

# Supporting Information

## A Convergent Approach to the Dioxadamantane Core of (+/-)-Tetrodotoxin

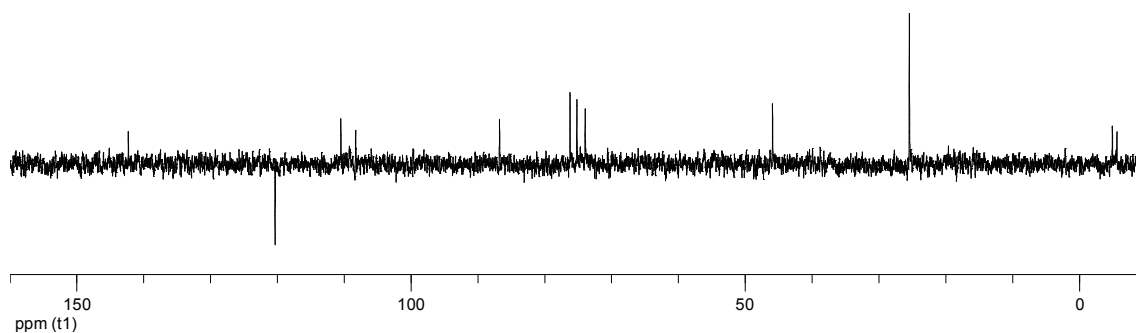
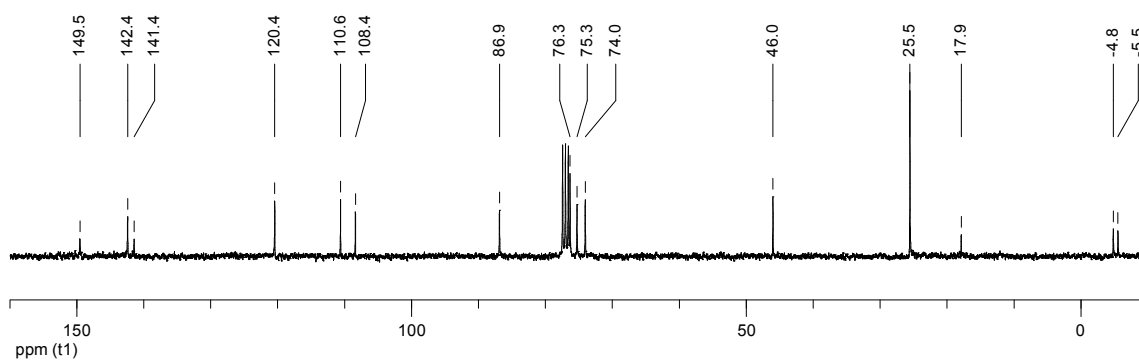
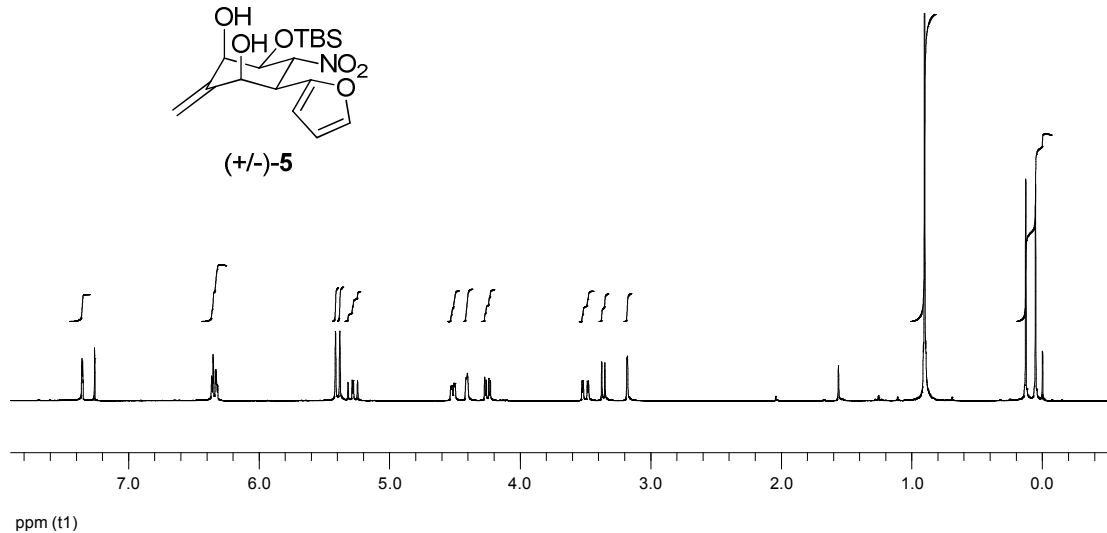
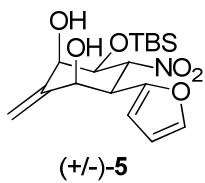
Hugo Lago-Santomé, Rubén Meana-Pañeda, and Ricardo Alonso\*

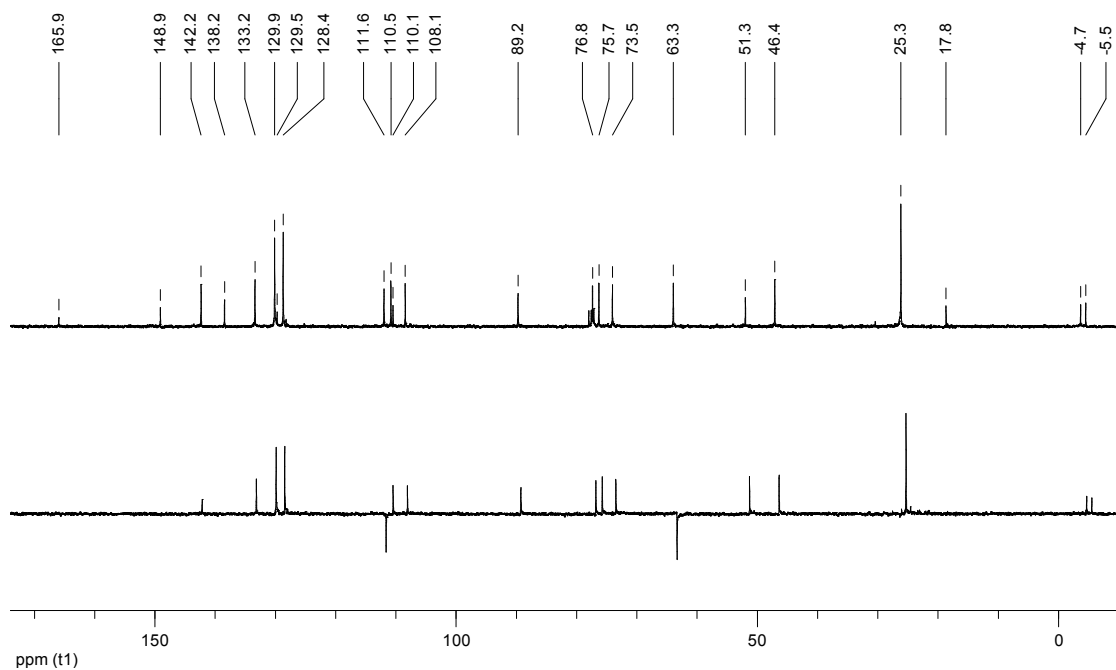
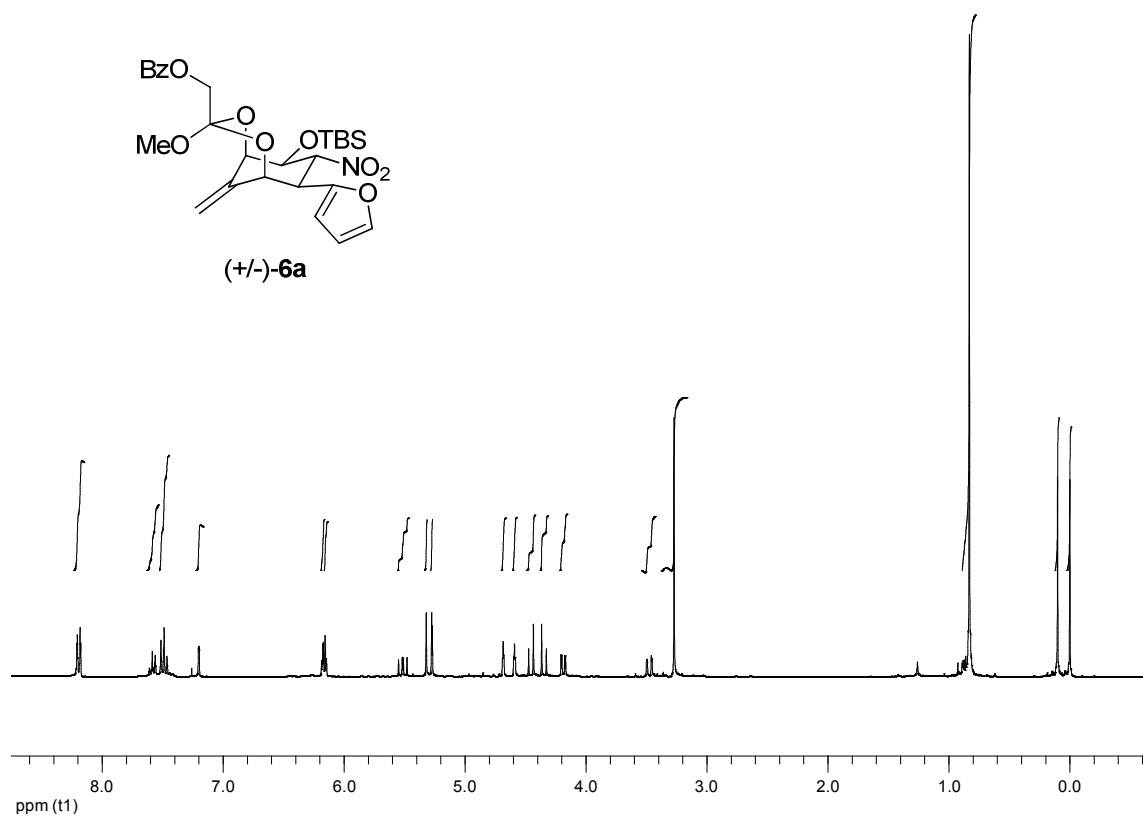
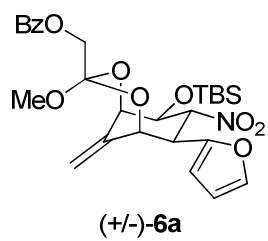
### Contents

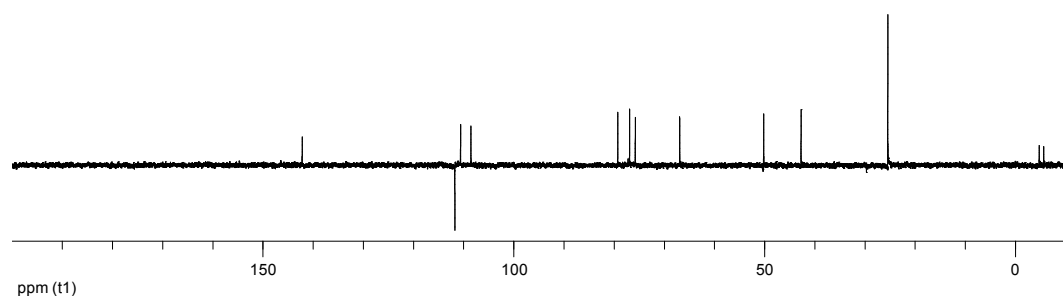
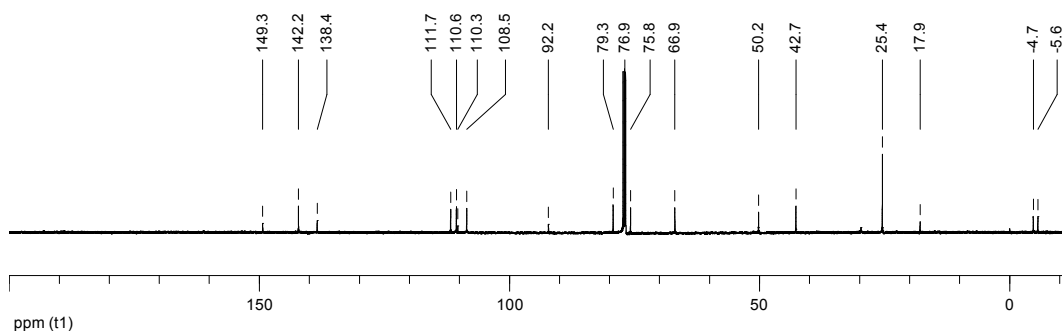
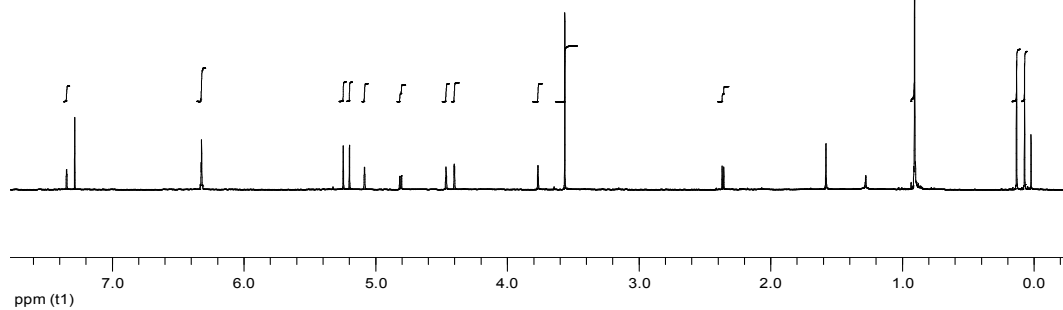
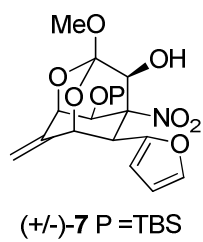
|                                                                                                                                                                                                                                 |         |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|
| General Remarks                                                                                                                                                                                                                 | S1      |
| Copies of NMR spectra for <b>5</b> , <b>6a</b> , <b>7</b> , <b>8</b> , <b>9</b> , <i>6-epi-9</i> , <b>10</b> ,<br><i>6-epi-10</i> , <b>11</b> , <i>6-epi-11</i> , <b>12</b> , <i>6-epi-12</i> , <b>13</b> and <i>6-epi-13</i> . | S2-S17  |
| Calculations                                                                                                                                                                                                                    | S18-S48 |

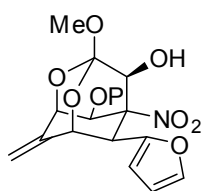
### General Remarks

Solvents for moisture-sensitive reactions were distilled and dried according to standard procedures. Anhydrous Na<sub>2</sub>SO<sub>4</sub> was used to dry organic solutions during workups. Reactions were monitored by TLC with pre-coated silica gel 60 F254 aluminum plates using UV light as the visualizing agent and by dipping the plate into a solution of (NH<sub>4</sub>)<sub>6</sub>Mo<sub>7</sub>O<sub>24</sub>·4 H<sub>2</sub>O (12.5 g) and Ce(SO<sub>4</sub>)<sub>2</sub>·4 H<sub>2</sub>O (5 g) in 10% aqueous H<sub>2</sub>SO<sub>4</sub> (500 mL), followed by heating. Flash column chromatography was performed with silica gel (0.035-0.070 mm, 60 Å). Solvent evaporations were carried out in a rotary evaporator. Chemical shifts are reported in ppm and coupling constants in Hz; multiplicities are given as follows: s (singlet), br s (broad singlet), d (doublet), t (triplet), and m (multiplet).



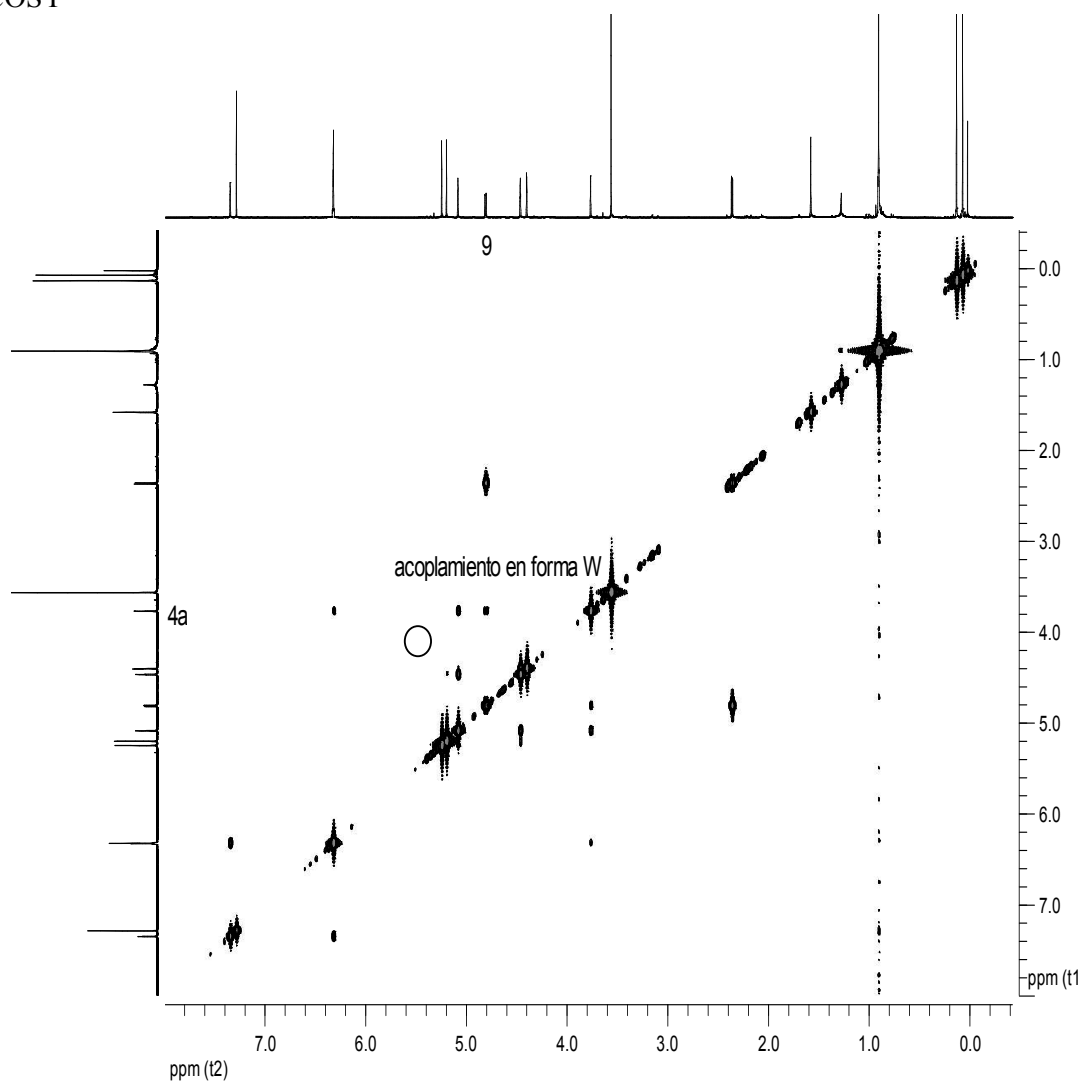


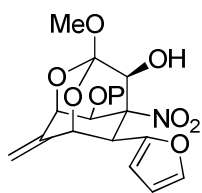




(+/-)-7 P = TBS

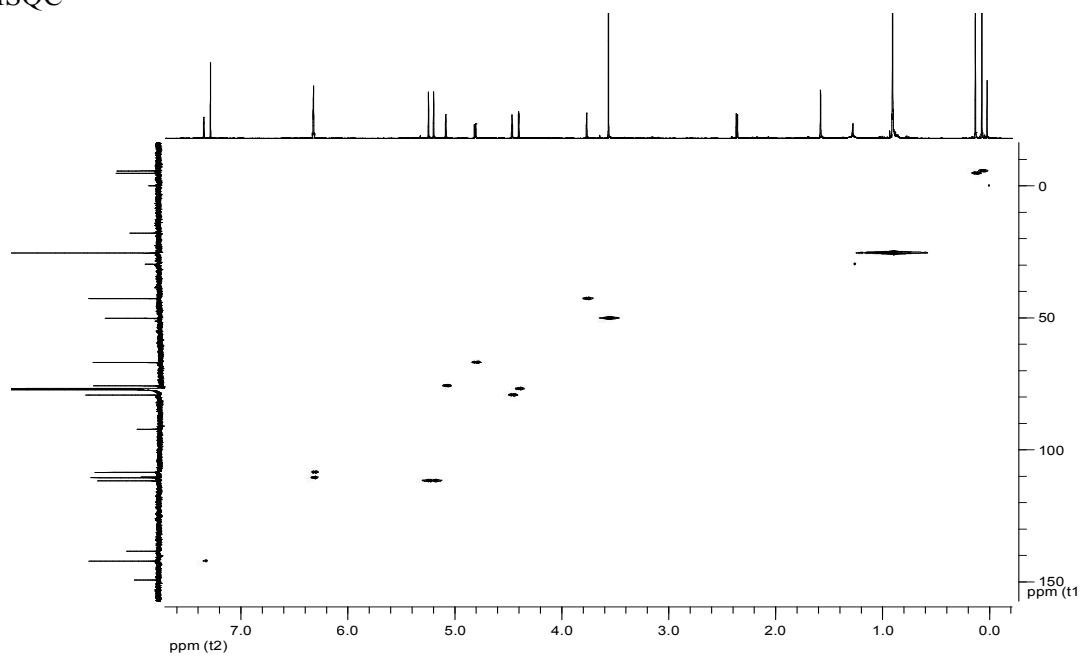
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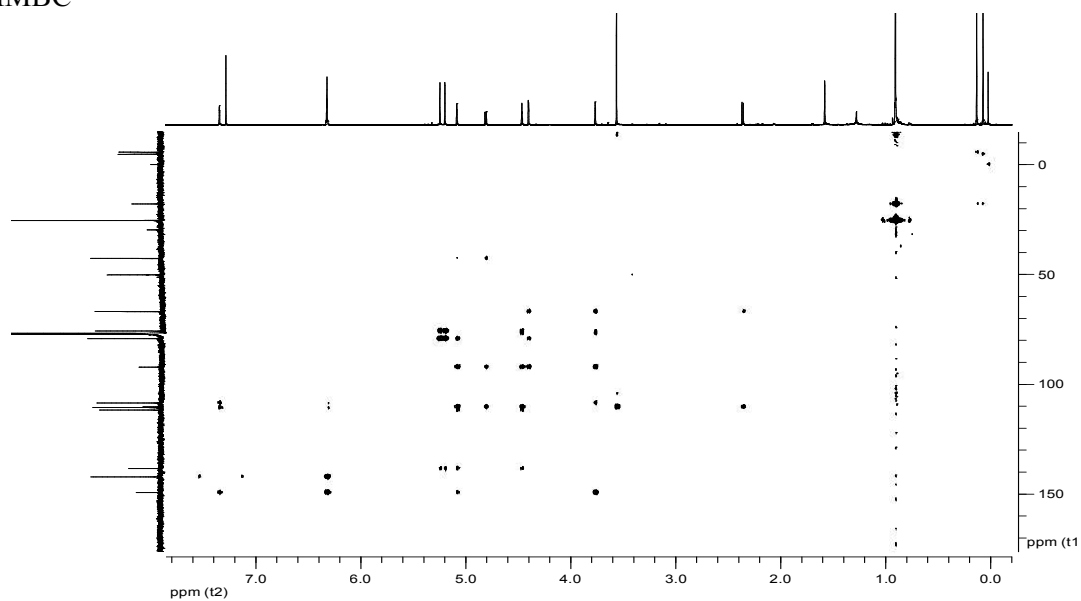


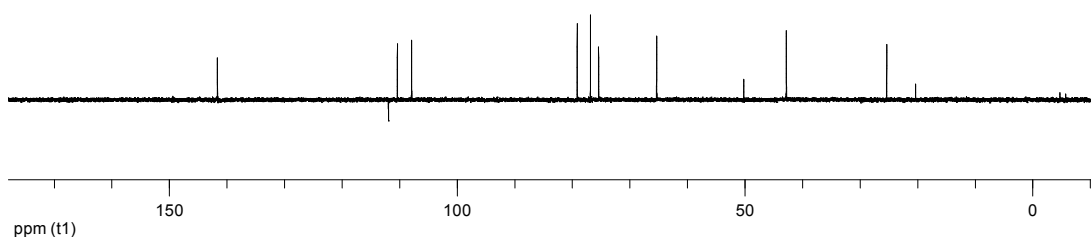
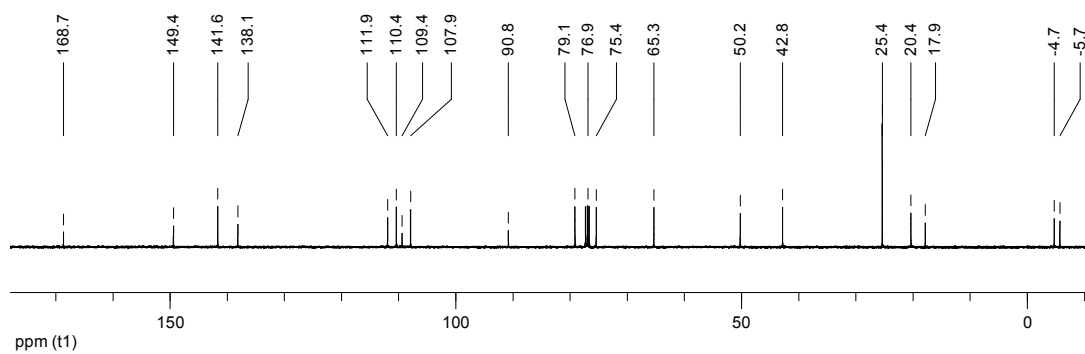
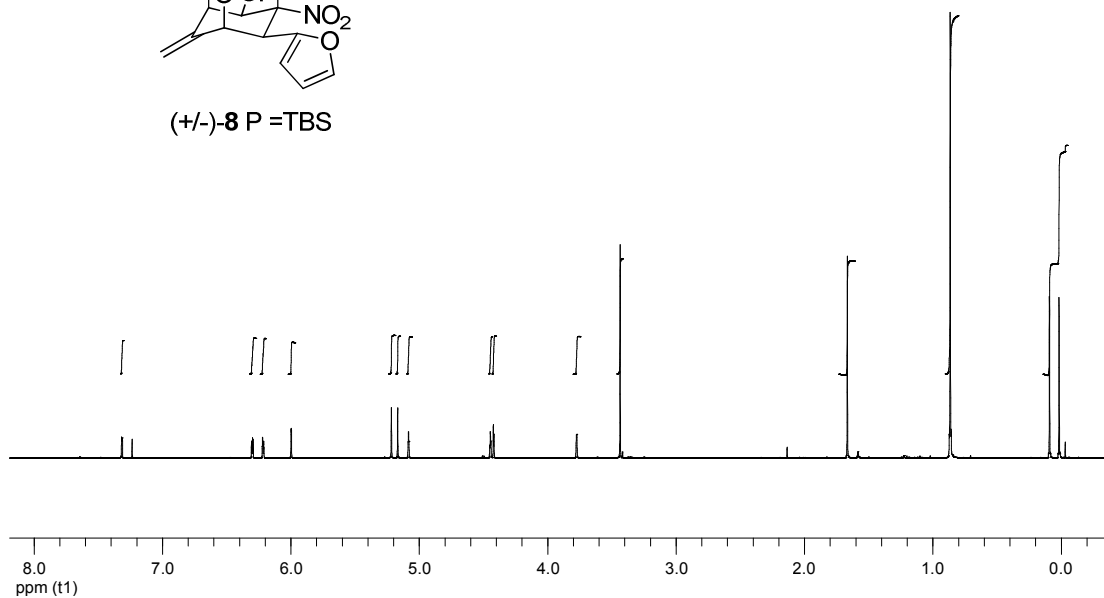
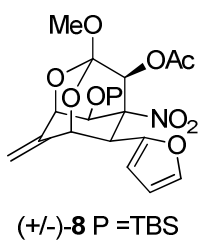
(+/-)-7 P =TBS

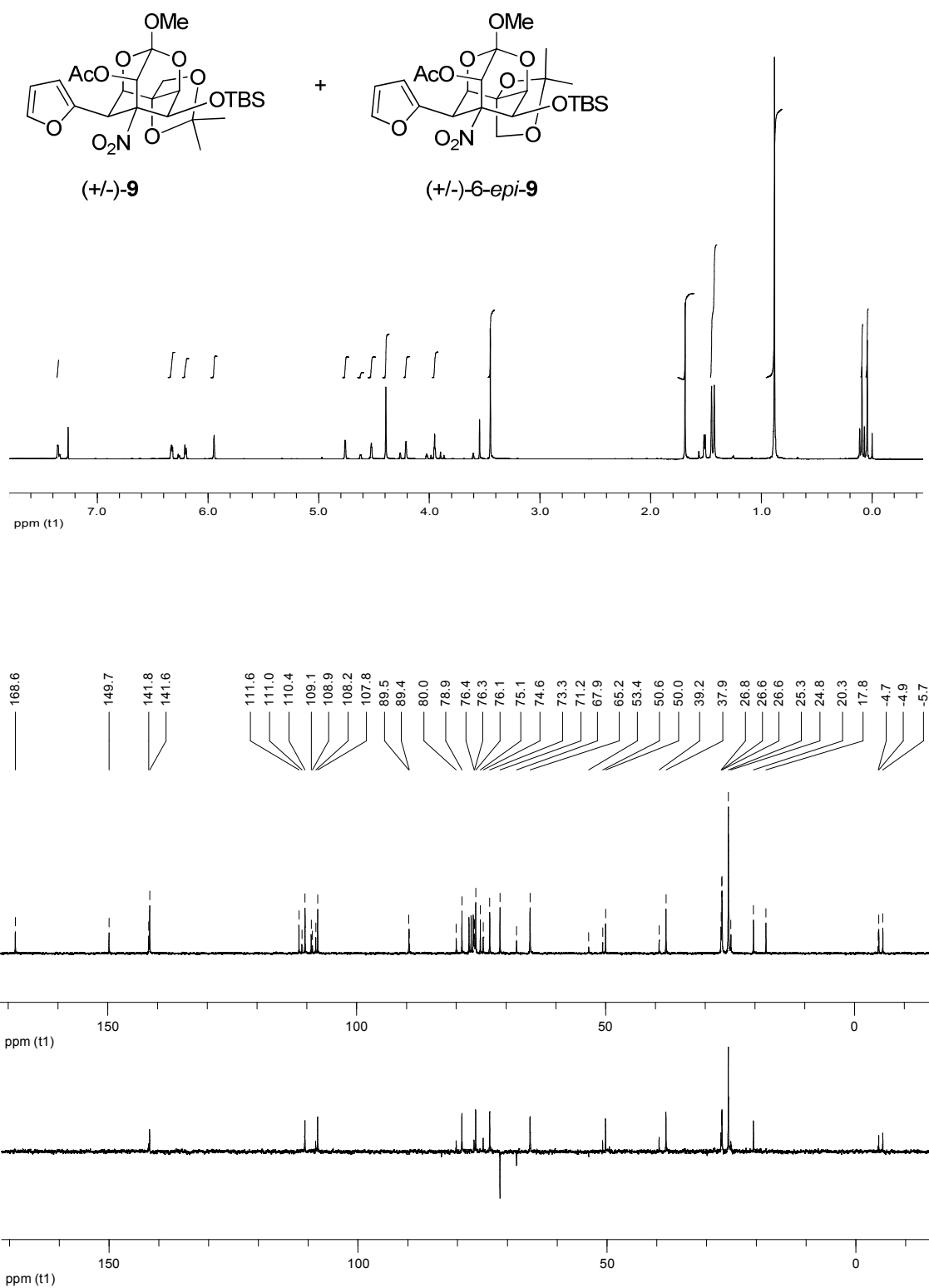
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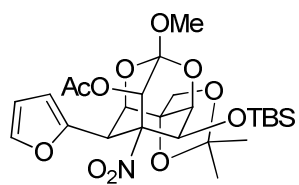


HMBC

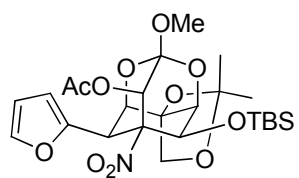
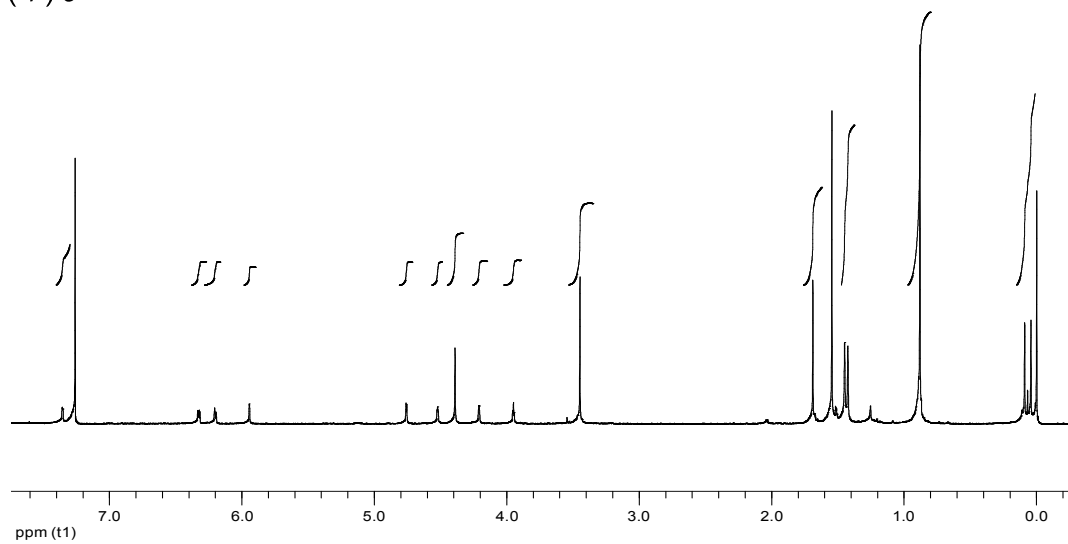




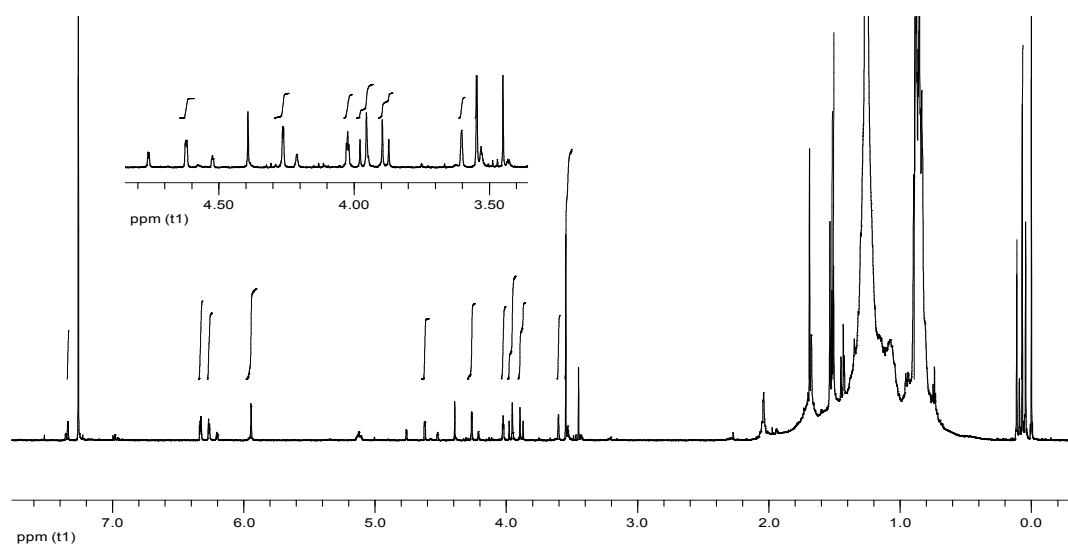


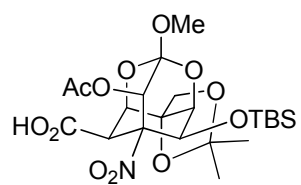


(+/-)-**9**

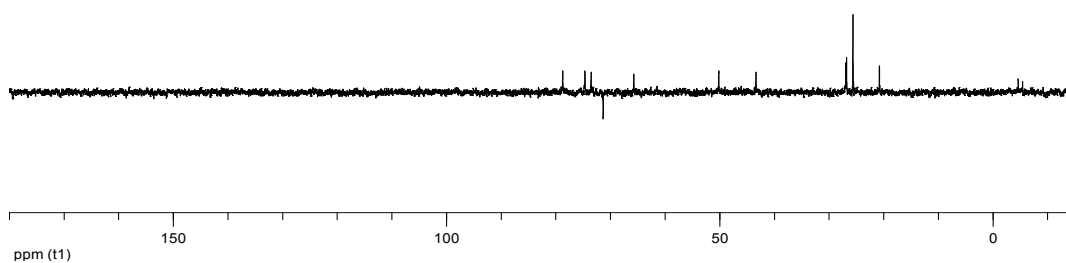
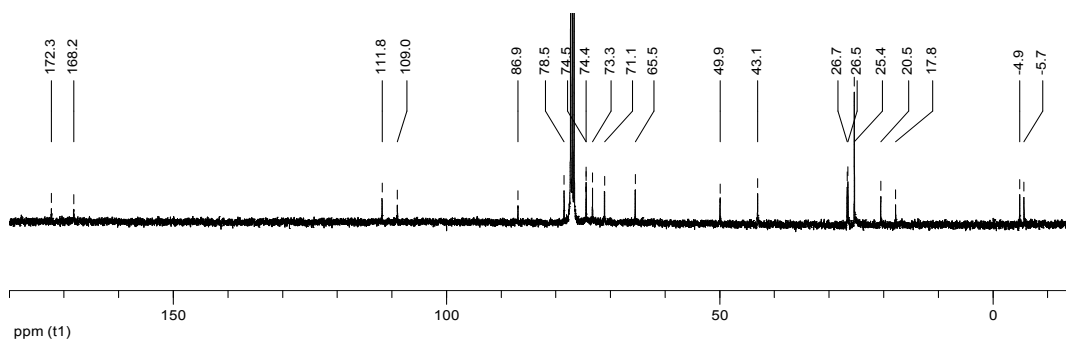
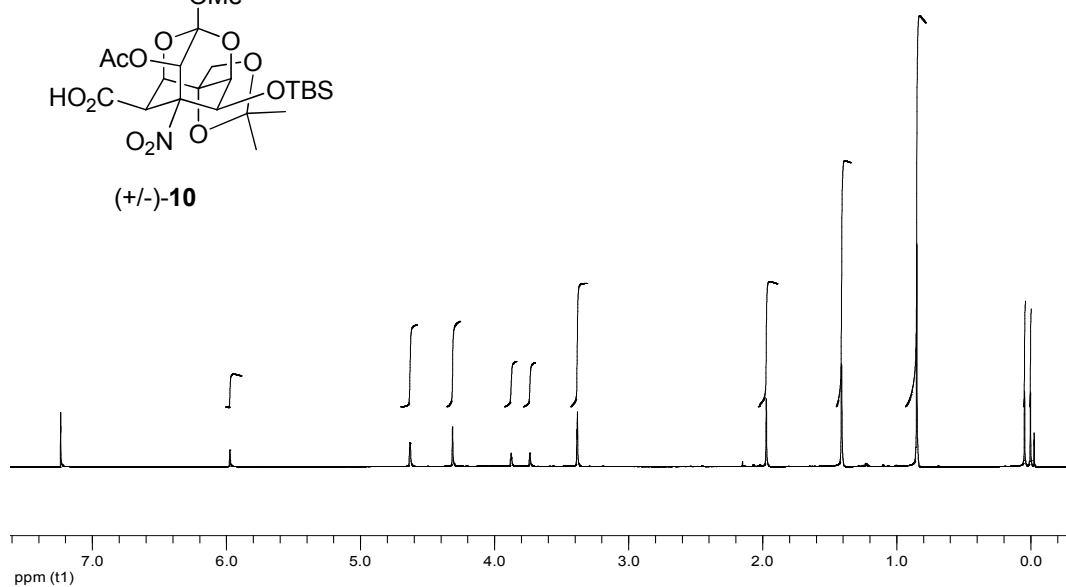


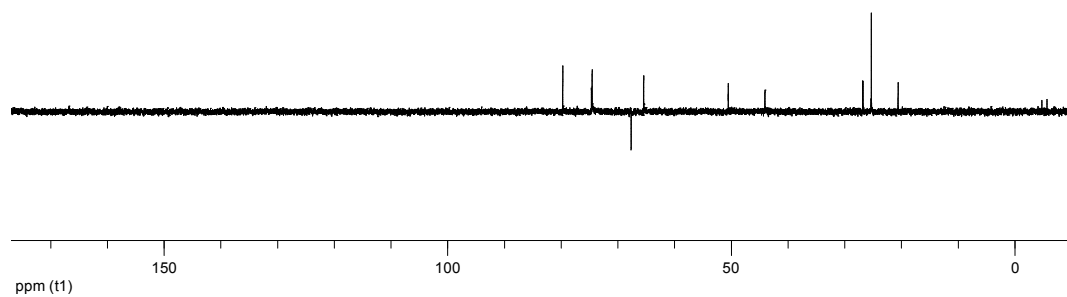
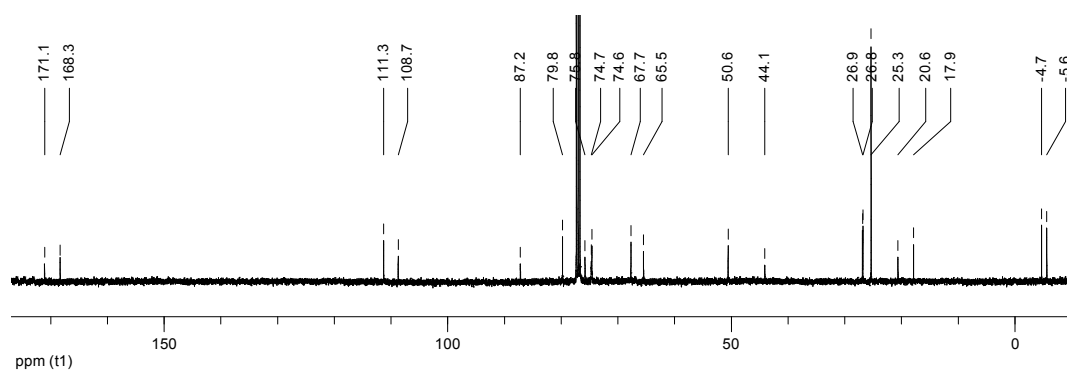
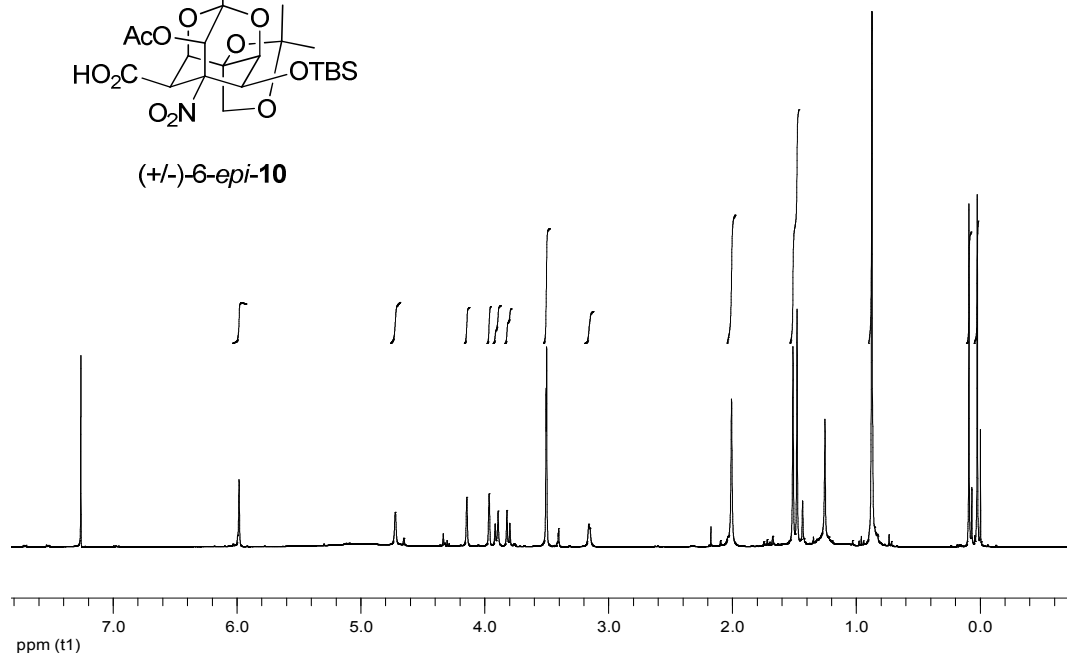
(+/-)-**6-epi-9**

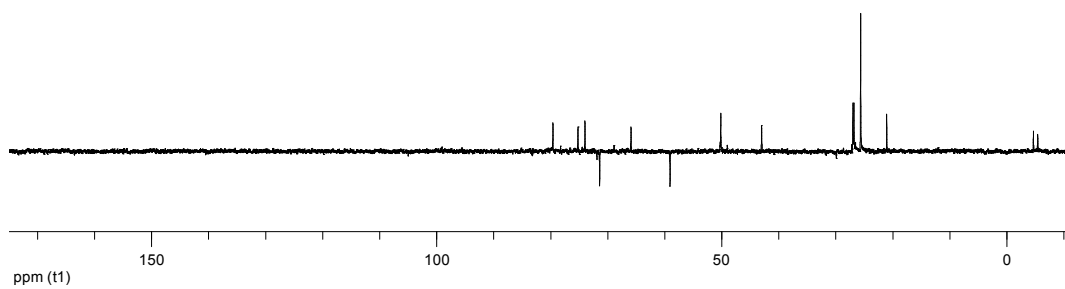
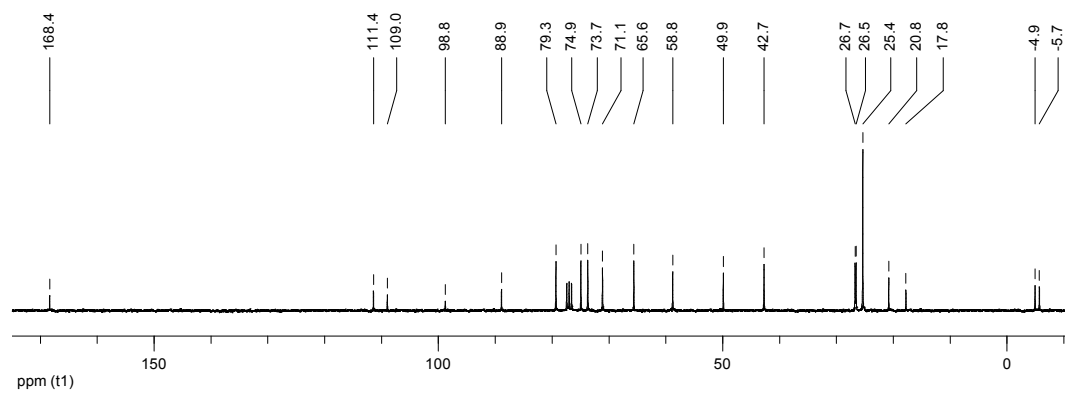
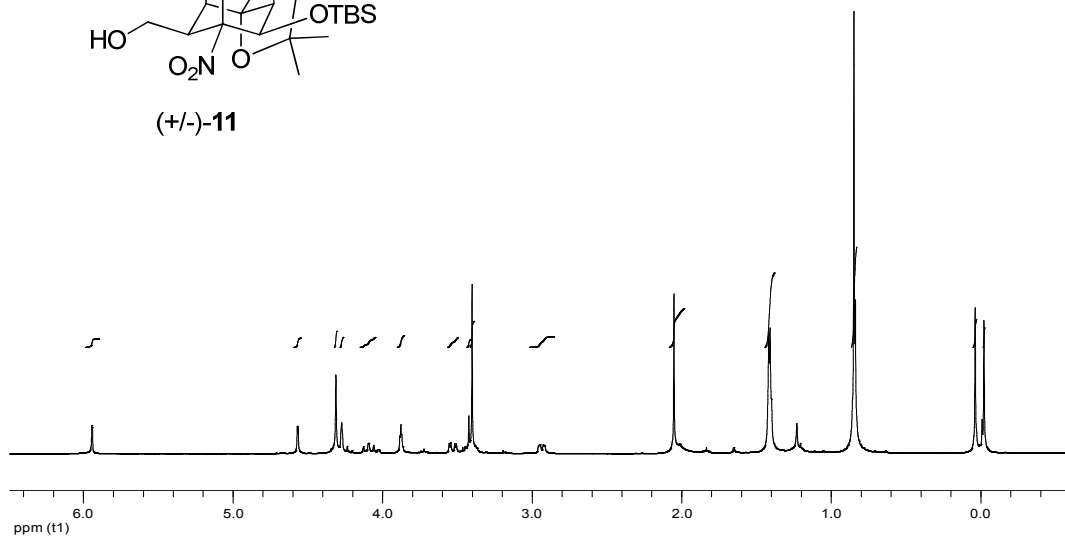


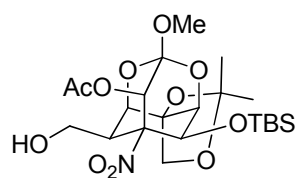


(+/-)-10

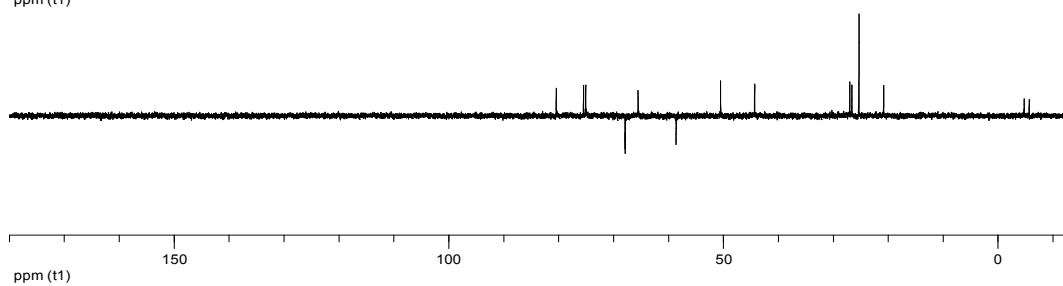
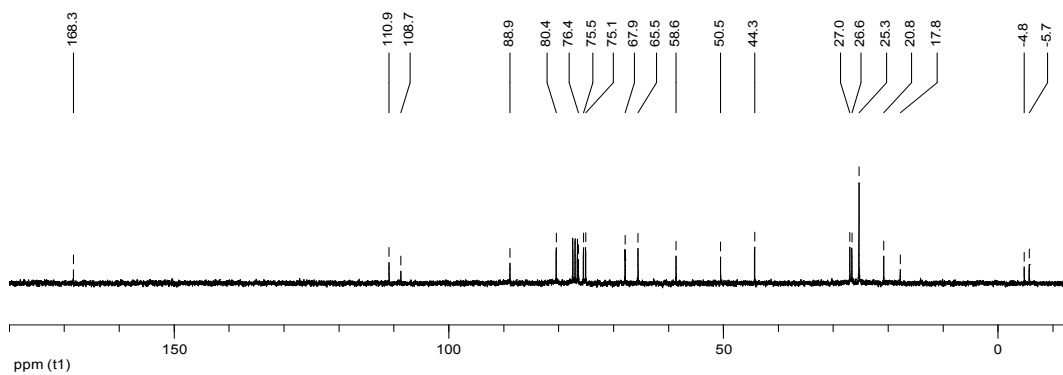
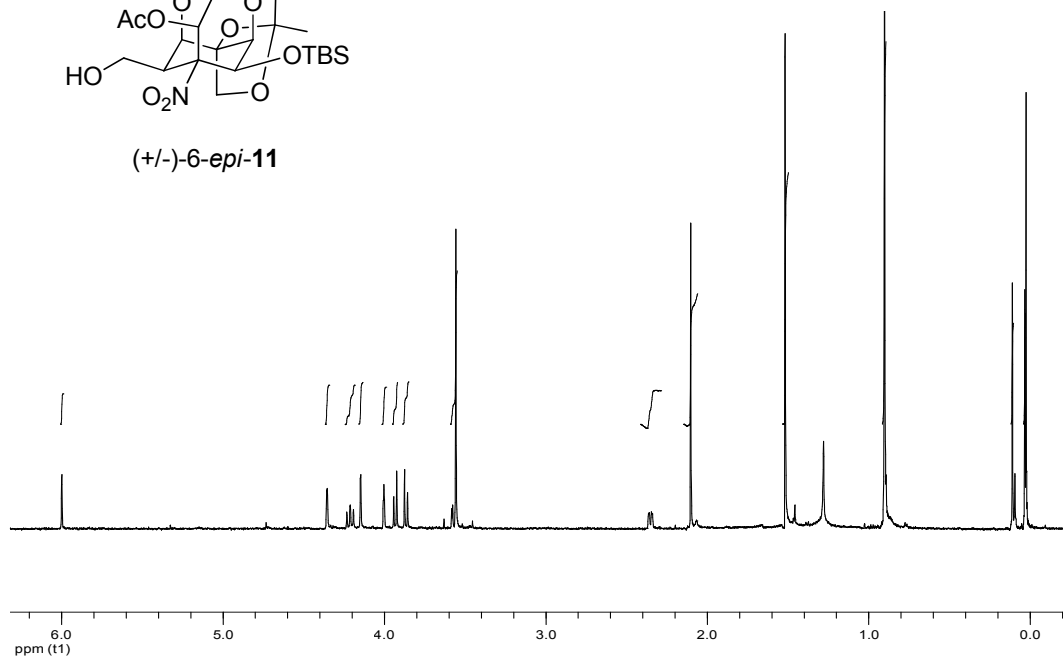


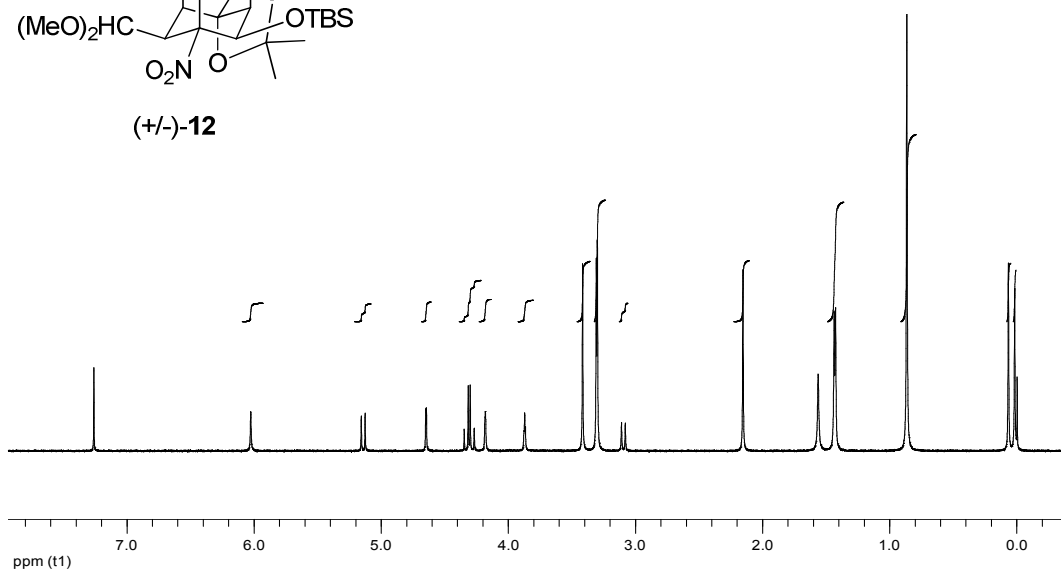


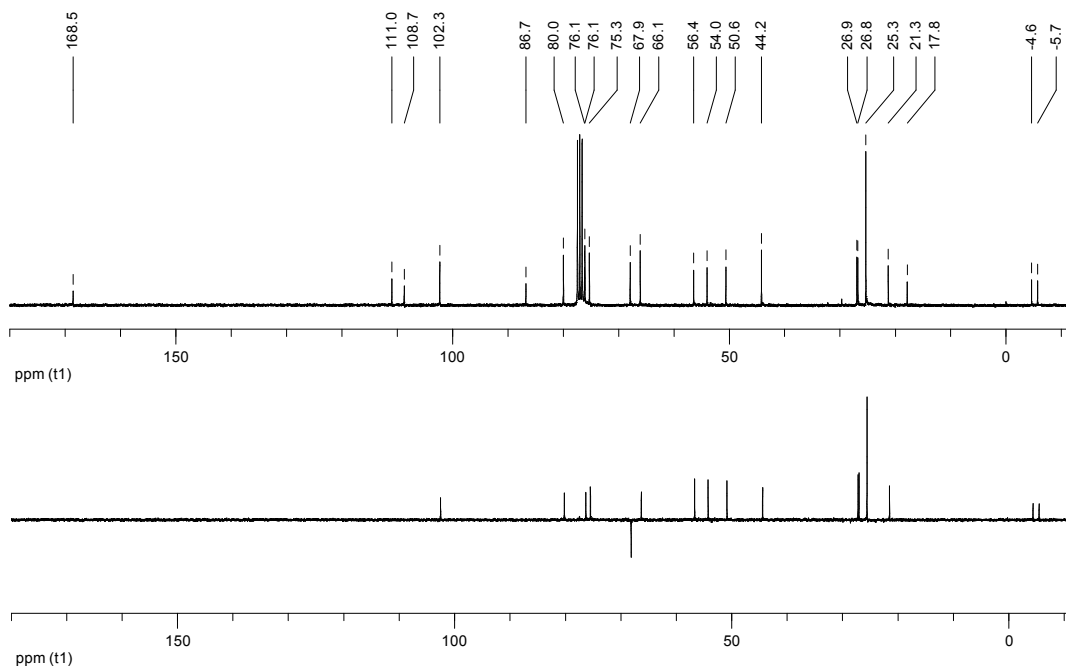
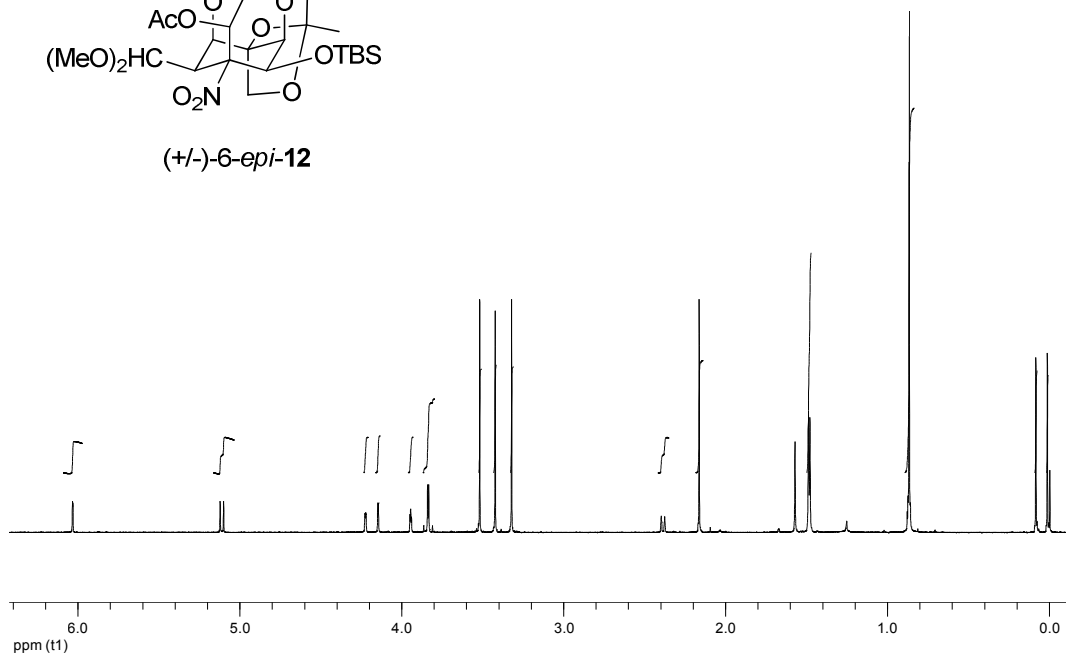
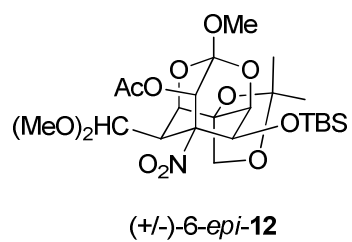


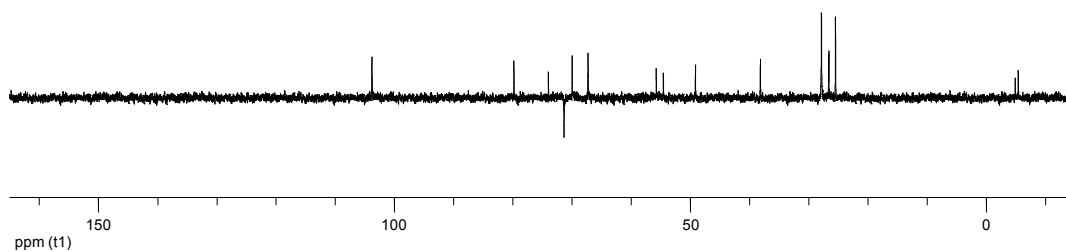
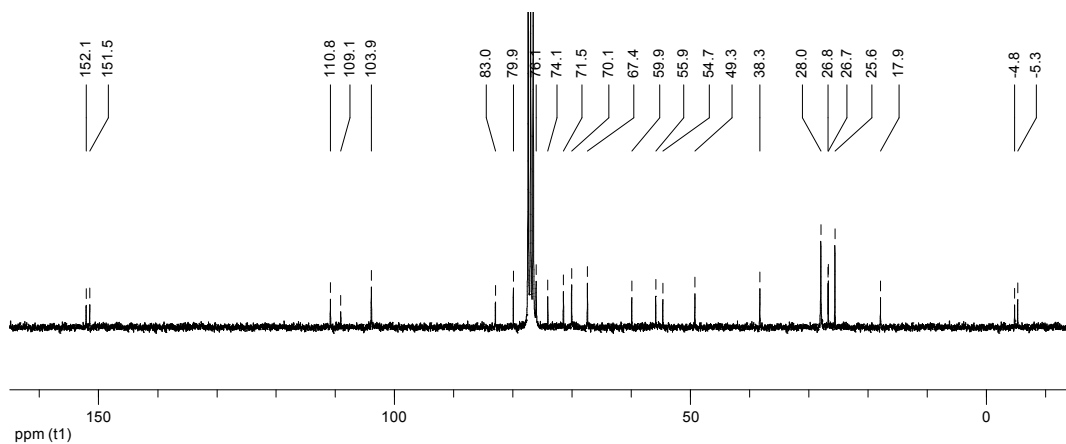
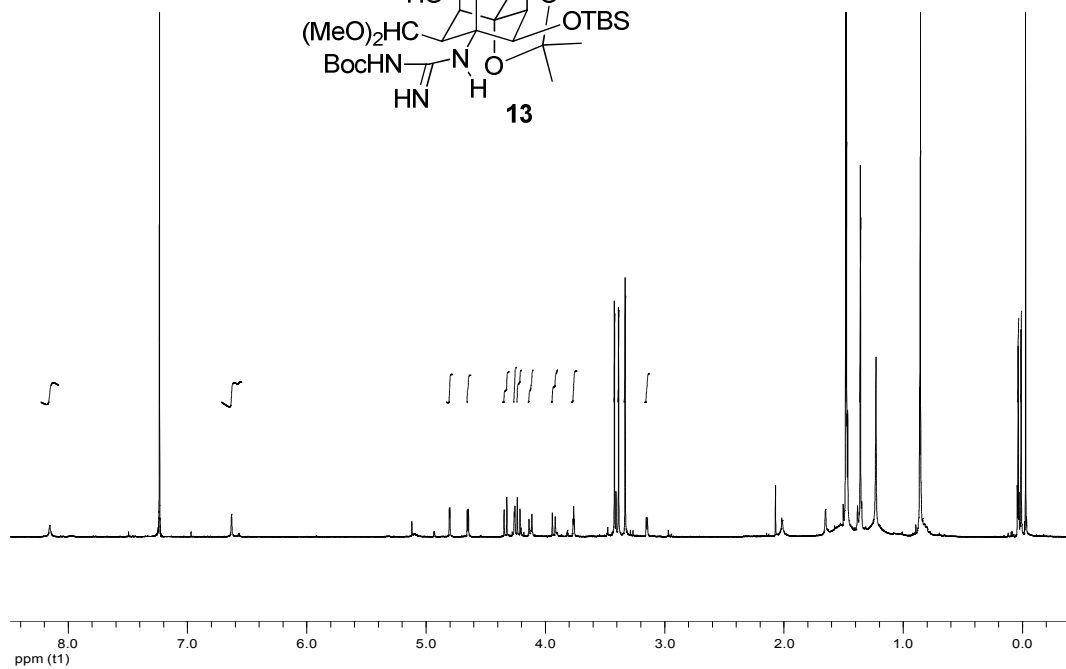
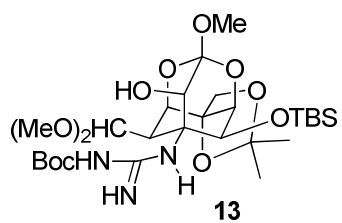


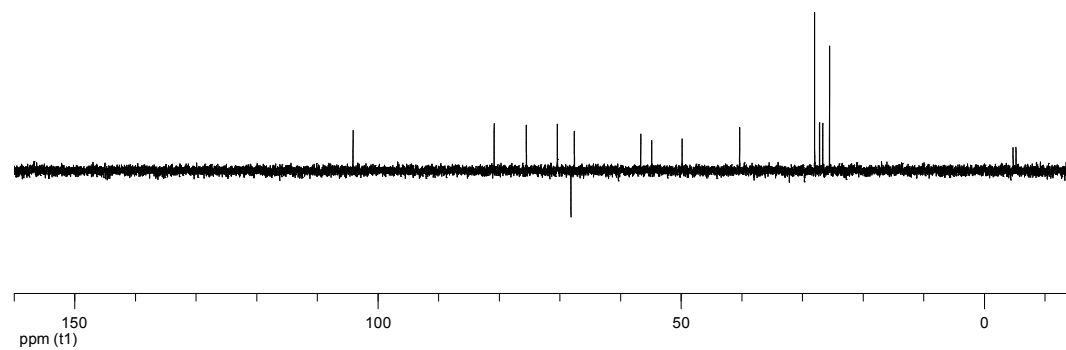
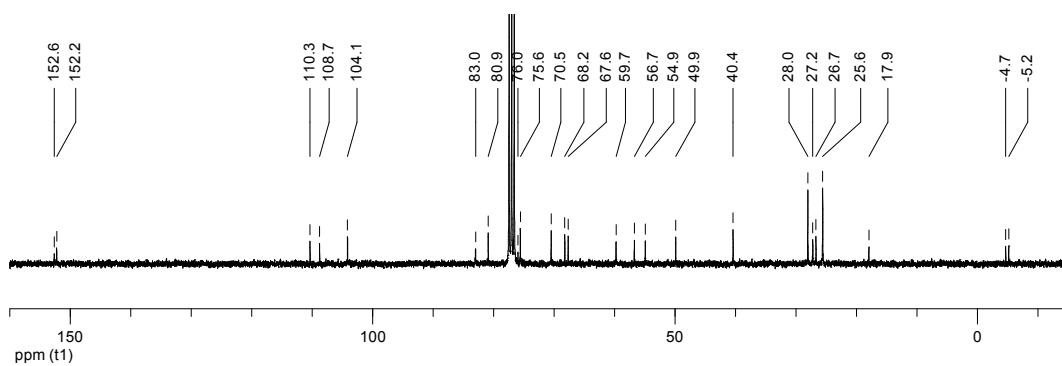
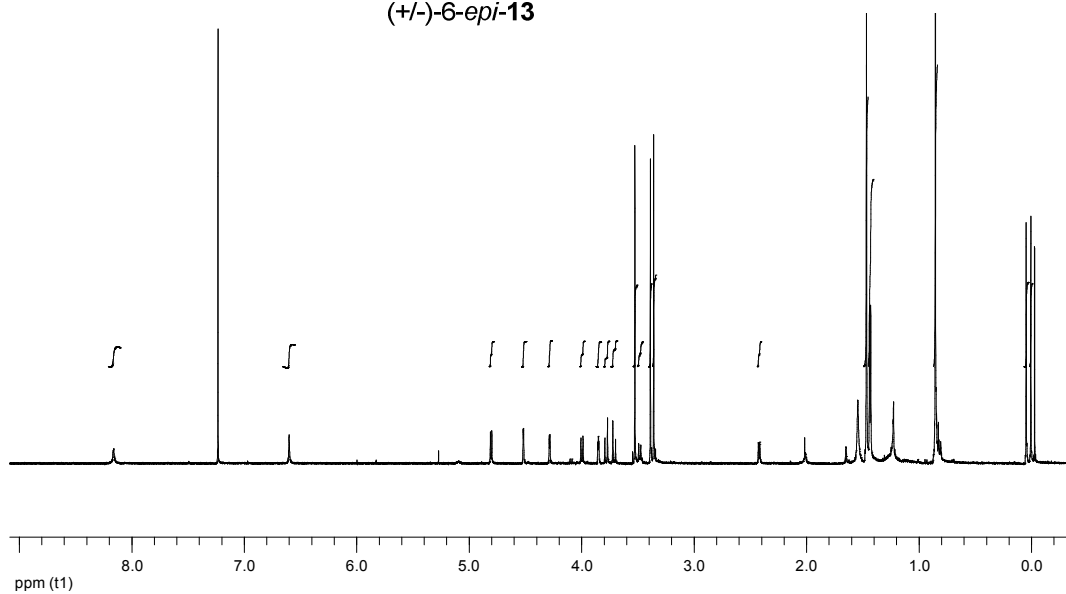
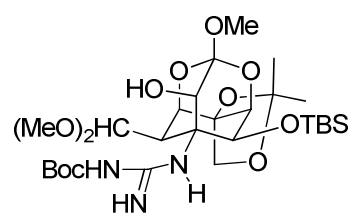
(+/-)-6-*epi*-11





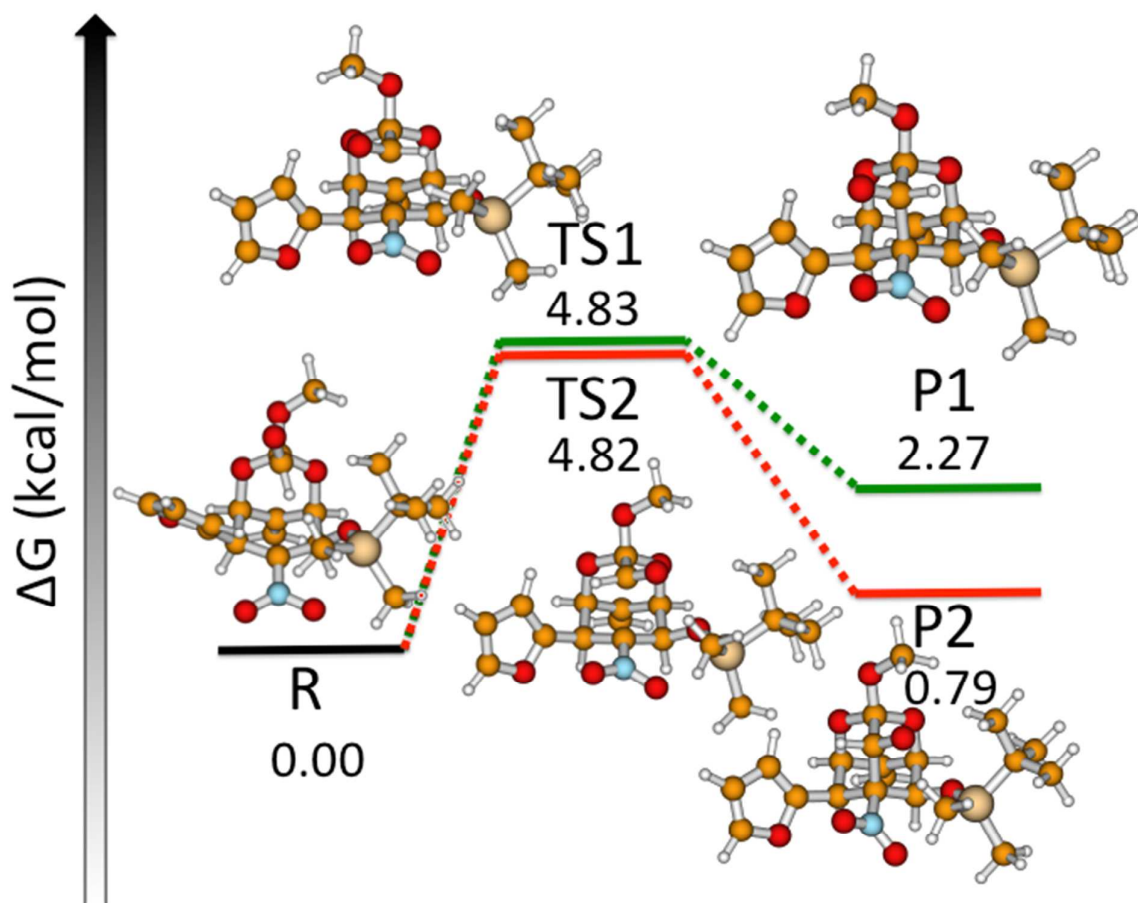




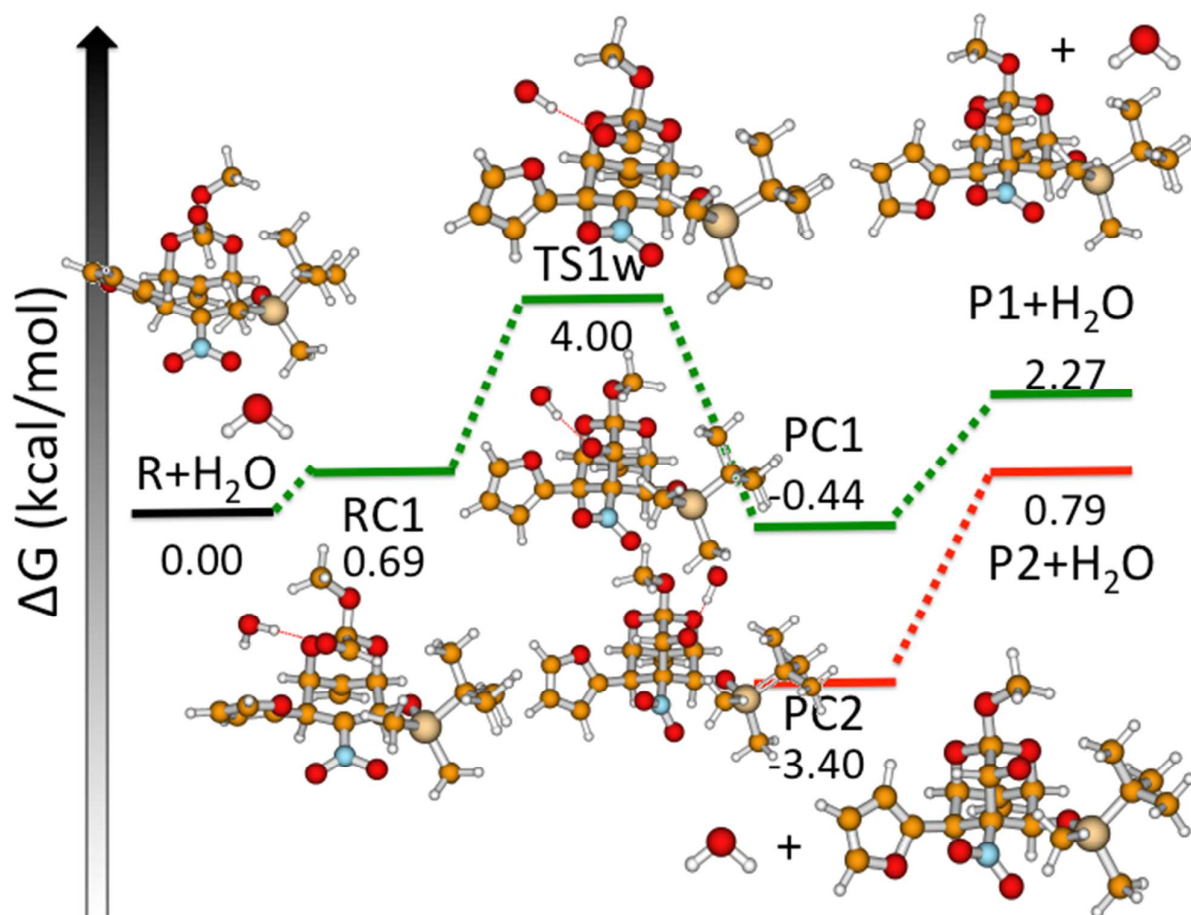


## DFT CALCULATIONS

**PROFILE S1.** Gibbs free energy profile (in kcal/mol) for the intramolecular nitroaldol reaction of **6c** (here denoted as **R**) in the gas phase at 289.15K computed at the M06-L/6-31G(d,p) level of theory. The two adducts, **P1** and **P2**, are epimers at C9. The Gibbs free energies of activation calculated for both reaction paths are roughly the same (4.8 kcal/mol).



**PROFILE S2.** Gibbs free energy profile (in kcal/mol) for the intramolecular nitroaldol reaction of **6c** in the presence of one water molecule ( $R + H_2O$ ) in the gas phase at 289.15K computed at the M06-L/6-31G(d,p) level of theory. The incorporation of a water molecule in the calculation reduces the free energy of activation for the formation of adduct P1, in line with the experimental result: the formation of  $\beta$ -hydroxy-nitroderivative **7**, where the oxygen at C9 is oriented towards the furan ring and away from the silyl substituent. In this case, neither the transition structure nor the pre-reactive complex for the formation of P2 could be located on the potential energy surface.



**Cartesian coordinates (in Å), electronic energies E (in hartree), enthalpies H (in hartree), Gibbs free energies G at 298.15K (in hartree), and frequencies (in cm<sup>-1</sup>) of the structures optimized by M06-L/6-31G(d,p) model chemistry in the gas-phase.**

Enthalpies and Gibbs free energies were computed using the rigid-rotor and harmonic-oscillator approximations.

**R**

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.614792  | -1.205015 | 0.882090  |
| C | 2.092395  | -0.956752 | 0.721764  |
| N | 0.227049  | -2.505986 | 0.849506  |
| C | 2.523232  | 0.437315  | 1.241978  |
| H | 2.627477  | -1.681101 | 1.364035  |
| C | 2.598047  | -1.173007 | -0.667096 |
| C | 1.709164  | 0.787415  | 2.444192  |
| H | 3.594196  | 0.411867  | 1.465219  |
| O | 2.429139  | 1.484994  | 0.259418  |
| C | 0.295768  | 1.028000  | 2.033580  |
| C | 2.162082  | 0.793543  | 3.695850  |
| C | -0.341513 | -0.305731 | 1.597735  |
| H | -0.306448 | 1.452345  | 2.843617  |
| O | 0.261997  | 2.060188  | 1.031322  |
| H | -0.652431 | -0.813513 | 2.529654  |
| O | -1.533470 | 0.040305  | 0.900034  |
| H | 3.199588  | 0.561715  | 3.924773  |
| H | 1.506399  | 1.010525  | 4.535824  |
| C | 1.174790  | 2.028718  | -0.041055 |
| O | 1.477718  | 3.336808  | -0.387817 |
| C | 0.353489  | 4.143113  | -0.690384 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 0.756035  | 5.105945  | -1.012145 |
| H  | -0.248455 | 3.722369  | -1.503715 |
| H  | -0.282022 | 4.293337  | 0.190152  |
| C  | 0.553335  | 1.249031  | -1.221417 |
| O  | 0.564757  | 1.654079  | -2.363717 |
| H  | 0.088810  | 0.286552  | -0.925848 |
| O  | -0.993521 | -2.776022 | 1.152779  |
| O  | 1.026322  | -3.421873 | 0.510031  |
| Si | -2.572915 | -0.906118 | -0.006093 |
| C  | -1.827477 | -1.726585 | -1.525113 |
| C  | -3.717481 | -2.041752 | 0.964691  |
| H  | -2.632325 | -2.180941 | -2.117023 |
| H  | -1.321361 | -1.003759 | -2.176753 |
| H  | -1.129211 | -2.523642 | -1.258984 |
| H  | -3.356812 | -3.071077 | 0.936435  |
| H  | -3.740650 | -1.735355 | 2.015475  |
| H  | -4.747142 | -2.007278 | 0.588119  |
| C  | -3.677788 | 0.534831  | -0.654638 |
| C  | -4.667575 | 0.040928  | -1.710033 |
| C  | -4.457794 | 1.139194  | 0.514996  |
| C  | -2.803829 | 1.630004  | -1.269371 |
| H  | -5.331431 | 0.855534  | -2.039976 |
| H  | -4.155536 | -0.338839 | -2.602626 |
| H  | -5.311487 | -0.764281 | -1.331879 |
| H  | -5.066749 | 1.995720  | 0.183889  |
| H  | -5.141703 | 0.413072  | 0.972393  |
| H  | -3.779089 | 1.496044  | 1.297708  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -3.418321 | 2.472385  | -1.626930 |
| H | -2.089082 | 2.019865  | -0.535779 |
| H | -2.227120 | 1.265967  | -2.128476 |
| C | 2.013606  | -1.531041 | -1.842476 |
| C | 3.049259  | -1.562521 | -2.820973 |
| C | 4.195010  | -1.224357 | -2.173011 |
| O | 3.942753  | -0.985338 | -0.855064 |
| H | 5.223340  | -1.105057 | -2.478254 |
| H | 2.953521  | -1.804401 | -3.870206 |
| H | 0.964827  | -1.763545 | -1.963693 |

$E = -1724.8177056$

$H = -1724.321520$

$G = -1724.412940$

#### Frequencies

3283.3 3272.3 3247.8 3237.6 3192.7 3188.8  
 3160.4 3146.2 3145.4 3142.2 3141.1 3138.9  
 3131.9 3130.2 3106.7 3103.9 3100.1 3093.0  
 3090.6 3052.2 3049.5 3048.9 3010.0 3003.6  
 3000.5 2978.2 2975.0 2963.5 1825.6 1756.7  
 1658.8 1566.3 1513.9 1506.5 1500.1 1496.9  
 1494.1 1490.3 1485.7 1481.3 1478.0 1472.1  
 1469.6 1464.1 1462.5 1450.1 1449.8 1431.1  
 1423.9 1411.6 1405.3 1384.6 1379.7 1377.6  
 1375.6 1364.2 1354.2 1331.0 1321.7 1300.5  
 1290.1 1278.9 1273.5 1262.9 1252.6 1239.2

1234.5 1232.3 1231.5 1224.8 1215.6 1209.1  
 1178.2 1175.9 1157.1 1149.7 1120.5 1113.7  
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 960.7 952.3 947.5 897.0 890.5 885.1  
 877.6 856.5 843.8 839.3 836.4 822.1  
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 666.1 648.2 646.8 630.2 610.8 605.9  
 569.8 527.3 495.0 478.1 469.7 437.2  
 411.0 402.9 393.4 389.3 383.7 366.5  
 350.5 321.0 315.7 309.2 300.6 299.1  
 295.0 290.2 285.2 267.4 258.6 253.0  
 245.3 239.3 221.7 214.1 210.3 201.1  
 188.5 178.0 166.7 161.5 149.0 130.2  
 117.8 105.9 101.6 94.6 89.0 80.9  
 74.9 71.3 57.7 50.5 46.1 38.5

## TS1

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.445057  | 0.638313  | -1.264198 |
| C | 0.592694  | -0.614268 | 0.442992  |
| C | -0.485546 | -0.020263 | 1.331603  |
| C | 2.035645  | -0.409455 | 0.928733  |
| C | 2.254048  | 1.084602  | 1.240755  |
| C | 1.245227  | 1.515181  | 2.259669  |
| C | -0.118418 | 1.438342  | 1.657579  |
| O | -0.147834 | 2.254211  | 0.481174  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| O  | 2.132060  | 1.890973  | 0.069317  |
| C  | 0.821437  | 1.920942  | -0.482551 |
| O  | 0.766504  | 3.023872  | -1.332329 |
| C  | 3.161631  | -0.921368 | 0.095180  |
| O  | 3.865080  | -1.953520 | 0.662007  |
| C  | 4.900308  | -2.235857 | -0.174228 |
| C  | 4.886121  | -1.393400 | -1.241956 |
| C  | 3.766943  | -0.531757 | -1.062103 |
| O  | -1.762114 | 0.058715  | 0.755916  |
| Si | -2.775633 | -1.026829 | -0.031548 |
| C  | -4.698376 | 0.785287  | 1.019337  |
| C  | -3.494638 | -2.362156 | 1.088191  |
| C  | -4.193775 | 0.248041  | -0.320532 |
| C  | -3.652058 | 1.415060  | -1.150010 |
| C  | -2.292068 | -1.642909 | -1.749964 |
| H  | -2.970887 | -1.267066 | -2.524187 |
| H  | -1.276572 | -1.354800 | -2.036849 |
| H  | -2.313038 | -2.736153 | -1.770367 |
| H  | -5.110437 | -0.014692 | 1.648870  |
| H  | -6.171825 | 0.341714  | -1.232279 |
| H  | -5.073696 | -0.777543 | -2.046884 |
| H  | -5.806615 | -1.225827 | -0.501251 |
| H  | -4.434209 | 2.169714  | -1.331883 |
| H  | -3.292735 | 1.080583  | -2.131908 |
| H  | -2.812050 | 1.907946  | -0.648327 |
| H  | -4.581439 | -2.451454 | 0.976996  |
| H  | -3.038826 | -3.334722 | 0.892474  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -3.292160 | -2.113839 | 2.135496  |
| H | -0.894110 | 1.855711  | 2.308174  |
| H | -0.660412 | 0.554598  | -1.298705 |
| O | 1.155986  | 0.220646  | -2.195351 |
| H | 1.496691  | 2.289923  | -3.148443 |
| H | 1.649190  | 4.046053  | -2.817431 |
| H | 2.731940  | 2.879004  | -2.012297 |
| H | 3.381802  | 0.226060  | -1.725588 |
| H | 5.586395  | -1.392432 | -2.066420 |
| H | 5.536988  | -3.050497 | 0.135155  |
| H | 2.141240  | -0.930362 | 1.897892  |
| H | 0.730160  | 2.095944  | 4.225039  |
| H | 2.538833  | 1.841650  | 3.898854  |
| H | 3.280353  | 1.236546  | 1.593773  |
| O | 1.163157  | -2.618540 | -0.532473 |
| O | -0.807664 | -2.440346 | 0.402978  |
| H | -0.544649 | -0.578402 | 2.290309  |
| H | -3.890583 | 1.267579  | 1.579526  |
| N | 0.326682  | -1.945248 | 0.090750  |
| C | -5.367256 | -0.391110 | -1.063190 |
| C | 1.714924  | 3.043550  | -2.385293 |
| C | 1.518166  | 1.834996  | 3.521955  |
| H | -5.499075 | 1.528410  | 0.874960  |

$E = -1724.8122851$

$H = -1724.317061$

$G = -1724.405244$

## Frequencies

3295.0 3280.1 3239.9 3234.0 3180.4 3175.8  
3158.5 3148.7 3145.9 3141.5 3140.1 3137.1  
3136.9 3126.3 3105.6 3093.4 3090.9 3088.9  
3085.8 3059.4 3055.6 3039.6 3004.1 2996.2  
2992.3 2977.4 2953.4 2908.6 1754.0 1655.2  
1652.2 1559.6 1528.4 1512.5 1505.1 1503.4  
1502.6 1487.5 1483.6 1482.7 1475.5 1469.0  
1462.2 1458.4 1457.0 1454.2 1449.3 1444.1  
1416.7 1399.0 1390.8 1389.5 1385.1 1371.5  
1363.5 1354.5 1331.8 1319.0 1310.2 1299.9  
1287.6 1281.5 1273.9 1261.3 1248.6 1239.2  
1229.9 1228.0 1226.2 1205.9 1202.7 1186.7  
1175.2 1172.5 1159.0 1147.3 1128.3 1120.5  
1117.5 1094.3 1067.9 1047.2 1043.0 1040.4  
1028.3 1019.5 1000.8 993.5 974.9 968.0  
961.3 955.2 954.8 934.1 905.0 882.6  
877.2 865.0 858.0 848.9 845.9 827.9  
819.6 809.4 802.8 799.8 794.6 772.4  
752.2 749.2 734.2 714.7 710.5 700.1  
667.7 655.9 644.8 638.7 617.8 612.7  
583.3 567.9 519.3 476.1 467.8 445.4  
437.9 421.2 407.8 398.7 392.9 358.3  
340.6 328.6 323.1 322.2 310.0 303.5  
302.3 295.8 286.1 275.3 269.1 257.3  
256.6 248.3 233.8 228.7 225.0 213.2

190.8 182.0 173.2 164.7 149.7 147.2  
 129.8 112.0 108.7 103.0 94.4 89.0  
 79.2 67.3 53.5 42.8 29.0 156.1i

## TS2

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 4.075140  | -0.218564 | -1.031414 |
| C | 3.396779  | -0.755487 | 0.025408  |
| O | 4.035378  | -1.885599 | 0.451664  |
| C | 5.096861  | -2.085730 | -0.373639 |
| C | 5.170047  | -1.091160 | -1.297740 |
| C | 2.227849  | -0.336874 | 0.853880  |
| C | 2.337061  | 1.164452  | 1.176716  |
| C | 1.287443  | 1.513584  | 2.183296  |
| C | -0.054724 | 1.358698  | 1.555217  |
| C | -0.324114 | -0.114081 | 1.187016  |
| C | 0.816924  | -0.631314 | 0.330598  |
| O | -0.109303 | 2.207634  | 0.400495  |
| C | 0.888223  | 1.966329  | -0.562998 |
| O | 2.188101  | 1.959691  | -0.001114 |
| C | 1.521152  | 1.820842  | 3.456669  |
| O | 0.953419  | 3.094676  | -1.387005 |
| C | -0.274790 | 3.503244  | -1.968044 |
| C | 0.634846  | 0.718855  | -1.440697 |
| H | 1.582516  | 0.271748  | -1.813134 |
| N | 0.640610  | -1.945800 | -0.107393 |
| O | 1.538090  | -2.528595 | -0.750022 |
| O | -1.578256 | -0.078537 | 0.573078  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| Si | -2.685526 | -1.203332 | 0.022188  |
| C  | -2.451470 | -1.906523 | -1.700340 |
| O  | -0.460383 | -2.526845 | 0.140159  |
| C  | -3.117821 | -2.500784 | 1.319731  |
| C  | -4.176702 | 0.010882  | -0.076036 |
| C  | -5.442131 | -0.684409 | -0.578483 |
| C  | -4.460508 | 0.598271  | 1.307346  |
| C  | -3.815804 | 1.153462  | -1.029785 |
| O  | -0.431558 | 0.583633  | -2.048380 |
| H  | 2.361661  | -0.861515 | 1.819966  |
| H  | 3.344899  | 1.388800  | 1.544463  |
| H  | -0.868490 | 1.708021  | 2.199193  |
| H  | -0.383952 | -0.687209 | 2.139636  |
| H  | 2.533451  | 1.885872  | 3.850205  |
| H  | 0.707440  | 2.010045  | 4.153177  |
| H  | -0.044558 | 4.419583  | -2.518465 |
| H  | -0.679058 | 2.746514  | -2.647855 |
| H  | -1.024690 | 3.720904  | -1.200150 |
| H  | -3.377731 | -1.867939 | -2.285496 |
| H  | -1.695208 | -1.307418 | -2.216274 |
| H  | -2.089552 | -2.935888 | -1.667805 |
| H  | -4.166419 | -2.812171 | 1.242145  |
| H  | -2.484637 | -3.384790 | 1.222070  |
| H  | -2.974615 | -2.098686 | 2.328872  |
| H  | -6.285368 | 0.022642  | -0.629287 |
| H  | -5.312079 | -1.100778 | -1.584493 |
| H  | -5.754182 | -1.506639 | 0.079389  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -5.285043 | 1.328230  | 1.266799  |
| H | -4.749112 | -0.175910 | 2.031097  |
| H | -3.577898 | 1.112599  | 1.702645  |
| H | -4.631333 | 1.893185  | -1.082524 |
| H | -2.901392 | 1.661239  | -0.705954 |
| H | -3.631145 | 0.790050  | -2.048140 |
| H | 5.687778  | -2.963806 | -0.164695 |
| H | 5.913947  | -0.990251 | -2.075850 |
| H | 3.808392  | 0.690211  | -1.549615 |

$E = -1724.812194$

$H = -1724.316881$

$G = -1724.405263$

#### Frequencies

3292.5 3285.7 3246.8 3231.9 3190.9 3188.3  
 3161.6 3158.6 3147.3 3144.8 3141.4 3141.2  
 3136.8 3120.1 3105.9 3103.8 3096.4 3096.2  
 3087.5 3056.7 3054.2 3039.2 3010.7 3005.4  
 3003.6 2954.1 2905.6 2872.7 1755.2 1689.0  
 1650.7 1562.7 1518.9 1517.0 1509.7 1504.7  
 1500.4 1487.1 1484.1 1480.4 1474.9 1468.9  
 1463.4 1457.8 1456.9 1453.2 1451.2 1447.5  
 1418.7 1410.9 1393.4 1384.3 1382.5 1373.3  
 1369.7 1357.5 1340.7 1327.4 1301.4 1299.9  
 1291.0 1285.3 1276.5 1265.9 1253.5 1239.7  
 1229.6 1223.1 1221.7 1213.2 1198.6 1193.9

1182.0 1177.9 1164.7 1151.8 1132.3 1124.6  
 1111.7 1090.9 1066.2 1055.9 1044.7 1035.9  
 1026.7 1023.6 998.6 992.7 962.2 960.4  
 960.1 953.7 941.2 935.0 905.4 889.0  
 883.2 873.3 852.9 843.5 843.0 832.2  
 822.1 805.0 803.3 798.8 792.9 772.8  
 760.0 753.0 737.8 717.6 714.6 703.6  
 680.8 664.5 653.7 634.5 613.3 608.6  
 578.0 570.1 508.7 474.8 452.4 445.8  
 435.4 425.8 397.1 393.0 383.8 360.0  
 342.9 329.0 321.6 315.9 310.8 305.0  
 294.8 288.1 284.0 273.6 266.6 261.7  
 254.2 243.9 232.7 221.6 217.0 196.1  
 186.2 170.6 157.8 154.4 142.1 136.9  
 124.9 116.1 108.4 104.7 95.0 90.4  
 80.5 71.6 55.6 47.4 35.0 68.2i

# **P1**

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 2.158781  | 1.991038  | 0.110322  |
| C | 2.208430  | 1.149333  | 1.255866  |
| C | 1.119113  | 1.541871  | 2.208185  |
| C | -0.194761 | 1.458632  | 1.500200  |
| O | -0.151514 | 2.296213  | 0.346314  |
| C | 0.886499  | 1.926654  | -0.548341 |
| C | 2.005853  | -0.335031 | 0.882291  |
| C | 0.634801  | -0.465773 | 0.164227  |
| C | -0.500386 | 0.009036  | 1.084259  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 3.217000  | -0.900297 | 0.230188  |
| O  | 3.757592  | -1.964897 | 0.909075  |
| C  | 4.894720  | -2.317248 | 0.251348  |
| C  | 5.099273  | -1.490214 | -0.810448 |
| C  | 4.016592  | -0.565346 | -0.820699 |
| N  | 0.431102  | -1.850151 | -0.227320 |
| O  | -0.638143 | -2.426774 | 0.119504  |
| O  | -1.762920 | 0.070607  | 0.486349  |
| Si | -2.894266 | -1.025854 | -0.068529 |
| C  | -3.340968 | -2.352095 | 1.189371  |
| C  | 1.289622  | 1.856449  | 3.489669  |
| O  | 0.847795  | 2.956945  | -1.464279 |
| C  | 1.851398  | 2.951483  | -2.468185 |
| C  | 0.659726  | 0.521439  | -1.205381 |
| O  | 1.529169  | 0.182773  | -2.093300 |
| O  | 1.287500  | -2.393948 | -0.925646 |
| C  | -4.370234 | 0.194271  | -0.174365 |
| C  | -4.681806 | 0.744507  | 1.218733  |
| C  | -2.584986 | -1.683188 | -1.801333 |
| C  | -3.981558 | 1.359864  | -1.088805 |
| C  | -5.622920 | -0.487127 | -0.726016 |
| H  | -0.423303 | 0.531074  | -1.503725 |
| H  | 1.915764  | -0.879830 | 1.836015  |
| H  | 3.203970  | 1.286067  | 1.693380  |
| H  | -1.025944 | 1.832070  | 2.108607  |
| H  | -0.528652 | -0.630646 | 1.987644  |
| H  | 2.278450  | 1.880638  | 3.943320  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.446118  | 2.099904  | 4.132134  |
| H | 1.787483  | 3.936596  | -2.942644 |
| H | 2.848327  | 2.824717  | -2.032231 |
| H | 1.689861  | 2.151919  | -3.195503 |
| H | -3.497395 | -1.677702 | -2.408387 |
| H | -1.845554 | -1.053415 | -2.308416 |
| H | -2.175504 | -2.694843 | -1.781312 |
| H | -4.393247 | -2.647604 | 1.105311  |
| H | -2.718575 | -3.241000 | 1.072571  |
| H | -3.192870 | -1.974141 | 2.206942  |
| H | -6.462317 | 0.222727  | -0.785072 |
| H | -5.465803 | -0.882552 | -1.736826 |
| H | -5.954330 | -1.321933 | -0.094465 |
| H | -5.499765 | 1.480623  | 1.178897  |
| H | -4.992341 | -0.047712 | 1.912736  |
| H | -3.806555 | 1.242393  | 1.649652  |
| H | -4.790230 | 2.105578  | -1.139471 |
| H | -3.074716 | 1.859876  | -0.731338 |
| H | -3.786253 | 1.022858  | -2.114615 |
| H | 5.426438  | -3.162268 | 0.661638  |
| H | 5.920792  | -1.543743 | -1.512330 |
| H | 3.759635  | 0.194410  | -1.543170 |

$E = -1724.8153485$

$H = -1724.319030$

$G = -1724.409321$

## Frequencies

3307.8 3283.1 3240.0 3232.7 3195.8 3188.2  
3153.2 3150.6 3147.6 3146.9 3142.3 3141.3  
3125.2 3122.7 3104.8 3100.1 3098.2 3091.8  
3060.0 3059.7 3054.5 3031.4 3028.7 3017.2  
3013.8 3010.0 2937.4 2769.7 1758.0 1654.8  
1580.7 1555.1 1512.1 1505.8 1503.1 1501.0  
1486.3 1482.3 1480.1 1473.0 1470.6 1465.0  
1460.5 1458.5 1454.4 1451.6 1448.3 1439.2  
1414.9 1391.2 1389.1 1380.3 1376.6 1368.5  
1356.8 1353.7 1338.8 1324.0 1296.0 1291.2  
1287.2 1286.0 1278.8 1270.6 1259.8 1246.9  
1242.3 1231.8 1228.6 1222.5 1211.2 1202.5  
1184.4 1179.0 1170.4 1151.2 1126.9 1118.4  
1107.1 1095.7 1070.8 1058.0 1037.9 1035.2  
1027.9 1024.1 1009.3 990.3 975.4 964.3  
959.4 954.3 951.9 941.2 915.1 897.5  
882.8 876.5 862.5 857.5 844.3 841.9  
829.5 812.6 800.5 791.2 785.9 773.7  
755.6 744.3 736.1 707.8 704.4 693.1  
671.1 668.1 658.2 654.2 628.4 612.6  
610.6 575.0 537.6 501.4 469.1 451.9  
438.5 428.7 404.0 393.5 386.4 361.3  
352.2 344.3 334.7 328.2 317.0 309.8  
300.5 293.5 291.7 283.9 274.4 266.7  
256.9 243.6 238.1 230.6 224.3 221.6  
186.5 177.7 171.4 164.0 157.0 141.7

128.9 116.3 104.8 101.6 96.9 93.8

78.0 68.7 65.8 45.0 41.3 22.2

**P2**

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 0.568523  | 0.408097  | -1.104583 |
| C  | 0.825829  | 1.876869  | -0.637524 |
| O  | 2.155296  | 2.061243  | -0.121699 |
| C  | 2.362058  | 1.330960  | 1.080692  |
| C  | 2.218906  | -0.184112 | 0.825362  |
| C  | 0.787190  | -0.422976 | 0.256407  |
| O  | -0.133398 | 2.283890  | 0.338143  |
| C  | -0.020815 | 1.526736  | 1.544826  |
| C  | 1.349411  | 1.745320  | 2.105709  |
| C  | -0.244075 | 0.017938  | 1.304730  |
| C  | 1.634297  | 2.187833  | 3.327551  |
| O  | 0.805965  | 2.798845  | -1.659915 |
| C  | -0.430919 | 2.970249  | -2.339594 |
| C  | 3.341259  | -0.690052 | -0.005380 |
| O  | 3.876182  | -1.889209 | 0.381154  |
| C  | 4.889503  | -2.169397 | -0.481664 |
| C  | 5.025796  | -1.169064 | -1.393351 |
| C  | 4.025353  | -0.204878 | -1.081557 |
| N  | 0.683321  | -1.896281 | 0.013472  |
| O  | 1.286518  | -2.359509 | -0.952417 |
| O  | -1.579689 | -0.141231 | 0.984429  |
| Si | -2.673594 | -1.156009 | 0.241592  |
| C  | -2.202201 | -2.258554 | -1.192468 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 1.468639  | 0.141276  | -1.719393 |
| O | 0.015546  | -2.578122 | 0.809241  |
| C | -3.368605 | -2.245673 | 1.618999  |
| C | -4.038500 | 0.063858  | -0.307763 |
| C | -5.352666 | -0.690323 | -0.527447 |
| C | -4.254556 | 1.131640  | 0.766268  |
| C | -3.625014 | 0.758115  | -1.607029 |
| O | -0.596526 | 0.238573  | -1.676573 |
| H | 2.281720  | -0.698381 | 1.798494  |
| H | 3.386140  | 1.556171  | 1.400884  |
| H | -0.813437 | 1.889255  | 2.207958  |
| H | -0.018360 | -0.507004 | 2.253645  |
| H | 2.662020  | 2.305886  | 3.665587  |
| H | 0.849827  | 2.447915  | 4.034976  |
| H | -0.301764 | 3.875043  | -2.944042 |
| H | -0.670443 | 2.104187  | -2.960641 |
| H | -1.252583 | 3.123780  | -1.631380 |
| H | -3.110455 | -2.502910 | -1.759044 |
| H | -1.506361 | -1.720335 | -1.844196 |
| H | -1.742419 | -3.192758 | -0.859911 |
| H | -4.118228 | -2.948779 | 1.238207  |
| H | -2.561568 | -2.835839 | 2.065067  |
| H | -3.834702 | -1.660646 | 2.419711  |
| H | -6.132110 | -0.008825 | -0.901935 |
| H | -5.247596 | -1.494390 | -1.267657 |
| H | -5.732542 | -1.141715 | 0.398029  |
| H | -5.076340 | 1.806695  | 0.479729  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.514418 | 0.696079  | 1.740528  |
| H | -3.352513 | 1.736457  | 0.901986  |
| H | -4.370123 | 1.519773  | -1.889511 |
| H | -2.635928 | 1.217400  | -1.508057 |
| H | -3.545606 | 0.045909  | -2.437181 |
| H | 5.399866  | -3.103935 | -0.308236 |
| H | 5.748892  | -1.127591 | -2.195967 |
| H | 3.803689  | 0.724012  | -1.586249 |

$$E = -1724.8198256$$

$$H = -1724.323190$$

$$G = -1724.411674$$

#### Frequencies

3288.1 3278.9 3250.6 3233.4 3179.9 3168.1  
 3158.5 3153.3 3142.4 3142.1 3140.2 3136.7  
 3134.5 3117.6 3103.0 3102.8 3098.6 3087.1  
 3085.8 3045.5 3035.4 3033.5 3021.7 3014.7  
 3004.7 3000.8 2947.8 2789.0 1757.8 1653.8  
 1625.0 1560.6 1512.7 1507.7 1504.0 1499.2  
 1499.0 1482.7 1477.8 1475.5 1466.9 1464.1  
 1455.1 1452.6 1452.3 1445.2 1443.9 1427.3  
 1419.5 1397.9 1394.3 1386.5 1378.2 1373.9  
 1364.4 1350.6 1339.4 1320.3 1303.1 1286.8  
 1284.2 1280.2 1275.5 1264.8 1262.4 1258.7  
 1247.9 1228.6 1225.0 1219.7 1216.1 1205.7  
 1200.1 1177.9 1173.2 1136.1 1125.1 1117.3

1100.4 1079.7 1072.3 1067.1 1051.2 1046.3  
 1028.8 1008.8 998.9 983.8 964.7 964.2  
 958.8 956.3 955.5 944.9 925.2 903.1  
 886.9 877.9 872.3 861.5 849.1 847.3  
 836.8 818.9 804.2 796.6 778.1 774.0  
 762.5 755.1 737.2 724.2 707.6 700.2  
 679.7 671.8 666.5 658.2 616.6 614.1  
 582.9 574.1 554.6 535.1 467.8 456.1  
 439.6 433.1 412.6 393.9 376.1 370.4  
 355.2 339.9 337.0 331.1 322.0 309.8  
 304.9 297.4 291.9 283.9 276.6 271.8  
 263.1 256.0 239.6 228.7 223.0 200.4  
 193.2 187.8 181.3 175.5 162.6 147.5  
 137.4 133.5 114.2 107.4 95.2 91.5  
 80.1 77.6 71.1 55.3 50.4 37.2

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

|   |          |           |           |
|---|----------|-----------|-----------|
| O | 0.000000 | 0.000000  | 0.118711  |
| H | 0.000000 | 0.754434  | -0.474846 |
| H | 0.000000 | -0.754434 | -0.474846 |

$$E = -76.4110228$$

$$H = -76.385395$$

$$G = -76.406815$$

## Frequencies

4010.7 3877.4 1702.5

**RC1**

|    |           |           |           |
|----|-----------|-----------|-----------|
| O  | 2.152160  | 1.507203  | 0.545304  |
| C  | 2.129649  | 0.544367  | 1.607838  |
| C  | 1.154751  | 0.950276  | 2.666774  |
| C  | -0.186302 | 1.158473  | 2.048067  |
| O  | -0.070737 | 2.156466  | 1.026489  |
| C  | 0.913820  | 1.981664  | 0.059194  |
| C  | 1.765438  | -0.882208 | 1.143903  |
| C  | 0.296166  | -0.995491 | 0.814818  |
| C  | -0.749057 | -0.174862 | 1.530379  |
| C  | 2.701396  | -1.370432 | 0.082994  |
| O  | 2.255325  | -1.490142 | -1.192273 |
| C  | 3.272045  | -1.998545 | -1.934773 |
| C  | 4.372433  | -2.195708 | -1.162200 |
| C  | 4.005282  | -1.777131 | 0.151418  |
| N  | -0.114229 | -2.283637 | 0.605676  |
| O  | 0.700695  | -3.220525 | 0.433794  |
| O  | -1.899250 | 0.153666  | 0.784757  |
| Si | -2.849917 | -0.829183 | -0.206851 |
| C  | -4.047341 | 0.599272  | -0.745162 |
| C  | -3.266561 | 1.758412  | -1.366311 |
| C  | 1.424047  | 1.006744  | 3.968619  |
| C  | 0.403588  | 1.149505  | -1.132599 |
| O  | 1.101444  | 0.892816  | -2.098862 |
| O  | 1.095285  | 3.295267  | -0.385160 |
| C  | 2.094507  | 3.513834  | -1.372086 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -1.380671 | -2.523502 | 0.619749  |
| C | -2.037307 | -1.404635 | -1.809455 |
| C | -3.993269 | -2.055415 | 0.661678  |
| C | -5.059648 | 0.088030  | -1.771154 |
| C | -4.803879 | 1.132210  | 0.472682  |
| O | 4.038593  | 1.031979  | -2.000658 |
| H | -2.331035 | -0.794637 | -2.671722 |
| H | -0.946004 | -1.364144 | -1.733256 |
| H | -2.297798 | -2.446095 | -2.019433 |
| H | -5.418417 | 0.355946  | 0.946320  |
| H | -5.755907 | 0.887172  | -2.071708 |
| H | -4.571418 | -0.272838 | -2.685331 |
| H | -5.668096 | -0.736951 | -1.378287 |
| H | -3.945217 | 2.561400  | -1.698128 |
| H | -2.695142 | 1.440258  | -2.248440 |
| H | -2.559135 | 2.192346  | -0.650911 |
| H | -5.049531 | -1.896453 | 0.418075  |
| H | -3.722234 | -3.086291 | 0.425984  |
| H | -3.880969 | -1.941478 | 1.744907  |
| H | -0.908653 | 1.589819  | 2.747819  |
| H | -0.681826 | 0.944214  | -1.110168 |
| H | 1.739561  | 3.248072  | -2.375976 |
| H | 2.300477  | 4.586701  | -1.341507 |
| H | 3.009973  | 2.950997  | -1.171003 |
| H | 3.058040  | -2.126143 | -2.983535 |
| H | 5.328941  | -2.575886 | -1.491735 |
| H | 1.988244  | -1.518255 | 2.023889  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.653153  | 1.245428  | 4.697517  |
| H | 2.421775  | 0.805625  | 4.352822  |
| H | 3.159524  | 0.541497  | 1.984342  |
| H | -1.076912 | -0.737200 | 2.430831  |
| H | -4.108321 | 1.513120  | 1.228502  |
| H | -5.481332 | 1.955437  | 0.192871  |
| H | 4.610905  | -1.809843 | 1.047402  |
| H | 4.170372  | 0.507776  | -1.202166 |
| H | 3.074123  | 0.978463  | -2.104656 |

$E = -1801.2460087$

$H = -1800.721800$

$G = -1800.818651$

#### Frequencies

3868.1 3714.4 3295.4 3257.8 3242.3 3240.3  
 3179.6 3172.3 3166.7 3155.6 3150.2 3145.6  
 3134.0 3130.0 3126.9 3125.1 3093.4 3092.4  
 3083.9 3083.4 3081.6 3058.5 3052.9 3049.2  
 3040.3 3010.3 3003.6 2997.4 2929.2 2889.4  
 1780.2 1757.4 1718.4 1635.5 1556.3 1512.6  
 1508.8 1502.9 1501.4 1498.8 1486.5 1485.1  
 1482.2 1478.8 1472.5 1471.2 1462.2 1457.2  
 1451.4 1449.5 1440.2 1418.3 1410.5 1399.3  
 1384.8 1382.6 1379.7 1370.4 1357.9 1342.3  
 1323.3 1321.2 1304.0 1292.7 1291.1 1285.1  
 1279.1 1263.5 1234.2 1232.6 1230.4 1229.2

1223.6 1222.0 1196.3 1192.2 1174.2 1170.8  
 1159.2 1122.3 1118.3 1105.3 1091.9 1071.1  
 1059.5 1038.5 1037.4 1036.4 1024.7 1000.6  
 989.0 962.6 962.0 956.5 948.9 934.3  
 927.0 897.9 884.7 867.0 853.5 845.0  
 842.9 825.4 821.8 818.7 806.1 795.1  
 787.8 776.2 769.6 760.4 745.1 728.1  
 717.9 710.4 697.3 674.6 653.2 644.2  
 639.7 626.2 621.2 608.2 562.7 539.1  
 497.4 483.1 472.0 448.0 437.1 412.8  
 407.1 395.1 388.9 369.9 342.2 339.0  
 333.8 324.3 321.0 308.1 300.5 291.9  
 284.5 279.5 275.2 266.7 255.8 252.2  
 246.3 242.7 233.8 223.2 218.3 205.4  
 198.9 186.0 174.3 169.4 150.1 148.7  
 143.5 133.0 120.4 114.1 106.9 98.5  
 92.7 87.1 81.4 75.0 68.0 56.3  
 52.9 43.3 34.7

# **TS1w**

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 2.026618  | 1.701370  | 0.584438  |
| C | 2.038268  | 0.750108  | 1.648717  |
| C | 0.967248  | 1.071514  | 2.646035  |
| C | -0.350598 | 1.095023  | 1.947555  |
| O | -0.279855 | 2.076722  | 0.909826  |
| C | 0.753653  | 1.900642  | -0.028344 |
| C | 1.780274  | -0.702514 | 1.174048  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 0.411724  | -0.758635 | 0.486041  |
| C  | -0.723512 | -0.284206 | 1.369015  |
| C  | 2.958582  | -1.289473 | 0.491478  |
| O  | 3.427215  | -0.676199 | -0.622083 |
| C  | 4.520043  | -1.365953 | -1.044822 |
| C  | 4.776085  | -2.398079 | -0.196075 |
| C  | 3.768274  | -2.341859 | 0.811042  |
| N  | 0.149358  | -1.981310 | -0.149343 |
| O  | 0.999702  | -2.503294 | -0.888834 |
| O  | -1.943700 | -0.062799 | 0.714712  |
| Si | -2.962045 | -0.964977 | -0.266056 |
| C  | -4.321318 | 0.387681  | -0.432901 |
| C  | -3.700556 | 1.642819  | -1.051637 |
| C  | 1.157960  | 1.232004  | 3.952992  |
| C  | 0.415374  | 0.803519  | -1.060837 |
| O  | 1.172146  | 0.524844  | -2.005433 |
| O  | 0.768432  | 3.154193  | -0.629279 |
| C  | 1.691187  | 3.360190  | -1.684587 |
| O  | -0.994417 | -2.516473 | 0.018252  |
| C  | -2.407104 | -1.349189 | -2.027186 |
| C  | -3.759464 | -2.426012 | 0.616299  |
| C  | -5.469759 | -0.095251 | -1.318898 |
| C  | -4.879259 | 0.741876  | 0.946060  |
| O  | 3.914070  | 1.246373  | -2.561382 |
| H  | -3.012017 | -0.817954 | -2.771073 |
| H  | -1.360206 | -1.092340 | -2.211016 |
| H  | -2.489235 | -2.423237 | -2.216757 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -5.342565 | -0.126425 | 1.433121  |
| H | -6.242728 | 0.682464  | -1.420929 |
| H | -5.132357 | -0.346757 | -2.331810 |
| H | -5.963879 | -0.985358 | -0.907751 |
| H | -4.449278 | 2.443904  | -1.157595 |
| H | -3.296982 | 1.444494  | -2.052932 |
| H | -2.876688 | 2.024345  | -0.438405 |
| H | -4.829471 | -2.502545 | 0.390180  |
| H | -3.275789 | -3.367315 | 0.348378  |
| H | -3.664627 | -2.304429 | 1.700644  |
| H | -1.167529 | 1.431055  | 2.594980  |
| H | -0.683200 | 0.714475  | -1.167295 |
| H | 1.409558  | 2.818798  | -2.593583 |
| H | 1.673611  | 4.436410  | -1.876429 |
| H | 2.705591  | 3.055898  | -1.416060 |
| H | 4.964115  | -0.975502 | -1.947885 |
| H | 5.579698  | -3.116050 | -0.283134 |
| H | 1.704429  | -1.285721 | 2.113037  |
| H | 0.326345  | 1.412045  | 4.630517  |
| H | 2.152230  | 1.185930  | 4.392379  |
| H | 3.039612  | 0.818997  | 2.089966  |
| H | -0.877062 | -0.985697 | 2.217577  |
| H | -4.088283 | 1.112282  | 1.606829  |
| H | -5.651190 | 1.524505  | 0.874318  |
| H | 3.628173  | -3.016723 | 1.644519  |
| H | 4.156758  | 1.308588  | -1.632487 |
| H | 3.001795  | 0.907590  | -2.466815 |

$$E = -1801.2418674$$

$$H = -1800.718295$$

$$G = -1800.813381$$

# Frequencies

3914.1 3633.9 3302.7 3256.8 3240.6 3235.8

3186.8 3175.3 3169.8 3162.0 3150.6 3145.0

3144.6 3144.0 3137.6 3129.0 3103.8 3095.8

3091.2 3086.9 3077.2 3062.8 3057.9 3048.2

3005.8 3001.8 3000.4 2958.4 2949.8 2902.8

1757.1 1749.0 1660.4 1652.6 1562.9 1529.2

1510.0 1503.9 1500.1 1493.6 1483.9 1481.5

1480.0 1476.0 1471.3 1466.4 1464.3 1460.6

1454.5 1447.5 1440.2 1413.9 1406.1 1395.4

1386.1 1385.4 1372.7 1366.7 1352.5 1332.0

1319.8 1305.5 1303.7 1297.2 1279.8 1273.0

1268.8 1244.7 1238.0 1235.5 1227.2 1226.7

1224.7 1202.7 1194.1 1183.7 1166.7 1165.6

1151.4 1131.8 1122.9 1113.7 1088.5 1069.3

1041.1 1037.1 1036.9 1022.5 1012.2 995.2

985.5 968.4 961.8 960.0 957.9 952.8

934.3 900.7 881.9 877.5 858.1 846.8

843.5 830.9 826.3 816.4 806.7 801.1

782.2 775.0 767.4 753.8 749.9 748.7

739.7 730.9 714.2 708.1 701.7 669.8

650.8 636.7 617.9 615.9 576.2 570.9

515.1 475.3 469.3 449.3 443.5 438.6  
 412.5 403.4 393.6 389.7 360.0 354.3  
 337.3 326.8 323.0 321.5 304.8 303.6  
 302.6 290.4 282.2 277.8 268.5 260.9  
 248.8 239.0 227.7 225.0 215.2 209.1  
 202.8 197.7 174.2 167.0 164.6 145.5  
 137.7 133.4 126.2 118.8 113.3 104.0  
 102.5 94.5 77.9 73.6 53.1 46.2  
 23.4 20.9 109.5i

# **PC1**

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | 2.074492  | 1.751283  | 0.610042  |
| C | 2.126595  | 0.794889  | 1.663033  |
| C | 1.067678  | 1.094428  | 2.681854  |
| C | -0.265952 | 1.114433  | 2.002998  |
| O | -0.214436 | 2.090369  | 0.959676  |
| C | 0.808184  | 1.788513  | -0.020080 |
| C | 1.893465  | -0.627855 | 1.110884  |
| C | 0.493404  | -0.640420 | 0.423164  |
| C | -0.590804 | -0.290761 | 1.454710  |
| C | 3.059531  | -1.104428 | 0.328503  |
| O | 3.538926  | -0.303794 | -0.651601 |
| C | 4.615670  | -0.917866 | -1.192289 |
| C | 4.857705  | -2.096073 | -0.551722 |
| C | 3.849404  | -2.212889 | 0.448750  |
| N | 0.279566  | -2.000767 | -0.103593 |
| O | 1.047272  | -2.403751 | -0.971714 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| O  | -1.897770 | -0.231341 | 0.963782  |
| Si | -2.854553 | -1.030858 | -0.158860 |
| C  | -4.170986 | 0.338751  | -0.404798 |
| C  | -3.473555 | 1.574720  | -0.979018 |
| C  | 1.284575  | 1.257891  | 3.984211  |
| C  | 0.404917  | 0.471448  | -0.776092 |
| O  | 1.022834  | 0.184045  | -1.884349 |
| O  | 0.923525  | 2.886862  | -0.833240 |
| C  | -0.019813 | 2.979787  | -1.891364 |
| O  | -0.683427 | -2.671769 | 0.345869  |
| C  | -2.129600 | -1.468002 | -1.840634 |
| C  | -3.703473 | -2.523715 | 0.606146  |
| C  | -5.273376 | -0.117614 | -1.360415 |
| C  | -4.804340 | 0.707259  | 0.937756  |
| O  | 3.212935  | 1.715807  | -2.653169 |
| H  | -2.865989 | -1.256491 | -2.625270 |
| H  | -1.207173 | -0.939259 | -2.111495 |
| H  | -1.892901 | -2.535152 | -1.879321 |
| H  | -5.334740 | -0.143695 | 1.384051  |
| H  | -6.015891 | 0.680733  | -1.511655 |
| H  | -4.880801 | -0.381829 | -2.349513 |
| H  | -5.814982 | -0.991282 | -0.975814 |
| H  | -4.189655 | 2.396601  | -1.136334 |
| H  | -3.000340 | 1.361667  | -1.946852 |
| H  | -2.685511 | 1.930362  | -0.304343 |
| H  | -4.534083 | -2.863521 | -0.023957 |
| H  | -3.005611 | -3.355750 | 0.719336  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -4.115546 | -2.286400 | 1.592444  |
| H | -1.078770 | 1.422847  | 2.670156  |
| H | -0.701079 | 0.611773  | -0.873358 |
| H | -1.044867 | 3.056960  | -1.505314 |
| H | 0.231130  | 3.899351  | -2.423902 |
| H | 0.069892  | 2.122035  | -2.566791 |
| H | 5.060309  | -0.383466 | -2.017218 |
| H | 5.649758  | -2.797974 | -0.773120 |
| H | 1.820994  | -1.302656 | 1.979099  |
| H | 0.467327  | 1.438730  | 4.678883  |
| H | 2.288045  | 1.217289  | 4.403008  |
| H | 3.134740  | 0.868214  | 2.085704  |
| H | -0.537500 | -1.014082 | 2.289048  |
| H | -4.047657 | 1.042927  | 1.654297  |
| H | -5.537398 | 1.519899  | 0.817107  |
| H | 3.697354  | -3.027169 | 1.144466  |
| H | 3.227631  | 2.184272  | -1.812873 |
| H | 2.479902  | 1.085780  | -2.467236 |

$E = -1801.2519704$

$H = -1800.726512$

$G = -1800.820449$

Frequencies

3903.2 3496.1 3305.6 3254.9 3238.4 3232.6

3188.4 3165.0 3164.4 3152.2 3150.6 3143.9

3142.0 3135.6 3135.4 3133.9 3098.1 3097.5

3096.0 3094.3 3086.8 3057.4 3052.6 3033.3  
 3025.6 3010.6 3006.6 3004.2 2978.7 2828.6  
 1770.3 1755.5 1640.0 1608.5 1548.1 1513.0  
 1506.5 1504.2 1501.5 1491.9 1485.8 1484.3  
 1475.6 1469.6 1467.0 1462.9 1460.2 1456.8  
 1447.4 1444.5 1436.0 1417.1 1392.4 1391.5  
 1384.5 1376.2 1369.2 1362.0 1353.5 1343.6  
 1325.5 1315.0 1303.8 1300.1 1281.4 1280.8  
 1278.4 1268.7 1257.9 1247.2 1243.1 1231.2  
 1229.7 1225.8 1215.9 1194.2 1188.0 1169.4  
 1146.1 1129.1 1126.3 1112.8 1083.5 1063.8  
 1054.6 1039.1 1035.2 1028.4 1012.3 992.6  
 974.1 971.8 960.9 960.4 955.1 942.4  
 924.4 913.1 896.7 882.3 879.6 864.3  
 858.3 848.3 838.4 828.1 826.4 811.0  
 803.6 780.8 771.3 767.6 759.2 754.5  
 749.4 735.2 712.2 707.5 700.0 693.8  
 671.4 654.5 628.9 619.7 615.8 576.3  
 549.3 521.9 487.0 481.7 461.1 441.8  
 417.7 412.4 396.7 395.7 391.3 370.3  
 351.3 336.9 330.8 322.9 314.8 313.3  
 304.8 294.9 289.5 279.9 274.4 267.3  
 263.7 251.5 243.1 242.6 231.9 220.0  
 209.1 203.1 195.5 189.4 169.6 168.4  
 150.4 143.6 133.5 121.8 109.7 109.1  
 100.0 93.2 80.1 73.5 67.6 60.6  
 50.9 47.8 36.8