

# Supporting Information

## Mechanistic Insights into the Gold(I)-Catalyzed [3,3]-Sigmatropic Rearrangement of Sulfoniums for the Formation of Chiral 1,4- Dicarbonyls or Formal $\alpha$ -Arylation of Carbonyl Compounds

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## **I. General information:**

Reactions were performed using oven dried glassware under an atmosphere of argon. All purifications were carried out under flash-chromatographic conditions on silica gel (Redi Sep prepacked column, 230–400 mesh) at medium pressure (20 psi) with use of a CombiFlash Companion or preparative HPLC. Reactions were monitored by thin-layer chromatography on Merck silica gel plates (60 F254 aluminum sheets) which were rendered visible by ultraviolet and spraying with KMnO<sub>4</sub> solution, followed by heating. Reagent-grade chemicals were obtained from diverse commercial suppliers and used as received. <sup>1</sup>H NMR (500 or 300 MHz) and <sup>13</sup>C NMR (125 or 75 MHz) spectra were recorded on Bruker Avance spectrometers at 298 K unless otherwise stated. Chemical shifts are given in ppm ( $\delta$ ) and are referenced to the internal solvent signal. Multiplicities are declared as follow: s (singlet), bs (broad singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets), m (multiplet). Coupling constants *J* are given in Hz. Carbon multiplicities were determined by DEPT-135 experiment. Infrared spectra (IR) were recorded on a Perkin-Elmer FT-IR system using diamond window Dura SamplIR II and the data are reported in reciprocal centimeters (cm<sup>-1</sup>). Melting points were recorded in open capillary tubes on a Büchi B-540 apparatus and are uncorrected. High-resolution mass spectrometry (HRMS) was performed using electrospray ionization (ESI) and time-of-flight (TOF) analyzer, in positive-ion or negative-ion detection mode. Vinyl sulfoxide substrates<sup>1</sup> [(*R,Z*)-**1a**, (*R,E*)-**1a**, (*R,E*)-**1b**, (*R,E*)-**1d**] and propargyl derivatives **2a**; **2c-d**<sup>2</sup> were prepared according to the literature or commercially available, as for **2b** [13361-64-3].

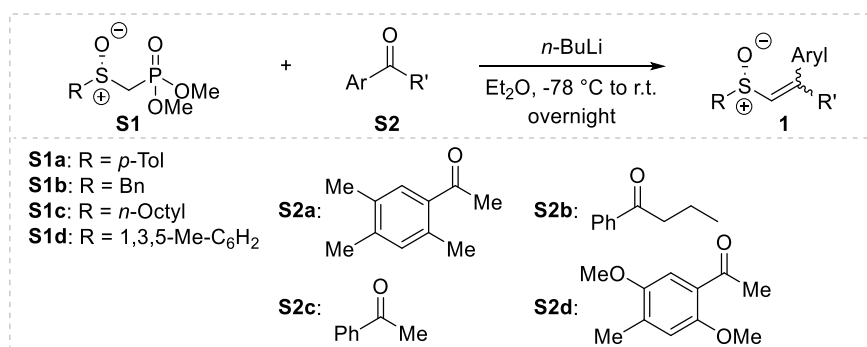
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<sup>1</sup> W. Zhou and A. Voituriez, *J. Am. Chem. Soc.*, 2021, **143**, 17348.

<sup>2</sup> (a) S. Iyer and L. S. Liebeskind, *J. Am. Chem. Soc.*, 1987, **109**, 2759; (b) L. F. Tietze, T. Neumann, M. Kajino and M. Pretor, *Synthesis*, 1995, **1995**, 1003.

## II. Experimental Procedures:

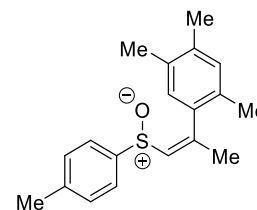
### A. General procedure for the synthesis of vinyl sulfoxide substrates.



A flask was charged with diethyl ((*p*-tolylsulfinyl)methyl)phosphonate **S1a-c** (1.3 equiv) and 10 mL of anhydrous diethyl ether (10 mL/mmol of **S2a-d**) under argon. This mixture was stirred vigorously and cooled to -78 °C. At this temperature, the solution of *n*BuLi (1.6 M in pentane, 1.3 equiv) was slowly added dropwise over 30 min and then this cold mixture was stirred for another 30 min. To this mixture was added the solution of ketone **S2a-d** (1.0 equiv) in 10 mL of diethyl ether dropwise over 30 min. This solution was then slowly warmed to room temperature overnight. Finally, this resulting mixture was quenched with saturated NH<sub>4</sub>Cl aqueous solution. The aqueous layer was extracted with ethyl acetate. The combined organic phase was dried over anhydrous MgSO<sub>4</sub> and then concentrated *in vacuo*. After flash chromatography, the corresponding (*R,Z*)- and/or (*R,E*)-vinylsulfoxides were separated and isolated in pure form.

#### II.1. (*Z*)-1,2,4-Trimethyl-5-(1-(*p*-tolylsulfinyl)prop-1-en-2-yl)benzene (**Z-1c**).

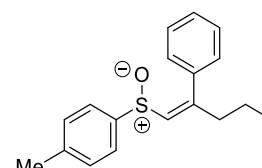
Compound **Z-1c** was obtained with the use of **S1a** and **S2a** (1.0 mmol) as substrates. Colorless oil; *R<sub>f</sub>* 0.34 (EtOAc/Petroleum ether = 1/2); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz) δ 7.43 (d, *J* = 7.9 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 7.03 (s, 1H), 6.33 (s, 1H), 2.40 (s, 3H), 2.26 (s, 6H), 2.21-2.30 (m, 3H), 2.09 (s, 3H); <sup>13</sup>C NMR



(CDCl<sub>3</sub>, 125 MHz) δ 142.0 (C), 141.2 (C), 136.8 (C), 136.3 (C), 134.9 (CH), 131.9 (CH), 131.4 (C), 130.0 (CH<sub>x</sub>3), 129.0 (C<sub>x</sub>2), 124.4 (CH<sub>x</sub>2), 25.8 (CH<sub>3</sub>), 21.5 (CH<sub>3</sub>), 19.6 (CH<sub>3</sub>), 19.4 (CH<sub>3</sub>), 19.1 (CH<sub>3</sub>); HRMS (ESI) calcd. for C<sub>19</sub>H<sub>23</sub>OS [M+H]<sup>+</sup>: 299.1470, found: 299.1466.

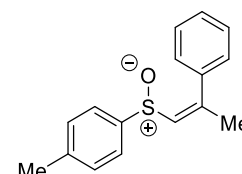
#### II.2. (*Z*)-1-Methyl-4-((2-phenylpent-1-en-1-yl)sulfinyl)benzene (**Z-1d**).

Compound **Z-1c** was obtained with the use of **S1a** and **S2b** (1.0 mmol) as substrates. Colorless oil; *R<sub>f</sub>* 0.18 (EtOAc/Petroleum ether = 1/3); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) δ 7.48-7.39 (m, 5H), 7.35-7.28 (m, 4H), 6.30 (t, *J* = 1.2 Hz, 1H), 2.53-2.43 (m, 2H), 2.40

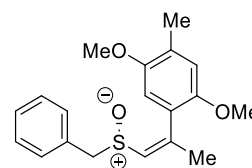


(s, 3H), 1.47-1.35 (m, 2H), 0.88 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  155.0 (C), 142.3 (C), 141.1 (C), 138.1 (C), 133.9 (CH), 130.1 ( $\text{CH}_2$ ), 128.8 (CH), 128.6 ( $\text{CH}_2$ ), 128.4 ( $\text{CH}_2$ ), 124.5 ( $\text{CH}_2$ ), 41.3 ( $\text{CH}_2$ ), 21.5 ( $\text{CH}_3$ ), 20.7 ( $\text{CH}_2$ ), 13.7 ( $\text{CH}_3$ ); IR (neat)  $\nu_{\text{max}} = 2960, 2923, 2853, 1716, 1492, 1457, 1377, 1081, 1022, 1010, 808, 772, 701$   $\text{cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{21}\text{OS}$   $[\text{M}+\text{H}]^+$ : 285.1313, found: 285.1308.

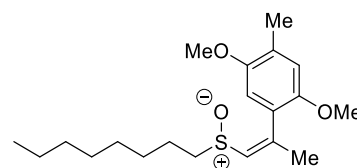
**II.3. (Z)-1-Methyl-4-((2-phenylprop-1-en-1-yl)sulfinyl)benzene (Z-1e).** Compound **Z-1e** was obtained with the use of **S1a** and **S2c** (1.0 mmol) as substrates. Yellow solid (229.6 mg, 30% yield); Mp 122-124 °C;  $R_f$  0.23 (EtOAc/Petroleum ether = 1/2);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.49 (d,  $J = 7.9$  Hz, 2H), 7.46-7.37 (m, 5H), 7.30 (d,  $J = 7.9$  Hz, 2H), 6.33 (s, 1H), 2.40 (s, 3H), 2.22 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  150.9 (C), 142.0 (C), 141.2 (C), 138.6 (C), 134.0 (CH), 130.1 ( $\text{CH}_2$ ), 129.0 (CH), 128.6 ( $\text{CH}_2$ ), 128.1 ( $\text{CH}_2$ ), 124.5 ( $\text{CH}_2$ ), 25.9 ( $\text{CH}_3$ ), 21.5 ( $\text{CH}_3$ ); HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{17}\text{OS}$   $[\text{M}+\text{H}]^+$ : 257.1000, found: 257.0995.



**II.4. (S,Z)-1-(1-(Benzylsulfinyl)prop-1-en-2-yl)-2,5-dimethoxy-4-methylbenzene ((S,Z)-1f).** Compound **1f** was obtained with the use of **S1b** and **S2d** (1.0 mmol) as substrates. White solid (125 mg, 34% yield); *E/Z* geometry of the double bond was assigned by NOESY analysis. Mp 106-108 °C;  $R_f$  0.18 (EtOAc/Petroleum ether = 2/1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.35-7.29 (m, 3H), 7.25 (d,  $J = 7.5$  Hz, 2H), 6.70 (s, 1H), 6.39 (s, 1H), 6.18 (q,  $J = 1.5$  Hz, 1H), 3.96 (d,  $J = 13.0$  Hz, 1H), 3.93 (d,  $J = 13.0$  Hz, 1H), 3.73 (s, 3H), 3.71 (s, 3H), 2.22 (s, 3H), 2.15 (d,  $J = 1.5$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  151.6 (C), 149.3 (C), 149.0 ( $\text{C}_2$ ), 132.1 (CH), 130.5 ( $\text{CH}_2+\text{C}$ ), 128.7 ( $\text{CH}_2$ ), 128.1 (CH), 125.3 (C), 114.4 (CH), 111.4 (CH), 59.8 ( $\text{CH}_2$ ), 56.23 ( $\text{CH}_3$ ), 56.18 ( $\text{CH}_3$ ), 25.3 ( $\text{CH}_3$ ), 16.6 ( $\text{CH}_3$ ); IR (neat)  $\nu_{\text{max}} = 2953, 2849, 1501, 1465, 1455, 1395, 1375, 1211, 1035, 866, 813, 763, 700$   $\text{cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{23}\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 331.1368, found: 331.1368;  $[\alpha]_D^{20} = -200.0$  ( $c$  0.12,  $\text{CHCl}_3$ ); 82% ee [HPLC analysis, Daicel Chiralpak IA column, heptane/*i*-PrOH = 90:10, 1.0 mL/min, 217.2 nm,  $t_R = 11.6$  min and 14.0 min].



**II.5. (Z)-1,4-Dimethoxy-2-methyl-5-(1-(octylsulfinyl)prop-1-en-2-yl)benzene (Z-1g).** Compound **1g** was obtained with the use of **S1c** and **S2d** (1.0 mmol) as substrates. Colorless oil (157 mg, 44% yield); *E/Z* geometry of the double bond was assigned by NOESY analysis.  $R_f$  0.25 (EtOAc/Petroleum ether = 2/1);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  6.71 (s, 1H), 6.64 (s, 1H), 6.27 (s, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 2.76 (dt,  $J = 13.0, 7.5$  Hz, 1H), 2.63 (dt,  $J$

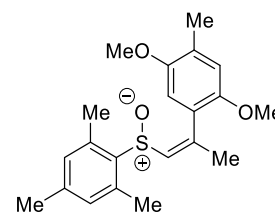


= 13.0, 8.0 Hz, 1H), 2.23 (s, 3H), 2.18 (s, 3H), 1.69-1.63 (m, 2H), 1.38-1.21 (m, 10H), 0.87 (t,  $J = 7.0$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  151.7 (C), 149.5 (C), 148.8 (C), 132.7 (CH), 128.1 (C), 125.5 (C), 114.3 (CH), 111.5 (CH), 56.2 ( $\text{CH}_3$ ), 56.0 ( $\text{CH}_3$ ), 54.0 ( $\text{CH}_2$ ), 31.9 ( $\text{CH}_2$ ), 29.3 ( $\text{CH}_2$ ), 29.2 ( $\text{CH}_2$ ), 29.1 ( $\text{CH}_2$ ), 25.3 ( $\text{CH}_3$ ), 22.8 ( $\text{CH}_2$ ), 22.6 ( $\text{CH}_2$ ), 16.6 ( $\text{CH}_3$ ), 14.2 ( $\text{CH}_3$ ); IR (neat)  $\nu_{\text{max}} = 2926, 2854, 1504, 1465, 1397, 1375, 1213, 1040, 863, 811, 726$   $\text{cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{20}\text{H}_{33}\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 353.2150, found: 353.2151.

**II.6. (Z)-2-((2-(2,5-Dimethoxy-4-methylphenyl)prop-1-en-1-yl)sulfinyl)-1,3,5-trimethylbenzene (Z-1h).** Compound **1h** was obtained with

the use of **S1d** and **S2d** (1.0 mmol) as substrates. Colorless oil (41.4 mg, 21% yield).  $R_f$  0.37 (EtOAc/Petroleum ether = 2/3);

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  6.80 (bs, 3H), 6.69 (s, 1H), 6.65 (bs, 1H), 3.76 (s, 3H), 3.67 (s, 3H), 2.34 (s, 6H), 2.25 (s, 3H),



2.24 (s, 3H), 2.13 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  151.5 (C), 149.5 (C), 140.8 (C), 138.6 ( $\text{C}_x2$ ), 136.8 (C), 131.5 (CH), 130.9 (C), 130.6 ( $\text{CH}_x2$ ), 127.7 (C), 125.4 (C), 114.1 (CH), 111.9 (CH), 56.1 ( $\text{CH}_3$ ), 55.9 ( $\text{CH}_3$ ), 25.1 ( $\text{CH}_3$ ), 21.2 ( $\text{CH}_3$ ), 19.2 ( $\text{CH}_3x2$ ), 16.6 ( $\text{CH}_3$ ); HRMS (ESI) calcd. for  $\text{C}_{21}\text{H}_{27}\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 359.1681, found: 359.1668.

**B. Investigation of the catalytic reaction.**

In a 15 mL-reaction tube,  $\text{Au}(\text{Johnphos})\text{SbF}_6 \cdot \text{MeCN}$  (0.010 mmol, 10 mol%) and water (0.30 mmol, 5.4  $\mu\text{L}$ , 3.0 equiv) were added in 1,2-dichloroethane (0.5 mL). Then a solution of sulfoxides **1a-h** (0.10 mmol, 1.0 equiv) and propargyl-silane **2a-d** (0.15 mmol, 1.5 equiv) in 1,2-dichloroethane (1.5 mL) were added dropwise over 5 min, at room temperature. The reaction mixture was kept at 40  $^\circ\text{C}$  and when the reaction was completed, the solvent was evaporated and NMR yields were determined by using dibromomethane as internal standard. The major and minor products **3-5** were obtained by flash chromatography (2-10% EtOAc/Petroleum ether as eluent) or preparative TLC (10 % EtOAc/ Petroleum ether).

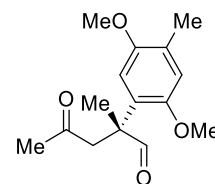
**II.7. (R)-2-(2-(2,5-Dimethoxy-4-methylphenyl)-2-methyl-4-oxopentanal ((R)-3a).**

Colorless oil (14.8 mg, 56% yield).  $R_f$  0.23 (EtOAc/Petroleum ether

= 1/5);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  9.52 (s, 1H), 6.74 (s, 1H), 6.71 (s, 1H), 3.81 (s, 3H), 3.74 (s, 3H), 3.15 (d,  $J = 16.0$  Hz, 1H),

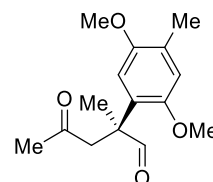
3.04 (d,  $J = 16.0$  Hz, 1H), 2.21 (s, 3H), 1.96 (s, 3H), 1.50 (s, 3H);

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  207.5 (C), 202.8 (CH), 151.2 (C), 150.2 (C), 127.4 (C), 127.3 (C), 114.5 (CH), 111.2 (CH), 56.4 ( $\text{CH}_3$ ), 56.0 ( $\text{CH}_3$ ), 50.3 (C), 48.3 ( $\text{CH}_2$ ), 31.5 ( $\text{CH}_3$ ), 20.0 ( $\text{CH}_3$ ), 16.3 ( $\text{CH}_3$ ); IR (neat)  $\nu_{\text{max}} = 2935, 2850, 1714, 1504, 1465, 1397,$

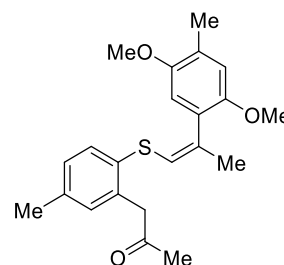


1375, 1359, 1211, 1181, 1041, 862  $\text{cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{15}\text{H}_{21}\text{O}_4$   $[\text{M}+\text{H}]^+$ : 265.1440, found: 265.1439;  $[\alpha]_D^{20} = -111.7$  ( $c$  0.6,  $\text{CHCl}_3$ ); 96% ee [HPLC analysis, Daicel Chiralpak IA column, heptane/*i*-PrOH = 80:20, 1.0 mL/min, 290.6 nm,  $t_R = 4.8$  min and 6.6 min].

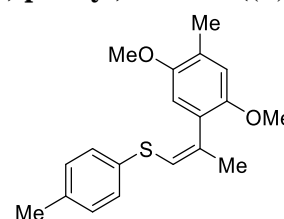
**II.8. (S)-2-(2,5-Dimethoxy-4-methylphenyl)-2-methyl-4-oxopentanal ((S)-3a).** Colorless oil (18.5 mg, 70% yield).  $[\alpha]_D^{20} = 125.5$  ( $c$  0.55,  $\text{CHCl}_3$ ); 99% ee [HPLC analysis, Daicel Chiralpak IA column, heptane/*i*-PrOH = 80:20, 1.0 mL/min, 290.6 nm,  $t_R = 4.8$  min and 6.6 min].



**II.9. (Z)-1-(2-((2-(2,5-Dimethoxy-4-methylphenyl)prop-1-en-1-yl)thio)-5-methylphenyl)propan-2-one (4a').** Colorless oil (16.5 mg, 44% yield).  $R_f$  0.28 (EtOAc/Petroleum ether = 1/50);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.39 (d,  $J = 8.0$  Hz, 1H), 7.05 (d,  $J = 8.0$  Hz, 1H), 6.95 (s, 1H), 6.76 (s, 1H), 6.66 (s, 1H), 6.05-6.01 (m, 1H), 3.80 (bs, 8H), 2.31 (s, 3H), 2.24 (s, 3H), 2.11 (s, 6H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  206.4 (C), 151.7 (C), 150.1 (C), 137.5 (C), 137.2 (C), 135.8 (C), 132.9 (C), 132.4 (CH), 131.7 (CH), 128.9 (CH), 127.4 (C), 127.0 (C), 121.9 (CH), 114.9 (CH), 112.2 (CH), 56.4 ( $\text{CH}_3$ ), 56.2 ( $\text{CH}_3$ ), 49.0 ( $\text{CH}_2$ ), 29.7 ( $\text{CH}_3$ ), 24.6 ( $\text{CH}_3$ ), 21.1 ( $\text{CH}_3$ ), 16.5 ( $\text{CH}_3$ ); IR (neat)  $\nu_{\text{max}} = 2995, 2917, 2849, 1721, 1709, 1501, 1465, 1396, 1211, 1158, 1041, 808, 756$   $\text{cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{22}\text{H}_{27}\text{O}_3\text{S}$   $[\text{M}+\text{H}]^+$ : 371.1681, found: 371.1685.

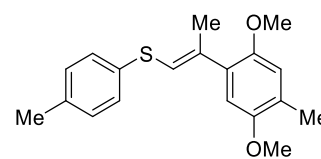


**II.10. (Z)-2-(2-(2,5-Dimethoxy-4-methylphenyl)prop-1-en-1-yl)(*p*-tolyl)sulfane ((Z)-5a).** Colorless oil (5.0 mg, 15% yield).  $R_f$  0.40 (EtOAc/Petroleum ether = 1/50);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.24 (d,  $J = 8.0$  Hz, 2H), 7.08 (d,  $J = 8.0$  Hz, 2H), 6.77 (s, 1H), 6.67 (s, 1H), 6.26-6.23 (m, 1H), 3.80 (s, 6H), 2.31 (s, 3H), 2.24 (s, 3H), 2.16 (d,  $J = 1.0$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  151.7 (C), 150.1 (C), 137.3 (C), 136.1 (C), 133.8 (C), 129.7 ( $\text{CH}_2$ ), 129.3 ( $\text{CH}_2$ ), 127.7 (C), 126.9 (C), 121.3 (CH), 115.2 (CH), 112.1 (CH), 56.7 ( $\text{CH}_3$ ), 56.2 ( $\text{CH}_3$ ), 24.8 ( $\text{CH}_3$ ), 21.1 ( $\text{CH}_3$ ), 16.5 ( $\text{CH}_3$ ); IR (neat)  $\nu_{\text{max}} = 3002, 2920, 2849, 1501, 1493, 1465, 1396, 1210, 1043, 1017, 864, 803, 753, 667$   $\text{cm}^{-1}$ ; HRMS (ESI) calcd for  $\text{C}_{19}\text{H}_{23}\text{O}_2\text{S}$   $[\text{M}+\text{H}]^+$ : 315.1419, found: 315.1422.



**II.11. (*E*)-2-(2,5-Dimethoxy-4-methylphenyl)prop-1-en-1-yl(*p*-tolyl)sulfane ((*E*)-5a).** Colorless oil (6.5 mg, 21% yield).  $R_f$  0.42

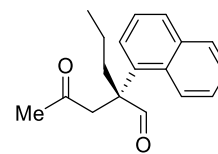
(EtOAc/Petroleum ether = 1/50);  $^1\text{H NMR}$  ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.31 (d,  $J = 8.0$  Hz, 2H), 7.12 (d,  $J = 8.0$  Hz, 2H), 6.71 (s, 1H), 6.67 (s, 1H), 6.35 (s, 1H), 3.79 (s, 3H), 3.78 (s, 3H),



2.33 (s, 3H), 2.22 (s, 3H), 2.18 (s, 3H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  151.7 (C), 150.5 (C), 136.6 (C), 136.3 (C), 133.1 (C), 130.4 (C), 129.9 (CH<sub>2</sub>), 129.3 (CH<sub>2</sub>), 126.5 (C), 123.2 (CH), 114.9 (CH), 112.1 (CH), 56.5 (CH<sub>3</sub>), 56.3 (CH<sub>3</sub>), 21.2 (CH<sub>3</sub>), 19.3 (CH<sub>3</sub>), 16.3 (CH<sub>3</sub>); IR (neat)  $\nu_{\text{max}} = 2920, 2848, 2828, 1493, 1463, 1395, 1373, 1207, 1179, 1043, 1004, 805, 756, 674$   $\text{cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{23}\text{O}_2\text{S}$   $[\text{M}+\text{H}]^+$ : 315.1419, found: 315.1413.

**II.12. (*R*)-2-(Naphthalen-1-yl)-4-oxo-2-propylpentanal ((*R*)-3b).** Colorless oil (10.5 mg, 39% yield).  $R_f$  0.30 (EtOAc/Petroleum ether = 1/5);  $^1\text{H NMR}$

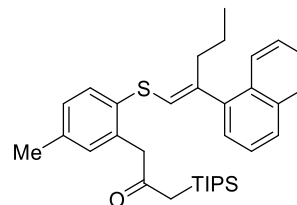
( $\text{CDCl}_3$ , 300 MHz)  $\delta$  9.99 (s, 1H), 7.93-7.88 (m, 1H), 7.83 (d,  $J = 7.8$  Hz, 1H), 7.80-7.75 (m, 1H), 7.52-7.42 (m, 4H), 3.54 (d,  $J = 17.1$  Hz, 1H), 3.36 (d,  $J = 17.1$  Hz, 1H), 2.44 (ddd,  $J = 14.1, 12.6,$



4.8 Hz, 1H), 2.14 (ddd,  $J = 13.8, 12.3, 4.5$  Hz, 1H), 1.94 (s, 3H), 1.26-1.17 (m, 1H), 1.11-1.02 (m, 1H), 0.88 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  206.5 (C), 205.4 (CH), 135.2 (C), 135.0 (C), 131.2 (C), 130.0 (CH), 129.2 (CH), 126.6 (CH), 126.4 (CH), 125.6 (CH), 125.3 (CH), 124.3 (CH), 56.3 (C), 48.8 (CH<sub>2</sub>), 36.2 (CH<sub>2</sub>), 31.0 (CH<sub>3</sub>), 17.5 (CH<sub>2</sub>), 14.6 (CH<sub>3</sub>); IR (neat)  $\nu_{\text{max}} = 2960, 2932, 2872, 1712, 1600, 1511, 1466, 1415, 1398, 1361, 1186, 1170, 803, 778$   $\text{cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{21}\text{O}_2$   $[\text{M}+\text{H}]^+$ : 269.1542, found: 269.1541;  $[\alpha]_D^{20} = -104.0$  ( $c$  0.35,  $\text{CHCl}_3$ ); 96% ee [HPLC analysis, Daicel Chiralpak IC column, heptane/*i*-PrOH = 80:20, 1.0 mL/min, 281.1 nm,  $t_R = 7.6$  min and 11.8 min].

**II.13. (*E*)-1-(5-Methyl-2-((2-(naphthalen-1-yl)pent-1-en-1-yl)thio)phenyl)-3-(triisopropylsilyl)propan-2-one ((*E*)-4b).** Brown oil (16.5 mg, 31% yield).  $R_f$  0.35 (EtOAc/Petroleum ether = 1/50);  $^1\text{H NMR}$

( $\text{CDCl}_3$ , 500 MHz)  $\delta$  8.02-7.99 (m, 1H), 7.86-7.83 (m, 1H), 7.76 (d,  $J = 8.0$  Hz, 1H), 7.51-7.46 (m, 2H), 7.42 (t,  $J = 7.5$  Hz, 1H), 7.36 (d,  $J = 8.0$  Hz, 1H), 7.28 (d,  $J = 7.0$  Hz, 1H),

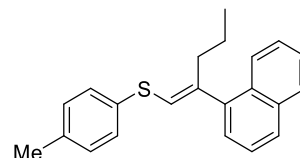


7.01 (d,  $J = 8.0$  Hz, 1H), 6.99 (bs, 1H), 6.13 (s, 1H), 3.99 (s, 2H), 2.75 (t,  $J = 7.5$  Hz, 2H), 2.35 (s, 2H), 2.28 (s, 3H), 1.47-1.38 (m, 2H), 1.27-1.19 (m, 3H), 1.14 (d,  $J = 7.0$  Hz, 18H), 0.93 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  207.3 (C), 142.3 (C), 140.9 (C), 137.3 (C), 135.5 (C), 133.9 (C), 132.5 (C), 131.8 (C), 131.6 (CH), 131.5 (CH), 128.9 (CH), 128.5 (CH), 127.6 (CH), 126.0 (CH), 125.91 (CH), 125.88 (CH), 125.82 (CH), 125.3 (CH), 124.9 (CH), 50.2 (CH<sub>2</sub>), 36.9 (CH<sub>2</sub>), 29.6 (CH<sub>2</sub>), 21.6 (CH<sub>2</sub>),

21.1 (CH<sub>3</sub>), 18.8 (CH<sub>3</sub>x6), 14.2 (CH<sub>3</sub>), 11.7 (CHx3); IR (neat)  $\nu_{\max}$  = 2942, 2891, 2866, 1694, 1463, 1232, 1107, 1044, 883, 794, 776, 758 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>34</sub>H<sub>47</sub>OSSi [M+H]<sup>+</sup>: 531.3117, found: 531.3118.

**II.14. (E)-(2-(Naphthalen-1-yl)pent-1-en-1-yl)(p-tolyl)sulfane ((E)-5b).** Brown oil (4.0 mg, 12% yield).  $R_f$  0.43 (EtOAc/Petroleum ether = 1/50);

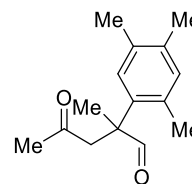
<sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz)  $\delta$  8.03 (d,  $J$  = 8.0 Hz, 1H), 7.87-7.84 (m, 1H), 7.77 (d,  $J$  = 8.0 Hz, 1H), 7.51-7.46 (m, 2H), 7.43 (t,  $J$  = 7.0 Hz, 1H), 7.31-7.19 (m, 3H), 7.10 (d,  $J$  = 8.0 Hz, 2H),



6.28 (s, 1H), 2.75 (t,  $J$  = 7.5 Hz, 2H), 2.31 (s, 3H), 1.42 (sx,  $J$  = 7.5 Hz, 2H), 0.93 (t,  $J$  = 7.5 Hz, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$  142.6 (C), 140.9 (C), 136.5 (C), 133.9 (C), 132.9 (C), 131.8 (C), 129.9 (CHx2), 129.4 (CHx2), 128.5 (CH), 127.6 (CH), 126.03 (CH), 125.97 (CH), 125.9 (CH), 125.8 (CH), 125.4 (CH), 124.2 (CH), 37.0 (CH<sub>2</sub>), 21.6 (CH<sub>2</sub>), 21.1 (CH<sub>3</sub>), 14.2 (CH<sub>3</sub>); IR (neat)  $\nu_{\max}$  = 3039, 2958, 2928, 2869, 1738, 1491, 1455, 1393, 1216, 1091, 1017, 793, 775, 756 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>22</sub>H<sub>23</sub>S [M+H]<sup>+</sup>: 319.1520, found: 319.1512.

**II.15. 2-Methyl-4-oxo-2-(2,4,5-trimethylphenyl)pentanal (3c).** Colorless oil (4.3 mg, 18% yield).  $R_f$  0.41 (EtOAc/Petroleum ether = 1/10); <sup>1</sup>H NMR

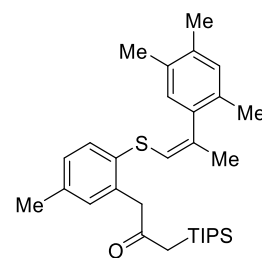
(CDCl<sub>3</sub>, 500 MHz)  $\delta$  9.65 (s, 1H), 6.99 (s, 1H), 6.95 (s, 1H), 3.13 (d,  $J$  = 16.2 Hz, 1H), 3.07 (d,  $J$  = 16.2 Hz, 1H), 2.24 (s, 3H), 2.21 (s, 3H), 2.20 (s, 3H), 1.97 (s, 3H), 1.56 (s, 3H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125



MHz)  $\delta$  206.9 (C), 203.2 (CH), 136.3 (C), 135.1 (C), 134.6 (C), 134.1 (CH), 133.1 (C), 128.9 (CH), 52.6 (C), 49.3 (CH<sub>2</sub>), 31.4 (CH<sub>3</sub>), 21.3 (CH<sub>3</sub>), 20.9 (CH<sub>3</sub>), 19.7 (CH<sub>3</sub>), 19.2 (CH<sub>3</sub>); HRMS (ESI) calcd. for C<sub>15</sub>H<sub>21</sub>O<sub>2</sub> [M+H]<sup>+</sup>: 233.1542, found: 233.1539.

**II.16. (Z)-1-(5-Methyl-2-((2-(2,4,5-trimethylphenyl)prop-1-en-1-yl)thio)phenyl)-3-(triisopropylsilyl)propan-2-one ((Z)-4c).** Colorless oil (20.7

mg, 42% yield).  $R_f$  0.63 (EtOAc/Petroleum ether = 1/40); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz)  $\delta$  7.34 (d,  $J$  = 7.9 Hz, 1H), 7.04 (d,  $J$  = 7.9 Hz, 1H), 6.99 (s, 1H), 6.95 (s, 1H), 6.84 (s, 1H), 6.05 (s, 1H), 3.83 (s, 2H), 2.29 (s, 3H), 2.24 (s, 3H), 2.23 (s, 6H), 2.21 (s, 2H), 2.03 (s, 3H), 1.17-1.08 (m, 3H), 1.05 (d,  $J$  = 6.7 Hz,

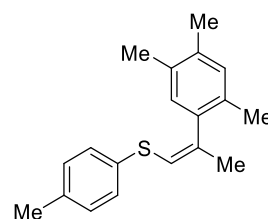


18H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$  207.6 (C), 138.6 (C), 138.3 (C), 137.1 (C), 135.6 (C), 135.5 (C), 134.0 (C), 132.9 (C), 132.1 (C), 131.70 (CH), 131.66 (CH), 131.5 (CH), 129.0 (CH), 128.7 (CH), 121.8 (CH), 49.8 (CH<sub>2</sub>), 29.6 (CH<sub>2</sub>), 25.6 (CH<sub>3</sub>), 21.1 (CH<sub>3</sub>), 19.6 (CH<sub>3</sub>), 19.5 (CH<sub>3</sub>), 18.74 (CH<sub>3</sub>), 18.68 (CH<sub>3</sub>x6), 11.6 (CHx3); HRMS (ESI) calcd. for C<sub>31</sub>H<sub>47</sub>OSSi [M+H]<sup>+</sup>: 495.3117, found: 495.3111.



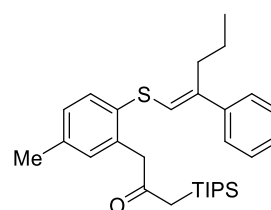
**II.17. (Z)-p-Tolyl(2-(2,4,5-trimethylphenyl)prop-1-en-1-yl)sulfane ((Z)-5c).**

Colorless oil (2.7 mg, 10% yield).  $R_f$  0.37 (100% Petroleum ether);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.22 (d,  $J = 7.9$  Hz, 2H), 7.09 (d,  $J = 7.9$  Hz, 2H), 7.01 (s, 1H), 6.86 (s, 1H), 6.22 (s, 1H), 2.31 (s, 3H), 2.23 (s, 6H), 2.20-2.23 (m, 3H), 2.07 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  139.2 (C), 138.4 (C), 136.1 (C), 135.7 (C), 134.1 (C), 133.6 (C), 132.0 (C), 131.7 (CH), 129.8 ( $\text{CH}_2$ ), 129.2 ( $\text{CH}_2$ ), 129.0 (CH), 121.0 (CH), 25.6 ( $\text{CH}_3$ ), 21.1 ( $\text{CH}_3$ ), 19.6 ( $\text{CH}_3$ ), 19.4 ( $\text{CH}_3$ ), 18.7 ( $\text{CH}_3$ ); HRMS (ESI) calcd. for  $\text{C}_{19}\text{H}_{23}\text{S}$   $[\text{M}+\text{H}]^+$ : 283.1520, found: 283.1514.



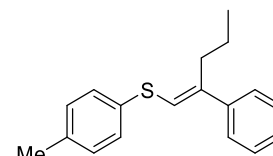
**II.18. (E)-1-(5-Methyl-2-((2-phenylpent-1-en-1-yl)thio)phenyl)-3-(triisopropylsilyl)propan-2-one ((E)-4d).**

Colorless oil (6.0 mg, 13% yield).  $R_f$  0.21 (EtOAc/Petroleum ether = 1/50);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.36 (d,  $J = 8.0$  Hz, 1H), 7.34 (d,  $J = 8.0$  Hz, 2H), 7.30 (t,  $J = 7.5$  Hz, 2H), 7.22 (t,  $J = 7.0$  Hz, 1H), 7.04 (d,  $J = 8.0$  Hz, 1H), 7.01 (bs, 1H), 6.30 (s, 1H), 3.97 (s, 2H), 2.70 (t,  $J = 7.5$  Hz, 2H), 2.31 (s, 3H), 2.30 (s, 2H), 1.55-1.47 (m, 2H), 1.22-1.15 (m, 3H), 1.10 (d,  $J = 7.0$  Hz, 18H), 0.95 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  207.3 (C), 141.2 (C), 137.6 (C), 136.0 (C), 132.5 (C), 132.2 (CH), 131.7 (CH), 128.9 (CH), 128.5 ( $\text{CH}_2+\text{C}$ ), 127.1 (CH), 126.0 ( $\text{CH}_2$ ), 123.7 (CH), 50.2 ( $\text{CH}_2$ ), 33.7 ( $\text{CH}_2$ ), 29.7 ( $\text{CH}_2$ ), 21.6 ( $\text{CH}_2$ ), 21.2 ( $\text{CH}_3$ ), 18.7 ( $\text{CH}_3 \times 6$ ), 14.1 ( $\text{CH}_3$ ), 11.7 ( $\text{CH}_3 \times 3$ ); IR (neat)  $\nu_{\text{max}} = 2941, 2891, 2866, 1694, 1463, 1443, 1233, 1192, 1106, 1043, 1017, 999, 882, 809, 752, 696 \text{ cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{30}\text{H}_{45}\text{OSSi}$   $[\text{M}+\text{H}]^+$ : 481.2960, found: 481.2957.



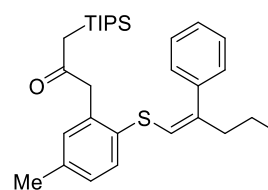
**II.19. (E)-(2-Phenylpent-1-en-1-yl)(p-tolyl)sulfane ((E)-5d).**

Colorless oil (4.0 mg, 14% yield).  $R_f$  0.18 (Pure petroleum ether);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.38 (d,  $J = 7.5$  Hz, 2H), 7.34-7.30 (m, 4H), 7.25 (t,  $J = 7.5$  Hz, 1H), 7.13 (d,  $J = 8.0$  Hz, 2H), 6.46 (s, 1H), 2.71 (t,  $J = 7.5$  Hz, 2H), 2.34 (s, 3H), 1.50 (sx,  $J = 7.5$  Hz, 2H), 0.96 (t,  $J = 7.0$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  142.0 (C), 141.4 (C), 136.6 (C), 133.0 (C), 130.0 ( $\text{CH}_2$ ), 129.6 ( $\text{CH}_2$ ), 128.5 ( $\text{CH}_2$ ), 127.2 (CH), 126.1 ( $\text{CH}_2$ ), 122.7 (CH), 33.9 ( $\text{CH}_2$ ), 21.6 ( $\text{CH}_2$ ), 21.2 ( $\text{CH}_3$ ), 14.1 ( $\text{CH}_3$ ); IR (neat)  $\nu_{\text{max}} = 2957, 2926, 2869, 1491, 1455, 1441, 1091, 1017, 821, 803, 752, 695 \text{ cm}^{-1}$ ; HRMS (ESI) calcd. for  $\text{C}_{18}\text{H}_{21}\text{S}$   $[\text{M}+\text{H}]^+$ : 269.1364, found: 269.1366.



**II.20. (Z)-1-(5-Methyl-2-((2-phenylpent-1-en-1-yl)thio)phenyl)-3-**

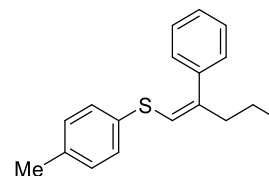
**(triisopropylsilyl)propan-2-one ((Z)-4d).** Colorless oil (6.0 mg, 12% yield).  $R_f$  0.12 (EtOAc/Petroleum ether = 1/50);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.37-7.28 (m, 6H), 7.05 (dd,  $J = 1.5$  Hz,  $J = 7.5$  Hz, 1H), 6.97 (d,  $J = 1.2$  Hz, 1H), 6.02 (t,  $J = 1.2$  Hz, 1H), 3.86 (s, 2H), 2.44 (dt,  $J = 7.5$ , 0.9 Hz, 2H), 2.30



(s, 3H), 2.21 (s, 2H), 1.41-1.33 (m, 2H), 1.17-1.12 (m, 3H), 1.06 (d,  $J = 5.7$  Hz, 18H), 0.87 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  207.5 (C), 141.6 (C), 139.8 (C), 137.6 (C), 136.1 (C), 133.0 (C), 132.4 (CH), 131.6 (CH), 128.8 (CH), 128.3 (CH<sub>x</sub>2), 128.2 (CH<sub>x</sub>2), 127.4 (CH), 122.0 (CH), 49.9 (CH<sub>2</sub>), 41.0 (CH<sub>2</sub>), 29.7 (CH<sub>2</sub>), 21.7 (CH<sub>2</sub>), 21.2 (CH<sub>3</sub>), 18.7 (CH<sub>3</sub>x6), 13.7 (CH<sub>3</sub>), 11.6 (CH<sub>x</sub>3); IR (neat)  $\nu_{\text{max}} = 2928$ , 2867, 1694, 1464, 1232, 1044, 883, 808, 699  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{30}\text{H}_{45}\text{OSSi}$  481.2960; Found 481.2968.

**II.21. (Z)-(2-Phenylpent-1-en-1-yl)(p-tolyl)sulfane ((Z)-5d).** Colorless oil (3.0 mg, 11% yield).  $R_f$  0.59 (EtOAc/Petroleum ether = 1/50);  $^1\text{H}$  NMR

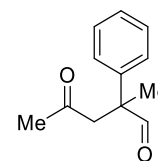
( $\text{CDCl}_3$ , 300 MHz)  $\delta$  7.41-7.28 (m, 5H), 7.25 (d,  $J = 8.1$  Hz, 2H), 7.10 (d,  $J = 7.8$  Hz, 2H), 6.22 (t,  $J = 0.9$  Hz, 1H), 2.49 (dt,  $J = 7.5$ , 0.9 Hz, 2H), 2.32 (s, 3H), 1.40 (sx,  $J = 7.5$  Hz, 2H),



0.90 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)  $\delta$  142.3 (C), 140.0 (C), 136.4 (C), 133.7 (C), 129.9 (CH<sub>x</sub>2), 129.6 (CH<sub>x</sub>2), 128.3 (CH<sub>x</sub>2), 128.2 (CH<sub>x</sub>2), 127.5 (CH), 121.0 (CH), 41.1 (CH<sub>2</sub>), 21.6 (CH<sub>2</sub>), 21.2 (CH<sub>3</sub>), 13.7 (CH<sub>3</sub>); IR (neat)  $\nu_{\text{max}} = 3020$ , 2958, 2927, 2870, 1492, 1456, 1441, 1092, 1018, 804, 699  $\text{cm}^{-1}$ ; HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calcd for  $\text{C}_{18}\text{H}_{21}\text{S}$  269.1364; Found 269.1354.

**II.22. 2-Methyl-4-oxo-2-phenylpentanal (3e).** Colorless oil (7.8 mg, 41% yield).  $R_f$

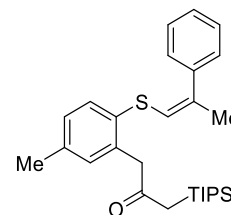
0.28 (EtOAc/Petroleum ether = 1/5);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  9.49 (s, 1H), 7.31 (t, d,  $J = 7.5$  Hz, 2H), 7.23-7.18 (m, 3H), 3.10 (d,  $J = 17.5$  Hz, 1H), 3.00 (d,  $J = 17.5$  Hz, 1H), 2.01 (s, 3H), 1.54 (s, 3H);  $^{13}\text{C}$  NMR



( $\text{CDCl}_3$ , 125 MHz)  $\delta$  206.2 (C), 201.2 (CH), 139.3 (C), 129.1 (CH<sub>x</sub>2), 127.6 (CH), 127.0 (CH<sub>x</sub>2), 52.0 (C), 50.6 (CH<sub>2</sub>), 31.1 (CH<sub>3</sub>), 20.0 (CH<sub>3</sub>); HRMS (ESI) calcd.  $\text{C}_{12}\text{H}_{15}\text{O}_2$  for  $[\text{M}+\text{H}]^+$ : 191.1072, found: 191.1064.

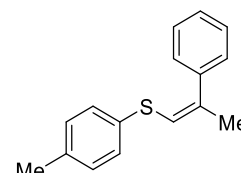
**II.23. (Z)-1-(5-Methyl-2-((2-phenylprop-1-en-1-yl)thio)phenyl)-3-**

**(triisopropylsilyl)propan-2-one ((Z)-4e).** Colorless oil (2.4 mg, 5% yield).  $R_f$  0.29 (EtOAc/Petroleum ether = 1/40);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.42-7.34 (m, 5H), 7.28 (d,  $J = 7.0$  Hz, 1H), 7.05 (d,  $J = 7.9$  Hz, 1H), 6.98 (s, 1H), 6.05 (s, 1H), 3.88 (s, 2H), 2.30 (s, 3H), 2.22 (s, 2H), 2.15 (s, 3H), 1.18-1.10 (m, 3H), 1.06



(d,  $J = 6.7$  Hz, 18H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  207.5 (C), 140.4 (C), 137.7 (C), 136.2 (Cx2), 132.9 (C), 132.6 (CH), 131.6 (CH), 128.8 (CH), 128.2 (CHx2), 127.7 (CHx2), 127.4 (CH), 122.3 (CH), 50.0 ( $\text{CH}_2$ ), 29.7 ( $\text{CH}_2$ ), 25.1 ( $\text{CH}_3$ ), 21.2 ( $\text{CH}_3$ ), 18.7 ( $\text{CH}_3$ x6), 11.6 ( $\text{CH}_3$ x3); HRMS (ESI) calcd. for  $\text{C}_{28}\text{H}_{41}\text{OSSi}$   $[\text{M}+\text{H}]^+$ : 453.2647, found: 453.2654.

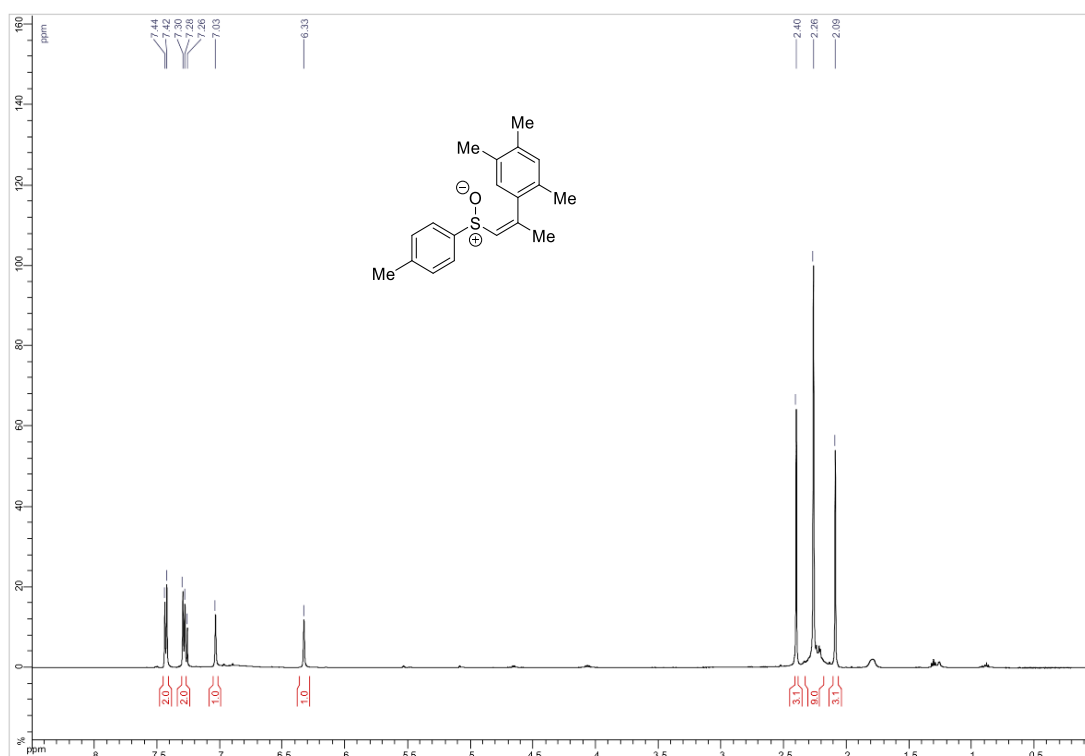
**II.24. (Z)-(2-Phenylprop-1-en-1-yl)(p-tolyl)sulfane ((Z)-5e).** Colorless oil (2.0 mg, 8% yield).  $R_f$  0.50 (100% Petroleum ether);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)  $\delta$  7.34–7.28 (m, 4H), 7.24–7.19 (m, 3H), 7.04 (d,  $J = 7.9$  Hz, 2H), 6.16 (s, 1H), 2.25 (s, 3H), 2.13 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)  $\delta$  140.5 (C), 137.1 (C), 136.6 (C), 133.5 (C), 129.9 ( $\text{CH}_2$ ), 129.6 ( $\text{CH}_2$ ), 128.3 ( $\text{CH}_2$ ), 127.8 ( $\text{CH}_2$ ), 127.5 (CH), 121.1 (C), 25.2 ( $\text{CH}_3$ ), 21.2 ( $\text{CH}_3$ ); HRMS (ESI) calcd. for  $\text{C}_{16}\text{H}_{17}\text{S}$   $[\text{M}+\text{H}]^+$ : 241.1051, found: 241.1053.



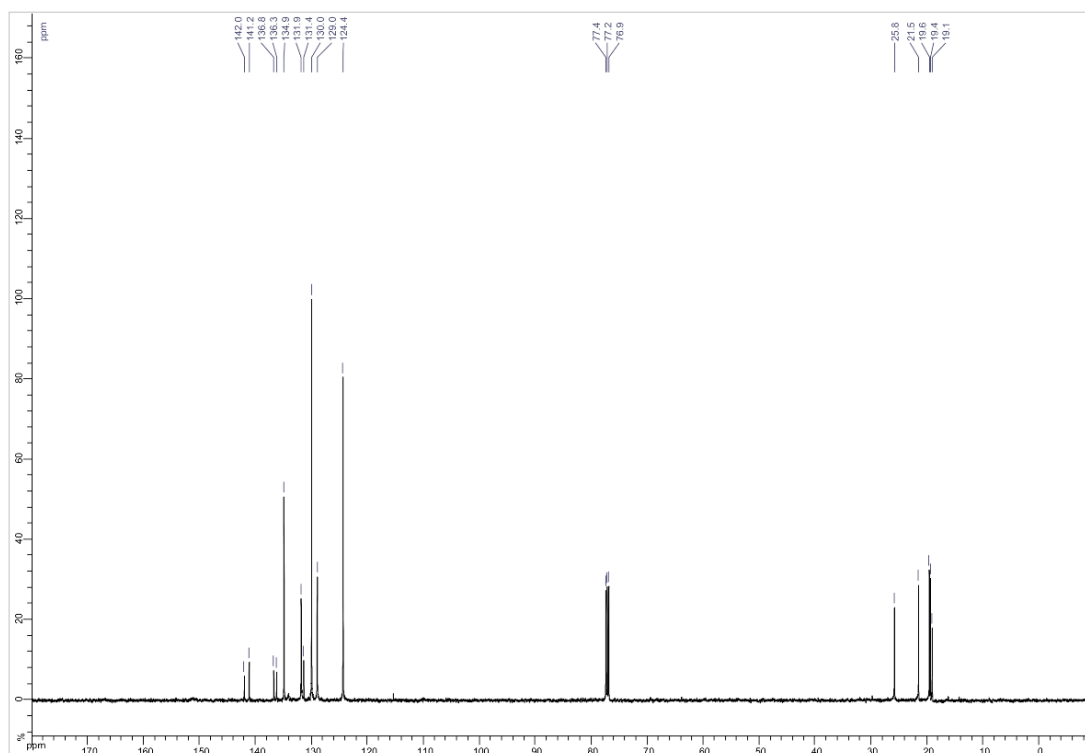
### III. NMR Spectra ( $^1\text{H}$ NMR and $^{13}\text{C}$ NMR):

#### III.1. (Z)-1c

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

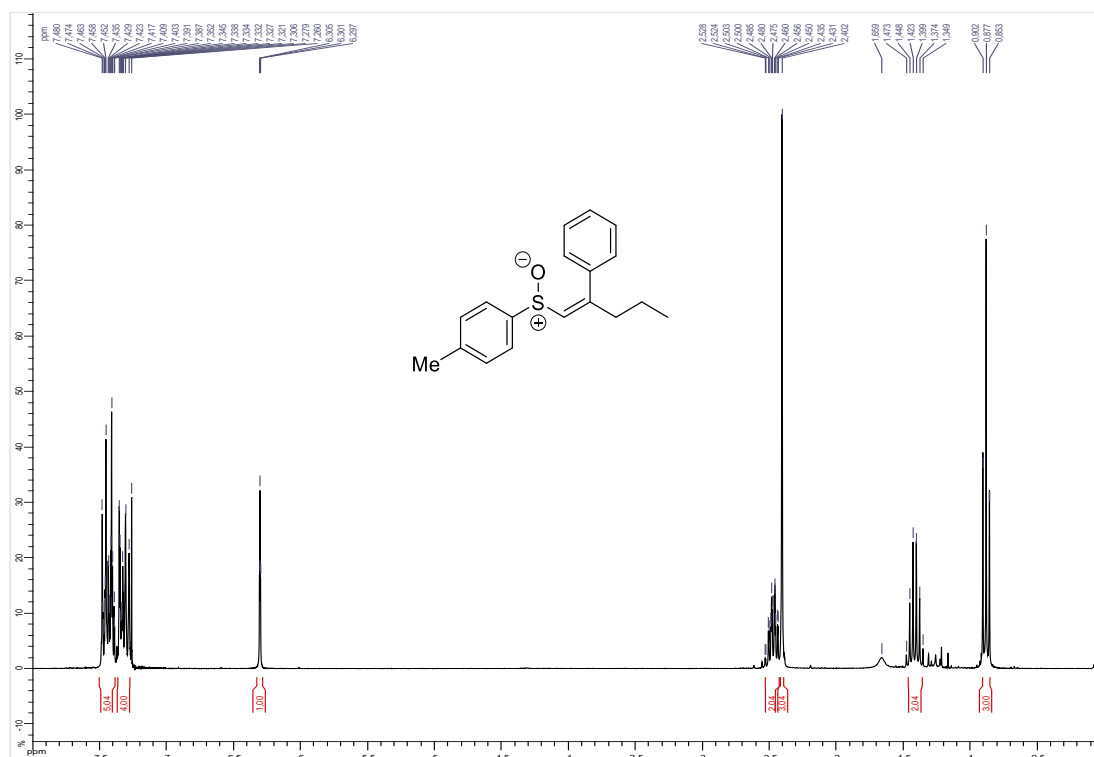


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

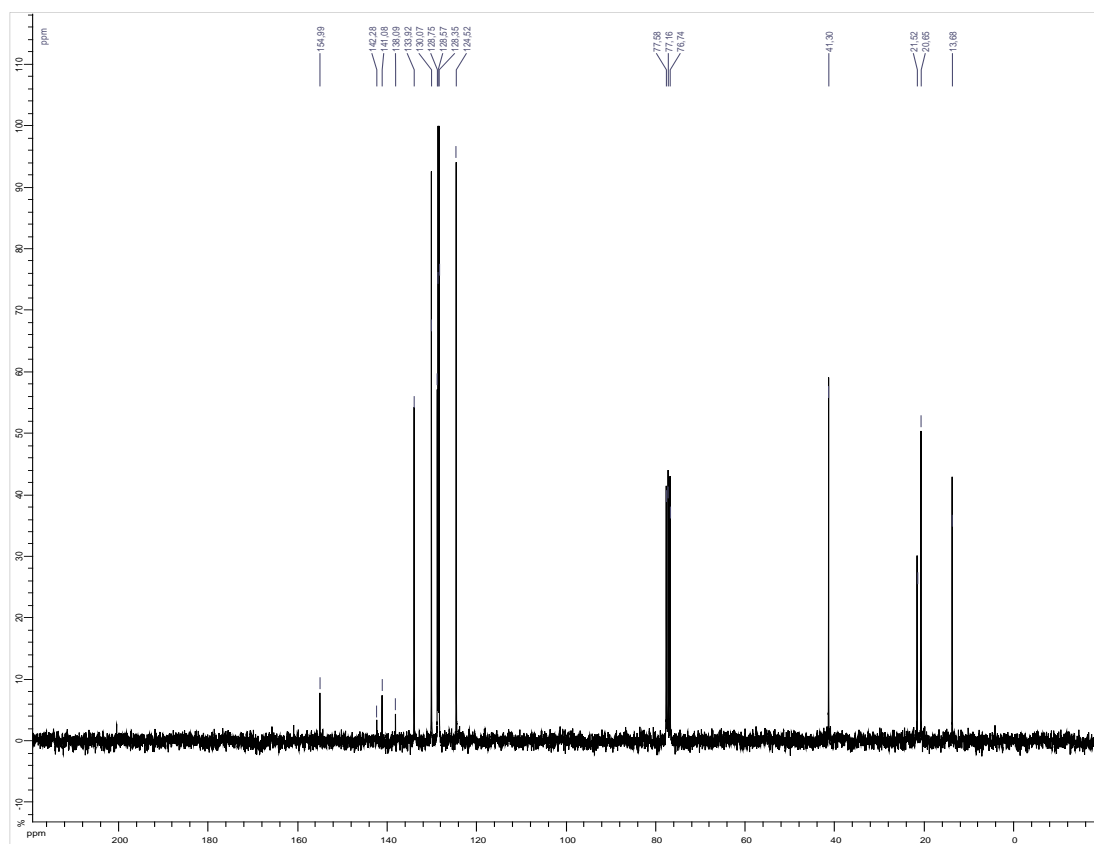


### III.2. (Z)-1d

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

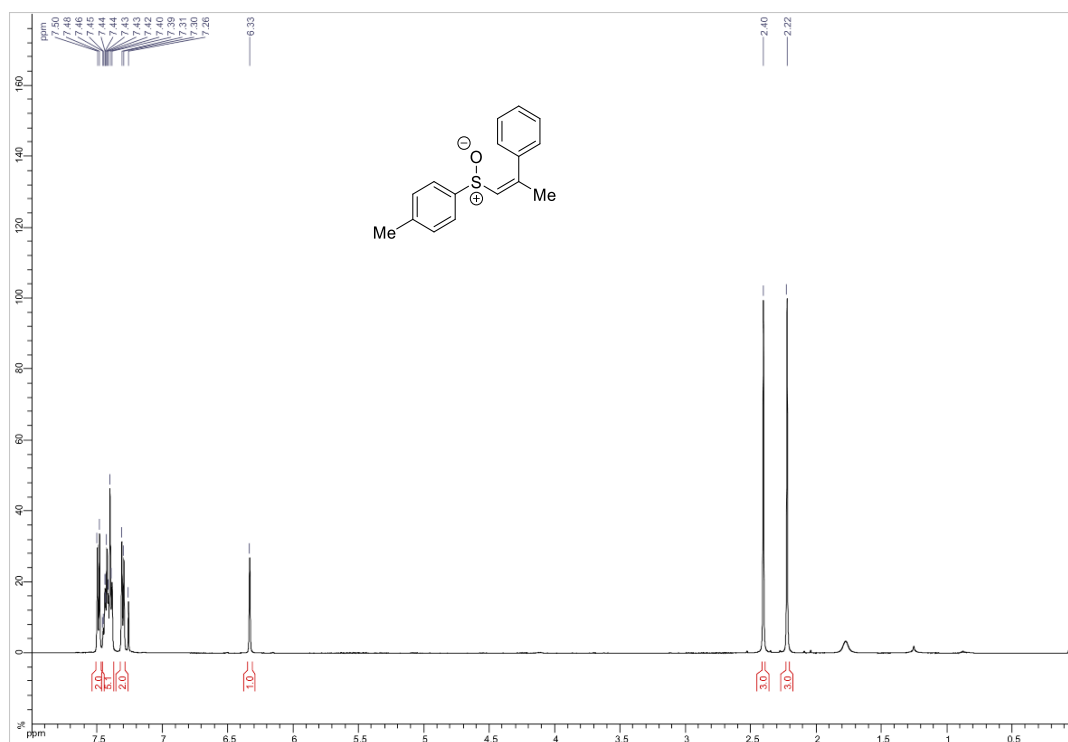


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)

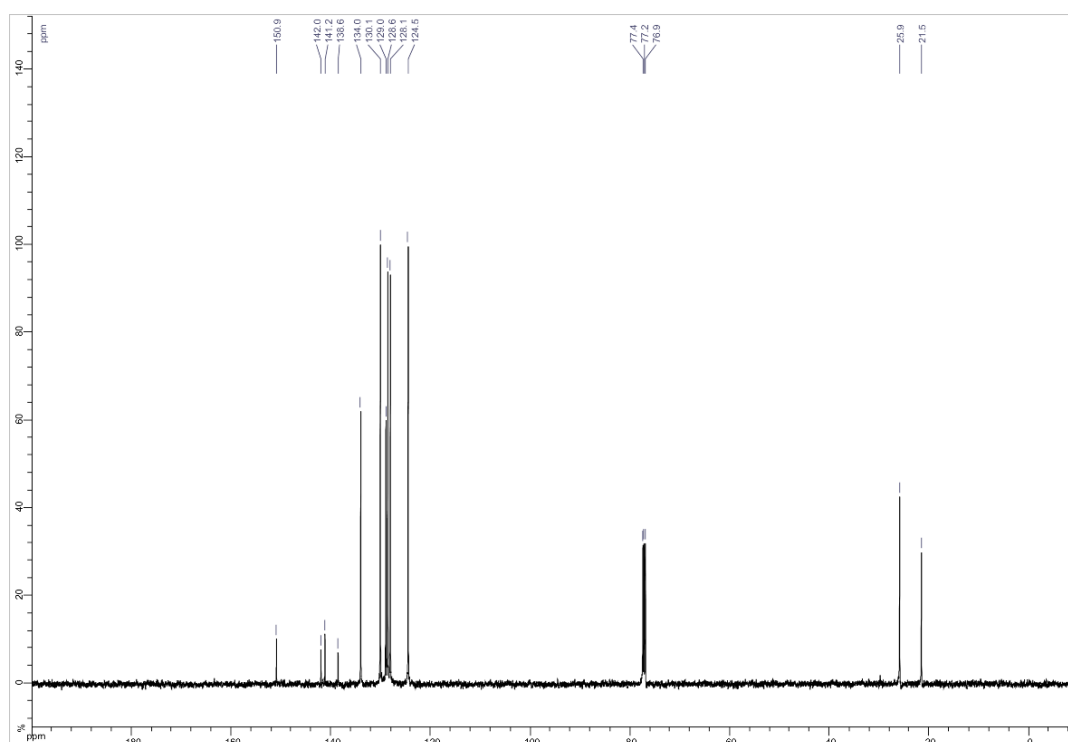


### III.3. (Z)-1e

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

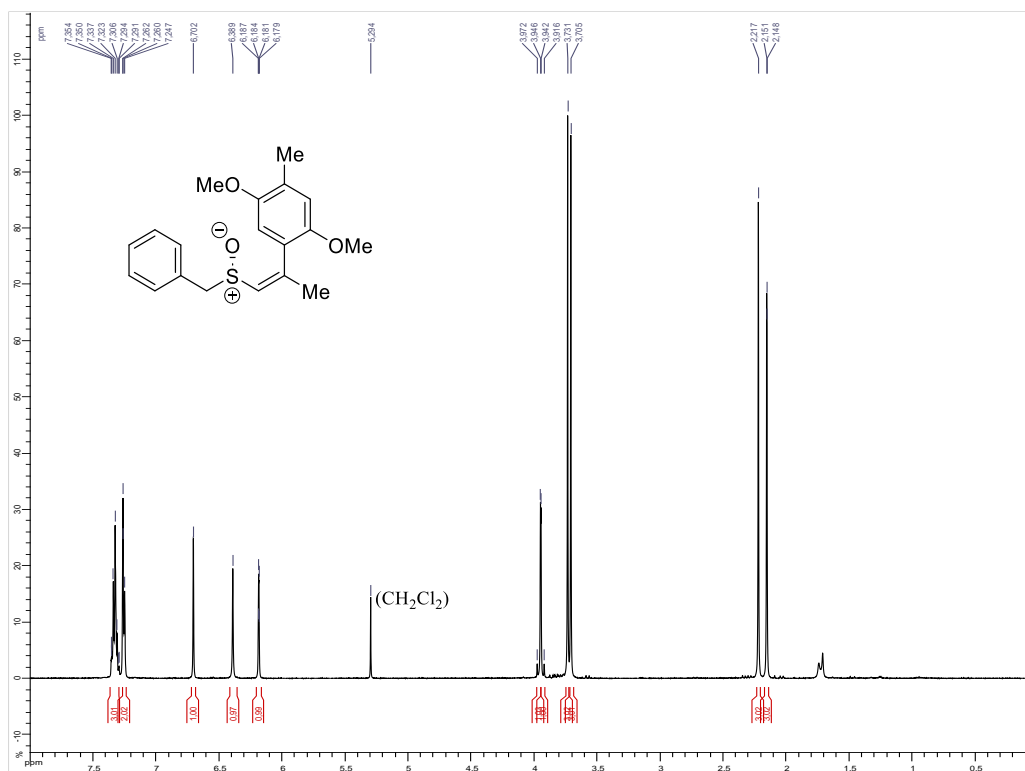


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

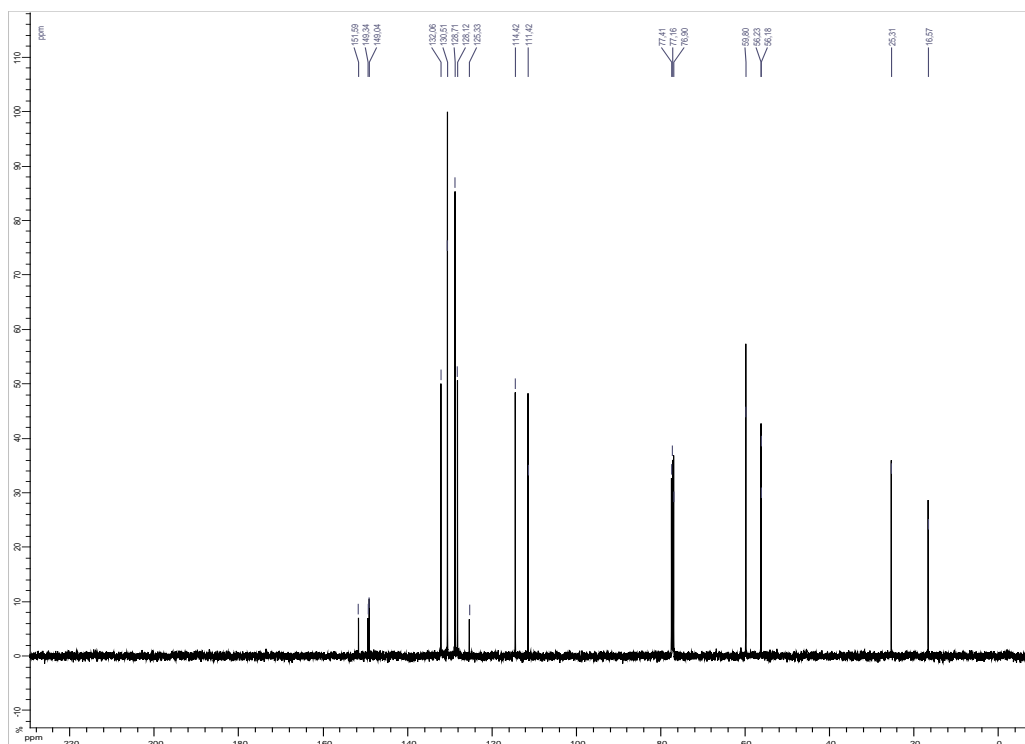


### III.4. (S,Z)-1f.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

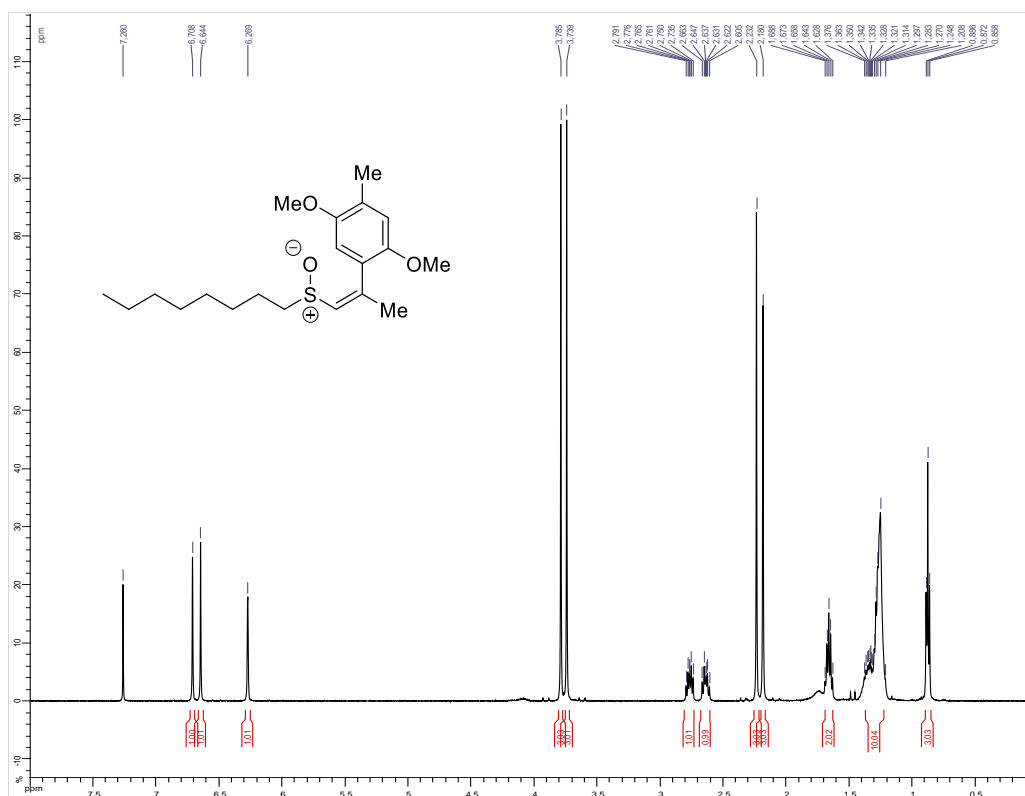


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

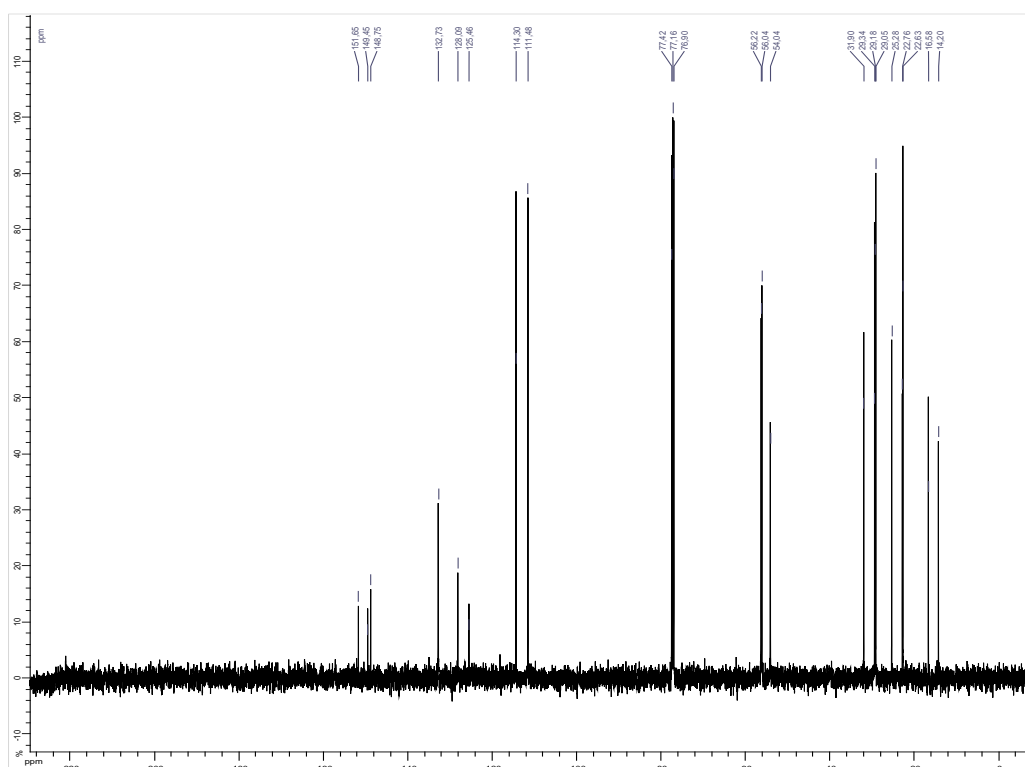


### III.5. (Z)-1g.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)



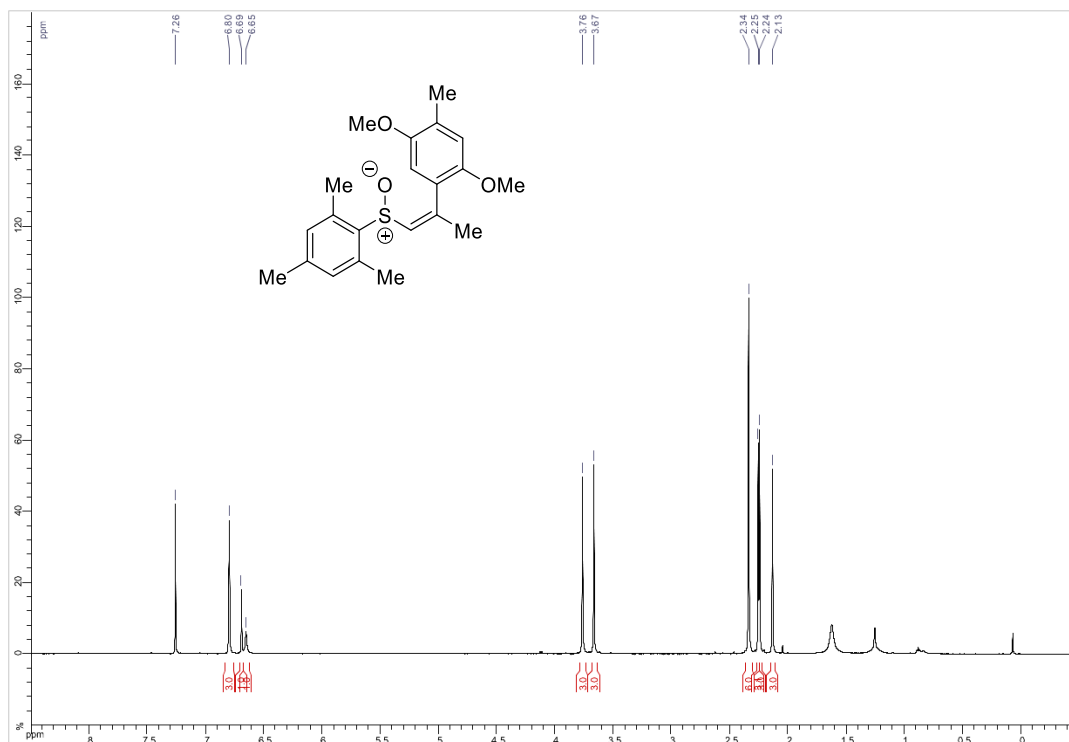
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)



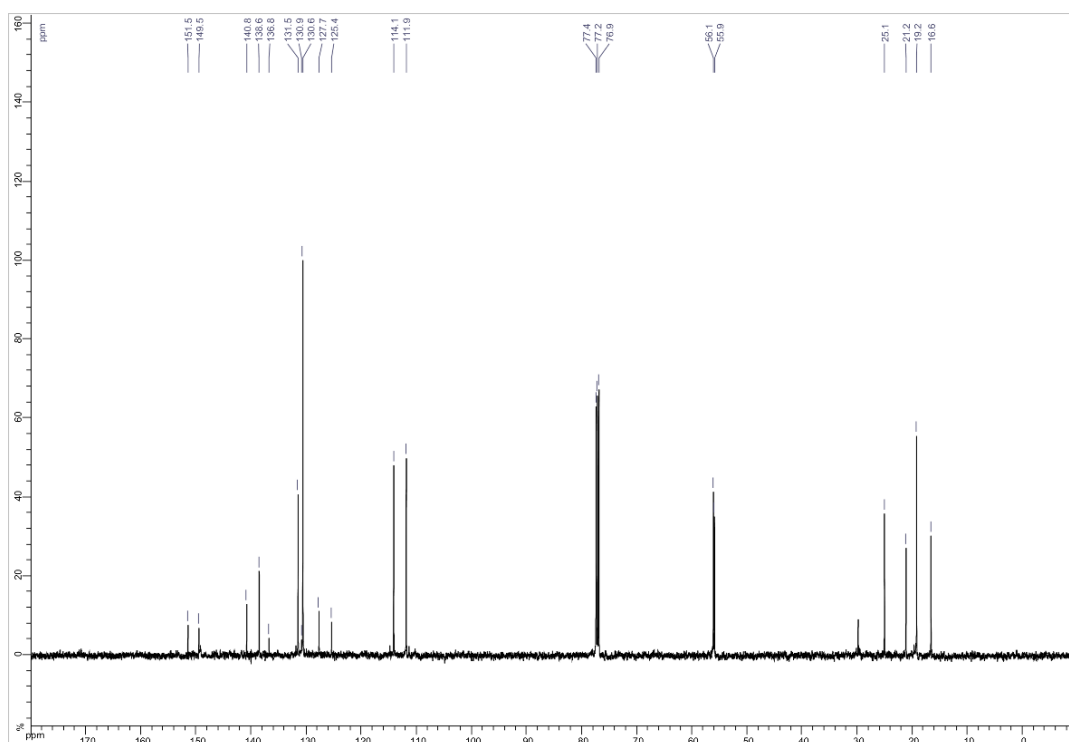


### III.6. (Z)-1h.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

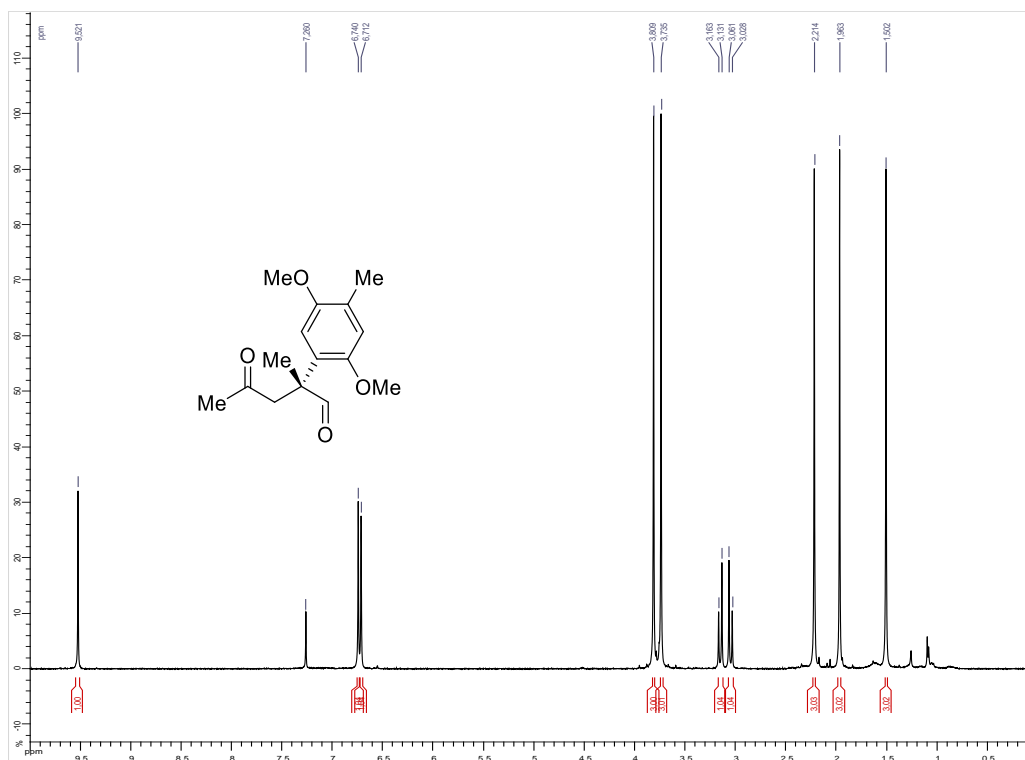


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

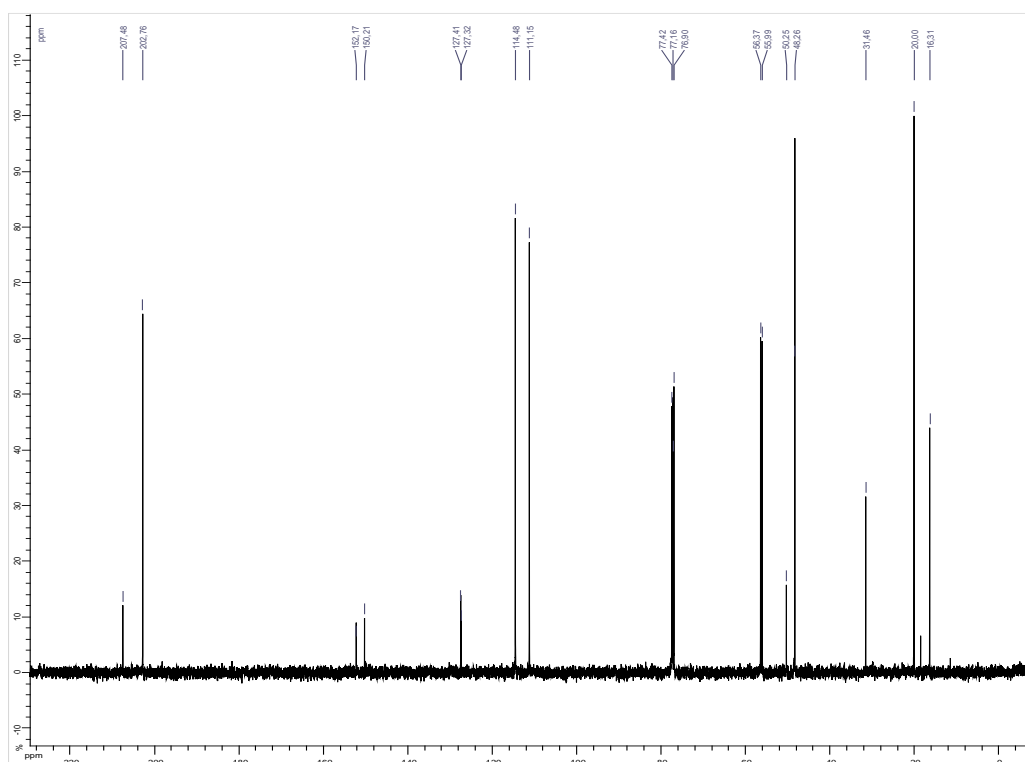


### III.7. 3a.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

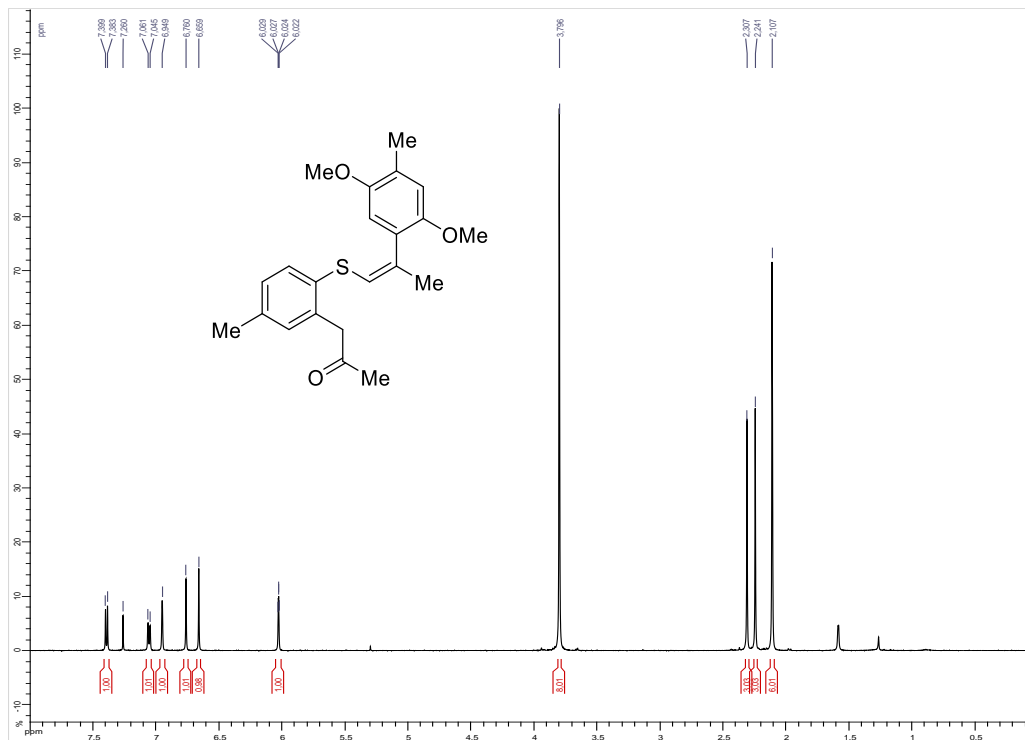


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

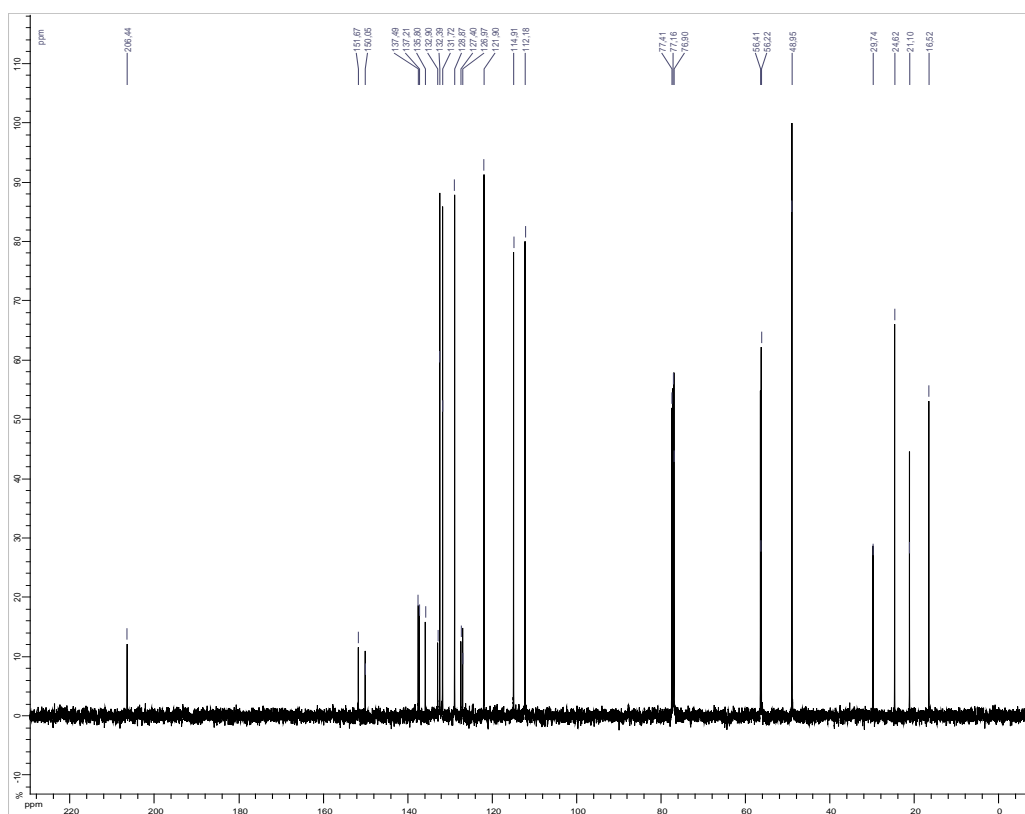


### III.8. 4a'

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

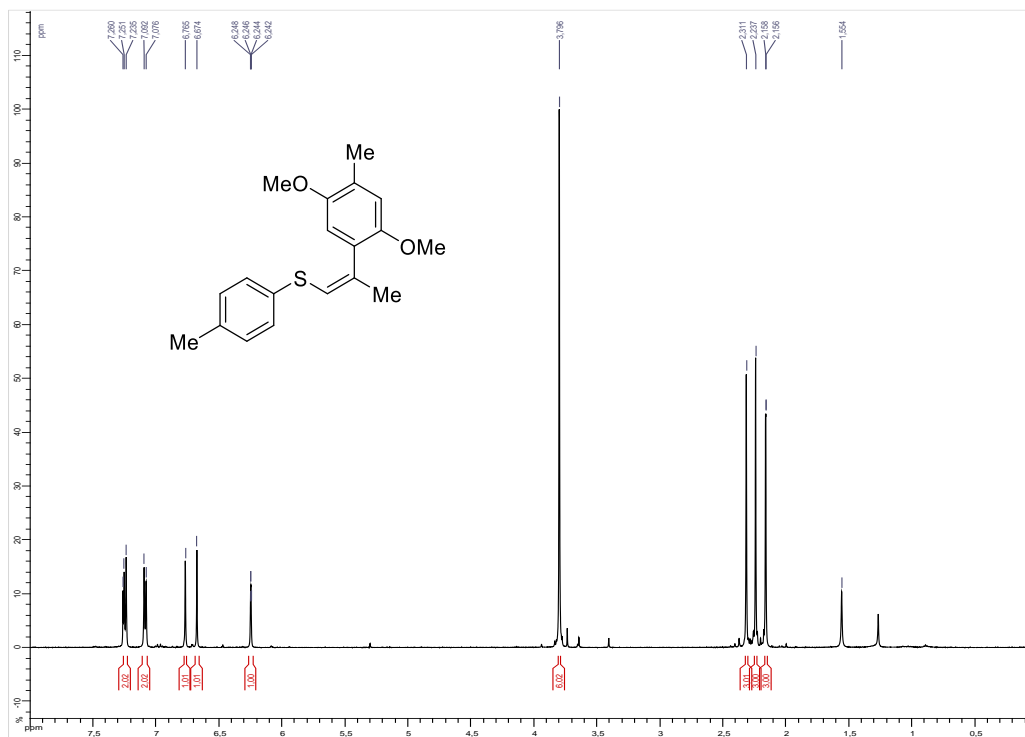


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

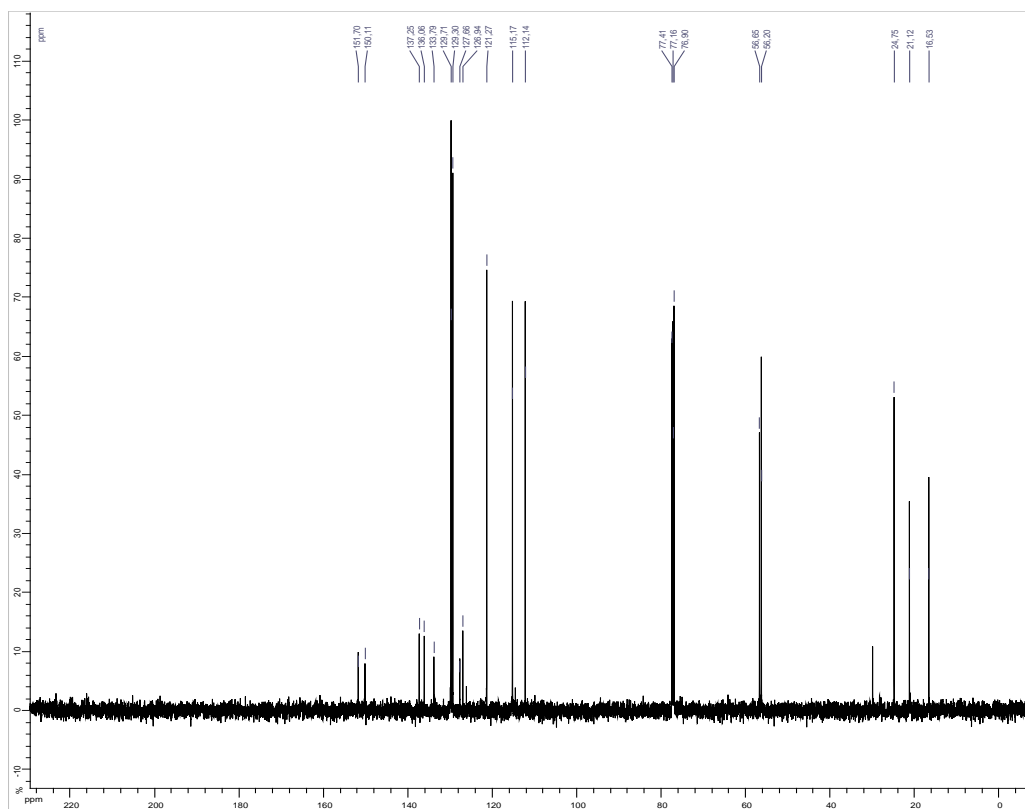


### III.9. (Z)-5a.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

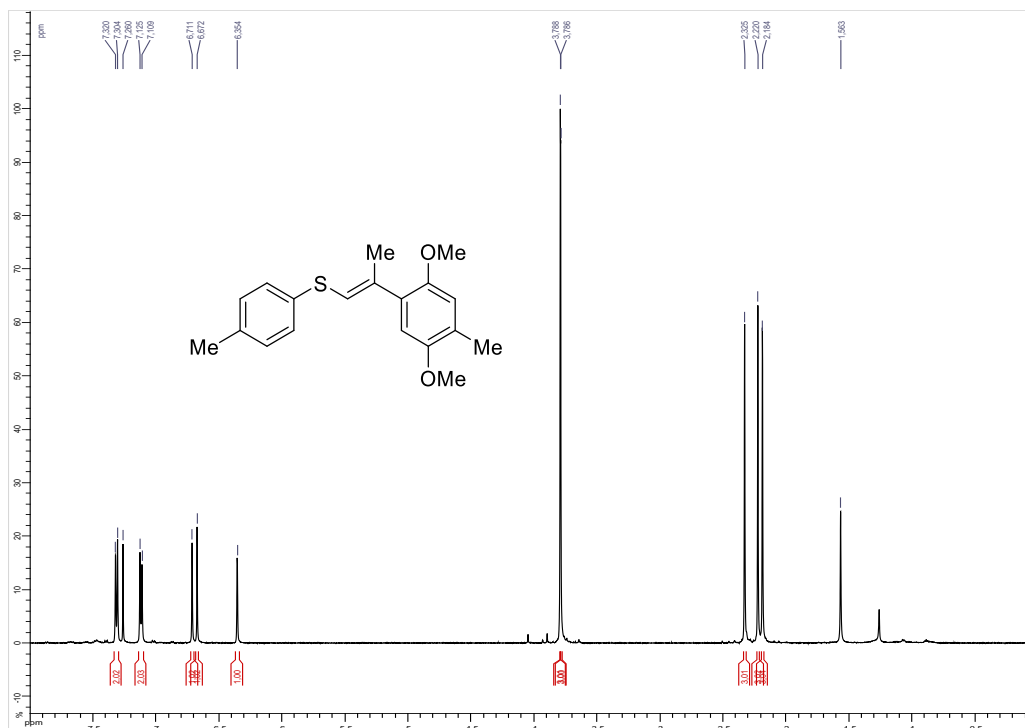


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

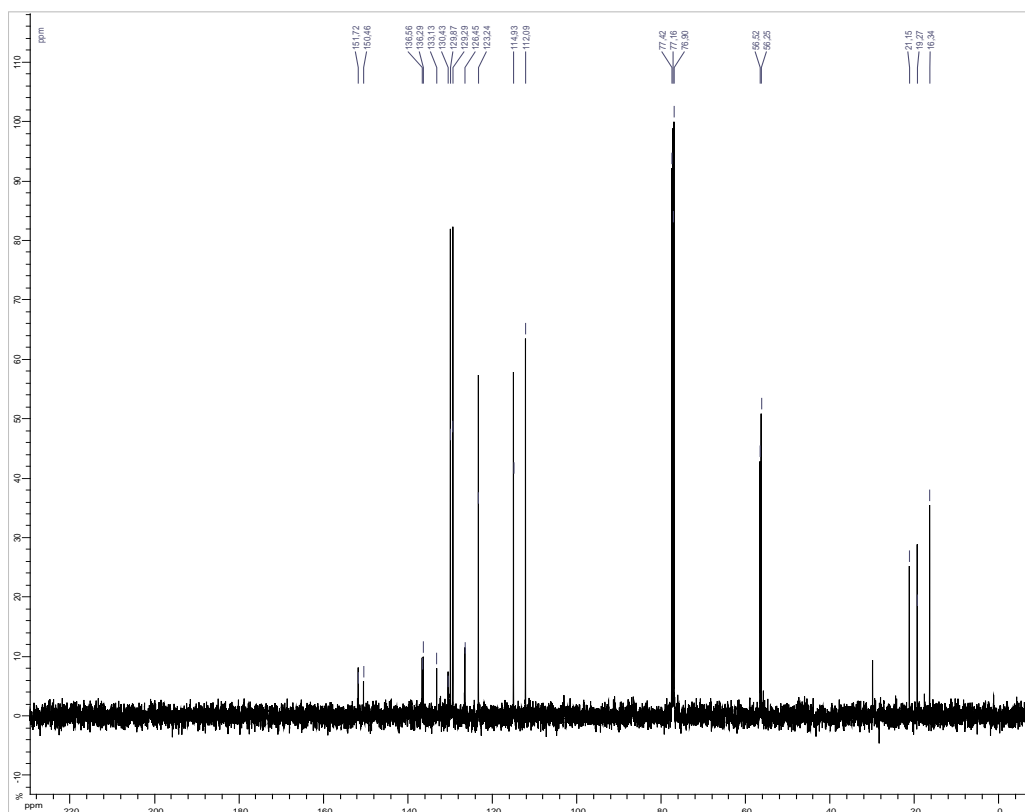


### III.10. (E)-5a.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)



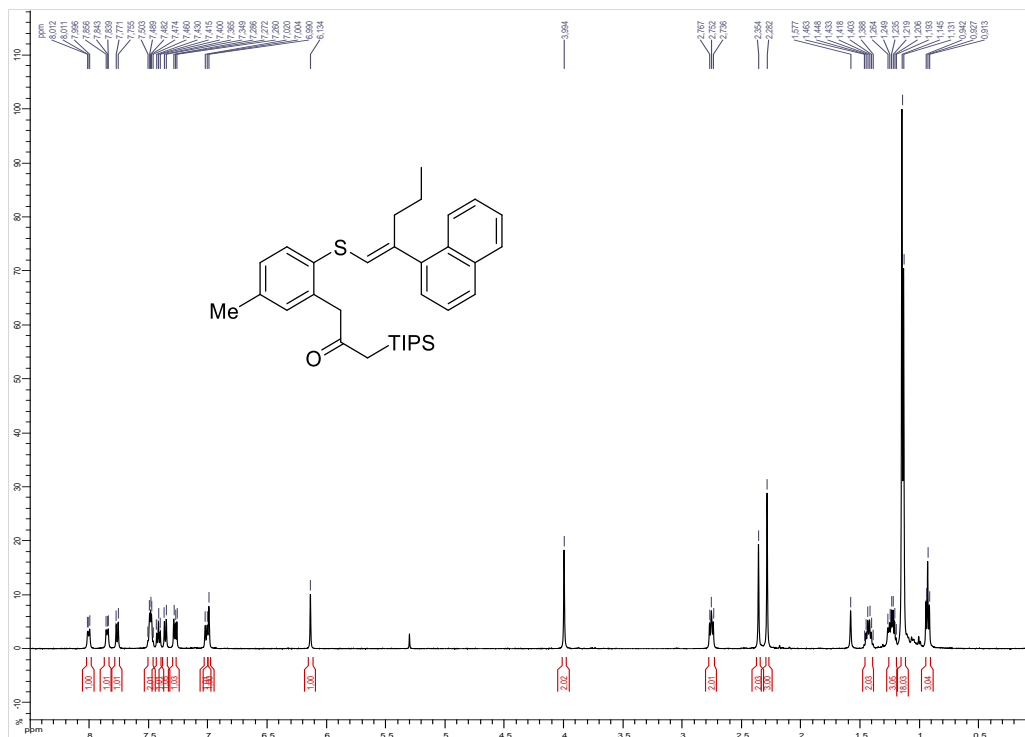
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)



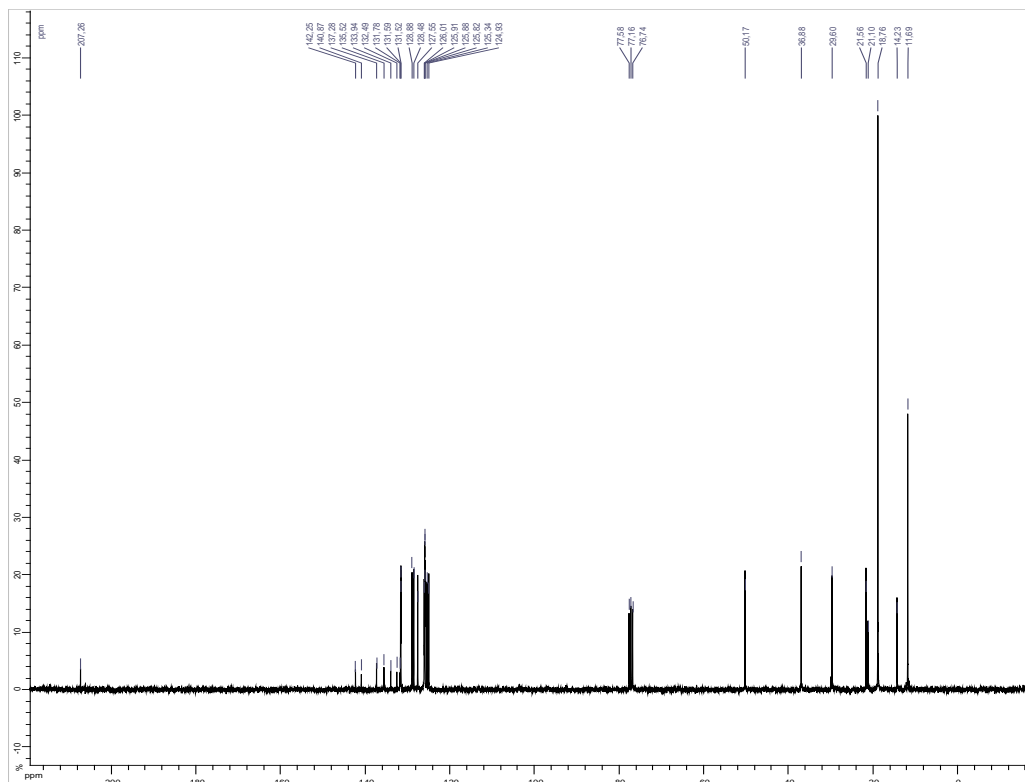


### III.12. (E)-4b.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

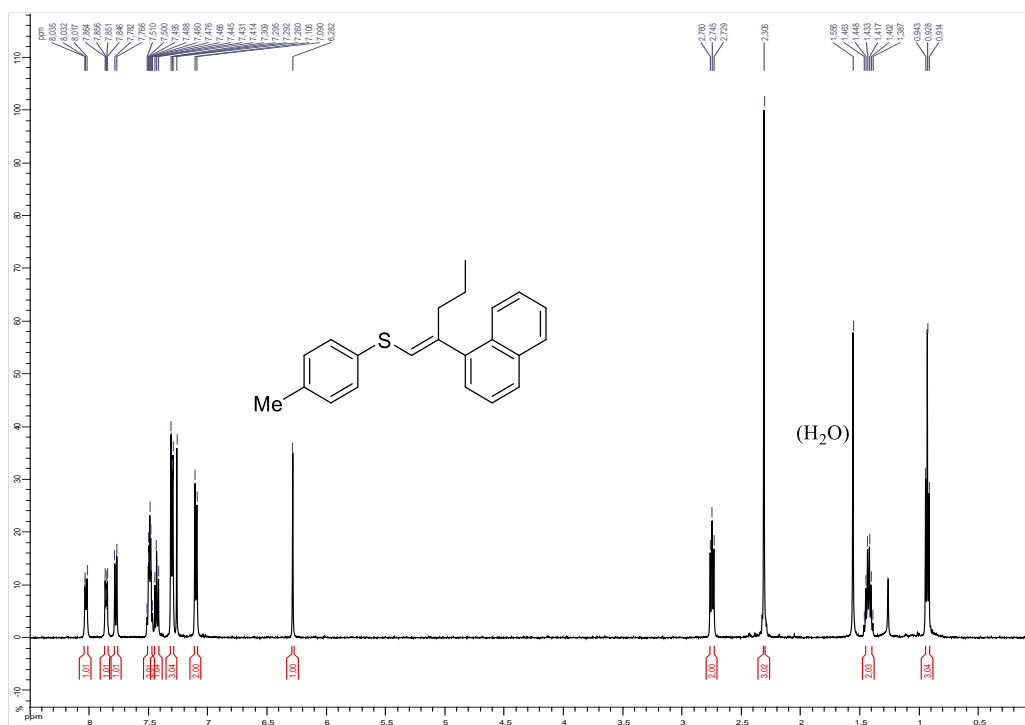


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)

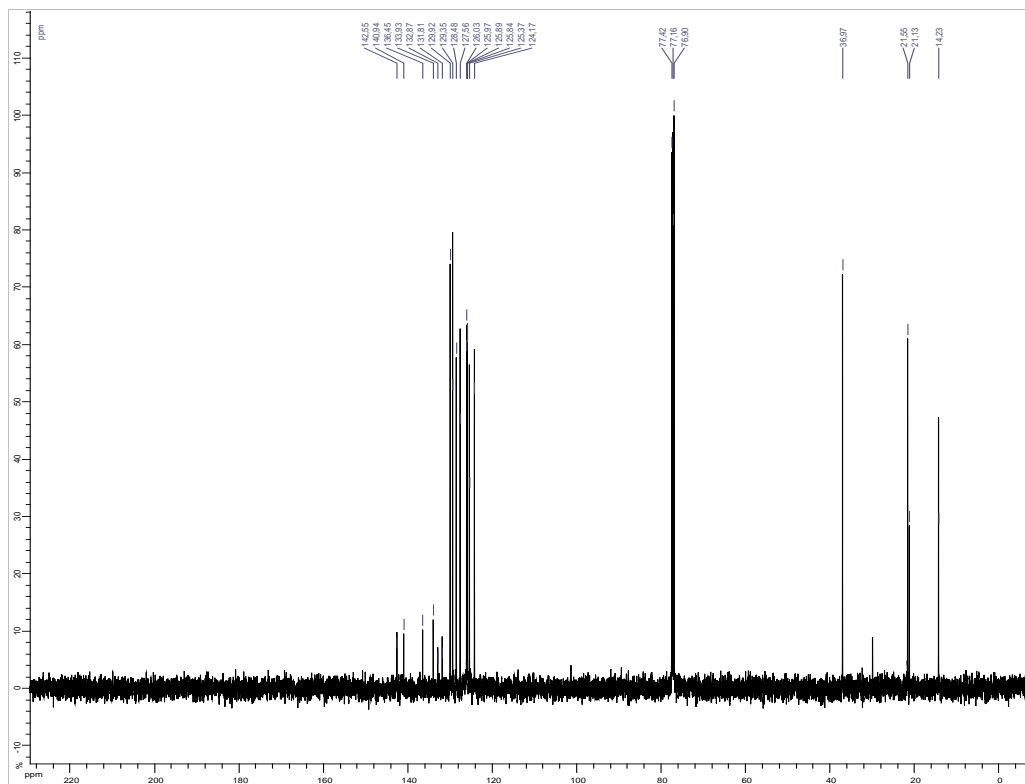


### III.13. (*E*)-5b.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz)



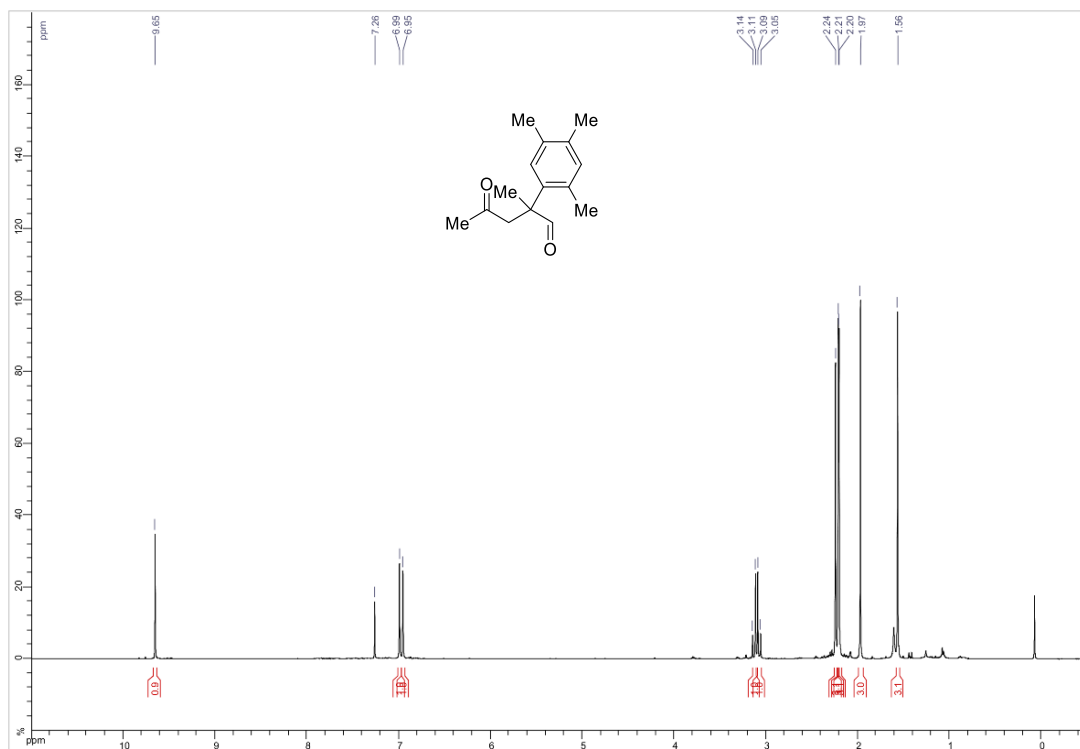
<sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)



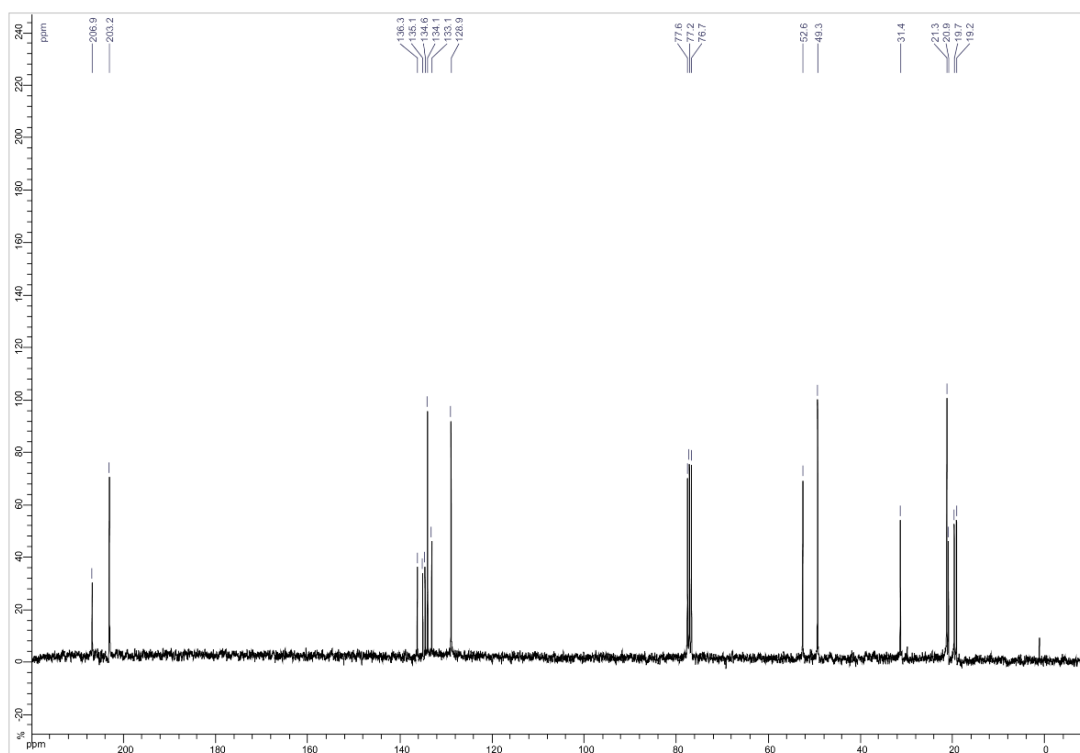


### III.14. 3c

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

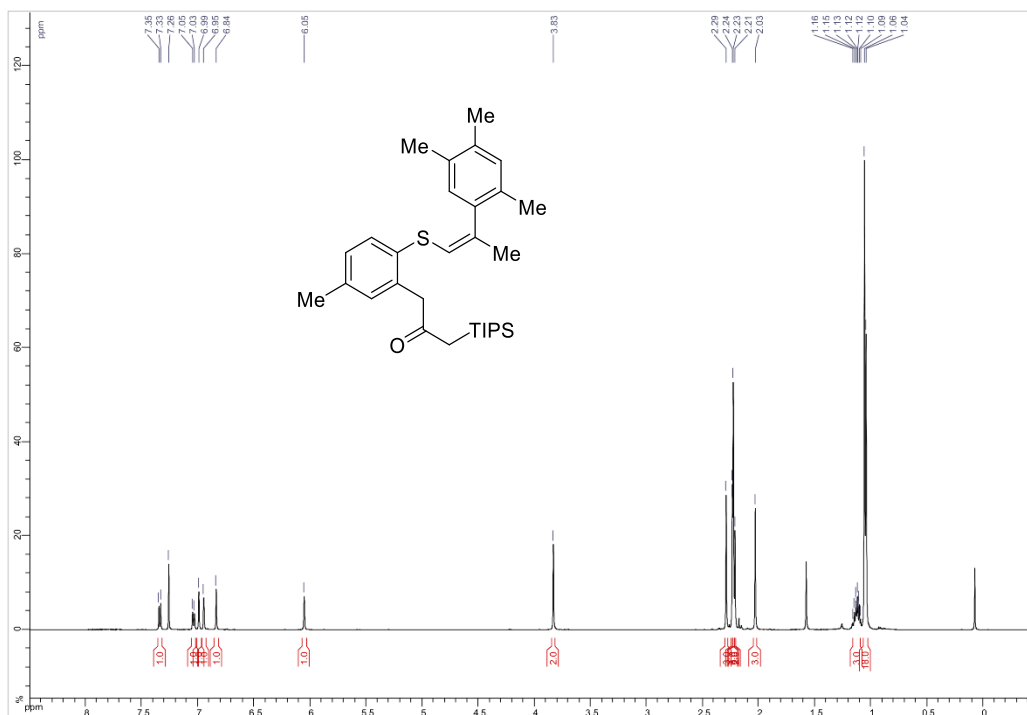


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

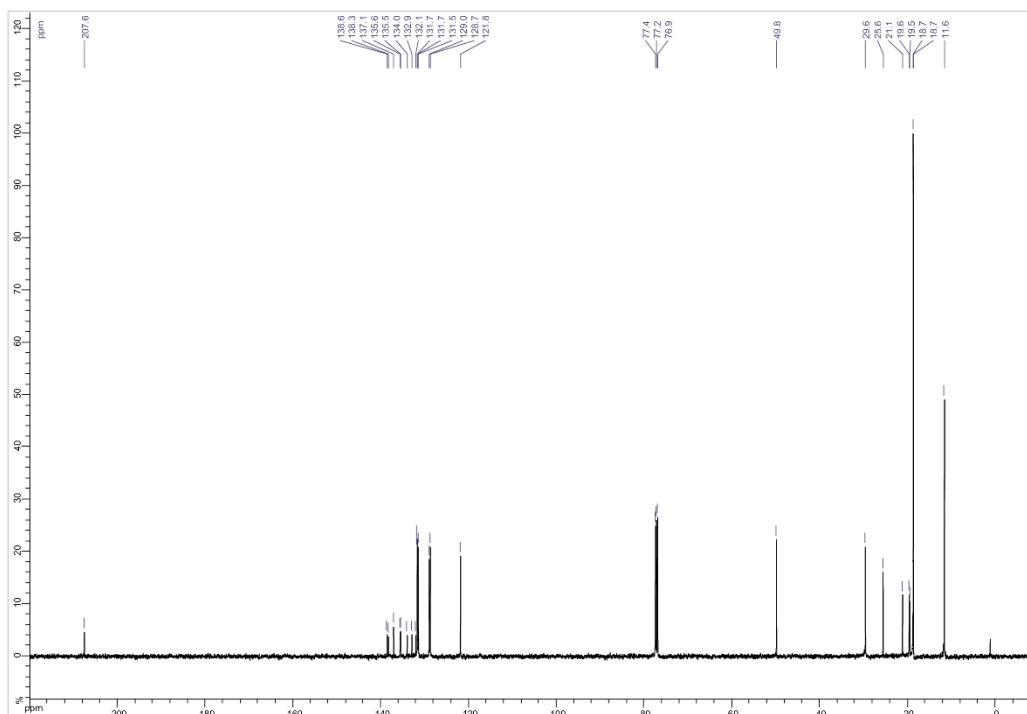


### III.15. (Z)-4c

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

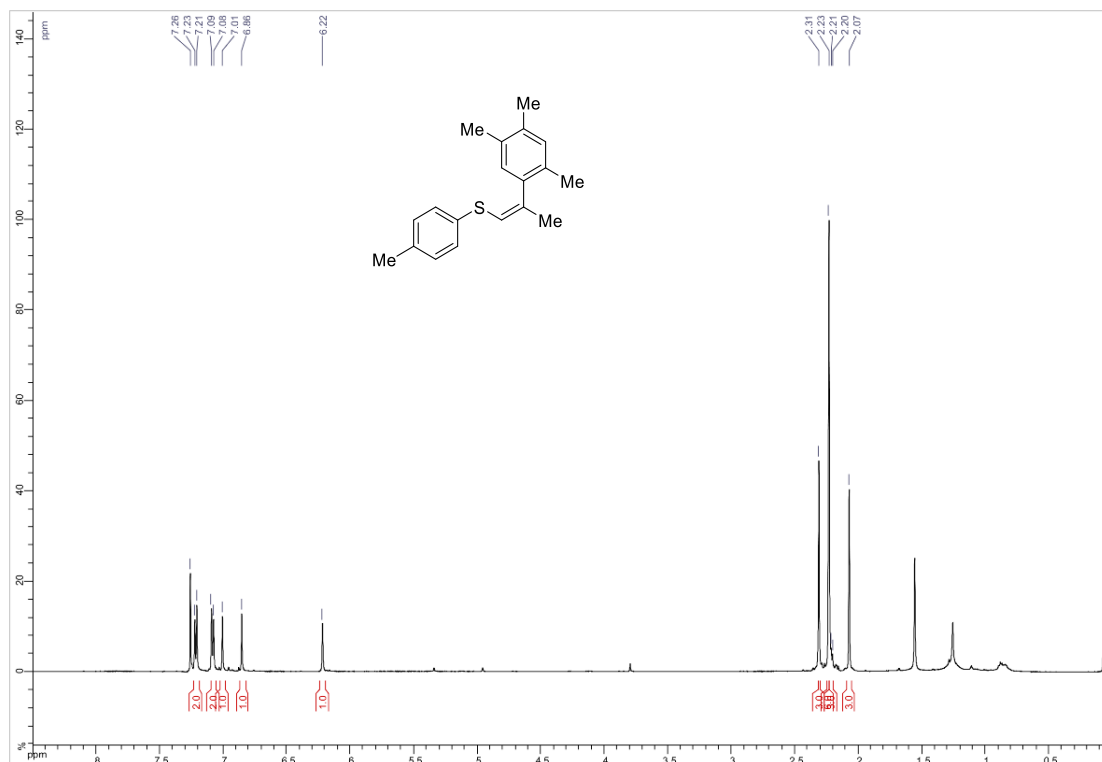


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

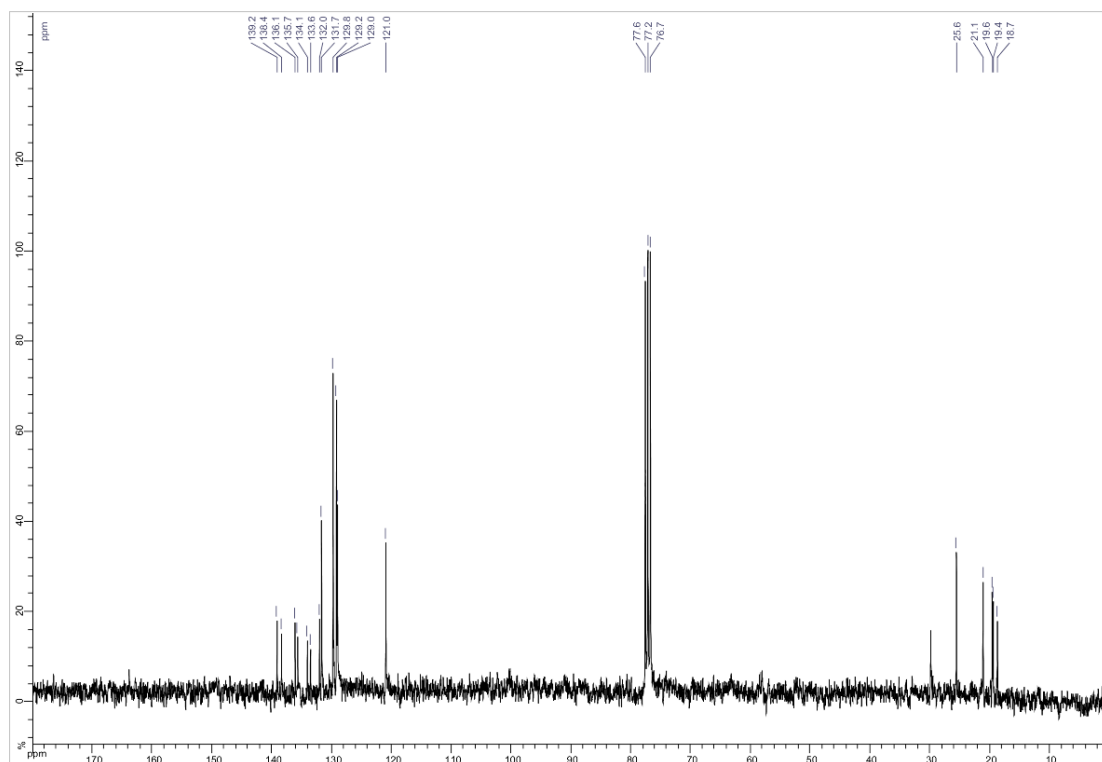


### III.16. (Z)-5c

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

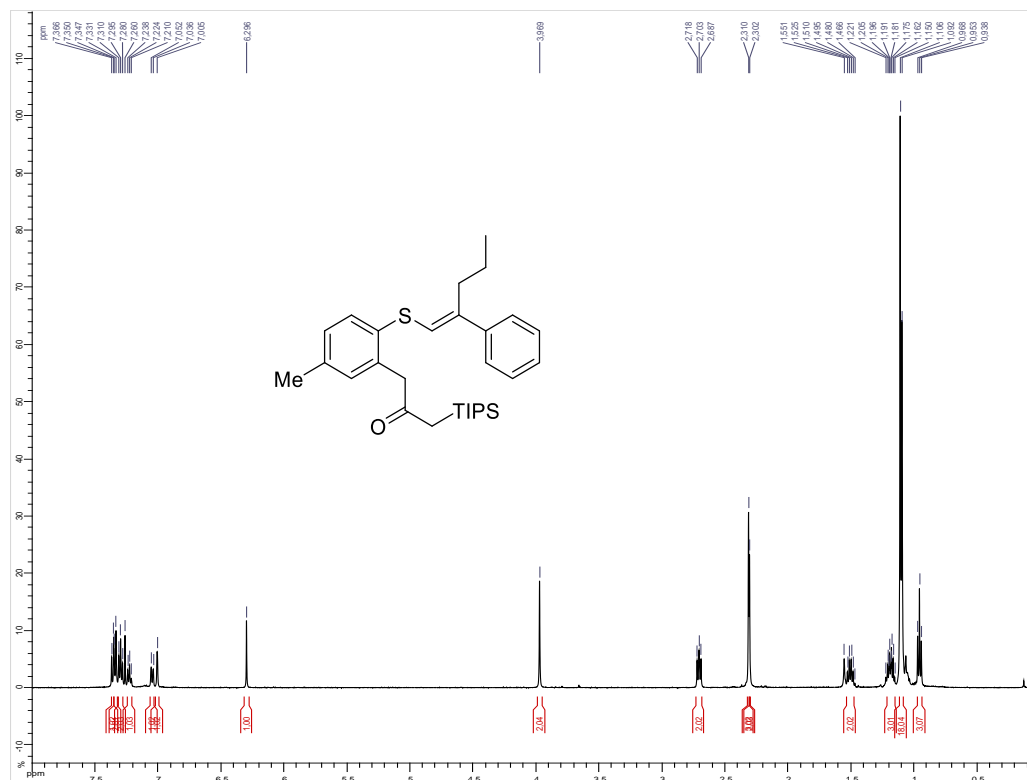


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)

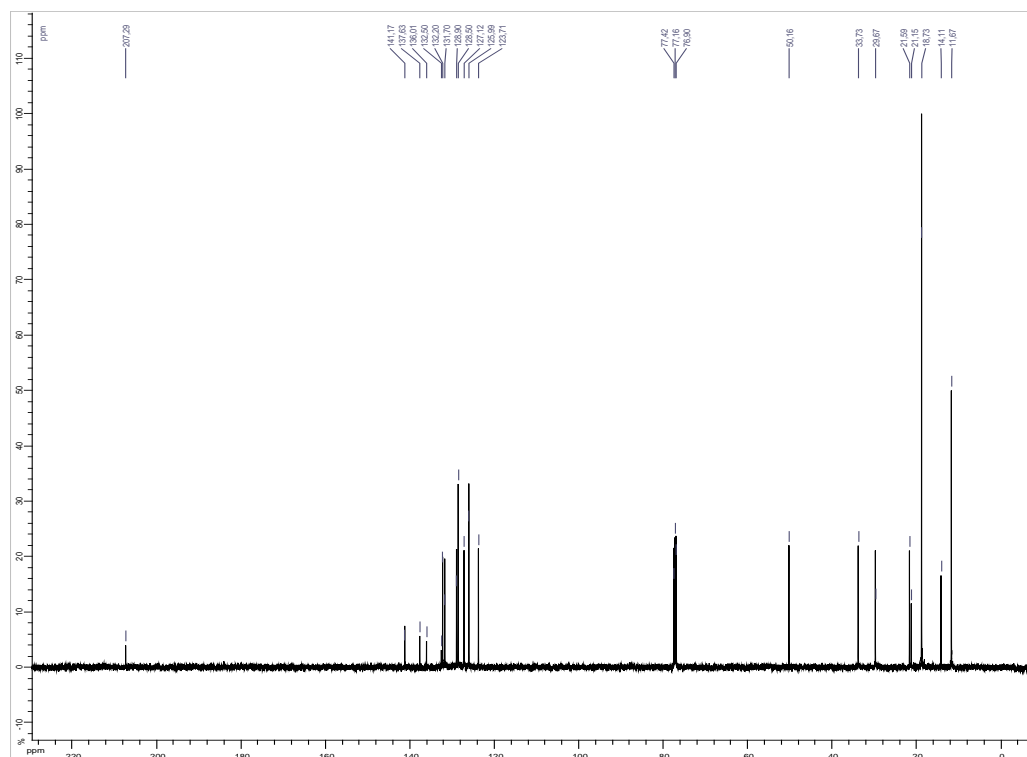


### III.17. (E)-4d.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

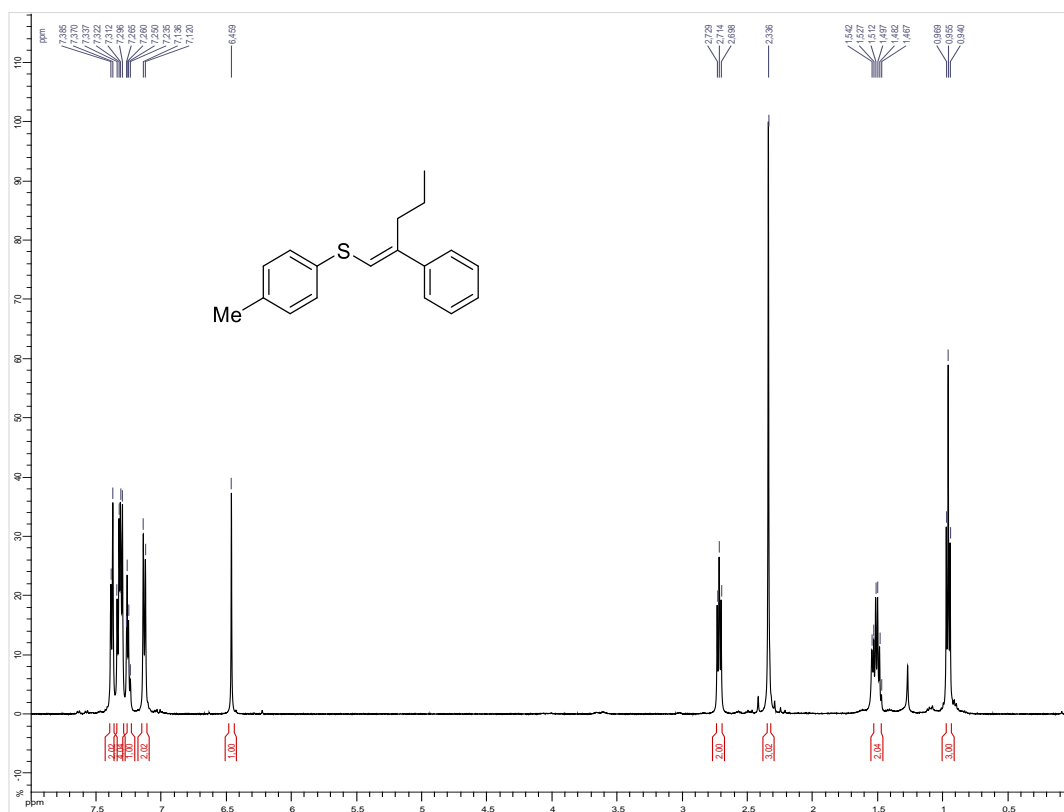


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

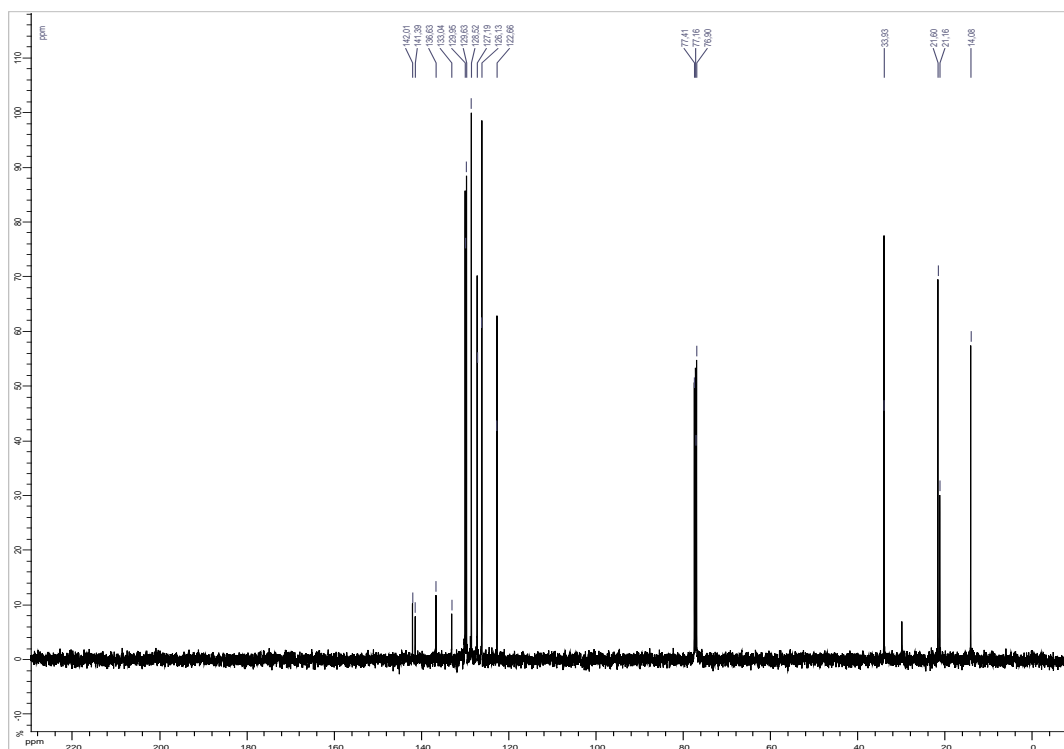


### III.18. (E)-5d.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

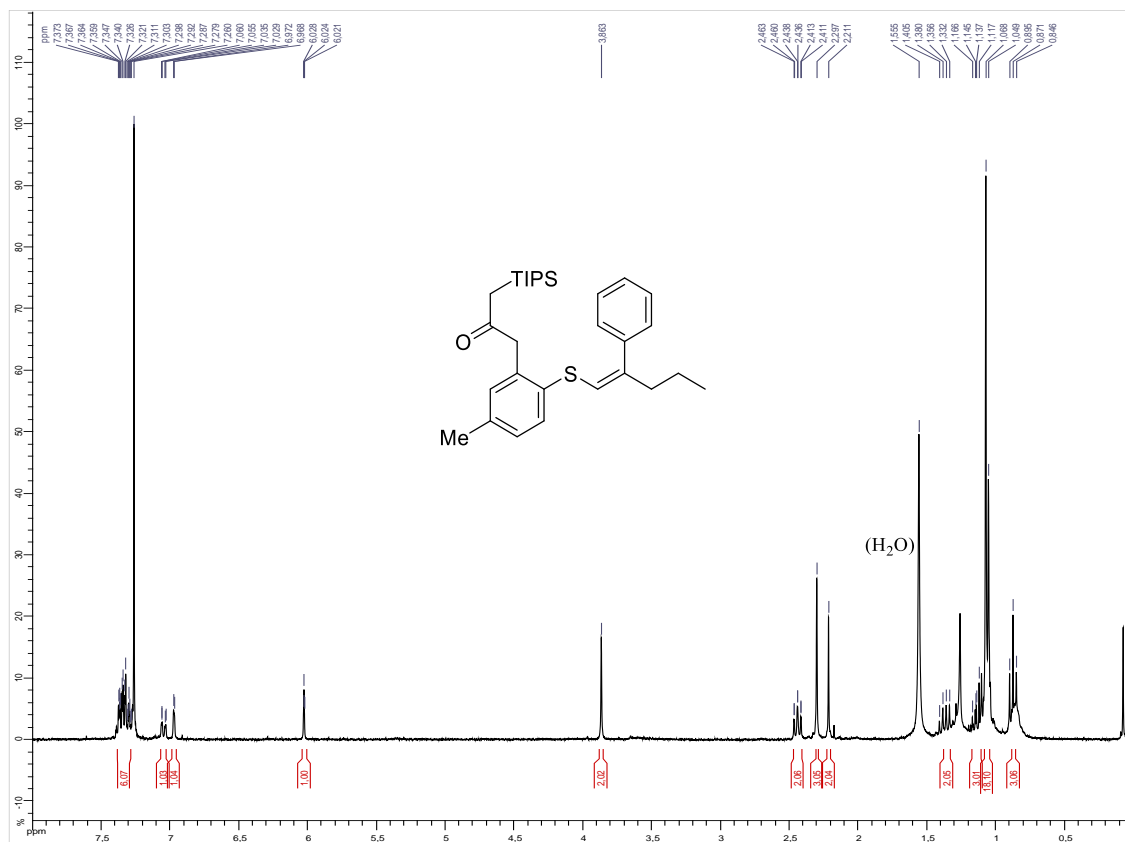


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

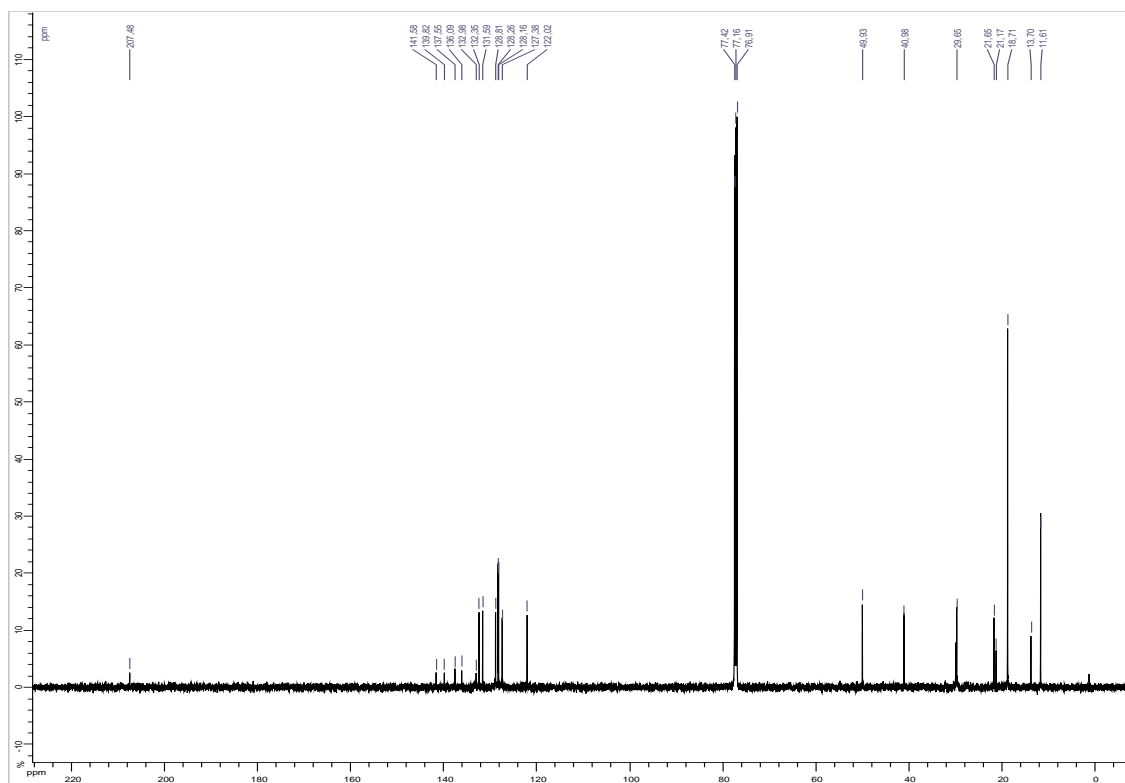


### III.19. (Z)-4d.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)

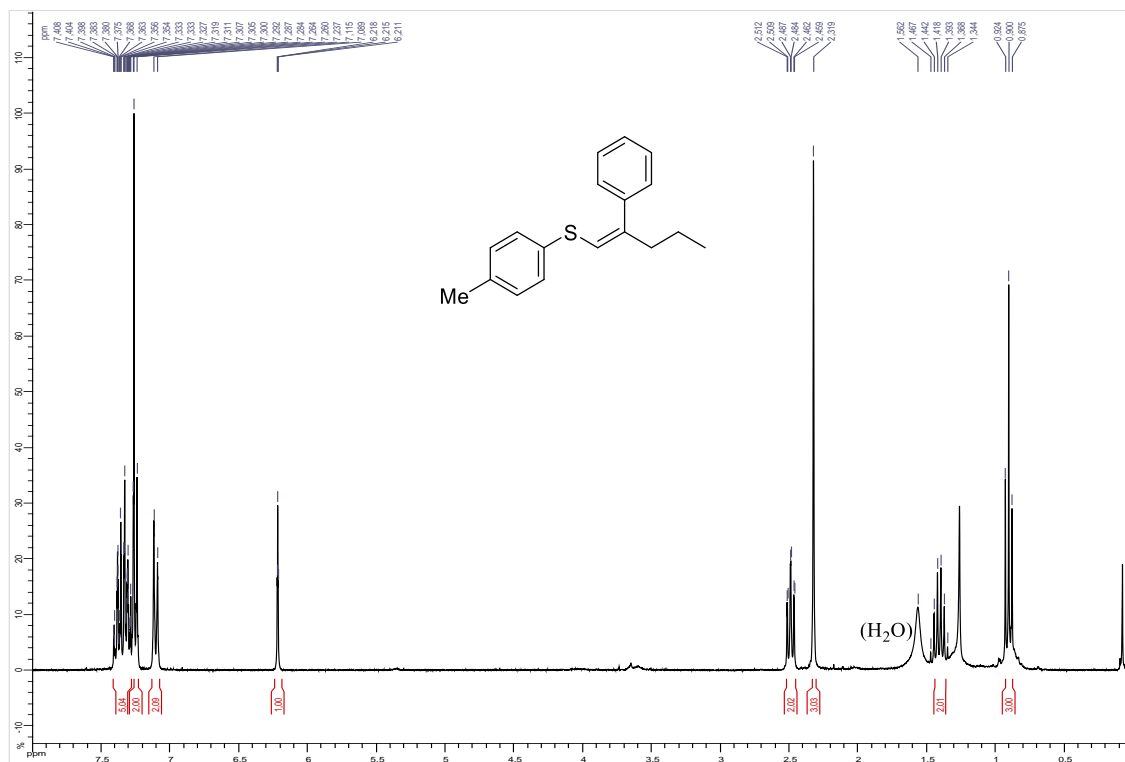


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

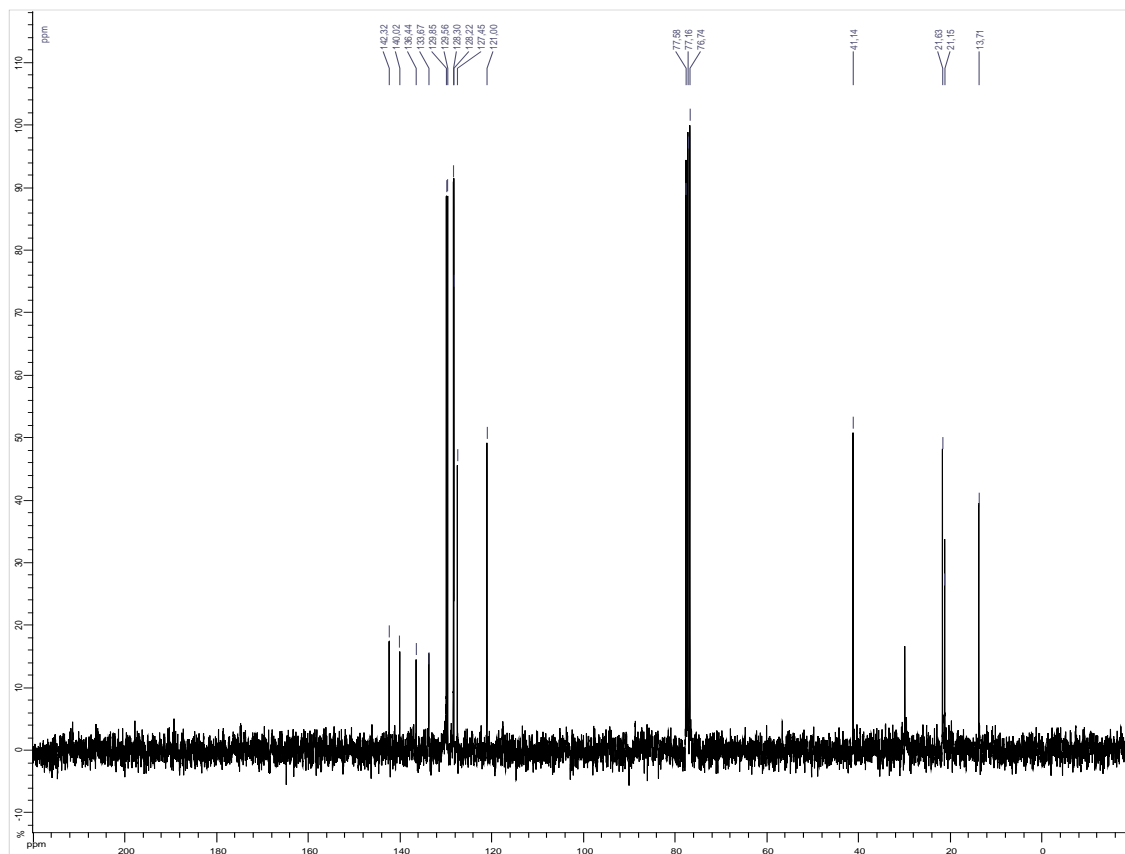


### III.20. (Z)-5d.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)

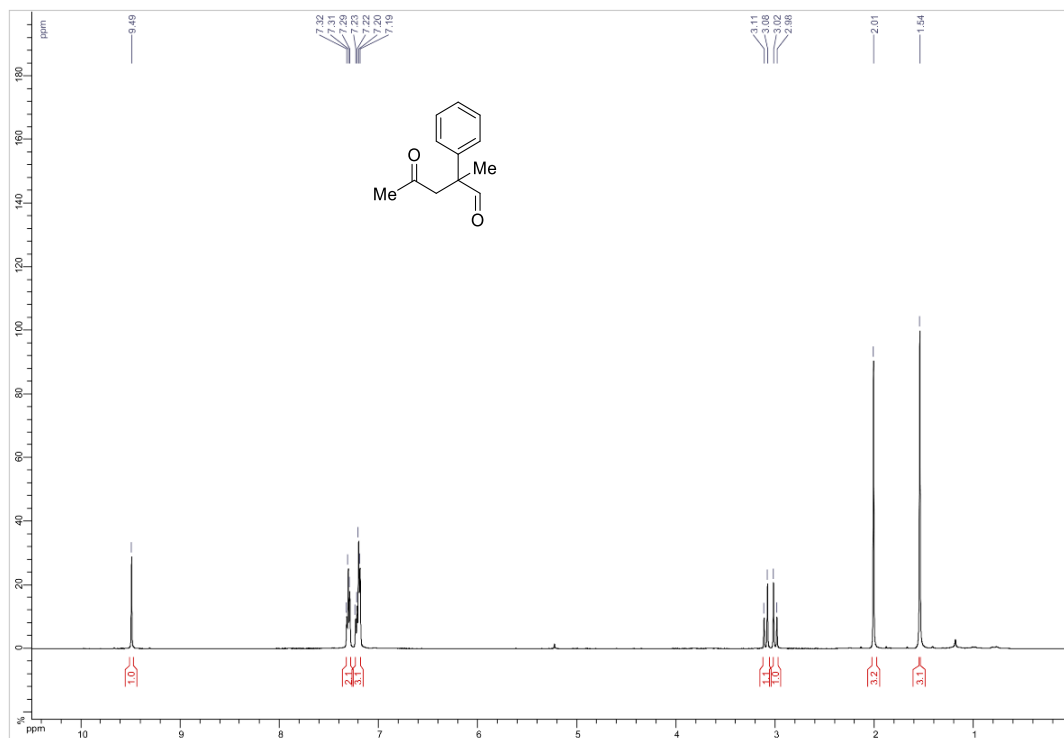


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz)

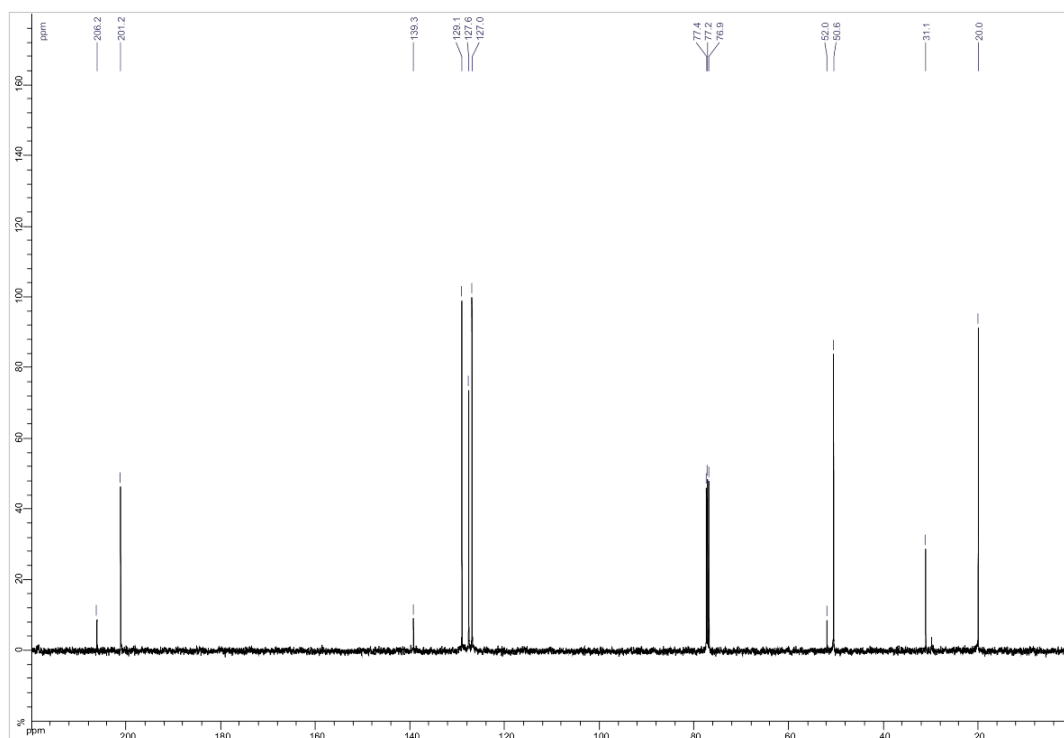


### III.21. 3e

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)



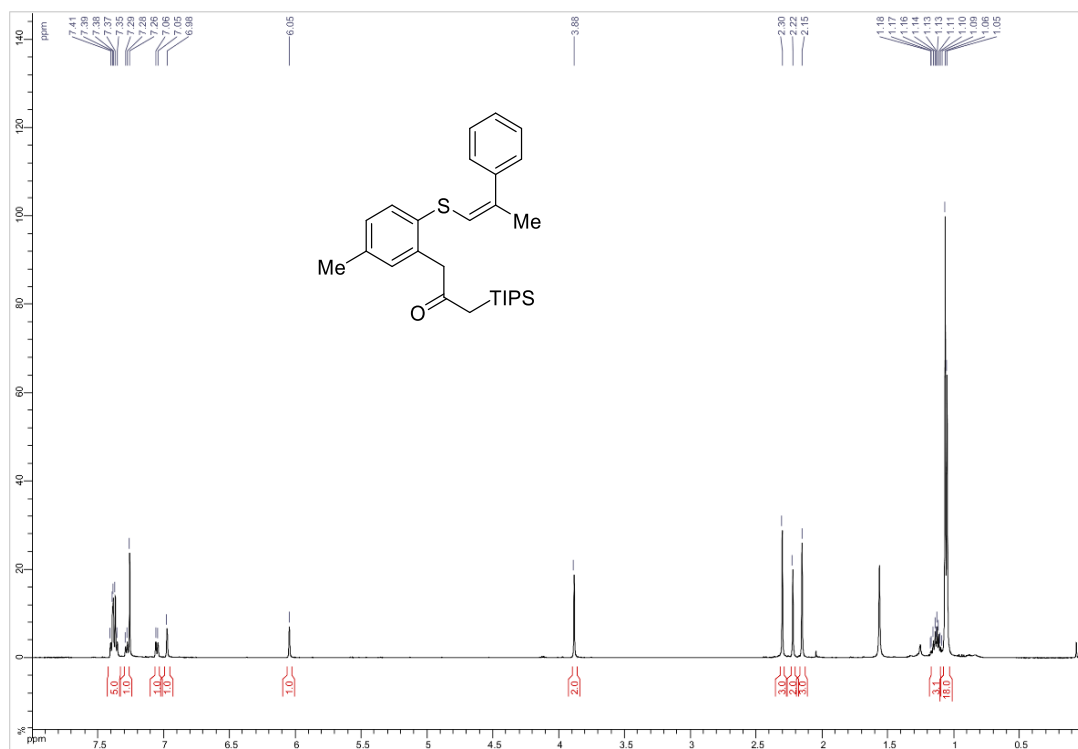
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)



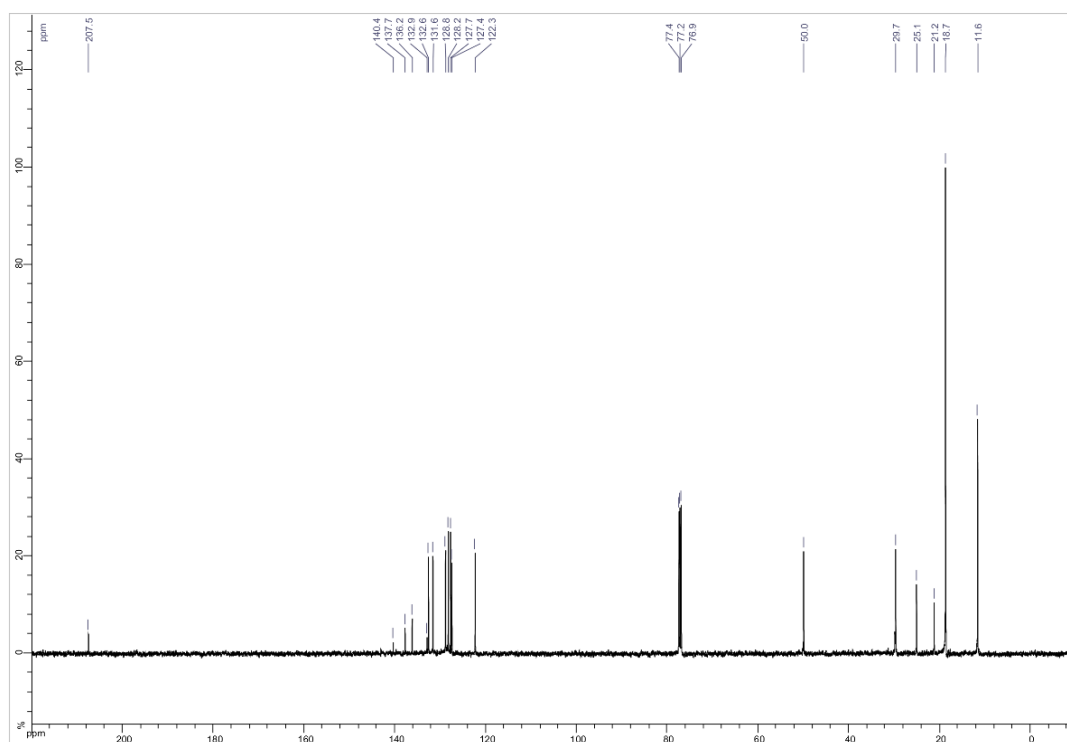


### III.22. (Z)-4e

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)

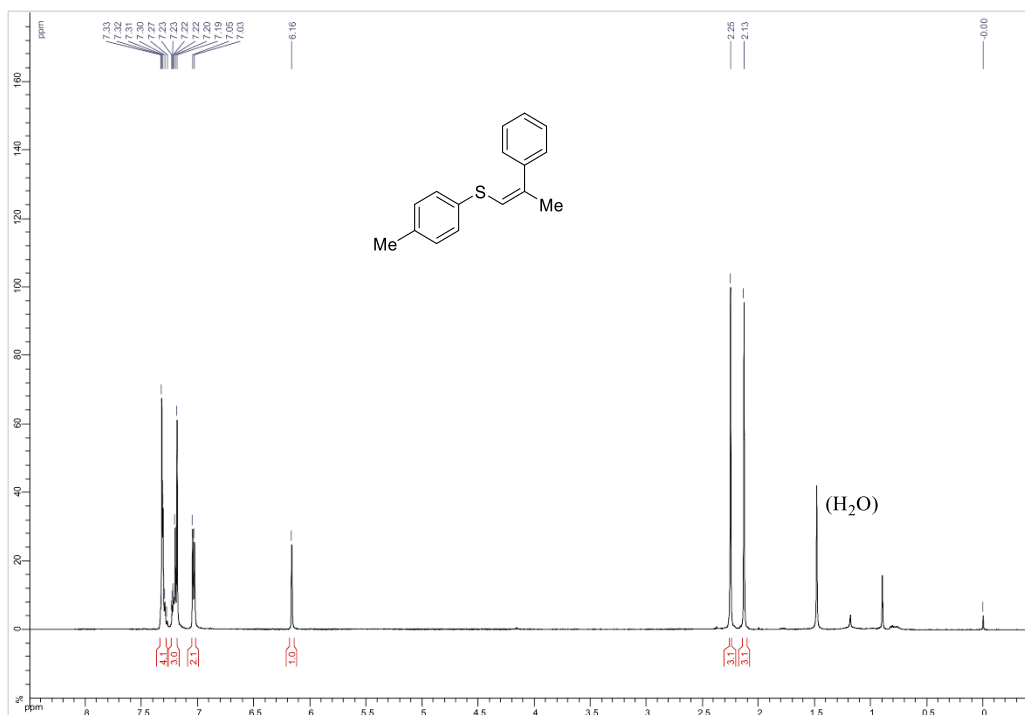


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)

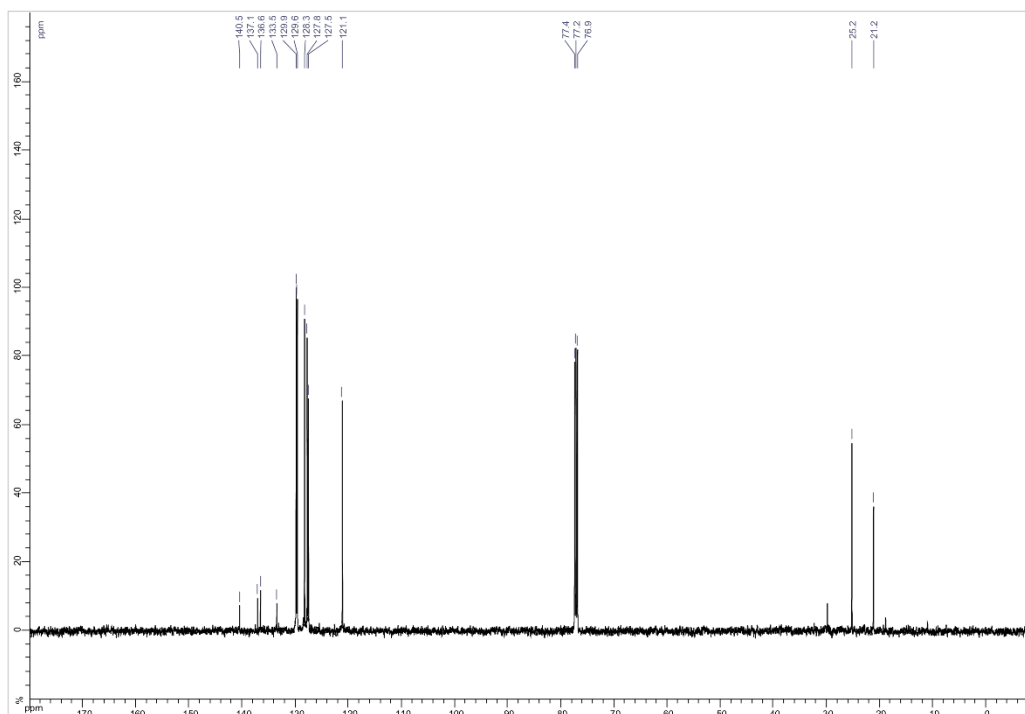


### III.23. (Z)-5e

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)



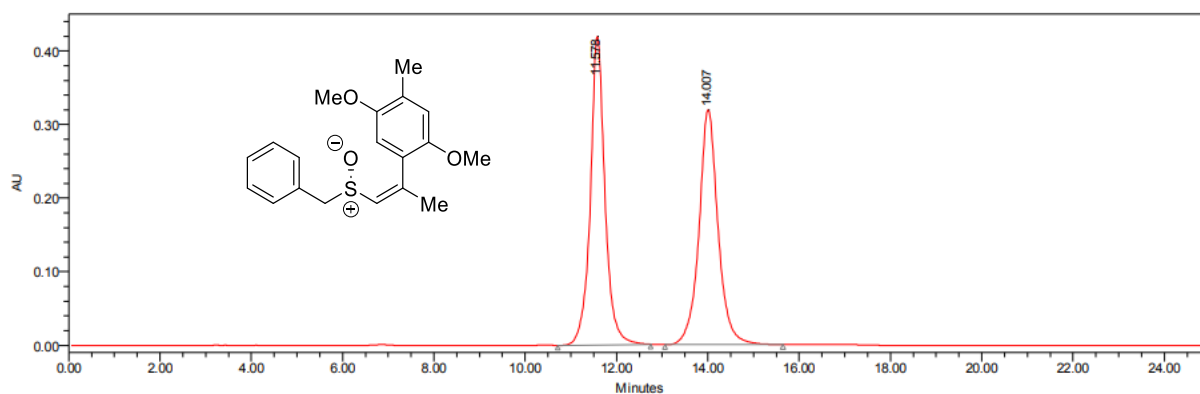
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz)



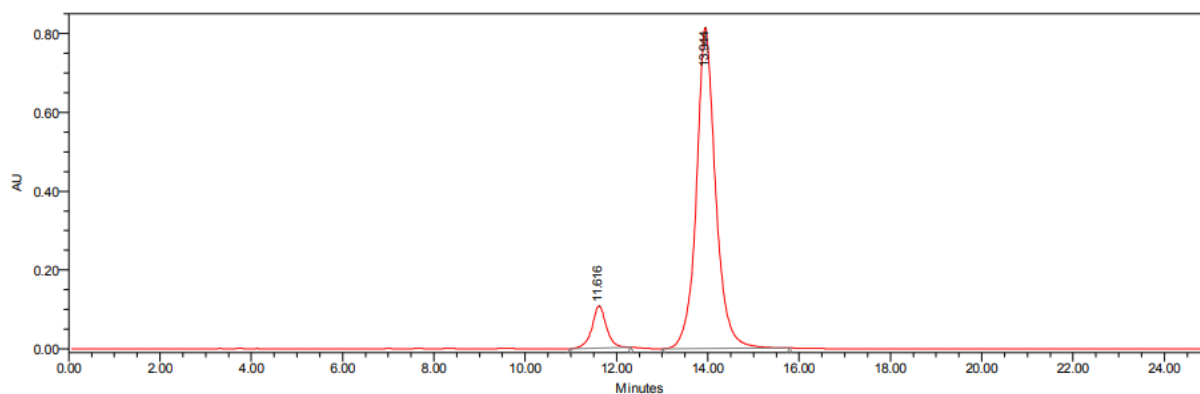
## IV. Chiral HPLC Spectra:

### IV.1. Compound (*S,Z*)-1d.

82% ee [Daicel Chiralpak IA column, heptane/*i*-PrOH = 90:10, 1.0 mL/min, 217.2 nm,  $t_R$  = 11.6 min and 14.0 min].



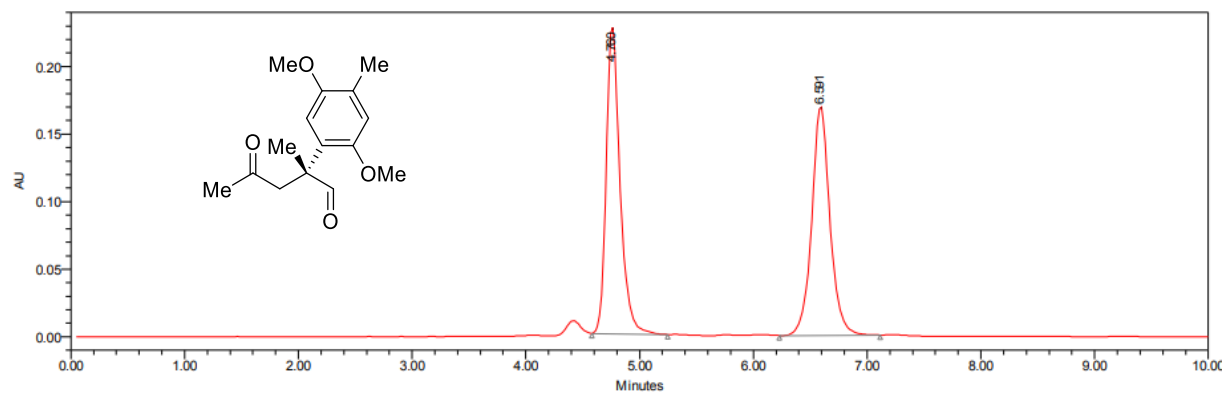
	Processed Channel Descr.	RT	Area	% Area
1	996 PDA 217.2 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	11.578	9338913	50.14
2	996 PDA 217.2 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	14.007	9286217	49.86



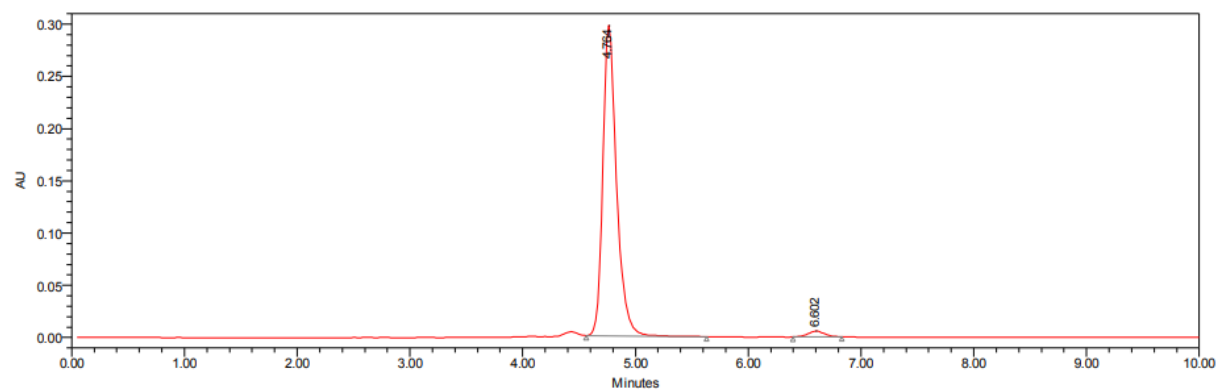
	Processed Channel Descr.	RT	Area	% Area
1	996 PDA 217.2 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	11.616	2332600	8.93
2	996 PDA 217.2 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	13.944	23782399	91.07

## IV.2. Compound (*R*)-3a.

96% ee [Daicel Chiralpak IA column, heptane/*i*-PrOH = 80:20, 1.0 mL/min, 290.6 nm,  $t_R$  = 4.8 min and 6.6 min].



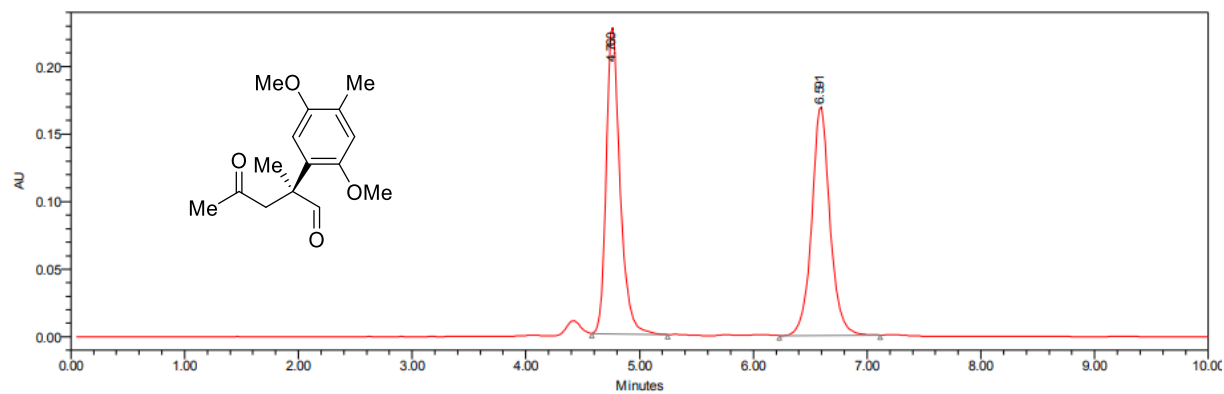
	Processed Channel Descr.	RT	Area	% Area
1	996 PDA 290.6 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	4.760	1909256	50.41
2	996 PDA 290.6 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	6.591	1878198	49.59



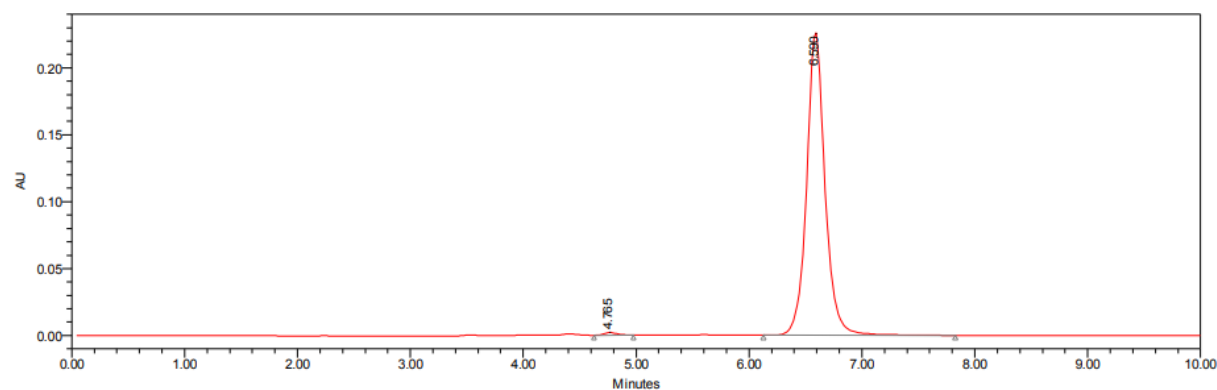
	Processed Channel Descr.	RT	Area	% Area
1	996 PDA 290.6 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	4.764	2510266	97.79
2	996 PDA 290.6 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	6.602	56631	2.21

### IV.3. Compound (*S*)-3a.

99% ee [Daicel Chiralpak IA column, heptane/*i*-PrOH = 80:20, 1.0 mL/min, 290.6 nm,  $t_R$  = 4.8 min and 6.6 min].



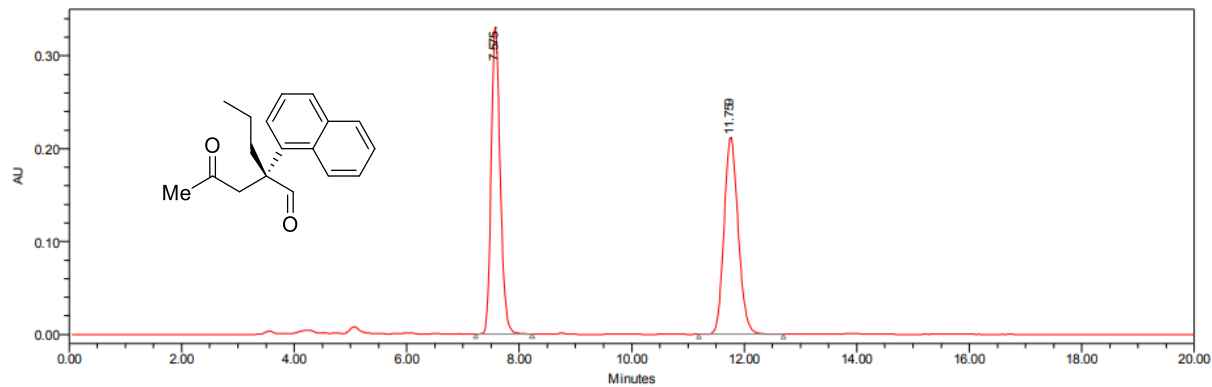
	Processed Channel Descr.	RT	Area	% Area
1	996 PDA 290.6 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	4.760	1909256	50.41
2	996 PDA 290.6 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	6.591	1878198	49.59



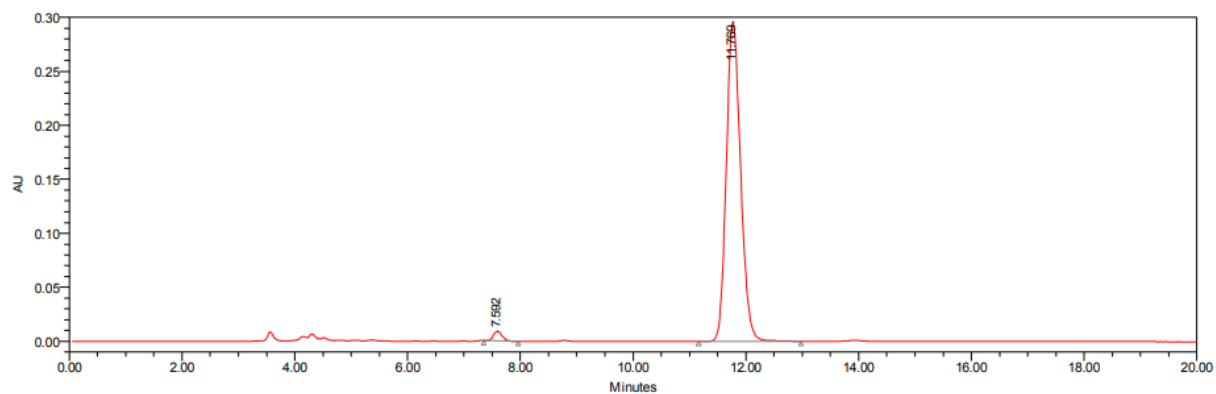
	Processed Channel Descr.	RT	Area	% Area
1	996 PDA 290.6 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	4.765	18202	0.70
2	996 PDA 290.6 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	6.590	2566592	99.30

#### IV.4. Compound (*R*)-3b.

96% ee [Daicel Chiralpak IC column, heptane/*i*-PrOH = 80:20, 1.0 mL/min, 281.1 nm,  $t_R$  = 7.6 min and 11.8 min].



	Processed Channel Descr.	RT	Area	% Area
1	996 PDA 281.1 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	7.575	3690943	49.89
2	996 PDA 281.1 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	11.759	3707950	50.11



	Processed Channel Descr.	RT	Area	% Area
1	996 PDA 281.1 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	7.592	94328	1.78
2	996 PDA 281.1 nm (PDA 200.0 to 400.0 nm at 2.4 nm)	11.769	5203913	98.22

## V. Computational details:

**Table S1.** Coordinates (x,y,z), energies (Hartree, uncorrected) and imaginary frequencies ( $\text{cm}^{-1}$ ) of the computed species.

<b>1</b>				<b>3</b>			
Thermal correction to Gibbs Free Energy= 0.222592				Thermal correction to Gibbs Free Energy= 0.290376			
E(RBMK) = -1092.42351353				E(RBMK) = -761.391472322			
C	1.662742	-0.995033	1.103969	C	-3.233151	-0.636346	-1.293682
C	0.464889	-1.316284	0.604036	C	-1.975776	-0.659027	-1.561766
C	2.575162	-0.015705	0.461906	H	-3.621094	-0.274583	-0.345416
C	2.153303	-1.621207	2.376558	H	-3.942297	-0.993608	-2.039166
S	-0.117225	-0.830988	-1.013611	C	-0.661912	-0.699261	-1.816601
H	-0.18547	-2.046667	1.080007	H	-0.251807	0.03658	-2.510043
O	-0.426015	-2.129211	-1.712181	H	-0.176126	-1.677319	-1.78638
C	-1.718556	-0.187973	-0.463663	Si	0.184901	0.098884	0.001792
C	-2.816411	-1.023028	-0.591264	C	1.984933	-0.33542	-0.382778
C	-1.861304	1.112322	0.004533	C	-0.634449	-0.79756	1.442893
C	3.843368	-0.413639	0.030748	C	-0.137869	1.957318	-0.101702
C	2.202515	1.320094	0.305475	H	2.481321	0.166204	0.466297
H	2.334526	-0.85219	3.134693	C	2.351844	-1.817274	-0.317899
H	1.439565	-2.346794	2.770211	C	2.499903	0.316291	-1.66837
H	3.109272	-2.128739	2.209835	H	-1.61497	-0.314281	1.561262
C	4.703752	0.496761	-0.56647	C	0.172985	-0.509334	2.720994
H	4.146475	-1.45027	0.138418	C	-0.864803	-2.301533	1.266675
H	5.677518	0.167905	-0.913935	H	0.017563	2.228058	-1.155796
C	4.319957	1.824118	-0.722304	C	0.90612	2.728097	0.72494
H	4.995291	2.535685	-1.185322	C	-1.55668	2.374762	0.292612
C	3.069044	2.234478	-0.280479	H	2.121168	-2.266667	0.649822
H	2.76478	3.269959	-0.391764	H	1.849046	-2.404936	-1.09417
H	1.234267	1.644485	0.671261	H	3.426505	-1.938577	-0.484563
H	-2.664808	-2.015004	-1.006862	H	3.588082	0.219938	-1.72504
C	-4.069767	-0.556387	-0.215318	H	2.09809	-0.178164	-2.559455
H	-4.933926	-1.206651	-0.317196	H	2.265762	1.382389	-1.734568
C	-4.241118	0.736617	0.278605	H	0.282703	0.559704	2.923594
C	-3.119027	1.563973	0.376148	H	-0.33371	-0.950139	3.584699
C	-5.593566	1.228955	0.705324	H	1.17404	-0.949329	2.675904
H	-3.235943	2.58116	0.738995	H	-1.383879	-2.698696	2.144308
H	-6.393411	0.648031	0.241097	H	-1.48234	-2.540117	0.396071
H	-5.737825	2.279562	0.44044	H	0.073378	-2.853225	1.174521
H	-5.713384	1.146621	1.791291	H	0.749627	3.803357	0.597335
H	-1.003107	1.774032	0.067235	H	0.817294	2.518044	1.794873
				H	1.933992	2.512605	0.422288

	H	-2.321649	1.928641	-0.348468			
	H	-1.782779	2.115468	1.33158			
	H	-1.663408	3.460009	0.203534			
<b>TS1</b>				<b>4</b>			
Thermal correction to Gibbs Free Energy= 0.536817				Thermal correction to Gibbs Free Energy= 0.539787			
E(RBMK) = -1853.82943173				E(RBMK) = -1853.88190649			
Frequency -165.3553							
C	-1.233179	-0.572175	-1.773578	C	-0.699049	-0.869889	2.896476
O	0.213021	0.505277	0.002682	C	2.593346	-2.437639	1.169946
C	-0.594008	-1.674065	-1.94336	C	-0.656095	-0.50638	1.618622
C	-2.077455	0.491317	-1.760855	H	0.037264	-0.51077	3.604143
S	1.642038	0.000575	-0.216295	H	-1.507455	-1.492441	3.258971
H	-0.220575	-2.289924	-1.127626	C	2.557333	-1.090778	1.249492
H	-0.386625	-1.995666	-2.963051	C	1.93802	-3.202988	0.089134
H	-2.958832	0.307783	-2.387897	C	3.358245	-3.215311	2.189248
H	-1.614164	1.473189	-1.856698	O	0.371036	0.409458	1.283268
Si	-3.187389	0.587117	-0.013072	C	-1.598351	-0.841193	0.528848
C	2.156225	-0.681014	1.341223	S	1.515819	-0.164024	0.208851
C	2.701318	1.444269	-0.225014	H	3.080796	-0.525308	2.01295
C	2.259021	-2.000307	1.553497	C	1.019897	-4.211816	0.396365
H	2.28523	0.04913	2.13499	C	2.2597	-2.955569	-1.249369
C	2.075438	-3.010857	0.480967	H	4.153666	-3.783393	1.696559
C	2.570868	-2.526147	2.921035	H	3.790594	-2.580097	2.962711
C	1.077814	-3.984479	0.60237	H	2.701806	-3.952436	2.662601
C	2.902757	-3.031869	-0.644304	H	-2.220511	-1.675517	0.86479
H	3.501603	-3.101769	2.896287	H	-1.057641	-1.202879	-0.355915
H	2.667844	-1.724078	3.653776	Si	-2.805724	0.566991	-0.026984
H	1.788133	-3.21394	3.256542	C	2.379424	1.34707	-0.048774
C	0.895049	-4.936378	-0.393586	C	0.410061	-4.932127	-0.620066
H	0.435882	-3.993198	1.477619	H	0.76099	-4.414617	1.430256
C	2.727356	-3.992576	-1.632699	C	1.661331	-3.693608	-2.261855
H	3.70566	-2.307343	-0.728308	H	3.016001	-2.215235	-1.492056
C	-4.872575	1.099217	-0.719311	C	2.756105	2.164101	1.017184
C	-2.352547	1.862863	1.100386	C	2.662847	1.68847	-1.366817
C	-3.274151	-1.156148	0.730634	H	2.491713	1.907178	2.03643
C	2.275472	2.616078	0.385016	C	3.439016	3.33303	0.741333
C	3.928608	1.374519	-0.872743	C	3.362077	2.861245	-1.615407
H	0.116193	-5.683909	-0.286739	H	2.342251	1.055199	-2.187
C	1.719869	-4.942824	-1.513599	H	3.728119	3.982855	1.561089
H	3.388517	-4.005944	-2.492508	C	3.760387	3.698597	-0.573546
H	-5.507405	1.100982	0.180815	H	3.591882	3.134148	-2.639708
C	-4.918078	2.503883	-1.32354	C	-4.297667	-0.314494	-0.816378
C	-5.459061	0.071744	-1.691347	C	-1.882254	1.739523	-1.214836



H	-1.510307	1.317721	1.542538	C	-3.367697	1.506347	1.536697
C	-3.339235	2.246924	2.214487	H	-5.013573	0.491863	-1.031272
C	-1.776259	3.100147	0.412436	C	-3.997744	-1.031459	-2.135036
H	-3.284954	-1.843644	-0.12786	C	-4.971115	-1.277854	0.167921
C	-4.570926	-1.387087	1.519633	H	-1.156813	2.253431	-0.566568
C	-2.058101	-1.489849	1.600482	C	-2.816724	2.80604	-1.796946
H	1.297526	2.652827	0.85254	C	-1.092617	1.062352	-2.337966
C	3.106844	3.726298	0.35951	H	-3.426054	0.73359	2.318366
C	4.748678	2.493604	-0.882943	C	-4.757338	2.142051	1.416635
H	4.241556	0.462335	-1.371229	C	-2.350513	2.55348	2.003548
H	1.588991	-5.69736	-2.281644	H	-0.313203	-5.701504	-0.373535
H	2.778834	4.648112	0.830102	C	0.730728	-4.676754	-1.949404
C	4.355475	3.683459	-0.266076	H	1.9314	-3.507803	-3.295502
H	5.70743	2.44646	-1.389635	H	-3.679982	-0.341998	-2.920663
C	5.258262	4.880355	-0.2623	H	-3.215691	-1.790997	-2.01942
H	5.916757	4.860565	0.612857	H	-4.891763	-1.548438	-2.501527
H	4.688517	5.810947	-0.222565	H	-5.918733	-1.64485	-0.240785
H	5.894195	4.904384	-1.149599	H	-4.347803	-2.159722	0.354033
H	-4.650551	3.278227	-0.601549	H	-5.18991	-0.81732	1.135812
H	-4.24711	2.602349	-2.184804	H	-3.318242	3.388497	-1.019594
H	-5.92765	2.728123	-1.683119	H	-2.259963	3.511892	-2.423762
H	-6.505049	0.309885	-1.90871	H	-3.592999	2.35895	-2.426967
H	-4.941152	0.083718	-2.658937	H	-0.484153	1.79998	-2.8749
H	-5.428168	-0.952598	-1.310413	H	-0.418085	0.278848	-1.976183
H	-3.712966	1.380545	2.768776	H	-1.751408	0.597378	-3.075871
H	-2.84352	2.901249	2.939206	H	-5.044901	2.608189	2.365543
H	-4.204372	2.794319	1.826932	H	-4.780284	2.928623	0.655866
H	-1.359663	3.777984	1.16597	H	-5.534451	1.41724	1.161684
H	-0.961516	2.835508	-0.265509	H	-1.346088	2.142331	2.135492
H	-2.527498	3.668479	-0.142652	H	-2.2778	3.380374	1.289128
H	-4.598368	-2.415176	1.895142	H	-2.658198	2.984777	2.962632
H	-4.637475	-0.72898	2.391431	H	0.263407	-5.252851	-2.740338
H	-5.471123	-1.236359	0.919253	C	4.508279	4.967193	-0.840818
H	-1.106901	-1.271583	1.109289	H	5.489432	4.946417	-0.356897
H	-2.0758	-0.909567	2.528661	H	3.967745	5.828388	-0.437387
H	-2.075331	-2.548257	1.882088	H	4.659598	5.129032	-1.908579
<b>TS2</b>				<b>5</b>			
Thermal correction to Gibbs Free Energy= 0.541440				Thermal correction to Gibbs Free Energy= 0.549024			
E(RBMK) = -1853.86415730				E(RBMK) = -1853.96022140			
Frequency -186.2971							
C	0.245223	0.63169	2.258772	C	-0.211848	-2.023675	1.071705
C	-1.137936	2.785324	1.195478	C	1.319843	-1.84871	1.13935
C	0.327699	0.06356	1.00713	C	-0.633634	-1.133849	-0.04055

H	-0.623207	0.439014	2.875532	H	-0.688412	-1.651286	1.988404
H	1.103982	1.109159	2.718734	H	-0.544393	-3.05313	0.928765
C	-2.106706	1.846866	0.902074	C	1.464916	-0.420756	0.560186
C	-0.161859	3.303228	0.218168	C	2.024302	-2.881577	0.259679
C	-1.27357	3.540819	2.482581	C	1.816086	-1.85569	2.584477
O	-0.743272	-0.545552	0.565787	O	0.261528	-0.2698	-0.336917
C	1.514087	0.16186	0.129112	C	-1.880214	-1.148791	-0.725298
S	-1.975739	0.776113	-0.398719	S	2.96648	-0.092951	-0.331814
H	-2.891283	1.627267	1.618089	H	1.312895	0.349978	1.319118
C	1.129428	3.664767	0.622728	C	1.427239	-3.372703	-0.905463
C	-0.537228	3.537965	-1.110826	C	3.30577	-3.336162	0.578082
H	-1.691777	4.529655	2.260597	H	2.855318	-1.528576	2.649687
H	-1.924375	3.035188	3.196547	H	1.218178	-1.176754	3.198975
H	-0.302356	3.716405	2.948151	H	1.74732	-2.858797	3.010465
H	2.176386	0.963265	0.46642	H	-2.370461	-2.119719	-0.648861
H	1.188783	0.401583	-0.891039	H	-1.783897	-0.809405	-1.759353
Si	2.605115	-1.430723	-0.015271	Si	-3.220096	0.150012	-0.012473
C	-3.395374	-0.248427	-0.298464	C	2.995314	1.691146	-0.24954
C	2.028773	4.205457	-0.28124	C	2.086054	-4.278327	-1.725767
H	1.441667	3.499261	1.648417	H	0.4286	-3.062333	-1.199277
C	0.36179	4.092303	-2.0114	C	3.965184	-4.24604	-0.238298
H	-1.554035	3.339069	-1.430097	H	3.808191	-2.981799	1.469514
C	-3.802736	-0.845115	0.895101	C	2.433017	2.445207	-1.276735
C	-4.07216	-0.487167	-1.49328	C	3.63512	2.331282	0.810473
H	-3.229859	-0.708352	1.804325	H	1.958032	1.946785	-2.114543
C	-4.923769	-1.652811	0.885215	C	2.495477	3.831006	-1.227455
C	-5.196126	-1.298127	-1.476933	C	3.687	3.71701	0.848134
H	-3.73463	-0.036701	-2.42068	H	4.098856	1.745817	1.597289
H	-5.244816	-2.124593	1.808382	H	2.057428	4.412306	-2.033103
C	-5.642326	-1.890181	-0.294372	C	3.121799	4.490144	-0.168369
H	-5.73472	-1.475899	-2.401539	H	4.187276	4.208148	1.677192
C	4.142159	-0.891801	-1.001529	C	-4.833299	-0.474204	-0.787316
C	1.59756	-2.810179	-0.853085	C	-2.657829	1.875243	-0.562937
C	3.124608	-1.93656	1.752832	C	-3.261567	-0.013843	1.884134
H	4.805258	-1.768595	-0.976172	H	-5.590928	0.191329	-0.345815
C	3.872392	-0.55999	-2.47087	C	-4.91157	-0.322843	-2.308009
C	4.88093	0.266054	-0.321699	C	-5.174015	-1.906944	-0.365327
H	0.901016	-3.152035	-0.074308	H	-1.864962	2.156487	0.144217
C	2.488057	-3.999556	-1.231905	C	-3.810029	2.875286	-0.383174
C	0.746898	-2.363786	-2.045116	C	-2.061866	1.96906	-1.970024
H	3.264122	-0.984601	2.288747	H	-3.095789	-1.081519	2.095559
C	4.457203	-2.691411	1.815034	C	-4.62763	0.353334	2.480239
C	2.039929	-2.729843	2.489593	C	-2.159405	0.794596	2.577817
H	3.028971	4.467058	0.045961	H	1.598964	-4.643186	-2.623355

C	1.648344	4.41872	-1.602958	C	3.359629	-4.720004	-1.39366
H	0.048848	4.284108	-3.031663	H	4.958391	-4.585221	0.034531
H	3.478385	-1.415484	-3.024663	H	-4.80669	0.715164	-2.631922
H	3.158928	0.265382	-2.578354	H	-4.143679	-0.91453	-2.819086
H	4.797191	-0.248626	-2.969694	H	-5.879698	-0.680427	-2.67365
H	5.840525	0.454619	-0.815349	H	-6.193752	-2.160365	-0.671669
H	4.304857	1.196396	-0.385261	H	-4.515556	-2.63651	-0.850017
H	5.090296	0.075896	0.735373	H	-5.110928	-2.06411	0.715391
H	3.036423	-4.401244	-0.374988	H	-4.20489	2.886089	0.637093
H	1.885463	-4.816943	-1.643283	H	-3.467919	3.890659	-0.607659
H	3.224288	-3.726396	-1.995202	H	-4.643203	2.65863	-1.059092
H	0.175167	-3.211614	-2.439813	H	-1.79015	3.006935	-2.189603
H	0.028715	-1.590592	-1.76045	H	-1.150679	1.373608	-2.074764
H	1.354878	-1.977381	-2.868108	H	-2.766702	1.653418	-2.744331
H	4.728804	-2.901438	2.855529	H	-4.618731	0.204098	3.564829
H	4.399432	-3.655754	1.300505	H	-4.875848	1.404456	2.304434
H	5.282511	-2.130384	1.369314	H	-5.44141	-0.252167	2.074679
H	1.067866	-2.227875	2.488816	H	-1.157938	0.61433	2.170633
H	1.898278	-3.716882	2.037541	H	-2.345208	1.868909	2.487162
H	2.325064	-2.89396	3.534818	H	-2.125423	0.564011	3.647848
H	2.349838	4.851533	-2.307489	H	3.874083	-5.432153	-2.029111
C	-6.841418	-2.785393	-0.281857	C	3.223011	5.98584	-0.141144
H	-7.406394	-2.715205	-1.212163	H	2.422196	6.452631	-0.718086
H	-7.508937	-2.538076	0.547569	H	4.174178	6.312538	-0.574921
H	-6.536425	-3.829078	-0.151781	H	3.181647	6.370874	0.88016
<b>6</b>				<b>TS3</b>			
Thermal correction to Gibbs Free Energy= 0.541223				Thermal correction to Gibbs Free Energy= 0.541935			
E(RBMK) = -1853.88100611				E(RBMK) = -1853.85060499			
Frequency				Frequency -152.2592			
C	-0.214176	-2.374896	-1.736281	C	0.731349	1.487636	-1.704387
C	3.224023	-1.959807	-0.920803	C	-1.043282	3.183045	-0.766979
C	-0.235194	-1.360216	-0.877464	C	0.599991	0.522648	-0.703739
C	2.6993	-1.229194	0.14689	C	-1.267254	2.439788	0.411679
C	3.979168	-3.0831	-0.646926	C	-0.344893	4.392105	-0.69474
C	-1.068677	-1.194429	0.340936	C	1.634486	0.289236	0.333844
C	2.900756	-1.626303	1.46561	C	-0.66127	2.857333	1.613038
C	4.22057	-3.496418	0.671501	C	0.209539	4.833248	0.495638
C	2.738031	1.202363	-1.104445	C	-3.278255	0.979792	-0.774975
C	3.669855	-2.753711	1.715869	C	0.050555	4.031646	1.64647
C	5.048914	-4.713768	0.93843	C	0.953942	6.127017	0.582703
C	-3.612666	-0.310095	1.79568	C	3.786874	-1.467019	1.610184
C	-2.886096	0.989023	-0.92949	C	1.803698	-2.726415	-0.436624
C	-3.788136	-2.023663	-0.905572	C	3.960077	-0.699855	-1.489044

C	2.779113	2.545539	-0.976	C	-4.222847	0.014619	-0.916504
C	-2.810448	0.766411	2.535466	C	2.828077	-1.751681	2.771572
C	-3.773171	-1.549984	2.678531	C	4.770106	-0.358626	1.992612
C	-4.131595	1.857614	-0.720849	C	2.48651	-4.046736	-0.061175
C	-2.622968	0.788228	-2.42557	C	1.34822	-2.769934	-1.899291
C	-5.277501	-1.716242	-1.101477	C	5.062193	-1.740239	-1.720594
C	-3.609281	-3.440831	-0.352345	C	4.55869	0.708353	-1.434733
C	1.841418	3.312633	-0.138629	C	-4.224116	-1.237154	-0.150667
C	3.807502	3.312456	-1.741425	C	-5.327975	0.240839	-1.898577
C	2.316222	4.25995	0.775504	C	-5.417897	-1.727047	0.399172
C	0.461137	3.136956	-0.287733	C	-3.044411	-1.97804	0.016973
C	1.426868	4.988704	1.549417	C	-5.421751	-2.902582	1.130564
C	-0.42467	3.889082	0.473229	C	-3.061519	-3.165639	0.735359
C	0.055519	4.808412	1.396855	C	-4.24423	-3.626233	1.299145
H	-4.617829	0.0953	1.610491	H	4.37158	-2.380962	1.43191
H	0.439848	-2.359815	-2.598218	H	0.0212	1.479321	-2.521638
H	-0.889328	-3.211735	-1.611899	H	1.617288	2.106103	-1.79693
H	3.03256	-1.663733	-1.946241	H	-1.539033	2.916234	-1.690984
O	0.585254	-0.267913	-1.234438	O	-0.487979	-0.151739	-0.692558
S	1.723769	0.21818	-0.092683	S	-2.099807	0.937333	0.481344
H	4.389351	-3.660273	-1.469432	H	-0.236577	4.989143	-1.594086
H	-1.104721	-2.140247	0.890275	H	2.244936	1.181359	0.500344
H	-0.626469	-0.454557	1.017345	H	1.135398	0.026266	1.272314
Si	-2.90233	-0.644823	0.06033	Si	2.846735	-1.180366	-0.020483
H	2.471729	-1.060463	2.286019	H	-0.795968	2.271539	2.516467
H	3.401042	0.653331	-1.762187	H	-3.295033	1.86883	-1.392101
H	-2.670498	1.676298	1.943747	H	2.094402	-2.529425	2.538599
H	-2.03094	1.541234	-0.511801	H	0.902392	-2.628625	0.186754
H	-3.313651	-1.997248	-1.897958	H	3.287868	-0.734904	-2.35982
H	3.312564	4.021753	-2.411775	H	-5.360523	-0.579938	-2.621351
H	4.465041	2.664255	-2.321075	H	-5.218808	1.185691	-2.431899
H	4.418405	3.908315	-1.055961	H	-6.297147	0.248563	-1.389639
H	3.383152	4.409361	0.902226	H	-6.341198	-1.170826	0.282201
H	0.083237	2.452302	-1.041268	H	-2.126752	-1.654116	-0.462381
H	1.804097	5.706817	2.268915	H	-6.346902	-3.259804	1.568945
H	-1.492964	3.766521	0.331241	H	-2.14772	-3.740124	0.840664
H	-0.637309	5.394596	1.990397	H	-4.254633	-4.554382	1.86004
H	3.839925	-3.06344	2.741357	H	0.483464	4.361586	2.585471
H	-1.817161	0.399884	2.819051	H	2.275733	-0.850516	3.06107
H	-3.315687	1.054446	3.463775	H	3.382058	-2.079666	3.657748
H	-4.151227	-1.268625	3.667835	H	5.243764	-0.582558	2.955066
H	-2.820462	-2.068042	2.837351	H	4.271833	0.611673	2.101019
H	-4.476929	-2.271055	2.257426	H	5.570766	-0.241827	1.258572
H	-4.030347	2.80751	-1.25885	H	1.823121	-4.892326	-0.275356

H	-4.312108	2.093045	0.331561	H	2.75198	-4.100683	0.997649
H	-5.033758	1.372951	-1.105509	H	3.402634	-4.209032	-0.637719
H	-1.707595	0.224034	-2.622801	H	0.802562	-1.871967	-2.200307
H	-2.532898	1.75473	-2.935173	H	0.68393	-3.625246	-2.067902
H	-3.449106	0.25302	-2.904525	H	2.198654	-2.889213	-2.578484
H	-5.444316	-0.764823	-1.613503	H	4.660933	-2.746156	-1.871767
H	-5.809915	-1.676394	-0.145146	H	5.756245	-1.785163	-0.874586
H	-5.755685	-2.496479	-1.703754	H	5.652145	-1.488906	-2.608887
H	-4.140653	-3.577592	0.592854	H	5.2803	0.81522	-0.620722
H	-2.562543	-3.706299	-0.174405	H	3.801454	1.487139	-1.299912
H	-4.015612	-4.17659	-1.055157	H	5.090746	0.932612	-2.36599
H	5.118771	-4.92842	2.00528	H	1.977872	5.962578	0.932426
H	6.06356	-4.582577	0.550176	H	0.475067	6.799463	1.30104
H	4.623814	-5.589643	0.439687	H	0.998778	6.634139	-0.381654
<b>7</b>				<b>8</b>			
Thermal correction to Gibbs Free Energy= 0.546175				Thermal correction to Gibbs Free Energy= 0.524316			
E(RBMK) = -1853.91809514				E(RBMK) = -1932.07017508			
C	0.385708	1.678901	1.235878	C	1.475655	-1.648969	-0.769903
C	-0.583953	2.84349	0.916968	C	2.105826	-0.71167	-0.262784
C	1.306676	1.402291	0.051819	C	2.873831	0.346258	0.289578
H	-0.168164	0.760088	1.45916	C	5.565367	1.71158	0.659716
H	0.957576	1.922779	2.135232	C	5.277238	-1.313842	1.339957
C	-1.483677	2.572398	-0.242579	C	5.16199	-0.40975	-1.698335
C	0.168479	4.125465	0.81937	C	5.196499	2.054124	2.106789
H	-1.229728	2.93789	1.808654	C	5.274196	2.892057	-0.268978
O	0.931179	1.726637	-1.056539	C	6.773169	-1.329443	1.676501
C	2.603804	0.737678	0.312234	C	4.81038	-2.707888	0.911477
S	-2.594215	1.293563	-0.335037	C	6.658896	-0.311276	-2.019064
C	-1.539418	3.479542	-1.319684	C	4.334254	0.356381	-2.735482
C	0.082207	4.978502	-0.221216	H	6.649533	1.526791	0.627624
H	0.817627	4.35426	1.660709	H	1.444119	-2.596215	-1.27367
H	2.944449	0.899604	1.338717	H	2.663788	1.290164	-0.224581
H	3.338036	1.163991	-0.378898	H	2.680605	0.465006	1.360206
Si	2.721634	-1.166231	-0.041441	Si	4.811846	0.058019	0.107888
C	-2.658608	0.557892	1.252131	H	5.433448	1.247513	2.806513
C	-0.793426	4.621249	-1.303424	H	4.737699	-1.05149	2.262559
H	-2.199496	3.271432	-2.154916	H	4.877653	-1.469811	-1.771413
C	0.84994	6.260694	-0.298418	H	4.129019	2.281977	2.207027
C	4.535578	-1.612494	0.317492	H	5.740123	2.944391	2.440015
C	2.355959	-1.442312	-1.894731	H	5.755691	3.800433	0.108851
C	1.453754	-2.076409	1.052609	H	4.201741	3.108944	-0.335507
C	-3.206175	-0.656033	1.457278	H	5.644821	2.726605	-1.283322
H	-2.40115	1.199888	2.087927	H	6.977582	-2.069359	2.457583

H	4.630461	-2.652269	-0.02765	H	7.134703	-0.363716	2.040125
C	5.495108	-0.758143	-0.519275	H	7.380178	-1.606646	0.809181
C	4.941509	-1.578899	1.792317	H	3.731965	-2.755184	0.734126
H	2.772165	-0.555398	-2.3936	H	5.043457	-3.443828	1.688458
C	3.058325	-2.673782	-2.478573	H	5.31598	-3.036457	-0.002414
C	0.860455	-1.48428	-2.221959	H	7.274026	-0.916388	-1.347619
H	0.47787	-1.785404	0.632131	H	7.017147	0.721382	-1.955384
C	1.573524	-3.597843	0.908596	H	6.854435	-0.657853	-3.039323
C	1.452134	-1.681411	2.532165	H	4.556173	1.427186	-2.728168
C	-3.590046	-1.568827	0.361666	H	3.257105	0.236366	-2.585147
C	-3.456942	-1.115204	2.860535	H	4.560819	-0.009874	-3.74267
C	-4.853392	-2.170878	0.354706	Au	-0.386094	-0.687083	-0.291388
C	-2.69295	-1.870674	-0.669307	P	-2.551105	0.068915	0.051615
H	-2.959301	-2.073318	3.037709	C	-3.166852	-0.299422	1.719647
H	-3.11301	-0.38934	3.598949	C	-4.492533	-0.683114	1.927915
H	-4.526271	-1.282864	3.023297	H	-5.165479	-0.804637	1.085704
C	-5.218142	-3.025562	-0.67469	C	-4.946871	-0.919556	3.219756
H	-5.565377	-1.952254	1.143128	H	-5.9759	-1.221994	3.379655
C	-3.055793	-2.739643	-1.688791	C	-4.086595	-0.772832	4.300928
H	-1.693276	-1.450599	-0.655709	H	-4.444775	-0.961242	5.307147
H	-6.206614	-3.471417	-0.677009	H	-2.091114	-0.284746	4.938389
C	-4.320854	-3.313669	-1.697548	C	-2.764363	-0.392562	4.095149
H	-2.344393	-2.973247	-2.47344	C	-2.301749	-0.160625	2.807989
H	-4.605838	-3.99075	-2.495233	H	-1.266548	0.126418	2.647654
H	-0.87459	5.303709	-2.144966	C	-2.684682	1.866198	-0.181574
H	5.239337	-0.745239	-1.583095	C	-3.424887	2.657631	0.696879
H	5.512312	0.279784	-0.169167	H	-3.912252	2.21134	1.557104
H	6.519164	-1.136808	-0.434506	H	-4.105681	4.639278	1.154132
H	6.006839	-1.81142	1.898434	C	-3.532006	4.024879	0.469009
H	4.78743	-0.590469	2.239883	C	-2.908105	4.601455	-0.629954
H	4.391727	-2.30747	2.392609	H	-2.994666	5.668505	-0.803755
H	2.86094	-2.747142	-3.553705	H	-1.678978	4.263373	-2.363262
H	4.142973	-2.641863	-2.349806	C	-2.168157	3.813371	-1.506357
H	2.700587	-3.603161	-2.023894	C	-2.049873	2.449709	-1.281946
H	0.340902	-0.577424	-1.90135	H	-1.467707	1.836927	-1.964414
H	0.710746	-1.576128	-3.303682	C	-3.71078	-0.701117	-1.115768
H	0.376143	-2.350184	-1.756378	C	-3.628502	-2.079607	-1.332385
H	1.469186	-3.927995	-0.128385	H	-2.866157	-2.667542	-0.829089
H	2.540702	-3.958357	1.274141	C	-4.525778	-2.700637	-2.188445
H	0.798379	-4.106508	1.492629	H	-4.461037	-3.770369	-2.354028
H	2.35634	-2.022225	3.042034	C	-5.501378	-1.950305	-2.83764
H	1.385054	-0.600317	2.688513	H	-6.198226	-2.436677	-3.511495
H	0.602778	-2.141127	3.051034	H	-6.339561	0.00589	-3.136397
H	1.507409	6.264228	-1.173043	C	-5.581274	-0.579484	-2.628165

H	0.172737	7.114461	-0.396781	C	-4.689325	0.049817	-1.767328
H	1.463765	6.4135	0.589987	H	-4.7531	1.12097	-1.6085
<b>TS4</b>				<b>9</b>			
Thermal correction to Gibbs Free Energy= 0.766676				Thermal correction to Gibbs Free Energy= 0.770342			
E(RBMK) = -3024.49927195				E(RBMK) = -3024.52308069			
Frequency -110.8277							
C	1.064803	0.679946	-0.199148	C	-0.613166	-0.465162	-1.068699
O	3.349333	0.395642	-0.217671	C	-2.337559	-3.413915	0.304255
C	0.582054	-0.391292	0.250812	C	-1.602251	0.052984	-0.33799
H	0.983675	-1.267912	0.738837	H	-0.946714	-1.008228	-1.954056
C	1.21016	2.008177	-0.707082	C	-3.202657	-2.75227	-0.488242
S	3.726104	-1.086003	-0.115979	C	-2.071032	-3.036531	1.712021
C	4.789783	-1.194324	1.298713	C	-1.618471	-4.613906	-0.217573
C	4.447829	-1.86663	2.405091	O	-2.934091	-0.134799	-0.850535
C	3.225726	-2.705787	2.49401	C	-1.567957	0.873982	0.898799
C	5.30547	-1.805507	3.631391	S	-3.859104	-1.219787	0.017283
H	5.685046	-0.582248	1.234517	H	-3.422157	-3.045944	-1.509025
C	2.216616	-2.379402	3.404197	C	-0.784772	-2.662687	2.10965
C	3.078175	-3.845352	1.700633	C	-3.092717	-3.097048	2.663012
H	5.654172	-2.808797	3.896094	H	-1.853271	-5.484867	0.40242
H	6.168332	-1.152354	3.494372	H	-1.86464	-4.829009	-1.257929
H	4.72232	-1.442631	4.484043	H	-0.538469	-4.454565	-0.135005
H	0.194356	2.350418	-0.946745	H	-0.549878	0.827714	1.294823
H	1.786564	1.994322	-1.635815	H	-2.216526	0.438974	1.673282
Si	1.896926	3.376333	0.497764	Si	-2.023341	2.733642	0.700537
C	4.944989	-1.372335	-1.397229	C	-5.352908	-1.077811	-0.907253
C	1.072937	-3.161868	3.496385	C	-0.533995	-2.333658	3.43387
H	2.319406	-1.498525	4.029956	H	0.007351	-2.585412	1.371957
C	1.939699	-4.634972	1.804345	C	-2.832318	-2.780888	3.990507
H	3.874759	-4.125339	1.018982	H	-4.085217	-3.421412	2.36563
C	5.666119	-0.302899	-1.910546	C	-5.339058	-1.036676	-2.300488
C	5.135041	-2.663446	-1.873062	C	-6.538594	-0.994953	-0.186931
H	5.475173	0.698988	-1.541826	H	-4.401671	-1.055729	-2.844312
C	6.605546	-0.542213	-2.902331	C	-6.54421	-0.928379	-2.969169
C	6.082889	-2.883754	-2.862517	C	-7.736238	-0.898919	-0.882237
H	4.550038	-3.489614	-1.481153	H	-6.531416	-1.002616	0.897748
H	7.175314	0.288921	-3.306813	H	-6.545693	-0.885685	-4.053736
C	6.831529	-1.831066	-3.392405	C	-7.760354	-0.865086	-2.276111
H	6.239338	-3.890988	-3.235783	H	-8.667228	-0.838166	-0.32881
C	0.911971	4.941082	0.030704	C	-1.327344	3.624562	2.238522
C	3.770648	3.570102	0.251038	C	-3.915737	2.910014	0.52141
C	1.458436	2.870934	2.284184	C	-1.145031	3.393921	-0.861884
H	1.244914	5.698991	0.754569	H	-1.518661	4.692286	2.059075

C	1.209841	5.479373	-1.370797	C	-2.00508	3.246678	3.557613
C	-0.597561	4.758515	0.219161	C	0.189608	3.442039	2.356834
H	4.192257	2.697361	0.766335	H	-4.12092	2.467575	-0.464275
C	4.293129	4.837838	0.935979	C	-4.357791	4.376147	0.473815
C	4.246267	3.495771	-1.201463	C	-4.753895	2.140794	1.545656
H	0.476757	2.379879	2.20215	H	-0.190162	2.846619	-0.886715
C	1.305107	4.05716	3.242378	C	-0.823351	4.891513	-0.823575
C	2.439842	1.848538	2.864665	C	-1.893918	3.052073	-2.154415
H	0.293023	-2.892893	4.200752	H	0.46388	-2.026783	3.728611
C	0.932348	-4.292194	2.698176	C	-1.55475	-2.395815	4.37701
H	1.844085	-5.524597	1.191084	H	-3.62872	-2.842006	4.724101
H	2.256098	5.770032	-1.489743	H	-3.06256	3.520208	3.573621
H	0.979681	4.742733	-2.149581	H	-1.935355	2.171302	3.758198
H	0.600221	6.36579	-1.580449	H	-1.525359	3.760729	4.398793
H	-1.119992	5.713216	0.091922	H	0.595045	4.075631	3.154144
H	-1.019712	4.073537	-0.526246	H	0.446422	2.407702	2.612398
H	-0.861037	4.370248	1.207303	H	0.716431	3.69658	1.432016
H	4.045107	4.872071	2.000949	H	-3.862728	4.9334	-0.325914
H	5.384511	4.896229	0.855699	H	-5.437996	4.453235	0.303241
H	3.88887	5.745057	0.47439	H	-4.143625	4.891525	1.416445
H	5.339614	3.572801	-1.243065	H	-5.812808	2.151926	1.260428
H	3.96689	2.547789	-1.667649	H	-4.450161	1.093628	1.645957
H	3.849259	4.309372	-1.81536	H	-4.688153	2.586314	2.541886
H	0.994019	3.708033	4.233666	H	-0.255799	5.18221	-1.715098
H	2.250649	4.591895	3.377091	H	-1.731874	5.502134	-0.811951
H	0.562449	4.784546	2.904806	H	-0.228725	5.176706	0.048335
H	2.589963	0.990957	2.205164	H	-2.104557	1.983742	-2.246683
H	3.421112	2.303715	3.036903	H	-2.847135	3.588366	-2.2158
H	2.080487	1.481244	3.833603	H	-1.302397	3.34742	-3.028735
H	0.045452	-4.910882	2.782668	H	-1.353119	-2.147334	5.413246
C	7.829199	-2.070484	-4.486036	C	-9.05133	-0.754201	-3.026946
H	8.680767	-1.391471	-4.403553	H	-9.198864	-1.624085	-3.674091
H	7.371933	-1.904125	-5.467398	H	-9.052264	0.130814	-3.669833
H	8.204871	-3.095427	-4.467713	H	-9.905158	-0.685332	-2.35181
Au	-1.487551	-0.348107	-0.099267	Au	1.390244	-0.295931	-0.738351
P	-3.782585	-0.415423	-0.415839	P	3.707739	-0.182178	-0.399471
C	-4.447826	1.18612	-0.970632	C	4.661811	-0.991447	-1.724647
C	-5.593662	1.741606	-0.402144	C	5.827454	-1.71244	-1.461718
H	-6.104076	1.231095	0.407526	H	6.174551	-1.833566	-0.440852
C	-6.079187	2.956862	-0.872655	C	6.540584	-2.283495	-2.509139
H	-6.968986	3.387609	-0.426647	H	7.444366	-2.845681	-2.300241
C	-5.429069	3.615902	-1.90784	C	6.097916	-2.135881	-3.818112
H	-5.811194	4.563481	-2.271792	H	6.656946	-2.583283	-4.632948
C	-4.285178	3.063621	-2.476493	H	4.585069	-1.30885	-5.104052



H	-3.775775	3.577814	-3.284246	C	4.935307	-1.420323	-4.083604
C	-3.790786	1.855602	-2.007098	C	4.214597	-0.854065	-3.04126
H	-2.895195	1.427815	-2.448921	H	3.300124	-0.305438	-3.247289
C	-4.293353	-1.632	-1.66751	C	4.357439	1.517463	-0.293157
C	-5.348933	-1.374088	-2.543388	C	5.559741	1.890557	-0.894274
H	-5.860711	-0.417831	-2.515161	H	6.129623	1.167655	-1.468289
C	-5.737717	-2.342642	-3.461101	H	6.956645	3.481609	-1.238336
H	-6.555585	-2.138234	-4.143376	C	6.023793	3.194692	-0.765153
C	-5.079994	-3.56575	-3.506827	C	5.296388	4.126975	-0.035877
H	-5.384912	-4.317993	-4.226266	H	5.66165	5.143665	0.061654
C	-4.025731	-3.823882	-2.637024	H	3.522496	4.486155	1.127724
H	-3.506795	-4.775308	-2.67734	C	4.095855	3.758977	0.562696
C	-3.628157	-2.859285	-1.722271	C	3.622853	2.461261	0.429413
H	-2.796737	-3.056654	-1.05184	H	2.678436	2.178998	0.885107
C	-4.678237	-0.840434	1.109606	C	4.239536	-1.000956	1.143452
C	-4.240425	-0.291826	2.31804	C	3.700157	-2.255009	1.444172
H	-3.360645	0.344918	2.337969	H	2.976885	-2.705764	0.770483
C	-4.927628	-0.562651	3.492661	C	4.091434	-2.925986	2.594011
H	-4.586646	-0.132929	4.428253	H	3.675567	-3.902707	2.817835
C	-6.045318	-1.390597	3.470112	C	5.013866	-2.34496	3.459116
H	-6.577615	-1.606848	4.390099	H	5.316587	-2.867669	4.360107
C	-6.476442	-1.946359	2.271948	H	6.263635	-0.639557	3.84218
H	-7.343925	-2.597017	2.254417	C	5.545736	-1.095308	3.168815
C	-5.797754	-1.673022	1.090163	C	5.16346	-0.422444	2.012996
H	-6.135092	-2.112771	0.157578	H	5.581748	0.553632	1.791211
<b>TS5</b>				<b>10</b>			
Thermal correction to Gibbs Free Energy= 0.772853				Thermal correction to Gibbs Free Energy= 0.779682			
E(RBMK) = -3024.51710733				E(RBMK) = -3024.58587311			
Frequency -185.5765							
C	-0.838945	-0.71045	-0.816049	C	-1.234274	-1.064909	-0.011451
C	-2.073171	-2.773215	1.258708	C	-1.626531	-1.863489	1.285584
C	-1.80601	0.079869	-0.253188	C	-1.846932	0.246481	-0.441353
H	-1.24699	-1.438559	-1.519039	H	-1.281129	-1.73385	-0.880478
C	-3.152972	-2.5959	0.450079	C	-2.960944	-1.997608	0.697036
C	-1.848438	-2.023628	2.512449	C	-1.520419	-1.221705	2.65419
C	-1.131483	-3.899823	0.96889	C	-0.899741	-3.213216	1.294656
O	-3.067288	-0.106944	-0.669326	O	-2.194203	0.348431	-1.608885
C	-1.600606	1.141445	0.766254	C	-2.008817	1.379807	0.512168
S	-4.114074	-1.17978	0.536816	S	-4.340455	-1.101252	1.046708
H	-3.330877	-3.231976	-0.40978	H	-3.086099	-2.750129	-0.077724
C	-0.585855	-1.505684	2.819559	C	-0.448505	-0.404643	3.008099
C	-2.878182	-1.892564	3.450737	C	-2.434351	-1.582853	3.646005
H	-1.181445	-4.63438	1.779753	H	-1.333638	-3.872618	2.050381

H	-1.355725	-4.392202	0.022021	H	-0.956221	-3.704588	0.318725
H	-0.102695	-3.532617	0.935349	H	0.15246	-3.049474	1.541601
H	-0.6084	1.030424	1.210424	H	-1.573537	1.170404	1.489121
H	-2.33497	1.01918	1.575595	H	-3.088726	1.516824	0.665762
Si	-1.74904	2.953888	0.140339	Si	-1.447859	3.114394	-0.117767
C	-5.426945	-1.45596	-0.598816	C	-5.436891	-1.564869	-0.282252
C	-0.367756	-0.848632	4.020354	C	-0.308528	0.063197	4.308371
H	0.214938	-1.578183	2.090202	H	0.28602	-0.126687	2.25597
C	-2.653319	-1.243471	4.657698	C	-2.30144	-1.109631	4.945607
H	-3.847123	-2.338104	3.251311	H	-3.252542	-2.25721	3.41424
C	-5.189307	-1.827896	-1.921681	C	-5.091685	-1.33731	-1.612837
C	-6.720026	-1.238084	-0.13197	C	-6.675359	-2.10271	0.056277
H	-4.175484	-1.934446	-2.288427	H	-4.140669	-0.880042	-1.870261
C	-6.26951	-2.013778	-2.764239	C	-5.995115	-1.689546	-2.605297
C	-7.788071	-1.433523	-0.995433	C	-7.56612	-2.433485	-0.953822
H	-6.892511	-0.927869	0.893069	H	-6.938837	-2.27282	1.094743
H	-6.092837	-2.299351	-3.79647	H	-5.727114	-1.519602	-3.643383
C	-7.583926	-1.825713	-2.318277	C	-7.24291	-2.235923	-2.297889
H	-8.798346	-1.274427	-0.633654	H	-8.528719	-2.860835	-0.691622
C	-1.049877	4.053698	1.534306	C	-1.507257	4.230098	1.4274
C	-3.563119	3.349611	-0.288283	C	-2.626056	3.704636	-1.492257
C	-0.647276	3.124501	-1.41395	C	0.354225	3.029491	-0.753268
H	-1.025218	5.067608	1.109429	H	-1.163019	5.213357	1.075472
C	-1.915983	4.102476	2.795288	C	-2.91285	4.413174	2.005085
C	0.38791	3.66912	1.89904	C	-0.542872	3.763841	2.522693
H	-3.740876	2.800121	-1.223376	H	-2.257667	3.203965	-2.397354
C	-3.763333	4.840835	-0.579163	C	-2.523152	5.21783	-1.715603
C	-4.598592	2.850695	0.721828	C	-4.08387	3.272906	-1.317754
H	0.190129	2.43369	-1.226953	H	0.861372	2.328852	-0.070739
C	-0.061201	4.523369	-1.627813	C	1.099131	4.36613	-0.672344
C	-1.344778	2.647378	-2.692032	C	0.470321	2.463128	-2.171887
H	0.612603	-0.43585	4.23403	H	0.530596	0.702368	4.561643
C	-1.40052	-0.71604	4.943566	C	-1.239618	-0.280592	5.280809
H	-3.457365	-1.161182	5.380777	H	-3.026665	-1.398598	5.698437
H	-2.905918	4.52281	2.602213	H	-3.606077	4.850768	1.282405
H	-2.055264	3.106778	3.23196	H	-3.339071	3.461226	2.342036
H	-1.443431	4.725757	3.563529	H	-2.889196	5.077159	2.876959
H	0.821105	4.399923	2.591423	H	-0.500643	4.495139	3.338163
H	0.424602	2.695471	2.399925	H	-0.870337	2.81569	2.963356
H	1.047375	3.615221	1.027167	H	0.47847	3.623511	2.154291
H	-3.101143	5.202853	-1.371094	H	-1.499228	5.542831	-1.922944
H	-4.792198	5.039947	-0.900382	H	-3.139275	5.524027	-2.568508
H	-3.57915	5.454088	0.309538	H	-2.875902	5.781408	-0.845454
H	-5.61338	3.050405	0.357791	H	-4.691988	3.646028	-2.149943

H	-4.517457	1.77316	0.888754	H	-4.177447	2.183755	-1.311173
H	-4.503367	3.344474	1.693002	H	-4.529842	3.66331	-0.397179
H	0.608844	4.528778	-2.496002	H	2.146106	4.236843	-0.969991
H	-0.843085	5.26303	-1.827897	H	0.662887	5.108745	-1.348235
H	0.509857	4.880841	-0.766352	H	1.095895	4.795439	0.332773
H	-1.752267	1.637598	-2.596505	H	-0.039745	1.503074	-2.291101
H	-2.169428	3.314297	-2.965086	H	0.035009	3.150449	-2.904797
H	-0.64297	2.641555	-3.534149	H	1.524771	2.332937	-2.445238
H	-1.226668	-0.208312	5.886016	H	-1.133738	0.089583	6.294519
C	-8.735492	-2.022117	-3.255357	C	-8.224323	-2.568815	-3.380651
H	-9.692761	-1.944809	-2.738216	H	-8.880582	-3.390455	-3.08669
H	-8.684893	-3.001999	-3.738158	H	-7.717925	-2.846367	-4.307305
H	-8.718597	-1.26886	-4.049382	H	-8.859147	-1.70344	-3.599615
Au	1.174941	-0.54273	-0.634546	Au	0.91861	-0.775929	-0.14233
P	3.516291	-0.418773	-0.425114	P	3.215738	-0.601424	-0.44162
C	4.372456	-1.852363	-1.153885	C	3.712652	-0.966659	-2.152076
C	5.511768	-2.408384	-0.569957	C	4.936408	-1.579937	-2.429202
H	5.893692	-2.012195	0.365216	H	5.592053	-1.882455	-1.619343
C	6.153722	-3.477321	-1.184089	C	5.309218	-1.813045	-3.74682
H	7.037366	-3.908319	-0.725984	H	6.258246	-2.29294	-3.959464
C	5.666365	-3.991851	-2.379446	C	4.468171	-1.437161	-4.787949
H	6.170104	-4.826198	-2.855551	H	4.762161	-1.623497	-5.815248
C	4.530484	-3.441195	-2.963242	C	3.247292	-0.830655	-4.51449
H	4.146475	-3.844108	-3.894134	H	2.586631	-0.543706	-5.325207
C	3.880763	-2.378267	-2.351392	C	2.865136	-0.599179	-3.199995
H	2.988225	-1.954405	-2.802541	H	1.907116	-0.13447	-2.98778
C	4.247297	1.049887	-1.217146	C	3.880393	1.04431	-0.040039
C	5.500659	1.004855	-1.829749	C	4.725861	1.725203	-0.915222
H	6.053846	0.072582	-1.872612	H	4.989822	1.28631	-1.87132
C	6.036149	2.154758	-2.396907	C	5.231625	2.971097	-0.559503
H	7.008192	2.114268	-2.876305	H	5.888115	3.497992	-1.24331
C	5.328631	3.350308	-2.354622	C	4.899912	3.537158	0.664337
H	5.749347	4.244935	-2.800935	H	5.297377	4.508388	0.938351
C	4.077802	3.398263	-1.749074	C	4.053227	2.86127	1.538276
H	3.518794	4.327386	-1.722512	H	3.790326	3.303479	2.493125
C	3.534611	2.251003	-1.186942	C	3.538794	1.622232	1.186507
H	2.550956	2.28569	-0.728251	H	2.875941	1.098373	1.869375
C	4.059329	-0.366721	1.317055	C	4.126883	-1.780885	0.604807
C	3.579612	-1.349955	2.187969	C	3.665292	-3.098427	0.675865
H	2.911386	-2.122458	1.817883	H	2.768598	-3.38936	0.136103
C	3.966557	-1.351728	3.520185	C	4.355542	-4.037125	1.428361
H	3.599684	-2.124108	4.187925	H	3.996358	-5.059288	1.47761
C	4.82433	-0.364396	3.997153	C	5.503181	-3.665696	2.12206
H	5.124539	-0.363991	5.039472	H	6.038932	-4.399227	2.71472

C	5.296542	0.618274	3.137494	C	5.961472	-2.356193	2.05813
H	5.96539	1.388416	3.506155	H	6.855496	-2.065135	2.598711
C	4.919154	0.619124	1.798345	C	5.278421	-1.411453	1.30009
H	5.294052	1.387597	1.130921	H	5.641068	-0.390252	1.252943
<b>TS6</b>				<b>11</b>			
Thermal correction to Gibbs Free Energy= 0.786006				Thermal correction to Gibbs Free Energy= 0.778791			
E(RBMK) = -3024.57999322				E(RBMK) = -3024.58141138			
Frequency -73.9464							
C	2.249692	-1.956305	0.722319	O	1.850661	-0.426924	-1.692631
C	1.030855	-0.787918	0.393088	C	2.527894	-2.017384	0.765642
C	0.852214	-2.34064	0.634379	C	1.062684	-2.109224	0.660857
C	1.31559	-0.050413	-0.889984	C	0.800201	-0.582004	0.437791
O	1.596039	-0.655576	-1.909525	C	1.367976	0.152058	-0.730201
H	1.032733	-0.176834	1.300951	H	0.984855	-0.031053	1.36836
C	0.414413	-3.263338	-0.476458	C	0.583985	-3.085583	-0.407732
C	0.186111	-2.660112	1.967989	C	0.476438	-2.483486	2.032522
S	3.438157	-2.462613	-0.456136	S	3.56317	-2.430031	-0.453776
H	2.65369	-1.736395	1.707256	H	2.954847	-1.600582	1.675799
C	4.955609	-1.889984	0.277496	C	5.166539	-1.98706	0.172396
C	5.842157	-1.173658	-0.52791	C	6.011504	-1.29263	-0.689529
C	5.326618	-2.224608	1.582715	C	5.603377	-2.373802	1.437511
C	1.210879	1.448629	-0.842523	C	1.244825	1.650985	-0.700415
H	0.455244	1.764592	-0.109913	H	0.478281	1.963079	0.01802
H	0.861837	1.757834	-1.834825	H	0.904172	1.954655	-1.697303
C	-0.405986	-2.887179	-1.539344	C	-0.120045	-2.702724	-1.546146
C	0.813819	-4.602	-0.376665	C	0.850864	-4.446526	-0.220901
H	0.455539	-3.673794	2.278205	H	0.747436	-3.500196	2.322695
H	0.502528	-1.966487	2.753548	H	0.821548	-1.794619	2.809275
H	-0.904244	-2.612496	1.878391	H	-0.613951	-2.418372	1.976945
C	-0.836783	-3.828636	-2.471419	C	-0.563917	-3.653222	-2.460212
H	-0.683974	-1.845445	-1.676957	H	-0.298746	-1.654651	-1.749633
H	-1.468327	-3.512845	-3.296523	H	-1.104682	-3.328885	-3.342996
C	-0.442225	-5.157539	-2.358528	C	-0.299705	-5.000459	-2.259167
H	-0.770104	-5.889295	-3.090628	H	-0.638778	-5.73902	-2.977543
C	0.389779	-5.541258	-1.309681	C	0.41639	-5.395224	-1.134948
H	0.71283	-6.573677	-1.217619	H	0.635556	-6.444099	-0.966885
H	1.467924	-4.911735	0.434205	H	1.407831	-4.777998	0.650699
H	5.566517	-0.928909	-1.549554	H	5.671073	-1.003357	-1.678352
C	7.074969	-0.776043	-0.019282	C	7.287825	-0.958056	-0.2617
H	7.757293	-0.21891	-0.656076	H	7.941998	-0.407672	-0.930266
C	7.447266	-1.071677	1.294569	C	7.742932	-1.311954	1.009809
C	6.549527	-1.798985	2.085172	C	6.879414	-2.02237	1.848127
C	8.786591	-0.659585	1.833545	C	9.135148	-0.97651	1.450609

H	6.824151	-2.056684	3.10495	H	7.218993	-2.321416	2.834752
H	8.726599	-0.386845	2.890843	H	9.182671	-0.804446	2.527902
H	9.195891	0.191316	1.283282	H	9.512077	-0.08726	0.94186
H	9.507141	-1.48149	1.750139	H	9.817449	-1.801726	1.219718
H	4.670961	-2.829843	2.202945	H	4.964559	-2.958153	2.091386
Au	-1.25591	-0.31544	0.296166	Au	-1.341537	-0.248523	0.304124
P	-3.465847	0.284333	0.270234	P	-3.620389	0.184448	0.212178
C	-3.680893	2.024871	-0.206415	C	-3.984976	1.944686	-0.075641
C	-4.584443	2.855555	0.463403	C	-5.009159	2.601908	0.606592
H	-5.154805	2.476963	1.306449	H	-5.594581	2.07417	1.35206
C	-4.74858	4.174947	0.047943	C	-5.274755	3.939203	0.334051
H	-5.448703	4.819147	0.570918	H	-6.069668	4.447967	0.868397
C	-4.018481	4.665578	-1.030589	C	-4.525898	4.62094	-0.616682
H	-4.148292	5.695331	-1.349418	H	-4.73581	5.664345	-0.825648
C	-3.11731	3.838731	-1.700333	C	-3.502914	3.96827	-1.297525
H	-2.545273	4.221434	-2.54005	H	-2.914645	4.500311	-2.037304
C	-2.943627	2.522574	-1.288891	C	-3.227729	2.635903	-1.025448
H	-2.236351	1.880456	-1.808883	H	-2.422896	2.129891	-1.551016
C	-4.424119	-0.70923	-0.909691	C	-4.456794	-0.729952	-1.11996
C	-5.494694	-0.147948	-1.615326	C	-5.498636	-0.158554	-1.852369
H	-5.739478	0.903292	-1.49377	H	-5.803535	0.864861	-1.660648
C	-6.24191	-0.940696	-2.481629	C	-6.140193	-0.901146	-2.836361
H	-7.070176	-0.503394	-3.030614	H	-6.946847	-0.453395	-3.406499
C	-5.925254	-2.286783	-2.647872	C	-5.748551	-2.210015	-3.090775
H	-6.508429	-2.899856	-3.328374	H	-6.251356	-2.78562	-3.86047
C	-4.857156	-2.84635	-1.949443	C	-4.70747	-2.779805	-2.36547
H	-4.602432	-3.893131	-2.084106	H	-4.394268	-3.798454	-2.567082
C	-4.104129	-2.06134	-1.083443	C	-4.057417	-2.042287	-1.38581
H	-3.262065	-2.498459	-0.552682	H	-3.233297	-2.484805	-0.833915
C	-4.234469	0.077732	1.903699	C	-4.477974	-0.262941	1.754505
C	-3.522728	0.476775	3.042586	C	-3.89357	0.098555	2.971775
H	-2.515291	0.874555	2.943544	H	-2.936807	0.612752	2.983169
C	-4.104702	0.365651	4.299751	C	-4.535407	-0.197276	4.16551
H	-3.551591	0.677319	5.180466	H	-4.080741	0.088492	5.107817
C	-5.392558	-0.15262	4.428227	C	-5.755566	-0.865981	4.152766
H	-5.843092	-0.245611	5.411734	H	-6.253198	-1.102566	5.087024
C	-6.099567	-0.556173	3.299139	C	-6.333777	-1.235849	2.945228
H	-7.100865	-0.963567	3.399382	H	-7.282393	-1.761426	2.934044
C	-5.526081	-0.442062	2.035248	C	-5.700114	-0.935316	1.744701
H	-6.079951	-0.760184	1.157018	H	-6.154089	-1.228251	0.804083
Si	2.717553	2.618147	-0.498181	Si	2.768679	2.773938	-0.357053
C	2.056547	4.352744	-0.949257	C	2.143313	4.552453	-0.640937
C	0.787298	4.70503	-0.163568	C	0.929938	4.875621	0.237935
H	0.902162	4.562478	0.916576	H	1.098142	4.648524	1.295326

H	0.509094	5.753535	-0.325184	H	0.675628	5.939342	0.169824
C	4.225886	2.080531	-1.522176	C	4.224016	2.291144	-1.484019
H	4.600042	1.18989	-0.995458	H	4.599785	1.353326	-1.048144
C	3.088054	2.589614	1.382286	C	3.245661	2.59021	1.488532
H	2.100065	2.487899	1.861667	H	2.284677	2.456229	2.008811
C	3.938418	1.387898	1.803687	C	4.092027	1.342494	1.747865
H	3.532903	0.436397	1.446501	H	3.656403	0.446694	1.294818
C	5.341137	3.132959	-1.491422	C	5.360604	3.317064	-1.417058
H	5.663169	3.376004	-0.473461	H	5.727233	3.474191	-0.398281
H	5.02939	4.067798	-1.971239	H	5.047346	4.291116	-1.807308
H	6.223932	2.774537	-2.035046	H	6.212644	2.989697	-2.024297
C	3.71465	3.885463	1.911662	C	3.923603	3.820836	2.098474
H	3.093888	4.764883	1.717318	H	3.312684	4.722593	2.009833
H	3.864382	3.824477	2.996581	H	4.12021	3.663233	3.165345
H	4.697555	4.071554	1.465243	H	4.887393	4.029703	1.623513
H	4.019621	1.327147	2.896168	H	4.205413	1.155903	2.822504
H	4.95808	1.460704	1.409973	H	5.098635	1.449954	1.331004
H	-0.066809	4.098052	-0.488602	H	0.044355	4.315707	-0.083036
C	1.837827	4.587477	-2.446346	C	1.849318	4.901548	-2.101304
H	1.444367	5.595915	-2.624747	H	1.477647	5.929587	-2.182496
H	1.112948	3.882514	-2.872312	H	1.081145	4.248866	-2.53179
H	2.763031	4.493941	-3.021447	H	2.737226	4.826867	-2.733483
C	3.905554	1.656791	-2.960454	C	3.83827	1.988386	-2.935234
H	3.158289	0.859071	-2.999948	H	3.092025	1.193089	-2.996803
H	3.538151	2.495031	-3.561309	H	3.443097	2.870868	-3.446422
H	4.812932	1.289427	-3.456899	H	4.720808	1.666035	-3.501581
H	2.850834	5.04073	-0.621814	H	2.973098	5.193739	-0.309982
<b>TS7</b>				<b>12</b>			
Thermal correction to Gibbs Free Energy= 0.778574				Thermal correction to Gibbs Free Energy= 0.781378			
E(RBMK) = -3024.57911944				E(RBMK) = -3024.61684289			
Frequency -33.7886							
O	2.030379	-0.166004	-1.454834	C	-0.732187	-0.228727	-1.19739
C	2.563584	-1.985651	0.775295	C	-1.387355	-1.617098	-1.37442
C	1.097415	-1.942678	0.873058	C	-1.475135	0.466125	-0.219374
C	0.813975	-0.411901	0.603313	H	-0.472721	0.325905	-2.101693
C	1.452763	0.353446	-0.508302	C	-2.682489	-1.425763	-0.539068
H	0.969064	0.143	1.535927	C	-0.516168	-2.738071	-0.806657
C	0.405165	-2.932117	-0.065112	C	-1.774156	-1.8534	-2.83237
C	0.731864	-2.177509	2.35169	S	-3.265328	-2.849053	0.378717
S	3.405096	-2.753462	-0.415278	H	-3.503168	-1.089597	-1.176703
H	3.140371	-1.437726	1.519422	O	-2.412921	-0.264602	0.336867
C	5.100917	-2.367451	-0.046329	C	-4.995486	-2.428124	0.524324
C	5.856205	-1.76646	-1.04963	C	-5.452863	-1.709777	1.62645

C	5.674773	-2.710188	1.175325	C	-5.904553	-2.869111	-0.435932
C	1.292099	1.845772	-0.425606	C	-1.351316	1.840002	0.258334
H	0.556896	2.12069	0.337594	H	-0.399985	2.271887	-0.058917
H	0.900317	2.178737	-1.394057	H	-1.376033	1.832762	1.353884
C	0.248064	-2.648974	-1.426419	Si	-2.780913	3.075423	-0.213862
C	-0.052434	-4.164536	0.409338	C	-0.144286	-2.709576	0.54524
H	1.035198	-3.165254	2.702304	C	-0.087808	-3.815119	-1.579575
H	1.215334	-1.432236	2.987788	H	-2.349666	-2.776376	-2.944231
H	-0.350869	-2.073911	2.465262	H	-2.384884	-1.025987	-3.201638
C	-0.347207	-3.570178	-2.279661	H	-0.888637	-1.921333	-3.468761
H	0.621418	-1.713704	-1.825458	C	-2.349576	4.712041	0.673031
H	-0.453893	-3.327736	-3.331608	C	-4.433438	2.39868	0.434796
C	-0.799549	-4.79078	-1.794594	C	-2.852313	3.252694	-2.10963
H	-1.257721	-5.511763	-2.463479	C	0.620578	-3.724887	1.101629
C	-0.651896	-5.082813	-0.445313	H	-0.490191	-1.904395	1.18724
H	-1.000746	-6.030804	-0.049832	H	0.879433	-3.68797	2.154259
H	0.043485	-4.426851	1.455641	C	1.040324	-4.791971	0.315488
H	5.401408	-1.503615	-1.998719	H	1.631343	-5.590576	0.750502
C	7.192168	-1.485137	-0.807385	C	0.686445	-4.830932	-1.025216
H	7.780241	-1.00573	-1.583379	H	1.000036	-5.662057	-1.648122
C	7.791556	-1.801794	0.413951	H	-0.361875	-3.884511	-2.625094
C	7.010899	-2.414517	1.39723	H	-3.340397	5.149561	0.867915
C	9.2452	-1.52582	0.649791	H	-4.585188	1.436041	-0.072756
H	7.460381	-2.677964	2.349347	H	-3.429151	4.173565	-2.281825
H	9.454485	-1.359779	1.708344	H	-4.749478	-1.381843	2.383595
H	9.581515	-0.651186	0.089501	C	-6.805268	-1.421962	1.751769
H	9.852071	-2.377526	0.32402	H	-7.152929	-0.863207	2.615725
H	5.092887	-3.213863	1.940004	C	-7.727589	-1.847819	0.794697
Au	-1.303774	-0.176398	0.317911	C	-7.253429	-2.573292	-0.299855
P	-3.592618	0.147902	0.086267	C	-9.192627	-1.569606	0.956005
C	-4.014083	1.857367	-0.380553	H	-7.953372	-2.920982	-1.053758
C	-5.081113	2.538457	0.20572	H	-9.366824	-0.679004	1.563453
H	-5.670426	2.063527	0.982977	H	-9.690484	-2.408977	1.453345
C	-5.384828	3.832273	-0.203149	H	-9.681259	-1.427412	-0.010571
H	-6.213365	4.359778	0.256846	H	-5.554735	-3.449064	-1.28336
C	-4.631152	4.446929	-1.194886	Au	1.30485	-0.18325	-0.404468
H	-4.870893	5.456568	-1.510532	P	3.525034	0.061899	0.217038
C	-3.56542	3.770554	-1.780239	C	3.713971	1.204496	1.622956
H	-2.973816	4.250387	-2.552397	C	4.696538	2.1944	1.636257
C	-3.252493	2.482093	-1.371998	H	5.357865	2.317964	0.785278
H	-2.414629	1.958304	-1.8232	C	4.824262	3.027604	2.742252
C	-4.348776	-0.917666	-1.179594	H	5.588047	3.797567	2.748317
C	-5.426179	-0.476378	-1.950412	C	3.979309	2.874821	3.833944
H	-5.803296	0.534231	-1.833095	H	4.082844	3.526242	4.694968

C	-6.009504	-1.330995	-2.87748	H	2.336243	1.769003	4.674235
H	-6.843774	-0.984178	-3.477478	C	2.997523	1.888619	3.822875
C	-5.523726	-2.623442	-3.037715	C	2.859688	1.05899	2.71963
H	-5.981136	-3.287369	-3.763434	H	2.089018	0.293416	2.709626
C	-4.446234	-3.062317	-2.276316	C	4.345166	-1.483543	0.710117
H	-4.057621	-4.066398	-2.406469	C	5.284027	-1.508544	1.743359
C	-3.853636	-2.212395	-1.352465	H	5.50009	-0.607088	2.307126
H	-2.998894	-2.553168	-0.775191	H	6.665691	-2.711993	2.857946
C	-4.49411	-0.18261	1.634369	C	5.938938	-2.694164	2.053137
C	-3.977802	0.33314	2.826731	C	5.664176	-3.851644	1.334392
H	-3.049083	0.896531	2.816551	H	6.17936	-4.774746	1.577475
C	-4.651084	0.128028	4.022196	H	4.500845	-4.734102	-0.245406
H	-4.249473	0.534282	4.944201	C	4.724014	-3.829813	0.309967
C	-5.834738	-0.603387	4.037946	C	4.058508	-2.651779	0.00059
H	-6.35715	-0.76834	4.974097	H	3.310149	-2.643974	-0.786385
C	-6.344605	-1.126605	2.856689	C	4.528693	0.754765	-1.135126
H	-7.264651	-1.700805	2.867948	C	3.988477	1.780825	-1.915183
C	-5.679392	-0.91738	1.653661	H	2.975326	2.12594	-1.729991
H	-6.080527	-1.32937	0.733895	C	4.742887	2.355986	-2.927463
Si	2.841963	2.943362	-0.13576	H	4.320073	3.152791	-3.52962
C	2.171056	4.719559	0.032169	C	6.034821	1.903296	-3.175336
C	1.16199	4.850576	1.178005	H	6.621077	2.348275	-3.972012
H	1.536919	4.448254	2.124205	H	7.576195	0.518648	-2.604835
H	0.905863	5.902097	1.349375	C	6.571532	0.876827	-2.40857
C	4.068355	2.741084	-1.578046	C	5.823824	0.30136	-1.38765
H	4.577928	1.788338	-1.374878	H	6.246061	-0.502903	-0.794799
C	3.651927	2.427758	1.520668	C	-5.592564	3.32436	0.044836
H	2.806125	2.150682	2.16889	H	-5.643357	3.513887	-1.03153
C	4.546831	1.195687	1.363488	H	-6.55023	2.884884	0.343942
H	4.071252	0.400441	0.780777	H	-5.516668	4.294953	0.546576
C	5.131378	3.845414	-1.577073	C	-4.453837	2.128829	1.940892
H	5.677067	3.903652	-0.630252	H	-5.409812	1.679607	2.231652
H	4.690472	4.830564	-1.761509	H	-3.664853	1.438	2.251862
H	5.869397	3.671767	-2.368559	H	-4.347568	3.053697	2.516909
C	4.423414	3.545149	2.229068	C	-1.666847	4.509402	2.029989
H	3.802149	4.420694	2.432835	H	-2.207748	3.818603	2.682575
H	4.818562	3.194015	3.189541	H	-0.646613	4.127987	1.909897
H	5.279514	3.881539	1.635515	H	-1.587614	5.463392	2.562312
H	4.832919	0.783859	2.339174	C	-1.566019	5.72929	-0.159485
H	5.474391	1.44891	0.839985	H	-1.469118	6.672338	0.389588
H	0.22607	4.330849	0.94465	H	-0.549619	5.380393	-0.372356
C	1.581344	5.29313	-1.258444	H	-2.051017	5.956408	-1.11254
H	1.219536	6.314834	-1.095059	C	-1.481577	3.436053	-2.768833
H	0.726176	4.704067	-1.609417	H	-0.855671	2.545116	-2.645607



H	2.312295	5.332782	-2.069724	H	-1.593126	3.598606	-3.846524
C	3.411166	2.603008	-2.954371	H	-0.927129	4.286006	-2.366252
H	2.751493	1.732938	-2.991958	C	-3.609519	2.103126	-2.781959
H	2.831054	3.489886	-3.227536	H	-3.669547	2.262779	-3.864298
H	4.17711	2.474084	-3.728388	H	-3.097269	1.145641	-2.631143
H	3.051058	5.325828	0.292122	H	-4.630779	1.993028	-2.409565
<b>13</b>				<b>TS8</b>			
Thermal correction to Gibbs Free Energy= 0.773277				Thermal correction to Gibbs Free Energy= 0.781958			
E(RBMK) = -3024.52470191				E(RBMK) = -3024.50779694			
				Frequency -92.9820			
C	-0.462021	0.725814	-0.969544	O	2.820619	-0.337977	-0.71272
C	-2.322783	3.506592	-0.093319	S	4.215155	-1.488817	0.277434
C	-1.522039	0.283798	-0.291315	C	1.646597	-0.239554	-0.123775
C	-3.187274	2.69536	0.641778	C	0.584125	-0.813931	-0.80252
C	-1.733253	4.587296	0.535801	C	1.564783	0.547541	1.138057
C	-1.616356	-0.482151	0.981326	H	0.919081	-1.422365	-1.645926
C	-3.437029	2.936347	1.989184	C	4.897439	-2.297765	-1.093833
C	-1.984429	4.871973	1.883891	C	5.995773	-1.849541	-1.750333
C	-4.867124	2.028576	-1.39028	C	6.637346	-0.552723	-1.473321
C	-2.841342	4.032327	2.596054	C	6.596135	-2.712912	-2.818766
C	-1.332215	6.049739	2.539834	C	8.032424	-0.461627	-1.346073
C	-2.656546	-3.014373	2.381744	C	5.868908	0.617482	-1.370537
C	-2.537265	-2.952016	-0.720091	C	8.636247	0.760916	-1.085881
C	0.155023	-3.043226	0.885851	C	6.482267	1.842617	-1.126969
C	-6.070253	1.574925	-1.792412	C	7.863529	1.916709	-0.977427
C	-4.082232	-2.453397	2.366358	C	3.135234	-2.677096	0.965246
C	-2.005164	-2.753919	3.742001	C	2.242055	-3.429502	0.191706
C	-3.187548	-4.337114	-0.641789	C	1.392562	-4.333008	0.820235
C	-1.642307	-2.85665	-1.960362	C	3.123081	-2.786992	2.363039
C	0.221349	-4.571276	0.980241	C	1.390166	-4.482346	2.209408
C	1.07797	-2.403652	1.925565	C	2.262647	-3.687174	2.968029
C	-6.668921	0.318317	-1.307154	C	0.494211	-5.481666	2.878026
C	-6.838136	2.35447	-2.811232	H	2.221673	-3.325184	-0.887868
C	-7.980917	0.292461	-0.821839	H	0.711011	-4.92612	0.216959
C	-5.942821	-0.874896	-1.378773	H	0.686784	0.241808	1.713164
C	-8.539503	-0.898639	-0.385211	H	2.452164	0.318974	1.74403
C	-6.516623	-2.069365	-0.961412	Si	1.552452	2.478507	0.981368
C	-7.810764	-2.081992	-0.457925	C	2.349021	2.980871	-0.685851
H	-2.7293	-4.103761	2.252933	C	2.99685	4.370776	-0.681899
H	-0.718025	1.260352	-1.885923	C	1.37833	2.856095	-1.866185
H	-2.103742	3.287194	-1.131638	C	-0.257253	3.086091	1.060969
O	-2.781521	0.51121	-0.939856	C	-0.338815	4.613488	1.17022
S	-3.990577	1.294285	-0.072537	C	-1.135365	2.425932	2.12785

H	-1.055688	5.222198	-0.026106	C	2.629587	3.142811	2.413125
H	-0.771968	-0.201216	1.615903	C	4.063402	2.603808	2.346563
H	-2.520448	-0.193601	1.535267	C	2.041258	2.90203	3.806595
Si	-1.642282	-2.409432	0.88081	H	2.676445	4.230836	2.254625
H	-4.095507	2.285031	2.554629	H	3.801381	-2.187634	2.963622
H	-4.408059	2.921879	-1.797003	H	4.426108	-3.237863	-1.359461
H	-4.590233	-2.598066	1.40824	H	4.530327	2.742734	1.365839
H	-3.343031	-2.214092	-0.8397	H	3.147449	2.239607	-0.838878
H	0.541864	-2.752176	-0.102103	H	-0.68	2.80213	0.084708
H	-7.007839	1.736308	-3.698034	H	6.6287	-2.170086	-3.769272
H	-6.326862	3.272294	-3.103041	H	6.040688	-3.642442	-2.957718
H	-7.826481	2.614427	-2.419153	H	7.631449	-2.97046	-2.569655
H	-8.557859	1.20925	-0.761079	H	8.645848	-1.354372	-1.42135
H	-4.945918	-0.871787	-1.808699	H	4.795613	0.572408	-1.532305
H	-9.55045	-0.906159	0.007002	H	9.714484	0.81443	-0.970845
H	-5.952393	-2.992121	-1.04258	H	5.877216	2.743015	-1.071743
H	-8.257777	-3.01449	-0.131248	H	8.341214	2.873255	-0.788304
H	-3.042711	4.234981	3.642566	H	2.271012	-3.785445	4.050035
H	-4.089617	-1.378222	2.580975	H	4.099395	1.530919	2.573062
H	-4.695541	-2.930285	3.139368	H	4.700476	3.101088	3.087922
H	-2.663593	-3.083598	4.554265	H	2.724465	3.264413	4.584808
H	-1.807506	-1.687646	3.902891	H	1.87461	1.83483	3.999702
H	-1.058616	-3.286853	3.856579	H	1.086852	3.416897	3.948276
H	-3.729807	-4.558923	-1.569288	H	3.484102	4.570481	-1.644837
H	-3.89624	-4.427538	0.186286	H	3.754205	4.483591	0.100088
H	-2.443066	-5.129555	-0.518366	H	2.257292	5.165264	-0.533539
H	-1.182201	-1.871248	-2.069252	H	0.90703	1.869187	-1.920938
H	-2.219077	-3.060026	-2.870446	H	1.898464	3.026816	-2.816879
H	-0.836421	-3.597372	-1.921311	H	0.578413	3.60304	-1.800293
H	-0.336553	-5.064419	0.179251	H	0.201721	5.119994	0.364112
H	-0.178847	-4.934772	1.933067	H	0.074587	4.973149	2.119657
H	1.260134	-4.915078	0.91474	H	-1.382646	4.948218	1.124624
H	0.770638	-2.630428	2.950255	H	-0.786655	2.638111	3.143641
H	1.120328	-1.314848	1.819882	H	-1.175822	1.337179	2.010534
H	2.100904	-2.777221	1.802188	H	-2.165389	2.795869	2.053209
H	-1.646654	6.157338	3.578696	H	0.101643	-5.095926	3.822872
H	-1.578734	6.97528	2.011348	H	1.048157	-6.399352	3.108183
H	-0.242894	5.947847	2.522301	H	-0.349148	-5.756283	2.240255
Au	1.518178	0.434274	-0.596373	Au	-1.393579	-0.47897	-0.583186
P	3.822792	0.129674	-0.29457	P	-3.715147	-0.137071	-0.409136
C	4.513353	1.001581	1.151084	C	-4.474634	-1.021776	0.992477
C	5.770986	1.605112	1.117902	C	-5.753857	-1.580582	0.906038
H	6.357427	1.591254	0.205288	H	-6.31248	-1.52164	-0.02356
C	6.27016	2.23284	2.253213	C	-6.309497	-2.21995	2.011089

H	7.246965	2.703293	2.220904	H	-7.301777	-2.65477	1.9378
C	5.522084	2.258478	3.423771	C	-5.596466	-2.302648	3.204184
H	5.915508	2.748292	4.308101	H	-6.033526	-2.802016	4.063778
H	3.678366	1.684433	4.371128	C	-4.320716	-1.749648	3.294108
C	4.266423	1.661388	3.459896	H	-3.761542	-1.816316	4.222634
C	3.759264	1.040933	2.326659	C	-3.757421	-1.116349	2.191597
H	2.773812	0.585493	2.351049	H	-2.758095	-0.693123	2.258891
C	4.278956	-1.622659	-0.070823	C	-4.146464	1.620875	-0.186095
C	5.165989	-2.041659	0.920198	C	-5.10116	2.041389	0.7443
H	5.607212	-1.318251	1.597558	H	-5.608356	1.314333	1.37165
H	6.168759	-3.712078	1.819143	C	-5.398328	3.39659	0.871068
C	5.480312	-3.390762	1.044962	H	-6.138895	3.718657	1.596976
C	4.9173	-4.322389	0.182082	C	-4.750199	4.333626	0.071166
H	5.165971	-5.373592	0.281294	H	-4.984926	5.389042	0.172577
H	3.590014	-4.632849	-1.483014	C	-3.799131	3.917843	-0.859756
C	4.032268	-3.907395	-0.808637	H	-3.291668	4.646844	-1.484428
C	3.707717	-2.563983	-0.931941	C	-3.492745	2.567429	-0.9856
H	3.007351	-2.242778	-1.697586	H	-2.743797	2.246002	-1.705882
C	4.806233	0.700029	-1.719945	C	-4.620119	-0.679002	-1.894926
C	4.418436	1.875898	-2.3671	C	-4.176772	-1.822129	-2.571041
H	3.528869	2.404868	-2.037779	H	-3.289453	-2.346104	-2.223514
C	5.163367	2.36293	-3.432039	C	-4.865649	-2.283418	-3.687574
H	4.857901	3.276192	-3.931174	H	-4.516847	-3.169413	-4.209478
C	6.291687	1.674674	-3.86495	C	-5.993755	-1.602984	-4.140956
H	6.8689	2.052118	-4.7022	H	-6.526632	-1.959798	-5.017259
H	7.550909	-0.042409	-3.571511	C	-6.434122	-0.461249	-3.476432
C	6.675077	0.49924	-3.230878	H	-7.309831	0.073007	-3.832449
C	5.937024	0.010319	-2.159344	C	-5.751583	0.002848	-2.355299
H	6.236507	-0.91126	-1.671234	H	-6.093958	0.897897	-1.843715
<b>14</b>				<b>TS9</b>			
Thermal correction to Gibbs Free Energy= 0.780118 E(RBMK) = -3024.56466953				Thermal correction to Gibbs Free Energy= 0.770188 E(RBMK) = -3024.51587469 Frequency -979.3399			
C	1.294465	-0.506465	0.627412	H	0.685883	-0.952756	1.878686
C	1.666606	-0.516996	2.160448	C	1.313097	-0.485697	0.70506
C	1.928097	0.583229	-0.185725	C	1.796233	-0.539617	2.224308
C	3.124694	-0.29426	2.381255	C	1.933354	0.64627	-0.128105
C	0.791042	0.315602	3.018821	C	2.859149	-1.408568	2.612454
C	1.931395	2.005591	0.287624	C	1.400021	0.503489	3.100942
C	3.556595	0.760041	3.208053	C	2.07645	2.0275	0.421687
C	1.234825	1.274963	3.864518	C	3.529205	-1.115437	3.800935
C	2.64819	1.500394	3.916893	C	2.067509	0.778609	4.277303
C	0.323416	2.102836	4.717377	C	3.159398	-0.04313	4.595403

H	1.671715	-1.437078	0.195203	C	1.644348	1.888541	5.191509
H	1.437687	-1.557964	2.446099	H	1.598088	-1.430013	0.24964
O	2.457104	0.285395	-1.245262	O	2.300023	0.316212	-1.231689
S	4.363666	-1.206206	1.669831	S	3.487321	-2.74807	1.673634
C	3.628179	-2.665946	1.048766	C	2.03225	-3.556973	1.087608
C	4.201019	-3.37343	0.059055	C	1.989427	-4.266587	-0.048883
C	5.329543	-2.855164	-0.742468	C	3.100735	-4.295128	-1.032462
C	3.686444	-4.738544	-0.273713	C	0.786727	-5.104745	-0.36535
C	6.512746	-3.592564	-0.857971	C	3.731573	-5.503019	-1.341418
C	5.208182	-1.638738	-1.424588	C	3.505519	-3.130557	-1.690511
C	7.568385	-3.105603	-1.613889	C	4.759867	-5.542453	-2.273209
C	6.264299	-1.167915	-2.194662	C	4.525662	-3.176849	-2.631766
C	7.445466	-1.893108	-2.285334	C	5.157851	-4.379691	-2.922315
H	-0.271458	0.104903	2.930586	H	0.52054	1.080497	2.827713
H	1.531844	2.115238	1.29802	H	1.217164	2.265422	1.056045
H	2.982101	2.320154	0.300297	H	2.938084	2.014336	1.105283
Si	1.09615	3.336133	-0.831036	Si	2.371478	3.464	-0.826234
C	1.497494	3.001728	-2.666967	C	4.206514	3.472177	-1.357155
C	1.541754	4.265056	-3.533664	C	4.731053	4.863981	-1.72876
C	0.564145	1.96504	-3.299064	C	4.520916	2.475487	-2.477212
C	-0.789925	3.315745	-0.542526	C	1.210051	3.258005	-2.31965
C	-1.474842	4.522554	-1.192091	C	1.20533	4.499376	-3.218146
C	-1.227994	3.167908	0.915741	C	-0.219765	2.836703	-1.974018
C	1.897818	4.989187	-0.311678	C	2.028263	5.039633	0.195903
C	3.417756	4.967575	-0.505135	C	2.908083	5.088391	1.450133
C	1.554566	5.460285	1.103074	C	0.560949	5.261829	0.568128
H	1.486144	5.727511	-1.0146	H	2.330098	5.872838	-0.453911
H	4.618394	0.95859	3.312658	H	4.34684	-1.757417	4.110737
H	2.785394	-3.05103	1.614688	H	1.204911	-3.57676	1.792915
H	3.716421	4.610341	-1.494931	H	3.970757	4.956069	1.225901
H	2.502656	2.560137	-2.652418	H	4.755441	3.146092	-0.460408
H	-1.137644	2.416398	-1.071985	H	1.660379	2.432559	-2.887104
H	3.356221	-4.76662	-1.316756	H	0.376943	-4.824759	-1.341033
H	2.860703	-5.03819	0.373843	H	0.006878	-5.00585	0.392731
H	4.48567	-5.480583	-0.178976	H	1.063224	-6.16193	-0.435366
H	6.618158	-4.53801	-0.335633	H	3.429343	-6.415263	-0.836601
H	4.274329	-1.084755	-1.387847	H	3.015617	-2.183986	-1.482865
H	8.488633	-3.675342	-1.682874	H	5.250022	-6.484603	-2.493789
H	6.155272	-0.232556	-2.732794	H	4.824539	-2.266679	-3.140787
H	8.268476	-1.520631	-2.885686	H	5.956886	-4.412288	-3.655088
H	3.021303	2.286991	4.567849	H	3.707153	0.136765	5.515933
H	3.904608	4.323874	0.236414	H	2.623291	4.309157	2.167065
H	3.839438	5.970656	-0.376303	H	2.800193	6.049646	1.965186
H	2.078944	6.394159	1.336959	H	0.451325	6.164539	1.180584

H	1.858306	4.726069	1.859368	H	0.15566	4.42856	1.155976
H	0.485733	5.64889	1.231062	H	-0.074367	5.387669	-0.312163
H	1.83261	4.009613	-4.559024	H	5.798258	4.813763	-1.971678
H	2.25737	5.006535	-3.169266	H	4.614839	5.592267	-0.921779
H	0.564466	4.755382	-3.593505	H	4.223495	5.266551	-2.611266
H	0.556895	1.024049	-2.742972	H	4.181903	1.4641	-2.243805
H	0.888011	1.734966	-4.320713	H	5.599887	2.441246	-2.665361
H	-0.463306	2.340692	-3.361163	H	4.041796	2.775194	-3.415667
H	-1.253693	4.599264	-2.260226	H	2.207413	4.759168	-3.570344
H	-1.164756	5.463137	-0.724122	H	0.801195	5.375523	-2.6994
H	-2.563991	4.452172	-1.090004	H	0.583156	4.333591	-4.105043
H	-0.906886	4.011356	1.534102	H	-0.757924	3.620505	-1.431897
H	-0.832563	2.252018	1.367942	H	-0.249652	1.926387	-1.362969
H	-2.322646	3.124457	0.978993	H	-0.791402	2.625595	-2.885306
H	-0.717708	1.804607	4.58673	H	0.770745	2.415256	4.803818
H	0.407731	3.164167	4.463471	H	2.449787	2.618056	5.317734
H	0.576855	1.999307	5.776694	H	1.394633	1.505389	6.185101
Au	-0.776154	-0.63488	0.236225	Au	-0.801327	-0.371139	0.331033
P	-3.053256	-0.945288	-0.206169	P	-3.082084	-0.282345	-0.163104
C	-4.071116	-0.808613	1.301191	C	-3.946281	1.024584	0.761963
C	-5.06688	-1.735834	1.607132	C	-5.173453	0.794842	1.383665
H	-5.246524	-2.579433	0.949355	H	-5.629137	-0.188881	1.346095
C	-5.828684	-1.58073	2.760307	C	-5.811569	1.830983	2.056702
H	-6.60018	-2.306095	2.994777	H	-6.764919	1.649229	2.54069
C	-5.605861	-0.502196	3.606439	C	-5.232682	3.09249	2.107906
H	-6.204334	-0.383456	4.503218	H	-5.734524	3.897994	2.632996
C	-4.613534	0.425256	3.304125	C	-4.008425	3.323908	1.487889
H	-4.440163	1.270264	3.962082	H	-3.555364	4.308686	1.526434
C	-3.842876	0.270323	2.160641	C	-3.362312	2.293493	0.820823
H	-3.067131	0.993607	1.926628	H	-2.406565	2.476282	0.337835
C	-3.759168	0.244737	-1.39049	C	-3.382155	0.053559	-1.923912
C	-4.993394	0.858492	-1.175108	C	-4.451342	0.849681	-2.337945
H	-5.553683	0.65445	-0.268874	H	-5.10566	1.309973	-1.605032
C	-5.505133	1.736046	-2.124541	C	-4.670241	1.0605	-3.693819
H	-6.464249	2.212588	-1.952986	H	-5.499531	1.681944	-4.013526
C	-4.793663	1.999152	-3.28841	C	-3.828756	0.480906	-4.635931
H	-5.197022	2.682842	-4.027601	H	-4.001723	0.650317	-5.693196
C	-3.562439	1.388515	-3.505444	C	-2.760495	-0.309794	-4.225646
H	-3.003536	1.593755	-4.412029	H	-2.098377	-0.756015	-4.959446
C	-3.041425	0.518615	-2.558082	C	-2.532686	-0.520777	-2.873111
H	-2.07556	0.051412	-2.726886	H	-1.690098	-1.128307	-2.555459
C	-3.413239	-2.592176	-0.896562	C	-3.935079	-1.841006	0.227097
C	-2.694773	-3.690767	-0.41814	C	-3.656984	-2.470386	1.443883
H	-1.91488	-3.544263	0.323533	H	-2.928859	-2.039267	2.125105

C	-2.9732	-4.965027	-0.892147	C	-4.313526	-3.643885	1.785075
H	-2.414097	-5.815259	-0.516735	H	-4.099043	-4.127011	2.732127
C	-3.960374	-5.149007	-1.854433	C	-5.240414	-4.202065	0.910058
H	-4.172129	-6.144208	-2.230226	H	-5.748512	-5.122952	1.174931
C	-4.670212	-4.057853	-2.340419	C	-5.511963	-3.583984	-0.303863
H	-5.435844	-4.199056	-3.095493	H	-6.231032	-4.020525	-0.988302
C	-4.401612	-2.780273	-1.863674	C	-4.863829	-2.40326	-0.648623
H	-4.955306	-1.93088	-2.24958	H	-5.07704	-1.925319	-1.598791
<b>15</b>							
Thermal correction to Gibbs Free Energy= 0.780474 E(RBMK) = -3024.63566832							
H	-2.421611	-0.383189	1.841557				
C	-2.131732	0.487228	1.237769				
C	-3.004113	1.655711	1.606338				
C	-2.181825	0.032962	-0.202504				
C	-2.930238	2.862106	0.894821				
C	-3.878838	1.570541	2.686186				
C	-3.45045	-0.058258	-0.92041				
C	-3.748462	3.929195	1.252757				
C	-4.696857	2.636019	3.064655				
C	-4.624335	3.813983	2.322974				
C	-5.613706	2.520487	4.245827				
H	-1.078982	0.692993	1.469955				
O	-1.149815	-0.394615	-0.757715				
S	-1.84899	3.018995	-0.510711				
C	-0.30309	3.213338	0.323909				
C	0.913192	3.365035	-0.229275				
C	1.1944	3.290069	-1.679163				
C	2.066097	3.702067	0.678941				
C	2.15992	4.126801	-2.253824				
C	0.546661	2.368797	-2.513647				
C	2.445156	4.065636	-3.611356				
C	0.840837	2.299744	-3.868858				
C	1.787093	3.151915	-4.426381				
H	-3.934663	0.640574	3.246423				
H	-4.18082	0.662081	-0.547479				
H	-3.259144	0.114751	-1.982388				
Si	-4.306082	-1.817817	-0.908474				
C	-2.942796	-3.152076	-0.977283				
C	-3.396889	-4.459794	-1.636689				
C	-2.318544	-3.446944	0.390239				
C	-5.347918	-1.986728	0.676368				
C	-6.181042	-3.274495	0.649429				

C	-6.23208	-0.78626	1.023714
C	-5.319195	-1.862278	-2.51799
C	-4.434701	-1.685976	-3.757055
C	-6.499212	-0.888957	-2.566427
H	-5.727147	-2.883459	-2.545304
H	-3.690907	4.852943	0.687871
H	-0.415942	3.307029	1.399925
H	-3.561238	-2.344505	-3.75945
H	-2.158355	-2.714649	-1.611245
H	-4.607494	-2.094114	1.484147
H	2.937242	3.073782	0.471067
H	1.793717	3.574663	1.728014
H	2.379384	4.743489	0.546895
H	2.683407	4.849308	-1.63802
H	-0.182533	1.682435	-2.097157
H	3.182487	4.739893	-4.034444
H	0.32831	1.574091	-4.491706
H	2.008263	3.10537	-5.487304
H	-5.257304	4.655292	2.587553
H	-4.0729	-0.655735	-3.847346
H	-5.006813	-1.896376	-4.666909
H	-7.006078	-0.954075	-3.535546
H	-6.176916	0.151258	-2.444875
H	-7.245315	-1.099632	-1.797084
H	-2.556416	-5.159173	-1.709714
H	-3.783774	-4.310729	-2.647603
H	-4.178014	-4.960613	-1.056587
H	-1.923056	-2.552881	0.882367
H	-1.483508	-4.149622	0.288433
H	-3.042096	-3.906628	1.071291
H	-5.568168	-4.169263	0.510352
H	-6.924229	-3.253706	-0.154528
H	-6.728537	-3.397946	1.590255
H	-7.024473	-0.637073	0.286006
H	-5.670474	0.148481	1.100862
H	-6.724036	-0.94836	1.989805
H	-5.897551	1.482782	4.433584
H	-6.525265	3.1039	4.099971
H	-5.125607	2.897842	5.150901
Au	0.853934	-0.540719	-0.077726
P	3.025371	-0.849689	0.496934
C	3.327498	-2.529229	1.124144
C	4.158712	-2.754192	2.221871
H	4.609656	-1.91896	2.747055

C	4.403455	-4.054994	2.647135
H	5.04722	-4.227515	3.502637
C	3.826027	-5.128162	1.980632
H	4.018861	-6.14136	2.316195
C	2.996306	-4.905448	0.886069
H	2.542296	-5.742599	0.367287
C	2.742031	-3.610312	0.459621
H	2.087958	-3.437745	-0.390135
C	4.143322	-0.611742	-0.913994
C	5.280623	-1.4074	-1.067825
H	5.487066	-2.209415	-0.366969
C	6.143952	-1.17611	-2.13141
H	7.024209	-1.797781	-2.253
C	5.877796	-0.156656	-3.038075
H	6.553127	0.017511	-3.868868
C	4.743326	0.633518	-2.888047
H	4.524272	1.423933	-3.597284
C	3.871994	0.406584	-1.831604
H	2.980631	1.01928	-1.731951
C	3.571217	0.290778	1.803719
C	2.745891	0.4894	2.913771
H	1.784612	-0.012741	2.973173
C	3.155952	1.325181	3.942086
H	2.515901	1.473392	4.805089
C	4.384173	1.975237	3.863334
H	4.701059	2.632606	4.665756
C	5.20332	1.784633	2.757937
H	6.15974	2.291955	2.694678
C	4.802428	0.941731	1.727142
H	5.443952	0.796647	0.864443