

# **Organocatalysis for the Asymmetric Michael Addition of Aldehydes and $\alpha, \beta$ -Unsaturated Nitroalkenes**

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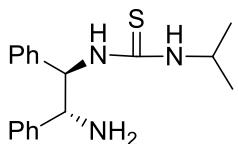
## **Supporting Information**

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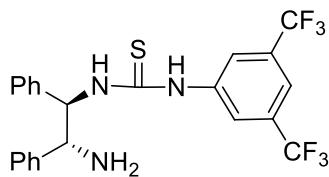
## 1. Compound Characterization Data

### 1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-isopropylthiourea (1a)<sup>1</sup>



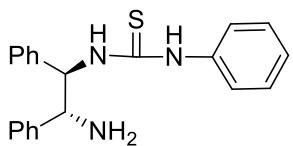
$[\alpha]_D^{25} +62.3$  (*c* 1.0, CHCl<sub>3</sub>); <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.37~7.21 (m, 11H), 6.04 (br s, 1H), 5.09(br s, 1H), 4.30 (s, 1H), 4.15 (br s, 1H), 1.73 (s, 2H), 1.09~1.03 (m, 6H) ppm; <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  180.68, 142.06, 129.00, 128.75, 127.88, 126.91, 64.12, 60.55, 46.39, 22.70 ppm; IR (KBr) 3335, 2966, 1527, 1326, 1273, 966, 695, 514 cm<sup>-1</sup>; HRMS (ESI+) for C<sub>18</sub>H<sub>23</sub>N<sub>3</sub>S [M + H]<sup>+</sup> Calcd: 314.1691, Found: 314.1627;

### 1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-[3,5-bis(trifluoromethyl)phenyl]thiourea(1b)<sup>1</sup>



$[\alpha]_D^{25} +13.5$  (*c* 1.0, CH<sub>3</sub>Cl); <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.25 (s, 2H), 7.78 (s, 1H), 7.32~7.15 (m, 13H), 5.99 (d, *J* = 3 Hz, 1H), 4.77 (d, *J* = 3 Hz, 1H) ppm; <sup>13</sup>C-NMR (125 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  180.51, 143.26, 142.48, 130.82, 130.56, 128.51, 128.29, 127.66, 127.55, 127.38, 124.78, 122.62, 121.34, 116.08, 63.66, 59.94 ppm; IR (KBr) 3305, 3032, 2963, 1652, 1601, 1557, 1383, 1277, 1262, 803, 700 cm<sup>-1</sup>; HRMS (FAB+) for C<sub>23</sub>H<sub>19</sub>F<sub>6</sub>N<sub>3</sub>S [M + H]<sup>+</sup> Calcd: 484.1282, Found: 484.1254;

**1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-phenylthiourea (**1c**)<sup>1</sup>**



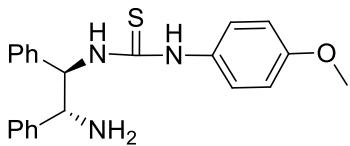
$[\alpha]_D^{20} = +62.0$  ( $c = 0.02$ ,  $\text{CH}_2\text{Cl}_2$ );  $^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (s, 1 H), 7.54~7.19 (m, 15 H), 5.54 (s, 1 H), 4.42 (d, 1 H,  $J = 5$  Hz), 1.35 (br s, 1 H);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{DMSO-d}_6$ )  $\delta$  182.09, 134.48, 133.93, 129.89, 128.70, 128.10, 127.91, 127.15, 126.94, 126.82, 126.74, 126.23, 125.59, 125.24, 122.98, 63.07, 59.09; IR (KBr) 3287.86, 3027.84, 1521.63, 1241.99, 1072.28, 939.20, 698.13  $\text{cm}^{-1}$ ; HRMS (FAB $^+$ ) for  $\text{C}_{21}\text{H}_{22}\text{N}_3\text{S}$  [ $\text{M} + \text{H}$ ] $^+$  Calcd: 348.4918, Found: 348.1534.

**1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-*p*-tolylthiourea (**1d**)<sup>1</sup>**



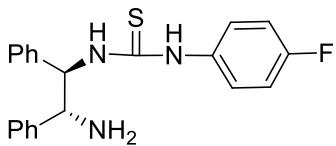
$[\alpha]_D^{22} +0.27$  ( $c 1.00$ ,  $\text{CH}_3\text{Cl}$ );  $^1\text{H-NMR}$  (300 MHz,  $\text{DMSO-d}_6$ )  $\delta$  9.79 (s, 1H), 7.13~7.38 (m, 15H), 5.50(s, 1H), 4.32 (d,  $J = 3$  Hz, 1H), 2.27(s, 3H) ppm;  $^{13}\text{C-NMR}$  (100 MHz,  $\text{DMSO-d}_6$ )  $\delta$  180.90, 143.72, 142.20, 137.14, 134.32, 129.86, 128.82, 128.59, 127.68, 127.61, 127.46, 127.39, 123.97, 63.88, 60.00, 21.23 ppm; IR (KBr) 3301.69, 2861.98, 1889.99, 1527.42, 1342.28, 964.28, 701.99, 524.56  $\text{cm}^{-1}$ ; HRMS (FAB $^+$ ) for  $\text{C}_{22}\text{H}_{24}\text{N}_3\text{S}$  [ $\text{M} + \text{H}$ ] $^+$  Calcd: 362.1691, Found: 362.2188

**1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-(4-methoxyphenyl)thiourea (**1e**)<sup>1</sup>**



$[\alpha]_D^{22} +0.327$  (*c* 1.00, CH<sub>3</sub>Cl); <sup>1</sup>H-NMR (300 MHz, DMSO-d<sub>6</sub>) δ 9.55 (s, 1H), 8.17 (s, 1H), 7.12~7.22 (m, 12H), 6.87(d, *J* = 6.0 Hz, 3H), 5.94 (s, 1H), 3.72 (s, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, DMSO-d<sub>6</sub>) δ 180.72, 156.54, 139.70, 131.67, 128.09, 127.97, 127.19, 125.61, 113.93, 62.38, 59.81, 55.24 ppm; IR (KBr) 3303.63, 3027.84, 1733.78, 1510.06, 1297.92, 1243.92, 1029.85, 831.21, 700.07, 568.93 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>22</sub>H<sub>24</sub>N<sub>3</sub>OS [M + H]<sup>+</sup> Calcd: 378.1640, Found: 378.1563

**1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-(4-fluorophenyl)thiourea (**1f**)<sup>1</sup>**



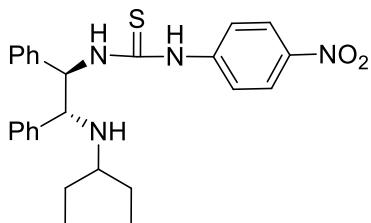
$[\alpha]_D^{22} +0.132$  (*c* 1.00, CH<sub>3</sub>Cl); <sup>1</sup>H-NMR (300 MHz, DMSO-d<sub>6</sub>) δ 9.93 (s, 1H), 7.08~7.46 (m, 15H), 5.52(s, 1H), 4.34 (d, *J* = 3 Hz, 1H) ppm; <sup>13</sup>C-NMR (100 MHz, DMSO-d<sub>6</sub>) δ 181.28, 160.71, 143.73, 142.10, 136.32, 128.79, 128.58, 127.70, 127.59, 127.49, 127.39, 125.79, 115.94, 115.71, 63.88, 60.06 ppm; IR (KBr) 3301.69, 3029.77, 1874.56, 1527.42, 1342.27, 1218.85, 840.85, 701.99 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>21</sub>H<sub>21</sub>FN<sub>3</sub>S [M + H]<sup>+</sup> Calcd: 366.1440, Found: 366.1440

**1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-(4-cyanophenyl)thiourea (1g)<sup>1</sup>**



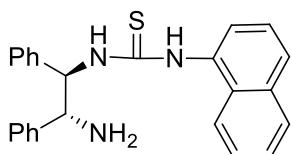
$[\alpha]_D^{22} +1.50$  (*c* 1.00, CH<sub>3</sub>Cl); <sup>1</sup>H-NMR (300 MHz, DMSO-d<sub>6</sub>)  $\delta$  10.50 (s, 1H), 7.07~7.88 (m, 15H), 5.56 (d, *J* = 3 Hz, 1H), 4.39 (d, *J* = 3 Hz, 1H) ppm; <sup>13</sup>C-NMR (100 MHz, DMSO-d<sub>6</sub>)  $\delta$  180.47, 145.05, 143.34, 141.61, 133.36, 128.83, 128.64 127.74, 127.68, 127.59, 127.50, 121.37, 119.85, 105.11, 63.74, 60.04 ppm; IR (KBr) 3263.1, 2219.7, 1646.9, 1592.9, 1361.5, 1091.5 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>22</sub>H<sub>20</sub>N<sub>4</sub>S [M + H]<sup>+</sup> Calcd: 372.1487, Found: 372.1400

**1-(4-Nitrophenyl)-3-[(1*R*,2*R*)-2-(pentan-3-ylamino)-1,2-diphenylethyl]thiourea (1h)<sup>2</sup>**



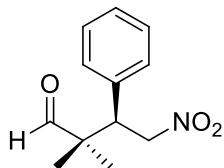
$[\alpha]_D^{20} +37.7$  (*c* 0.20, CHCl<sub>3</sub>); <sup>1</sup>H-NMR (300 MHz, DMSO-d<sub>6</sub>)  $\delta$  10.5 (s, 1H), 8.16 (m, 2H), 7.90 (d, *J* = 9.1 Hz, 2H), 7.37~7.15 (m, 10H), 5.54 (br s, 1H), 4.16 (d, *J* = 5.5 Hz, 1H), 2.07 (m, 1H), 1.30~1.15 (m, 4H), 0.75 (t, *J* = 7.4 Hz, 3H), 0.50 (t, *J* = 7.4 Hz, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, DMSO-d<sub>6</sub>)  $\delta$  179.85, 146.27, 141.82, 141.25, 140.25, 128.00, 127.86, 127.04, 126.98, 126.87, 124.60, 124.46, 120.28, 63.71, 63.14, 55.72, 26.04, 23.36, 10.32, 7.97 ppm; IR (KBr) 3330.5, 2960.2, 2599.6, 2456.4, 2345.0, 1951.6, 1743.3, 1496.5, 1346.1, 1110.8, 1072.2, 852.4, 700.0, 586.3 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>26</sub>H<sub>31</sub>N<sub>4</sub>O<sub>2</sub>S [M + H]<sup>+</sup> Calcd: 463.2168, Found: 463.2186.

**1-[(1*R*,2*R*)-2-Amino-1,2-diphenylethyl]-3-(naphthalene-1-yl)thiourea (1i)<sup>1</sup>**



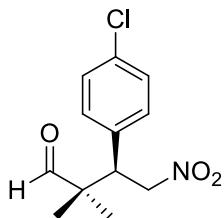
$[\alpha]_D^{25} +0.157$  (*c* 1.00, CH<sub>3</sub>Cl); <sup>1</sup>H-NMR (300 MHz, DMSO-d<sub>6</sub>) δ 9.93 (s, 1H), 7.22~7.99 (m, 18H), 5.51(s, 1H), 4.34 (d, *J* = 3 Hz, 1H) ppm; <sup>13</sup>C-NMR (100 MHz, DMSO-d<sub>6</sub>) δ 182.70, 143.47, 142.08, 135.06, 134.65, 130.66, 128.84, 128.55, 127.69, 127.61, 127.45, 126.99, 126.32, 126.00, 123.65, 64.01, 59.88 ppm; IR (KBr) 3340.26, 3116.55, 1951.70, 1511.99, 1249.70, 941.13, 701.99, 632.56 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>25</sub>H<sub>24</sub>N<sub>3</sub>S [M + H]<sup>+</sup> Calcd: 398.1691, Found: 398.551

**(*R*)-2,2,-Dimethyl-4-nitro-3-phenylbutanal (2a)<sup>3</sup>**



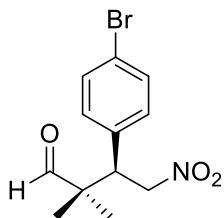
$[\alpha]_D^{20} +11.26$  (*c* 0.3, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.50 (s, 1H), 7.18~7.34 (m, 5H), 4.81~4.89 (dd, *J* = 9.0, 12 Hz, 1H), 4.66~4.71 (dd, *J* = 3.0, 12 Hz, 1H), 3.76~3.81 (dd, *J* = 3.0 12 Hz, 1H) 1.10 (s, 3H), 0.97 (s, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 204.25, 135.30, 129.06, 128.71, 128.15, 76.30, 48.45, 48.22, 21.70, 18.88 ppm; IR(neat) 3033, 2974, 2933, 2819, 2721, 1725, 1555, 1496, 1455, 1379, 882, 750, 705 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>12</sub>H<sub>15</sub>NO<sub>3</sub> [M+Na]<sup>+</sup> Calcd: 244.0950 Found: 244.0950; HPLC [Chiralcel OD-H, hexane/2-propanol = 80/20, flow rate = 0.7 mL/min,  $\lambda$  = 254nm, retention times: (major) 18.3 min, (minor) 31.1 min].

**(R)-3-(4-Chlorophenyl)-2,2-dimethyl-4-nitrobutanal (2b)<sup>5</sup>**



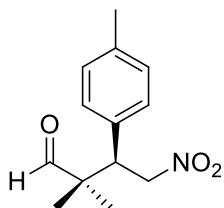
$[\alpha]_D^{22} -5.83$  (*c* 0.2, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.50 (s, 1H), 7.31 (d, *J* = 6.0 Hz, 2H), 7.15 (d, *J* = 6.0 Hz, 2H), 4.79~4.85 (dd, *J* = 6.0, 9.0 Hz, 1H), 4.67~4.71 (dd, *J* = 3.0, 9.0 Hz, 1H), 3.75~3.79 (dd, *J* = 3.0, 9.0 Hz, 1H), 1.12 (s, 3H), 1.00 (s, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 204.07, 134.34, 134.20, 130.61, 129.16, 76.35, 48.39, 48.07, 21.95, 19.10 ppm; IR (KBr) 2926, 1728, 1556, 1494, 1378, 1094, 835 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>12</sub>H<sub>14</sub>ClNO<sub>3</sub> [M+Na]<sup>+</sup> Calcd: 278.0560 Found: 278.0562; HPLC [Chiralcel OD-H, hexane/2-propanol = 80/20, flow rate = 0.7 mL/min, λ = 254nm, retention times: (major) 16.1 min, (minor) 25.4 min].

**(R)-3-(4-Bromophenyl)-2,2-dimethyl-4-nitrobutanal (2c)<sup>3</sup>**



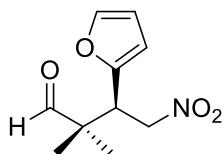
$[\alpha]_D^{23} -14.86$  (*c* 0.1, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.49 (s, 1H), 7.47 (d, *J* = 6.0 Hz, 2H), 7.09 (d, *J* = 6.0 Hz, 2H), 4.79~4.85 (dd, *J* = 9.0, 9.0 Hz, 1H), 4.67~4.71 (dd, *J* = 3.0, 9.0 Hz, 1H), 3.74~3.78 (dd, *J* = 3.0, 9.0 Hz, 1H), 1.12 (s, 3H), 1.01 (s, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 204.04, 134.73, 132.12, 130.95, 122.49, 76.28, 48.33, 48.15, 21.98, 19.11 ppm; IR (KBr) 2924, 2857, 1727, 1555, 1457, 1377, 1009 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>12</sub>H<sub>14</sub>BrNO<sub>3</sub> [M+Na]<sup>+</sup> Calcd: 322.0055 Found: 322.0053; HPLC [Chiralcel OD-H, hexane/2-propanol = 80/20, flow rate = 0.7 mL/min, λ = 254nm, retention times: (major) 21.9 min, (minor) 31.7 min].

**(R)-2,2-Dimethyl-4-nitro-3-p-tolylbutanal (2d)<sup>4</sup>**



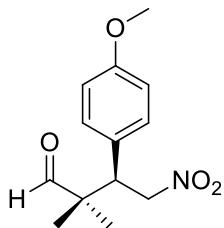
$[\alpha]_D^{22} -15.07$  (*c* 0.4, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.50 (s, 1H), 7.05~7.12 (m, 4H), 4.78~4.84 (dd, *J* = 9.0, 12.0 Hz, 1H), 4.63~4.67 (dd, *J* = 3.0, 9.0 Hz, 1H) 2.29 (s, 3H), 1.09 (s, 3H), 0.97 (s, 3H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 204.65, 138.07, 132.38, 129.60, 129.13, 76.60, 48.46, 48.34, 21.75, 21.23, 19.05 ppm; IR (KBr) 2973, 2925, 1726, 1556, 1516, 1381, 1120, 824 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>13</sub>H<sub>17</sub>NO<sub>3</sub> [M+Na]<sup>+</sup> Calcd: 258.1106 Found: 258.1107; HPLC [Chiralcel OD-H, hexane/2-propanol = 80/20, flow rate = 0.7 mL/min,  $\lambda$  = 254nm, retention times: (major) 14.2 min, (minor) 21.1 min].

**(R)-3-(Furan-2-yl)-2,2-dimethyl-4-nitrobutanal (2e)<sup>3</sup>**



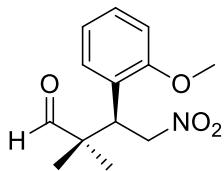
$[\alpha]_D^{22} -12.06$  (*c* 0.3, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.51 (s, 1H), 7.37 (d, *J* = 0.6 Hz, 1H), 6.31~6.32 (dd, *J* = 3.0, 3.3 Hz, 1H), 6.23 (d, *J* = 3.0 Hz, 1H), 4.73~4.79 (dd, *J* = 9.0, 12 Hz, 1H), 4.58~4.62 (dd, *J* = 3.0, 9.0 Hz, 1H), 3.91~3.95 (dd, *J* = 3.0, 9.0 Hz, 1H), 1.17 (s, 3H), 1.04 (s, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 203.76, 150.02, 142.92, 110.62, 109.82, 75.09, 48.36, 42.39, 21.31, 19.21 ppm; IR (KBr) 2925, 1728, 1557, 1376, 1148, 740 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>10</sub>H<sub>13</sub>NO<sub>4</sub> [M+Na]<sup>+</sup> Calcd: 234.0742 Found: 234.0742; HPLC [Chiralcel OD-H, hexane/2-propanol = 90/10, flow rate = 0.7 mL/min,  $\lambda$  = 254nm, retention times: (major) 14.7 min, (minor) 21.2 min].

**(R)-3-(4-Methoxyphenyl)-2,2-dimethyl-4-nitrobutanal (2f)<sup>3</sup>**



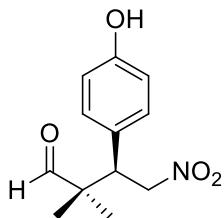
$[\alpha]_D^{22} -9.55$  (*c* 0.2, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.51 (s, 1H), 7.12 (d, *J* = 9.0 Hz, 2H), 6.85 (d, *J* = 6.0, 2H), 4.78~4.84 (dd, *J* = 9.0, 12 Hz, 1H), 4.64~4.68 (dd, *J* = 3.0, 9.0 Hz, 1H), 3.77 (s, 3H), 3.71~3.75 (dd, *J* = 3.0, 9.0 Hz, 1H), 1.11 (s, 3H), 0.98 (s, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 204.73, 159.47, 130.32, 127.30, 114.26, 76.69, 55.41, 48.57, 47.98, 21.71, 19.10 ppm; IR (KBr) 2927, 1725, 1611, 1556, 1514, 1465, 1380, 1252, 1033, 836 cm<sup>-1</sup>; HRMS(FAB<sup>+</sup>) for C<sub>13</sub>H<sub>17</sub>NO<sub>4</sub> [M+Na]<sup>+</sup> Calcd: 274.1055 Found: 274.1055; HPLC [Chiralcel OD-H, hexane/2-propanol = 80/20, flow rate = 0.7 mL/min,  $\lambda$  = 254nm, retention times: (major) 18.2 min, (minor) 25.7 min].

**(R)-3-(2-Methoxyphenyl)-2,2-dimethyl-4-nitrobutanal (2g)<sup>6</sup>**



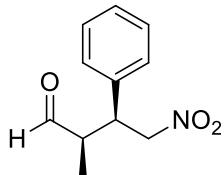
$[\alpha]_D^{20} -14.39$  (*c* 0.3, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.50 (s, 1H), 7.23~7.29 (m, 1H), 7.11~7.14 (dd, *J* = 3.0, 9.0 Hz, 1H), 6.87~6.95 (m, 2H), 4.86~4.94 (dd, *J* = 12, 15 Hz, 1H), 4.69~4.75 (dd, *J* = 3.0, 12 Hz, 1H), 4.22 (d, *J* = 9.0 Hz, 1H), 3.81 (s, 3H), 1.09 (s, 3H), 1.05 (s, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 204.13, 157.36, 129.79, 129.28, 124.00, 120.76, 111.29, 75.81, 55.34, 48.37, 21.00, 19.96 ppm; HRMS (FAB<sup>+</sup>) for C<sub>13</sub>H<sub>17</sub>NO<sub>4</sub> [M+Na]<sup>+</sup> Calcd: 274.1055 Found: 274.1056; IR (KBr) 2927, 1725, 1611, 1556, 1514, 1465, 1380, 1252, 1033, 836 cm<sup>-1</sup>; HPLC [Chiralcel OD-H, hexane/2-propanol = 90/10, flow rate = 0.7 mL/min,  $\lambda$  = 254nm, retention times: (major) 15.4 min, (minor) 25.2 min].

**(R)-3-(4-Hydroxyphenyl)-2,2-dimethyl-4-nitrobutanal (2h)<sup>5</sup>**



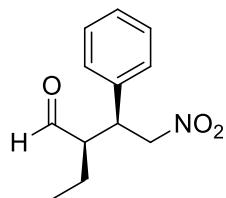
$[\alpha]_D^{22} -13.37$  (*c* 0.2, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.52(s, 1H), 7.04~7.07 (m, 2H), 6.74~6.77 (m, 2H), 5.47 (br s, 1H), 4.77~4.85 (dd, *J* = 12, 12 Hz, 1H), 4.64~4.69 (dd, *J* = 3.0, 12.0 Hz, 1H), 3.69~3.75 (dd, *J* = 6.0, 12.0 Hz), 1.12 (s, 3H), 1.00 (s, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 205.71, 155.80, 130.47, 127.07, 115.8, 76.71, 48.67, 48.01, 21.40, 19.07 ppm; IR (KBr) 2925, 1726, 1638, 1556, 1456, 1380, 705 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>12</sub>H<sub>15</sub>NO<sub>4</sub> [M+Na]<sup>+</sup> Calcd: 260.0899 Found: 260.0899; HPLC [Chiralcel OD-H, hexane/2-propanol = 80/20, flow rate = 0.7 mL/min,  $\lambda$  = 254nm, retention times: (major) 16.1 min, (minor) 24.9 min].

**(2*R*,3*S*)-2-Methyl-4-nitro-3-phenylbutanal (2i)<sup>4</sup>**



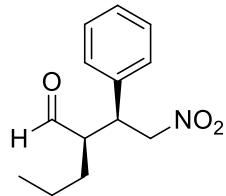
$[\alpha]_D^{20} -9.00$  (*c* 0.2, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.71 (s, 1H), 7.15~7.36 (m, 5H), 4.77~4.83 (dd, *J* = 6.0, 12 Hz, 1H), 4.64~4.71 (dd, *J* = 9.0, 12 Hz, 1H), 3.77~3.87 (m, 1H), 2.72~2.83 (m, 1H), 1.00 (d, *J* = 9.0 Hz, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 202.53, 136.75, 129.30, 128.35, 128.28, 78.33, 48.65, 44.24, 12.36 ppm; IR (neat) 3031, 2975, 2933, 2827, 2729, 1724, 1603, 1551, 1496, 1433, 1459, 1380, 1203, 914, 853, 757, 702 cm<sup>-1</sup>; LRMS (FAB<sup>+</sup>) for C<sub>11</sub>H<sub>13</sub>NO<sub>3</sub> [M+Na]<sup>+</sup> Calcd: 230.1 Found: 230.1; HPLC [Chiralcel OD-H, hexane/2-propanol = 90/10, flow rate = 1.0 mL/min,  $\lambda$  = 254nm, retention times: (major) 35.4 min, (minor) 25.4 min].

**(2*R*,3*S*)-2-Ethyl-4-nitro-3-phenylbutanal (2j)<sup>4</sup>**



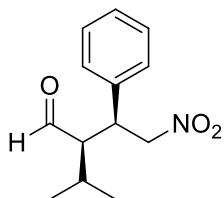
$[\alpha]_D^{20} +8.10$  (*c* 0.4, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.72 (d, *J* = 3.0 Hz, 1H), 7.28~7.35 (m, 3H), 7.16~7.20 (m, 2H), 4.74~4.81 (dd, *J* = 9.0, 18 Hz), 4.63~4.71 (dd, *J* = 3.0, 15 Hz), 3.75~3.83 (m, 1H), 2.64~2.72 (m, 1H), 1.46~1.56 (m, 2H), 0.83 (t, *J* = 9.0 Hz, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 203.32, 136.75, 129.11, 128.21, 127.99, 78.55, 54.98, 42.68, 20.36, 10.66 ppm; IR (neat) 3031, 2969, 2878, 2738, 1719, 1551, 1496, 1456, 1432, 1379, 1206, 757, 702 cm<sup>-1</sup>; LRMS (FAB<sup>+</sup>) for C<sub>12</sub>H<sub>15</sub>NO<sub>3</sub> [M+Na]<sup>+</sup> Calcd: 244.1 Found: 244.1; HPLC [Chiralcel OD-H, hexane/2-propanol = 90/10, flow rate = 0.8 mL/min, λ = 215nm, retention times: (major) 34.5 min, (minor) 29.9 min].

**(*R*)-2-[*(S*)-2-Nitro-1-phenylethyl]pentanal (2k)<sup>4</sup>**



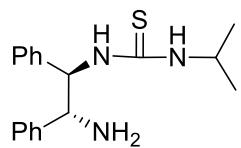
$[\alpha]_D^{20} +15.40$  (*c* 0.2, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.70 (d, *J* = 3.0 Hz, 1H), 7.27~7.37 (m, 3H), 7.16~7.19 (m, 3H), 4.60~4.81 (m, 2H), 3.73~3.81 (m, 3H), 2.60~2.74 (m, 3H), 1.12~1.55 (m, 4H), 0.79 (t, *J* = 6.0 Hz, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 203.28, 136.77, 129.11, 128.22, 127.98, 78.42, 53.78, 43.13, 29.44, 19.75, 13.93 ppm; IR (neat) 2968, 1719, 1553, 1379 cm<sup>-1</sup>; LRMS (FAB<sup>+</sup>) for C<sub>13</sub>H<sub>17</sub>NO<sub>3</sub> [M+Na]<sup>+</sup> Calcd: 258.1 Found: 258.1; HPLC [Chiralcel OD-H, hexane/2-propanol = 80/20, flow rate = 1.0 mL/min, λ = 254nm, retention times: (major) 19.3 min, (minor) 14.1 min].

**(2*R*,3*S*)-2-Isopropyl-4-nitro-3-phenylbutanal (2l)<sup>4</sup>**



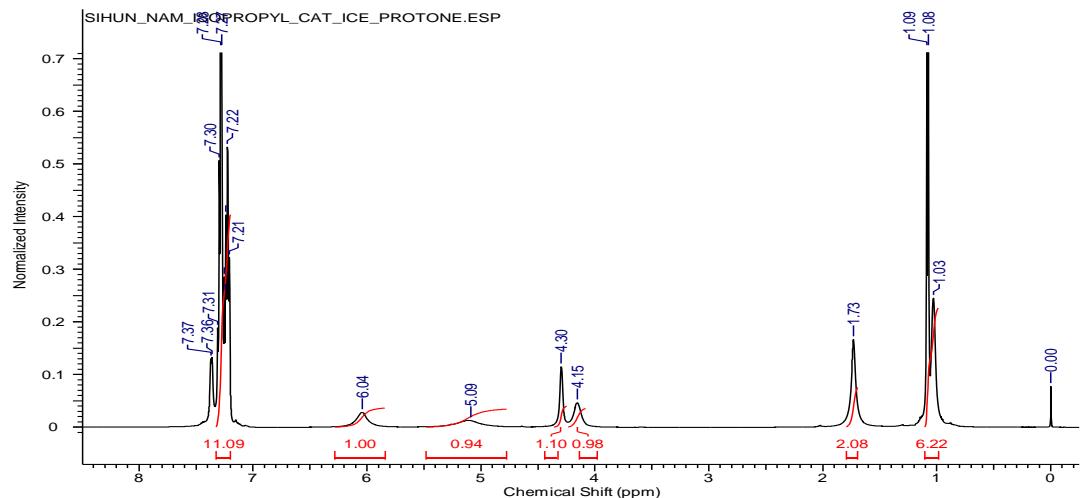
$[\alpha]_D^{20} +19.81$  (*c* 0.5, CH<sub>2</sub>Cl<sub>2</sub>); <sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>) δ 9.93 (d, *J* = 1.8 Hz, 1H), 7.28~7.37 (m, 3H), 7.15~7.20 (m, 2H), 4.65~4.69 (dd, *J* = 3.0, 9.0 Hz, 1H), 4.55~4.60 (dd, *J* = 6.0, 9.0 Hz, 1H), 3.87~3.93 (m, 1H), 2.75~2.80 (m, 1H), 1.68~1.76 (m, 1H), 1.11 (d, *J* = 6.0 Hz, 3H), 0.89 (d, *J* = 6.0 Hz, 3H) ppm; <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 204.59, 137.26, 129.37, 128.32, 128.16, 79.21, 58.95, 42.13, 28.13, 21.88, 17.18 ppm; IR (neat) 2964, 1717, 1553, 1379 cm<sup>-1</sup>; HRMS (FAB<sup>+</sup>) for C<sub>13</sub>H<sub>17</sub>NO<sub>3</sub> [M + H]<sup>+</sup> Calcd: 236.1208 Found: 236.1287; HPLC [Chiralcel AD-H, hexane/2-propanol = 99.5/0.5, flow rate = 0.3 mL/min, λ = 254nm, retention times: (major) 24.1 min, (minor) 29.6 min].

## 2. Copy of HPLC, NMR and MASS Spectra

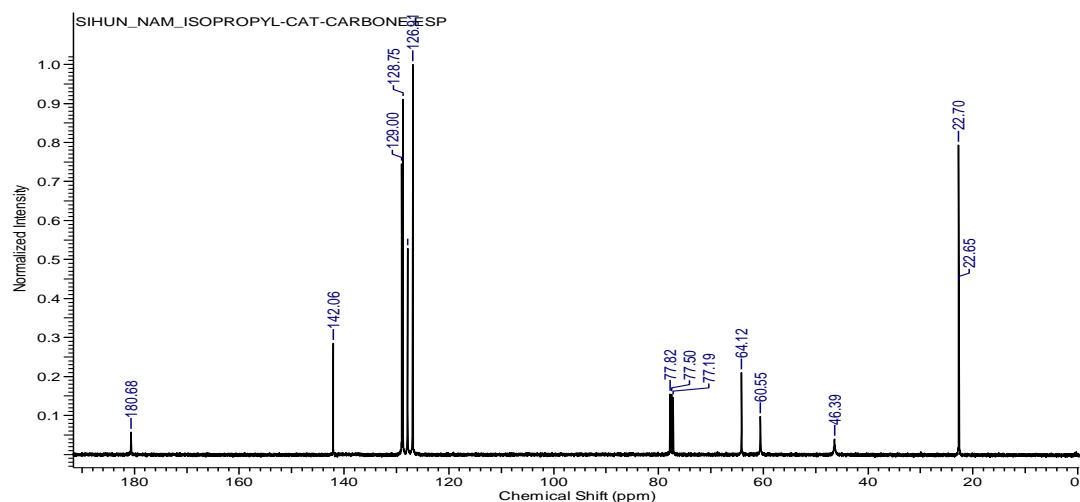


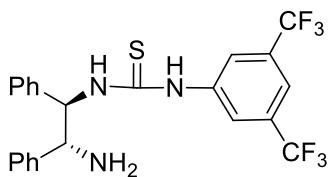
**1a**

### <sup>1</sup>H-NMR



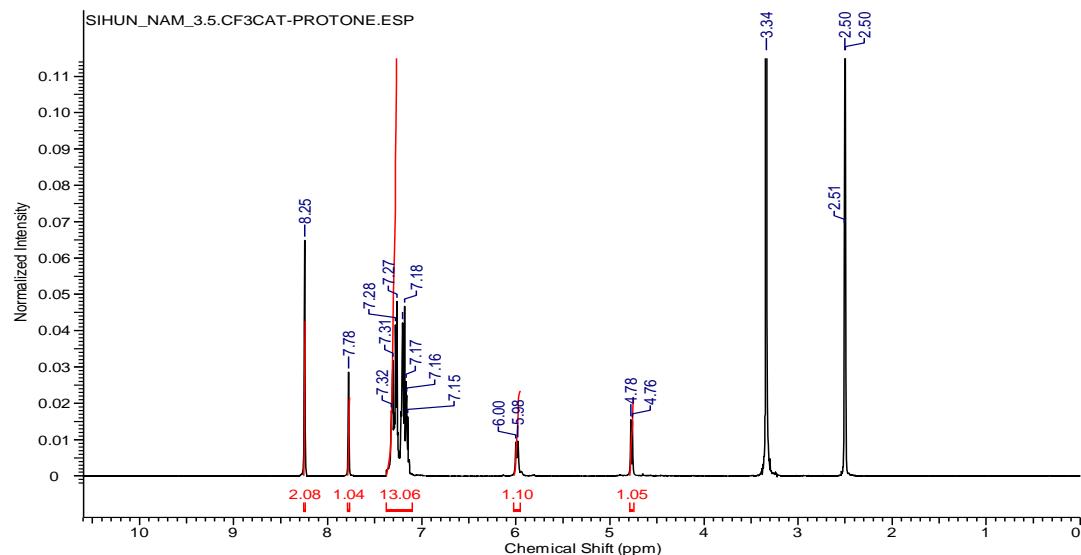
### <sup>13</sup>C-NMR



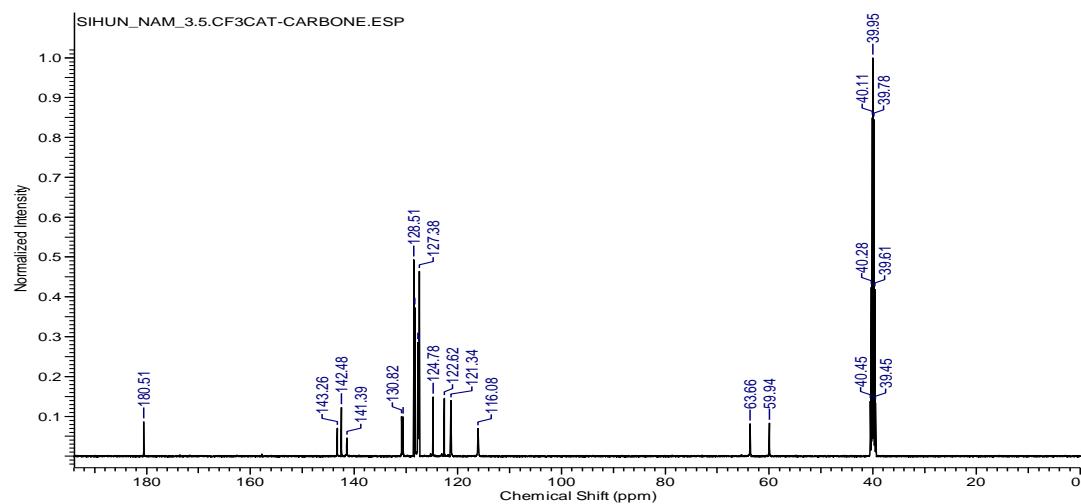


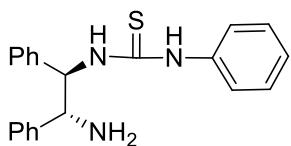
**1b**

**<sup>1</sup>H-NMR**



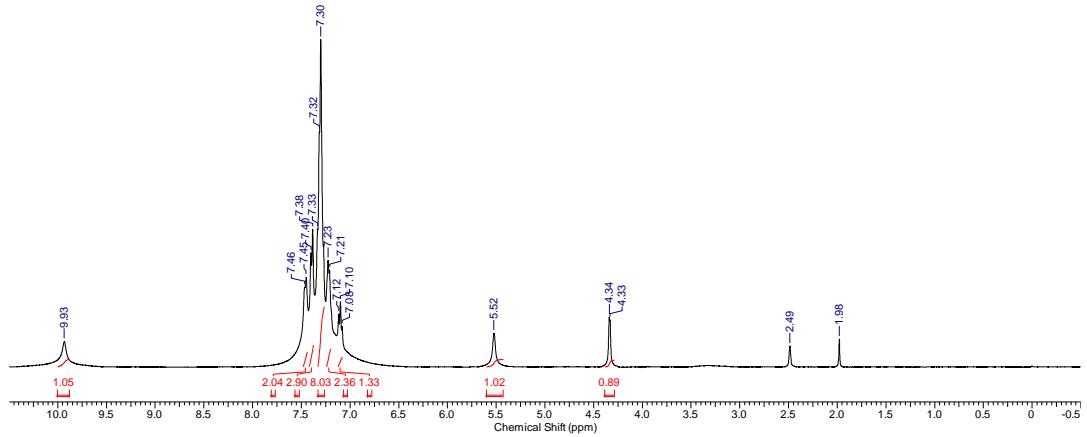
**<sup>13</sup>C-NMR**



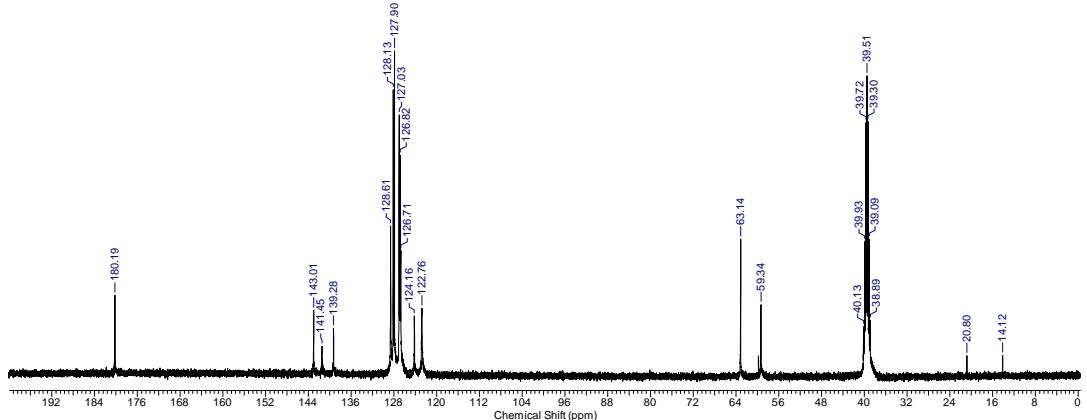


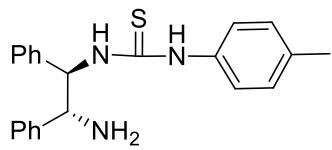
**1c**

**<sup>1</sup>H-NMR**



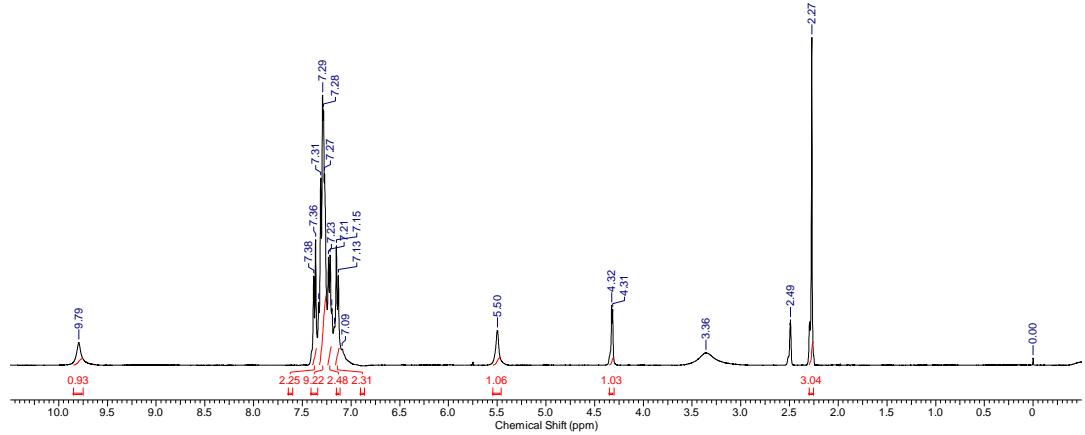
**<sup>13</sup>C-NMR**



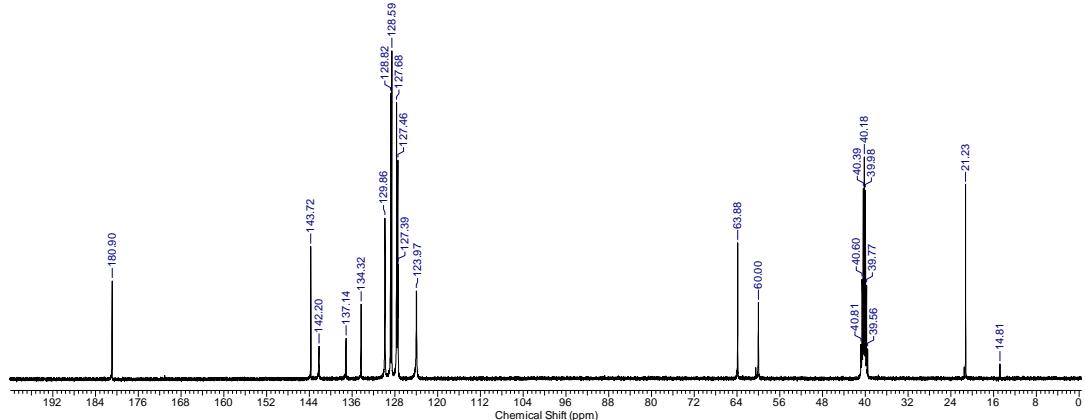


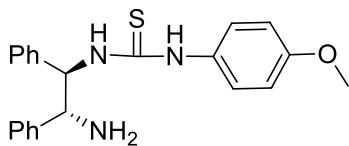
1d

## **<sup>1</sup>H-NMR**

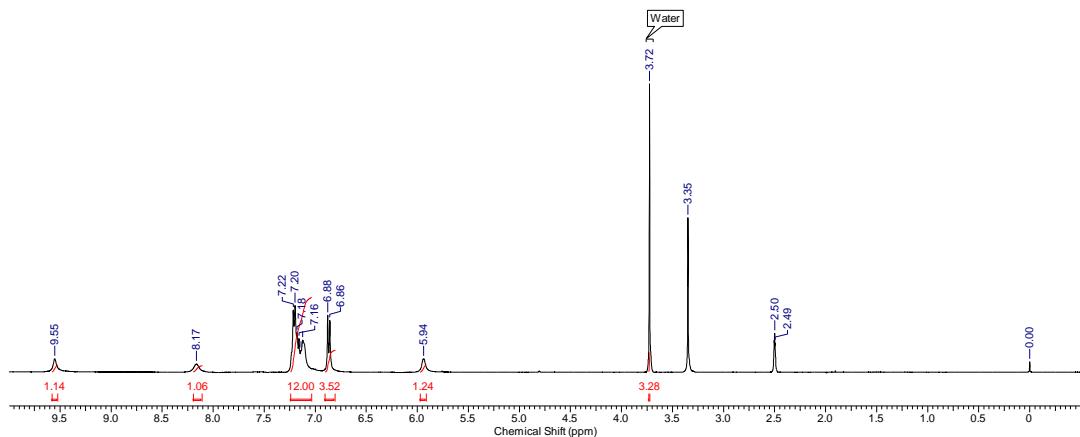


## **<sup>13</sup>C-NMR**

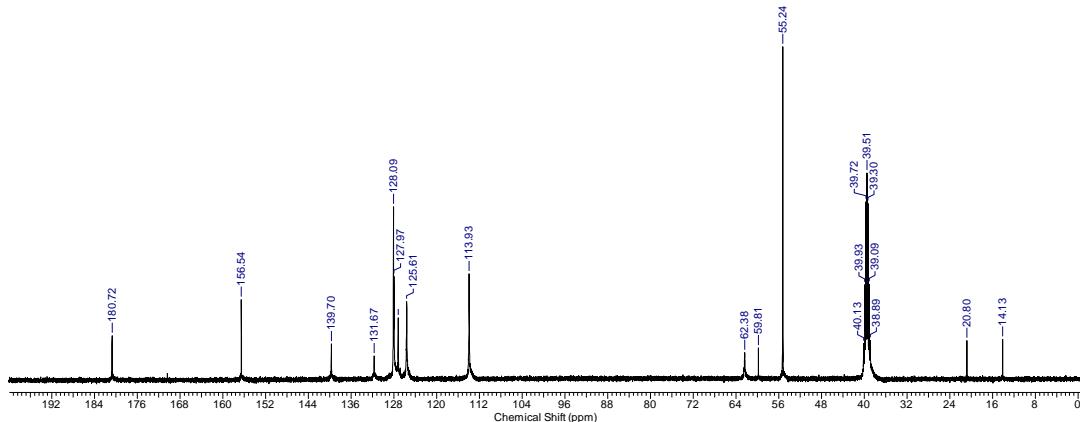


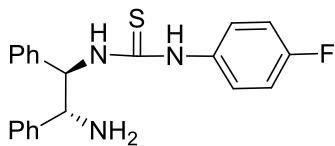


**<sup>1</sup>H-NMR**

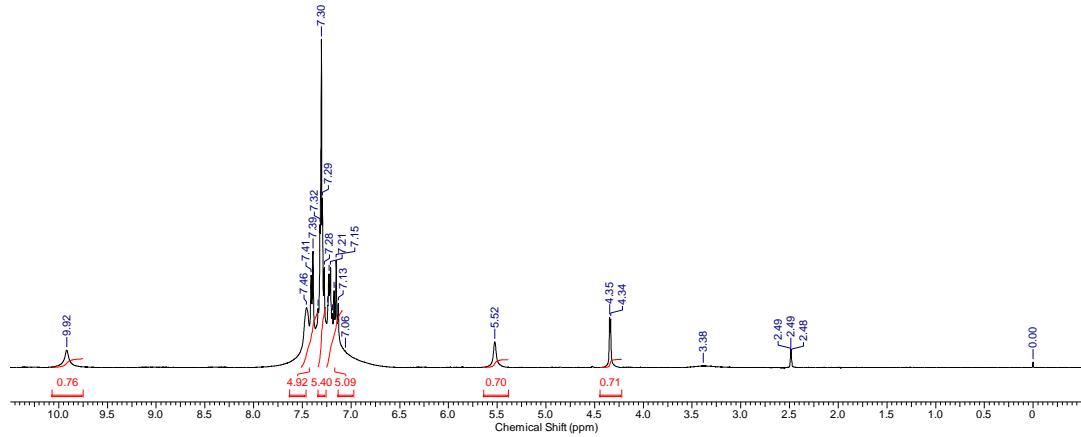


**<sup>13</sup>C-NMR**

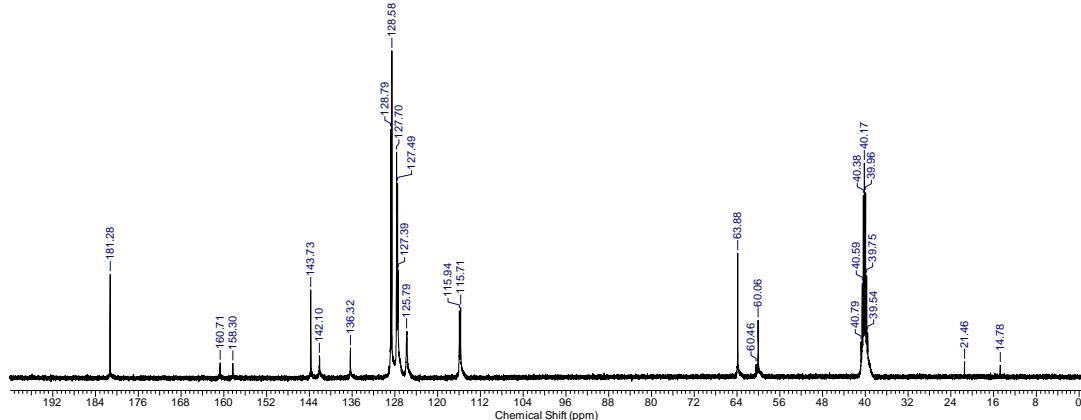


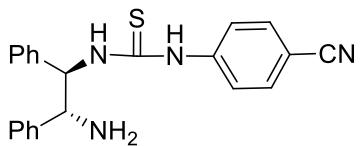


**<sup>1</sup>H-NMR**

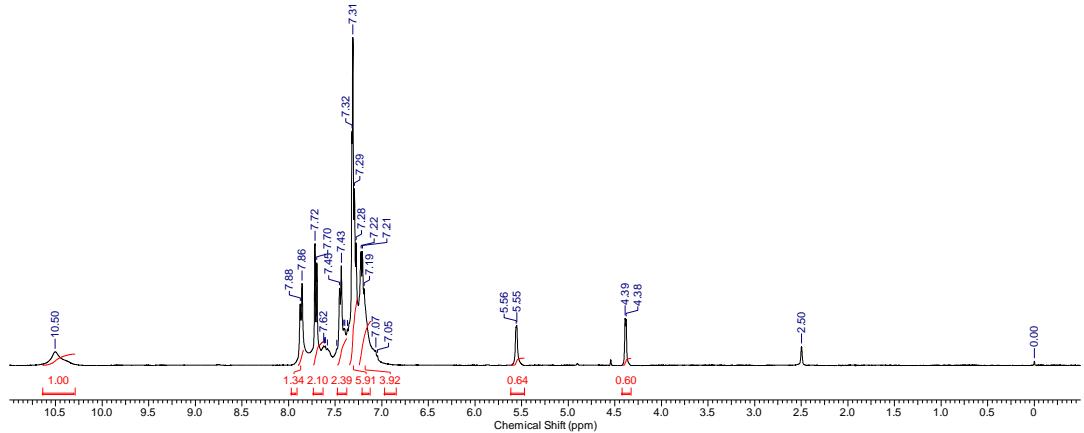


**<sup>13</sup>C-NMR**

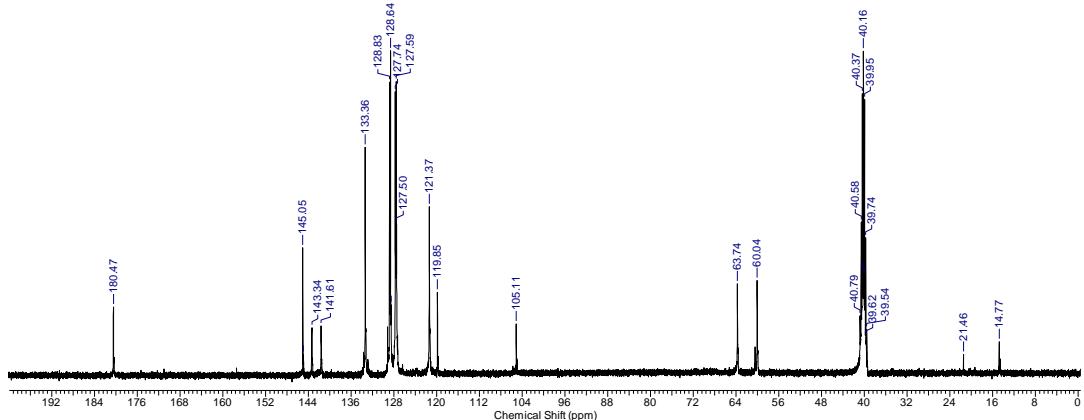


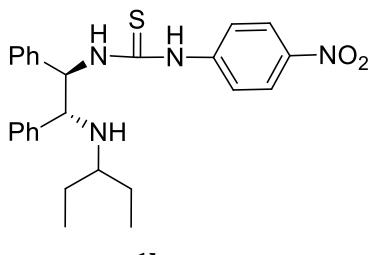


**<sup>1</sup>H-NMR**



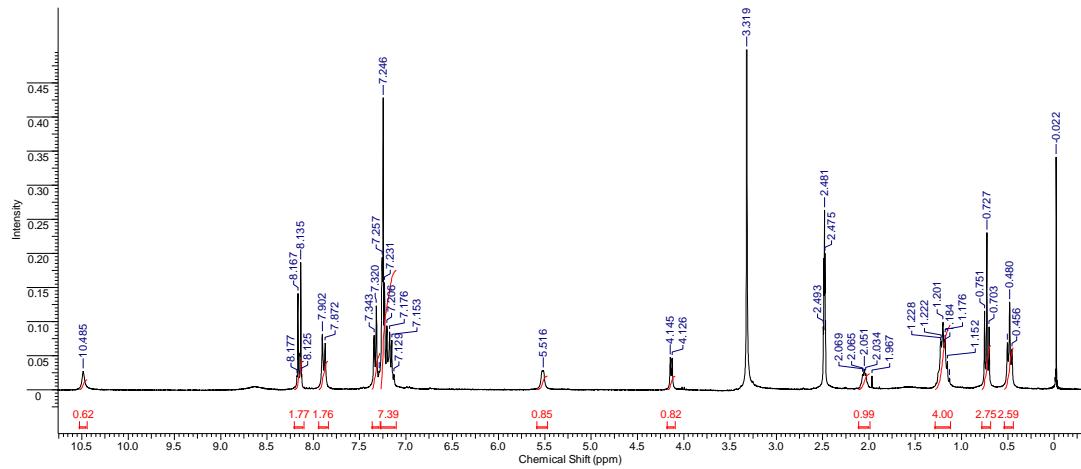
**<sup>13</sup>C-NMR**



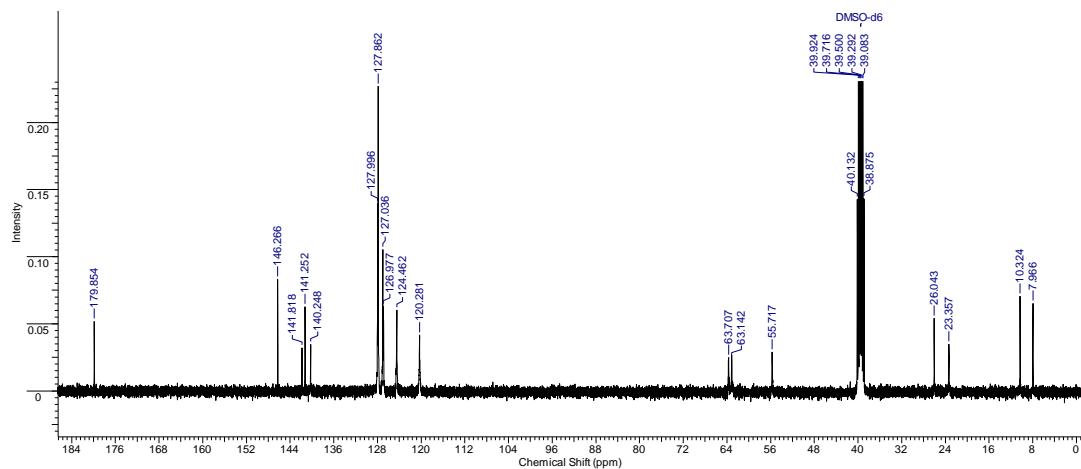


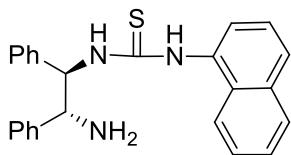
**1h**

**<sup>1</sup>H-NMR**



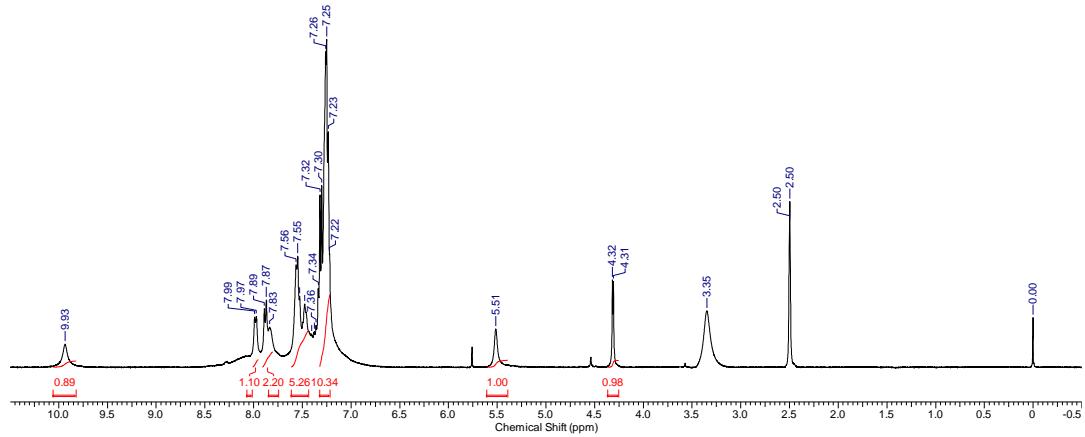
**<sup>13</sup>C-NMR**



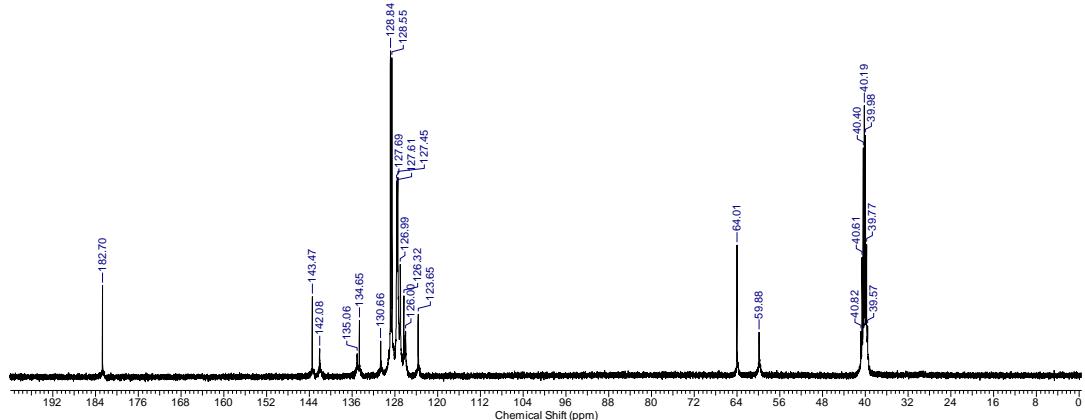


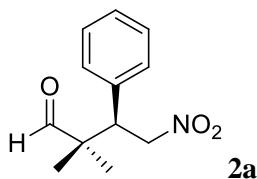
**1i**

**<sup>1</sup>H-NMR**



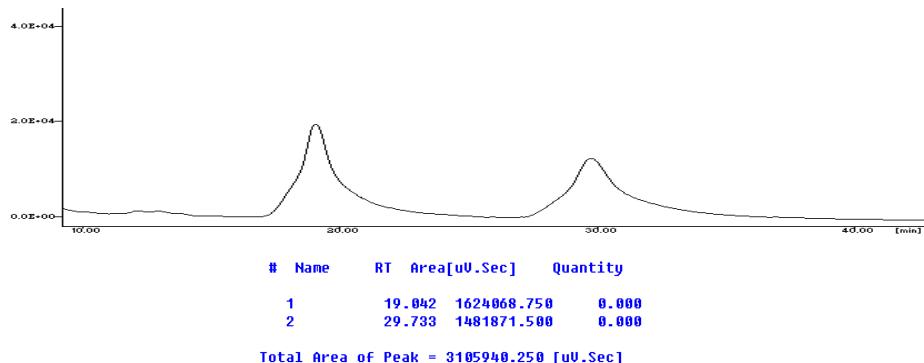
**<sup>13</sup>C-NMR**



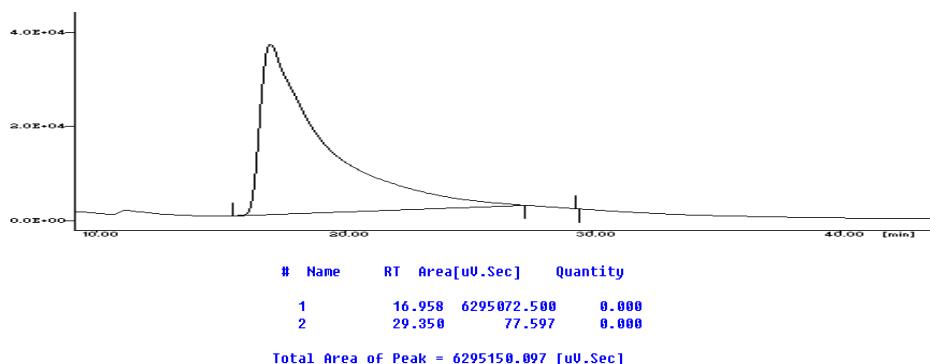


LC data

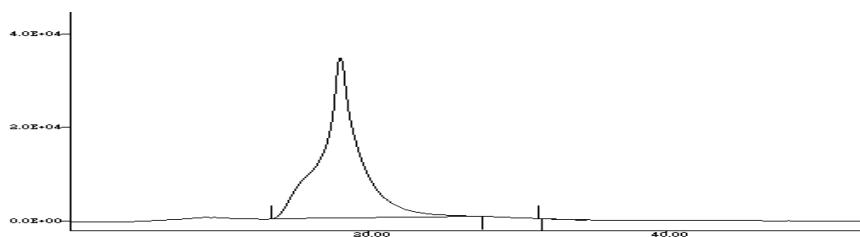
Racemic



Asymmetric-Table 1-1



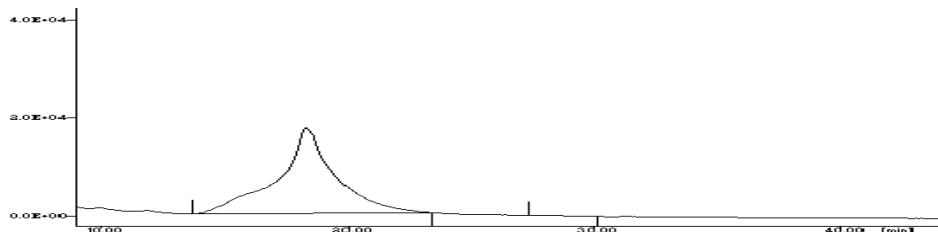
Asymmetric-Table 1-2



#	Name	RT	Area[uV.Sec]	Quantity
1		18.058	5582896.344	0.000
2		31.458	272.098	0.000

Total Area of Peak = 5583168.442 [uV.Sec]

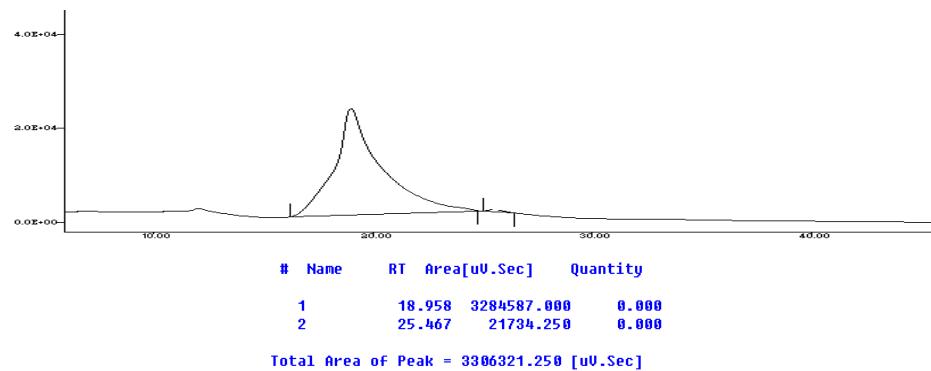
Asymmetric-Table 1-3



#	Name	RT	Area[uV.Sec]	Quantity
1		18.317	2699551.000	0.000
2		27.367	3158.500	0.000

Total Area of Peak = 2702709.500 [uV.Sec]

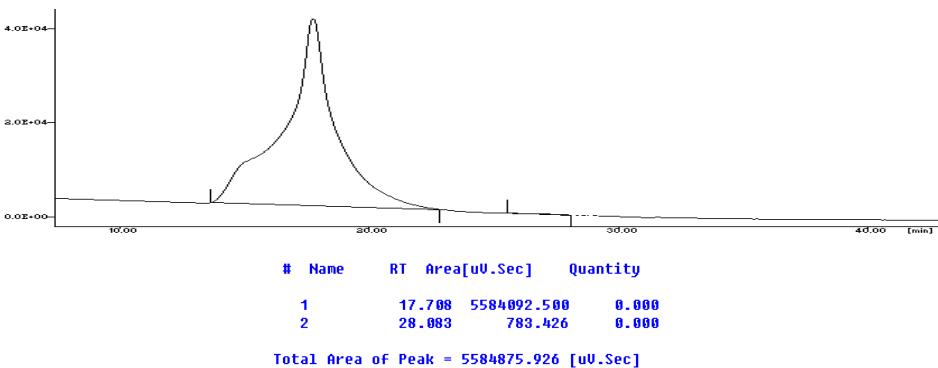
Asymmetric-Table 1-4



#	Name	RT	Area[uV.Sec]	Quantity
1		18.958	3284587.000	0.000
2		25.467	21734.250	0.000

Total Area of Peak = 3306321.250 [uV.Sec]

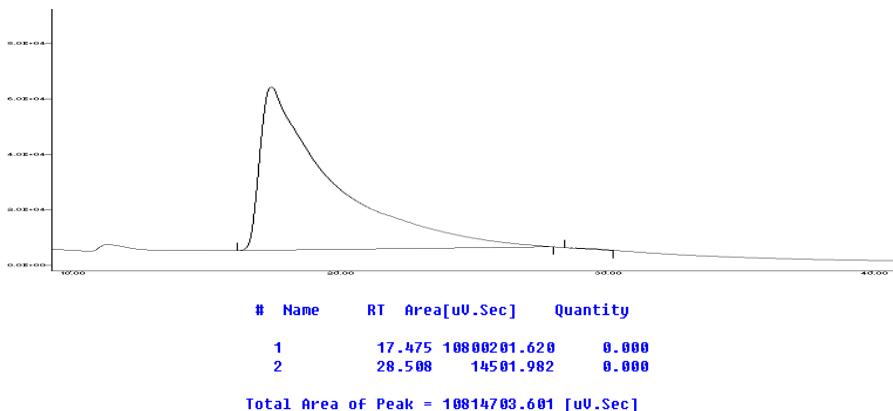
Asymmetric-Table 1-5



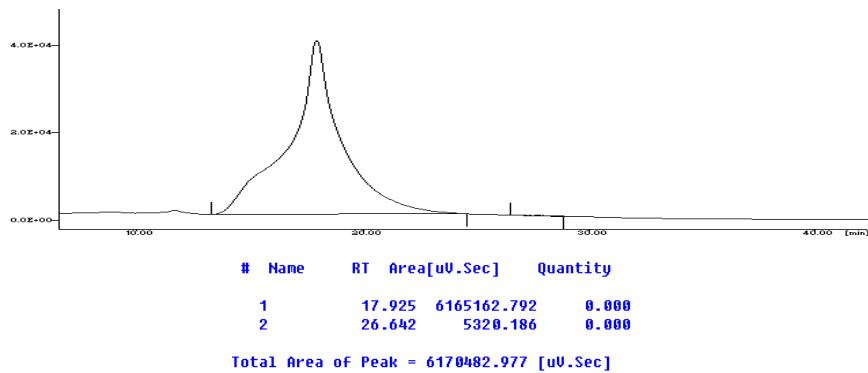
#	Name	RT	Area[uV.Sec]	Quantity
1		17.708	5584092.500	0.000
2		28.083	783.426	0.000

Total Area of Peak = 5584875.926 [uV.Sec]

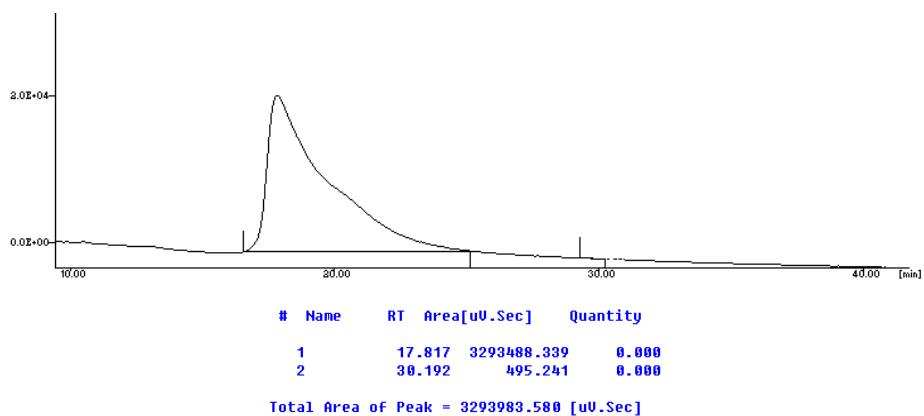
Asymmetric-Table 1-6



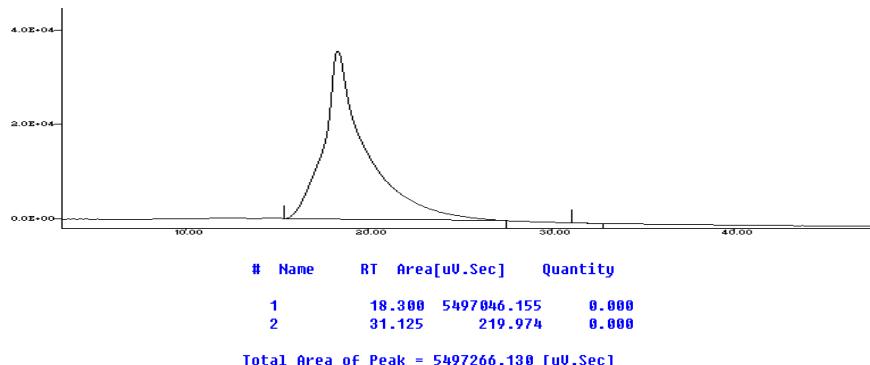
Asymmetric-Table 1-7



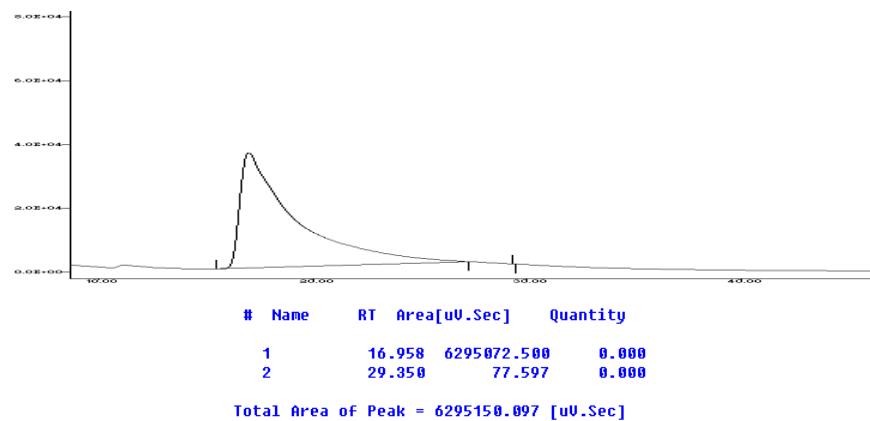
Asymmetric-Table 1-9



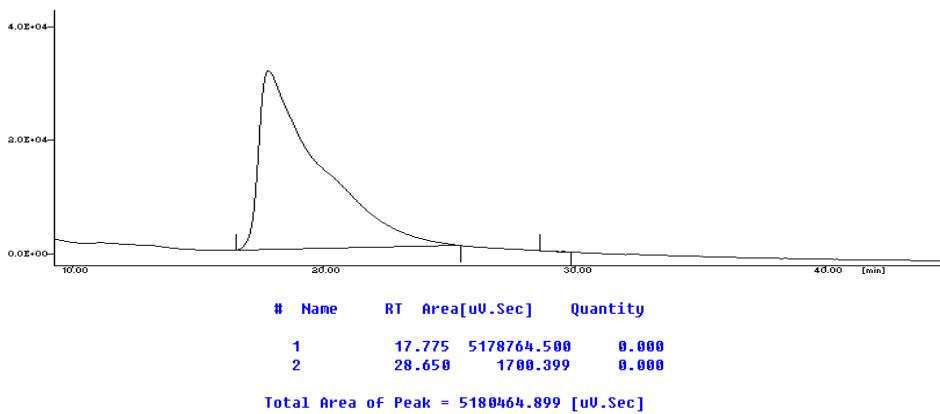
Asymmetric-Table 1-10



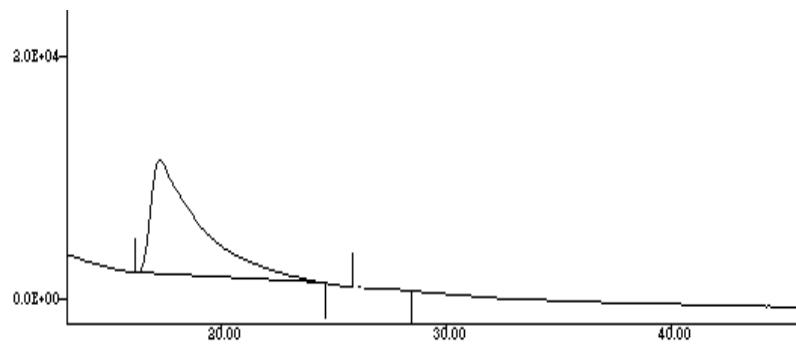
Asymmetric-Table 1-11



Asymmetric-Table 1-12



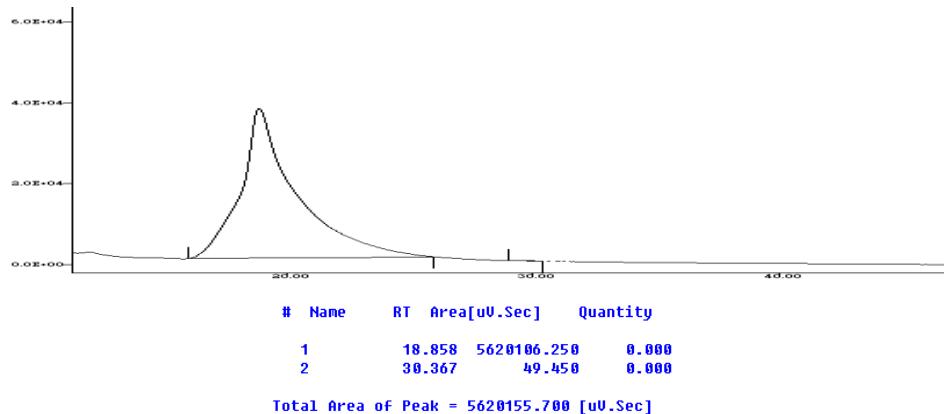
Asymmetric-Table 1-13



#	Name	RT	Area[uV.Sec]	Quantity
1		17.275	1119681.596	0.000
2		26.092	12541.344	0.000

Total Area of Peak = 1132142.948 [uV.Sec]

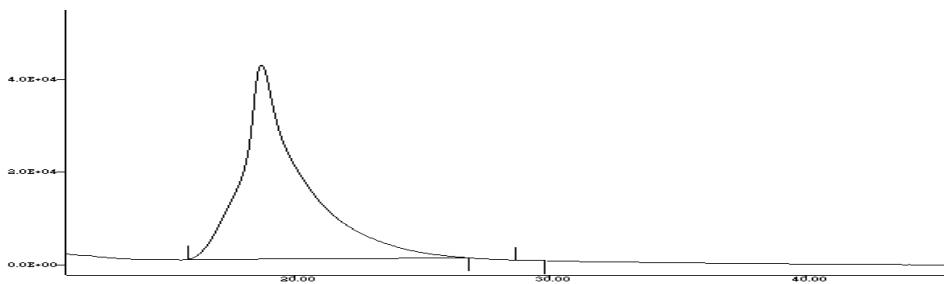
Asymmetric-Table 2-1



#	Name	RT	Area[uV.Sec]	Quantity
1		18.858	5620106.250	0.000
2		30.367	49.450	0.000

Total Area of Peak = 5620155.700 [uV.Sec]

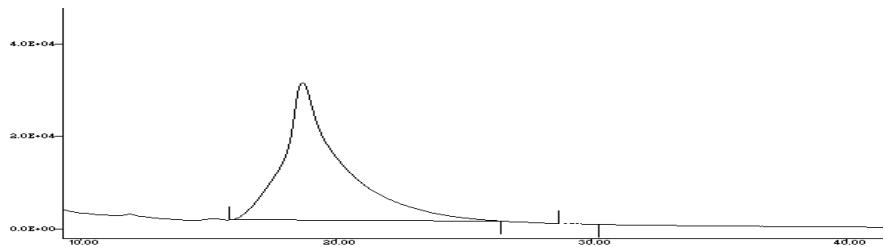
Asymmetric-Table 2-2



#	Name	RT	Area[uV.Sec]	Quantity
1		18.692	6583836.000	0.000
2		28.658	782.495	0.000

Total Area of Peak = 6584618.495 [uV.Sec]

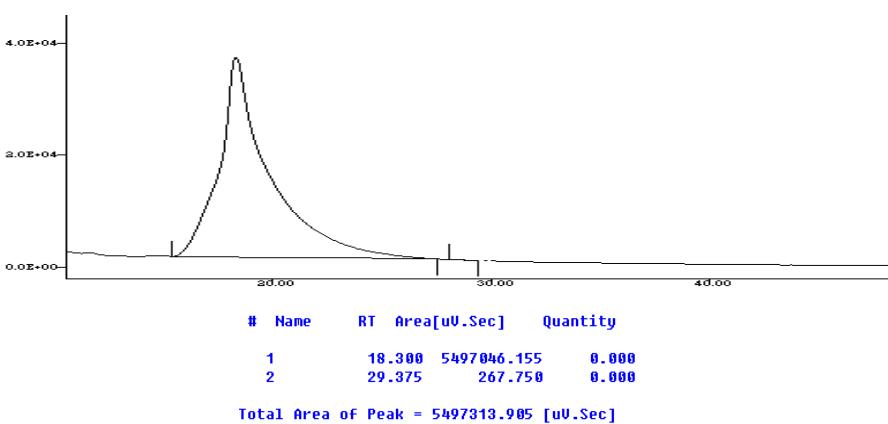
Asymmetric-Table 2-3



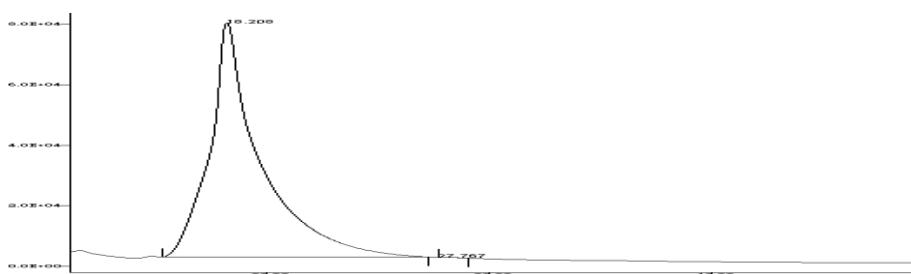
#	Name	RT	Area[uV.Sec]	Quantity
1		18.642	4538044.500	0.000
2		28.717	110327.500	0.000

Total Area of Peak = 4648372.000 [uV.Sec]

Asymmetric-Table 2-4



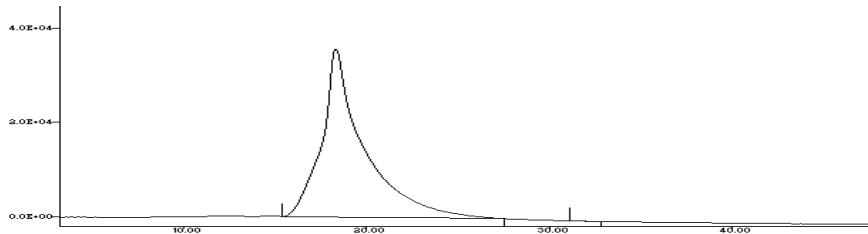
Asymmetric-Table 2-5



#	Name	RT	Area[uV.Sec]	Quantity
1		18.208	11757129.538	0.000
2		27.767	220453.000	0.000

Total Area of Peak = 11977582.538 [uV.Sec]

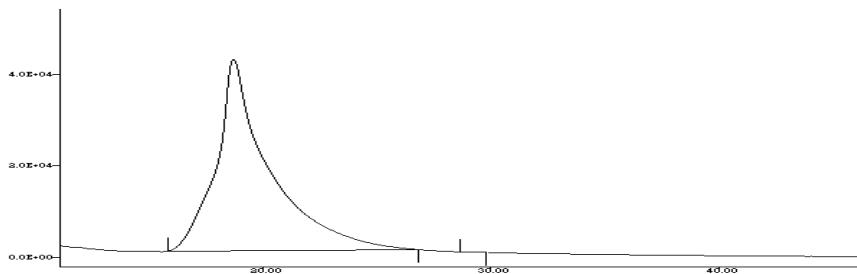
Asymmetric-Table 2-6



#	Name	RT	Area[uV.Sec]	Quantity
1		18.300	5497046.155	0.000
2		31.125	219.974	0.000

Total Area of Peak = 5497266.130 [uV.Sec]

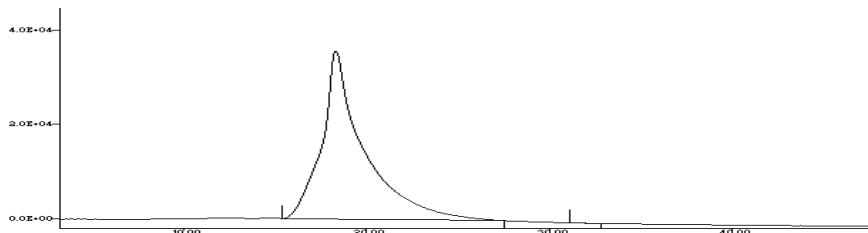
Asymmetric-Table 2-7



#	Name	RT	Area[uV.Sec]	Quantity
1		18.692	6583836.000	0.000
2		28.658	782.435	0.000

Total Area of Peak = 6584618.435 [uV.Sec]

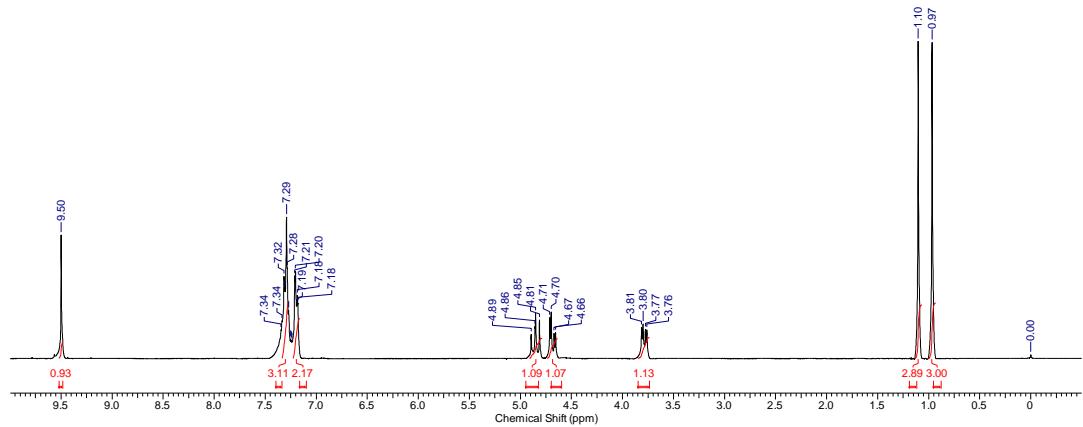
Asymmetric-Table 2-8



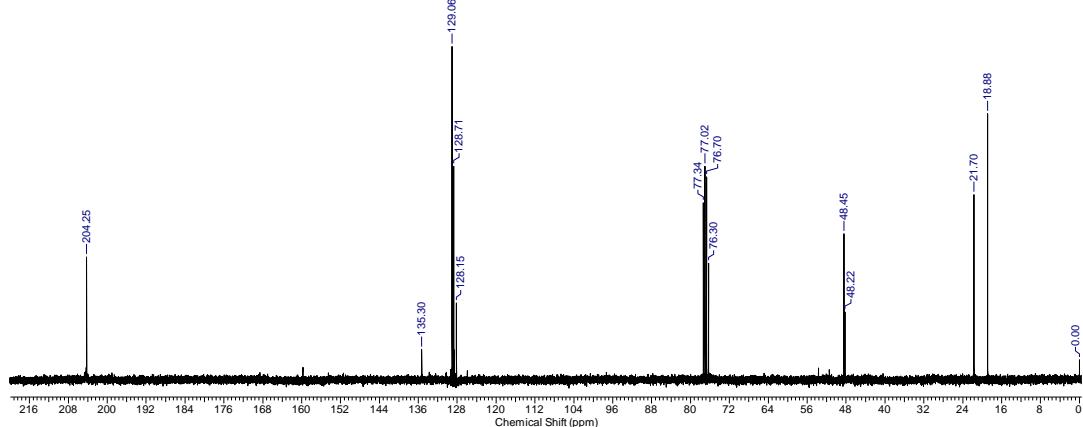
#	Name	RT	Area[uV.Sec]	Quantity
1		18.300	5497046.155	0.000
2		31.125	219.974	0.000

Total Area of Peak = 5497266.130 [uV.Sec]

### <sup>1</sup>H-NMR



### <sup>13</sup>C-NMR



### MASS

Note : with NBA+Na

Inlet : Direct

RT : 0.29 min

Elements : C 12/0, H 15/0, O 3/0, N 1/0, Na 1/0

Mass Tolerance : 100mmu

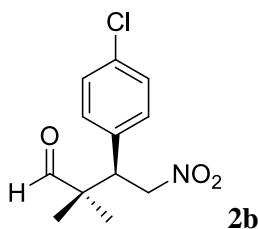
Unsaturation (U.S.) : -10.0 - 10.0

Ion Mode : FAB+

Scan# : (3,6) - (11,13)

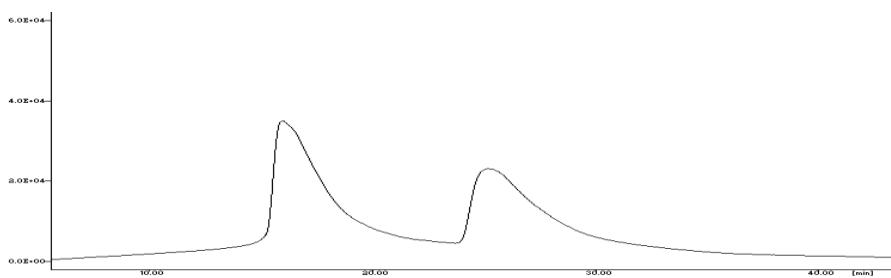
Observed m/z	Int%
244.0950	19.3

Estimated m/z	Error [ppm]	U.S.	C	H	O	N	Na
244.0950	+0.2	5.5	12	15	3	1	1



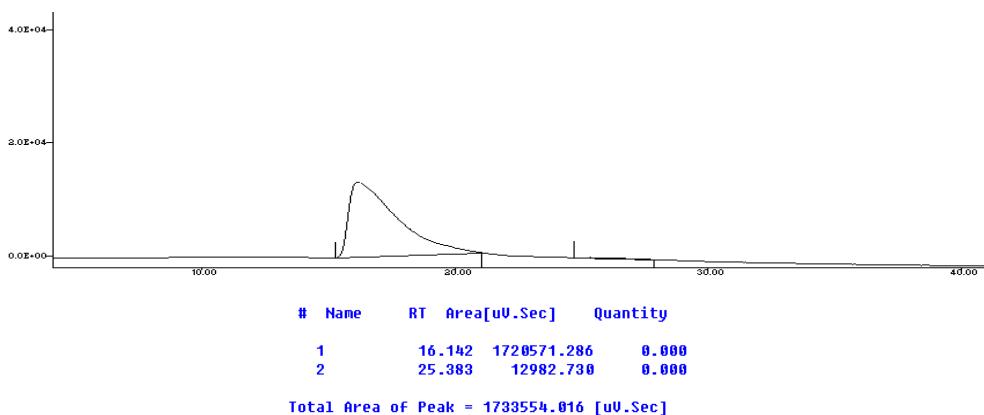
LC data

Racemic

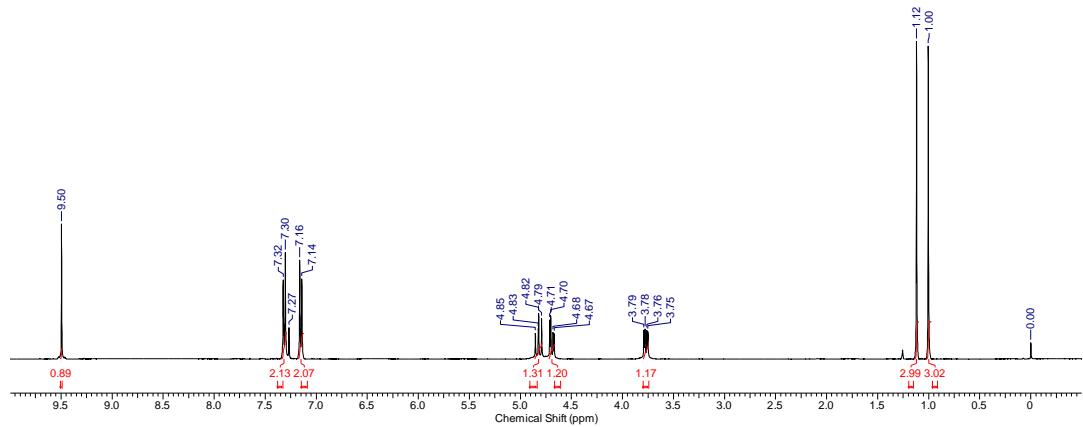


#	Name	RT	Area[uV.Sec]	Quantity
1		15.925	3551639.000	0.000
2		25.167	3361446.500	0.000
Total Area of Peak = 6913085.500 [uV.Sec]				

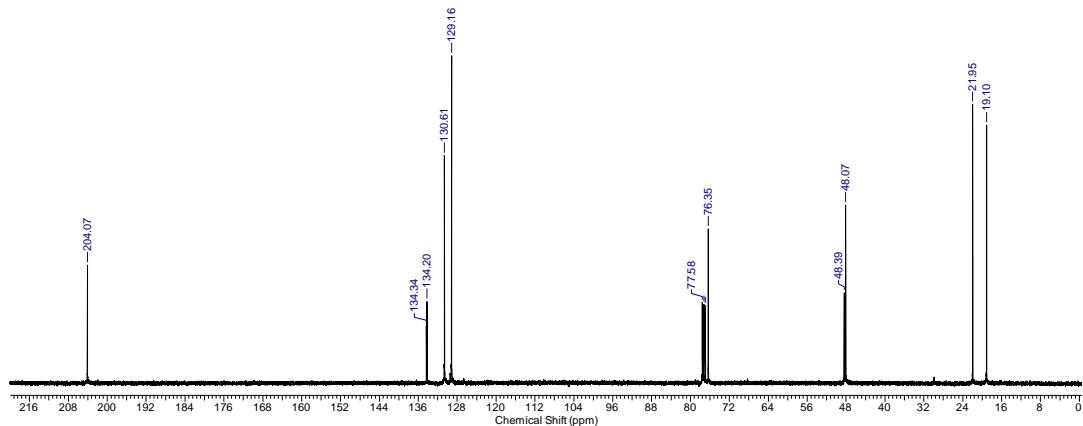
Asymmetric-Table 3-2



### <sup>1</sup>H-NMR



### <sup>13</sup>C-NMR



### MASS

Note : with NBA+Na

Inlet : Direct

Ion Mode : FAB+

RT : 0.38 min

Scan# : (3,8) - (10,11)

Elements : C 12/0, H 14/0, O 3/0, N 1/0, Cl 1/0, Na 1/0

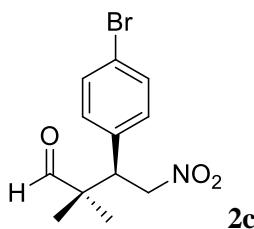
Mass Tolerance : 100mmu

Unsaturation (U.S.) : -10.0 - 10.0

Observed m/z Int%

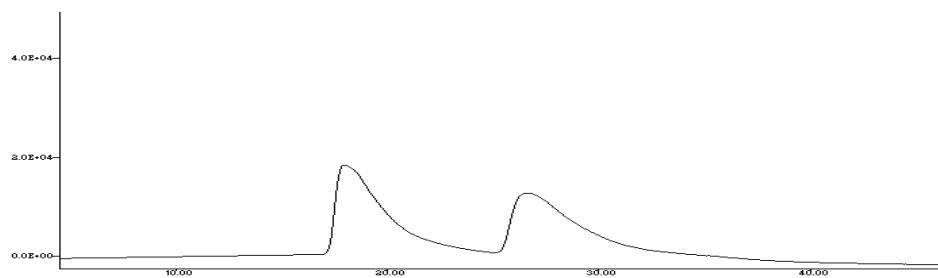
278.0562 100.0

Estimated m/z	Error [ppm]	U.S.	C	H	O	N	Cl	Na
278.0560	+0.8	5.5	12	14	3	1	1	1



LC data

Racemic

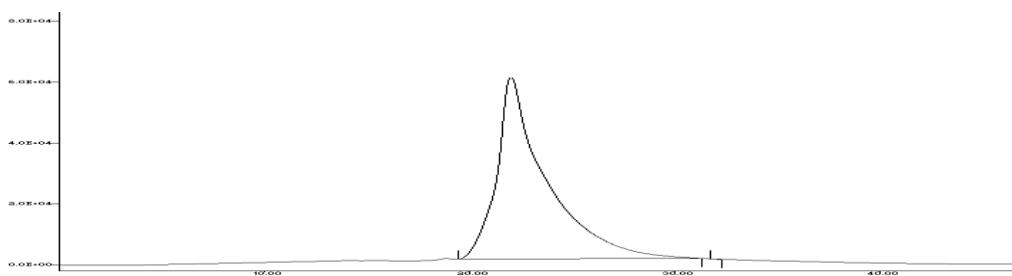


# Name RT Area[uV.Sec] Quantity

1	17.942	2751283.821	0.000
2	26.608	2620466.372	0.000

Total Area of Peak = 5371670.192 [uV.Sec]

### Asymmetric-Table 3-3

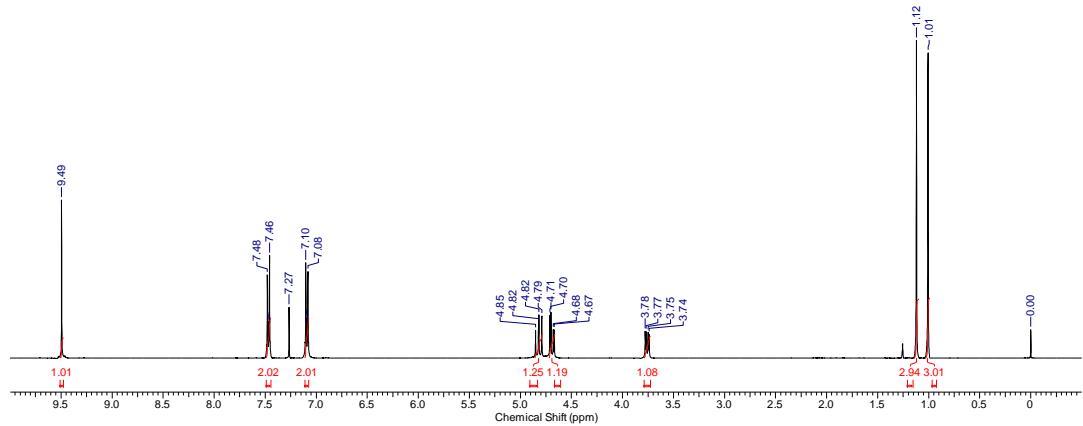


# Name RT Area[uV.Sec] Quantity

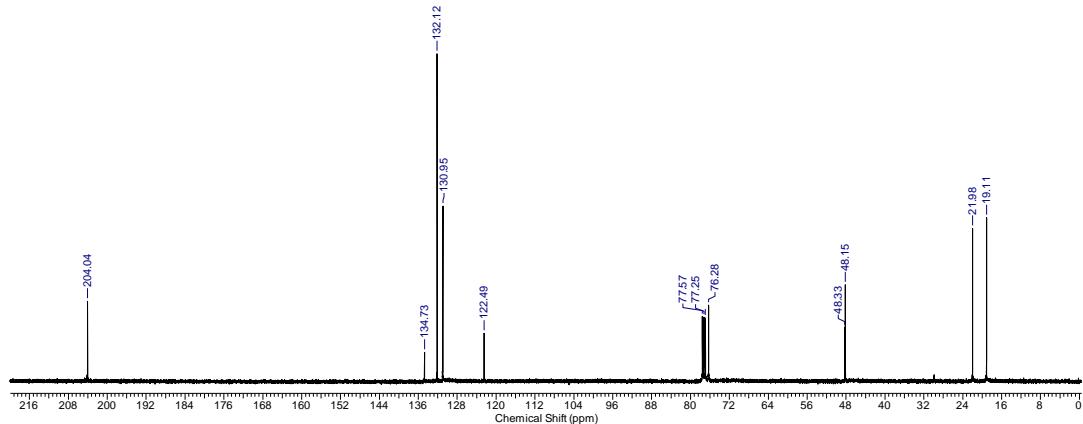
1	21.983	9675147.784	0.000
2	31.775	592.250	0.000

Total Area of Peak = 9675740.034 [uV.Sec]

### <sup>1</sup>H-NMR



### <sup>13</sup>C-NMR



### MASS

Note : with NBA+Na

Inlet : Direct

Ion Mode : FAB+

RT : 0.29 min

Scan# : (4,5)-17

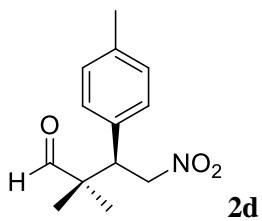
Elements : C 12/0, H 14/0, O 3/0, N 1/0, Br 1/0, Na 1/0

Mass Tolerance : 100mmu

Unsaturation (U.S.) : -10.0 - 10.0

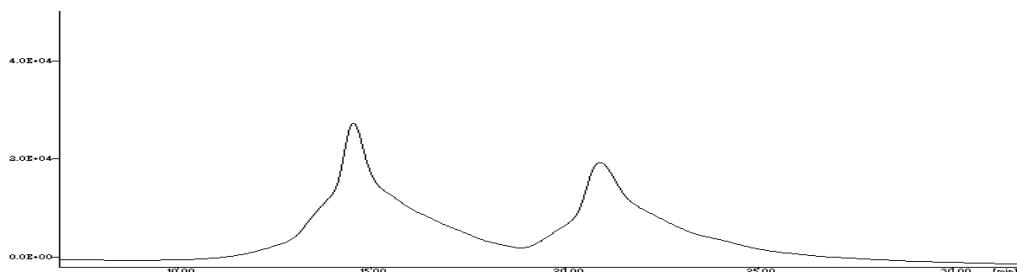
Observed m/z	Int%
322.0053	46.4

Estimated m/z	Error [ppm]	U.S.	C	H	O	N	Br	Na
322.0055	-0.5	5.5	12	14	3	1	1	1



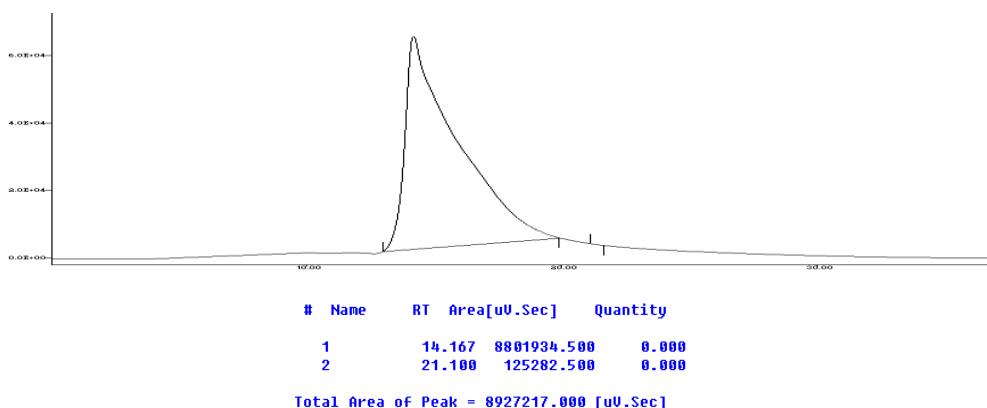
LC data

Racemic



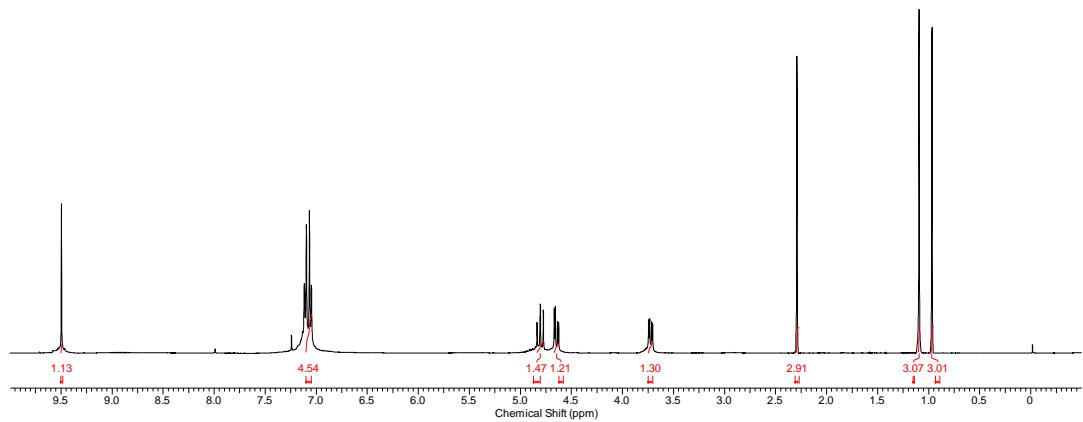
#	Name	RT	Area[uV.Sec]	Quantity
1		14.517	1876288.000	0.000
2		20.883	1886939.752	0.000
Total Area of Peak = 3763227.752 [uV.Sec]				

Asymmetric-Table 3-4

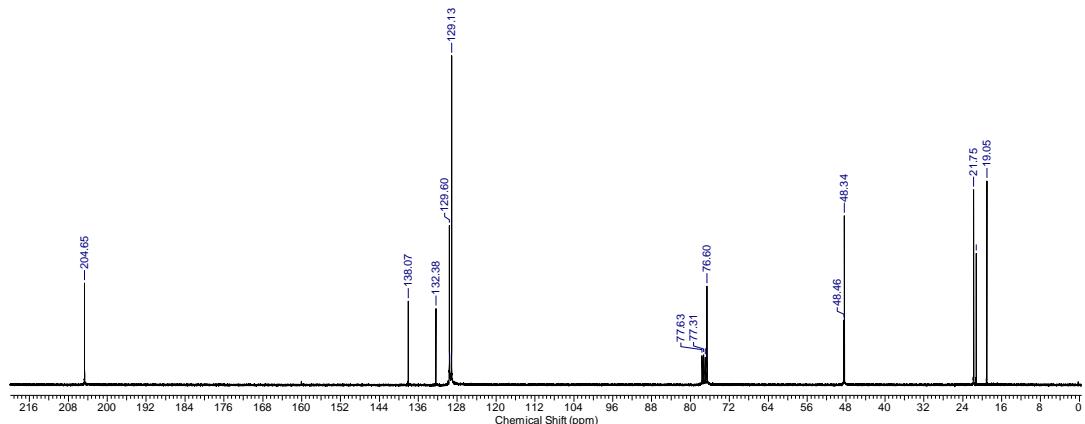


#	Name	RT	Area[uV.Sec]	Quantity
1		14.167	8801934.500	0.000
2		21.100	125282.500	0.000
Total Area of Peak = 8927217.000 [uV.Sec]				

### <sup>1</sup>H-NMR



### <sup>13</sup>C-NMR



### MASS

Note : with NBA+Na

Inlet : Direct

Ion Mode : FAB+

RT : 1.00 min

Scan# : (10,16)

Elements : C 13/0, H 17/0, O 3/0, N 1/0, Na 1/0

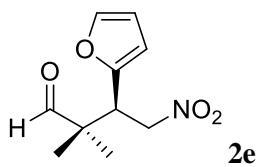
Mass Tolerance : 100mmu

Unsaturation (U.S.) : -10.0 - 10.0

Observed m/z      Int%

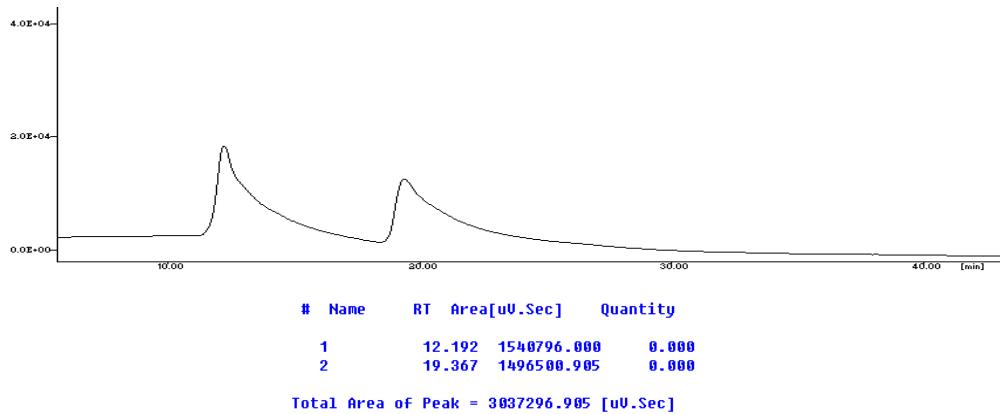
258.1107      100.0

Estimated m/z	Error [ppm]	U.S.	C	H	O	N	Na
258.1106	+0.2	5.5	13	17	3	1	1

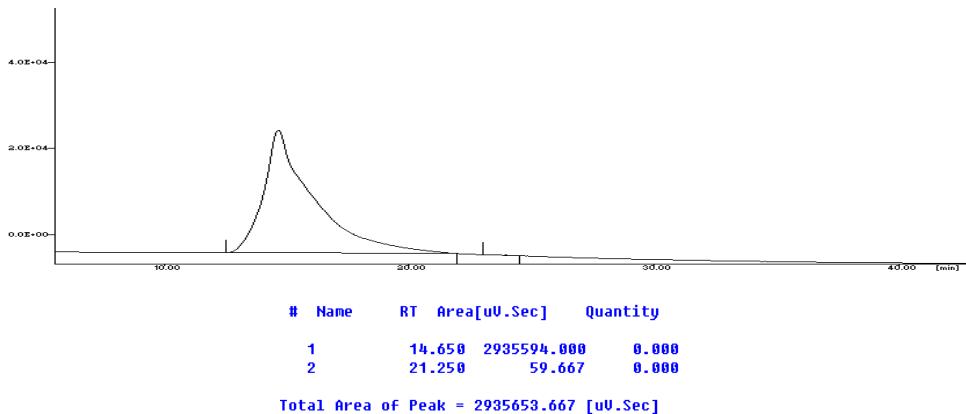


LC data

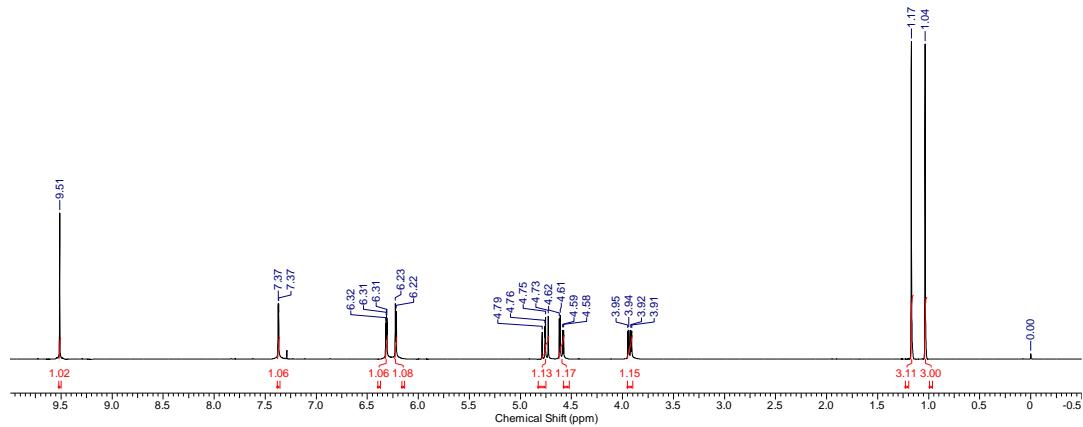
Racemic



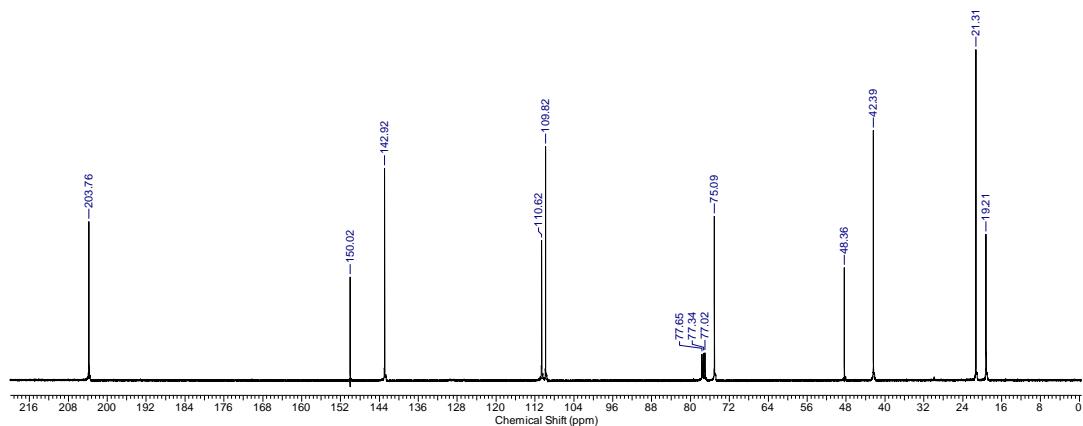
Asymmetric-Table 3-5



### <sup>1</sup>H-NMR



### <sup>13</sup>C-NMR



### MASS

Note : with NBA+Na

Inlet : Direct

Ion Mode : FAB+

RT : 1.09 min

Scan# : (11,17) - (5,7)

Elements : C 10/0, H 13/0, O 4/0, N 1/0, Na 1/0

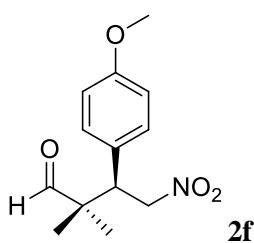
Mass Tolerance : 100mmu

Unsaturation (U.S.) : -10.0 - 10.0

Observed m/z Int%

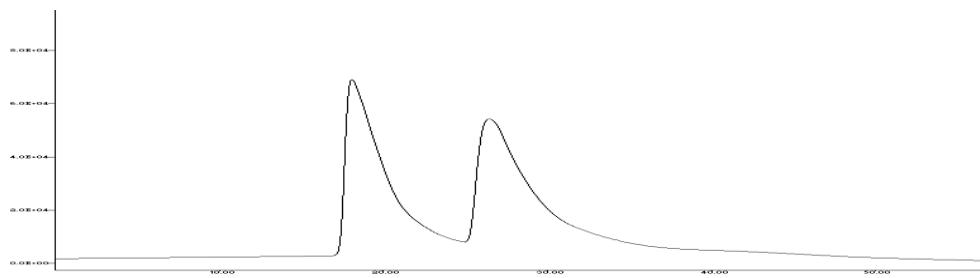
234.0742 100.0

Estimated m/z	Error [ppm]	U.S.	C	H	O	N	Na
234.0742	+0.0	4.5	10	13	4	1	1

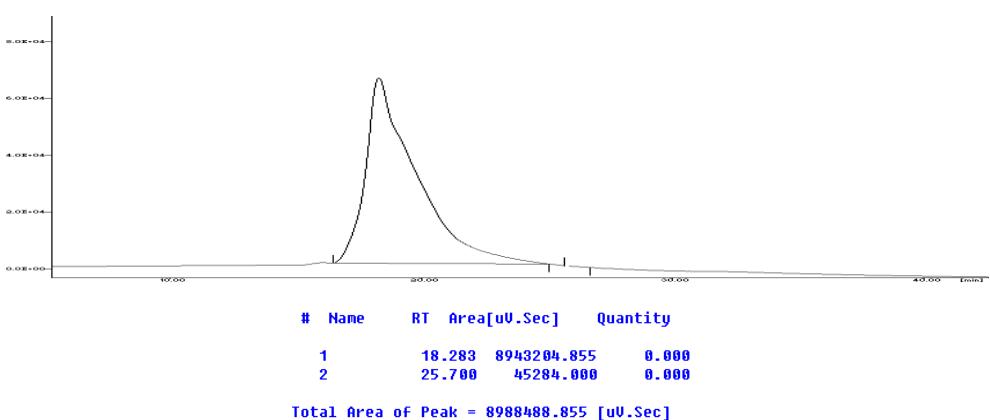


LC data

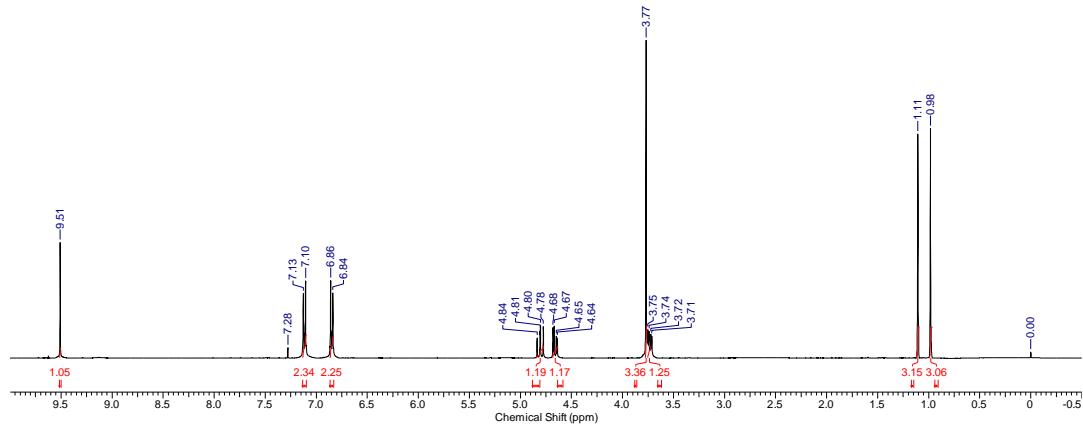
Racemic



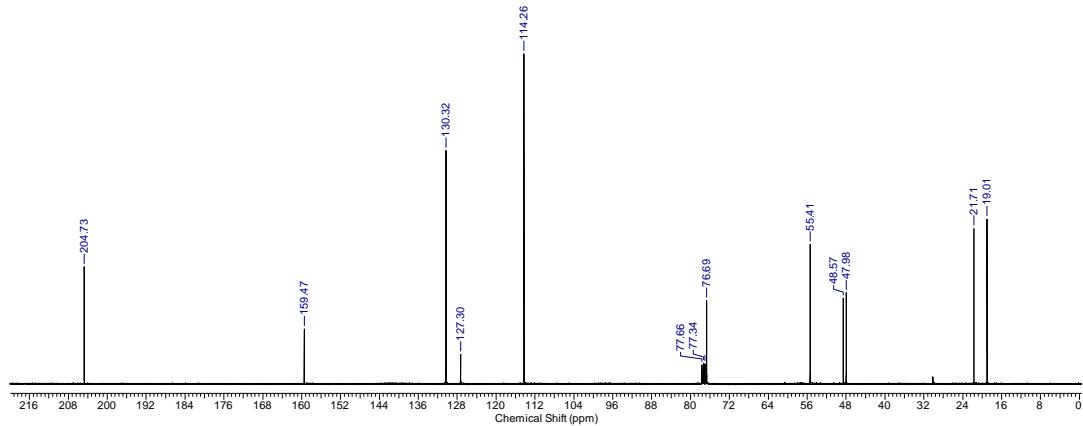
### Asymmetric-Table 3-6



### <sup>1</sup>H-NMR



### <sup>13</sup>C-NMR



### MASS

Note : with NBA+Na

Inlet : Direct

RT : 0.96 min

Elements : C 13/0, H 17/0, O 4/0, N 1/0, Na 1/0

Mass Tolerance : 100mmu

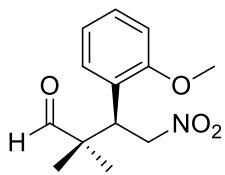
Unsaturation (U.S.) : -10.0 - 10.0

Ion Mode : FAB+  
Scan#: (10,15)-(5,6)

Observed m/z Int%

274.1055 100.0

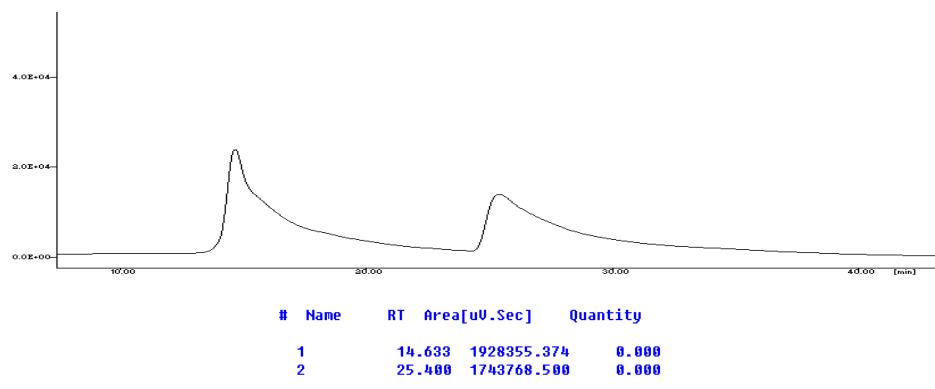
Estimated m/z	Error [ppm]	U.S.	C	H	O	N	Na
274.1055	-0.1	5.5	13	17	4	1	1



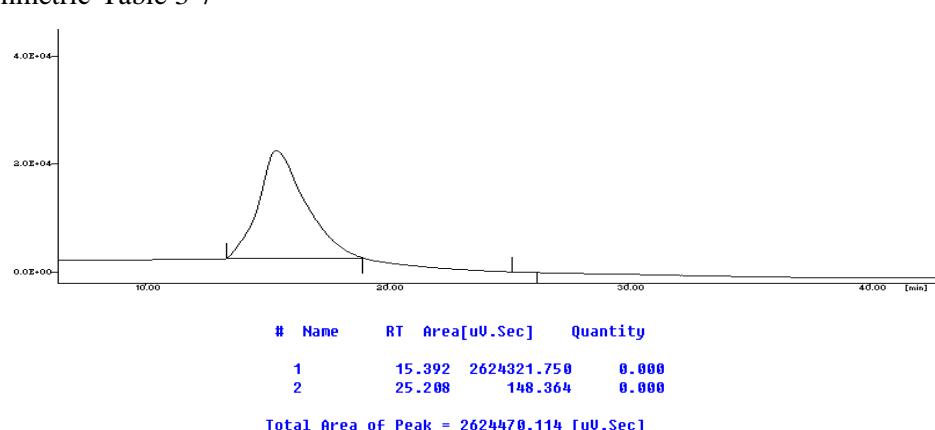
**2g**

LC data

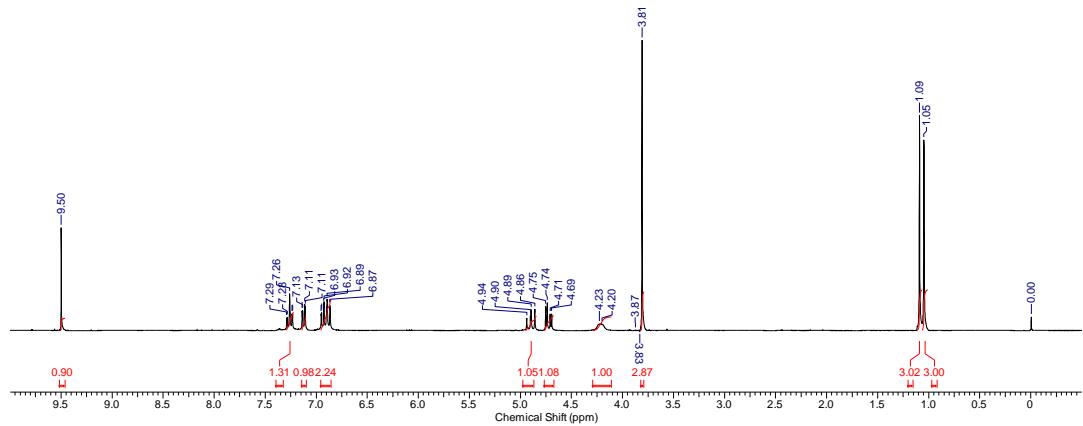
Racemic



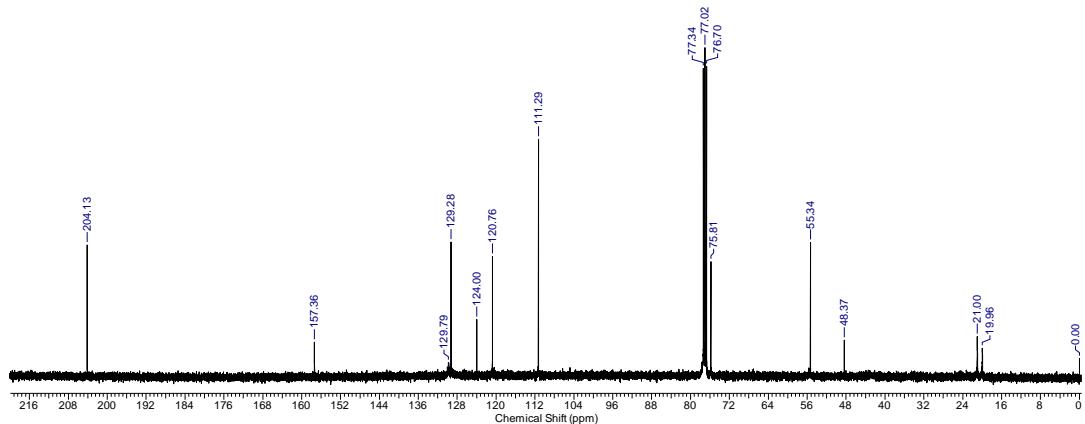
Asymmetric-Table 3-7



### <sup>1</sup>H-NMR



### <sup>13</sup>C-NMR



### MASS

Note : with NBA+Na

Inlet : Direct

Ion Mode : FAB+

RT : 1.29 min

Scan# : (16, 17) - 9

Elements : C 13/0, H 17/0, O 4/0, N 1/0, Na 1/0

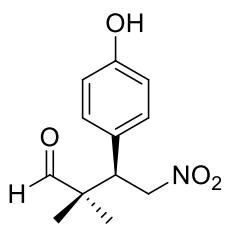
Mass Tolerance : 100mmu

Unsaturation (U.S.) : -10.0 - 10.0

Observed m/z      Int%

274.1056      100.0

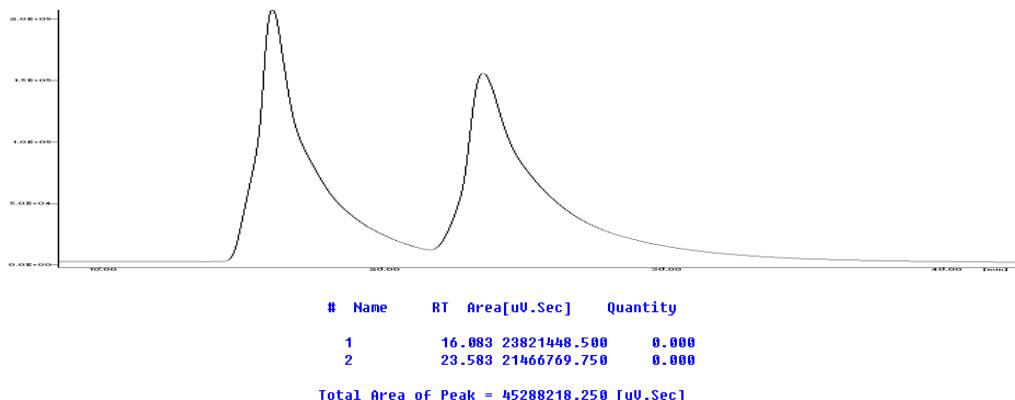
Estimated m/z	Error [ppm]	U.S.	C	H	O	N	Na
274.1055	+0.2	5.5	13	17	4	1	1



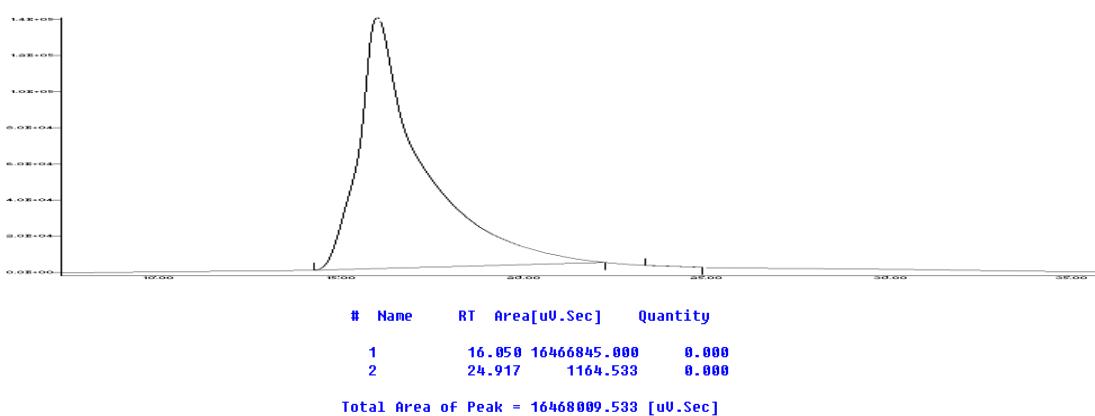
**2h**

LC data

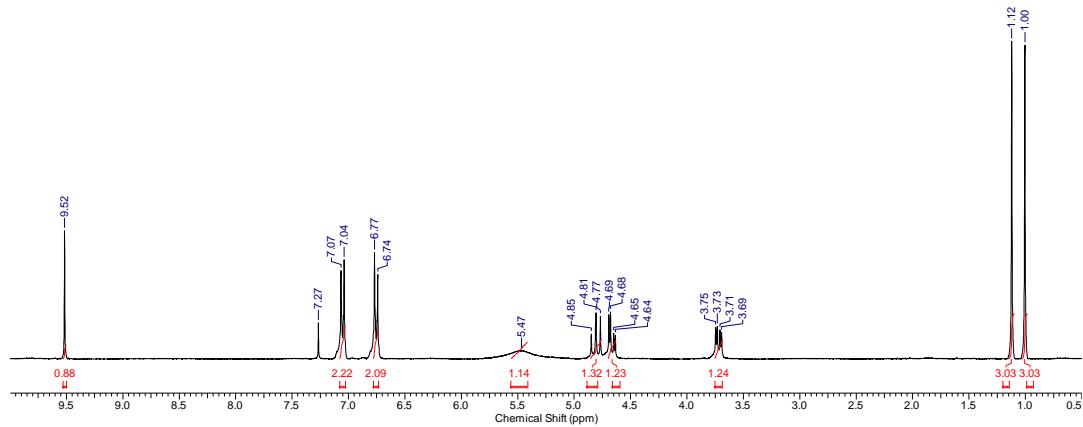
Racemic



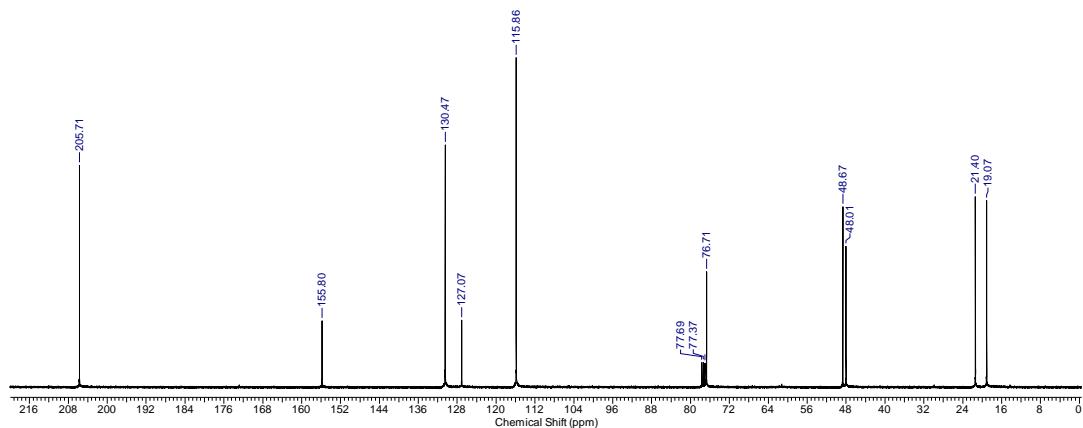
Asymmetric-Table 3-2



### <sup>1</sup>H-NMR



### <sup>13</sup>C-NMR



### MASS

Note : with NBA+Na

Inlet : Direct

Ion Mode : FAB+

RT : 0.21 min

Scan# : (1,6)-(18,22)-24

Elements : C 12/0, H 15/0, O 4/0, N 1/0, Na 1/0

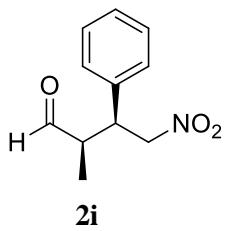
Mass Tolerance : 100mmu

Unsaturation (U.S.) : -10.0 - 10.0

Observed m/z Int%

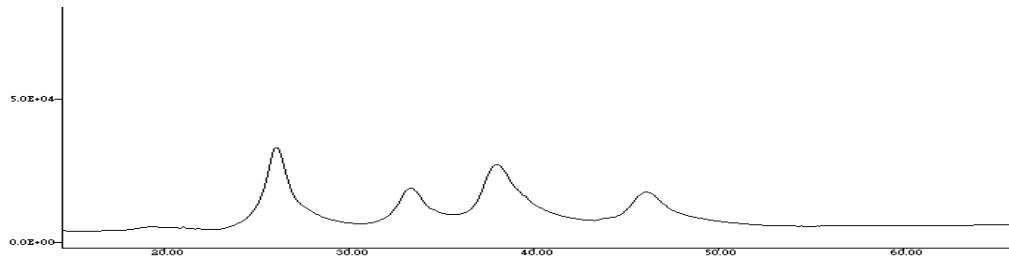
260.0899 100.0

Estimated m/z	Error [ppm]	U.S.	C	H	O	N	Na
260.0899	+0.0	5.5	12	15	4	1	1



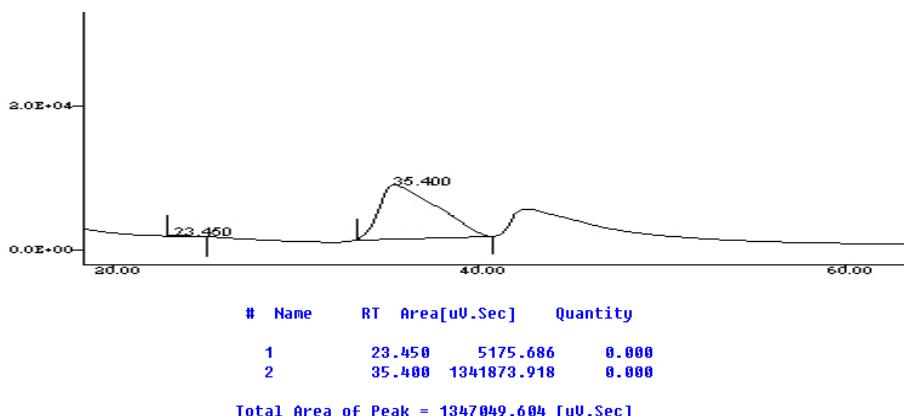
LC data

Racemic

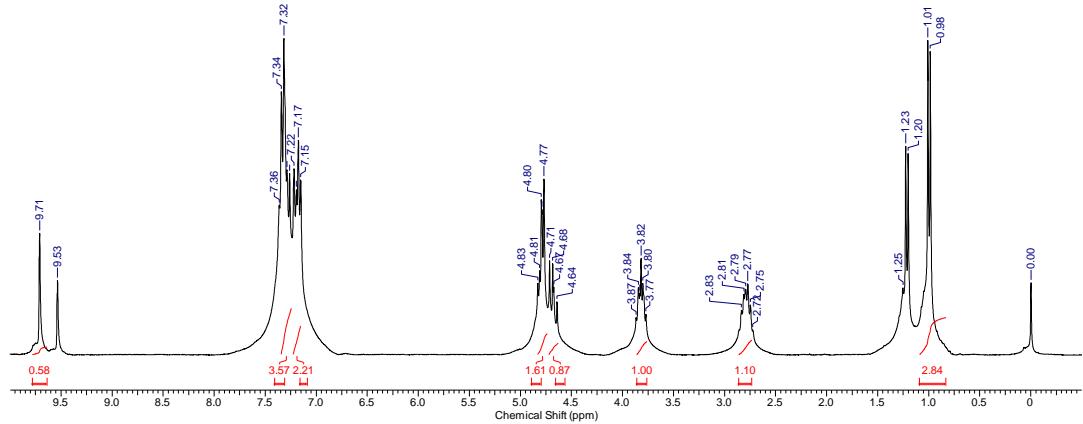


Total Area of Peak = 4796732.559 [uV.Sec]

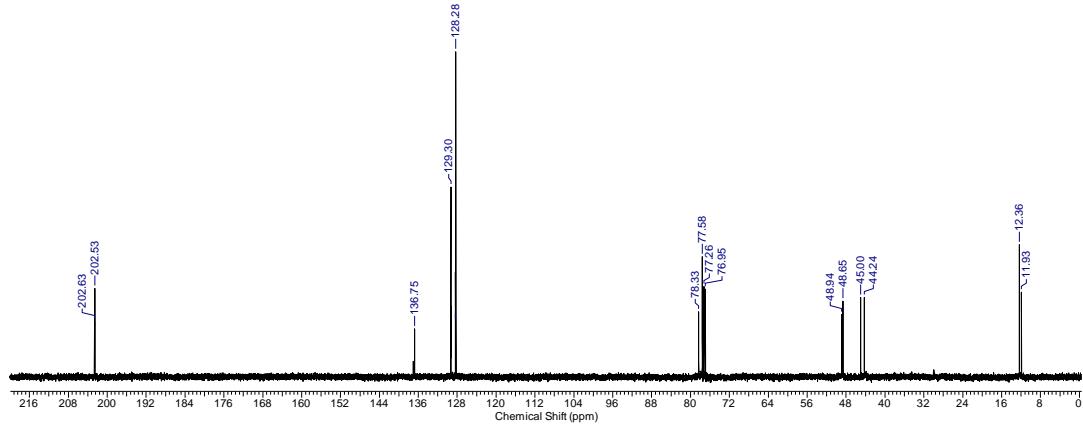
Asymmetric-Table 4-1



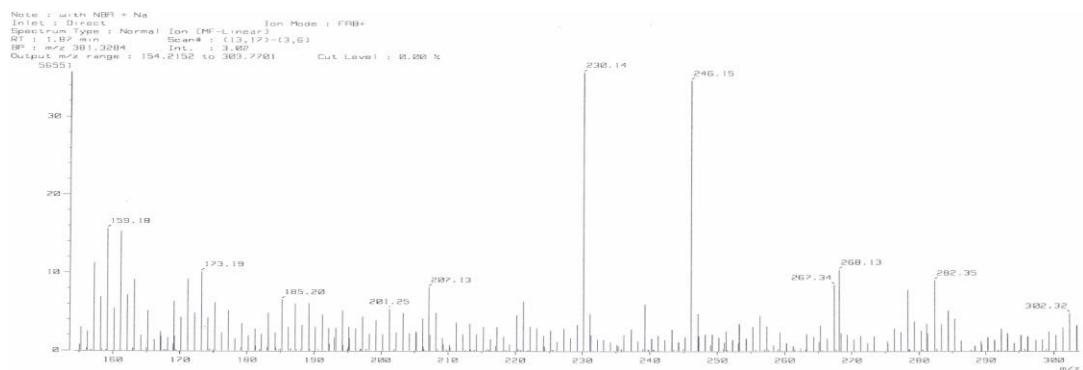
## <sup>1</sup>H-NMR

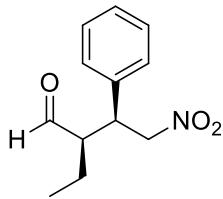


## <sup>13</sup>C-NMR



## MASS

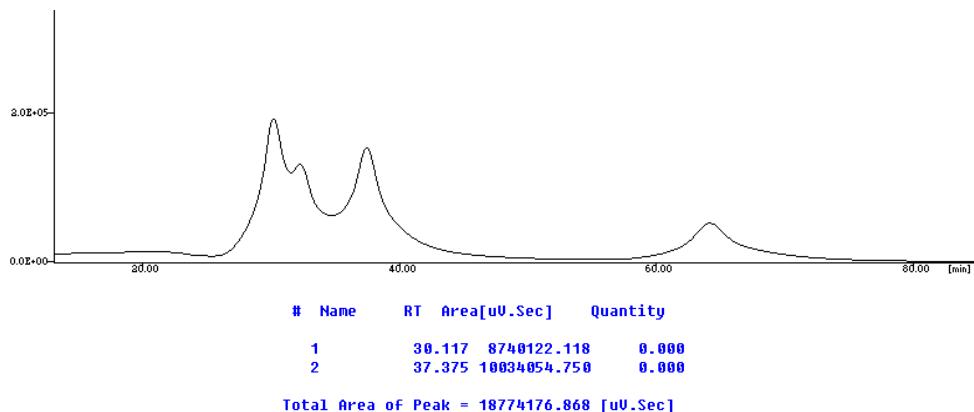




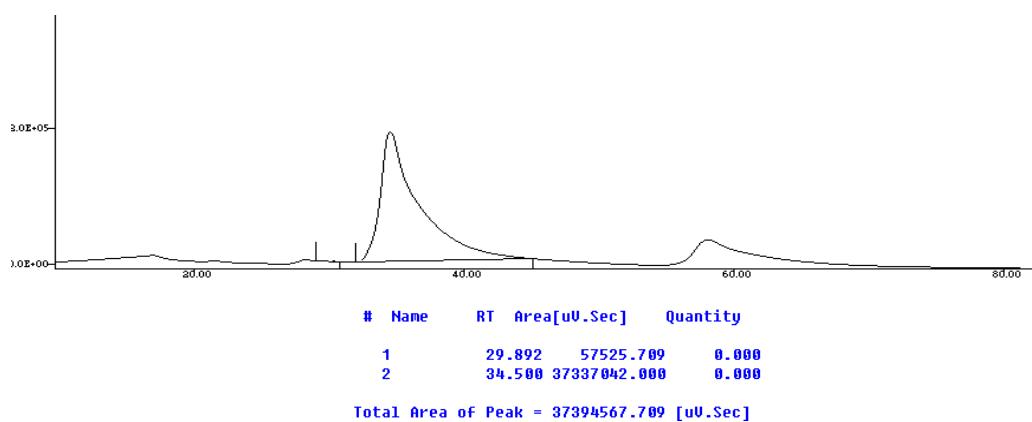
**2j**

LC data

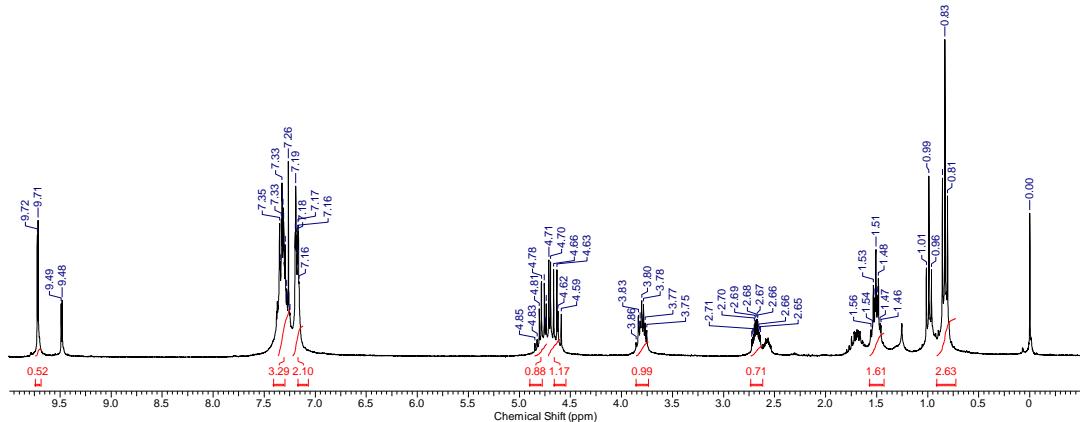
Racemic



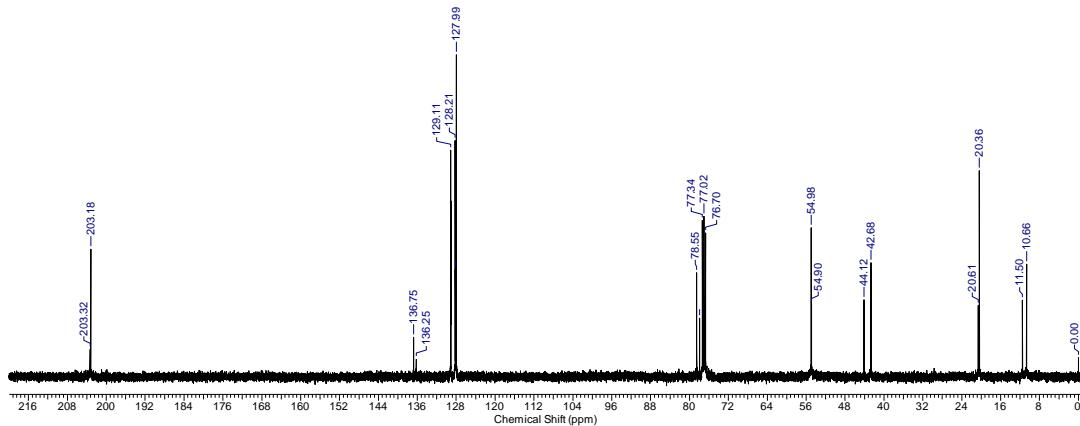
Asymmetric-Table 4-2



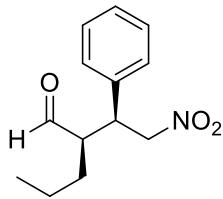
## **<sup>1</sup>H-NMR**



## **<sup>13</sup>C-NMR**



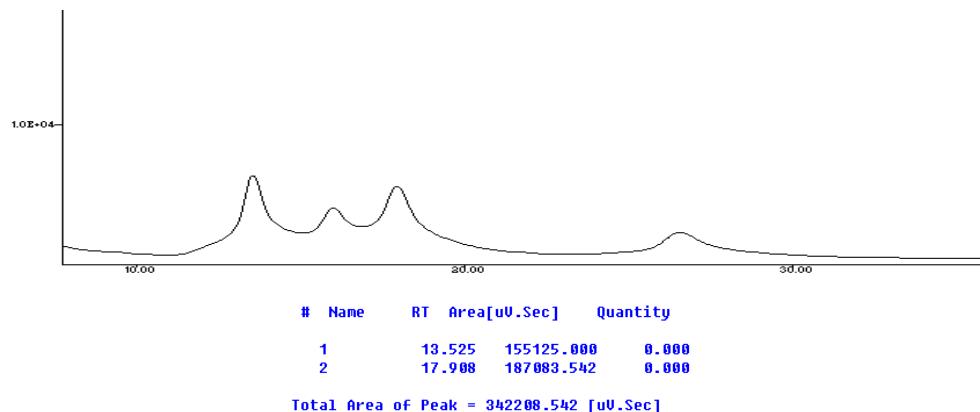
MASS



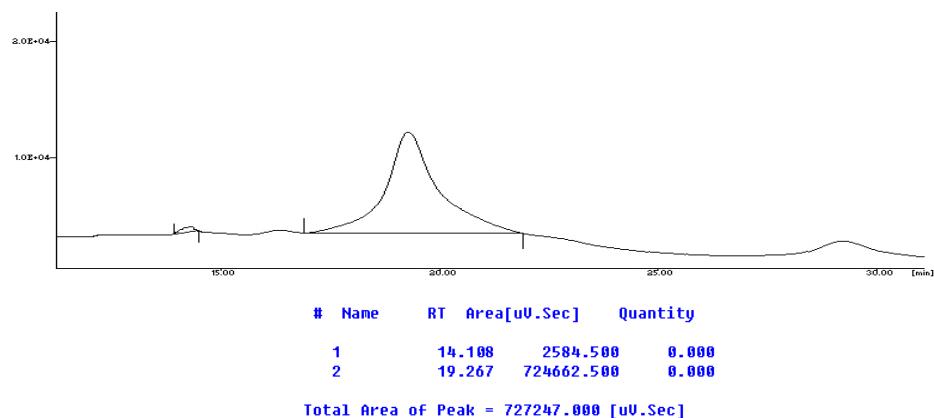
### **2k**

LC data

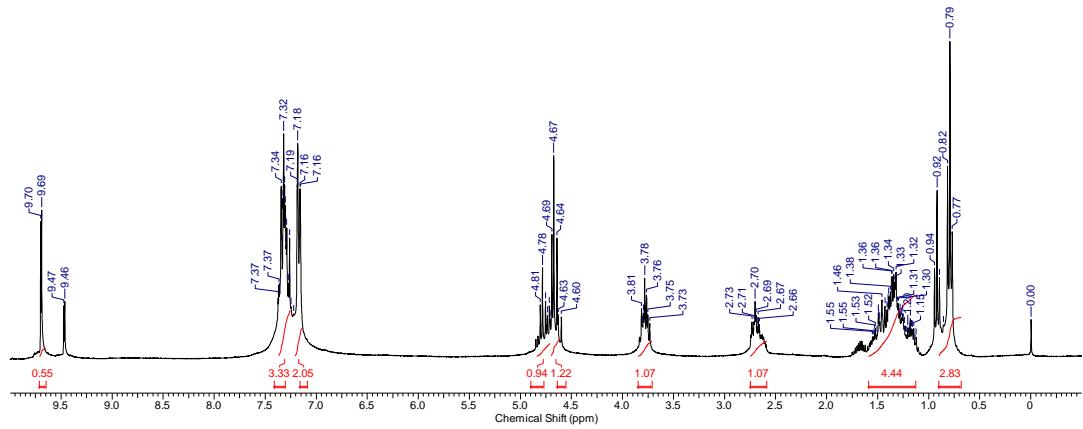
Racemic



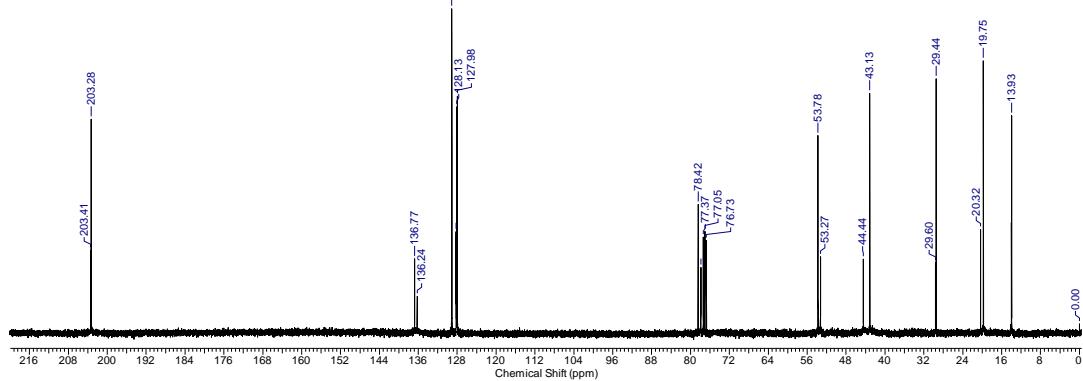
Asymmetric-Table 4-3



## <sup>1</sup>H-NMR

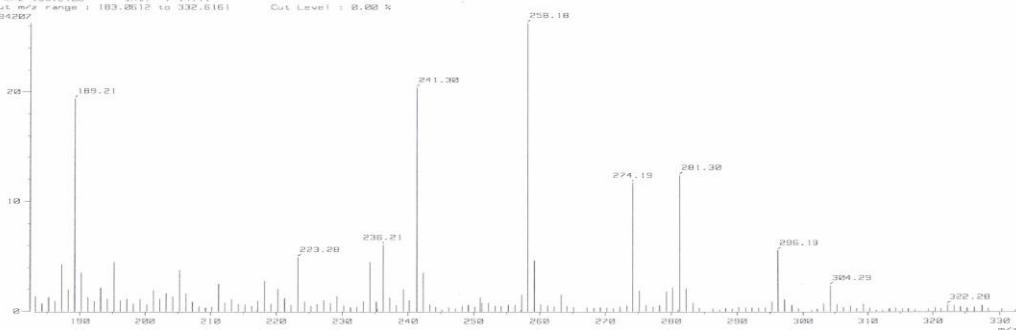


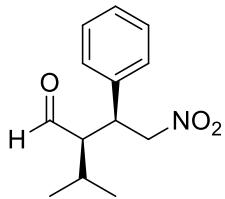
## <sup>13</sup>C-NMR



## MASS

Note: i = with NBF<sub>3</sub> + Na  
 Intens.: Direct.  
 Spectrum Type: Normal Ion Mode: ESI(+)  
 RT: 10.00 min Ion Source: ESI(+)-QTOF-QQQ  
 DRP: i m/z 159.2186 Int.: i 14.11  
 Output m/z range: i 183.0612 to 332.6161 Cut Level: i 0.000 %  
 184.0202

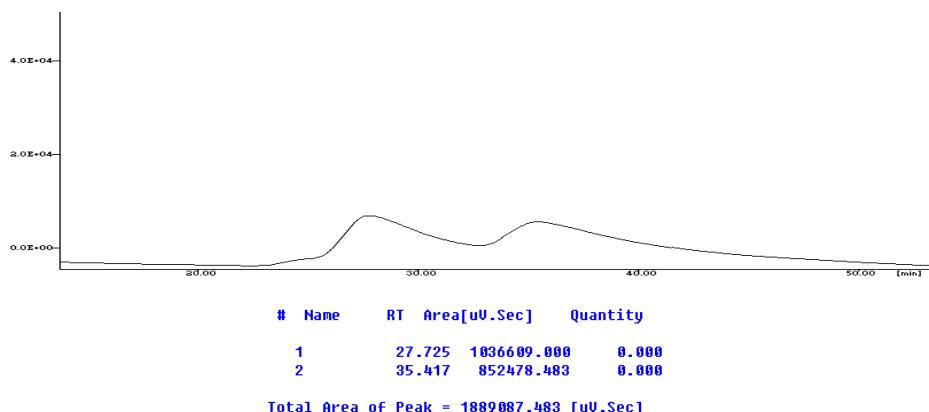




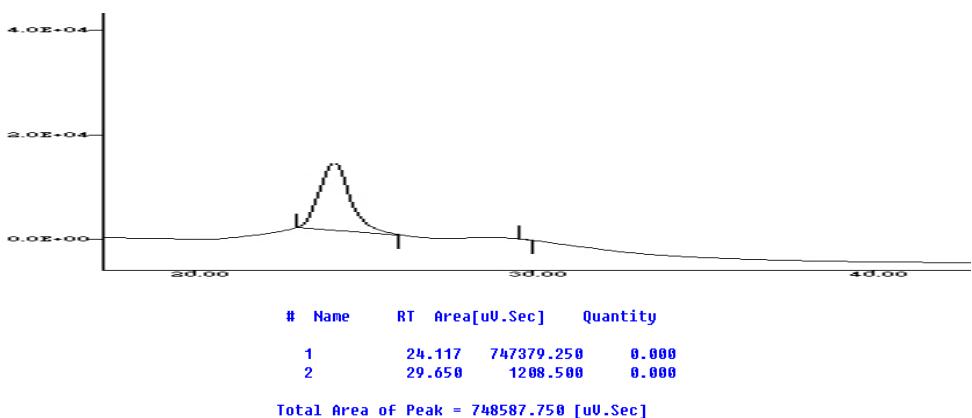
**2l**

LC data

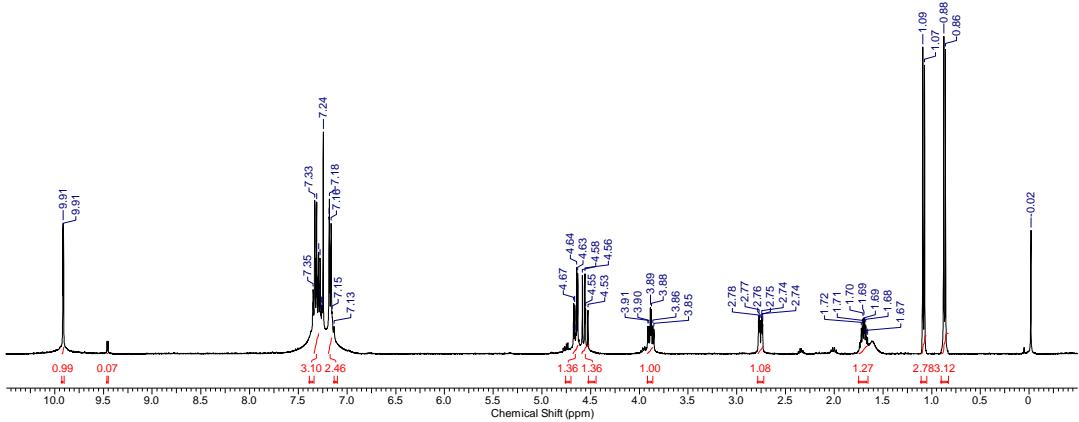
Racemic



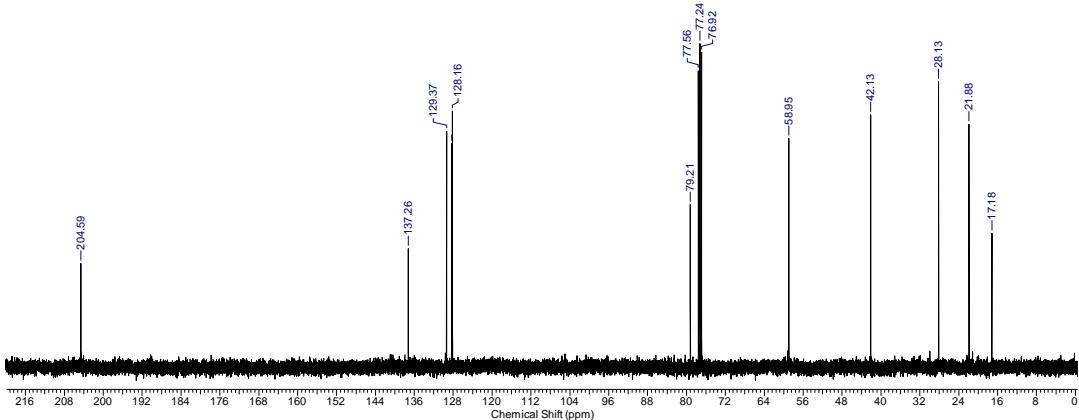
Asymmetric-Table 4-4



## **<sup>1</sup>H-NMR**



## **<sup>13</sup>C-NMR**



MASS

Note : with NBA

Inlet : Direct

RT : 1.17 min

Ion Mode : FAB+

Scan#: (13, 17) - (4, 5)

Elements : C 13/0, H 18/0, O 3/0, N 1/0

Mass Tolerance : 100mmu

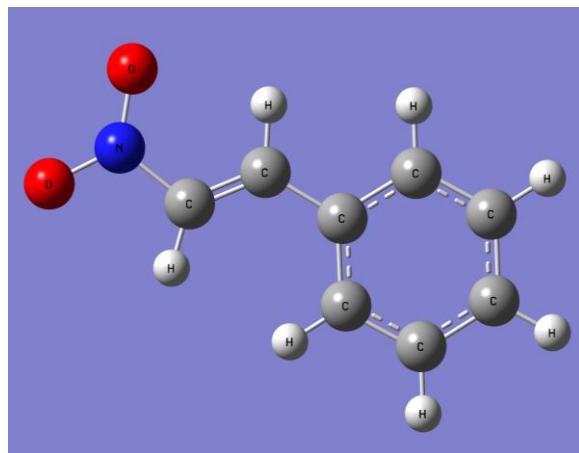
Unsaturation (U.S.) : -20.0 = 20.0

Observed m/z	Int%							
Estimated m/z	Error [ppm]	U.S.	C	H	O	N		
236.1287	31.0							
236.1287	+0.1	5.5	13	18	3	1		

### 3. DFT Calculations for all Calculated Structures

**Figure 4.**

**Nitrostyrene(1)**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -511.28944 Hartree

RMS Gradient Norm = 4.727e-06 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 5.5828134 Debye

Polarizability (?) = 97.877333 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -511.28944 Hartree

Zero-point Energy Correction = 0.136109 Hartree

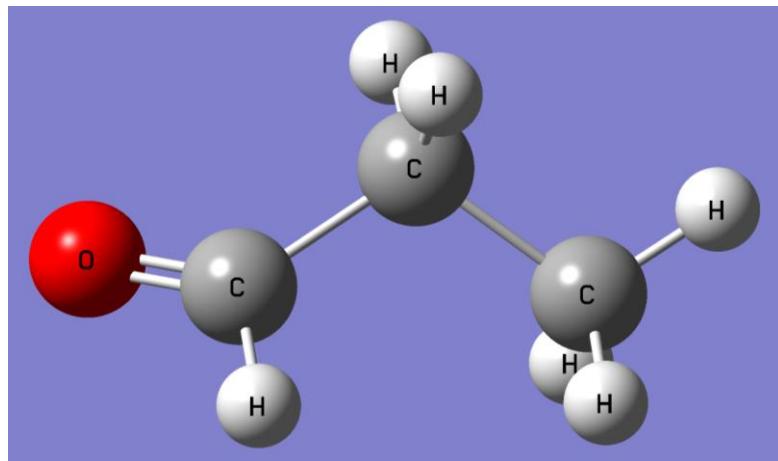
Thermal Correction to Energy = 0.145175 Hartree  
 Thermal Correction to Enthalpy = 0.14612 Hartree  
 Thermal Correction to Free Energy = 0.100523 Hartree  
 EE + Zero-point Energy = -511.15333 Hartree  
 EE + Thermal Energy Correction = -511.14426 Hartree  
 EE + Thermal Enthalpy Correction = -511.14332 Hartree  
 EE + Thermal Free Energy Correction = -511.18892 Hartree  
 E (Thermal) = 91.099 kcal/mol  
 Heat Capacity (Cv) = 33.914 cal/mol-kelvin  
 Entropy (S) = 95.966 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	-0.28529	2.22435	1.01636
O	1.24132	0.90584	2.11211
N	0.93242	1.97372	1.41043
C	1.94956	2.88334	1.02661
C	3.25227	2.55156	1.14184
H	3.5089	1.5712	1.52801
H	1.56434	3.78061	0.56984
C	4.26989	4.78373	0.59551
C	4.36825	3.38219	0.72182
C	5.593	2.74793	0.41897
C	6.68157	3.5008	-0.01228
C	6.57382	4.88925	-0.13008
C	5.36622	5.5284	0.17669
H	3.34466	5.28489	0.85534
H	5.66166	1.66897	0.47786
H	7.61351	3.00601	-0.25703
H	7.42608	5.47338	-0.45644
H	5.28771	6.60569	0.09403

## Ethylaldehyde(2)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -192.08015 Hartree

RMS Gradient Norm = 3.571e-06 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 2.6295358 Debye

Polarizability (?) = 31.647333 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -192.08015 Hartree

Zero-point Energy Correction = 0.085185 Hartree

Thermal Correction to Energy = 0.090228 Hartree

Thermal Correction to Enthalpy = 0.091172 Hartree

Thermal Correction to Free Energy = 0.057632 Hartree

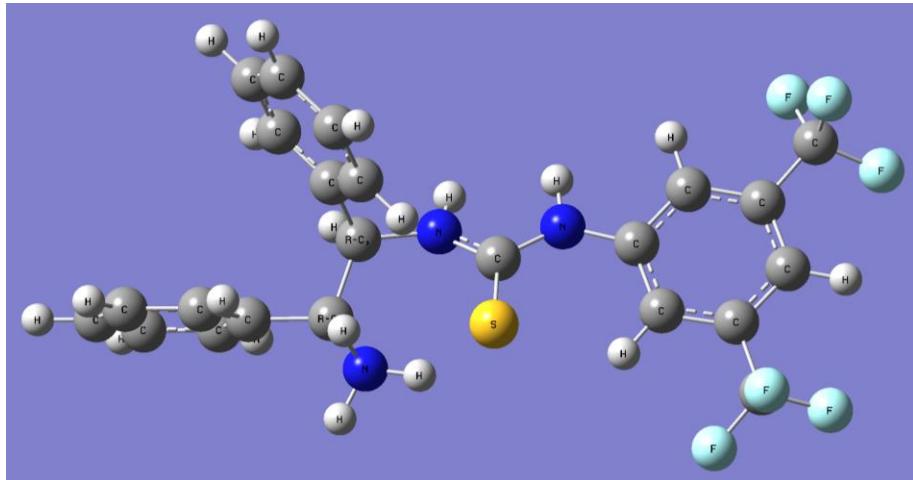
EE + Zero-point Energy = -191.99497 Hartree  
EE + Thermal Energy Correction = -191.98993 Hartree  
EE + Thermal Enthalpy Correction = -191.98898 Hartree  
EE + Thermal Free Energy Correction = -192.02252 Hartree  
E (Thermal) = 56.619 kcal/mol  
Heat Capacity (Cv) = 15.761 cal/mol-kelvin  
Entropy (S) = 70.592 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	-1.83716	0.0216	-0.23052
H	-0.64826	-1.29663	0.70102
C	0.46142	0.5657	0.16
C	1.69618	-0.24466	-0.15931
H	0.33892	1.38691	-0.57383
H	0.56816	1.06034	1.14628
H	1.63136	-0.70504	-1.15385
H	2.59539	0.38439	-0.14832
H	1.85326	-1.05379	0.56687
C	-0.76453	-0.31252	0.21697

## Catalyst 1b.(3)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2038.4342 Hartree

RMS Gradient Norm = 2.73e-07 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 5.7831636 Debye

Polarizability (?) = 259.51567 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2038.4342 Hartree

Zero-point Energy Correction = 0.390498 Hartree

Thermal Correction to Energy = 0.419537 Hartree

Thermal Correction to Enthalpy = 0.420482 Hartree

Thermal Correction to Free Energy = 0.325242 Hartree

EE + Zero-point Energy = -2038.0437 Hartree  
 EE + Thermal Energy Correction = -2038.0147 Hartree  
 EE + Thermal Enthalpy Correction = -2038.0138 Hartree  
 EE + Thermal Free Energy Correction = -2038.109 Hartree  
 E (Thermal) = 263.264 kcal/mol  
 Heat Capacity (Cv) = 110.445 cal/mol-kelvin  
 Entropy (S) = 200.448 cal/mol-kelvin

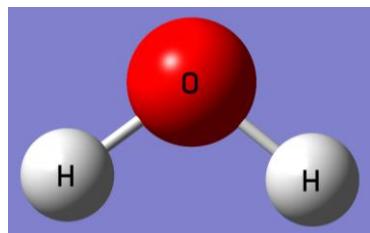
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	5.35849	1.33787	-1.80781
C	4.82708	1.14638	-0.52483
C	5.69825	0.95831	0.5539
C	7.08048	0.9594	0.3547
C	7.60459	1.1496	-0.92613
C	6.73965	1.33999	-2.00723
H	4.67012	1.50429	-2.62759
H	5.29272	0.8047	1.54752
H	7.74614	0.81433	1.19782
H	8.67773	1.1541	-1.07954
H	7.1414	1.49523	-3.00239
C	3.29335	-1.35884	0.35108
C	4.2752	-2.28379	-0.02492
C	4.73342	-3.24351	0.88009
C	4.21062	-3.28913	2.17354
C	3.23141	-2.36846	2.55692
C	2.77436	-1.40784	1.65364
H	4.69377	-2.24224	-1.0248
H	5.49665	-3.95033	0.57561
H	4.56373	-4.03365	2.87769
H	2.82295	-2.39699	3.56063

H	2.01493	-0.69495	1.95103
C	3.3155	1.12842	-0.32606
C	2.81394	-0.3166	-0.65186
N	1.33778	-0.45595	-0.89719
N	2.68733	2.05148	-1.30251
H	3.24995	-0.54539	-1.62815
H	3.07939	1.35208	0.7202
H	3.151	2.9666	-1.25754
H	1.69517	2.17017	-1.06525
H	1.14702	-1.08786	-1.67474
C	0.25972	0.03025	-0.23611
C	-2.73205	0.98572	0.09707
C	-4.09709	1.1922	0.26486
C	-5.03531	0.22018	-0.05727
C	-4.57426	-0.9948	-0.54801
C	-3.217	-1.22889	-0.71787
C	-2.27072	-0.24091	-0.40093
H	-2.03806	1.77115	0.34469
H	-6.0936	0.41447	0.04014
H	-2.90295	-2.18378	-1.12204
N	-0.92225	-0.55008	-0.67028
S	0.33444	1.23285	1.01256
H	-0.81622	-1.3929	-1.23506
F	-5.79041	-2.88065	0.25434
F	-5.05699	-2.91949	-1.82873
F	-6.75108	-1.57598	-1.24681
F	-3.69111	3.50442	0.54004
F	-5.8118	2.80855	0.3756
F	-4.65299	2.43695	2.21884
C	-5.54204	-2.08849	-0.84265
C	-4.55983	2.48514	0.84774

## H<sub>2</sub>O



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -75.973965 Hartree

RMS Gradient Norm = 0.000115305 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 2.2397 Debye

Polarizability (?) = 4.2726667 a.u.

Point Group = C2V

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -75.973965 Hartree

Zero-point Energy Correction = 0.019746 Hartree

Thermal Correction to Energy = 0.022581 Hartree

Thermal Correction to Enthalpy = 0.023525 Hartree

Thermal Correction to Free Energy = 0.002 Hartree

EE + Zero-point Energy = -75.954218 Hartree

EE + Thermal Energy Correction = -75.951384 Hartree

EE + Thermal Enthalpy Correction = -75.95044 Hartree

EE + Thermal Free Energy Correction = -75.971965 Hartree

E (Thermal) = 14.17 kcal/mol

Heat Capacity (Cv) = 5.999 cal/mol-kelvin

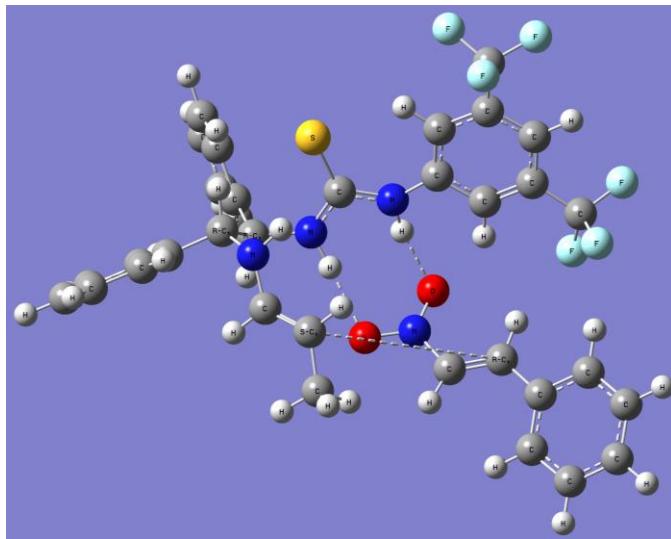
Entropy (S) = 45.304 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	-0.0579	2.33917	-0.16269
H	0.9021	2.33917	-0.16269
H	-0.37836	3.24411	-0.16269

## TS1(syn major)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2665.8507 Hartree

RMS Gradient Norm = 2.88e-07 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 9.5833983 Debye

Polarizability (?) = 485.66567 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2665.8507 Hartree

Zero-point Energy Correction = 0.591917 Hartree

Thermal Correction to Energy = 0.634748 Hartree

Thermal Correction to Enthalpy = 0.635693 Hartree  
 Thermal Correction to Free Energy = 0.510051 Hartree  
 EE + Zero-point Energy = -2665.2588 Hartree  
 EE + Thermal Energy Correction = -2665.2159 Hartree  
 EE + Thermal Enthalpy Correction = -2665.215 Hartree  
 EE + Thermal Free Energy Correction = -2665.3406 Hartree  
 E (Thermal) = 398.311 kcal/mol  
 Heat Capacity (Cv) = 161.557 cal/mol-kelvin  
 Entropy (S) = 264.434 cal/mol-kelvin

Symbolic Z-matrix:

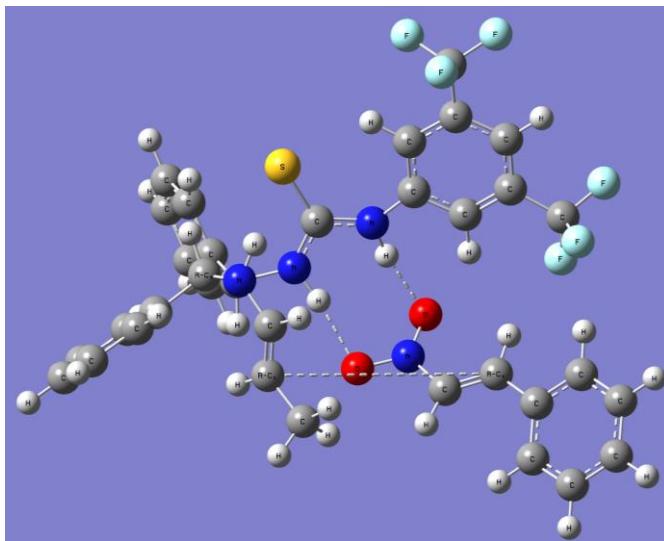
Charge = 0 Multiplicity = 1

C	-5.84016	0.76666	-2.07859
C	-5.34509	0.33945	-0.83189
C	-6.20308	0.37265	0.27693
C	-7.51451	0.85184	0.15055
C	-7.99269	1.28478	-1.0878
C	-7.14983	1.23141	-2.20647
H	-5.17524	0.75444	-2.93648
H	-5.87238	0.02513	1.24753
H	-8.16039	0.87835	1.02349
H	-9.00928	1.65344	-1.18475
H	-7.51279	1.56018	-3.17604
C	-3.97454	-1.51098	1.46624
C	-4.20642	-1.32901	2.84128
C	-4.78308	-2.34451	3.6084
C	-5.13076	-3.56107	3.00764
C	-4.89399	-3.75236	1.64267
C	-4.31331	-2.73619	0.87473
H	-3.94161	-0.38161	3.30852
H	-4.96358	-2.18817	4.66786

H	-5.58383	-4.35085	3.59887
H	-5.15778	-4.69483	1.1726
H	-4.12405	-2.90882	-0.17804
C	-3.89454	-0.17012	-0.77754
C	-3.35258	-0.35195	0.68526
N	-1.8637	-0.42664	0.78297
N	-3.0045	0.64558	-1.63363
H	-3.58173	0.56838	1.2337
H	-3.87298	-1.15798	-1.24637
H	-1.46397	0.34135	1.32909
C	-1.00515	-1.28102	0.17627
C	1.76128	-2.22873	-0.99568
C	3.06487	-2.53973	-1.38712
C	4.173	-2.25157	-0.5906
C	3.92883	-1.66371	0.65273
C	2.63971	-1.36764	1.0888
C	1.52572	-1.61853	0.25111
H	5.17542	-2.50138	-0.91863
H	2.47201	-0.95333	2.0741
N	0.27606	-1.22351	0.74412
S	-1.42151	-2.34059	-1.13632
H	0.33204	-0.72929	1.6579
F	5.9405	-2.38035	1.79302
F	4.71649	-0.75524	2.73872
F	5.93734	-0.34944	0.96875
F	3.43278	-2.12294	-3.73719
F	4.45847	-3.89012	-2.81274
F	2.23393	-3.93274	-3.17485
C	5.10566	-1.29494	1.51476
C	3.28669	-3.11969	-2.74986
C	-2.52374	1.94447	-1.32016

O	-0.45469	2.10919	1.25266
O	0.96382	0.76642	2.42978
N	0.74664	1.83415	1.67528
C	1.8164	2.66438	1.25132
H	-2.31799	0.06461	-2.11884
H	0.92369	-2.47165	-1.63395
C	-1.28035	2.31883	-1.7
C	-0.71959	3.71838	-1.5406
H	-0.64469	1.59485	-2.21397
H	-0.71563	4.21133	-2.49028
H	0.28041	3.66122	-1.16425
C	3.06511	2.13146	1.18602
H	3.15824	1.10615	1.51317
H	1.47864	3.6047	0.84055
C	4.5059	4.06409	0.50633
C	4.29177	2.67856	0.66297
C	5.25389	1.68212	0.30792
C	6.47978	2.20429	-0.1783
C	6.7086	3.57498	-0.34407
C	5.72302	4.51061	0.00285
H	3.7435	4.77898	0.80174
H	5.51163	0.59599	0.62168
H	7.27435	1.52181	-0.47322
H	7.65267	3.92166	-0.75545
H	5.9117	5.57197	-0.12118
H	-1.32778	4.27033	-0.85478
H	-3.14625	2.62867	-0.78234

## TS2(anti major)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2665.8493 Hartree

RMS Gradient Norm = 5.49e-07 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 9.5146664 Debye

Polarizability (?) = 490.43133 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2665.8493 Hartree

Zero-point Energy Correction = 0.592417 Hartree

Thermal Correction to Energy = 0.635076 Hartree

Thermal Correction to Enthalpy = 0.63602 Hartree  
 Thermal Correction to Free Energy = 0.511378 Hartree  
 EE + Zero-point Energy = -2665.2568 Hartree  
 EE + Thermal Energy Correction = -2665.2142 Hartree  
 EE + Thermal Enthalpy Correction = -2665.2132 Hartree  
 EE + Thermal Free Energy Correction = -2665.3379 Hartree  
 E (Thermal) = 398.516 kcal/mol  
 Heat Capacity (Cv) = 161.451 cal/mol-kelvin  
 Entropy (S) = 262.331 cal/mol-kelvin

Symbolic Z-matrix:

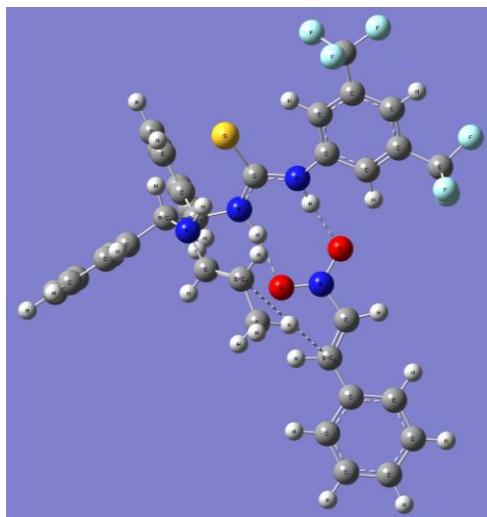
Charge = 0 Multiplicity = 1

C	5.71851	1.27437	2.40903
C	5.3043	0.95726	1.10473
C	6.13162	1.31749	0.03281
C	7.33796	1.98724	0.25997
C	7.73744	2.3021	1.55814
C	6.92208	1.93943	2.63426
H	5.07368	1.00439	3.2355
H	5.85485	1.05553	-0.97899
H	7.96473	2.25665	-0.58264
H	8.67313	2.82101	1.73176
H	7.22367	2.17638	3.64838
C	4.1259	-0.52662	-1.60537
C	4.21848	0.02644	-2.89301
C	4.85477	-0.66117	-3.92582
C	5.40801	-1.92143	-3.68527
C	5.31699	-2.48209	-2.41073
C	4.68005	-1.79228	-1.37579
H	3.79049	1.00617	-3.08265
H	4.91987	-0.21621	-4.91213

H	5.905	-2.45982	-4.48391
H	5.73905	-3.46145	-2.21762
H	4.59598	-2.2504	-0.40094
C	3.98997	0.18559	0.92959
C	3.40299	0.28266	-0.52739
N	1.93525	0.03717	-0.57647
N	2.98615	0.65544	1.90687
H	3.48261	1.33898	-0.80782
H	4.15557	-0.86654	1.16466
H	1.3842	0.87473	-0.80619
C	1.25537	-1.07683	-0.20749
C	-1.23437	-2.96334	0.4814
C	-2.46252	-3.57045	0.7422
C	-3.66847	-3.03909	0.3022
C	-3.62454	-1.84793	-0.41851
C	-2.41923	-1.2311	-0.6969
C	-1.1963	-1.76539	-0.24737
H	-4.60013	-3.55301	0.49341
H	-2.40325	-0.32566	-1.2821
N	-0.06577	-1.01216	-0.59342
S	1.94752	-2.39798	0.68926
H	-0.30016	-0.22389	-1.21811
F	-5.78006	-2.07035	-1.3942
F	-4.62969	-0.19277	-1.80069
F	-5.53867	-0.53923	0.17563
F	-2.57991	-4.53124	2.91937
F	-3.56884	-5.59289	1.25377
F	-1.33672	-5.54434	1.40066
C	-4.88016	-1.1883	-0.8626
C	-2.48247	-4.80849	1.57398
C	2.53787	1.97344	1.85132

O	0.29441	2.53162	-0.73125
O	-1.15007	1.21376	-1.93537
N	-0.90173	2.24095	-1.15399
C	-1.96742	3.0689	-0.71517
H	2.30532	-0.06652	2.14976
H	-0.31935	-3.42386	0.81764
C	-3.25152	2.69069	-0.87347
H	-3.46085	1.73216	-1.33556
H	-1.62775	3.94517	-0.18675
C	-4.36967	4.8326	-0.18238
C	-4.40809	3.44152	-0.41277
C	-5.60978	2.73796	-0.18003
C	-6.73496	3.41255	0.28586
C	-6.6864	4.79147	0.50759
C	-5.50188	5.49966	0.27031
H	-3.46233	5.38849	-0.38836
H	-5.63406	1.66468	-0.32035
H	-7.64932	2.86401	0.47629
H	-7.56687	5.31509	0.86064
H	-5.46924	6.57015	0.43314
C	3.64346	2.97756	1.47579
C	3.03177	4.38314	1.32818
H	2.15957	4.3295	0.71069
H	2.76284	4.75826	2.29351
H	3.7479	5.03826	0.87777
H	4.67677	2.736	1.33866
H	1.52611	2.25951	2.04982

## TS3(anti minor)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2665.8409 Hartree

RMS Gradient Norm = 3.25e-07 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 14.735089 Debye

Polarizability (?) = 488.39233 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2665.8409 Hartree

Zero-point Energy Correction = 0.590917 Hartree

Thermal Correction to Energy = 0.634358 Hartree

Thermal Correction to Enthalpy = 0.635302 Hartree

Thermal Correction to Free Energy = 0.504485 Hartree

EE + Zero-point Energy = -2665.25 Hartree

EE + Thermal Energy Correction = -2665.2066 Hartree

EE + Thermal Enthalpy Correction = -2665.2056 Hartree

EE + Thermal Free Energy Correction = -2665.3365 Hartree

E (Thermal) = 398.065 kcal/mol

Heat Capacity (Cv) = 161.818 cal/mol-kelvin

Entropy (S) = 275.328 cal/mol-kelvin

Symbolic Z-matrix:

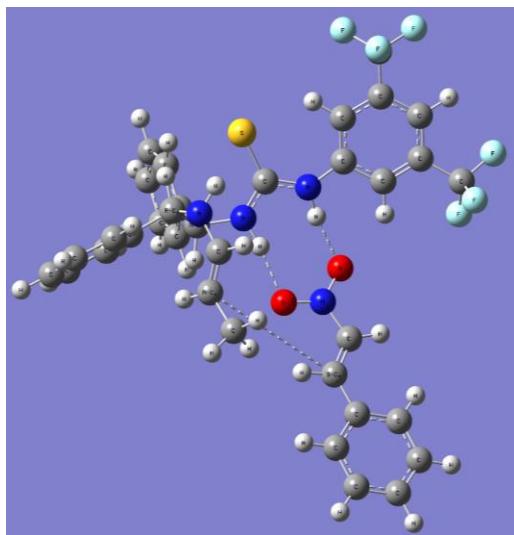
Charge = 0 Multiplicity = 1

C	5.71851	1.27437	2.40903
C	5.3043	0.95726	1.10473
C	6.13162	1.31749	0.03281
C	7.33796	1.98724	0.25997
C	7.73744	2.3021	1.55814
C	6.92208	1.93943	2.63426
H	5.07368	1.00439	3.2355
H	5.85485	1.05553	-0.97899
H	7.96473	2.25665	-0.58264
H	8.67313	2.82101	1.73176
H	7.22367	2.17638	3.64838
C	4.1259	-0.52662	-1.60537
C	4.21848	0.02644	-2.89301
C	4.85477	-0.66117	-3.92582
C	5.40801	-1.92143	-3.68527
C	5.31699	-2.48209	-2.41073
C	4.68005	-1.79228	-1.37579
H	3.79049	1.00617	-3.08265
H	4.91987	-0.21621	-4.91213
H	5.905	-2.45982	-4.48391

H	5.73905	-3.46145	-2.21762
H	4.59598	-2.2504	-0.40094
C	3.98997	0.18559	0.92959
C	3.40299	0.28266	-0.52739
N	1.93525	0.03717	-0.57647
N	2.98615	0.65544	1.90687
H	3.48261	1.33898	-0.80782
H	4.15557	-0.86654	1.16466
H	1.3842	0.87473	-0.80619
C	1.25537	-1.07683	-0.20749
C	-1.23437	-2.96334	0.4814
C	-2.46252	-3.57045	0.7422
C	-3.66847	-3.03909	0.3022
C	-3.62454	-1.84793	-0.41851
C	-2.41923	-1.2311	-0.6969
C	-1.1963	-1.76539	-0.24737
H	-4.60013	-3.55301	0.49341
H	-2.40325	-0.32566	-1.2821
N	-0.06577	-1.01216	-0.59342
S	1.94752	-2.39798	0.68926
H	-0.30016	-0.22389	-1.21811
F	-5.78006	-2.07035	-1.3942
F	-4.62969	-0.19277	-1.80069
F	-5.53867	-0.53923	0.17563
F	-2.57991	-4.53124	2.91937
F	-3.56884	-5.59289	1.25377
F	-1.33672	-5.54434	1.40066
C	-4.88016	-1.1883	-0.8626
C	-2.48247	-4.80849	1.57398
C	2.53787	1.97344	1.85132
O	0.29415	2.53146	-0.7315

O	-1.15141	1.21143	-1.93193
N	-0.90245	2.23971	-1.15219
C	-1.96791	3.06773	-0.71291
H	2.30532	-0.06652	2.14976
H	-0.31935	-3.42386	0.81764
C	1.29524	2.41619	2.12164
C	0.92821	3.87957	2.13404
H	0.51181	1.70547	2.3768
H	0.47722	4.18001	3.0889
H	0.20965	4.09834	1.3336
H	1.81275	4.50432	1.96624
H	3.31846	2.68239	1.58618
C	-1.48226	4.32052	0.03959
H	-0.45135	4.41629	0.30969
C	-2.48034	5.43546	0.40335
C	-3.20973	5.35875	1.59018
C	-2.65509	6.52203	-0.45361
C	-4.11413	6.3681	1.91959
H	-3.0723	4.50161	2.26521
C	-3.55901	7.53226	-0.12378
H	-2.08017	6.58274	-1.38898
C	-4.2886	7.4554	1.06253
H	-4.68954	6.30739	2.85474
H	-3.69627	8.38906	-0.79944
H	-5.0017	8.25114	1.32249
H	-3.00002	2.84506	-0.88628

## TS4(syn minor)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -2665.8396 Hartree

RMS Gradient Norm = 3.67e-07 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 14.360848 Debye

Polarizability (?) = 502.50933 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2665.8396 Hartree

Zero-point Energy Correction = 0.591305 Hartree

Thermal Correction to Energy = 0.634625 Hartree

Thermal Correction to Enthalpy = 0.635569 Hartree

Thermal Correction to Free Energy = 0.505209 Hartree

EE + Zero-point Energy = -2665.2483 Hartree

EE + Thermal Energy Correction = -2665.205 Hartree

EE + Thermal Enthalpy Correction = -2665.204 Hartree

EE + Thermal Free Energy Correction = -2665.3344 Hartree

E (Thermal) = 398.233 kcal/mol

Heat Capacity (Cv) = 161.764 cal/mol-kelvin

Entropy (S) = 274.366 cal/mol-kelvin

Symbolic Z-matrix:

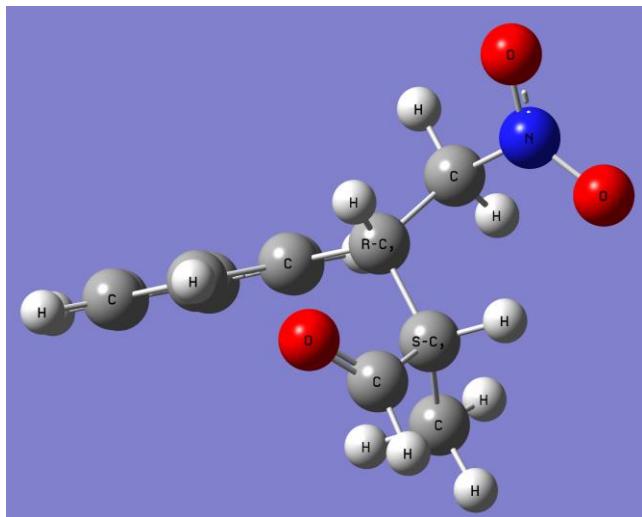
Charge = 0 Multiplicity = 1

C	-4.32266	-3.02493	-2.49368
C	-3.87364	-2.88691	-1.17023
C	-4.80182	-3.03055	-0.12957
C	-6.14661	-3.29265	-0.40752
C	-6.58377	-3.42007	-1.72572
C	-5.66348	-3.288	-2.76928
H	-3.60543	-2.9105	-3.29601
H	-4.47681	-2.96457	0.89959
H	-6.84861	-3.40233	0.41147
H	-7.62685	-3.62404	-1.93885
H	-5.99038	-3.39005	-3.79806
C	-2.18754	-2.90315	1.69336
C	-2.7411	-2.37731	2.87224
C	-2.85906	-3.15795	4.02177
C	-2.41916	-4.48389	4.01018
C	-1.86272	-5.01466	2.84571
C	-1.7454	-4.23211	1.69405
H	-3.08599	-1.34771	2.88361
H	-3.29262	-2.73505	4.92086

H	-2.50931	-5.09595	4.90012
H	-1.51307	-6.04039	2.83055
H	-1.28467	-4.64706	0.80937
C	-2.37802	-2.64443	-0.92471
C	-2.08646	-1.98141	0.47577
N	-0.82702	-1.19329	0.49431
N	-1.8026	-1.82334	-2.00872
H	-2.85273	-1.2072	0.59908
H	-1.84815	-3.59707	-0.97017
H	-1.00036	-0.18282	0.56485
C	0.43685	-1.59991	0.22844
C	3.58649	-1.53916	-0.16377
C	4.94246	-1.29046	-0.35552
C	5.49084	-0.02386	-0.20788
C	4.63545	1.01901	0.13053
C	3.28	0.80299	0.32181
C	2.72564	-0.48558	0.18058
H	6.55264	0.14031	-0.31989
H	2.64663	1.6332	0.60604
N	1.34738	-0.58475	0.42701
S	0.83621	-3.19395	-0.35499
H	0.95294	0.29108	0.8026
F	6.47899	2.4032	0.64211
F	4.42609	3.16157	1.11004
F	5.13539	3.07114	-0.97774
F	5.88932	-2.5407	-2.15034
F	7.11374	-2.21791	-0.341
F	5.3688	-3.6171	-0.29336
C	5.16753	2.40475	0.22861
C	5.82287	-2.41566	-0.78027
C	-2.21772	-0.50407	-2.18048

O	-1.61286	1.57544	0.39464
O	0.46697	2.00271	1.27645
N	-0.69183	2.39262	0.81475
C	-0.91439	3.79807	0.80244
H	-0.81371	-2.02661	-2.16923
H	3.20391	-2.54221	-0.2585
C	-2.09993	4.29136	0.40012
H	-2.83781	3.55982	0.08409
C	-2.48446	5.68873	0.34118
C	-1.61944	6.74053	0.714
C	-3.78241	6.00656	-0.11097
C	-2.04364	8.06084	0.63577
H	-0.61741	6.5213	1.0626
C	-4.20333	7.33093	-0.18788
H	-4.45288	5.20502	-0.40077
C	-3.3358	8.36063	0.18516
H	-1.37232	8.86071	0.92341
H	-5.20221	7.56121	-0.53737
H	-3.66127	9.39223	0.12558
H	-0.06029	4.35342	1.15291
C	-3.51198	-0.16703	-1.96169
H	-1.51456	0.2427	-2.4851
H	-4.27648	-0.91333	-2.02062
C	-3.88241	1.29009	-1.62824
H	-3.16179	1.95002	-2.06424
H	-4.85242	1.51063	-2.02236
H	-3.8904	1.42202	-0.56643

## Products



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -703.40279 Hartree

RMS Gradient Norm = 6.73e-07 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 4.0645582 Debye

Polarizability (?) = 114.528 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -703.40279 Hartree

Zero-point Energy Correction = 0.226592 Hartree

Thermal Correction to Energy = 0.240738 Hartree

Thermal Correction to Enthalpy = 0.241682 Hartree

Thermal Correction to Free Energy = 0.184233 Hartree  
 EE + Zero-point Energy = -703.1762 Hartree  
 EE + Thermal Energy Correction = -703.16206 Hartree  
 EE + Thermal Enthalpy Correction = -703.16111 Hartree  
 EE + Thermal Free Energy Correction = -703.21856 Hartree  
 E (Thermal) = 151.065 kcal/mol  
 Heat Capacity (Cv) = 52.226 cal/mol-kelvin  
 Entropy (S) = 120.912 cal/mol-kelvin

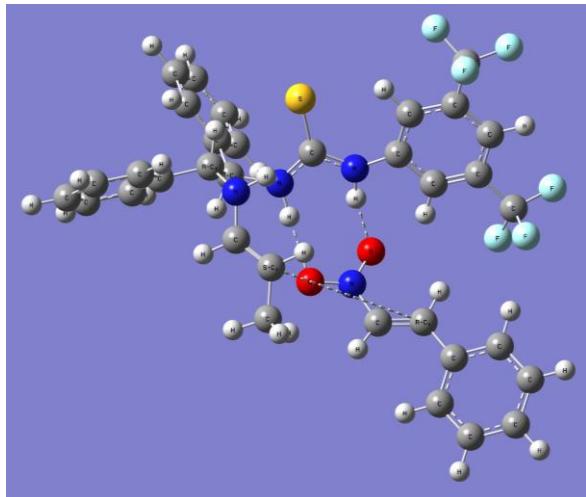
Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	2.73014	-2.10935	-0.92973
O	3.05613	-0.51405	0.66634
N	2.31855	-1.30881	-0.03044
C	0.82443	-1.27353	0.23795
C	0.17775	0.03028	-0.28403
H	0.4535	0.13086	-1.34064
H	0.42943	-2.1391	-0.2891
C	-1.98832	-0.53144	0.9753
C	-1.34033	-0.08269	-0.18537
C	-2.12368	0.30712	-1.28188
C	-3.51676	0.25772	-1.22003
C	-4.15121	-0.18873	-0.05864
C	-3.38269	-0.58444	1.03747
H	-1.41058	-0.84431	1.83725
H	-1.63477	0.64821	-2.18836
H	-4.10483	0.56173	-2.07824
H	-5.23286	-0.23136	-0.00978
H	-3.86692	-0.93518	1.94161
C	0.71054	1.32426	0.40244
C	0.89478	1.2718	1.92876

H	-0.03915	0.99581	2.42668
H	1.68444	0.56069	2.17658
H	1.19011	2.25987	2.30144
H	0.71924	-1.38089	1.31681
C	-0.31969	2.42293	0.0813
H	-0.5583	2.96042	0.97521
O	0.22927	3.32359	-0.88428
H	1.6456	1.58866	-0.04551

**Figure 5.**  
**TS1(Only water)**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2665.8732 Hartree

RMS Gradient Norm = 3.54e-07 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 14.828325 Debye

Polarizability (?) = 591.778 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2665.8732 Hartree

Zero-point Energy Correction = 0.59078 Hartree

Thermal Correction to Energy = 0.633828 Hartree

Thermal Correction to Enthalpy = 0.634772 Hartree  
 Thermal Correction to Free Energy = 0.507944 Hartree  
 EE + Zero-point Energy = -2665.2825 Hartree  
 EE + Thermal Energy Correction = -2665.2394 Hartree  
 EE + Thermal Enthalpy Correction = -2665.2385 Hartree  
 EE + Thermal Free Energy Correction = -2665.3653 Hartree  
 E (Thermal) = 397.733 kcal/mol  
 Heat Capacity (Cv) = 161.905 cal/mol-kelvin  
 Entropy (S) = 266.932 cal/mol-kelvin

Symbolic Z-matrix:

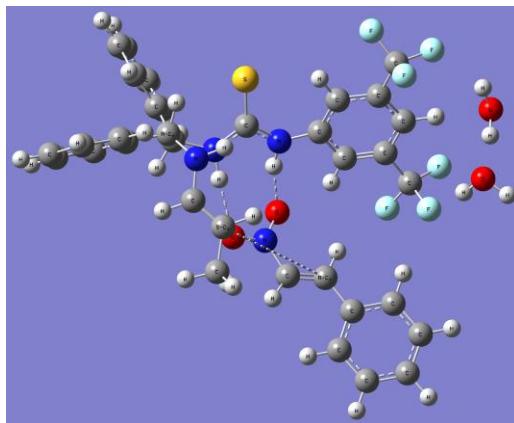
Charge = 0 Multiplicity = 1

C	5.71851	1.27437	2.40903
C	5.3043	0.95726	1.10473
C	6.13162	1.31749	0.03281
C	7.33796	1.98724	0.25997
C	7.73744	2.3021	1.55814
C	6.92208	1.93943	2.63426
H	5.07368	1.00439	3.2355
H	5.85485	1.05553	-0.97899
H	7.96473	2.25665	-0.58264
H	8.67313	2.82101	1.73176
H	7.22367	2.17638	3.64838
C	4.1259	-0.52662	-1.60537
C	4.21848	0.02644	-2.89301
C	4.85477	-0.66117	-3.92582
C	5.40801	-1.92143	-3.68527
C	5.31699	-2.48209	-2.41073
C	4.68005	-1.79228	-1.37579
H	3.79049	1.00617	-3.08265
H	4.91987	-0.21621	-4.91213

H	5.905	-2.45982	-4.48391
H	5.73905	-3.46145	-2.21762
H	4.59598	-2.2504	-0.40094
C	3.98997	0.18559	0.92959
C	3.40299	0.28266	-0.52739
N	1.93525	0.03717	-0.57647
N	2.98615	0.65544	1.90687
H	3.48261	1.33898	-0.80782
H	4.15557	-0.86654	1.16466
H	1.3842	0.87473	-0.80619
C	1.25537	-1.07683	-0.20749
C	-1.23437	-2.96334	0.4814
C	-2.46252	-3.57045	0.7422
C	-3.66847	-3.03909	0.3022
C	-3.62454	-1.84793	-0.41851
C	-2.41923	-1.2311	-0.6969
C	-1.1963	-1.76539	-0.24737
H	-4.60013	-3.55301	0.49341
H	-2.40325	-0.32566	-1.2821
N	-0.06577	-1.01216	-0.59342
S	1.94752	-2.39798	0.68926
H	-0.30016	-0.22389	-1.21811
F	-5.78006	-2.07035	-1.3942
F	-4.62969	-0.19277	-1.80069
F	-5.53867	-0.53923	0.17563
F	-2.57991	-4.53124	2.91937
F	-3.56884	-5.59289	1.25377
F	-1.33672	-5.54434	1.40066
C	-4.88016	-1.1883	-0.8626
C	-2.48247	-4.80849	1.57398
C	2.53787	1.97344	1.85132

O	0.29441	2.53162	-0.73125
O	-1.15007	1.21376	-1.93537
N	-0.90173	2.24095	-1.15399
C	-1.96742	3.0689	-0.71517
H	2.30532	-0.06652	2.14976
H	-0.31935	-3.42386	0.81764
C	1.29524	2.41619	2.12164
C	0.92821	3.87957	2.13404
H	0.51181	1.70547	2.3768
H	0.47722	4.18001	3.0889
H	0.20965	4.09834	1.3336
C	-3.25152	2.69069	-0.87347
H	-3.46085	1.73216	-1.33556
H	-1.62775	3.94517	-0.18675
C	-4.36967	4.8326	-0.18238
C	-4.40809	3.44152	-0.41277
C	-5.60978	2.73796	-0.18003
C	-6.73496	3.41255	0.28586
C	-6.6864	4.79147	0.50759
C	-5.50188	5.49966	0.27031
H	-3.46233	5.38849	-0.38836
H	-5.63406	1.66468	-0.32035
H	-7.64932	2.86401	0.47629
H	-7.56687	5.31509	0.86064
H	-5.46924	6.57015	0.43314
H	1.81275	4.50432	1.96624
H	3.31846	2.68239	1.58618

## TS1+2H<sub>2</sub>O(water)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2817.8903 Hartree

RMS Gradient Norm = 1.595e-06 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 17.580323 Debye

Polarizability (?) = 607.342 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2817.8903 Hartree

Zero-point Energy Correction = 0.64028 Hartree

Thermal Correction to Energy = 0.688449 Hartree

Thermal Correction to Enthalpy = 0.689393 Hartree

Thermal Correction to Free Energy = 0.551398 Hartree

EE + Zero-point Energy = -2817.25 Hartree

EE + Thermal Energy Correction = -2817.2019 Hartree

EE + Thermal Enthalpy Correction = -2817.2009 Hartree

EE + Thermal Free Energy Correction = -2817.3389 Hartree

E (Thermal) = 432.008 kcal/mol

Heat Capacity (C<sub>v</sub>) = 179.397 cal/mol-kelvin

Entropy (S) = 290.435 cal/mol-kelvin

Symbolic Z-matrix:

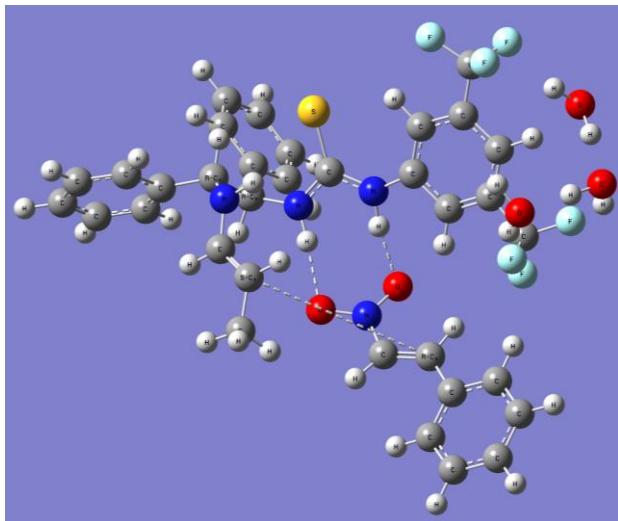
Charge = 0 Multiplicity = 1

C	-6.14947	0.76697	-2.49577
C	-5.73349	0.51519	-1.17779
C	-6.61846	0.80105	-0.1298
C	-7.88351	1.3353	-0.39361
C	-8.28455	1.58696	-1.70502
C	-7.41125	1.29712	-2.75747
H	-5.46178	0.55414	-3.30421
H	-6.33867	0.58455	0.89182
H	-8.55433	1.54861	0.43095
H	-9.2658	2.0008	-1.90704
H	-7.71329	1.48545	-3.7816
C	-4.46457	-0.79395	1.58109
C	-4.66373	-0.2283	2.85111
C	-5.24863	-0.96406	3.88117
C	-5.64164	-2.28575	3.65584
C	-5.44293	-2.85902	2.39924
C	-4.85783	-2.12107	1.36692
H	-4.36048	0.79907	3.02902
H	-5.39797	-0.50892	4.85359
H	-6.09799	-2.86189	4.45239
H	-5.7398	-3.88552	2.21835
H	-4.68633	-2.58686	0.40727

C	-4.34964	-0.11044	-0.96165
C	-3.80708	0.07094	0.50468
N	-2.32325	-0.0151	0.58712
N	-3.37812	0.4476	-1.9253
H	-4.00489	1.11695	0.76474
H	-4.39811	-1.17772	-1.18101
H	-1.87145	0.88006	0.81493
C	-1.51778	-1.05388	0.24937
C	1.17354	-2.68406	-0.33568
C	2.46383	-3.17552	-0.5415
C	3.60496	-2.53605	-0.06634
C	3.40572	-1.33328	0.61308
C	2.13872	-0.82033	0.83518
C	0.99061	-1.4857	0.36918
H	4.60715	-2.98232	-0.17722
H	2.01528	0.10005	1.3842
N	-0.22303	-0.84496	0.66634
S	-2.0429	-2.44926	-0.65054
H	-0.08894	-0.02491	1.27879
F	5.6071	-1.24132	1.55563
F	4.23407	0.48876	1.91655
F	5.14105	0.17766	-0.06794
F	2.6984	-4.07215	-2.73189
F	3.75713	-5.09634	-1.08922
F	1.53404	-5.23401	-1.2574
C	4.56599	-0.5188	1.03113
C	2.60946	-4.39214	-1.3931
C	-3.07588	1.80556	-1.88957
O	-0.9786	2.64727	0.70998
O	0.58189	1.52298	1.96724
N	0.23452	2.4985	1.15766

C	1.21113	3.42838	0.71333
H	-2.62058	-0.20328	-2.14133
H	0.31959	-3.23297	-0.69916
C	-1.88358	2.37586	-2.15129
C	-1.67879	3.86987	-2.19017
H	-1.0242	1.74986	-2.38243
H	-1.25077	4.19922	-3.14609
H	-0.99921	4.18271	-1.38685
C	2.52453	3.19801	0.90565
H	2.82304	2.28035	1.40035
H	0.78785	4.24842	0.15583
C	3.42271	5.42739	0.16925
C	3.60445	4.05657	0.44596
C	4.88056	3.48173	0.26266
C	5.93852	4.25923	-0.19987
C	5.74734	5.61743	-0.46826
C	4.48777	6.19924	-0.28063
H	2.45587	5.88771	0.33646
H	5.01449	2.42229	0.44068
H	6.91185	3.80871	-0.35167
H	6.57497	6.2224	-0.81895
H	4.34383	7.25429	-0.47972
H	-2.62849	4.397	-2.04513
H	-3.93204	2.43097	-1.64866
O	6.22808	-3.77758	-0.4867
H	5.88058	-4.31349	-1.24553
H	6.70326	-2.95707	-0.85547
O	7.33501	-1.412	-0.78718
H	7.52154	-1.49088	0.18793
H	6.57228	-0.77315	-0.82931

## TS1+3H<sub>2</sub>O(water)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2893.9059 Hartree

RMS Gradient Norm = 3.82e-07 Hartree/Bohr

Imaginary Freq = 0

Dipole Moment = 18.087444 Debye

Polarizability (?) = 620.80367 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2893.9059 Hartree

Zero-point Energy Correction = 0.665479 Hartree

Thermal Correction to Energy = 0.715589 Hartree

Thermal Correction to Enthalpy = 0.716533 Hartree

Thermal Correction to Free Energy = 0.574474 Hartree  
 EE + Zero-point Energy = -2893.2404 Hartree  
 EE + Thermal Energy Correction = -2893.1903 Hartree  
 EE + Thermal Enthalpy Correction = -2893.1894 Hartree  
 EE + Thermal Free Energy Correction = -2893.3314 Hartree  
 E (Thermal) = 449.039 kcal/mol  
 Heat Capacity (Cv) = 186.791 cal/mol-kelvin  
 Entropy (S) = 298.987 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

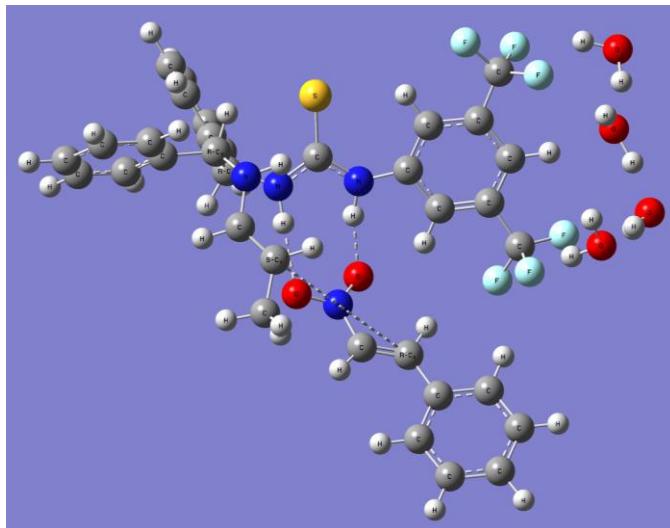
C	-6.35548	0.4337	-2.55236
C	-5.8569	0.50269	-1.2398
C	-6.65881	1.08416	-0.24956
C	-7.92966	1.58234	-0.56267
C	-8.41587	1.50334	-1.86756
C	-7.62215	0.92369	-2.86457
H	-5.72718	0.00691	-3.3247
H	-6.3155	1.14059	0.77513
H	-8.53464	2.02973	0.21761
H	-9.40025	1.88778	-2.10805
H	-7.9901	0.85838	-3.8822
C	-4.58493	-0.82403	1.53081
C	-4.1225	-0.75242	2.85477
C	-4.68674	-1.54516	3.85421
C	-5.72926	-2.42542	3.54609
C	-6.19918	-2.5007	2.23378
C	-5.63239	-1.70454	1.23315
H	-3.30975	-0.07724	3.09661
H	-4.31577	-1.47576	4.87041
H	-6.16965	-3.04271	4.3204

H	-7.00659	-3.17917	1.98325
H	-6.01812	-1.77373	0.22496
C	-4.45884	-0.07764	-0.98683
C	-3.95211	0.10989	0.48907
N	-2.47072	0.07883	0.58068
N	-3.5115	0.50964	-1.95957
H	-4.19231	1.14074	0.77402
H	-4.46993	-1.14944	-1.19576
H	-2.03005	0.99655	0.73878
C	-1.66342	-0.98416	0.34664
C	1.0018	-2.69084	-0.11499
C	2.28303	-3.21156	-0.29051
C	3.44182	-2.50933	0.03725
C	3.26797	-1.22534	0.55078
C	2.00661	-0.6895	0.75772
C	0.84399	-1.40764	0.4292
H	4.426	-2.98849	-0.08251
H	1.9	0.29322	1.18984
N	-0.36123	-0.73346	0.68946
S	-2.23845	-2.49171	-0.33189
H	-0.2053	0.14947	1.21068
F	5.56869	-1.04814	1.15169
F	4.18517	0.59679	1.78741
F	4.78775	0.42559	-0.31064
F	3.32846	-4.64464	-1.87817
F	2.88496	-5.48615	0.11091
F	1.22449	-5.08077	-1.30049
C	4.43478	-0.34762	0.80935
C	2.41956	-4.59625	-0.82785
C	-3.28992	1.89544	-1.93078
O	-1.12366	2.78145	0.72329

O	0.45173	1.62646	1.91504
N	0.08573	2.64978	1.17415
C	1.03706	3.63921	0.82635
H	-2.68725	-0.0737	-2.11102
H	0.13823	-3.27148	-0.39211
C	-2.12495	2.52561	-2.15019
C	-1.98511	4.02948	-2.16574
H	-1.2201	1.94478	-2.31871
H	-1.5177	4.38946	-3.09174
H	-1.3608	4.35339	-1.32371
C	2.35095	3.41831	1.04648
H	2.63996	2.47272	1.49209
H	0.60516	4.49107	0.32722
C	3.25924	5.66723	0.37811
C	3.44128	4.30172	0.68838
C	4.74199	3.74984	0.64265
C	5.8281	4.54304	0.2856
C	5.63628	5.89577	-0.01529
C	4.35152	6.4548	0.03328
H	2.27139	6.10891	0.42978
H	4.87088	2.69586	0.85502
H	6.82068	4.11236	0.24238
H	6.48329	6.51504	-0.28489
H	4.20978	7.50406	-0.19407
H	-2.96298	4.51484	-2.06727
H	-4.19287	2.46947	-1.73812
O	5.84061	-4.13716	-0.51407
H	5.34039	-4.37181	-1.33951
H	6.49398	-3.36883	-0.77405
O	7.29878	-2.05792	-1.00023
H	6.80077	-1.53505	-1.74326

H	7.07425	-1.58455	-0.15616
O	5.8318	-0.69526	-2.64862
H	5.18068	-1.28992	-3.10522
H	5.31426	-0.17303	-1.97732

## TS1+4H<sub>2</sub>O(water)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2969.9179 Hartree

Dipole Moment = 22.550253 Debye

Polarizability (?) = 624.734 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2969.9179 Hartree

Zero-point Energy Correction = 0.689487 Hartree

Thermal Correction to Energy = 0.742132 Hartree

Thermal Correction to Enthalpy = 0.743076 Hartree

Thermal Correction to Free Energy = 0.595014 Hartree

EE + Zero-point Energy = -2969.2284 Hartree

EE + Thermal Energy Correction = -2969.1757 Hartree

EE + Thermal Enthalpy Correction = -2969.1748 Hartree

EE + Thermal Free Energy Correction = -2969.3228 Hartree

E (Thermal) = 465.695 kcal/mol

Heat Capacity (Cv) = 195.252 cal/mol-kelvin

Entropy (S) = 311.624 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

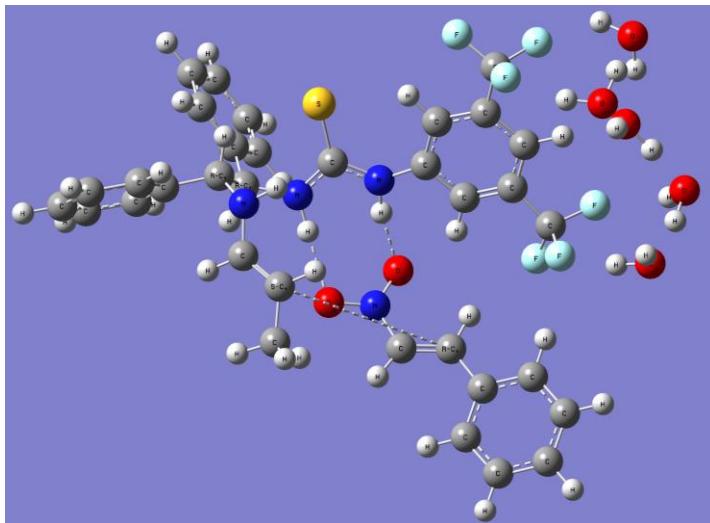
C	-6.35549	0.43365	-2.55235
C	-5.85689	0.5027	-1.2398
C	-6.65878	1.08423	-0.24957
C	-7.92962	1.58242	-0.5627
C	-8.41585	1.50337	-1.86758
C	-7.62215	0.92365	-2.86457
H	-5.7272	0.00682	-3.32468
H	-6.31547	1.1407	0.77511
H	-8.53459	2.02986	0.21757
H	-9.40022	1.88782	-2.10807
H	-7.99011	0.85831	-3.88219
C	-4.58494	-0.82402	1.53083
C	-4.12246	-0.75245	2.85478
C	-4.68671	-1.54519	3.85422
C	-5.72929	-2.42539	3.54611
C	-6.19925	-2.50063	2.23382
C	-5.63245	-1.70448	1.23318
H	-3.30968	-0.07732	3.0966
H	-4.31571	-1.47582	4.8704
H	-6.16967	-3.04268	4.32042
H	-7.00669	-3.17906	1.98329
H	-6.0182	-1.77363	0.225

C	-4.45884	-0.07765	-0.98682
C	-3.95211	0.10989	0.48908
N	-2.47072	0.07882	0.58069
N	-3.51149	0.50961	-1.95957
H	-4.1923	1.14074	0.77402
H	-4.46994	-1.14945	-1.19573
H	-2.03004	0.99654	0.73878
C	-1.66342	-0.98416	0.34665
C	1.0018	-2.69084	-0.115
C	2.28302	-3.21156	-0.29052
C	3.44181	-2.50933	0.03724
C	3.26797	-1.22534	0.55077
C	2.00661	-0.6895	0.75772
C	0.84398	-1.40765	0.4292
H	4.426	-2.98849	-0.08253
H	1.9	0.29322	1.18983
N	-0.36123	-0.73346	0.68946
S	-2.23846	-2.49172	-0.33186
H	-0.20529	0.14947	1.21068
F	5.56869	-1.04814	1.15167
F	4.18517	0.59679	1.7874
F	4.78774	0.42559	-0.31066
F	3.32845	-4.64464	-1.87819
F	2.88496	-5.48616	0.11089
F	1.22448	-5.08077	-1.3005
C	4.43478	-0.34762	0.80933
C	2.41955	-4.59625	-0.82786
C	-3.28991	1.89541	-1.93079
O	-1.12366	2.78144	0.72328
O	0.45173	1.62646	1.91503
N	0.08573	2.64978	1.17415

C	1.03706	3.63921	0.82635
H	-2.68725	-0.07374	-2.111
H	0.13823	-3.27149	-0.39211
C	-2.12493	2.52557	-2.1502
C	-1.98508	4.02944	-2.16578
H	-1.22009	1.94474	-2.31871
H	-1.51766	4.3894	-3.09178
H	-1.36078	4.35336	-1.32375
C	2.35095	3.41831	1.04649
H	2.63996	2.47272	1.49211
H	0.60516	4.49107	0.32722
C	3.25924	5.66722	0.37812
C	3.44128	4.30172	0.6884
C	4.742	3.74985	0.6427
C	5.82811	4.54305	0.28566
C	5.63629	5.89578	-0.01524
C	4.35153	6.4548	0.0333
H	2.27139	6.1089	0.42977
H	4.87088	2.69587	0.85508
H	6.82069	4.11237	0.24246
H	6.4833	6.51505	-0.28483
H	4.20978	7.50405	-0.19406
H	-2.96295	4.5148	-2.06732
H	-4.19285	2.46945	-1.73815
O	5.8406	-4.13716	-0.5141
H	5.34039	-4.37181	-1.33954
H	6.49398	-3.36883	-0.77408
O	7.29878	-2.05792	-1.00026
H	6.80077	-1.53505	-1.74328
H	7.07425	-1.58455	-0.15619
O	5.8318	-0.69525	-2.64865

H	5.18067	-1.28992	-3.10524
H	5.31425	-0.17303	-1.97733
O	4.18948	-6.01677	1.77342
H	5.14948	-6.01677	1.77342
H	3.86902	-5.11183	1.77342

## TS1+5H<sub>2</sub>O(water)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -3045.9502 Hartree

Dipole Moment = 19.509388 Debye

Polarizability (?) = 630.27033 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3045.9502 Hartree

Zero-point Energy Correction = 0.716343 Hartree

Thermal Correction to Energy = 0.770331 Hartree

Thermal Correction to Enthalpy = 0.771276 Hartree

Thermal Correction to Free Energy = 0.619969 Hartree

EE + Zero-point Energy = -3045.2338 Hartree

EE + Thermal Energy Correction = -3045.1798 Hartree

EE + Thermal Enthalpy Correction = -3045.1789 Hartree

EE + Thermal Free Energy Correction = -3045.3302 Hartree

E (Thermal) = 483.39 kcal/mol

Heat Capacity (Cv) = 200.35 cal/mol-kelvin

Entropy (S) = 318.451 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

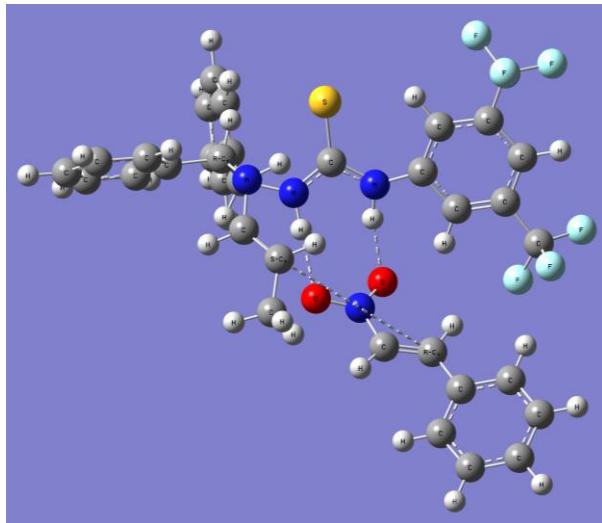
C	-6.75133	-0.24289	-2.56072
C	-6.27143	-0.04018	-1.25507
C	-7.13736	0.51201	-0.30255
C	-8.45213	0.85086	-0.64577
C	-8.91884	0.6397	-1.94308
C	-8.06107	0.08849	-2.90246
H	-6.07511	-0.64616	-3.30456
H	-6.80847	0.66784	0.71657
H	-9.10653	1.27816	0.10538
H	-9.93718	0.90078	-2.20666
H	-8.41322	-0.07825	-3.91412
C	-4.868	-0.99735	1.60876
C	-4.42456	-0.75652	2.91932
C	-4.89704	-1.51986	3.98688
C	-5.82688	-2.54035	3.76174
C	-6.27781	-2.78435	2.46339
C	-5.80321	-2.01729	1.39424
H	-3.69836	0.02823	3.0976
H	-4.54247	-1.31883	4.99134
H	-6.19564	-3.13539	4.58908
H	-6.99847	-3.5723	2.27703
H	-6.17293	-2.21939	0.39797

C	-4.82282	-0.45568	-0.96408
C	-4.34063	-0.091	0.48692
N	-2.86469	0.04566	0.57185
N	-3.93612	0.13352	-1.9912
H	-4.69226	0.9278	0.68637
H	-4.72841	-1.53751	-1.07913
H	-2.52478	1.01446	0.65828
C	-1.94715	-0.93966	0.4229
C	0.89681	-2.32799	-0.0079
C	2.23176	-2.70664	-0.16008
C	3.30265	-1.89454	0.20962
C	2.97719	-0.64652	0.74271
C	1.66302	-0.24779	0.91827
C	0.59035	-1.07606	0.54234
H	4.35059	-2.22068	0.09566
H	1.44415	0.71283	1.35661
N	-0.6841	-0.52821	0.75993
S	-2.34892	-2.54587	-0.1435
H	-0.6344	0.39294	1.23331
F	5.13918	-0.26794	1.6728
F	3.60008	1.33441	1.9182
F	4.53361	1.00085	-0.04443
F	3.00089	-3.90833	-2.08243
F	3.49355	-4.71981	-0.08438
F	1.40558	-4.82397	-0.85489
C	4.04685	0.32361	1.08834
C	2.51486	-4.02823	-0.78108
C	-3.84506	1.53272	-2.07668
O	-1.79277	2.86825	0.51735
O	-0.15202	1.98281	1.84212
N	-0.58966	2.89487	1.00262

C	0.27186	3.93736	0.58229
H	-3.05842	-0.37869	-2.09314
H	0.10614	-2.99987	-0.29715
C	-2.74131	2.24772	-2.3449
C	-2.73832	3.75186	-2.48303
H	-1.78547	1.74044	-2.46227
H	-2.29628	4.07664	-3.43417
H	-2.15421	4.19804	-1.66854
C	1.59656	3.86001	0.83269
H	1.96465	2.98652	1.35884
H	-0.22892	4.6984	0.00645
C	2.30283	6.12128	-0.01244
C	2.60635	4.80872	0.41053
C	3.95351	4.37979	0.41916
C	4.96572	5.24012	0.00469
C	4.65328	6.53984	-0.40795
C	3.32155	6.97762	-0.41381
H	1.27771	6.47104	-0.00385
H	4.17964	3.36362	0.71718
H	5.99458	4.9024	0.0033
H	5.44274	7.2119	-0.72211
H	3.08556	7.98687	-0.72763
H	-3.75708	4.15253	-2.42696
H	-4.79941	2.03359	-1.93401
O	6.09258	-2.7407	-0.24794
H	6.03209	-2.71899	-1.27687
H	6.81656	-2.06919	0.1159
O	7.71016	-0.9896	0.66916
H	7.62012	-0.21765	-0.02418
H	7.18418	-0.68809	1.45571
O	7.164	0.88512	-1.00426

H	7.18017	0.56912	-1.94503
H	6.20752	1.0279	-0.76601
O	6.20878	-5.19319	-0.80062
H	6.27632	-4.2514	-0.32305
H	5.27526	-5.478	-0.60741
O	5.80095	-3.50605	-2.70027
H	6.03822	-4.35921	-2.14206
H	4.80602	-3.52226	-2.73747

## TS1(Only toluene)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=toluene

E(RB3LYP) = -2665.8597 Hartree

Dipole Moment = 11.792022 Debye

Polarizability (?) = 543.95733 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2665.8597 Hartree

Zero-point Energy Correction = 0.591481 Hartree

Thermal Correction to Energy = 0.634384 Hartree

Thermal Correction to Enthalpy = 0.635328 Hartree

Thermal Correction to Free Energy = 0.509479 Hartree

EE + Zero-point Energy = -2665.2682 Hartree

EE + Thermal Energy Correction = -2665.2253 Hartree

EE + Thermal Enthalpy Correction = -2665.2243 Hartree

EE + Thermal Free Energy Correction = -2665.3502 Hartree

E (Thermal) = 398.082 kcal/mol

Heat Capacity (Cv) = 161.714 cal/mol-kelvin

Entropy (S) = 264.871 cal/mol-kelvin

Symbolic Z-matrix:

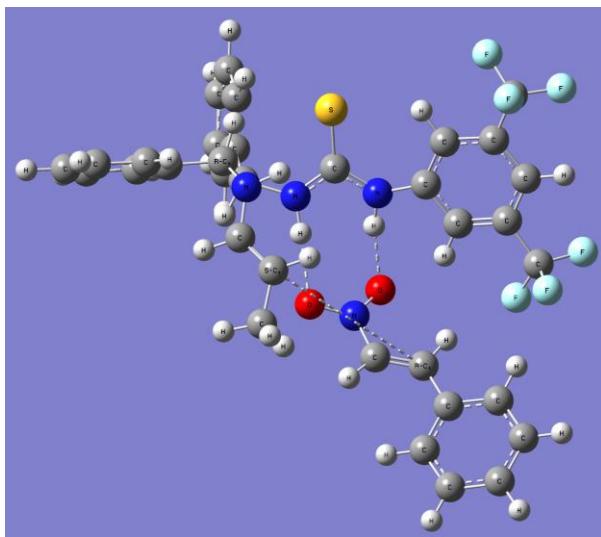
Charge = 0 Multiplicity = 1

C	5.71851	1.27437	2.40903
C	5.3043	0.95726	1.10473
C	6.13162	1.31749	0.03281
C	7.33796	1.98724	0.25997
C	7.73744	2.3021	1.55814
C	6.92208	1.93943	2.63426
H	5.07368	1.00439	3.2355
H	5.85485	1.05553	-0.97899
H	7.96473	2.25665	-0.58264
H	8.67313	2.82101	1.73176
H	7.22367	2.17638	3.64838
C	4.1259	-0.52662	-1.60537
C	4.21848	0.02644	-2.89301
C	4.85477	-0.66117	-3.92582
C	5.40801	-1.92143	-3.68527
C	5.31699	-2.48209	-2.41073
C	4.68005	-1.79228	-1.37579
H	3.79049	1.00617	-3.08265
H	4.91987	-0.21621	-4.91213
H	5.905	-2.45982	-4.48391
H	5.73905	-3.46145	-2.21762
H	4.59598	-2.2504	-0.40094

C	3.98997	0.18559	0.92959
C	3.40299	0.28266	-0.52739
N	1.93525	0.03717	-0.57647
N	2.98615	0.65544	1.90687
H	3.48261	1.33898	-0.80782
H	4.15557	-0.86654	1.16466
H	1.3842	0.87473	-0.80619
C	1.25537	-1.07683	-0.20749
C	-1.23437	-2.96334	0.4814
C	-2.46252	-3.57045	0.7422
C	-3.66847	-3.03909	0.3022
C	-3.62454	-1.84793	-0.41851
C	-2.41923	-1.2311	-0.6969
C	-1.1963	-1.76539	-0.24737
H	-4.60013	-3.55301	0.49341
H	-2.40325	-0.32566	-1.2821
N	-0.06577	-1.01216	-0.59342
S	1.94752	-2.39798	0.68926
H	-0.30016	-0.22389	-1.21811
F	-5.78006	-2.07035	-1.3942
F	-4.62969	-0.19277	-1.80069
F	-5.53867	-0.53923	0.17563
F	-2.57991	-4.53124	2.91937
F	-3.56884	-5.59289	1.25377
F	-1.33672	-5.54434	1.40066
C	-4.88016	-1.1883	-0.8626
C	-2.48247	-4.80849	1.57398
C	2.53787	1.97344	1.85132
O	0.29441	2.53162	-0.73125
O	-1.15007	1.21376	-1.93537
N	-0.90173	2.24095	-1.15399

C	-1.96742	3.0689	-0.71517
H	2.30532	-0.06652	2.14976
H	-0.31935	-3.42386	0.81764
C	1.29524	2.41619	2.12164
C	0.92821	3.87957	2.13404
H	0.51181	1.70547	2.3768
H	0.47722	4.18001	3.0889
H	0.20965	4.09834	1.3336
C	-3.25152	2.69069	-0.87347
H	-3.46085	1.73216	-1.33556
H	-1.62775	3.94517	-0.18675
C	-4.36967	4.8326	-0.18238
C	-4.40809	3.44152	-0.41277
C	-5.60978	2.73796	-0.18003
C	-6.73496	3.41255	0.28586
C	-6.6864	4.79147	0.50759
C	-5.50188	5.49966	0.27031
H	-3.46233	5.38849	-0.38836
H	-5.63406	1.66468	-0.32035
H	-7.64932	2.86401	0.47629
H	-7.56687	5.31509	0.86064
H	-5.46924	6.57015	0.43314
H	1.81275	4.50432	1.96624
H	3.31846	2.68239	1.58618

## TS1(Only gas)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=toluene

E(RB3LYP) = -2665.8597 Hartree

Dipole Moment = 11.792022 Debye

Polarizability (?) = 543.95733 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2665.8597 Hartree

Zero-point Energy Correction = 0.591481 Hartree

Thermal Correction to Energy = 0.634384 Hartree

Thermal Correction to Enthalpy = 0.635328 Hartree

Thermal Correction to Free Energy = 0.509479 Hartree

EE + Zero-point Energy = -2665.2682 Hartree  
 EE + Thermal Energy Correction = -2665.2253 Hartree  
 EE + Thermal Enthalpy Correction = -2665.2243 Hartree  
 EE + Thermal Free Energy Correction = -2665.3502 Hartree  
 E (Thermal) = 398.082 kcal/mol  
 Heat Capacity (Cv) = 161.714 cal/mol-kelvin  
 Entropy (S) = 264.871 cal/mol-kelvin

Symbolic Z-matrix:

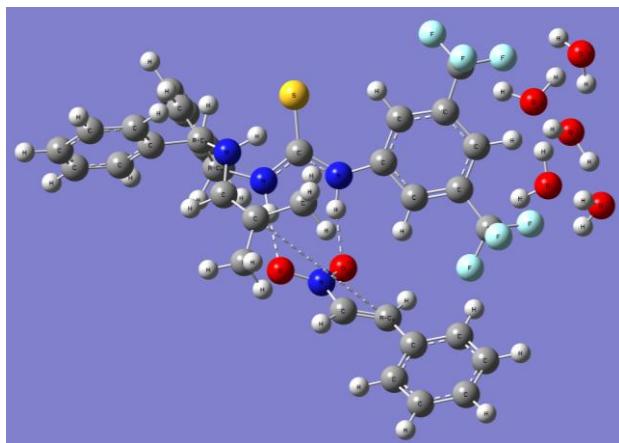
Charge = 0 Multiplicity = 1

C	-5.84016	0.76666	-2.07859
C	-5.34509	0.33945	-0.83189
C	-6.20308	0.37265	0.27693
C	-7.51451	0.85184	0.15055
C	-7.99269	1.28478	-1.0878
C	-7.14983	1.23141	-2.20647
H	-5.17524	0.75444	-2.93648
H	-5.87238	0.02513	1.24753
H	-8.16039	0.87835	1.02349
H	-9.00928	1.65344	-1.18475
H	-7.51279	1.56018	-3.17604
C	-3.97454	-1.51098	1.46624
C	-4.20642	-1.32901	2.84128
C	-4.78308	-2.34451	3.6084
C	-5.13076	-3.56107	3.00764
C	-4.89399	-3.75236	1.64267
C	-4.31331	-2.73619	0.87473
H	-3.94161	-0.38161	3.30852
H	-4.96358	-2.18817	4.66786
H	-5.58383	-4.35085	3.59887
H	-5.15778	-4.69483	1.1726

H	-4.12405	-2.90882	-0.17804
C	-3.89454	-0.17012	-0.77754
C	-3.35258	-0.35195	0.68526
N	-1.8637	-0.42664	0.78297
N	-3.0045	0.64558	-1.63363
H	-3.58173	0.56838	1.2337
H	-3.87298	-1.15798	-1.24637
H	-1.46397	0.34135	1.32909
C	-1.00515	-1.28102	0.17627
C	1.76128	-2.22873	-0.99568
C	3.06487	-2.53973	-1.38712
C	4.173	-2.25157	-0.5906
C	3.92883	-1.66371	0.65273
C	2.63971	-1.36764	1.0888
C	1.52572	-1.61853	0.25111
H	5.17542	-2.50138	-0.91863
H	2.47201	-0.95333	2.0741
N	0.27606	-1.22351	0.74412
S	-1.42151	-2.34059	-1.13632
H	0.33204	-0.72929	1.6579
F	5.9405	-2.38035	1.79302
F	4.71649	-0.75524	2.73872
F	5.93734	-0.34944	0.96875
F	3.43278	-2.12294	-3.73719
F	4.45847	-3.89012	-2.81274
F	2.23393	-3.93274	-3.17485
C	5.10566	-1.29494	1.51476
C	3.28669	-3.11969	-2.74986
C	-2.52374	1.94447	-1.32016
O	-0.45469	2.10919	1.25266
O	0.96382	0.76642	2.42978

N	0.74664	1.83415	1.67528
C	1.8164	2.66438	1.25132
H	-2.31799	0.06461	-2.11884
H	0.92369	-2.47165	-1.63395
C	-1.28035	2.31883	-1.7
C	-0.71959	3.71838	-1.5406
H	-0.64469	1.59485	-2.21397
H	-0.71563	4.21133	-2.49028
H	0.28041	3.66122	-1.16425
C	3.06511	2.13146	1.18602
H	3.15824	1.10615	1.51317
H	1.47864	3.6047	0.84055
C	4.5059	4.06409	0.50633
C	4.29177	2.67856	0.66297
C	5.25389	1.68212	0.30792
C	6.47978	2.20429	-0.1783
C	6.7086	3.57498	-0.34407
C	5.72302	4.51061	0.00285
H	3.7435	4.77898	0.80174
H	5.51163	0.59599	0.62168
H	7.27435	1.52181	-0.47322
H	7.65267	3.92166	-0.75545
H	5.9117	5.57197	-0.12118
H	-1.32778	4.27033	-0.85478
H	-3.14625	2.62867	-0.78234

**Figure 6.**



**TS1+Gas(1)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = None

E(RB3LYP) = -3085.0361 Hartree

Dipole Moment = 11.178062 Debye

Polarizability (?) = 529.562 a.u.

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0361 Hartree

Zero-point Energy Correction = 0.74761 Hartree

Thermal Correction to Energy = 0.801733 Hartree

Thermal Correction to Enthalpy = 0.802677 Hartree

Thermal Correction to Free Energy = 0.654197 Hartree

EE + Zero-point Energy = -3084.2884 Hartree

EE + Thermal Energy Correction = -3084.2343 Hartree

EE + Thermal Enthalpy Correction = -3084.2334 Hartree

EE + Thermal Free Energy Correction = -3084.3819 Hartree

E (Thermal) = 503.095 kcal/mol

Heat Capacity (Cv) = 203.218 cal/mol-kelvin

Entropy (S) = 312.503 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-6.69631	-0.24736	-2.51098
C	-6.22526	-0.07239	-1.19814
C	-7.098	0.45896	-0.24003
C	-8.41057	0.80476	-0.58489
C	-8.86832	0.62131	-1.88955
C	-8.00377	0.09086	-2.85457
H	-6.0152	-0.63475	-3.25889
H	-6.77651	0.59312	0.78454
H	-9.07022	1.21574	0.17076
H	-9.88493	0.8877	-2.15446
H	-8.34897	-0.05447	-3.87192
C	-4.84234	-1.1087	1.64913
C	-4.40082	-0.91247	2.96775
C	-4.88119	-1.70607	4.00943
C	-5.81725	-2.7126	3.74991
C	-6.26614	-2.91251	2.44334
C	-5.78369	-2.11522	1.40015
H	-3.66992	-0.13869	3.1724
H	-4.52787	-1.5393	5.02058
H	-6.19225	-3.33092	4.55712
H	-6.99148	-3.68937	2.23039
H	-6.15214	-2.28322	0.39707
C	-4.77773	-0.49331	-0.90696

C	-4.30918	-0.16863	0.55824
N	-2.83538	-0.02785	0.65684
N	-3.88408	0.12496	-1.90981
H	-4.66645	0.84265	0.78403
H	-4.68112	-1.5715	-1.05062
H	-2.50266	0.94126	0.76651
C	-1.91233	-1.00283	0.47759
C	0.94016	-2.36616	0.0109
C	2.27693	-2.73143	-0.15678
C	3.3438	-1.91273	0.21004
C	3.0122	-0.67216	0.75638
C	1.69625	-0.2868	0.94794
C	0.62786	-1.12188	0.57503
H	4.39391	-2.2287	0.0861
H	1.47217	0.66779	1.39713
N	-0.64926	-0.58805	0.81152
S	-2.30592	-2.59913	-0.12142
H	-0.60293	0.32481	1.3013
F	5.19027	-0.28299	1.64261
F	3.6349	1.29299	1.95805
F	4.52869	1.01238	-0.03134
F	3.05113	-3.91069	-2.09056
F	3.54967	-4.73847	-0.10067
F	1.46183	-4.84691	-0.87027
C	4.07644	0.30488	1.09846
C	2.56667	-4.04565	-0.79026
C	-3.79693	1.52535	-1.95643
O	-1.80785	2.80571	0.6482
O	-0.13966	1.90716	1.93231
N	-0.59537	2.83115	1.11543
C	0.25288	3.88793	0.70381

H	-3.02218	-0.40047	-2.052
H	0.15272	-3.0421	-0.27765
C	-2.71108	2.28248	-2.20751
C	-2.82969	3.7908	-2.29637
H	-2.4357	4.16909	-3.24985
H	-2.25164	4.25086	-1.48457
C	1.58101	3.81879	0.94013
H	1.96248	2.93876	1.44548
H	-0.26125	4.65731	0.15118
C	2.25744	6.10137	0.12763
C	2.57746	4.78546	0.52771
C	3.92929	4.37122	0.5212
C	4.92969	5.24884	0.1145
C	4.60083	6.55148	-0.27559
C	3.26443	6.97481	-0.26638
H	1.22878	6.44006	0.14779
H	4.16785	3.35291	0.80162
H	5.96208	4.92225	0.10151
H	5.38101	7.23692	-0.58397
H	3.01565	7.98624	-0.56281
H	-3.87156	4.11638	-2.20263
H	-4.75537	2.01073	-1.79266
O	6.13652	-2.73257	-0.26218
H	6.07675	-2.70783	-1.29093
H	6.85722	-2.05887	0.10573
O	7.75556	-0.98996	0.6664
H	7.64332	-0.19295	0.00491
H	7.26229	-0.71612	1.48332
O	7.17802	0.94264	-0.92747
H	7.21026	0.67155	-1.8816
H	6.21731	1.06878	-0.69686

O	6.2693	-5.18252	-0.82154
H	6.33009	-4.24119	-0.34171
H	5.338	-5.47472	-0.62861
O	5.84851	-3.4933	-2.71661
H	6.09185	-4.34622	-2.16055
H	4.85355	-3.51486	-2.75081
C	-1.32118	1.72245	-2.43065
H	-0.5899	2.29983	-1.85105
H	-1.23665	0.67556	-2.12107
H	-1.02808	1.78945	-3.48771

## **TS1+n-Hexane(2)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=n-hexane

E(RB3LYP) = -3085.0468 Hartree

Dipole Moment = 12.25269 Debye

Polarizability (?) = 591.247 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0468 Hartree

Zero-point Energy Correction = 0.747194 Hartree

Thermal Correction to Energy = 0.801274 Hartree

Thermal Correction to Enthalpy = 0.802218 Hartree

Thermal Correction to Free Energy = 0.654424 Hartree

EE + Zero-point Energy = -3084.2996 Hartree

EE + Thermal Energy Correction = -3084.2455 Hartree

EE + Thermal Enthalpy Correction = -3084.2446 Hartree

EE + Thermal Free Energy Correction = -3084.3924 Hartree

E (Thermal) = 502.807 kcal/mol

Heat Capacity (Cv) = 203.273 cal/mol-kelvin

Entropy (S) = 311.057 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C                            -6.43142    0.16134   -2.66671

C                            -6.07751    0.12844   -1.30712

C	-7.02238	0.54207	-0.35936
C	-8.28948	0.9797	-0.76102
C	-8.62956	1.00776	-2.11274
C	-7.69375	0.59391	-3.06676
H	-5.69502	-0.13922	-3.40171
H	-6.79362	0.50327	0.69765
H	-9.00738	1.2943	-0.01224
H	-9.61165	1.34614	-2.4221
H	-7.94823	0.61112	-4.12041
C	-4.90436	-1.18355	1.554
C	-4.53315	-1.09558	2.90471
C	-5.08425	-1.95261	3.85568
C	-6.02207	-2.91524	3.47097
C	-6.40072	-3.00802	2.13172
C	-5.8471	-2.14762	1.17926
H	-3.79669	-0.35886	3.20403
H	-4.78222	-1.87158	4.89362
H	-6.45077	-3.58475	4.20753
H	-7.12477	-3.75241	1.82131
H	-6.16086	-2.23445	0.14774
C	-4.67947	-0.39012	-0.94491
C	-4.29889	-0.1737	0.56891
N	-2.83554	-0.05516	0.76615
N	-3.67375	0.23182	-1.82911
H	-4.66715	0.82348	0.83945
H	-4.6232	-1.46205	-1.14543
H	-2.49666	0.90613	0.91182
C	-1.91574	-1.03129	0.5484
C	0.93199	-2.41663	0.15572
C	2.26991	-2.79724	0.03718
C	3.32642	-2.02147	0.50659

C	2.99345	-0.79205	1.0752
C	1.67705	-0.38887	1.21291
C	0.61257	-1.19358	0.76436
H	4.36632	-2.35999	0.44738
H	1.44612	0.55707	1.67744
N	-0.66156	-0.64793	0.96326
S	-2.29308	-2.55744	-0.1938
H	-0.62669	0.24178	1.49273
F	5.1561	-0.4107	2.02666
F	3.59786	1.17992	2.27179
F	4.56494	0.8574	0.32268
F	2.83577	-3.73029	-2.08155
F	3.71301	-4.66825	-0.28473
F	1.54029	-4.92036	-0.7427
C	4.0567	0.17338	1.4444
C	2.57324	-4.03009	-0.7352
C	-3.52446	1.61393	-1.84644
O	-1.77682	2.75629	0.76341
O	-0.15129	1.83658	2.10427
N	-0.56665	2.74911	1.24792
C	0.32618	3.75916	0.81015
H	-2.85195	-0.35098	-1.98105
H	0.14623	-3.06216	-0.20331
C	-2.39355	2.32722	-2.05361
C	-2.45446	3.83535	-2.16329
H	-2.03136	4.1841	-3.11551
H	-1.87862	4.29167	-1.34778
C	1.64822	3.6725	1.06624
H	2.01359	2.80642	1.60665
H	-0.1539	4.51921	0.21504
C	2.35797	5.94399	0.25352

C	2.6591	4.6159	0.6232
C	3.99696	4.16827	0.54967
C	4.99935	5.02459	0.10364
C	4.6891	6.33923	-0.25711
C	3.36739	6.79636	-0.17878
H	1.34115	6.31015	0.33309
H	4.22508	3.14003	0.80075
H	6.02054	4.67011	0.036
H	5.47225	7.00702	-0.59541
H	3.13166	7.81822	-0.44991
H	-3.48519	4.19881	-2.09404
H	-4.46203	2.14311	-1.7012
O	6.15588	-2.72044	-0.05073
H	5.73954	-2.37511	-0.90539
H	6.85621	-1.95929	0.20161
O	7.48389	-0.60586	0.21971
H	7.07343	-0.30542	-0.70633
H	6.949	-0.14754	0.91995
O	6.14528	-0.10969	-1.90149
H	5.86405	-1.00415	-2.34618
H	5.3293	0.27493	-1.48889
O	6.25844	-4.59162	-1.71101
H	6.45184	-4.00484	-0.85604
H	5.4375	-5.09899	-1.46814
O	5.30082	-2.44998	-2.59273
H	5.78161	-3.4037	-2.45899
H	4.32511	-2.62783	-2.6149
C	-1.02943	1.70239	-2.24985
H	-0.27781	2.25371	-1.66915
H	-0.99824	0.65704	-1.92475
H	-0.71905	1.74107	-3.30341

## **TS1+Benzene(3)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=benzene

E(RB3LYP) = -3085.0496 Hartree

Dipole Moment = 12.534454 Debye

Polarizability (?) = 606.17733 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0496 Hartree

Zero-point Energy Correction = 0.747065 Hartree

Thermal Correction to Energy = 0.801152 Hartree

Thermal Correction to Enthalpy = 0.802097 Hartree

Thermal Correction to Free Energy = 0.654241 Hartree

EE + Zero-point Energy = -3084.3026 Hartree

EE + Thermal Energy Correction = -3084.2485 Hartree

EE + Thermal Enthalpy Correction = -3084.2475 Hartree

EE + Thermal Free Energy Correction = -3084.3954 Hartree

E (Thermal) = 502.731 kcal/mol

Heat Capacity (Cv) = 203.293 cal/mol-kelvin

Entropy (S) = 311.189 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C                          -6.48427    0.03502   -2.65179

C                          -6.10301    0.07075   -1.29947

C	-7.03262	0.52251	-0.354
C	-8.31211	0.92923	-0.75053
C	-8.67989	0.88736	-2.09497
C	-7.7589	0.43563	-3.04697
H	-5.75913	-0.29292	-3.38633
H	-6.78193	0.54156	0.69854
H	-9.01731	1.27547	-0.00363
H	-9.67124	1.20153	-2.40029
H	-8.03444	0.39933	-4.09484
C	-4.88749	-1.14429	1.57518
C	-4.51151	-1.01105	2.92128
C	-5.05063	-1.84372	3.90107
C	-5.98109	-2.82691	3.55043
C	-6.36498	-2.96424	2.21601
C	-5.82355	-2.12795	1.23488
H	-3.78296	-0.25681	3.19555
H	-4.74607	-1.72675	4.93484
H	-6.40098	-3.47672	4.30937
H	-7.08442	-3.72364	1.93224
H	-6.14171	-2.24853	0.20808
C	-4.69025	-0.41459	-0.94602
C	-4.29424	-0.16034	0.55657
N	-2.82754	-0.03795	0.73486
N	-3.71268	0.20586	-1.86281
H	-4.65784	0.84323	0.80751
H	-4.62033	-1.48941	-1.12546
H	-2.48897	0.92504	0.8728
C	-1.9092	-1.01761	0.54474
C	0.94007	-2.40511	0.15424
C	2.2777	-2.7892	0.0433
C	3.33272	-2.01027	0.50956

C	3.00091	-0.77461	1.0642
C	1.68494	-0.36932	1.19565
C	0.62054	-1.17754	0.75278
H	4.3701	-2.3524	0.45852
H	1.45519	0.58163	1.65015
N	-0.65389	-0.62794	0.94508
S	-2.29193	-2.57093	-0.14725
H	-0.61616	0.27124	1.45929
F	5.16789	-0.39134	2.00009
F	3.61155	1.20219	2.2487
F	4.56506	0.87225	0.295
F	2.84215	-3.7372	-2.06862
F	3.72585	-4.65755	-0.2658
F	1.55254	-4.92046	-0.71843
C	4.06586	0.19467	1.42142
C	2.58345	-4.02697	-0.72002
C	-3.58172	1.59509	-1.88896
O	-1.76707	2.77603	0.74174
O	-0.1376	1.86197	2.07343
N	-0.55711	2.77549	1.22227
C	0.32893	3.79137	0.78621
H	-2.87676	-0.35892	-2.00512
H	0.15558	-3.05234	-0.20372
C	-2.46305	2.32195	-2.0998
C	-2.54066	3.83078	-2.20263
H	-2.11281	4.19007	-3.14879
H	-1.97593	4.28681	-1.37934
C	1.65262	3.70291	1.03716
H	2.01807	2.83499	1.57454
H	-0.15615	4.55436	0.1992
C	2.36513	5.96683	0.20622

C	2.66482	4.64365	0.59633
C	4.00514	4.1979	0.54787
C	5.01227	5.05171	0.10783
C	4.70362	6.36169	-0.27242
C	3.37928	6.81653	-0.22021
H	1.34628	6.33095	0.26321
H	4.23148	3.17319	0.81485
H	6.03541	4.69987	0.06058
H	5.49009	7.02784	-0.60606
H	3.14535	7.83422	-0.50761
H	-3.57616	4.18228	-2.14038
H	-4.52774	2.11059	-1.7482
O	6.17044	-2.76054	-0.02551
H	5.74776	-2.42	-0.87887
H	6.86839	-1.99375	0.21752
O	7.5028	-0.64507	0.23038
H	7.08412	-0.34807	-0.69576
H	6.96952	-0.18454	0.93098
O	6.16836	-0.14977	-1.88968
H	5.87779	-1.04929	-2.31931
H	5.35764	0.2499	-1.48019
O	6.28038	-4.63821	-1.68055
H	6.46268	-4.04568	-0.82679
H	5.45408	-5.14193	-1.44732
O	5.32643	-2.49403	-2.57452
H	5.80214	-3.44608	-2.43509
H	4.34932	-2.66503	-2.6002
C	-1.08784	1.71765	-2.28932
H	-0.3481	2.28247	-1.70697
H	-1.04157	0.67375	-1.96122
H	-0.77406	1.758	-3.34178

## **TS1+Toluene(4)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=toluene

E(RB3LYP) = -3085.0503 Hartree

Dipole Moment = 12.599236 Debye

Polarizability (?) = 609.469 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0503 Hartree

Zero-point Energy Correction = 0.747034 Hartree

Thermal Correction to Energy = 0.801124 Hartree

Thermal Correction to Enthalpy = 0.802068 Hartree

Thermal Correction to Free Energy = 0.654184 Hartree

EE + Zero-point Energy = -3084.3032 Hartree

EE + Thermal Energy Correction = -3084.2491 Hartree

EE + Thermal Enthalpy Correction = -3084.2482 Hartree

EE + Thermal Free Energy Correction = -3084.3961 Hartree

E (Thermal) = 502.713 kcal/mol

Heat Capacity (Cv) = 203.298 cal/mol-kelvin

Entropy (S) = 311.249 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-6.43142	0.16134	-2.66671
C	-6.07751	0.12844	-1.30712

C	-7.02238	0.54207	-0.35936
C	-8.28948	0.9797	-0.76102
C	-8.62956	1.00776	-2.11274
C	-7.69375	0.59391	-3.06676
H	-5.69502	-0.13922	-3.40171
H	-6.79362	0.50327	0.69765
H	-9.00738	1.2943	-0.01224
H	-9.61165	1.34614	-2.4221
H	-7.94823	0.61112	-4.12041
C	-4.90436	-1.18355	1.554
C	-4.53315	-1.09558	2.90471
C	-5.08425	-1.95261	3.85568
C	-6.02207	-2.91524	3.47097
C	-6.40072	-3.00802	2.13172
C	-5.8471	-2.14762	1.17926
H	-3.79669	-0.35886	3.20403
H	-4.78222	-1.87158	4.89362
H	-6.45077	-3.58475	4.20753
H	-7.12477	-3.75241	1.82131
H	-6.16086	-2.23445	0.14774
C	-4.67947	-0.39012	-0.94491
C	-4.29889	-0.1737	0.56891
N	-2.83554	-0.05516	0.76615
N	-3.67375	0.23182	-1.82911
H	-4.66715	0.82348	0.83945
H	-4.6232	-1.46205	-1.14543
H	-2.49666	0.90613	0.91182
C	-1.91574	-1.03129	0.5484
C	0.93199	-2.41663	0.15572
C	2.26991	-2.79724	0.03718
C	3.32642	-2.02147	0.50659

C	2.99345	-0.79205	1.0752
C	1.67705	-0.38887	1.21291
C	0.61257	-1.19358	0.76436
H	4.36632	-2.35999	0.44738
H	1.44612	0.55707	1.67744
N	-0.66156	-0.64793	0.96326
S	-2.29308	-2.55744	-0.1938
H	-0.62669	0.24178	1.49273
F	5.1561	-0.4107	2.02666
F	3.59786	1.17992	2.27179
F	4.56494	0.8574	0.32268
F	2.83577	-3.73029	-2.08155
F	3.71301	-4.66825	-0.28473
F	1.54029	-4.92036	-0.7427
C	4.0567	0.17338	1.4444
C	2.57324	-4.03009	-0.7352
C	-3.52446	1.61393	-1.84644
O	-1.77682	2.75629	0.76341
O	-0.15129	1.83658	2.10427
N	-0.56665	2.74911	1.24792
C	0.32618	3.75916	0.81015
H	-2.85195	-0.35098	-1.98105
H	0.14623	-3.06216	-0.20331
C	-2.39355	2.32722	-2.05361
C	-2.45446	3.83535	-2.16329
H	-2.03136	4.1841	-3.11551
H	-1.87862	4.29167	-1.34778
C	1.64822	3.6725	1.06624
H	2.01359	2.80642	1.60665
H	-0.1539	4.51921	0.21504
C	2.35797	5.94399	0.25352

C	2.6591	4.6159	0.6232
C	3.99696	4.16827	0.54967
C	4.99935	5.02459	0.10364
C	4.6891	6.33923	-0.25711
C	3.36739	6.79636	-0.17878
H	1.34115	6.31015	0.33309
H	4.22508	3.14003	0.80075
H	6.02054	4.67011	0.036
H	5.47225	7.00702	-0.59541
H	3.13166	7.81822	-0.44991
H	-3.48519	4.19881	-2.09404
H	-4.46203	2.14311	-1.7012
O	6.15588	-2.72044	-0.05073
H	5.73954	-2.37511	-0.90539
H	6.85621	-1.95929	0.20161
O	7.48389	-0.60586	0.21971
H	7.07343	-0.30542	-0.70633
H	6.949	-0.14754	0.91995
O	6.14528	-0.10969	-1.90149
H	5.86405	-1.00415	-2.34618
H	5.3293	0.27493	-1.48889
O	6.25844	-4.59162	-1.71101
H	6.45184	-4.00484	-0.85604
H	5.4375	-5.09899	-1.46814
O	5.30082	-2.44998	-2.59273
H	5.78161	-3.4037	-2.45899
H	4.32511	-2.62783	-2.6149
C	-1.02943	1.70239	-2.24985
H	-0.27781	2.25371	-1.66915
H	-0.99824	0.65704	-1.92475
H	-0.71905	1.74107	-3.30341

## **TS1+Chloroform(5)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=chloroform

E(RB3LYP) = -3085.0586 Hartree

Dipole Moment = 13.51022 Debye

Polarizability (?) = 647.57933 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0586 Hartree

Zero-point Energy Correction = 0.74654 Hartree

Thermal Correction to Energy = 0.800749 Hartree

Thermal Correction to Enthalpy = 0.801693 Hartree

Thermal Correction to Free Energy = 0.65265 Hartree

EE + Zero-point Energy = -3084.312 Hartree

EE + Thermal Energy Correction = -3084.2578 Hartree

EE + Thermal Enthalpy Correction = -3084.2569 Hartree

EE + Thermal Free Energy Correction = -3084.4059 Hartree

E (Thermal) = 502.477 kcal/mol

Heat Capacity (Cv) = 203.396 cal/mol-kelvin

Entropy (S) = 313.687 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-6.48428	0.035	-2.65178
C	-6.10302	0.07073	-1.29946

C	-7.03262	0.52249	-0.35399
C	-8.31211	0.9292	-0.75052
C	-8.6799	0.88733	-2.09495
C	-7.75892	0.43561	-3.04696
H	-5.75914	-0.29293	-3.38633
H	-6.78193	0.54154	0.69855
H	-9.01731	1.27544	-0.00361
H	-9.67126	1.2015	-2.40027
H	-8.03446	0.39931	-4.09482
C	-4.88749	-1.14431	1.57517
C	-4.51151	-1.01106	2.92128
C	-5.05062	-1.84374	3.90107
C	-5.98107	-2.82693	3.55042
C	-6.36496	-2.96426	2.21601
C	-5.82354	-2.12797	1.23488
H	-3.78296	-0.25682	3.19555
H	-4.74606	-1.72677	4.93484
H	-6.40096	-3.47674	4.30937
H	-7.0844	-3.72366	1.93224
H	-6.1417	-2.24855	0.20808
C	-4.69025	-0.4146	-0.94602
C	-4.29424	-0.16035	0.55657
N	-2.82754	-0.03796	0.73486
N	-3.71269	0.20585	-1.86281
H	-4.65784	0.84321	0.80752
H	-4.62033	-1.48942	-1.12547
H	-2.48897	0.92503	0.8728
C	-1.90919	-1.01761	0.54473
C	0.94008	-2.40511	0.15423
C	2.27771	-2.78919	0.0433
C	3.33273	-2.01026	0.50956

C	3.00092	-0.7746	1.06418
C	1.68494	-0.36931	1.19563
C	0.62055	-1.17753	0.75276
H	4.37011	-2.35239	0.45852
H	1.45519	0.58164	1.65013
N	-0.65389	-0.62794	0.94507
S	-2.29193	-2.57094	-0.14726
H	-0.61616	0.27125	1.45928
F	5.1679	-0.39131	2.00007
F	3.61155	1.20221	2.24868
F	4.56505	0.87227	0.29497
F	2.84218	-3.7372	-2.06862
F	3.72585	-4.65755	-0.26578
F	1.55255	-4.92045	-0.71844
C	4.06586	0.19469	1.4214
C	2.58346	-4.02696	-0.72001
C	-3.58174	1.59509	-1.88895
O	-1.76708	2.77603	0.74174
O	-0.1376	1.86197	2.07343
N	-0.55712	2.77549	1.22227
C	0.32892	3.79138	0.78621
H	-2.87677	-0.35891	-2.00512
H	0.15559	-3.05234	-0.20372
C	-2.46307	2.32196	-2.0998
C	-2.54069	3.83078	-2.20262
H	-2.11284	4.19008	-3.14878
H	-1.97596	4.28682	-1.37933
C	1.6526	3.70292	1.03716
H	2.01806	2.83501	1.57453
H	-0.15617	4.55437	0.19921
C	2.3651	5.96685	0.20622

C	2.66479	4.64367	0.59633
C	4.00512	4.19793	0.54786
C	5.01225	5.05174	0.10783
C	4.70359	6.36172	-0.27242
C	3.37925	6.81655	-0.2202
H	1.34626	6.33097	0.26322
H	4.23147	3.17321	0.81484
H	6.03539	4.6999	0.06057
H	5.49006	7.02787	-0.60606
H	3.14532	7.83424	-0.5076
H	-3.57619	4.18229	-2.14037
H	-4.52776	2.11058	-1.74819
O	6.17045	-2.76056	-0.02549
H	5.74778	-2.42001	-0.87885
H	6.86841	-1.99378	0.21755
O	7.50284	-0.64511	0.23041
H	7.08417	-0.34811	-0.69573
H	6.96956	-0.18457	0.93101
O	6.16842	-0.14979	-1.88965
H	5.87784	-1.0493	-2.31929
H	5.3577	0.2499	-1.48016
O	6.28038	-4.63822	-1.68054
H	6.46268	-4.0457	-0.82678
H	5.45408	-5.14193	-1.44732
O	5.32646	-2.49403	-2.57451
H	5.80216	-3.44609	-2.43507
H	4.34935	-2.66502	-2.60019
C	-1.08786	1.71767	-2.28932
H	-0.34812	2.2825	-1.70697
H	-1.04158	0.67377	-1.96122
H	-0.77409	1.75802	-3.34178

## **TS1+THF(6)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=thf

E(RB3LYP) = -3085.0626 Hartree

Dipole Moment = 14.078182 Debye

Polarizability (?) = 661.33833 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0626 Hartree

Zero-point Energy Correction = 0.746413 Hartree

Thermal Correction to Energy = 0.800652 Hartree

Thermal Correction to Enthalpy = 0.801596 Hartree

Thermal Correction to Free Energy = 0.652211 Hartree

EE + Zero-point Energy = -3084.3162 Hartree

EE + Thermal Energy Correction = -3084.2619 Hartree

EE + Thermal Enthalpy Correction = -3084.261 Hartree

EE + Thermal Free Energy Correction = -3084.4104 Hartree

E (Thermal) = 502.417 kcal/mol

Heat Capacity (Cv) = 203.377 cal/mol-kelvin

Entropy (S) = 314.407 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C                            -6.5159    -0.04415    -2.63721

C                            -6.11723    0.03132    -1.29149

C	-7.03798	0.50166	-0.34645
C	-8.32615	0.88697	-0.7368
C	-8.71151	0.8046	-2.07454
C	-7.79917	0.33449	-3.02626
H	-5.79757	-0.38562	-3.37235
H	-6.77342	0.55334	0.70157
H	-9.02413	1.24861	0.00958
H	-9.70952	1.10194	-2.37497
H	-8.08822	0.26711	-4.06893
C	-4.87358	-1.13252	1.58351
C	-4.4963	-0.97646	2.92695
C	-5.02658	-1.79955	3.91985
C	-5.94919	-2.79584	3.58523
C	-6.33431	-2.95586	2.25349
C	-5.80184	-2.12906	1.2593
H	-3.77445	-0.21154	3.18926
H	-4.72167	-1.66457	4.95132
H	-6.36245	-3.43787	4.35436
H	-7.04802	-3.72521	1.98227
H	-6.12086	-2.26696	0.23495
C	-4.69441	-0.43055	-0.94661
C	-4.28926	-0.15936	0.54953
N	-2.82102	-0.03289	0.71654
N	-3.7361	0.19757	-1.87919
H	-4.65195	0.84633	0.79249
H	-4.61119	-1.50557	-1.119
H	-2.48455	0.93137	0.85165
C	-1.90145	-1.01233	0.53741
C	0.95002	-2.39975	0.15497
C	2.2879	-2.78431	0.04905
C	3.34178	-1.99953	0.50775

C	3.00936	-0.75722	1.04677
C	1.69302	-0.35185	1.17342
C	0.62933	-1.16665	0.7409
H	4.37805	-2.34388	0.46425
H	1.46258	0.60407	1.61685
N	-0.64607	-0.61718	0.93
S	-2.28392	-2.57766	-0.13195
H	-0.60845	0.28694	1.43593
F	5.17945	-0.36329	1.96838
F	3.62153	1.2293	2.21416
F	4.56378	0.8888	0.25746
F	2.85416	-3.75339	-2.05249
F	3.73734	-4.65471	-0.2399
F	1.56435	-4.9236	-0.69117
C	4.07392	0.21811	1.39023
C	2.59514	-4.02947	-0.70149
C	-3.62257	1.59071	-1.90443
O	-1.76995	2.78785	0.73024
O	-0.13324	1.87668	2.05175
N	-0.55931	2.79227	1.20709
C	0.31999	3.81518	0.77427
H	-2.89	-0.35247	-2.01951
H	0.16662	-3.05121	-0.1973
C	-2.51453	2.33141	-2.11695
C	-2.6089	3.84036	-2.20892
H	-2.1845	4.21177	-3.15194
H	-2.04874	4.29511	-1.38177
C	1.64483	3.72842	1.02102
H	2.01246	2.85843	1.55345
H	-0.17035	4.57994	0.19405
C	2.35396	5.99314	0.18921

C	2.65545	4.67143	0.58348
C	3.99741	4.22901	0.54342
C	5.00479	5.08499	0.10829
C	4.69443	6.39363	-0.2757
C	3.36837	6.84493	-0.23238
H	1.33371	6.35421	0.23839
H	4.22464	3.20557	0.81463
H	6.02925	4.73621	0.06809
H	5.48096	7.06163	-0.60547
H	3.13334	7.86138	-0.52311
H	-3.64823	4.18017	-2.14423
H	-4.57509	2.09335	-1.76059
O	6.18113	-2.78928	-0.00366
H	5.75788	-2.4513	-0.85789
H	6.88274	-2.02336	0.23272
O	7.52875	-0.68155	0.23879
H	7.11317	-0.3861	-0.69038
H	6.99657	-0.21215	0.93464
O	6.20447	-0.18128	-1.88414
H	5.9025	-1.08179	-2.30391
H	5.39965	0.23176	-1.47572
O	6.29138	-4.67167	-1.65442
H	6.46891	-4.0766	-0.80113
H	5.46262	-5.17353	-1.42579
O	5.34589	-2.52476	-2.55547
H	5.816	-3.47807	-2.41296
H	4.36781	-2.68925	-2.58627
C	-1.13182	1.74504	-2.31081
H	-0.39802	2.31942	-1.73077
H	-1.07097	0.70189	-1.98257
H	-0.8219	1.78905	-3.36427

## **TS1+Dichloromethane(7)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=dichloromethane

E(RB3LYP) = -3085.0639 Hartree

Dipole Moment = 14.285918 Debye

Polarizability (?) = 663.788 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0639 Hartree

Zero-point Energy Correction = 0.746411 Hartree

Thermal Correction to Energy = 0.800645 Hartree

Thermal Correction to Enthalpy = 0.80159 Hartree

Thermal Correction to Free Energy = 0.652135 Hartree

EE + Zero-point Energy = -3084.3175 Hartree

EE + Thermal Energy Correction = -3084.2632 Hartree

EE + Thermal Enthalpy Correction = -3084.2623 Hartree

EE + Thermal Free Energy Correction = -3084.4117 Hartree

E (Thermal) = 502.413 kcal/mol

Heat Capacity (Cv) = 203.362 cal/mol-kelvin

Entropy (S) = 314.553 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C -6.515 -0.08747 -2.6453

C -6.1158 0.00984 -1.30117

C	-7.03883	0.48759	-0.36207
C	-8.33002	0.85836	-0.75664
C	-8.71611	0.75382	-2.09268
C	-7.80132	0.27649	-3.0385
H	-5.79489	-0.43427	-3.37618
H	-6.77321	0.5565	0.68464
H	-9.02973	1.22619	-0.01491
H	-9.71646	1.03979	-2.39634
H	-8.09083	0.19219	-4.07982
C	-4.87594	-1.09121	1.59211
C	-4.52483	-0.8872	2.93622
C	-5.05737	-1.68936	3.94505
C	-5.9556	-2.71257	3.62547
C	-6.31388	-2.92075	2.29277
C	-5.7791	-2.11482	1.28275
H	-3.82185	-0.10099	3.1872
H	-4.77349	-1.51707	4.97695
H	-6.37081	-3.33833	4.40687
H	-7.00833	-3.71152	2.03338
H	-6.07656	-2.29056	0.25771
C	-4.68957	-0.43693	-0.951
C	-4.28631	-0.14155	0.54008
N	-2.81715	-0.02113	0.70689
N	-3.73633	0.18598	-1.89299
H	-4.64345	0.87046	0.76391
H	-4.59826	-1.51343	-1.10944
H	-2.47602	0.943	0.83136
C	-1.90298	-1.00855	0.54939
C	0.94587	-2.4019	0.16859
C	2.28296	-2.78892	0.0616
C	3.33882	-2.00361	0.51471

C	3.00941	-0.75837	1.04876
C	1.69397	-0.35059	1.17634
C	0.62814	-1.16571	0.74948
H	4.37427	-2.34959	0.4704
H	1.46617	0.60802	1.61523
N	-0.64586	-0.61204	0.93552
S	-2.29272	-2.58759	-0.08456
H	-0.60546	0.29779	1.43092
F	5.1827	-0.36446	1.96171
F	3.62771	1.23124	2.20761
F	4.56313	0.88361	0.24907
F	2.84027	-3.76628	-2.03836
F	3.73085	-4.66066	-0.22591
F	1.55589	-4.93091	-0.66725
C	4.07623	0.21716	1.38515
C	2.58695	-4.03702	-0.68533
C	-3.62744	1.58054	-1.92627
O	-1.75741	2.79575	0.70923
O	-0.12601	1.88882	2.03893
N	-0.54869	2.80157	1.1902
C	0.33218	3.82301	0.75736
H	-2.88597	-0.35931	-2.02592
H	0.16094	-3.05388	-0.17926
C	-2.52127	2.32316	-2.139
C	-2.61831	3.83178	-2.23571
H	-2.19149	4.20159	-3.17827
H	-2.0612	4.28915	-1.4079
C	1.65644	3.7342	1.00691
H	2.02133	2.86411	1.54108
H	-0.15625	4.58737	0.17502
C	2.37168	5.99611	0.17312

C	2.66977	4.67462	0.57086
C	4.01121	4.22993	0.53688
C	5.02164	5.08368	0.10449
C	4.7147	6.39223	-0.28277
C	3.38911	6.84566	-0.24567
H	1.35176	6.35868	0.21739
H	4.23551	3.20659	0.81093
H	6.04574	4.73339	0.06909
H	5.50357	7.05857	-0.61028
H	3.15683	7.86198	-0.539
H	-3.65848	4.16988	-2.17517
H	-4.58231	2.08052	-1.78856
O	6.17696	-2.80355	-0.00062
H	5.74909	-2.4672	-0.85325
H	6.87988	-2.037	0.23003
O	7.52835	-0.69656	0.23001
H	7.10982	-0.4029	-0.69878
H	6.99896	-0.22418	0.92604
O	6.19946	-0.19817	-1.89008
H	5.89227	-1.0997	-2.3039
H	5.3979	0.21982	-1.48013
O	6.28076	-4.68876	-1.64885
H	6.46055	-4.09189	-0.79719
H	5.45231	-5.18988	-1.41737
O	5.33275	-2.54229	-2.54963
H	5.80218	-3.49563	-2.40751
H	4.35436	-2.70514	-2.57859
C	-1.13607	1.73953	-2.32502
H	-0.40512	2.3229	-1.75066
H	-1.07209	0.70039	-1.98472
H	-0.8252	1.77252	-3.37859

## **TS1+EtOH(8)**

Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=ethanol

E(RB3LYP) = -3085.0686 Hartree

Dipole Moment = 14.990209 Debye

Polarizability (?) = 670.97967 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0686 Hartree

Zero-point Energy Correction = 0.746229 Hartree

Thermal Correction to Energy = 0.800531 Hartree

Thermal Correction to Enthalpy = 0.801475 Hartree

Thermal Correction to Free Energy = 0.651711 Hartree

EE + Zero-point Energy = -3084.3223 Hartree

EE + Thermal Energy Correction = -3084.268 Hartree

EE + Thermal Enthalpy Correction = -3084.2671 Hartree

EE + Thermal Free Energy Correction = -3084.4169 Hartree

E (Thermal) = 502.341 kcal/mol

Heat Capacity (Cv) = 203.381 cal/mol-kelvin

Entropy (S) = 315.205 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C                          -6.5159    -0.04407    -2.63723

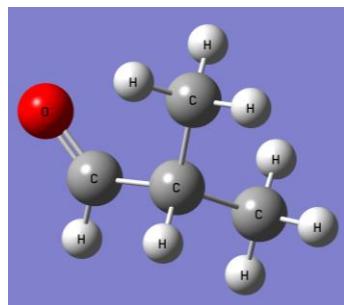
C                          -6.11725    0.03133    -1.2915

C	-7.03801	0.50157	-0.34644
C	-8.32619	0.88688	-0.73677
C	-8.71154	0.80458	-2.07452
C	-7.79918	0.33457	-3.02626
H	-5.79756	-0.38547	-3.37239
H	-6.77346	0.55319	0.70159
H	-9.02419	1.24845	0.00963
H	-9.70955	1.10192	-2.37494
H	-8.08822	0.26725	-4.06894
C	-4.87357	-1.13247	1.58351
C	-4.49637	-0.97629	2.92696
C	-5.02662	-1.79937	3.91988
C	-5.94913	-2.79576	3.58527
C	-6.33416	-2.95591	2.25353
C	-5.80173	-2.12911	1.25931
H	-3.7746	-0.21129	3.18926
H	-4.72179	-1.6643	4.95136
H	-6.36237	-3.43779	4.35442
H	-7.04779	-3.72533	1.98231
H	-6.12068	-2.2671	0.23495
C	-4.69442	-0.43054	-0.94663
C	-4.28926	-0.15932	0.5495
N	-2.82102	-0.03286	0.7165
N	-3.73611	0.19758	-1.87922
H	-4.65195	0.84637	0.79245
H	-4.61119	-1.50556	-1.11901
H	-2.48454	0.9314	0.85161
C	-1.90146	-1.01232	0.5374
C	0.95	-2.39974	0.15493
C	2.28787	-2.78431	0.04902
C	3.34176	-1.99955	0.50774

C	3.00934	-0.75725	1.04679
C	1.69301	-0.35188	1.17345
C	0.62932	-1.16665	0.74089
H	4.37803	-2.34391	0.46424
H	1.46258	0.60403	1.6169
N	-0.64608	-0.61717	0.92999
S	-2.28396	-2.57766	-0.13192
H	-0.60846	0.28694	1.43592
F	5.17944	-0.36336	1.96841
F	3.62152	1.22923	2.21424
F	4.56377	0.88879	0.25753
F	2.85412	-3.75337	-2.05254
F	3.7373	-4.65472	-0.23996
F	1.56431	-4.92359	-0.69123
C	4.0739	0.21806	1.39029
C	2.5951	-4.02947	-0.70155
C	-3.62256	1.59071	-1.90446
O	-1.76991	2.78785	0.73021
O	-0.13322	1.87667	2.05175
N	-0.55928	2.79226	1.20708
C	0.32004	3.81516	0.77426
H	-2.89002	-0.35247	-2.01954
H	0.1666	-3.05119	-0.19735
C	-2.51451	2.3314	-2.11698
C	-2.60886	3.84035	-2.20894
H	-2.18445	4.21176	-3.15196
H	-2.04869	4.29509	-1.3818
C	1.64488	3.72838	1.02102
H	2.01251	2.85839	1.55344
H	-0.17028	4.57992	0.19403
C	2.354	5.99312	0.18924

C	2.6555	4.6714	0.58348
C	3.99745	4.22898	0.5434
C	5.00483	5.08496	0.10827
C	4.69447	6.39362	-0.27569
C	3.36841	6.84491	-0.23235
H	1.33376	6.35419	0.23845
H	4.22468	3.20553	0.81457
H	6.02929	4.73619	0.06805
H	5.481	7.06162	-0.60546
H	3.13337	7.86137	-0.52305
H	-3.64818	4.18018	-2.14426
H	-4.57508	2.09337	-1.76062
O	6.18111	-2.78929	-0.00365
H	5.75785	-2.4513	-0.85787
H	6.88273	-2.02338	0.23273
O	7.52874	-0.68158	0.23882
H	7.11316	-0.38611	-0.69034
H	6.99658	-0.21218	0.93468
O	6.20444	-0.18125	-1.88409
H	5.90247	-1.08175	-2.30386
H	5.39964	0.23177	-1.47563
O	6.29137	-4.67164	-1.65447
H	6.46889	-4.07659	-0.80117
H	5.4626	-5.17352	-1.42585
O	5.34585	-2.52471	-2.55545
H	5.81596	-3.47802	-2.41297
H	4.36777	-2.68921	-2.58627
C	-1.13181	1.745	-2.31084
H	-0.39801	2.31938	-1.73079
H	-1.07098	0.70186	-1.9826
H	-0.82189	1.78901	-3.36429

**Figure 7.**  
**Isobutyraldehyde(1)**



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -231.19058 Hartree

Dipole Moment = 3.0664175 Debye

Polarizability (?) = 50.257333 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -231.19058 Hartree

Zero-point Energy Correction = 0.113758 Hartree

Thermal Correction to Energy = 0.119987 Hartree

Thermal Correction to Enthalpy = 0.120931 Hartree

Thermal Correction to Free Energy = 0.084489 Hartree

EE + Zero-point Energy = -231.07683 Hartree

EE + Thermal Energy Correction = -231.0706 Hartree

EE + Thermal Enthalpy Correction = -231.06965 Hartree

EE + Thermal Free Energy Correction = -231.10609 Hartree

E (Thermal) = 75.293 kcal/mol

Heat Capacity (Cv) = 21.001 cal/mol-kelvin

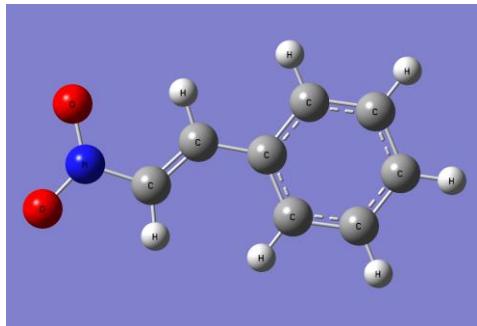
Entropy (S) = 76.699 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	-1.8992	-0.10315	-0.26595
H	-0.91113	-1.73269	0.47759
C	0.43632	0.01567	0.43676
C	1.54479	-0.81135	-0.26368
H	0.61992	-0.02198	1.52255
H	1.40682	-0.78259	-1.35008
H	2.52952	-0.39606	-0.02739
H	1.5247	-1.85767	0.06339
C	-0.90422	-0.65864	0.19693
C	0.40064	1.47363	-0.04454
H	-0.41764	2.01768	0.43591
H	1.34567	1.97845	0.17845
H	0.23052	1.50422	-1.12573

## Nitrostyrene(2)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -511.29897 Hartree

Dipole Moment = 6.926932 Debye

Polarizability (?) = 133.89933 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -511.29897 Hartree

Zero-point Energy Correction = 0.136251 Hartree

Thermal Correction to Energy = 0.145263 Hartree

Thermal Correction to Enthalpy = 0.146207 Hartree

Thermal Correction to Free Energy = 0.100918 Hartree

EE + Zero-point Energy = -511.16272 Hartree

EE + Thermal Energy Correction = -511.15371 Hartree

EE + Thermal Enthalpy Correction = -511.15277 Hartree

EE + Thermal Free Energy Correction = -511.19806 Hartree

E (Thermal) = 91.154 kcal/mol

Heat Capacity (Cv) = 33.849 cal/mol-kelvin

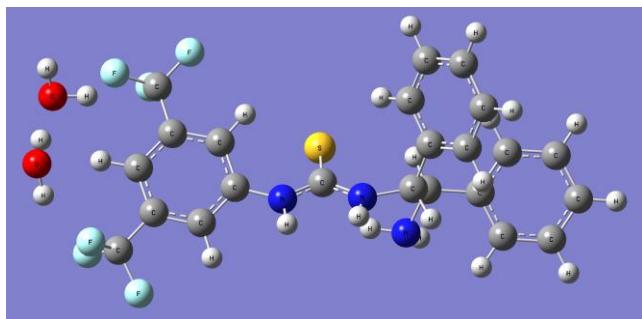
Entropy (S) = 95.319 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	-3.86253	-0.96939	0.00039
O	-3.23129	1.23612	-0.00044
N	-2.98359	-0.02858	0.00002
C	-1.60189	-0.47685	0.00018
C	-0.61632	0.42568	-0.00011
H	-0.93718	1.46382	-0.00042
H	-1.51986	-1.55135	0.00052
C	1.3633	-1.13399	-0.00025
C	0.81932	0.16615	-0.00006
C	1.69957	1.26503	0.00019
C	3.07954	1.0732	0.00024
C	3.60397	-0.22098	0.00004
C	2.74089	-1.32319	-0.0002
H	0.70486	-1.99449	-0.00045
H	1.29049	2.26944	0.00036
H	3.74361	1.92917	0.00043
H	4.67679	-0.37292	0.00008
H	3.14666	-2.32782	-0.00036

## Catalyst 1b.(3)



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2190.4759 Hartree

Dipole Moment = 7.6290985 Debye

Polarizability (?) = 344.08367 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2190.4759 Hartree

Zero-point Energy Correction = 0.439304 Hartree

Thermal Correction to Energy = 0.473472 Hartree

Thermal Correction to Enthalpy = 0.474417 Hartree

Thermal Correction to Free Energy = 0.368328 Hartree

EE + Zero-point Energy = -2190.0366 Hartree

EE + Thermal Energy Correction = -2190.0024 Hartree

EE + Thermal Enthalpy Correction = -2190.0014 Hartree

EE + Thermal Free Energy Correction = -2190.1075 Hartree

E (Thermal) = 297.108 kcal/mol

Heat Capacity (C<sub>v</sub>) = 128.135 cal/mol-kelvin

Entropy (S) = 223.281 cal/mol-kelvin

Symbolic Z-matrix:

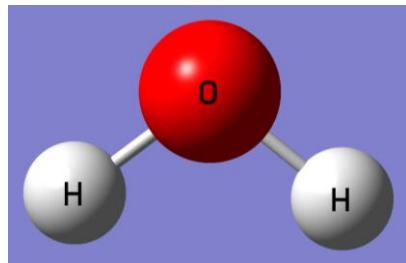
Charge = 0 Multiplicity = 1

C	5.95702	-2.0257	-0.99747
C	5.31343	-0.78977	-1.15311
C	6.08417	0.35455	-1.3923
C	7.4772	0.26852	-1.46758
C	8.11327	-0.96582	-1.30522
C	7.34877	-2.11364	-1.07154
H	5.34877	-2.90778	-0.84029
H	5.59286	1.31319	-1.51709
H	8.06328	1.16099	-1.65527
H	9.19349	-1.03345	-1.36527
H	7.83615	-3.07477	-0.95197
C	3.89545	0.58264	1.1739
C	4.94237	0.48821	2.10013
C	5.41299	1.6259	2.76155
C	4.83664	2.8724	2.50476
C	3.78736	2.97356	1.5853
C	3.31822	1.83683	0.92364
H	5.39328	-0.47753	2.30146
H	6.22394	1.53746	3.47528
H	5.19895	3.75603	3.01732
H	3.33395	3.93758	1.38433
H	2.50024	1.91008	0.21708
C	3.79434	-0.70344	-1.05643
C	3.40676	-0.67122	0.45678
N	1.9588	-0.92522	0.7652
N	3.20105	-1.93013	-1.64968

H	3.90898	-1.5372	0.89565
H	3.45423	0.22643	-1.5242
H	3.5871	-2.07576	-2.59057
H	1.85504	-1.45948	1.62979
C	0.82062	-0.50323	0.18225
C	-2.09556	0.64191	0.19432
C	-3.45486	0.89091	0.02454
C	-4.42239	-0.08562	0.23553
C	-3.98211	-1.35313	0.6043
C	-2.63084	-1.6402	0.76007
C	-1.66918	-0.63958	0.56089
H	-1.38016	1.43301	0.04259
H	-5.49698	0.11274	0.11464
H	-2.32892	-2.64378	1.02737
N	-0.31601	-0.96901	0.80595
H	-0.18708	-1.68947	1.51789
F	-5.87206	-2.51813	-0.24276
F	-5.77538	-2.18874	1.9346
F	-4.40485	-3.65399	0.98784
F	-2.95742	3.20037	-0.2284
F	-4.0937	2.21453	-1.85513
F	-5.0932	2.6085	0.07102
C	-4.99283	-2.42396	0.82923
C	-3.88315	2.22416	-0.46421
S	0.74853	0.4812	-1.26775
O	-6.86435	1.94786	-2.06896
H	-7.01316	2.73572	-1.48077
H	-5.88504	1.95701	-2.2495
O	-7.31491	0.03044	-0.31199
H	-7.12805	-0.86465	-0.70079
H	-7.20109	0.70903	-1.07468

H 2.18444 -1.80902 -1.73222

## H<sub>2</sub>O



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -75.981704 Hartree

Dipole Moment = 2.4259 Debye

Polarizability (?) = 4.43 a.u.

Point Group = C2V

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -75.981704 Hartree

Zero-point Energy Correction = 0.019862 Hartree

Thermal Correction to Energy = 0.022697 Hartree

Thermal Correction to Enthalpy = 0.023641 Hartree

Thermal Correction to Free Energy = 0.002118 Hartree

EE + Zero-point Energy = -75.961842 Hartree

EE + Thermal Energy Correction = -75.959007 Hartree

EE + Thermal Enthalpy Correction = -75.958063 Hartree

EE + Thermal Free Energy Correction = -75.979586 Hartree

E (Thermal) = 14.243 kcal/mol

Heat Capacity (C<sub>v</sub>) = 5.998 cal/mol-kelvin

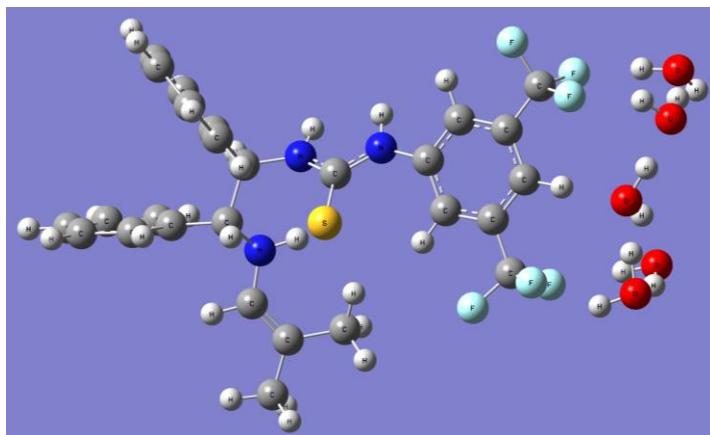
Entropy (S) = 45.3 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	-2.30435	1.26087	0.
H	-1.34435	1.26087	0.
H	-2.6248	2.16581	0.

## IM1



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -2573.7169 Hartree

Dipole Moment = 15.954455 Debye

Polarizability (?) = 422.96 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -2573.7169 Hartree

Zero-point Energy Correction = 0.604658 Hartree

Thermal Correction to Energy = 0.650152 Hartree

Thermal Correction to Enthalpy = 0.651096 Hartree

Thermal Correction to Free Energy = 0.519036 Hartree

EE + Zero-point Energy = -2573.1122 Hartree

EE + Thermal Energy Correction = -2573.0667 Hartree

EE + Thermal Enthalpy Correction = -2573.0658 Hartree

EE + Thermal Free Energy Correction = -2573.1978 Hartree

E (Thermal) = 407.976 kcal/mol

Heat Capacity (C<sub>v</sub>) = 168.118 cal/mol-kelvin

Entropy (S) = 277.943 cal/mol-kelvin

Symbolic Z-matrix:

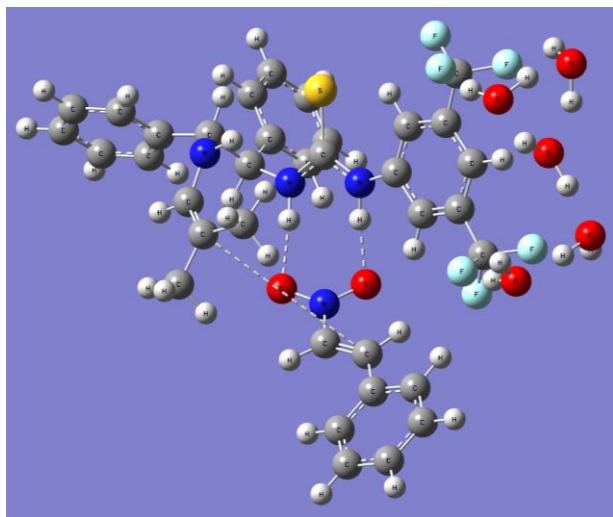
Charge = 0 Multiplicity = 1

C	-6.74597	-0.75461	-2.10271
C	-6.1044	-0.0241	-1.08912
C	-6.84012	0.9552	-0.40338
C	-8.18652	1.17783	-0.70588
C	-8.81747	0.43119	-1.70419
C	-8.09144	-0.53644	-2.40491
H	-6.18459	-1.50335	-2.65267
H	-6.37099	1.54947	0.37235
H	-8.74043	1.93449	-0.16221
H	-9.86224	0.60296	-1.9351
H	-8.57071	-1.11798	-3.18397
C	-4.83748	-1.36328	1.53886
C	-4.48332	-1.38942	2.89751
C	-5.03201	-2.33603	3.76259
C	-5.95239	-3.27378	3.28292
C	-6.31507	-3.25092	1.93491
C	-5.76368	-2.30082	1.06905
H	-3.76443	-0.66892	3.2706
H	-4.74417	-2.34134	4.80775
H	-6.38139	-4.01031	3.95238
H	-7.0273	-3.9727	1.55149
H	-6.06367	-2.29574	0.03096
C	-4.62077	-0.25805	-0.84473

C	-4.23554	-0.25182	0.67023
N	-2.76832	-0.15359	0.86125
N	-3.70555	0.74491	-1.49966
H	-4.59979	0.69839	1.07577
H	-4.32873	-1.22818	-1.25471
H	-2.43358	0.81294	0.97453
C	-1.84438	-1.10403	0.58773
C	1.02454	-2.41105	0.02845
C	2.36343	-2.74417	-0.18358
C	3.42337	-1.91037	0.16936
C	3.08166	-0.68849	0.75071
C	1.76413	-0.33651	0.98894
C	0.70222	-1.18572	0.62813
H	4.47597	-2.20179	0.01179
H	1.53516	0.60329	1.46596
N	-0.57664	-0.68514	0.9124
S	-2.22394	-2.67186	-0.08276
H	-0.53389	0.21175	1.42611
F	5.27605	-0.26637	1.57972
F	3.69724	1.26998	1.96824
F	4.53864	1.04196	-0.05066
F	3.12736	-3.86955	-2.15285
F	3.66647	-4.73268	-0.18853
F	1.57006	-4.85662	-0.93061
C	4.13414	0.30576	1.07891
C	2.6633	-4.03988	-0.84938
C	-4.16812	1.7902	-2.06812
H	0.24226	-3.09555	-0.25425
C	-3.25843	2.84333	-2.66883
C	-3.43875	4.15907	-1.85867
H	-2.89931	4.94947	-2.33738

H	-3.06336	4.02112	-0.86622
H	-5.23795	2.01878	-2.13578
O	6.22178	-2.66952	-0.37389
H	6.14808	-2.6374	-1.40144
H	6.9382	-1.99013	-0.00845
O	7.8326	-0.91866	0.55465
H	7.68704	-0.10835	-0.0838
H	7.35928	-0.67357	1.39223
O	7.17893	1.03829	-0.979
H	7.20249	0.79244	-1.94012
H	6.21946	1.13897	-0.73136
O	6.38318	-5.11292	-0.95313
H	6.43663	-4.17395	-0.46753
H	5.45925	-5.42043	-0.74896
O	5.90911	-3.41669	-2.8288
H	6.17312	-4.26997	-2.28257
H	4.91398	-3.45073	-2.8445
C	-1.7825	2.41007	-2.66265
H	-1.46084	2.25963	-1.62901
H	-1.64565	1.47112	-3.2078
H	-1.15933	3.184	-3.12424
H	-2.71791	0.58856	-1.48862
H	-4.47761	4.41161	-1.81515

## TS1



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -3085.0549 Hartree

Dipole Moment = 19.506576 Debye

Polarizability (?) = 671.26133 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0549 Hartree

Zero-point Energy Correction = 0.744372 Hartree

Thermal Correction to Energy = 0.799909 Hartree

Thermal Correction to Enthalpy = 0.800853 Hartree

Thermal Correction to Free Energy = 0.646074 Hartree

EE + Zero-point Energy = -3084.3105 Hartree  
 EE + Thermal Energy Correction = -3084.255 Hartree  
 EE + Thermal Enthalpy Correction = -3084.254 Hartree  
 EE + Thermal Free Energy Correction = -3084.4088 Hartree  
 E (Thermal) = 501.951 kcal/mol  
 Heat Capacity (Cv) = 205.996 cal/mol-kelvin  
 Entropy (S) = 325.76 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

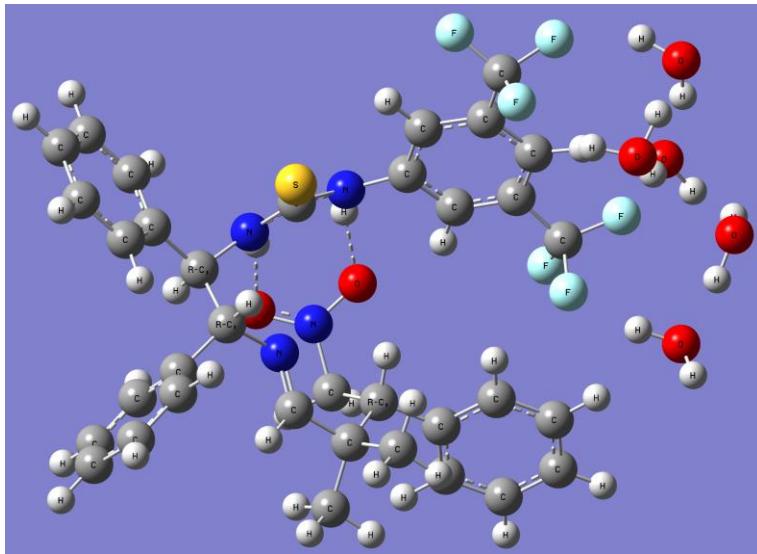
C	-6.6963	-0.24736	-2.51099
C	-6.22525	-0.07239	-1.19815
C	-7.098	0.45895	-0.24003
C	-8.41057	0.80475	-0.58489
C	-8.86831	0.62131	-1.88956
C	-8.00376	0.09087	-2.85458
H	-6.01519	-0.63474	-3.25889
H	-6.77651	0.59311	0.78453
H	-9.07022	1.21573	0.17075
H	-9.88492	0.8877	-2.15447
H	-8.34896	-0.05446	-3.87192
C	-4.84234	-1.10872	1.64912
C	-4.40082	-0.91248	2.96775
C	-4.8812	-1.70609	4.00942
C	-5.81725	-2.71262	3.74989
C	-6.26614	-2.91253	2.44332
C	-5.78369	-2.11523	1.40013
H	-3.66992	-0.1387	3.1724
H	-4.52788	-1.53933	5.02058
H	-6.19226	-3.33094	4.5571

H	-6.99148	-3.68938	2.23037
H	-6.15213	-2.28323	0.39706
C	-4.77772	-0.49331	-0.90696
C	-4.30918	-0.16864	0.55825
N	-2.83538	-0.02785	0.65684
N	-3.88407	0.12496	-1.9098
H	-4.66645	0.84264	0.78403
H	-4.68111	-1.57151	-1.05063
H	-2.50266	0.94125	0.76652
C	-1.91233	-1.00283	0.47759
C	0.94017	-2.36617	0.01091
C	2.27693	-2.73144	-0.15677
C	3.3438	-1.91273	0.21004
C	3.0122	-0.67215	0.75637
C	1.69625	-0.28679	0.94793
C	0.62787	-1.12188	0.57503
H	4.39391	-2.2287	0.0861
H	1.47217	0.6678	1.39711
N	-0.64926	-0.58806	0.81152
S	-2.30591	-2.59913	-0.12142
H	-0.60293	0.32481	1.3013
F	5.19029	-0.28297	1.64257
F	3.6349	1.293	1.95803
F	4.52867	1.01239	-0.03138
F	3.05113	-3.91072	-2.09054
F	3.54969	-4.73847	-0.10064
F	1.46184	-4.84693	-0.87022
C	4.07644	0.30489	1.09843
C	2.56667	-4.04566	-0.79023
C	-3.79693	1.52536	-1.95642
O	-1.80786	2.8057	0.64821

O	-0.13965	1.90716	1.93231
N	-0.59538	2.83115	1.11544
C	0.25286	3.88794	0.70381
H	-3.02217	-0.40046	-2.052
H	0.15272	-3.04211	-0.27763
C	-2.71107	2.28249	-2.20749
C	-2.82969	3.79081	-2.29636
H	-2.4357	4.1691	-3.24984
H	-2.25165	4.25087	-1.48455
C	1.581	3.8188	0.94013
H	1.96247	2.93877	1.44548
H	-0.26126	4.65731	0.15119
C	2.25742	6.10138	0.12764
C	2.57744	4.78548	0.52771
C	3.92928	4.37124	0.5212
C	4.92967	5.24887	0.1145
C	4.60081	6.55151	-0.27558
C	3.26441	6.97483	-0.26637
H	1.22876	6.44007	0.1478
H	4.16784	3.35293	0.80162
H	5.96206	4.92228	0.1015
H	5.38098	7.23695	-0.58396
H	3.01562	7.98626	-0.5628
H	-3.87156	4.11639	-2.20262
H	-4.75537	2.01073	-1.79265
O	6.13652	-2.73256	-0.26218
H	6.07674	-2.70785	-1.29093
H	6.85722	-2.05886	0.10572
O	7.75557	-0.98995	0.66637
H	7.64331	-0.19294	0.00487
H	7.26232	-0.71611	1.48329

O	7.178	0.94264	-0.92751
H	7.21023	0.67155	-1.88164
H	6.2173	1.06878	-0.69689
O	6.26931	-5.18252	-0.82151
H	6.3301	-4.24119	-0.34169
H	5.33802	-5.47473	-0.62857
O	5.8485	-3.49334	-2.7166
H	6.09185	-4.34625	-2.16053
H	4.85355	-3.5149	-2.7508
C	-1.32118	1.72247	-2.43063
H	-0.58989	2.29985	-1.85104
H	-1.23665	0.67558	-2.12105
H	-1.02807	1.78946	-3.4877

## IM2



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -3085.0641 Hartree

Dipole Moment = 19.432765 Debye

Polarizability (?) = 538.81167 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -3085.0641 Hartree

Zero-point Energy Correction = 0.747732 Hartree

Thermal Correction to Energy = 0.801393 Hartree

Thermal Correction to Enthalpy = 0.802337 Hartree

Thermal Correction to Free Energy = 0.656847 Hartree

EE + Zero-point Energy = -3084.3164 Hartree  
 EE + Thermal Energy Correction = -3084.2627 Hartree  
 EE + Thermal Enthalpy Correction = -3084.2618 Hartree  
 EE + Thermal Free Energy Correction = -3084.4073 Hartree  
 E (Thermal) = 502.882 kcal/mol  
 Heat Capacity (Cv) = 203.484 cal/mol-kelvin  
 Entropy (S) = 306.211 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

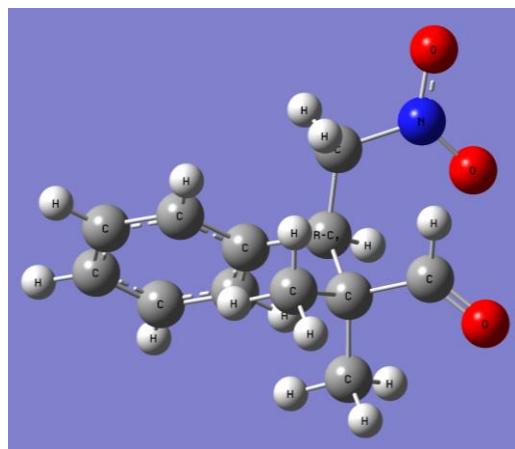
C	-4.66605	0.34328	-2.93101
C	-4.79851	0.04508	-1.56462
C	-6.05563	0.19233	-0.96563
C	-7.15808	0.6152	-1.71755
C	-7.01705	0.89855	-3.07673
C	-5.76321	0.76119	-3.68334
H	-3.68974	0.25392	-3.39339
H	-6.19483	-0.02908	0.08493
H	-8.12401	0.72165	-1.23724
H	-7.87213	1.22293	-3.65834
H	-5.64289	0.98048	-4.73813
C	-4.54344	-2.35327	0.60886
C	-4.77192	-2.96679	1.85082
C	-5.47101	-4.17098	1.93765
C	-5.95816	-4.78294	0.77819
C	-5.73842	-4.17877	-0.46136
C	-5.03747	-2.97161	-0.5457
H	-4.38903	-2.50003	2.75152
H	-5.63658	-4.62955	2.90589
H	-6.50255	-5.71798	0.84154
H	-6.11	-4.64521	-1.36662

H	-4.88216	-2.51734	-1.51431
C	-3.53113	-0.37688	-0.817
C	-3.80305	-1.00991	0.59723
N	-2.53481	-1.08921	1.37799
N	-2.59837	0.78098	-0.79719
H	-4.40049	-0.29689	1.17577
H	-3.02507	-1.15086	-1.40073
H	-2.49102	-0.40531	2.14223
C	-1.41247	-1.76503	1.0434
C	1.63372	-2.73759	0.96706
C	2.95167	-2.70921	0.50457
C	3.70836	-1.53861	0.47327
C	3.10712	-0.38783	0.97188
C	1.80353	-0.38493	1.44965
C	1.03869	-1.55467	1.4196
H	4.71831	-1.48336	0.03697
H	1.3691	0.53465	1.8162
N	-0.31976	-1.43465	1.82231
S	-1.31621	-2.9171	-0.26527
H	-0.46376	-0.65787	2.48283
F	5.13779	0.86718	0.85749
F	3.33335	1.85798	1.71402
F	3.44855	1.45027	-0.46337
F	3.56269	-3.9713	-1.43637
F	4.86502	-4.10586	0.34726
F	2.85546	-5.0746	0.34385
C	3.77345	0.92264	0.82128
C	3.5421	-3.95774	-0.04214
C	-3.09451	2.05428	-0.22246
O	-2.66602	1.36636	2.85976
O	-0.40937	1.19656	2.90694

N	-1.4921	1.85528	2.68232
C	-1.33652	3.24468	2.10634
H	1.0786	-3.66058	0.96063
C	-2.1024	3.24583	-0.42077
C	-2.91189	4.55151	-0.23499
H	-2.27421	5.42861	-0.36997
H	-3.39238	4.60778	0.7485
C	-0.89528	3.14738	0.59797
H	-0.4463	2.15609	0.47339
H	-2.2925	3.73588	2.25797
C	0.13034	5.50576	0.70786
C	0.23662	4.15136	0.34972
C	1.44642	3.69785	-0.19798
C	2.51908	4.57057	-0.40815
C	2.39001	5.91996	-0.07034
C	1.1963	6.38303	0.49101
H	-0.7748	5.88111	1.17035
H	1.56881	2.65305	-0.44529
H	3.45345	4.19303	-0.81167
H	3.21646	6.60318	-0.22805
H	1.0965	7.42544	0.77083
H	-3.70266	4.58775	-0.99221
H	-4.00788	2.3031	-0.76934
O	6.2545	-1.13723	-0.96832
H	5.87569	-1.43408	-1.87942
H	6.63295	-0.16091	-0.99189
O	7.18522	1.26613	-0.9327
H	6.52528	1.98004	-1.27778
H	7.28272	1.44282	0.03855
O	5.32131	2.95875	-1.65991
H	5.22935	3.0841	-2.64094

H	4.56193	2.38337	-1.36675
O	7.25545	-3.43248	-1.1803
H	7.06302	-2.42825	-0.91138
H	6.62454	-3.94867	-0.6089
O	5.61457	-2.61818	-2.98873
H	6.35252	-3.13205	-2.45479
H	4.76463	-3.02595	-2.66902
C	-1.54913	3.21453	-1.86354
H	-0.91037	4.08282	-2.0475
H	-0.97918	2.30044	-2.04601
H	-2.38775	3.23573	-2.568
H	-0.55014	3.69805	2.70693

## Products



Calculation Type = FREQ

Calculation Method = RB3LYP

Basis Set = 6-31G(d,p)

Charge = 0

Spin = Singlet

Solvation = scrf=solvent=water

E(RB3LYP) = -742.51173 Hartree

Dipole Moment = 6.5962025 Debye

Polarizability (?) = 162.24867 a.u.

Point Group = C1

Temperature = 298.15 Kelvin

Pressure = 1 atm

Frequencies scaled by = 1

Electronic Energy (EE) = -742.51173 Hartree

Zero-point Energy Correction = 0.254743 Hartree

Thermal Correction to Energy = 0.270076 Hartree

Thermal Correction to Enthalpy = 0.271021 Hartree

Thermal Correction to Free Energy = 0.211644 Hartree

EE + Zero-point Energy = -742.25699 Hartree

EE + Thermal Energy Correction = -742.24166 Hartree

EE + Thermal Enthalpy Correction = -742.24071 Hartree

EE + Thermal Free Energy Correction = -742.30009 Hartree

E (Thermal) = 169.476 kcal/mol

Heat Capacity (Cv) = 58.104 cal/mol-kelvin

Entropy (S) = 124.969 cal/mol-kelvin

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.53796	2.87382	1.52481
O	2.54528	1.98745	-1.55763
O	0.46011	1.39761	-2.21711
N	1.30275	2.2465	-1.74377
C	0.76043	3.61115	-1.36161
C	0.38374	3.83509	1.23021
C	0.9757	5.27231	1.28476
H	0.18199	6.00321	1.10814
H	1.77461	5.42701	0.55214
C	-0.24557	3.47677	-0.16557
H	-0.53387	2.42088	-0.1245
H	1.63665	4.21785	-1.15389
C	-1.51567	5.58187	-0.92321
C	-1.52759	4.25931	-0.45285
C	-2.76379	3.62958	-0.24892
C	-3.96614	4.30265	-0.48364
C	-3.9421	5.62375	-0.93841
C	-2.71615	6.25799	-1.16174
H	-0.5765	6.08873	-1.11441
H	-2.79564	2.60305	0.0851
H	-4.90611	3.7841	-0.31803
H	-4.86895	6.1531	-1.12646
H	-2.6916	7.27881	-1.52514

H	1.39318	5.44231	2.28224
C	-0.66379	3.68647	2.35549
H	-1.41758	4.47362	2.28884
H	-1.16342	2.71305	2.29677
H	-0.1466	3.75025	3.31606
H	2.08096	2.46421	0.66493
H	0.24565	3.95375	-2.25902
O	1.87951	2.55583	2.67167