

## Enantioselective Gold(I)-Catalyzed Rearrangement of Cyclopropyl-Substituted 1,6-Enynes into 2-Oxocyclobutyl-cyclopentanes

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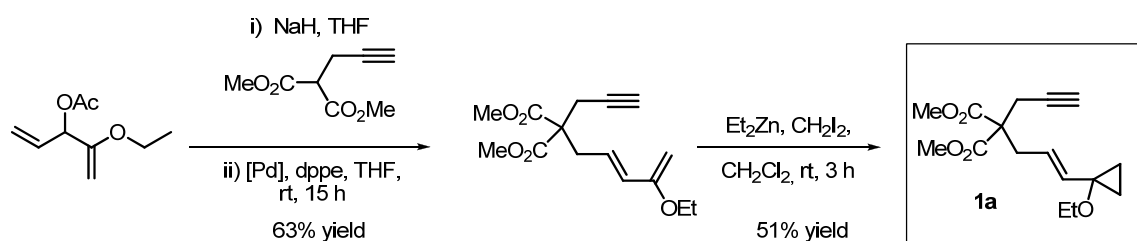
## **I. General information**

All non-aqueous reactions were run under an inert atmosphere (argon), by using standard techniques for manipulating air-sensitive compounds. Anhydrous solvents were obtained by filtration through drying columns (THF, Et<sub>2</sub>O, CH<sub>2</sub>Cl<sub>2</sub>, DMF). All reagents and solvents were of commercial quality and were used without further purification. Analytical thin-layer chromatography (TLC) was performed on plates precoated with silica gel (Merck 60 F<sub>254</sub>). The developed chromatograms were visualized by UV absorbance. Flash column chromatography was performed using 40-63 mesh silica gel. Purifications have been performed on a CombiFlash Companion TS Chromatography system, unless otherwise stated. NMR spectra (<sup>1</sup>H, <sup>13</sup>C, <sup>31</sup>P) were recorded on either Bruker AV 500 or AV 300 spectrometers. Chemical shifts are reported in parts per million relative to an internal standard of residual chloroform ( $\delta = 7.26$  ppm for <sup>1</sup>H NMR and 77.16 ppm for <sup>13</sup>C NMR). IR spectra have been recorded on a Perkin-Elmer FT-IR spectrophotometer and are reported in reciprocal centimeters (cm<sup>-1</sup>). High resolution mass spectra (HRMS-ESI) and MS (FAB+) data have been recorded with the mass spectrometer Vg Analytical 7070 EQ. Optical rotations have been determined on a JASCO P-1010 polarimeter. Data are reported as follows:  $[\alpha]_D^{\text{temp}}$  ( $c$  in g/100 mL, solvent). HPLC was performed at a column temperature of 20-35 °C on a Waters 2695 Separations Module equipped with a diode array UV detector. Data are reported as follows: column type, eluent, flow rate, retention time ( $t_r$ ).

## II. Experimental Procedures

### II.1. Synthesis of substrates:

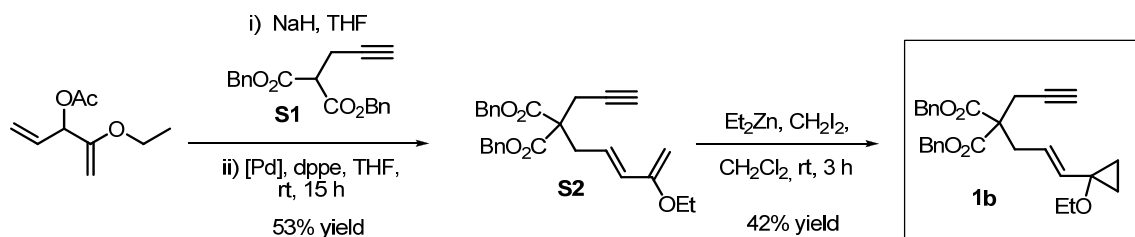
#### 1. Substrate 1a:



Compound **1a** was synthesized according to the described procedures.<sup>1</sup>

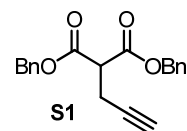
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 5.47-5.26 (m, 2H), 3.68 (s, 6H), 3.38 (q, *J* = 6.9 Hz, 2H), 2.78-2.68 (m, 4H), 1.98 (t, *J* = 2.7 Hz, 1H), 1.08 (t, *J* = 6.9 Hz, 3H), 0.97 (dd, *J* = 7.5, 5.4 Hz, 2H), 0.64 (dd, *J* = 7.5, 5.4 Hz, 2H).

#### 2. Substrate 1b:



Compound **S1** was synthesized according to the described procedure.<sup>2</sup>

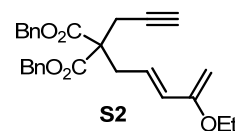
Purification by flash column chromatography of the filtrate (silica gel; petroleum ether/ MTBE/ 95/5) gave the desired compound as colorless oil (43% yield). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.36-7.25 (m, 10H), 5.18 (s, 4H), 3.71 (t, *J* = 7.8 Hz, 1H), 2.83 (dd, *J* = 7.8, 2.7 Hz, 2H), 2.00 (m, 1H).



To a dry schlenk charged with allylpalladium chloride dimer (32 mg, 0.086 mmol) and dppe (85 mg, 0.22 mmol) in 10 mL of dry THF, the acetic acid 2-ethoxy-1-vinyl-allyl ester (363 mg, 2.2 mmol) was slowly added under argon.

The resulting solution was stirred at room temperature for 30 min before the

sodium salt solution of dibenzyl propargylmalonate [which was previously prepared by addition of malonate (690 mg, 2.2 mmol) to NaH (86 mg, 2.2 mmol, 60% dispersion mineral oil) in 15 mL THF] was added. The mixture was stirred at room temperature for 16 h then quenched with 20 mL saturated NH<sub>4</sub>Cl solution, extracted with EtOAc and washed with brine before drying over MgSO<sub>4</sub>. The solvent was removed under reduced pressure and the crude was purified by chromatography on silica gel with (10/1/0.5 petroleum ether/ MTBE/triethylamine) afforded diene **S2** as a colorless oil (531 mg, 53% yield). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.37-7.24 (m, 10H), 5.98-5.79 (m, 2H), 5.15 (s, 4H), 4.08 (s, 1H), 4.01 (s, 1H), 3.78 (q, *J* = 6.9 Hz, 2H), 2.91 (d, *J* = 7.2 Hz, 2H), 2.87 (d, *J* = 2.7 Hz, 2H), 2.02 (t, *J* = 2.4 Hz, 1H), 1.33 (t, *J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 169.4 (C), 157.6

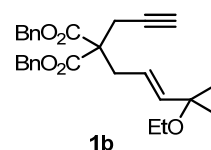


<sup>1</sup> a) P. A. Wender, A. J. Dyckman, C. O. Husfeld, D. Kadereit, J. A. Love, H. Rieck, *J. Am. Chem. Soc.* **1999**, *121*, 10442-10443; b) E. Jimenez-Nunez, C. K. Claverie, C. Nieto-Oberhuber, A. M. Echavarren *Angew. Chem. Int. Ed.* **2006**, *45*, 5452-5455.

<sup>2</sup> C. Kourra, F. Klotter, F. Sladojevich, D. J. Dixon, *Org. Lett.*, **2012**, *14*, 1016-1019.

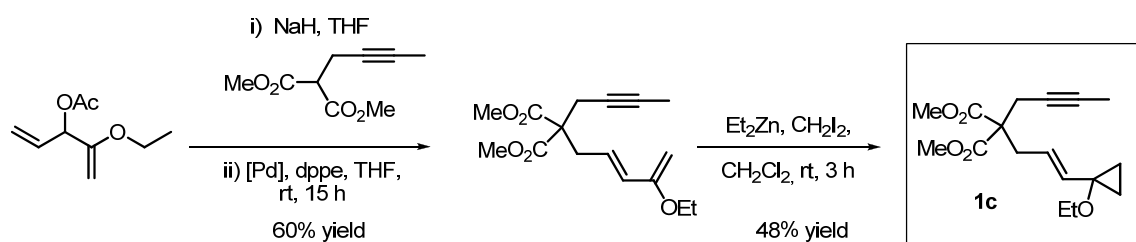
(C), 135.2 (C), 131.4 (CH), 128.5 (CH), 128.3 (CH), 128.2 (CH), 122.9 (CH), 86.5 (CH<sub>2</sub>), 78.8 (C), 71.8 (CH), 67.4 (CH<sub>2</sub>), 62.7 (CH<sub>2</sub>), 57.2 (C), 35.0 (CH<sub>2</sub>), 22.7 (CH<sub>2</sub>), 14.5 (CH<sub>3</sub>); **HRMS** (ESI) calcd. for C<sub>27</sub>H<sub>28</sub>NaO<sub>5</sub> [M+ Na]<sup>+</sup>: 455.1834, found: 455.1951.

**S2** (530 mg, 1.23 mmol) was dissolved in 10 mL anhydrous CH<sub>2</sub>Cl<sub>2</sub> under argon. The diethylzinc (1.1 mL, 1.0 M in hexanes, 1.1 mmol) and diiodomethane (294 mg, 1.1 mmol) was sequentially added to this solution. The resulting reaction mixture was stirred at room for 3 h then quenched with 10 mL saturated NH<sub>4</sub>Cl.



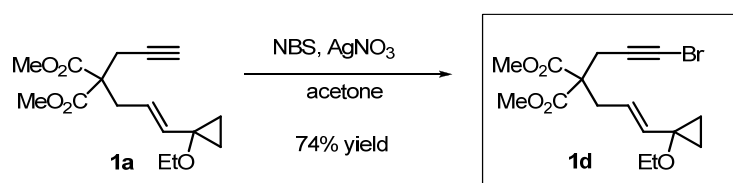
The organic layer was washed with 10 mL saturated NaHCO<sub>3</sub> and 10 mL H<sub>2</sub>O and then dried over MgSO<sub>4</sub>. The solvent was removed in *vacuo* and the residue was purified by flash chromatography (petroleum ether/ EtOAc 90/10) gave the desired compound as colorless oil (42% yield, 225 mg). **<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 7.36-7.20 (m, 10H), 5.44-5.25 (m, 2H), 5.13 (s, 4H), 3.40 (q, *J* = 6.9 Hz, 2H), 2.55-2.58 (m, 4H), 1.99 (t, *J* = 2.7 Hz, 1H), 1.12 (t, *J* = 7.2 Hz, 3H), 0.94 (dd, *J* = 7.5, 5.4 Hz, 2H), 0.56 (dd, *J* = 7.5, 5.4 Hz, 2H); **<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 169.6 (C), 136.8 (CH), 135.4 (C), 128.7 (CH), 128.5 (CH), 128.3 (CH), 120.9 (CH), 78.9 (C), 71.8 (CH), 67.5 (CH<sub>2</sub>), 63.1 (CH<sub>2</sub>), 60.9 (C), 57.3 (C), 34.9 (CH<sub>2</sub>), 22.7 (CH<sub>2</sub>), 15.6 (CH<sub>3</sub>), 14.5 (CH<sub>2</sub>); **IR**: *v*<sub>max</sub> = 3291, 3034, 2973, 1733, 1498, 1456, 1279, 1245, 1217, 1191, 1169, 1061, 968, 946, 906, 745, 736, 696 cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>28</sub>H<sub>30</sub>NaO<sub>5</sub> [M+ Na]<sup>+</sup>: 469.1991, found: 469.2032.

### 3. Substrate 1c:



Compound **1c** was synthesized according to the described procedures.<sup>3</sup> Purification by flash column chromatography on silica gel (petroleum ether/ EtOAc 80/20) gave the desired compound as colorless oil (48% yield). **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 5.39-5.26 (m, 2H), 3.65 (s, 6H), 3.37 (q, *J* = 7.0 Hz, 2H), 2.69 (d, *J* = 7.0 Hz, 2H), 2.65 (d, *J* = 2.5 Hz, 2H), 1.70-1.65 (m, 3H), 1.07 (t, *J* = 7.5 Hz, 3H), 0.88 (dd, *J* = 7.0, 5.0 Hz, 2H), 0.56 (dd, *J* = 7.0, 5.0 Hz, 2H); **<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 170.5 (C), 136.0 (CH), 121.4 (CH), 78.9 (C), 73.2 (C), 62.8 (CH<sub>2</sub>), 60.8 (C), 57.5 (C), 52.6 (CH<sub>3</sub>), 35.0 (CH<sub>2</sub>), 23.0 (CH<sub>2</sub>), 15.4 (CH<sub>3</sub>), 14.2 (CH<sub>2</sub>), 3.4 (CH<sub>3</sub>); **IR**: *v*<sub>max</sub> = 2976, 2953, 1737, 1438, 1326, 1286, 1229, 1203, 1181, 1063, 1029, 973 cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>17</sub>H<sub>24</sub>NaO<sub>5</sub> [M+ Na]<sup>+</sup>: 331.1521, found: 331.1600.

### 4. Substrate 1d:

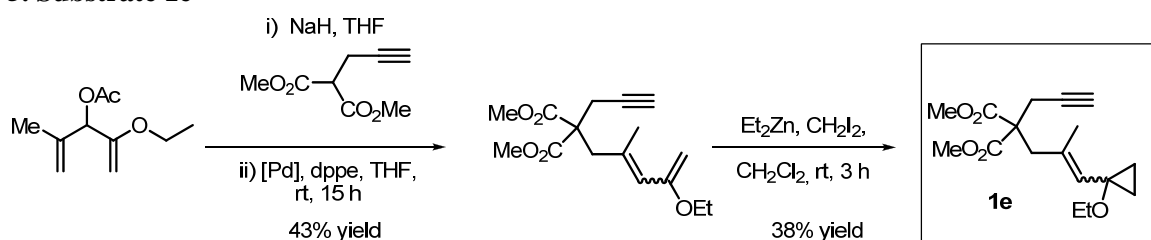


NBS (103 mg, 0.58 mmol) and AgNO<sub>3</sub> (17.3 mg, 0.1 mmol) were added to the solution of **1a** (100 mg,

<sup>3</sup> B. M. Trost, H. C. Shen, D. B. Horne, F. D. Toste, B. G. Steinmetz, C. Koradin, *Chem. Eur. J.* **2005**, *11*, 2577-2590.

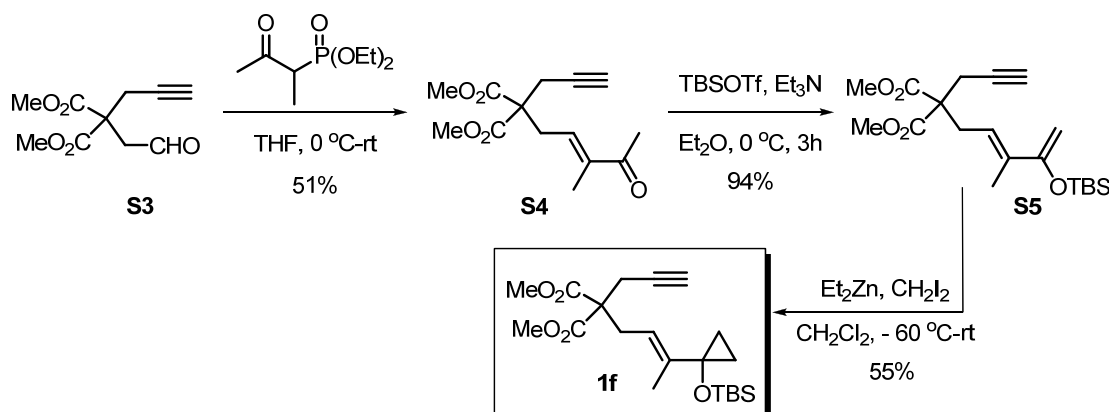
0.34 mmol) in acetone (4 mL) under argon. The reaction mixture was stirred at room temperature for 4 hours then quenched with sat. NaHCO<sub>3</sub> solution. The mixture was extracted with EtOAc, the combined organic layers were washed with brine and dried over MgSO<sub>4</sub>. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel using PE/EtOAc (90/10) as eluent to give the desired product **1d** as colorless oil (90 mg, 74% yield). **<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 5.46-5.26 (m, 2H), 3.72 (s, 6H), 3.42 (q, *J* = 6.9 Hz, 2H), 2.82-2.72 (m, 4H), 1.13 (t, *J* = 6.9 Hz, 3H), 0.95 (dd, *J* = 7.5, 5.4 Hz, 2H), 0.62 (dd, *J* = 7.5, 5.4 Hz, 2H); **<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) 170.2 (C), 136.7 (CH), 120.9 (CH), 74.9 (C), 63.0 (CH<sub>2</sub>), 60.9 (C), 57.2 (C), 52.9 (CH<sub>3</sub>), 41.6 (C), 35.3 (CH<sub>2</sub>), 24.0 (CH<sub>2</sub>), 15.6 (CH<sub>3</sub>), 14.4 (CH<sub>2</sub>); **IR**:  $\nu_{max}$  = 2975, 2955, 1737, 1437, 1285, 1227, 1202, 1181, 1062, 973 cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>16</sub>H<sub>22</sub>BrO<sub>5</sub> [M+H]<sup>+</sup>: 373.0651, found: 373.0645.

### 5. Substrate 1e

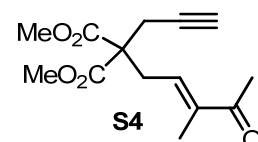


Compound **1e** was synthesized according to the procedure described for **1a**.<sup>1</sup> The crude was purified by flash column chromatography with 15/1 (petroleum ether /EtOAc) gave product **1e** (mixture *E/Z* 8:1) as a colorless oil (38% yield). **<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ 5.42 (s, 1H), 3.73 (s, 6H), 3.42 (q, *J* = 7.2 Hz, 2H), 2.82 (s, 2H), 2.78 (d, *J* = 2.7 Hz, 2H), 2.03 (t, *J* = 2.7 Hz, 1H), 1.76 (d, *J* = 0.6 Hz, 3H), 1.11 (t, *J* = 7.2 Hz, 3H), 0.93 (dd, *J* = 6.9, 4.5 Hz, 2H), 0.54 (dd, *J* = 6.9, 4.8 Hz, 2H); **HRMS** (ESI) calcd. for C<sub>17</sub>H<sub>24</sub>NaO<sub>5</sub> [M+ Na]<sup>+</sup>: 331.1521, found: 331.1581.

### 6. Substrate 1f:



Diethyl 3-oxobutan-2-ylphosphonate (375 mg, 1.8 mmol) in dry THF (3 mL) was added to a stirring suspension of NaH (72mg, 1.8 mmol) in dry THF (5 mL) at 0 °C under argon. After 1 hour stirring at 0 °C, a solution of aldehyde **S3**<sup>4</sup> (191 mg, 0.9 mmol) in dry THF (5 mL) was added dropwise to the resulting mixture. The solution was stirred at room temperature for another 4 hours then quenched by the addition of

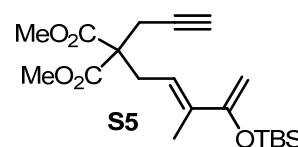


<sup>4</sup> a) E. Dunach, R. L. Halterman, K. P. C. Vollhardt, *J. Am. Chem. Soc.*, **1985**, *107*, 1664-1671 ; b) F. Cambeiro, S. Lopez, J. A. Varela, C. Saa, *Angew. Chem. Int. Ed.* **2014**, *53*, 5959-5963.

saturated  $\text{NH}_4\text{Cl}$  (10 mL). After extracted by with diethyl ether, the combined organic layers were dried over  $\text{MgSO}_4$  and concentrated under reduced pressure. The crude was purified by flash column chromatography on silica gel (PE/ethyl acetate 80/20) to obtain compound **S4** (120 mg, 51% yield) as a white solid.  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  6.45 (t,  $J = 7.2$  Hz, 1H), 3.76 (s, 6H), 3.01 (d,  $J = 7.5$  Hz, 2H), 2.83 (d,  $J = 2.4$  Hz, 2H), 2.28 (s, 3H), 2.06 (t,  $J = 2.4$  Hz, 1H), 1.81 (s, 3H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 199.4 (C), 169.9 (C), 141.0 (C), 135.5 (CH), 78.4 (C), 72.1 (CH), 56.6 (C), 53.1 ( $\text{CH}_3$ ), 32.0 ( $\text{CH}_2$ ), 25.6 ( $\text{CH}_3$ ), 23.5 ( $\text{CH}_2$ ), 11.4 ( $\text{CH}_3$ ); **IR**:  $\nu_{\text{max}} = 2956, 1733, 1670, 1436, 1291, 1200, 1183, 1054, 975 \text{ cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{14}\text{H}_{19}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 267.1232, found: 267.1310.

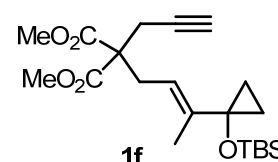
Compound **S5** was synthesized according to the same procedure used for **S10**.

(160 mg, 94%).  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  5.79 (t,  $J = 8.0$  Hz, 1H), 4.43 (s, 1H), 4.26 (s, 1H), 3.72 (s, 6H), 2.93 (d,  $J = 7.5$  Hz, 2H), 2.77 (s, 2H), 1.99 (s, 1H), 1.80 (s, 3H), 0.94 (s, 9H), 0.14 (s, 6H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 170.3 (C), 156.8 (C), 135.4 (C), 120.6 (CH), 92.1 ( $\text{CH}_2$ ), 79.1 (C), 71.5 (CH), 57.1 (C), 52.9 ( $\text{CH}_3$ ), 31.2 ( $\text{CH}_2$ ), 25.9 ( $\text{CH}_3$ ), 22.9 ( $\text{CH}_2$ ), 18.3 (C), 13.5 ( $\text{CH}_3$ ), -4.6 ( $\text{CH}_3$ ); **IR**:  $\nu_{\text{max}} = 3292, 2955, 1739, 1596, 1436, 1253, 1211, 1046, 1016, 1005, 832, 781 \text{ cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{20}\text{H}_{33}\text{O}_5\text{Si}$   $[\text{M}+\text{H}]^+$ : 381.2097, found: 381.2157.

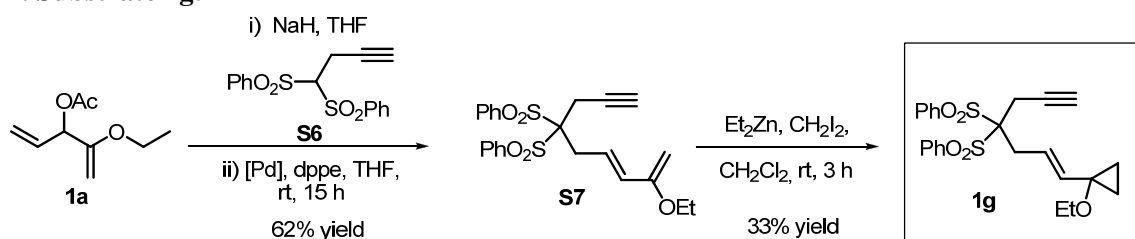


Compound **1f** was prepared following the same procedure for the synthesis

of **1j** (88 mg, 55%).  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  5.19 (t,  $J = 7.2$  Hz, 1H), 3.72 (s, 6H), 2.84-2.72 (m, 4H), 2.00 (bs, 1H), 1.72 (s, 3H), 0.83 (s, 9H), 0.78 (m, 2H), 0.67 (m, 2H), 0.36 (s, 6H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 170.5 (C), 141.6 (C), 116.8 (CH), 79.2 (C), 71.5 (CH), 61.0 (C), 57.1 (C), 52.9 ( $\text{CH}_3$ ), 30.6 ( $\text{CH}_2$ ), 25.9 ( $\text{CH}_3$ ), 22.8 ( $\text{CH}_2$ ), 17.9 (C), 14.1 ( $\text{CH}_3$ ), 13.5 ( $\text{CH}_2$ ), -3.6 ( $\text{CH}_3$ ); **IR**:  $\nu_{\text{max}} = 2955, 2931, 2857, 1738, 1437, 1287, 1238, 1212, 1025, 836, 776 \text{ cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{21}\text{H}_{35}\text{O}_5\text{Si}$   $[\text{M}+\text{H}]^+$ : 395.2254, found: 395.2353.

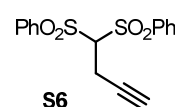


## 7. Substrate **1g**:

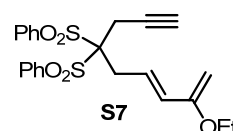


Compound **1g** was synthesized according to the described procedure.<sup>5</sup>

The crude was purified by flash chromatography (silica gel: petroleum ether/ EtOAc 60/40) to give 480 mg of **S6** as a white solid (60% yield),  $R_f = 0.61$  (60% of petroleum ether/ EtOAc).  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (d,  $J = 7.5$  Hz, 4H), 7.73 (t,  $J = 7.5$  Hz, 2H), 7.59 (t,  $J = 7.8$  Hz, 4H), 4.60 (t,  $J = 6.3$  Hz, 1H), 3.13 (dd,  $J = 6.3, 2.7$  Hz, 2H), 1.94 (t,  $J = 2.7$  Hz, 1H).



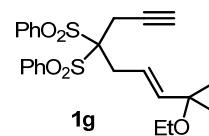
Compound **S7** was synthesized according to the procedure described for **S2**. Purification by flash column chromatography of the filtrate (6/4/0.5 petroleum ether/ MTBE/triethylamine) gave the desired compound as colorless oil (62% yield, 270 mg).  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.11 (d,  $J = 7.5$  Hz, 4H), 7.69 (t,



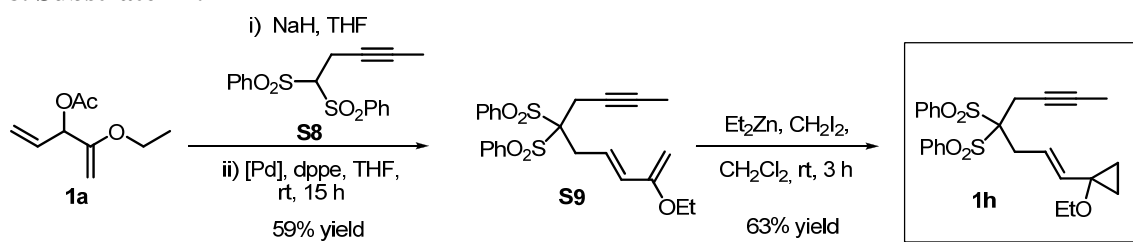
<sup>5</sup> J. R. Rodriguez, L. Castedo, J. L. Mascarenas, *J. Org. Chem.* **2000**, *65*, 2528-2531

$J = 7.5$  Hz, 2H), 7.56 (t,  $J = 7.5$  Hz, 4H), 6.21-6.13 (m, 1H), 6.01 (d,  $J = 15.5$  Hz, 1H), 4.12 (s, 1H), 4.08 (s, 1H), 3.79 (q,  $J = 7.0$  Hz, 2H), 3.19-3.12 (m, 4H), 2.12 (t,  $J = 3.0$  Hz, 1H), 1.33 (t,  $J = 7.0$  Hz, 3H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )  $\delta$  157.5 (C), 136.5 (C), 134.9 (CH), 132.8 (CH), 131.6 (CH), 128.6 (CH), 120.7 (CH), 89.0 (C), 87.1 ( $\text{CH}_2$ ), 75.8 (C), 74.5 (CH), 62.9 ( $\text{CH}_2$ ), 32.2 ( $\text{CH}_2$ ), 21.0 ( $\text{CH}_2$ ), 14.5 ( $\text{CH}_3$ ); **HRMS** (ESI) calcd. for  $\text{C}_{23}\text{H}_{24}\text{NaO}_5\text{S}_2$  [ $\text{M} + \text{Na}$ ] $^+$ : 467.0963, found: 467.1053.

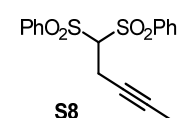
Compound **1g** was synthesized according to the procedure described for **1b**. Purification by flash column chromatography of the filtrate (petroleum ether/EtOAc 60/40) gave the desired compound as colorless oil (33% yield, 120 mg).  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.14-8.07 (m, 4H), 7.75-7.66 (m, 2H), 7.62-7.52 (m, 4H), 5.85-5.70 (m, 1H), 5.51 (d,  $J = 15.3$  Hz, 1H), 3.53 (q,  $J = 6.9$  Hz, 2H), 3.16 (d,  $J = 2.7$  Hz, 2H), 3.10 (dd,  $J = 6.9, 0.6$  Hz, 2H), 2.07 (t,  $J = 2.7$  Hz, 1H), 1.18 (t,  $J = 6.9$  Hz, 3H), 1.02 (dd,  $J = 7.5, 5.4$  Hz, 2H), 0.69 (dd,  $J = 7.5, 5.4$  Hz, 2H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 138.4 (CH), 136.7 (C), 134.9 (CH), 131.6 (CH), 128.7 (CH), 118.4 (CH), 89.0 (C), 76.0 (C), 74.4 (CH), 63.3 ( $\text{CH}_2$ ), 61.0 (C), 32.0 ( $\text{CH}_2$ ), 20.9 ( $\text{CH}_2$ ), 15.6 ( $\text{CH}_3$ ), 14.5 ( $\text{CH}_2$ ); **IR**:  $\nu_{\text{max}} = 3275, 2968, 1584, 1448, 1331, 1310, 1144, 1077, 1060, 1021, 910, 801, 725, 685$   $\text{cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{24}\text{H}_{26}\text{NaO}_5\text{S}_2$  [ $\text{M} + \text{Na}$ ] $^+$ : 481.1119, found: 481.1183.



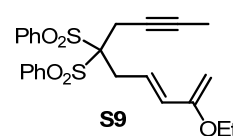
## 8. Substrate 1h:



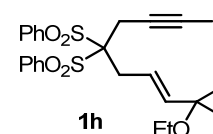
Compound **S8** was prepared according to the known procedure.<sup>6</sup> Purification by flash column chromatography (petroleum ether/EtOAc 60/40) to give the 1,1-bis(phenylsulfonyl)-pent-3-yne (532 mg, 52% yield) as a white solid.  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (d,  $J = 7.2$  Hz, 4H), 7.71 (t,  $J = 7.5$  Hz, 2H), 7.59 (t,  $J = 7.8$  Hz, 4H), 4.54 (t,  $J = 6.0$  Hz, 1H), 3.08 (ddd,  $J = 8.4, 5.1, 2.4$  Hz, 2H), 1.52 (t,  $J = 2.7$  Hz, 3H).



Compound **S9** was synthesized according to the procedure described for **S2**. Purification by flash column chromatography (6/4/0.5 petroleum ether/MTBE/triethylamine) gave the desired compound as colorless oil (410 mg, 59% yield).  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 (d,  $J = 7.5$  Hz, 4H), 7.64 (t,  $J = 7.5$  Hz, 2H), 7.52 (t,  $J = 7.8$  Hz, 4H), 6.24-6.08 (m, 1H), 5.96 (d,  $J = 15.3$  Hz, 1H), 4.09 (s, 1H), 4.05 (s, 1H), 3.75 (q,  $J = 6.9$  Hz, 2H), 3.19-3.01 (m, 4H), 1.59 (s, 3H), 1.29 (t,  $J = 6.9$  Hz, 3H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 157.5 (C), 136.9 (C), 134.6 (CH), 132.1 (CH), 131.4 (CH), 128.4 (CH), 121.1 (CH), 89.2 (C), 86.8 ( $\text{CH}_2$ ), 81.9 (C), 70.7 (C), 62.8 ( $\text{CH}_2$ ), 32.6 ( $\text{CH}_2$ ), 21.4 ( $\text{CH}_2$ ), 14.4 ( $\text{CH}_3$ ), 3.5 ( $\text{CH}_3$ ); **HRMS** (ESI) calcd. for  $\text{C}_{24}\text{H}_{26}\text{NaO}_5\text{S}_2$  [ $\text{M} + \text{Na}$ ] $^+$ : 481.1119, found: 481.1162.



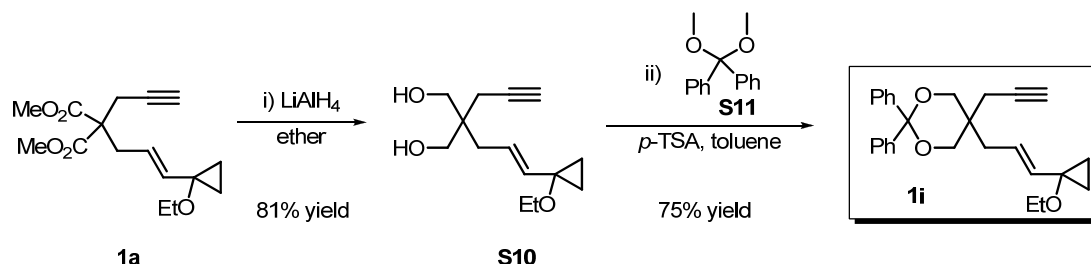
Compound **1h** was synthesized according to the procedure described for **1b**. Purification by flash column chromatography (petroleum ether/EtOAc 60/40) gave the desired compound as colorless oil (63% yield, 260 mg).  $^1\text{H NMR}$  (300



<sup>6</sup> B. P. Peppers, S. T. Diver, *J. Am. Chem. Soc.* **2004**, *126*, 9524-9525.

MHz, CDCl<sub>3</sub>) δ 8.12-8.05 (m, 4H), 7.70 (tt, *J* = 7.5, 1.2 Hz, 2H), 7.62-7.52 (m, 4H), 5.86-5.72 (m, 1H), 5.50 (d, *J* = 18.3 Hz, 1H), 3.54 (q, *J* = 7.2 Hz, 2H), 3.15 (dd, *J* = 5.4, 2.7 Hz, 2H), 3.06 (dd, *J* = 7.2, 1.2 Hz, 2H), 1.62 (t, *J* = 2.7 Hz, 3H), 1.19 (t, *J* = 7.2 Hz, 3H), 1.02 (dd, *J* = 7.2, 5.1 Hz, 2H), 0.69 (dd, *J* = 7.2, 4.8 Hz, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 137.8 (CH), 137.3 (C), 134.7 (CH), 131.7 (CH), 128.6 (CH), 119.1 (CH), 89.5 (C), 81.9 (C), 70.9 (C), 63.4 (CH<sub>2</sub>), 61.1 (C), 32.5 (CH<sub>2</sub>), 21.4 (CH<sub>2</sub>), 15.7 (CH<sub>3</sub>), 14.5 (CH<sub>2</sub>), 3.8 (CH<sub>3</sub>); IR: *v*<sub>max</sub> = 3065, 2974, 2920, 1583, 1448, 1332, 1311, 1145, 1078, 1062, 757, 727, 689 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>25</sub>H<sub>28</sub>NaO<sub>5</sub>S<sub>2</sub> [M+Na]<sup>+</sup>: 495.1276, found: 495.1331.

## 9. Substrate 1i:



Compound **S10** was prepared according to the well known procedure.<sup>1b</sup> The crude mixture was purified by flash column chromatography (silica gel, 60/40 PE/EtOAc), to afford diol **S10** as a colorless oil (80 mg, 81%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 5.58-5.49 (m, 1H), 5.43 (d, *J* = 15.5 Hz, 1H), 3.61 (m, 4H), 3.46 (q, *J* = 7.0 Hz, 2H), 2.86 (bs, 2H), 2.22 (d, *J* = 2.5 Hz, 2H), 2.11 (d, *J* = 7.5 Hz, 2H), 2.00 (t, *J* = 2.5 Hz, 1H), 1.14 (t, *J* = 7.0 Hz, 3H), 0.95 (dd, *J* = 7.0, 5.0 Hz, 2H), 0.63 (dd, *J* = 7.5, 5.0 Hz, 2H).

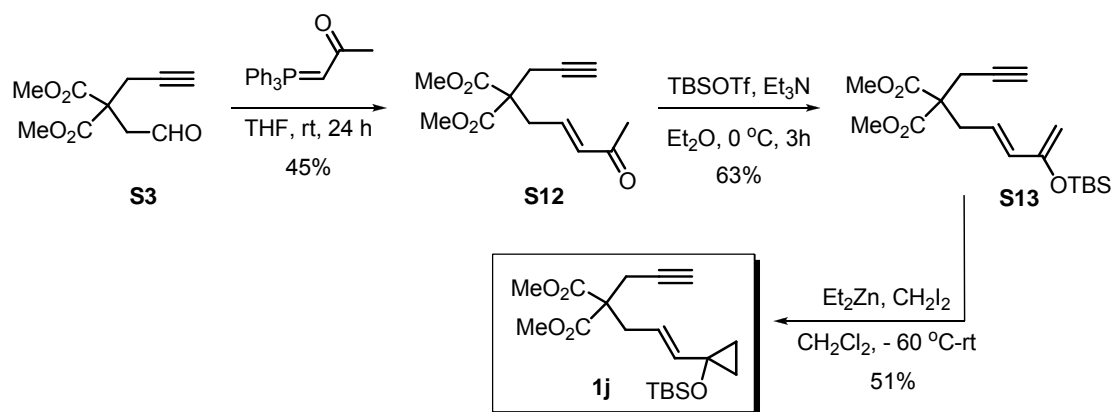
Compound **S11** was prepared according to the described procedure.<sup>7</sup> <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.54-7.47 (m, 4H), 7.34-7.17 (m, 6H), 3.13 (s, 6H).

The diol **S10** (80 mg, 0.34 mmol) and **S11** (1.14g, 5 mmol) were dissolved in anhydrous toluene (10 mL) under argon. *p*-TSA (57 mg, 0.068 mmol) was added to the solution under argon. The resulting mixture was stirred at rt for 8 hours. The reaction mixture was stopped by the addition of 5 drops of Et<sub>3</sub>N and extracted with MTBE. The combined organic layers were washed with sat. aq. NaHCO<sub>3</sub> (5 ml) and brine (5 ml) and dried over MgSO<sub>4</sub>. The solvent was removed under reduced pressure and the crude mixture was purified by flash column chromatography (silica gel, 90/10 Petroleum ether/EtOAc) to give the desired product **1i** as a colorless oil (102 mg, 75%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.56-7.46 (m, 4H), 7.42-7.21 (m, 6H), 5.56-5.53 (m, 1H), 5.35 (d, *J* = 15.6 Hz, 1H), 3.90-3.70 (m, 4H), 3.40 (q, *J* = 6.9 Hz, 2H), 2.50 (d, *J* = 2.7 Hz, 2H), 2.13 (d, *J* = 7.2 Hz, 2H), 2.00 (t, *J* = 2.7 Hz, 1H), 1.14 (t, *J* = 7.2 Hz, 3H), 0.95 (dd, *J* = 7.2, 5.1 Hz, 2H), 0.61 (dd, *J* = 7.2, 5.1 Hz, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 142.8 (C), 140.5 (C), 135.4 (CH), 128.7 (CH), 128.3 (CH), 128.05 (CH), 127.97 (CH), 127.1 (CH), 126.1 (CH), 121.4 (CH), 101.4 (C), 80.7 (C), 71.1 (CH), 68.4 (CH<sub>2</sub>), 63.0 (CH<sub>2</sub>), 61.0 (C), 35.9 (C), 35.0 (CH<sub>2</sub>), 22.5 (CH<sub>2</sub>), 15.6 (CH<sub>3</sub>), 14.4 (CH<sub>2</sub>); IR: *v*<sub>max</sub> = 3301, 2972, 2870, 1491, 1452, 1287, 1261, 1198, 1118, 1093, 1065, 1029, 977, 770, 748, 707, 694 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>27</sub>H<sub>31</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 403.2273, found: 403.2322.

## 10. Substrate 1j:

<sup>7</sup> M. Aepkers, B. Wünsch, *Arch. Pharm. Pharm. Med. Chem.* **2004**, 337, 67-75





2-(2-oxoethyl)-2-(prop-2-yn-1-yl)malonate **S12** was prepared according to the well known procedure with a slight modification.<sup>8</sup> The dimethyl 2-((1,3-dioxolan-2-yl)methyl)-2-(prop-2-ynyl)malonate<sup>9</sup> (1.12 g, 4.4 mmol) was dissolved in conc. formic acid (4 ml), and the resulting solution was stirred at room temperature for 16 hours. After neutralization with *sat.* NaHCO<sub>3</sub>, the mixture was extracted with diethyl ether; the organic layers were collected, dried over MgSO<sub>4</sub> and concentrated under reduced pressure. The crude was purified by flash column chromatography (silica gel, 80/20 PE/EtOAc) afforded the aldehyde **S3** as a white solid (810 mg, 88%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 9.73 (s, 1H), 3.76 (s, 6H), 3.26 (s, 2H), 2.97 (d, *J* = 2.7 Hz, 2H), 2.03 (t, *J* = 2.7 Hz, 1H).

2-(2-oxoethyl)-2-(prop-2-yn-1-yl)malonate **S3** (490 mg, 2.31 mmol) and 1-(triphenylphosphoranylidene)-2-propanone (768 mg, 2.43 mmol) were dissolved in 30 mL THF under argon at rt. The resulting mixture was stirred at rt for 24 hours, then quenched by the addition of 15 mL of H<sub>2</sub>O. The aqueous solution was extracted with diethyl ether and the combined organic layers were dried over MgSO<sub>4</sub> and concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel using PE/EtOAc (80/20) as the eluent to give 251 mg of the compound **S12** (45% yield). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 6.68-6.54 (m, 1H), 6.16 (d, *J* = 15.6 Hz, 1H), 3.76 (s, 6H), 2.95 (dd, *J* = 7.5, 1.2 Hz, 2H), 2.81 (d, *J* = 2.7 Hz, 2H), 2.23 (s, 3H), 2.06 (t, *J* = 2.7 Hz, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 198.1 (C), 169.7 (C), 140.8 (CH), 135.1 (CH), 78.3 (C), 72.3 (CH), 56.8 (C), 53.2 (CH<sub>3</sub>), 35.6 (CH<sub>2</sub>), 27.2 (CH<sub>3</sub>), 23.5 (CH<sub>2</sub>); IR:  $\nu_{max}$  = 3283, 2957, 1734, 1676, 1630, 1437, 1254, 1207, 1182, 982 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>13</sub>H<sub>17</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 253.1076, found: 253.1097.

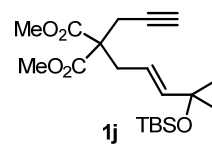
Anhydrous ether was added to a 100 mL flask charged with compound **S12** (165 mg, 0.66 mmol) under argon. Triethylamine (199 mg, 1.96 mmol) and TBSOTf (349 mg, 1.32 mmol) was sequentially added to the resulting solution at 0 °C. The mixture was stirred at 0 °C for 2 hours and then quenched by the addition of 5 mL brine. The resulting mixture was extracted by ether and the combined organic layers were washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, and concentrated. The crude was purified by flash column chromatography on silica gel using PE/MTBE/Et<sub>3</sub>N (10/1/0.5) as the eluent to produce the silylenol ether **S13** (85 mg, 63% yield) as a white solid. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 6.01 (d, *J* = 15.0 Hz, 1H), 5.83-5.67 (m, 1H), 4.26 (d, *J* = 3.6 Hz, 2H), 3.73 (s, 6H), 2.85 (d, *J* = 7.8 Hz,

<sup>8</sup> a) E. Dunach, R. L. Halterman, K. P. C. Vollhardt, *J. Am. Chem. Soc.*, **1985**, *107*, 1664-1671 ; b) F. Cambeiro, S. Lopez, J. A. Varela, C. Saa, *Angew. Chem. Int. Ed.* **2014**, *53*, 5959-5963.

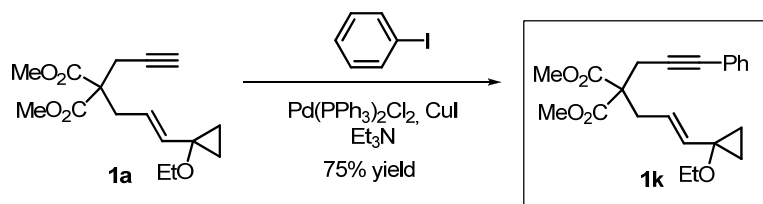
<sup>9</sup> a) F. Cambeiro, S. Lopez, J. A. Varela, C. Saa, *Angew. Chem. Int. Ed.* **2012**, *51*, 723-727; b) L. Escalante, C. Gonzalez-Rodriguez, J. A. Varela, C. Saa, *Angew. Chem. Int. Ed.* **2012**, *51*, 12316-12320.

2H), 2.77 (d,  $J = 2.4$  Hz, 2H), 2.02 (t,  $J = 2.4$  Hz, 1H), 0.95 (s, 9H), 0.15 (s, 6H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 170.2 (C), 154.5 (C), 132.8 (CH), 123.9 (CH), 95.8 ( $\text{CH}_2$ ), 78.9 (C), 71.6 (CH), 57.1 (C), 52.9 ( $\text{CH}_3$ ), 34.9 ( $\text{CH}_2$ ), 25.9 ( $\text{CH}_3$ ), 22.9 ( $\text{CH}_2$ ), 18.3 (C), -4.6 ( $\text{CH}_3$ ); **IR**:  $\nu_{\text{max}} = 3287, 2956, 2931, 2860, 1741, 1595, 1437, 1292, 1207, 1179, 1027, 968, 839, 782 \text{ cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{19}\text{H}_{31}\text{O}_5\text{Si}$   $[\text{M}+\text{H}]^+$ : 367.1941, found: 367.1953.

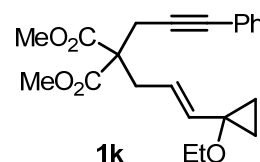
$\text{ZnEt}_2$  (1M in Hexane, 0.3 mL, 0.30 mmol) and  $\text{CH}_2\text{I}_2$  (30  $\mu\text{L}$ , 0.30 mmol) was sequentially added to a flask charged with anhydrous  $\text{CH}_2\text{Cl}_2$  (5 mL) at  $-60^\circ\text{C}$  under argon. The resulting mixture was warmed to  $0^\circ\text{C}$  until a white precipitate appeared. The solution was cooled down to  $-60^\circ\text{C}$  again and silylenol ether **S13** (38 mg, 0.1 mmol) in dry  $\text{CH}_2\text{Cl}_2$  (2 mL) was added dropwise. The resulting solution was stirred at rt for 3 hours and then quenched with saturated  $\text{NH}_4\text{Cl}$ . The mixture was extracted with  $\text{Et}_2\text{O}$  and the combined organic layers were washed with brine, dried over  $\text{MgSO}_4$  and concentrated *in vacuo*. The crude mixture was purified by flash column chromatography on silica gel using (PE/MTBE 80/20) to afford substrate **1j** (18 mg, 51% yield) as a colorless oil.  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  5.44-5.34 (m, 2H), 3.73 (s, 6H), 2.81-2.78 (m, 4H), 2.00 (t,  $J = 3.0$  Hz, 1H), 0.99 (dd,  $J = 7.5, 5.5$  Hz, 2H), 0.87 (s, 9H), 0.67 (dd,  $J = 7.5, 5.5$  Hz, 2H), 0.09 (s, 6H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 170.3 (C), 140.4 (CH), 119.2 (CH), 79.0 (C), 71.5 (CH), 57.1 (C), 56.6 (C), 52.9 ( $\text{CH}_3$ ), 35.0 ( $\text{CH}_2$ ), 26.0 ( $\text{CH}_3$ ), 22.8 ( $\text{CH}_2$ ), 18.1 (C), 15.9 ( $\text{CH}_2$ ), -3.4 ( $\text{CH}_3$ ); **IR**:  $\nu_{\text{max}} = 3295, 2955, 2930, 1739, 1437, 1285, 1202, 1180, 1035, 836, 777 \text{ cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{20}\text{H}_{32}\text{NaO}_5\text{Si}$   $[\text{M}+\text{Na}]^+$ : 403.1917, found: 403.1968.



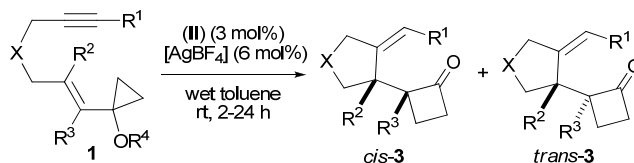
### 11. Substrate 1k:



Anhydrous  $\text{Et}_3\text{N}$  (8 mL) was added to a flask charged with iodobenzene (84 mg, 0.41 mmol),  $\text{PdCl}_2(\text{PPh}_3)_2$  (12 mg, 0.017 mmol) and  $\text{CuI}$  (5.2 mg, 0.027 mmol) under argon. Compound **1a** (100 mg, 0.34 mmol) was slowly added to this mixture at rt. The resulting solution was stirred at room temperature for 6 hours then quenched with sat.  $\text{NH}_4\text{Cl}$  solution. The mixture was extracted with  $\text{Et}_2\text{O}$  and the combined organic layers were washed with brine, dried over  $\text{MgSO}_4$ . The solvent was evaporated *in vacuo* and the residue was purified by flash column chromatography (PE/ $\text{EtOAc}$  90/10) to give the desired product **1k** as a yellow oil (93 mg, 75% yield).  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40-7.31 (m, 2H), 7.30-7.23 (m, 3H), 5.53-5.34 (m, 2H), 3.74 (s, 6H), 3.44 (q,  $J = 6.9$  Hz, 2H), 3.00 (s, 2H), 2.85 (d,  $J = 6.3$  Hz, 2H), 1.14 (t,  $J = 6.9$  Hz, 3H), 0.96 (dd,  $J = 7.2, 5.1$  Hz, 2H), 0.63 (dd,  $J = 7.2, 5.1$  Hz, 2H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 170.5 (C), 136.5 (CH), 131.8 (CH), 128.3 (CH), 128.1 (CH), 123.3 (C), 121.3 (CH), 84.3 (C), 83.7 (C), 63.1 ( $\text{CH}_2$ ), 60.9 (C), 57.7 (C), 52.9 ( $\text{CH}_3$ ), 35.4 ( $\text{CH}_2$ ), 23.8 ( $\text{CH}_2$ ), 15.6 ( $\text{CH}_3$ ), 14.4 ( $\text{CH}_2$ ); **IR**:  $\nu_{\text{max}} = 2976, 2953, 1737, 1437, 1285, 1202, 1181, 1062, 757, 693 \text{ cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{22}\text{H}_{27}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 371.1858, found: 371.1870.



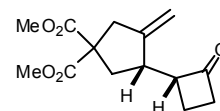
## II.2. General procedure for Au(I)-catalyzed cyclizations of 1,6-enynes.



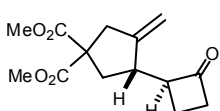
To a solution of the chiral gold(I) catalyst (2.5 mg, 0.0015 mmol, 3 mol%) and the substrates (0.05 mmol, 1 equiv.) in toluene (saturated of water or 5 mol% of water or extreme dry, 1.0 mL), AgBF<sub>4</sub> (0.6 mg, 0.003 mmol, 6 mol%) and another 0.5 ml of toluene were added sequentially. The mixture was stirred at room temperature for 2-24 hours. The reaction was monitored by <sup>1</sup>H NMR. Volatiles were removed under reduced pressure and the final product was purified by flash column chromatography (petroleum ether/ethyl acetate = 90/10 to 60/40). Enantiomeric excesses have been measured by chiral HPLC or chiral SFC. Samples of racemic compounds have been obtained *via* (acetonitrile)[(2-biphenyl)di-*tert*-butylphosphine]gold(I) hexafluoroantimonate promoted cycloadditions.

**1.** *cis*-**3a** and *trans*-**3a** were separated by preparative HPLC on sunfire silica column (19\*150 mm, 5 μm), heptane/EtOAc (92/8), 25 °C 17 mL/min, 297nm, retention times: 12.0 min (major diastereoisomers) and 13.3 min (minor diastereoisomers), (87% yield, 4.9/1 d.r.).

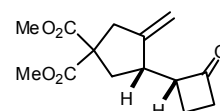
*cis*-**3a**. Colorless oil; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 4.97 (dd, *J* = 4.2, 2.1 Hz, 1H), 4.85 (dd, *J* = 4.2, 2.1 Hz, 1H), 3.73 (s, 6H), 3.45-3.33 (m, 1H), 3.13-2.98 (m, 1H), 2.98-2.83 (m, 4H), 2.72 (dd, *J* = 13.2, 8.1 Hz, 1H), 2.25 (dq, *J* = 10.5, 5.1 Hz, 1H), 1.98 (dd, *J* = 13.2, 10.2 Hz, 1H), 1.92-1.79 (m, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 210.4 (C), 172.1 (C), 149.7 (C), 108.0 (CH<sub>2</sub>), 63.7 (CH), 58.6 (C), 53.02 (CH<sub>3</sub>), 52.98 (CH<sub>3</sub>), 45.1 (CH<sub>2</sub>), 42.7 (CH), 41.3 (CH<sub>2</sub>), 38.3 (CH<sub>2</sub>), 16.1 (CH<sub>2</sub>); IR: *v*<sub>max</sub> = 2955, 2928, 1777, 1732, 1435, 1270, 1250, 1201, 1166, 1082, 891 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>14</sub>H<sub>19</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 267.1232, found: 267.1233; HPLC Analysis: 99% ee, [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: 45.0 min (major) and 47.7 min (minor)]; [α]<sub>D</sub><sup>20</sup> = -27 (*c* 0.5 in CHCl<sub>3</sub>).



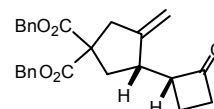
*trans*-**3a**. Colorless oil; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 5.06 (dd, *J* = 4.5, 2.4 Hz, 1H), 5.00 (dd, *J* = 4.5, 2.4 Hz, 1H), 3.73 (s, 6H), 3.62-3.50 (m, 1H), 3.11-2.79 (m, 5H), 2.52 (dd, *J* = 13.2, 7.8 Hz, 1H), 2.13 (dd, *J* = 10.5, 5.1 Hz, 1H), 1.92 (dd, *J* = 13.2, 10.8 Hz, 1H), 1.84-1.70 (m, 1H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 210.1 (C), 172.1 (C), 149.0 (C), 108.4 (CH<sub>2</sub>), 62.7 (CH), 58.3 (C), 53.1 (CH<sub>3</sub>), 53.0 (CH<sub>3</sub>), 44.3 (CH<sub>2</sub>), 41.5 (CH), 41.1 (CH<sub>2</sub>), 37.0 (CH<sub>2</sub>), 13.9 (CH<sub>2</sub>); IR: *v*<sub>max</sub> = 2955, 2928, 1776, 1731, 1657, 1434, 1269, 1250, 1201, 1166, 1081, 891 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>14</sub>H<sub>19</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 267.1232, found: 267.1238; HPLC Analysis: 95% ee, [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: 23.5 min (minor) and 38.5 min (major)].



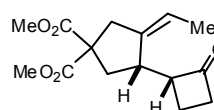
**2.** *cis*-**3a** (from OTBS substrate **1j**). (94% yield, 10/1 d.r.); colorless oil; the NMR data of compound **10j** was the same as compound **10a**. HPLC Analysis: 97% ee, [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: 45.4 min (major) and 48.2 min (minor)].



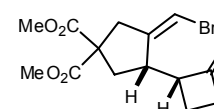
**3. *cis*-3b** (92% yield, 5.2/1 d.r.); colorless oil;  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.35-7.18 (m, 10H), 5.15-5.05 (m, 4H), 4.95 (dd,  $J = 4.2, 2.1$  Hz, 1H), 4.84 (dd,  $J = 4.2, 2.1$  Hz, 1H), 3.42-3.30 (m, 1H), 3.11-2.95 (m, 3H), 2.95-2.81 (m, 2H), 2.73 (dd,  $J = 13.2, 8.7$  Hz, 1H), 2.21 (dd,  $J = 10.2, 5.1$  Hz, 1H), 2.02 (dd,  $J = 13.2, 9.6$  Hz, 1H), 1.89-1.78 (m, 1H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 210.4 (C), 171.3 (C), 171.2 (C), 149.6 (C), 135.5 (C), 128.7 (CH), 128.4 (CH), 128.1 (CH), 108.1 ( $\text{CH}_2$ ), 67.4 ( $\text{CH}_2$ ), 63.6 (CH), 58.9 (C), 45.1 ( $\text{CH}_2$ ), 42.7 (CH), 41.2 ( $\text{CH}_2$ ), 38.2 ( $\text{CH}_2$ ), 16.1 ( $\text{CH}_2$ ); **IR**:  $\nu_{\text{max}} = 3037, 2957, 1777, 1731, 1456, 1265, 1225, 1160, 1082, 903, 738, 697$   $\text{cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{26}\text{H}_{27}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 419.1858, found: 419.1893; **HPLC** Analysis: major diastereoisomers: 98% ee, minor diastereoisomers: 95% ee [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: minor diastereoisomer, 19.7 min (minor) and 27.7 min (major)]; major diastereoisomer, 30.2 min (minor) and 32.8 min (major)].



**4. *cis*-3c** (85% yield, >40/1 d.r.); colorless oil;  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  5.41 (q,  $J = 7.0$  Hz, 1H), 3.72 (s, 3H), 3.69 (s, 3H), 3.49-3.41 (m, 1H), 3.10-3.01 (m, 2H), 3.00-2.93 (m, 1H), 2.83 (dddd,  $J = 9.5, 7.5, 4.5, 2.5$  Hz, 1H), 2.78-2.69 (m, 2H), 2.17-2.08 (m, 2H), 1.84-1.75 (m, 1H), 1.60 (dd,  $J = 7.0, 2.5$  Hz, 3H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 210.8 (C), 172.4 (C), 172.2 (C), 140.3 (C), 119.0 (CH), 64.0 (CH), 58.6 (C), 52.9 ( $\text{CH}_3$ ), 44.6 ( $\text{CH}_2$ ), 42.0 ( $\text{CH}_2$ ), 38.8 (CH), 37.7 ( $\text{CH}_2$ ), 15.9 ( $\text{CH}_2$ ), 14.9 ( $\text{CH}_3$ ); **IR**:  $\nu_{\text{max}} = 2955, 2929, 1776, 1733, 1450, 1435, 1289, 1261, 1201, 1172, 1084, \text{cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{15}\text{H}_{21}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 281.1389, found: 281.1449; **HPLC** Analysis: 99% ee, [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: 37.0 min (major) and 42.4 min (minor)];  $[\alpha]_{\text{D}}^{20} = +33$  ( $c$  0.9 in  $\text{CHCl}_3$ ). This structure was confirmed by HMQC, HMBC, COSY, and NOESY experiments.

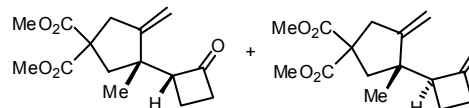


**5. *cis*-3d** (87% yield, 2.4/1 d.r.); colorless oil;  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  6.08 (s, 1H), 3.91-3.84 (m, 1H), 3.74 (s, 3H), 3.72 (s, 3H), 3.14-2.80 (m, 5H), 2.73 (dd,  $J = 13.0, 8.0$  Hz, 1H), 2.20 (dd,  $J = 10.5, 4.5$  Hz, 1H), 2.14 (dd,  $J = 14.0, 6.5$  Hz, 1H), 1.98-1.92 (m, 1H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 210.0 (C), 171.4 (C), 146.1 (C), 100.0 (CH), 61.7 (CH), 59.1 (C), 53.14 ( $\text{CH}_3$ ), 53.12 ( $\text{CH}_3$ ), 45.1 ( $\text{CH}_2$ ), 41.96 ( $\text{CH}_2$ ), 41.91 (CH), 36.4 ( $\text{CH}_2$ ), 15.6 ( $\text{CH}_2$ ); **IR**:  $\nu_{\text{max}} = 2954, 1775, 1734, 1435, 1276, 1245, 1205, 1168, 1082, \text{cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{14}\text{H}_{18}\text{BrO}_5$   $[\text{M}+\text{H}]^+$ : 345.0338, found: 345.0363; **HPLC** Analysis: major diastereoisomers: 99% ee, [CHIRALPAK® IC, 25 °C, 30% *i*PrOH/*n*-heptane, 0.8 mL/min, 218 nm, retention times: major diastereoisomers, 10.7 min (major) and 11.9 min (minor)];  $[\alpha]_{\text{D}}^{20} = -43$  ( $c$  0.3 in  $\text{CHCl}_3$ ).



**6. Mixture of *cis*-3e (major diastereoisomer) and *trans*-3e**

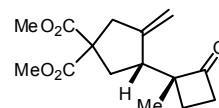
(minor diastereoisomer) (84% yield, 1.3/1 d.r.); colorless oil;  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  4.99-4.95 (m, 1H, major + 1H, minor), 4.93 (t,  $J = 2.1$  Hz, 1H, minor), 4.80 (t,  $J = 1.8$  Hz, 1H, major), 3.76-3.70 (m, 6H, major + 6H, minor), 3.49-3.35 (m, 1H, major + 1H, minor), 3.21-2.84 (m, 3H, major + 3H, minor), 2.83-2.69 (m, 1H, major + 1H, minor), 2.53-2.22 (m, 2H, major + 2H, minor), 2.05 (q,  $J = 10.8, 5.1$  Hz, 1H, major + 1H, minor), 1.90-1.75 (m, 1H, major + 1H, minor), 1.15 (s, 3H, minor), 1.14 (s, 3H, major);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 210.8 (C, major), 210.4 (C, minor), 172.44 (C, major), 172.38 (C, minor), 154.42 (C, minor), 154.38 (C, major), 107.6 ( $\text{CH}_2$ , minor), 107.3 ( $\text{CH}_2$ , major), 69.2 (CH, major), 68.9 (CH, minor), 57.7 (C, major + minor), 53.1 ( $\text{CH}_3$ , major), 53.0 ( $\text{CH}_3$ , minor), 45.6 ( $\text{CH}_2$ , major), 45.5 (C, major + minor), 44.4 ( $\text{CH}_2$ , major), 44.1 ( $\text{CH}_2$ , minor), 43.8 ( $\text{CH}_2$ , minor), 42.1 ( $\text{CH}_2$ , major), 41.7 ( $\text{CH}_2$ , minor), 25.9 ( $\text{CH}_3$ , minor), 24.3 ( $\text{CH}_3$ , major), 14.0 ( $\text{CH}_2$ , major), 13.7 ( $\text{CH}_2$ , minor); **IR**:  $\nu_{\text{max}} = 2957, 1776, 1734, 1435, 1261, 1244, 1200,$



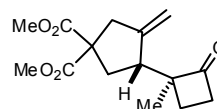
1174, 1081, 897  $\text{cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{15}\text{H}_{21}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 281.1389, found: 281.1389; **HPLC** Analysis: major diastereoisomer: 89% ee, minor diastereoisomer: 92% ee [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: minor diastereoisomer, 18.2 min (minor) and 32.2 min (major)]; major diastereoisomer, 23.2 min (major) and 26.7 min (minor)].

**7.** *cis*-**3f** and *trans*-**3f** was separated by prepare HPLC on sunfire silica column (19\*150 mm, 5  $\mu\text{m}$ ), heptane/EtOAc (95/5), 25 °C 17 mL/min, 305 nm, retention times: 19.3 min (major diastereoisomer) and 21.4 min (minor diastereoisomer); (80% yield, 4.5/1 d.r.).

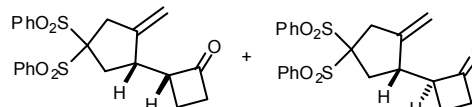
*cis*-**3f**. Colorless oil;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  5.06 (bs, 1H), 4.83 (bs, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 3.14-2.80 (m, 5H), 2.69-2.56 (m, 1H), 2.10-1.97 (m, 1H), 1.92-1.69 (m, 2H), 1.19 (s, 3H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 215.3 (C), 171.8 (C), 171.7 (C), 148.0 (C), 110.0 ( $\text{CH}_2$ ), 66.9 (C), 58.4 (C), 53.0 ( $\text{CH}_3$ ), 45.6 (CH), 43.2 ( $\text{CH}_2$ ), 42.8 ( $\text{CH}_2$ ), 36.4 ( $\text{CH}_2$ ), 22.8 ( $\text{CH}_2$ ), 19.2 ( $\text{CH}_3$ ); **IR**:  $\nu_{\text{max}}$  = 2957, 1776, 1734, 1436, 1271, 1204, 1167, 1062  $\text{cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{15}\text{H}_{21}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 281.1389, found: 281.1470; **HPLC** Analysis: 87% ee, [CHIRALPAK® IC, 25 °C, 2% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: 46.2 min (minor) and 50.4 min (major)];  $[\alpha]_{\text{D}}^{20}$  = +12 (*c* 0.4 in  $\text{CHCl}_3$ ).



*trans*-**3f**. Colorless oil;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  5.14 (bs, 1H), 5.08 (bs, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 3.12-2.78 (m, 5H), 2.68-2.54 (m, 1H), 2.08-1.88 (m, 2H), 1.80-1.68 (m, 1H), 1.24 (s, 3H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 213.5 (C), 171.9 (C), 171.8 (C), 147.1 (C), 111.0 ( $\text{CH}_2$ ), 66.2 (C), 58.4 (C), 53.0 ( $\text{CH}_3$ ), 52.9 ( $\text{CH}_3$ ), 45.6 (CH), 43.0 ( $\text{CH}_2$ ), 42.4 ( $\text{CH}_2$ ), 36.2 ( $\text{CH}_2$ ), 23.0 ( $\text{CH}_2$ ), 18.1 ( $\text{CH}_3$ ); **IR**:  $\nu_{\text{max}}$  = 2957, 1776, 1734, 1435, 1271, 1204, 1167, 1062  $\text{cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{15}\text{H}_{21}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 281.1389, found: 281.1465. **HPLC** Analysis: 75% ee, [CHIRALPAK® IC, 25 °C, 2% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: 38.0 min (minor) and 40.3 min (major)];  $[\alpha]_{\text{D}}^{20}$  = -17 (*c* 0.5 in  $\text{CHCl}_3$ ).

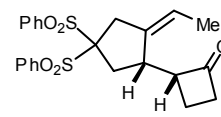


**8.** *cis*-**3g** and *trans*-**3g** were separated by chiral HPLC, [CHIRALPAK® IC, 25 °C, 35% *i*PrOH/*n*-heptane, 0.8 mL/min, 222 nm, retention times: minor diastereoisomer, 36.6 min (enantiomers I), 41.8 min (enantiomers II); major diastereoisomer, 48.7 min; (82% yield, 2.0/1 d.r.); pale yellow oil;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (major)  $\delta$  8.07-7.96 (m, 4H), 7.76-7.68 (m, 2H), 7.65-7.55 (m, 4H), 4.84 (d,  $J$  = 1.8 Hz, 1H), 4.79 (dd,  $J$  = 1.8 Hz, 1H), 3.41-3.26 (m, 2H), 3.17-2.85 (m, 5H), 2.60-2.47 (m, 1H), 2.27 (dq,  $J$  = 10.5, 4.8 Hz, 1H), 1.87-1.72 (m, 1H); (minor)  $\delta$  8.07-8.00 (m, 4H), 7.77-7.68 (m, 2H), 7.61 (t,  $J$  = 7.5 Hz, 4H), 5.01 (d,  $J$  = 2.1 Hz, 1H), 4.91 (d,  $J$  = 2.1 Hz, 1H), 3.61-3.49 (m, 1H), 3.28-3.18 (m, 2H), 3.15-2.99 (m, 2H), 2.93-2.77 (m, 1H), 2.68 (dd,  $J$  = 14.7, 8.1 Hz, 1H), 2.40 (dd,  $J$  = 15.0, 10.2 Hz, 1H), 2.15 (dd,  $J$  = 10.5, 5.1 Hz, 1H), 1.80-1.65 (m, 1H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) 209.4 (C, major), 208.8 (C, minor), 147.6 (C, major), 146.7 (C, minor), 136.6 (C, major), 136.0 (C, minor), 135.0 (CH, major), 134.8 (CH, minor), 131.5 (CH, major), 131.4 (CH, minor), 128.96 (CH, major + minor), 109.2 ( $\text{CH}_2$ , minor), 108.5 ( $\text{CH}_2$ , major), 91.6 (C, major), 91.1 (C, minor), 63.2 (CH, major), 62.1 (CH, minor), 45.3 ( $\text{CH}_2$ , major), 44.6 ( $\text{CH}_2$ , minor), 43.7 (CH, major), 42.2 (CH, minor), 38.7 ( $\text{CH}_2$ , minor), 38.4 ( $\text{CH}_2$ , major), 35.9 ( $\text{CH}_2$ , major), 34.4 ( $\text{CH}_2$ , minor), 16.5 ( $\text{CH}_2$ , major), 13.9 ( $\text{CH}_2$ , minor); **IR** (major):  $\nu_{\text{max}}$  = 2962, 2924, 1774, 1447, 1328, 1310, 1143, 1077, 1024, 754, 730, 687  $\text{cm}^{-1}$ ; **HRMS** (ESI) (major) calcd. for  $\text{C}_{22}\text{H}_{23}\text{O}_5\text{S}_2$   $[\text{M}+\text{H}]^+$ : 431.0987, found: 431.1036; **HPLC** Analysis: major diastereoisomer: 74% ee, [CHIRALPAK® ID, 35 °C, 35% *i*PrOH/*n*-heptane, 0.7 mL/min, 222 nm, retention times: 45.7 min

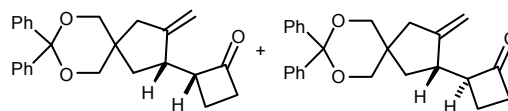


(minor) and 50.3 min (major)]; minor diastereoisomer: 95% ee [CHIRALPAK® ID, 35 °C, 35% *i*PrOH/*n*-heptane, 0.7 mL/min, 222 nm, retention times: 34.9 min (minor) and 45.1 min (major)].

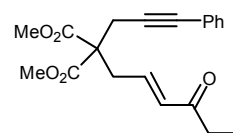
**9. *cis*-3h** (77% yield, 4.1/1 d.r.); light yellow oil;  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.11 (d,  $J = 7.5$  Hz, 2H), 7.92 (d,  $J = 7.5$  Hz, 2H), 7.78-7.70 (m, 1H), 7.69-7.65 (m, 1H), 7.62 (t,  $J = 7.5$  Hz, 2H), 7.54 (t,  $J = 7.5$  Hz, 2H), 5.16-5.03 (m, 1H), 3.62-3.45 (m, 2H), 3.11-2.68 (m, 6H), 2.13 (dq,  $J = 10.5, 5.0$  Hz, 1H), 1.80-1.67 (m, 1H), 1.44 (dd,  $J = 7.0, 2.5$  Hz, 3H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 210.3 (C), 137.9 (C), 137.2 (C), 136.4 (C), 134.8 (CH), 134.7 (CH), 131.5 (CH), 131.2 (CH), 128.9 (CH), 120.2 (CH), 91.7 (C), 63.5 (CH), 44.5 (CH<sub>2</sub>), 39.5 (CH), 39.0 (CH<sub>2</sub>), 35.1 (CH<sub>2</sub>), 16.4 (CH<sub>2</sub>), 15.2 (CH<sub>3</sub>); **IR**:  $\nu_{\text{max}} = 2923, 1774, 1448, 1329, 1311, 1144, 1077, 753, 725, 688$  cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>23</sub>H<sub>25</sub>O<sub>5</sub>S<sub>2</sub> [M+H]<sup>+</sup>: 445.1143, found: 445.1204; **HPLC** Analysis: 91% ee, [CHIRALPAK® IC, 35 °C, 40% EtOH/*n*-heptane, 0.7 mL/min, 222 nm, retention times: 30.8 min (major) and 38.9 min (minor)];  $[\alpha]_{\text{D}}^{20} = +10$  (c 0.6 in  $\text{CHCl}_3$ ).



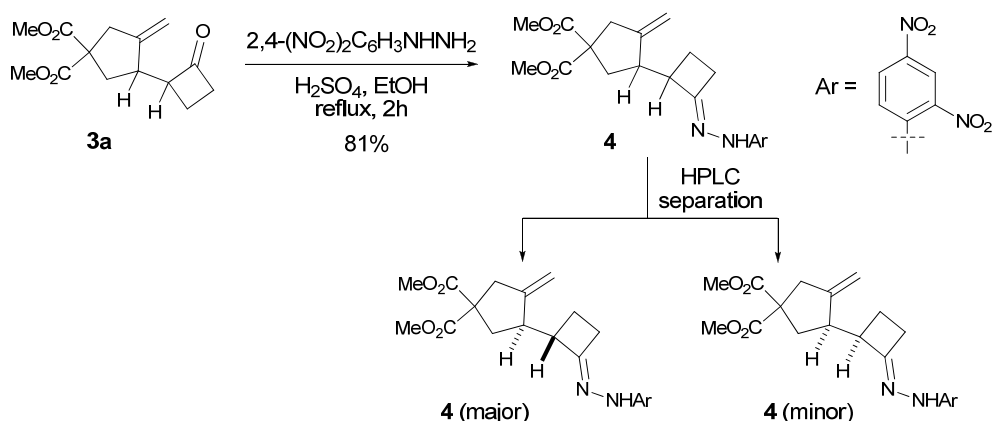
**10.** Mixture of *cis*-3i (major diastereoisomer) and *trans*-3i (minor diastereoisomer). (84% yield, 3.9/1 d.r.); colorless oil;  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.53-7.45 (m, 4H, major + 4H, minor), 7.38-7.31 (m, 4H, major + 4H, minor), 7.31-7.24 (m, 2H, major + 2H, minor), 5.00 (dd,  $J = 4.2, 2.4$  Hz, 1H, minor), 4.94 (m, 1H, major + 1H, minor), 4.84 (dd,  $J = 4.2, 2.4$  Hz, 1H, major), 3.80-3.64 (m, 4H, major + 4H, minor), 3.62-3.51 (m, 1H, minor), 3.43-3.31 (m, 1H, major), 3.10-2.94 (m, 1H, major + 1H, minor), 2.94-2.74 (m, 2H, major + 2H, minor), 2.55-1.96 (m, 4H, major + 4H, minor), 1.91-1.67 (m, 1H, major + 1H, minor), 1.31-1.19 (m, 1H, major + 1H, minor);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 211.1 (C, major), 210.8 (C, minor), 151.4 (C, major), 150.8 (C, minor), 142.4 (C, major), 141.8 (C, minor), 141.3 (C, major), 140.7 (C, minor), 128.6, 128.55, 128.46, 128.1, 127.1, 126.8, 126.6 (10 CH, major + 10 CH, minor), 108.0 (CH<sub>2</sub>, minor), 107.9 (CH<sub>2</sub>, major), 101.4 (C, major + minor), 71.0 (CH<sub>2</sub>, minor), 70.9 (CH<sub>2</sub>, major), 69.5 (CH<sub>2</sub>, minor), 69.4 (CH<sub>2</sub>, major), 64.8 (CH, major), 63.0 (CH, minor), 45.0 (CH<sub>2</sub>, major), 44.4 (CH<sub>2</sub>, minor), 42.0 (CH, major), 41.3 (CH<sub>2</sub>, major), 40.9 (CH, minor), 40.8 (CH<sub>2</sub>, minor), 40.4 (C, major), 40.0 (C, minor), 37.1 (CH<sub>2</sub>, major), 35.9 (CH<sub>2</sub>, minor), 16.0 (CH<sub>2</sub>, major), 13.9 (CH<sub>2</sub>, minor); **IR**:  $\nu_{\text{max}} = 3061, 2956, 2865, 1776, 1491, 1451, 1259, 1198, 1101, 1086, 1028, 1001, 771, 749, 708, 696$  cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>25</sub>H<sub>27</sub>O<sub>3</sub> [M+H]<sup>+</sup>: 375.1960, found: 375.1969; **SFC** Analysis: major diastereoisomers: 87% ee, minor diastereoisomers: 85% ee [CHIRAL SFC AD-H, 30 °C, 5% MeOH/CO<sub>2</sub>, 4 mL/min, pressure: 150 bar, 214 nm, retention times: minor diastereoisomer, 8.3 min (major) and 9.5 min (minor)]; major diastereoisomer, 7.0 min (major) and 14.3 min (minor)].



**11. S15.** 88% yield; colorless oil;  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39-7.26 (m, 5H), 6.70 (dt,  $J = 15.6, 7.8$  Hz, 1H), 6.20 (d,  $J = 15.6$  Hz, 1H), 3.78 (s, 6H), 3.03 (s, 2H), 2.99 (d,  $J = 7.8$  Hz, 2H), 2.55 (q,  $J = 7.5$  Hz, 2H), 1.07 (t,  $J = 7.5$  Hz, 3H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 200.7 (C), 170.0 (C), 139.7 (CH), 134.0 (CH), 131.8 (CH), 128.4 (CH), 128.3 (CH), 123.0 (C), 84.4 (C), 83.7 (C), 57.2 (C), 53.2 (CH<sub>3</sub>), 35.8 (CH<sub>2</sub>), 33.5 (CH<sub>2</sub>), 24.4 (CH<sub>2</sub>), 8.1 (CH<sub>3</sub>); **HRMS** (ESI) calcd. for C<sub>20</sub>H<sub>23</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 343.1545, found: 343.1554.



## 12. Synthesis of compound 4.



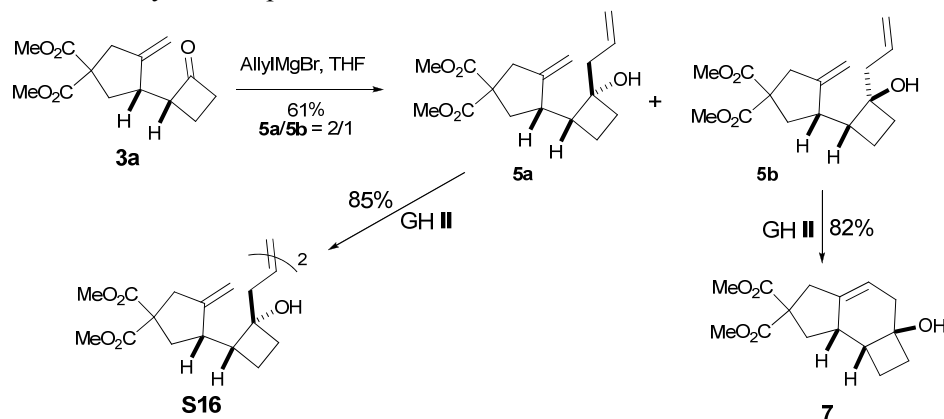
To a solution of **3a** (15 mg, 0.056 mmol) in EtOH (2 mL) was added (2,4-dinitrophenyl)hydrazine (17 mg, 0.085 mmol) and 0.5 N H<sub>2</sub>SO<sub>4</sub> (0.056 mL, 0.028 mmol). The red reaction mixture was heated to reflux and stirred at this temperature for 4 hours. The EtOH was removed under reduced pressure and the crude mixture was purified by flash column chromatography (heptanes/EtOAc 80/20, R<sub>f</sub> = 0.28) to afford **4** as a mixture of two diastereoisomers (20 mg, 81% yield). The two diastereoisomers were separated by preparative HPLC<sup>10</sup> to produce the two diastereoisomers **4a** (major) and **4b** (minor).

**4a** (major diastereoisomer). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 10.74 (bs, 1H), 9.12 (d, *J* = 2.7 Hz, 1H), 8.32 (dd, *J* = 9.6, 2.1 Hz, 1H), 7.85 (d, *J* = 9.6 Hz, 1H), 5.00 (dd, *J* = 4.2, 2.1 Hz, 1H), 4.90 (dd, *J* = 4.2, 2.1 Hz, 1H), 3.75 (s, 6H), 3.53-3.40 (m, 1H), 3.04-2.89 (m, 5H), 2.79 (d, *J* = 13.2, 7.8 Hz, 1H), 2.43-2.31 (m, 1H), 2.16-1.97 (m, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 172.2 (C), 162.9 (C), 149.7 (C), 145.0 (C), 130.3 (CH), 129.6 (C), 123.7 (CH), 116.4 (CH), 108.1 (CH<sub>2</sub>), 58.6 (C), 53.1 (CH<sub>3</sub>), 50.6 (CH), 44.8 (CH), 41.6 (CH<sub>2</sub>), 38.7 (CH<sub>2</sub>), 29.1 (CH<sub>2</sub>), 20.1 (CH<sub>2</sub>); IR:  $\nu_{\text{max}}$  = 2956, 2924, 2853, 1733, 1618, 1592, 1519, 1426, 1337, 1312, 1273, 1136, 1072, 759 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>20</sub>H<sub>23</sub>N<sub>4</sub>O<sub>8</sub> [M+H]<sup>+</sup>: 447.1516, found: 447.1544; [α]<sub>D</sub><sup>20</sup> = -12 (*c* 0.1 in CHCl<sub>3</sub>); [α]<sub>D</sub><sup>20</sup> = -12 (*c* 0.1 in CHCl<sub>3</sub>).

**4b** (minor diastereoisomer). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 10.73 (bs, 1H), 9.12 (d, *J* = 2.7 Hz, 1H), 8.31 (dd, *J* = 9.6, 2.1 Hz, 1H), 7.86 (d, *J* = 9.6 Hz, 1H), 5.17 (dd, *J* = 4.2, 2.1 Hz, 1H), 5.07 (dd, *J* = 4.2, 2.1 Hz, 1H), 3.75 (s, 6H), 3.68-3.55 (m, 1H), 3.08-2.88 (m, 5H), 2.70-2.59 (m, 1H), 2.34-2.19 (m, 1H), 2.06-1.91 (m, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) 172.1 (C), 163.0 (C), 149.2 (C), 145.0 (C), 130.2 (CH + C), 123.7 (CH), 116.4 (CH), 108.8 (CH<sub>2</sub>), 58.3 (C), 53.1 (CH<sub>3</sub>), 49.7 (CH), 43.6 (CH), 41.7 (CH<sub>2</sub>), 37.1 (CH<sub>2</sub>), 29.1 (CH<sub>2</sub>), 18.0 (CH<sub>2</sub>); IR:  $\nu_{\text{max}}$  = 2955, 2923, 2853, 1733, 1618, 1592, 1519, 1337, 1312, 1272, 1137, 1072, 759 cm<sup>-1</sup>; HRMS (ESI) calcd. for C<sub>20</sub>H<sub>23</sub>N<sub>4</sub>O<sub>8</sub> [M+H]<sup>+</sup>: 447.1516, found: 447.1566; [α]<sub>D</sub><sup>20</sup> = -21 (*c* 0.2 in CHCl<sub>3</sub>).

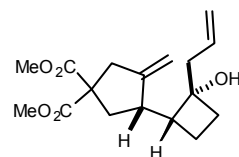
<sup>10</sup> HPLC conditions : Heptane/ Ethyl acetate 90/10-65/35, 14 ml/min, retention times 21.2min and 24.1 min.

### 13. Synthesis of the tricyclic compounds.

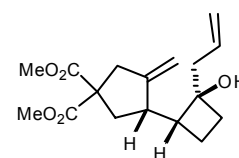


Compounds **5a** and **5b**. Allylmagnesium bromide (1.0M in THF) (0.18 mL, 0.18 mmol) was added to a solution of **3a** (25 mg, 0.09 mmol) in THF 4 mL at  $-78\text{ }^{\circ}\text{C}$  under argon. The resulting mixture was warmed to rt and stirred at this temperature for 1.5 hours. Water (3mL) was added, the mixture was extracted with EtOAc and the combined organic layers were dried over  $\text{MgSO}_4$  and concentrated in *vacuo*. The crude was purified by flash column chromatography on silica gel using PE/EtOAc (85/15) as eluent, to provide the two diastereoisomers **5a** (10 mg) and **5b** (7 mg) in 61% overall yield.

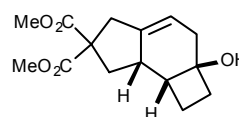
**5a** (major).  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  5.87-5.77 (m, 1H), 5.20-5.13 (m, 2H), 4.85 (d,  $J = 0.9$  Hz, 1H), 4.81 (d,  $J = 0.9$  Hz, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 2.96 (d,  $J = 9.6$  Hz, 1H), 2.90 (dd,  $J = 9.6, 1.2$  Hz, 1H), 2.86-2.78 (m, 1H), 2.70 (dd,  $J = 8.1, 5.1$  Hz, 1H), 2.34 (dq,  $J = 8.1, 4.5$  Hz, 2H), 2.23-2.16 (m, 1H), 2.06-1.98 (m, 1H), 1.97-1.84 (m, 4H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 172.7 (C), 151.6 (C), 133.3 (CH), 119.3 ( $\text{CH}_2$ ), 106.8 ( $\text{CH}_2$ ), 76.5 (C), 58.7 (C), 52.94 ( $\text{CH}_3$ ), 52.88 ( $\text{CH}_3$ ), 48.6 (CH), 46.8 ( $\text{CH}_2$ ), 46.3 (CH), 41.2 ( $\text{CH}_2$ ), 39.5 ( $\text{CH}_2$ ), 32.5 ( $\text{CH}_2$ ), 20.8 ( $\text{CH}_2$ ); **IR**:  $\nu_{\text{max}} = 3353, 2957, 2923, 1735, 1640, 1435, 1260, 1093, 1023, 801\text{ cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{17}\text{H}_{25}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 309.1702, found: 309.1720.



**5b** (minor).  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  5.96-5.87 (m, 1H), 5.25-5.18 (m, 2H), 4.86 (d,  $J = 1.5$  Hz, 1H), 4.79 (d,  $J = 1.5$  Hz, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 3.01 (dq,  $J = 16.5, 2.5$  Hz, 1H), 2.88 (dd,  $J = 16.5, 1.0$  Hz, 1H), 2.66-2.58 (m, 2H), 2.47 (dd,  $J = 13.5, 6.5$  Hz, 1H), 2.32-2.24 (m, 2H), 2.07-1.98 (m, 3H), 1.96-1.88 (m, 1H), 1.79-1.71 (m, 1H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 175.5 (C), 151.1 (C), 133.4 (CH), 119.5 ( $\text{CH}_2$ ), 107.2 ( $\text{CH}_2$ ), 75.8 (C), 59.2 (C), 52.9 ( $\text{CH}_3$ ), 52.8 ( $\text{CH}_3$ ), 43.5 (CH), 41.1 ( $\text{CH}_2$ ), 38.9 (CH), 38.8 ( $\text{CH}_2$ ), 33.1 ( $\text{CH}_2$ ), 19.3 ( $\text{CH}_2$ ); **IR**:  $\nu_{\text{max}} = 3353, 2957, 2923, 1735, 1640, 1435, 1260, 1093, 1023, 801\text{ cm}^{-1}$ ; **HRMS** (ESI) calcd. for  $\text{C}_{17}\text{H}_{25}\text{O}_5$   $[\text{M}+\text{H}]^+$ : 309.1702, found: 309.1709.



**14. Compound 7.** To a stirring solution of **5b** (5 mg, 0.016 mmol) in anhydrous  $\text{CH}_2\text{Cl}_2$  (1.6 mL) was added the Hoveyda-Grubbs Catalyst 2nd Generation (1 mg, 0.0016 mmol) under argon at room temperature. The resulting solution was stirred at  $40\text{ }^{\circ}\text{C}$  for 4 hours and the solvent was removed under reduced pressure. The crude was purified by flash column chromatography on silica gel using PE/EtOAc (60/40) as eluent, to provide compound **7** (3.8 mg, 82% yield).  $^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  5.66 (d,  $J = 2.0$  Hz, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 3.10 (d,  $J = 17.0$  Hz, 1H), 2.84 (d,  $J = 17.0$  Hz, 1H), 2.73-2.66 (m, 1H), 2.66-2.55 (m, 1H), 2.43 (dd,  $J = 12.5, 7.0$  Hz, 1H), 2.29 (dd,  $J = 15.5, 7.0$  Hz, 1H), 2.07-1.94 (m, 2H), 1.90-1.81 (m, 1H), 1.77-1.60 (m, 3H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ) 172.3 (C), 141.9 (C), 116.2 (CH), 75.4 (C), 59.9 (C), 52.95 ( $\text{CH}_3$ ), 52.86 ( $\text{CH}_3$ ), 46.3 (CH), 40.8 (CH), 39.3

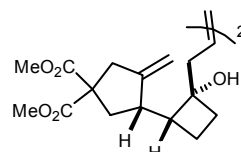




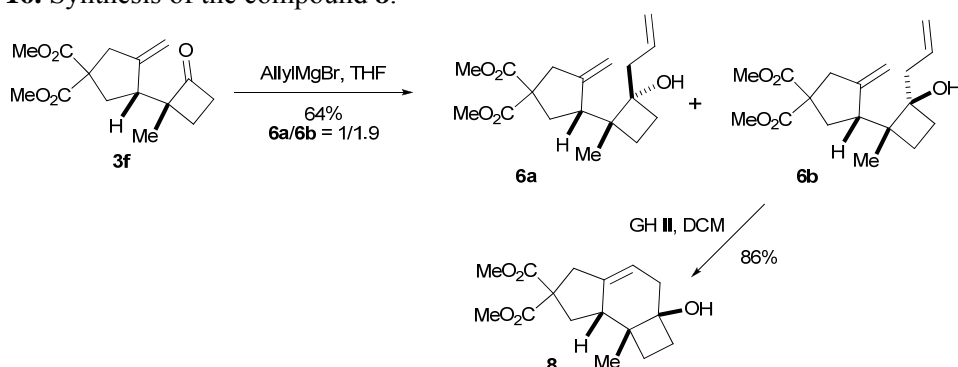
(CH<sub>2</sub>), 38.0 (CH<sub>2</sub>), 36.2 (CH<sub>2</sub>), 35.0 (CH<sub>2</sub>), 13.4 (CH<sub>2</sub>); **IR**:  $\nu_{max}$  = 3373, 2956, 2926, 1731, 1668, 1435, 1283, 1256, 1168, 1093, 1015, 798, 754 cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>15</sub>H<sub>21</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 281.1389, found: 281.1392; [ $\alpha$ ]<sub>D</sub><sup>20</sup> = -10 (*c* 0.45 in CHCl<sub>3</sub>).

**15. Compound S16.** Compound **5a** was subjected to the ruthenium-catalyzed ring-closing metathesis reaction according to the same procedure used for **5b**.

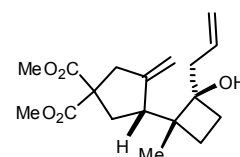
The dimer of compound **S16** was obtained in 86% yield. **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>)  $\delta$  5.53-5.45 (m, 2H), 4.85 (bs, 2H), 4.81 (bs, 2H), 3.72 (bs, 12H), 2.99-2.85 (m, 4H), 2.85-2.76 (m, 2H), 2.69 (dd, *J* = 13.0, 8.0 Hz, 2H), 2.40-2.27 (m, 4H), 2.22-2.14 (m, 2H), 2.06-1.97 (m, 2H), 1.95-1.84 (m, 8H); **IR**:  $\nu_{max}$  = 3464, 2952, 2923, 2852, 1731, 1664, 1435, 1258, 1202, 1168, 1071, 1016, 886, 799 cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>32</sub>H<sub>45</sub>O<sub>10</sub> [M+H]<sup>+</sup>: 589.3013, found: 589.3073.



**16. Synthesis of the compound 8.**

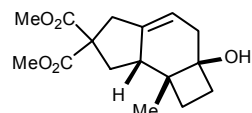


Compound **6a/6b** were prepared according to the same procedure used for the synthesized of compound **5a** and **5b**. Only the diastereoisomer **6b** was characterized and used for the next step (5 mg, 44% yield). **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>)  $\delta$  5.98-5.83 (m, 1H), 5.24-5.17 (m, 2H), 4.92 (d, *J* = 1.5 Hz, 1H), 4.76 (d, *J* = 1.5 Hz, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 2.88-2.84 (m, 2H), 2.62-2.55 (m, 2H), 2.35-2.28 (m, 1H), 2.06-2.00 (m, 1H), 1.96-1.88 (m, 2H), 1.64-1.59 (m, 2H), 1.14 (s, 3H), 0.95-0.86 (m, 1H); **<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) 172.3 (C), 172.0 (C), 150.2 (C), 134.1 (CH), 119.3 (CH<sub>2</sub>), 107.9 (CH<sub>2</sub>), 76.2 (C), 59.2 (C), 52.94 (CH<sub>3</sub>), 52.88 (CH<sub>3</sub>), 49.4 (C), 47.6 (CH), 43.0 (CH<sub>2</sub>), 40.1 (CH<sub>2</sub>), 36.0 (CH<sub>2</sub>), 31.7 (CH<sub>2</sub>), 27.6 (CH<sub>2</sub>), 14.7 (CH<sub>3</sub>); **IR**:  $\nu_{max}$  = 3519, 2952, 2928, 1735, 1457, 1435, 1269, 1250, 1203, 1167, 1068, 881 cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>18</sub>H<sub>26</sub>NaO<sub>5</sub> [M+ Na]<sup>+</sup>: 345.1678, found: 345.1718.



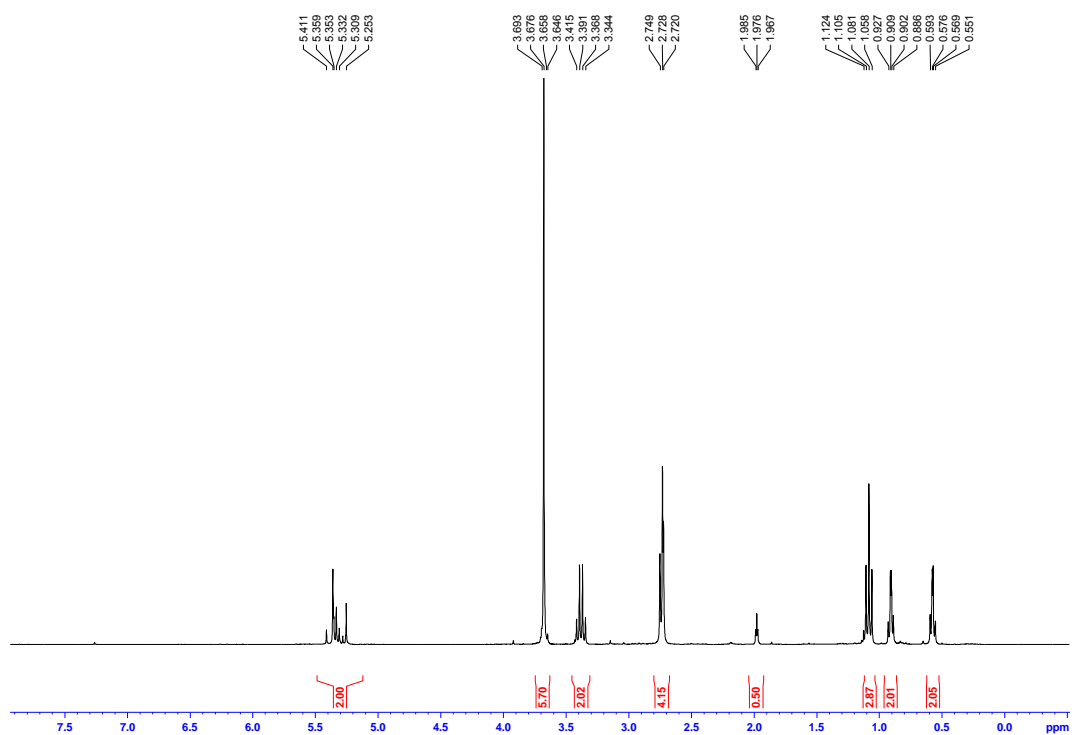
**17. Compound 8** was synthesized according to the same procedure used for the synthesized of compound **7** (3.9 mg, 86% yield). **<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>)

$\delta$  5.68-5.64 (m, 1H), 3.73 (s, 3H), 3.72 (s, 3H), 3.10 (d, *J* = 17.0 Hz, 1H), 2.85 (dm, *J* = 17.0 Hz, 1H), 2.47 (dd, *J* = 11.0, 6.0 Hz, 1H), 2.40-2.35 (m, 1H), 2.31 (dd, *J* = 15.0, 7.0 Hz, 1H), 2.05-1.95 (m, 2H), 1.88-1.77 (m, 2H), 1.74-1.68 (m, 2H), 1.18 (s, 3H); **<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) 172.5 (C), 143.7 (C), 116.0 (CH), 60.0 (C), 53.0 (CH<sub>3</sub>), 52.9 (CH<sub>3</sub>), 47.6 (CH), 39.6 (CH<sub>2</sub>), 38.4 (CH<sub>2</sub>), 35.3 (CH<sub>2</sub>), 33.1 (CH<sub>2</sub>), 22.1 (CH<sub>2</sub>), 20.2 (CH<sub>3</sub>); **IR**:  $\nu_{max}$  = 3396, 2956, 2927, 1730, 1670, 1435, 1283, 1248, 1170, 1073, 1024, 907, 799, 729 cm<sup>-1</sup>; **HRMS** (ESI) calcd. for C<sub>16</sub>H<sub>23</sub>O<sub>5</sub> [M+H]<sup>+</sup>: 295.1545, found: 295.1654; [ $\alpha$ ]<sub>D</sub><sup>20</sup> = -6 (*c* 0.15 in CHCl<sub>3</sub>).

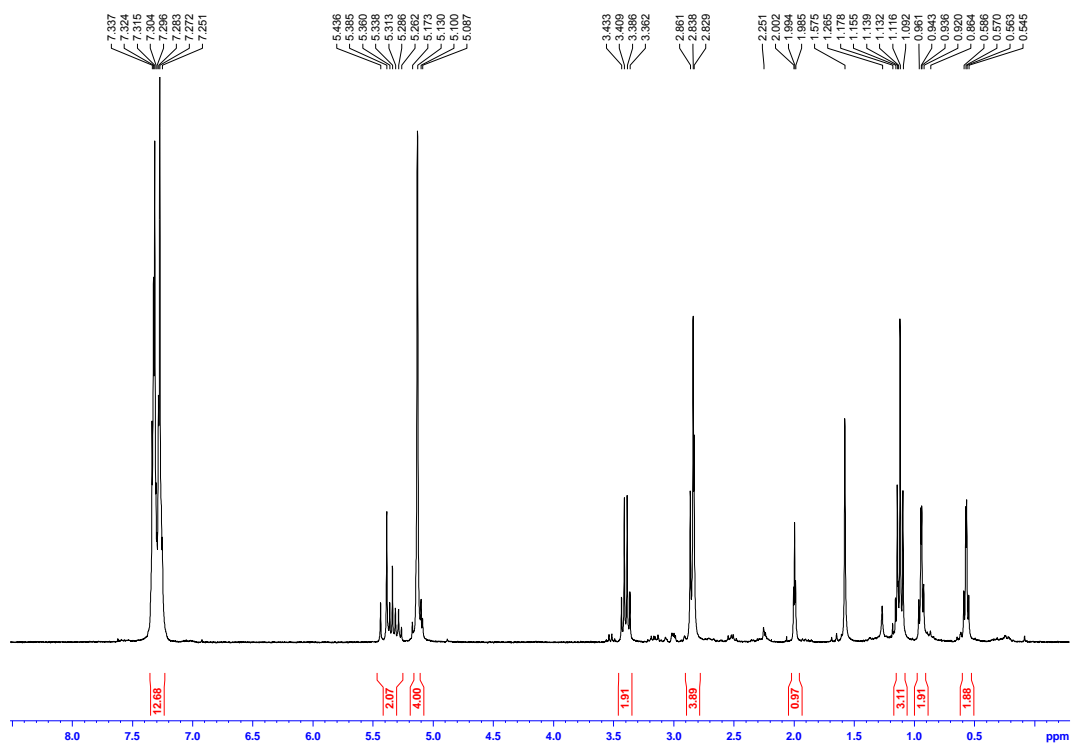


### III. NMR Spectra ( $^1\text{H}$ , $^{13}\text{C}$ )

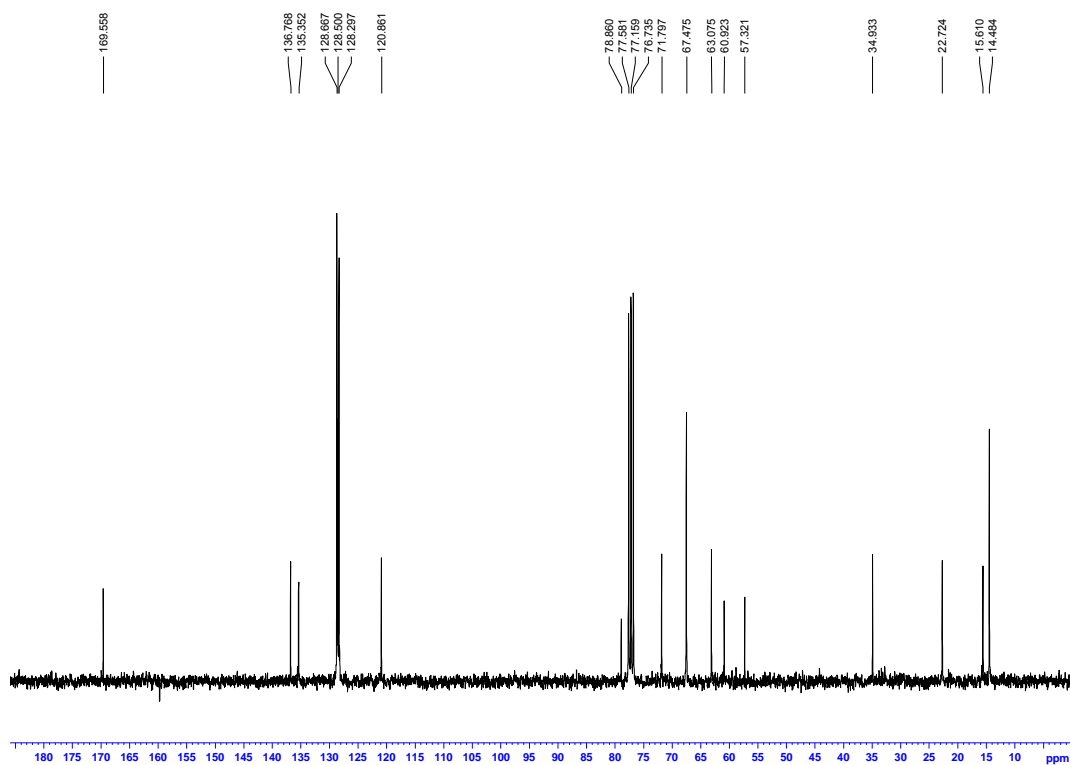
#### $^1\text{H}$ NMR (300 MHz, $\text{CDCl}_3$ ) (1a):



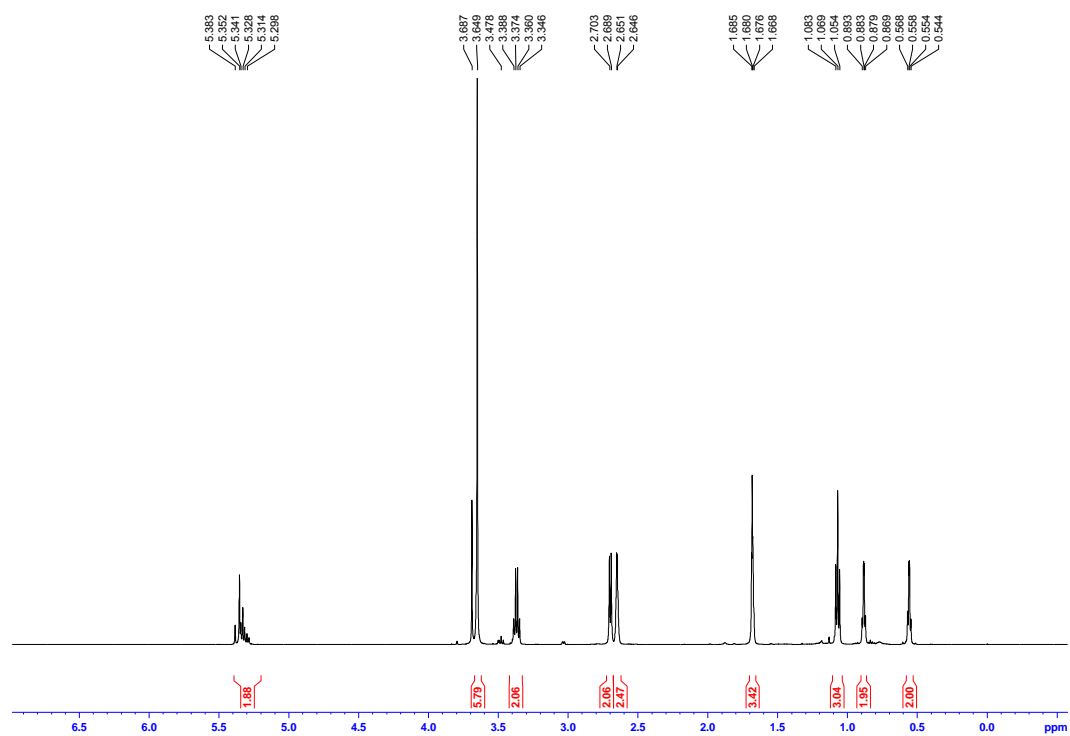
#### $^1\text{H}$ NMR (300 MHz, $\text{CDCl}_3$ ) (1b):



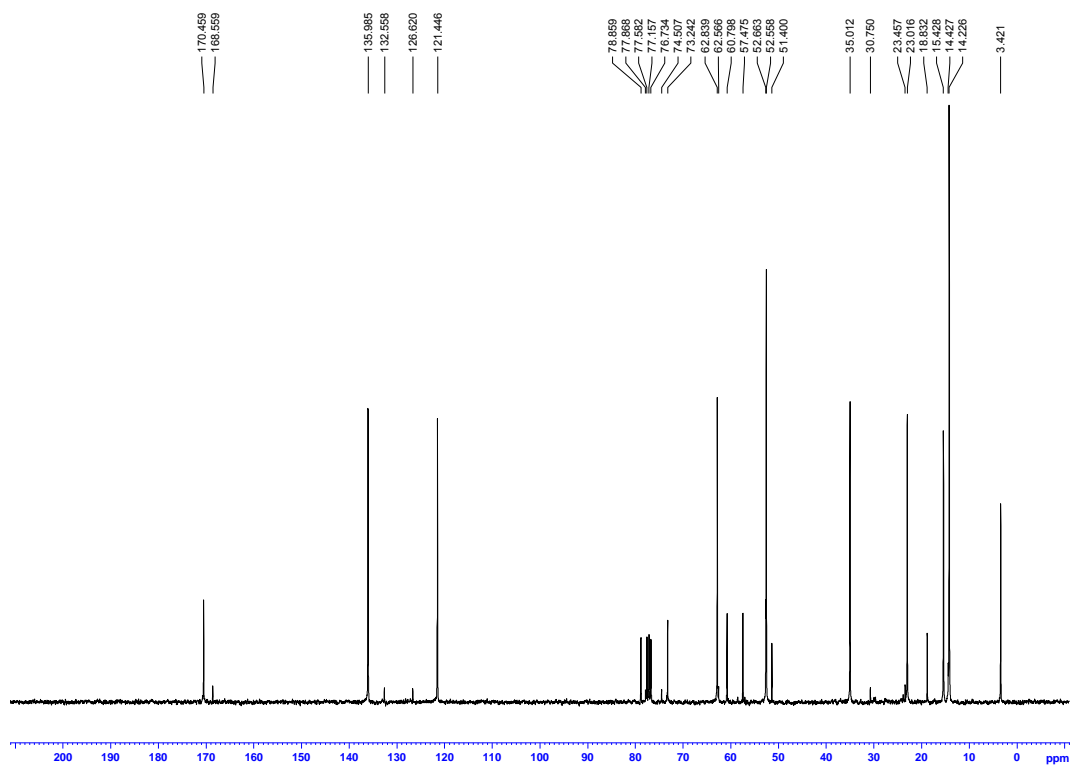
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (1b):



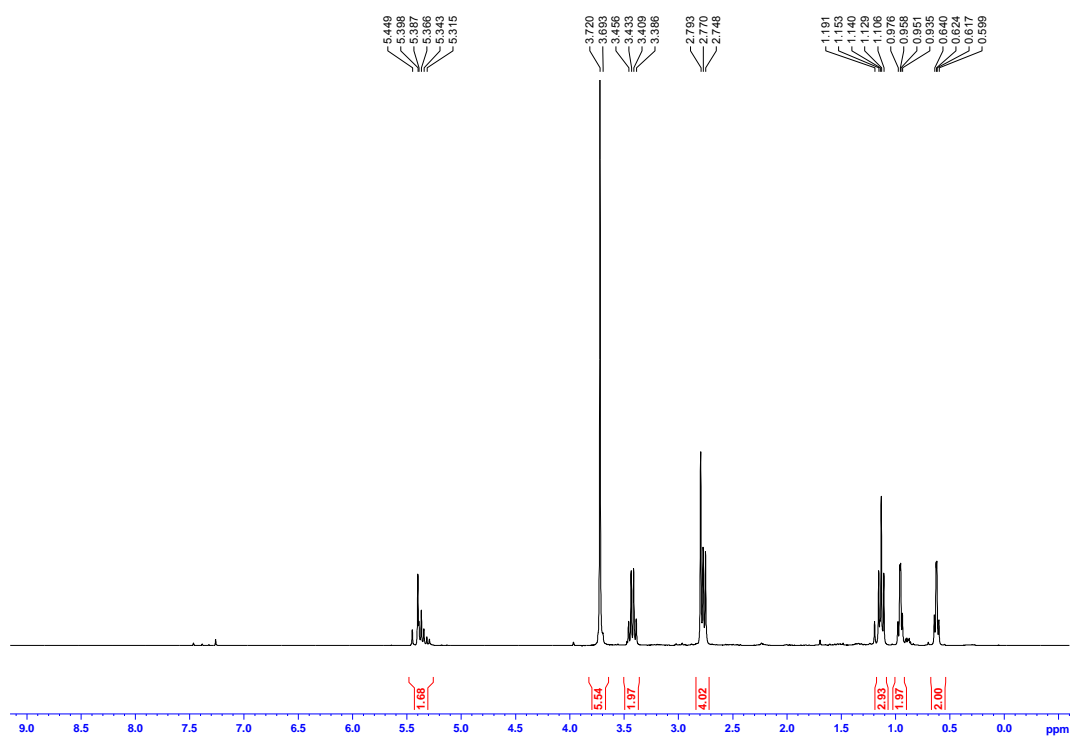
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) (1c):



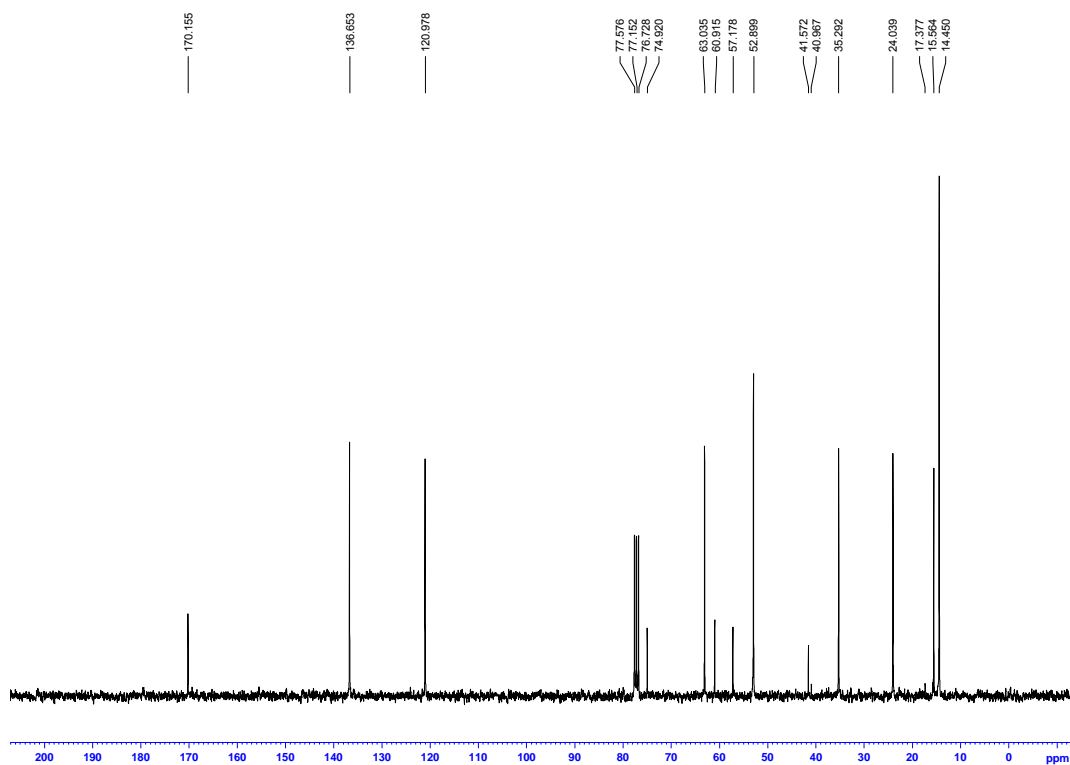
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (1c):**



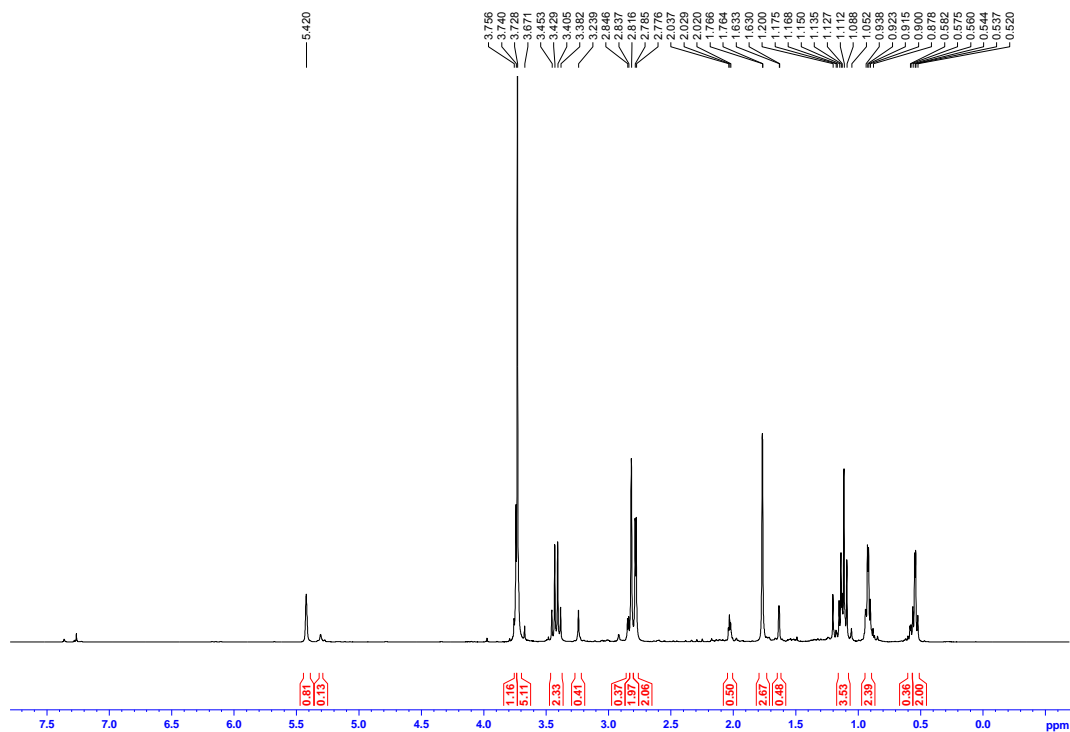
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (1d):**



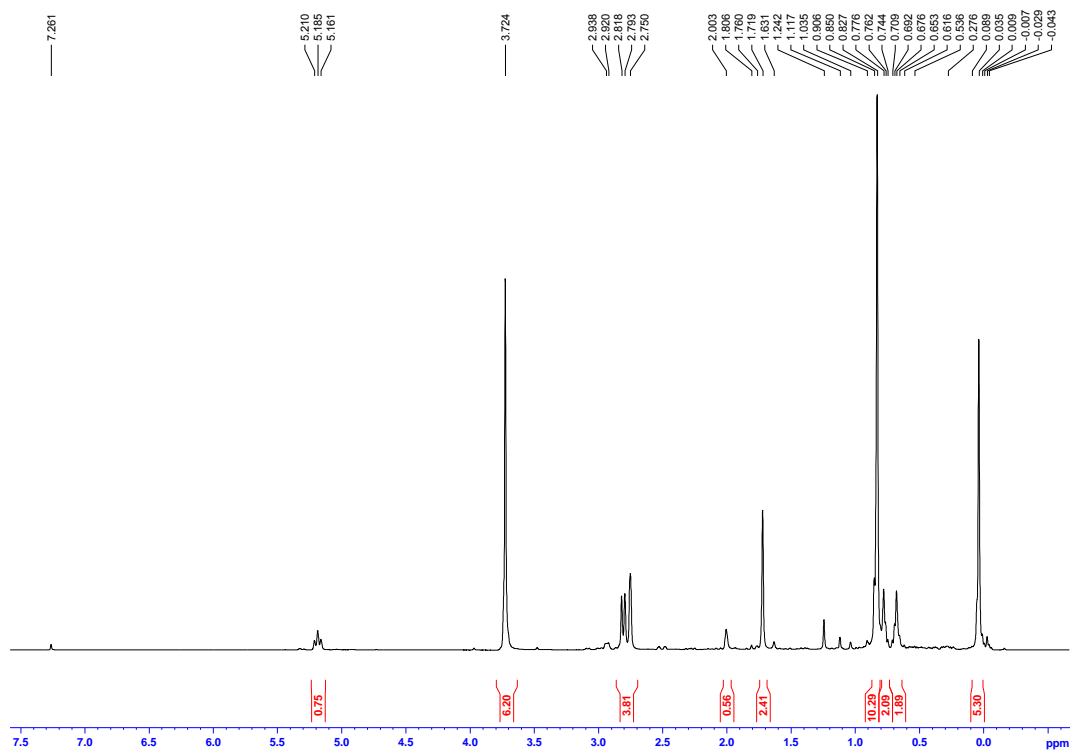
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (1d):**



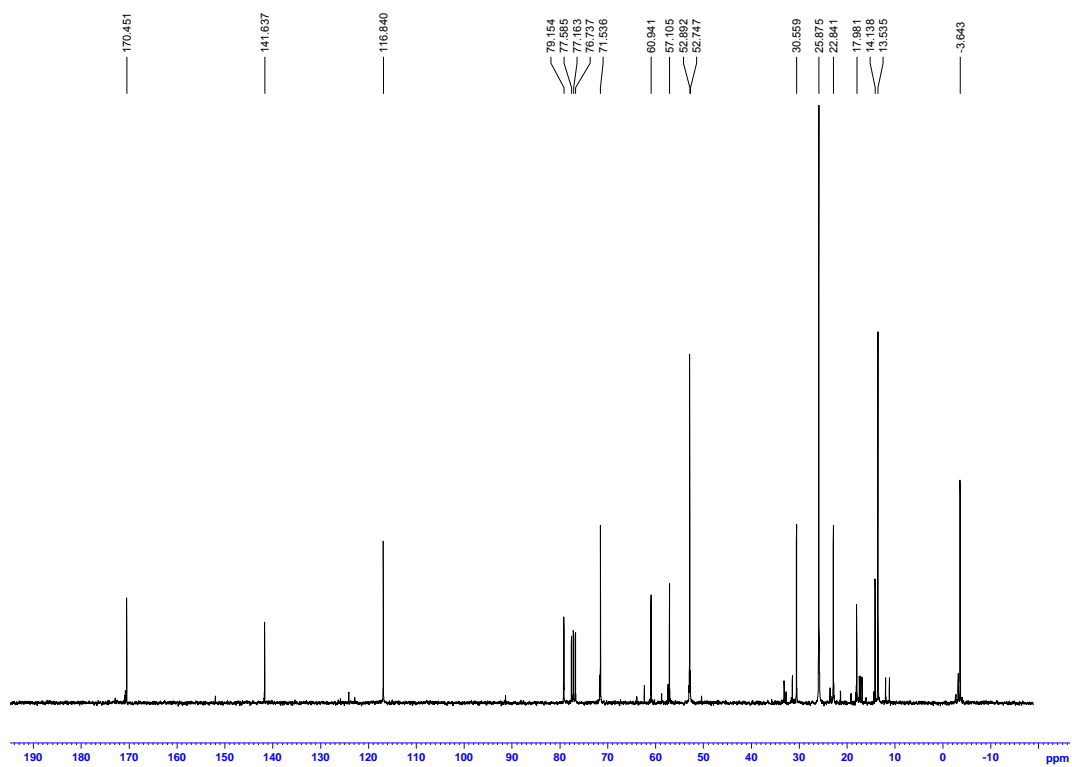
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (1e):**



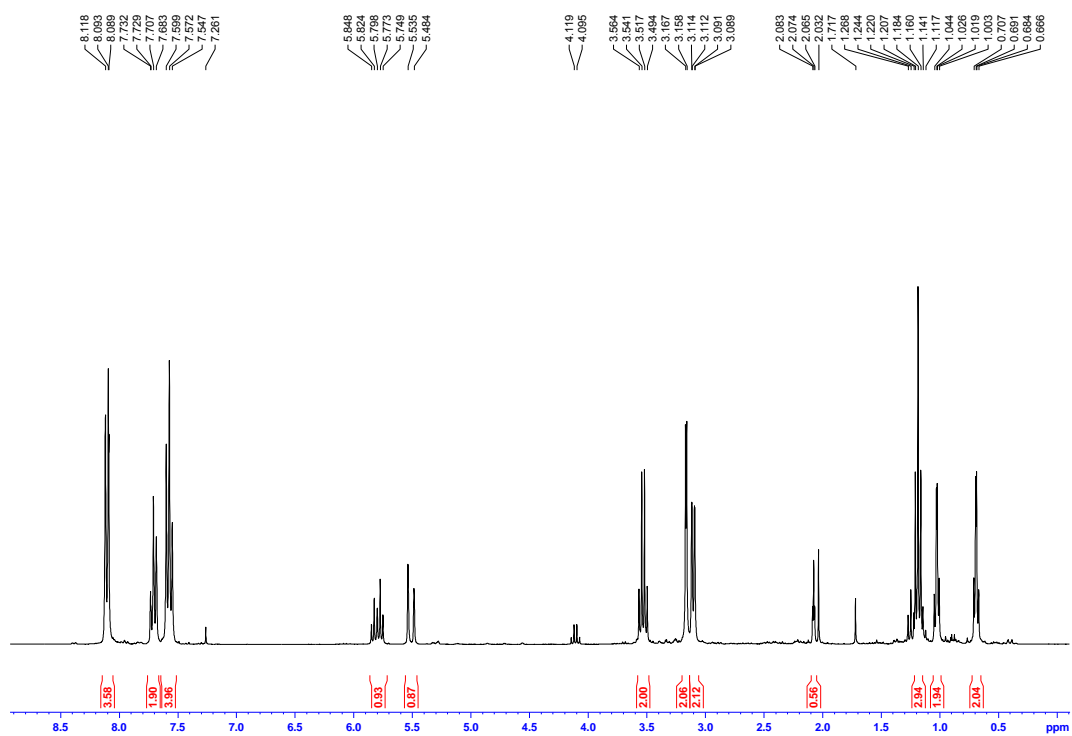
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (1f):**



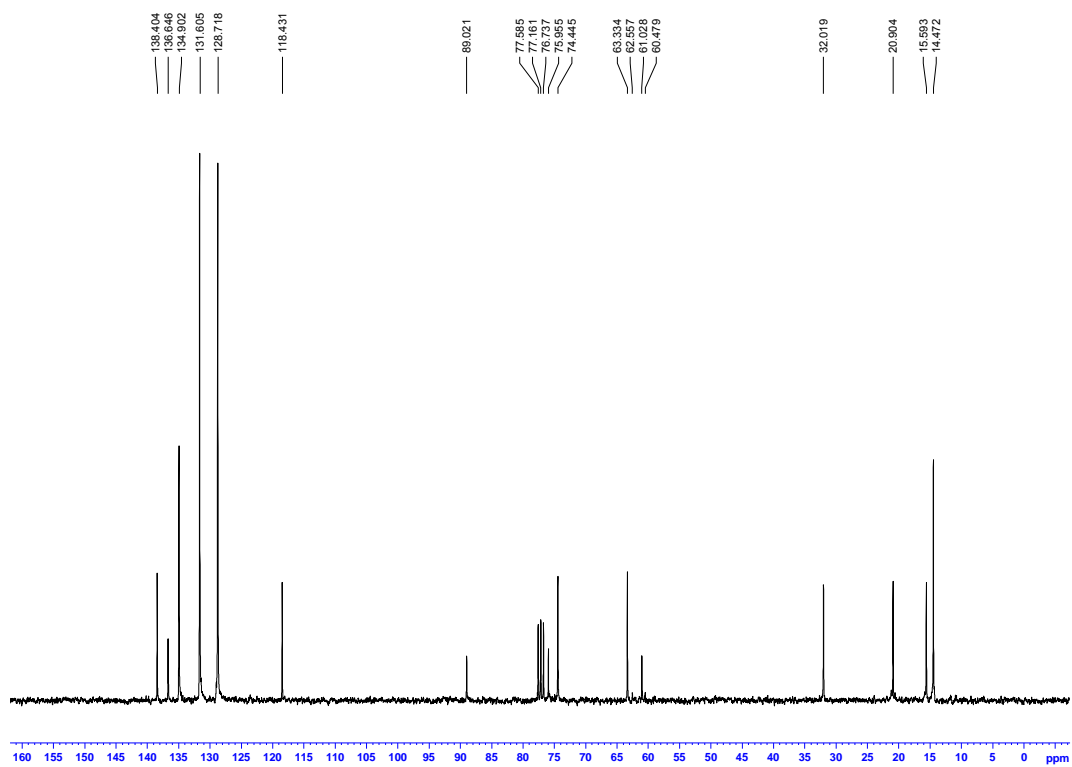
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) (1f):**



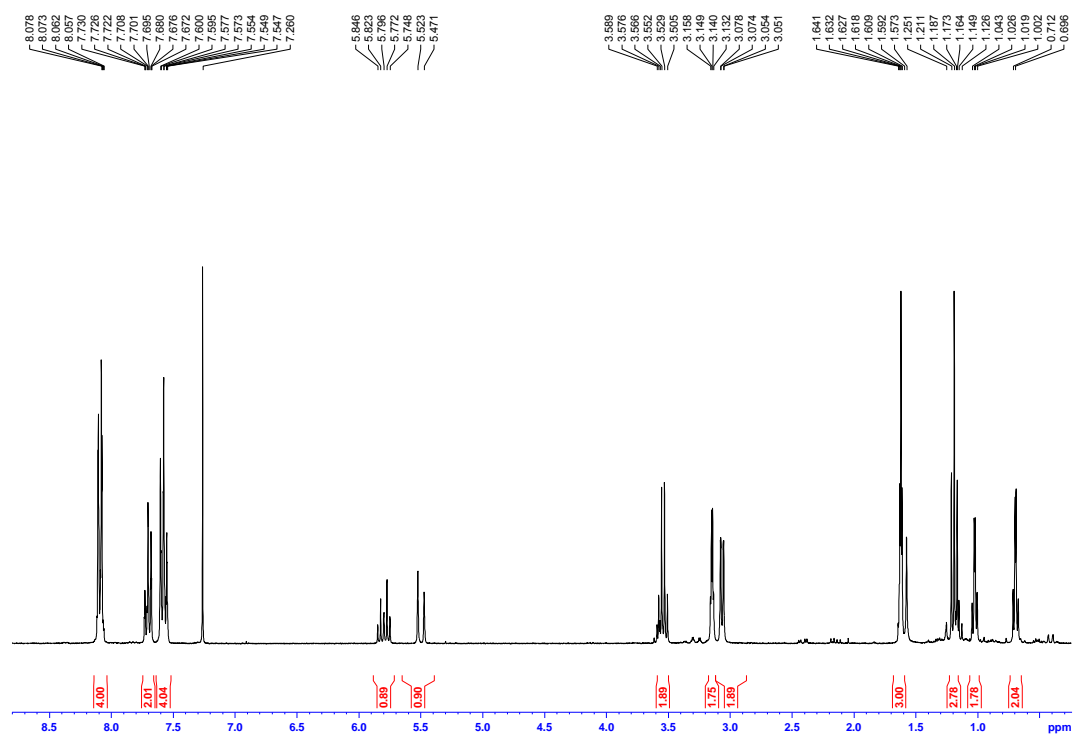
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (1g):**



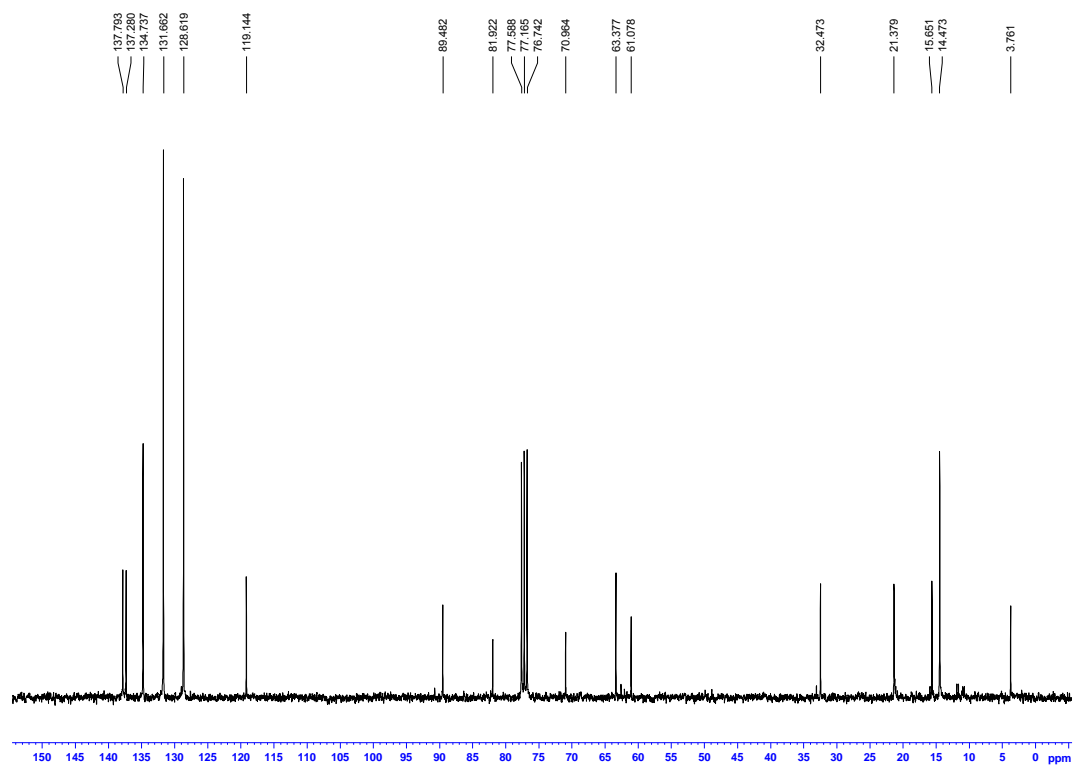
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (1g):**



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

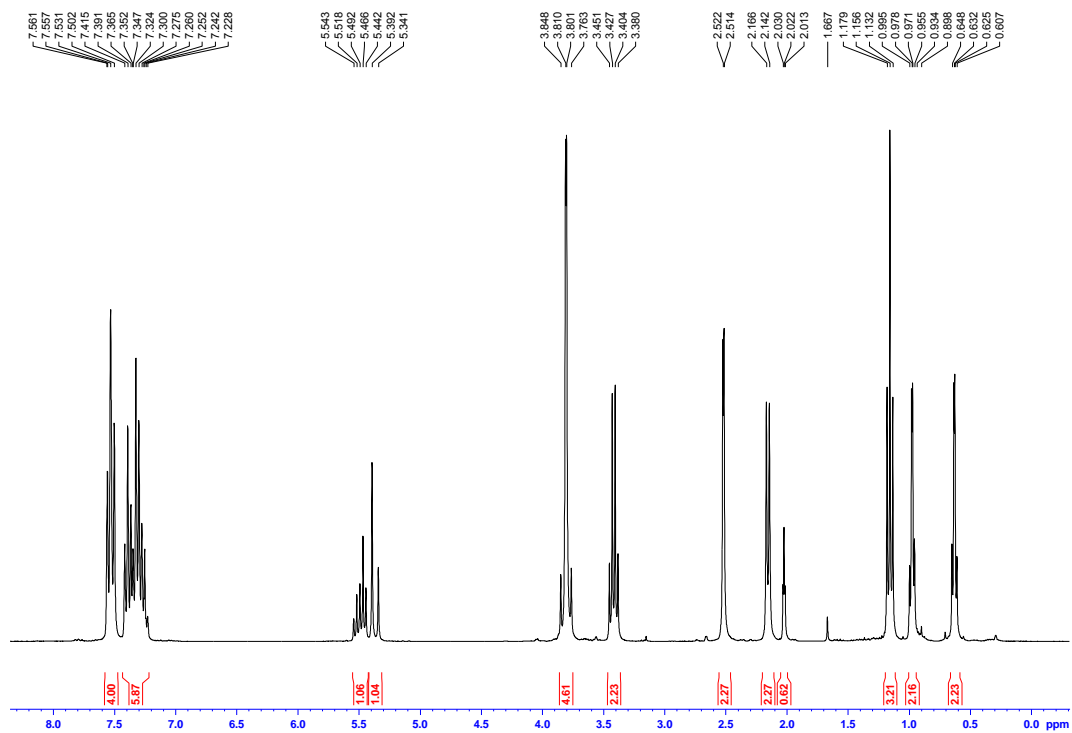


**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (1h):**

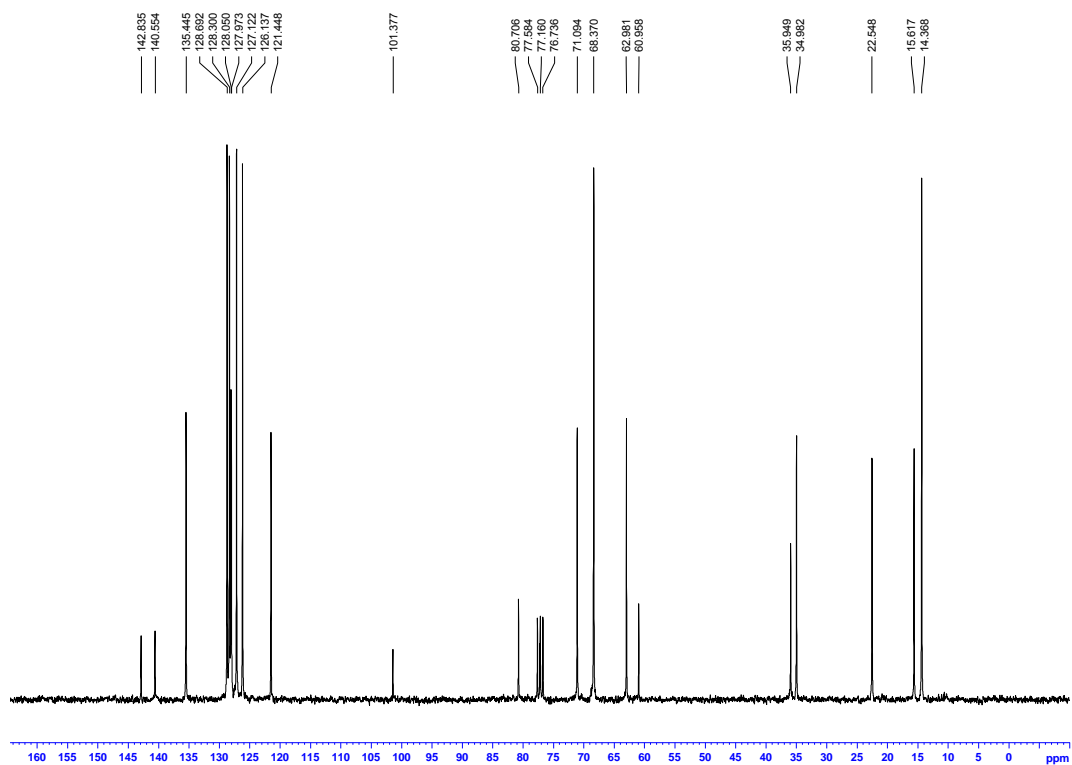




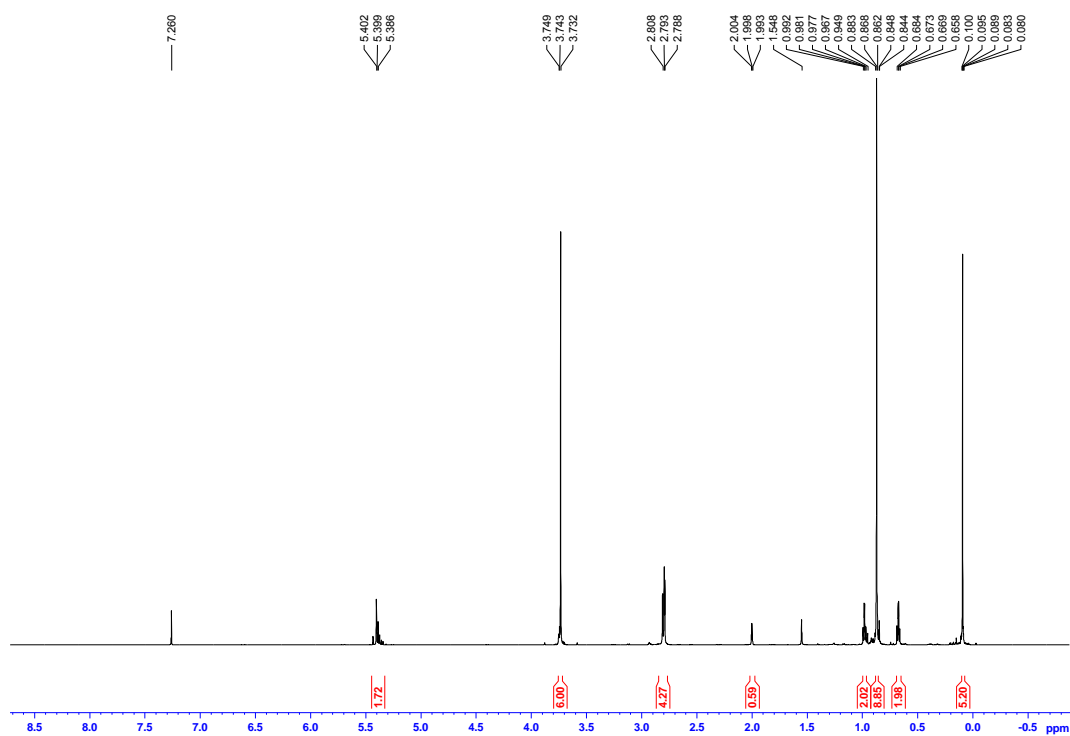
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (1i):**



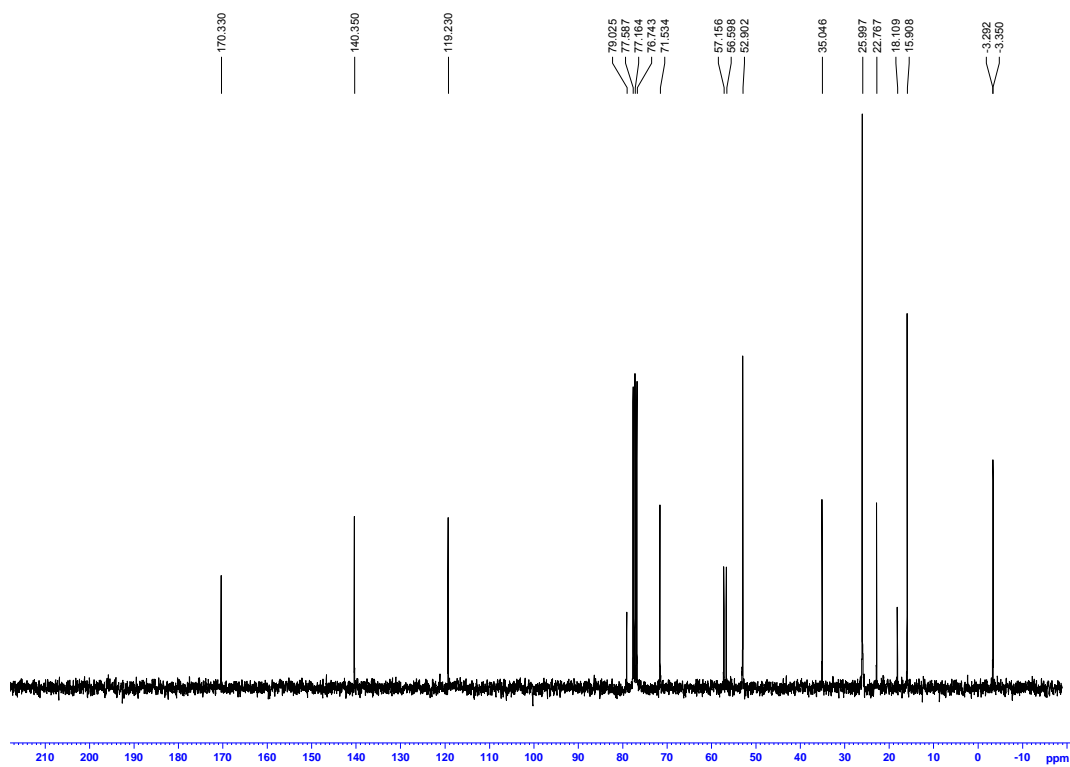
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (1i):**



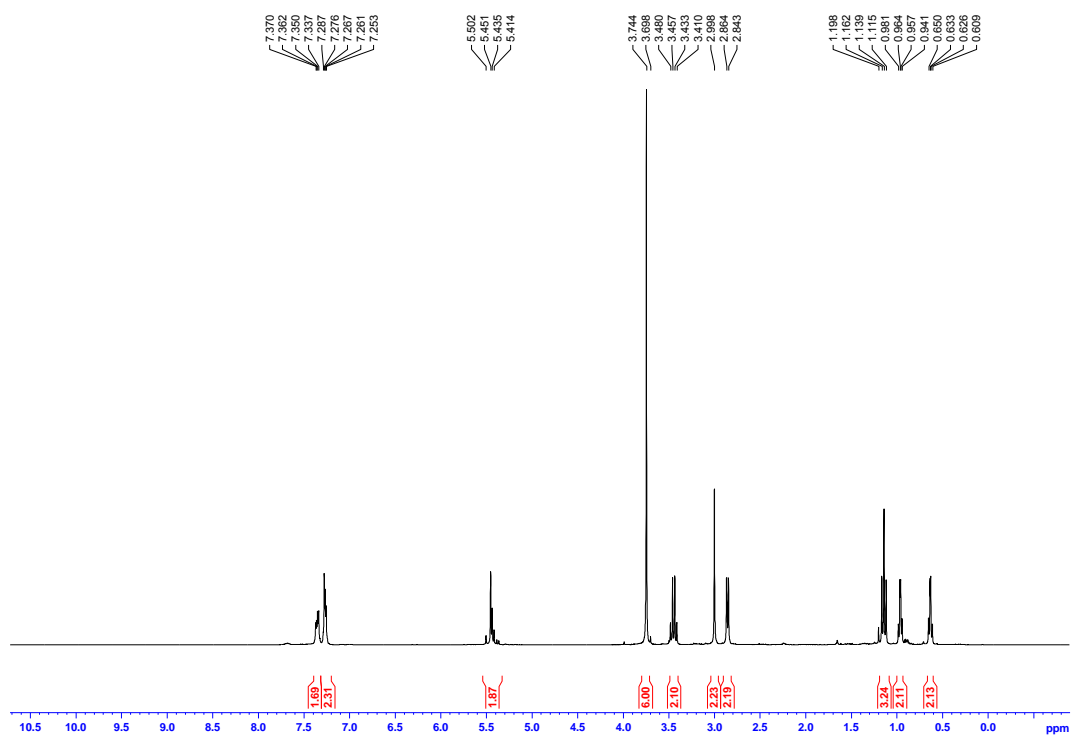
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (1j):**



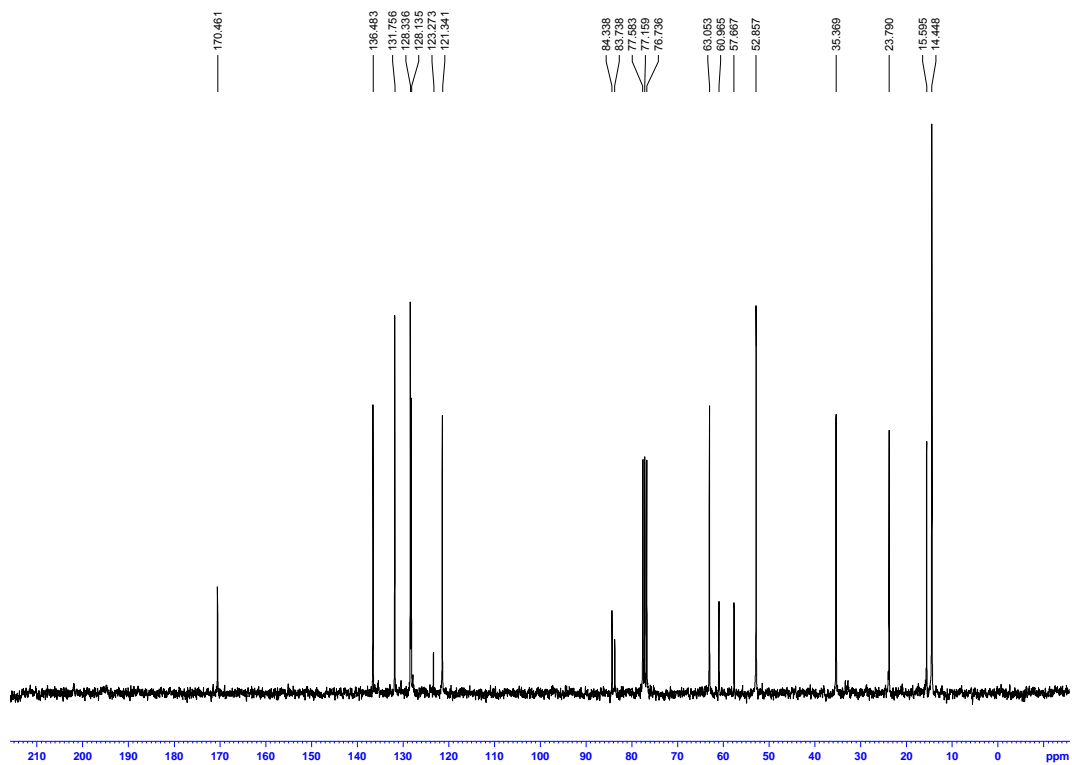
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) (1j):**



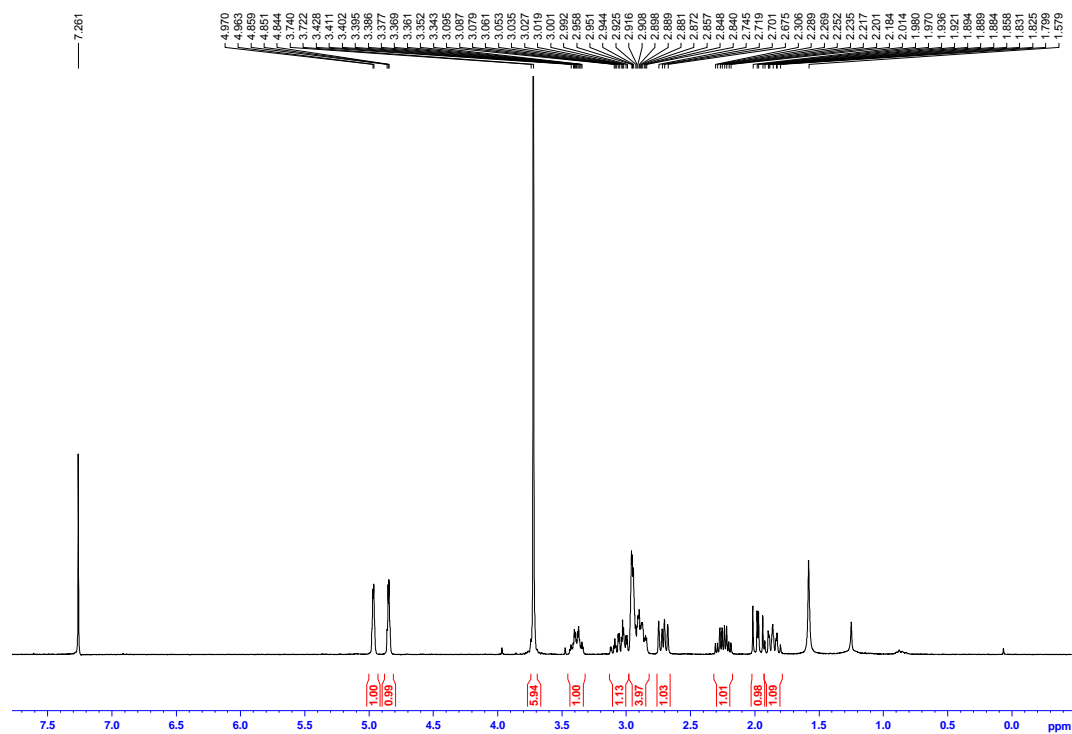
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (1k):**



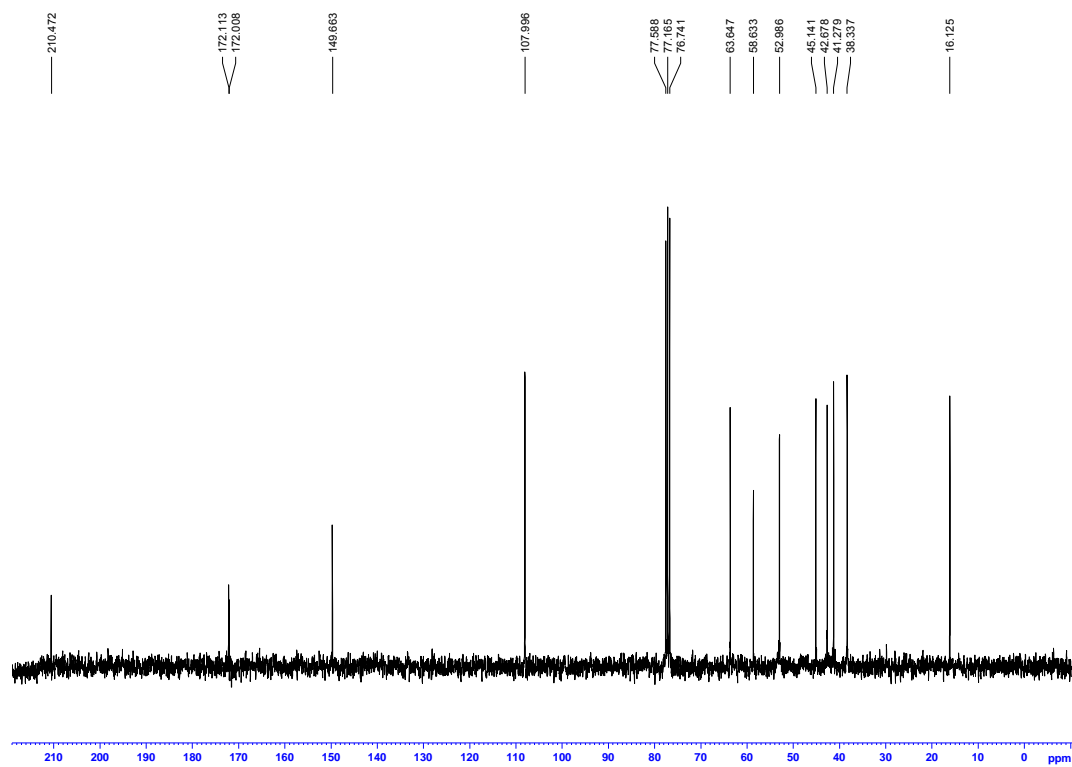
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (1k):**



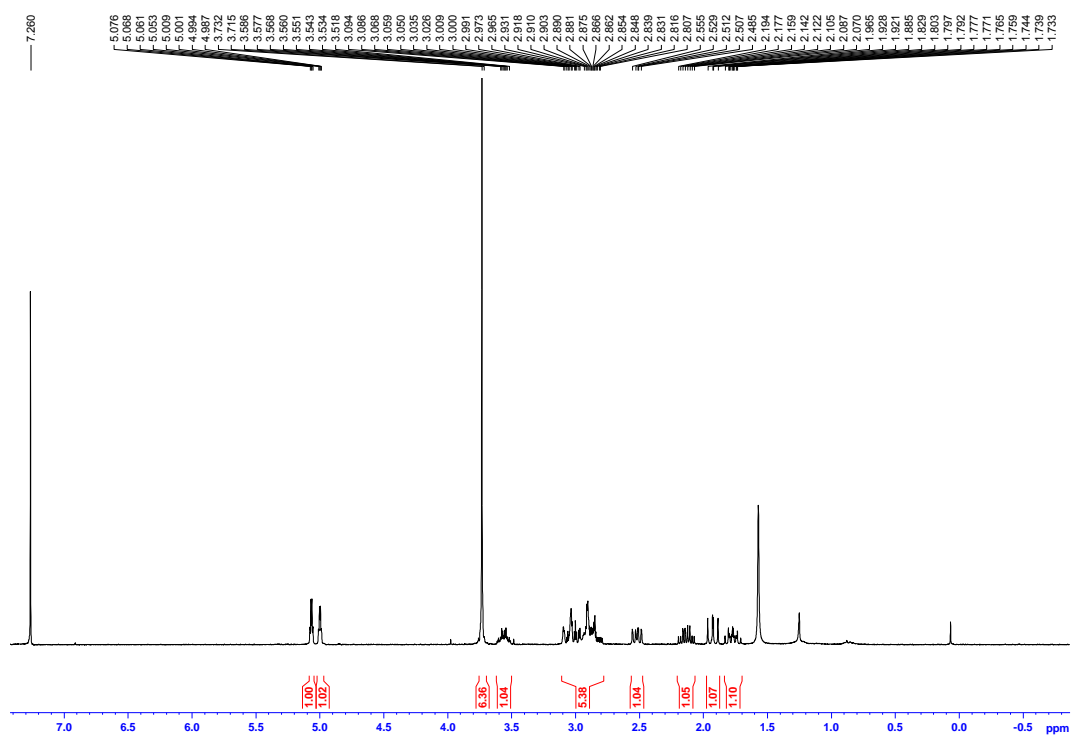
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (*cis*-3a):**



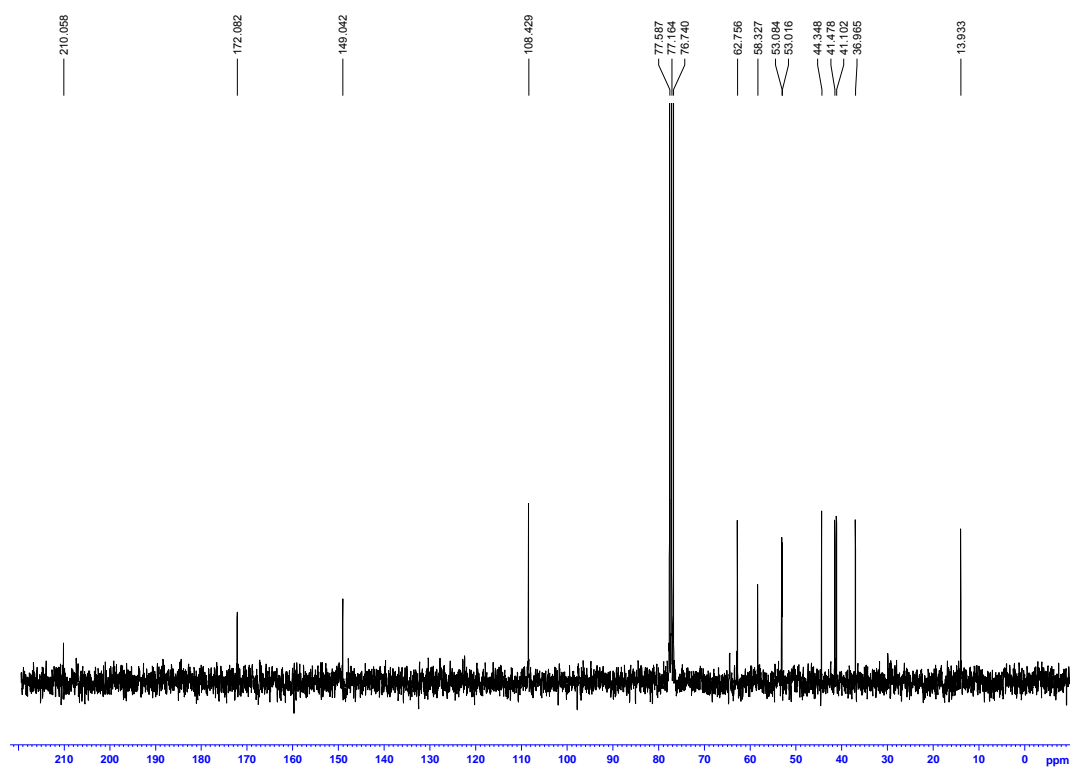
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) (*cis*-3a):**



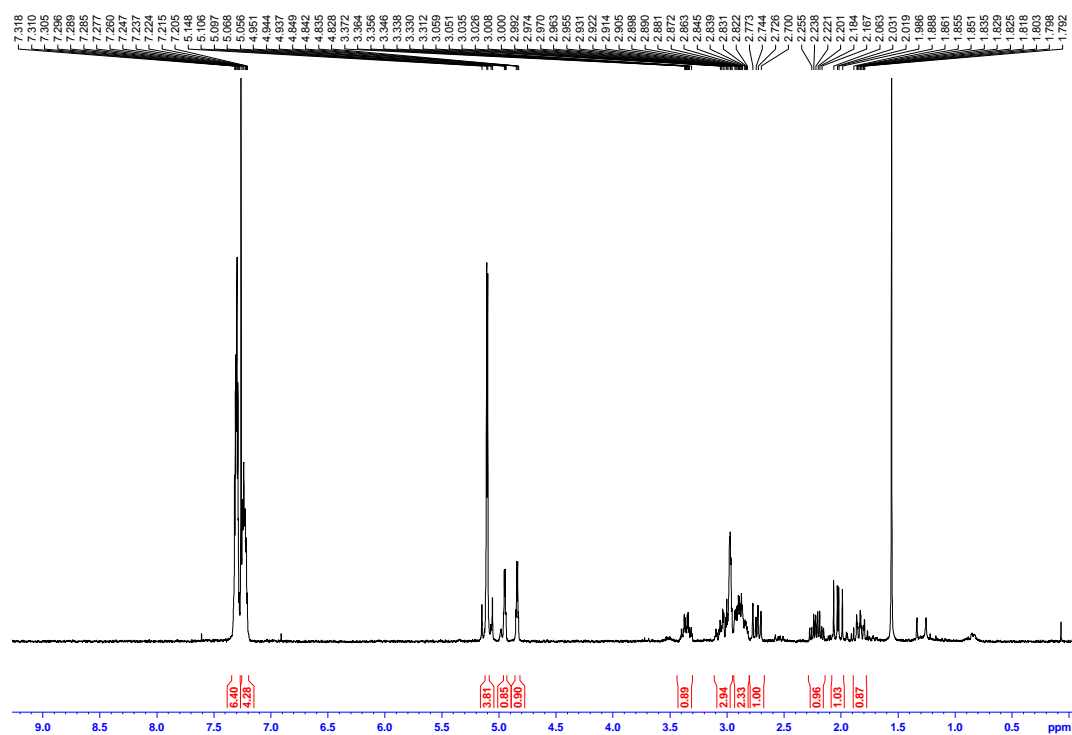
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (*trans*-3a):**



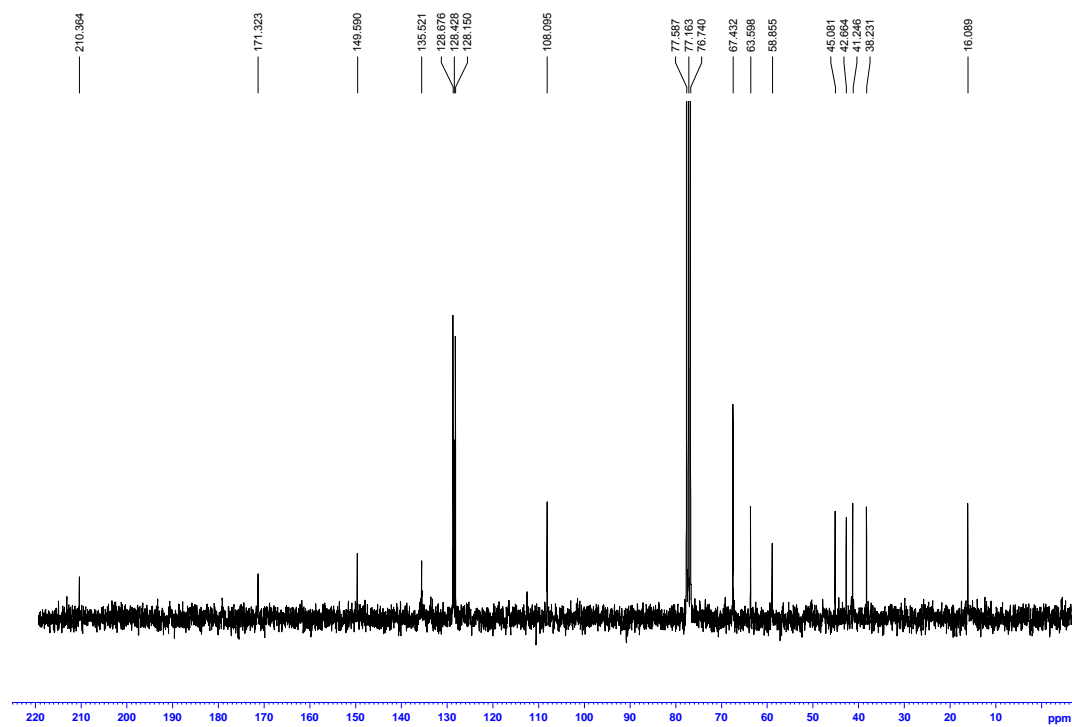
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (*trans*-3a):**



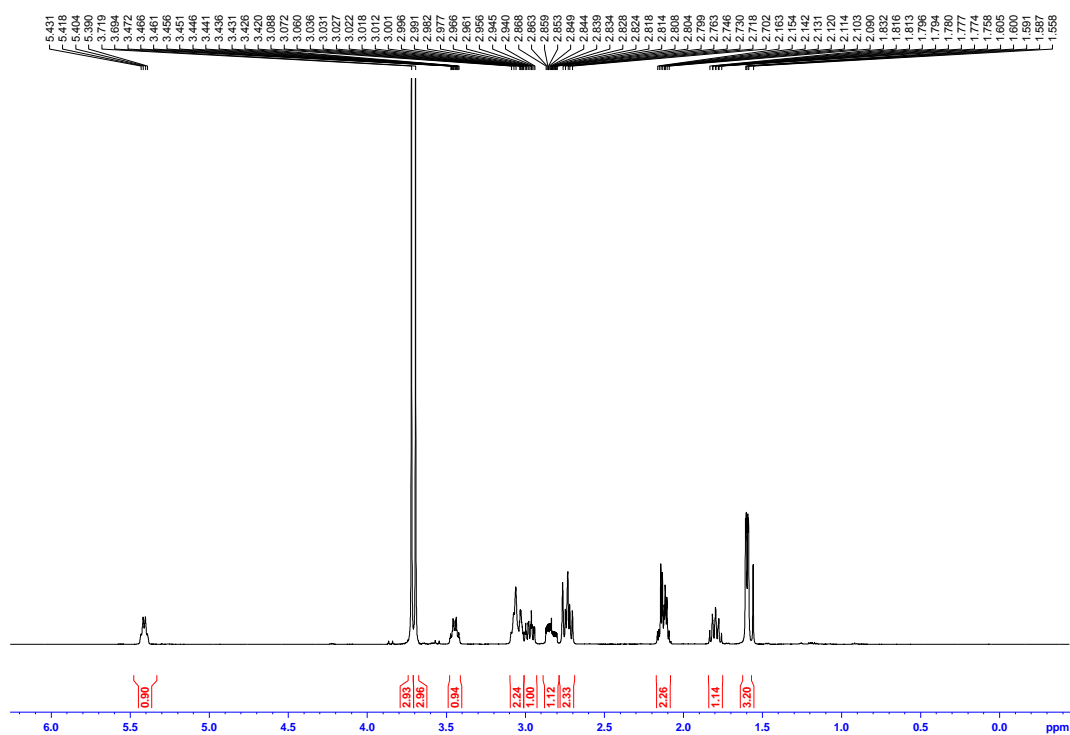
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (*cis*-3b):**



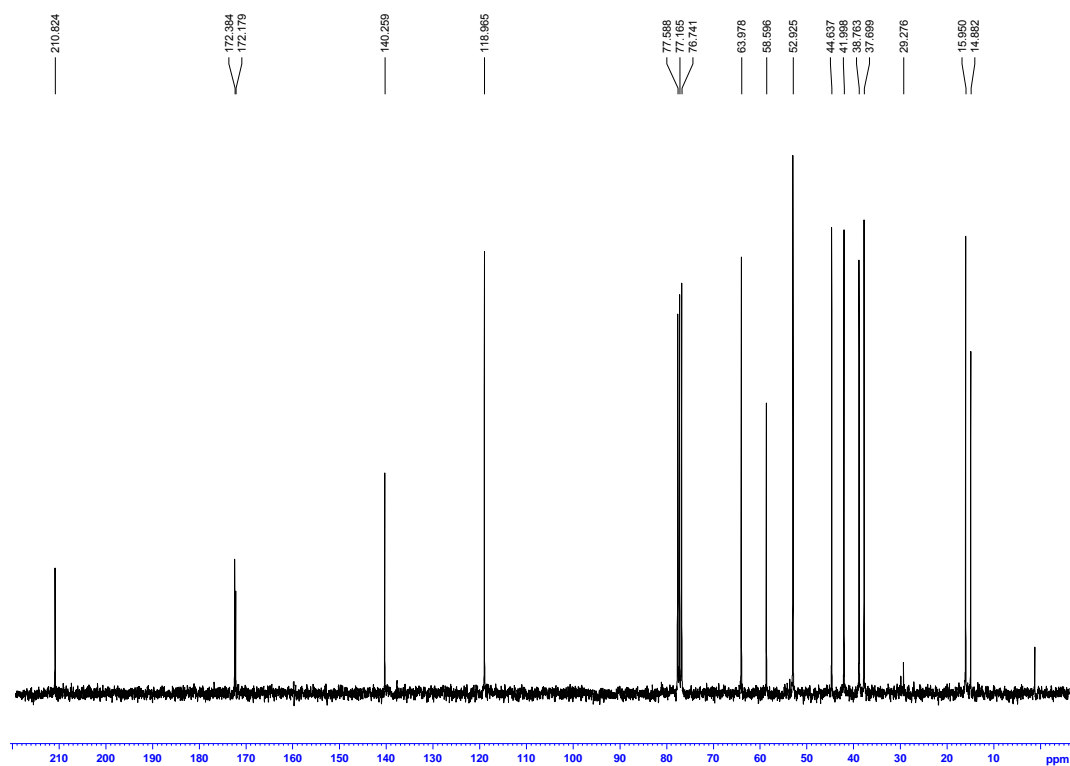
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) (*cis*-3b):**



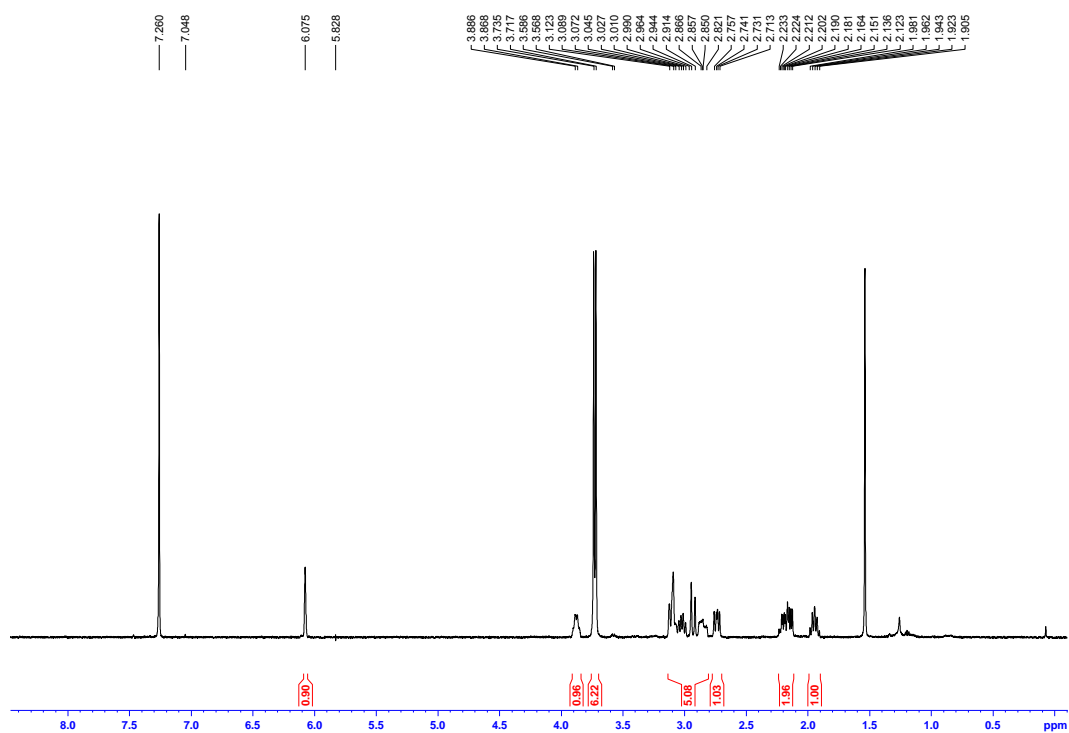
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) (*cis*-3c):**



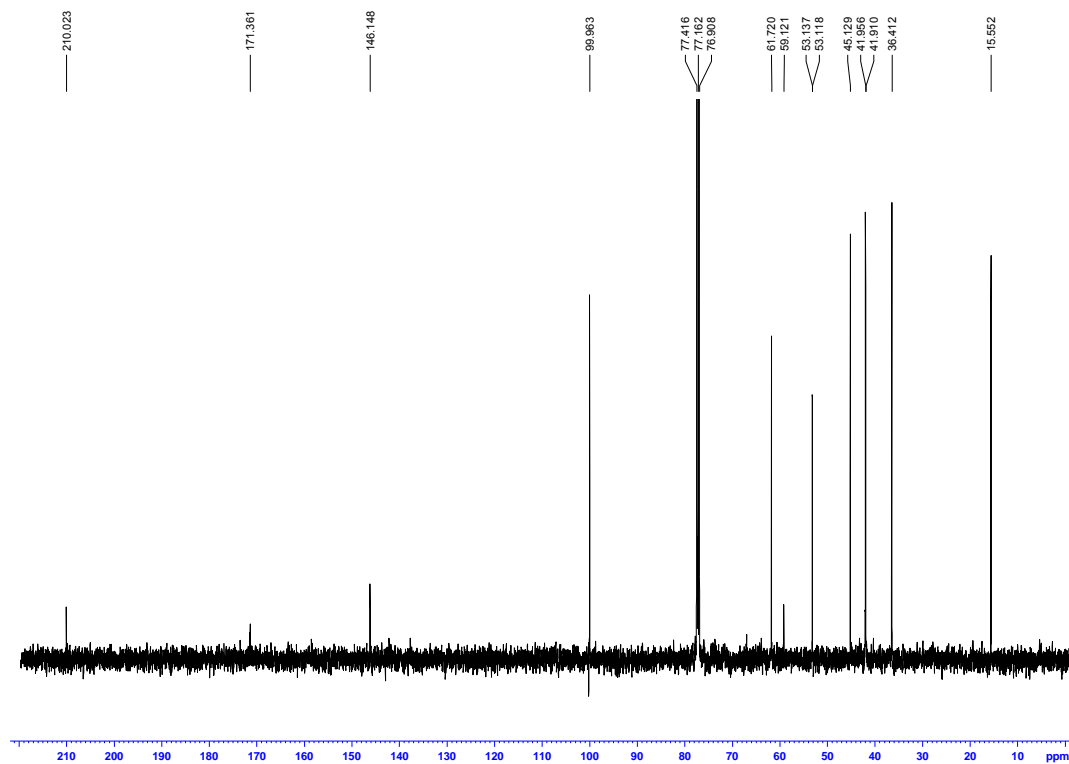
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) (*cis*-3c):**



**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (*cis*-3d):**

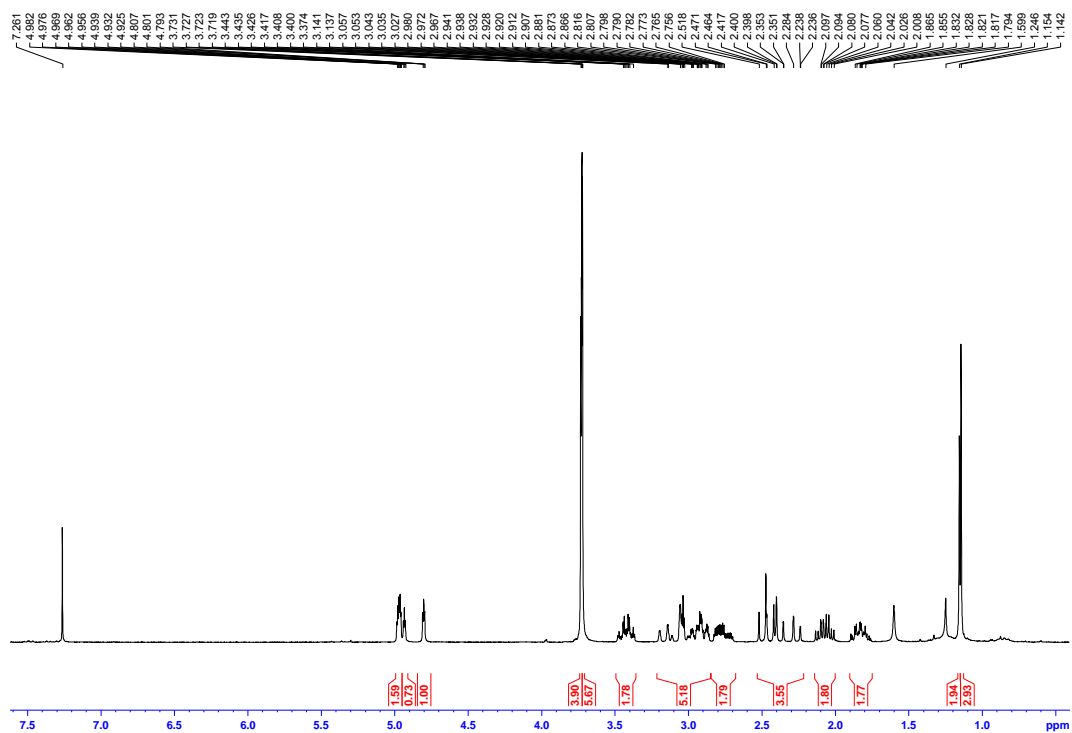


**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (*cis*-3d):**

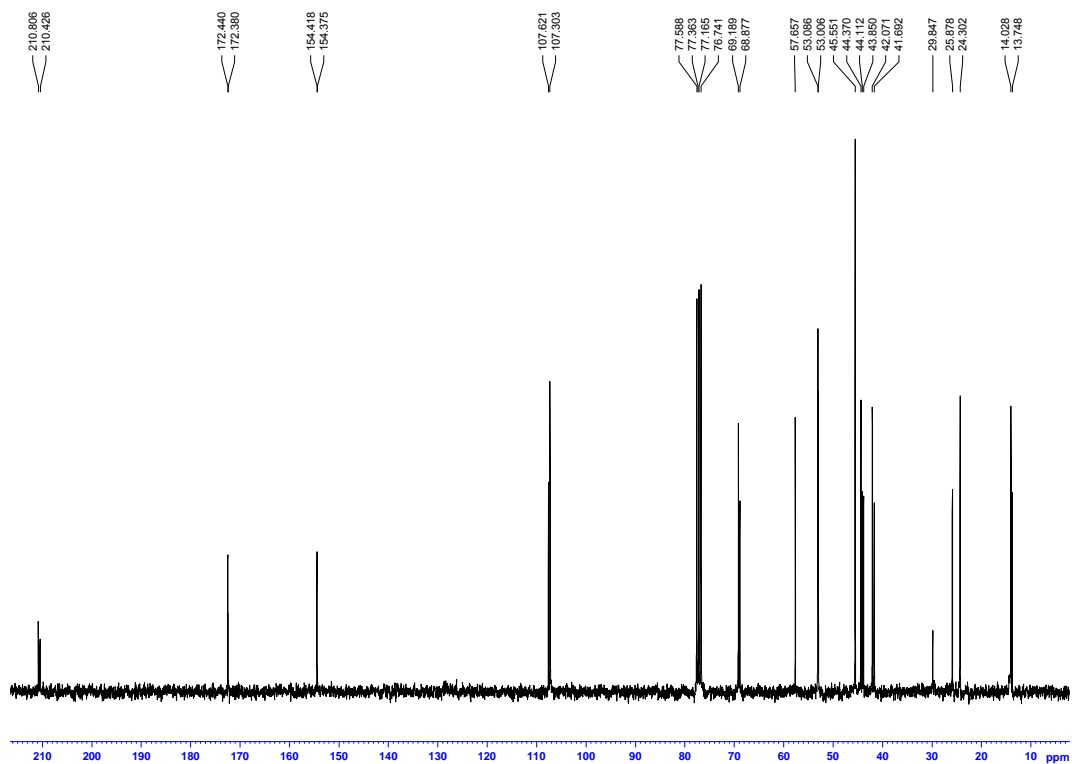




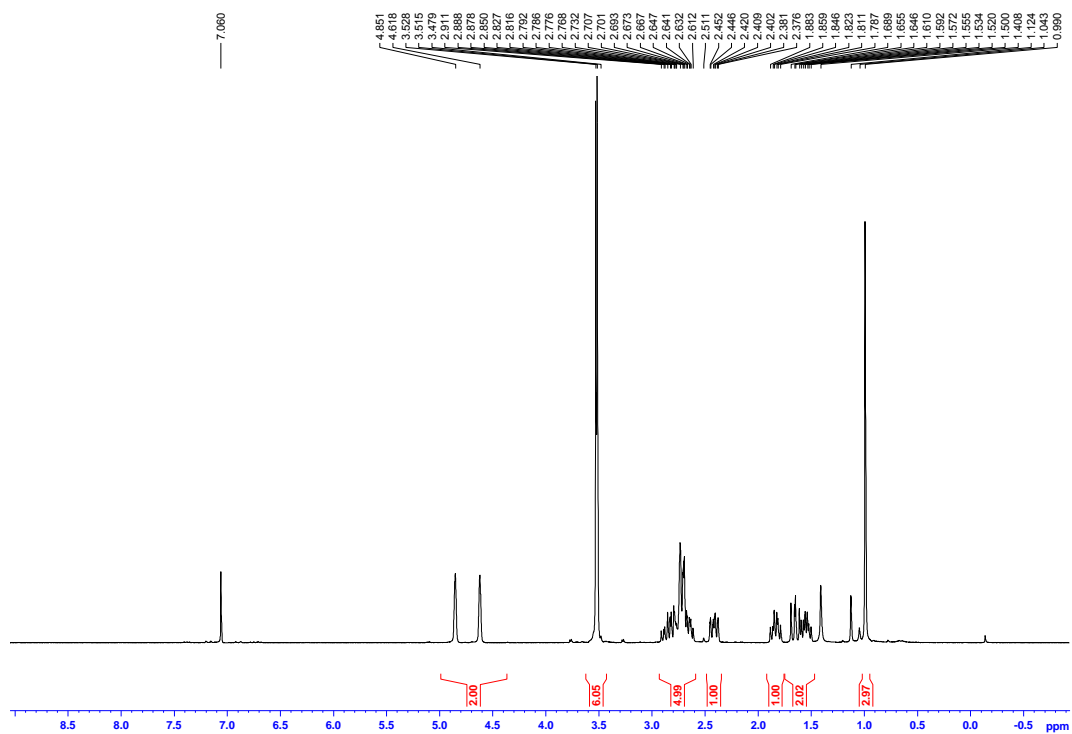
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (*cis*-**3e** + *trans*-**3e**):**



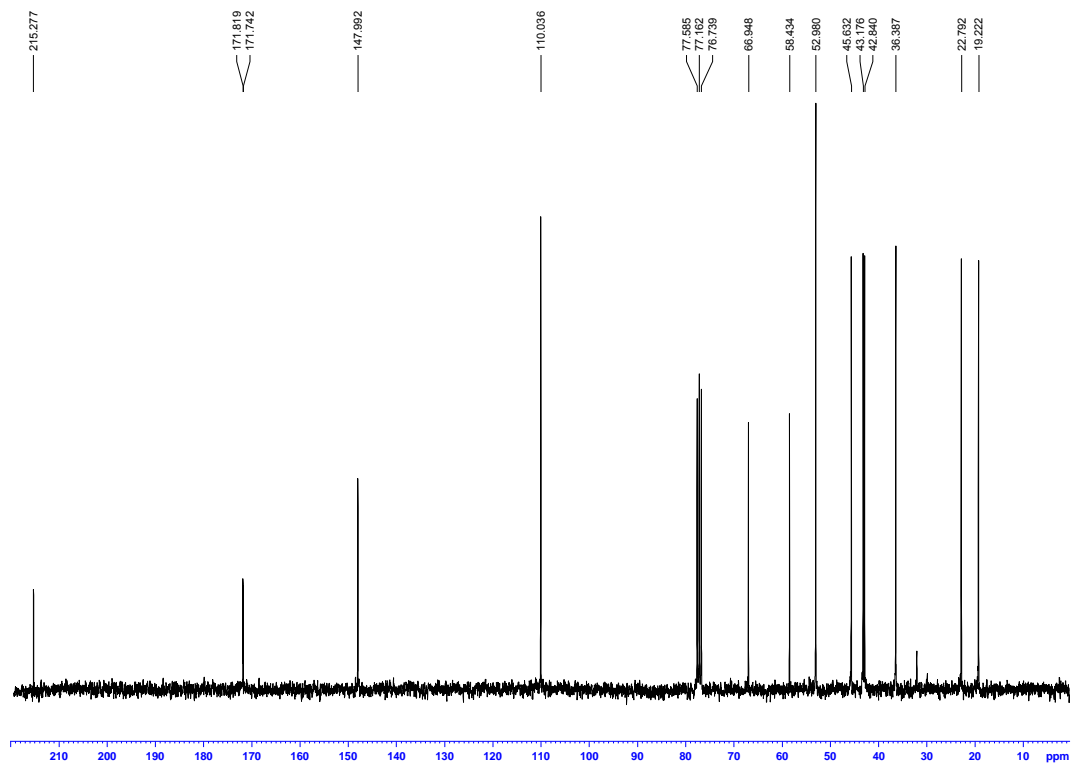
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) (*cis*-**3e** + *trans*-**3e**):**



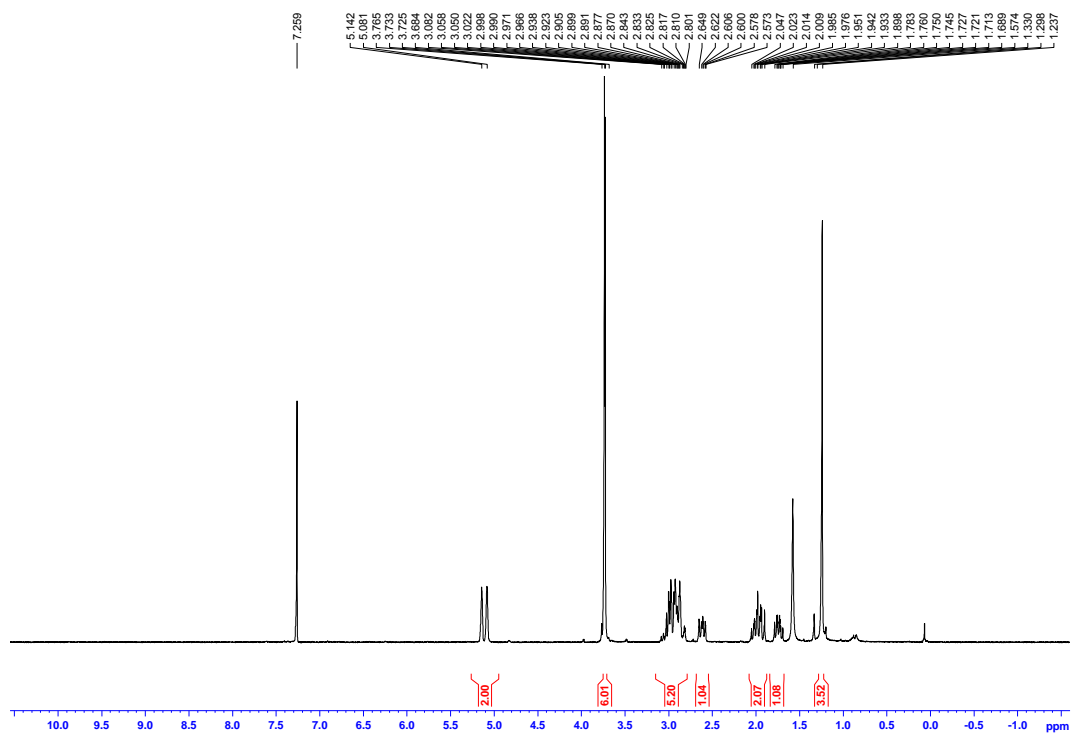
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (*cis*-3f):**



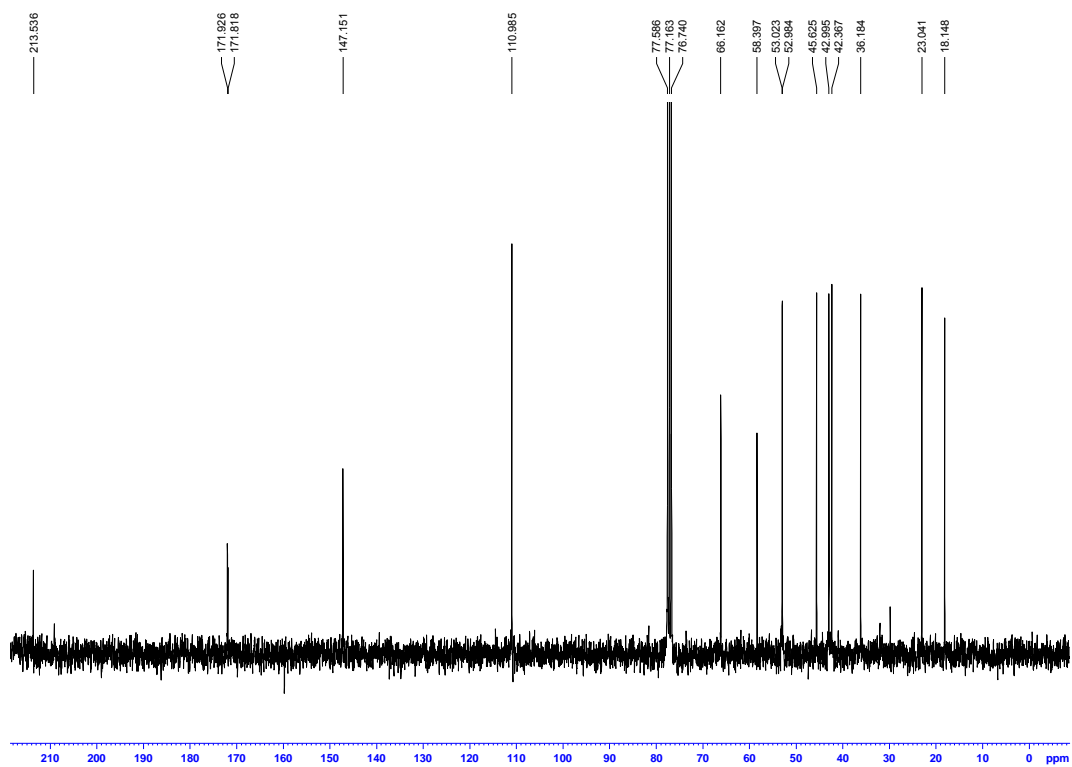
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) (*cis*-3f):**



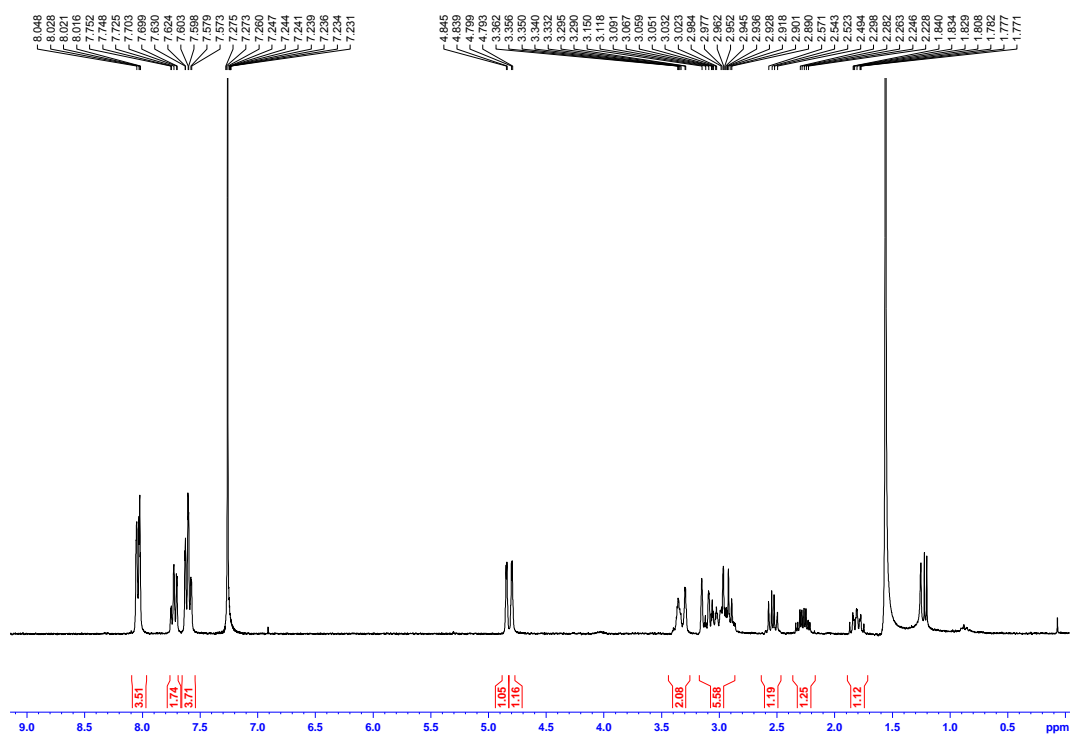
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (*trans*-3f):**



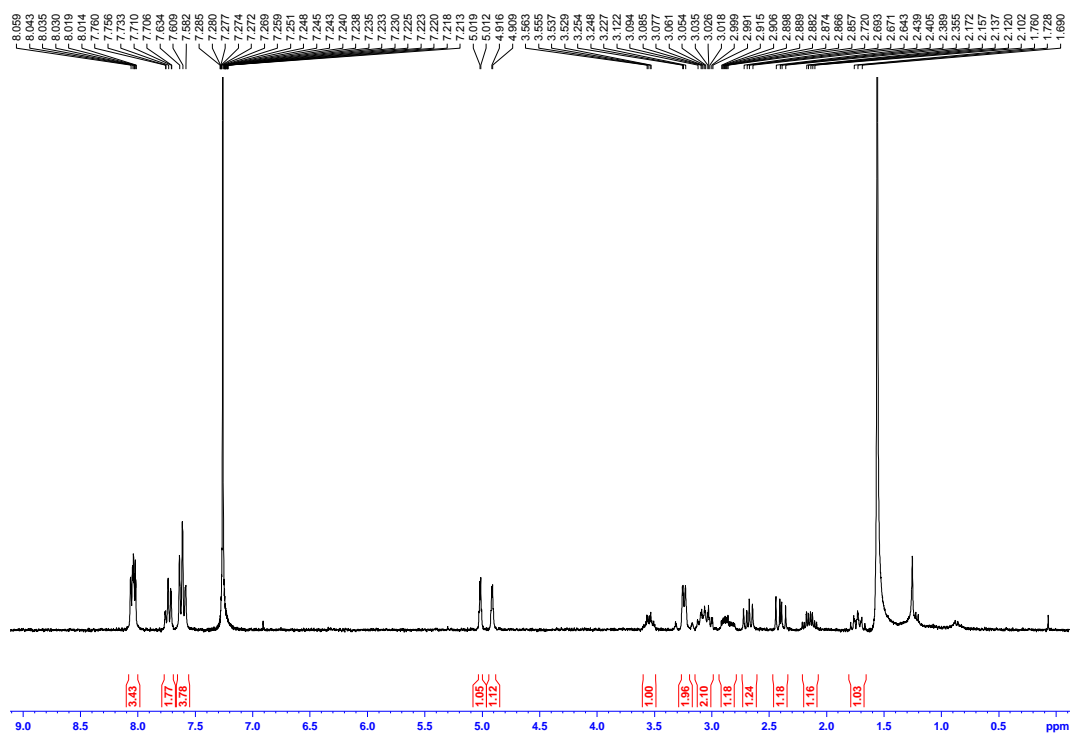
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (*trans*-3f):**



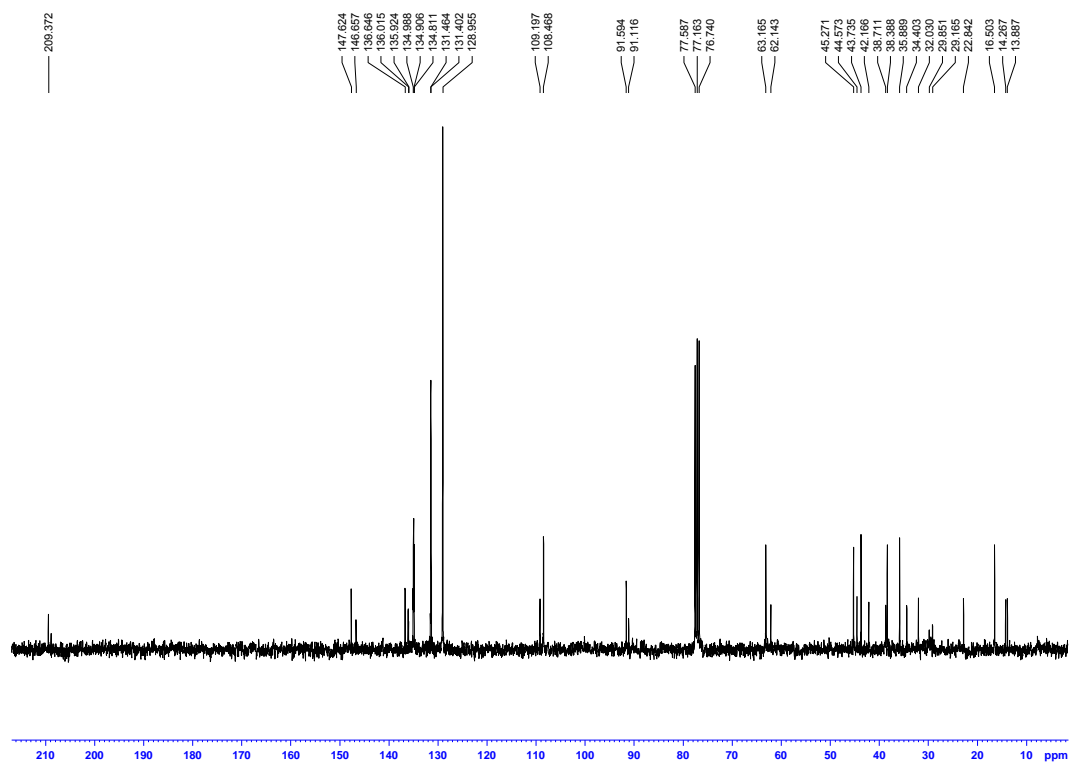
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (*cis*-3g):**



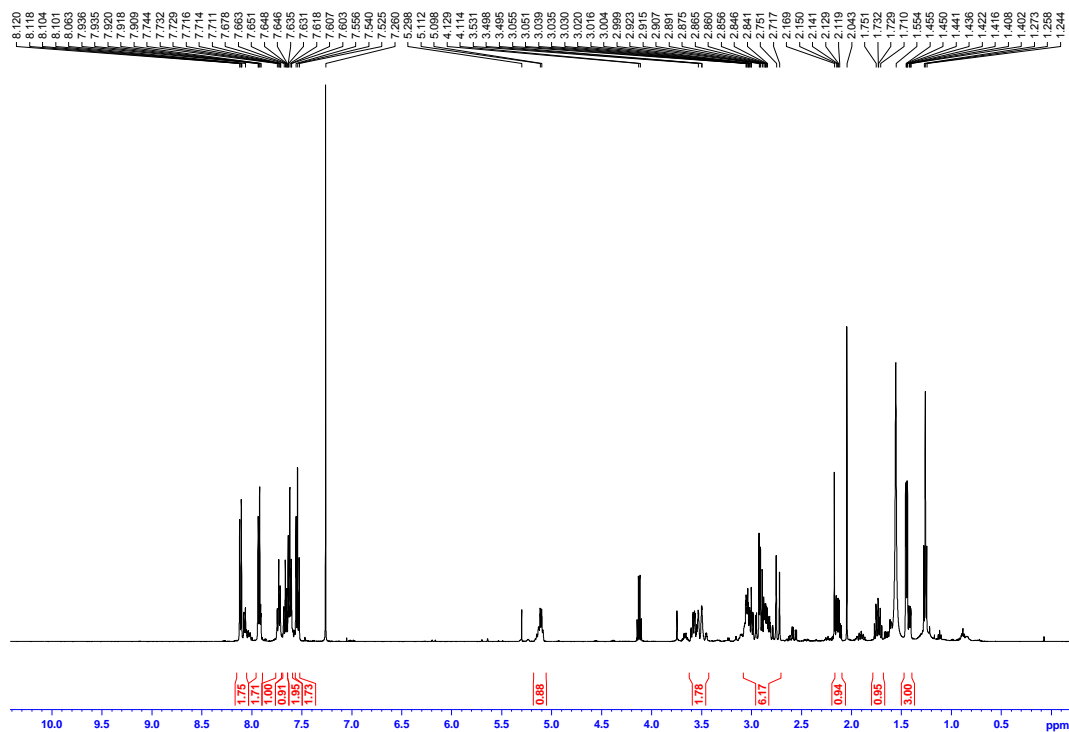
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (*trans*-3g):**



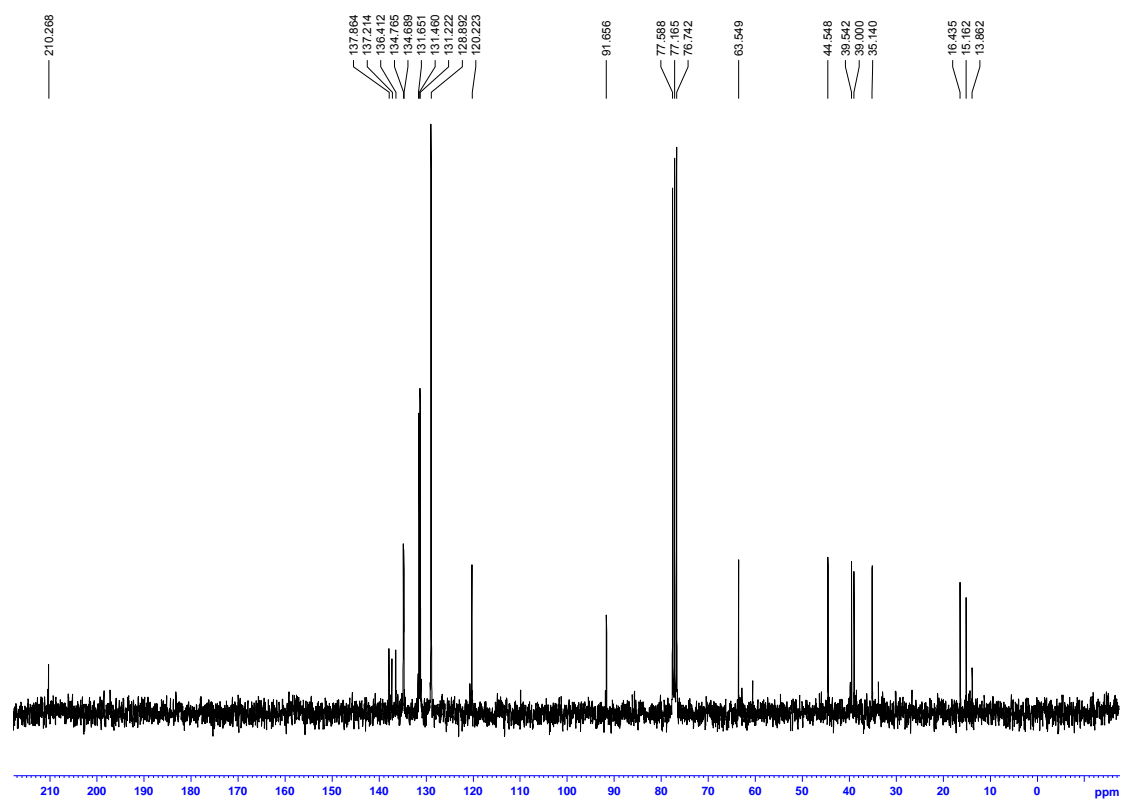
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (*cis*-**3g** + *trans*-**3g**):



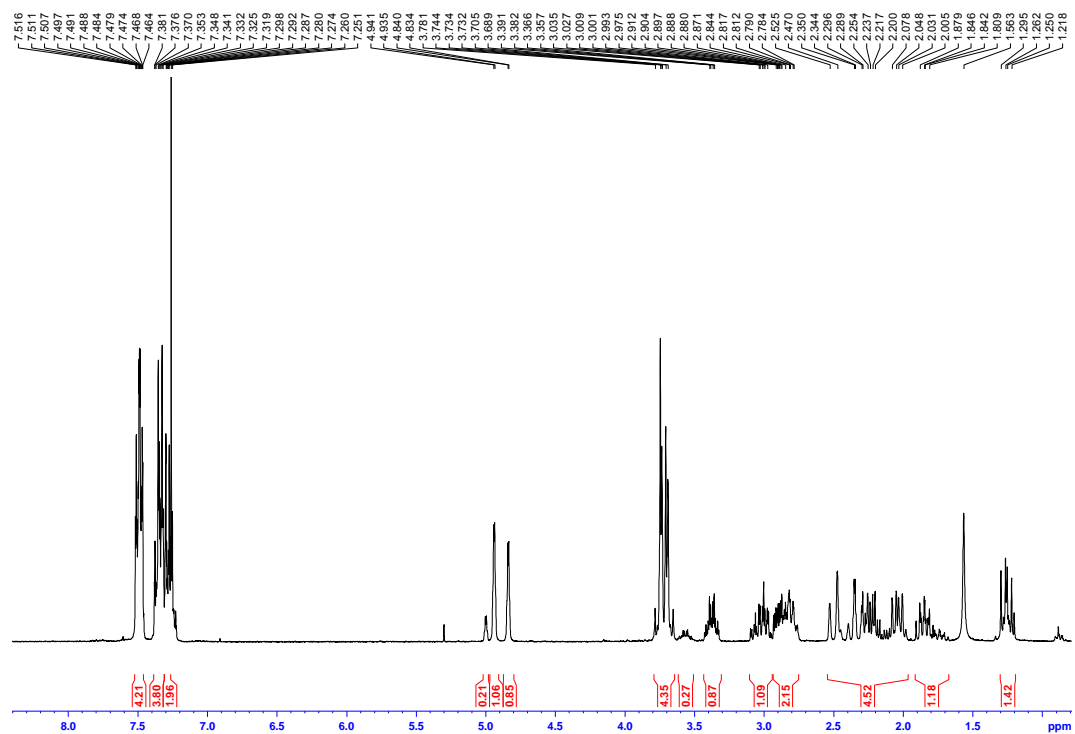
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (*cis*-**3h**):



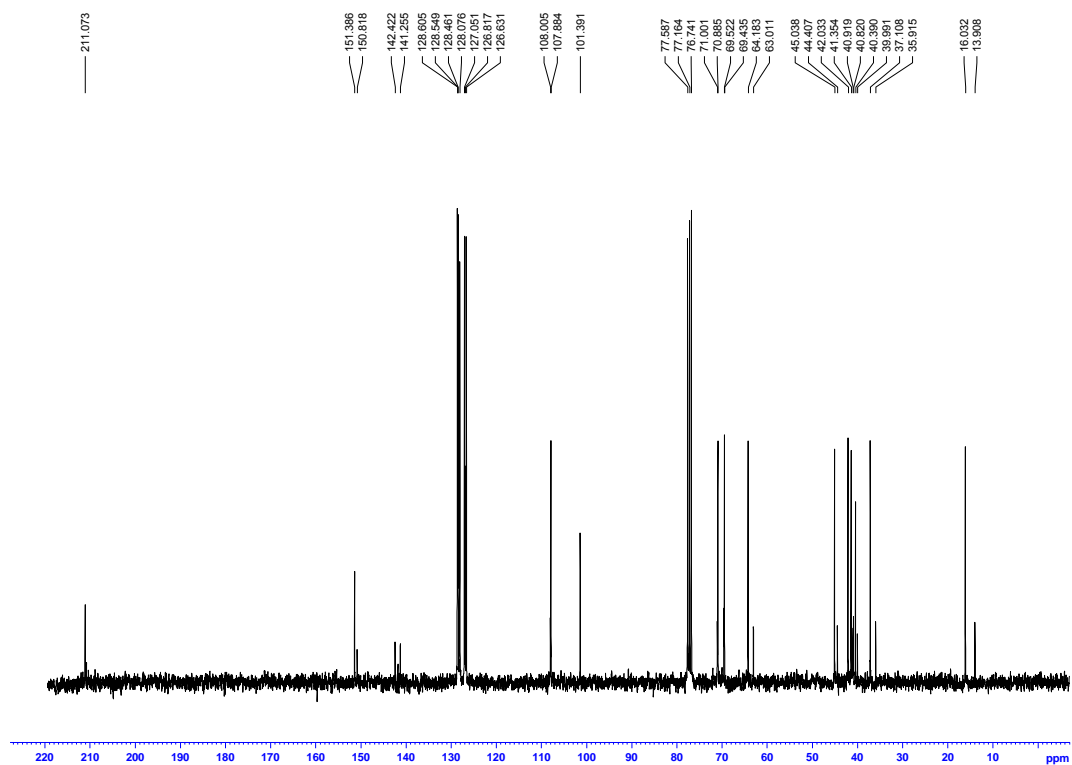
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (*cis*-3h):



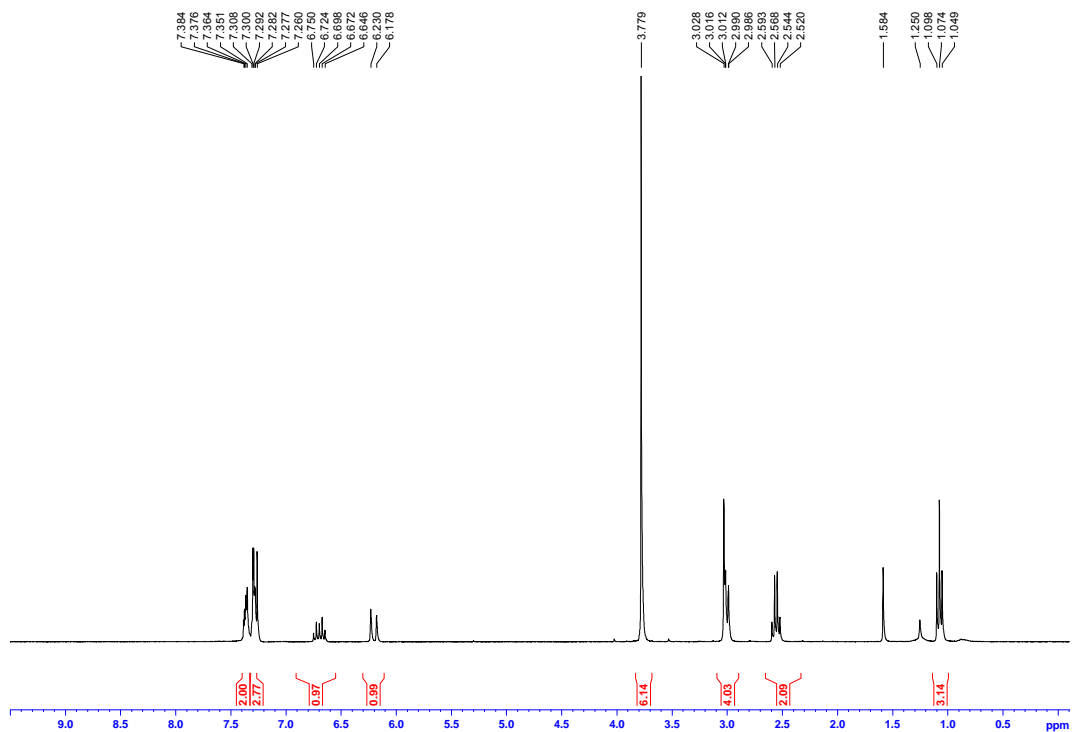
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (*cis*-3i + *trans*-3i):



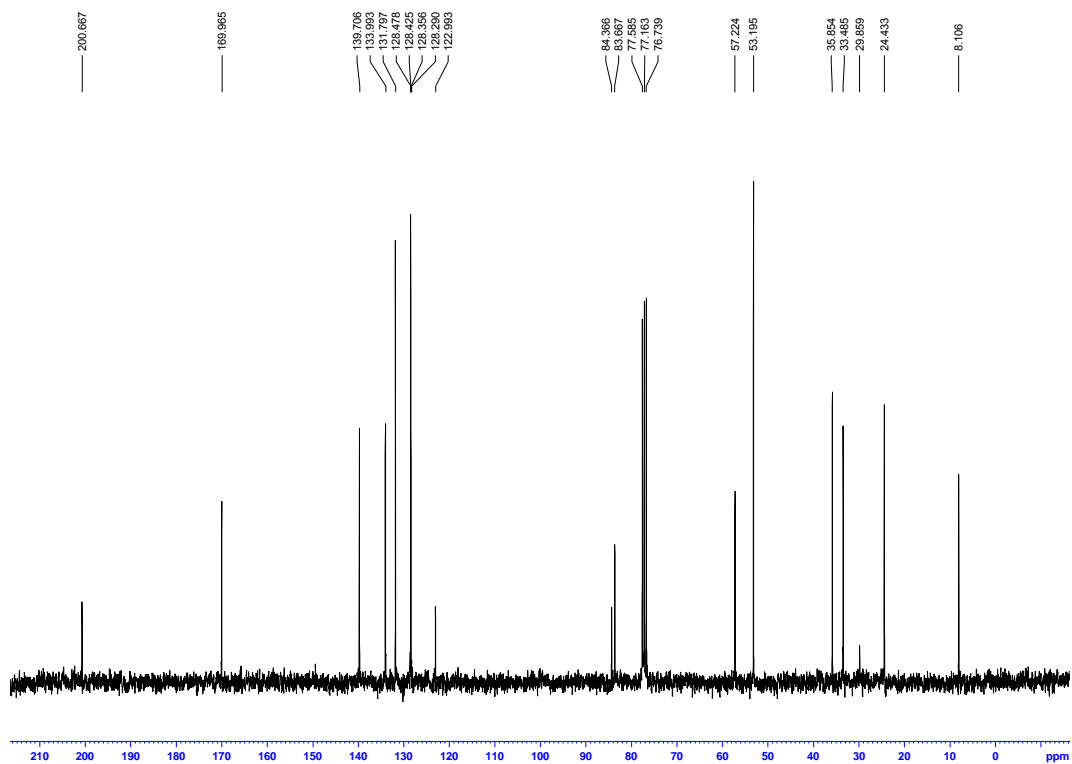
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (*cis*-**3i** + *trans*-**3i**):



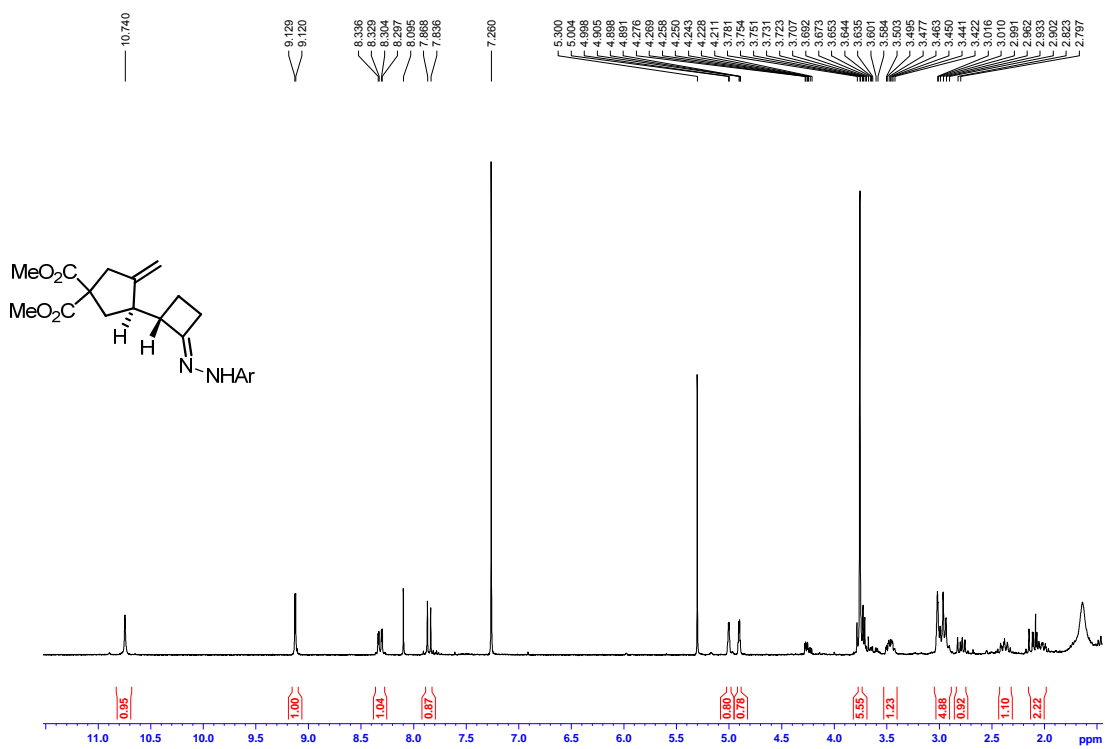
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (S15):



**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (S15):**

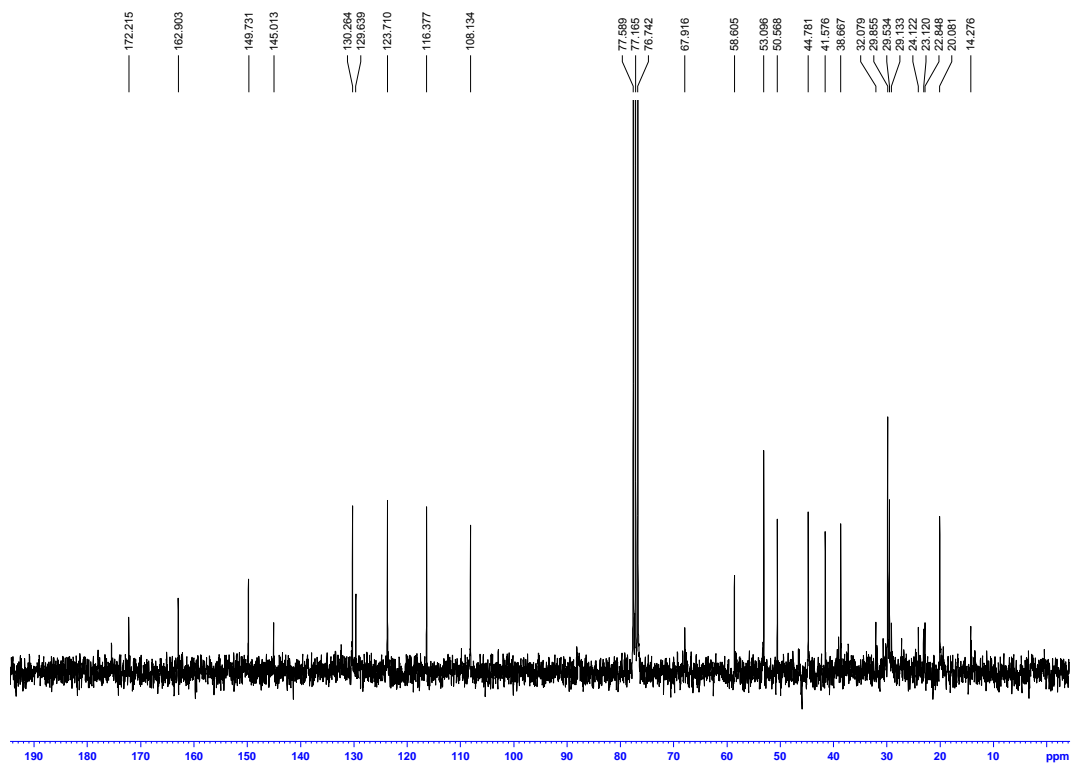


**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (4-major diastereoisomer):**

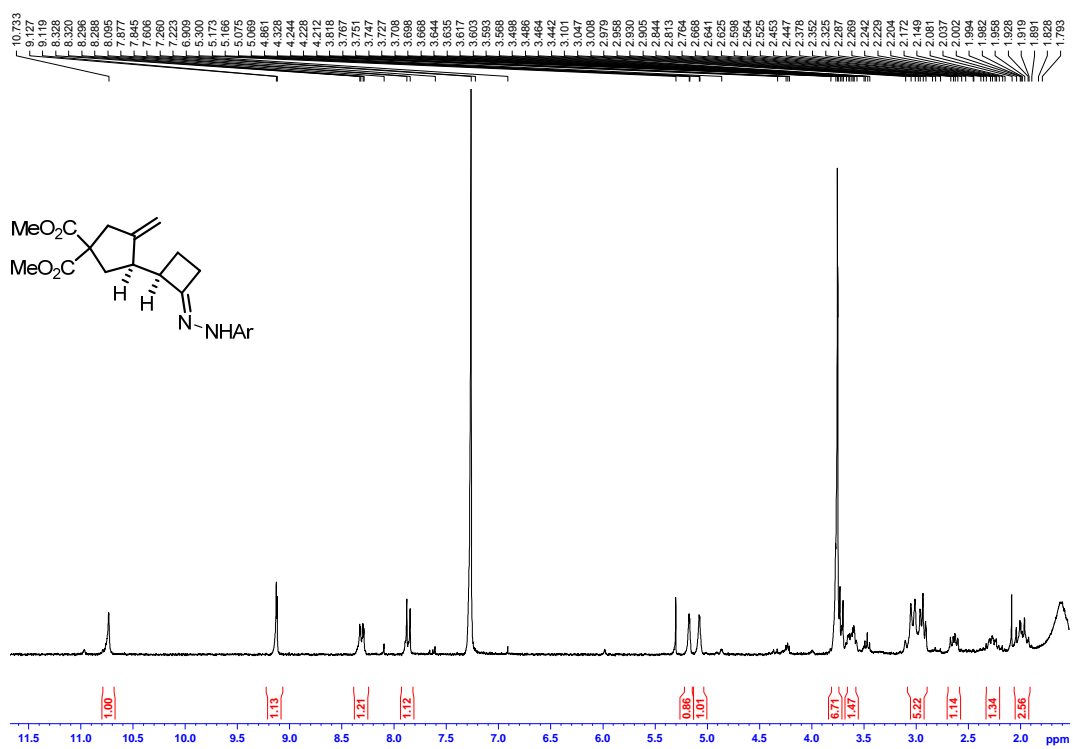




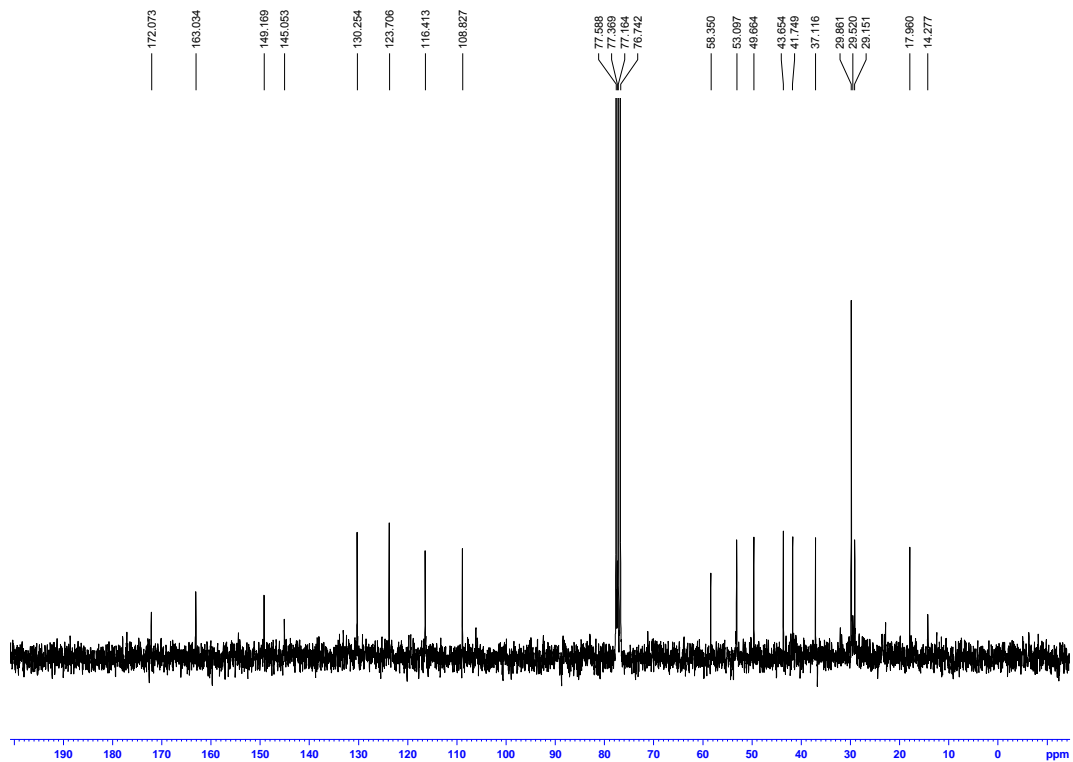
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) (4-major diastereoisomer):



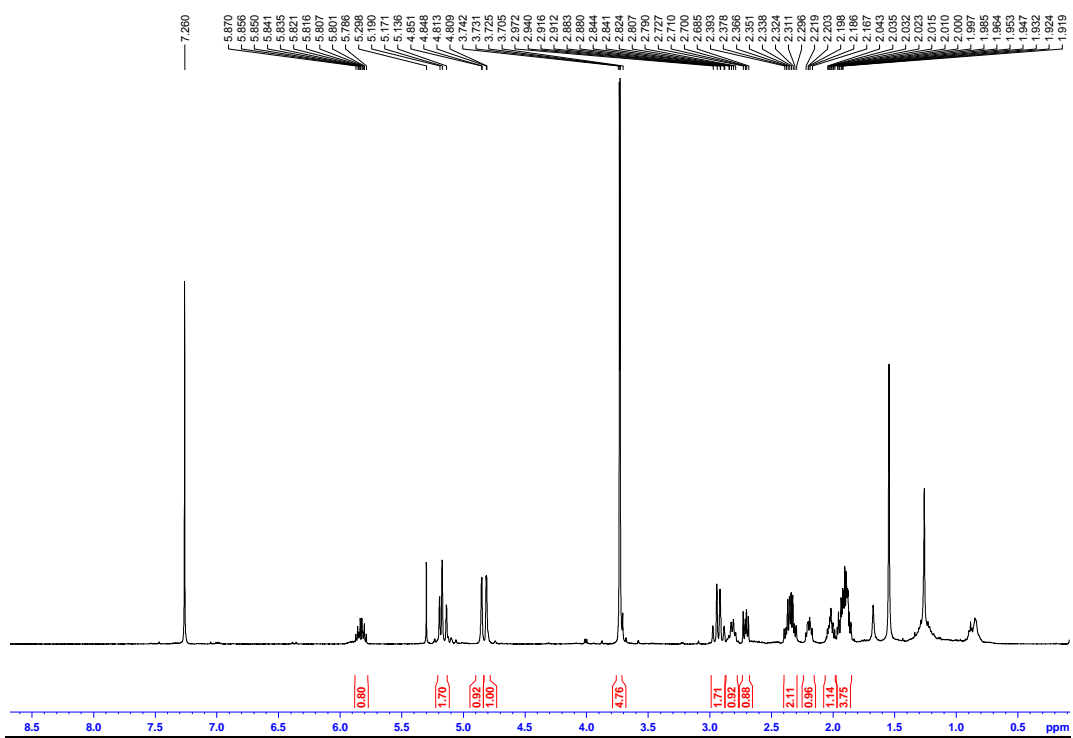
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) (4-minor diastereoisomer):



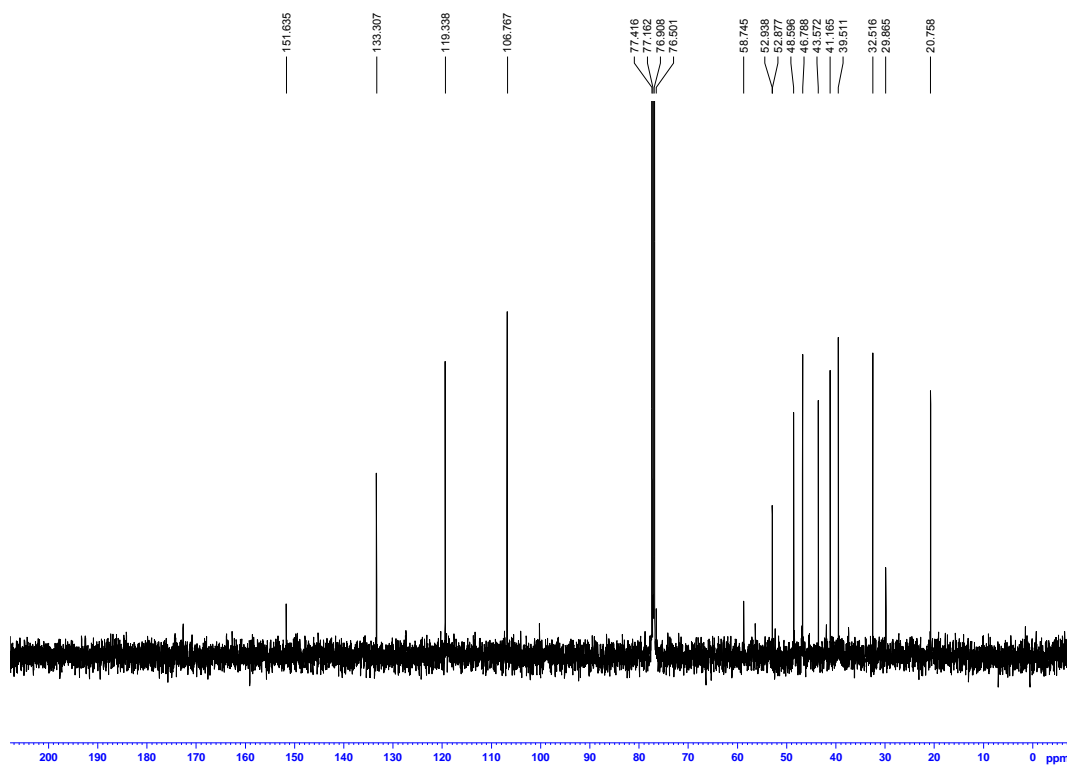
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (4-minor diastereoisomer):**



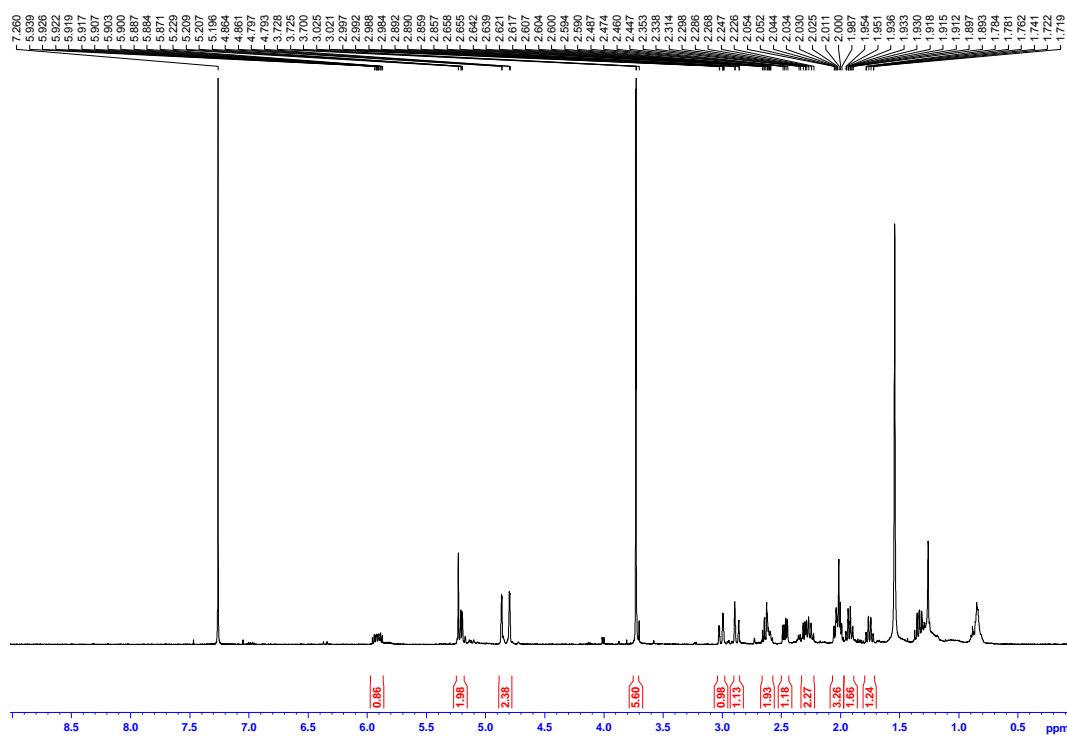
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (5a):**



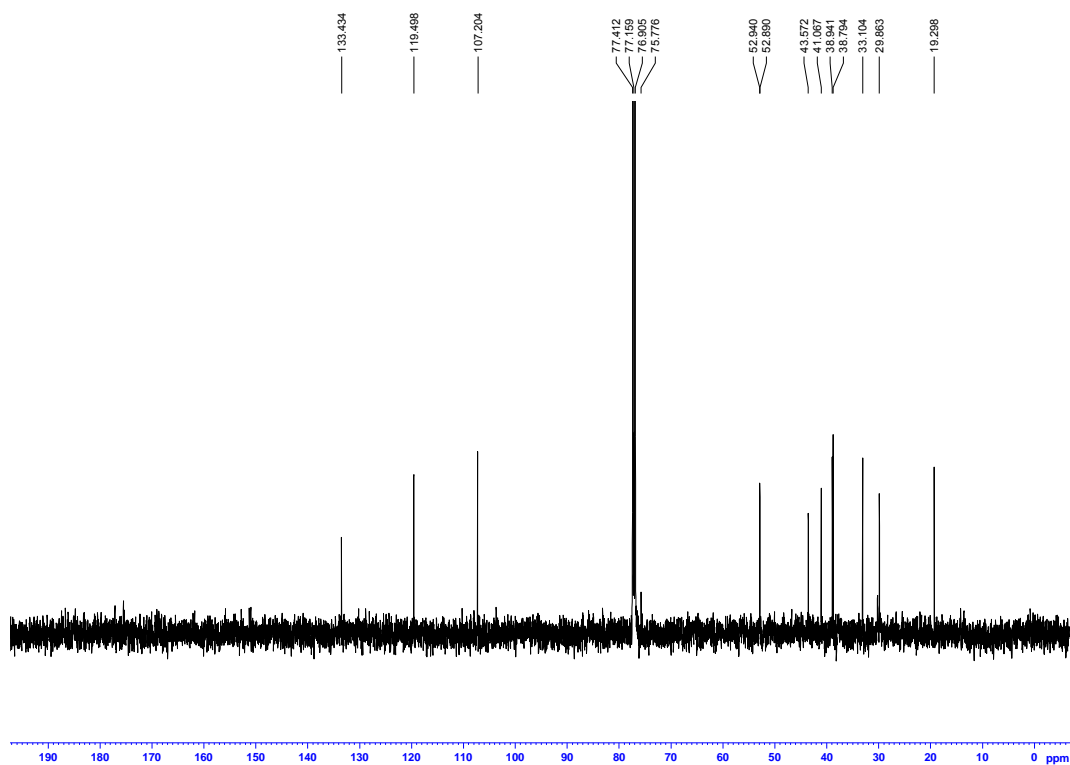
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (5a):



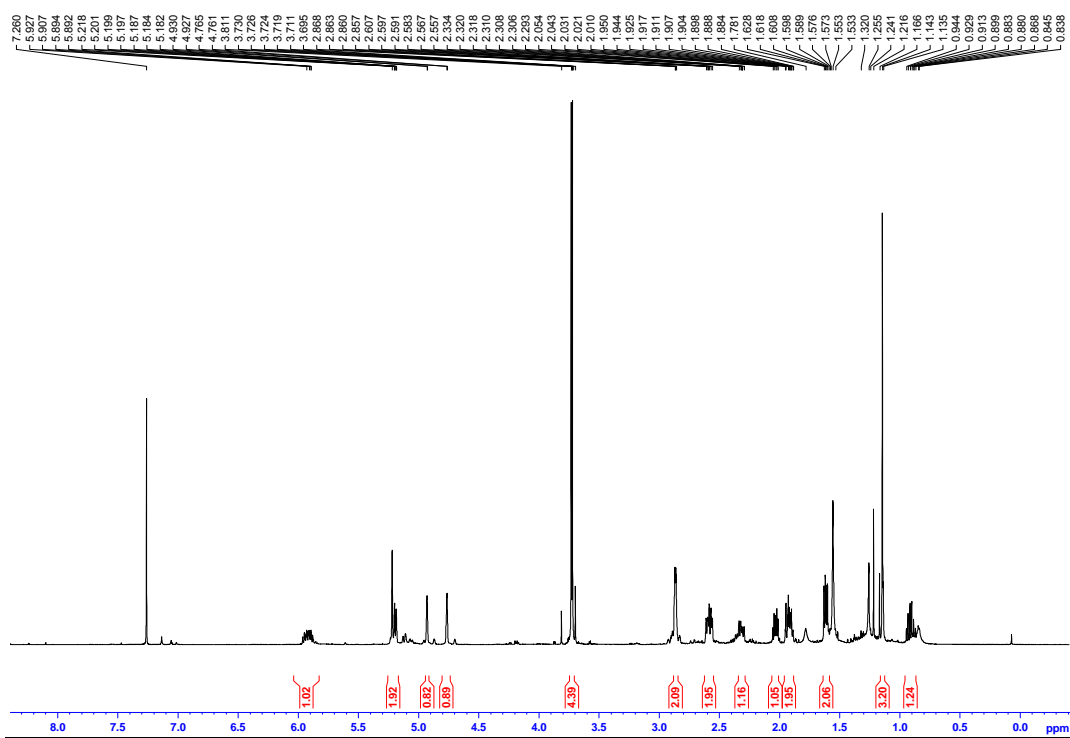
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) (5b):



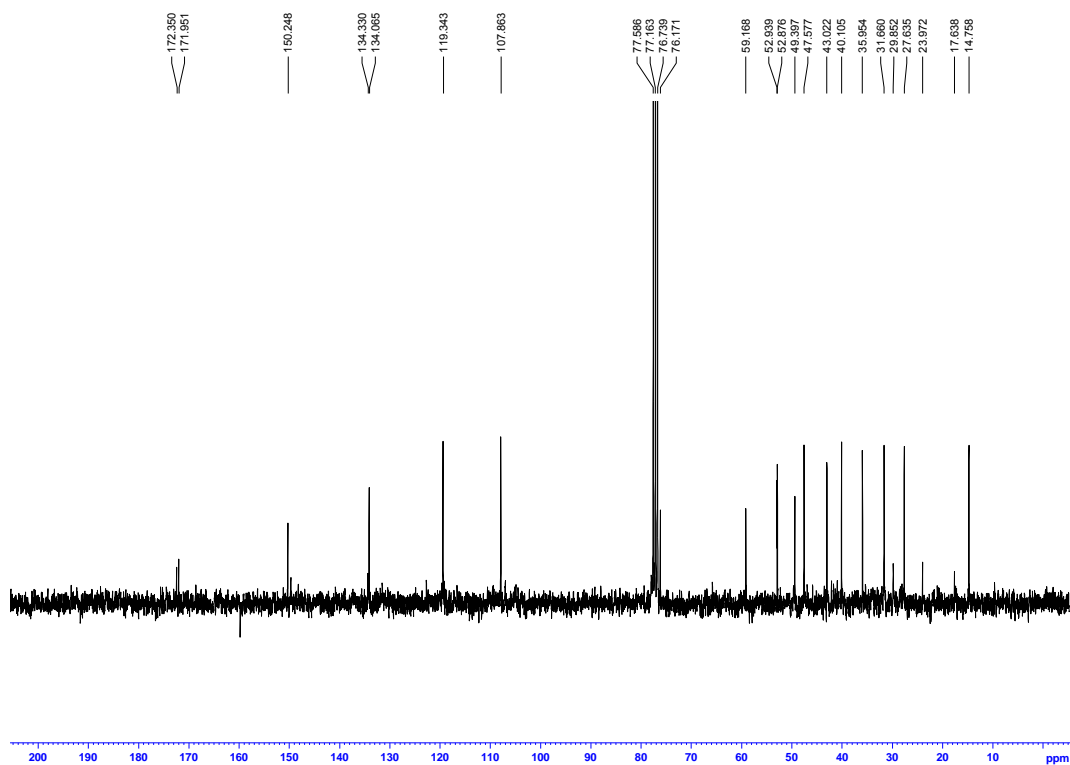
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (5b):



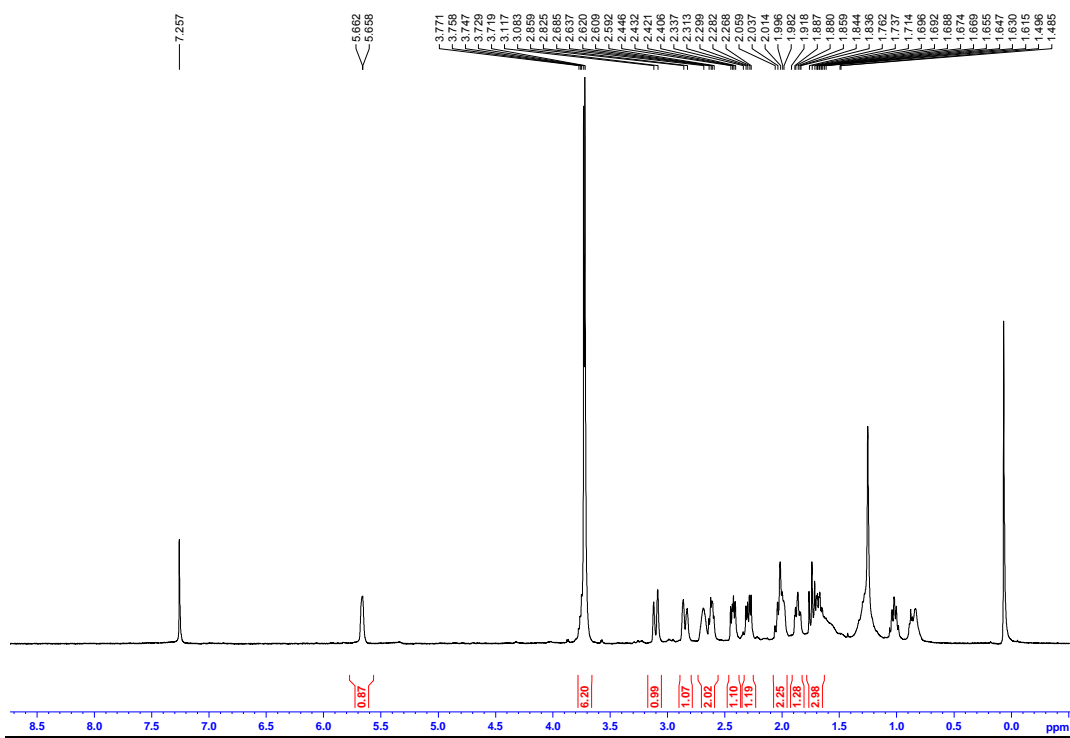
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (6b):



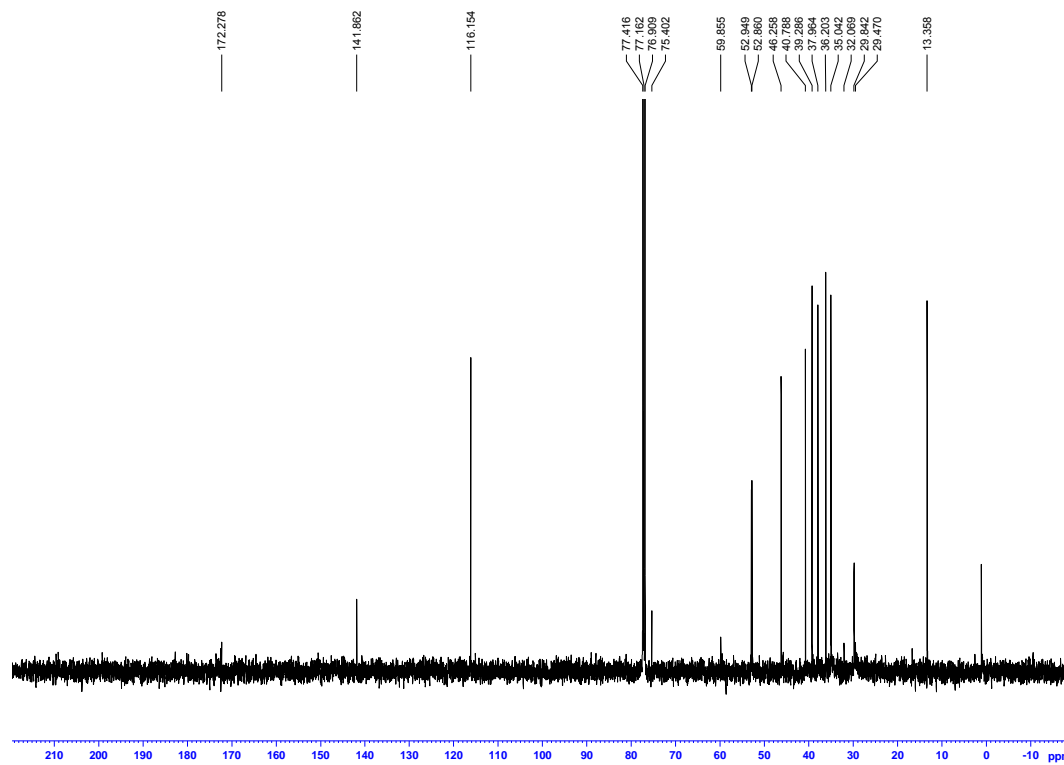
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (6b):**



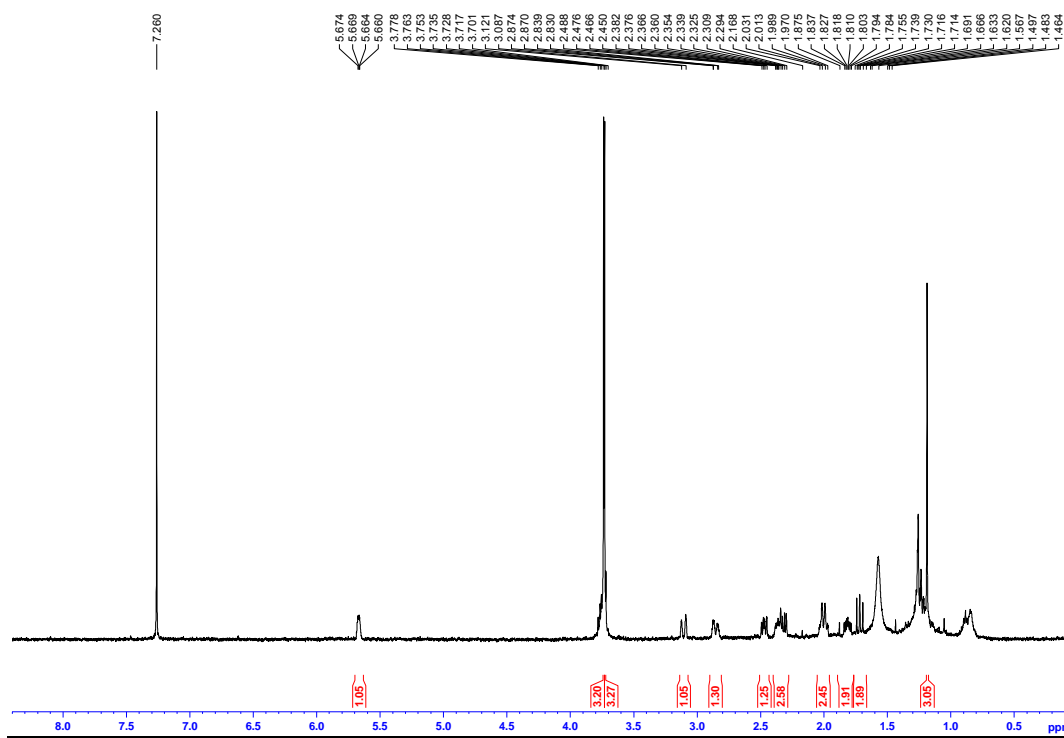
**$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) (7):**



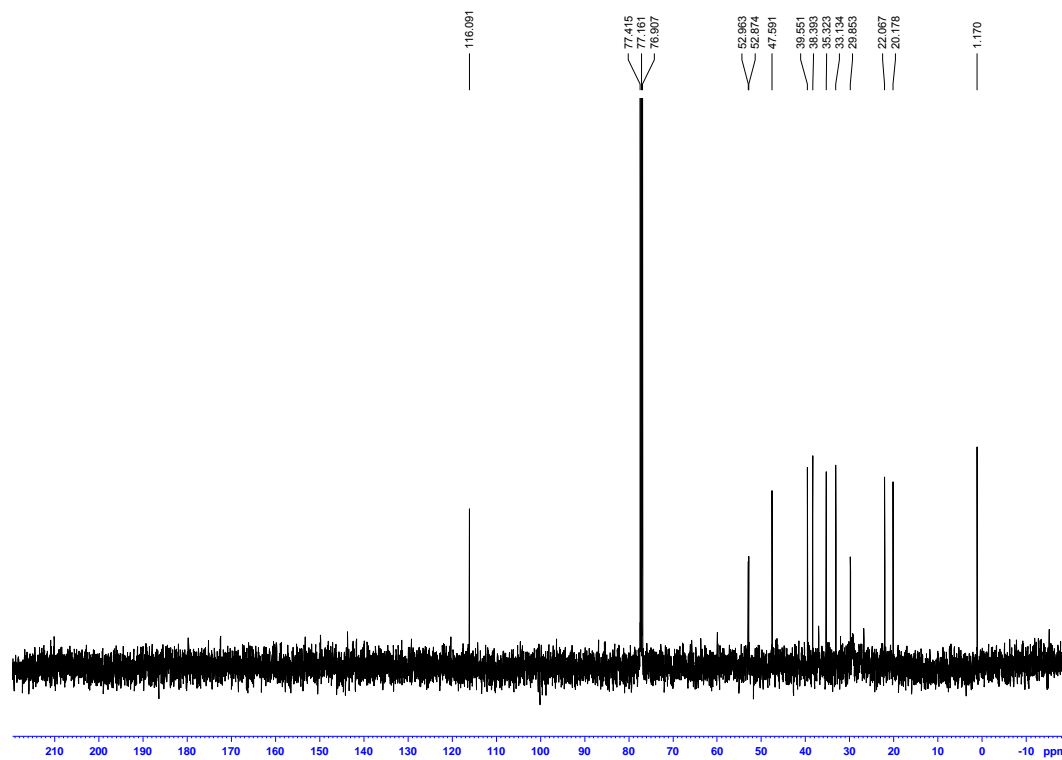
**$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) (7):**



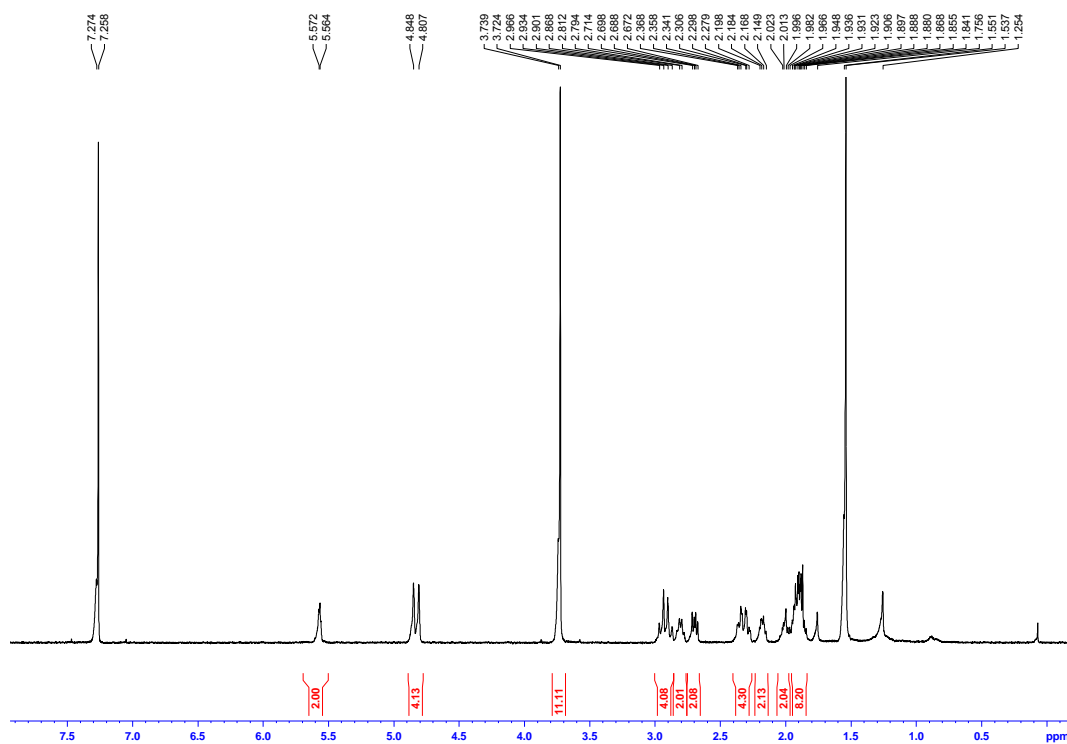
**$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) (8):**



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) (8):



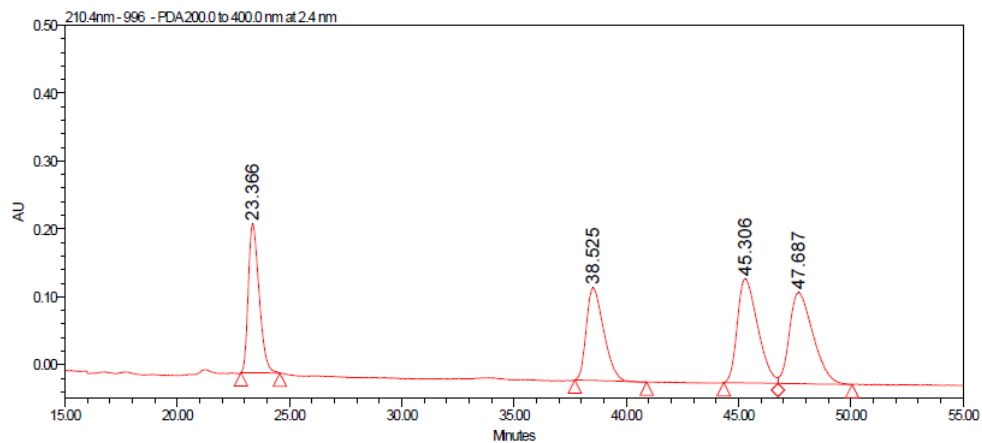
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) (S16):



## IV. HPLC Data.

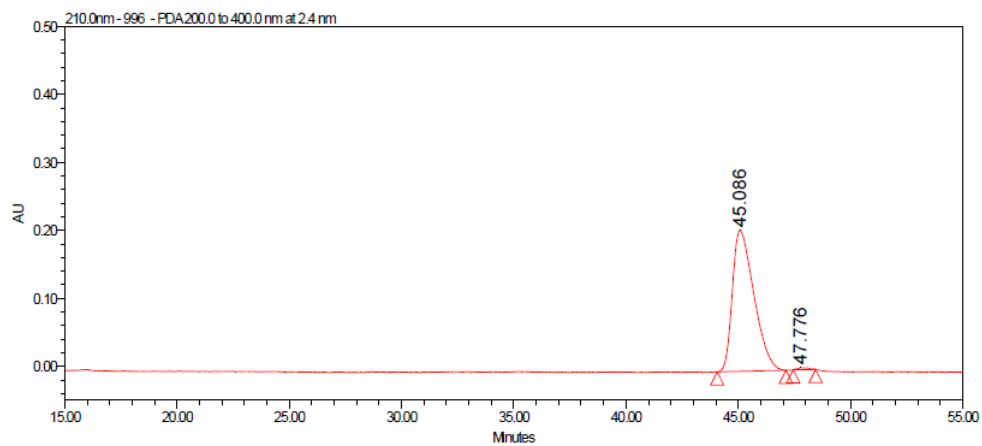
### IV. (*cis*-**3a** and *trans*-**3a**)

HPLC Analysis: major diastereoisomer: 99% ee, minor diastereoisomer: 95% ee [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: minor diastereoisomer, 23.5 min (minor) and 38.5 min (major)]; major diastereoisomer, 45.1 min (major) and 47.8 min (minor)].



Peak Results

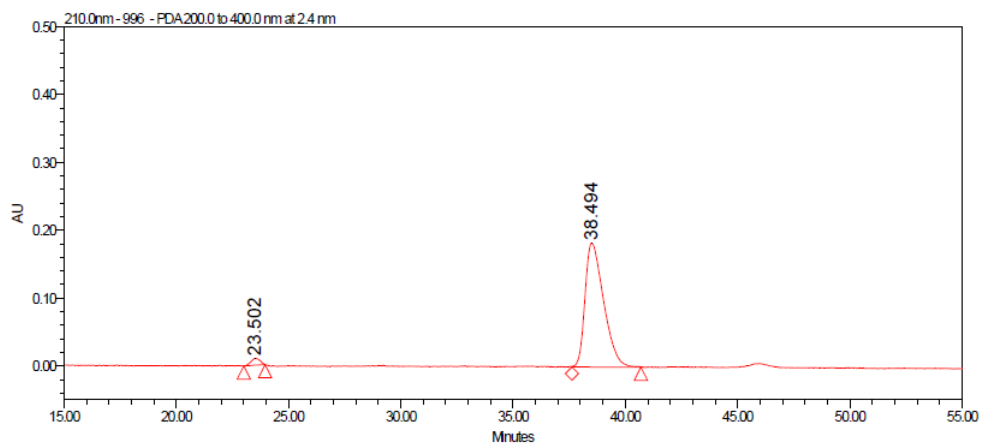
	RT	Height	Area	%Area
1	23.366	219291	7335806	21.45
2	38.525	136314	7347438	21.48
3	45.306	153550	9678718	28.30
4	47.687	134638	9844450	28.78



Peak Results

	RT	Height	Area	%Area
1	45.086	208271	13794887	99.30
2	47.776	2947	97738	0.70



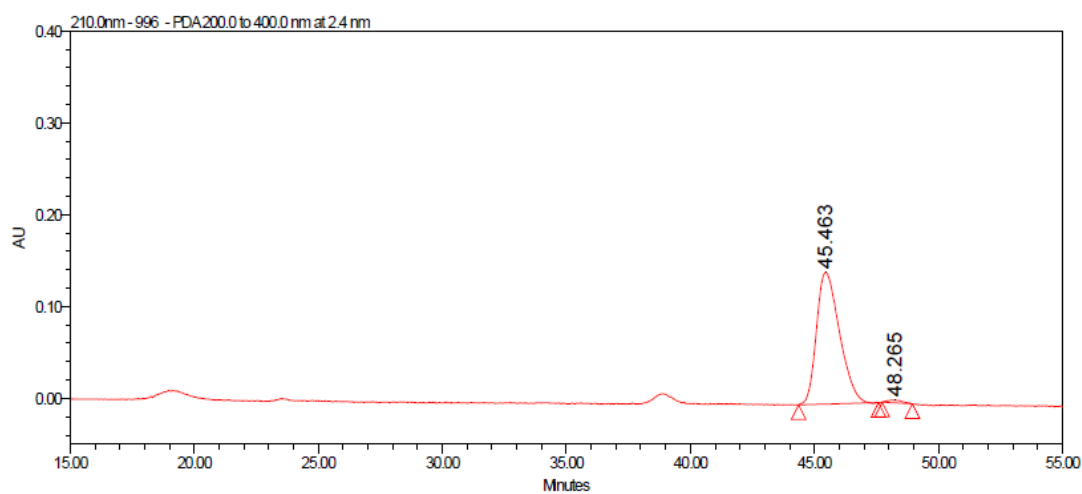


**Peak Results**

	RT	Height	Area	%Area
1	23.502	9960	276246	2.57
2	38.494	182658	10489496	97.43

### Synthesis of product 3a from OTBS Substrate 1j.

HPLC Analysis: 97% ee, [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: 45.4 min (major) and 48.2 min (minor)]

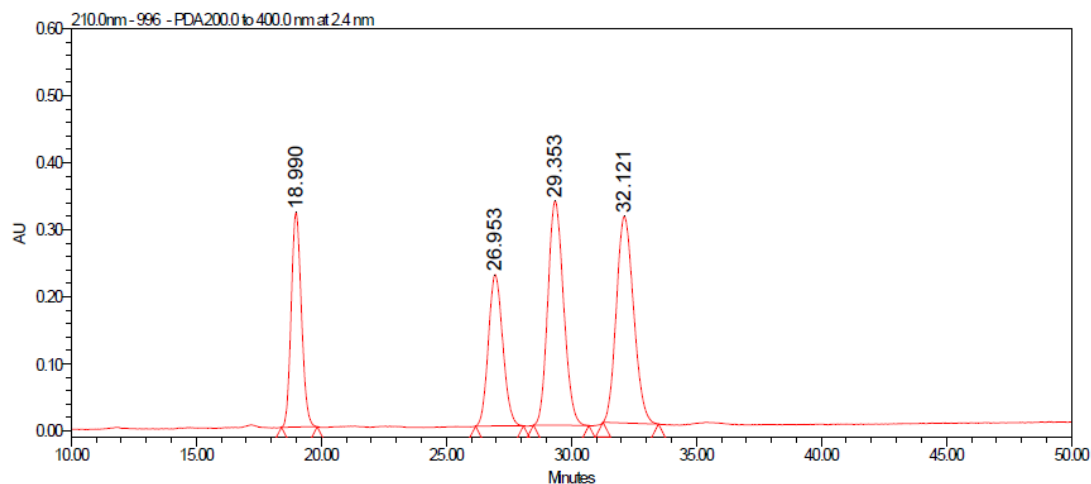


**Peak Results**

	RT	Height	Area	%Area
1	45.463	143960	9255744	98.64
2	48.265	3317	127944	1.36

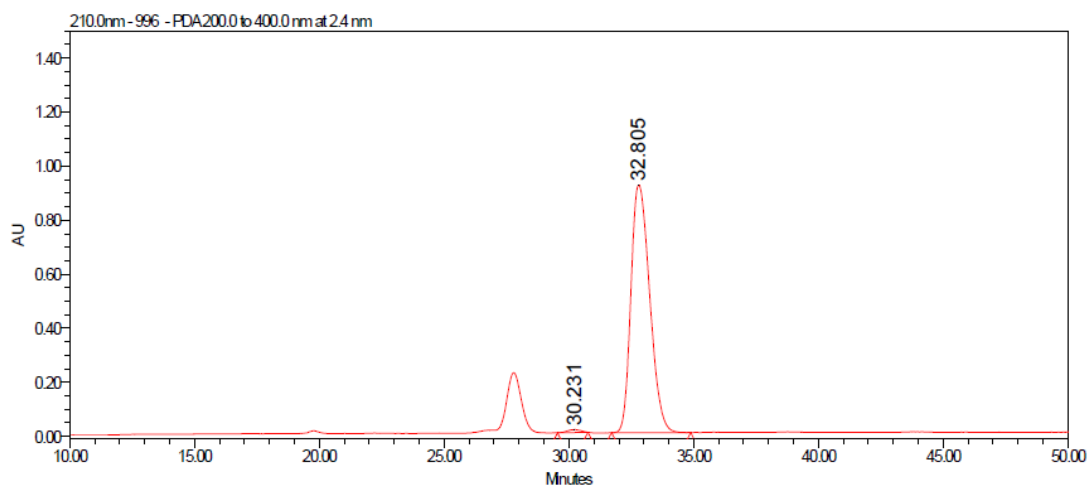
**(cis-3b and trans-3b)**

HPLC Analysis: major diastereoisomer: 98% ee, minor diastereoisomer: 95% ee [CHIRALPAK® IC, 25 °C, 4% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: minor diastereoisomer, 19.7 min (minor) and 27.7 min (major)]; major diastereoisomer, 30.2 min (minor) and 32.8 min (major)].



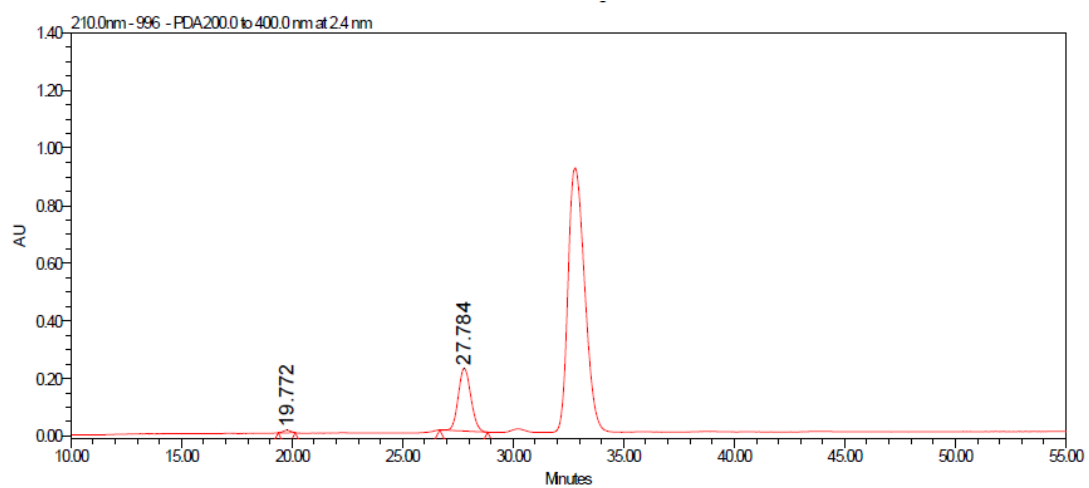
**Peak Results**

	RT	Height	Area	%Area
1	18.990	320061	9041997	18.99
2	26.953	225664	9056874	19.02
3	29.353	334656	14689801	30.85
4	32.121	308667	14826438	31.14



**Peak Results**

	RT	Height	Area	%Area
1	30.231	11104	404220	0.84
2	32.805	917660	47967605	99.16

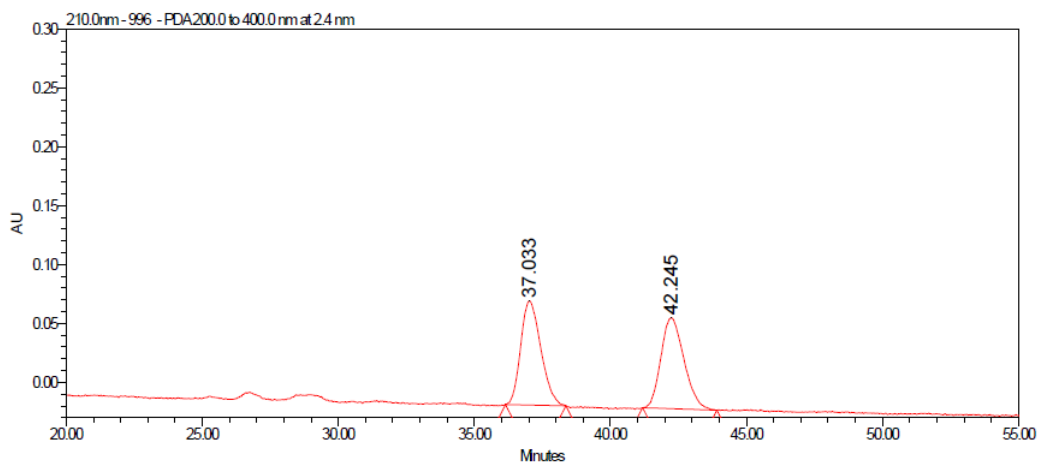


Peak Results

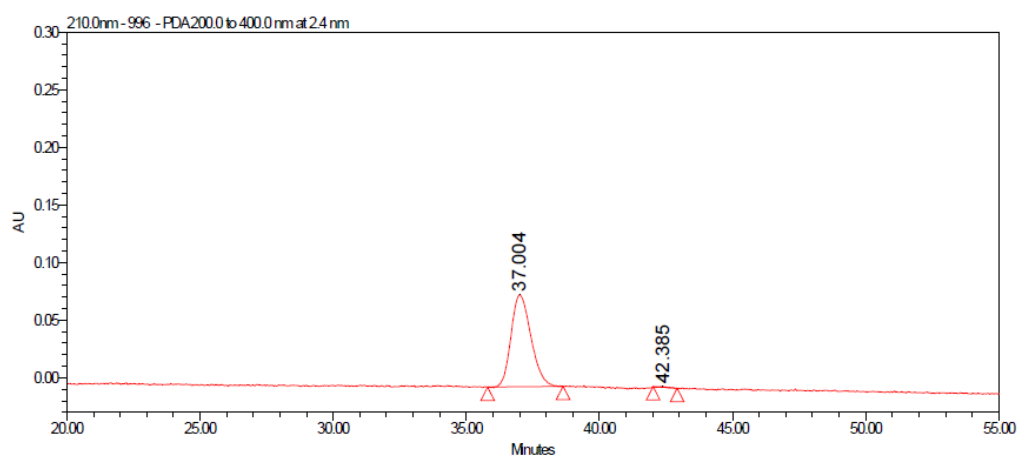
	RT	Height	Area	%Area
1	19.772	9030	211823	2.40
2	27.784	218293	6619215	97.60

**(cis-3c)**

HPLC Analysis: 99% ee, [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: 37.0 min (major) and 42.4 min (minor)]



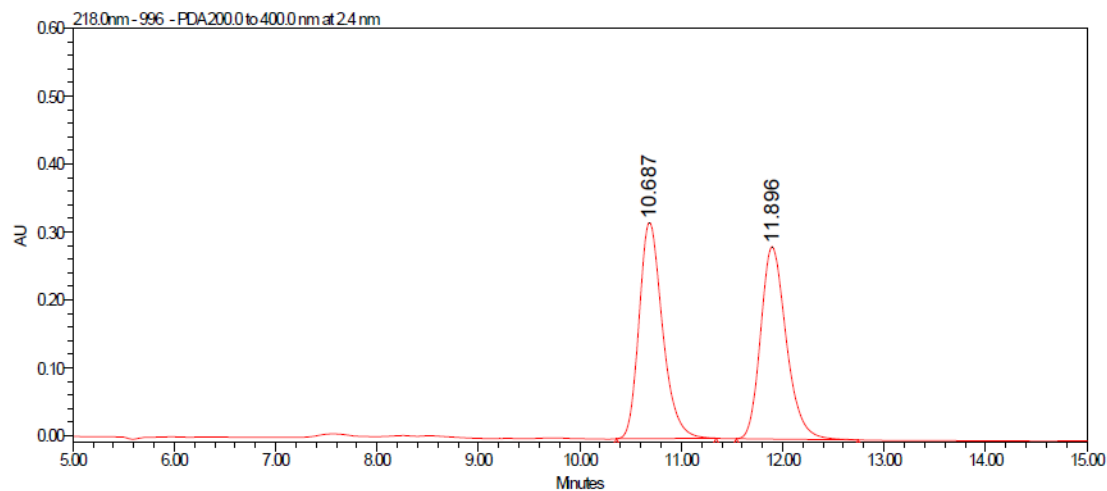
Peak Results				
	RT	Height	Area	%Area
1	37.033	88257	4538958	49.95
2	42.245	77144	4547351	50.05



Peak Results				
	RT	Height	Area	%Area
1	37.004	80086	4139945	99.57
2	42.385	695	17960	0.43

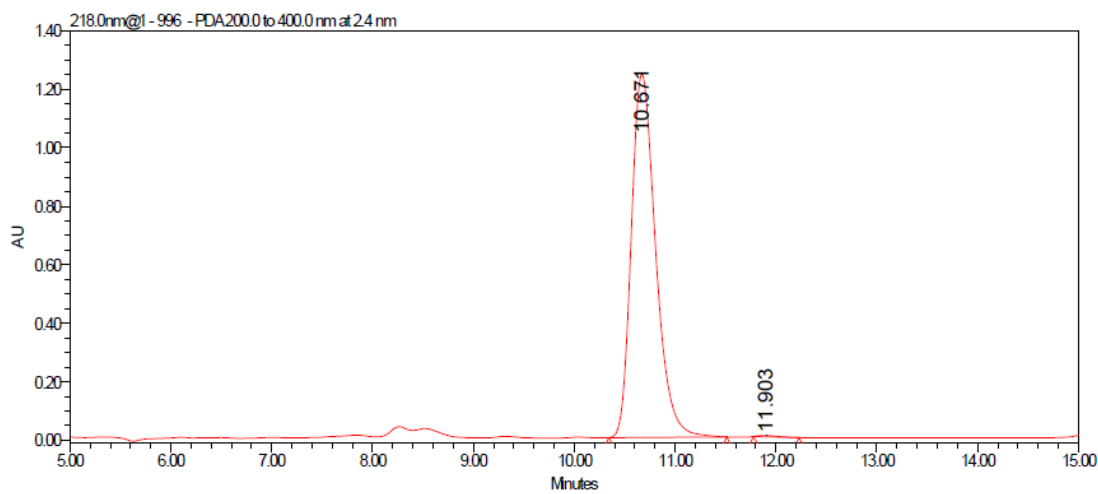
**(cis-3d)**

HPLC Analysis: 99% ee, [CHIRALPAK® IC, 25 °C, 30% *i*PrOH/*n*-heptane, 0.8 mL/min, 218 nm, retention times: 10.7 min (major) and 11.9 min (minor)]



**Peak Results**

	RT	Height	Area	%Area
1	10.687	319170	5102966	50.58
2	11.896	283357	4966922	49.42

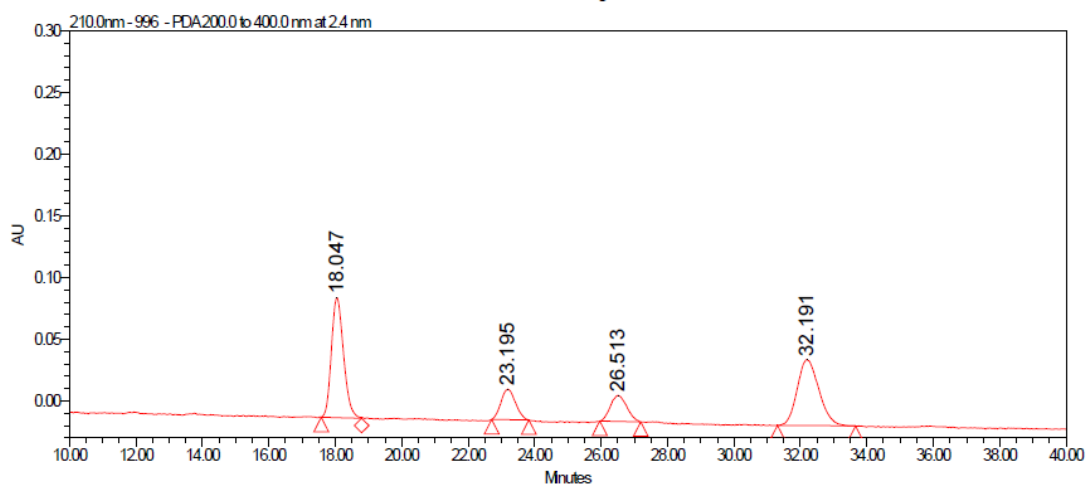


**Peak Results**

	RT	Height	Area	%Area
1	10.671	1242361	20773634	99.76
2	11.903	4407	50744	0.24

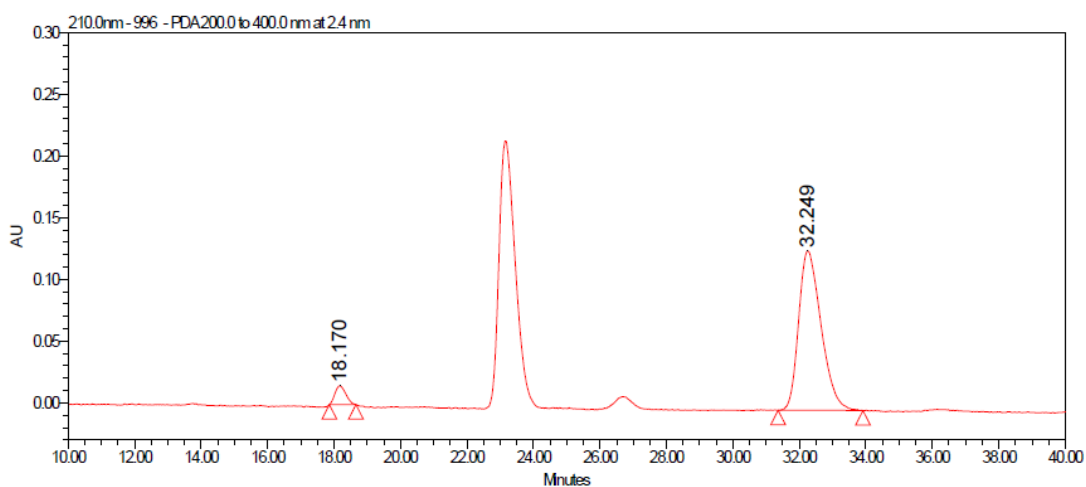
(*cis-3e* and *trans-3e*)

HPLC Analysis: major diastereoisomer: 89% ee, minor diastereoisomer: 92% ee [CHIRALPAK® IC, 25 °C, 6% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: major diastereoisomer, 18.2 min (minor) and 32.2 min (major); minor diastereoisomers, 23.2 min (major) and 26.7 min (minor)].



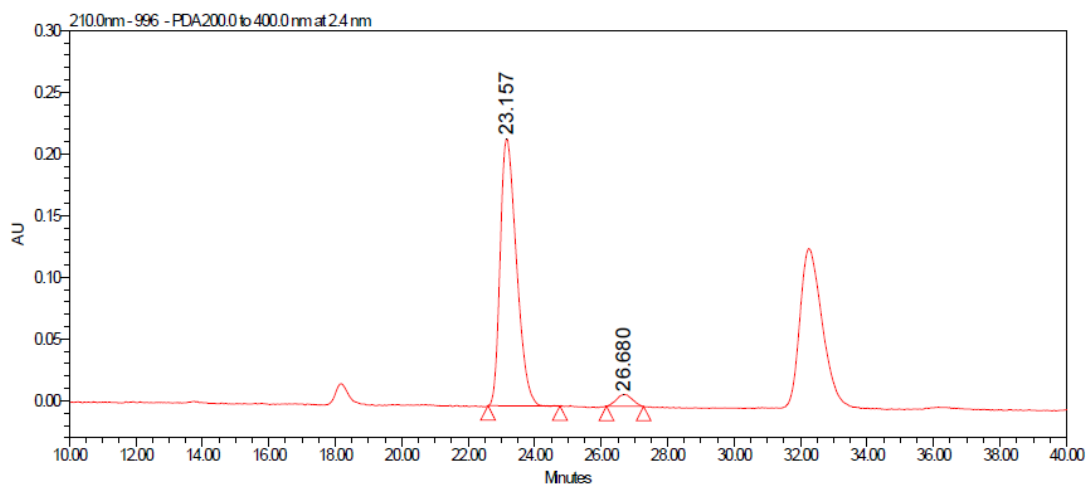
Peak Results

	RT	Height	Area	%Area
1	18.047	97610	2465326	38.79
2	23.195	24689	746759	11.75
3	26.513	21064	719734	11.33
4	32.191	53458	2423229	38.13



Peak Results

	RT	Height	Area	%Area
1	18.170	15278	343955	5.38
2	32.249	129246	6053493	94.62

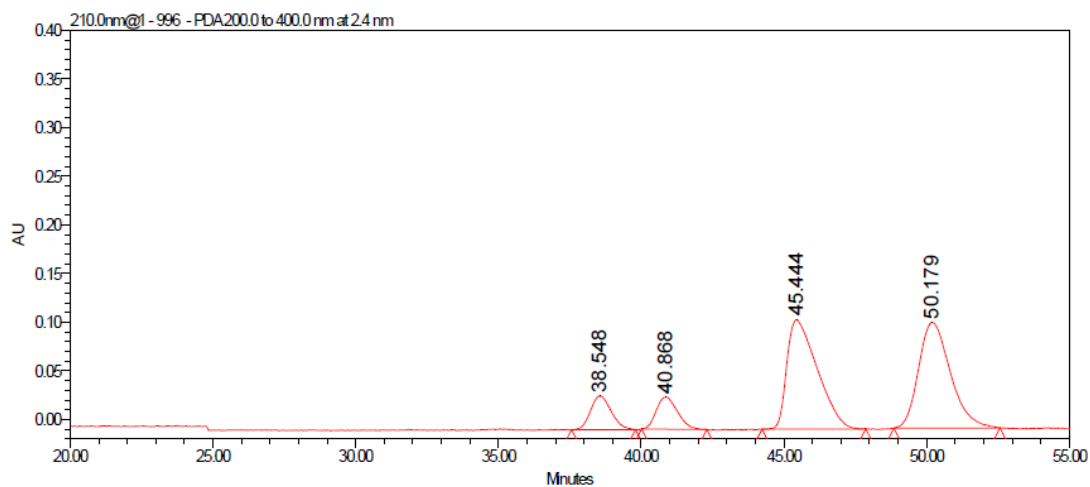


**Peak Results**

	RT	Height	Area	%Area
1	23.157	216512	7363302	95.93
2	26.680	9518	312586	4.07

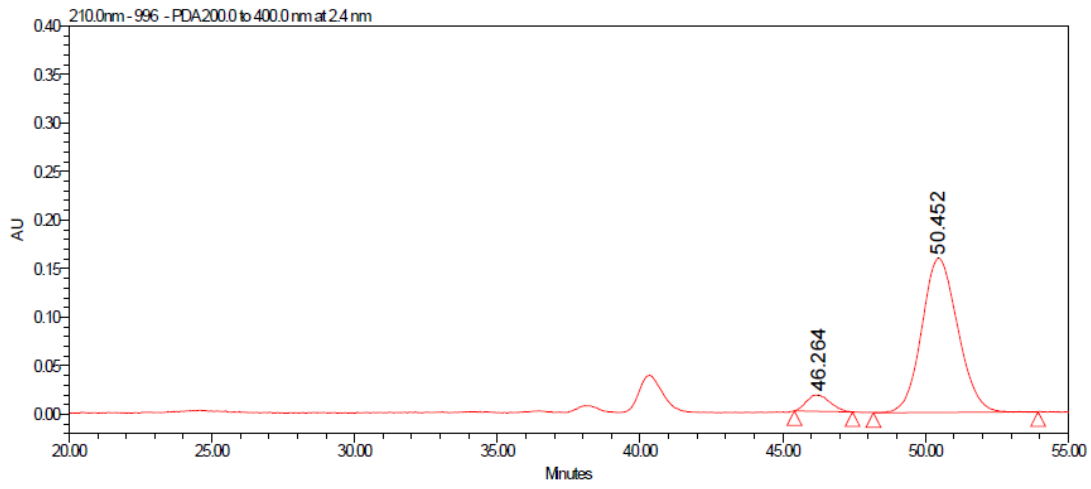
(*cis*-**3f** and *trans*-**3f**).

HPLC Analysis: major diastereoisomer: 87% ee, minor diastereoisomer: 75% ee [CHIRALPAK® IC, 25 °C, 2% *i*PrOH/*n*-heptane, 1 mL/min, 210 nm, retention times: minor diastereoisomer, 38.0 min (minor) and 40.3 min (major)]; major diastereoisomer, 46.2 min (minor) and 50.4 min (major)].



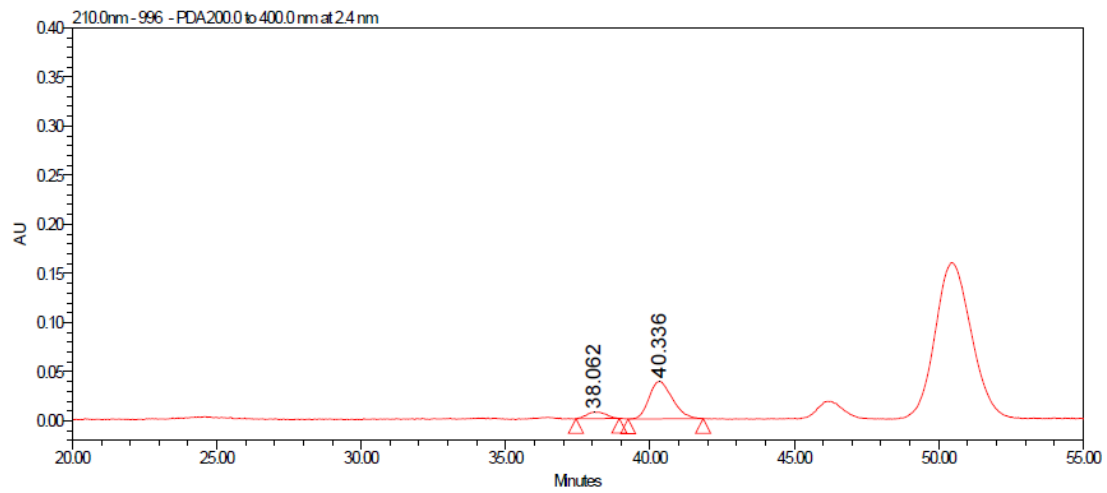
**Peak Results**

	RT	Height	Area	%Area
1	38.548	34528	1731278	8.59
2	40.868	33114	1698572	8.43
3	45.444	112738	8298368	41.18
4	50.179	108738	8421591	41.79



**Peak Results**

	RT	Height	Area	%Area
1	46.264	16823	964561	6.48
2	50.452	158949	13916564	93.52



**Peak Results**

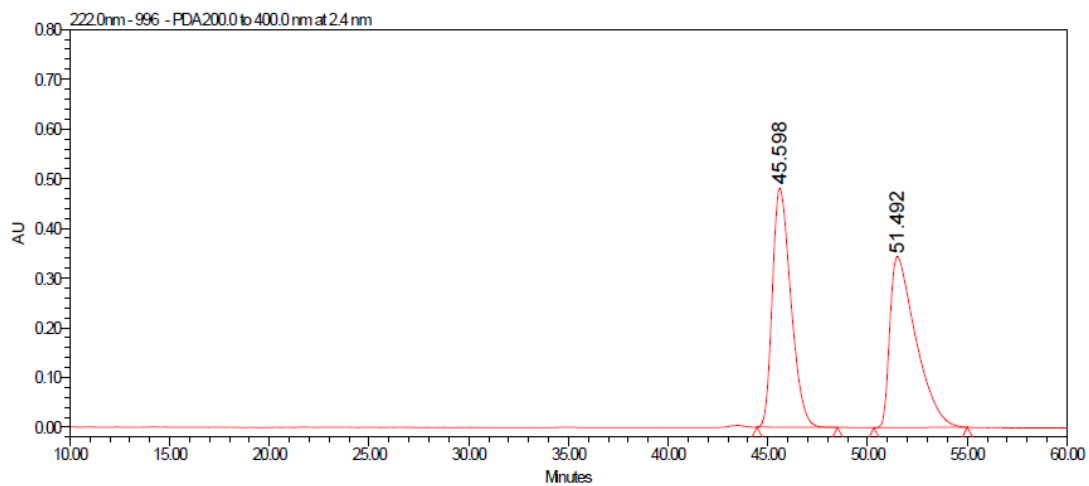
	RT	Height	Area	%Area
1	38.062	6811	307365	12.62
2	40.336	38121	2127681	87.38



(*cis*-**3g** and *trans*-**3g**).

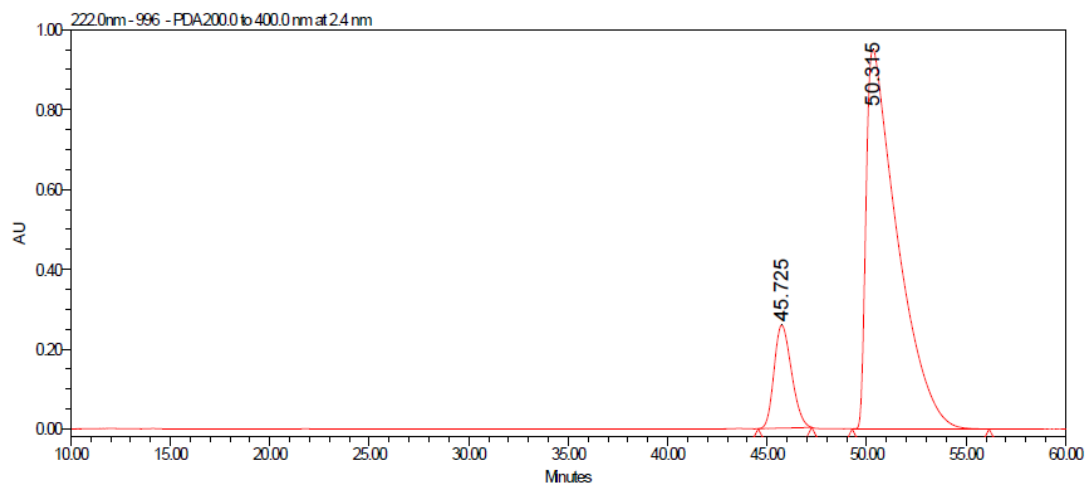
(*cis*-**3g**) major diastereoisomer:

74% ee, [CHIRALPAK® ID, 35 °C, 35% *i*PrOH/*n*-heptane, 0.7 mL/min, 222 nm, retention times: 45.7 min (minor) and 50.3 min (major)].



Peak Results

	RT	Height	Area	%Area
1	45.598	480583	30907195	49.83
2	51.492	343905	31115378	50.17

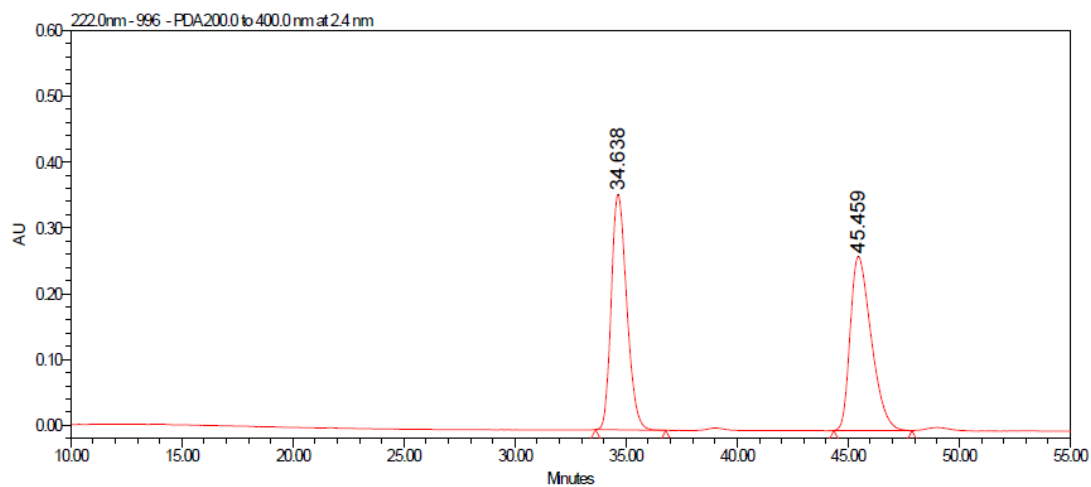


Peak Results

	RT	Height	Area	%Area
1	45.725	258341	15693048	13.13
2	50.315	950815	103845357	86.87

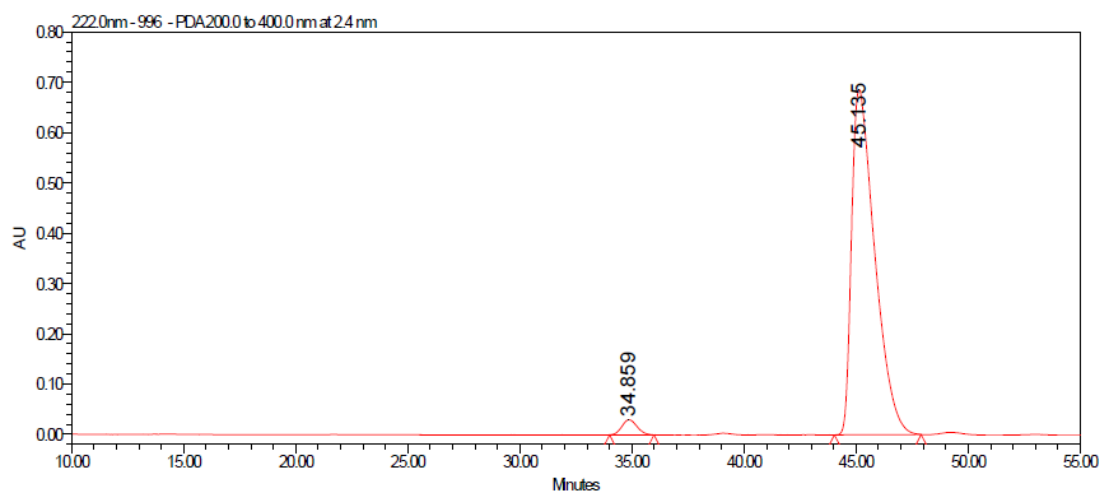
(*trans*-**3g**) minor diastereoisomer:

95% ee [CHIRALPAK® ID, 35 °C, 35% *i*PrOH/*n*-heptane, 0.7 mL/min, 222 nm, retention times: 34.9 min (minor) and 45.1 min (major)].



Peak Results

	RT	Height	Area	%Area
1	34.638	357754	17339900	49.93
2	45.459	264220	17388851	50.07

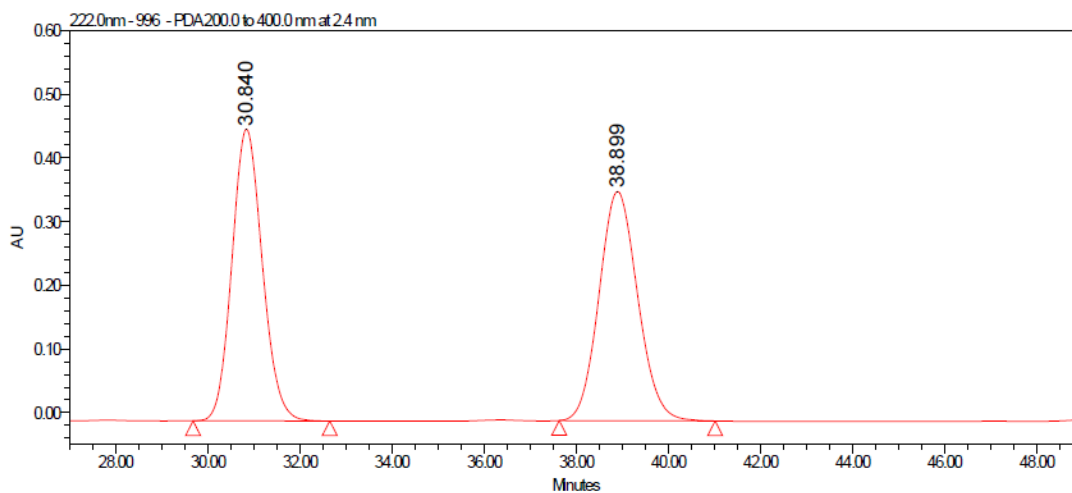


Peak Results

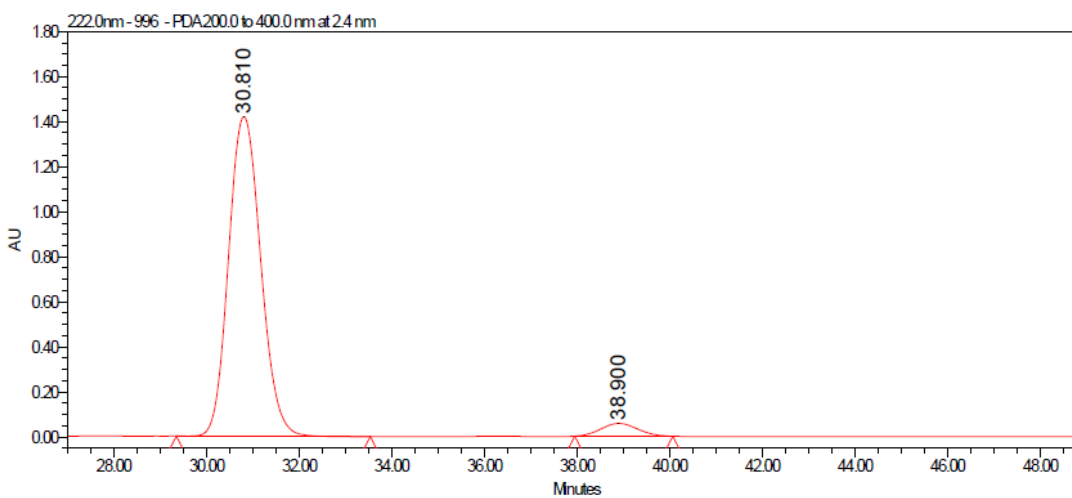
	RT	Height	Area	%Area
1	34.859	30201	1415444	2.79
2	45.135	686325	49302735	97.21

(*cis*-**3h**) :

HPLC Analysis: 91% ee, [CHIRALPAK® IC, 35 °C, 40% EtOH/*n*-heptane, 0.7 mL/min, 222 nm, retention times: 30.8 min (major) and 38.9 min (minor)].



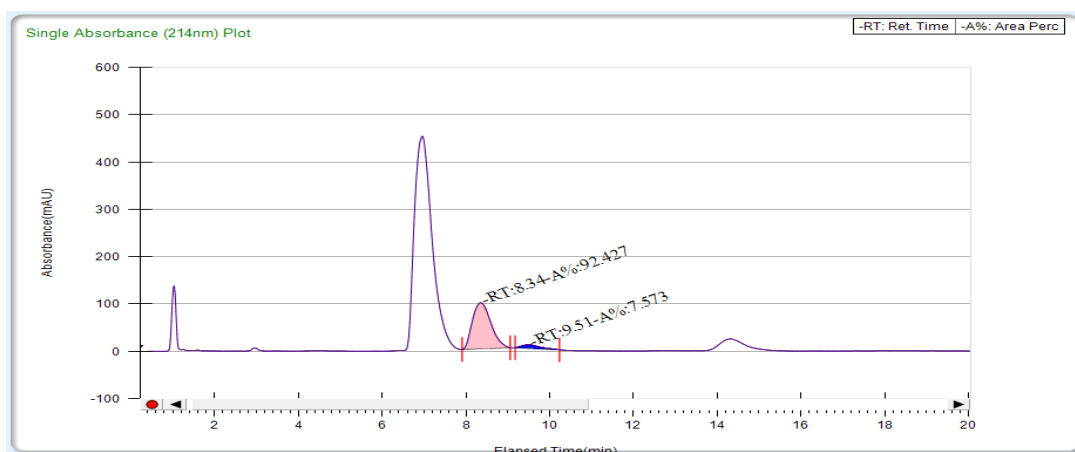
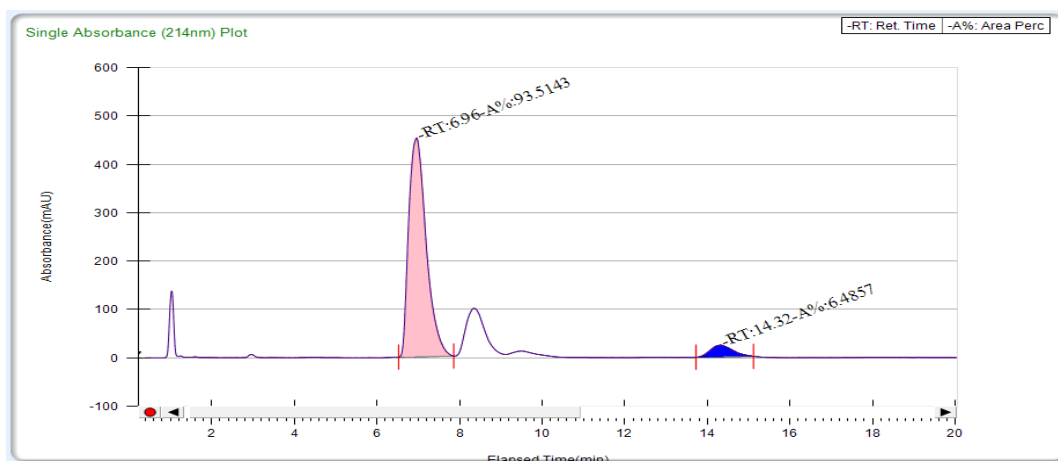
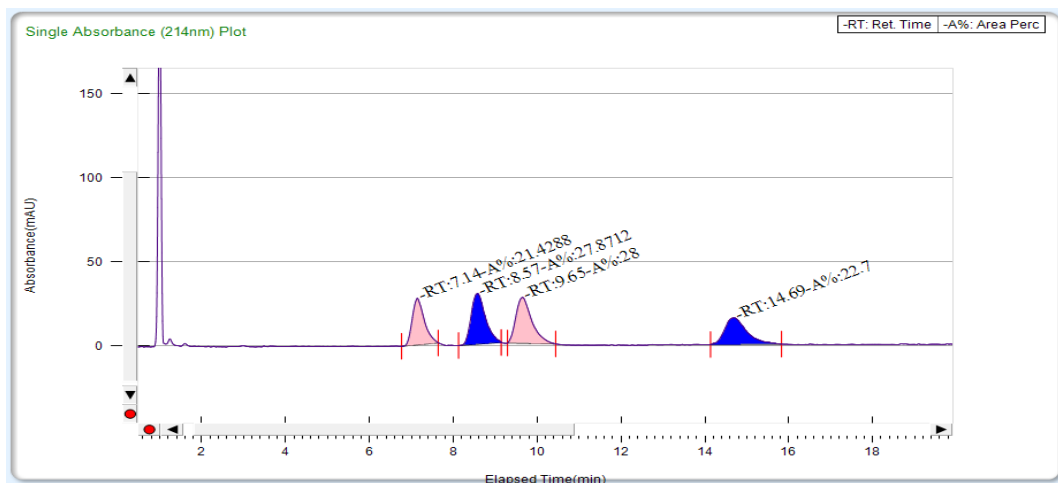
Peak Results				
	RT	Height	%Area	
1	30.840	457883	20981806	50.00
2	38.899	359686	20979251	50.00



Peak Results				
	RT	Height	%Area	
1	30.810	1419065	68499773	95.63
2	38.900	56877	3127967	4.37

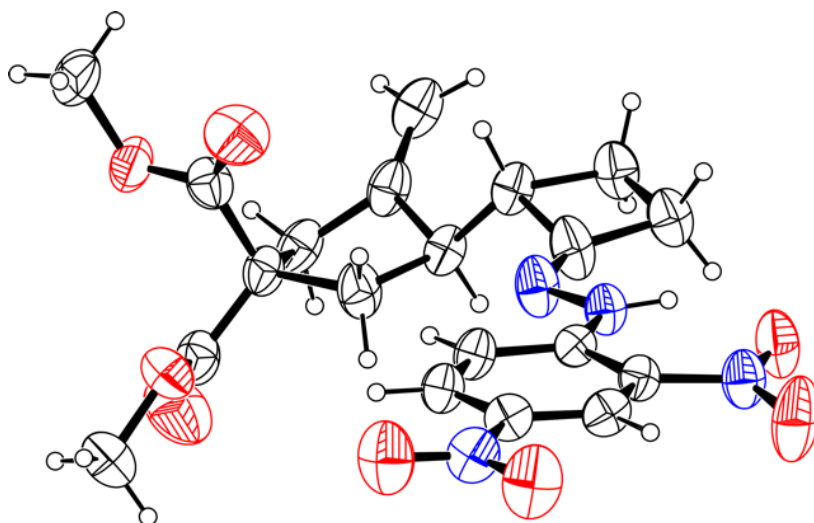
(*cis-3i* and *trans-3i*).

SFC Analysis: major diastereoisomers: 87% ee, minor diastereoisomers: 85% ee [CHIRAL SFC AD-H, 30 °C, 5% MeOH/CO<sub>2</sub>, 4 mL/min, pressure: 150 bar, 214 nm, retention times: minor diastereoisomers, 8.3 min (major) and 9.5 min (minor)]; major diastereoisomers, 7.0 min (major) and 14.3 min (minor)].



## V. X-Ray crystal structure determination of compound 4

The Ortep drawing of 4. (one conformer without disorder is shown for clarity).



**Table S1.** Crystal data and structure refinement for compound 4.

CCDC deposit number	<b>1520299</b>	
Empirical formula	$C_{20}H_{22}N_4O_8$	
Formula weight	446.41	
Temperature / K	293	
Wavelength / Å	1.54187	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	$a / \text{Å}, \alpha / ^\circ$	10.5093 (3) 105.992 (7)
	$b / \text{Å}, \beta / ^\circ$	13.2957 (4) 97.837 (7)
	$c / \text{Å}, \gamma / ^\circ$	17.9828 (12) 111.220 (8)
Volume / Å <sup>3</sup>	2172.2 (2)	
Z	4	
Density (calculated) / Mg/m <sup>3</sup>	1.365	
Absorption coefficient / mm <sup>-1</sup>	0.909	
F(000)	936	
Crystal size / mm <sup>3</sup>	0.58 x 0.20 x 0.16	
$\theta$ range for data collection / °	6.699 to 68.205	
	SI61	

Index ranges	-8 ≤ h ≤ 12, -16 ≤ k ≤ 15, -21 ≤ l ≤ 21
Reflections collected	24719
Independent reflections	7638 [R(int) = 0.0458]
Completeness to θ = 67.687°	96.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.768
Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	7638 / 26 / 642
Goodness-of-fit on $F^2$	1.065
Final R indices [ $I > 2\sigma(I)$ ]	R <sub>1</sub> = 0.0676, wR <sub>2</sub> = 0.1812
R indices (all data)	R <sub>1</sub> = 0.0946, wR <sub>2</sub> = 0.2033
Largest diff. peak / hole / e.Å <sup>-3</sup>	0.252 / -0.238

$$R_1 = \sum ||F_o| - |F_c|| / \sum |F_o| ; wR_2 = [\sum w (F_o^2 - F_c^2)^2 / \sum w (F_o^2)^2]^{1/2}$$

## VI. DFT Computations.

All structures were optimized using the Gaussian 09 software package<sup>11</sup> at the B3LYP<sup>12</sup> level of density functional theory (DFT). The effective-core potential of Hay and Wadt with a double- $\xi$  valence basis set (LANL2DZ) was used to describe Au.<sup>13</sup> The other atoms were described by the 6-31G(d,p) basis set. Thermal corrections to the Gibbs free energy were obtained at the same level of theory. Single-point energy calculations were carried out at the M06<sup>14</sup> level with the quadruple- $\zeta$  valence def2-QZVP basis set on Au and the 6-311+G(2d,p) basis set on other elements. The values presented herein are Gibbs free energies (kcal/mol) obtained from the M06/def2-QZVP(Au)-6-311+G(2d,p)//B3LYP/LANL2DZ(Au)-6-31G(d,p) calculations ( $\Delta G_{298}$ , kcal/mol).

DFT computations were carried out to gain some insight into the factors governing the course and stereoselectivity of the title reaction. However, the ligands used in this study are too large to allow calculations at a high level of theory. To get extrapolation elements, we focused then on an achiral active catalyst, JohnPhosAu<sup>+</sup>, which has been used by Echavarren to generate type **2** tricyclic products (Scheme 1b), and by us to set up the reaction conditions favoring the formation of the cyclobutanones (Table 1, Entries 1 and 2). The model enyne used in the computations is displayed in Scheme S1, as well as the key steps studied computationally.

After coordination of the substrate to the cationic gold complex, we considered conformers **Int1** and **Int1'**, which differ by the relative orientation of the ethoxycyclopropyl group (see Figure S3 for the geometries). The latter is more stable by 0.5 kcal/mol and has been taken as the reference for energy calculations. Interconversion of these conformers requires an activation energy of 1.3 kcal/mol. The cyclization of **Int1** into the cyclopropylcarbene **Int2** requires 9.0 kcal/mol of free energy of activation (relatively to **Int1'**) and releases 3.5 kcal/mol. This step is, as expected for this kind of transformation, stereospecific, *i.e.* the two *trans* hydrogen atoms of the alkene moiety of **Int1** are found in a *trans* relationship in **Int2**. The conversion of **Int2** into **Int3**, which shows the framework of the isolated *trans* cyclobutanone products, is virtually thermoneutral and is achieved through **TS<sub>2-3</sub>**, which lies 12.1 kcal/mol above **Int1'**. The final step, not observed experimentally with our ligands but which takes place with JohnPhosAu<sup>+</sup>, leads to **Int4**. The corresponding transition state **TS<sub>3-4</sub>** lies 2.1 kcal/mol below **Int1**. This step is strongly exergonic ( $\Delta G_{298}(\mathbf{Int1}'-\mathbf{Int4}) = -41.4$  kcal/mol). The cyclization of **Int1'** into **Int2'** requires a slightly higher free energy of activation than that of **Int1** (10.3 kcal/mol vs 9.0 kcal/mol). This transformation is endergonic by 3.0 kcal/mol. Interestingly, the geometry of **Int2'** is markedly different from that of **Int2** in the

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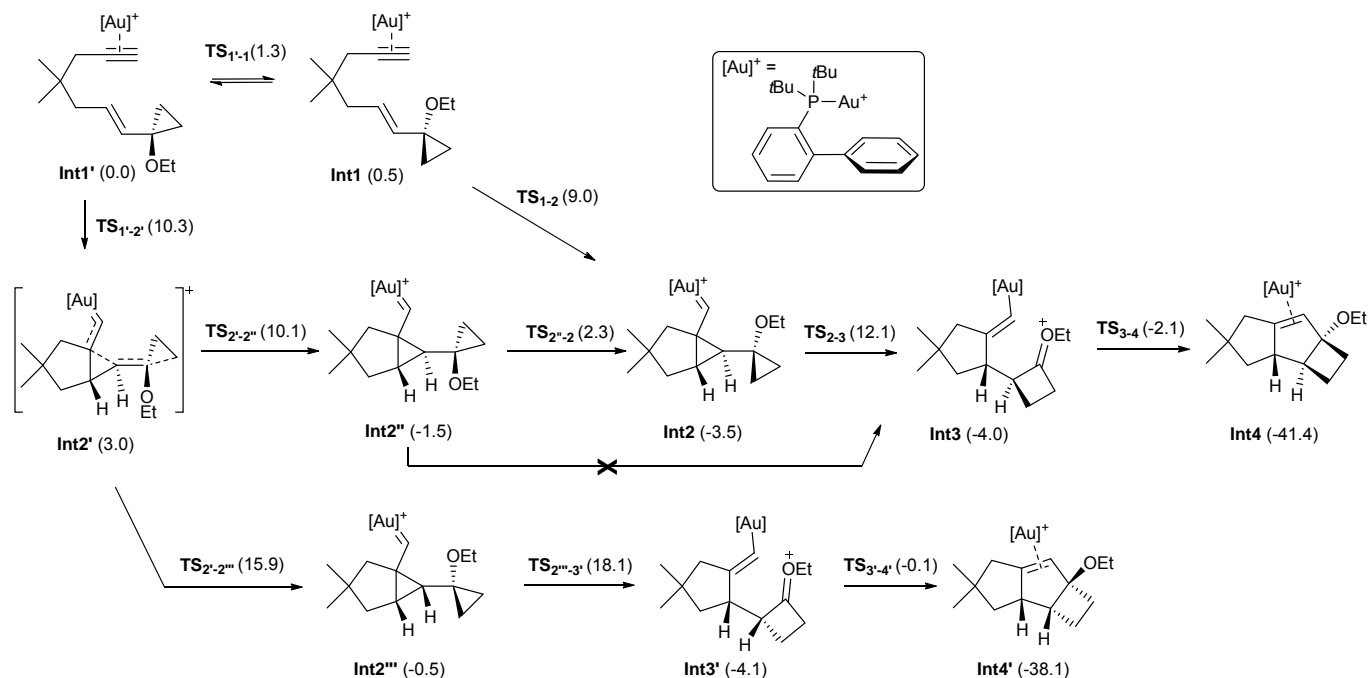
<sup>11</sup> Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

<sup>12</sup> (a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648; (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, **1988**, *37*, 785; (c) S. H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* **1980**, *58*, 1200; (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623.

<sup>13</sup> P. J. Hay, W. R. Wadt, *J. Chem. Phys.* **1985**, *82*, 299.

<sup>14</sup> Y. Zhao, D. G. Truhlar, The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements. *Theor. Chem. Acc.* **2008**, *120*, 215.

sense that it displays elongated bonds in the two cyclopropane units. Thus, **Int2'** has more a carbocationic than a cyclopropylcarbene character.



**Scheme S1.** Computed intermediates and transition states with their relative free energy at the M06/def2-QZVP(Au)-6-311+G(2d,p) (other elements) level of theory ( $\Delta G_{298}$ , kcal/mol).

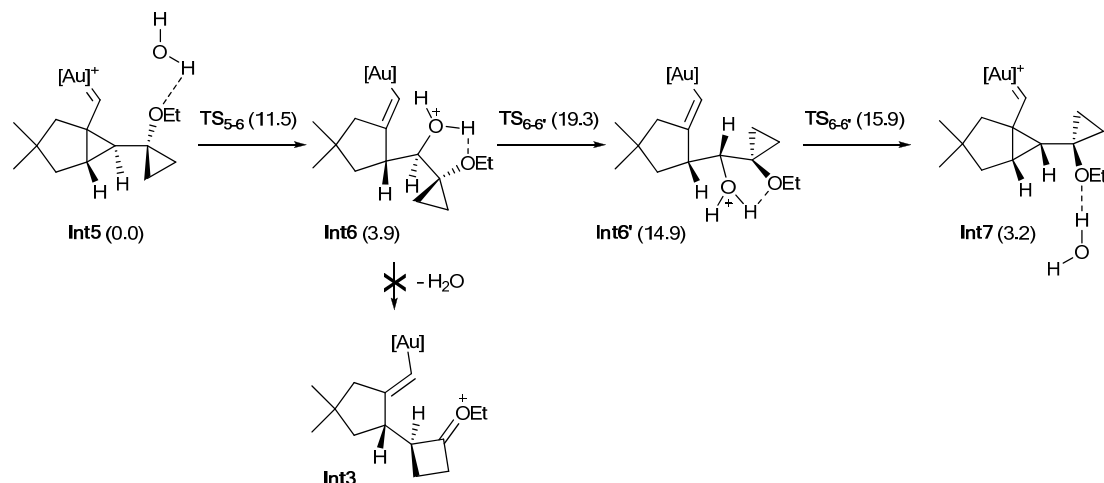
Nevertheless, the cyclopropylcarbene isomer **Int2''** also exists and could be connected to **Int2'** by a transition state lying 10.1 kcal/mol above **Int1'**. These calculation results are consistent with those reported by Echavarren in a related study.<sup>15</sup> Complex **Int2''** could not be transformed into a cyclobutanone such as **Int3**. However, **TS<sub>2-2''</sub>**, which lies 2.3 kcal/mol above **Int1'**, was found to connect the two conformers **Int2''** and **Int2** by simple rotation of the C-C bond between the two cyclopropyl rings. Of particular interest, although an inversion of configuration is not possible from the cyclopropylcarbene intermediates, it becomes feasible from the carbocationic complex **Int2'**. A transition state corresponding to the rotation of the C-C bond holding to the two *trans* hydrogen, **TS<sub>2-2'''</sub>**, could be located. This step requires 12.9 kcal/mol of free energy of activation and leads to the cyclopropylcarbene **Int2'''**, which is more stable than **Int1'** by 0.5 kcal/mol. It displays a *cis* configuration of the two hydrogens and can be converted into the cyclobutanone precursor **Int3'**, and then the *cis* tricyclic product **Int4'**. The transition state corresponding to the formation of **Int3'** is significantly less stable than **TS<sub>2-3</sub>** by 6.0 kcal/mol. On the other hand, the final step in the *cis* series, achieved through **TS<sub>3'-4'</sub>**, is more energetically demanding than the corresponding one in the *trans* series (**TS<sub>3-4</sub>**) by 2.0 kcal/mol. Of note, the formation of this third stereocenter leads necessarily to a *cis* 5/4 ring fusion. Attaining a geometry of a transition state giving rise to a *trans* ring fusion is geometrically unworkable.

Although calculations reveal that the final step **Int3/Int4** is highly favored with the Echavarren's catalyst, it might be slowed down by, for instance, bulky ligands such as those used in this study. In this case, the cyclobutanone intermediates **Int3,3'** might evolve then into the observed cyclobutanone derivatives *trans*-**3a** and *cis*-**3a** respectively, by reaction with water and subsequent protodemetalation. If **Int3,3'** are formed reversibly, then the proportion of the *trans* and *cis* cyclobutanone products might be in fact dictated by the ease by which the solvent- or the water-assisted deethylation (adventitious or intentionally added

<sup>15</sup> C. Nieto-Oberhuber, S. López, M-P. Muñoz, D.J. Cárdenas, E. Buñuel, C. Nevado and A. M. Echavarren, *Angew. Chem. Int. Ed.* 2005, **44**, 6146.



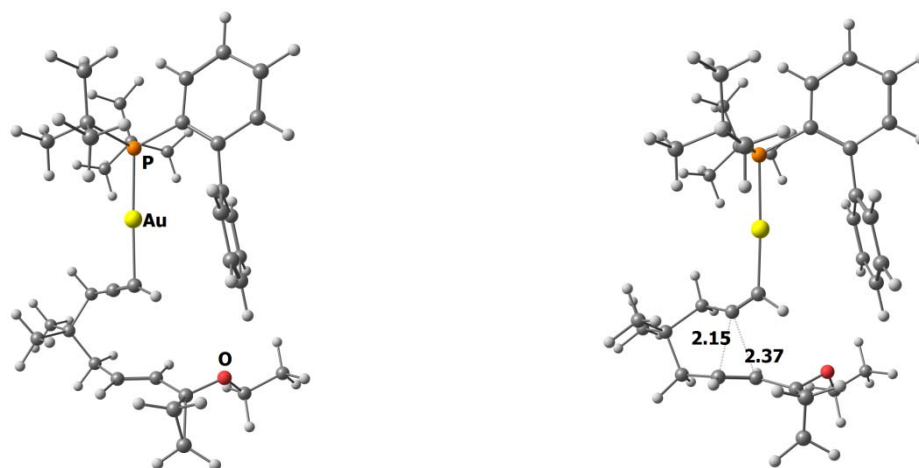
water), and the following protodemetalation by  $\text{EtOH}_2^+$ , are achieved from these intermediates. Unfortunately, the water-promoted deethylation process could not be computed. Nevertheless, we checked whether water could affect the diastereoselectivity (according to the Echavarren's disclosure) by changing the ratios of diastereomeric intermediates (Scheme S2).



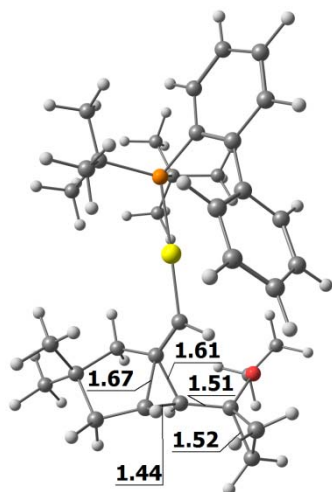
**Scheme S2.** Computed  $\text{H}_2\text{O}$ -assisted stereomutation ( $\Delta G_{298}$ , kcal/mol).

The addition of water to **Int2** was studied, starting from the H-bonded complex **Int5**. The latter undergoes a ring opening of the cyclopropylcarbene framework to give the water adduct **Int6**. This step requires 11.5 kcal/mol of free energy of activation and is endergonic by 3.9 kcal/mol. Of note, it was not possible to compute a pinacol-type expansion of the cyclopropyl unit of **Int6** to give rise to **Int3** with elimination of water. On the other hand, the stereodetermining C-C bond is now free to rotate to give **Int6'**. From this complex, cyclization reaction provides the *cis* cyclopropylcarbene **Int7**. The rotation step is achieved at a quite high free energy cost of 15.4 kcal/mol (19.3 kcal/mol relatively to **Int5**) and is strongly endergonic by 11 kcal/mol. On the other hand, ring closing requires only 1 kcal/mol to reach **TS<sub>6-6'</sub>** (15.9 kcal/mol relatively to **Int5**). The *cis* complex **Int7** is slightly less stable than **Int5** by 3.2 kcal/mol, which is in line with the calculation results summarized in Scheme S2. Thus, a scenario involving water as stereomutating agent seems also plausible. As in the case shown in Scheme S2, such a process would cross a quite high barrier (but surmountable at room temperature), yet they are in the same range (18.1 vs 19.3 kcal/mol), so both mechanisms can actually coexist.

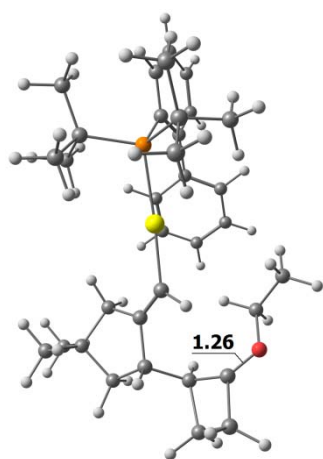
**Figure S3.** Geometries of the computed species (selected distances in Å)



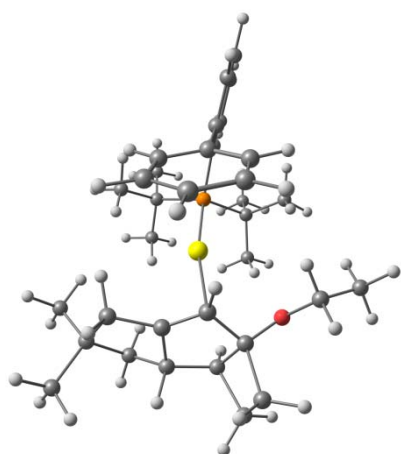
Int1



Int2

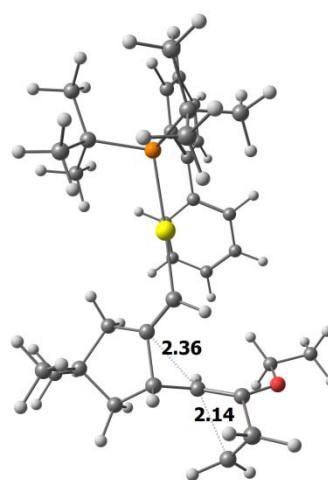


Int3

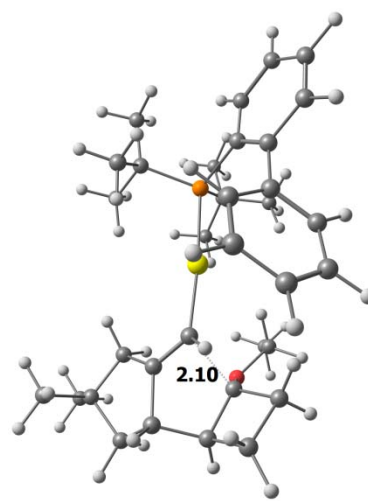


Int4

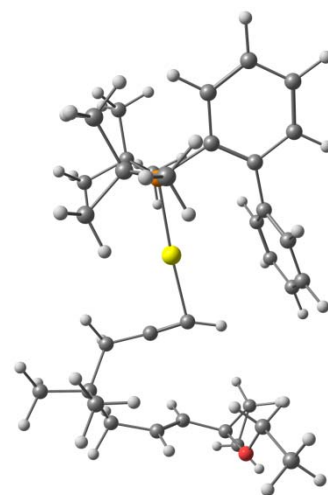
TS<sub>1-2</sub>



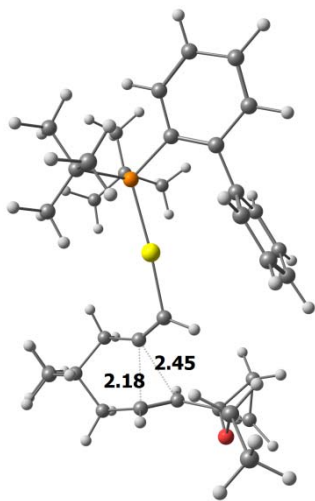
TS<sub>2-3</sub>



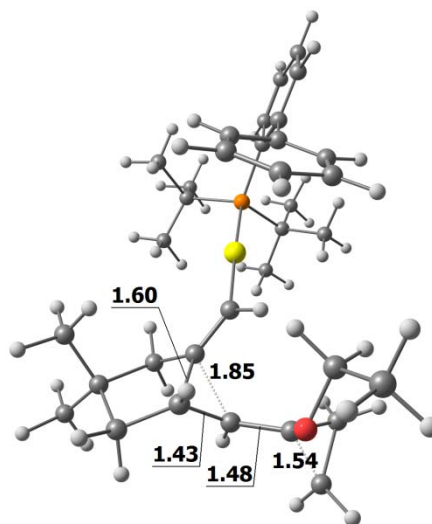
TS<sub>3-4</sub>



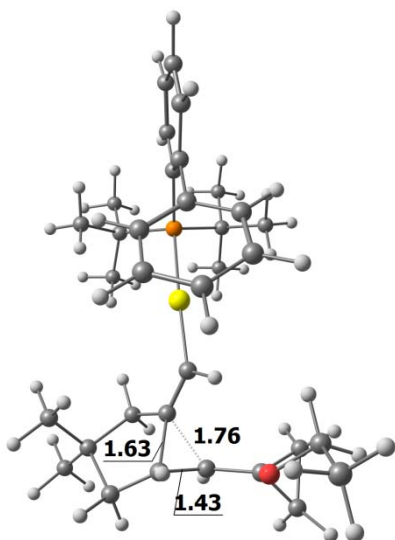
Int1'



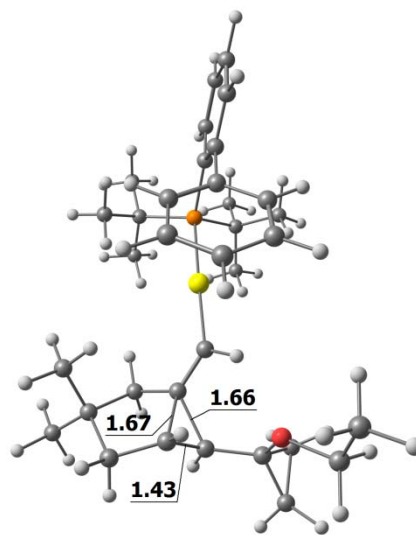
TS<sub>1'-2'</sub>



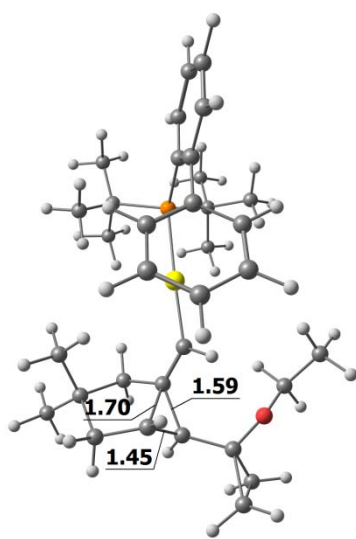
Int2'



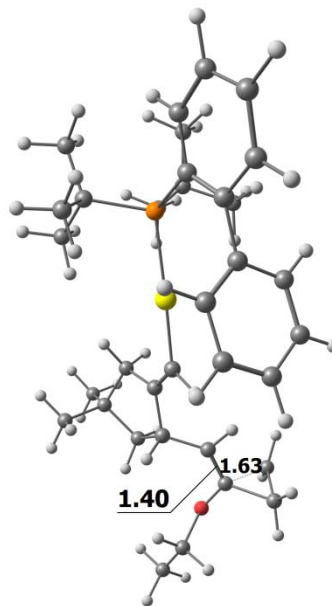
TS<sub>2'-2''</sub>



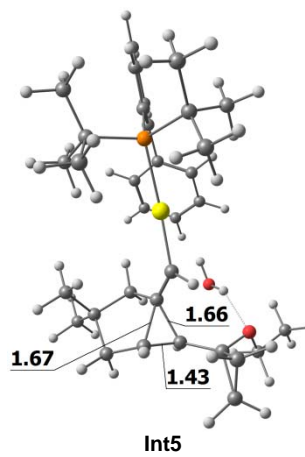
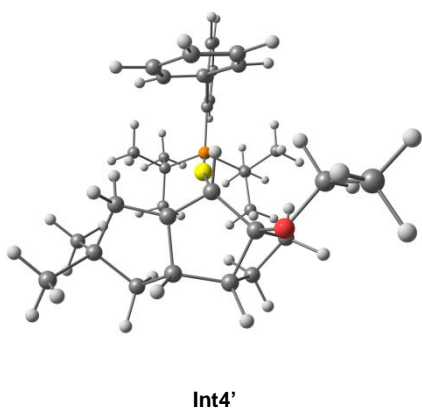
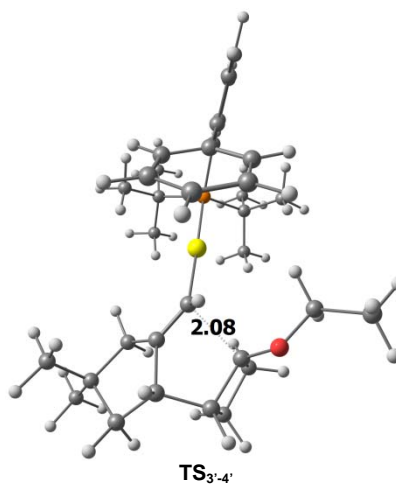
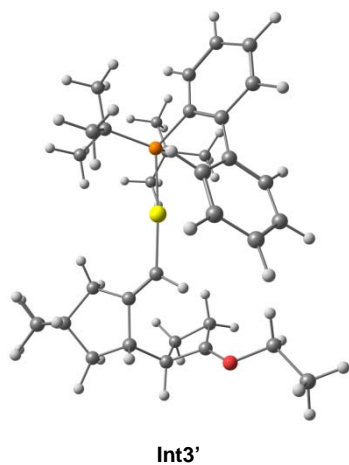
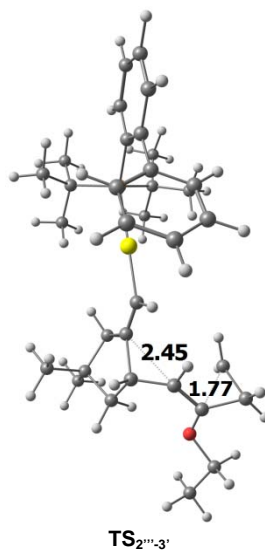
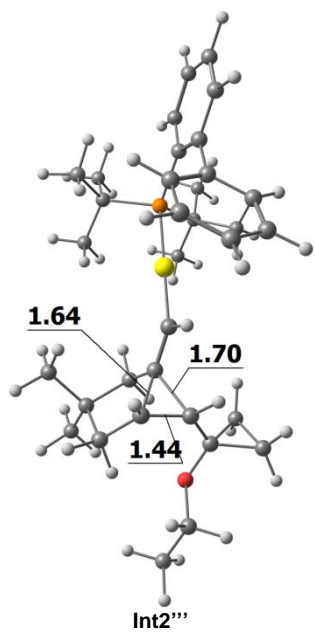
Int2''

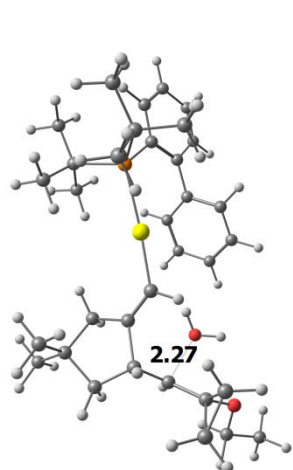


TS<sub>2-2''</sub>

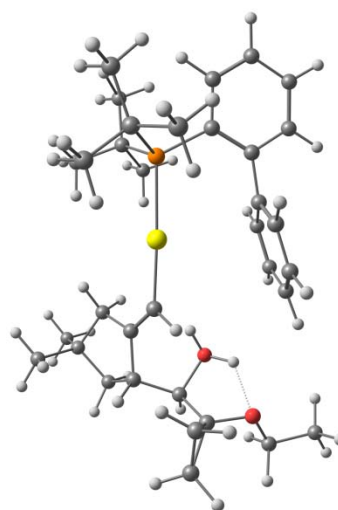


TS<sub>2'-2'''</sub>

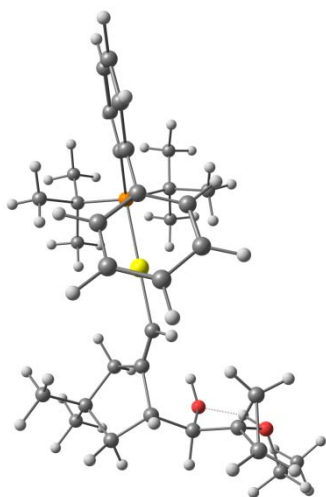




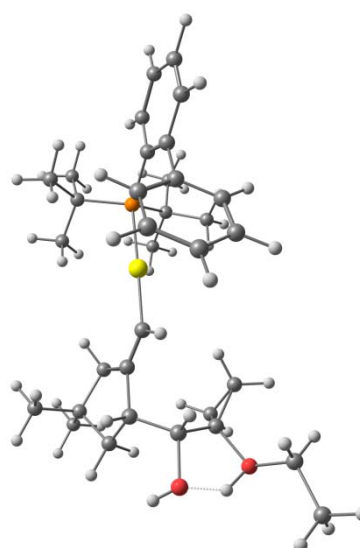
**TS<sub>5-6</sub>**



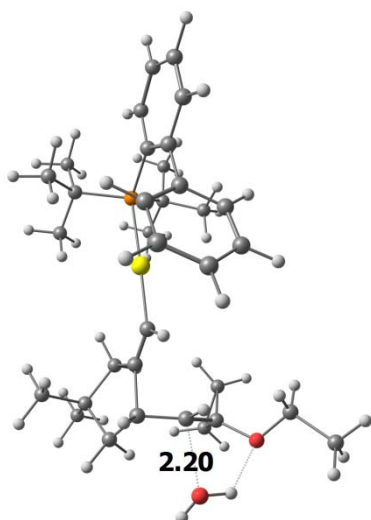
**Int6**



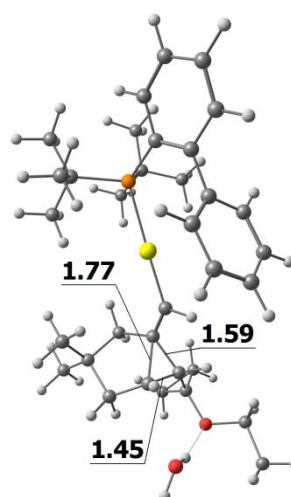
**TS<sub>6-6'</sub>**



**Int6'**



**TS<sub>6'-7</sub>**



**Int7**

**Table S1.** Coordinates (x,y,z) and energy (Hartree) of the computed species

Int1 E(RM06) = -1876.51247703				TS <sub>1,2</sub> E(RM06) = -1876.50091039 Frequency -223.1887			
C	-4.990104000	-1.313200000	-0.245196000	C	4.598510000	-1.205434000	0.698945000
C	-1.929443000	-1.454510000	-0.002245000	C	2.601691000	-1.077299000	-0.088267000
C	-5.027884000	-0.088042000	0.294529000	C	4.733837000	-0.040624000	-0.013077000
C	-5.231998000	1.205474000	-0.421801000	C	4.694350000	1.335324000	0.514282000
C	-6.435766000	1.400109000	-1.333691000	C	5.747479000	1.720494000	1.569145000
C	-5.049260000	1.315666000	-1.915983000	C	4.305208000	1.635419000	1.950895000
H	-7.107706000	0.556810000	-1.457970000	H	6.431091000	0.950326000	1.910752000
H	-6.915841000	2.373612000	-1.327576000	H	6.184462000	2.706764000	1.452774000
H	-4.901845000	0.012985000	1.372382000	H	4.968080000	-0.119462000	-1.073651000
C	-4.814065000	-2.586280000	0.537486000	C	4.942654000	-2.556156000	0.122251000
H	-5.126957000	-1.428145000	-1.319866000	H	4.413262000	-1.151141000	1.768559000
C	-1.630877000	-0.405574000	-0.581156000	C	1.775929000	-0.210395000	0.400570000
C	-2.245182000	-2.701152000	0.688285000	C	2.750052000	-2.297765000	-0.919675000
Au	0.527304000	-0.563343000	-0.139366000	Au	-0.291344000	-0.389306000	0.127528000
H	-1.856185000	0.521142000	-1.076869000	H	2.080239000	0.661544000	0.968199000
C	-3.549134000	-3.435205000	0.214808000	C	3.653643000	-3.350315000	-0.238331000
H	-1.401941000	-3.387748000	0.545411000	H	1.738975000	-2.686201000	-1.086186000
H	-2.314168000	-2.499480000	1.764604000	H	3.158487000	-2.033998000	-1.904646000
O	-4.777802000	2.333528000	0.292383000	O	4.319143000	2.320066000	-0.404976000
H	-4.607020000	2.240774000	-2.271430000	H	3.764693000	2.565807000	2.084399000
H	-4.763428000	0.428026000	-2.472554000	H	3.978281000	0.824811000	2.593715000
C	-5.658180000	2.789428000	1.326727000	C	5.318503000	2.698877000	-1.366022000
P	2.881296000	-0.537214000	0.078833000	P	-2.661033000	-0.688178000	-0.066385000
C	3.582449000	-1.414704000	-1.475605000	C	-3.214023000	-1.616674000	1.520727000
C	3.593597000	1.169132000	0.089030000	C	-3.674778000	0.863283000	-0.121967000
C	3.314368000	-1.365675000	1.758993000	C	-2.998258000	-1.642246000	-1.704375000
C	5.116639000	-1.370803000	-1.621726000	C	-4.732819000	-1.815303000	1.687936000
C	3.113647000	-2.884009000	-1.473567000	C	-2.510980000	-2.988925000	1.557895000
C	2.960532000	-0.683028000	-2.686484000	C	-2.709400000	-0.755403000	2.700659000
C	2.831756000	2.354692000	-0.073940000	C	-3.132100000	2.165780000	0.019841000
C	4.991669000	1.284579000	0.237945000	C	-5.071407000	0.737097000	-0.275333000
C	4.779575000	-1.821433000	1.899809000	C	-4.347458000	-2.382414000	-1.778883000
C	2.397093000	-2.592326000	1.958835000	C	-1.869268000	-2.676781000	-1.912970000

C	2.986131000	-0.324826000	2.850064000	C	-2.913954000	-0.599074000	-2.839316000
H	5.487220000	-0.355263000	-1.772008000	H	-5.261155000	-0.865256000	1.786997000
H	5.387989000	-1.948217000	-2.512540000	H	-4.903874000	-2.379884000	2.611580000
H	5.643903000	-1.817424000	-0.776208000	H	-5.185051000	-2.384797000	0.873409000
H	3.352367000	-3.329540000	-2.445529000	H	-2.663650000	-3.438138000	2.545742000
H	3.622982000	-3.480104000	-0.711550000	H	-2.921281000	-3.684280000	0.820482000
H	2.032720000	-2.973894000	-1.324969000	H	-1.432095000	-2.902451000	1.394574000
H	3.355710000	-1.127999000	-3.606378000	H	-2.993137000	-1.242105000	3.640713000
H	3.214803000	0.380936000	-2.697550000	H	-3.156779000	0.243115000	2.697075000
H	1.870848000	-0.779303000	-2.710376000	H	-1.620946000	-0.645367000	2.692403000
C	3.510056000	3.586948000	-0.108805000	C	-4.010059000	3.264915000	0.038341000
C	1.338856000	2.459743000	-0.183619000	C	-1.677794000	2.514204000	0.119435000
C	5.638296000	2.516518000	0.216337000	C	-5.920143000	1.840125000	-0.272979000
H	5.595149000	0.396088000	0.363719000	H	-5.514541000	-0.242479000	-0.391306000
C	4.891222000	3.677937000	0.032500000	C	-5.385821000	3.115663000	-0.103929000
H	2.923431000	4.491199000	-0.236841000	H	-3.585888000	4.257756000	0.151587000
C	0.733188000	2.723948000	-1.422885000	C	-1.119843000	2.900811000	1.347313000
C	0.542988000	2.498248000	0.976482000	C	-0.892992000	2.618574000	-1.041466000
H	5.376578000	4.648579000	0.005512000	H	-6.031524000	3.988334000	-0.090889000
H	6.715982000	2.562874000	0.336818000	H	-6.989295000	1.698531000	-0.396452000
C	-0.633462000	3.008889000	-1.501662000	C	0.196757000	3.363552000	1.415948000
H	1.340752000	2.730204000	-2.323270000	H	-1.725366000	2.853192000	2.247811000
C	-0.821364000	2.781459000	0.893910000	C	0.421942000	3.080941000	-0.970921000
H	1.006176000	2.337017000	1.945589000	H	-1.325895000	2.360343000	-2.003485000
C	-1.416775000	3.040117000	-0.344412000	C	0.971551000	3.454416000	0.257713000
H	-1.079462000	3.225524000	-2.468355000	H	0.607342000	3.669047000	2.374362000
H	-2.480075000	3.254755000	-0.393967000	H	1.995603000	3.810973000	0.302546000
H	-1.420201000	2.814583000	1.798954000	H	1.014143000	3.161107000	-1.877455000
H	5.491320000	-0.997298000	1.825170000	H	-5.207329000	-1.716245000	-1.690741000
H	5.048975000	-2.589058000	1.170528000	H	-4.431951000	-3.168023000	-1.024106000
H	4.908114000	-2.262410000	2.894625000	H	-4.422442000	-2.867591000	-2.758828000
H	2.544396000	-3.360779000	1.197502000	H	-1.840039000	-3.433697000	-1.126352000
H	2.625445000	-3.042525000	2.931355000	H	-2.040130000	-3.194150000	-2.863958000
H	1.339857000	-2.310984000	1.963214000	H	-0.887853000	-2.196459000	-1.963558000
H	3.645221000	0.545202000	2.803826000	H	-3.730494000	0.125445000	-2.798745000

H	1.949307000	0.020562000	2.779908000	H	-1.965355000	-0.052166000	-2.814652000
H	3.113388000	-0.792809000	3.832392000	H	-2.971424000	-1.118104000	-3.802684000
C	-5.040811000	4.019065000	1.969403000	C	4.751995000	3.824559000	-2.211893000
H	-5.810466000	1.998365000	2.075813000	H	5.583672000	1.839952000	-1.999815000
H	-6.642436000	3.025518000	0.899765000	H	6.231722000	3.017483000	-0.845708000
H	-4.894638000	4.810427000	1.228549000	H	4.501931000	4.688300000	-1.589604000
H	-4.070807000	3.781190000	2.416892000	H	3.848168000	3.499718000	-2.735188000
H	-5.695851000	4.402040000	2.757542000	H	5.487255000	4.139006000	-2.958241000
H	-4.821628000	-2.362417000	1.611890000	H	5.543401000	-2.422549000	-0.784418000
H	-5.680572000	-3.237512000	0.354630000	H	5.552784000	-3.122170000	0.834516000
C	-3.456123000	-3.774027000	-1.282637000	C	2.980344000	-3.910283000	1.027581000
H	-2.604246000	-4.433709000	-1.481197000	H	2.062273000	-4.449415000	0.771222000
H	-4.360230000	-4.296728000	-1.610995000	H	3.645787000	-4.614239000	1.537409000
H	-3.339710000	-2.881950000	-1.904354000	H	2.711739000	-3.121728000	1.737304000
C	-3.625129000	-4.740554000	1.031296000	C	3.983199000	-4.494838000	-1.206756000
H	-4.513207000	-5.313660000	0.748502000	H	4.681537000	-5.202328000	-0.748292000
H	-2.750180000	-5.374688000	0.852846000	H	3.081091000	-5.052532000	-1.478739000
H	-3.686916000	-4.540290000	2.106649000	H	4.440730000	-4.121869000	-2.129492000
<b>Int2</b> E(RM06) = -1876.52486710				<b>TS<sub>2-3</sub></b> E(RM06) = -1876.52649642 Frequency -253.7244			
C	-4.237611000	-0.528202000	-1.194850000	C	-6.407044000	0.302035000	-1.319714000
C	-2.996972000	-0.649487000	-0.090589000	C	-4.581608000	0.253311000	-0.197991000
C	-4.427140000	0.072187000	0.104755000	C	-4.189401000	-1.170945000	-0.112052000
C	-4.473020000	1.558625000	0.354449000	C	-2.659037000	-1.050501000	0.189194000
C	-5.801242000	2.260973000	0.146415000	C	-1.773052000	-0.482897000	-0.648584000
C	-4.630277000	2.553899000	-0.762793000	C	-2.420697000	-1.710505000	1.533773000
H	-6.635704000	1.693659000	-0.255163000	C	-4.768806000	-1.940119000	1.101276000
H	-6.071578000	3.013246000	0.880037000	H	-4.355902000	-1.702258000	-1.052775000
H	-4.991421000	-0.524471000	0.820903000	C	-4.791959000	1.005551000	-1.373173000
C	-4.671241000	-1.962214000	-1.453890000	H	-4.516219000	0.809045000	0.733424000
H	-4.014167000	0.119871000	-2.035354000	C	-5.494046000	0.342972000	-2.507914000
C	-1.894975000	0.164434000	-0.295910000	O	-4.726714000	2.337758000	-1.464187000
C	-2.973487000	-2.117291000	0.310940000	H	-5.745785000	1.032549000	-3.308084000
Au	0.074402000	-0.217776000	0.000040000	H	-5.114526000	-0.614475000	-2.850621000
H	-2.134178000	1.157736000	-0.678054000	H	-6.671559000	-0.650012000	-0.875815000



C	-3.565691000	-2.915710000	-0.885410000	H	-7.084442000	1.131356000	-1.146603000
H	-1.951813000	-2.426893000	0.543923000	Au	0.266583000	-0.400829000	-0.477569000
H	-3.577765000	-2.279068000	1.212174000	P	2.688047000	-0.537726000	-0.505390000
O	-3.663366000	2.012169000	1.400974000	H	-2.195403000	-0.056860000	-1.564934000
H	-4.113495000	3.496938000	-0.620592000	C	-3.576241000	-2.726264000	1.709879000
H	-4.681902000	2.212621000	-1.791715000	H	-1.429672000	-2.171841000	1.573120000
C	-4.060331000	1.596991000	2.716756000	H	-2.456884000	-0.965146000	2.342040000
P	2.411316000	-0.740190000	0.384015000	C	3.222226000	-0.368208000	-2.351489000
C	2.841987000	-2.281270000	-0.674798000	C	3.662333000	0.740241000	0.426673000
C	3.621611000	0.577516000	-0.099091000	C	3.153972000	-2.225005000	0.286442000
C	2.613257000	-1.012970000	2.281490000	C	4.613530000	-0.919150000	-2.717636000
C	4.327513000	-2.689797000	-0.674549000	C	2.176206000	-1.088874000	-3.232877000
C	1.983073000	-3.469926000	-0.197303000	C	3.164773000	1.141288000	-2.673883000
C	2.441818000	-1.923226000	-2.123441000	H	5.425666000	-0.430155000	-2.177324000
C	3.249220000	1.793959000	-0.724772000	H	4.787850000	-0.734758000	-3.784254000
C	4.983874000	0.375964000	0.206524000	H	4.688194000	-1.998689000	-2.564169000
C	3.858977000	-1.808577000	2.715840000	C	3.068982000	1.776607000	1.189834000
C	1.361207000	-1.752989000	2.805628000	C	5.069607000	0.710122000	0.333554000
C	2.647402000	0.392469000	2.920400000	C	3.903474000	2.728480000	1.805124000
H	4.962572000	-1.922558000	-1.121711000	C	1.603867000	1.983946000	1.436957000
H	4.435219000	-3.595227000	-1.282690000	C	5.289150000	2.680616000	1.694297000
H	4.708076000	-2.922432000	0.321997000	H	3.438775000	3.517813000	2.387952000
H	2.088629000	-4.292803000	-0.913390000	C	5.877903000	1.658438000	0.953344000
H	2.301912000	-3.847834000	0.777597000	H	5.900359000	3.432304000	2.184398000
H	0.920607000	-3.212057000	-0.140657000	H	6.957161000	1.596028000	0.853787000
H	2.672555000	-2.773668000	-2.775170000	H	5.552401000	-0.071422000	-0.235984000
H	3.000660000	-1.060396000	-2.498627000	C	0.914935000	2.996759000	0.752336000
H	1.372190000	-1.711087000	-2.214263000	C	0.951231000	1.316777000	2.485312000
C	4.248661000	2.743542000	-1.005089000	C	-0.391614000	3.336022000	1.108701000
C	1.865083000	2.195657000	-1.139752000	H	1.417208000	3.538402000	-0.043883000
C	5.957261000	1.327794000	-0.081781000	C	-1.026947000	2.672151000	2.159988000
H	5.298699000	-0.543917000	0.679500000	H	-0.897298000	4.141185000	0.582503000
C	5.586279000	2.524115000	-0.691940000	C	-0.354181000	1.656803000	2.843130000
H	3.954516000	3.671816000	-1.484948000	H	-2.028781000	2.961943000	2.466140000
C	1.363662000	1.837690000	-2.401283000	H	-0.832446000	1.147682000	3.675051000

C	1.120644000	3.082620000	-0.345359000	H	1.481594000	0.552024000	3.044175000
H	6.329850000	3.280272000	-0.924155000	C	4.659168000	-2.514950000	0.440458000
H	6.994714000	1.132502000	0.170966000	C	2.502236000	-3.351468000	-0.541616000
C	0.146186000	2.350813000	-2.855111000	C	2.523851000	-2.204473000	1.696597000
H	1.943934000	1.180306000	-3.041430000	H	5.144506000	-1.813664000	1.122117000
C	-0.097832000	3.593735000	-0.797983000	H	5.197148000	-2.508856000	-0.509857000
H	1.511889000	3.390736000	0.619913000	H	4.775019000	-3.516619000	0.870772000
C	-0.585402000	3.233217000	-2.056331000	H	2.989444000	-3.482187000	-1.511549000
H	-0.214638000	2.081843000	-3.843763000	H	2.604585000	-4.297303000	0.002820000
H	-1.516967000	3.655594000	-2.422151000	H	1.435355000	-3.174766000	-0.710281000
H	-0.653369000	4.288494000	-0.175217000	H	2.959114000	-1.418946000	2.322069000
H	4.796279000	-1.324633000	2.435998000	H	1.440712000	-2.055727000	1.656974000
H	3.859328000	-2.828752000	2.324031000	H	2.718516000	-3.164348000	2.189100000
H	3.856618000	-1.884274000	3.809205000	H	2.456555000	-0.956123000	-4.284389000
H	1.249508000	-2.751956000	2.378731000	H	2.127000000	-2.162301000	-3.039082000
H	1.453522000	-1.867961000	3.891679000	H	1.173656000	-0.675048000	-3.096192000
H	0.443719000	-1.192217000	2.606016000	H	3.314064000	1.279453000	-3.750806000
H	3.547799000	0.948781000	2.650213000	H	3.940970000	1.705512000	-2.151731000
H	1.774397000	0.990018000	2.636110000	H	2.191478000	1.572779000	-2.415538000
H	2.632601000	0.284287000	4.010711000	C	-4.372831000	3.138554000	-0.301621000
C	-3.207074000	2.346484000	3.724066000	C	-4.253052000	4.574308000	-0.771625000
H	-3.920949000	0.511539000	2.827957000	H	-3.428113000	2.766309000	0.108933000
H	-5.127075000	1.815768000	2.863918000	H	-5.162191000	3.030697000	0.453223000
H	-3.349751000	3.425797000	3.623326000	H	-5.196580000	4.928311000	-1.194570000
H	-2.146575000	2.122799000	3.575468000	H	-3.471331000	4.669970000	-1.529338000
H	-3.482265000	2.054038000	4.741710000	H	-3.995149000	5.214725000	0.076724000
H	-5.624413000	-2.149679000	-0.946838000	H	-5.149499000	-1.229846000	1.846428000
H	-4.829967000	-2.131545000	-2.522148000	H	-5.604519000	-2.589787000	0.820044000
C	-2.481391000	-3.146268000	-1.954726000	C	-3.299501000	-4.001440000	0.890209000
H	-1.678347000	-3.777380000	-1.559965000	H	-2.434567000	-4.537431000	1.294359000
H	-2.901932000	-3.650898000	-2.830669000	H	-4.156896000	-4.682557000	0.921216000
H	-2.029554000	-2.207152000	-2.292157000	H	-3.082336000	-3.776876000	-0.159666000
C	-4.159610000	-4.260428000	-0.446584000	C	-3.829830000	-3.092196000	3.177195000
H	-4.612355000	-4.786480000	-1.293529000	H	-4.693930000	-3.758135000	3.277164000
H	-3.384074000	-4.912501000	-0.031169000	H	-2.965488000	-3.610237000	3.605731000

H	-4.932047000	-4.126993000	0.318703000	H	-4.020414000	-2.200298000	3.784864000
<b>Int3</b> E(RM06) = -1876.52649642				<b>TS<sub>3-4</sub></b> E(RM06) = -1876.52724590 Frequency -122.5674			
C	6.420734000	0.704248000	0.951694000	C	-1.980191000	0.670970000	-0.450454000
C	4.983892000	0.721029000	0.290592000	C	-3.158294000	1.319686000	1.158915000
C	4.386799000	-0.706680000	0.110311000	Au	-0.065726000	-0.058567000	-0.155028000
C	2.879693000	-0.704901000	-0.201590000	C	-3.105839000	-0.081080000	-0.728794000
C	1.933761000	-0.268306000	0.644312000	H	-2.017942000	1.693050000	-0.826704000
C	2.696832000	-1.373829000	-1.551081000	O	-3.089267000	0.490472000	2.184267000
C	5.052089000	-1.435618000	-1.083456000	C	-4.466362000	1.545414000	0.368369000
H	4.570726000	-1.258483000	1.041125000	C	-2.840371000	2.817062000	1.186501000
C	4.606159000	1.466670000	1.528092000	P	2.136523000	-1.045455000	0.061056000
H	4.850316000	1.290819000	-0.633966000	C	-4.499881000	0.558079000	-0.806504000
C	5.781064000	1.052538000	2.341388000	C	-3.256371000	-1.566055000	-0.658060000
O	3.867367000	2.463533000	1.771116000	C	-1.984830000	0.634766000	3.125000000
H	6.219449000	1.822888000	2.978525000	C	-4.001305000	3.025194000	0.164646000
H	5.581997000	0.153637000	2.933682000	H	-5.349060000	1.477863000	1.012673000
H	6.933315000	-0.255771000	0.896365000	H	-3.090404000	3.208684000	2.180535000
H	7.064392000	1.504266000	0.585269000	H	-1.837863000	3.151324000	0.917776000
Au	-0.110394000	-0.333664000	0.471028000	C	2.317234000	-2.332427000	-1.352401000
P	-2.520813000	-0.646491000	0.554138000	C	3.586687000	0.102891000	-0.098382000
H	2.309587000	0.132320000	1.597656000	C	2.252364000	-1.813896000	1.828215000
C	3.927257000	-2.303229000	-1.712890000	C	-5.471714000	-0.638708000	-0.668785000
H	1.742383000	-1.903144000	-1.620826000	H	-4.647750000	1.070102000	-1.765205000
H	2.706604000	-0.621688000	-2.354439000	C	-4.686489000	-1.879080000	-1.175017000
C	-3.036316000	-0.213148000	2.365847000	H	-2.448913000	-2.095677000	-1.174366000
C	-3.633843000	0.379763000	-0.527006000	H	-3.172458000	-1.837311000	0.409414000
C	-2.846641000	-2.477603000	0.064599000	C	-2.200578000	-0.360965000	4.245625000
C	-4.405367000	-0.735222000	2.840235000	H	-1.977362000	1.665158000	3.495769000
C	-1.959109000	-0.755121000	3.332924000	H	-1.057037000	0.448895000	2.573910000
C	-3.021889000	1.329402000	2.443697000	H	-3.652829000	3.232560000	-0.849218000
H	-5.239287000	-0.334239000	2.262437000	H	-4.733477000	3.784884000	0.442139000
H	-4.556842000	-0.414581000	3.877654000	H	-2.204884000	-1.385756000	3.864828000
H	-4.460162000	-1.826615000	2.832617000	H	-3.147555000	-0.174991000	4.759085000
C	-3.176058000	1.384115000	-1.418222000	H	-1.391101000	-0.268077000	4.975473000

C	-5.027072000	0.207426000	-0.388033000	C	1.243125000	-3.424872000	-1.170935000
C	-4.127525000	2.170119000	-2.097230000	C	2.034587000	-1.562349000	-2.661842000
C	-1.754241000	1.709447000	-1.757510000	C	3.700701000	-2.998595000	-1.484498000
C	-5.496268000	1.984548000	-1.936854000	C	3.472380000	1.490640000	-0.368228000
H	-3.767618000	2.932480000	-2.781066000	C	4.876048000	-0.424304000	0.124043000
C	-5.950746000	0.987090000	-1.077861000	C	0.893283000	-2.467545000	2.165426000
H	-6.197390000	2.607865000	-2.483371000	C	2.478119000	-0.629950000	2.794289000
H	-7.013593000	0.815098000	-0.938801000	C	3.352573000	-2.869350000	2.051108000
H	-5.406826000	-0.552374000	0.279221000	H	1.205884000	-4.038983000	-2.077812000
C	-1.244706000	2.980790000	-1.447170000	H	1.471484000	-4.094815000	-0.337822000
C	-0.978318000	0.854908000	-2.555974000	H	0.246654000	-3.000284000	-1.013168000
C	0.003123000	3.387465000	-1.923637000	H	2.099512000	-2.260596000	-3.504135000
H	-1.846620000	3.662536000	-0.852978000	H	2.772205000	-0.772637000	-2.832948000
C	0.761044000	2.531424000	-2.726231000	H	1.036344000	-1.114411000	-2.670671000
H	0.362625000	4.388987000	-1.701177000	H	4.479883000	-2.277524000	-1.739470000
C	0.266190000	1.263865000	-3.038630000	H	3.654185000	-3.727026000	-2.302253000
H	1.714467000	2.860179000	-3.130645000	H	4.005323000	-3.541651000	-0.587469000
H	0.835906000	0.598926000	-3.680863000	C	4.640433000	2.276253000	-0.374636000
H	-1.370227000	-0.117358000	-2.835511000	C	2.215977000	2.245923000	-0.681720000
C	-4.318859000	-2.929561000	0.012870000	C	6.019528000	0.368595000	0.102855000
C	-2.075803000	-3.392349000	1.039288000	H	4.995856000	-1.480051000	0.320538000
C	-2.251024000	-2.638209000	-1.352477000	H	0.682414000	-3.339354000	1.543327000
H	-4.882247000	-2.410044000	-0.764584000	H	0.916352000	-2.805321000	3.207995000
H	-4.839895000	-2.808427000	0.965215000	H	0.062357000	-1.765983000	2.052087000
H	-4.341384000	-3.997849000	-0.232358000	H	3.456861000	-0.164805000	2.656277000
H	-2.543319000	-3.425874000	2.026958000	H	1.712777000	0.145015000	2.676885000
H	-2.082600000	-4.414828000	0.644418000	H	2.424071000	-0.997908000	3.825328000
H	-1.031993000	-3.085783000	1.158190000	H	4.359790000	-2.476898000	1.903460000
H	-2.769118000	-2.009413000	-2.083406000	H	3.220345000	-3.749497000	1.417289000
H	-1.183843000	-2.397903000	-1.378112000	H	3.296703000	-3.211962000	3.090951000
H	-2.370610000	-3.679740000	-1.672284000	H	-5.729460000	-0.782286000	0.387992000
H	-2.206722000	-0.424464000	4.348471000	H	-6.408251000	-0.483029000	-1.212187000
H	-1.914960000	-1.845873000	3.345758000	C	-4.687847000	-1.937355000	-2.715199000
H	-0.961663000	-0.379846000	3.088238000	C	-5.238798000	-3.190001000	-0.602398000
H	-3.177922000	1.633647000	3.485132000	C	5.900189000	1.734681000	-0.141935000

H	-3.812422000	1.782058000	1.840235000	H	4.543160000	3.337005000	-0.583825000
H	-2.060477000	1.740508000	2.117078000	C	1.708157000	3.170412000	0.244940000
C	2.851635000	2.977862000	0.788145000	C	1.642440000	2.195063000	-1.962420000
C	1.690410000	3.504724000	1.595750000	H	6.991698000	-0.081014000	0.279321000
H	2.574463000	2.149285000	0.136706000	H	6.778134000	2.373064000	-0.159231000
H	3.382457000	3.761522000	0.242435000	C	0.653956000	4.019490000	-0.099344000
H	1.999851000	4.305289000	2.271954000	H	2.162823000	3.241889000	1.228893000
H	1.218170000	2.702310000	2.167293000	C	0.589227000	3.044177000	-2.307577000
H	0.947146000	3.898812000	0.897599000	H	2.047787000	1.513521000	-2.703156000
H	5.393187000	-0.701551000	-1.825418000	C	0.093617000	3.961713000	-1.378393000
H	5.925307000	-2.028518000	-0.792839000	H	0.295627000	4.750132000	0.620815000
C	3.730584000	-3.600339000	-0.904895000	H	0.176178000	3.006544000	-3.311396000
H	2.909985000	-4.192619000	-1.323245000	H	-0.702471000	4.646046000	-1.657796000
H	4.633810000	-4.219741000	-0.930390000	H	-4.296477000	-1.018551000	-3.166908000
H	3.486763000	-3.399434000	0.143696000	H	-4.070039000	-2.767623000	-3.073701000
C	4.226432000	-2.643965000	-3.177699000	H	-5.702658000	-2.088885000	-3.096767000
H	5.134266000	-3.250696000	-3.267647000	H	-4.640243000	-4.047304000	-0.928813000
H	3.404408000	-3.215931000	-3.621460000	H	-5.241178000	-3.176952000	0.493127000
H	4.367035000	-1.738213000	-3.778516000	H	-6.266909000	-3.360619000	-0.938129000
<b>Int4</b>				<b>Int1'</b>			
E(RM06) = -1876.59288372				E(RM06) = -1876.51206685			
C	-2.276018000	1.045686000	-0.622312000	C	-5.157405000	1.130532000	0.067172000
C	-2.780617000	1.689071000	0.675748000	C	-2.023840000	1.132983000	-0.389811000
Au	-0.308318000	-0.024099000	0.013214000	C	-5.337377000	0.183280000	-0.862193000
C	-2.839483000	-0.205048000	-0.733809000	C	-5.752762000	-1.217218000	-0.594331000
H	-1.829620000	1.599143000	-1.447208000	C	-5.396318000	-2.308122000	-1.597537000
O	-1.795770000	2.369054000	1.429239000	C	-6.814426000	-1.816453000	-1.493433000
C	-3.441193000	0.532429000	1.501105000	H	-4.810572000	-2.038476000	-2.471921000
C	-4.172604000	2.420701000	0.682293000	H	-5.182827000	-3.292992000	-1.193913000
P	1.824851000	-0.704241000	0.789873000	H	-5.231356000	0.438332000	-1.917647000
C	-3.742213000	-0.531647000	0.425627000	C	-4.869429000	2.575481000	-0.235569000
C	-2.869752000	-1.344816000	-1.716231000	H	-5.309149000	0.862275000	1.110513000
C	-1.323343000	3.600872000	0.866893000	C	-1.698573000	-0.051157000	-0.247442000
C	-4.623696000	1.480667000	1.834025000	C	-2.327345000	2.547376000	-0.589708000
H	-2.845811000	0.141171000	2.331815000	Au	0.472393000	0.361127000	-0.174793000
H	-4.148474000	3.489903000	0.901826000	H	-1.898578000	-1.104105000	-0.161383000

H	-4.735170000	2.271489000	-0.243869000	C	-3.506690000	3.149454000	0.247704000
C	1.892679000	-2.620473000	0.769441000	H	-1.418096000	3.109742000	-0.344055000
C	3.239141000	-0.109896000	-0.244760000	H	-2.516000000	2.712120000	-1.658342000
C	2.034164000	0.080765000	2.539618000	O	-5.872142000	-1.590636000	0.751783000
C	-3.577135000	-2.050207000	0.566983000	H	-7.532862000	-2.458513000	-0.995350000
H	-4.762035000	-0.350682000	0.045069000	H	-7.220194000	-1.201946000	-2.290777000
C	-3.505909000	-2.553858000	-0.917501000	C	-4.663433000	-1.971081000	1.406228000
H	-3.491446000	-1.070856000	-2.579033000	P	2.809860000	0.659972000	-0.014803000
H	-1.879288000	-1.577825000	-2.115498000	C	3.117092000	1.678522000	1.589995000
C	-0.618375000	4.389074000	1.957802000	C	3.738696000	-0.928217000	0.156493000
H	-2.166186000	4.179156000	0.466096000	C	3.407261000	1.490682000	-1.635310000
H	-0.640100000	3.387753000	0.031804000	C	4.495783000	2.361607000	1.677005000
H	-5.629368000	1.056572000	1.768600000	C	2.029341000	2.770961000	1.705363000
H	-4.503275000	1.952092000	2.811559000	C	2.944717000	0.693518000	2.765950000
H	0.221639000	3.822862000	2.369451000	C	3.135823000	-2.211759000	0.133645000
H	-1.308552000	4.618370000	2.774151000	C	5.129975000	-0.844940000	0.375674000
H	-0.233621000	5.330788000	1.554518000	C	4.936929000	1.638069000	-1.761167000
C	0.804065000	-3.161631000	1.717620000	C	2.744963000	2.877098000	-1.758620000
C	1.574566000	-3.049370000	-0.678761000	C	2.914997000	0.585513000	-2.786211000
C	3.257539000	-3.226097000	1.154257000	H	5.327058000	1.655086000	1.654931000
C	3.108799000	0.621919000	-1.452554000	H	4.556408000	2.890809000	2.634493000
C	4.537355000	-0.357230000	0.249650000	H	4.641801000	3.105188000	0.889822000
C	0.656948000	0.079801000	3.242166000	H	2.195061000	3.325958000	2.635342000
C	2.466881000	1.545753000	2.317135000	H	2.060159000	3.490916000	0.884648000
C	3.050337000	-0.623915000	3.459856000	H	1.024484000	2.341098000	1.751016000
H	0.733495000	-4.247723000	1.592258000	H	2.977927000	1.257903000	3.704217000
H	1.036156000	-2.971439000	2.768653000	H	3.736888000	-0.057532000	2.797189000
H	-0.179881000	-2.735822000	1.498777000	H	1.979437000	0.177032000	2.725569000
H	1.579960000	-4.143721000	-0.732338000	C	3.951152000	-3.339712000	0.340971000
H	2.326480000	-2.682059000	-1.383428000	C	1.687350000	-2.528690000	-0.100143000
H	0.590787000	-2.701573000	-1.006648000	C	5.916871000	-1.975443000	0.572803000
H	4.039215000	-2.962650000	0.439103000	H	5.615864000	0.121057000	0.396188000
H	3.160243000	-4.317453000	1.139479000	C	5.321278000	-3.234758000	0.558400000
H	3.586765000	-2.945358000	2.156016000	H	3.485297000	-4.319892000	0.321523000
C	4.278143000	1.075850000	-2.091573000	C	0.877174000	-2.929256000	0.976557000

C	1.837395000	0.977400000	-2.163868000	C	1.174533000	-2.636311000	-1.405347000
C	5.679388000	0.094563000	-0.404055000	H	5.916273000	-4.129500000	0.712510000
H	4.665608000	-0.909786000	1.170212000	H	6.984170000	-1.867989000	0.738149000
H	0.245010000	-0.924754000	3.364749000	C	-0.408411000	-3.428418000	0.754264000
H	0.781866000	0.506366000	4.244061000	H	1.270476000	-2.876275000	1.987588000
H	-0.073752000	0.694101000	2.709552000	C	-0.109899000	-3.137561000	-1.626655000
H	3.481300000	1.624850000	1.920754000	H	1.799597000	-2.363505000	-2.249824000
H	1.788609000	2.071183000	1.637052000	C	-0.902508000	-3.541671000	-0.548382000
H	2.438313000	2.066997000	3.280355000	H	-1.011866000	-3.752237000	1.597168000
H	4.062267000	-0.648277000	3.051515000	H	-1.888534000	-3.961892000	-0.724227000
H	2.748155000	-1.642654000	3.713837000	H	-0.480367000	-3.235649000	-2.642690000
H	3.102839000	-0.062433000	4.399346000	H	5.441522000	0.670443000	-1.794009000
H	-2.638530000	-2.271196000	1.091069000	H	5.379217000	2.239383000	-0.964422000
H	-4.387406000	-2.531739000	1.121662000	H	5.152452000	2.146569000	-2.707507000
C	-4.923020000	-2.845057000	-1.449673000	H	3.139191000	3.590530000	-1.030468000
C	-2.650469000	-3.821952000	-1.040320000	H	2.955320000	3.280191000	-2.755173000
C	5.548312000	0.821759000	-1.584988000	H	1.657432000	2.824964000	-1.644592000
H	4.172225000	1.633333000	-3.016854000	H	3.358165000	-0.413422000	-2.735532000
C	1.414387000	2.316715000	-2.199921000	H	1.825648000	0.483534000	-2.796298000
C	1.167990000	0.040152000	-2.969575000	H	3.219074000	1.032589000	-3.739111000
H	6.659239000	-0.118517000	0.011321000	C	-5.015107000	-2.386792000	2.825237000
H	6.425372000	1.186587000	-2.110396000	H	-3.950411000	-1.133629000	1.414106000
C	0.348003000	2.708139000	-3.013097000	H	-4.189031000	-2.804588000	0.864760000
H	1.944915000	3.057977000	-1.609157000	H	-5.722472000	-3.220424000	2.816102000
C	0.105748000	0.433184000	-3.787162000	H	-5.475402000	-1.556402000	3.368014000
H	1.509500000	-0.989914000	-2.988879000	H	-4.116547000	-2.698892000	3.367147000
C	-0.306682000	1.768161000	-3.813108000	H	-4.955683000	2.751495000	-1.315659000
H	0.048819000	3.751826000	-3.042599000	H	-5.651070000	3.188032000	0.235471000
H	-0.379060000	-0.298537000	-4.426976000	C	-3.282611000	2.903171000	1.748664000
H	-1.114592000	2.077486000	-4.469575000	H	-2.350505000	3.369127000	2.088096000
H	-5.585242000	-1.976449000	-1.362358000	H	-4.099569000	3.341476000	2.330549000
H	-4.890438000	-3.128489000	-2.507214000	H	-3.234821000	1.837590000	1.989493000
H	-5.383934000	-3.670781000	-0.898201000	C	-3.497821000	4.665689000	-0.031851000
H	-2.600139000	-4.167904000	-2.078574000	H	-4.306067000	5.157204000	0.517583000
H	-1.626778000	-3.649151000	-0.691322000	H	-2.554711000	5.125507000	0.283214000

H	-3.073544000	-4.636055000	-0.442183000	H	-3.641929000	4.879938000	-1.096586000
<b>TS<sub>1-2'</sub></b> E(RM06) = -1876.49946985 Frequency -207.1800				<b>Int2'</b> E(RM06) = -1876.51328126			
C	4.749836000	0.930027000	-0.158180000	C	-4.368246000	0.579505000	0.633693000
C	2.614870000	1.013400000	0.285073000	C	-2.861110000	0.898309000	0.197957000
C	4.782439000	0.038449000	0.883220000	C	-4.343232000	0.405453000	-0.789804000
C	4.912132000	-1.414852000	0.745029000	C	-4.561541000	-0.881651000	-1.480258000
C	4.188574000	-2.337600000	1.734211000	C	-3.925427000	-1.142913000	-2.836020000
C	5.648791000	-2.105128000	1.904965000	C	-5.358298000	-0.725978000	-2.791226000
H	3.489196000	-1.885949000	2.430386000	H	-3.178547000	-0.437061000	-3.186462000
H	3.875964000	-3.295059000	1.331500000	H	-3.712348000	-2.180350000	-3.071208000
H	4.809152000	0.422977000	1.901879000	H	-4.438752000	1.290611000	-1.412841000
C	5.007207000	2.406160000	0.011737000	C	-4.898362000	1.886024000	1.246994000
H	4.787210000	0.523366000	-1.164598000	H	-4.496583000	-0.338989000	1.199371000
C	1.837728000	0.002000000	0.076068000	C	-1.864933000	-0.027769000	0.070768000
C	2.658378000	2.456786000	0.633064000	C	-2.726767000	2.408553000	0.301360000
Au	-0.243717000	0.285260000	0.048693000	Au	0.146434000	0.271560000	-0.087561000
H	2.166661000	-1.016757000	-0.091367000	H	-2.200474000	-1.063553000	0.029866000
C	3.707298000	3.228740000	-0.195169000	C	-3.677972000	2.833668000	1.451057000
H	1.648015000	2.845687000	0.463114000	H	-1.684916000	2.681265000	0.485865000
H	2.871937000	2.573839000	1.704388000	H	-3.025092000	2.898137000	-0.635948000
O	5.253731000	-1.907227000	-0.512901000	O	-4.972027000	-1.952167000	-0.690003000
H	6.331832000	-2.882314000	1.580880000	H	-6.117873000	-1.487402000	-2.928412000
H	6.000135000	-1.492108000	2.728388000	H	-5.635621000	0.270169000	-3.120170000
C	4.203999000	-2.306329000	-1.406082000	C	-4.025699000	-2.967272000	-0.314826000
P	-2.588131000	0.773831000	0.005194000	P	2.505615000	0.704422000	-0.447481000
C	-2.906352000	1.792466000	-1.598926000	C	2.950007000	2.351815000	0.447136000
C	-3.734585000	-0.680223000	-0.056769000	C	3.697181000	-0.578386000	0.162946000
C	-2.989815000	1.696928000	1.639134000	C	2.735635000	0.756403000	-2.354349000
C	-4.217516000	2.600462000	-1.630217000	C	4.213487000	3.073542000	-0.058434000
C	-1.730816000	2.773029000	-1.810220000	C	1.752671000	3.319431000	0.313417000
C	-2.898764000	0.771943000	-2.758457000	C	3.118870000	1.998936000	1.940534000
C	-3.299539000	-2.028485000	-0.029905000	C	3.297848000	-1.794528000	0.772312000
C	-5.119878000	-0.429123000	-0.148643000	C	5.076903000	-0.347229000	-0.017876000
C	-4.476392000	2.026759000	1.877021000	C	4.184616000	0.907157000	-2.854981000



C	-2.168035000	3.000767000	1.688729000	C	1.879330000	1.905731000	-2.924717000
C	-2.518161000	0.756848000	2.771439000	C	2.186210000	-0.591609000	-2.873873000
H	-5.107685000	1.975122000	-1.546561000	H	5.119603000	2.474543000	0.047395000
H	-4.282419000	3.115614000	-2.595409000	H	4.359747000	3.976973000	0.544848000
H	-4.250884000	3.368782000	-0.853896000	H	4.123088000	3.395148000	-1.098943000
H	-1.887342000	3.303680000	-2.756272000	H	1.986133000	4.242653000	0.856025000
H	-1.661050000	3.524701000	-1.021104000	H	1.540392000	3.591117000	-0.722789000
H	-0.771999000	2.250977000	-1.873732000	H	0.843279000	2.895398000	0.748379000
H	-2.951571000	1.316625000	-3.707801000	H	3.248262000	2.925271000	2.511462000
H	-3.750770000	0.089465000	-2.716077000	H	3.992169000	1.368346000	2.122654000
H	-1.978871000	0.177375000	-2.769793000	H	2.234396000	1.488687000	2.336532000
C	-4.264174000	-3.051061000	-0.090653000	C	4.287463000	-2.727687000	1.132269000
C	-1.881768000	-2.512244000	0.050426000	C	1.896643000	-2.197583000	1.120590000
C	-6.057129000	-1.455821000	-0.211177000	C	6.041017000	-1.275936000	0.362791000
H	-5.482601000	0.589028000	-0.167915000	H	5.413141000	0.573517000	-0.473985000
C	-5.625717000	-2.780023000	-0.180171000	C	5.642365000	-2.482701000	0.933531000
H	-3.922122000	-4.081087000	-0.067915000	H	3.971811000	-3.658061000	1.594107000
C	-1.192885000	-2.864155000	-1.121370000	C	1.305008000	-1.748182000	2.312505000
C	-1.297965000	-2.809835000	1.292116000	C	1.227189000	-3.168346000	0.360047000
H	-6.340377000	-3.595949000	-0.226123000	H	6.377943000	-3.224067000	1.230029000
H	-7.113912000	-1.218100000	-0.282049000	H	7.092729000	-1.056443000	0.207581000
C	0.048068000	-3.500656000	-1.053490000	C	0.074725000	-2.258115000	2.733438000
H	-1.648254000	-2.667215000	-2.087441000	H	1.829826000	-1.024144000	2.928591000
C	-0.057094000	-3.446559000	1.359947000	C	-0.004871000	-3.675616000	0.779257000
H	-1.833310000	-2.570416000	2.206026000	H	1.687145000	-3.544045000	-0.549345000
C	0.614263000	-3.801027000	0.187537000	C	-0.580964000	-3.226767000	1.969734000
H	0.555188000	-3.787824000	-1.970110000	H	-0.355625000	-1.918649000	3.671091000
H	1.558766000	-4.335151000	0.240826000	H	-1.521310000	-3.647227000	2.314787000
H	0.368414000	-3.691483000	2.328820000	H	-0.497893000	-4.442813000	0.188868000
H	-5.084926000	1.126660000	1.980867000	H	4.802280000	0.047805000	-2.587906000
H	-4.908122000	2.655098000	1.095203000	H	4.670949000	1.814985000	-2.492878000
H	-4.556689000	2.581574000	2.818842000	H	4.165651000	0.964844000	-3.949419000
H	-2.538530000	3.750850000	0.984806000	H	2.297025000	2.888306000	-2.688794000
H	-2.248550000	3.431545000	2.693120000	H	1.853679000	1.819152000	-4.016937000
H	-1.106626000	2.825437000	1.486116000	H	0.846579000	1.870114000	-2.563112000

H	-3.060198000	-0.193556000	2.762570000	H	2.734543000	-1.442427000	-2.458293000
H	-1.446792000	0.543838000	2.708880000	H	1.124559000	-0.719268000	-2.641738000
H	-2.712202000	1.239058000	3.736243000	H	2.300065000	-0.623843000	-3.963439000
C	4.851730000	-3.015111000	-2.583012000	C	-4.807061000	-4.230900000	0.002674000
H	3.638185000	-1.428029000	-1.747045000	H	-3.454419000	-2.640171000	0.565503000
H	3.501224000	-2.972363000	-0.887439000	H	-3.310538000	-3.139997000	-1.128726000
H	5.398779000	-3.899869000	-2.246837000	H	-5.347161000	-4.585230000	-0.879313000
H	5.554022000	-2.351652000	-3.094865000	H	-5.533472000	-4.045405000	0.798491000
H	4.087821000	-3.328900000	-3.300711000	H	-4.126917000	-5.021380000	0.334352000
H	5.391153000	2.597665000	1.020356000	H	-5.629793000	2.341359000	0.571274000
H	5.781250000	2.726944000	-0.694461000	H	-5.415664000	1.680327000	2.188031000
C	3.309186000	3.271366000	-1.681327000	C	-3.015831000	2.550455000	2.812730000
H	2.379520000	3.833962000	-1.817359000	H	-2.118574000	3.164473000	2.943726000
H	4.085368000	3.767370000	-2.272765000	H	-3.702289000	2.782913000	3.633423000
H	3.154500000	2.270669000	-2.095968000	H	-2.719029000	1.500705000	2.911710000
C	3.881363000	4.656360000	0.341755000	C	-4.082214000	4.310248000	1.360772000
H	4.675483000	5.179294000	-0.200608000	H	-4.800836000	4.569219000	2.145351000
H	2.961662000	5.238007000	0.220045000	H	-3.212232000	4.963881000	1.483907000
H	4.144473000	4.657792000	1.405274000	H	-4.543133000	4.542028000	0.394114000
<b>TS<sub>2-2</sub>"</b> E(RM06) = -1876.50763608 Frequency -70.8891				<b>Int2"</b> E(RM06) = -1876.52097889			
C	-4.319931000	-0.638877000	-0.791421000	C	4.258175000	0.527688000	-0.863577000
C	-2.862790000	-0.952148000	-0.121731000	C	2.865590000	0.935513000	-0.045397000
C	-4.379849000	-0.480134000	0.629778000	C	4.368440000	0.567512000	0.565190000
C	-4.610321000	0.818628000	1.316673000	C	4.601675000	-0.641001000	1.418265000
C	-4.131827000	0.961044000	2.747583000	C	4.326139000	-0.523943000	2.897886000
C	-5.599082000	0.779931000	2.485920000	C	5.755075000	-0.528889000	2.401799000
H	-3.555859000	0.147052000	3.177749000	H	3.899013000	0.402385000	3.271172000
H	-3.808715000	1.950666000	3.054246000	H	3.974007000	-1.414637000	3.409027000
H	-4.623057000	-1.354915000	1.227651000	H	4.734362000	1.489282000	1.011646000
C	-4.744389000	-1.953977000	-1.451639000	C	4.584583000	1.755547000	-1.703194000
H	-4.355160000	0.278319000	-1.370215000	H	4.220755000	-0.453742000	-1.322149000
C	-1.877714000	-0.000787000	-0.030709000	C	1.876390000	-0.014598000	0.096670000
C	-2.703137000	-2.459858000	-0.218974000	C	2.673643000	2.419372000	-0.324140000
Au	0.132364000	-0.256007000	0.161178000	Au	-0.133238000	0.242879000	0.234715000

H	-2.241832000	1.026914000	-0.041515000	H	2.255357000	-1.035099000	0.171443000
C	-3.498886000	-2.895104000	-1.479751000	C	3.333388000	2.694475000	-1.704594000
H	-1.644782000	-2.724447000	-0.281460000	H	1.608806000	2.664943000	-0.322774000
H	-3.107339000	-2.954101000	0.674330000	H	3.148947000	3.030369000	0.453570000
O	-4.623042000	1.919486000	0.454402000	O	4.311173000	-1.813410000	0.701849000
H	-6.250674000	1.640746000	2.583700000	H	6.350058000	-1.414674000	2.591830000
H	-6.063321000	-0.167817000	2.739951000	H	6.326928000	0.393943000	2.424129000
C	-4.079271000	3.171236000	0.897884000	C	4.920825000	-3.046551000	1.101165000
P	2.498499000	-0.617355000	0.563976000	P	-2.514042000	0.608781000	0.549138000
C	2.886646000	-2.330404000	-0.218382000	C	-2.953324000	2.296660000	-0.251537000
C	3.665997000	0.587970000	-0.225120000	C	-3.644059000	-0.644171000	-0.220399000
C	2.814152000	-0.525387000	2.459663000	C	-2.819292000	0.531828000	2.449824000
C	4.244257000	-2.980745000	0.108638000	C	-4.449418000	2.663617000	-0.264068000
C	1.803416000	-3.387879000	0.084677000	C	-2.164805000	3.409578000	0.468605000
C	2.822842000	-2.067895000	-1.738878000	C	-2.469566000	2.200702000	-1.715530000
C	3.245275000	1.726388000	-0.956109000	C	-3.188862000	-1.739735000	-0.997245000
C	5.051469000	0.356103000	-0.100268000	C	-5.029406000	-0.529587000	0.019874000
C	4.287202000	-0.814088000	2.805450000	C	-4.139833000	1.150180000	2.946308000
C	1.887695000	-1.573798000	3.112945000	C	-1.650727000	1.244876000	3.167474000
C	2.409119000	0.905524000	2.878848000	C	-2.775868000	-0.965375000	2.826832000
H	5.090903000	-2.356663000	-0.182950000	H	-5.036876000	1.970396000	-0.868975000
H	4.335998000	-3.868345000	-0.527945000	H	-4.556466000	3.657143000	-0.714508000
H	4.343619000	-3.313444000	1.144451000	H	-4.886516000	2.714783000	0.735434000
H	2.023895000	-4.290327000	-0.496792000	H	-2.253925000	4.336350000	-0.109451000
H	1.722394000	-3.646895000	1.143067000	H	-2.558765000	3.614092000	1.467633000
H	0.823805000	-3.054907000	-0.271086000	H	-1.099849000	3.172755000	0.557786000
H	2.957205000	-3.030214000	-2.245774000	H	-2.669485000	3.153378000	-2.219267000
H	3.652878000	-1.447554000	-2.087508000	H	-2.999670000	1.419249000	-2.268260000
H	1.864121000	-1.651592000	-2.064586000	H	-1.395229000	2.002990000	-1.781318000
C	4.220436000	2.605178000	-1.463421000	C	-4.132818000	-2.662708000	-1.483372000
C	1.828549000	2.125900000	-1.240169000	C	-1.767464000	-2.035781000	-1.370900000
C	6.001293000	1.203654000	-0.664428000	C	-5.946897000	-1.452029000	-0.474559000
H	5.403400000	-0.526104000	0.416176000	H	-5.407565000	0.295968000	0.606651000
C	5.582417000	2.352371000	-1.332475000	C	-5.494581000	-2.530495000	-1.231570000
H	3.889819000	3.521647000	-1.942230000	H	-3.774780000	-3.497387000	-2.077976000

C	1.130576000	1.570343000	-2.324575000	C	-1.163001000	-1.412321000	-2.473969000
C	1.241703000	3.187863000	-0.534344000	C	-1.076175000	-3.070474000	-0.720332000
H	6.305982000	3.040078000	-1.759242000	H	-6.193687000	-3.262018000	-1.624950000
H	7.054714000	0.945247000	-0.620834000	H	-7.004621000	-1.326024000	-0.265465000
C	-0.124148000	2.062996000	-2.691432000	C	0.103659000	-1.809391000	-2.910255000
H	1.587821000	0.773188000	-2.902816000	H	-1.699298000	-0.636255000	-3.011245000
C	-0.013763000	3.678307000	-0.899734000	C	0.190212000	-3.465583000	-1.155762000
H	1.783619000	3.644635000	0.288726000	H	-1.545027000	-3.580034000	0.116533000
C	-0.697849000	3.120761000	-1.982083000	C	0.782462000	-2.838753000	-2.254107000
H	-0.638488000	1.637669000	-3.548387000	H	0.545509000	-1.331490000	-3.779962000
H	-1.660137000	3.522685000	-2.285839000	H	1.756102000	-3.164071000	-2.608668000
H	-0.442948000	4.513878000	-0.354135000	H	0.701553000	-4.280033000	-0.650694000
H	4.965166000	-0.055805000	2.409893000	H	-5.023234000	0.662147000	2.531228000
H	4.617183000	-1.766629000	2.384979000	H	-4.200661000	2.222271000	2.743418000
H	4.407153000	-0.878764000	3.893079000	H	-4.191635000	1.025880000	4.034151000
H	2.198160000	-2.588017000	2.850919000	H	-1.611715000	2.314683000	2.953500000
H	1.933968000	-1.491794000	4.204840000	H	-1.785923000	1.131007000	4.249073000
H	0.854431000	-1.484617000	2.763957000	H	-0.683110000	0.809169000	2.902830000
H	2.980156000	1.650650000	2.318428000	H	-3.617266000	-1.522999000	2.409016000
H	1.356724000	1.111644000	2.658322000	H	-1.846658000	-1.440585000	2.494016000
H	2.608676000	1.058974000	3.945441000	H	-2.821376000	-1.055409000	3.917999000
C	-4.695171000	4.234300000	0.004882000	C	4.362708000	-4.144670000	0.213285000
H	-2.983744000	3.088691000	0.869391000	H	4.699965000	-3.259881000	2.156146000
H	-4.418783000	3.374787000	1.921356000	H	6.010233000	-2.975438000	0.988005000
H	-5.782886000	4.245580000	0.116653000	H	4.581873000	-3.940042000	-0.838582000
H	-4.509436000	3.986091000	-1.043801000	H	3.278980000	-4.228467000	0.334903000
H	-4.279216000	5.224044000	0.215229000	H	4.815319000	-5.104537000	0.477955000
H	-5.555211000	-2.413489000	-0.876135000	H	5.445600000	2.275769000	-1.268827000
H	-5.129760000	-1.764332000	-2.457102000	H	4.861417000	1.460987000	-2.719067000
C	-2.670477000	-2.619629000	-2.748738000	C	2.375573000	2.279934000	-2.837247000
H	-1.759174000	-3.225882000	-2.784348000	H	1.473713000	2.901133000	-2.828377000
H	-3.267601000	-2.864263000	-3.633368000	H	2.855231000	2.402963000	-3.813947000
H	-2.419049000	-1.558699000	-2.852912000	H	2.060962000	1.234938000	-2.745497000
C	-3.950790000	-4.360671000	-1.457584000	C	3.736311000	4.165107000	-1.872621000
H	-4.559212000	-4.597637000	-2.336653000	H	4.241885000	4.327505000	-2.830306000

H	-3.089338000	-5.036789000	-1.462480000	H	2.856684000	4.817046000	-1.850631000
H	-4.547848000	-4.582858000	-0.566205000	H	4.414599000	4.488260000	-1.075309000
<b>TS<sub>2-2"</sub></b> E(RM06) = -1876.51939777 Frequency -17.0197				<b>TS<sub>2-2"</sub></b> E(RM06) = -1876.48996848 Frequency -33.1750			
C	4.098844000	0.410530000	-1.107630000	C	4.363831000	0.951850000	-0.505367000
C	3.015806000	0.717416000	0.160321000	C	3.991224000	-0.237563000	0.256689000
C	4.504490000	0.176887000	0.266025000	C	2.501375000	-0.653515000	0.104561000
C	4.914723000	-1.186357000	0.810406000	C	5.645482000	1.402690000	-0.842033000
C	6.023699000	-1.218718000	1.838384000	H	3.534516000	1.566854000	-0.858928000
C	6.301651000	-1.632253000	0.412860000	C	4.835505000	-1.527805000	0.048339000
H	6.427756000	-0.276110000	2.196746000	H	4.105604000	0.094081000	1.310608000
H	5.995665000	-2.001856000	2.587863000	C	1.474646000	0.190176000	0.241700000
H	5.113041000	0.977329000	0.684966000	C	2.506364000	-2.146007000	-0.165077000
C	4.328999000	1.768388000	-1.743458000	C	3.849854000	-2.676533000	0.399799000
H	3.847512000	-0.446353000	-1.724576000	H	5.135294000	-1.603291000	-1.002435000
C	1.938366000	-0.150695000	0.049572000	H	5.745909000	-1.553186000	0.651333000
C	2.907726000	2.235098000	0.223896000	Au	-0.532111000	-0.186804000	0.054637000
Au	-0.051906000	0.191935000	0.238817000	H	1.724798000	1.232226000	0.482365000
H	2.237325000	-1.176967000	-0.161207000	H	1.635546000	-2.643555000	0.269989000
C	3.253975000	2.773011000	-1.198633000	H	2.474938000	-2.328556000	-1.250033000
H	1.900261000	2.528587000	0.529732000	C	5.680498000	1.904287000	-2.396107000
H	3.605839000	2.640144000	0.965164000	O	6.790614000	0.758496000	-0.464580000
O	3.949024000	-2.201337000	0.832491000	C	5.804578000	2.890929000	-1.342490000
H	6.417571000	-2.691879000	0.211367000	H	6.573260000	1.484037000	-2.847743000
H	6.900826000	-0.978278000	-0.214272000	H	4.763180000	1.813380000	-2.965736000
C	3.211848000	-2.349919000	2.060028000	C	7.295015000	1.087635000	0.857997000
P	-2.417238000	0.579534000	0.621348000	H	4.979116000	3.564897000	-1.139462000
C	-2.805245000	2.390947000	0.126742000	H	6.793129000	3.267176000	-1.099943000
C	-3.575851000	-0.495163000	-0.349225000	C	3.755733000	-2.849312000	1.927572000
C	-2.731572000	0.180691000	2.480369000	C	4.284530000	-3.995818000	-0.250355000
C	-4.290285000	2.799877000	0.176266000	P	-2.870526000	-0.767561000	-0.203197000
C	-1.987897000	3.338623000	1.028274000	C	-3.263813000	-2.124564000	1.109566000
C	-2.318895000	2.537428000	-1.332873000	C	-4.133482000	0.573520000	0.046960000
C	-3.150397000	-1.463418000	-1.293908000	C	-3.098900000	-1.343852000	-2.021155000
C	-4.957428000	-0.381720000	-0.088067000	C	8.623539000	0.379933000	1.031436000

C	-4.030707000	0.752166000	3.079227000	H	6.567569000	0.762977000	1.612309000
C	-1.540667000	0.713602000	3.309102000	H	7.407516000	2.176540000	0.938200000
C	-2.746285000	-1.359888000	2.588877000	H	9.342533000	0.712477000	0.278271000
H	-4.895274000	2.234537000	-0.535245000	H	8.503409000	-0.702930000	0.942789000
H	-4.363849000	3.856863000	-0.104332000	H	9.031654000	0.602314000	2.021416000
H	-4.731159000	2.699648000	1.170208000	C	-4.519540000	-2.981417000	0.862224000
H	-2.059670000	4.356302000	0.628155000	C	-2.046506000	-3.071437000	1.209080000
H	-2.370382000	3.366951000	2.051716000	C	-3.404141000	-1.379320000	2.455117000
H	-0.927947000	3.067419000	1.062222000	C	-3.799566000	1.922496000	0.323941000
H	-2.492349000	3.568002000	-1.663000000	C	-5.499696000	0.234453000	-0.040957000
H	-2.868784000	1.878518000	-2.011643000	C	-4.533335000	-1.698097000	-2.456188000
H	-1.250002000	2.325936000	-1.434622000	C	-2.179322000	-2.557100000	-2.271142000
C	-4.119972000	-2.274263000	-1.912298000	C	-2.613202000	-0.160125000	-2.888778000
C	-1.740695000	-1.723451000	-1.733372000	H	-5.440382000	-2.396323000	0.836106000
C	-5.900405000	-1.188738000	-0.717443000	H	-4.621307000	-3.693347000	1.689846000
H	-5.311124000	0.351295000	0.623496000	H	-4.449135000	-3.568288000	-0.057110000
C	-5.477412000	-2.147575000	-1.635349000	H	-2.238508000	-3.806193000	1.999923000
H	-3.786358000	-3.012889000	-2.634525000	H	-1.866171000	-3.623384000	0.284174000
C	-1.131112000	-0.920784000	-2.710949000	H	-1.132745000	-2.528921000	1.466304000
C	-1.074433000	-2.882724000	-1.303437000	H	-3.495137000	-2.116132000	3.261412000
H	-6.196044000	-2.789529000	-2.135383000	H	-4.289167000	-0.739058000	2.483512000
H	-6.954310000	-1.067660000	-0.487427000	H	-2.523680000	-0.763303000	2.667090000
C	0.114990000	-1.266631000	-3.240842000	C	-4.837361000	2.858713000	0.486695000
H	-1.650524000	-0.043044000	-3.082603000	C	-2.417444000	2.483927000	0.481533000
C	0.172714000	-3.225970000	-1.830107000	C	-6.512271000	1.173875000	0.130194000
H	-1.549554000	-3.528364000	-0.570438000	H	-5.784882000	-0.786165000	-0.253382000
C	0.769214000	-2.420667000	-2.803364000	H	-5.198270000	-0.832882000	-2.424765000
H	0.557375000	-0.649236000	-4.017549000	H	-4.975501000	-2.500640000	-1.862337000
H	1.723888000	-2.705788000	-3.236078000	H	-4.502520000	-2.044634000	-3.495910000
H	0.665321000	-4.135354000	-1.498643000	H	-2.546784000	-3.461467000	-1.778299000
H	-4.929281000	0.374205000	2.588688000	H	-2.150205000	-2.764007000	-3.347317000
H	-4.052163000	1.844666000	3.062895000	H	-1.153962000	-2.369144000	-1.937181000
H	-4.090974000	0.445758000	4.129799000	H	-3.227460000	0.732916000	-2.737715000
H	-1.458257000	1.801894000	3.282089000	H	-1.570978000	0.098681000	-2.680009000
H	-1.686556000	0.421128000	4.355172000	H	-2.690436000	-0.439634000	-3.946076000

H	-0.588722000	0.292393000	2.973652000	C	-6.178344000	2.500399000	0.393619000
H	-3.609753000	-1.802440000	2.087244000	H	-4.569976000	3.889775000	0.696897000
H	-1.837744000	-1.805586000	2.169402000	C	-1.824420000	2.556888000	1.751498000
H	-2.792926000	-1.638168000	3.647678000	C	-1.773309000	3.103622000	-0.599698000
C	2.298055000	-3.553262000	1.911072000	H	-7.551205000	0.867704000	0.055500000
H	2.632814000	-1.439510000	2.271508000	H	-6.952359000	3.249871000	0.528139000
H	3.908400000	-2.495213000	2.893854000	C	-0.614782000	3.228750000	1.935213000
H	2.880884000	-4.451929000	1.691041000	H	-2.326751000	2.104354000	2.601357000
H	1.574987000	-3.405055000	1.103322000	C	-0.562432000	3.773746000	-0.416711000
H	1.746112000	-3.719476000	2.841243000	H	-2.235053000	3.078677000	-1.582277000
H	5.333797000	2.116793000	-1.476832000	C	0.017473000	3.842442000	0.851774000
H	4.285300000	1.699893000	-2.833463000	H	-0.178717000	3.288082000	2.928210000
C	2.010818000	2.724543000	-2.105813000	H	-0.087643000	4.263029000	-1.262771000
H	1.223436000	3.379382000	-1.718324000	H	0.944191000	4.390018000	1.000707000
H	2.260272000	3.064542000	-3.116471000	H	3.041072000	-3.639645000	2.178764000
H	1.596421000	1.713771000	-2.182311000	H	4.725321000	-3.128586000	2.354374000
C	3.805594000	4.204267000	-1.148782000	H	3.412650000	-1.936822000	2.428087000
H	4.083370000	4.554447000	-2.148371000	H	4.358192000	-3.898516000	-1.339108000
H	3.055761000	4.897587000	-0.753631000	H	5.259410000	-4.324768000	0.126294000
H	4.693184000	4.269839000	-0.510231000	H	3.563179000	-4.790883000	-0.033834000
<b>Int2'''</b> E(RM06) = -1876.52065430				<b>TS<sub>2'''-3'</sub></b> E(RM06) = -1876.48829413 Frequency -128.7058			
C	-3.942314000	1.266959000	0.137984000	C	-4.350649000	1.276614000	-0.189799000
C	-3.975350000	0.835046000	-1.239177000	C	-4.247038000	1.482879000	2.044702000
C	-2.715403000	0.212289000	-0.397521000	C	-4.006092000	0.160084000	-1.081832000
C	-4.766797000	0.811450000	1.310746000	C	-5.405544000	1.475639000	0.712260000
H	-3.499753000	2.247371000	0.285413000	H	-3.641803000	2.100278000	-0.229457000
C	-4.743542000	-0.380554000	-1.750227000	C	-2.562408000	-0.338216000	-0.621925000
H	-3.671831000	1.578018000	-1.970987000	C	-4.874543000	-1.113158000	-1.128174000
C	-1.479057000	0.814326000	-0.428906000	H	-3.875029000	0.599083000	-2.081438000
C	-3.024516000	-1.266780000	-0.255217000	C	-1.475151000	0.436909000	-0.561448000
C	-3.858594000	-1.649286000	-1.508918000	C	-2.711187000	-1.827262000	-0.380502000
H	-5.683269000	-0.486295000	-1.209981000	O	-6.435762000	0.614958000	0.777764000
H	-4.970665000	-0.250352000	-2.811759000	C	-5.205048000	2.565241000	1.750569000
Au	0.367966000	0.030375000	-0.108572000	C	-3.872313000	-2.286796000	-1.296142000

H	-1.502712000	1.887907000	-0.638722000	H	-5.415887000	-1.241047000	-0.188746000
H	-2.093168000	-1.834195000	-0.185667000	H	-5.619595000	-1.074611000	-1.929000000
H	-3.600789000	-1.460381000	0.655236000	Au	0.455786000	-0.097696000	-0.119305000
C	-4.049042000	0.464107000	2.598111000	H	-1.606023000	1.496053000	-0.811337000
O	-5.906384000	0.049227000	1.054505000	H	-1.770613000	-2.349867000	-0.575577000
C	-4.806973000	1.754816000	2.512636000	H	-2.978749000	-2.024354000	0.669108000
H	-4.496387000	-0.342073000	3.170157000	C	-3.394167000	-2.395643000	-2.756432000
H	-2.963527000	0.490110000	2.596732000	C	-4.485051000	-3.618639000	-0.847381000
C	-7.061726000	0.796821000	0.626294000	P	2.694440000	-0.828061000	0.449922000
H	-4.254787000	2.688094000	2.455771000	H	-4.553866000	0.643114000	2.659174000
H	-5.752563000	1.819867000	3.039895000	H	-3.182214000	1.604717000	1.889030000
C	-2.928715000	-1.877376000	-2.714328000	C	-7.719206000	1.073220000	1.292731000
C	-4.723618000	-2.892290000	-1.265406000	H	-4.788999000	3.502877000	1.391651000
P	2.537965000	-0.956015000	0.327683000	H	-6.041474000	2.693824000	2.429476000
C	2.767462000	-2.402933000	-0.922525000	C	-8.760952000	0.059407000	0.864813000
C	3.998802000	0.166132000	0.117880000	H	-7.933051000	2.066787000	0.884637000
C	2.537658000	-1.489238000	2.170790000	H	-7.664008000	1.140328000	2.385800000
C	-8.233163000	-0.163859000	0.534903000	H	-2.659350000	-3.200675000	-2.862294000
H	-6.863414000	1.272146000	-0.345436000	H	-4.231472000	-2.618278000	-3.426751000
H	-7.266300000	1.596968000	1.348564000	H	-2.916947000	-1.473190000	-3.104408000
H	-8.422536000	-0.632220000	1.504446000	H	-4.826195000	-3.570875000	0.193192000
H	-8.042663000	-0.954779000	-0.196480000	H	-5.344034000	-3.890420000	-1.470842000
H	-9.134532000	0.374964000	0.228603000	H	-3.754798000	-4.431385000	-0.922575000
C	3.824967000	-3.455919000	-0.541400000	C	3.070091000	-2.392926000	-0.609148000
C	1.410082000	-3.120543000	-1.100422000	C	4.096867000	0.351165000	0.144318000
C	3.148347000	-1.747190000	-2.267658000	C	2.703429000	-1.148510000	2.344812000
C	3.892492000	1.536999000	-0.225867000	C	4.205491000	-3.304300000	-0.106880000
C	5.288122000	-0.374480000	0.306133000	C	1.781030000	-3.240774000	-0.705975000
C	3.874931000	-2.027713000	2.713621000	C	3.411142000	-1.876859000	-2.024407000
C	1.438504000	-2.551291000	2.376558000	C	3.919252000	1.666274000	-0.353587000
C	2.170470000	-0.218406000	2.970551000	C	5.410489000	-0.077290000	0.428017000
H	4.829304000	-3.039147000	-0.448843000	C	4.054162000	-1.537769000	2.976108000
H	3.866652000	-4.208351000	-1.337333000	C	1.664250000	-2.244129000	2.661251000
H	3.574978000	-3.981454000	0.383591000	C	2.243865000	0.181675000	2.983602000
H	1.526580000	-3.902817000	-1.859161000	H	-8.526671000	-0.931454000	1.262177000



H	1.062346000	-3.602399000	-0.184106000	H	-8.819765000	-0.002976000	-0.224493000
H	0.629923000	-2.434831000	-1.443474000	H	-9.739609000	0.361286000	1.248612000
H	3.162370000	-2.518279000	-3.046054000	H	5.176374000	-2.806245000	-0.084247000
H	4.136468000	-1.282610000	-2.236339000	H	4.301102000	-4.151388000	-0.796230000
H	2.419007000	-0.987204000	-2.568689000	H	3.998122000	-3.718012000	0.882988000
C	5.069759000	2.297402000	-0.348040000	H	1.972076000	-4.091160000	-1.371100000
C	2.625994000	2.292915000	-0.501535000	H	1.466879000	-3.643694000	0.259321000
C	6.440995000	0.393461000	0.171676000	H	0.949168000	-2.666629000	-1.123017000
H	5.400992000	-1.417318000	0.568326000	H	3.503185000	-2.733813000	-2.701491000
H	4.655928000	-1.265095000	2.707437000	H	4.355453000	-1.327623000	-2.048692000
H	4.235610000	-2.904213000	2.171742000	H	2.622018000	-1.227255000	-2.417653000
H	3.725408000	-2.330398000	3.756369000	C	5.050611000	2.484904000	-0.526064000
H	1.704649000	-3.512969000	1.929637000	C	2.619043000	2.303110000	-0.746184000
H	1.305249000	-2.719418000	3.451150000	C	6.518042000	0.744774000	0.241596000
H	0.475111000	-2.231198000	1.967166000	H	5.578274000	-1.074326000	0.810283000
H	2.903061000	0.581179000	2.824124000	H	4.791723000	-0.737007000	2.894990000
H	1.181878000	0.165924000	2.701060000	H	4.480788000	-2.450772000	2.554477000
H	2.157303000	-0.463733000	4.038612000	H	3.893632000	-1.720978000	4.045176000
C	6.331126000	1.743601000	-0.154055000	H	2.002286000	-3.235445000	2.346850000
H	4.978302000	3.347147000	-0.609140000	H	1.509809000	-2.284282000	3.745847000
C	2.136920000	2.395382000	-1.814073000	H	0.696860000	-2.040943000	2.191134000
C	2.015743000	3.055207000	0.506695000	H	2.941925000	0.996577000	2.768524000
H	7.414140000	-0.062956000	0.323360000	H	1.250160000	0.478453000	2.635188000
H	7.217860000	2.360867000	-0.260252000	H	2.202994000	0.059223000	4.072334000
C	1.062408000	3.237038000	-2.110359000	C	6.336543000	2.040846000	-0.235793000
H	2.621299000	1.835627000	-2.608816000	H	4.902374000	3.491220000	-0.905609000
C	0.940783000	3.896907000	0.210611000	C	2.147415000	2.197340000	-2.064003000
H	2.403683000	3.009796000	1.520047000	C	1.950369000	3.158158000	0.142502000
C	0.464732000	3.994225000	-1.099382000	H	7.511601000	0.372348000	0.471412000
H	0.711593000	3.320134000	-3.134992000	H	7.186357000	2.699962000	-0.385020000
H	0.495563000	4.496910000	0.999146000	C	1.031585000	2.924848000	-2.481238000
H	-0.348052000	4.675270000	-1.335804000	H	2.672918000	1.560444000	-2.769501000
H	-2.270853000	-2.735457000	-2.539782000	C	0.833668000	3.885190000	-0.274517000
H	-3.510011000	-2.081963000	-3.619456000	H	2.322077000	3.270459000	1.156794000
H	-2.294393000	-1.006405000	-2.914055000	C	0.373874000	3.773858000	-1.588455000

H	-5.388243000	-2.746114000	-0.407716000	H	0.689483000	2.842269000	-3.508723000
H	-5.341297000	-3.119283000	-2.140961000	H	0.340695000	4.557968000	0.421963000
H	-4.100183000	-3.770930000	-1.067721000	H	-0.476936000	4.361483000	-1.922175000
<b>Int3'</b> E(RM06) = -1876.52516593				<b>TS<sub>3-4'</sub></b> E(RM06) = -1876.52223973 Frequency -166.1114			
C	-1.920381000	-0.056175000	-0.172021000	C	-2.010931000	0.491728000	-0.300766000
C	-4.300996000	1.562451000	0.943924000	C	-3.137005000	1.446212000	1.164018000
Au	0.105409000	-0.325787000	0.004337000	Au	-0.070082000	-0.129374000	0.056105000
C	-2.899421000	-0.971096000	-0.240356000	C	-3.107247000	-0.316557000	-0.521371000
H	-2.235114000	0.995815000	-0.243427000	H	-2.095674000	1.473048000	-0.773227000
O	-4.408324000	2.651093000	0.298784000	O	-2.775345000	2.717300000	1.144949000
C	-4.986388000	0.269328000	0.691667000	C	-4.577331000	1.066625000	0.738273000
C	-3.725435000	1.179489000	2.261980000	C	-3.173093000	0.587236000	2.428090000
P	2.462978000	-0.834821000	0.282130000	P	2.165812000	-0.945531000	0.490920000
C	-4.388943000	-0.641798000	-0.432690000	C	-4.511577000	0.287062000	-0.588740000
C	-2.765073000	-2.485047000	-0.217950000	C	-3.228982000	-1.804012000	-0.509285000
C	-3.681631000	3.874847000	0.740356000	C	-1.559067000	3.139242000	1.827506000
C	-4.628979000	-0.095041000	2.174487000	C	-4.651331000	0.232605000	2.062451000
H	-6.051776000	0.417129000	0.472969000	H	-5.261864000	1.918850000	0.710566000
H	-2.660857000	0.924095000	2.149584000	H	-2.478572000	-0.252967000	2.453531000
H	-3.849838000	1.885900000	3.088535000	H	-3.054216000	1.171942000	3.345181000
C	2.869750000	-2.271143000	-0.926242000	C	2.266402000	-2.733272000	-0.200150000
C	3.702430000	0.505244000	-0.074832000	C	3.556376000	-0.005189000	-0.302673000
C	2.710597000	-1.284959000	2.142975000	C	2.458899000	-0.831537000	2.393401000
C	-5.104774000	-2.009467000	-0.487295000	C	-5.469867000	-0.909178000	-0.793681000
H	-4.538460000	-0.095035000	-1.371890000	H	-4.576797000	0.997237000	-1.422285000
C	-4.021607000	-3.020208000	-0.953480000	C	-4.569062000	-2.100568000	-1.245718000
H	-1.827648000	-2.821837000	-0.669797000	H	-2.351486000	-2.303586000	-0.931150000
H	-2.769624000	-2.852379000	0.819933000	H	-3.300910000	-2.136116000	0.541768000
C	-4.360856000	5.062367000	0.099635000	C	-1.650260000	4.635701000	2.050135000
H	-2.652638000	3.732913000	0.400274000	H	-0.720008000	2.868776000	1.179095000
H	-3.713420000	3.901077000	1.831797000	H	-1.467109000	2.590874000	2.770129000
H	-5.486266000	-0.058876000	2.847345000	H	-5.379045000	0.624200000	2.774682000
H	-4.088702000	-1.032787000	2.297317000	H	-4.835214000	-0.835681000	1.935162000
H	-5.396421000	5.158586000	0.434816000	H	-2.497035000	4.888643000	2.693527000

H	-4.344273000	4.984542000	-0.990057000	H	-1.764552000	5.165059000	1.100528000
H	-3.823019000	5.970649000	0.387163000	H	-0.734343000	4.988519000	2.533181000
C	1.994347000	-3.485910000	-0.554668000	C	1.23251000	-3.607913000	0.542507000
C	2.456331000	-1.764656000	-2.326639000	C	1.859363000	-2.629757000	-1.686927000
C	4.343511000	-2.715823000	-0.997554000	C	3.649332000	-3.409677000	-0.131761000
C	3.356056000	1.814733000	-0.496859000	C	3.365833000	1.111346000	-1.156441000
C	5.065257000	0.227095000	0.159859000	C	4.879214000	-0.386726000	0.004543000
C	1.488394000	-2.103376000	2.617441000	C	1.142345000	-1.204040000	3.113398000
C	2.713650000	0.059283000	2.903647000	C	2.767152000	0.651641000	2.693249000
C	3.983592000	-2.076848000	2.495837000	C	3.581942000	-1.715481000	2.968305000
H	2.067227000	-4.233092000	-1.353205000	H	1.151351000	-4.571443000	0.026988000
H	2.328569000	-3.965455000	0.369155000	H	1.536575000	-3.818370000	1.572108000
H	0.939830000	-3.214727000	-0.444570000	H	0.241540000	-3.148796000	0.558052000
H	2.639085000	-2.558665000	-3.059848000	H	1.873943000	-3.632432000	-2.129505000
H	3.045244000	-0.894202000	-2.632600000	H	2.558297000	-2.009307000	-2.255850000
H	1.395255000	-1.501465000	-2.370379000	H	0.852476000	-2.219591000	-1.810110000
H	4.993244000	-1.925237000	-1.377959000	H	4.388495000	-2.893834000	-0.747701000
H	4.414702000	-3.556874000	-1.697100000	H	3.553675000	-4.427800000	-0.526711000
H	4.735638000	-3.061959000	-0.038665000	H	4.037701000	-3.494132000	0.885232000
C	4.378650000	2.772168000	-0.639845000	C	4.497480000	1.796113000	-1.636949000
C	1.986571000	2.318622000	-0.837396000	C	2.054307000	1.656479000	-1.637599000
C	6.062123000	1.185662000	0.002968000	C	5.985119000	0.299616000	-0.488351000
H	5.361642000	-0.762193000	0.477281000	H	5.057465000	-1.240050000	0.643725000
H	1.415104000	-3.075014000	2.124941000	H	0.839210000	-2.237370000	2.932681000
H	1.588349000	-2.286599000	3.693768000	H	1.289563000	-1.087622000	4.193453000
H	0.550453000	-1.567114000	2.449368000	H	0.318299000	-0.551428000	2.811790000
H	3.596331000	0.661958000	2.676878000	H	3.730356000	0.965541000	2.285195000
H	1.822120000	0.653650000	2.675600000	H	1.992537000	1.314183000	2.291946000
H	2.712624000	-0.142485000	3.981070000	H	2.798227000	0.794731000	3.779369000
H	4.902378000	-1.539583000	2.255211000	H	4.565114000	-1.480575000	2.557891000
H	4.011379000	-3.057189000	2.013573000	H	3.386539000	-2.781300000	2.827571000
H	3.993723000	-2.251878000	3.578085000	H	3.640926000	-1.540564000	4.048931000
C	5.714904000	2.474043000	-0.395663000	C	5.792716000	1.405936000	-1.312717000
H	4.104081000	3.770058000	-0.967455000	H	4.341700000	2.649192000	-2.290077000
C	1.397202000	3.311234000	-0.038978000	C	1.564567000	2.866680000	-1.119860000

C	1.355397000	1.963917000	-2.040460000	C	1.392502000	1.077405000	-2.731680000
H	7.098082000	0.923771000	0.194729000	H	6.985758000	-0.029543000	-0.226067000
H	6.474820000	3.239075000	-0.522211000	H	6.641101000	1.957848000	-1.705514000
C	0.212651000	3.935917000	-0.435009000	C	0.435529000	3.474429000	-1.673807000
H	1.887460000	3.613184000	0.881976000	H	2.090938000	3.344290000	-0.298106000
C	0.171449000	2.587040000	-2.437158000	C	0.265113000	1.686191000	-3.286908000
H	1.812423000	1.220116000	-2.684617000	H	1.781110000	0.163126000	-3.169057000
C	-0.400488000	3.580314000	-1.638896000	C	-0.216762000	2.886768000	-2.760426000
H	-0.203999000	4.729153000	0.181106000	H	0.084344000	4.422636000	-1.276121000
H	-0.289614000	2.312568000	-3.381130000	H	-0.221042000	1.233826000	-4.146354000
H	-1.299156000	4.093009000	-1.971995000	H	-1.077152000	3.374056000	-3.209878000
H	-5.987781000	-2.000105000	-1.134949000	H	-6.250653000	-0.694059000	-1.528130000
H	-5.443953000	-2.294166000	0.517628000	H	-5.979394000	-1.164848000	0.141291000
C	-4.373501000	-4.458669000	-0.556155000	C	-5.159552000	-3.460268000	-0.855735000
H	-5.294271000	-4.791997000	-1.047401000	H	-6.121200000	-3.625085000	-1.352785000
H	-3.576548000	-5.151415000	-0.847442000	H	-4.494025000	-4.279728000	-1.147627000
H	-4.517409000	-4.550781000	0.526411000	H	-5.326017000	-3.530262000	0.225122000
C	-3.825483000	-2.933397000	-2.479459000	C	-4.337408000	-2.044093000	-2.768594000
H	-3.036639000	-3.619599000	-2.805402000	H	-3.640222000	-2.825980000	-3.088262000
H	-4.744534000	-3.207485000	-3.008854000	H	-5.277634000	-2.192861000	-3.308978000
H	-3.536623000	-1.927167000	-2.801431000	H	-3.920855000	-1.080558000	-3.085346000
<b>Int4'</b> E(RM06) = -1876.58516266				<b>Int5</b> E(RM06) = -1952.94969423			
C	-2.334370000	0.695806000	-0.073754000	C	4.340202000	-0.513627000	-0.218231000
C	-3.125544000	0.868307000	1.249143000	O	3.274328000	2.433117000	0.605086000
Au	-0.170074000	-0.137553000	0.154544000	C	3.924254000	-1.514762000	-1.157443000
C	-2.763140000	-0.447674000	-0.710787000	C	4.721604000	-0.783890000	1.207490000
H	-1.903915000	1.549445000	-0.599774000	H	4.821433000	0.369948000	-0.632880000
O	-4.058537000	1.915026000	1.143361000	H	3.425242000	1.718295000	1.243982000
C	-3.764280000	-0.543462000	1.471427000	H	2.318833000	2.447570000	0.467888000
C	-2.354742000	0.701111000	2.589548000	C	2.758132000	-0.399710000	-0.710436000
P	2.111867000	-0.668140000	0.524672000	C	4.109108000	-1.294186000	-2.652652000
C	-3.749161000	-1.235905000	0.105806000	H	3.730027000	-2.519885000	-0.796654000
C	-2.539600000	-1.163502000	-2.013805000	C	1.782064000	-0.806955000	0.171999000
C	-3.537284000	3.237426000	1.296345000	C	2.565642000	0.470747000	-1.939901000
				C	2.929546000	-0.404812000	-3.170055000

C	-2.680245000	-0.819884000	2.550964000	H	5.064972000	-0.787515000	-2.823817000
H	-4.762127000	-0.472481000	1.907056000	H	4.146295000	-2.251775000	-3.178893000
H	-1.304775000	1.007151000	2.628922000	Au	-0.228192000	-0.502308000	0.217599000
H	-2.899903000	1.202438000	3.394184000	H	2.151149000	-1.472821000	0.953171000
C	2.446658000	-2.395487000	-0.245255000	H	1.535064000	0.833099000	-1.982471000
C	3.301140000	0.508825000	-0.269055000	H	3.212019000	1.352052000	-1.868744000
C	2.396517000	-0.546108000	2.427148000	C	5.859721000	-1.759383000	1.466319000
C	-3.365962000	-2.686546000	-0.219411000	C	4.457204000	-2.107445000	1.885308000
H	-4.724503000	-1.042375000	-0.372440000	O	4.617189000	0.337252000	2.050325000
C	-3.037234000	-2.644789000	-1.755102000	H	6.291835000	-2.278223000	0.616253000
H	-3.146321000	-0.678762000	-2.790940000	H	6.569118000	-1.497654000	2.243345000
H	-1.504426000	-1.116000000	-2.359676000	H	4.219306000	-2.039649000	2.941537000
C	-4.700867000	4.211091000	1.218375000	H	3.943074000	-2.904441000	1.356927000
H	-2.800359000	3.454066000	0.507545000	C	5.752727000	1.239731000	2.058287000
H	-3.020575000	3.327670000	2.263327000	C	3.357685000	0.441771000	-4.375643000
H	-3.035498000	-1.263105000	3.483476000	C	1.738610000	-1.302034000	-3.554508000
H	-1.851976000	-1.428685000	2.177567000	P	-2.647980000	-0.786569000	0.338442000
H	-5.428092000	4.003179000	2.007843000	C	-3.001123000	-1.548711000	2.075006000
H	-5.209211000	4.128825000	0.253607000	C	-3.778617000	0.670058000	0.149889000
H	-4.344798000	5.238870000	1.337119000	C	-3.073582000	-1.947594000	-1.134029000
C	1.558933000	-3.437695000	0.463738000	C	5.490868000	2.312088000	3.099944000
C	2.032306000	-2.285418000	-1.728640000	H	5.876799000	1.688849000	1.064924000
C	3.914838000	-2.862679000	-0.193984000	H	6.659753000	0.672906000	2.295566000
C	2.930475000	1.627648000	-1.057823000	H	5.322137000	1.863870000	4.083070000
C	4.673744000	0.297463000	-0.015630000	H	4.621663000	2.914423000	2.824669000
C	1.226343000	-1.238176000	3.157967000	H	6.357708000	2.976148000	3.167140000
C	2.365514000	0.961672000	2.761617000	C	-4.319104000	-2.336721000	2.208337000
C	3.713864000	-1.157347000	2.943391000	C	-1.838849000	-2.497191000	2.448690000
H	1.584646000	-4.371184000	-0.109052000	C	-3.001052000	-0.369589000	3.071518000
H	1.918717000	-3.667307000	1.469938000	C	-3.339550000	1.980965000	-0.158857000
H	0.514937000	-3.117054000	0.533485000	C	-5.166107000	0.445374000	0.273008000
H	2.194481000	-3.254700000	-2.213045000	C	-4.567935000	-2.265361000	-1.333451000
H	2.633556000	-1.544872000	-2.264273000	C	-2.297576000	-3.270615000	-0.970096000
H	0.976116000	-2.027028000	-1.845200000	C	-2.566315000	-1.210624000	-2.394036000
H	4.568846000	-2.232637000	-0.799355000	H	-5.205401000	-1.725175000	2.032225000

H	3.963264000	-3.874472000	-0.611753000	H	-4.393776000	-2.709631000	3.236289000
H	4.313542000	-2.914254000	0.821012000	H	-4.355011000	-3.207921000	1.549274000
C	3.944721000	2.480001000	-1.533507000	H	-2.028048000	-2.901361000	3.449671000
C	1.547423000	2.026300000	-1.480055000	H	-1.744587000	-3.343912000	1.765463000
C	5.659207000	1.149770000	-0.503714000	H	-0.878952000	-1.974119000	2.478623000
H	4.988982000	-0.550027000	0.575933000	H	-3.083298000	-0.766747000	4.089380000
H	1.195456000	-2.315211000	2.982584000	H	-3.838858000	0.312189000	2.908371000
H	1.354412000	-1.086317000	4.235368000	H	-2.070289000	0.205669000	3.018034000
H	0.259484000	-0.815943000	2.876859000	C	-4.304600000	2.985408000	-0.364885000
H	3.208096000	1.501172000	2.322581000	C	-1.922686000	2.455714000	-0.259497000
H	1.437642000	1.436226000	2.424669000	C	-6.102419000	1.457366000	0.085796000
H	2.421180000	1.080060000	3.849267000	H	-5.531245000	-0.544130000	0.508113000
H	4.600391000	-0.678206000	2.526132000	H	-5.147744000	-1.377672000	-1.592141000
H	3.773301000	-2.234208000	2.768503000	H	-5.024782000	-2.742369000	-0.463927000
H	3.754478000	-1.007053000	4.028003000	H	-4.659054000	-2.965869000	-2.171514000
C	5.291076000	2.255531000	-1.266146000	H	-2.692171000	-3.881271000	-0.153545000
H	3.653697000	3.333525000	-2.137561000	H	-2.399565000	-3.855666000	-1.890995000
C	0.941300000	3.154438000	-0.902845000	H	-1.229316000	-3.106847000	-0.796826000
C	0.936247000	1.431962000	-2.597909000	H	-3.071891000	-0.250573000	-2.535009000
H	6.703026000	0.948199000	-0.284894000	H	-1.487986000	-1.028493000	-2.357096000
H	6.042783000	2.935758000	-1.654194000	H	-2.774822000	-1.828497000	-3.274863000
C	-0.244924000	3.673559000	-1.426967000	C	-5.667997000	2.738472000	-0.247181000
H	1.420317000	3.644112000	-0.059844000	H	-3.959482000	3.986643000	-0.602845000
C	-0.248099000	1.953676000	-3.123404000	C	-1.174305000	2.725694000	0.897062000
H	1.415923000	0.587995000	-3.084394000	C	-1.405287000	2.848621000	-1.505041000
C	-0.840520000	3.078035000	-2.542071000	H	-7.160519000	1.240234000	0.193323000
H	-0.686827000	4.559944000	-0.981451000	H	-6.381404000	3.541285000	-0.405520000
H	-0.690634000	1.500101000	-4.005481000	C	0.049881000	3.395486000	0.811147000
H	-1.746564000	3.499057000	-2.967384000	H	-1.579576000	2.464343000	1.870077000
H	-4.153786000	-3.409528000	0.008764000	C	-0.178433000	3.507392000	-1.591973000
H	-2.474373000	-2.975603000	0.351028000	H	-1.985967000	2.663581000	-2.404215000
C	-1.958634000	-3.671942000	-2.123389000	C	0.545577000	3.797967000	-0.432489000
H	-2.291750000	-4.687697000	-1.884956000	H	0.599529000	3.632650000	1.717712000
H	-1.731023000	-3.642652000	-3.194782000	H	0.196515000	3.823252000	-2.561110000
H	-1.028609000	-3.489400000	-1.574232000	H	1.482655000	4.343350000	-0.494311000

C	-4.308004000	-2.922643000	-2.581328000	H	3.662394000	-0.191388000	-5.215580000
H	-4.106287000	-2.818974000	-3.652960000	H	2.531483000	1.071796000	-4.721454000
H	-4.669836000	-3.941091000	-2.407773000	H	4.197784000	1.098030000	-4.124262000
H	-5.121166000	-2.232589000	-2.330605000	H	2.006658000	-1.972958000	-4.377456000
				H	1.403018000	-1.918758000	-2.713498000
				H	0.888319000	-0.694830000	-3.882054000
<b>TS<sub>5-6</sub></b> E(RM06) = -1952.92780272 Frequency -118.5264				<b>Int6</b> E(RM06) = -1952.94500758			
C	4.697459000	-0.085237000	0.001804000	C	4.508509000	0.005276000	-0.250418000
O	3.402444000	1.656312000	-0.651474000	O	3.440987000	0.764861000	-1.013115000
C	3.912744000	-1.319415000	0.146842000	C	3.953643000	-1.405412000	0.053217000
C	5.329735000	0.635665000	1.071150000	C	4.879497000	0.938376000	0.897694000
H	5.015331000	0.171197000	-1.001914000	H	5.323603000	-0.047279000	-0.974966000
H	3.597271000	2.366009000	-0.022069000	H	3.541966000	1.702696000	-0.682517000
H	2.496621000	1.341416000	-0.469473000	H	2.543260000	0.335149000	-0.698646000
C	2.385425000	-1.103675000	-0.241825000	C	2.407135000	-1.465035000	-0.045179000
C	4.396575000	-2.427087000	-0.844768000	C	4.441850000	-2.479184000	-0.948607000
H	3.933921000	-1.672070000	1.180121000	H	4.266743000	-1.673776000	1.067268000
C	1.513283000	-0.438659000	0.527312000	C	1.548704000	-0.608564000	0.555682000
C	2.146474000	-1.915884000	-1.494746000	C	2.049980000	-2.602301000	-0.987905000
C	3.119143000	-3.113743000	-1.398493000	C	3.298008000	-3.519830000	-1.037487000
H	4.947441000	-1.970036000	-1.675684000	H	4.582587000	-2.019789000	-1.936243000
H	5.079406000	-3.128664000	-0.355285000	H	5.400035000	-2.922289000	-0.657823000
Au	-0.535077000	-0.353800000	0.334510000	Au	-0.495675000	-0.511044000	0.379851000
H	1.929199000	0.050797000	1.413651000	H	1.998718000	0.115978000	1.241126000
H	1.097081000	-2.211333000	-1.574534000	H	1.143883000	-3.120208000	-0.661566000
H	2.388600000	-1.321492000	-2.388730000	H	1.845712000	-2.204710000	-1.992817000
C	6.084297000	-0.238307000	2.144236000	C	5.892384000	0.546306000	1.935902000
C	4.862825000	0.494643000	2.525982000	C	4.444363000	0.737115000	2.324029000
O	5.874789000	1.879388000	0.793311000	O	4.818544000	2.282873000	0.442313000
H	6.058180000	-1.317195000	2.039094000	H	6.295646000	-0.461935000	1.904661000
H	7.049224000	0.185640000	2.401769000	H	6.604365000	1.301965000	2.250270000
H	4.975729000	1.418870000	3.082422000	H	4.189493000	1.642604000	2.864152000
H	3.951250000	-0.058942000	2.719126000	H	3.852724000	-0.132837000	2.586326000
C	7.035526000	1.911264000	-0.066175000	C	6.007817000	2.802750000	-0.211205000

C	3.383849000	-3.772531000	-2.758525000	C	3.373811000	-4.342542000	-2.329533000
C	2.593693000	-4.161921000	-0.399299000	C	3.321112000	-4.461535000	0.182511000
P	-2.953084000	-0.529431000	0.316401000	P	-2.907801000	-0.493523000	0.228399000
C	-3.468217000	-0.881011000	2.143134000	C	-3.596283000	-0.865489000	1.987957000
C	-3.948160000	0.949351000	-0.207711000	C	-3.711229000	1.087186000	-0.326268000
C	-3.405524000	-1.932096000	-0.914354000	C	-3.376474000	-1.799094000	-1.101516000
C	7.544998000	3.339502000	-0.101967000	C	5.741046000	4.247912000	-0.585497000
H	6.764150000	1.572164000	-1.074806000	H	6.242868000	2.199573000	-1.098383000
H	7.796299000	1.225378000	0.329811000	H	6.850060000	2.722647000	0.483233000
H	7.824117000	3.677391000	0.899466000	H	5.496724000	4.838376000	0.301356000
H	6.780754000	4.014436000	-0.496790000	H	4.915049000	4.330305000	-1.298728000
H	8.425594000	3.403100000	-0.747364000	H	6.632007000	4.678363000	-1.051492000
C	-4.876124000	-1.467461000	2.360085000	C	-5.064605000	-1.324883000	2.060928000
C	-2.444202000	-1.855043000	2.769282000	C	-2.715323000	-1.952023000	2.646157000
C	-3.356442000	0.474336000	2.875699000	C	-3.426221000	0.443220000	2.789820000
C	-3.375089000	2.176654000	-0.626029000	C	-2.992309000	2.254704000	-0.687248000
C	-5.353945000	0.871621000	-0.120897000	C	-5.117910000	1.120660000	-0.425625000
C	-4.908115000	-2.194024000	-1.132165000	C	-4.870421000	-1.925208000	-1.456386000
C	-2.729022000	-3.237206000	-0.446732000	C	-2.852925000	-3.173729000	-0.637145000
C	-2.795883000	-1.504746000	-2.268419000	C	-2.615896000	-1.372676000	-2.378060000
H	-5.673187000	-0.808628000	2.012383000	H	-5.764430000	-0.579054000	1.679685000
H	-5.029317000	-1.607363000	3.436533000	H	-5.323187000	-1.493122000	3.112844000
H	-4.997069000	-2.447176000	1.890578000	H	-5.232030000	-2.268323000	1.535459000
H	-2.688614000	-1.980522000	3.830517000	H	-3.053845000	-2.095238000	3.678887000
H	-2.467592000	-2.845141000	2.309212000	H	-2.788565000	-2.917848000	2.142028000
H	-1.421807000	-1.473795000	2.701971000	H	-1.661049000	-1.662971000	2.675719000
H	-3.506575000	0.310415000	3.948899000	H	-3.695750000	0.256461000	3.835481000
H	-4.108841000	1.190706000	2.537476000	H	-4.068404000	1.244885000	2.416267000
H	-2.366847000	0.925352000	2.744565000	H	-2.388215000	0.792116000	2.773311000
C	-4.227652000	3.259570000	-0.912339000	C	-3.706213000	3.372225000	-1.158619000
C	-1.917777000	2.464583000	-0.825150000	C	-1.510052000	2.468741000	-0.586882000
C	-6.180190000	1.951303000	-0.418464000	C	-5.806920000	2.242283000	-0.878126000
H	-5.820984000	-0.051992000	0.189348000	H	-5.695037000	0.248848000	-0.151590000
H	-5.416083000	-1.334261000	-1.573419000	H	-5.259520000	-1.020007000	-1.926277000
H	-5.431104000	-2.479370000	-0.216863000	H	-5.497832000	-2.172234000	-0.597284000



H	-5.013314000	-3.027762000	-1.836181000	H	-4.982685000	-2.739208000	-2.181996000
H	-3.209607000	-3.654494000	0.442268000	H	-3.449348000	-3.583833000	0.182155000
H	-2.815394000	-3.985748000	-1.242780000	H	-2.920715000	-3.879874000	-1.472666000
H	-1.665236000	-3.096129000	-0.231179000	H	-1.806948000	-3.130313000	-0.317718000
H	-3.249927000	-0.582053000	-2.642572000	H	-2.934182000	-0.387079000	-2.731467000
H	-1.713801000	-1.356496000	-2.203733000	H	-1.533311000	-1.349725000	-2.221221000
H	-2.987608000	-2.290117000	-3.008638000	H	-2.828397000	-2.094476000	-3.175178000
C	-5.611339000	3.160222000	-0.812251000	C	-5.093719000	3.376381000	-1.258700000
H	-3.778516000	4.194844000	-1.231826000	H	-3.146081000	4.259915000	-1.435885000
C	-1.243941000	3.309023000	0.071093000	C	-0.936539000	2.886606000	0.625521000
C	-1.259269000	2.066085000	-1.999093000	C	-0.710743000	2.457331000	-1.739668000
H	-7.257573000	1.844813000	-0.338046000	H	-6.890801000	2.223056000	-0.935850000
H	-6.236454000	4.016930000	-1.044750000	H	-5.610015000	4.259633000	-1.621990000
C	0.054240000	3.745504000	-0.199785000	C	0.398467000	3.287804000	0.682538000
H	-1.751814000	3.644119000	0.970813000	H	-1.552338000	2.931386000	1.518555000
C	0.036819000	2.505390000	-2.272295000	C	0.625895000	2.860680000	-1.685499000
H	-1.778762000	1.439840000	-2.717431000	H	-1.147240000	2.159851000	-2.688439000
C	0.695029000	3.352621000	-1.377289000	C	1.181391000	3.285285000	-0.475215000
H	0.549887000	4.417044000	0.496025000	H	0.816223000	3.633721000	1.623539000
H	0.521903000	2.207959000	-3.197455000	H	1.217061000	2.876039000	-2.597325000
H	1.692547000	3.713836000	-1.608193000	H	2.202643000	3.658439000	-0.434553000
H	4.134182000	-4.566214000	-2.675816000	H	4.292253000	-4.938311000	-2.364992000
H	2.469495000	-4.225492000	-3.155568000	H	2.529411000	-5.036030000	-2.402941000
H	3.742936000	-3.043533000	-3.493475000	H	3.356304000	-3.697665000	-3.215322000
H	3.323486000	-4.966235000	-0.257105000	H	4.248402000	-5.043768000	0.210316000
H	2.375431000	-3.724424000	0.580565000	H	3.236233000	-3.918275000	1.130166000
H	1.668133000	-4.615291000	-0.769019000	H	2.486069000	-5.168361000	0.138265000
<b>TS<sub>6'</sub></b> E(RM06) = -1952.92382092 Frequency -28.1258				<b>Int6'</b> E(RM06) = -1952.92784106			
C	4.888525000	-0.030375000	-0.115103000	O	-5.997981000	0.625373000	-0.943768000
O	4.634441000	0.744215000	1.093200000	C	-4.590518000	0.543596000	-0.518404000
C	3.881379000	0.288779000	-1.245173000	C	-3.930169000	-0.714413000	-1.091421000
C	5.004961000	-1.466591000	0.404536000	C	-4.648460000	0.753130000	1.010434000
H	5.892227000	0.276991000	-0.432333000	H	-4.122166000	1.426637000	-0.963138000
H	5.290795000	-0.353802000	1.920353000	H	-6.318955000	-0.272556000	-1.124500000

H	3.663524000	0.796253000	1.185973000	C	-2.477622000	-0.960183000	-0.624399000
C	2.481561000	0.670619000	-0.716716000	C	-4.676017000	-2.043633000	-0.813887000
C	4.338811000	1.541775000	-2.063302000	H	-3.924185000	-0.543036000	-2.175848000
H	3.832794000	-0.592861000	-1.887886000	C	-3.524723000	1.050670000	1.946219000
C	1.448779000	-0.171991000	-0.567185000	C	-4.349869000	-0.206828000	2.120028000
C	2.431380000	2.191177000	-0.652807000	O	-5.908796000	1.527822000	1.237430000
C	3.267652000	2.671821000	-1.869800000	H	-6.385871000	1.219094000	0.355012000
H	5.330908000	1.887778000	-1.736313000	C	-1.493178000	-0.048585000	-0.668417000
H	4.434989000	1.280396000	-3.122403000	C	-2.374017000	-2.422029000	-0.210887000
Au	-0.483109000	0.188067000	0.010533000	C	-3.574510000	-3.141117000	-0.878283000
H	1.645994000	-1.220141000	-0.815808000	H	-5.124459000	-2.045750000	0.187274000
H	1.400123000	2.548642000	-0.685459000	H	-5.480355000	-2.248435000	-1.533620000
H	2.880130000	2.600464000	0.261316000	Au	0.484633000	-0.260300000	-0.173220000
C	5.300861000	-2.716259000	-0.358131000	H	-1.771055000	0.944886000	-1.038998000
C	3.992647000	-2.565402000	0.398552000	H	-1.411506000	-2.855215000	-0.497170000
O	5.672708000	-1.310783000	1.732426000	H	-2.445858000	-2.528782000	0.882801000
H	5.300807000	-2.640943000	-1.441855000	C	-3.996753000	-4.413532000	-0.133972000
H	6.036778000	-3.412076000	0.038444000	C	-3.243393000	-3.481704000	-2.344442000
H	3.888887000	-3.132861000	1.313078000	P	2.802945000	-0.625716000	0.458957000
H	3.075572000	-2.398511000	-0.147846000	H	-2.525406000	0.949246000	1.535239000
C	7.168842000	-1.299982000	1.794355000	H	-3.653253000	1.841089000	2.679079000
C	3.937384000	4.030188000	-1.602358000	H	-5.055902000	-0.239658000	2.943688000
C	2.367586000	2.766776000	-3.120901000	H	-3.895119000	-1.154578000	1.862128000
P	-2.764223000	0.609341000	0.717073000	C	-5.835305000	3.023047000	1.250239000
C	-3.244397000	2.369307000	0.094184000	C	-7.249148000	3.557092000	1.202734000
C	-4.085568000	-0.538843000	0.091435000	H	-5.227582000	3.332272000	0.396628000
C	-2.796973000	0.430437000	2.627860000	H	-5.322789000	3.270961000	2.178159000
C	7.573296000	-0.895859000	3.194034000	H	-4.874911000	-4.875624000	-0.598801000
H	7.524832000	-0.606696000	1.028317000	H	-3.191579000	-5.155673000	-0.144566000
H	7.466044000	-2.317075000	1.545950000	H	-4.241777000	-4.203375000	0.913706000
H	7.144144000	-1.567076000	3.938061000	H	-4.119601000	-3.885552000	-2.863933000
H	7.276886000	0.136352000	3.421438000	H	-2.890218000	-2.607604000	-2.901146000
H	8.663554000	-0.949054000	3.269836000	H	-2.452618000	-4.237454000	-2.390274000
C	-4.408896000	3.067685000	0.825967000	C	3.404805000	-2.209511000	-0.462378000
C	-1.996082000	3.273741000	0.217347000	C	4.043081000	0.703664000	0.068129000

C	-3.591938000	2.221954000	-1.404835000	C	2.830501000	-0.788009000	2.372974000
C	-3.807326000	-1.672299000	-0.711466000	C	4.628397000	-2.931804000	0.133233000
C	-5.428726000	-0.273648000	0.425676000	C	2.231934000	-3.215168000	-0.514738000
C	-4.168575000	0.557971000	3.313188000	C	3.722686000	-1.769151000	-1.908101000
C	-1.827331000	1.465204000	3.233600000	C	3.697430000	1.946993000	-0.518059000
C	-2.254951000	-0.989954000	2.910597000	C	5.398438000	0.476801000	0.385597000
H	-5.354199000	2.532729000	0.720052000	C	4.212256000	-0.940201000	3.036098000
H	-4.555018000	4.058322000	0.381606000	C	1.941453000	-1.983614000	2.773244000
H	-4.202532000	3.220932000	1.889593000	C	2.187221000	0.514616000	2.901442000
H	-2.231532000	4.256450000	-0.208070000	H	-7.838304000	3.195079000	2.048762000
H	-1.687216000	3.427789000	1.253620000	H	-7.753126000	3.289095000	0.269214000
H	-1.143347000	2.867122000	-0.335995000	H	-7.209743000	4.649088000	1.256304000
H	-3.750745000	3.223501000	-1.825926000	H	5.526384000	-2.311640000	0.152049000
H	-4.504966000	1.641151000	-1.561204000	H	4.858274000	-3.800241000	-0.495473000
H	-2.781156000	1.749742000	-1.964670000	H	4.440695000	-3.308877000	1.141815000
C	-4.877385000	-2.484523000	-1.130824000	H	2.550314000	-4.094203000	-1.087735000
C	-2.456570000	-2.108970000	-1.195856000	H	1.927469000	-3.560657000	0.475601000
C	-6.474428000	-1.083922000	-0.006539000	H	1.355725000	-2.787559000	-1.009481000
H	-5.670207000	0.585254000	1.038029000	H	3.940294000	-2.658808000	-2.510229000
H	-4.860992000	-0.227844000	3.001361000	H	4.591689000	-1.108718000	-1.958139000
H	-4.646486000	1.528126000	3.141780000	H	2.871491000	-1.257899000	-2.369983000
H	-4.026164000	0.453075000	4.393734000	C	4.709033000	2.901681000	-0.731379000
H	-2.223092000	2.482714000	3.181691000	C	2.332331000	2.366084000	-0.975204000
H	-1.674894000	1.229692000	4.292497000	C	6.387189000	1.428707000	0.153897000
H	-0.850764000	1.443480000	2.739163000	H	5.694185000	-0.462220000	0.831900000
H	-2.872299000	-1.760605000	2.439351000	H	4.836844000	-0.056639000	2.890784000
H	-1.227140000	-1.112238000	2.556305000	H	4.760615000	-1.817286000	2.686833000
H	-2.269241000	-1.168399000	3.991392000	H	4.065479000	-1.058855000	4.116218000
C	-6.195297000	-2.204095000	-0.790061000	H	2.406773000	-2.942788000	2.529682000
H	-4.651965000	-3.351144000	-1.748615000	H	1.787568000	-1.964674000	3.858580000
C	-1.968431000	-1.657193000	-2.433605000	H	0.959243000	-1.940942000	2.292062000
C	-1.746093000	-3.110415000	-0.514452000	H	2.770219000	1.397643000	2.621906000
H	-7.496608000	-0.842163000	0.270114000	H	1.166886000	0.644574000	2.528832000
H	-6.996758000	-2.851249000	-1.138802000	H	2.150372000	0.474806000	3.996581000
C	-0.796973000	-2.190500000	-2.973283000	C	6.038522000	2.656821000	-0.403641000

H	-2.521940000	-0.900190000	-2.982231000	H	4.431628000	3.851422000	-1.178341000
C	-0.574986000	-3.640501000	-1.054913000	C	1.882051000	2.036142000	-2.262985000
H	-2.127465000	-3.488288000	0.429157000	C	1.560225000	3.238912000	-0.194598000
C	-0.099669000	-3.185749000	-2.287115000	H	7.418735000	1.209570000	0.412045000
H	-0.442743000	-1.840600000	-3.939477000	H	6.793100000	3.415502000	-0.587914000
H	-0.048908000	-4.428185000	-0.523843000	C	0.686456000	2.561316000	-2.755638000
H	0.798366000	-3.622377000	-2.721750000	H	2.485034000	1.384777000	-2.888530000
H	4.530622000	4.364540000	-2.463285000	C	0.362549000	3.761835000	-0.686017000
H	3.186928000	4.807711000	-1.402452000	H	1.911434000	3.523183000	0.793171000
H	4.603532000	3.981140000	-0.731060000	C	-0.075263000	3.428071000	-1.969271000
H	2.962738000	2.996389000	-4.013895000	H	0.360698000	2.305755000	-3.759640000
H	1.840516000	1.823484000	-3.300156000	H	-0.213723000	4.449973000	-0.073502000
H	1.620017000	3.557095000	-3.005502000	H	-0.992767000	3.856381000	-2.363244000
<b>TS<sub>g-7</sub></b> E(RM06) = -1952.92175125 Frequency -73.8571				<b>Int7</b> E(RM06) = -1952.94382367			
O	-6.249587000	1.183777000	-1.220206000	O	-6.084416000	1.100425000	-2.062350000
C	-4.340221000	0.527970000	-0.350858000	C	-3.941051000	0.334091000	0.218859000
C	-3.967719000	-0.573947000	-1.238729000	C	-3.775531000	-0.117425000	-1.146300000
C	-4.810815000	0.622670000	1.051310000	C	-5.124333000	0.006641000	1.119384000
H	-3.996737000	1.492427000	-0.714375000	H	-3.701379000	1.388376000	0.341097000
H	-6.882131000	0.453806000	-1.285357000	H	-6.843918000	0.889599000	-2.618829000
C	-2.539529000	-0.844826000	-0.628312000	C	-2.578086000	-0.471043000	0.106989000
C	-4.698326000	-1.934526000	-1.207142000	C	-4.219477000	-1.488073000	-1.586155000
H	-3.875920000	-0.181521000	-2.252601000	H	-3.434310000	0.595923000	-1.885432000
C	-3.998579000	0.109664000	2.242454000	C	-4.966260000	-0.358617000	2.572529000
C	-5.311890000	-0.521659000	1.913622000	C	-5.590783000	-1.338241000	1.602838000
O	-5.515265000	1.830988000	1.258116000	O	-6.200424000	0.860228000	0.773301000
H	-6.475544000	1.666154000	-0.401052000	H	-6.381667000	0.956468000	-1.147349000
C	-1.499028000	0.004828000	-0.742452000	C	-1.438565000	0.292330000	-0.067624000
C	-2.590505000	-2.250308000	-0.060670000	C	-2.575682000	-1.988503000	0.194658000
C	-3.603076000	-3.013860000	-0.953600000	C	-3.146267000	-2.542687000	-1.148519000
H	-5.455607000	-1.965702000	-0.420252000	H	-5.179678000	-1.715648000	-1.114249000
H	-5.223194000	-2.105266000	-2.151983000	H	-4.369915000	-1.500592000	-2.667671000
Au	0.452273000	-0.265308000	-0.188526000	Au	0.537640000	-0.167306000	0.042434000
H	-1.711848000	0.957271000	-1.234485000	H	-1.638292000	1.350851000	-0.260173000

H	-1.590315000	-2.692987000	-0.061326000	H	-1.549134000	-2.328581000	0.353419000
H	-2.940840000	-2.263170000	0.981383000	H	-3.158096000	-2.345440000	1.046731000
C	-4.174798000	-4.260253000	-0.266907000	C	-3.770696000	-3.934475000	-0.981657000
C	-2.936437000	-3.408723000	-2.285777000	C	-2.029568000	-2.604880000	-2.207320000
P	2.744805000	-0.674225000	0.482666000	P	2.890753000	-0.706165000	0.279158000
H	-3.077169000	-0.419525000	2.036474000	H	-3.962808000	-0.564937000	2.933791000
H	-3.959679000	0.790519000	3.086199000	H	-5.615426000	0.123638000	3.295325000
H	-6.165258000	-0.277873000	2.537348000	H	-6.669438000	-1.448830000	1.642042000
H	-5.310095000	-1.523988000	1.504714000	H	-5.058562000	-2.244743000	1.350172000
C	-4.734064000	3.020933000	1.518128000	C	-6.183246000	2.197289000	1.317208000
C	-5.698372000	4.182784000	1.667940000	C	-7.353914000	2.953156000	0.714271000
H	-4.029673000	3.197176000	0.693824000	H	-5.237006000	2.698155000	1.072704000
H	-4.147457000	2.873293000	2.431954000	H	-6.260850000	2.144202000	2.409736000
H	-4.933089000	-4.743387000	-0.892359000	H	-4.186806000	-4.293150000	-1.928823000
H	-3.388905000	-4.998295000	-0.075425000	H	-3.019160000	-4.661482000	-0.656029000
H	-4.640393000	-4.014738000	0.694910000	H	-4.578327000	-3.932609000	-0.241956000
H	-3.661215000	-3.874144000	-2.962087000	H	-2.431860000	-2.928871000	-3.172717000
H	-2.503180000	-2.543239000	-2.798407000	H	-1.544231000	-1.634137000	-2.352651000
H	-2.128882000	-4.128349000	-2.115263000	H	-1.257129000	-3.321406000	-1.909514000
C	3.328863000	-2.264248000	-0.437054000	C	3.310110000	-2.058915000	-1.024773000
C	3.994789000	0.641477000	0.089481000	C	4.077840000	0.690872000	-0.001682000
C	2.743771000	-0.833446000	2.395760000	C	3.137786000	-1.247724000	2.104282000
C	4.544174000	-2.993212000	0.167075000	C	4.595430000	-2.868461000	-0.769230000
C	2.147242000	-3.259247000	-0.492732000	C	2.123525000	-3.044952000	-1.104710000
C	3.657745000	-1.827719000	-1.881681000	C	3.422168000	-1.323920000	-2.378323000
C	3.667548000	1.871205000	-0.534229000	C	3.678267000	2.017250000	-0.301731000
C	5.344578000	0.406688000	0.425299000	C	5.458415000	0.416882000	0.092287000
C	4.118663000	-0.991137000	3.072218000	C	4.588502000	-1.538072000	2.532820000
C	1.847046000	-2.025772000	2.788370000	C	2.269568000	-2.494108000	2.372228000
C	2.100916000	0.472955000	2.915403000	C	2.610949000	-0.071412000	2.957768000
H	-6.404785000	3.996703000	2.481140000	H	-8.299460000	2.460433000	0.957368000
H	-6.263454000	4.350324000	0.746304000	H	-7.252648000	3.006242000	-0.373476000
H	-5.142860000	5.096755000	1.896441000	H	-7.385140000	3.972321000	1.110085000
H	5.445163000	-2.377590000	0.189465000	H	5.494248000	-2.249831000	-0.746864000
H	4.772390000	-3.863991000	-0.458716000	H	4.723298000	-3.581898000	-1.591545000

H	4.348450000	-3.367038000	1.175322000	H	4.544704000	-3.450572000	0.154265000
H	2.460887000	-4.142204000	-1.061958000	H	2.338644000	-3.788487000	-1.880788000
H	1.834813000	-3.600423000	0.496615000	H	1.959050000	-3.584247000	-0.169637000
H	1.277747000	-2.826244000	-0.995000000	H	1.193263000	-2.538325000	-1.375822000
H	3.865903000	-2.720548000	-2.482223000	H	3.533049000	-2.066468000	-3.176445000
H	4.535963000	-1.179496000	-1.928172000	H	4.286846000	-0.657258000	-2.416818000
H	2.816268000	-1.304670000	-2.348473000	H	2.523350000	-0.736771000	-2.595813000
C	4.693519000	2.804047000	-0.773176000	C	4.670486000	2.999749000	-0.473335000
C	2.308979000	2.300010000	-1.003874000	C	2.272160000	2.507917000	-0.483983000
C	6.346428000	1.339077000	0.172259000	C	6.424288000	1.402097000	-0.090103000
H	5.625904000	-0.522677000	0.900454000	H	5.792902000	-0.585908000	0.318650000
H	4.746916000	-0.108920000	2.935562000	H	5.216283000	-0.646484000	2.486091000
H	4.667551000	-1.869257000	2.726305000	H	5.059066000	-2.330064000	1.946933000
H	3.960249000	-1.111925000	4.150246000	H	4.576680000	-1.871589000	3.576794000
H	2.312134000	-2.986802000	2.552313000	H	2.668734000	-3.388163000	1.885587000
H	1.681732000	-2.003588000	3.871763000	H	2.256793000	-2.690558000	3.450270000
H	0.869353000	-1.982577000	2.298182000	H	1.233975000	-2.351977000	2.046988000
H	2.688131000	1.353440000	2.636797000	H	3.182932000	0.845199000	2.785108000
H	1.082258000	0.605656000	2.538587000	H	1.554918000	0.138719000	2.762532000
H	2.057844000	0.436988000	4.010264000	H	2.712807000	-0.329947000	4.017896000
C	6.017532000	2.552124000	-0.428695000	C	6.026778000	2.707530000	-0.370521000
H	4.431715000	3.743665000	-1.249820000	H	4.355203000	4.013441000	-0.700378000
C	1.894583000	2.021933000	-2.316057000	C	1.684486000	2.507170000	-1.759593000
C	1.512069000	3.137064000	-0.208421000	C	1.593932000	3.139357000	0.570294000
H	7.373058000	1.115981000	0.445823000	H	7.476567000	1.147775000	-0.010244000
H	6.783165000	3.294565000	-0.632106000	H	6.763926000	3.491790000	-0.512497000
C	0.710479000	2.563983000	-2.819195000	C	0.448370000	3.120852000	-1.974940000
H	2.517698000	1.399527000	-2.951374000	H	2.214252000	2.051213000	-2.590857000
C	0.327017000	3.678233000	-0.711247000	C	0.356282000	3.750848000	0.355617000
H	1.835570000	3.383194000	0.798745000	H	2.051080000	3.174595000	1.554826000
C	-0.074637000	3.397249000	-2.019060000	C	-0.217007000	3.748388000	-0.918449000
H	0.414550000	2.352065000	-3.842497000	H	0.020340000	3.132105000	-2.973195000
H	-0.267230000	4.340223000	-0.087474000	H	-0.144560000	4.252643000	1.178585000
H	-0.980397000	3.842904000	-2.420805000	H	-1.162455000	4.254242000	-1.093016000