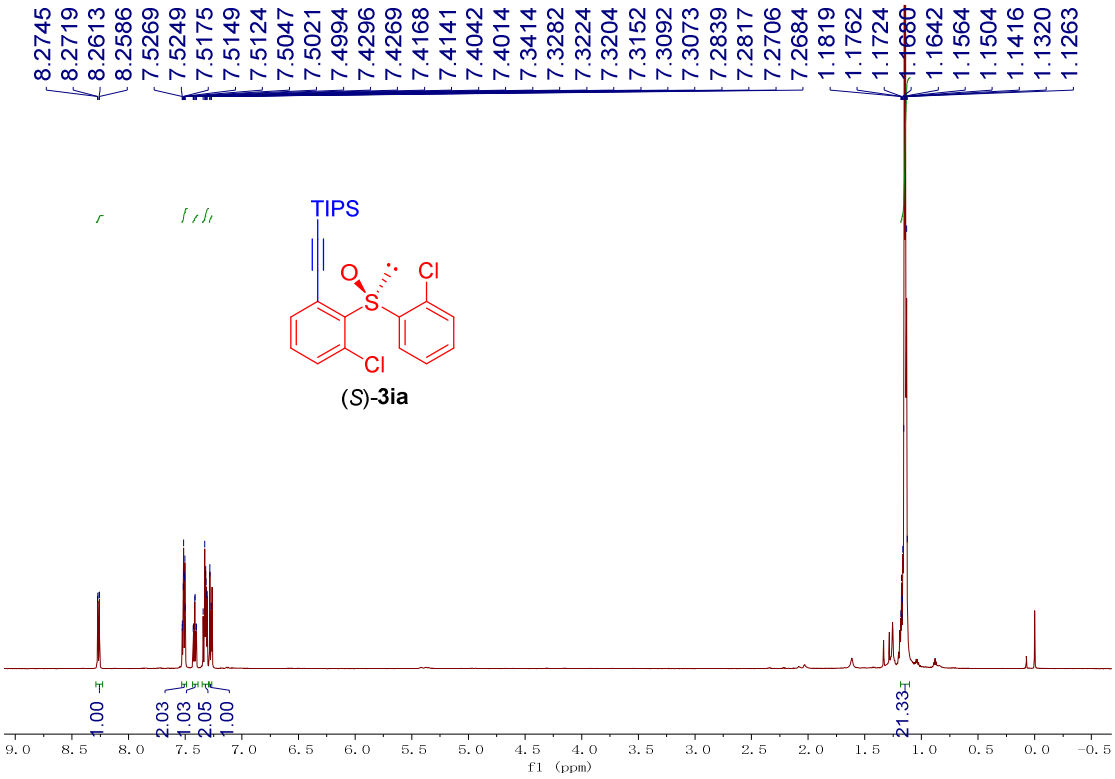
101.0017
100.6666
18.7621
11.4529
f1 (ppm)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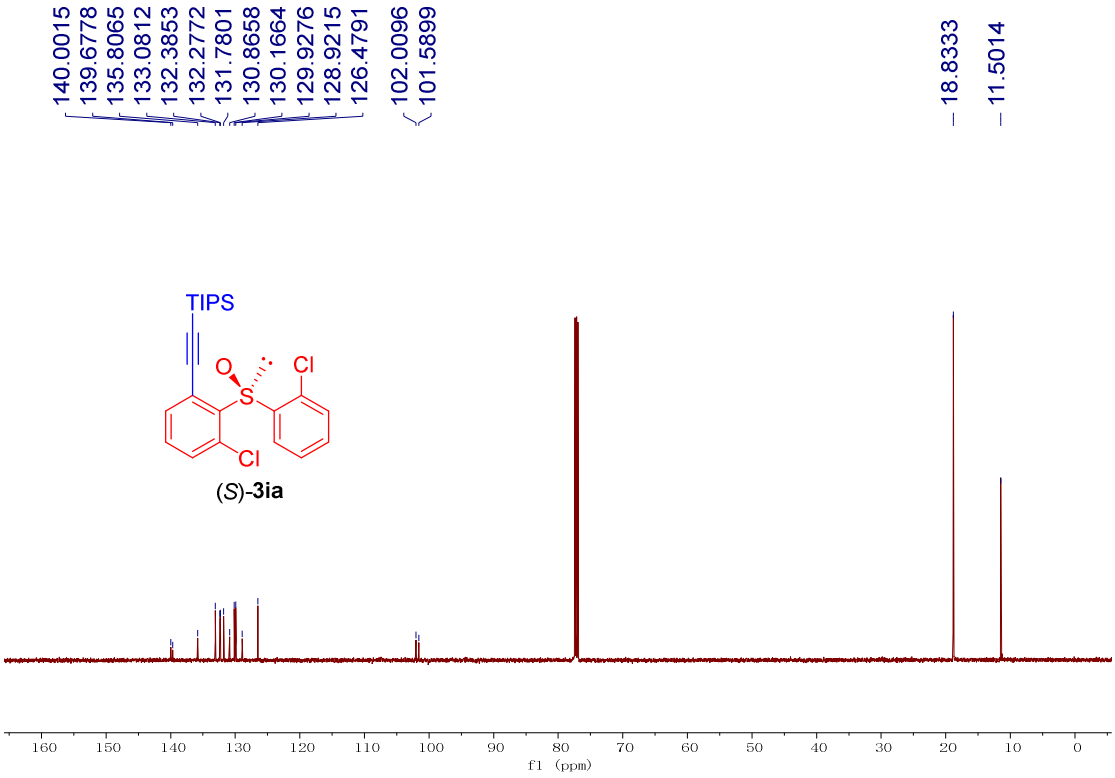
7.5249
7.5175
7.5149
7.5124
7.5047
7.5021
7.4994
7.4296
7.4269
7.4168
7.4141
7.4042
7.4014
7.3414
7.3282
7.3224
7.3204
7.3152
7.3092
7.3073
7.2839
7.2817
7.2706
7.2684
1.1819
1.1762
1.1724
1.1680
1.1642
1.1564
1.1504
1.1416
1.1320
1.1263
TIPS
O
S
Cl
Cl
(S)-3ia
1.00
2.03
1.03
2.05
1.00
21.33
f1 (ppm)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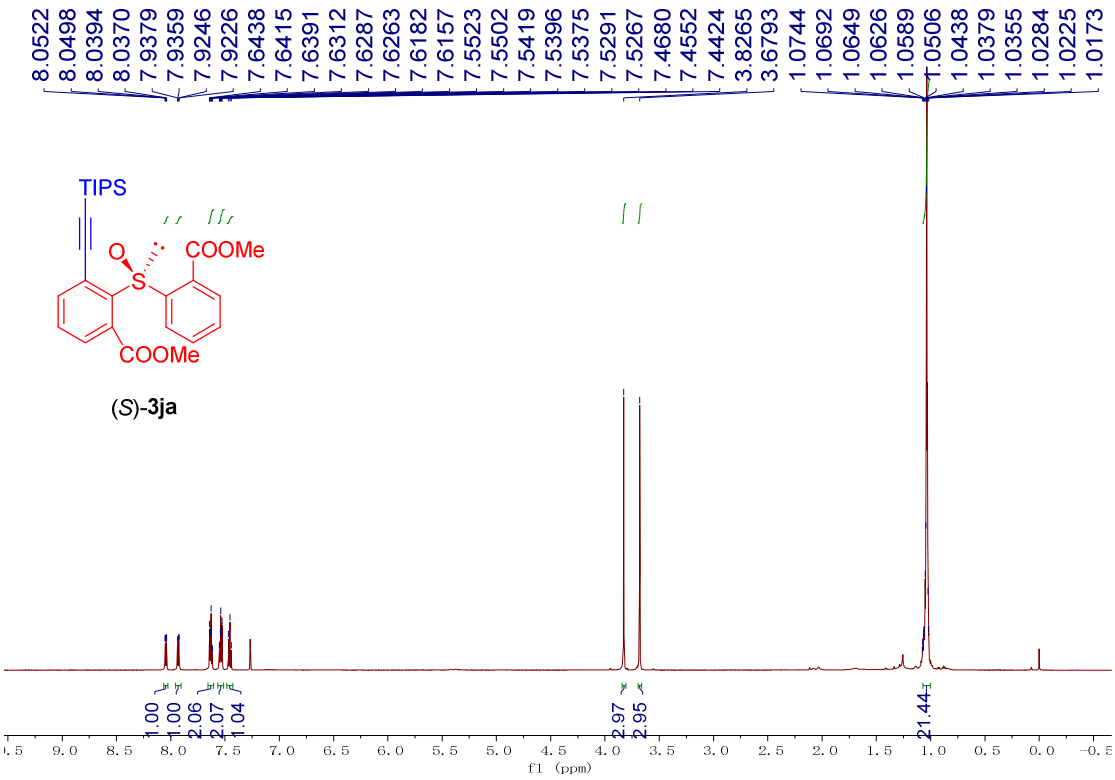
131.7801
130.8658
130.1664
129.9276
128.9215
126.4791
102.0096
101.5899
18.8333
11.5014
TIPS
O
S
Cl
Cl
(S)-3ia
f1 (ppm)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7.9359
7.9246
7.9226
7.6438
7.6415
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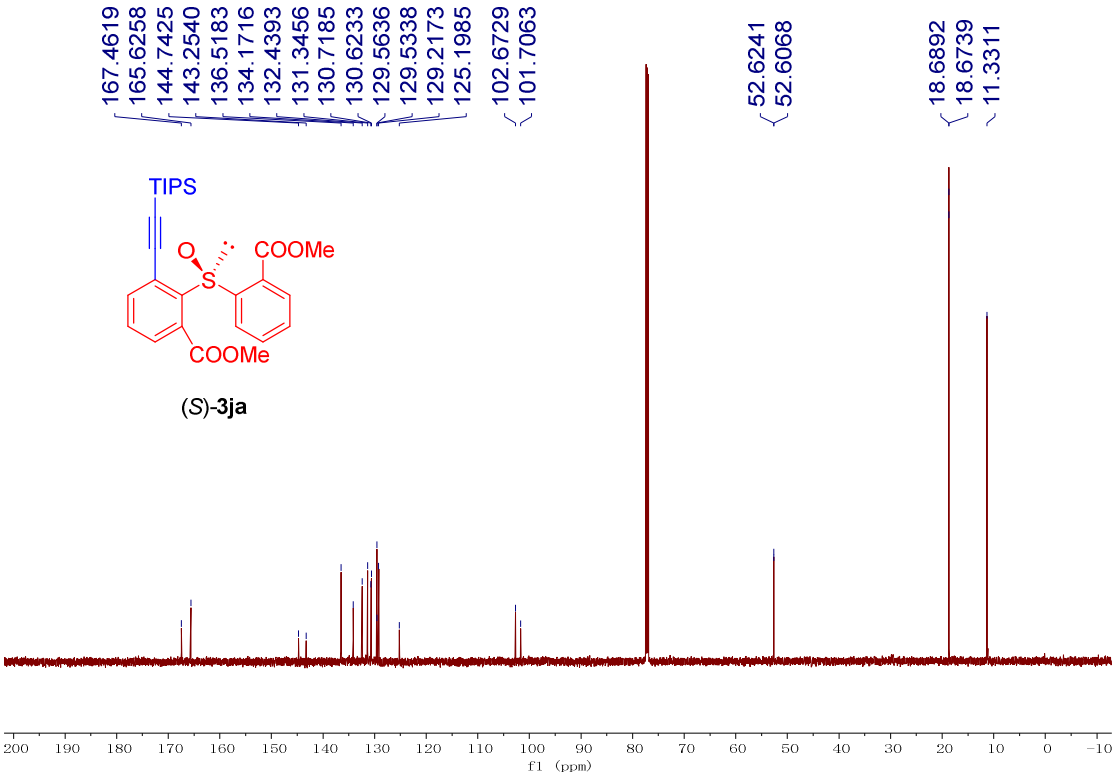
7.6312
7.6287
7.6263
7.6182
7.6157
7.5523
7.5502
7.5419
7.5396
7.5375
7.5291
7.5267
7.4680
7.4552
7.4424
3.8265
3.6793
1.0744
1.0692
1.0649
1.0626
1.0589
1.0506
1.0438
1.0379
1.0355
1.0284
1.0225
1.0173
TIPS
O
S
COOMe
COOMe
(S)-3ja
1.00
1.00
2.06
2.07
1.04
2.97
2.95
21.44
f1 (ppm)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143.2540
136.5183
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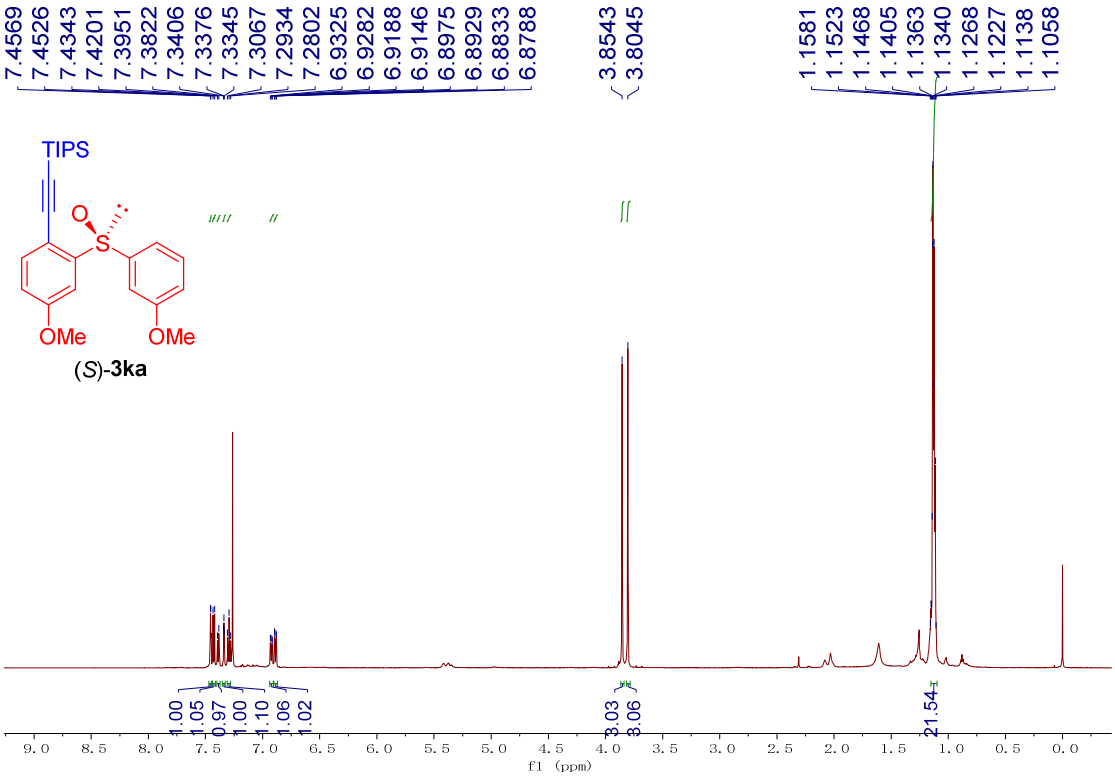
129.5338
129.2173
125.1985
102.6729
101.7063
52.6241
52.6068
18.6892
18.6739
11.3311
TIPS
O
S
COOMe
COOMe
(S)-3ja
f1 (ppm)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7.2934
7.2802
6.9325
6.9282
6.9188
6.9146
6.8975
6.8929
6.8833
6.8788
3.8543
3.8045
1.1581
1.1523
1.1468
1.1405
1.1363
1.1340
1.1268
1.1227
1.1138
1.1058
TIPS
O
S
OMe
OMe
(S)-3ka
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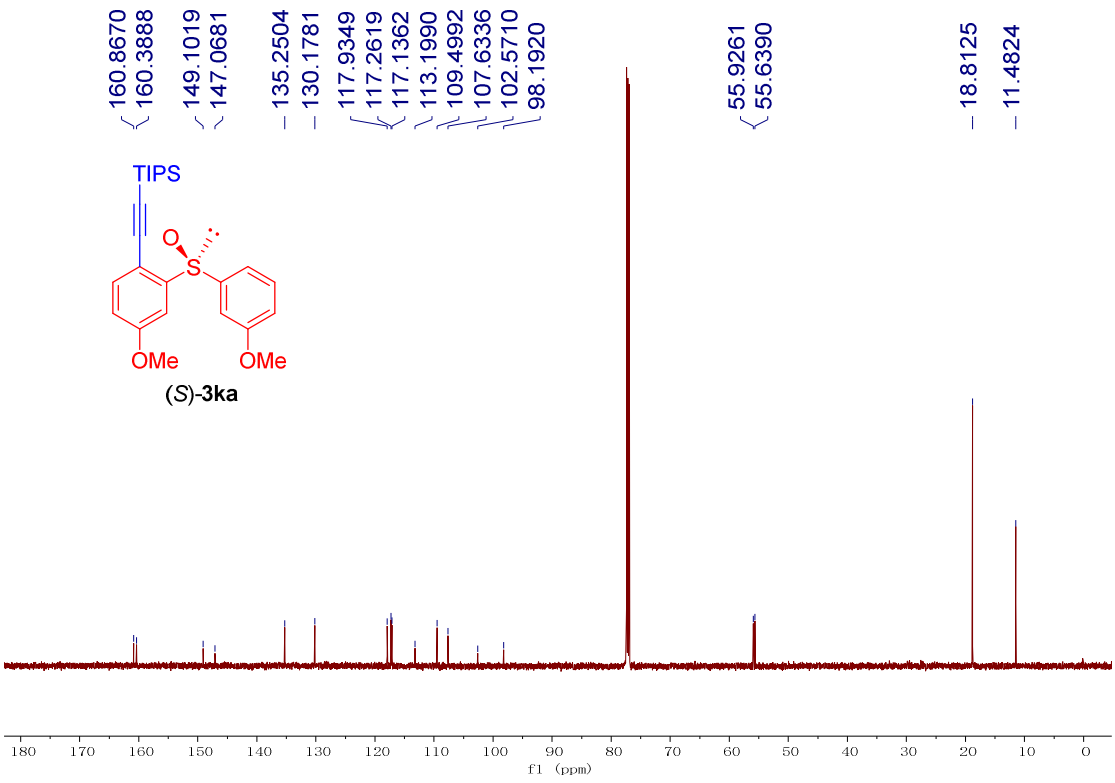
1.05
0.97
1.00
1.10
1.06
1.02
3.03
3.06
21.54
f1 (ppm)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117.2619
117.1362
113.1990
109.4992
107.6336
102.5710
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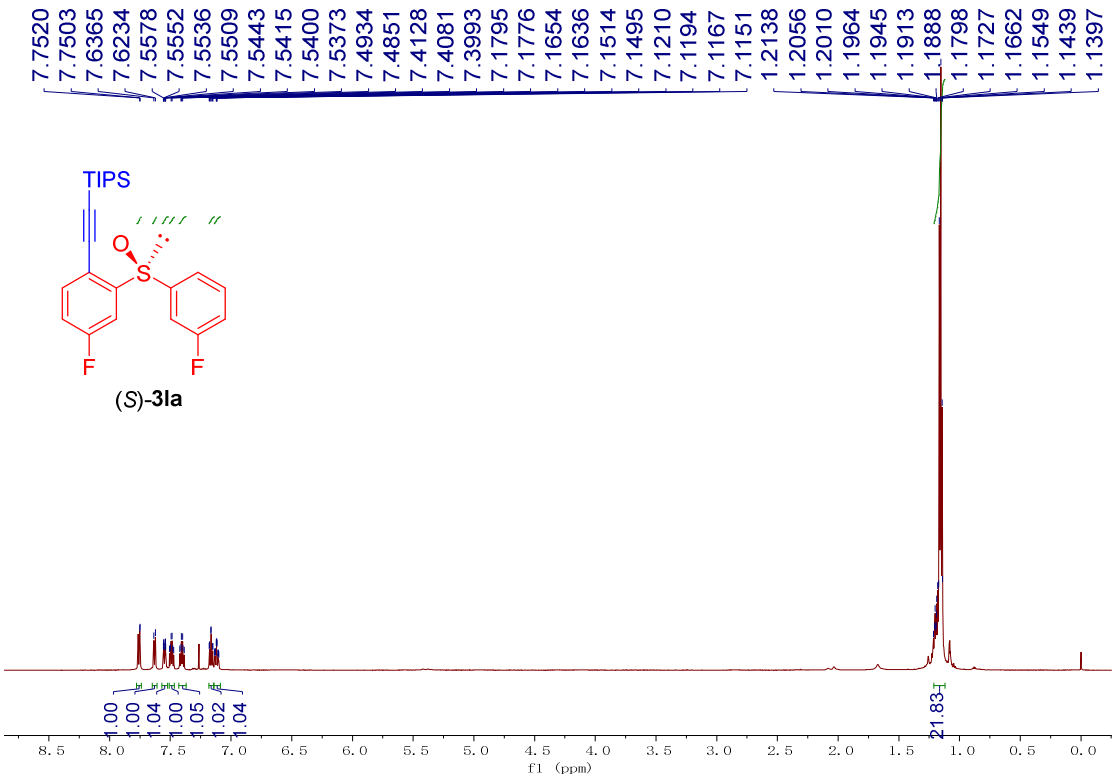
55.6390
18.8125
11.4824
TIPS
O
S
OMe
OMe
(S)-3ka
f1 (ppm)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7.5578
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7.5536
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7.5443
7.5415
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7.5373
7.4934
7.4851
7.4128
7.4081
7.3993
7.1795
7.1776
7.1654
7.1636
7.1514
7.1495
7.1210
7.1194
7.1167
7.1151
1.2138
1.2056
1.2010
1.1964
1.1945
1.1913
1.1888
1.1798
1.1727
1.1662
1.1549
1.1439
1.1397
TIPS
O
S
F
F
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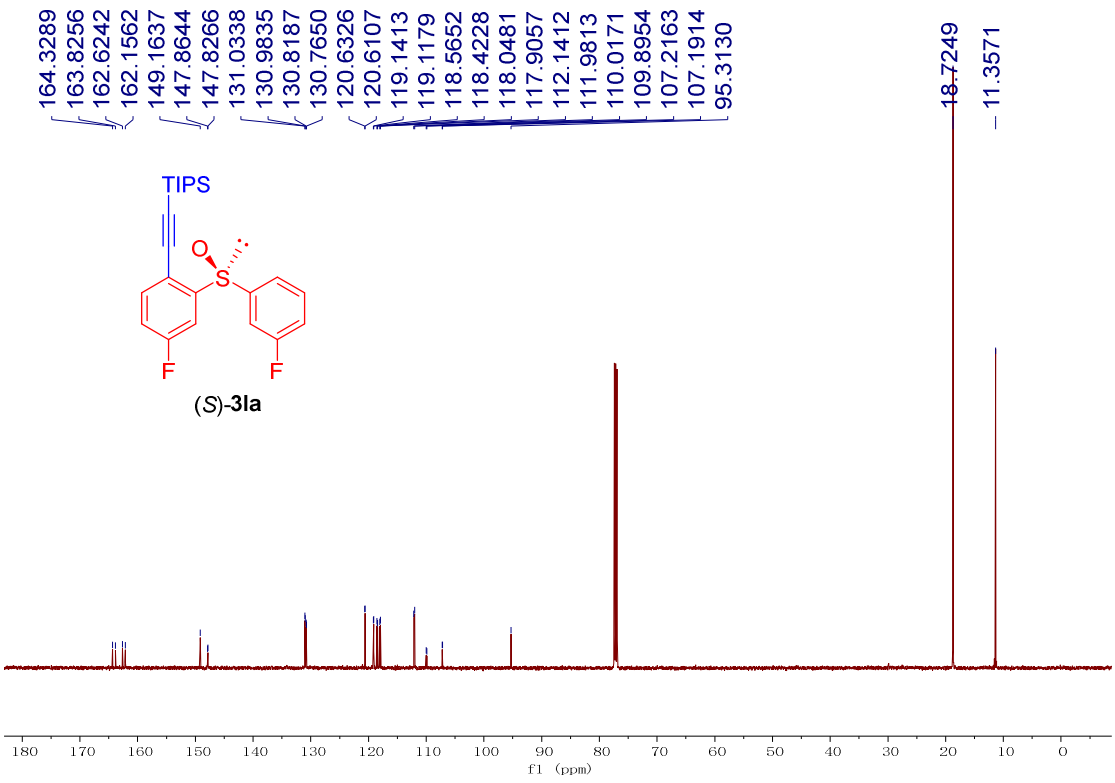
1.00
1.04
1.00
1.05
1.02
1.04
21.83
f1 (ppm)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120.6107
119.1413
119.1179
118.5652
118.4228
118.0481
117.9057
112.1412
111.9813
110.0171
109.8954
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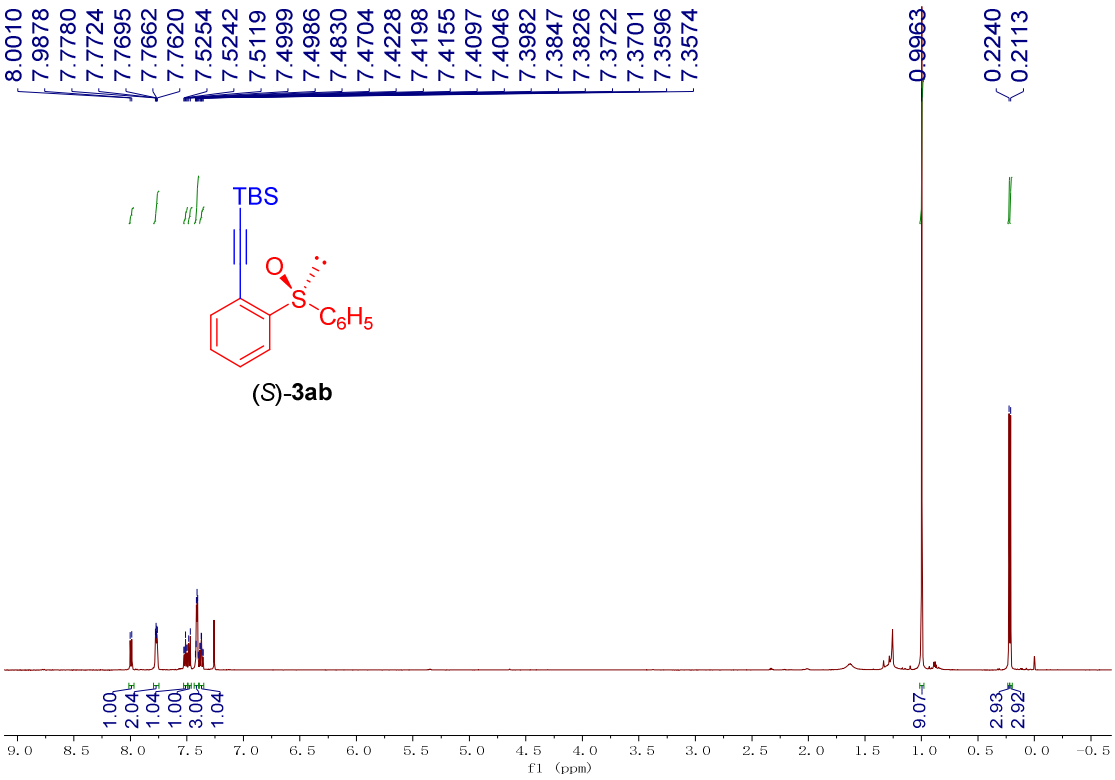
95.3130
18.7249
11.3571
TIPS
O
S
F
F
(S)-3la
f1 (ppm)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7.4830
7.4704
7.4228
7.4198
7.4155
7.4097
7.4046
7.3982
7.3847
7.3826
7.3722
7.3701
7.3596
7.3574
0.9963
0.2240
0.2113
TBS
O
S
C6H5
(S)-3ab
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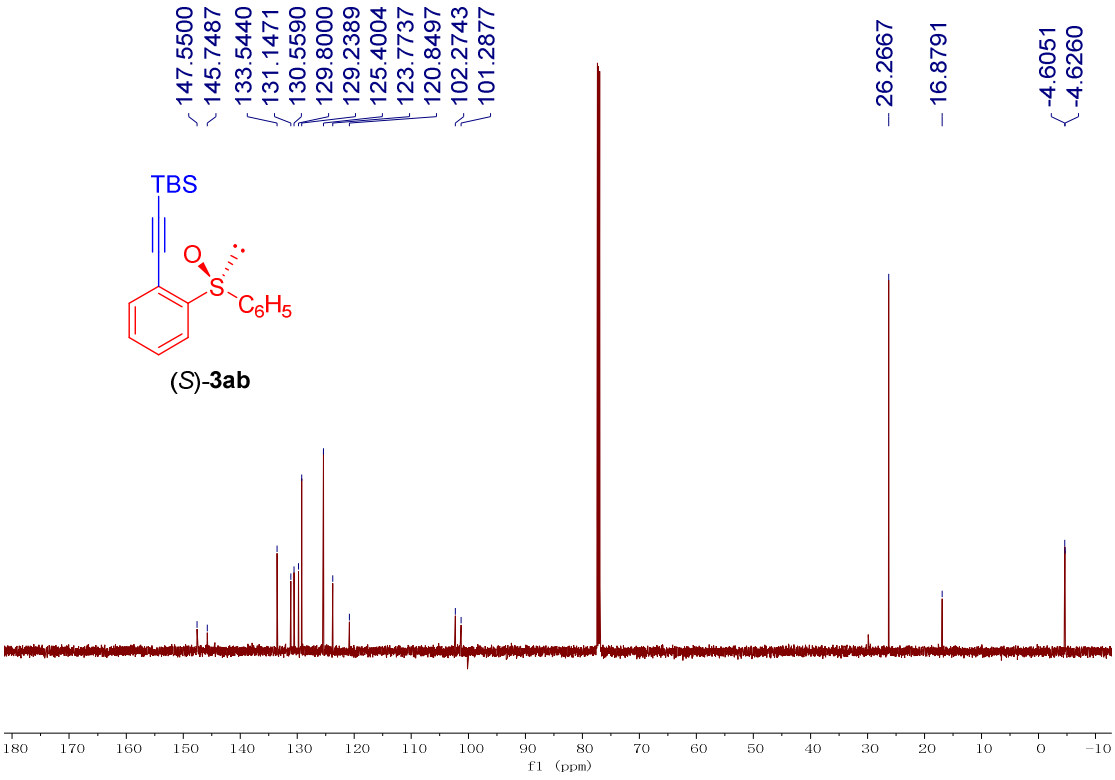
2.04
1.04
1.00
3.00
1.04
9.07
2.93
2.92
f1 (ppm)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102.2743
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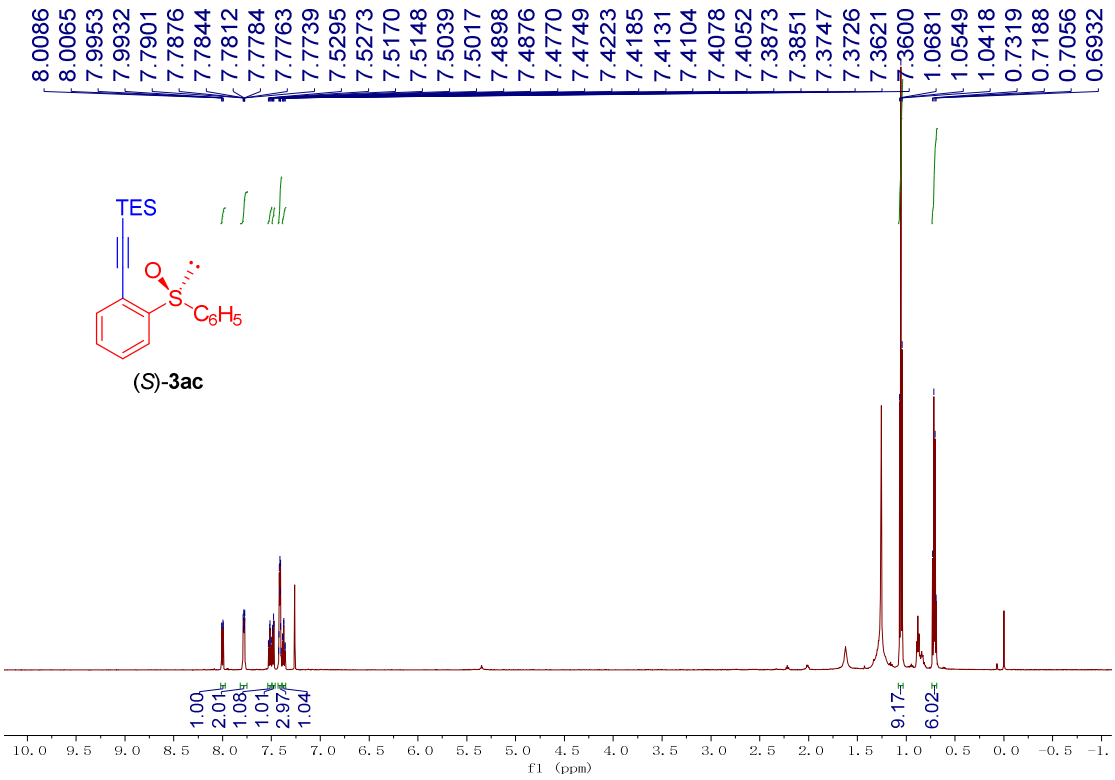
-4.6051
-4.6260
TBS
O
S
C6H5
(S)-3ab
f1 (ppm)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7.5273
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7.5148
7.5039
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7.4876
7.4770
7.4749
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7.4185
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7.3873
7.3851
7.3747
7.3726
7.3621
7.3600
1.0681
1.0549
1.0418
0.7319
0.7188
0.7056
0.6932
TES
O
S
C6H5
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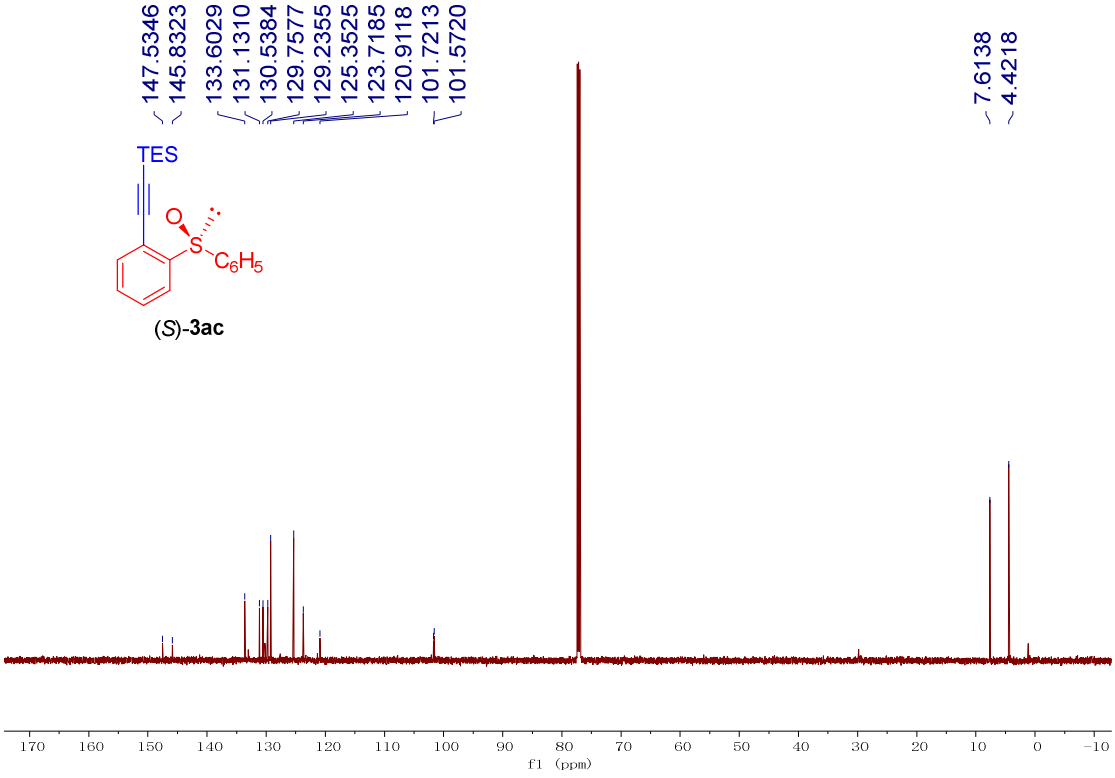
2.01
1.08
1.01
2.97
1.04
9.17
6.02
f1 (ppm)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123.7185
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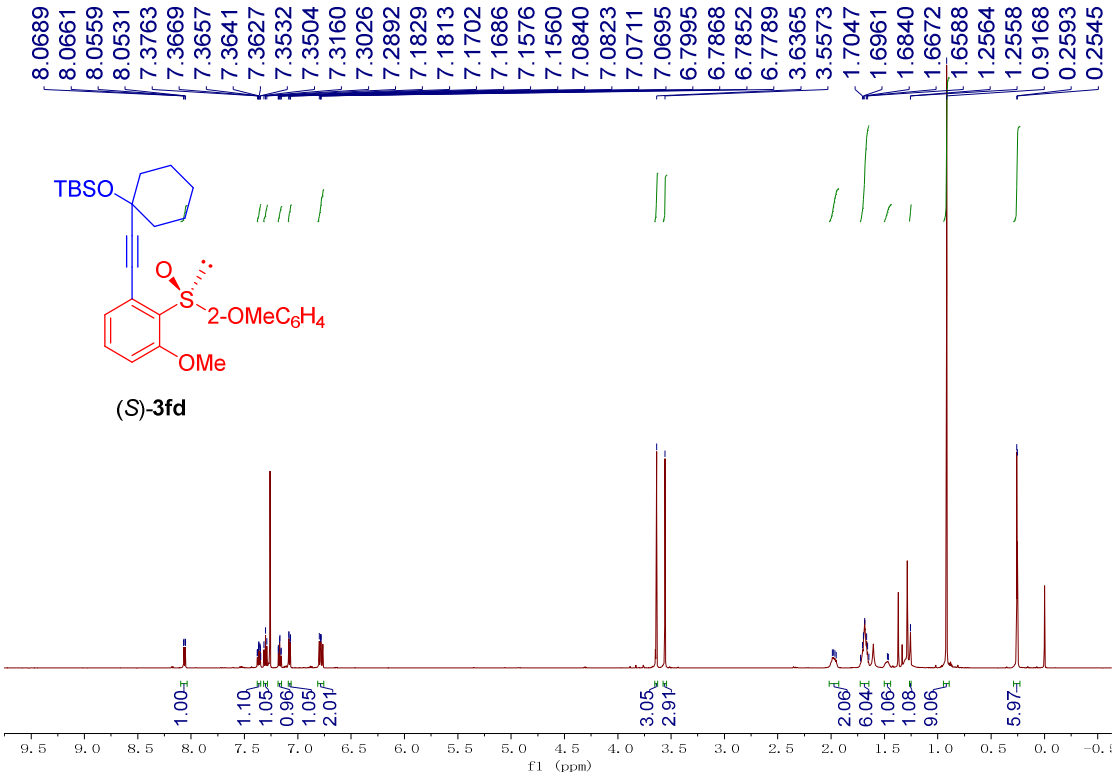
101.5720
7.6138
4.4218
TES
O
S
C6H5
(S)-3ac
f1 (ppm)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7.3627
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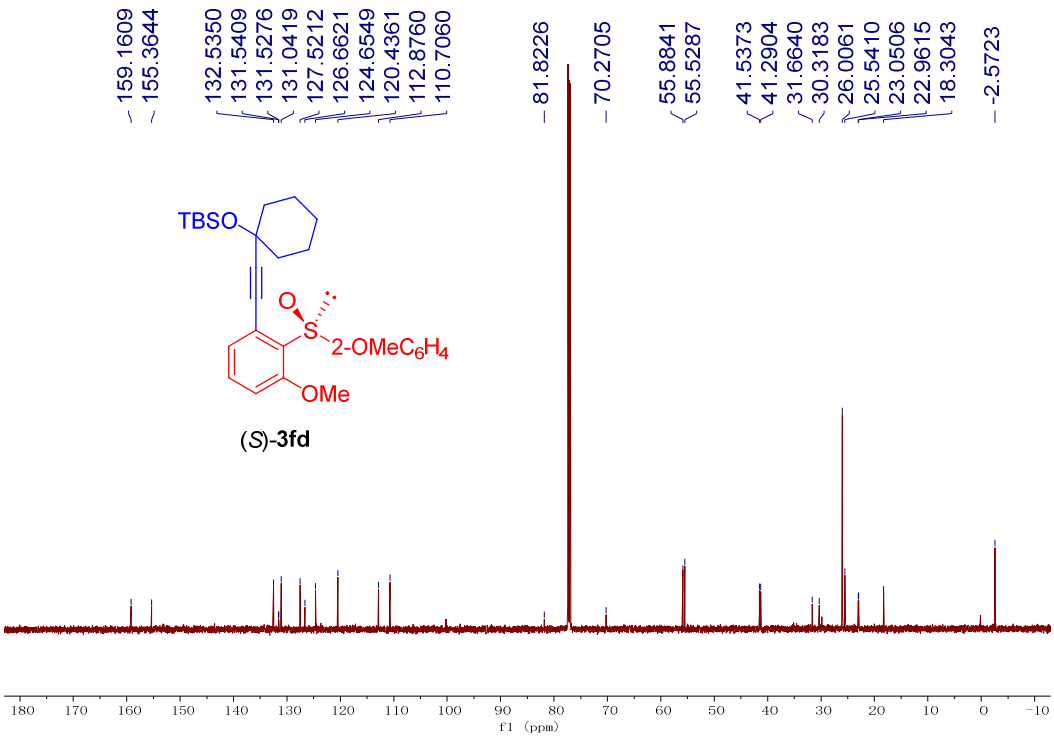
7.3504
7.3160
7.3026
7.2892
7.1829
7.1813
7.1702
7.1686
7.1576
7.1560
7.0840
7.0823
7.0711
7.0695
6.7995
6.7868
6.7852
6.7789
3.6365
3.5573
1.7047
1.6961
1.6840
1.6672
1.6588
1.2564
1.2558
0.9168
0.2593
0.2545
TBSO
O
S
2-OMeC6H4
OMe
(S)-3fd
1.00
1.10
1.05
0.96
1.05
2.01
3.05
2.91
2.06
6.04
1.06
1.08
9.06
5.97
f1 (ppm)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127.5212
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112.8760
110.7060
81.8226
70.2705
55.8841
55.5287
41.5373
41.2904
31.6640
30.3183
26.0061
25.5410
23.0506
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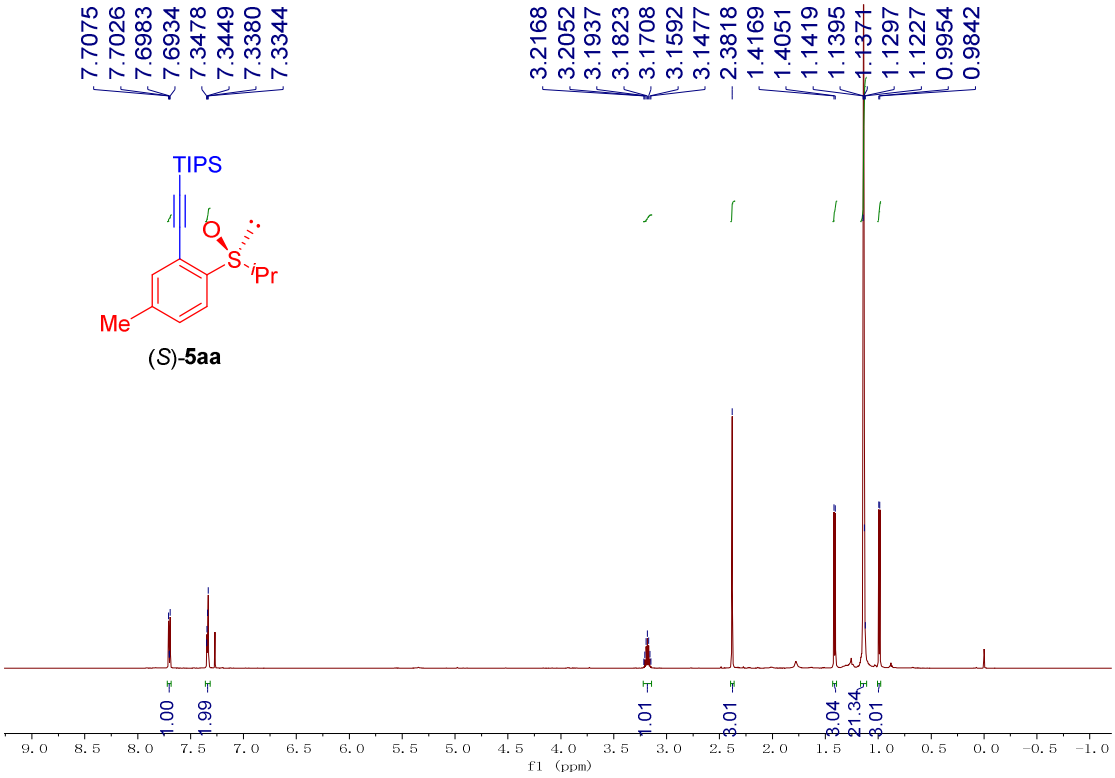
-2.5723
TBSO
O
S
2-OMeC6H4
OMe
(S)-3fd
f1 (ppm)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7.3380
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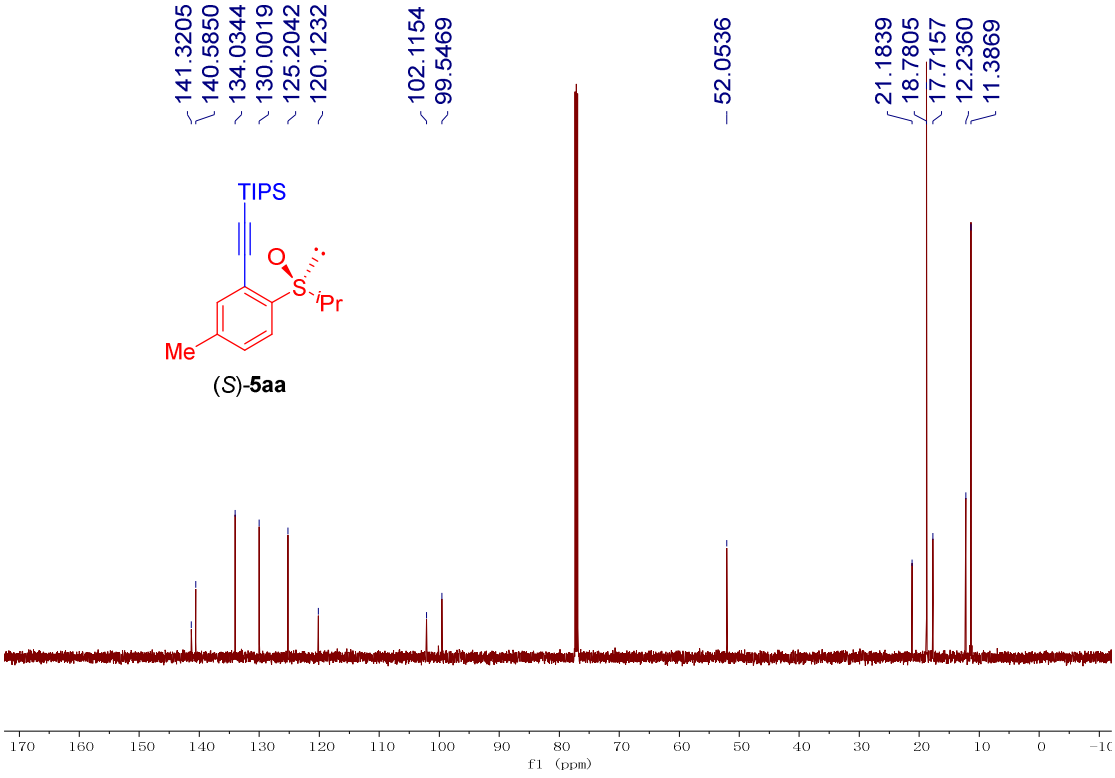
3.2052
3.1937
3.1823
3.1708
3.1592
3.1477
2.3818
1.4169
1.4051
1.1419
1.1395
1.1371
1.1297
1.1227
0.9954
0.9842
TIPS
O
S
iPr
Me
(S)-5aa
1.00
1.99
1.01
3.01
3.04
21.34
3.01
f1 (ppm)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130.0019
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120.1232
102.1154
99.5469
52.0536
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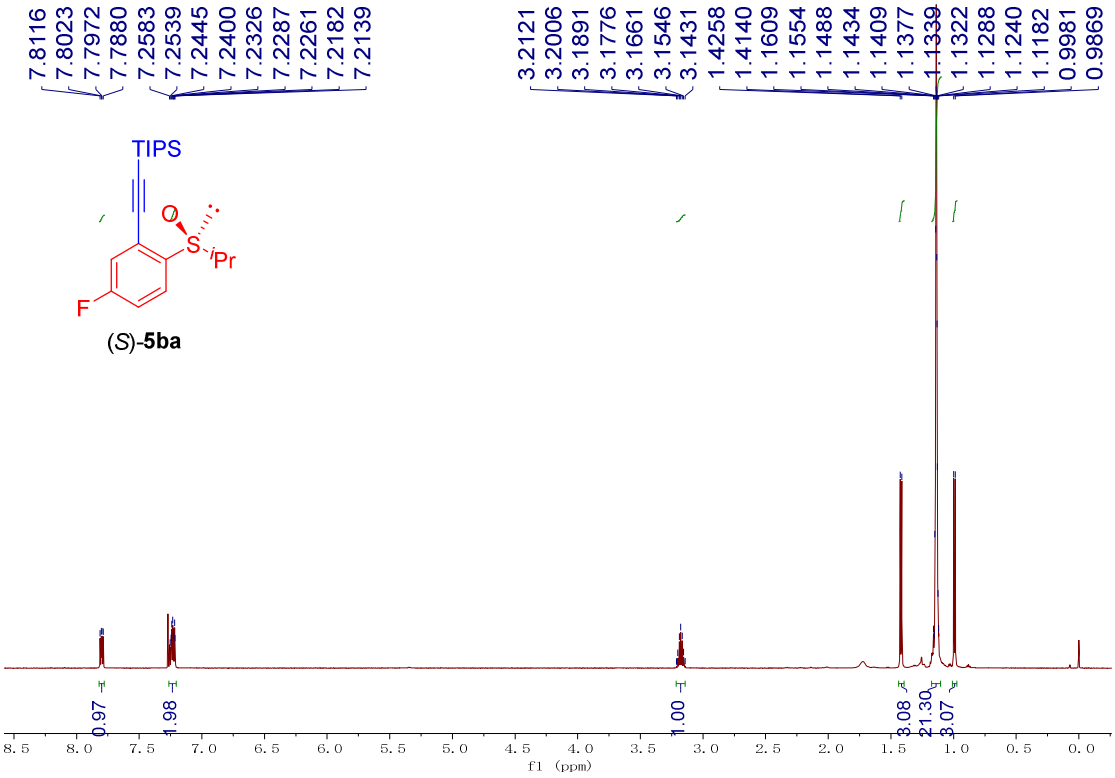
18.7805
17.7157
12.2360
11.3869
TIPS
O
S
iPr
Me
(S)-5aa
f1 (ppm)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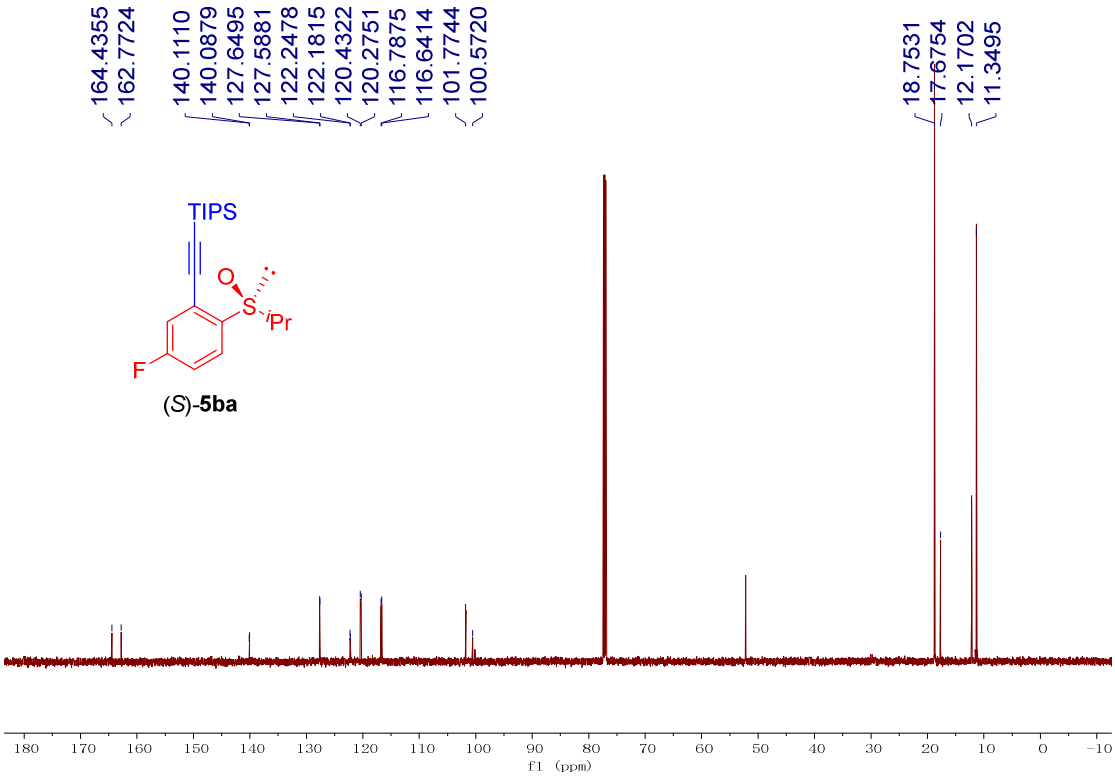
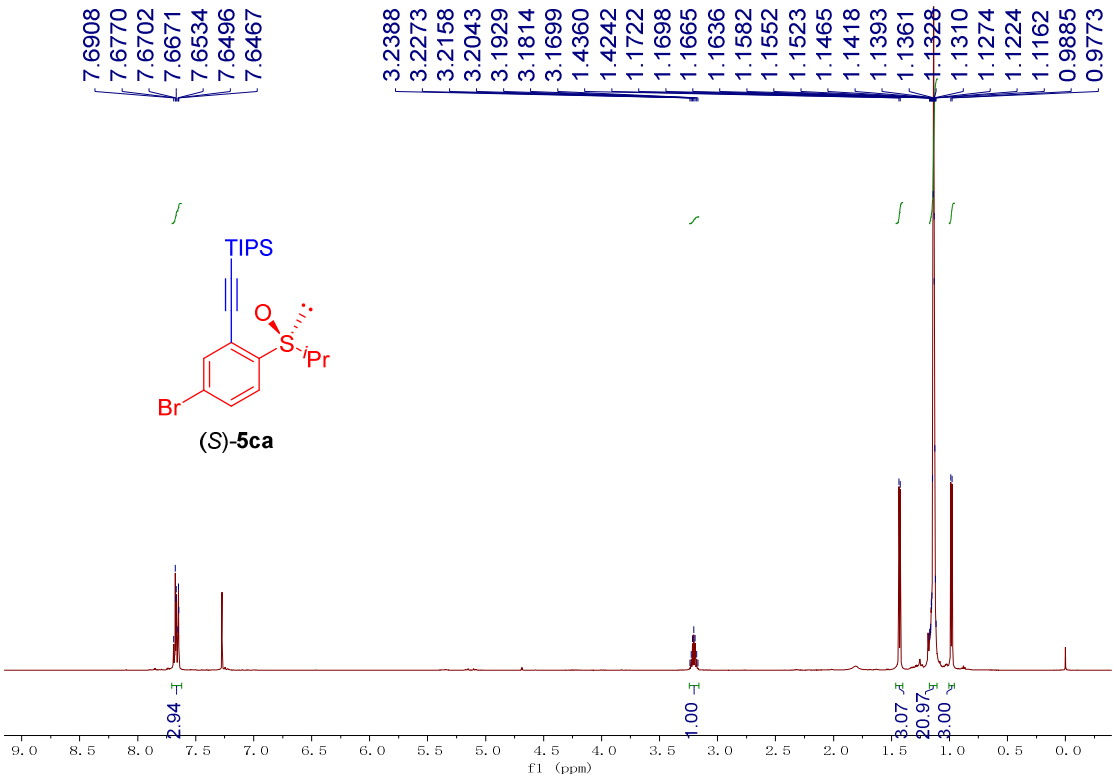
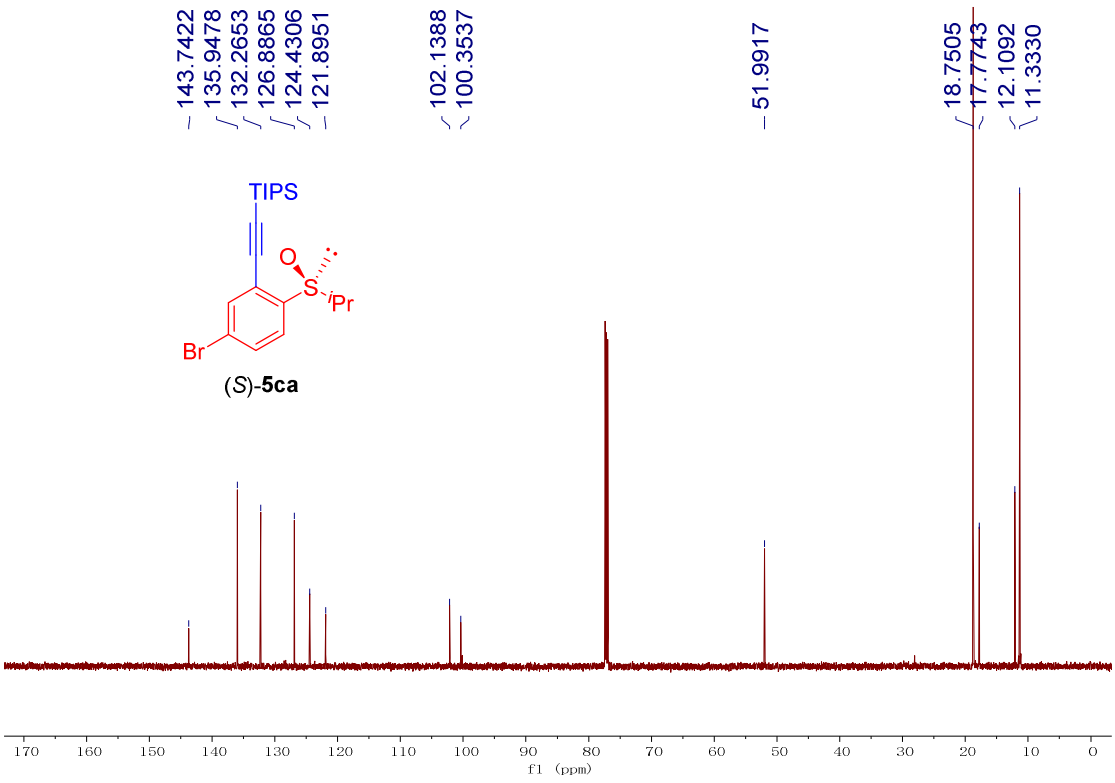
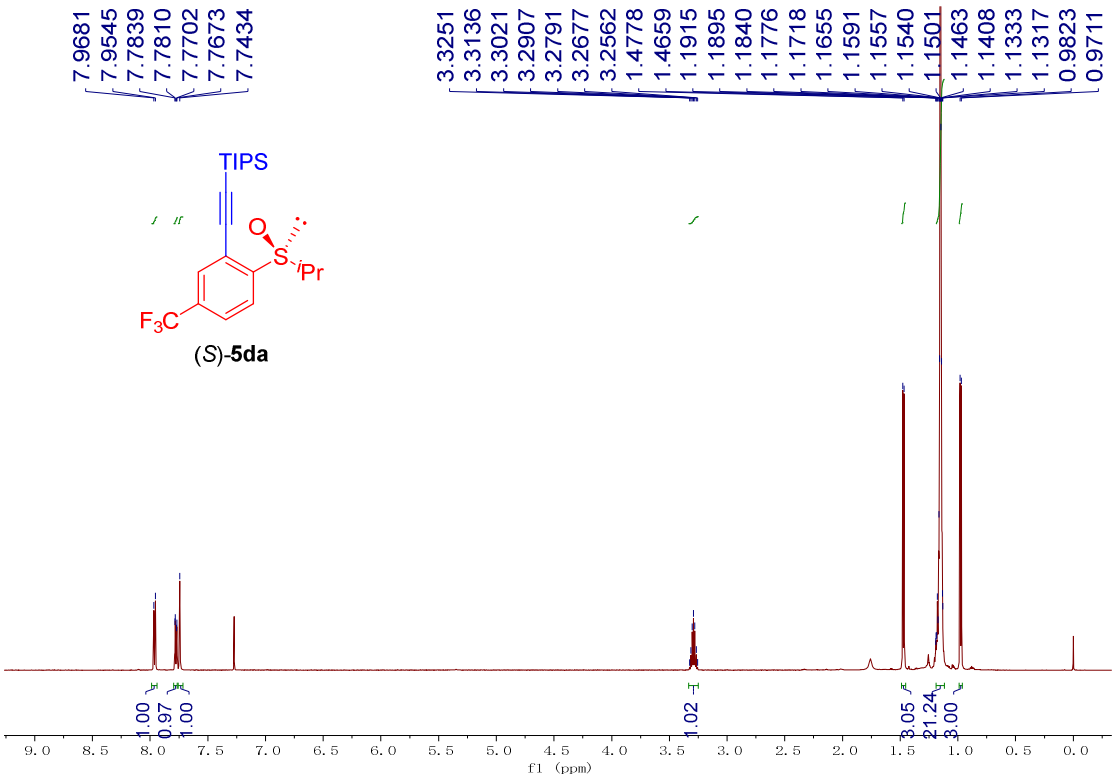
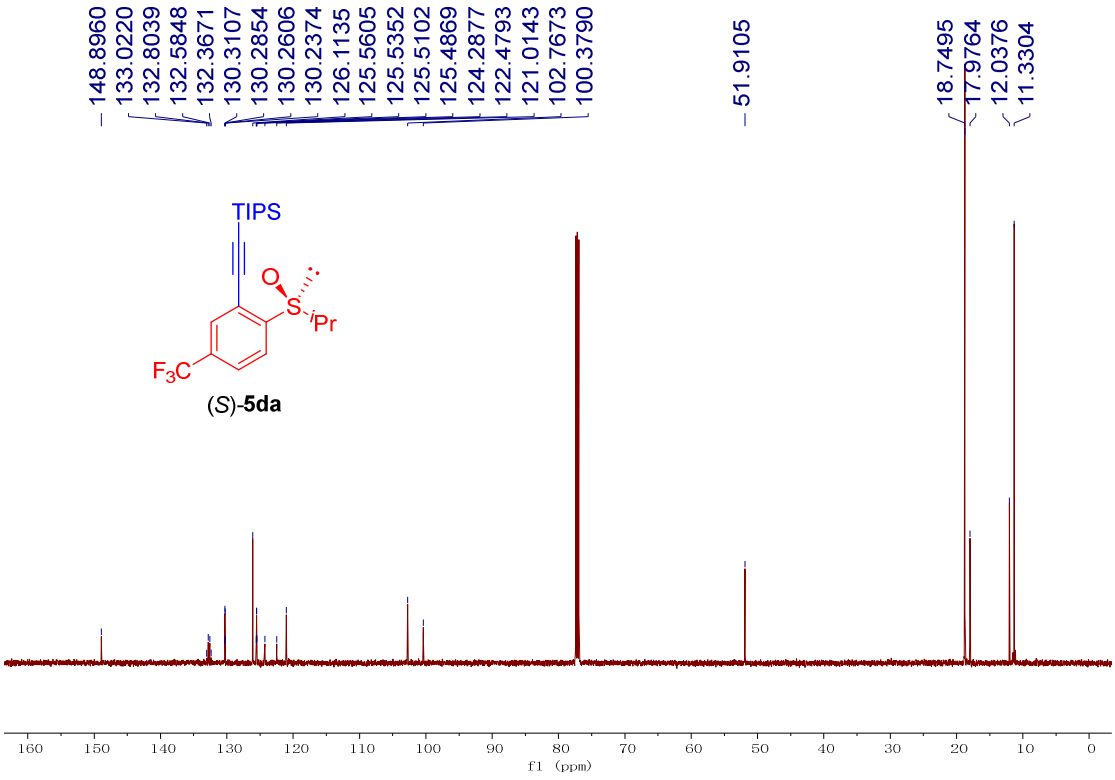
7.2182
7.2139
3.2121
3.2006
3.1891
3.1776
3.1661
3.1546
3.1431
1.4258
1.4140
1.1609
1.1554
1.1488
1.1434
1.1409
1.1377
1.1339
1.1322
1.1288
1.1240
1.1182
0.9981
0.9869
TIPS
O
S
iPr
F
(S)-5ba
0.97
1.98
1.00
3.08
21.30
3.07
f1 (ppm)

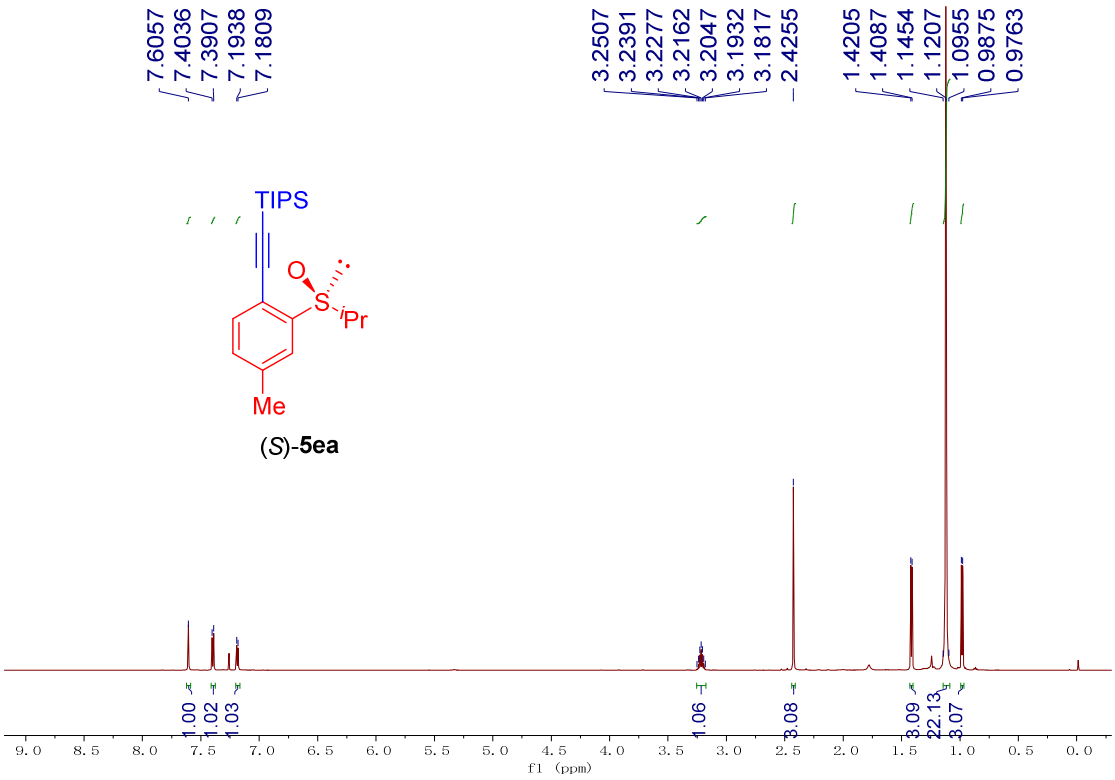

164.4355
162.7724
140.1110
140.0879
127.6495
127.5881
122.2478
122.1815
120.4322
120.2751
116.7875
116.6414
101.7744
100.5720
18.7531
17.6754
12.1702
11.3495
TIPS
O
S
iPr
F
(S)-5ba
f1 (ppm)


7.6908
7.6770
7.6702
7.6671
7.6534
7.6496
7.6467
3.2388
3.2273
3.2158
3.2043
3.1929
3.1814
3.1699
1.4360
1.4242
1.1722
1.1698
1.1665
1.1636
1.1582
1.1552
1.1523
1.1465
1.1418
1.1393
1.1361
1.1328
1.1310
1.1274
1.1224
1.1162
0.9885
0.9773
TIPS
O
S
iPr
Br
(S)-5ca
2.94
1.00
3.07
20.97
3.00
f1 (ppm)

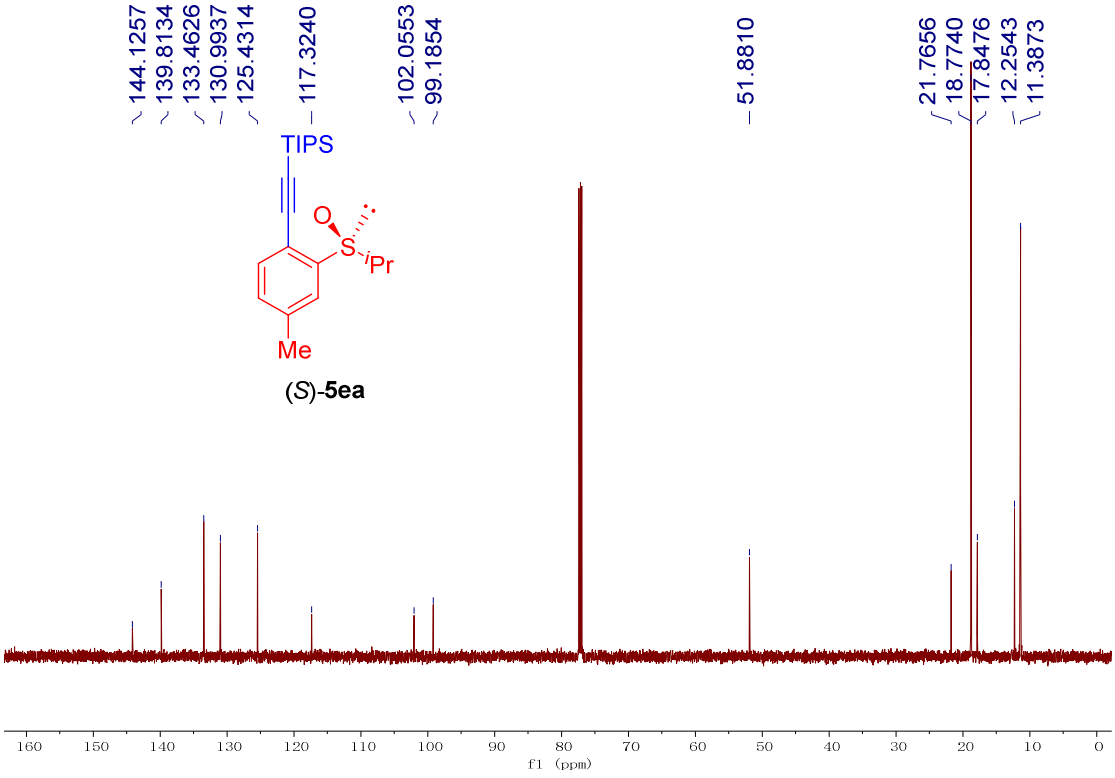

143.7422
135.9478
132.2653
126.8865
124.4306
121.8951
102.1388
100.3537
51.9917
18.7505
17.7743
12.1092
11.3330
TIPS
O
S
iPr
Br
(S)-5ca
f1 (ppm)


7.9681
7.9545
7.7839
7.7810
7.7702
7.7673
7.7434
3.3251
3.3136
3.3021
3.2907
3.2791
3.2677
3.2562
1.4778
1.4659
1.1915
1.1895
1.1840
1.1776
1.1718
1.1655
1.1591
1.1557
1.1540
1.1501
1.1463
1.1408
1.1333
1.1317
0.9823
0.9711
TIPS
O
S
iPr
F3C
(S)-5da
1.00
0.97
1.00
1.02
3.05
21.24
3.00
f1 (ppm)

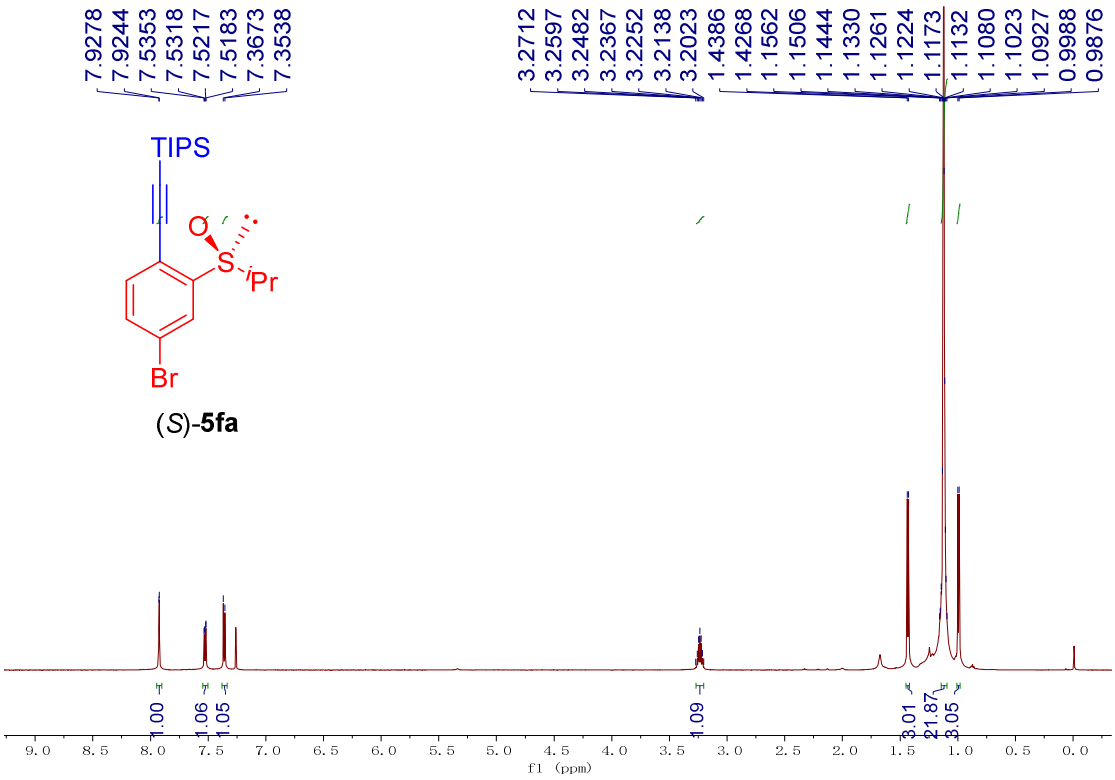

148.8960
133.0220
132.8039
132.5848
132.3671
130.3107
130.2854
130.2606
130.2374
126.1135
125.5605
125.5352
125.5102
125.4869
124.2877
122.4793
121.0143
102.7673
100.3790
51.9105
18.7495
17.9764
12.0376
11.3304
TIPS
O
S
iPr
F3C
(S)-5da
f1 (ppm)

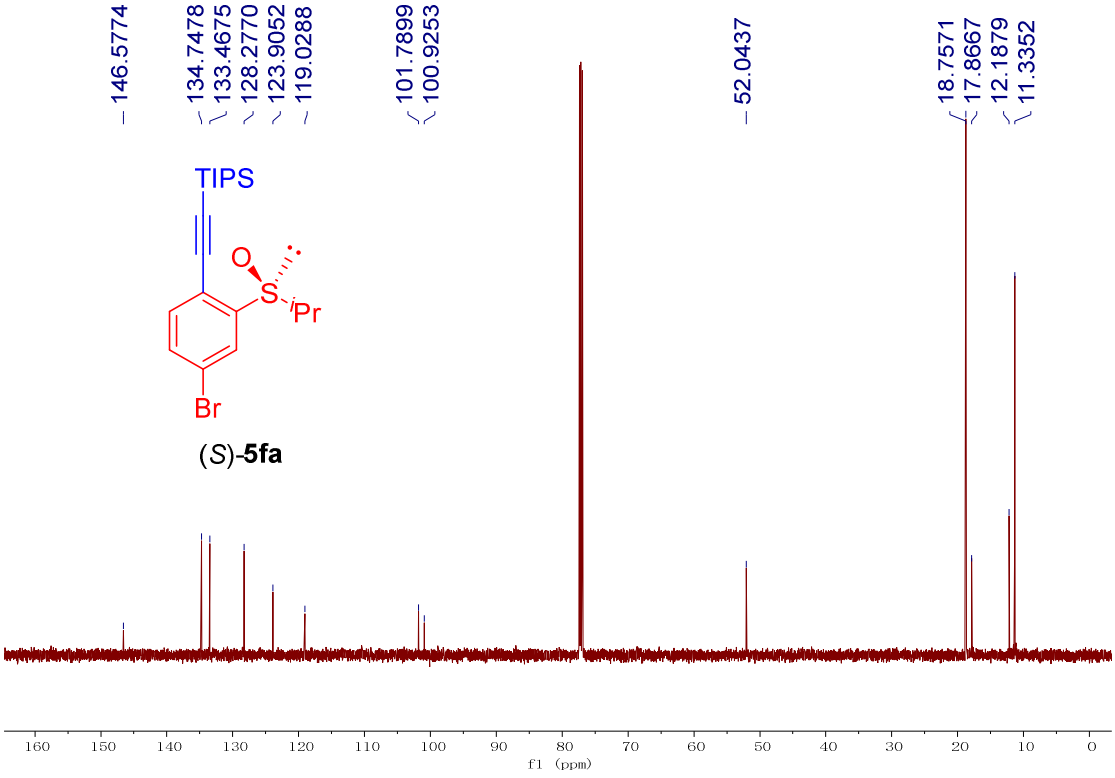

7.6057
7.4036
7.3907
7.1938
7.1809
3.2507
3.2391
3.2277
3.2162
3.2047
3.1932
3.1817
2.4255
1.4205
1.4087
1.1454
1.1207
1.0955
0.9875
0.9763
TIPS
O
S
iPr
Me
1.00
1.02
1.03
1.06
3.08
3.09
22.13
3.07
f1 (ppm)

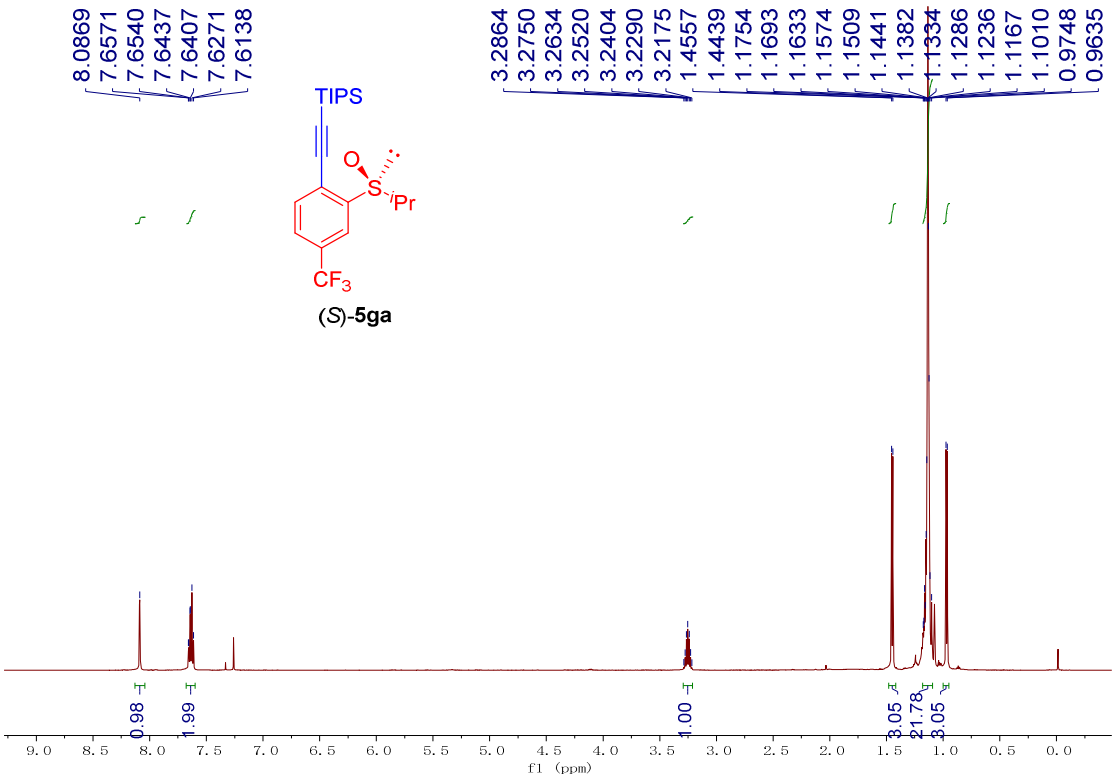
(*S*)-**5ea**

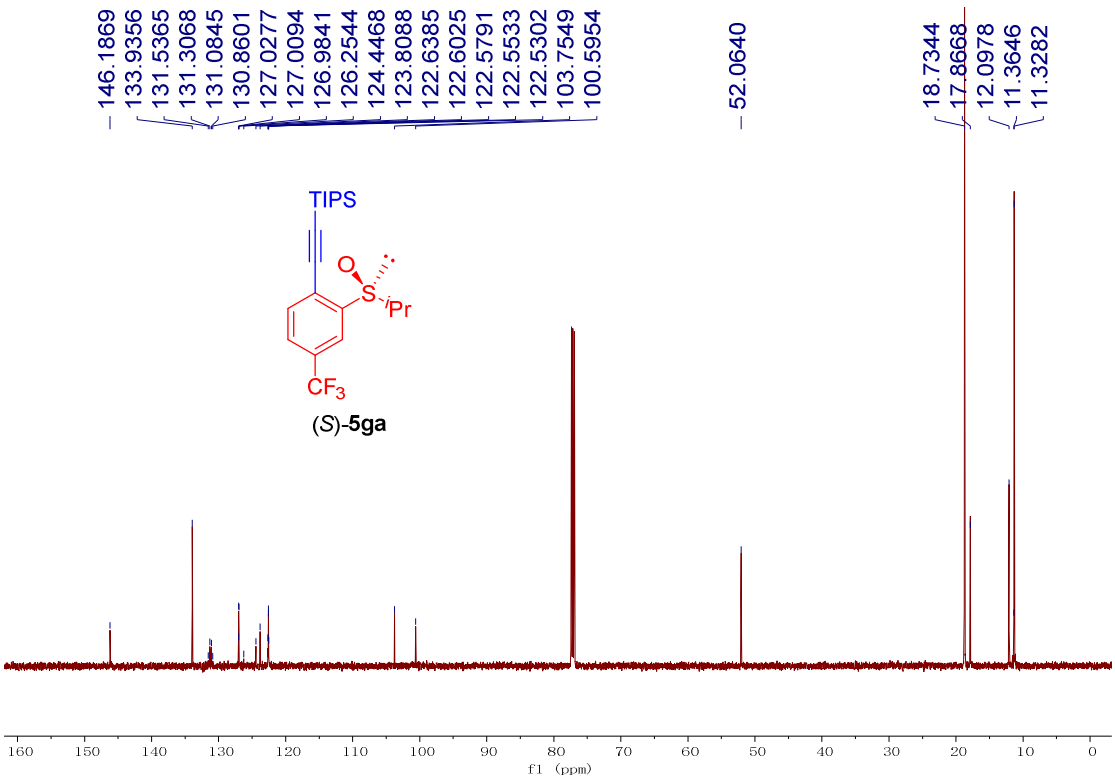

144.1257
139.8134
133.4626
130.9937
125.4314
117.3240
102.0553
99.1854
51.8810
21.7656
18.7740
17.8476
12.2543
11.3873
TIPS
O
S
iPr
Me
f1 (ppm)

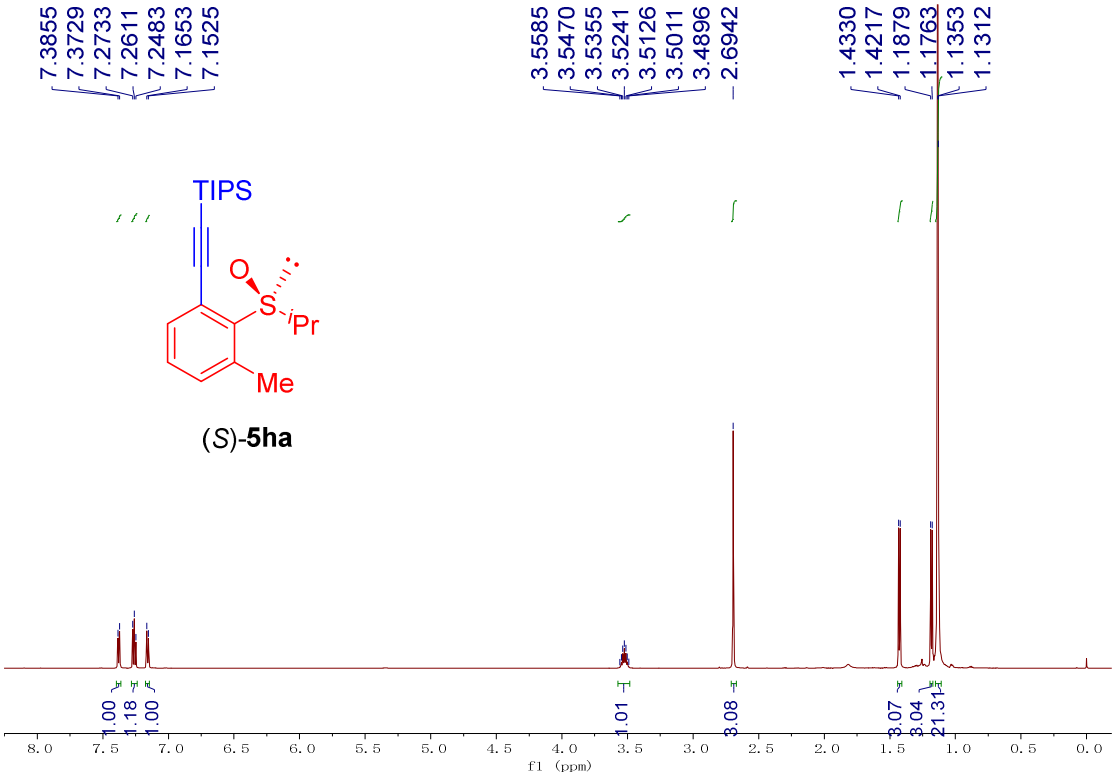
(*S*)-**5ea**


7.9278
7.9244
7.5353
7.5318
7.5217
7.5183
7.3673
7.3538
3.2712
3.2597
3.2482
3.2367
3.2252
3.2138
3.2023
1.4386
1.4268
1.1562
1.1506
1.1444
1.1330
1.1261
1.1224
1.1173
1.1132
1.1080
1.1023
1.0927
0.9988
0.9876
TIPS
O
S
iPr
Br
(S)-5fa
1.00
1.06
1.05
1.09
3.01
21.87
3.05
f1 (ppm)

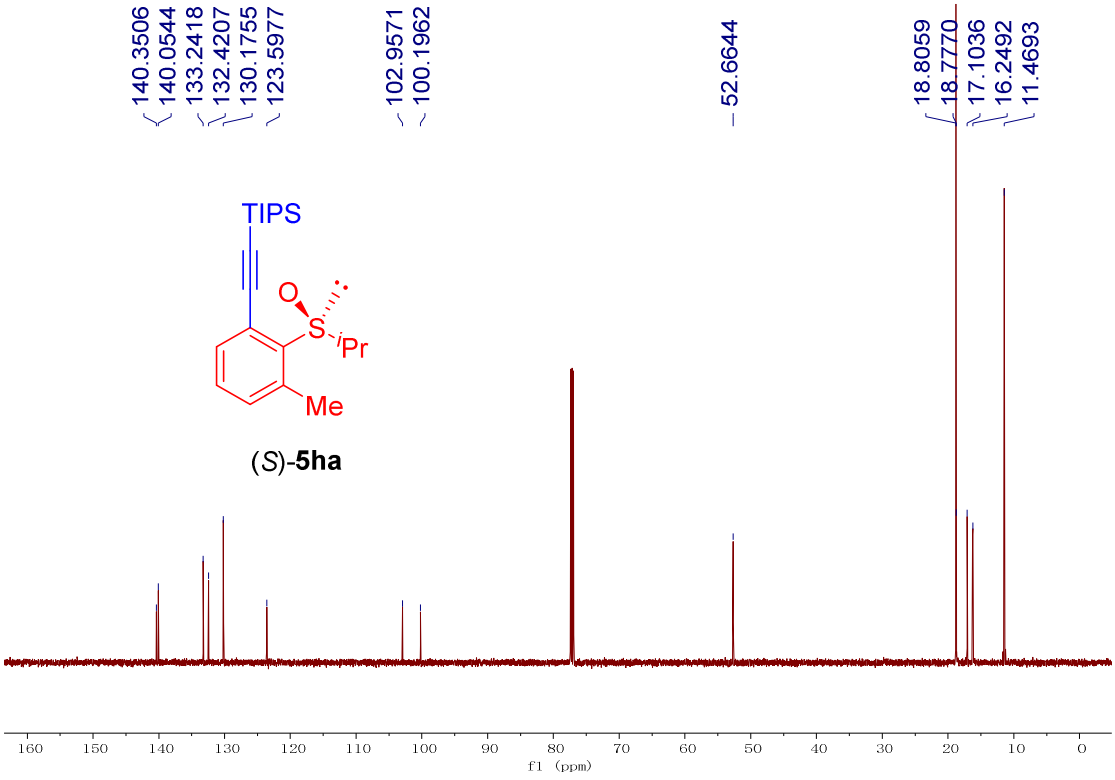

146.5774
134.7478
133.4675
128.2770
123.9052
119.0288
101.7899
100.9253
52.0437
18.7571
17.8667
12.1879
11.3352
TIPS
O
S
iPr
Br
(S)-5fa
f1 (ppm)


8.0869
7.6571
7.6540
7.6437
7.6407
7.6271
7.6138
3.2864
3.2750
3.2634
3.2520
3.2404
3.2290
3.2175
1.4557
1.4439
1.1754
1.1693
1.1633
1.1574
1.1509
1.1441
1.1382
1.1334
1.1286
1.1236
1.1167
1.1010
0.9748
0.9635
TIPS
O
S
iPr
CF3
(S)-5ga
0.98
1.99
1.00
3.05
21.78
3.05
f1 (ppm)

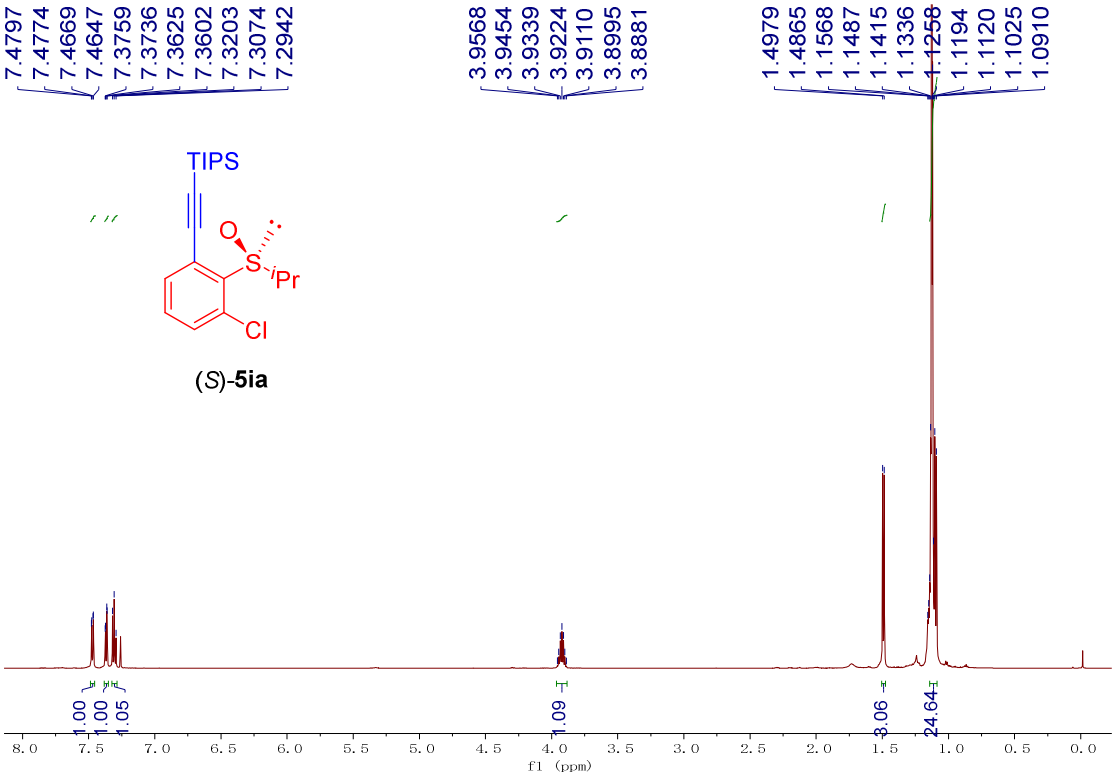

146.1869
133.9356
131.5365
131.3068
131.0845
130.8601
127.0277
127.0094
126.9841
126.2544
124.4468
123.8088
122.6385
122.6025
122.5791
122.5533
122.5302
103.7549
100.5954
52.0640
18.7344
17.8668
12.0978
11.3646
11.3282
TIPS
O
S
iPr
CF3
(S)-5ga
f1 (ppm)


7.3855
7.3729
7.2733
7.2611
7.2483
7.1653
7.1525
3.5585
3.5470
3.5355
3.5241
3.5126
3.5011
3.4896
2.6942
1.4330
1.4217
1.1879
1.1763
1.1353
1.1312
TIPS
O
S
iPr
Me
1.00
1.18
1.00
1.01
3.08
3.07
3.04
21.31
f1 (ppm)

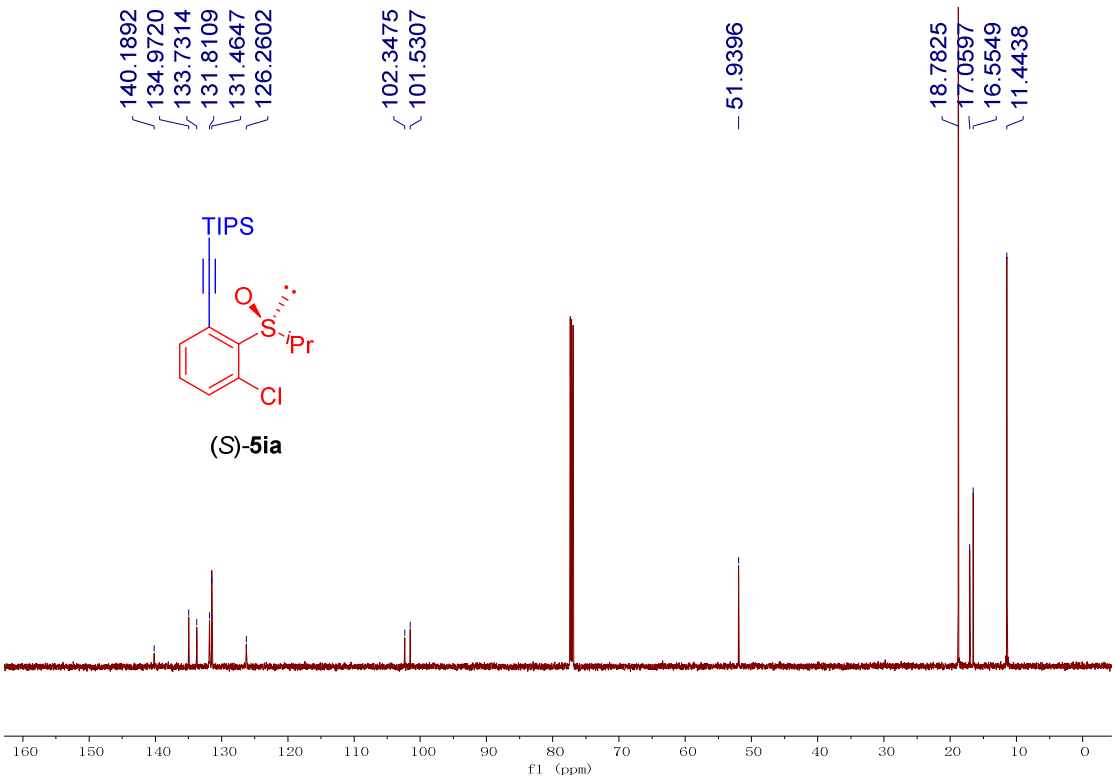
(*S*)-**5ha**


140.3506
140.0544
133.2418
132.4207
130.1755
123.5977
102.9571
100.1962
52.6644
18.8059
18.7770
17.1036
16.2492
11.4693
TIPS
O
S
iPr
Me
f1 (ppm)

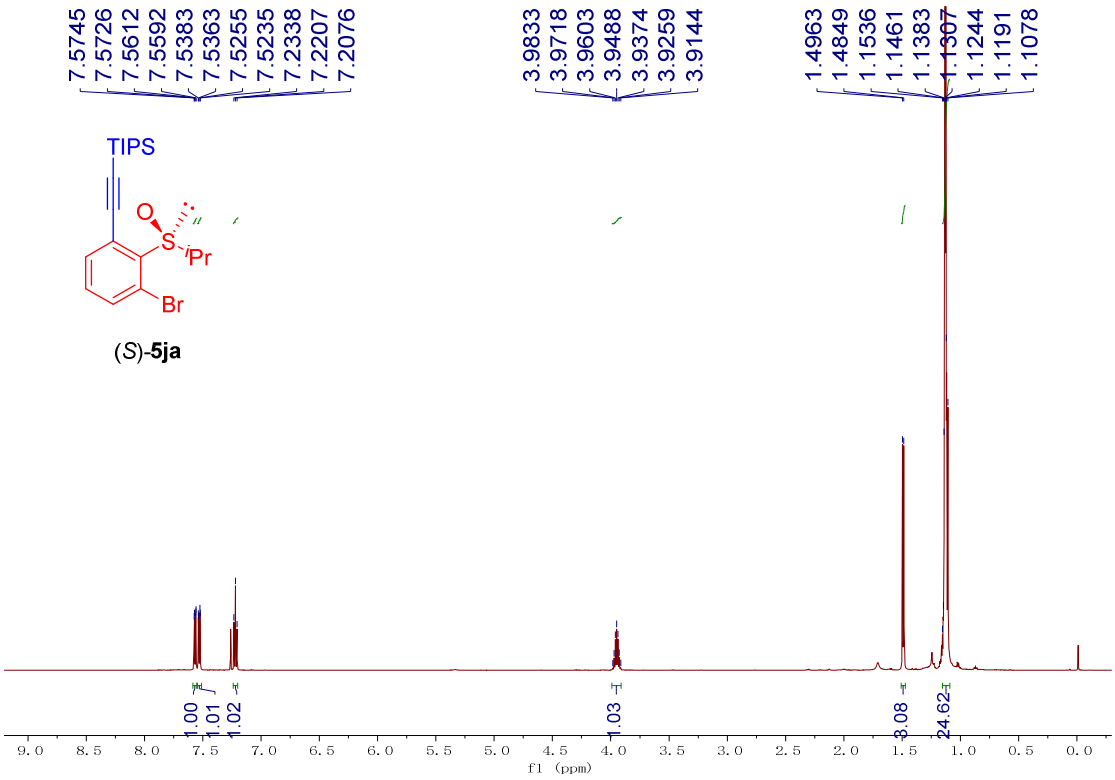
(*S*)-**5ha**


7.4797
7.4774
7.4669
7.4647
7.3759
7.3736
7.3625
7.3602
7.3203
7.3074
7.2942
3.9568
3.9454
3.9339
3.9224
3.9110
3.8995
3.8881
1.4979
1.4865
1.1568
1.1487
1.1415
1.1336
1.1258
1.1194
1.1120
1.1025
1.0910
TIPS
O
S
iPr
Cl
1.00
1.00
1.05
1.09
3.06
24.64
f1 (ppm)

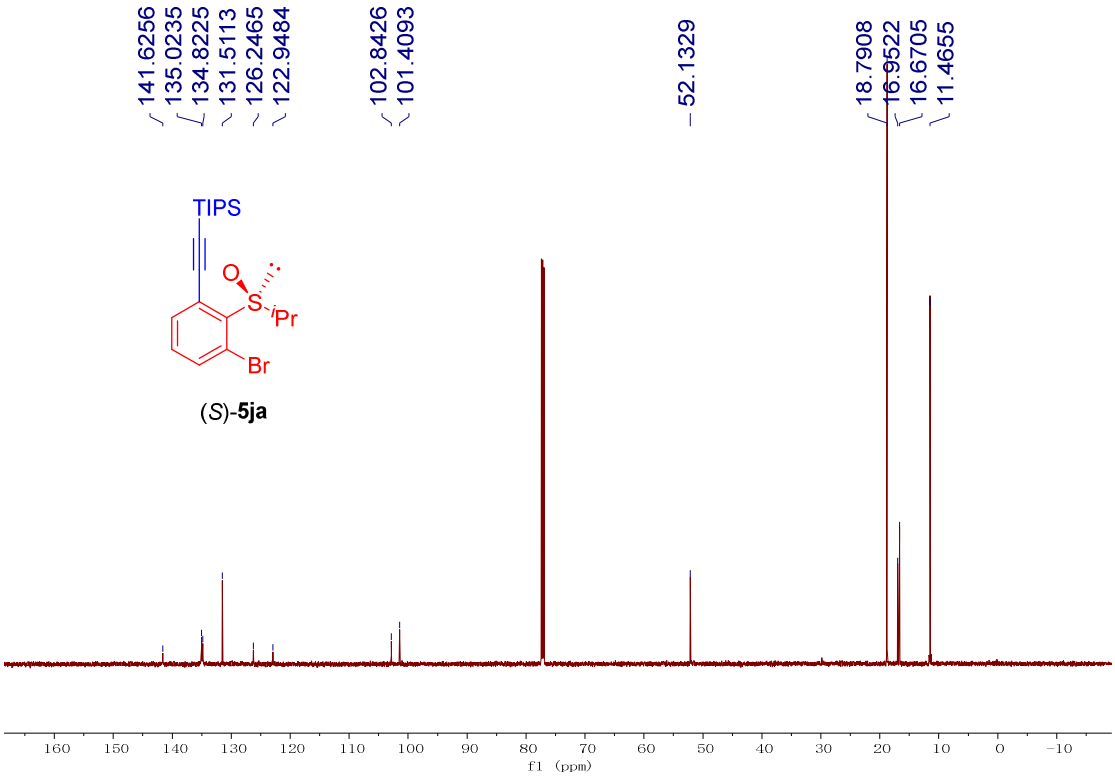
(*S*)-**5ia**


140.1892
134.9720
133.7314
131.8109
131.4647
126.2602
102.3475
101.5307
51.9396
18.7825
17.0597
16.5549
11.4438
TIPS
O
S
iPr
Cl
f1 (ppm)

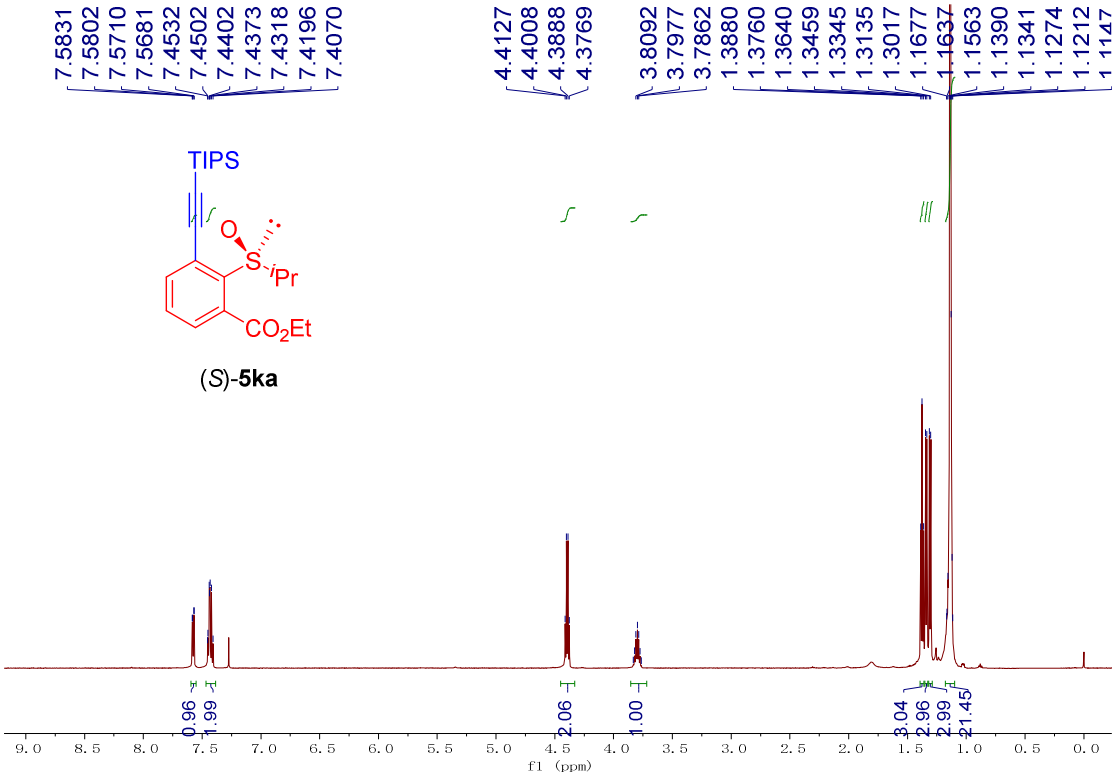
(*S*)-**5ia**

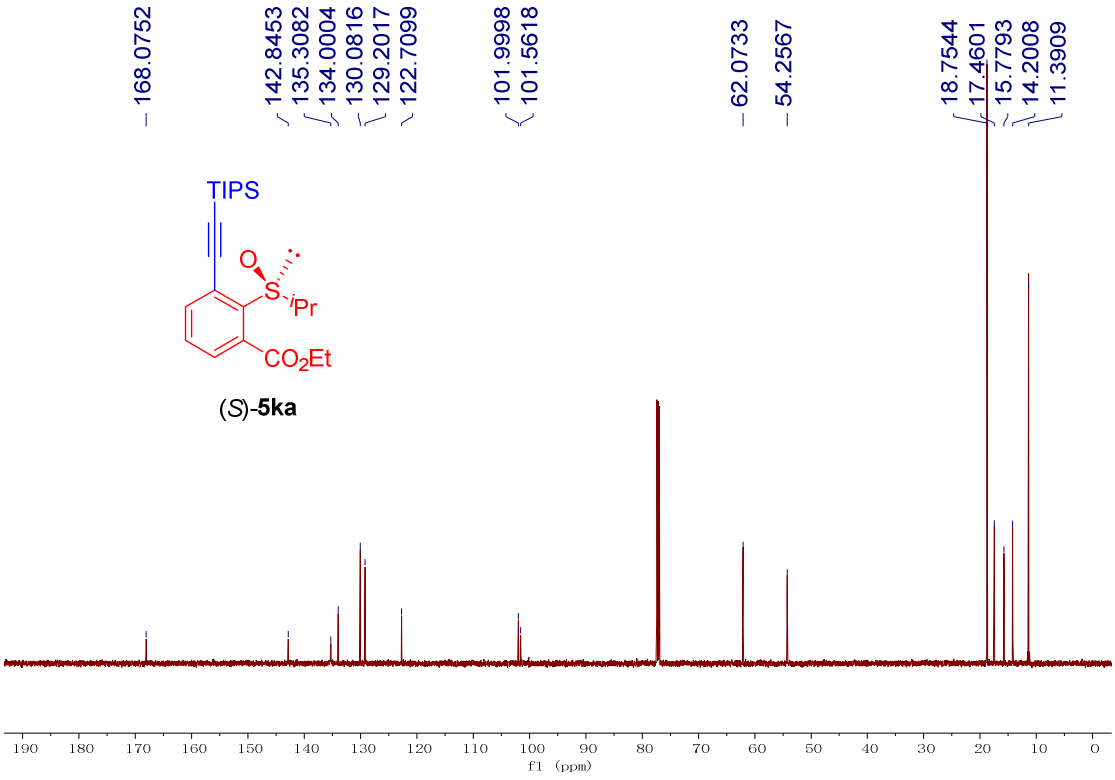

7.5745
7.5726
7.5612
7.5592
7.5383
7.5363
7.5255
7.5235
7.2338
7.2207
7.2076
3.9833
3.9718
3.9603
3.9488
3.9374
3.9259
3.9144
1.4963
1.4849
1.1536
1.1461
1.1383
1.1307
1.1244
1.1191
1.1078
TIPS
O
S
iPr
Br
1.00
1.01
1.02
1.03
3.08
24.62
f1 (ppm)

(*S*)-**5ja**


141.6256
135.0235
134.8225
131.5113
126.2465
122.9484
102.8426
101.4093
52.1329
18.7908
16.9522
16.6705
11.4655
TIPS
O
S
iPr
Br
f1 (ppm)

(*S*)-**5ja**


7.5831
7.5802
7.5710
7.5681
7.4532
7.4502
7.4402
7.4373
7.4318
7.4196
7.4070
4.4127
4.4008
4.3888
4.3769
3.8092
3.7977
3.7862
1.3880
1.3760
1.3640
1.3459
1.3345
1.3135
1.3017
1.1677
1.1637
1.1563
1.1390
1.1341
1.1274
1.1212
1.1147
TIPS
O
S
iPr
CO2Et
(S)-5ka
0.96
1.99
2.06
1.00
3.04
2.96
2.99
21.45
f1 (ppm)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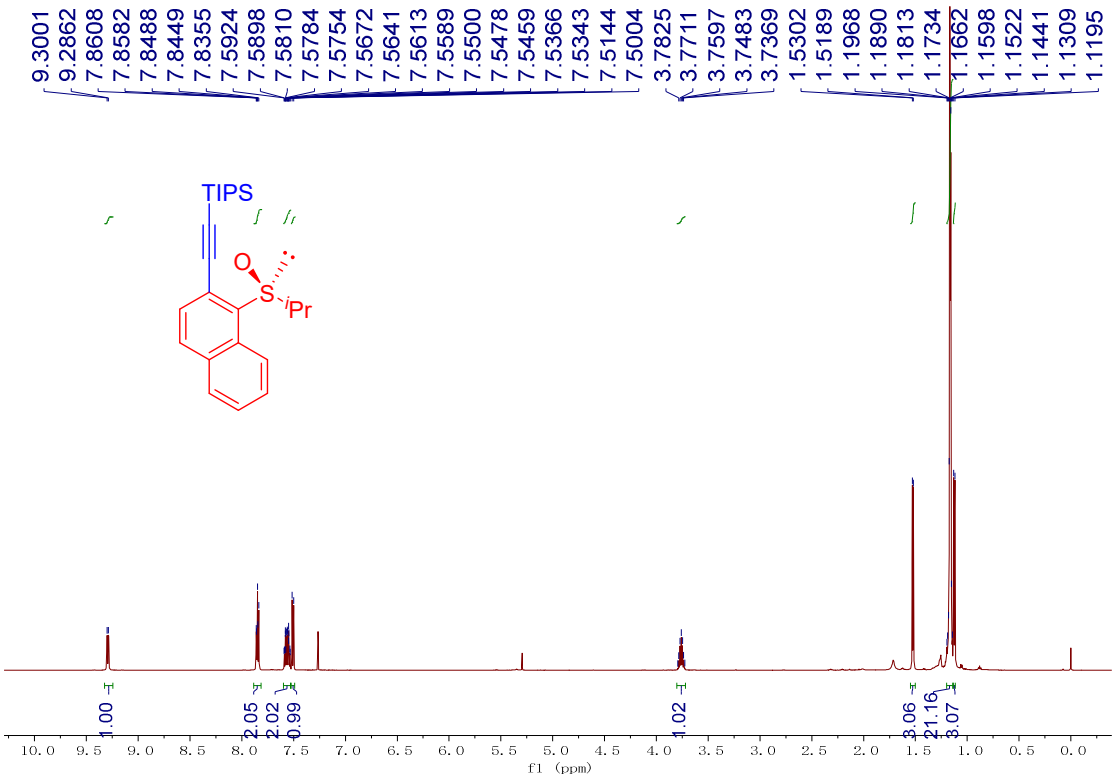
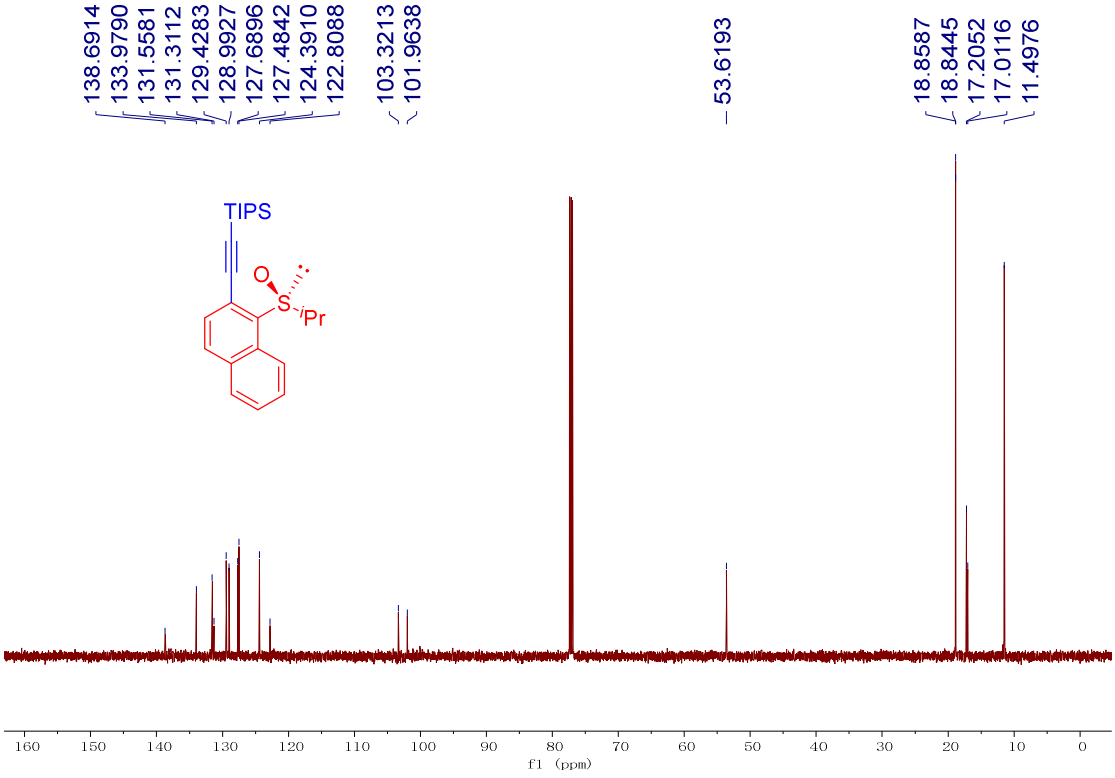
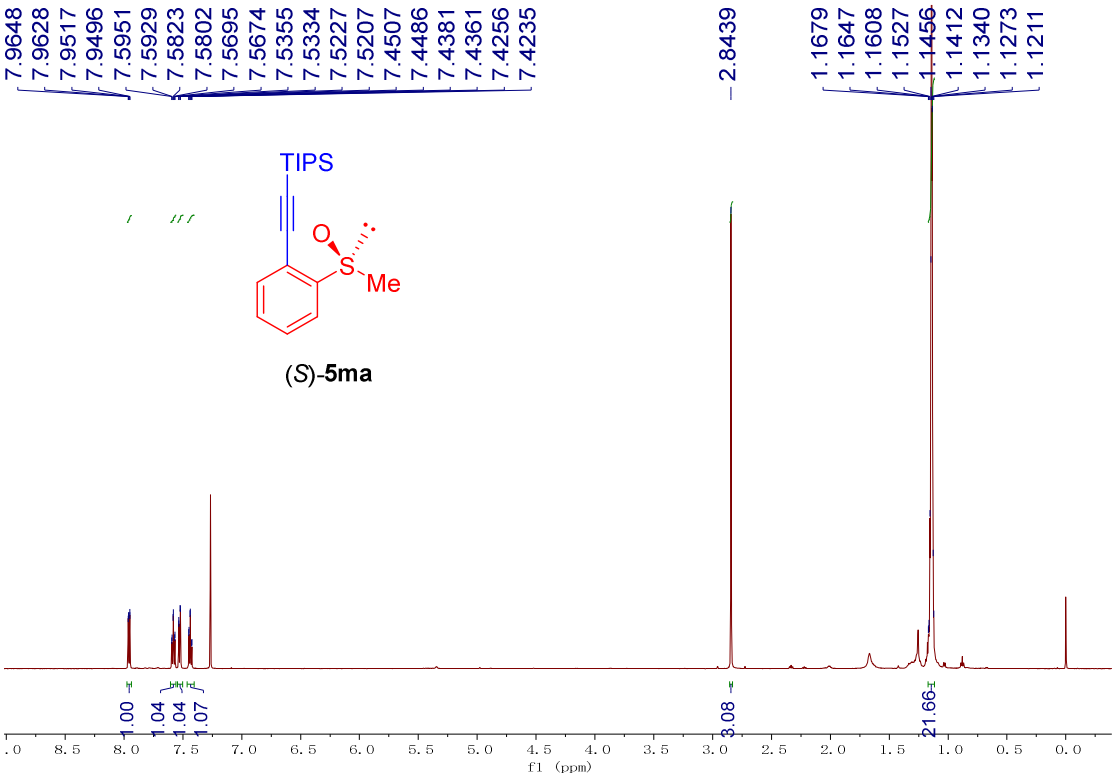
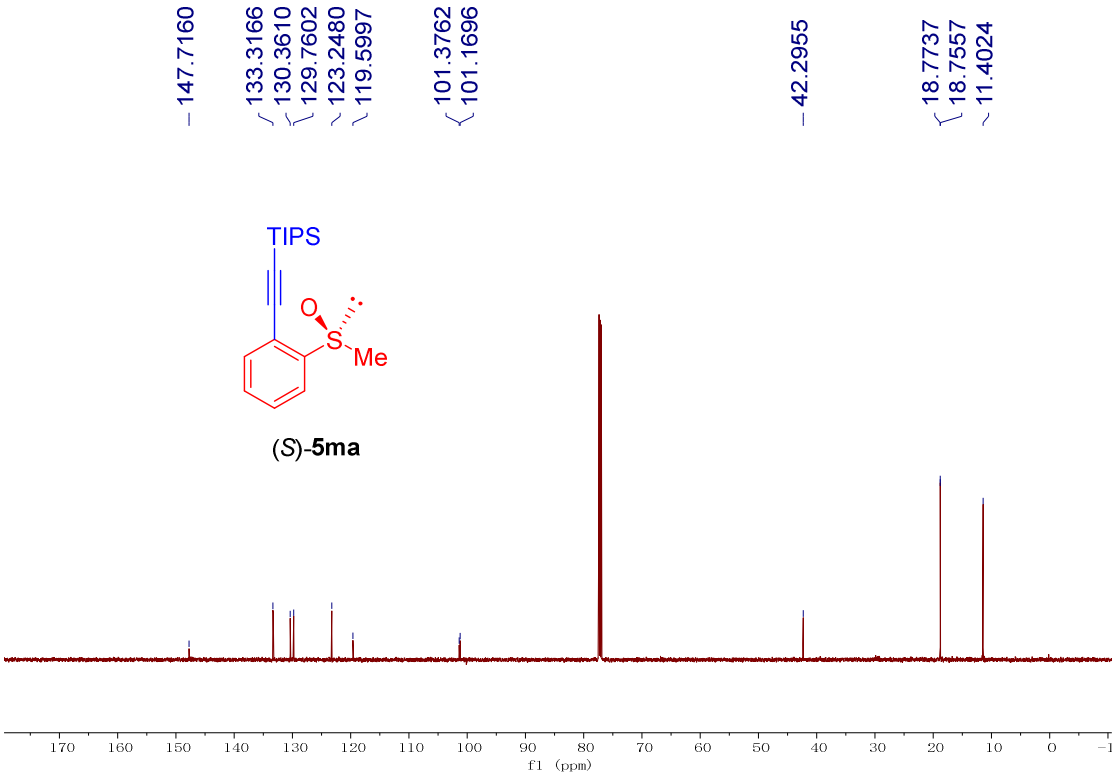
135.3082
134.0004
130.0816
129.2017
122.7099
101.9998
101.5618
62.0733
54.2567
18.7544
17.4601
15.7793
14.2008
11.3909
TIPS
O
S
iPr
CO2Et
(S)-5ka
f1 (ppm)


9.3001
9.2862
7.8608
7.8582
7.8488
7.8449
7.8355
7.5924
7.5898
7.5810
7.5784
7.5754
7.5672
7.5641
7.5613
7.5589
7.5500
7.5478
7.5459
7.5366
7.5343
7.5144
7.5004
3.7825
3.7711
3.7597
3.7483
3.7369
1.5302
1.5189
1.1968
1.1890
1.1813
1.1734
1.1662
1.1598
1.1522
1.1441
1.1309
1.1195
TIPS
O
S
iPr
1.00
2.05
2.02
0.99
1.02
3.06
21.16
3.07
f1 (ppm)

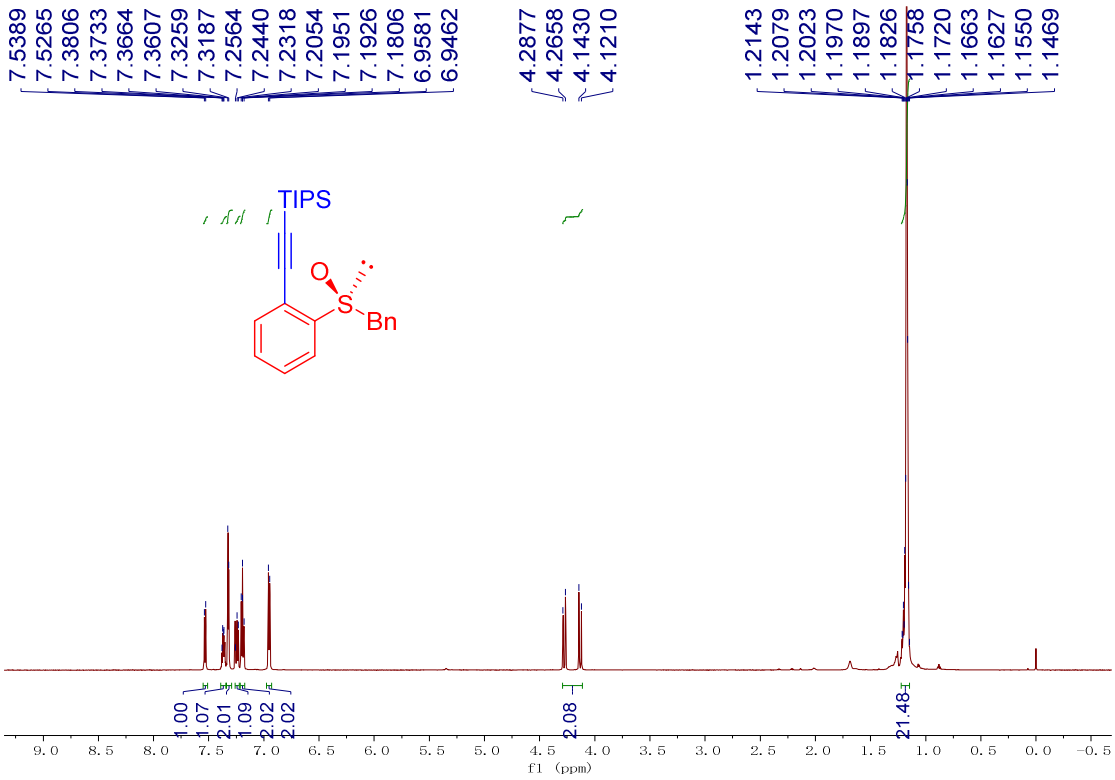

138.6914
133.9790
131.5581
131.3112
129.4283
128.9927
127.6896
127.4842
124.3910
122.8088
103.3213
101.9638
53.6193
18.8587
18.8445
17.2052
17.0116
11.4976
TIPS
O
S
iPr
f1 (ppm)

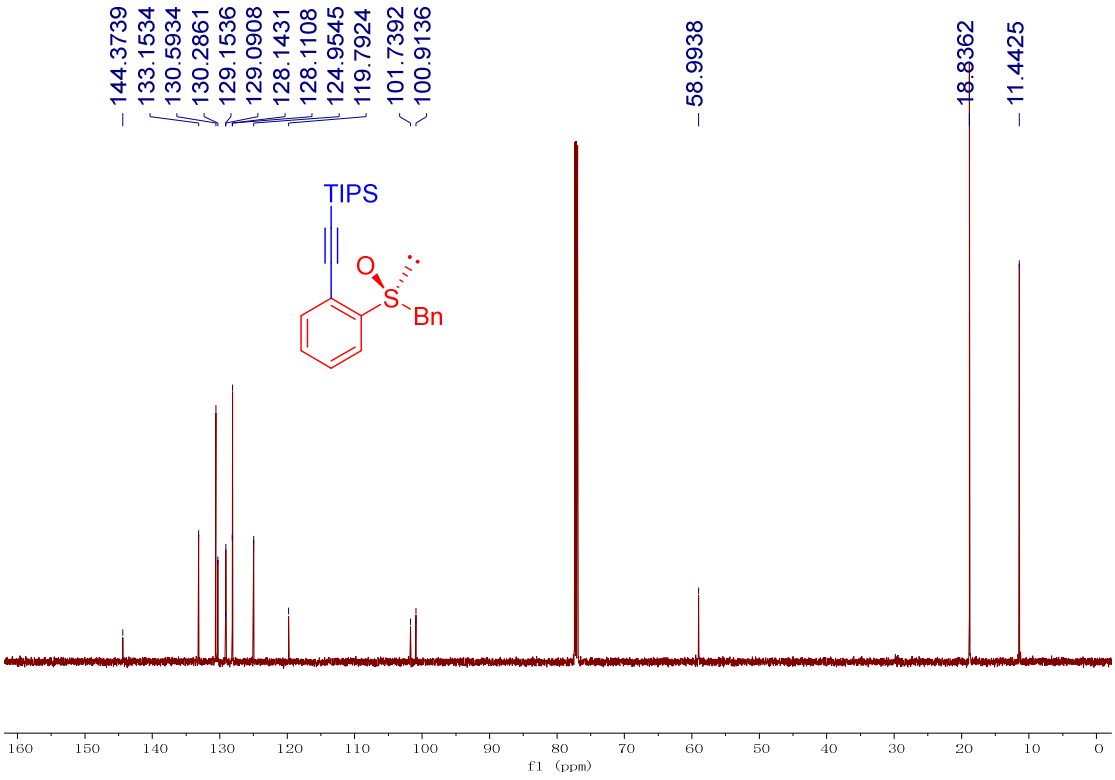

7.9648
7.9628
7.9517
7.9496
7.5951
7.5929
7.5823
7.5802
7.5695
7.5674
7.5355
7.5334
7.5227
7.5207
7.4507
7.4486
7.4381
7.4361
7.4256
7.4235
2.8439
1.1679
1.1647
1.1608
1.1527
1.1456
1.1412
1.1340
1.1273
1.1211
TIPS
O
S
Me
1.00
1.04
1.04
1.07
3.08
21.66
f1 (ppm)

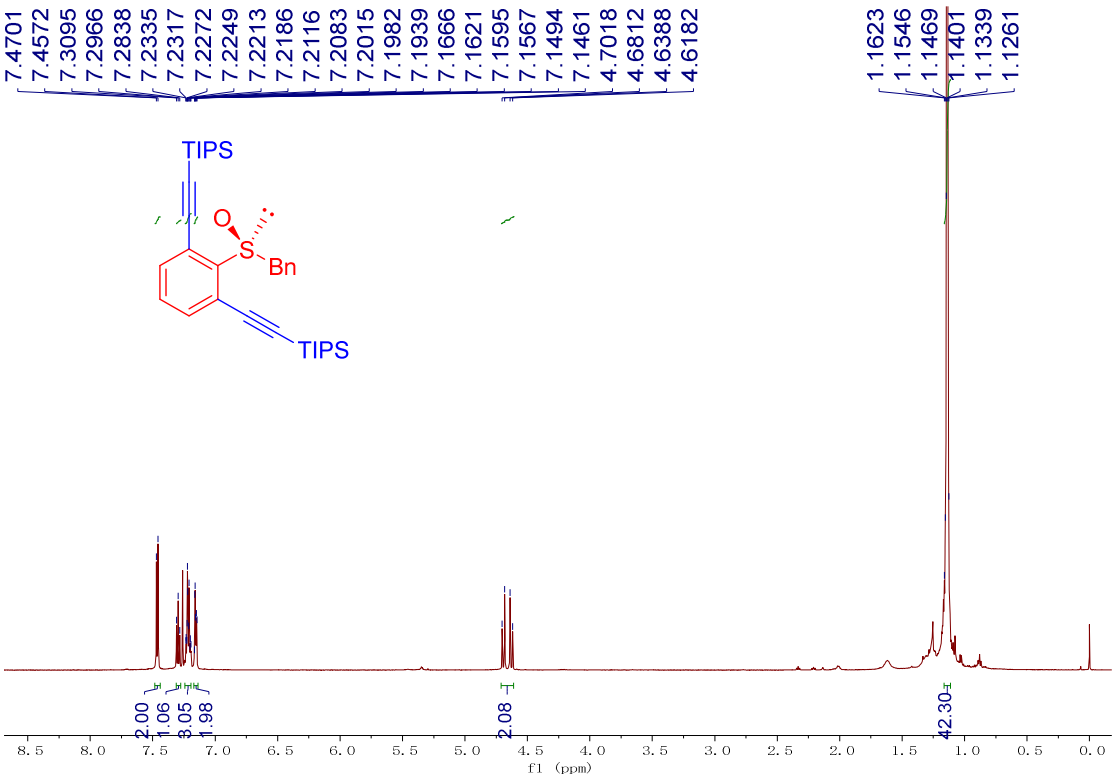
(*S*)-**5ma**

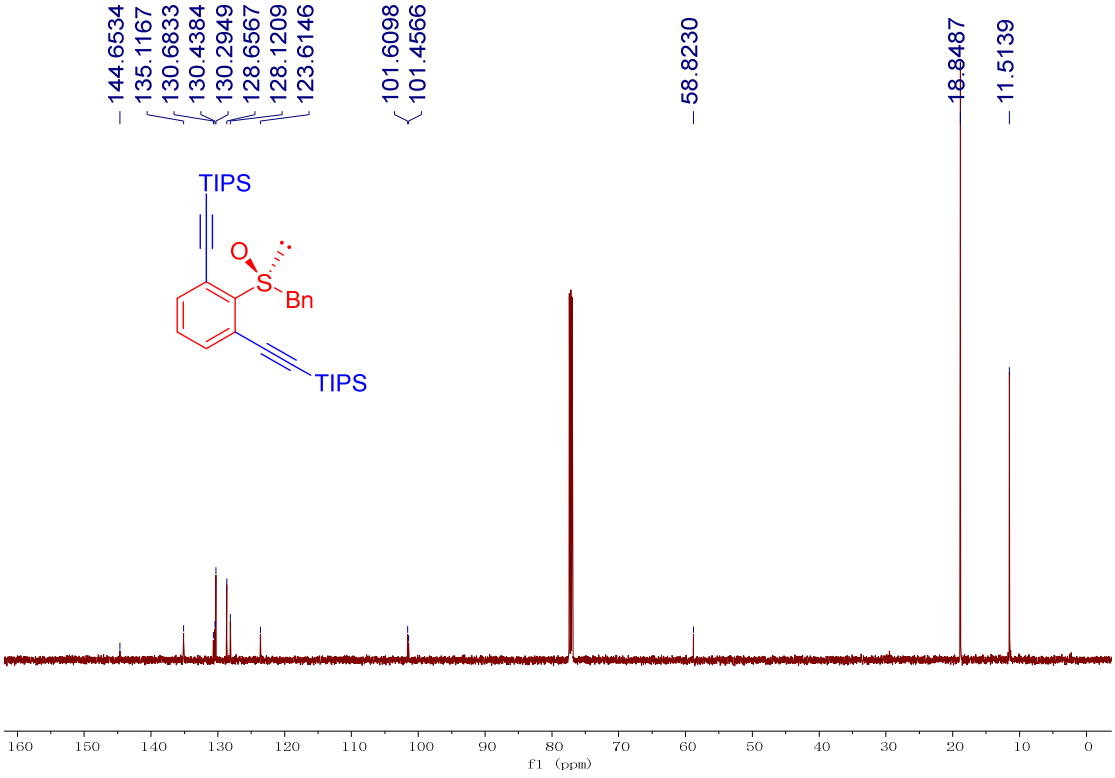

147.7160
133.3166
130.3610
129.7602
123.2480
119.5997
101.3762
101.1696
42.2955
18.7737
18.7557
11.4024
TIPS
O
S
Me
f1 (ppm)

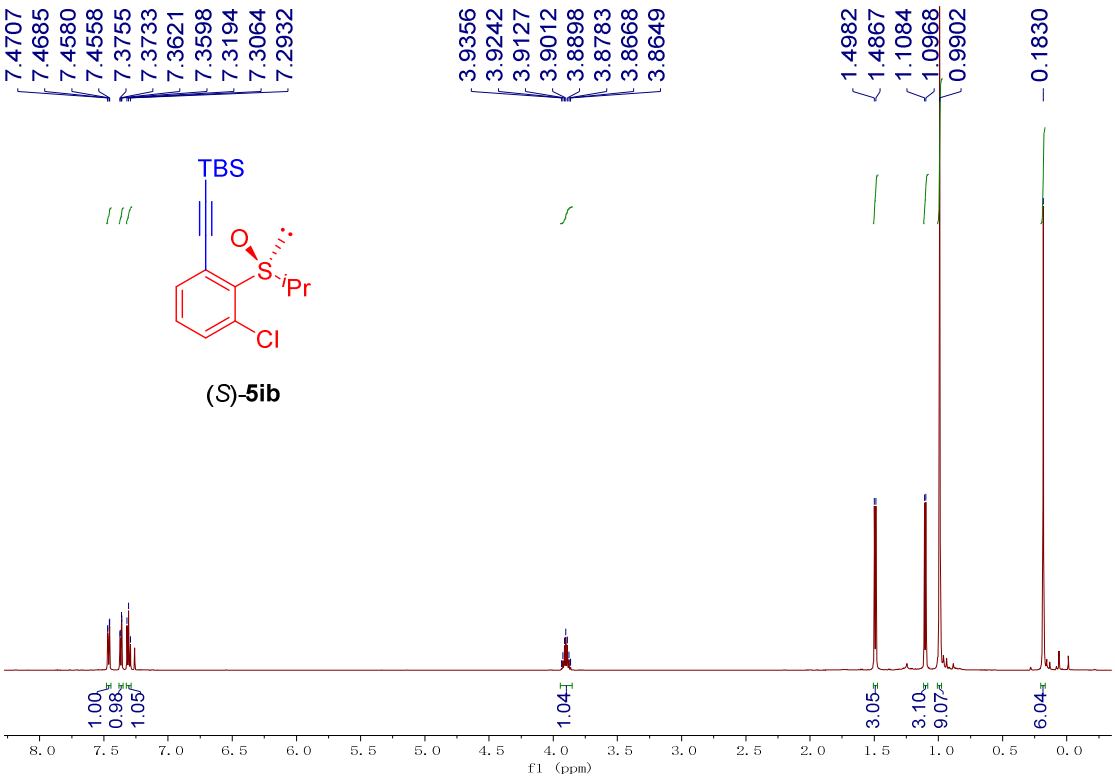
(*S*)-**5ma**


7.5389
7.5265
7.3806
7.3733
7.3664
7.3607
7.3259
7.3187
7.2564
7.2440
7.2318
7.2054
7.1951
7.1926
7.1806
6.9581
6.9462
4.2877
4.2658
4.1430
4.1210
1.2143
1.2079
1.2023
1.1970
1.1897
1.1826
1.1758
1.1720
1.1663
1.1627
1.1550
1.1469
TIPS
O
S
Bn
1.00
1.07
2.01
1.09
2.02
2.02
2.08
21.48
f1 (ppm)

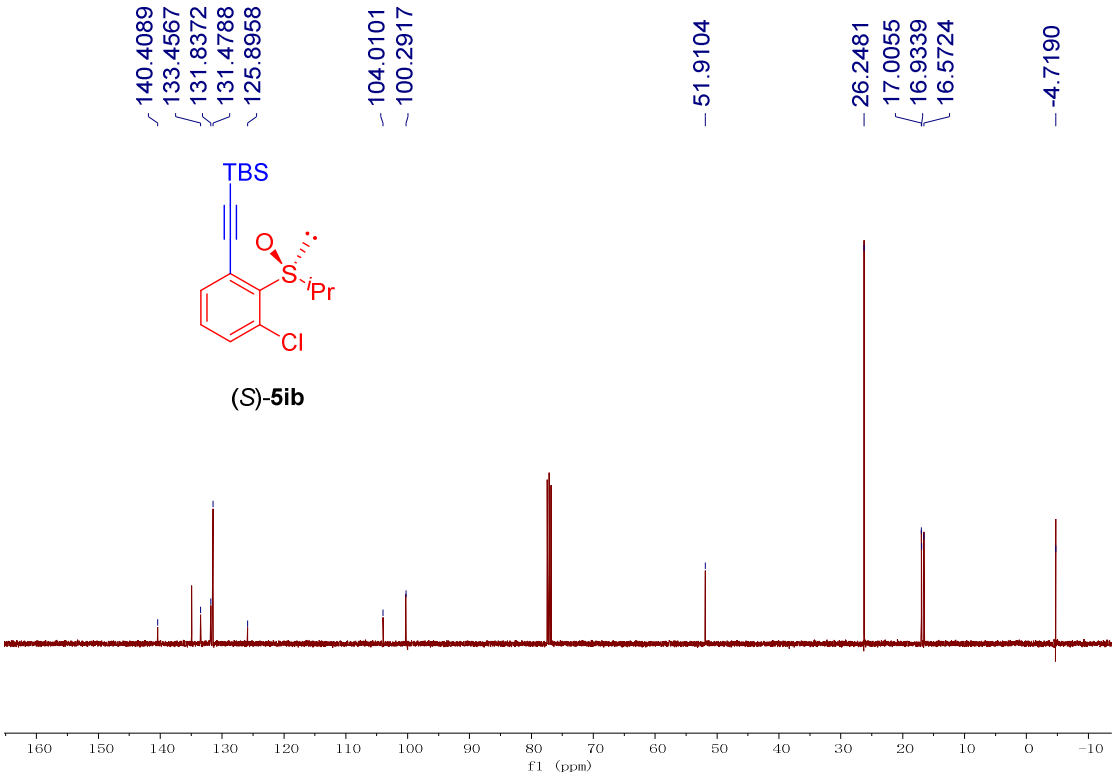

144.3739
133.1534
130.5934
130.2861
129.1536
129.0908
128.1431
128.1108
124.9545
119.7924
101.7392
100.9136
58.9938
18.8362
11.4425
TIPS
O
S
Bn
f1 (ppm)


7.4701
7.4572
7.3095
7.2966
7.2838
7.2335
7.2317
7.2272
7.2249
7.2213
7.2186
7.2116
7.2083
7.2015
7.1982
7.1939
7.1666
7.1621
7.1595
7.1567
7.1494
7.1461
7.1401
4.7018
4.6812
4.6388
4.6182
1.1623
1.1546
1.1469
1.1401
1.1339
1.1261
TIPS
O
S
Bn
TIPS
2.00
1.06
3.05
1.98
2.08
42.30
f1 (ppm)

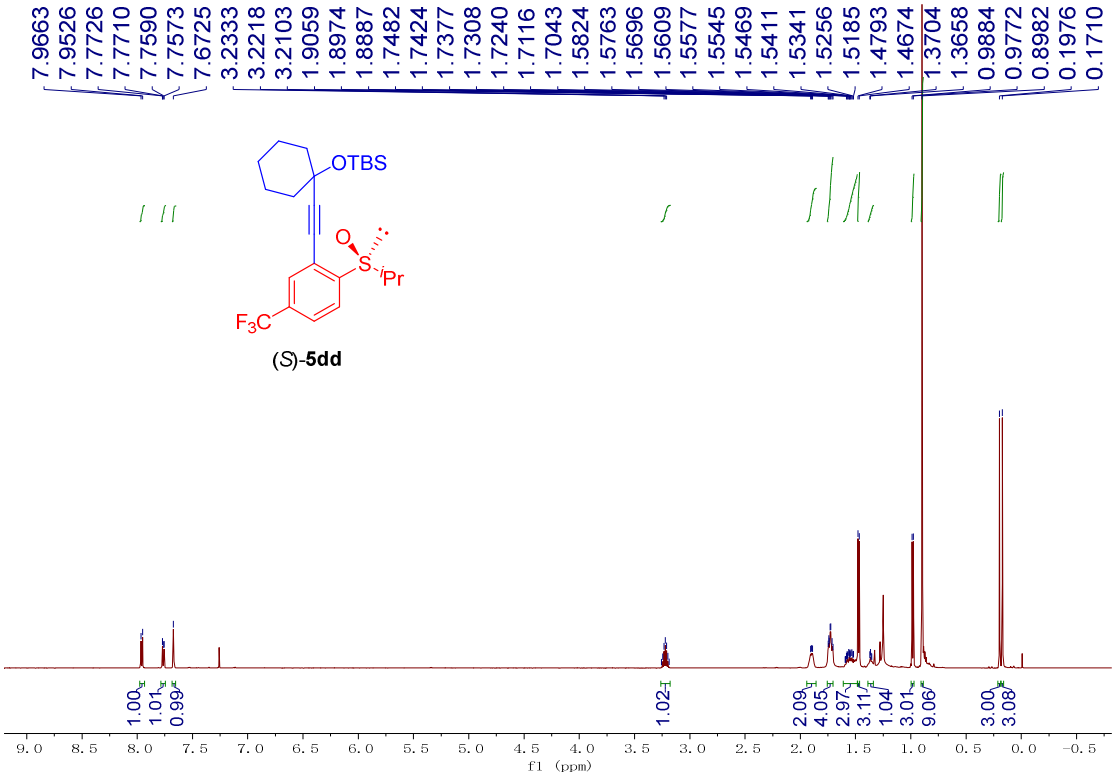

144.6534
135.1167
130.6833
130.4384
130.2949
128.6567
128.1209
123.6146
101.6098
101.4566
58.8230
18.8487
11.5139
TIPS
O
S
Bn
TIPS
f1 (ppm)


7.4707
7.4685
7.4580
7.4558
7.3755
7.3733
7.3621
7.3598
7.3194
7.3064
7.2932
3.9356
3.9242
3.9127
3.9012
3.8898
3.8783
3.8668
3.8649
1.4982
1.4867
1.1084
1.0968
0.9902
0.1830
TBS
O
S
iPr
Cl
1.00
0.98
1.05
1.04
3.05
3.10
9.07
6.04
f1 (ppm)

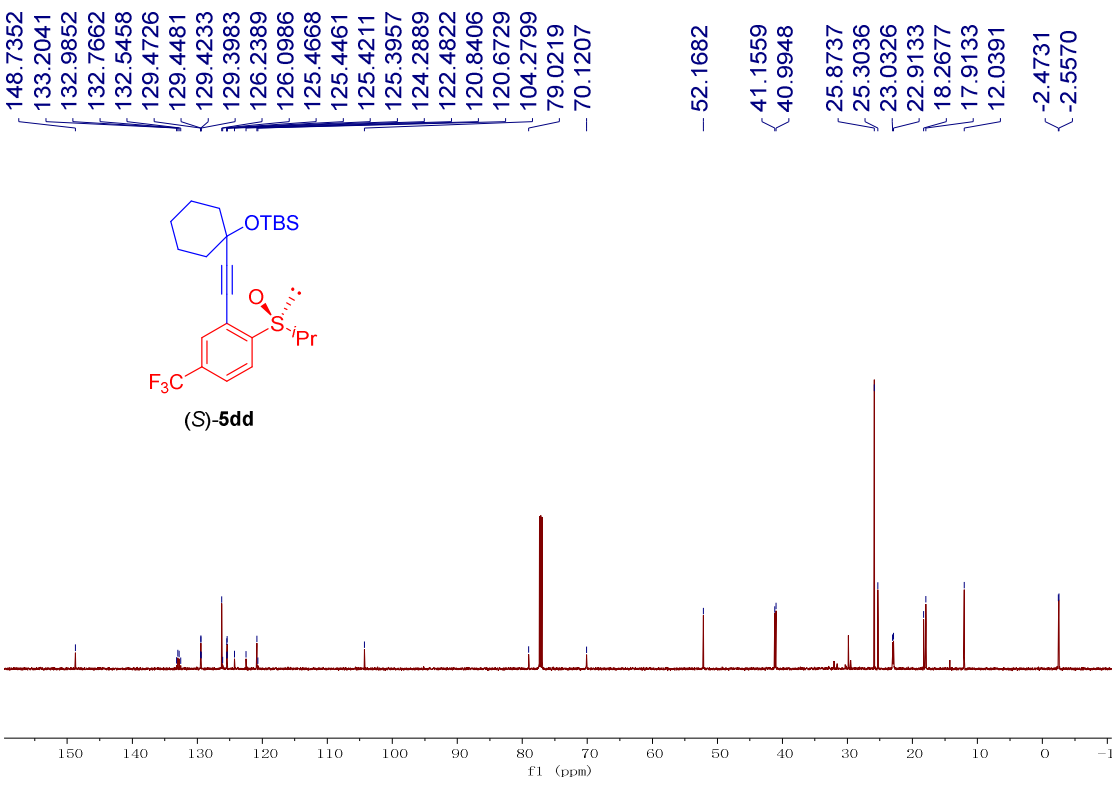
(*S*)-**5ib**


140.4089
133.4567
131.8372
131.4788
125.8958
104.0101
100.2917
51.9104
26.2481
17.0055
16.9339
16.5724
-4.7190
TBS
O
S
iPr
Cl
f1 (ppm)

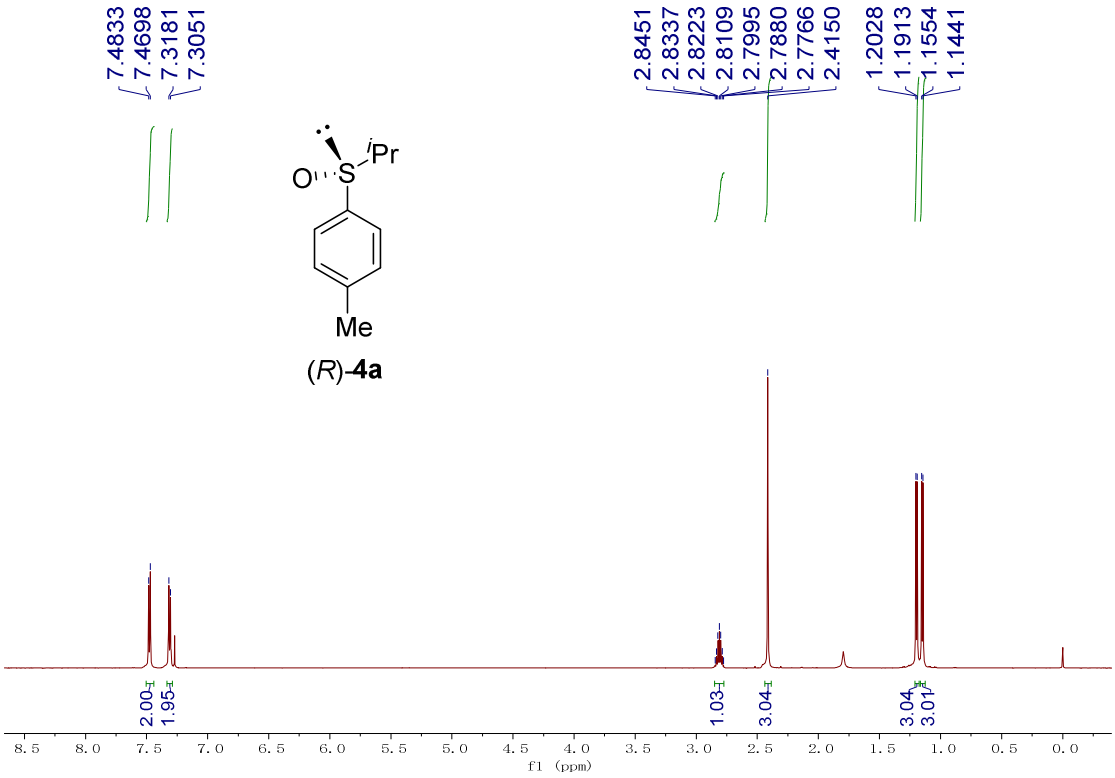
(*S*)-**5ib**

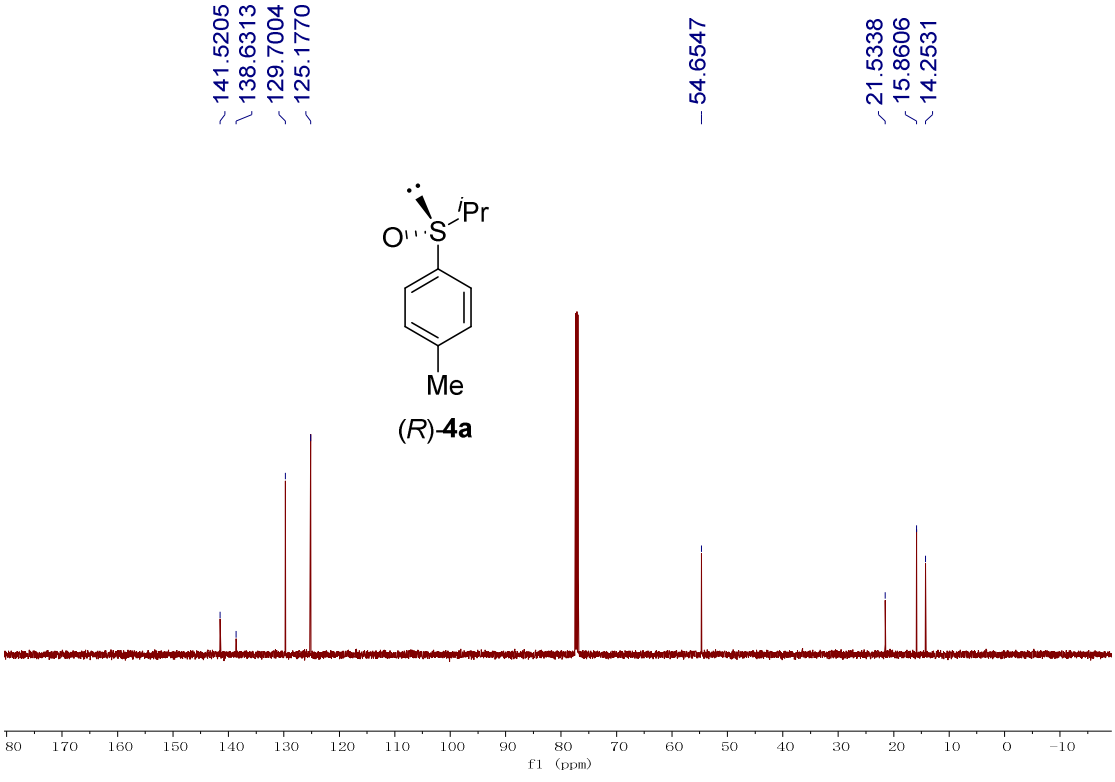

7.9663
7.9526
7.7726
7.7710
7.7590
7.7573
7.6725
3.2333
3.2218
3.2103
1.9059
1.8974
1.8887
1.7482
1.7424
1.7377
1.7308
1.7240
1.7116
1.7043
1.5824
1.5763
1.5696
1.5609
1.5577
1.5545
1.5469
1.5411
1.5341
1.5256
1.5185
1.4793
1.4674
1.3704
1.3658
0.9884
0.9772
0.8982
0.1976
0.1710
OTBS
O
S
iPr
F3C
1.00
1.01
0.99
1.02
2.09
4.05
2.97
3.11
1.04
3.01
9.06
3.00
3.08
f1 (ppm)

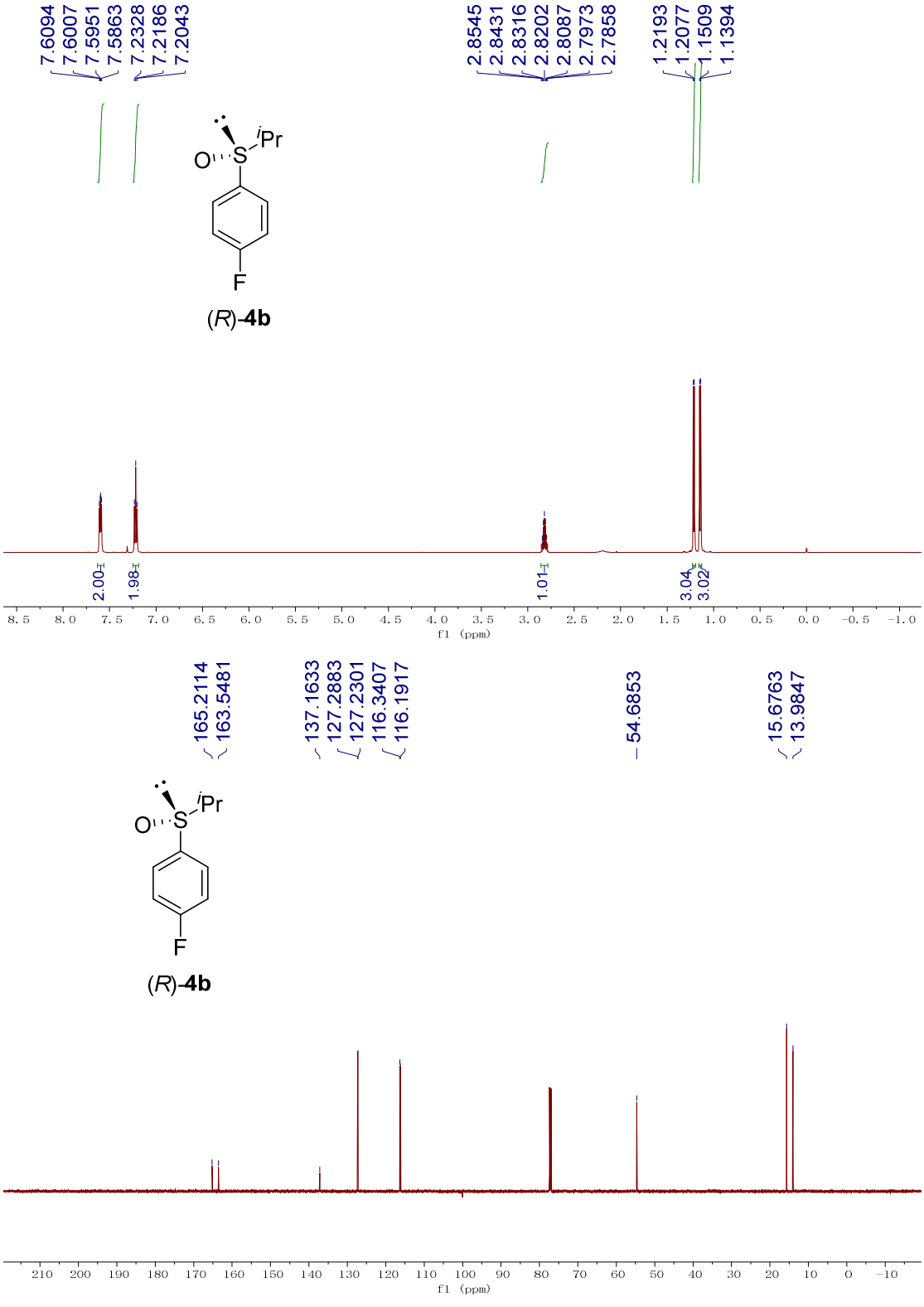
(*S*)-**5dd**

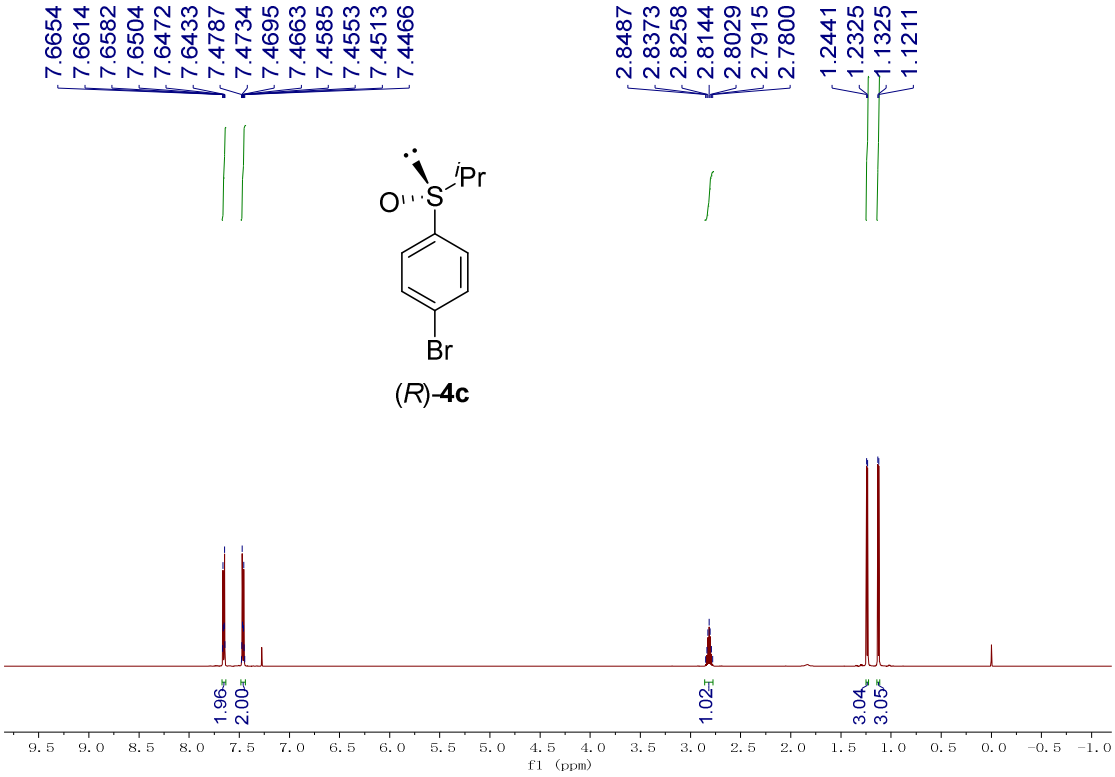

148.7352
133.2041
132.9852
132.7662
132.5458
129.4726
129.4481
129.4233
129.3983
126.2389
126.0986
125.4668
125.4461
125.4211
125.3957
124.2889
122.4822
120.8406
120.6729
104.2799
79.0219
70.1207
52.1682
41.1559
40.9948
25.8737
25.3036
23.0326
22.9133
18.2677
17.9133
12.0391
-2.4731
-2.5570
OTBS
O
S
iPr
F3C
f1 (ppm)

(*S*)-**5dd**

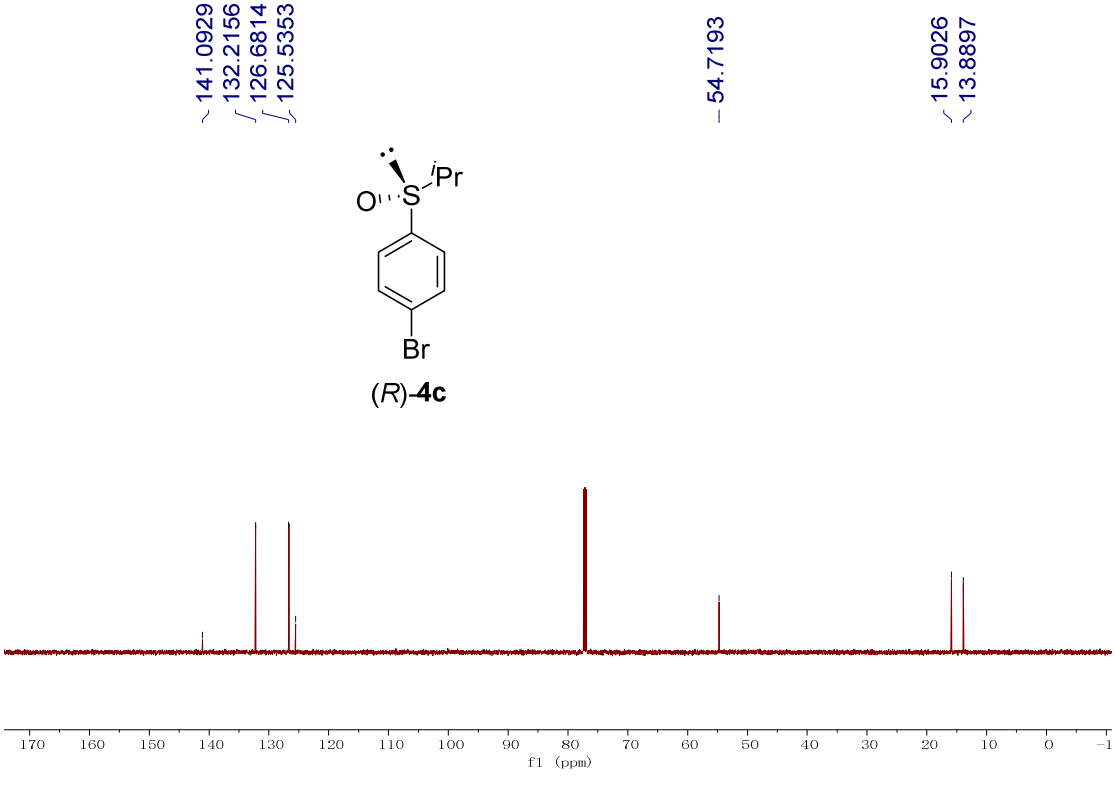

7.4833
7.4698
7.3181
7.3051
2.8451
2.8337
2.8223
2.8109
2.7995
2.7880
2.7766
2.4150
1.2028
1.1913
1.1554
1.1441
O
S
iPr
Me
(R)-4a
2.00
1.95
1.03
3.04
3.04
3.01
f1 (ppm)


141.5205
138.6313
129.7004
125.1770
54.6547
21.5338
15.8606
14.2531
O
S
iPr
Me
(R)-4a
f1 (ppm)

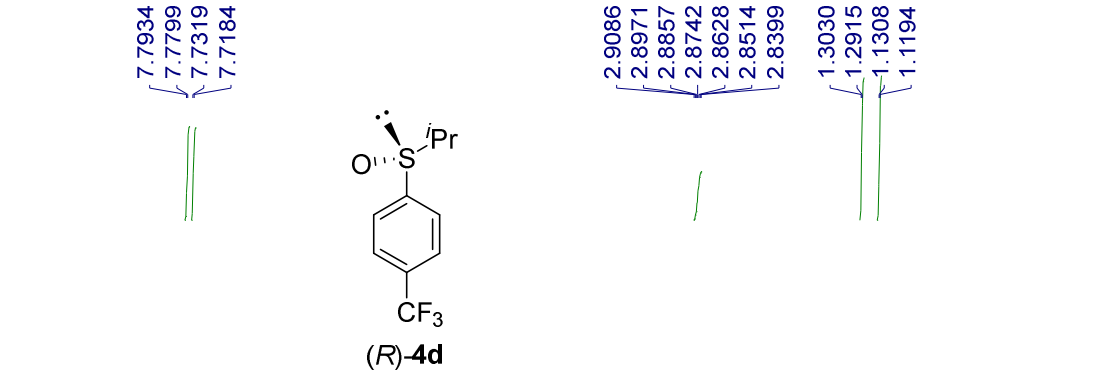

7.6094
7.6007
7.5951
7.5863
7.2328
7.2186
7.2043
2.8545
2.8431
2.8316
2.8202
2.8087
2.7973
2.7858
1.2193
1.2077
1.1509
1.1394
O
S
iPr
F
(R)-4b
2.00
1.98
1.01
3.04
3.02
f1 (ppm)
165.2114
163.5481
137.1633
127.2883
127.2301
116.3407
116.1917
54.6853
15.6763
13.9847
O
S
iPr
F
(R)-4b
f1 (ppm)


7.6654
7.6614
7.6582
7.6504
7.6472
7.6433
7.4787
7.4734
7.4695
7.4663
7.4585
7.4553
7.4513
7.4466
2.8487
2.8373
2.8258
2.8144
2.8029
2.7915
2.7800
1.2441
1.2325
1.1325
1.1211
O
S
iPr
Br
1.96
2.00
1.02
3.04
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0
f1 (ppm)

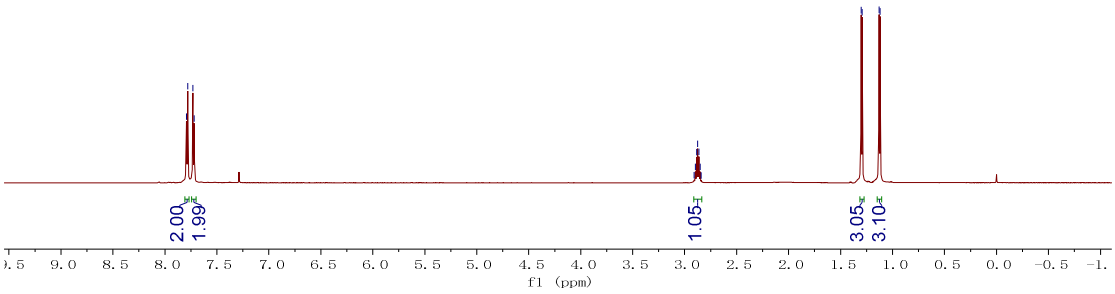
(*R*)-**4c**

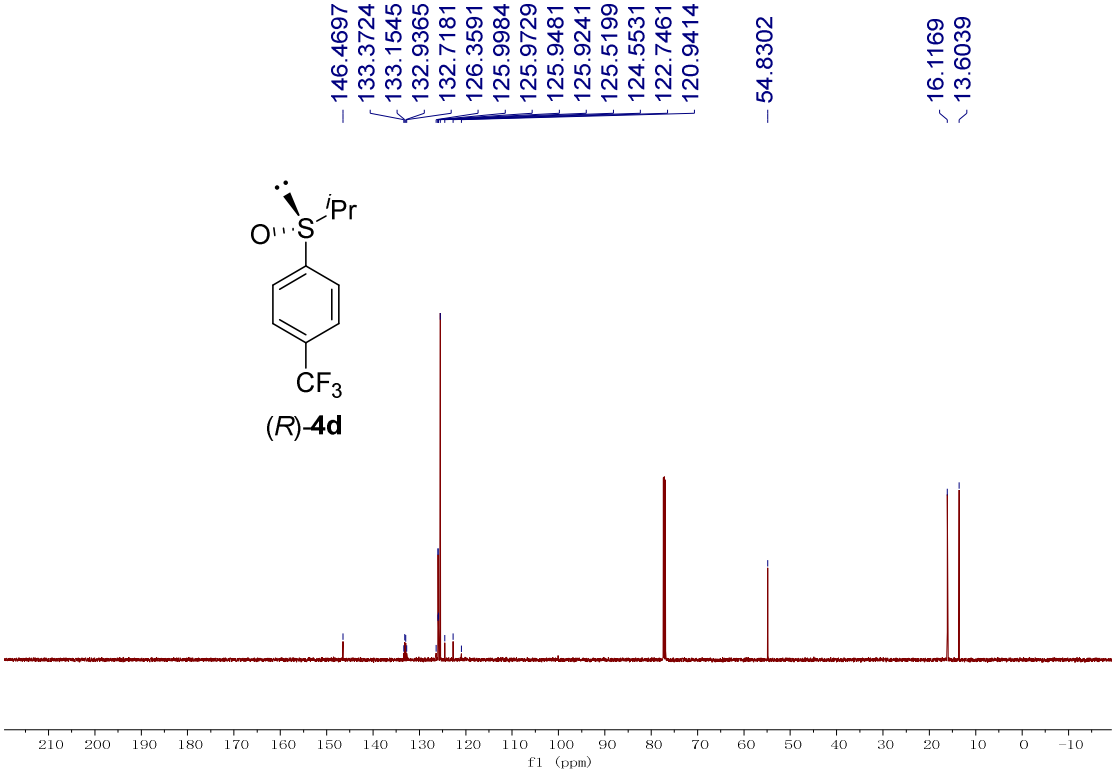

141.0929
132.2156
126.6814
125.5353
54.7193
15.9026
13.8897
O
S
iPr
Br
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −1
f1 (ppm)

(*R*)-**4c**

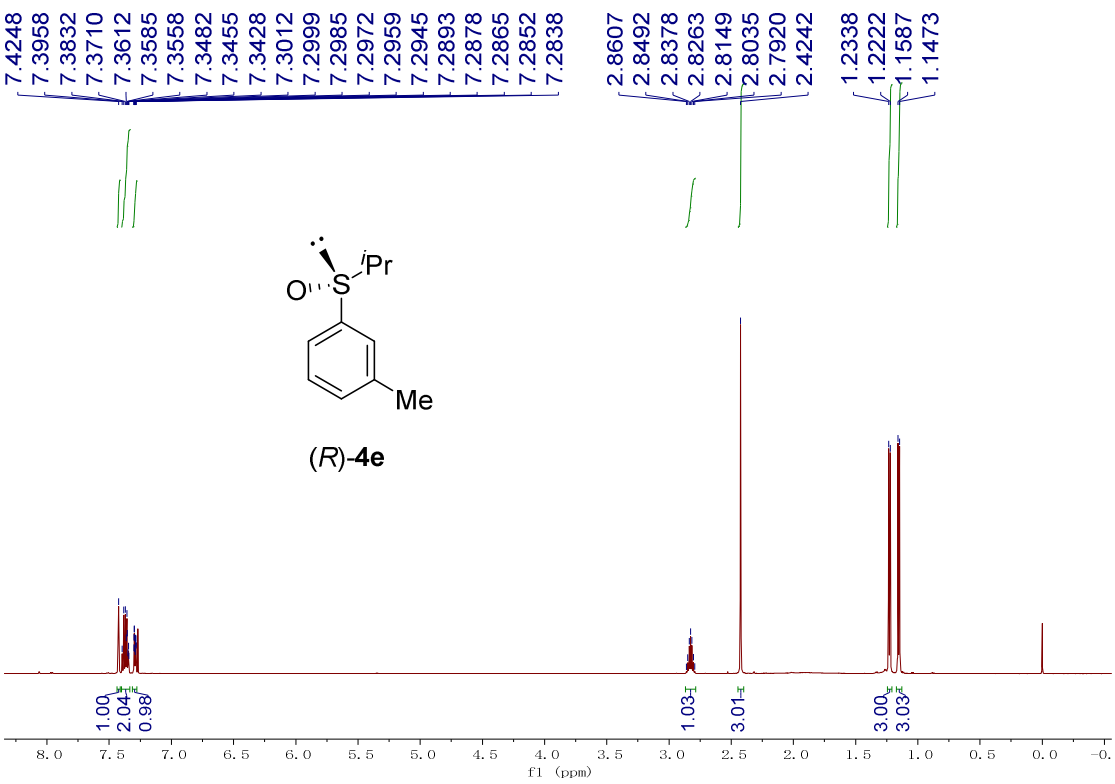

7.7934
7.7799
7.7319
7.7184
2.9086
2.8971
2.8857
2.8742
2.8628
2.8514
2.8399
1.3030
1.2915
1.1308
1.1194
O
S
iPr
CF3

(*R*)-**4d**

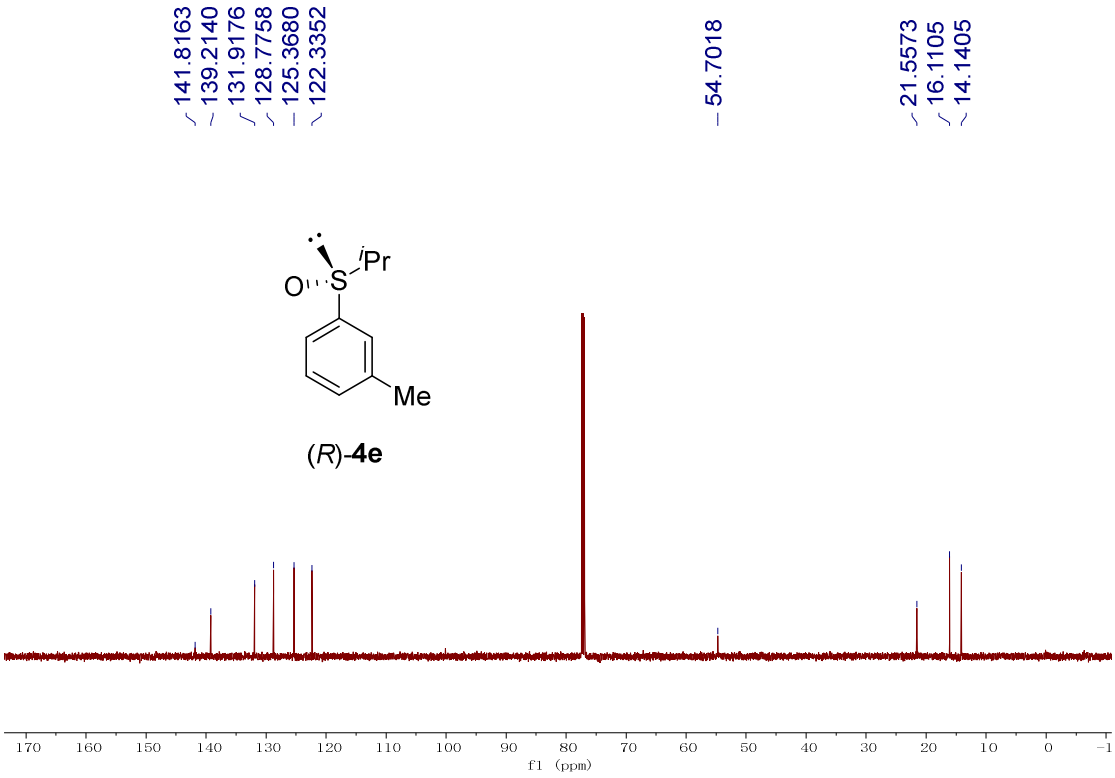

2.00
1.99
1.05
3.05
3.10
f1 (ppm)


146.4697
133.3724
133.1545
132.9365
132.7181
126.3591
125.9984
125.9729
125.9481
125.9241
125.5199
124.5531
122.7461
120.9414
54.8302
16.1169
13.6039
O
S
iPr
CF3
f1 (ppm)

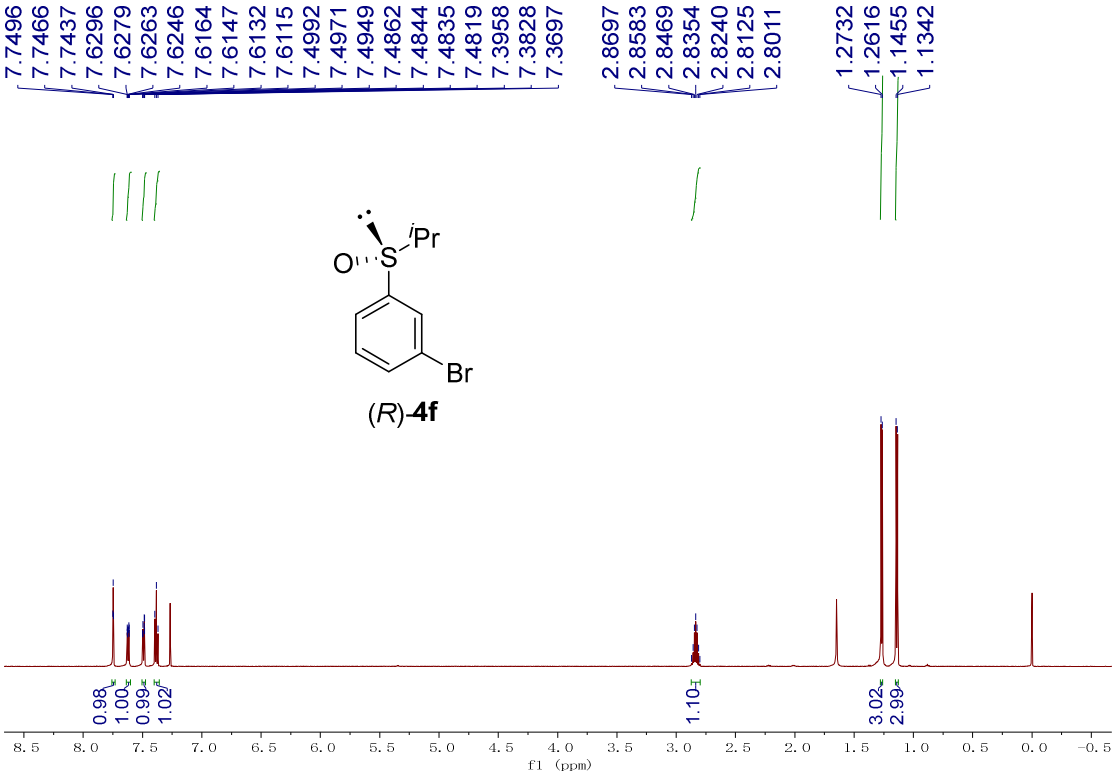
(*R*)-**4d**


7.4248
7.3958
7.3832
7.3710
7.3612
7.3585
7.3558
7.3482
7.3455
7.3428
7.3012
7.2999
7.2985
7.2972
7.2959
7.2945
7.2893
7.2878
7.2865
7.2852
7.2838
2.8607
2.8492
2.8378
2.8263
2.8149
2.8035
2.7920
2.4242
1.2338
1.2222
1.1587
1.1473
iPr
O
S
Me
1.00
2.04
0.98
1.03
3.01
3.00
3.03
f1 (ppm)

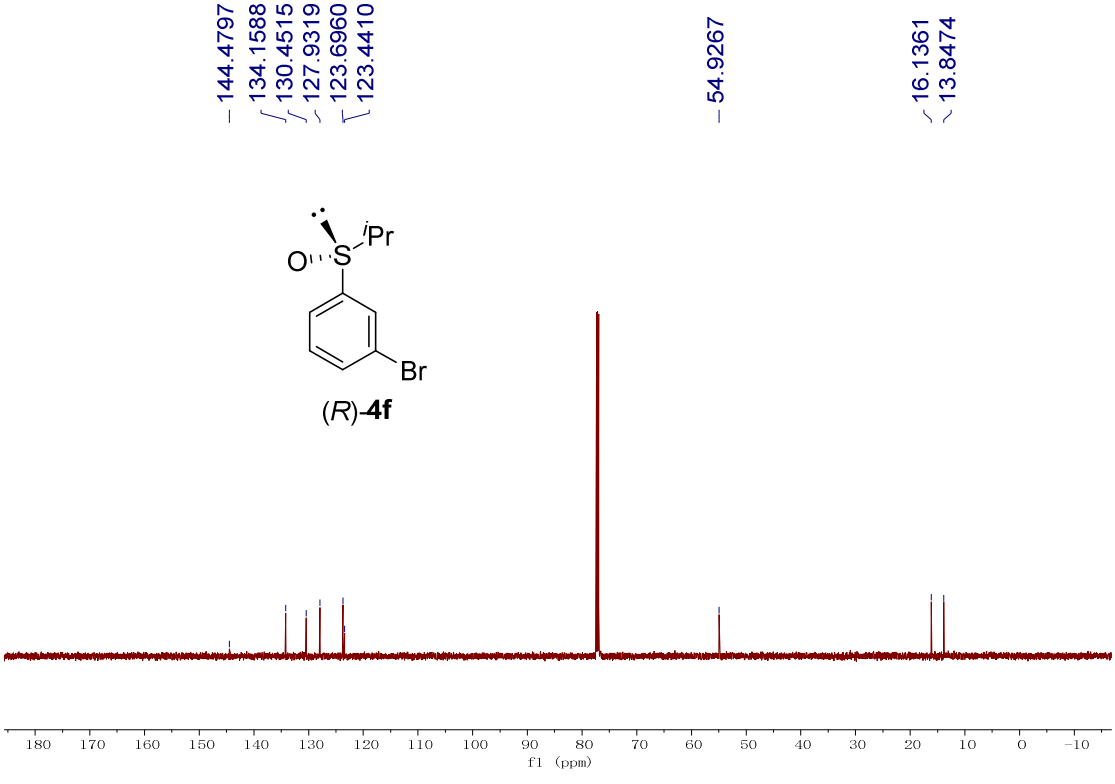
(*R*)-**4e**


141.8163
139.2140
131.9176
128.7758
125.3680
122.3352
54.7018
21.5573
16.1105
14.1405
iPr
O
S
Me
f1 (ppm)

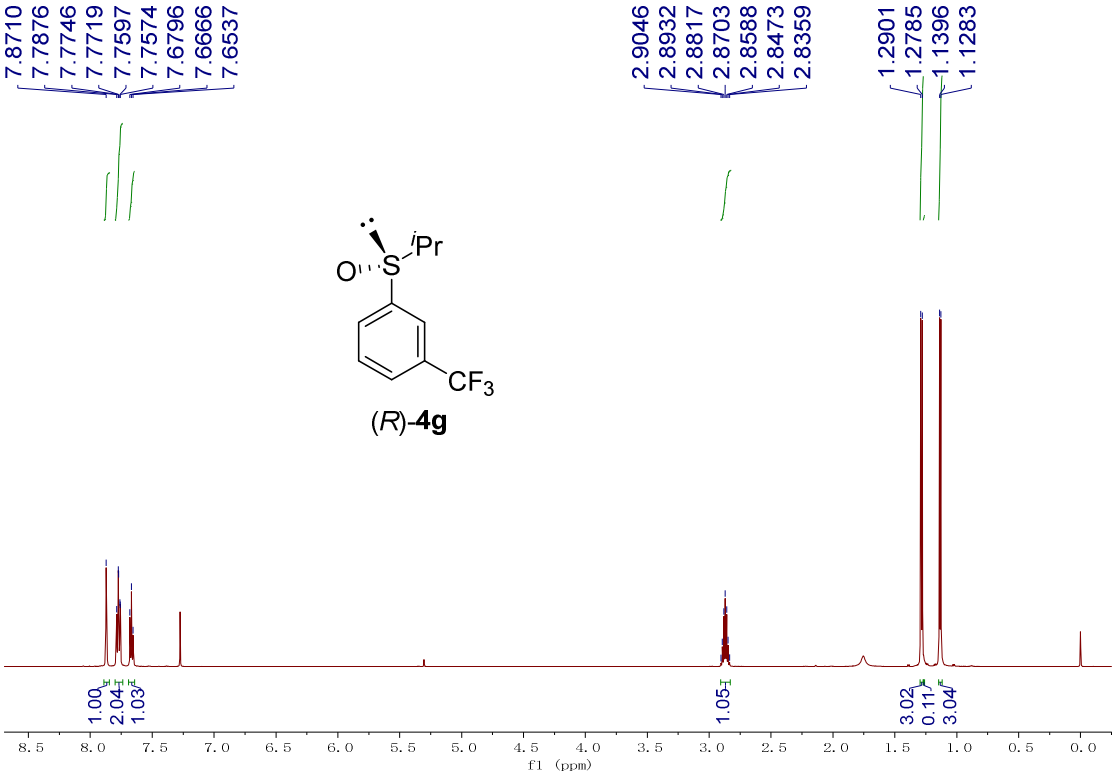
(*R*)-**4e**


7.7496
7.7466
7.7437
7.6296
7.6279
7.6263
7.6246
7.6164
7.6147
7.6132
7.6115
7.4992
7.4971
7.4949
7.4862
7.4844
7.4835
7.4819
7.3958
7.3828
7.3697
2.8697
2.8583
2.8469
2.8354
2.8240
2.8125
2.8011
1.2732
1.2616
1.1455
1.1342
O
S
iPr
Br
0.98
1.00
0.99
1.02
1.10
3.02
2.99
f1 (ppm)

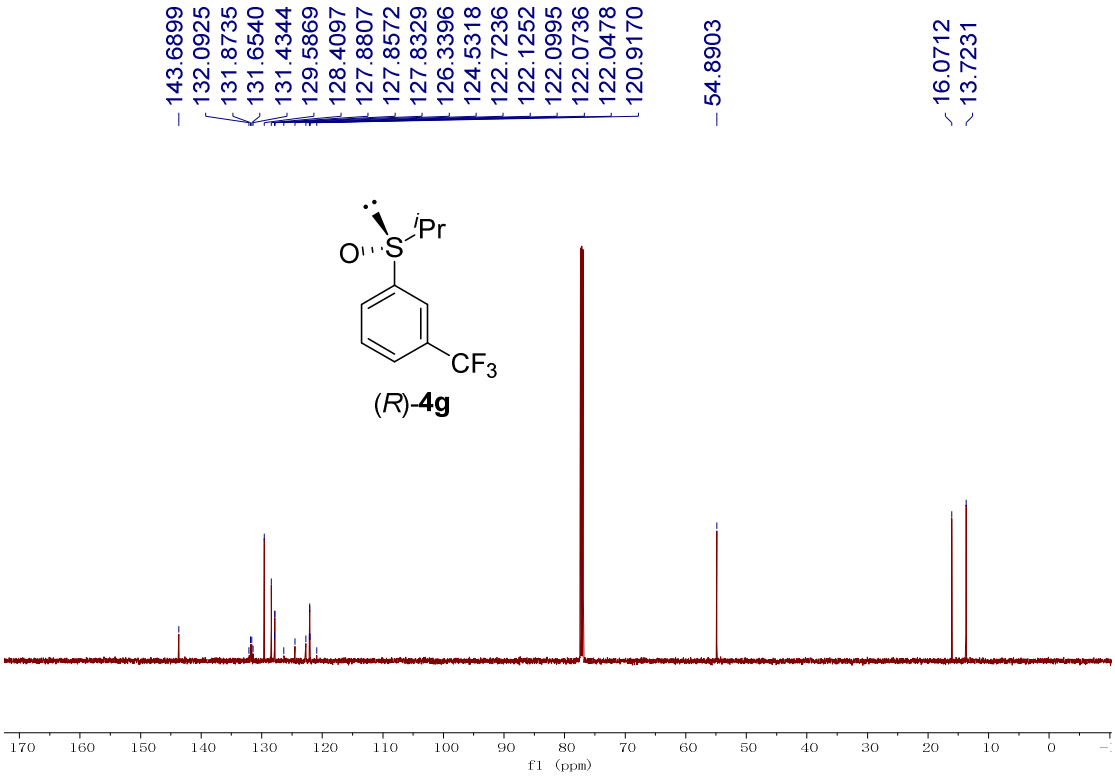
(*R*)-**4f**


144.4797
134.1588
130.4515
127.9319
123.6960
123.4410
54.9267
16.1361
13.8474
O
S
iPr
Br
f1 (ppm)

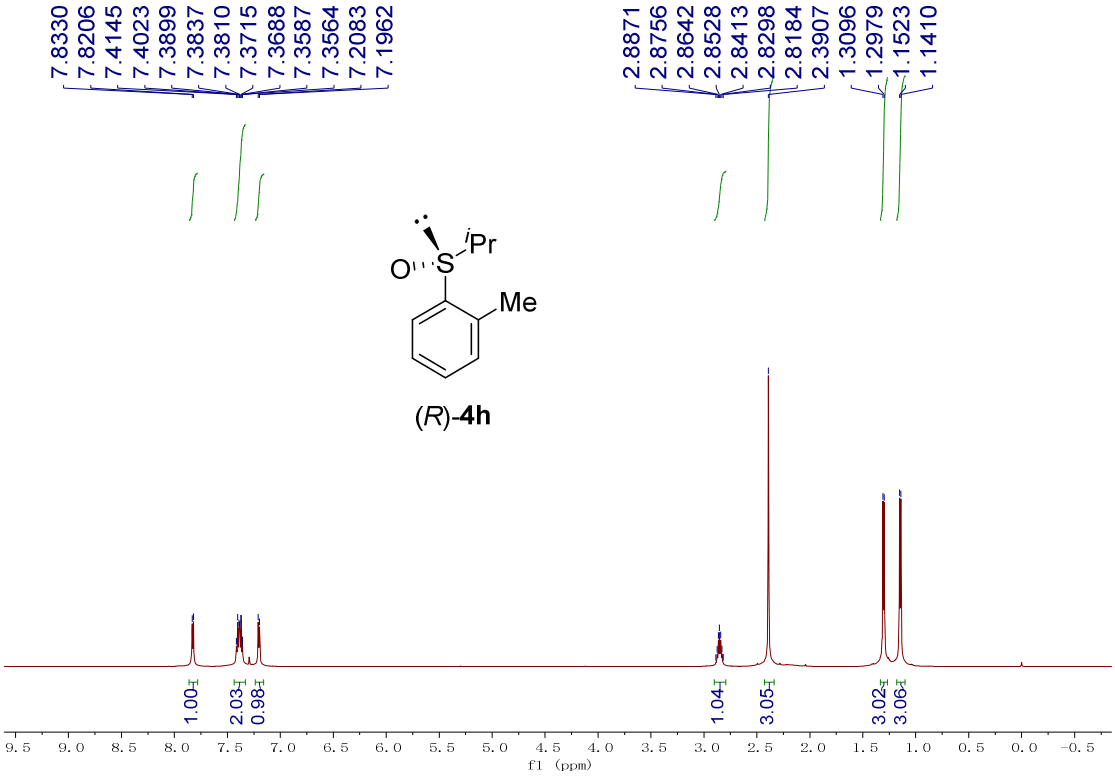
(*R*)-**4f**


7.8710
7.7876
7.7746
7.7719
7.7597
7.7574
7.6796
7.6666
7.6537
2.9046
2.8932
2.8817
2.8703
2.8588
2.8473
2.8359
1.2901
1.2785
1.1396
1.1283
iPr
O
S
CF3
1.00
2.04
1.03
1.05
3.02
0.11
3.04
f1 (ppm)

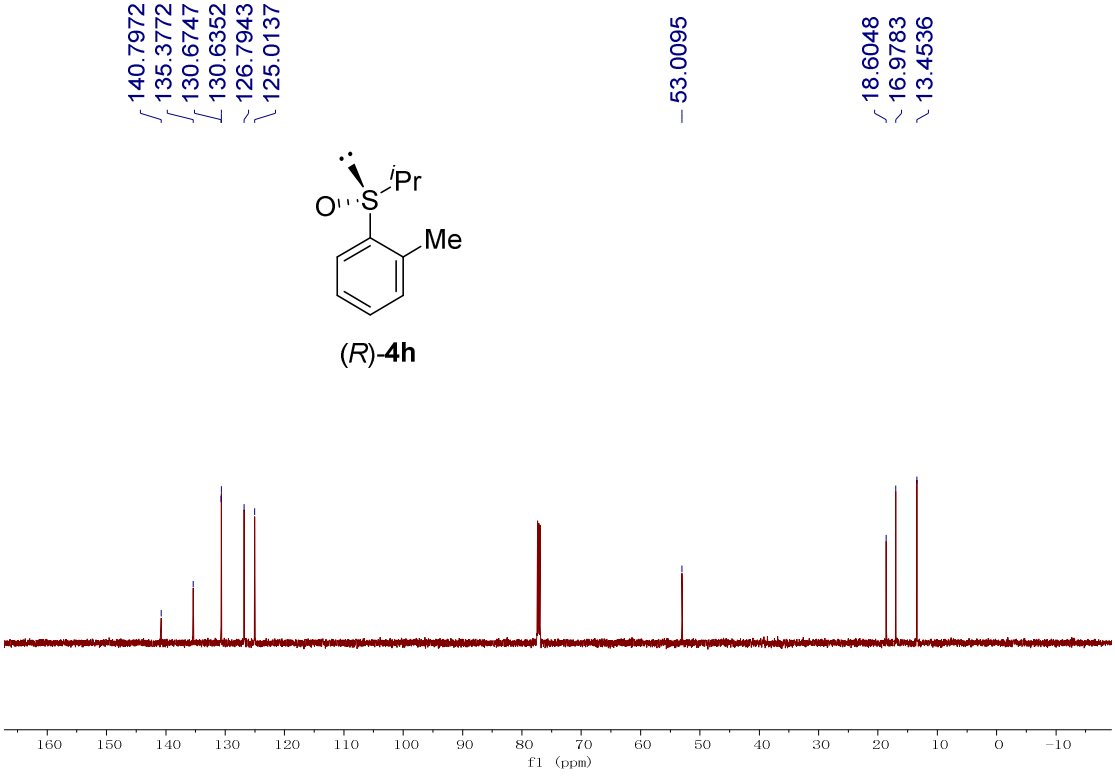
(*R*)-**4g**


143.6899
132.0925
131.8735
131.6540
131.4344
129.5869
128.4097
127.8807
127.8572
127.8329
126.3396
124.5318
122.7236
122.1252
122.0995
122.0736
122.0478
120.9170
54.8903
16.0712
13.7231
iPr
O
S
CF3
f1 (ppm)

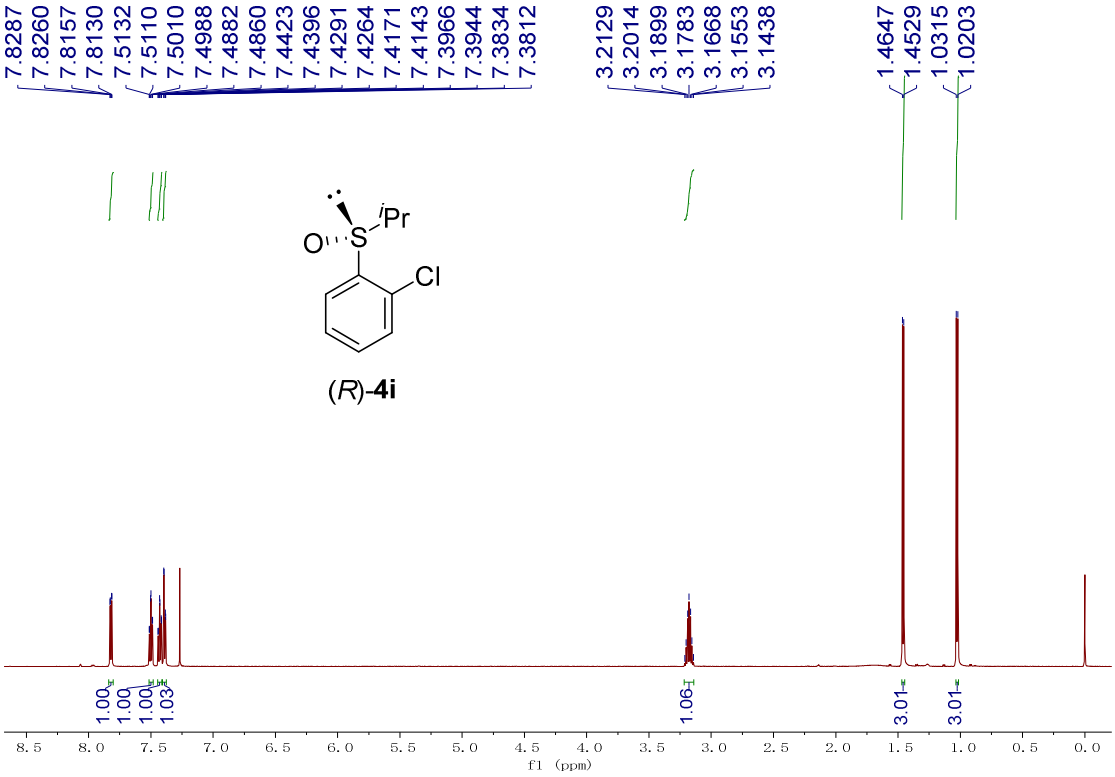
(*R*)-**4g**


7.8330
7.8206
7.4145
7.4023
7.3899
7.3837
7.3810
7.3715
7.3688
7.3587
7.3564
7.2083
7.1962
2.8871
2.8756
2.8642
2.8528
2.8413
2.8298
2.8184
2.3907
1.3096
1.2979
1.1523
1.1410
O
S
iPr
Me
1.00
2.03
0.98
1.04
3.05
3.02
3.06
f1 (ppm)

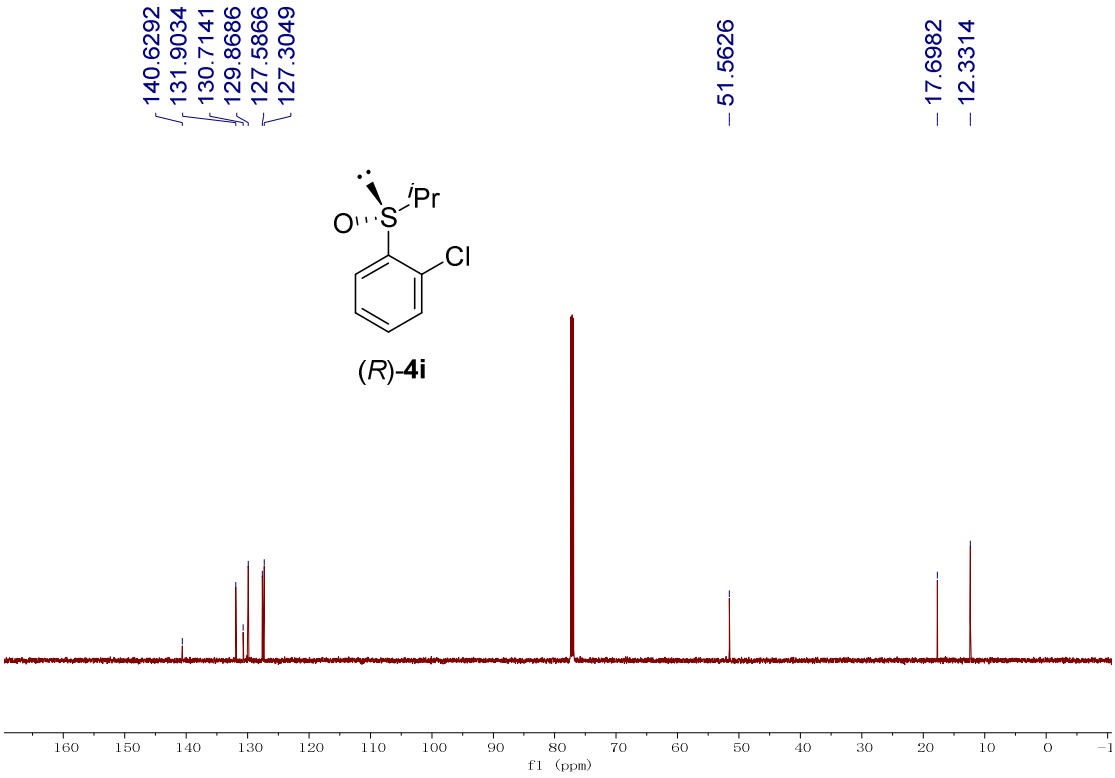
(*R*)-**4h**


140.7972
135.3772
130.6747
130.6352
126.7943
125.0137
53.0095
18.6048
16.9783
13.4536
O
S
iPr
Me
f1 (ppm)

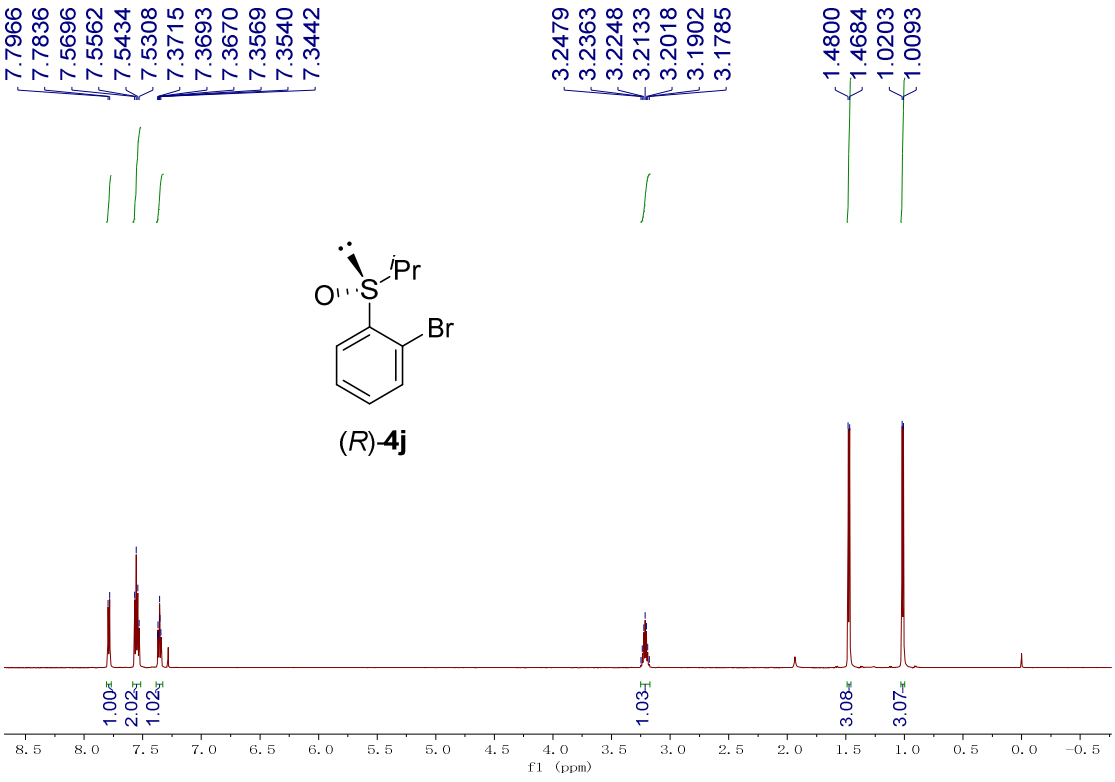
(*R*)-**4h**


7.8287
7.8260
7.8157
7.8130
7.5132
7.5110
7.5010
7.4988
7.4882
7.4860
7.4423
7.4396
7.4291
7.4264
7.4171
7.4143
7.3966
7.3944
7.3834
7.3812
3.2129
3.2014
3.1899
3.1783
3.1668
3.1553
3.1438
1.4647
1.4529
1.0315
1.0203
O
S
iPr
Cl
1.00
1.00
1.00
1.03
1.06
3.01
3.01
f1 (ppm)

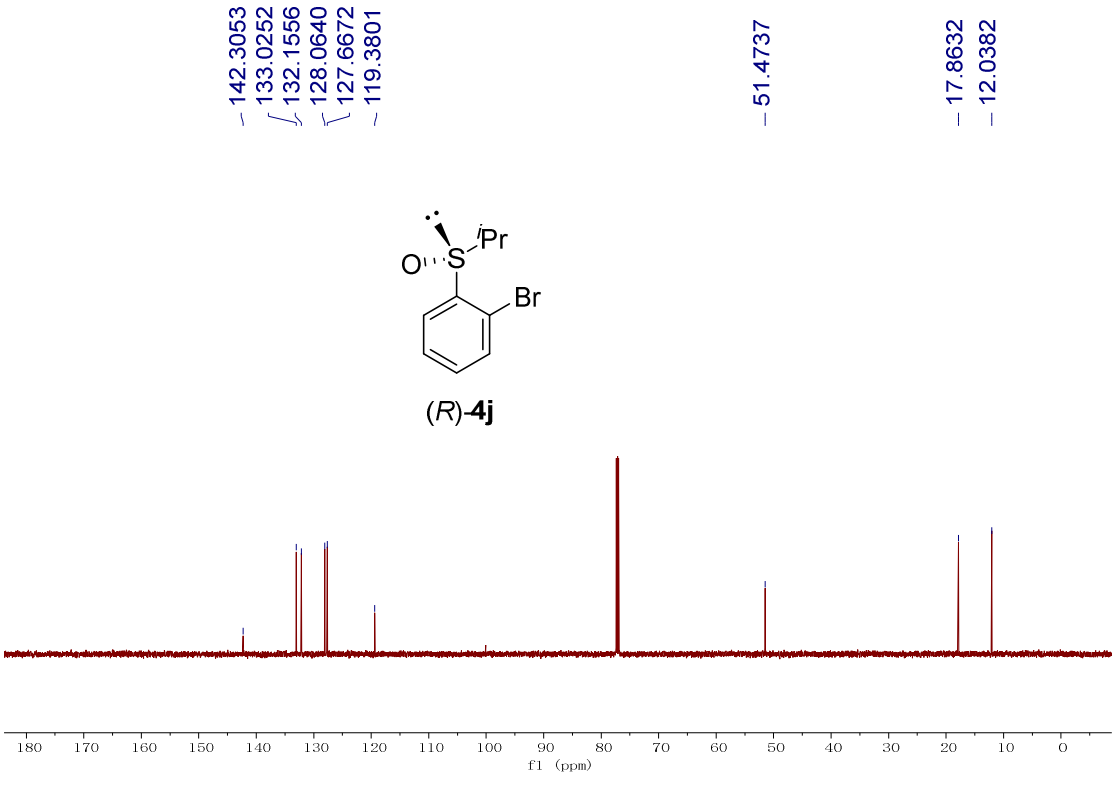
(*R*)-**4i**


140.6292
131.9034
130.7141
129.8686
127.5866
127.3049
51.5626
17.6982
12.3314
O
S
iPr
Cl
f1 (ppm)

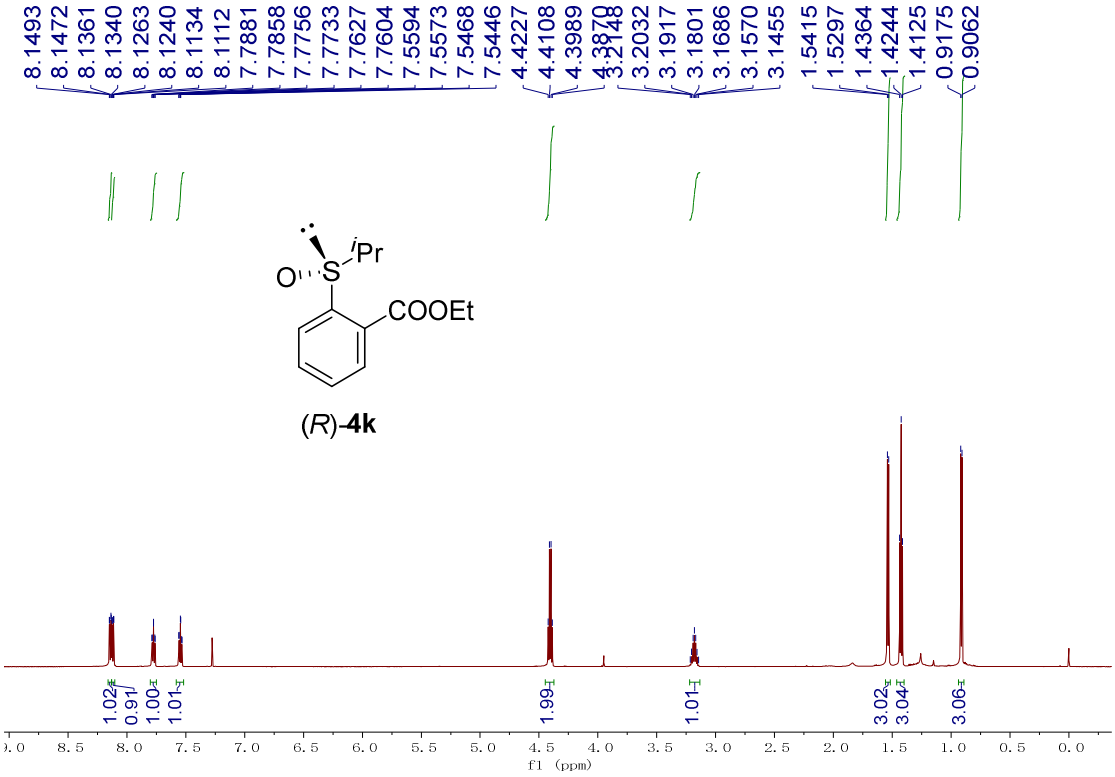
(*R*)-**4i**

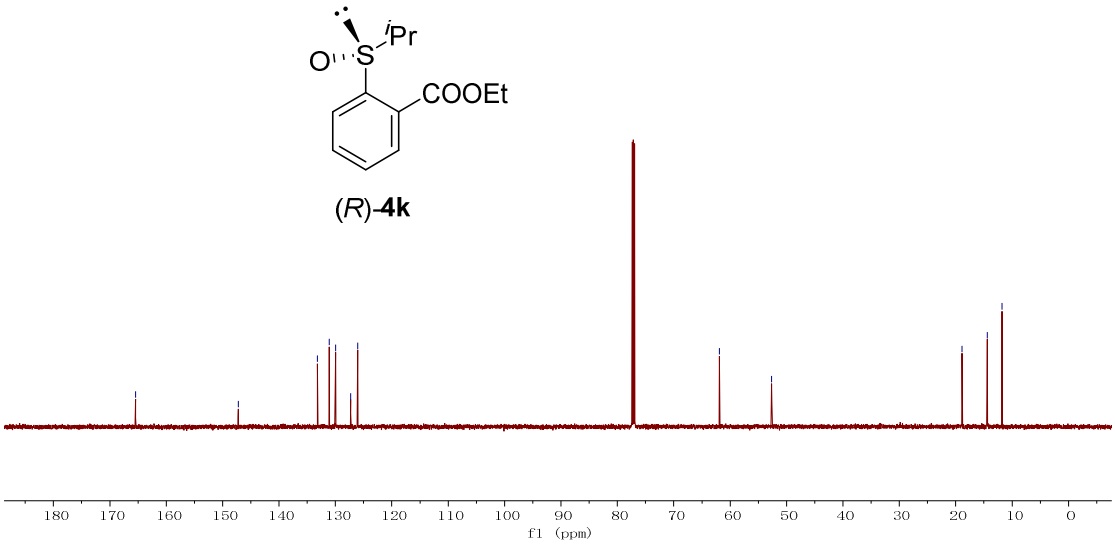

7.7966
7.7836
7.5696
7.5562
7.5434
7.5308
7.3715
7.3693
7.3670
7.3569
7.3540
7.3442
3.2479
3.2363
3.2248
3.2133
3.2018
3.1902
3.1785
1.4800
1.4684
1.0203
1.0093
iPr
O
S
Br
1.00
2.02
1.02
1.03
3.08
3.07
f1 (ppm)

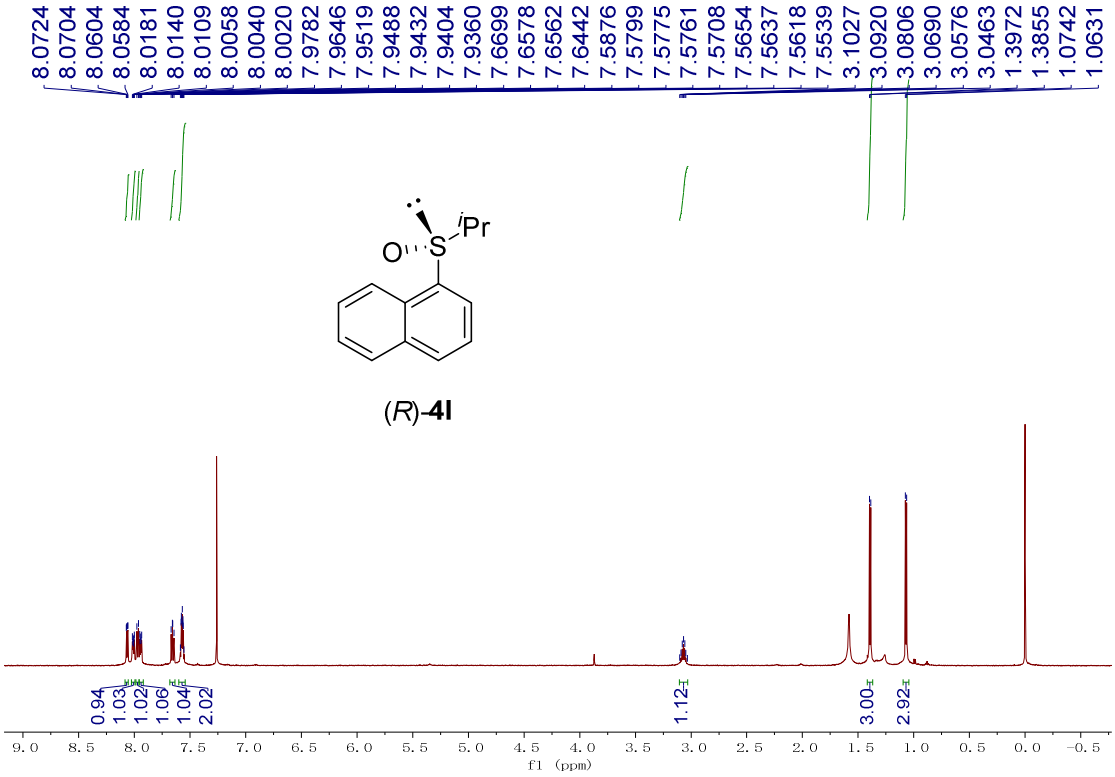
(*R*)-**4j**


142.3053
133.0252
132.1556
128.0640
127.6672
119.3801
51.4737
17.8632
12.0382
iPr
O
S
Br
f1 (ppm)

(*R*)-**4j**

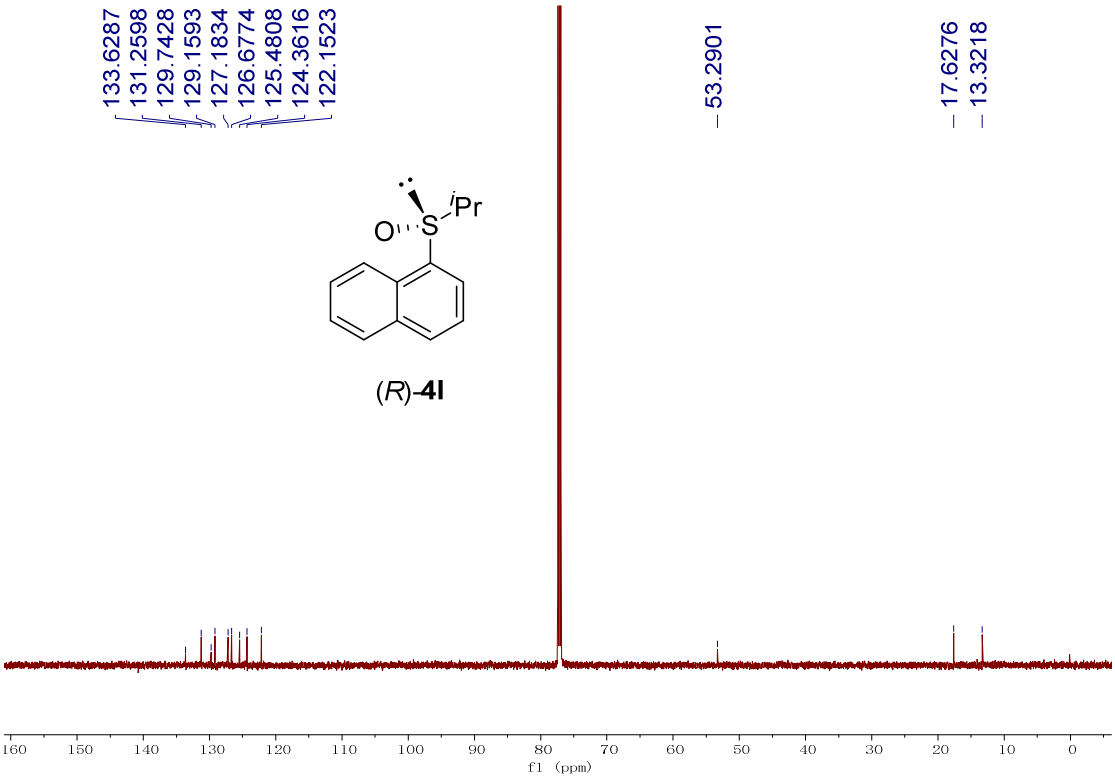

8.1493
8.1472
8.1361
8.1340
8.1263
8.1240
8.1134
8.1112
7.7881
7.7858
7.7756
7.7733
7.7627
7.7604
7.5594
7.5573
7.5468
7.5446
4.4227
4.4108
4.3989
4.3870
3.2148
3.2032
3.1917
3.1801
3.1686
3.1570
3.1455
1.5415
1.5297
1.4364
1.4244
1.4125
0.9175
0.9062
iPr
O
S
COOEt
(R)-4k
1.02
0.91
1.00
1.01
1.99
1.01
3.02
3.04
3.06
f1 (ppm)


165.4247
147.2270
133.1684
131.0759
129.9742
127.2938
126.0706
61.8992
52.6310
18.8975
14.4037
11.7786
iPr
O
S
COOEt
(R)-4k
f1 (ppm)

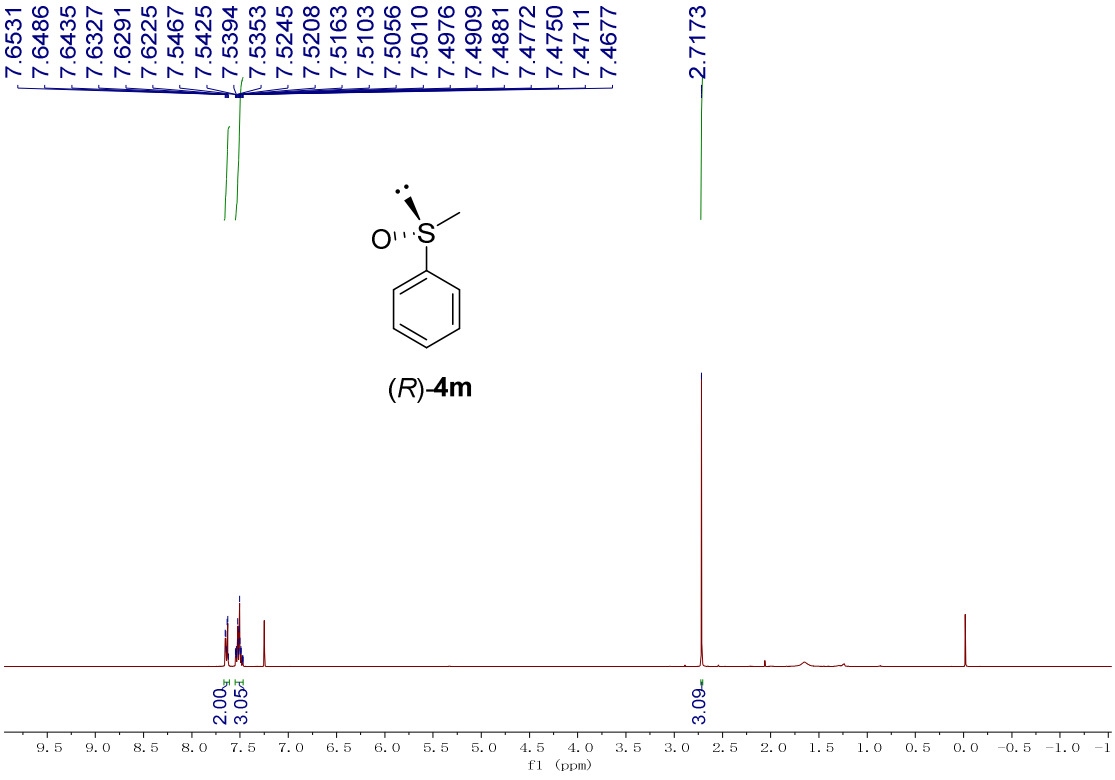

8.0724
8.0704
8.0604
8.0584
8.0181
8.0140
8.0109
8.0058
8.0040
8.0020
7.9782
7.9646
7.9519
7.9488
7.9432
7.9404
7.9360
7.6699
7.6578
7.6562
7.6442
7.5876
7.5799
7.5775
7.5761
7.5708
7.5654
7.5637
7.5618
7.5539
3.1027
3.0920
3.0806
3.0690
3.0576
3.0463
1.3972
1.3855
1.0742
1.0631
O
S
iPr

(*R*)-**4l**

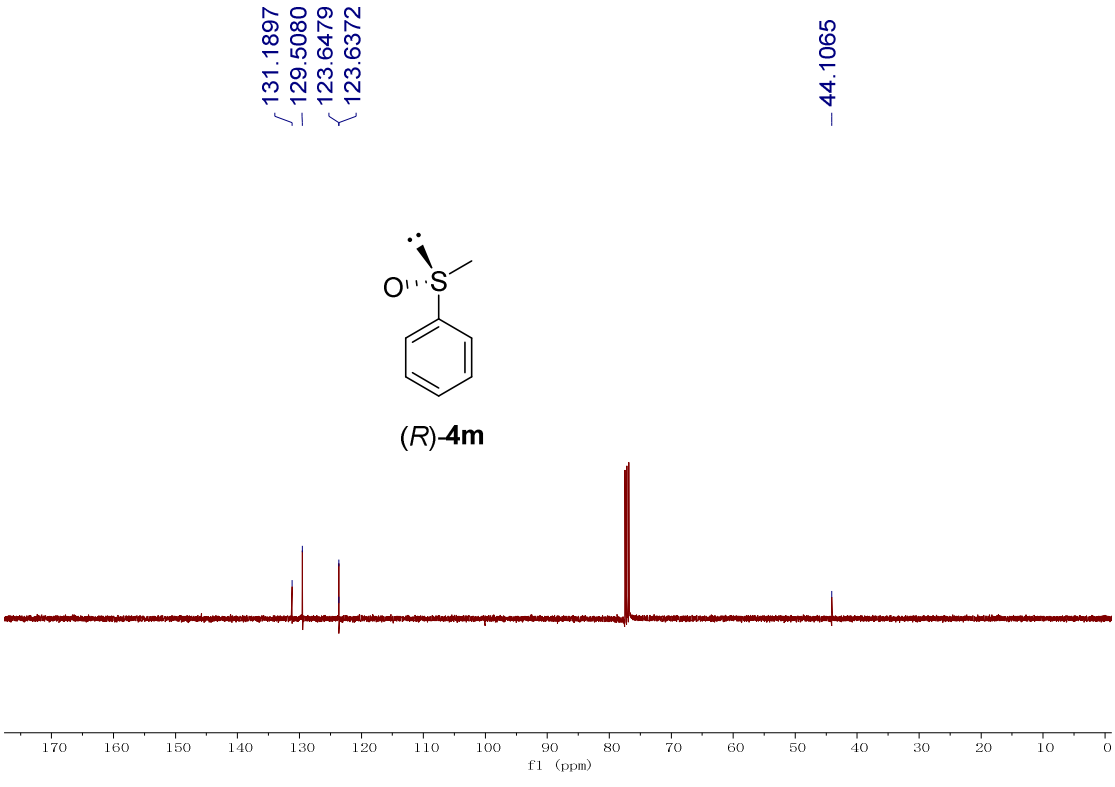
0.94
1.03
1.02
1.06
1.04
2.02
1.12
3.00
2.92
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


133.6287
131.2598
129.7428
129.1593
127.1834
126.6774
125.4808
124.3616
122.1523
53.2901
17.6276
13.3218
O
S
iPr
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

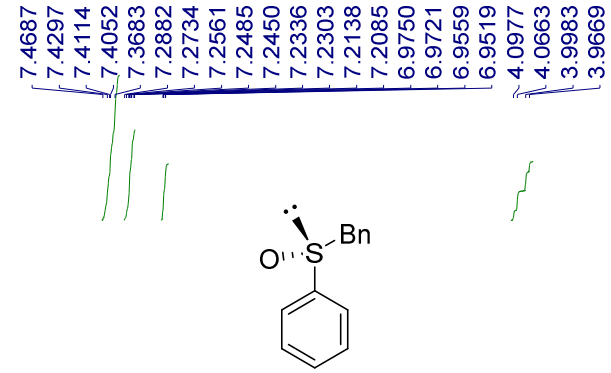
(*R*)-**4l**


7.6531
7.6486
7.6435
7.6327
7.6291
7.6225
7.5467
7.5425
7.5394
7.5353
7.5245
7.5208
7.5163
7.5103
7.5056
7.5010
7.4976
7.4909
7.4881
7.4772
7.4750
7.4711
7.4677
2.7173
O
S
2.00
3.05
3.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1
f1 (ppm)

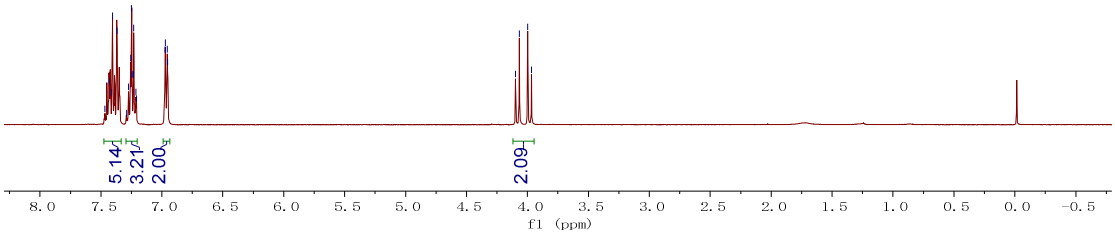
(*R*)-**4m**


131.1897
129.5080
123.6479
123.6372
44.1065
O
S
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

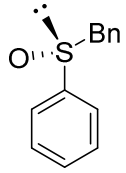
(*R*)-**4m**


7.4687
7.4297
7.4114
7.4052
7.3683
7.2882
7.2734
7.2561
7.2485
7.2450
7.2336
7.2303
7.2138
7.2085
6.9750
6.9721
6.9559
6.9519
4.0977
4.0663
3.9983
3.9669
O
S
Bn

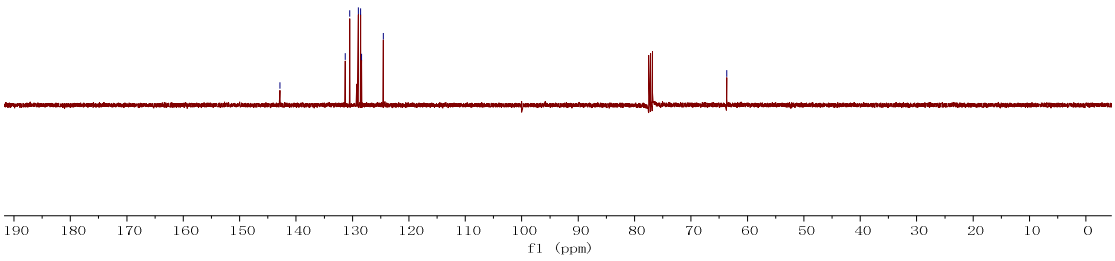
(*R*)-**4n**

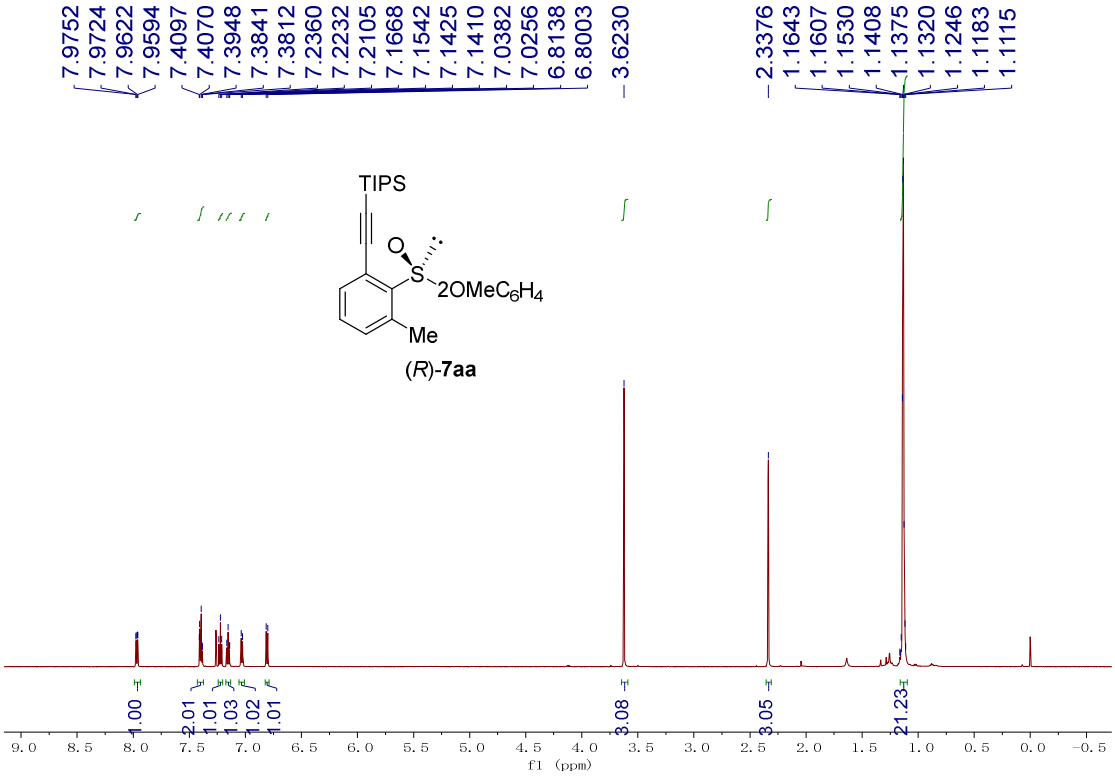

5.14
3.21
2.00
2.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

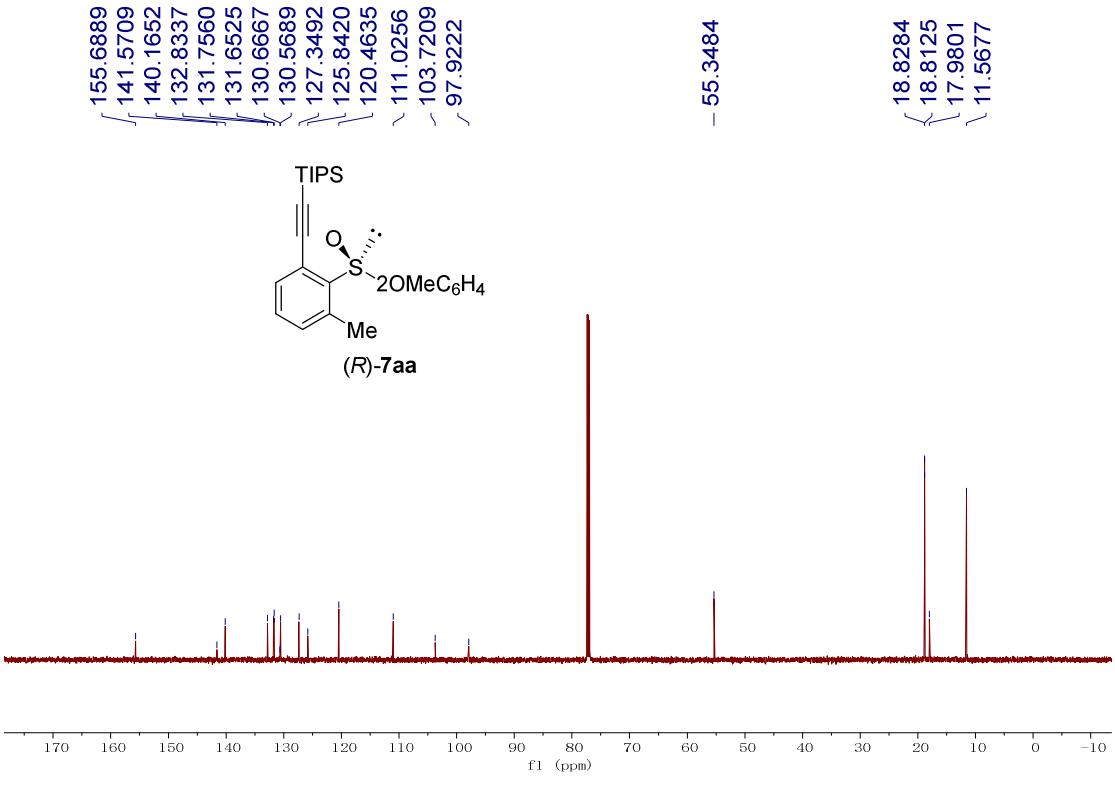

142.8418
131.2950
130.4804
128.9713
128.5734
128.3719
124.5584
63.6879

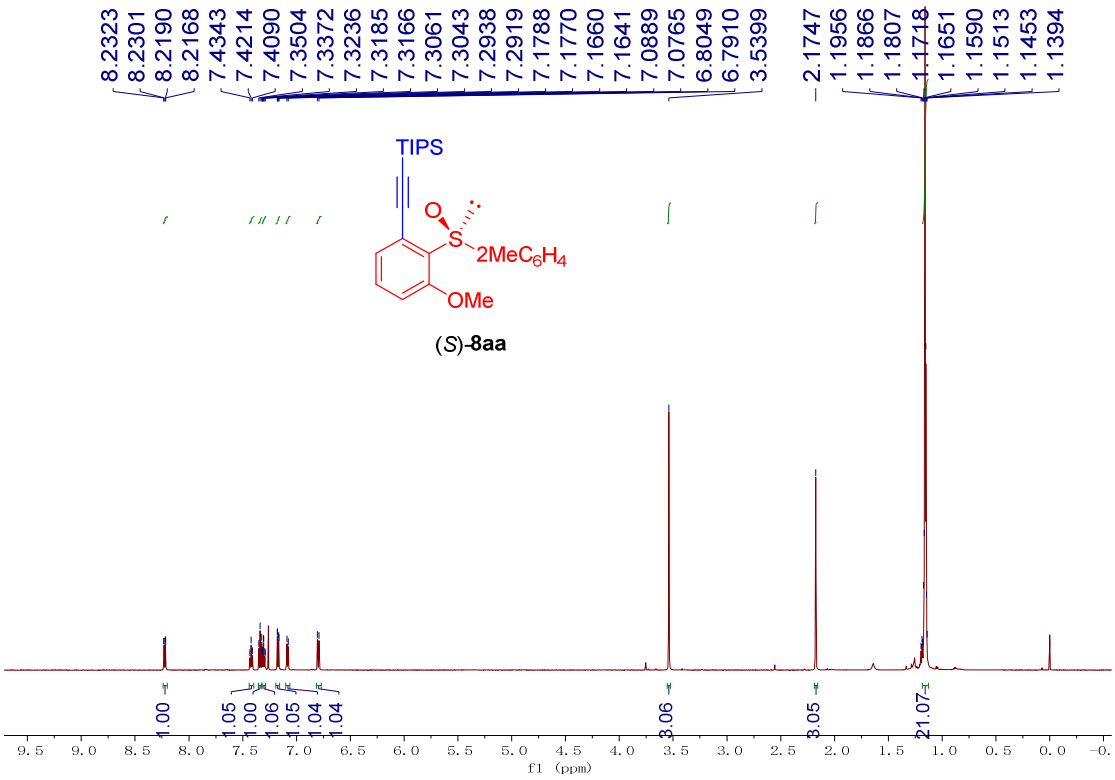

O
S
Bn

(*R*)-**4n**

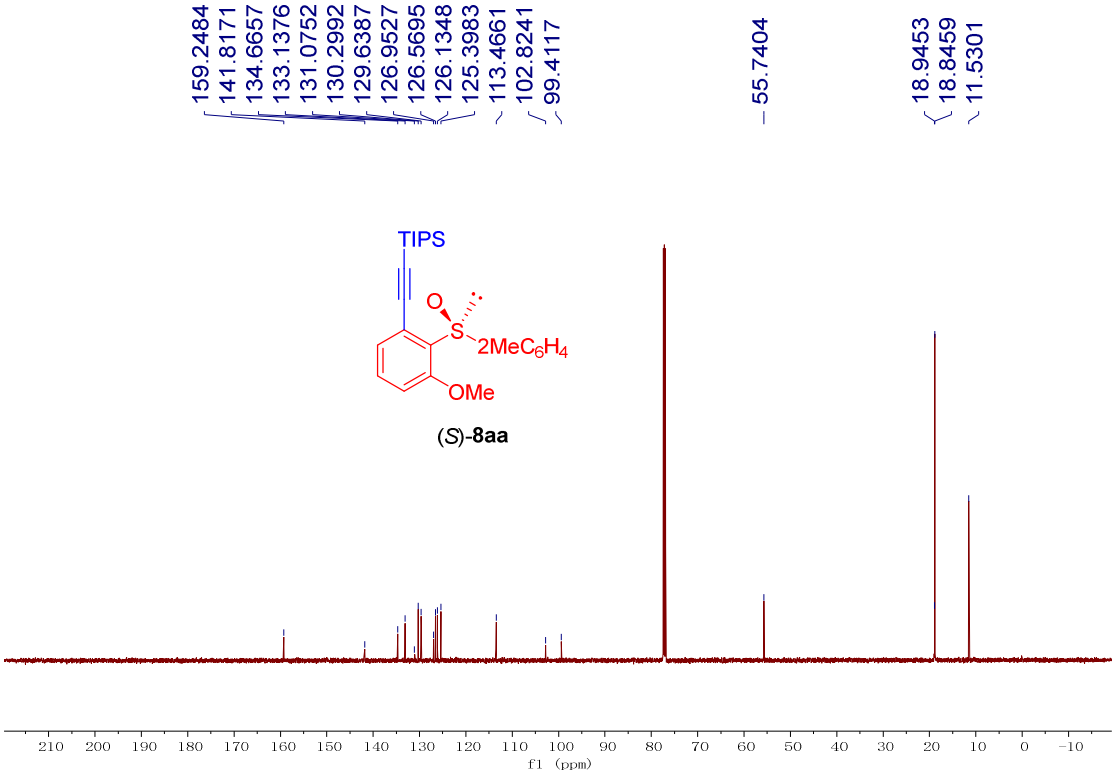

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.9752
7.9724
7.9622
7.9594
7.4097
7.4070
7.3948
7.3841
7.3812
7.2360
7.2232
7.2105
7.1668
7.1542
7.1425
7.1410
7.0382
7.0256
6.8138
6.8003
3.6230
2.3376
1.1643
1.1607
1.1530
1.1408
1.1375
1.1320
1.1246
1.1183
1.1115
TIPS
O
S
2OMeC6H4
Me
(R)-7aa
1.00
2.01
1.01
1.03
1.02
1.01
3.08
3.05
21.23
f1 (ppm)

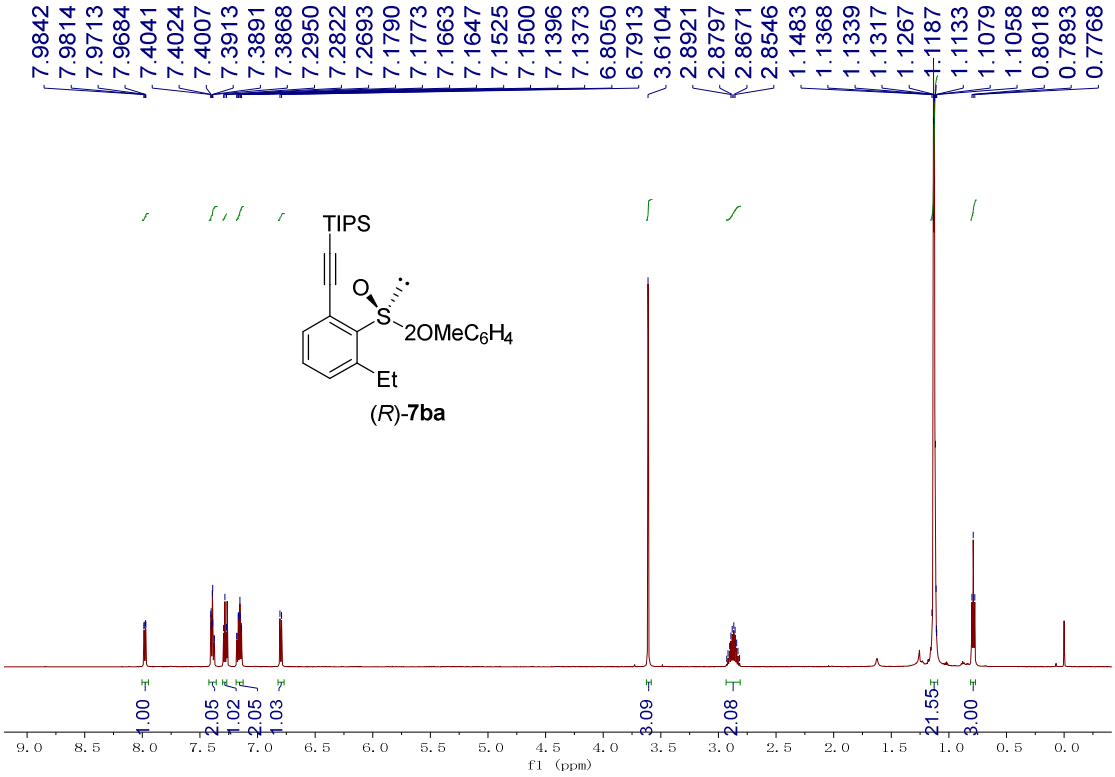

155.6889
141.5709
140.1652
132.8337
131.7560
131.6525
130.6667
130.5689
127.3492
125.8420
120.4635
111.0256
103.7209
97.9222
55.3484
18.8284
18.8125
17.9801
11.5677
TIPS
O
S
2OMeC6H4
Me
(R)-7aa
f1 (ppm)

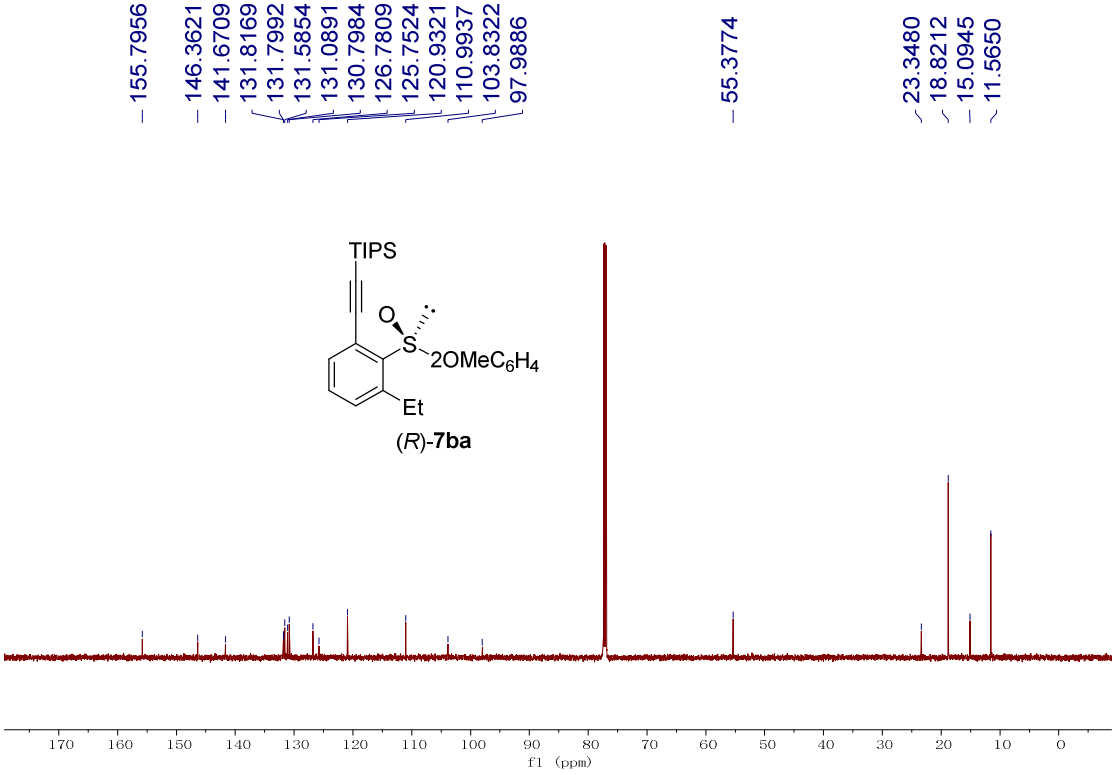

8.2323
8.2301
8.2190
8.2168
7.4343
7.4214
7.4090
7.3504
7.3372
7.3236
7.3185
7.3166
7.3061
7.3043
7.2938
7.2919
7.1788
7.1770
7.1660
7.1641
7.0889
7.0765
6.8049
6.7910
3.5399
2.1747
1.1956
1.1866
1.1807
1.1718
1.1651
1.1590
1.1513
1.1453
1.1394
TIPS
O
S
2MeC6H4
OMe
1.00
1.05
1.00
1.06
1.05
1.04
1.04
3.06
3.05
21.07
f1 (ppm)

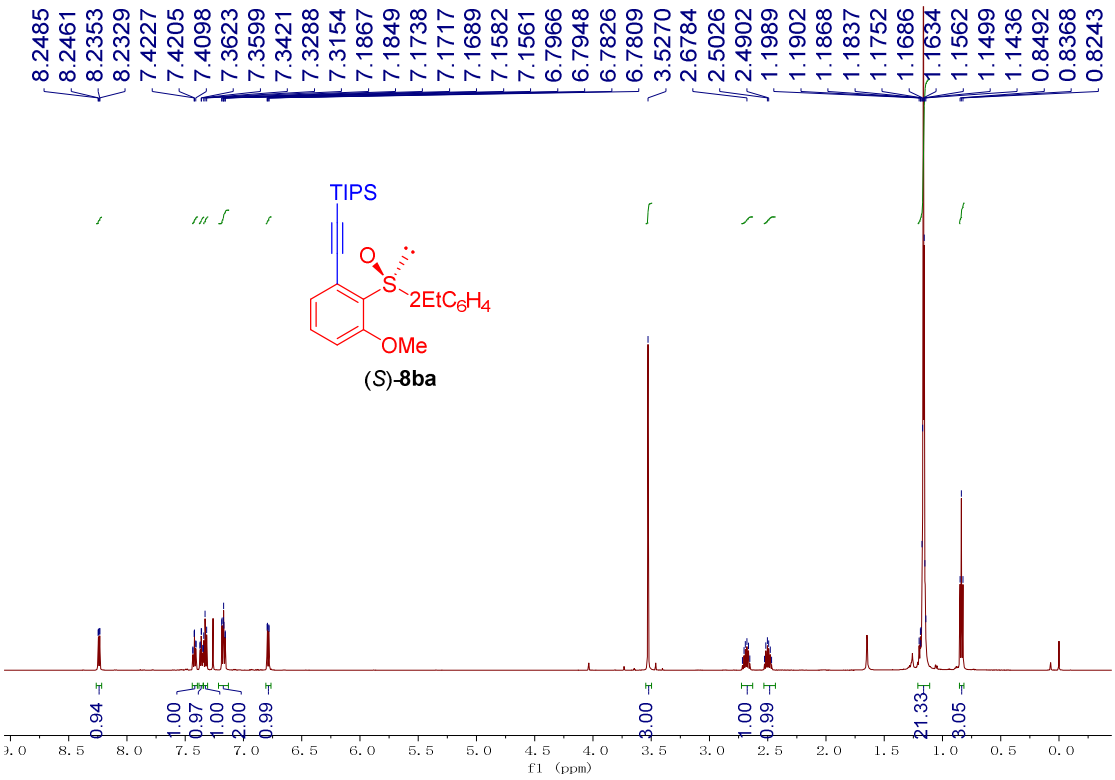
(*S*)-**8aa**


159.2484
141.8171
134.6657
133.1376
131.0752
130.2992
129.6387
126.9527
126.5695
126.1348
125.3983
113.4661
102.8241
99.4117
55.7404
18.9453
18.8459
11.5301
TIPS
O
S
2MeC6H4
OMe
f1 (ppm)

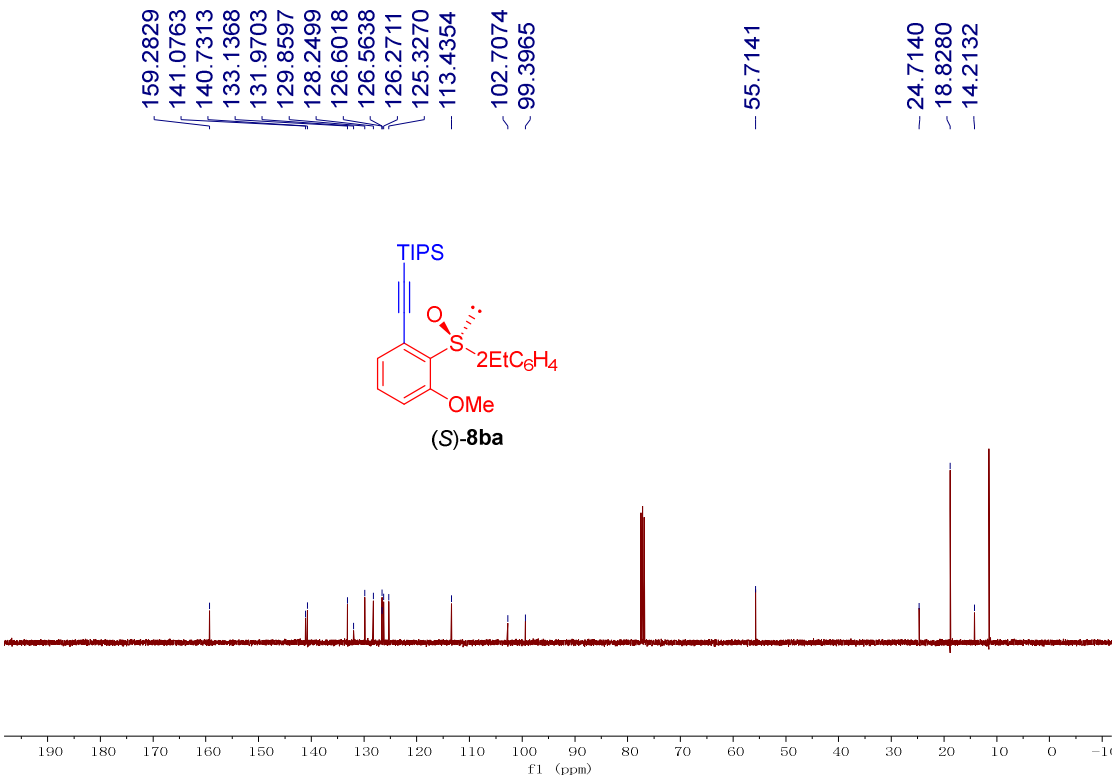
(*S*)-**8aa**


7.9842
7.9814
7.9713
7.9684
7.4041
7.4024
7.4007
7.3913
7.3891
7.3868
7.2950
7.2822
7.2693
7.1790
7.1773
7.1663
7.1647
7.1525
7.1500
7.1396
7.1373
6.8050
6.7913
3.6104
2.8921
2.8797
2.8671
2.8546
1.1483
1.1368
1.1339
1.1317
1.1267
1.1187
1.1133
1.1079
1.1058
0.8018
0.7893
0.7768
TIPS
O
S
2OMeC6H4
Et
(R)-7ba
1.00
2.05
1.02
2.05
1.03
3.09
2.08
21.55
3.00
f1 (ppm)

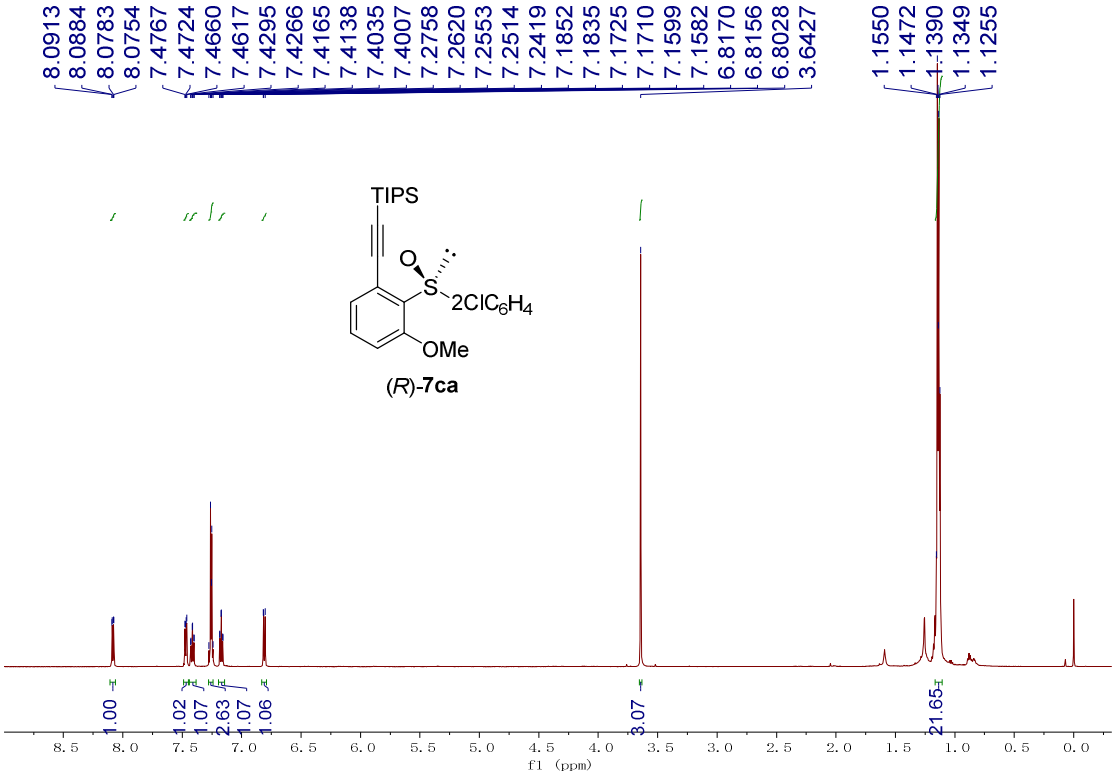

155.7956
146.3621
141.6709
131.8169
131.7992
131.5854
131.0891
130.7984
126.7809
125.7524
120.9321
110.9937
103.8322
97.9886
55.3774
23.3480
18.8212
15.0945
11.5650
TIPS
O
S
2OMeC6H4
Et
(R)-7ba
f1 (ppm)

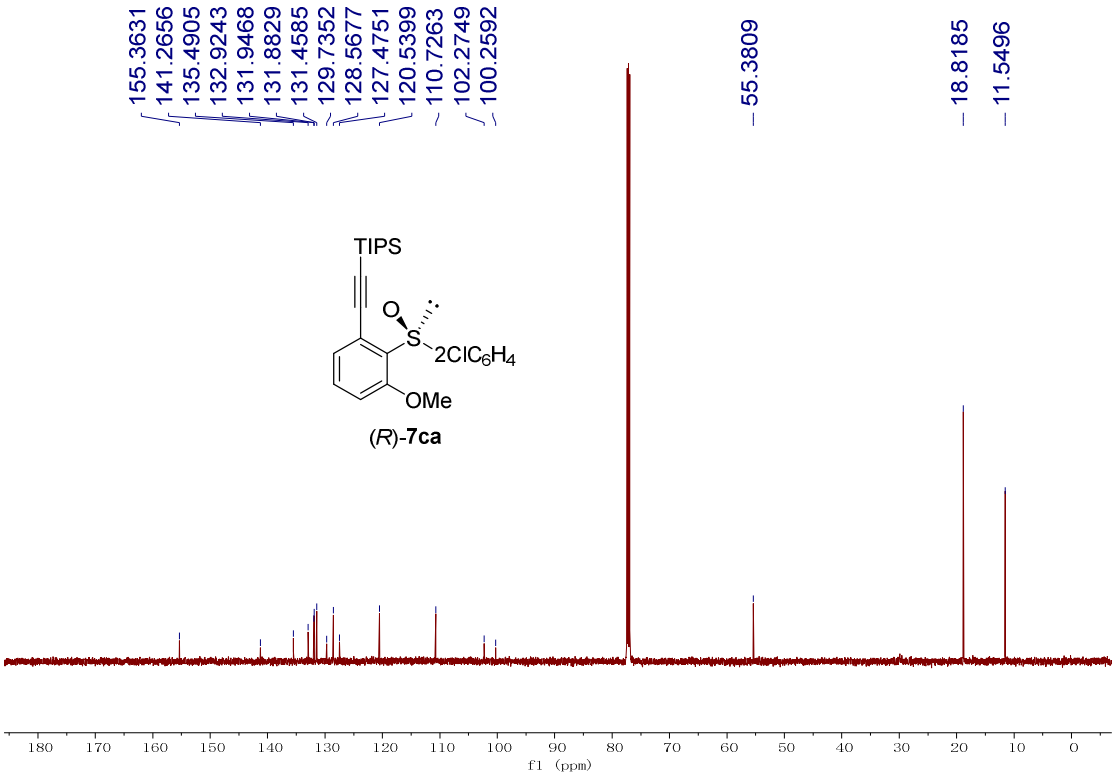

8.2485
8.2461
8.2353
8.2329
7.4227
7.4205
7.4098
7.3623
7.3599
7.3421
7.3288
7.3154
7.1867
7.1849
7.1738
7.1717
7.1689
7.1582
7.1561
6.7966
6.7948
6.7826
6.7809
3.5270
2.6784
2.5026
2.4902
1.1989
1.1902
1.1868
1.1837
1.1752
1.1686
1.1634
1.1562
1.1499
1.1436
0.8492
0.8368
0.8243
TIPS
O
S
2EtC6H4
OMe
0.94
1.00
0.97
1.00
2.00
0.99
3.00
1.00
0.99
21.33
3.05
f1 (ppm)

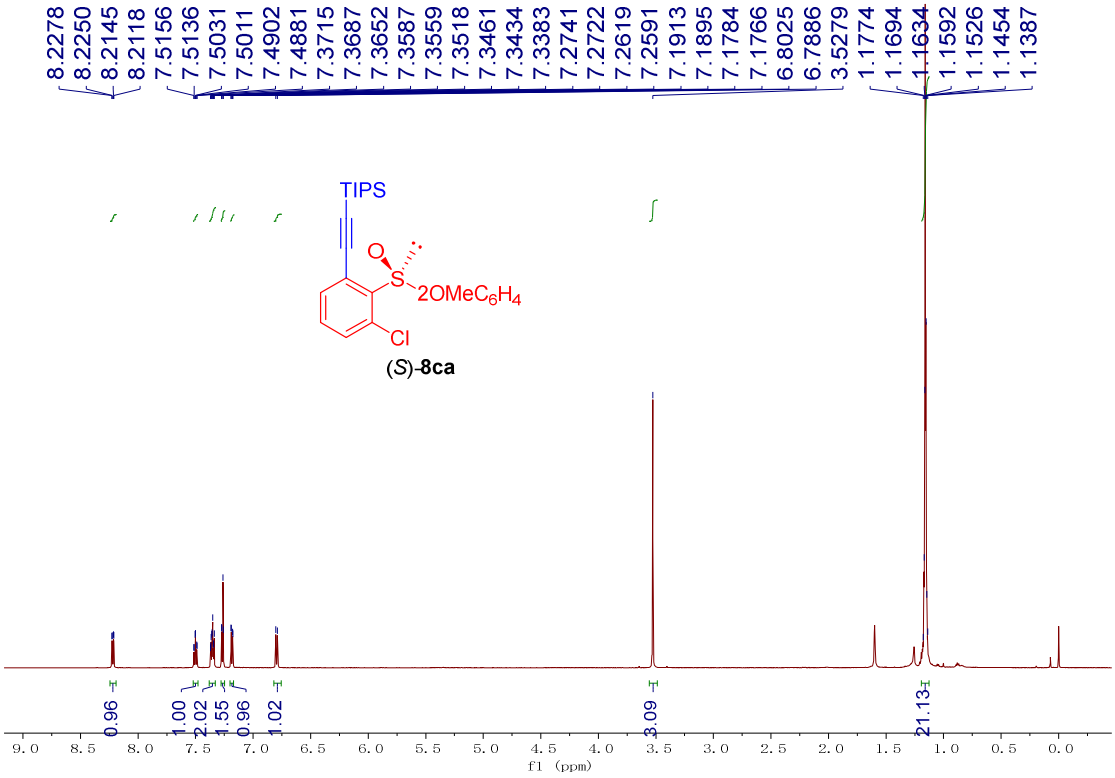
(*S*)-**8ba**


159.2829
141.0763
140.7313
133.1368
131.9703
129.8597
128.2499
126.6018
126.5638
126.2711
125.3270
113.4354
102.7074
99.3965
55.7141
24.7140
18.8280
14.2132
TIPS
O
S
2EtC6H4
OMe
f1 (ppm)

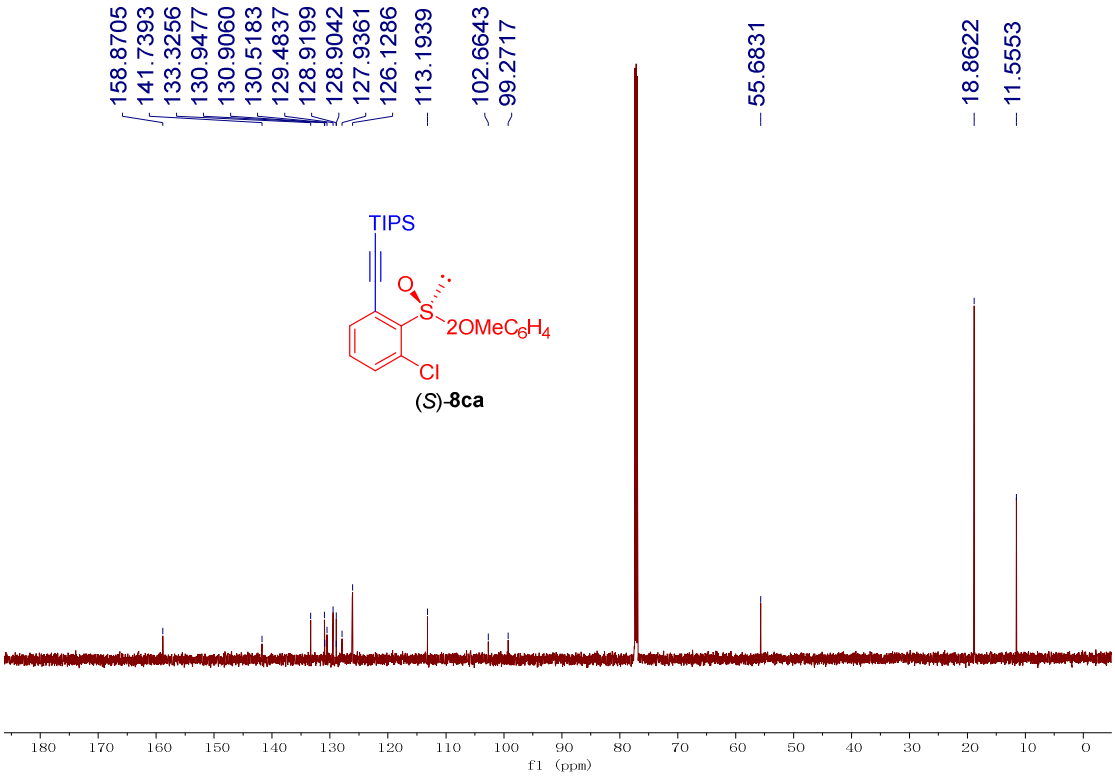
(*S*)-**8ba**


8.0913
8.0884
8.0783
8.0754
7.4767
7.4724
7.4660
7.4617
7.4295
7.4266
7.4165
7.4138
7.4035
7.4007
7.2758
7.2620
7.2553
7.2514
7.2419
7.1852
7.1835
7.1725
7.1710
7.1599
7.1582
6.8170
6.8156
6.8028
3.6427
1.1550
1.1472
1.1390
1.1349
1.1255
TIPS
O
S
2ClC6H4
OMe
(R)-7ca
1.00
1.02
1.07
2.63
1.07
1.06
3.07
21.65
f1 (ppm)

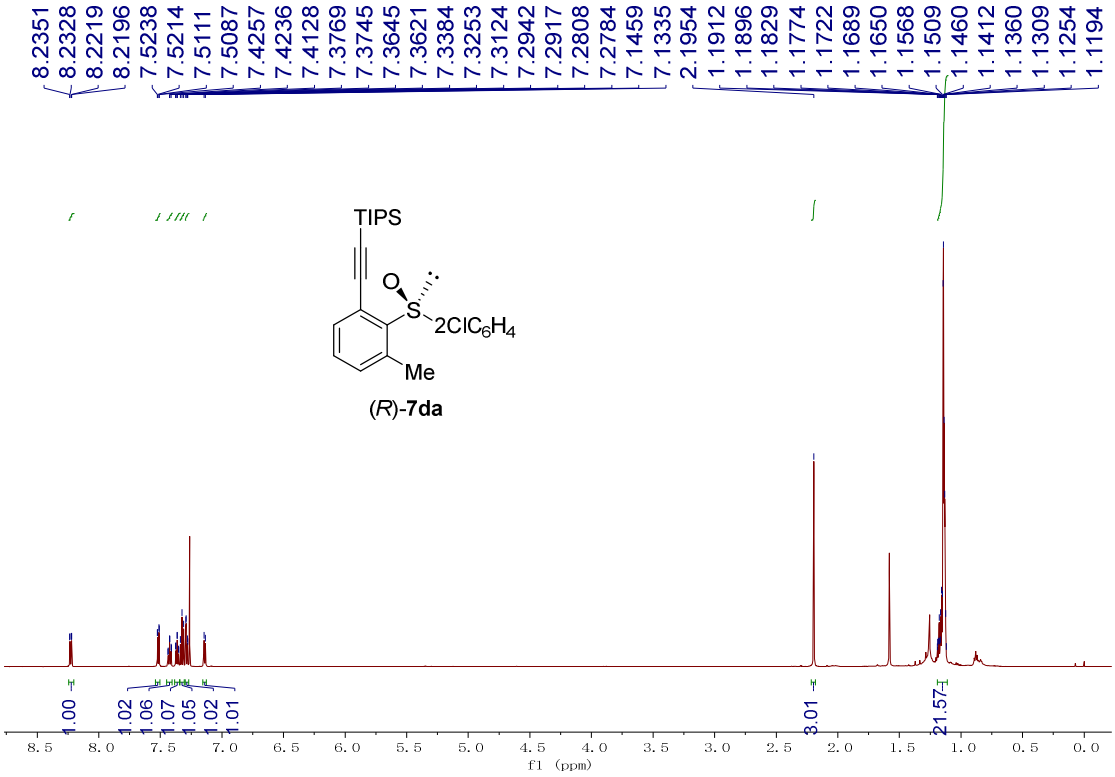

155.3631
141.2656
135.4905
132.9243
131.9468
131.8829
131.4585
129.7352
128.5677
127.4751
120.5399
110.7263
102.2749
100.2592
55.3809
18.8185
11.5496
TIPS
O
S
2ClC6H4
OMe
(R)-7ca
f1 (ppm)

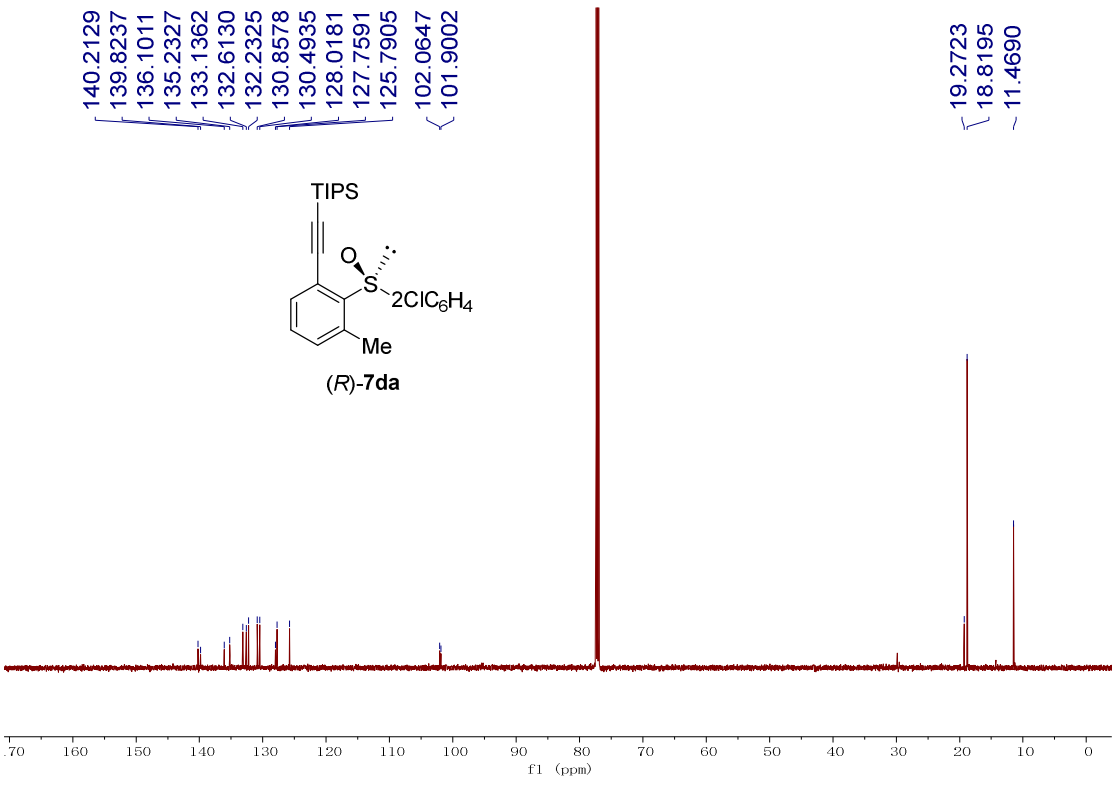

8.2278
8.2250
8.2145
8.2118
7.5156
7.5136
7.5031
7.5011
7.4902
7.4881
7.3715
7.3687
7.3652
7.3587
7.3559
7.3518
7.3461
7.3434
7.3383
7.2741
7.2722
7.2619
7.2591
7.1913
7.1895
7.1784
7.1766
6.8025
6.7886
3.5279
1.1774
1.1694
1.1634
1.1592
1.1526
1.1454
1.1387
TIPS
O
S
2OMeC6H4
Cl
0.96
1.00
2.02
1.55
0.96
1.02
3.09
21.13
f1 (ppm)

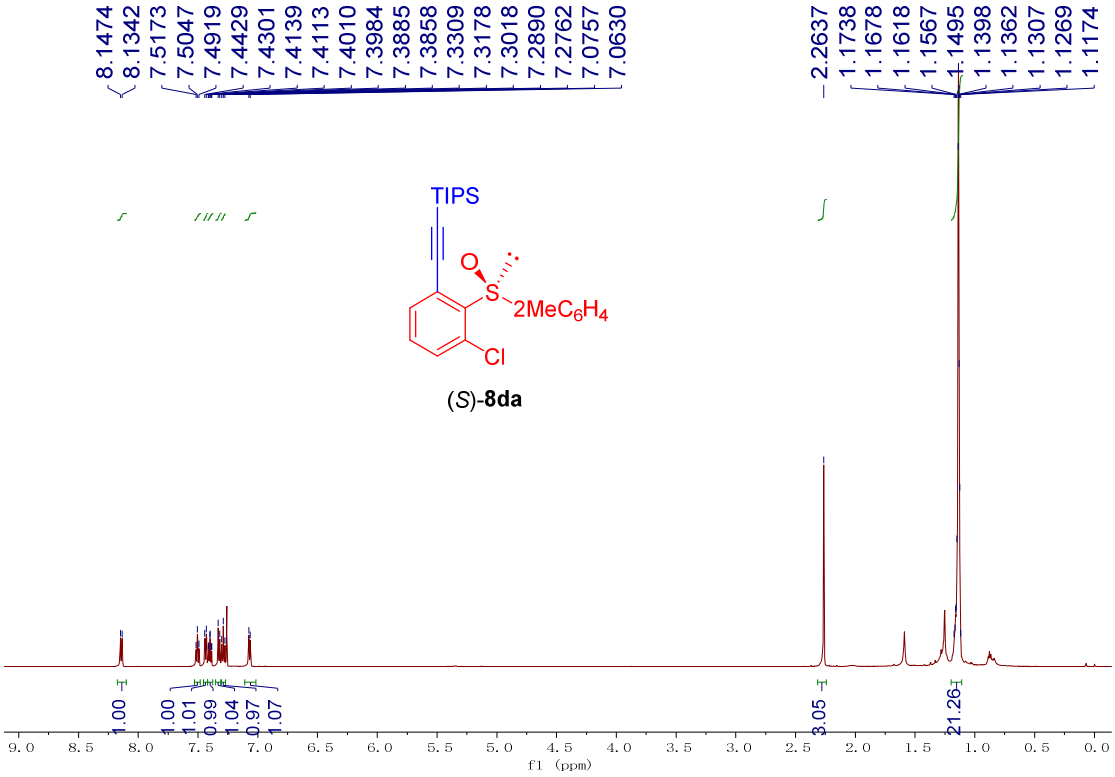
(*S*)-**8ca**

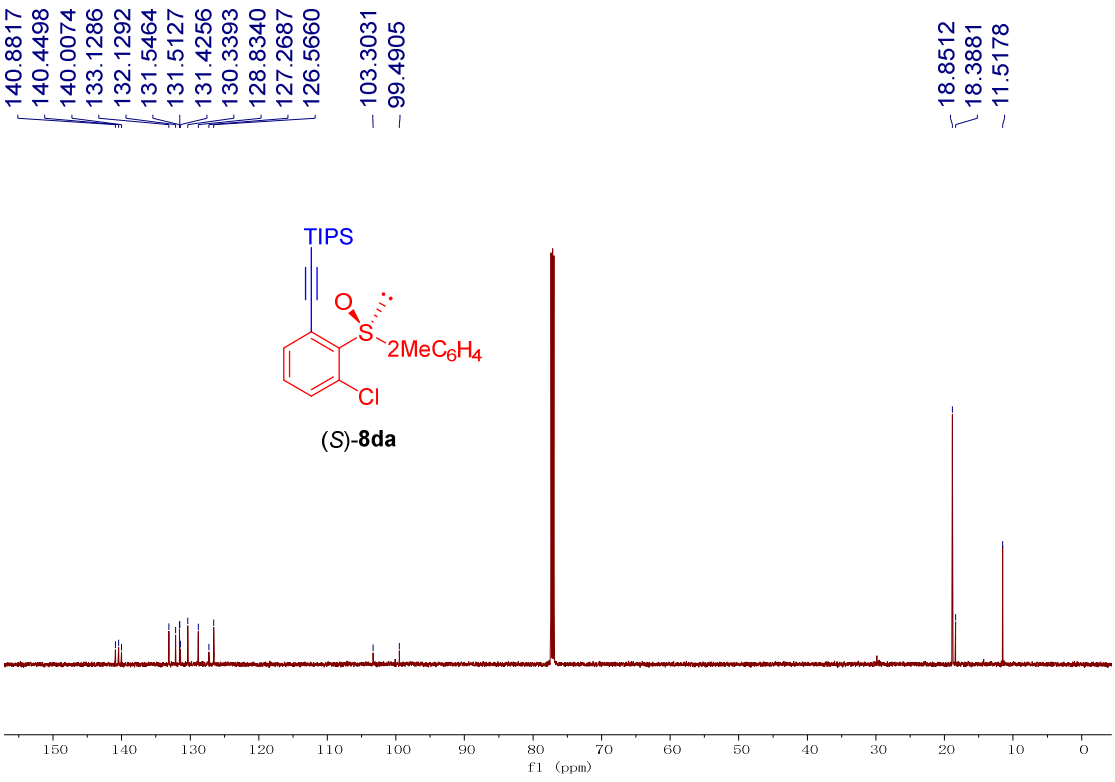

158.8705
141.7393
133.3256
130.9477
130.9060
130.5183
129.4837
128.9199
128.9042
127.9361
126.1286
113.1939
102.6643
99.2717
55.6831
18.8622
11.5553
TIPS
O
S
2OMeC6H4
Cl
f1 (ppm)

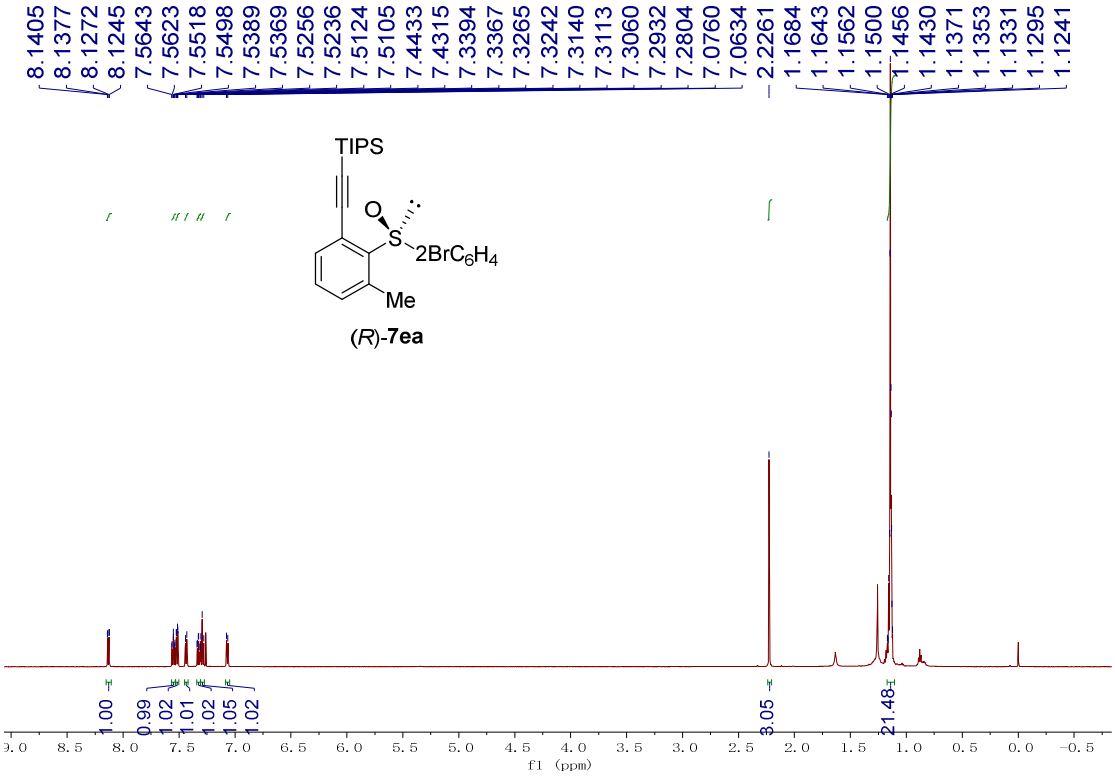
(*S*)-**8ca**


8.2351
8.2328
8.2219
8.2196
7.5238
7.5214
7.5111
7.5087
7.4257
7.4236
7.4128
7.3769
7.3745
7.3645
7.3621
7.3384
7.3253
7.3124
7.2942
7.2917
7.2808
7.2784
7.1459
7.1335
2.1954
1.1912
1.1896
1.1829
1.1774
1.1722
1.1689
1.1650
1.1568
1.1509
1.1460
1.1412
1.1360
1.1309
1.1254
1.1194
TIPS
O
S
2ClC6H4
Me
(R)-7da
1.00
1.02
1.06
1.07
1.05
1.02
1.01
3.01
21.57
f1 (ppm)

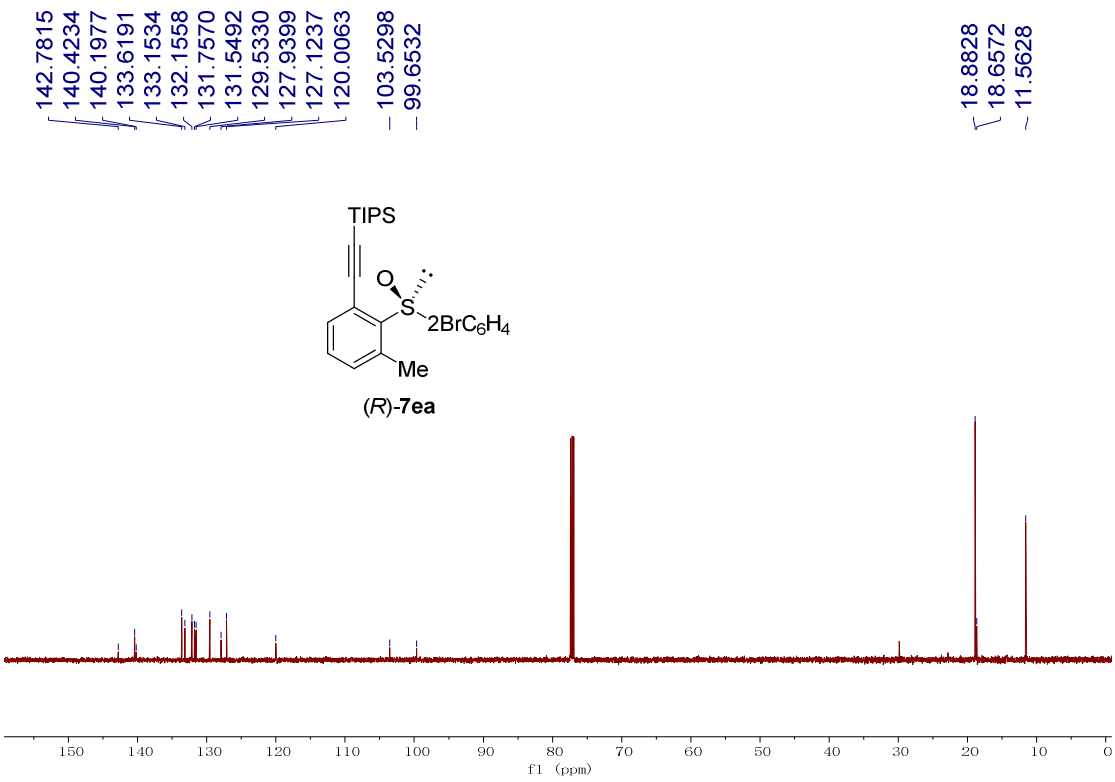

140.2129
139.8237
136.1011
135.2327
133.1362
132.6130
132.2325
130.8578
130.4935
128.0181
127.7591
125.7905
102.0647
101.9002
19.2723
18.8195
11.4690
TIPS
O
S
2ClC6H4
Me
(R)-7da
f1 (ppm)


8.1474
8.1342
7.5173
7.5047
7.4919
7.4429
7.4301
7.4139
7.4113
7.4010
7.3984
7.3885
7.3858
7.3309
7.3178
7.3018
7.2890
7.2762
7.0757
7.0630
2.2637
1.1738
1.1678
1.1618
1.1567
1.1495
1.1398
1.1362
1.1307
1.1269
1.1174
TIPS
O
S
2MeC6H4
Cl
(S)-8da
1.00
1.00
1.01
0.99
1.04
0.97
1.07
3.05
21.26
f1 (ppm)

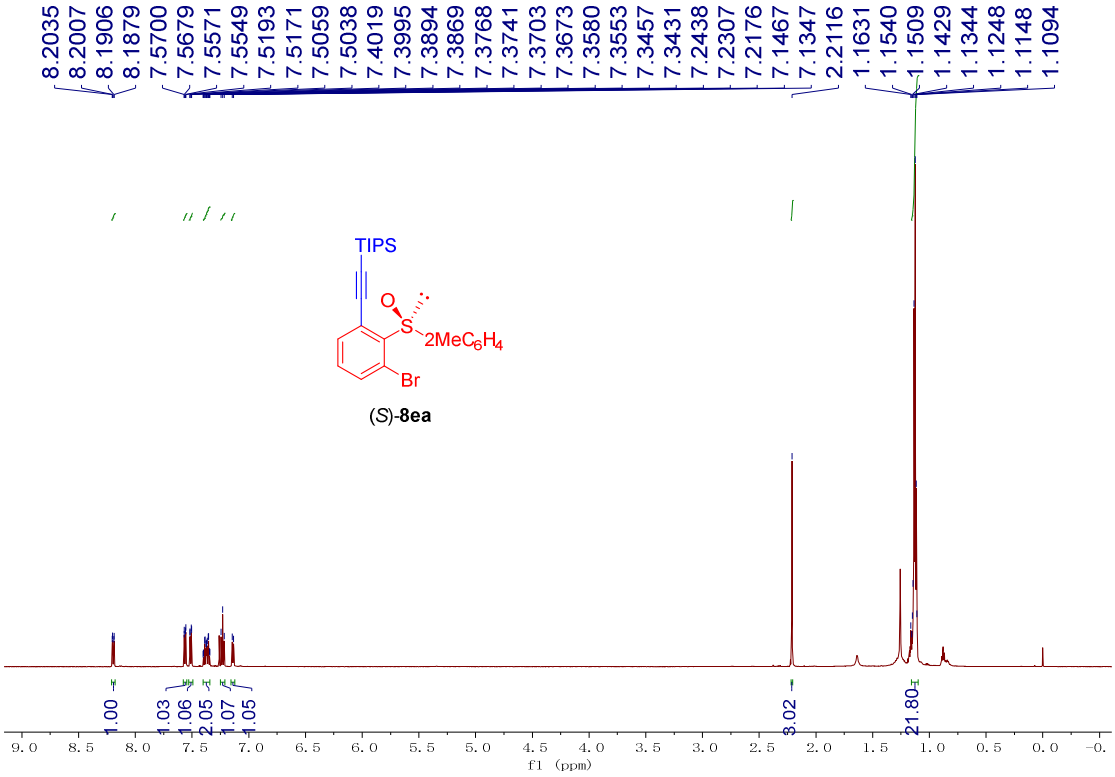

140.8817
140.4498
140.0074
133.1286
132.1292
131.5464
131.5127
131.4256
130.3393
128.8340
127.2687
126.5660
103.3031
99.4905
18.8512
18.3881
11.5178
TIPS
O
S
2MeC6H4
Cl
(S)-8da
f1 (ppm)


8.1405
8.1377
8.1272
8.1245
7.5643
7.5623
7.5518
7.5498
7.5389
7.5369
7.5256
7.5236
7.5124
7.5105
7.4433
7.4315
7.3394
7.3367
7.3265
7.3242
7.3140
7.3113
7.3060
7.2932
7.2804
7.0760
7.0634
2.2261
1.1684
1.1643
1.1562
1.1500
1.1456
1.1430
1.1371
1.1353
1.1331
1.1295
1.1241
TIPS
O
S
2BrC6H4
Me
1.00
0.99
1.02
1.01
1.02
1.05
1.02
3.05
21.48
f1 (ppm)

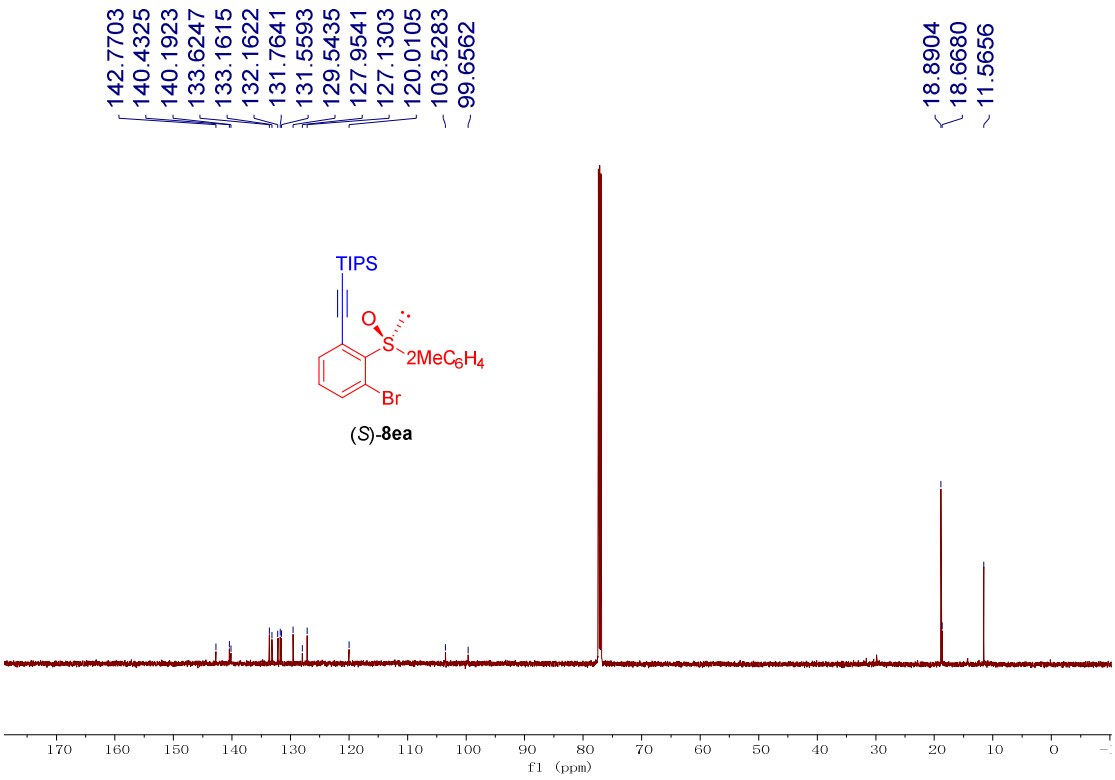
(*R*)-**7ea**


142.7815
140.4234
140.1977
133.6191
133.1534
132.1558
131.7570
131.5492
129.5330
127.9399
127.1237
120.0063
103.5298
99.6532
18.8828
18.6572
11.5628
TIPS
O
S
2BrC6H4
Me
f1 (ppm)

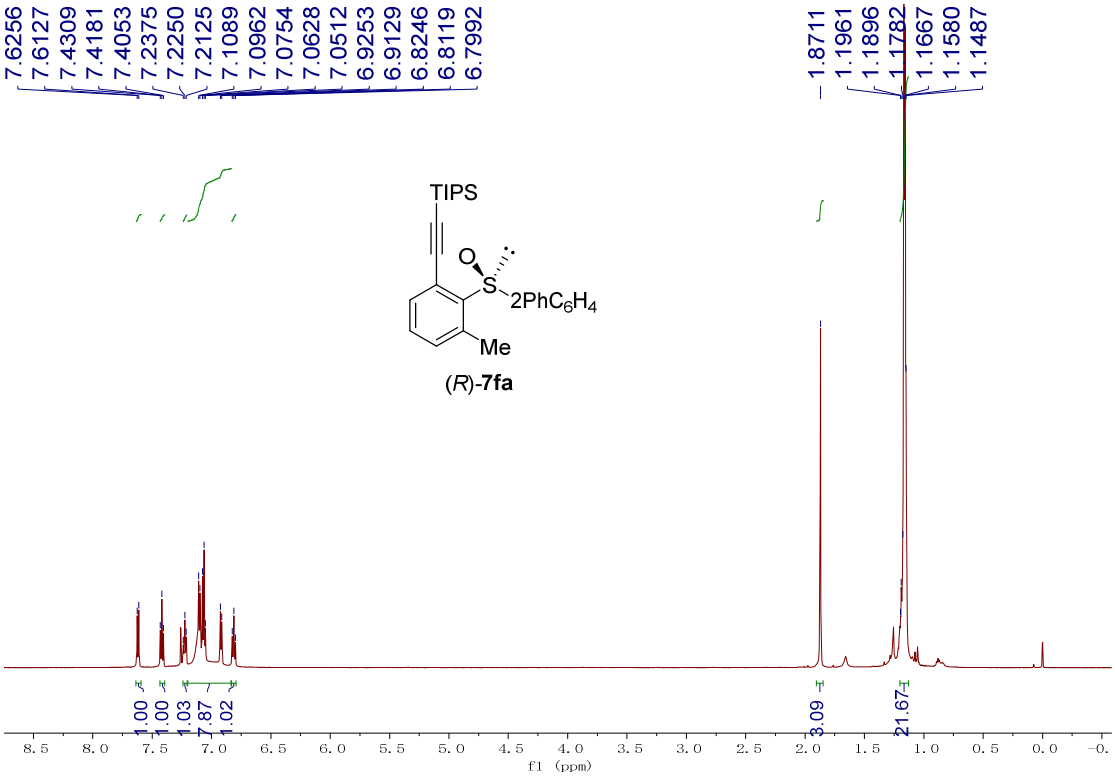
(*R*)-**7ea**


8.2035
8.2007
8.1906
8.1879
7.5700
7.5679
7.5571
7.5549
7.5193
7.5171
7.5059
7.5038
7.4019
7.3995
7.3894
7.3869
7.3768
7.3741
7.3703
7.3673
7.3580
7.3553
7.3457
7.3431
7.2438
7.2307
7.2176
7.1467
7.1347
2.2116
1.1631
1.1540
1.1509
1.1429
1.1344
1.1248
1.1148
1.1094
TIPS
O
S
2MeC6H4
Br
1.00
1.03
1.06
2.05
1.07
1.05
3.02
21.80
f1 (ppm)

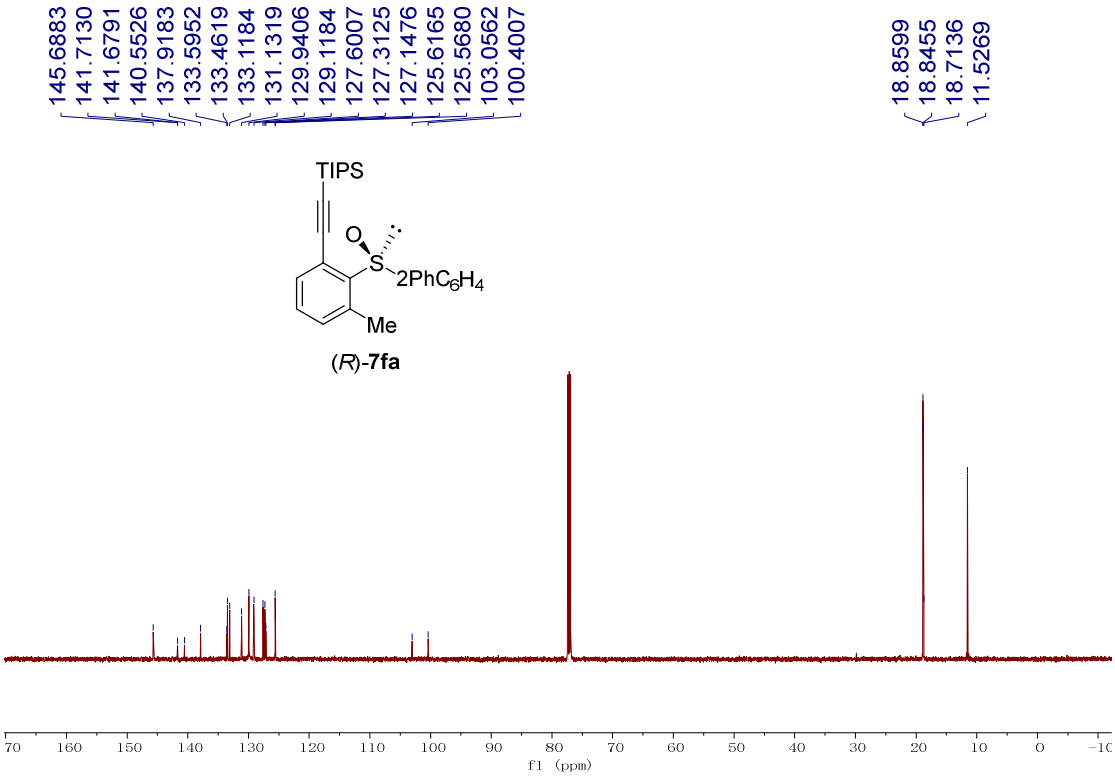
(*S*)-**8ea**


142.7703
140.4325
140.1923
133.6247
133.1615
132.1622
131.7641
131.5593
129.5435
127.9541
127.1303
120.0105
103.5283
99.6562
18.8904
18.6680
11.5656
TIPS
O
S
2MeC6H4
Br
f1 (ppm)

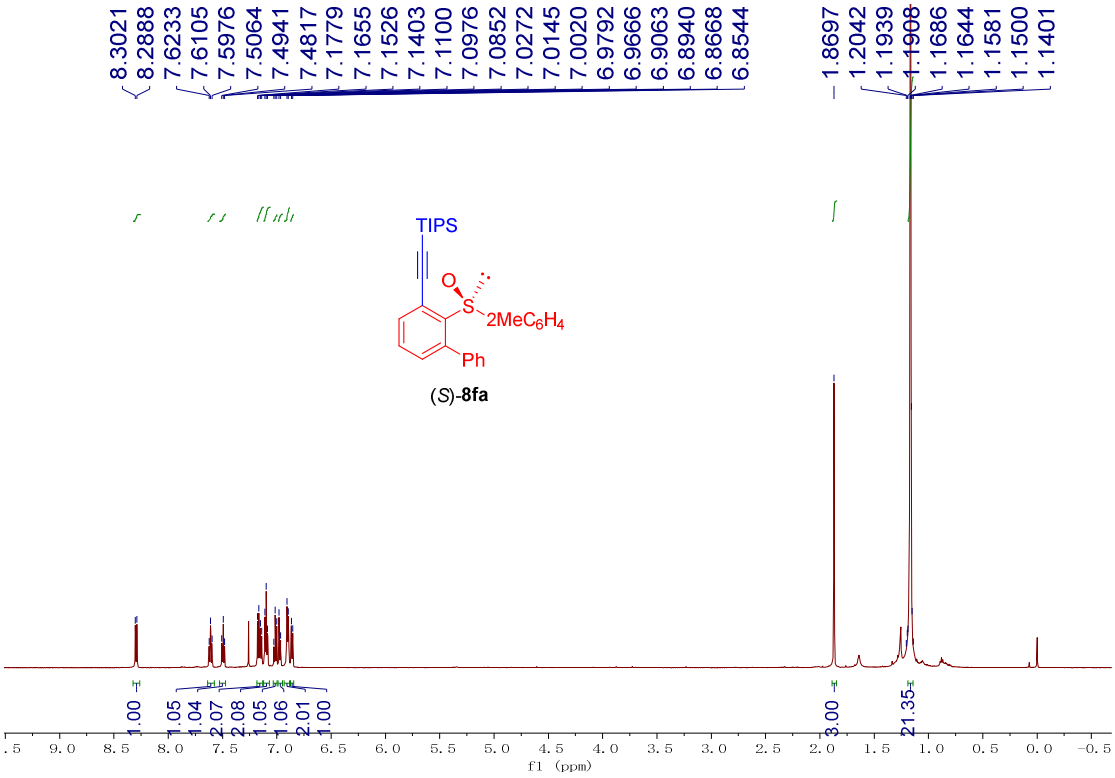
(*S*)-**8ea**

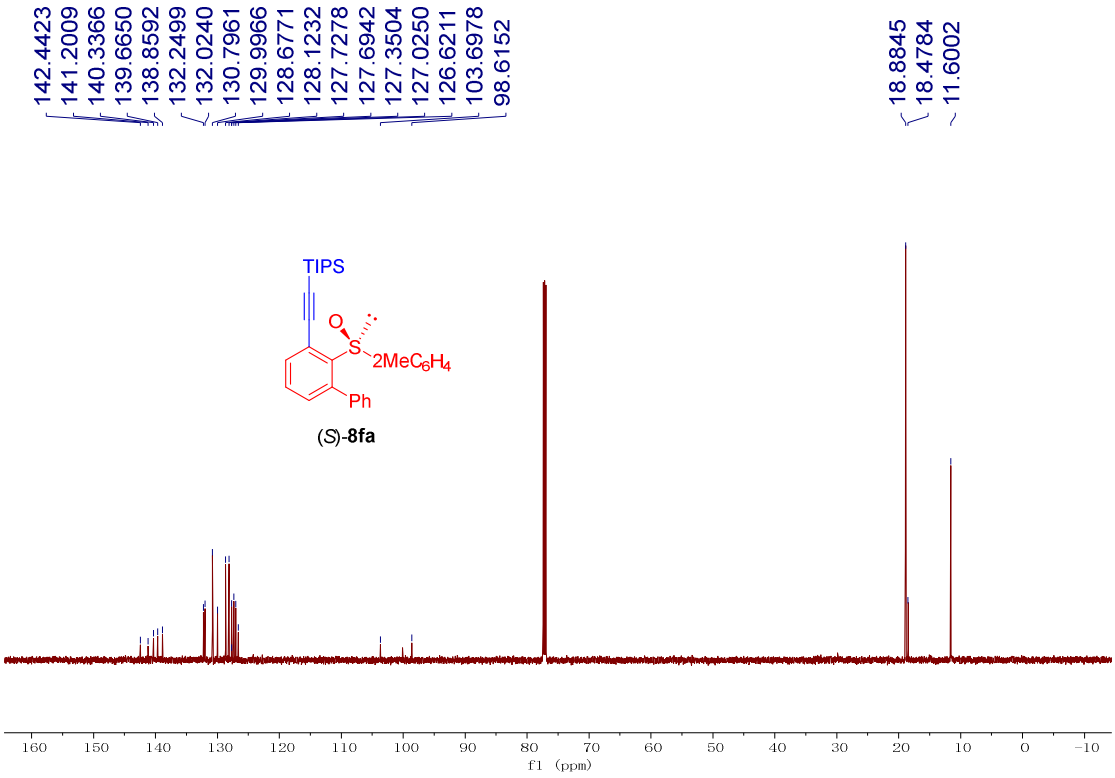

7.6256
7.6127
7.4309
7.4181
7.4053
7.2375
7.2250
7.2125
7.1089
7.0962
7.0754
7.0628
7.0512
6.9253
6.9129
6.8246
6.8119
6.7992
1.8711
1.1961
1.1896
1.1782
1.1667
1.1580
1.1487
TIPS
O
S
2PhC6H4
Me
1.00
1.00
1.03
7.87
1.02
3.09
21.67
f1 (ppm)

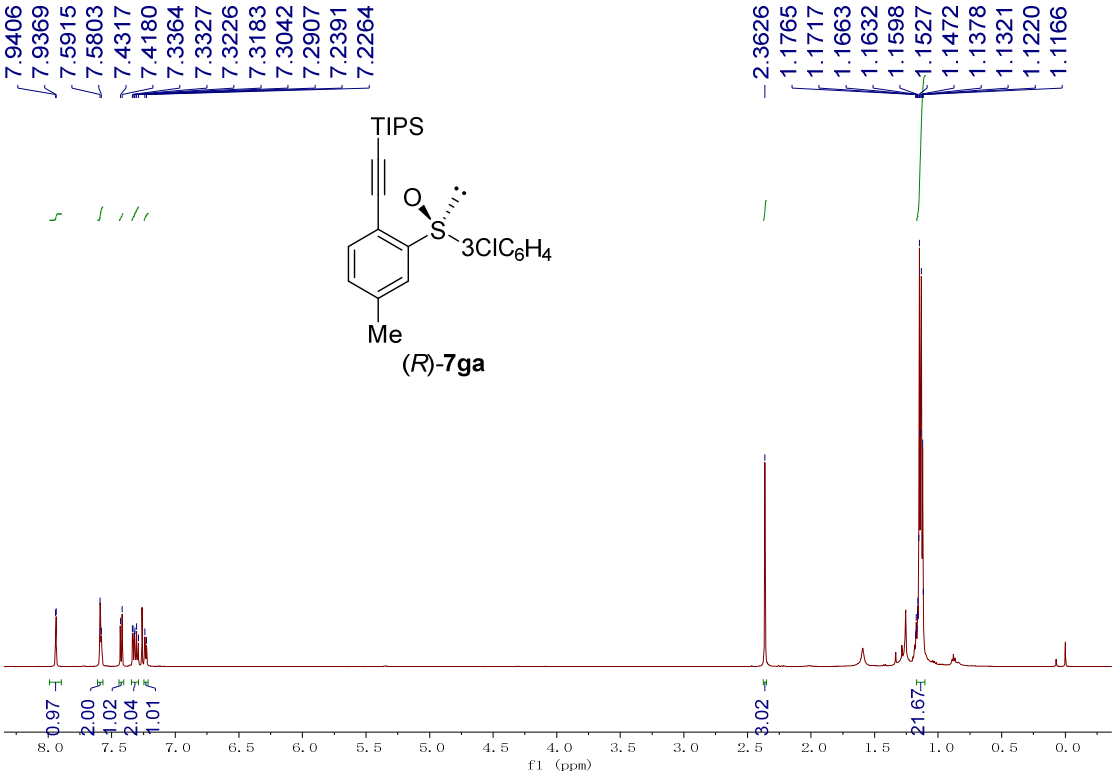
(*R*)-**7fa**

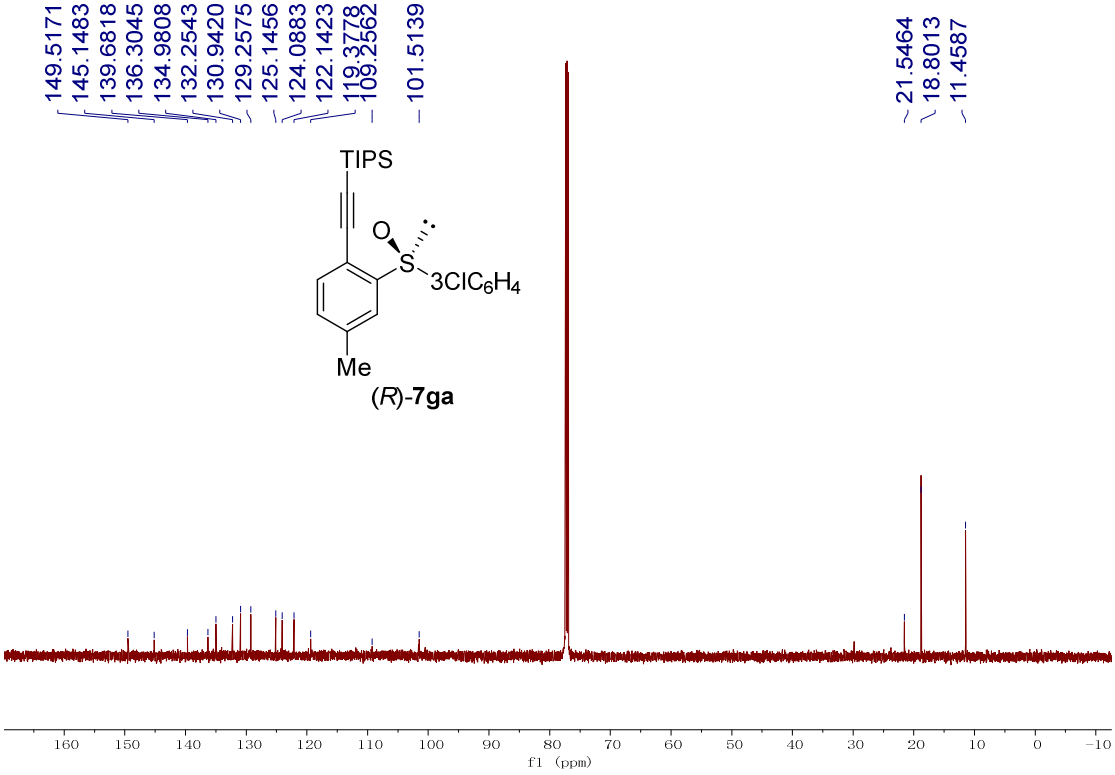

145.6883
141.7130
141.6791
140.5526
137.9183
133.5952
133.4619
133.1184
131.1319
129.9406
129.1184
127.6007
127.3125
127.1476
125.6165
125.5680
103.0562
100.4007
18.8599
18.8455
18.7136
11.5269
TIPS
O
S
2PhC6H4
Me
f1 (ppm)

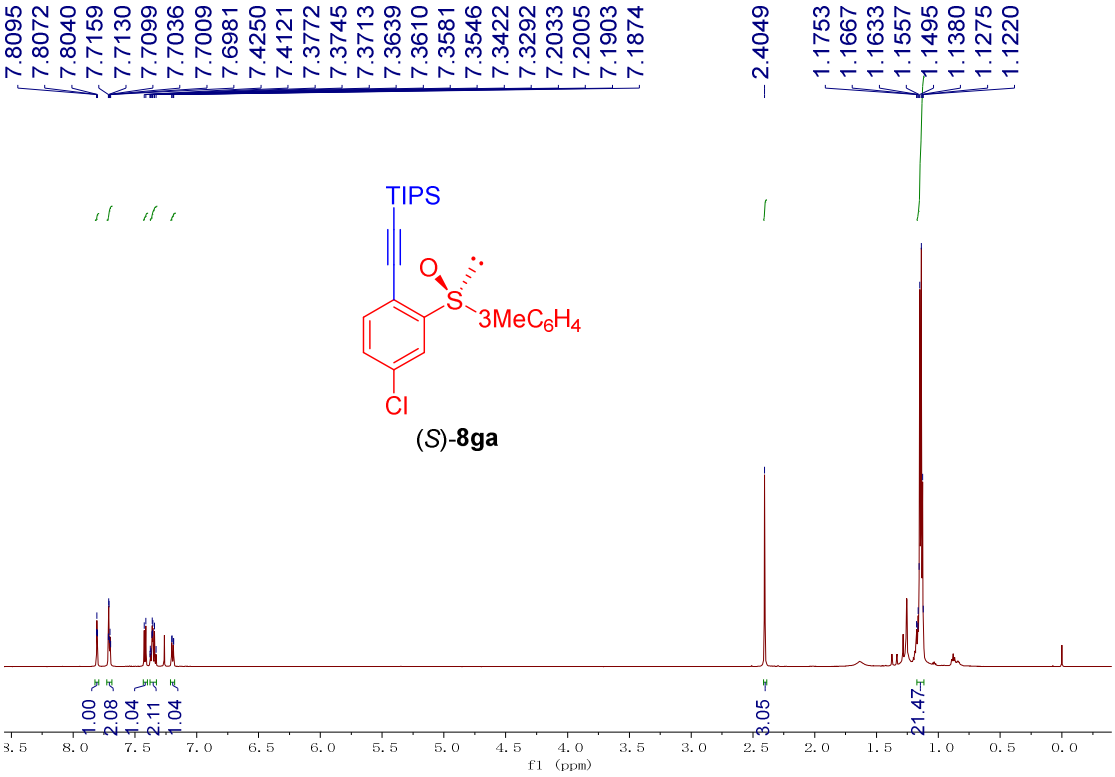
(*R*)-**7fa**


8.3021
8.2888
7.6233
7.6105
7.5976
7.5064
7.4941
7.4817
7.1779
7.1655
7.1526
7.1403
7.1100
7.0976
7.0852
7.0272
7.0145
7.0020
6.9792
6.9666
6.9063
6.8940
6.8668
6.8544
1.8697
1.2042
1.1939
1.1908
1.1686
1.1644
1.1581
1.1500
1.1401
TIPS
O
S
2MeC6H4
Ph
(S)-8fa
1.00
1.05
1.04
2.07
2.08
1.05
1.06
2.01
1.00
3.00
21.35
f1 (ppm)

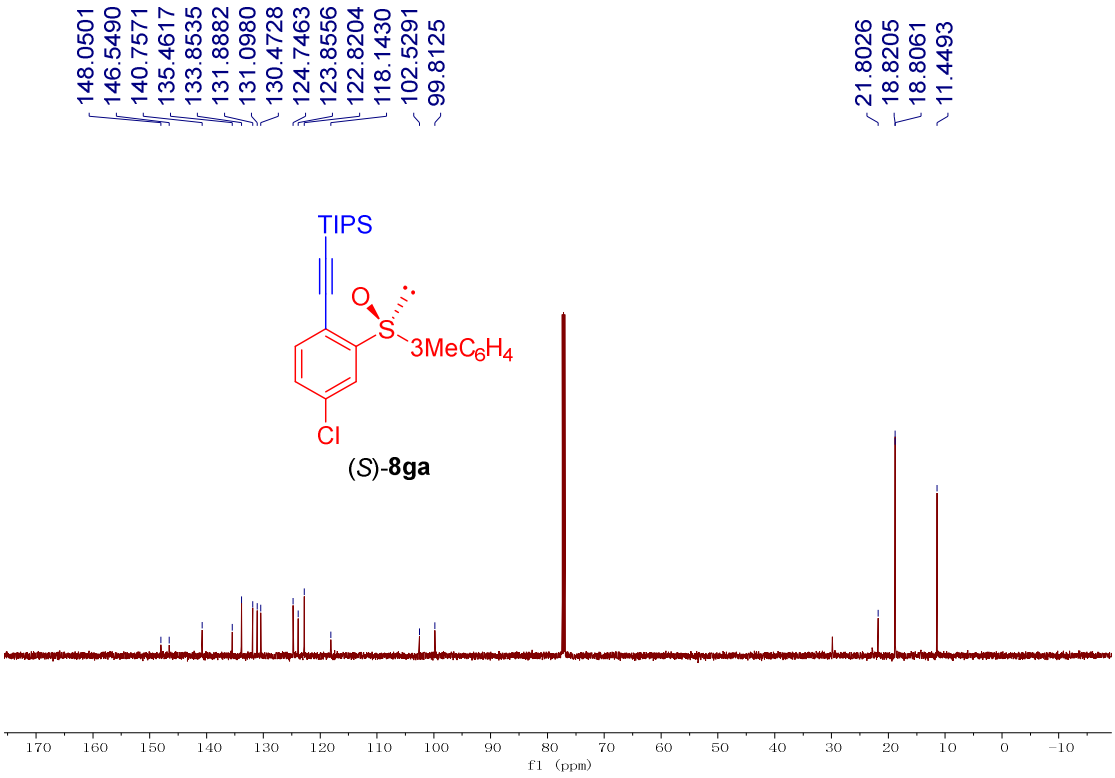

142.4423
141.2009
140.3366
139.6650
138.8592
132.2499
132.0240
130.7961
129.9966
128.6771
128.1232
127.7278
127.6942
127.3504
127.0250
126.6211
103.6978
98.6152
18.8845
18.4784
11.6002
TIPS
O
S
2MeC6H4
Ph
(S)-8fa
f1 (ppm)


7.9406
7.9369
7.5915
7.5803
7.4317
7.4180
7.3364
7.3327
7.3226
7.3183
7.3042
7.2907
7.2391
7.2264
2.3626
1.1765
1.1717
1.1663
1.1632
1.1598
1.1527
1.1472
1.1378
1.1321
1.1220
1.1166
TIPS
O
S
3ClC6H4
Me
(R)-7ga
0.97
2.00
1.02
2.04
1.01
3.02
21.67
f1 (ppm)

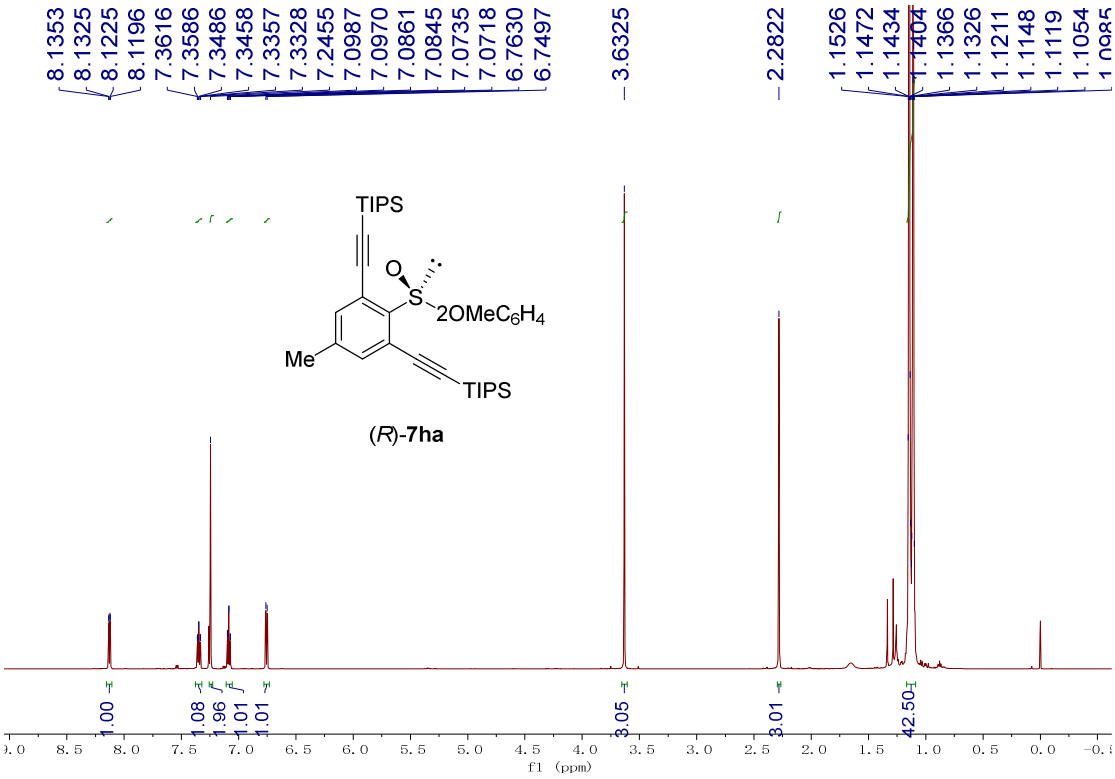

149.5171
145.1483
139.6818
136.3045
134.9808
132.2543
130.9420
129.2575
125.1456
124.0883
122.1423
119.3778
109.2562
101.5139
21.5464
18.8013
11.4587
TIPS
O
S
3ClC6H4
Me
(R)-7ga
f1 (ppm)


7.8095
7.8072
7.8040
7.7159
7.7130
7.7099
7.7036
7.7009
7.6981
7.4250
7.4121
7.3772
7.3745
7.3713
7.3639
7.3610
7.3581
7.3546
7.3422
7.3292
7.2033
7.2005
7.1903
7.1874
2.4049
1.1753
1.1667
1.1633
1.1557
1.1495
1.1380
1.1275
1.1220
TIPS
O
S
3MeC6H4
Cl
1.00
2.08
1.04
2.11
1.04
3.05
21.47
f1 (ppm)

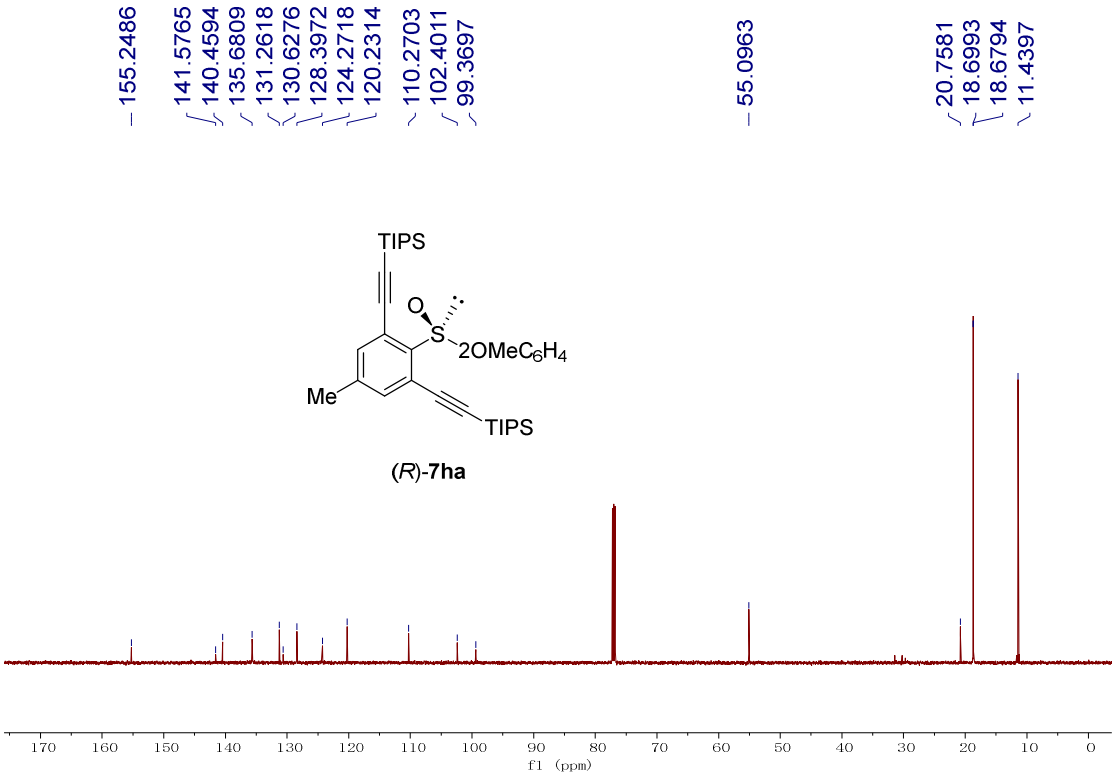
(*S*)-**8ga**


148.0501
146.5490
140.7571
135.4617
133.8535
131.8882
131.0980
130.4728
124.7463
123.8556
122.8204
118.1430
102.5291
99.8125
21.8026
18.8205
18.8061
11.4493
TIPS
O
S
3MeC6H4
Cl
f1 (ppm)

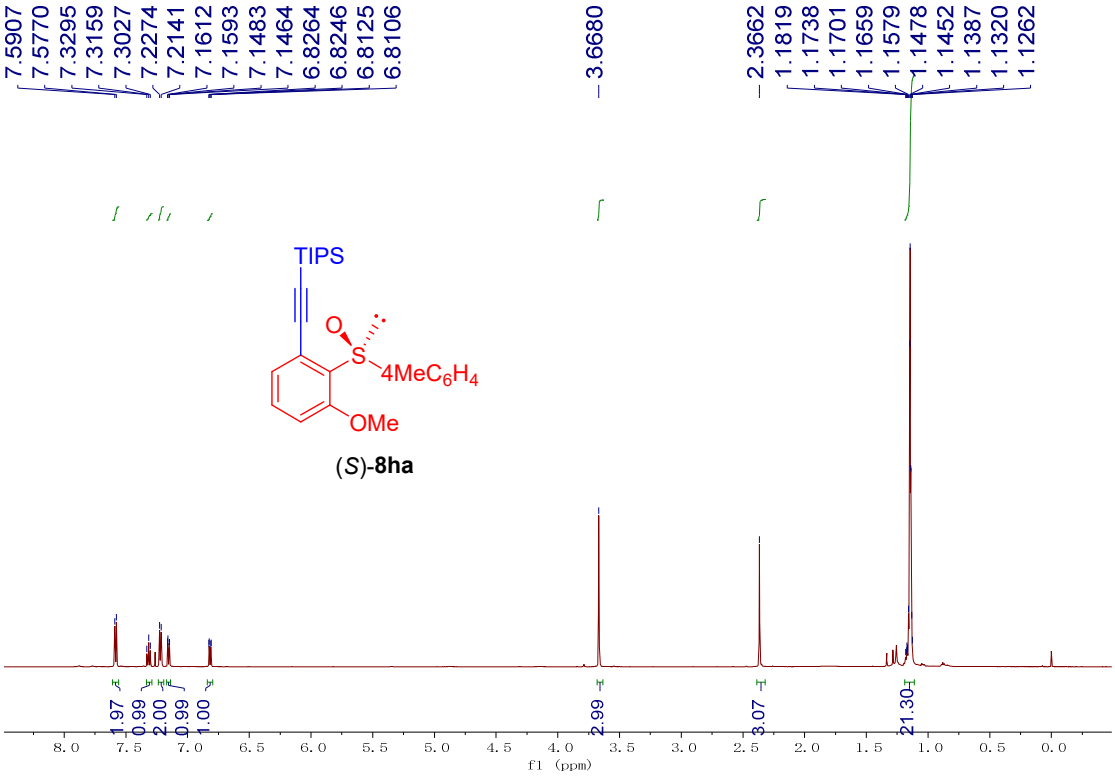
(*S*)-**8ga**


8.1353
8.1325
8.1225
8.1196
7.3616
7.3586
7.3486
7.3458
7.3357
7.3328
7.2455
7.0987
7.0970
7.0861
7.0845
7.0735
7.0718
6.7630
6.7497
3.6325
2.2822
1.1526
1.1472
1.1434
1.1404
1.1366
1.1326
1.1211
1.1148
1.1119
1.1054
TIPS
O
S
2OMeC6H4
Me
TIPS
1.00
1.08
1.96
1.01
1.01
3.05
3.01
42.50
f1 (ppm)

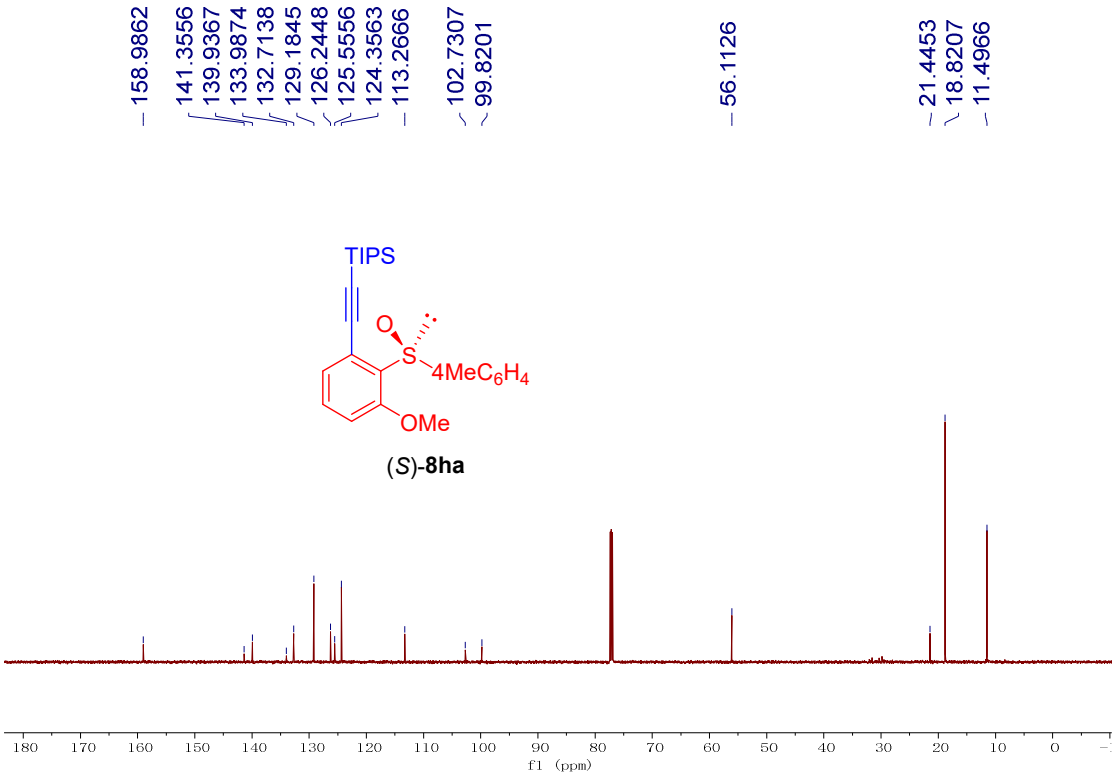
(*R*)-**7ha**


155.2486
141.5765
140.4594
135.6809
131.2618
130.6276
128.3972
124.2718
120.2314
110.2703
102.4011
99.3697
55.0963
20.7581
18.6993
18.6794
11.4397
TIPS
O
S
2OMeC6H4
Me
TIPS
f1 (ppm)

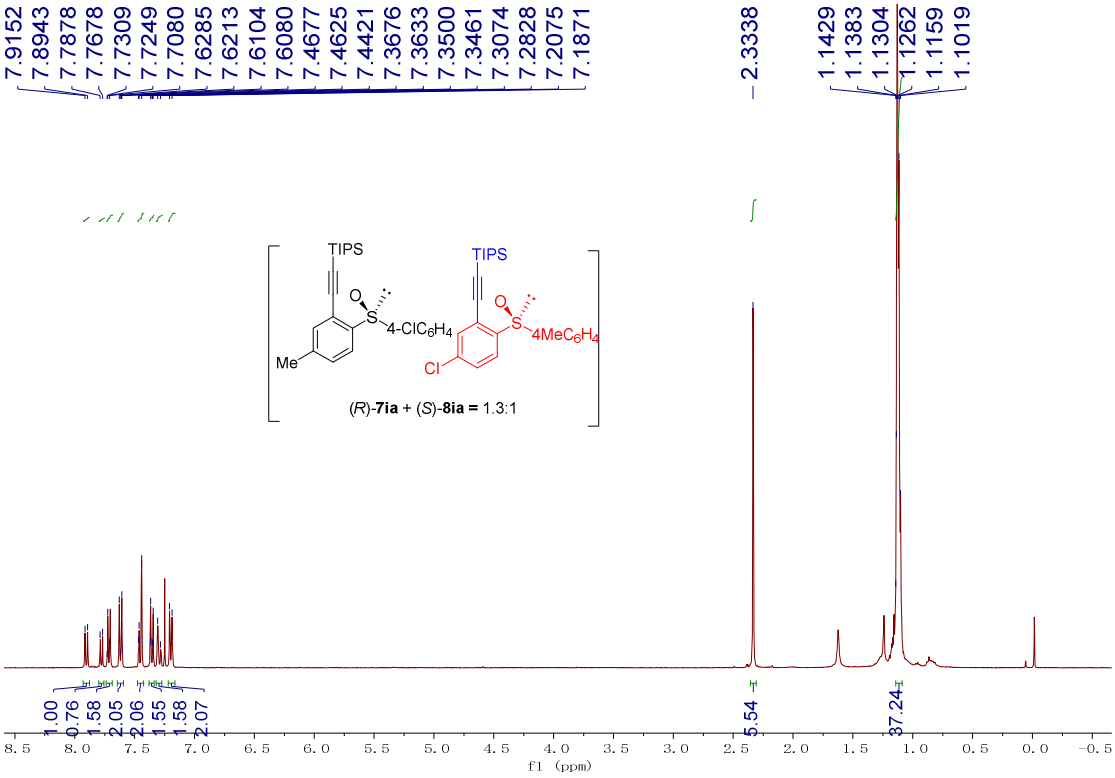
(*R*)-**7ha**

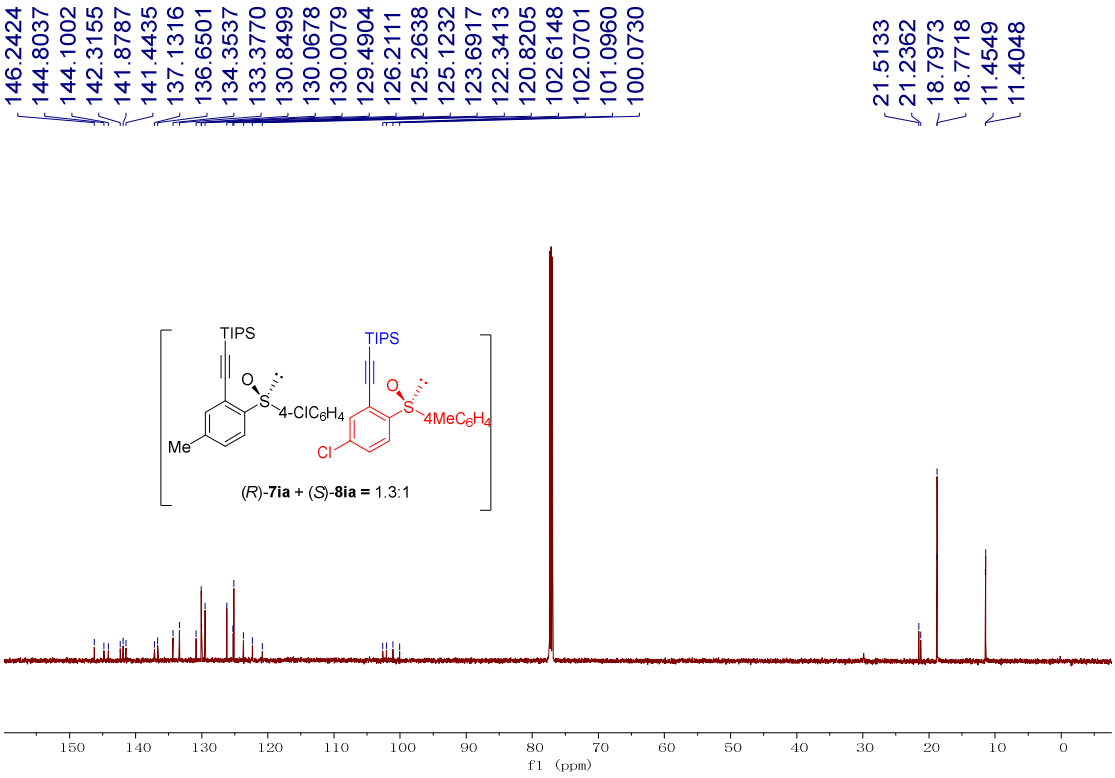

7.5907
7.5770
7.3295
7.3159
7.3027
7.2274
7.2141
7.1612
7.1593
7.1483
7.1464
6.8264
6.8246
6.8125
6.8106
3.6680
2.3662
1.1819
1.1738
1.1701
1.1659
1.1579
1.1478
1.1452
1.1387
1.1320
1.1262
TIPS
O
S
4MeC6H4
OMe
1.97
0.99
2.00
0.99
1.00
2.99
3.07
21.30
f1 (ppm)

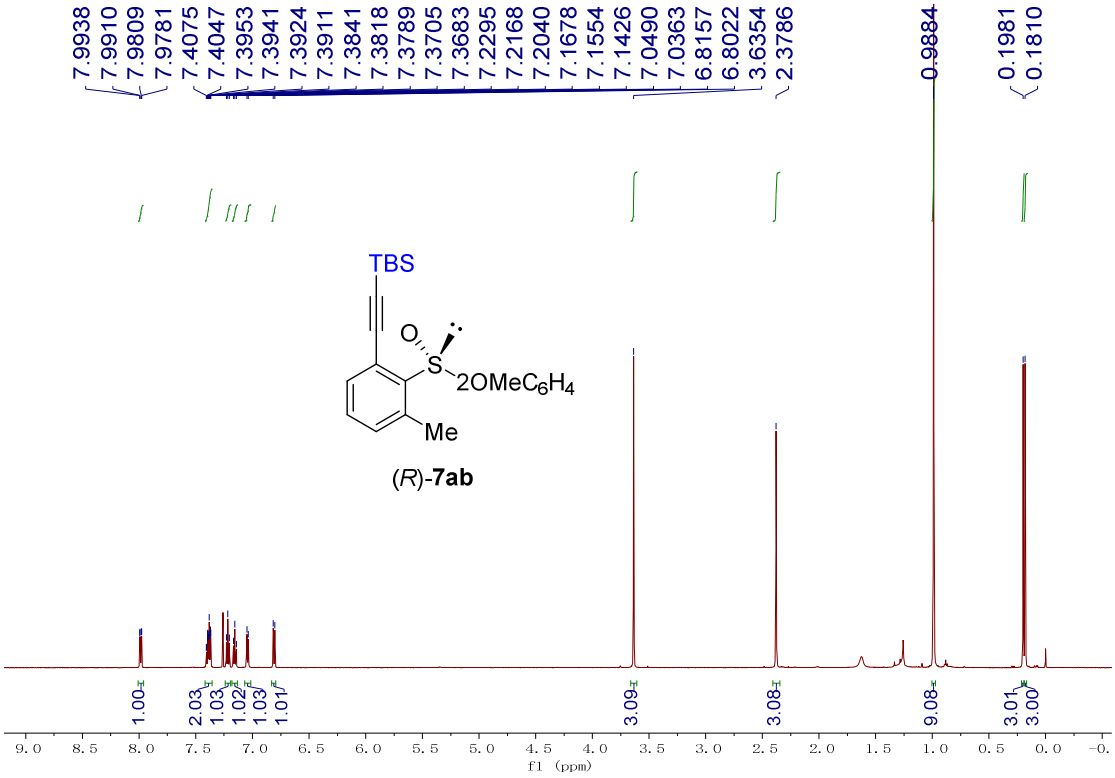
(*S*)-**8ha**

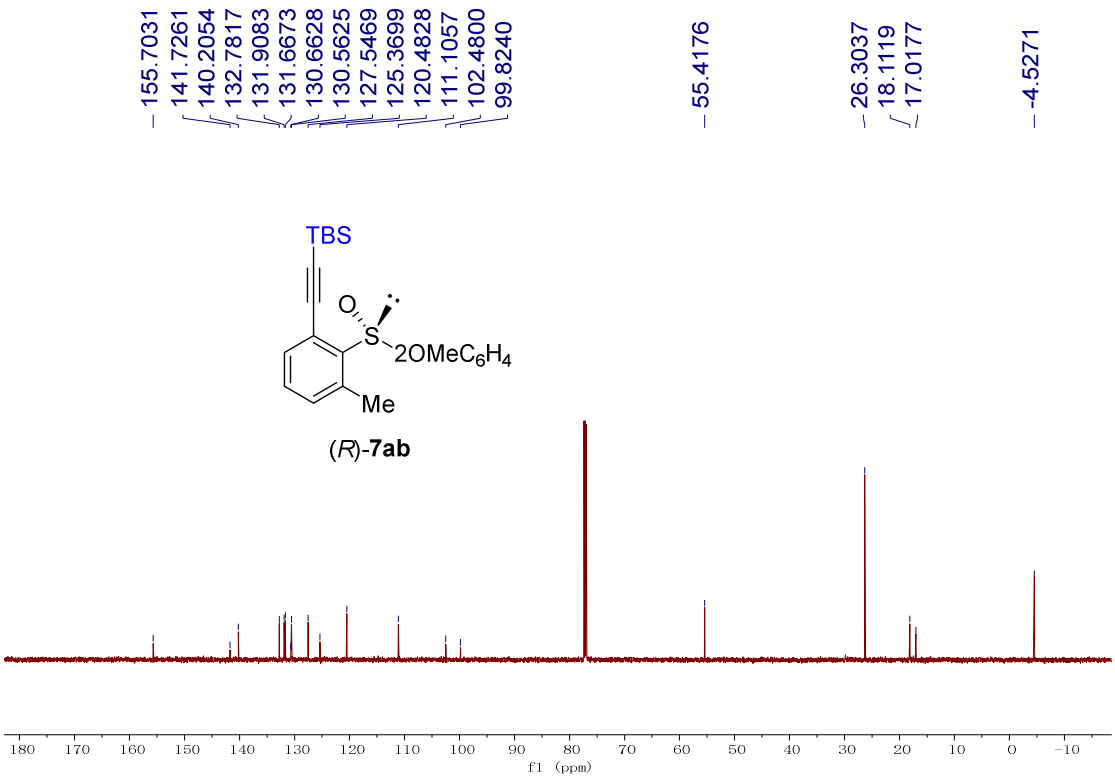

158.9862
141.3556
139.9367
133.9874
132.7138
129.1845
126.2448
125.5556
124.3563
113.2666
102.7307
99.8201
56.1126
21.4453
18.8207
11.4966
TIPS
O
S
4MeC6H4
OMe
f1 (ppm)

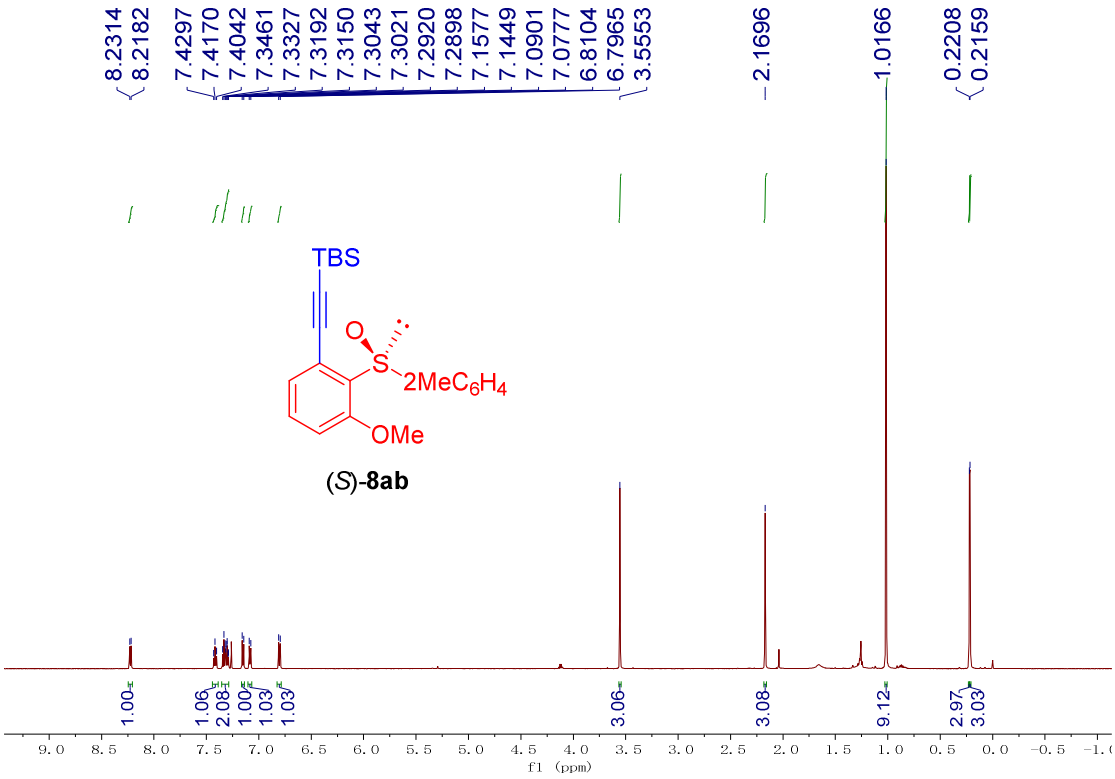
(*S*)-**8ha**

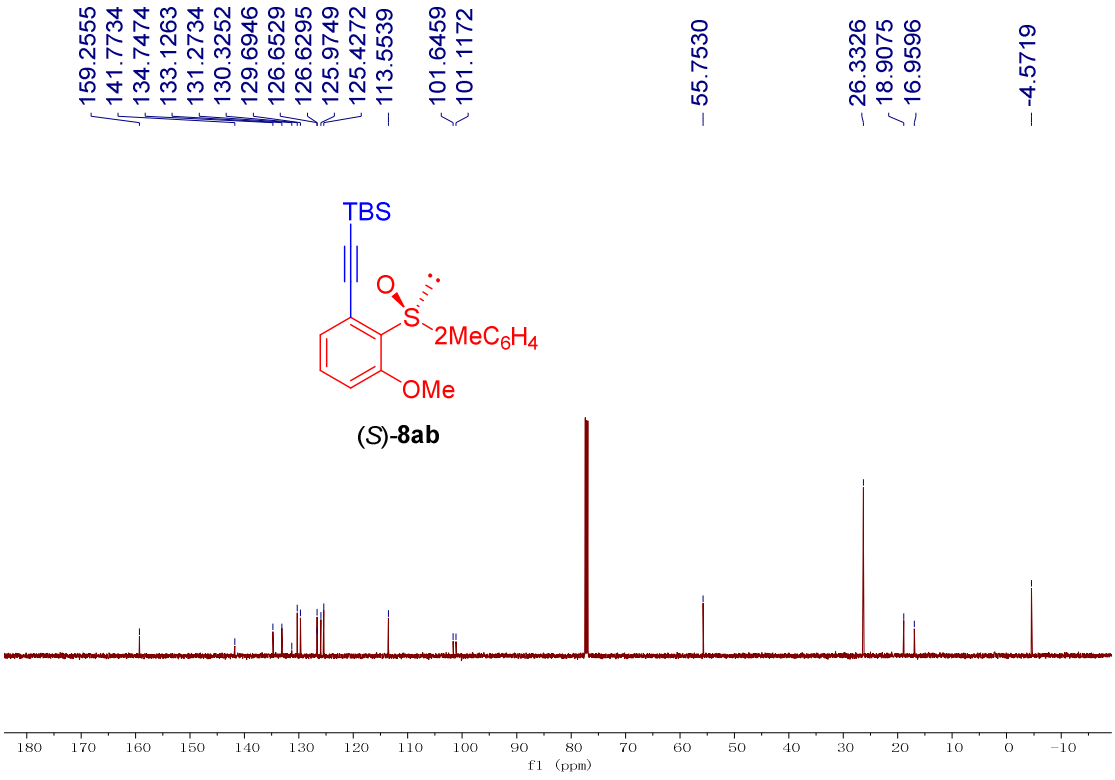

7.9152
7.8943
7.7878
7.7678
7.7309
7.7249
7.7080
7.6285
7.6213
7.6104
7.6080
7.4677
7.4625
7.4421
7.3676
7.3633
7.3500
7.3461
7.3074
7.2828
7.2075
7.1871
2.3338
1.1429
1.1383
1.1304
1.1262
1.1159
1.1019
TIPS
TIPS
4-ClC6H4
4MeC6H4
Me
Cl
(R)-7ia + (S)-8ia = 1.3:1
1.00
0.76
1.58
2.05
2.06
1.55
1.58
2.07
5.54
37.24
f1 (ppm)

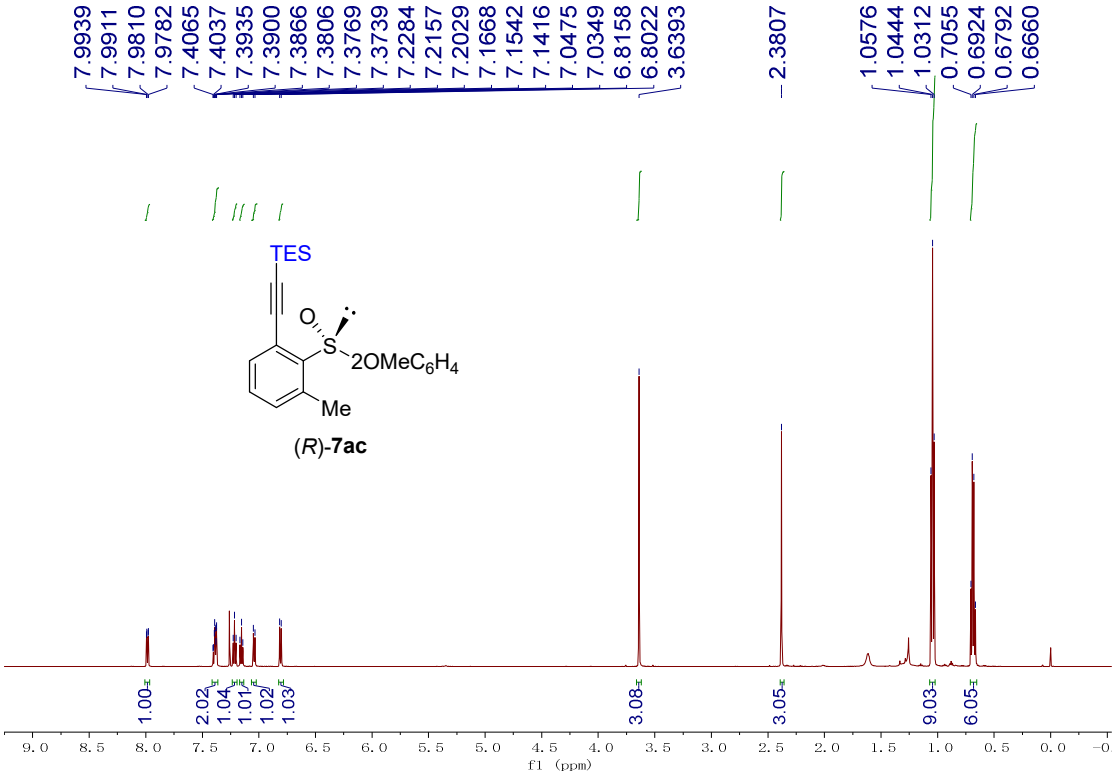

146.2424
144.8037
144.1002
142.3155
141.8787
141.4435
137.1316
136.6501
134.3537
133.3770
130.8499
130.0678
130.0079
129.4904
126.2111
125.2638
125.1232
123.6917
122.3413
120.8205
102.6148
102.0701
101.0960
100.0730
21.5133
21.2362
18.7973
18.7718
11.4549
11.4048
TIPS
TIPS
4-ClC6H4
4MeC6H4
Me
Cl
(R)-7ia + (S)-8ia = 1.3:1
f1 (ppm)


7.9938
7.9910
7.9809
7.9781
7.4075
7.4047
7.3953
7.3941
7.3924
7.3911
7.3841
7.3818
7.3789
7.3705
7.3683
7.2295
7.2168
7.2040
7.1678
7.1554
7.1426
7.0490
7.0363
6.8157
6.8022
3.6354
2.3786
0.9884
0.1981
0.1810
TBS
O
S
2OMeC6H4
Me
(R)-7ab
1.00
2.03
1.03
1.02
1.03
1.01
3.09
3.08
9.08
3.01
3.00
f1 (ppm)

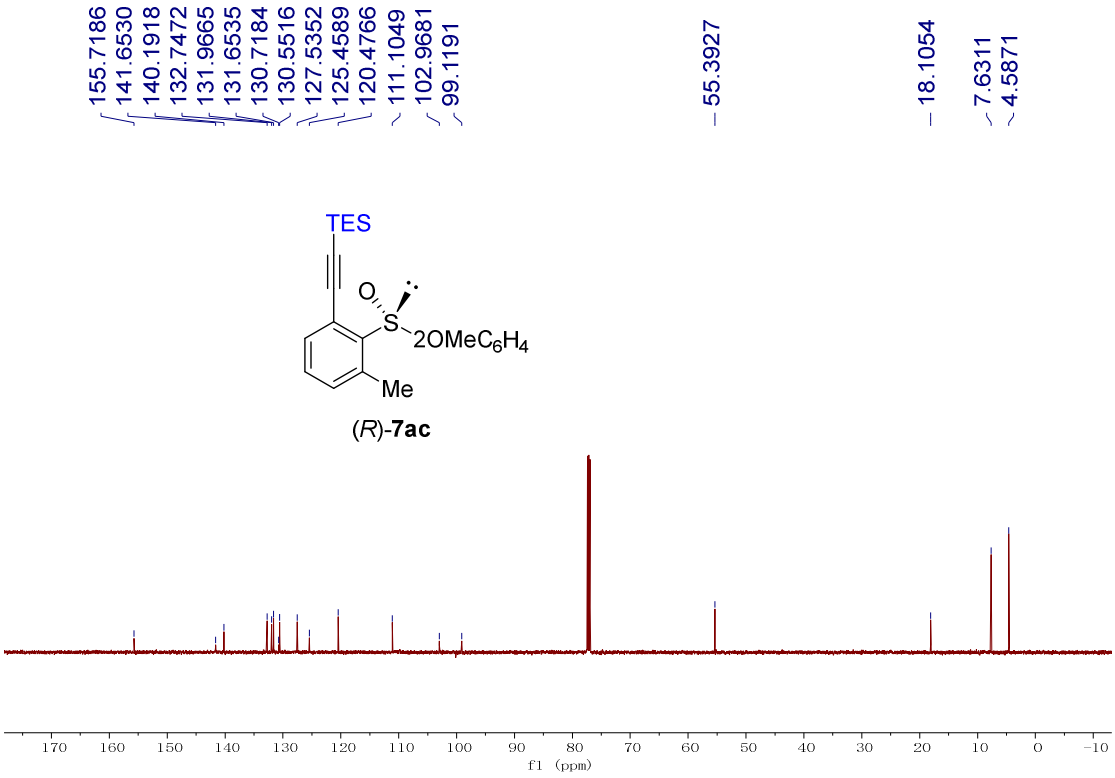

155.7031
141.7261
140.2054
132.7817
131.9083
131.6673
130.6628
130.5625
127.5469
125.3699
120.4828
111.1057
102.4800
99.8240
55.4176
26.3037
18.1119
17.0177
-4.5271
TBS
O
S
2OMeC6H4
Me
(R)-7ab
f1 (ppm)


8.2314
8.2182
7.4297
7.4170
7.4042
7.3461
7.3327
7.3192
7.3150
7.3043
7.3021
7.2920
7.2898
7.1577
7.1449
7.0901
7.0777
6.8104
6.7965
3.5553
2.1696
1.0166
0.2208
0.2159
TBS
O
S
2MeC6H4
OMe
(S)-8ab
1.00
1.06
2.08
1.00
1.03
1.03
3.06
3.08
9.12
2.97
3.03
f1 (ppm)

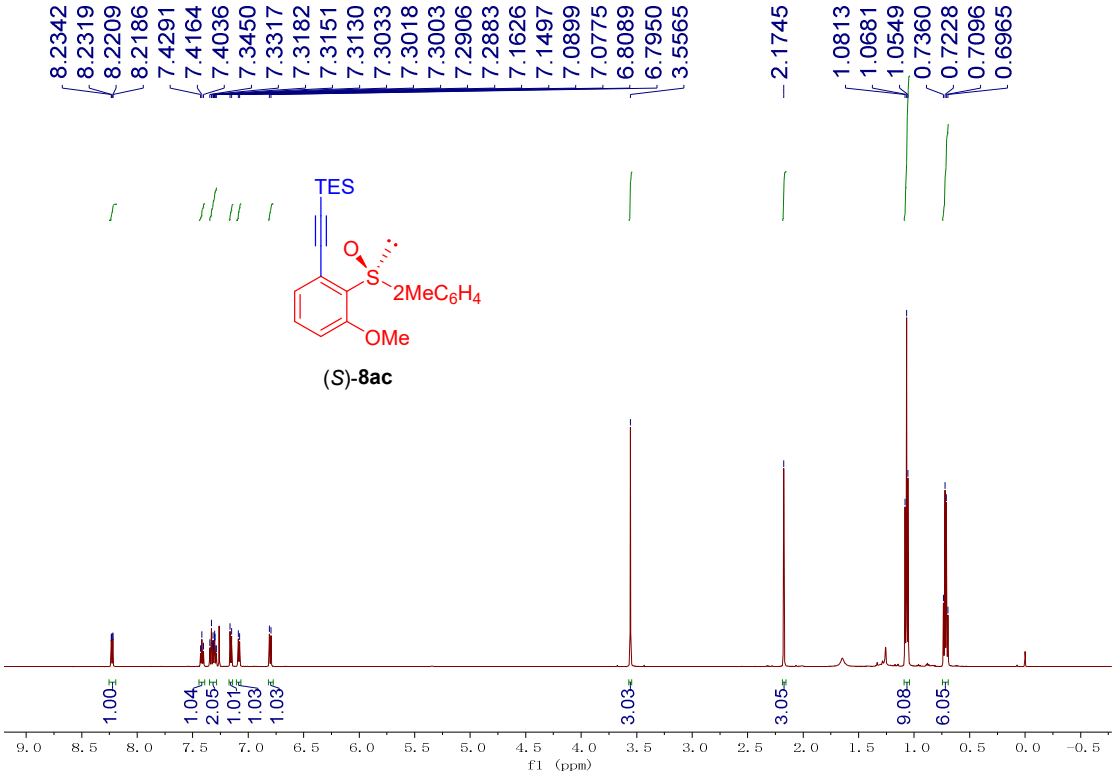

159.2555
141.7734
134.7474
133.1263
131.2734
130.3252
129.6946
126.6529
126.6295
125.9749
125.4272
113.5539
101.6459
101.1172
55.7530
26.3326
18.9075
16.9596
-4.5719
TBS
O
S
2MeC6H4
OMe
(S)-8ab
f1 (ppm)


7.9939
7.9911
7.9810
7.9782
7.4065
7.4037
7.3935
7.3900
7.3866
7.3806
7.3769
7.3739
7.2284
7.2157
7.2029
7.1668
7.1542
7.1416
7.0475
7.0349
6.8158
6.8022
3.6393
2.3807
1.0576
1.0444
1.0312
0.7055
0.6924
0.6792
0.6660
TES
O
S
2OMeC6H4
Me
1.00
2.02
1.04
1.01
1.02
1.03
3.08
3.05
9.03
6.05
f1 (ppm)

(*R*)-**7ac**


155.7186
141.6530
140.1918
132.7472
131.9665
131.6535
130.7184
130.5516
127.5352
125.4589
120.4766
111.1049
102.9681
99.1191
55.3927
18.1054
7.6311
4.5871
TES
O
S
2OMeC6H4
Me
f1 (ppm)

(*R*)-**7ac**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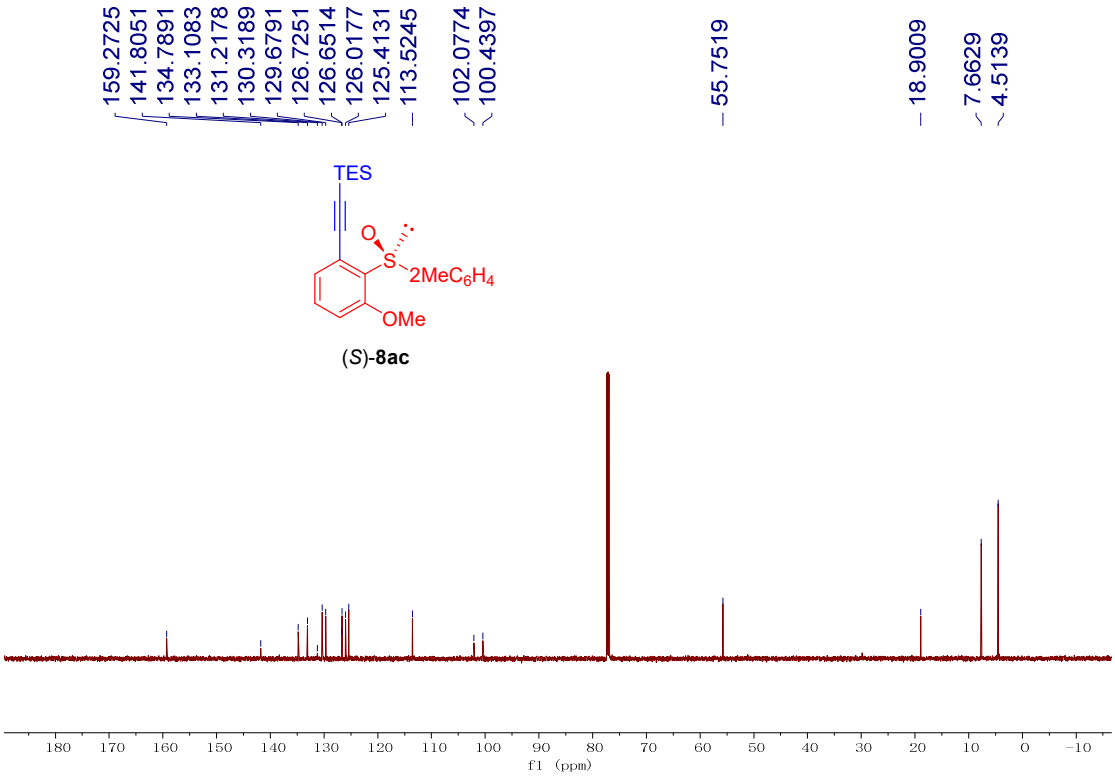
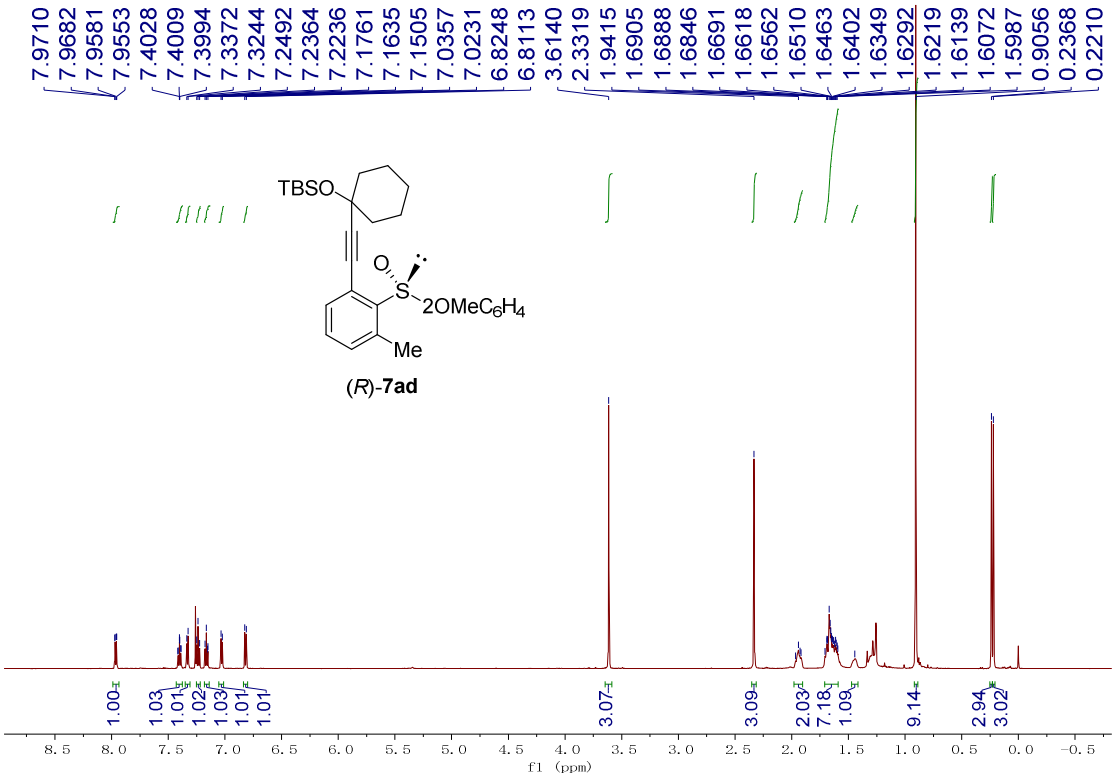
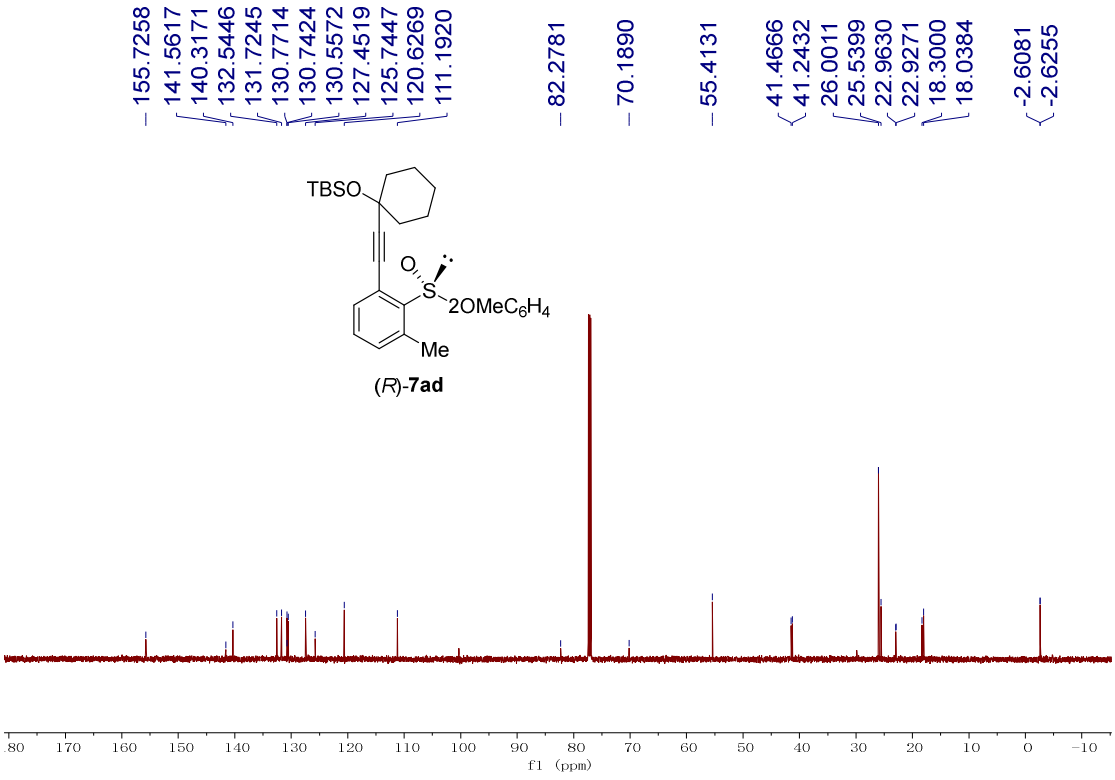
8.2319
8.2209
8.2186
7.4291
7.4164
7.4036
7.3450
7.3317
7.3182
7.3151
7.3130
7.3033
7.3018
7.3003
7.2906
7.2883
7.1626
7.1497
7.0899
7.0775
6.8089
6.7950
3.5565
2.1745
1.0813
1.0681
1.0549
0.7360
0.7228
0.7096
0.6965
TES
O
S
2MeC6H4
OMe
1.00
1.04
2.05
1.01
1.03
1.03
3.03
3.05
9.08
6.05
f1 (ppm)

(*S*)-**8ac**


159.2725
141.8051
134.7891
133.1083
131.2178
130.3189
129.6791
126.7251
126.6514
126.0177
125.4131
113.5245
102.0774
100.4397
55.7519
18.9009
7.6629
4.5139
TES
O
S
2MeC6H4
OMe
f1 (ppm)

(*S*)-**8ac**


7.9710
7.9682
7.9581
7.9553
7.4028
7.4009
7.3994
7.3372
7.3244
7.2492
7.2364
7.2236
7.1761
7.1635
7.1505
7.0357
7.0231
6.8248
6.8113
3.6140
2.3319
1.9415
1.6905
1.6888
1.6846
1.6691
1.6618
1.6562
1.6510
1.6463
1.6402
1.6349
1.6292
1.6219
1.6139
1.6072
1.5987
0.9056
0.2368
0.2210
TBSO
O
S
2OMeC6H4
Me
(R)-7ad
1.00
1.03
1.01
1.02
1.03
1.01
1.01
3.07
3.09
2.03
7.18
1.09
9.14
2.94
3.02
f1 (ppm)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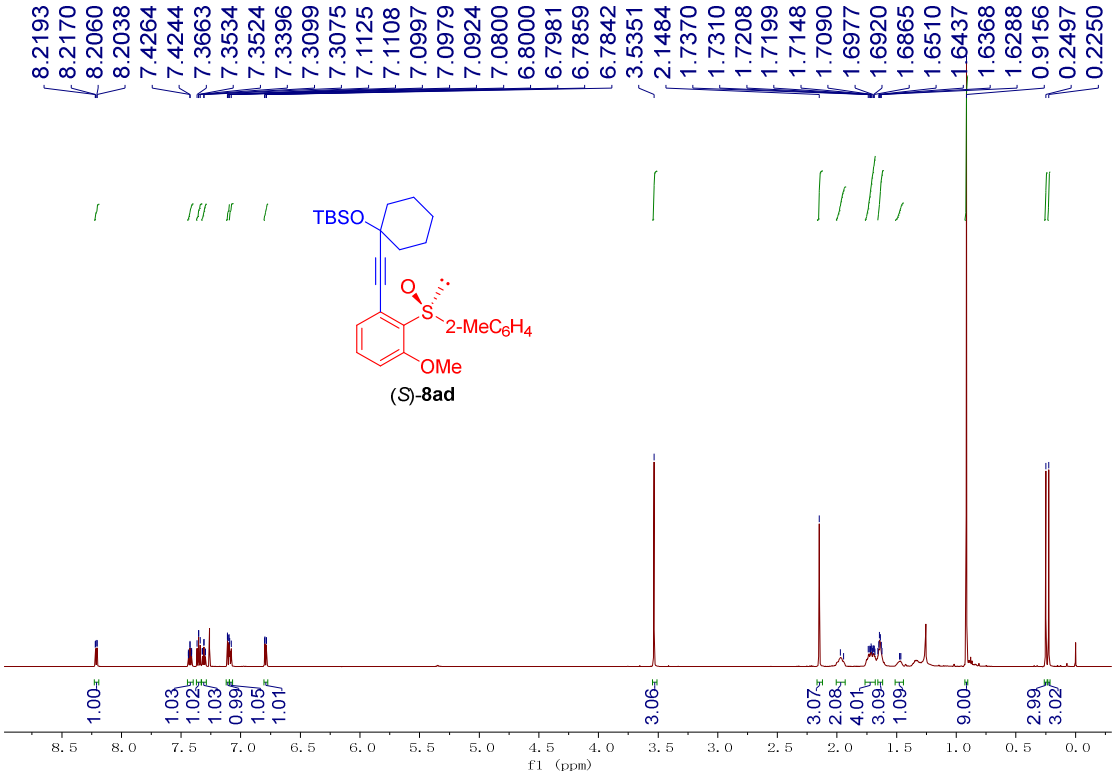
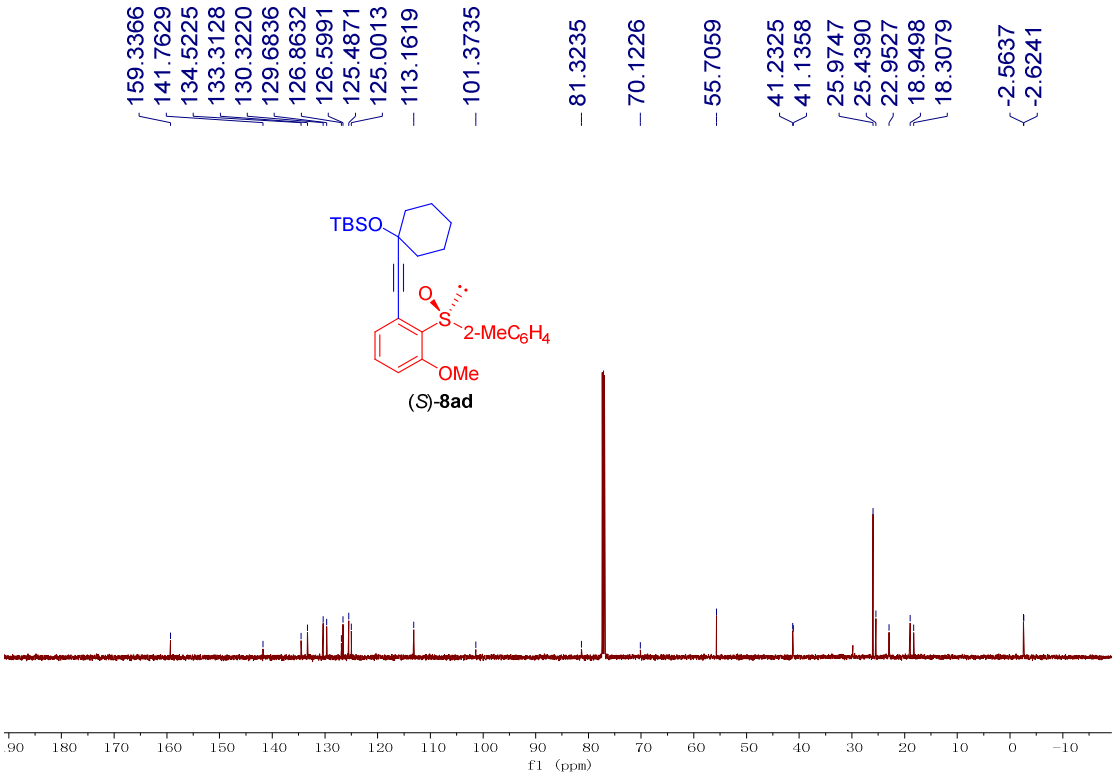
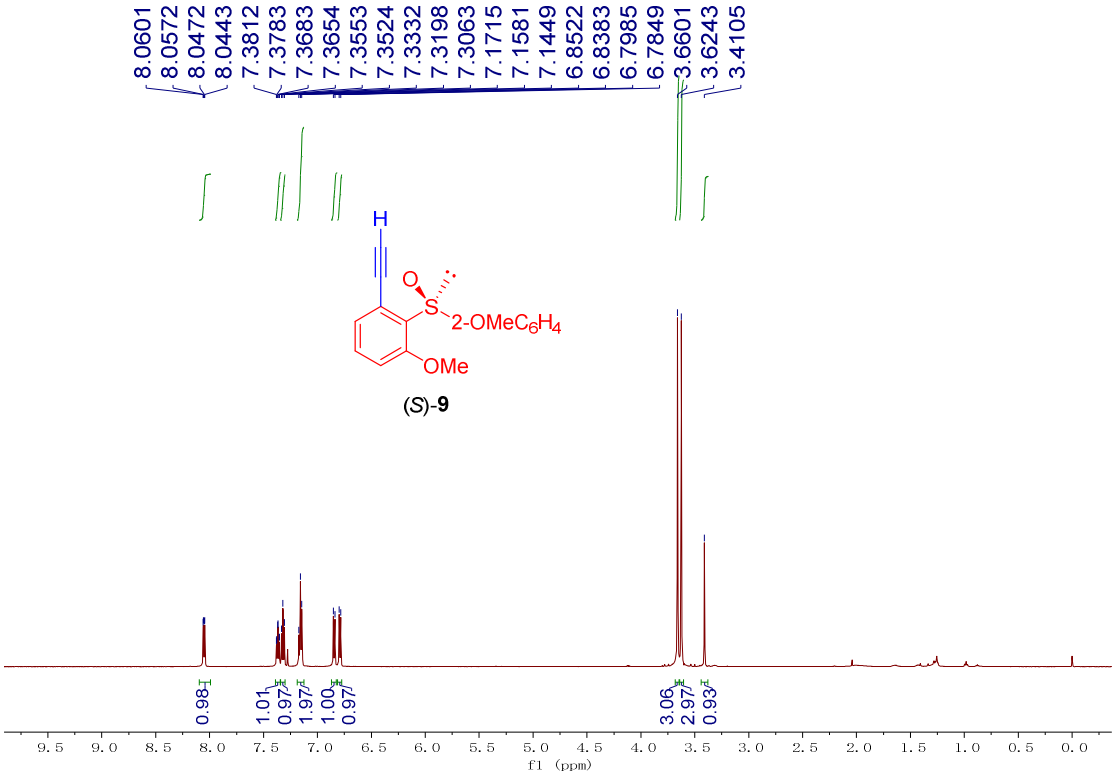
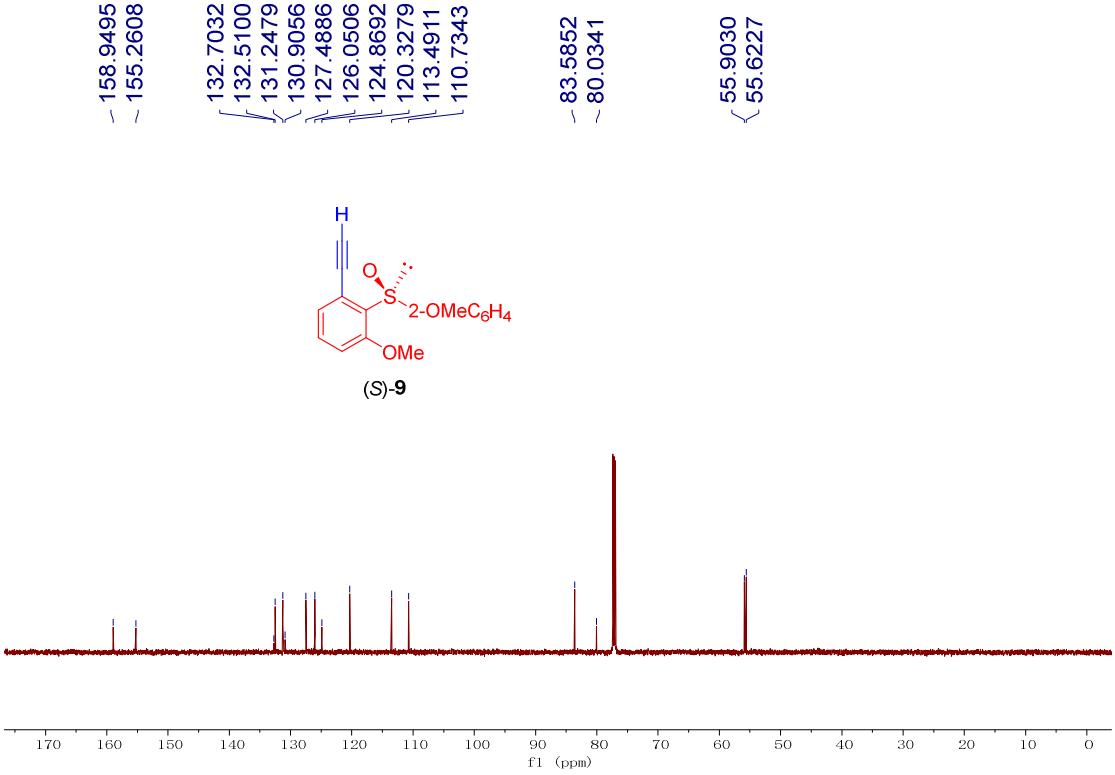
141.5617
140.3171
132.5446
131.7245
130.7714
130.7424
130.5572
127.4519
125.7447
120.6269
111.1920
82.2781
70.1890
55.4131
41.4666
41.2432
26.0011
25.5399
22.9630
22.9271
18.3000
18.0384
-2.6081
-2.6255
TBSO
O
S
2OMeC6H4
Me
(R)-7ad
f1 (ppm)


8.2193
8.2170
8.2060
8.2038
7.4264
7.4244
7.3663
7.3534
7.3524
7.3396
7.3099
7.3075
7.1125
7.1108
7.0997
7.0979
7.0924
7.0800
6.8000
6.7981
6.7859
6.7842
3.5351
2.1484
1.7370
1.7310
1.7208
1.7199
1.7148
1.7090
1.6977
1.6920
1.6865
1.6510
1.6437
1.6368
1.6288
0.9156
0.2497
0.2250
TBSO
O
S
2-MeC6H4
OMe
(S)-8ad
1.00
1.03
1.02
1.03
0.99
1.05
1.01
3.06
3.07
2.08
4.01
3.09
1.09
9.00
2.99
3.02
f1 (ppm)

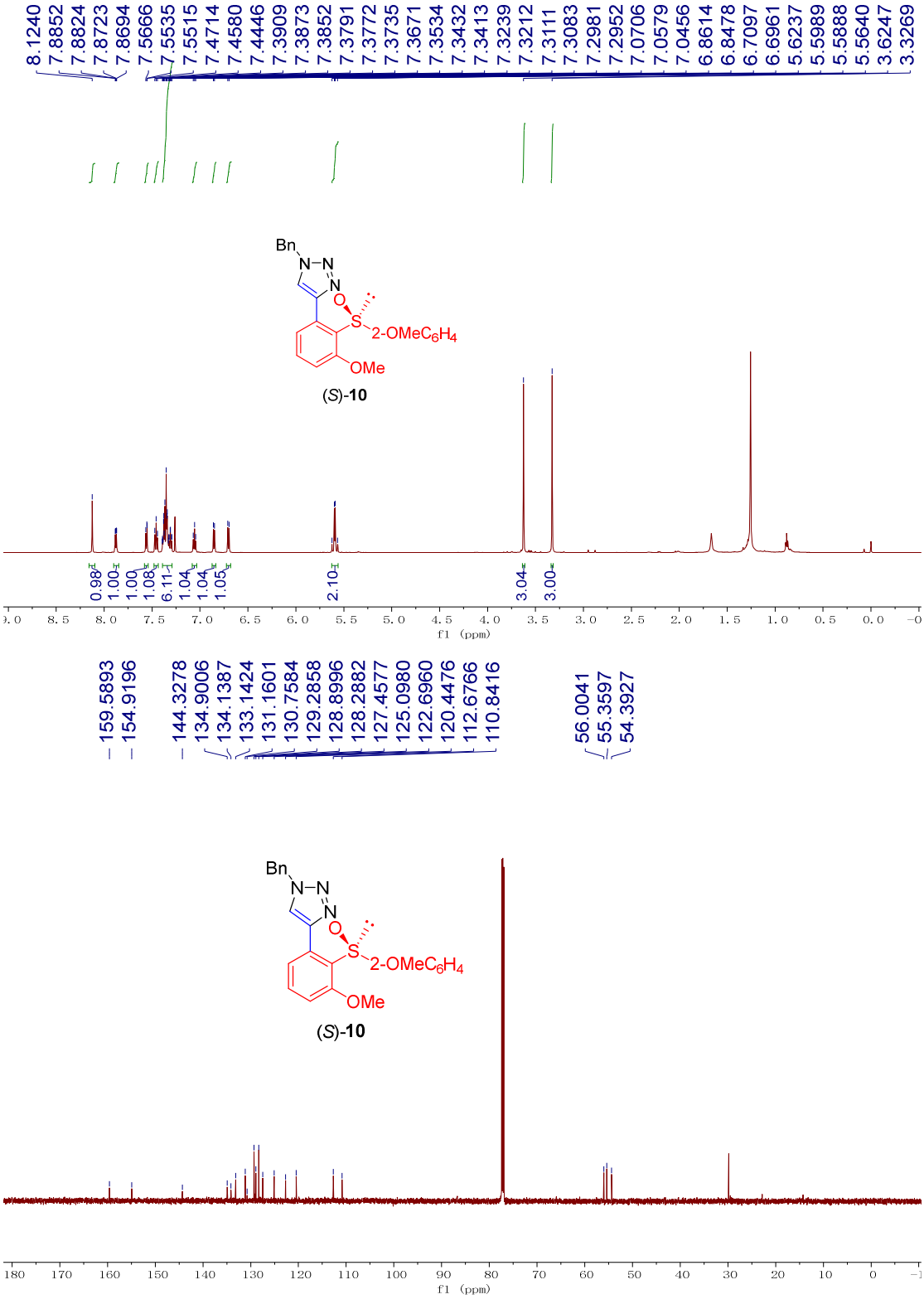

159.3366
141.7629
134.5225
133.3128
130.3220
129.6836
126.8632
126.5991
125.4871
125.0013
113.1619
101.3735
81.3235
70.1226
55.7059
41.2325
41.1358
25.9747
25.4390
22.9527
18.9498
18.3079
-2.5637
-2.6241
TBSO
O
S
2-MeC6H4
OMe
(S)-8ad
f1 (ppm)

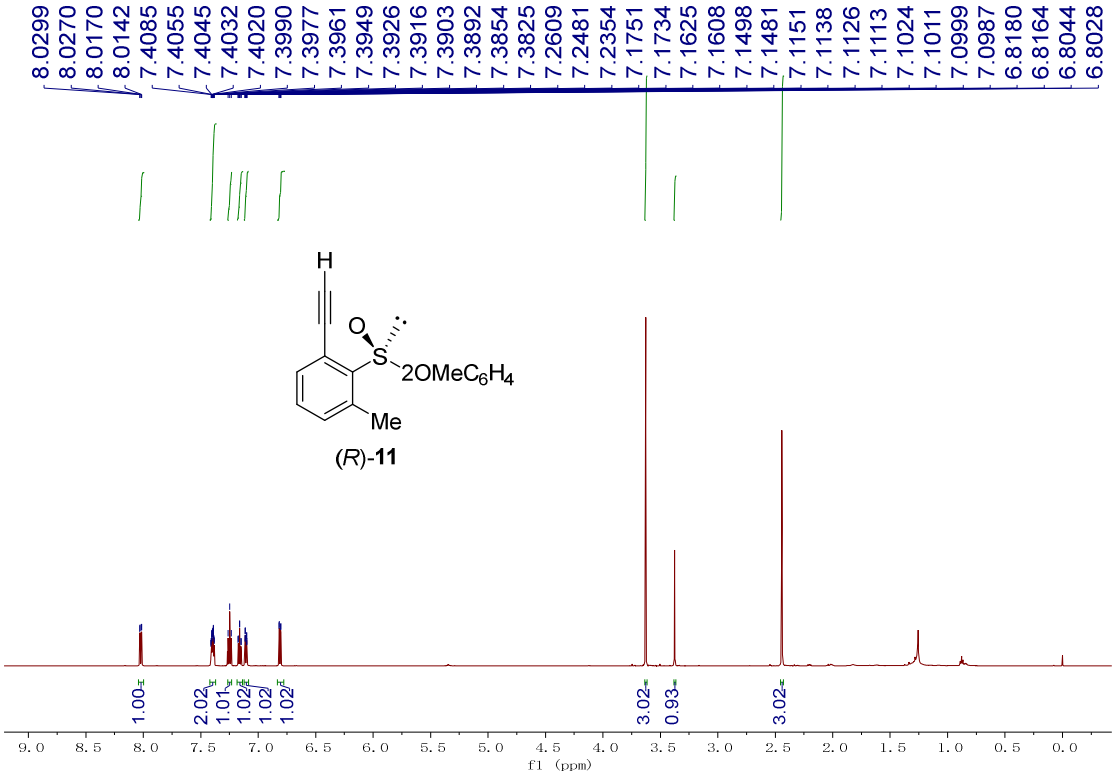

8.0601
8.0572
8.0472
8.0443
7.3812
7.3783
7.3683
7.3654
7.3553
7.3524
7.3332
7.3198
7.3063
7.1715
7.1581
7.1449
6.8522
6.8383
6.7985
6.7849
3.6601
3.6243
3.4105
H
O
S
2-OMeC6H4
OMe
0.98
1.01
0.97
1.97
1.00
0.97
3.06
2.97
0.93
f1 (ppm)

(*S*)-**9**


158.9495
155.2608
132.7032
132.5100
131.2479
130.9056
127.4886
126.0506
124.8692
120.3279
113.4911
110.7343
83.5852
80.0341
55.9030
55.6227
H
O
S
2-OMeC6H4
OMe
f1 (ppm)

(*S*)-**9**


8.1240
7.8852
7.8824
7.8723
7.8694
7.5666
7.5535
7.5515
7.4714
7.4580
7.4446
7.3909
7.3873
7.3852
7.3791
7.3772
7.3735
7.3671
7.3534
7.3432
7.3413
7.3239
7.3212
7.3111
7.3083
7.2981
7.2952
7.0706
7.0579
7.0456
6.8614
6.8478
6.7097
6.6961
5.6237
5.5989
5.5888
5.5640
3.6247
3.3269
Bn
2-OMeC6H4
OMe
(S)-10
0.98
1.00
1.00
1.08
6.11
1.04
1.04
1.05
2.10
3.04
3.00
f1 (ppm)
159.5893
154.9196
144.3278
134.9006
134.1387
133.1424
131.1601
130.7584
129.2858
128.8996
128.2882
127.4577
125.0980
122.6960
120.4476
112.6766
110.8416
56.0041
55.3597
54.3927
Bn
2-OMeC6H4
OMe
(S)-10
f1 (ppm)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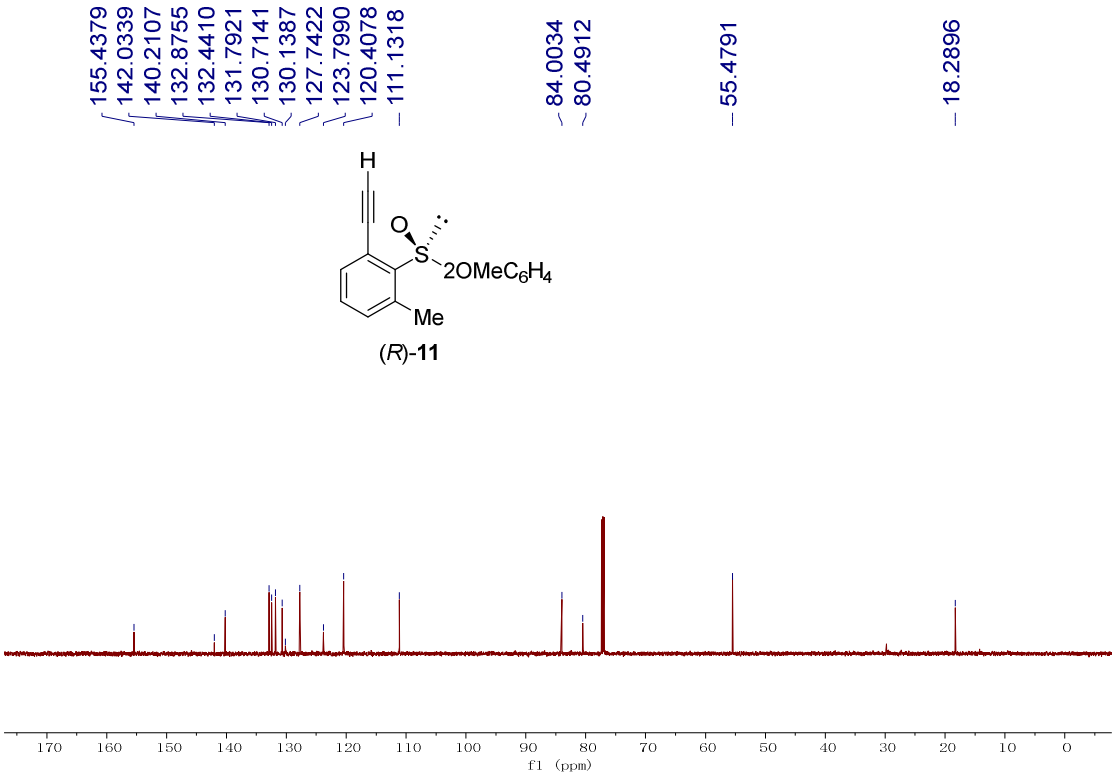
8.0270
8.0170
8.0142
7.4085
7.4055
7.4045
7.4032
7.4020
7.3990
7.3977
7.3961
7.3949
7.3926
7.3916
7.3903
7.3892
7.3854
7.3825
7.2609
7.2481
7.2354
7.1751
7.1734
7.1625
7.1608
7.1498
7.1481
7.1151
7.1138
7.1126
7.1113
7.1024
7.1011
7.0999
7.0987
6.8180
6.8164
6.8044
6.8028
H
O
S
2OMeC6H4
Me
1.00
2.02
1.01
1.02
1.02
1.02
3.02
0.93
3.02
f1 (ppm)

(*R*)-**11**


155.4379
142.0339
140.2107
132.8755
132.4410
131.7921
130.7141
130.1387
127.7422
123.7990
120.4078
111.1318
84.0034
80.4912
55.4791
18.2896
H
O
S
2OMeC6H4
Me
f1 (ppm)

(*R*)-**11**