

## Metal-free cycloisomerizations of *o*-alkynylbiaryls

Jingyi Zhang,<sup>a</sup> Siqi Li,<sup>a</sup> Yan Qiao,<sup>b</sup> Cheng Peng,<sup>a</sup> Xiao-Na Wang<sup>\*,a</sup> and Junbiao Chang<sup>\*,a</sup>

<sup>a</sup> Collaborative Innovation Center of New Drug Research and Safety Evaluation, Henan Province, Key Laboratory of Advanced Drug Preparation Technologies, Ministry of Education, School of Pharmaceutical Sciences, and College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450001, P. R. China

<sup>b</sup> School of Basic Medical Sciences, Zhengzhou University, Zhengzhou 450001, P. R. China

### *Supporting Information Part 3*

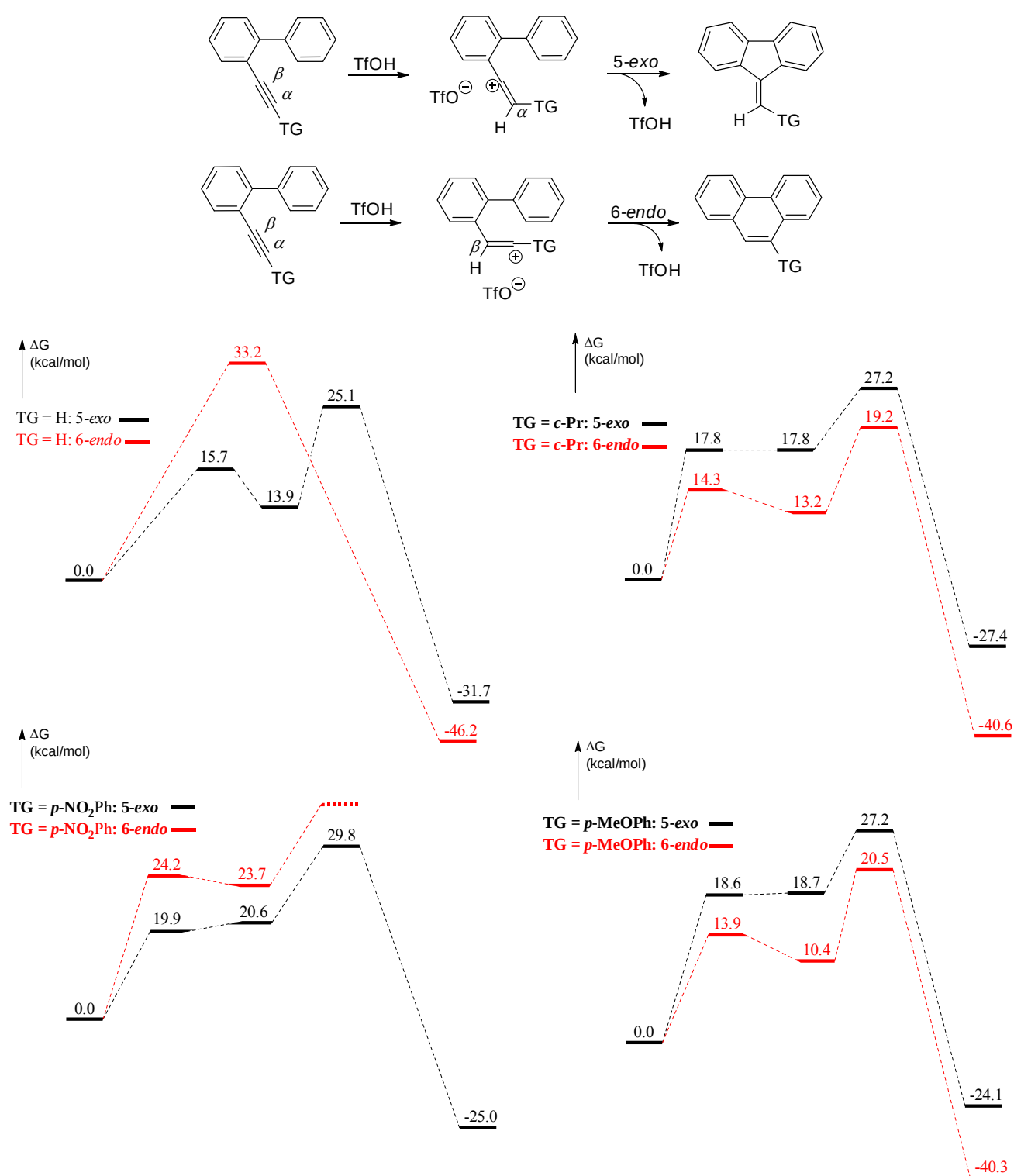
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## Computational Details

The Gaussian09<sup>1</sup> software was used for all theoretical calculations in the present study. The B3LYP method<sup>2</sup> with 6-31G(d,p) basis set was chosen for all geometrical optimizations in solvent using IEFPCM solvation model.<sup>3</sup> For transition states, the Berny algorithm was employed for both minimizations and optimizations.<sup>4</sup> The corresponding vibrational frequencies were calculated at the same level to identify the structures to be real minima or saddle points and to obtain the thermodynamic energy corrections. It was confirmed that all minima had no imaginary frequencies, and each saddle point had only one imaginary frequency. Intrinsic reaction coordinate (IRC) calculations,<sup>5</sup> at the same level of theory, were also performed for the key saddle point to ensure that it can lead to the expected reactants and products. Afterwards, the single-point energies were refined using M062X method<sup>6</sup> with 6-31++G(d,p) basis set. Finally, the Gibbs free energies, which is evaluated as the sum of the single-point energy at M062X/6-31++G(d,p) level and the thermal correction at B3LYP/6-31G(d,p) level, were used in the following discussion.

## Results and Discussion

In general, the reaction consists of two reaction steps. The first reaction step involves proton transfer from TfOH to  $C_\alpha/C_\beta$  atom generating the acetylene-cation, which is very unstable. Then, the intramolecular cyclization accompanied by hydrogen transfer gives rise to 5-*exo*/6-*endo* products. According to the calculated results, the first reaction step is reversible, while the second reaction step is irreversible and rate-determining. Noteworthy, for *o*-alkynylbiaryl **1a** in which TG = H, the proton transferred from TfOH to  $C_\beta$  atom is concerted with the intramolecular cyclization. However, the free energy barrier associated with the transition state is 33.2 kcal/mol (as shown in Figure S1), indicating that the 6-*endo* pathway can not occur. In contrast, the 5-*exo* pathway only requires the free energy of 25.1 kcal/mol, which is consistent with the experimental result that only the 5-*exo* product is observed. For *o*-alkynylbiaryls **5h** and **5q** in which TG = *c*-Pr and *p*-MeOC<sub>6</sub>H<sub>4</sub> substituents, the 6-*endo* pathway is more preferred. For *o*-alkynylbiaryl **5i** with *p*-NO<sub>2</sub>Ph substituent, the 5-*exo* pathway requires the free energy of 29.8 kcal/mol, which is possible at the experimental temperature 100 °C. However, for the 6-*endo* pathway, the cyclization transition state can not be obtained after many attempts. Coordinate scan between the forming C–C bond can not give the 6-*endo* product, which is consistent with the experimental results that the 6-*endo* cyclization product was not observed. These results agree well with the experimental observations, indicating that the calculated results are reliable.



**Figure S1.** The free energy profiles for generating the acetylenecations.

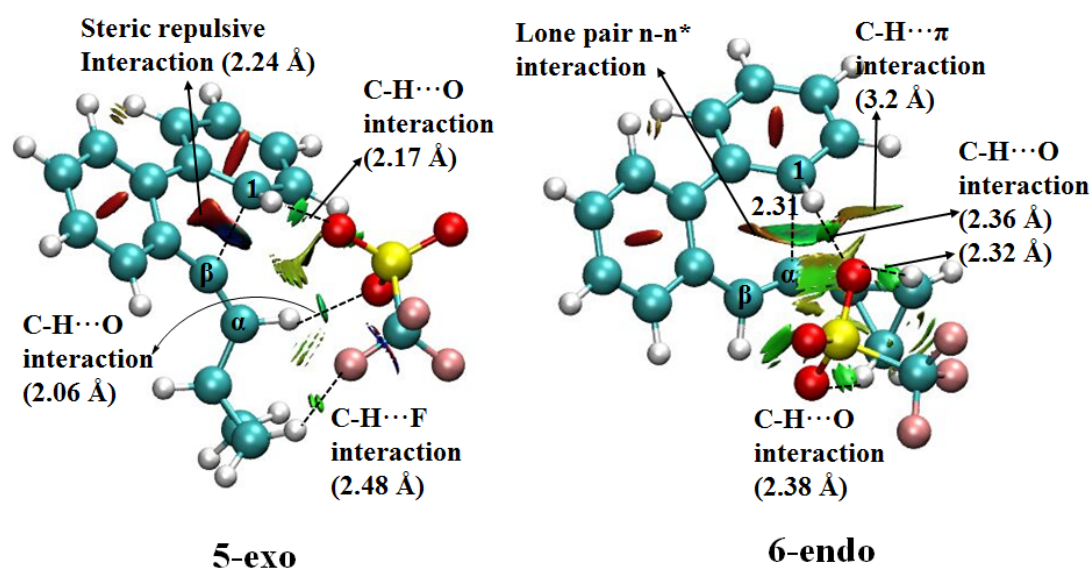
In order to explain the reaction selectivity observed, we then calculated the local reactivity indexes (electrophilic ( $P_k^+$ ) and nucleophilic ( $P_k^-$ ) Parr functions<sup>7</sup>) of  $C_\alpha$  and  $C_\beta$  in the four representative reactants, which are summarized in Table S1. Obviously, the  $P_k^-$  values of the  $C_\alpha$  atoms in *o*-alkynylbiaryls **1a** and **5i** are higher than those of  $C_\beta$ , while  $P_k^-$  values of the  $C_\alpha$  atoms in *o*-alkynylbiaryl **5q** is lower than that of  $C_\beta$ , indicating that the nucleophilicity of  $C_\alpha$  atom in

*o*-alkynylbiaryls **1a** and **5i** are higher than  $C_\beta$ , while for *o*-alkynylbiaryl **5q**, it is  $C_\beta$  that has higher nucleophilicity. This prediction is consistent with the free energy profile shown in Figure 1, which can satisfactorily explain the observed 5-*exo* regioselectivity for *o*-alkynylbiaryls **1a** and **5i**, and the 6-*endo* regioselectivity for *o*-alkynylbiaryl **5q**.

**Table S1** Electrophilic and Nucleophilic Parr Functions ( $P_k^+$  and  $P_k^-$ ) for the  $C_\alpha/C_\beta$  atoms of *o*-alkynylbiaryls.

| Parr function | <b>1a</b><br>TG = H |           | <b>5h</b><br>TG = <i>c</i> -Pr |           | <b>5i</b><br>TG = <i>p</i> -NO <sub>2</sub> C <sub>6</sub> H <sub>4</sub> |           | <b>5q</b><br>TG = <i>p</i> -MeOC <sub>6</sub> H <sub>4</sub> |           |
|---------------|---------------------|-----------|--------------------------------|-----------|---------------------------------------------------------------------------|-----------|--------------------------------------------------------------|-----------|
|               | $C_\alpha$          | $C_\beta$ | $C_\alpha$                     | $C_\beta$ | $C_\alpha$                                                                | $C_\beta$ | $C_\alpha$                                                   | $C_\beta$ |
| $P_k^+$       | 0.20                | -0.05     | 0.18                           | -0.05     | 0.00                                                                      | 0.11      | 0.13                                                         | 0.04      |
| $P_k^-$       | 0.24                | -0.05     | 0.21                           | 0.06      | 0.17                                                                      | 0.04      | 0.07                                                         | 0.13      |

Of note, for *o*-alkynylbiaryl **5h**, although the nucleophilicity of  $C_\alpha$  atom is higher than  $C_\beta$ , the 6-*endo* but not the 5-*exo* pathway is more preferred. To explain the unexpected regioselectivity for **5h**, we performed NCI analyses on the rate-determining transition states. As shown in Figure S2, the advantageous C–H···O hydrogen bond interactions and C–H··· $\pi$  interactions as well as the lone pair n–n\* interaction between  $C_1$  and  $C_\alpha$  determine that the 6-*endo* transition state have lower free energy. In contrast, the steric repulsion interaction between  $C_1$  and  $C_\beta$  results the 5-*exo* transition state with higher free energy.



**Figure S2.** Interaction analyses on the 5-*exo* and 6-*endo* cyclization transition states for **5h**.

## References

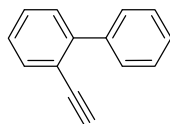
1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09*, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2010.
2. (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B: Condens. Matter*, 1988, **37**, 785.
3. (a) V. Barone, M. Cossi and J. Tomasi, *J. Comput. Chem.*, 1998, **19**, 404; (b) J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.* 2005, **105**, 2999; (c) M. Cossi and V. Barone, *J. Chem. Phys.*, 2000, **112**, 2427.
4. X. Li and M. J. Frisch, *J. Chem. Theory Comput.*, 2006, **2**, 835.
5. (a) C. Gonzalez and H. B. Schlegel, *J. Chem. Phys.*, 1989, **90**, 2154; (b) C. Gonzalez and H. B. Schlegel, *J. Phys. Chem.*, 1990, **94**, 5523.
6. (a) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157-167; (b) Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput.*, 2008, **4**, 1849.
7. (a) L. R. Domingo, P. Perez and J. A. Saez, *RSC Adv.*, 2013, **3**, 1486; (b) X. Li, Y. Wang, Y. Wang, M. Tang, L.-B. Qu, Z. Li and D. Wei, *J. Org. Chem.*, 2018, **83**, 8543.

## Calculated Energies of All Stationary Points

**Table S2.** The  $\delta G$  and  $G$  of SP (stationary points) at the B3LYP/6-31G(d,p) level in solvent, and E/B2 represents the single-point energy at M062X/6-31++G (d,p) level in solvent (unit: a.u.)

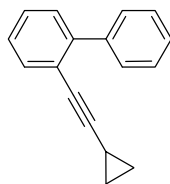
| SP                             | $\delta G$ | $G$          | E/B2           |
|--------------------------------|------------|--------------|----------------|
| <b>1a</b>                      | 0.153097   | -539.314065  | -539.249353418 |
| <b>5h</b>                      | 0.210055   | -655.973287  | -655.914763407 |
| <b>5i</b>                      | 0.225132   | -974.820658  | -974.664922054 |
| <b>5q</b>                      | 0.256081   | -884.813834  | -884.713611924 |
| TfOH                           | 0.005175   | -962.005547  | -961.811321166 |
| <b>1a-TS1<sub>5-exo</sub></b>  | 0.170667   | -1501.301245 | -1501.04809088 |
| <b>1a-M1<sub>5-exo</sub></b>   | 0.174487   | -1501.301899 | -1501.05473103 |
| <b>1a-TS2<sub>5-exo</sub></b>  | 0.178856   | -1501.285582 | -1501.04119368 |
| <b>1a-M2<sub>5-exo</sub></b>   | 0.179571   | -1501.370327 | -1501.13255540 |
| <b>1a-TS1<sub>6-endo</sub></b> | 0.173856   | -1501.273052 | -1501.02333868 |
| <b>1a-M1<sub>6-endo</sub></b>  | 0.181206   | -1501.394233 | -1501.15720019 |
| <b>5h-TS1<sub>5-exo</sub></b>  | 0.232246   | -1617.952980 | -1617.71469618 |
| <b>5h-M1<sub>5-exo</sub></b>   | 0.233829   | -1617.954593 | -1617.71633147 |
| <b>5h-TS2<sub>5-exo</sub></b>  | 0.237501   | -1617.941183 | -1617.70493391 |
| <b>5h-M2<sub>5-exo</sub></b>   | 0.238247   | -1618.021439 | -1617.79270561 |
| <b>5h-TS1<sub>6-endo</sub></b> | 0.231325   | -1617.956774 | -1617.71938989 |
| <b>5h-M1<sub>6-endo</sub></b>  | 0.234795   | -1617.957183 | -1617.72466774 |
| <b>5h-TS2<sub>6-endo</sub></b> | 0.237789   | -1617.944190 | -1617.71802456 |
| <b>5h-M2<sub>6-endo</sub></b>  | 0.240500   | -1618.039709 | -1617.81601601 |
| <b>5i-TS1<sub>5-exo</sub></b>  | 0.245111   | -1936.795724 | -1936.45932633 |
| <b>5i-M1<sub>5-exo</sub></b>   | 0.249653   | -1936.793923 | -1936.46277773 |
| <b>5i-TS2<sub>5-exo</sub></b>  | 0.251103   | -1936.781986 | -1936.44960369 |
| <b>5i-M2<sub>5-exo</sub></b>   | 0.253172   | -1936.862046 | -1936.53898143 |
| <b>5i-TS1<sub>6-endo</sub></b> | 0.245804   | -1936.787707 | -1936.45319669 |
| <b>5i-M1<sub>6-endo</sub></b>  | 0.245978   | -1936.787614 | -1936.45419834 |
| <b>5q-TS1<sub>5-exo</sub></b>  | 0.277552   | -1846.791213 | -1846.51164385 |
| <b>5q-M1<sub>5-exo</sub></b>   | 0.279863   | -1846.792297 | -1846.51369246 |
| <b>5q-TS2<sub>5-exo</sub></b>  | 0.282061   | -1846.780192 | -1846.50234924 |
| <b>5q-M2<sub>5-exo</sub></b>   | 0.285108   | -1846.855035 | -1846.58715248 |
| <b>5q-TS1<sub>6-endo</sub></b> | 0.275766   | -1846.798080 | -1846.51735799 |
| <b>5q-M1<sub>6-endo</sub></b>  | 0.279199   | -1846.801162 | -1846.52637832 |
| <b>5q-TS2<sub>6-endo</sub></b> | 0.282653   | -1846.787074 | -1846.51369811 |
| <b>5q-M2<sub>6-endo</sub></b>  | 0.285297   | -1846.876181 | -1846.61319520 |

# Cartesian Coordinates of All Stationary Points at M06-2X/6-31G(d, p) Level



**1a**

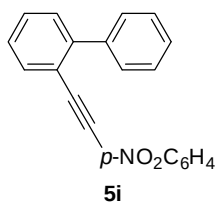
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| C | 2.87941200  | 0.56137400  | -0.05906100 |
| C | 3.45081900  | -0.69424000 | 0.11535000  |
| C | 2.62705300  | -1.81243000 | 0.25706900  |
| C | 1.24214400  | -1.66172200 | 0.22976600  |
| C | -0.84794900 | -0.31504500 | 0.04789400  |
| C | -1.53656800 | 0.61465500  | 0.84437300  |
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| C | -2.99183400 | -1.15676600 | -0.74419000 |
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| H | 3.06010700  | -2.79831000 | 0.39650800  |
| H | 0.60550800  | -2.53112500 | 0.36138900  |
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| H | -3.44437600 | 1.37661000  | 1.47656300  |
| H | -4.74912200 | -0.19232000 | 0.05373800  |
| H | -3.55194500 | -1.84531600 | -1.37020900 |
| H | -1.08117800 | -1.91823800 | -1.37522900 |
| C | 0.96618200  | 2.04282000  | -0.32398900 |
| C | 0.59375900  | 3.17556100  | -0.53640300 |
| H | 0.24541400  | 4.16622900  | -0.72172400 |



**5h**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.55899700 | -0.05794500 | -0.04520300 |
| C | -0.95727700 | -1.34543300 | -0.08361900 |
| C | -1.78022400 | -2.49043600 | -0.07848700 |
| C | -3.16584800 | -2.38271600 | -0.03018000 |
| C | -3.75961800 | -1.12012600 | 0.02075000  |
| C | -2.95883800 | 0.02040400  | 0.01363000  |
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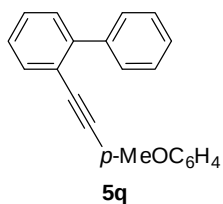
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| C | 0.24134900  | 1.42467100  | -1.01462600 |
| H | -1.30837900 | -3.46741200 | -0.10272200 |
| H | -3.77811700 | -3.27940000 | -0.02879900 |
| H | -4.84035600 | -1.02216400 | 0.05744000  |
| H | -3.42360700 | 1.00156800  | 0.03146500  |
| H | -1.80357700 | 2.05715700  | 1.62432000  |
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| H | 1.22328400  | 4.56122700  | -0.12117400 |
| H | 1.71418700  | 2.78429100  | -1.79197000 |
| H | 0.45817500  | 0.65821800  | -1.75060900 |
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| C | 1.65883800  | -1.73042500 | -0.06984600 |
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| H | 4.75071800  | -1.96140400 | 1.43116100  |
| H | 3.41467000  | -0.77570300 | 1.82679500  |



|   |             |             |             |
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| C | -2.33556200 | -1.46880800 | 0.04711500  |
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| C | -4.66574300 | -0.81297500 | -0.02814300 |
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| C | -2.07641000 | 1.53018700  | 1.00793700  |
| C | -1.78328600 | 2.89343900  | 1.03660800  |
| C | -2.36507500 | 3.75899200  | 0.10737500  |
| C | -3.24773800 | 3.25191100  | -0.84783000 |
| C | -3.54561800 | 1.88945600  | -0.87358500 |
| H | -1.98147700 | -3.59234900 | 0.04505400  |
| H | -4.38415900 | -4.20455600 | -0.02153600 |
| H | -6.11009400 | -2.40507600 | -0.07851300 |
| H | -5.42200300 | -0.03429900 | -0.03350000 |



|   |             |             |             |
|---|-------------|-------------|-------------|
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| H | -1.10626200 | 3.28103600  | 1.79235500  |
| H | -2.13419000 | 4.81984000  | 0.12974500  |
| H | -3.70293100 | 3.91570400  | -1.57697200 |
| H | -4.22264000 | 1.49942200  | -1.62784900 |
| C | -0.93943900 | -1.18562000 | 0.03689000  |
| C | 0.26217300  | -0.99222200 | 0.01011800  |
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| H | 4.69842600  | -2.27383300 | 0.01926100  |
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| N | 5.80832500  | 0.14437900  | -0.08530200 |
| O | 6.15673500  | 1.32689800  | -0.13870900 |
| O | 6.59726700  | -0.80379100 | -0.05049000 |



|   |             |             |             |
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| C | -1.44401700 | 2.90824300  | 1.02219000  |
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| H | -5.16671700 | 0.08389400  | -0.02117700 |
| H | -1.32810300 | 0.87766200  | 1.71888000  |
| H | -0.74641800 | 3.27667300  | 1.76894400  |
| H | -1.76126000 | 4.84611100  | 0.12628800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.37399100 | 3.98388300  | -1.56174100 |
| H | -3.95047300 | 1.58096900  | -1.61225400 |
| C | -0.71490600 | -1.20056300 | 0.03499700  |
| C | 0.49304500  | -1.04957100 | 0.00979300  |
| C | 1.89916300  | -0.82873600 | -0.01553900 |
| C | 2.42049300  | 0.47753000  | -0.05807400 |
| C | 2.80889800  | -1.90966900 | 0.00067000  |
| C | 3.79413400  | 0.70810000  | -0.08336200 |
| H | 1.73585200  | 1.31940900  | -0.07139100 |
| C | 4.17586800  | -1.68751000 | -0.02433000 |
| H | 2.42734300  | -2.92498200 | 0.03300100  |
| C | 4.68146500  | -0.37711200 | -0.06704500 |
| H | 4.15972700  | 1.72703900  | -0.11632100 |
| H | 4.87783900  | -2.51473300 | -0.01224800 |
| O | 6.03806600  | -0.26808600 | -0.09010800 |
| C | 6.61306700  | 1.03518300  | -0.13567200 |
| H | 6.34086900  | 1.62486800  | 0.74749100  |
| H | 7.69280000  | 0.88509400  | -0.15014800 |
| H | 6.30995200  | 1.57596000  | -1.03976200 |

#### TfOH

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.47750400 | 1.89993900  | -0.19641000 |
| S | -0.85220600 | -0.14336900 | 0.06496300  |
| O | -1.25658100 | 0.03465300  | 1.45297500  |
| O | -1.21786800 | -1.30748600 | -0.71962300 |
| O | -1.26651200 | 1.16297600  | -0.79959200 |
| C | 1.01109500  | 0.01159000  | -0.00170800 |
| F | 1.53819500  | -1.00798400 | 0.67006700  |
| F | 1.37579700  | 1.16156900  | 0.56280800  |
| F | 1.41644300  | -0.01988600 | -1.26652300 |

#### 1a-TS1<sub>5-exo</sub>

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.24489400 | 1.00671700  | -0.23133100 |
| C | 1.26814000 | 1.54821900  | 0.66642800  |
| C | 0.82059200 | 2.88979900  | 0.52344800  |
| C | 1.30042500 | 3.68076400  | -0.50432900 |
| C | 2.23620200 | 3.14556200  | -1.39927900 |
| C | 2.69856600 | 1.83659500  | -1.26242400 |
| C | 2.78164600 | -0.36482300 | -0.09035300 |
| C | 3.20649500 | -0.85949100 | 1.15513500  |
| C | 3.73448800 | -2.14484000 | 1.26416700  |
| C | 3.84286300 | -2.95752100 | 0.13432900  |
| C | 3.42749700 | -2.47562800 | -1.10938400 |
| C | 2.90762000 | -1.18844400 | -1.22354700 |
| H | 0.07330500 | 3.26237700  | 1.21406300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.95064300  | 4.70055300  | -0.61939000 |
| H | 2.62012700  | 3.76102200  | -2.20707900 |
| H | 3.44778900  | 1.45972200  | -1.95012000 |
| H | 3.15789800  | -0.22356300 | 2.03302100  |
| H | 4.06859900  | -2.50784800 | 2.23120200  |
| H | 4.25167700  | -3.95949800 | 0.22126700  |
| H | 3.50354400  | -3.10457100 | -1.99094500 |
| H | 2.56816100  | -0.82677300 | -2.18910400 |
| C | 0.66115000  | 0.77247100  | 1.65243000  |
| C | -0.03611300 | 0.10544100  | 2.45373800  |
| H | 0.10676500  | -0.23041600 | 3.47233300  |
| S | -2.99446900 | 0.15572300  | 0.46001000  |
| O | -4.44190500 | 0.32952000  | 0.60262200  |
| O | -2.17533600 | 1.31997900  | 0.09075600  |
| O | -2.39109400 | -0.62704800 | 1.63583900  |
| C | -2.77765900 | -1.05337200 | -0.93779700 |
| F | -3.26777200 | -0.52983200 | -2.06766900 |
| F | -3.42070000 | -2.19576600 | -0.67543700 |
| F | -1.47707500 | -1.32066900 | -1.11562700 |
| H | -1.18123700 | -0.23447200 | 1.97206200  |

# **1a-M1<sub>5-exo</sub>**

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.25468900 | 0.79969400  | -0.27795400 |
| C | 1.46022900 | 1.58666600  | 0.63281900  |
| C | 1.33038900 | 2.99964500  | 0.45032700  |
| C | 1.93732200 | 3.62032100  | -0.61943600 |
| C | 2.67957700 | 2.84605400  | -1.52694800 |
| C | 2.83471100 | 1.46988600  | -1.35826900 |
| C | 2.47625600 | -0.64514000 | -0.08927900 |
| C | 2.81184500 | -1.17330900 | 1.17087000  |
| C | 3.04286800 | -2.53830700 | 1.32565700  |
| C | 2.93541500 | -3.39642000 | 0.22963600  |
| C | 2.60661400 | -2.88258400 | -1.02765800 |
| C | 2.38792600 | -1.51763700 | -1.19028300 |
| H | 0.72111100 | 3.55645400  | 1.15258900  |
| H | 1.83478000 | 4.68925000  | -0.76690900 |
| H | 3.15826500 | 3.32953900  | -2.37303100 |
| H | 3.44716800 | 0.91265300  | -2.05808300 |
| H | 2.93573000 | -0.50834200 | 2.01907500  |
| H | 3.31455900 | -2.93012700 | 2.30072100  |
| H | 3.11125200 | -4.46049100 | 0.35294200  |
| H | 2.51493400 | -3.54678600 | -1.88113600 |
| H | 2.10996300 | -1.12635400 | -2.16357900 |
| C | 0.69325100 | 1.01052100  | 1.61313600  |
| C | 0.00004800 | 0.53734800  | 2.58395200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.44968800  | 0.36733400  | 3.56106800  |
| S | -2.69990700 | 0.54030000  | 0.27075700  |
| O | -3.85016300 | 1.31565800  | -0.22377500 |
| O | -1.36072600 | 1.09365700  | -0.07331800 |
| O | -2.80170000 | 0.08605400  | 1.68821400  |
| C | -2.77234000 | -1.04764100 | -0.69367700 |
| F | -2.65787600 | -0.80636300 | -2.00921600 |
| F | -3.93573500 | -1.68018400 | -0.47983700 |
| F | -1.77333800 | -1.86873000 | -0.32968600 |
| H | -1.06849400 | 0.29204400  | 2.42655500  |

**1a-TS<sub>5-exo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.99254800  | -0.51722800 | -0.18724300 |
| C | 1.98843800  | -1.31808800 | 0.43088500  |
| C | 2.04095600  | -2.73229000 | 0.35774600  |
| C | 3.15848200  | -3.32034300 | -0.20523500 |
| C | 4.19011300  | -2.52750500 | -0.74978100 |
| C | 4.11359100  | -1.14019400 | -0.75025000 |
| C | 2.66923700  | 0.89656200  | -0.18409500 |
| C | 1.28195300  | 1.21338500  | -0.09860600 |
| C | 0.87647800  | 2.52993600  | 0.20992000  |
| C | 1.83197900  | 3.52431500  | 0.33074300  |
| C | 3.19979000  | 3.22445700  | 0.15945200  |
| C | 3.62149100  | 1.92721800  | -0.09404600 |
| H | 1.24068400  | -3.32682400 | 0.78275400  |
| H | 3.24262500  | -4.40140800 | -0.23178400 |
| H | 5.04580100  | -3.01407400 | -1.20677000 |
| H | 4.88769000  | -0.54818500 | -1.22644000 |
| H | 0.52433000  | 0.57236800  | -0.57083100 |
| H | -0.18406400 | 2.74215000  | 0.29177200  |
| H | 1.53027300  | 4.54728000  | 0.53127200  |
| H | 3.93632200  | 4.01527400  | 0.26184800  |
| H | 4.68012800  | 1.69553500  | -0.14551300 |
| C | 0.96835500  | -0.63413500 | 1.10404100  |
| C | 0.02125700  | -0.49082100 | 1.98506700  |
| H | -0.80446100 | 0.20885500  | 1.83185600  |
| S | -2.52851300 | 0.59873500  | -0.56360200 |
| O | -2.14287200 | 1.33987000  | 0.67357300  |
| O | -3.41621800 | 1.33579500  | -1.48147500 |
| O | -1.39853800 | -0.12709700 | -1.20150700 |
| C | -3.59165600 | -0.77642400 | 0.10063600  |
| F | -4.67656100 | -0.28652700 | 0.71951200  |
| F | -2.90324700 | -1.51723900 | 0.99143200  |
| F | -3.99995900 | -1.58818600 | -0.88645200 |
| H | 0.05772000  | -1.08478200 | 2.89892300  |

**1a-M2<sub>5-exo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.61157800  | 0.23433100  | -0.48384800 |
| C | 2.56170800  | -0.46362300 | 0.74621300  |
| C | 3.39344100  | -1.55943000 | 0.96758000  |
| C | 4.27353100  | -1.95473800 | -0.04418600 |
| C | 4.32126800  | -1.26350600 | -1.26132400 |
| C | 3.49047200  | -0.16327100 | -1.49086800 |
| C | 1.63444800  | 1.33220100  | -0.43055700 |
| C | 0.99577600  | 1.29683400  | 0.83197200  |
| C | 0.01571500  | 2.23615500  | 1.15346800  |
| C | -0.32793400 | 3.21026100  | 0.20324700  |
| C | 0.30463700  | 3.23881100  | -1.04976700 |
| C | 1.28964500  | 2.30231500  | -1.37302200 |
| H | 3.36378800  | -2.10268900 | 1.90777300  |
| H | 4.92697000  | -2.80710800 | 0.11525400  |
| H | 5.01155200  | -1.58612800 | -2.03496500 |
| H | 3.53356600  | 0.36782000  | -2.43734100 |
| H | -1.73348700 | 1.54511800  | -0.27439500 |
| H | -0.47725500 | 2.22178600  | 2.12081400  |
| H | -1.07752700 | 3.95759600  | 0.44569500  |
| H | 0.02617100  | 3.99944300  | -1.77242000 |
| H | 1.77379000  | 2.33328900  | -2.34452600 |
| C | 1.54610800  | 0.16897000  | 1.61969800  |
| C | 1.18970900  | -0.20030500 | 2.85943400  |
| H | 0.42238200  | 0.32978000  | 3.41393400  |
| S | -2.99462300 | -0.17038900 | 0.14642800  |
| O | -2.60739800 | -0.00284600 | 1.54162200  |
| O | -4.36714200 | -0.42407600 | -0.25433300 |
| O | -2.46006100 | 1.06252000  | -0.73787800 |
| C | -1.95111900 | -1.55293300 | -0.55785900 |
| F | -2.23838700 | -2.67340200 | 0.10094000  |
| F | -0.66100400 | -1.25801400 | -0.40377700 |
| F | -2.22550000 | -1.70654100 | -1.84987000 |
| H | 1.65094500  | -1.04827600 | 3.35531700  |

**1a-TS1<sub>6-endo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.72827400 | 0.95642800  | -0.12077900 |
| C | -1.36963800 | 1.29133300  | -0.36661900 |
| C | -0.96609800 | 2.62889000  | -0.42422900 |
| C | -1.90281300 | 3.64841100  | -0.25638100 |
| C | -3.23898000 | 3.33087600  | -0.01498100 |
| C | -3.64553700 | 1.99556900  | 0.05922100  |
| C | -3.12932400 | -0.46534500 | -0.00291300 |
| C | -2.84923800 | -1.37581000 | -1.05152500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.17594000 | -2.73750800 | -0.91698900 |
| C | -3.76231100 | -3.20098200 | 0.25488200  |
| C | -4.04888500 | -2.30154500 | 1.29029100  |
| C | -3.73324900 | -0.94949500 | 1.16622200  |
| H | 0.08082900  | 2.85990700  | -0.58845500 |
| H | -1.58591700 | 4.68500200  | -0.30389600 |
| H | -3.97055300 | 4.12107900  | 0.12133200  |
| H | -4.68798100 | 1.75593800  | 0.24328900  |
| H | -2.53384200 | -0.99822500 | -2.01939100 |
| H | -2.98379400 | -3.41693700 | -1.74155500 |
| H | -4.01146300 | -4.25150200 | 0.36345700  |
| H | -4.51281900 | -2.66066800 | 2.20372600  |
| H | -3.93648300 | -0.26478200 | 1.98321100  |
| C | -0.40739700 | 0.20254400  | -0.50709900 |
| C | -0.53075300 | -1.05316300 | -0.61689900 |
| H | -0.24103500 | -2.08041100 | -0.70990200 |
| S | 3.04168200  | 0.61987600  | 0.49256000  |
| O | 4.24016900  | 1.46235400  | 0.53426700  |
| O | 2.37554500  | 0.27378900  | 1.75490000  |
| O | 2.06149000  | 1.07766300  | -0.59366400 |
| C | 3.60351200  | -1.01114500 | -0.20515000 |
| F | 4.44347800  | -1.61461800 | 0.64118000  |
| F | 4.21886000  | -0.84237100 | -1.37916100 |
| F | 2.53810900  | -1.81504100 | -0.39479000 |
| H | 0.80402500  | 0.51605600  | -0.52417200 |

**1a-Ml<sub>6-endo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.18189800  | 0.23647800  | -0.14804700 |
| C | 3.32455400  | -1.08091600 | 0.38283700  |
| C | 4.44832700  | -1.86179900 | 0.02328100  |
| C | 5.41132900  | -1.36919900 | -0.83501900 |
| C | 5.27524200  | -0.07079800 | -1.36220000 |
| C | 4.18542000  | 0.71154000  | -1.02536100 |
| C | 2.01960500  | 1.02910200  | 0.23243300  |
| C | 1.05659800  | 0.46517400  | 1.12187000  |
| C | -0.07783000 | 1.22800200  | 1.49714100  |
| C | -0.26700900 | 2.51400700  | 1.01513000  |
| C | 0.68309000  | 3.07271700  | 0.13401100  |
| C | 1.79595900  | 2.34462600  | -0.24315500 |
| H | 4.54015000  | -2.86257900 | 0.43651500  |
| H | 6.26900800  | -1.97834000 | -1.10349800 |
| H | 6.02957000  | 0.32063100  | -2.03797700 |
| H | 4.11032700  | 1.70648400  | -1.44895900 |
| H | -1.42287300 | 1.22306700  | -0.37303400 |
| H | -0.79776000 | 0.79168700  | 2.18392800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.13201900 | 3.09209400  | 1.32615200  |
| H | 0.54097200  | 4.07916700  | -0.24643800 |
| H | 2.50758200  | 2.80211900  | -0.92052000 |
| C | 2.32774100  | -1.60264600 | 1.27393800  |
| C | 1.24113500  | -0.86497200 | 1.62736600  |
| H | 0.49221200  | -1.27097700 | 2.30108600  |
| S | -3.40678300 | 0.37505900  | -0.47336200 |
| O | -3.64571200 | 1.01204000  | 0.81636100  |
| O | -4.38338300 | 0.39643500  | -1.54712500 |
| O | -2.00646800 | 0.86906300  | -1.08892000 |
| C | -2.99875900 | -1.41588900 | -0.12718800 |
| F | -4.06713900 | -1.99525400 | 0.41469400  |
| F | -1.97443800 | -1.47537400 | 0.72719000  |
| F | -2.67491900 | -2.03255200 | -1.25863500 |
| H | 2.46052700  | -2.60855100 | 1.66253700  |

# **5h-TS1<sub>5-exo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.67197700  | -0.02368200 | -0.15840700 |
| C | 2.17006100  | 1.30026000  | 0.05694500  |
| C | 2.81344500  | 2.41621300  | -0.54085300 |
| C | 3.91883100  | 2.23867100  | -1.35407100 |
| C | 4.39435700  | 0.94169900  | -1.58624900 |
| C | 3.78100800  | -0.16522400 | -0.99963200 |
| C | 2.05963600  | -1.21787200 | 0.46688500  |
| C | 1.78227400  | -1.26191300 | 1.84372000  |
| C | 1.22894300  | -2.40499200 | 2.41819200  |
| C | 0.93850500  | -3.51813600 | 1.62700500  |
| C | 1.21101400  | -3.48565200 | 0.25757900  |
| C | 1.77316200  | -2.34805800 | -0.31801900 |
| H | 2.40799100  | 3.40567100  | -0.36025700 |
| H | 4.40579200  | 3.09250900  | -1.81216900 |
| H | 5.26003100  | 0.79233900  | -2.22434900 |
| H | 4.18386500  | -1.15679700 | -1.17582900 |
| H | 2.02856200  | -0.41052200 | 2.47003100  |
| H | 1.03078300  | -2.42780200 | 3.48545400  |
| H | 0.50398600  | -4.40651000 | 2.07521700  |
| H | 0.98020100  | -4.34452600 | -0.36506700 |
| H | 1.96064900  | -2.31789200 | -1.38649300 |
| C | 1.00697200  | 1.52747200  | 0.79607500  |
| C | -0.12457100 | 1.73857800  | 1.29961400  |
| S | -1.84835900 | 0.50198100  | -1.61773800 |
| O | -2.73513100 | 0.76960700  | -2.75302000 |
| O | -0.44305900 | 0.16351400  | -1.88215200 |
| O | -1.99450100 | 1.56348900  | -0.51834200 |
| C | -2.55572700 | -0.99927600 | -0.77598100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -2.46737100 | -2.06404900 | -1.57935800 |
| F | -3.83979300 | -0.79918600 | -0.45897500 |
| F | -1.87326700 | -1.25286700 | 0.35316500  |
| H | -0.93495000 | 1.63747600  | 0.31720600  |
| C | -0.79293200 | 2.01200100  | 2.58011700  |
| C | -2.11670700 | 2.76136200  | 2.59690300  |
| C | -2.09870200 | 1.29805400  | 2.90606100  |
| H | -0.11692300 | 2.19192100  | 3.41006800  |
| H | -2.52490700 | 3.07248400  | 1.64156700  |
| H | -2.26240600 | 3.46621900  | 3.40874500  |
| H | -2.22494300 | 0.97787600  | 3.93511700  |
| H | -2.48784700 | 0.61086600  | 2.16388600  |

### 5h-M1<sub>5-exo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.42252800  | -1.22058400 | -0.49339700 |
| C | 1.43774000  | -0.72294500 | -1.42515900 |
| C | 0.96511400  | -1.55521700 | -2.49023500 |
| C | 1.40777800  | -2.85481500 | -2.60726100 |
| C | 2.33805300  | -3.34606200 | -1.67602800 |
| C | 2.83520900  | -2.54689200 | -0.64605200 |
| C | 2.99718500  | -0.37374800 | 0.56546700  |
| C | 3.38371600  | 0.95540800  | 0.30957600  |
| C | 3.94127300  | 1.73684300  | 1.31926700  |
| C | 4.11762900  | 1.20756900  | 2.59880400  |
| C | 3.74285400  | -0.11264600 | 2.86423600  |
| C | 3.19588600  | -0.90068600 | 1.85615500  |
| H | 0.22350800  | -1.14912400 | -3.16764600 |
| H | 1.03813800  | -3.49361900 | -3.40112700 |
| H | 2.69367600  | -4.36794500 | -1.76649100 |
| H | 3.58312600  | -2.95013900 | 0.02737600  |
| H | 3.29284500  | 1.36063800  | -0.69277700 |
| H | 4.24698000  | 2.75564100  | 1.10340400  |
| H | 4.55000900  | 1.81839800  | 3.38514200  |
| H | 3.87150200  | -0.52611500 | 3.85948000  |
| H | 2.88307800  | -1.91663800 | 2.07451600  |
| C | 0.82731400  | 0.49353300  | -1.25741000 |
| C | 0.14008200  | 1.57262400  | -1.13105900 |
| S | -2.91665800 | -0.21820100 | -0.24415000 |
| O | -4.16408600 | -0.53230200 | -0.96423200 |
| O | -1.73558700 | -1.04278400 | -0.59549300 |
| O | -2.60775200 | 1.24391000  | -0.13888000 |
| C | -3.28099100 | -0.68851000 | 1.51797800  |
| F | -3.55629900 | -1.99947200 | 1.60821100  |
| F | -4.33494000 | -0.00285200 | 1.98603900  |
| F | -2.22543100 | -0.42760400 | 2.30760900  |



|   |             |            |             |
|---|-------------|------------|-------------|
| H | -0.85488400 | 1.40832900 | -0.64661700 |
| C | 0.45165900  | 2.95976200 | -1.54255600 |
| C | -0.70758200 | 3.84434200 | -1.97836000 |
| C | -0.04402800 | 4.09602400 | -0.66042400 |
| H | 1.40113800  | 3.10156900 | -2.04732600 |
| H | -1.69780800 | 3.40143000 | -1.97052800 |
| H | -0.51413000 | 4.52330700 | -2.80218700 |
| H | 0.61563400  | 4.95148800 | -0.55880600 |
| H | -0.58537300 | 3.82875300 | 0.24083700  |

# **5h-TS2<sub>5-exo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.14030100  | -0.18765400 | -0.62325500 |
| C | 2.11884000  | -1.16246700 | -0.40902000 |
| C | 2.18557200  | -2.42699300 | -1.05074500 |
| C | 3.32309500  | -2.74732900 | -1.76697500 |
| C | 4.36573600  | -1.80859600 | -1.91685100 |
| C | 4.27883200  | -0.53884700 | -1.36102500 |
| C | 2.81977800  | 1.10628600  | -0.05611600 |
| C | 1.43327700  | 1.37450000  | 0.13187700  |
| C | 1.02601000  | 2.45863200  | 0.93830400  |
| C | 1.98193200  | 3.31100100  | 1.46397100  |
| C | 3.35188100  | 3.09412800  | 1.20537700  |
| C | 3.77300100  | 2.00597700  | 0.45581700  |
| H | 1.37436200  | -3.13598400 | -0.93115000 |
| H | 3.41292700  | -3.72587200 | -2.22656000 |
| H | 5.23662500  | -2.07429200 | -2.50748200 |
| H | 5.06181300  | 0.19112200  | -1.53707900 |
| H | 0.68526700  | 0.98302100  | -0.57083200 |
| H | -0.03485800 | 2.63160200  | 1.08425100  |
| H | 1.67905400  | 4.16876200  | 2.05592700  |
| H | 4.08878200  | 3.77053700  | 1.62710300  |
| H | 4.83176800  | 1.80628100  | 0.32782300  |
| C | 1.07703400  | -0.80924400 | 0.45337900  |
| C | 0.05677400  | -1.03922700 | 1.24506400  |
| H | -0.74027500 | -0.28568500 | 1.28020800  |
| S | -2.38131400 | 1.17005200  | -0.67752000 |
| O | -2.06286200 | 1.22118300  | 0.78025700  |
| O | -3.12596400 | 2.33291800  | -1.19410600 |
| O | -1.25066800 | 0.69855000  | -1.51804500 |
| C | -3.59920800 | -0.23262700 | -0.78274200 |
| F | -4.68968400 | 0.02058500  | -0.04449200 |
| F | -3.04517300 | -1.37669300 | -0.32695100 |
| F | -3.98435300 | -0.43965100 | -2.05033800 |
| C | -0.07306900 | -2.22669200 | 2.11702800  |
| C | -0.77295800 | -2.06621600 | 3.46132300  |

|                              |             |             |             |
|------------------------------|-------------|-------------|-------------|
| C                            | -1.47187000 | -2.78686400 | 2.35292100  |
| H                            | 0.74094900  | -2.94255000 | 2.07308300  |
| H                            | -1.12307100 | -1.07449100 | 3.72802700  |
| H                            | -0.36602800 | -2.64100100 | 4.28678100  |
| H                            | -1.55202500 | -3.86802000 | 2.39910900  |
| H                            | -2.29516200 | -2.29025000 | 1.85228700  |
| <b>5h-M2<sub>5-exo</sub></b> |             |             |             |
| C                            | -3.05714100 | -0.62542800 | -0.38989700 |
| C                            | -2.56567300 | 0.66638200  | -0.05893900 |
| C                            | -3.23411800 | 1.79249300  | -0.54989100 |
| C                            | -4.36396500 | 1.62655200  | -1.35560200 |
| C                            | -4.83664300 | 0.34976600  | -1.67962700 |
| C                            | -4.18387300 | -0.78530400 | -1.19612500 |
| C                            | -2.20261200 | -1.62950500 | 0.24883400  |
| C                            | -1.19597800 | -0.95085700 | 0.97489600  |
| C                            | -0.25105500 | -1.68274700 | 1.70544800  |
| C                            | -0.31187000 | -3.08423500 | 1.68836000  |
| C                            | -1.30294200 | -3.74912900 | 0.95378400  |
| C                            | -2.25683600 | -3.02473400 | 0.23637000  |
| H                            | -2.90101600 | 2.79642100  | -0.31707000 |
| H                            | -4.88115300 | 2.50340600  | -1.73372100 |
| H                            | -5.71595500 | 0.24236800  | -2.30764600 |
| H                            | -4.55131800 | -1.77704400 | -1.44420700 |
| H                            | 1.29224100  | -1.90401100 | 0.21250400  |
| H                            | 0.50140700  | -1.18354400 | 2.30987400  |
| H                            | 0.41237900  | -3.65782300 | 2.25901100  |
| H                            | -1.33356800 | -4.83420300 | 0.95167100  |
| H                            | -3.02877800 | -3.54461500 | -0.32387500 |
| C                            | -1.36359000 | 0.50971200  | 0.79428200  |
| C                            | -0.49580700 | 1.41689100  | 1.30354400  |
| H                            | 0.34156700  | 1.01565800  | 1.87391800  |
| S                            | 3.08908300  | -0.72328100 | -0.06940400 |
| O                            | 2.76592800  | -0.10200300 | 1.21128700  |
| O                            | 4.43354200  | -1.15958200 | -0.40027100 |
| O                            | 2.09575700  | -1.95140000 | -0.36343800 |
| C                            | 2.54653900  | 0.47336100  | -1.40136200 |
| F                            | 3.14916600  | 1.64161600  | -1.17684800 |
| F                            | 1.22615300  | 0.63321700  | -1.34316800 |
| F                            | 2.89376000  | 0.00853800  | -2.59635000 |
| C                            | -0.47154300 | 2.87593600  | 1.17578100  |
| C                            | 0.16354500  | 3.69798900  | 2.29544500  |
| C                            | 0.88929000  | 3.55588200  | 0.99912300  |
| H                            | -1.29490700 | 3.35161300  | 0.65964000  |
| H                            | 0.53831200  | 3.15592000  | 3.15821400  |
| H                            | -0.30691700 | 4.64755300  | 2.52967200  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 0.92228000 | 4.40361200 | 0.32220100 |
| H | 1.76220100 | 2.91256600 | 0.96038600 |

**5h-TS1**<sub>6-endo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.67197700  | -0.02368200 | -0.15840700 |
| C | 2.17006100  | 1.30026000  | 0.05694500  |
| C | 2.81344500  | 2.41621300  | -0.54085300 |
| C | 3.91883100  | 2.23867100  | -1.35407100 |
| C | 4.39435700  | 0.94169900  | -1.58624900 |
| C | 3.78100800  | -0.16522400 | -0.99963200 |
| C | 2.05963600  | -1.21787200 | 0.46688500  |
| C | 1.78227400  | -1.26191300 | 1.84372000  |
| C | 1.22894300  | -2.40499200 | 2.41819200  |
| C | 0.93850500  | -3.51813600 | 1.62700500  |
| C | 1.21101400  | -3.48565200 | 0.25757900  |
| C | 1.77316200  | -2.34805800 | -0.31801900 |
| H | 2.40799100  | 3.40567100  | -0.36025700 |
| H | 4.40579200  | 3.09250900  | -1.81216900 |
| H | 5.26003100  | 0.79233900  | -2.22434900 |
| H | 4.18386500  | -1.15679700 | -1.17582900 |
| H | 2.02856200  | -0.41052200 | 2.47003100  |
| H | 1.03078300  | -2.42780200 | 3.48545400  |
| H | 0.50398600  | -4.40651000 | 2.07521700  |
| H | 0.98020100  | -4.34452600 | -0.36506700 |
| H | 1.96064900  | -2.31789200 | -1.38649300 |
| C | 1.00697200  | 1.52747200  | 0.79607500  |
| C | -0.12457100 | 1.73857800  | 1.29961400  |
| S | -1.84835900 | 0.50198100  | -1.61773800 |
| O | -2.73513100 | 0.76960700  | -2.75302000 |
| O | -0.44305900 | 0.16351400  | -1.88215200 |
| O | -1.99450100 | 1.56348900  | -0.51834200 |
| C | -2.55572700 | -0.99927600 | -0.77598100 |
| F | -2.46737100 | -2.06404900 | -1.57935800 |
| F | -3.83979300 | -0.79918600 | -0.45897500 |
| F | -1.87326700 | -1.25286700 | 0.35316500  |
| H | -0.93495000 | 1.63747600  | 0.31720600  |
| C | -0.79293200 | 2.01200100  | 2.58011700  |
| C | -2.11670700 | 2.76136200  | 2.59690300  |
| C | -2.09870200 | 1.29805400  | 2.90606100  |
| H | -0.11692300 | 2.19192100  | 3.41006800  |
| H | -2.52490700 | 3.07248400  | 1.64156700  |
| H | -2.26240600 | 3.46621900  | 3.40874500  |
| H | -2.22494300 | 0.97787600  | 3.93511700  |
| H | -2.48784700 | 0.61086600  | 2.16388600  |

**5h-M1<sub>6-endo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.23241400 | 1.68264100  | -0.05190900 |
| C | -0.89492100 | 1.37716400  | -0.39899000 |
| C | 0.07321700  | 2.39149100  | -0.45666600 |
| C | -0.27401900 | 3.70868800  | -0.16698700 |
| C | -1.58841000 | 4.01779000  | 0.18380700  |
| C | -2.55548900 | 3.01116200  | 0.24132000  |
| C | -3.27577600 | 0.62083200  | 0.00576800  |
| C | -3.75184000 | 0.02151000  | -1.17535800 |
| C | -4.74737600 | -0.95498000 | -1.12358200 |
| C | -5.27827400 | -1.34867500 | 0.10636000  |
| C | -4.81774000 | -0.75554300 | 1.28516800  |
| C | -3.82673100 | 0.22467800  | 1.23640800  |
| H | 1.09722300  | 2.12989400  | -0.70134700 |
| H | 0.48043200  | 4.48750200  | -0.20925600 |
| H | -1.86545100 | 5.04213700  | 0.41302600  |
| H | -3.57884300 | 3.25694300  | 0.50711400  |
| H | -3.35035400 | 0.33834500  | -2.13327700 |
| H | -5.11369200 | -1.40001200 | -2.04374000 |
| H | -6.05440100 | -2.10696500 | 0.14655200  |
| H | -5.23390500 | -1.05336700 | 2.24284300  |
| H | -3.47175200 | 0.68798800  | 2.15205100  |
| C | -0.46510000 | 0.00008600  | -0.66042900 |
| C | -1.05549000 | -1.14152500 | -0.55195800 |
| S | 3.14312800  | -0.92683300 | -0.38988300 |
| O | 4.20838900  | -1.78297900 | -0.93965700 |
| O | 2.35067800  | -0.18199600 | -1.42157700 |
| O | 2.30669000  | -1.52780200 | 0.67725200  |
| C | 4.05030100  | 0.43973700  | 0.48655800  |
| F | 4.90094500  | 1.05654400  | -0.34630500 |
| F | 4.74780000  | -0.04252600 | 1.52514300  |
| F | 3.18183400  | 1.35629500  | 0.95323000  |
| H | 0.59962800  | -0.14050500 | -0.99201000 |
| C | -1.44099700 | -2.44858900 | -0.43576000 |
| C | -0.36673300 | -3.36506900 | 0.34044600  |
| C | -1.63068900 | -3.07185000 | 0.99215900  |
| H | -1.96789300 | -2.92757800 | -1.25474400 |
| H | 0.54194500  | -2.84760400 | 0.63325300  |
| H | -0.23918000 | -4.30658600 | -0.18317800 |
| H | -2.41229400 | -3.82369300 | 1.00168300  |
| H | -1.65187600 | -2.35505100 | 1.80427100  |

**5h-TS2<sub>6-endo</sub>**

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -2.64859300 | 1.13986000 | -0.08059000 |
| C | -1.59407600 | 1.40916900 | 0.82428100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.27398400 | 2.73535000  | 1.14787600  |
| C | -1.98817100 | 3.79055400  | 0.58699900  |
| C | -3.04354700 | 3.52847100  | -0.28920700 |
| C | -3.37361900 | 2.21293700  | -0.61351200 |
| C | -2.97173000 | -0.25483100 | -0.42397100 |
| C | -1.92130500 | -1.14464000 | -0.75710400 |
| C | -2.21543700 | -2.48819000 | -1.07843200 |
| C | -3.52210500 | -2.94623200 | -1.04660900 |
| C | -4.56140900 | -2.06202400 | -0.70867900 |
| C | -4.29219200 | -0.73296700 | -0.40077900 |
| H | -0.45899200 | 2.93177600  | 1.83669500  |
| H | -1.72657400 | 4.81309500  | 0.83842500  |
| H | -3.60625500 | 4.34743200  | -0.72578400 |
| H | -4.17883100 | 2.01197300  | -1.31297100 |
| H | -0.93559100 | -0.74451000 | -0.99789700 |
| H | -1.40812500 | -3.15451700 | -1.36414900 |
| H | -3.74834800 | -3.97830000 | -1.29387300 |
| H | -5.58546200 | -2.42171600 | -0.68041100 |
| H | -5.09933100 | -0.06269500 | -0.12384200 |
| C | -0.88772000 | 0.32417300  | 1.49988900  |
| C | -0.85476300 | -0.96764600 | 1.28603200  |
| S | 2.28030500  | 0.79685400  | -0.35995400 |
| O | 2.53475800  | 2.08987200  | -1.02441100 |
| O | 2.08200500  | 0.86634900  | 1.11263100  |
| O | 1.33027800  | -0.10274400 | -1.07150600 |
| C | 3.89464500  | -0.11622200 | -0.51305000 |
| F | 4.88774700  | 0.55885200  | 0.08725300  |
| F | 4.22838900  | -0.29589200 | -1.80082100 |
| F | 3.81047300  | -1.33135200 | 0.06597800  |
| H | -0.27553100 | 0.60271100  | 2.36104900  |
| C | -0.32834900 | -2.23818900 | 1.53687400  |
| C | 0.85789600  | -2.80007700 | 0.72713900  |
| C | 1.16886200  | -2.23707400 | 2.04819900  |
| H | -0.98855900 | -2.97147200 | 1.99181000  |
| H | 1.15206300  | -2.21482000 | -0.13786400 |
| H | 0.82643300  | -3.87821000 | 0.60805800  |
| H | 1.31403800  | -2.89094000 | 2.90182100  |
| H | 1.65195100  | -1.26628400 | 2.08066000  |

# 5h-M2<sub>6-endo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.21856200 | -0.66868600 | -0.03282100 |
| C | -3.46974300 | 0.67378600  | -0.43570800 |
| C | -4.60910900 | 0.96698900  | -1.22183600 |
| C | -5.48134000 | -0.03145800 | -1.60873400 |
| C | -5.23497900 | -1.36098800 | -1.21715900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.12818400 | -1.67004200 | -0.44653500 |
| C | -2.04291500 | -0.94115100 | 0.78381900  |
| C | -1.16724700 | 0.13079600  | 1.14062900  |
| C | -0.02476400 | -0.15591700 | 1.92865400  |
| C | 0.24780000  | -1.44301700 | 2.36831500  |
| C | -0.61811400 | -2.49833700 | 2.01807200  |
| C | -1.73275600 | -2.24453700 | 1.24168300  |
| H | -4.78591800 | 1.99719500  | -1.51901600 |
| H | -6.35168100 | 0.20548000  | -2.21315100 |
| H | -5.91600500 | -2.15014300 | -1.52111800 |
| H | -3.96655100 | -2.70388700 | -0.16390300 |
| H | 1.51942600  | -1.54366900 | 0.57608600  |
| H | 0.64517200  | 0.65288500  | 2.19625100  |
| H | 1.11265800  | -1.63192700 | 2.99831300  |
| H | -0.41185400 | -3.50796800 | 2.35890800  |
| H | -2.38247500 | -3.07300400 | 0.98548400  |
| C | -2.57178400 | 1.71755300  | -0.03774300 |
| C | -1.45323700 | 1.48736800  | 0.70916700  |
| S | 2.70701000  | -0.90273000 | -1.12942500 |
| O | 3.51481200  | -1.67679900 | -2.05437300 |
| O | 1.56257700  | -0.11183800 | -1.56216400 |
| O | 2.29680300  | -1.88833500 | 0.07335300  |
| C | 3.85671300  | 0.25901500  | -0.22107500 |
| F | 4.22542400  | 1.22743400  | -1.05496500 |
| F | 4.92654400  | -0.40351300 | 0.20574500  |
| F | 3.21242900  | 0.78872200  | 0.82367200  |
| H | -2.80950400 | 2.73068900  | -0.34829100 |
| C | -0.54159800 | 2.60314400  | 1.11791600  |
| C | 0.74320800  | 2.88569300  | 0.35721900  |
| C | -0.40022000 | 3.86502400  | 0.30407400  |
| H | -0.46803100 | 2.74066800  | 2.19612700  |
| H | 0.93390400  | 2.28828500  | -0.52823000 |
| H | 1.62918900  | 3.14456200  | 0.92874000  |
| H | -0.30537900 | 4.80281400  | 0.84249000  |
| H | -0.94723800 | 3.94228900  | -0.63010700 |

**5i-TS1<sub>5-exo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.28890000 | -2.23953200 | -0.01628500 |
| C | -1.37296400 | -2.07103400 | -1.10747100 |
| C | -1.65161400 | -2.64545500 | -2.37924200 |
| C | -2.81961400 | -3.35508200 | -2.58441600 |
| C | -3.72954000 | -3.49471900 | -1.52701300 |
| C | -3.46824800 | -2.94626800 | -0.27129000 |
| C | -2.02568300 | -1.68820500 | 1.33052000  |
| C | -0.79266400 | -1.88784500 | 1.97524700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.57110200 | -1.37452300 | 3.25184800  |
| C | -1.57273900 | -0.64957200 | 3.90026300  |
| C | -2.80242600 | -0.44682300 | 3.26951000  |
| C | -3.03167000 | -0.96810400 | 1.99836000  |
| H | -0.93963600 | -2.49726900 | -3.18347000 |
| H | -3.03407800 | -3.78979000 | -3.55429000 |
| H | -4.65075400 | -4.04790400 | -1.68189600 |
| H | -4.17877700 | -3.09169900 | 0.53502500  |
| H | -0.01913500 | -2.47532800 | 1.49109700  |
| H | 0.38199000  | -1.54683200 | 3.74220800  |
| H | -1.39698700 | -0.24681000 | 4.89302200  |
| H | -3.58244200 | 0.12253600  | 3.76529400  |
| H | -3.97998600 | -0.78836900 | 1.50217500  |
| C | -0.23507100 | -1.28379400 | -0.98487300 |
| C | 0.70512000  | -0.44149000 | -0.95815500 |
| S | -1.61772800 | 2.28053700  | -1.30641500 |
| O | -2.05230600 | 3.39843800  | -2.14734000 |
| O | -2.42531700 | 1.05174500  | -1.29027900 |
| O | -0.12196700 | 1.98107200  | -1.48178900 |
| C | -1.67430600 | 2.91918700  | 0.44035400  |
| F | -2.93629800 | 3.21351100  | 0.77298000  |
| F | -0.92575200 | 4.02089700  | 0.56139900  |
| F | -1.21153300 | 1.98737600  | 1.28415900  |
| H | 0.19411900  | 0.68519900  | -1.25336300 |
| C | 2.13609700  | -0.39114200 | -0.65722600 |
| C | 2.78695700  | 0.85133500  | -0.57333200 |
| C | 2.86966500  | -1.57623200 | -0.45195600 |
| C | 4.14544700  | 0.91501300  | -0.28276900 |
| H | 2.22458800  | 1.76356300  | -0.73490400 |
| C | 4.22574900  | -1.52173200 | -0.16252600 |
| H | 2.37364100  | -2.53774200 | -0.52731100 |
| C | 4.84391500  | -0.27327400 | -0.08067300 |
| H | 4.66265200  | 1.86301200  | -0.21267800 |
| H | 4.80567300  | -2.42125100 | -0.00194200 |
| N | 6.27855900  | -0.21237600 | 0.22618900  |
| O | 6.87616300  | -1.27563800 | 0.40192800  |
| O | 6.80801000  | 0.89768400  | 0.29251300  |

# 5i-M1<sub>5-exo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.81615600 | -2.39312600 | -0.14500900 |
| C | -0.99558500 | -1.95251800 | -1.25146100 |
| C | -1.23391200 | -2.44735000 | -2.57592900 |
| C | -2.27154300 | -3.31941300 | -2.81379600 |
| C | -3.09372000 | -3.71248200 | -1.74206100 |
| C | -2.87142200 | -3.25975600 | -0.44194100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.56766400 | -1.95822100 | 1.23833400  |
| C | -0.26693300 | -1.93379100 | 1.77603500  |
| C | -0.05484800 | -1.53259000 | 3.09248000  |
| C | -1.13350200 | -1.14294400 | 3.88893800  |
| C | -2.42968600 | -1.16585100 | 3.36711300  |
| C | -2.64877500 | -1.57907700 | 2.05678400  |
| H | -0.59705100 | -2.09645000 | -3.37986100 |
| H | -2.46230000 | -3.69071900 | -3.81408700 |
| H | -3.91514300 | -4.39815200 | -1.92622000 |
| H | -3.50661600 | -3.61467700 | 0.36172800  |
| H | 0.57306700  | -2.27203900 | 1.17828300  |
| H | 0.95162800  | -1.53201700 | 3.49853300  |
| H | -0.96562200 | -0.82599500 | 4.91346700  |
| H | -3.26971700 | -0.85480700 | 3.97980100  |
| H | -3.65343200 | -1.56773300 | 1.64714500  |
| C | -0.06732000 | -0.96144600 | -1.10094900 |
| C | 0.76634300  | 0.01904800  | -1.02338800 |
| S | -1.98926800 | 2.30617800  | -1.15422200 |
| O | -2.81283900 | 3.28392600  | -1.88391200 |
| O | -2.26160900 | 0.87567800  | -1.43953800 |
| O | -0.52526600 | 2.62644600  | -1.11857000 |
| C | -2.50288800 | 2.50009700  | 0.62225400  |
| F | -3.81167500 | 2.23873100  | 0.76355100  |
| F | -2.27162200 | 3.74831100  | 1.05423300  |
| F | -1.81812300 | 1.64878400  | 1.40480600  |
| H | 0.28104400  | 1.01669100  | -1.18056000 |
| C | 2.20481200  | 0.02850100  | -0.71444900 |
| C | 2.82258100  | 1.27128700  | -0.49795600 |
| C | 2.96443600  | -1.15277800 | -0.63254300 |
| C | 4.17826100  | 1.33894900  | -0.19589000 |
| H | 2.23275300  | 2.17903000  | -0.56398600 |
| C | 4.31815900  | -1.09550100 | -0.33158300 |
| H | 2.49816600  | -2.11504900 | -0.81771900 |
| C | 4.90445800  | 0.15257900  | -0.11625600 |
| H | 4.67193100  | 2.28656100  | -0.02426600 |
| H | 4.92126800  | -1.99156600 | -0.26542400 |
| N | 6.33723200  | 0.21563200  | 0.20168400  |
| O | 6.95974800  | -0.84560600 | 0.26811300  |
| O | 6.83870300  | 1.32512000  | 0.38556300  |

# 5i-TS2<sub>5-exo</sub>

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -2.29640200 | -2.69130900 | 0.61386600 |
| C | -1.13579300 | -1.98244500 | 1.05639200 |
| C | -0.56743500 | -2.25200900 | 2.33129100 |
| C | -1.07002700 | -3.30667500 | 3.06662000 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.16589000 | -4.05926400 | 2.59000900  |
| C | -2.78098500 | -3.75802800 | 1.38194400  |
| C | -2.86254600 | -2.14957900 | -0.60365300 |
| C | -2.57268100 | -0.77772900 | -0.86597600 |
| C | -2.81309300 | -0.23801300 | -2.14805900 |
| C | -3.42136600 | -1.02368300 | -3.11174200 |
| C | -3.78806900 | -2.35538300 | -2.82184300 |
| C | -3.51430700 | -2.91899600 | -1.58466800 |
| H | 0.27426000  | -1.66726200 | 2.68355800  |
| H | -0.62321200 | -3.55827100 | 4.02237800  |
| H | -2.55571500 | -4.86834600 | 3.19920500  |
| H | -3.66000400 | -4.30683000 | 1.06188800  |
| H | -2.47956300 | -0.05731500 | -0.04340500 |
| H | -2.56382000 | 0.80139400  | -2.33257600 |
| H | -3.64556200 | -0.60889700 | -4.08915800 |
| H | -4.26043000 | -2.95810400 | -3.59110500 |
| H | -3.72853100 | -3.96647300 | -1.40049900 |
| C | -0.60942000 | -1.03361200 | 0.18180500  |
| C | 0.30330700  | -0.22527000 | -0.30731000 |
| H | -0.05908500 | 0.72298300  | -0.72962000 |
| S | -1.69557200 | 2.92587300  | 0.01933300  |
| O | -1.04204000 | 2.39497200  | -1.21647700 |
| O | -2.66102400 | 4.01590800  | -0.20585200 |
| O | -2.12214800 | 1.86081000  | 0.96323100  |
| C | -0.27443900 | 3.73902200  | 0.90331400  |
| F | 0.22100600  | 4.75329200  | 0.18024200  |
| F | 0.72016400  | 2.84918600  | 1.10659000  |
| F | -0.65610500 | 4.21453900  | 2.09669400  |
| C | 1.75407400  | -0.46727700 | -0.36211300 |
| C | 2.58602400  | 0.63080700  | -0.64753500 |
| C | 2.32726100  | -1.73440800 | -0.14589400 |
| C | 3.96575800  | 0.47379800  | -0.70405300 |
| H | 2.14426700  | 1.60816800  | -0.80575900 |
| C | 3.70322800  | -1.90198600 | -0.20475100 |
| H | 1.69385800  | -2.59149700 | 0.05579100  |
| C | 4.50369200  | -0.79242600 | -0.48204700 |
| H | 4.62039000  | 1.30874100  | -0.91743000 |
| H | 4.16192800  | -2.86923000 | -0.04629900 |
| N | 5.95960100  | -0.96824700 | -0.54654000 |
| O | 6.41325400  | -2.09659600 | -0.34694400 |
| O | 6.64973700  | 0.02094600  | -0.79593500 |

# 5i-M2<sub>5-exo</sub>

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.28759800 | -3.23199300 | 0.41386200 |
| C | -0.07429400 | -2.50548100 | 0.28909700 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 1. 04245100  | -2. 90963400 | 1. 02546700  |
| C | 0. 95241700  | -4. 03999800 | 1. 84329800  |
| C | -0. 23962800 | -4. 76533000 | 1. 93844200  |
| C | -1. 37170400 | -4. 35983300 | 1. 22733400  |
| C | -2. 31928000 | -2. 56904200 | -0. 39242900 |
| C | -1. 73907700 | -1. 43397400 | -0. 99999000 |
| C | -2. 50303300 | -0. 62453900 | -1. 84763000 |
| C | -3. 85360500 | -0. 94248400 | -2. 05454900 |
| C | -4. 42706300 | -2. 06062600 | -1. 43509100 |
| C | -3. 66092300 | -2. 88539200 | -0. 60780800 |
| H | 1. 97442400  | -2. 36051900 | 0. 97991500  |
| H | 1. 82149600  | -4. 35556800 | 2. 41234700  |
| H | -0. 28827800 | -5. 64293500 | 2. 57588900  |
| H | -2. 30301300 | -4. 91125200 | 1. 31725500  |
| H | -3. 26622400 | 0. 87631600  | -0. 42301500 |
| H | -2. 06194500 | 0. 22168400  | -2. 36649400 |
| H | -4. 45489400 | -0. 32266700 | -2. 71251900 |
| H | -5. 47289600 | -2. 29310200 | -1. 60928400 |
| H | -4. 10850200 | -3. 75766800 | -0. 14072700 |
| C | -0. 31091400 | -1. 34253300 | -0. 60526400 |
| C | 0. 47878200  | -0. 30694300 | -0. 98143700 |
| H | -0. 01592800 | 0. 50763800  | -1. 50745600 |
| S | -2. 48536300 | 2. 87243600  | -0. 10842200 |
| O | -1. 65299600 | 2. 62082800  | -1. 28079600 |
| O | -3. 20725700 | 4. 11707700  | 0. 07833100  |
| O | -3. 53151200 | 1. 66894700  | 0. 10270200  |
| C | -1. 38950900 | 2. 62675500  | 1. 38804500  |
| F | -0. 33325100 | 3. 43169000  | 1. 26283300  |
| F | -0. 97985400 | 1. 35946700  | 1. 43121200  |
| F | -2. 05746100 | 2. 92485500  | 2. 49541200  |
| C | 1. 91354700  | -0. 07796900 | -0. 76617200 |
| C | 2. 34853800  | 1. 21260100  | -0. 40134700 |
| C | 2. 88113300  | -1. 07503000 | -0. 99705000 |
| C | 3. 69764100  | 1. 49221600  | -0. 22942400 |
| H | 1. 61486200  | 1. 99428600  | -0. 23339300 |
| C | 4. 23543700  | -0. 80710500 | -0. 83958600 |
| H | 2. 56661600  | -2. 05900300 | -1. 32598000 |
| C | 4. 62596400  | 0. 47397100  | -0. 44935200 |
| H | 4. 03866800  | 2. 47616200  | 0. 06544600  |
| H | 4. 98603400  | -1. 56512400 | -1. 02283900 |
| N | 6. 05132600  | 0. 76138000  | -0. 27785800 |
| O | 6. 85468100  | -0. 15420900 | -0. 47144400 |
| O | 6. 37652100  | 1. 90400700  | 0. 05308300  |

5i-TS1<sub>6-endo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.75177900  | 3.21871300  | 0.00746700  |
| C | 1.47188400  | 2.05010300  | -0.34543700 |
| C | 2.85882700  | 2.10150600  | -0.54639100 |
| C | 3.54173900  | 3.30706100  | -0.40745200 |
| C | 2.84010000  | 4.46695400  | -0.07815500 |
| C | 1.45894400  | 4.41941200  | 0.12625000  |
| C | -0.71771400 | 3.17911600  | 0.24837000  |
| C | -1.61279700 | 3.73555500  | -0.68122500 |
| C | -2.98606000 | 3.71231500  | -0.44067500 |
| C | -3.48499900 | 3.14093800  | 0.73439900  |
| C | -2.60523500 | 2.59401400  | 1.66923400  |
| C | -1.23046000 | 2.60840100  | 1.42789000  |
| H | 3.38929600  | 1.19284000  | -0.80804600 |
| H | 4.61524400  | 3.34005700  | -0.56196100 |
| H | 3.36539800  | 5.41139100  | 0.02458400  |
| H | 0.91967100  | 5.32234900  | 0.39454800  |
| H | -1.22519500 | 4.18386600  | -1.59103900 |
| H | -3.66750400 | 4.14490800  | -1.16693600 |
| H | -4.55436500 | 3.13076900  | 0.92180500  |
| H | -2.98592800 | 2.16052000  | 2.58890100  |
| H | -0.54470800 | 2.19588600  | 2.16189200  |
| C | 0.76468600  | 0.78722900  | -0.54578100 |
| C | -0.41702200 | 0.34343700  | -0.40949700 |
| S | 2.44981700  | -2.36305800 | -0.41161900 |
| O | 2.67118500  | -3.64978700 | -1.08261900 |
| O | 2.40389600  | -1.18988800 | -1.37800200 |
| O | 1.38793000  | -2.29874800 | 0.61105500  |
| C | 4.02180400  | -2.02766200 | 0.52404300  |
| F | 5.07741400  | -2.06556800 | -0.29778800 |
| F | 4.19126700  | -2.94158600 | 1.48686600  |
| F | 3.96938500  | -0.81197700 | 1.09344800  |
| H | 1.41875700  | -0.12708400 | -0.95218200 |
| C | -1.60607600 | -0.38797300 | -0.31146600 |
| C | -1.73924900 | -1.37388800 | 0.69902200  |
| C | -2.66457500 | -0.14672800 | -1.22255000 |
| C | -2.91187900 | -2.10885700 | 0.78924800  |
| H | -0.90444200 | -1.56860100 | 1.36060700  |
| C | -3.84446000 | -0.86647400 | -1.11365700 |
| H | -2.54739900 | 0.60750400  | -1.99127500 |
| C | -3.94049800 | -1.83252000 | -0.11168900 |
| H | -3.04223400 | -2.87897000 | 1.53795000  |
| H | -4.67491900 | -0.70355900 | -1.78752200 |
| N | -5.19807400 | -2.60516100 | -0.00202400 |
| O | -6.08797100 | -2.36066400 | -0.81391300 |
| O | -5.27594700 | -3.44073200 | 0.89526800  |

**5i-M1<sub>6-endo</sub>**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.75185400  | 3.19673300  | 0.00531900  |
| C | 1.48644500  | 2.05993900  | -0.40886200 |
| C | 2.86965500  | 2.14096200  | -0.62130700 |
| C | 3.53277700  | 3.35109500  | -0.43277300 |
| C | 2.81571100  | 4.48179700  | -0.04006000 |
| C | 1.43744300  | 4.40269500  | 0.17701900  |
| C | -0.71344700 | 3.10220500  | 0.25813300  |
| C | -1.64104900 | 3.55705000  | -0.69645500 |
| C | -3.00919000 | 3.48198200  | -0.44171100 |
| C | -3.47129200 | 2.95905000  | 0.77120600  |
| C | -2.56048300 | 2.51288700  | 1.73012200  |
| C | -1.19030000 | 2.58011400  | 1.47611600  |
| H | 3.41131100  | 1.25254200  | -0.92726300 |
| H | 4.60382600  | 3.41066800  | -0.59615300 |
| H | 3.32719300  | 5.42864400  | 0.10237300  |
| H | 0.88657300  | 5.28304000  | 0.49250100  |
| H | -1.28109100 | 3.96998900  | -1.63388500 |
| H | -3.71630800 | 3.83761300  | -1.18486700 |
| H | -4.53765500 | 2.90903700  | 0.96884300  |
| H | -2.91444600 | 2.11718700  | 2.67696300  |
| H | -0.47946800 | 2.24288000  | 2.22442200  |
| C | 0.79648500  | 0.79216000  | -0.64475300 |
| C | -0.40484600 | 0.38360900  | -0.48901400 |
| S | 2.47719400  | -2.37396800 | -0.45726500 |
| O | 2.74601100  | -3.69300900 | -1.04824300 |
| O | 2.51087100  | -1.24365500 | -1.45931800 |
| O | 1.34031200  | -2.27895300 | 0.48318900  |
| C | 3.96831800  | -2.00902100 | 0.59149700  |
| F | 5.08796600  | -2.05964500 | -0.14219200 |
| F | 4.06993000  | -2.89730800 | 1.58911600  |
| F | 3.86923400  | -0.77951000 | 1.12689900  |
| H | 1.43441700  | -0.07771100 | -1.05896400 |
| C | -1.59896300 | -0.32609100 | -0.36203200 |
| C | -1.73086000 | -1.28453200 | 0.67759300  |
| C | -2.66266800 | -0.10774100 | -1.27533700 |
| C | -2.90414800 | -2.01334700 | 0.79326400  |
| H | -0.89176600 | -1.46474300 | 1.33771400  |
| C | -3.84214300 | -0.82382400 | -1.14265500 |
| H | -2.54634300 | 0.62224000  | -2.06686000 |
| C | -3.93498700 | -1.76010700 | -0.11259900 |
| H | -3.03329400 | -2.76267400 | 1.56293900  |
| H | -4.67471400 | -0.68069600 | -1.81836600 |
| N | -5.19450100 | -2.52757700 | 0.02367700  |
| O | -6.08682500 | -2.30311300 | -0.79091300 |

|                               |             |             |             |
|-------------------------------|-------------|-------------|-------------|
| O                             | -5.26935400 | -3.33739500 | 0.94408800  |
| <b>5q-TS1<sub>5-exo</sub></b> |             |             |             |
| C                             | -2.73578700 | -1.75084100 | 0.04588800  |
| C                             | -1.81708600 | -1.89667100 | -1.04440100 |
| C                             | -2.24614600 | -2.46900400 | -2.27261700 |
| C                             | -3.56054600 | -2.86574800 | -2.44070100 |
| C                             | -4.46655100 | -2.69370200 | -1.38557800 |
| C                             | -4.06013700 | -2.14736200 | -0.16827400 |
| C                             | -2.32543100 | -1.20408600 | 1.35821500  |
| C                             | -1.18486500 | -1.68383700 | 2.02450000  |
| C                             | -0.82690100 | -1.17414100 | 3.27142500  |
| C                             | -1.59838000 | -0.17548000 | 3.86870100  |
| C                             | -2.73474300 | 0.30769100  | 3.21570100  |
| C                             | -3.10056900 | -0.20617900 | 1.97357100  |
| H                             | -1.52678000 | -2.56611800 | -3.07827500 |
| H                             | -3.88770700 | -3.29670500 | -3.38049300 |
| H                             | -5.50068300 | -3.00015000 | -1.51007200 |
| H                             | -4.77582200 | -2.05046000 | 0.64099800  |
| H                             | -0.59515800 | -2.47913700 | 1.57976000  |
| H                             | 0.05155200  | -1.56164400 | 3.77814600  |
| H                             | -1.31658100 | 0.22354000  | 4.83836500  |
| H                             | -3.33356300 | 1.09070400  | 3.67053300  |
| H                             | -3.96918200 | 0.18909300  | 1.45714900  |
| C                             | -0.51180700 | -1.41376800 | -0.96068100 |
| C                             | 0.59658500  | -0.81209900 | -0.97654400 |
| S                             | -0.90227700 | 2.45687200  | -1.30698600 |
| O                             | -1.09913800 | 3.70854700  | -2.04441600 |
| O                             | -2.08107100 | 1.65213100  | -0.95616500 |
| O                             | 0.22704500  | 1.61449700  | -1.91231700 |
| C                             | -0.15627800 | 2.95035000  | 0.32432900  |
| F                             | -0.99582600 | 3.74335700  | 0.99829900  |
| F                             | 0.99680300  | 3.60521700  | 0.13247800  |
| F                             | 0.09295500  | 1.85757300  | 1.06111100  |
| H                             | 0.29724000  | 0.32756800  | -1.44054200 |
| C                             | 2.00601700  | -0.98053900 | -0.64657800 |
| C                             | 2.87875700  | 0.11616000  | -0.66957400 |
| C                             | 2.51862000  | -2.24619800 | -0.29107200 |
| C                             | 4.22644700  | -0.03088200 | -0.34591800 |
| H                             | 2.49912900  | 1.09641500  | -0.93621500 |
| C                             | 3.85576000  | -2.40088400 | 0.02891400  |
| H                             | 1.85835200  | -3.10756100 | -0.27466000 |
| C                             | 4.72320300  | -1.29318200 | 0.00532000  |
| H                             | 4.87338400  | 0.83688900  | -0.37088600 |
| H                             | 4.25818000  | -3.37078400 | 0.30144900  |

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 6.01404900 | -1.55177500 | 0.33636300  |
| C | 6.94737300 | -0.47211400 | 0.33516000  |
| H | 6.66329000 | 0.30146700  | 1.05739100  |
| H | 7.90397200 | -0.90572500 | 0.62661700  |
| H | 7.03914000 | -0.02477100 | -0.66092200 |

# 5q-M1<sub>5-exo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.59562400 | -2.55045500 | -0.59058200 |
| C | -0.90571200 | -1.67371200 | -1.50929900 |
| C | -1.30618900 | -1.60872900 | -2.88320600 |
| C | -2.37778200 | -2.34745600 | -3.33418100 |
| C | -3.06676300 | -3.17200700 | -2.42861500 |
| C | -2.68312000 | -3.27203700 | -1.09146700 |
| C | -1.18352700 | -2.70071900 | 0.81535400  |
| C | 0.17276300  | -2.80345100 | 1.17672700  |
| C | 0.54070600  | -2.95539800 | 2.51148700  |
| C | -0.43663500 | -3.00368500 | 3.50705600  |
| C | -1.78743100 | -2.90825900 | 3.16124300  |
| C | -2.16015800 | -2.76672200 | 1.82807700  |
| H | -0.76576100 | -0.94036900 | -3.54344800 |
| H | -2.69197000 | -2.28897100 | -4.36996400 |
| H | -3.91030000 | -3.75933500 | -2.77845800 |
| H | -3.21744900 | -3.94890800 | -0.43443900 |
| H | 0.93890500  | -2.80783400 | 0.40911600  |
| H | 1.59061300  | -3.04403800 | 2.77169000  |
| H | -0.14838300 | -3.11884600 | 4.54727300  |
| H | -2.55088300 | -2.93646800 | 3.93217900  |
| H | -3.20906300 | -2.66362200 | 1.56994400  |
| C | 0.05721300  | -0.79317800 | -1.09011300 |
| C | 0.90089800  | 0.12736600  | -0.76735900 |
| S | -1.77274500 | 2.61932100  | -0.58322800 |
| O | -2.30819900 | 3.71675100  | -1.40864700 |
| O | -2.15281700 | 1.24714500  | -0.99623700 |
| O | -0.32149800 | 2.75044500  | -0.23717000 |
| C | -2.61133600 | 2.83978700  | 1.06200600  |
| F | -3.94298300 | 2.72962200  | 0.93025200  |
| F | -2.33697900 | 4.04734200  | 1.57891300  |
| F | -2.19855700 | 1.90548900  | 1.93467300  |
| H | 0.38545700  | 1.10317800  | -0.57179500 |
| C | 2.35643300  | 0.12181300  | -0.60046800 |
| C | 2.97771000  | 1.27874800  | -0.11043300 |
| C | 3.15508100  | -0.99693900 | -0.91270100 |
| C | 4.35727000  | 1.32949200  | 0.07873300  |
| H | 2.37083100  | 2.14729700  | 0.12500800  |
| C | 4.52567600  | -0.95589000 | -0.72912100 |

|   |            |             |             |
|---|------------|-------------|-------------|
| H | 2.69772200 | -1.89629400 | -1.31507100 |
| C | 5.13974400 | 0.20787200  | -0.22823400 |
| H | 4.80686000 | 2.23769000  | 0.45991300  |
| H | 5.15008600 | -1.80976100 | -0.96941200 |
| O | 6.48705700 | 0.14251900  | -0.08395700 |
| C | 7.17629700 | 1.28842700  | 0.41603400  |
| H | 6.83744600 | 1.54837800  | 1.42508900  |
| H | 8.22975500 | 1.01075800  | 0.44801200  |
| H | 7.04728900 | 2.15184200  | -0.24606400 |

# 5q-TS2<sub>5-exo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.88757500  | -2.01887600 | -0.57570900 |
| C | 1.55686700  | -1.72434300 | -1.00917800 |
| C | 1.09179200  | -2.19508200 | -2.26773200 |
| C | 1.89369200  | -3.05482400 | -2.99201600 |
| C | 3.17961600  | -3.40388400 | -2.52546200 |
| C | 3.67956600  | -2.88949900 | -1.33676700 |
| C | 3.26546800  | -1.30745400 | 0.62690700  |
| C | 2.54720400  | -0.10447700 | 0.88610600  |
| C | 2.61883700  | 0.50163600  | 2.15880300  |
| C | 3.46450200  | -0.03006700 | 3.11707900  |
| C | 4.24162300  | -1.17263500 | 2.83031500  |
| C | 4.14764200  | -1.80935400 | 1.60218500  |
| H | 0.10323100  | -1.91768100 | -2.61529900 |
| H | 1.53719900  | -3.45961200 | -3.93325700 |
| H | 3.80093300  | -4.06028800 | -3.12623400 |
| H | 4.69247900  | -3.11930300 | -1.02376600 |
| H | 2.21233000  | 0.53520800  | 0.05925200  |
| H | 2.04806100  | 1.40622700  | 2.33979100  |
| H | 3.55502600  | 0.44776700  | 4.08736600  |
| H | 4.89750000  | -1.57795800 | 3.59444000  |
| H | 4.69116400  | -2.73076400 | 1.42061300  |
| C | 0.75781700  | -0.97487600 | -0.14597500 |
| C | -0.36655000 | -0.45173000 | 0.29885100  |
| H | -0.29084900 | 0.56996800  | 0.69519200  |
| S | 0.60208700  | 3.17876200  | -0.05435800 |
| O | 0.13337300  | 2.49309600  | 1.18781700  |
| O | 1.15326100  | 4.53079400  | 0.14917800  |
| O | 1.37133900  | 2.29319700  | -0.96558400 |
| C | -0.98808500 | 3.46464700  | -0.97669100 |
| F | -1.81026200 | 4.26199200  | -0.27755500 |
| F | -1.62544100 | 2.29540900  | -1.18896500 |
| F | -0.75900300 | 4.03536100  | -2.16845000 |
| C | -1.68704000 | -1.07650300 | 0.36832600  |
| C | -2.77274000 | -0.27491500 | 0.75819900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.92791300 | -2.43211100 | 0.05812600  |
| C | -4.06367200 | -0.79086400 | 0.82929400  |
| H | -2.60126800 | 0.77069400  | 0.99292200  |
| C | -3.20503000 | -2.95549500 | 0.13150900  |
| H | -1.10506000 | -3.07881600 | -0.23047500 |
| C | -4.28716200 | -2.13915100 | 0.51587700  |
| H | -4.87844700 | -0.14339800 | 1.12778700  |
| H | -3.39879700 | -3.99761200 | -0.09884800 |
| O | -5.49557000 | -2.75059900 | 0.55515600  |
| C | -6.63744800 | -1.98493000 | 0.94240400  |
| H | -7.48240900 | -2.67207400 | 0.90335900  |
| H | -6.52921800 | -1.59740700 | 1.96135300  |
| H | -6.81149800 | -1.15317800 | 0.25102500  |

### 5q-M2<sub>5-exo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.16408500  | -3.28464500 | -0.38623000 |
| C | -0.06829600 | -2.58811600 | -0.26110800 |
| C | -1.18321100 | -3.04851800 | -0.96912100 |
| C | -1.07203300 | -4.19911700 | -1.75464000 |
| C | 0.13873600  | -4.89470000 | -1.84767900 |
| C | 1.26789600  | -4.43480700 | -1.16758700 |
| C | 2.18862800  | -2.56787400 | 0.37794100  |
| C | 1.58471000  | -1.42904200 | 0.95812600  |
| C | 2.34311000  | -0.57276800 | 1.76584900  |
| C | 3.70570200  | -0.84556600 | 1.95722300  |
| C | 4.30125800  | -1.96696000 | 1.36368500  |
| C | 3.54329900  | -2.83874700 | 0.57933800  |
| H | -2.13007600 | -2.52549200 | -0.92384300 |
| H | -1.94046200 | -4.55606300 | -2.30031400 |
| H | 0.20258800  | -5.79007800 | -2.45876500 |
| H | 2.21418600  | -4.96095400 | -1.25586800 |
| H | 3.06747100  | 0.91114400  | 0.33168500  |
| H | 1.88667900  | 0.27298700  | 2.27219800  |
| H | 4.29976200  | -0.18882200 | 2.58571400  |
| H | 5.35611800  | -2.16462100 | 1.52664500  |
| H | 4.00654000  | -3.71406400 | 0.13312900  |
| C | 0.15069600  | -1.38913300 | 0.58651100  |
| C | -0.65876700 | -0.35526600 | 0.93529100  |
| H | -0.16020300 | 0.48901500  | 1.41025900  |
| S | 2.33725500  | 2.93551800  | 0.06453000  |
| O | 1.60900200  | 2.73123800  | 1.31259000  |
| O | 3.08695600  | 4.14856700  | -0.20610800 |
| O | 3.31009600  | 1.68974800  | -0.22778000 |
| C | 1.09632300  | 2.72701700  | -1.31964300 |
| F | 0.09652200  | 3.58448600  | -1.10912300 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 0.62323300  | 1.48165100  | -1.30805200 |
| F | 1.67159200  | 2.98115100  | -2.48912600 |
| C | -2.10009400 | -0.16070200 | 0.76441000  |
| C | -2.58580500 | 1.12263100  | 0.45784200  |
| C | -3.04867800 | -1.18184800 | 0.98103600  |
| C | -3.94802300 | 1.37940300  | 0.31722900  |
| H | -1.87991000 | 1.93371500  | 0.30246000  |
| C | -4.40808600 | -0.93813900 | 0.86036900  |
| H | -2.71125300 | -2.16895200 | 1.27839400  |
| C | -4.87091100 | 0.34301900  | 0.51606200  |
| H | -4.27702000 | 2.37943400  | 0.06282900  |
| H | -5.13600200 | -1.72229800 | 1.04087800  |
| O | -6.22071200 | 0.47727900  | 0.41481800  |
| C | -6.75241300 | 1.75742800  | 0.08174000  |
| H | -7.83504700 | 1.63290200  | 0.05302500  |
| H | -6.49322000 | 2.50762100  | 0.83763500  |
| H | -6.39984200 | 2.09469300  | -0.89986300 |

# 5q-TS1<sub>6-endo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.05729400 | 3.30692000  | 0.04365400  |
| C | 0.83368500  | 2.22684400  | -0.19527200 |
| C | 2.21235200  | 2.47413500  | -0.30638400 |
| C | 2.71950400  | 3.76537900  | -0.19318300 |
| C | 1.84796800  | 4.83328100  | 0.01802400  |
| C | 0.47745000  | 4.59895200  | 0.13292000  |
| C | -1.52783600 | 3.12423500  | 0.19528200  |
| C | -2.41386100 | 3.75761100  | -0.69079000 |
| C | -3.79382100 | 3.62813000  | -0.53149300 |
| C | -4.31064800 | 2.86964500  | 0.52104700  |
| C | -3.43950600 | 2.24227500  | 1.41362500  |
| C | -2.05916100 | 2.36681600  | 1.25207600  |
| H | 2.88342100  | 1.64125900  | -0.48103100 |
| H | 3.78818400  | 3.93490300  | -0.27762600 |
| H | 2.23064400  | 5.84602200  | 0.09990000  |
| H | -0.19850700 | 5.42883500  | 0.31480100  |
| H | -2.01459000 | 4.34655400  | -1.51130900 |
| H | -4.46471700 | 4.12039600  | -1.22939600 |
| H | -5.38478200 | 2.77197300  | 0.64711300  |
| H | -3.83342300 | 1.66044100  | 2.24168800  |
| H | -1.38672100 | 1.89267500  | 1.96054800  |
| C | 0.34625000  | 0.86615000  | -0.38904400 |
| C | -0.66528800 | 0.12177000  | -0.34168800 |
| S | 2.59244000  | -1.94325300 | -0.26124100 |
| O | 2.84263000  | -3.17693400 | -1.01034900 |
| O | 2.21842900  | -0.77392100 | -1.19172100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.73688400  | -2.00330100 | 0.93211800  |
| C | 4.26115800  | -1.39334700 | 0.35387200  |
| F | 5.12832400  | -1.30814700 | -0.65909000 |
| F | 4.72216700  | -2.27131800 | 1.25049100  |
| F | 4.16376100  | -0.19065500 | 0.94019900  |
| H | 1.25029100  | -0.02112100 | -0.78187600 |
| C | -1.62416100 | -0.88929900 | -0.32875800 |
| C | -1.67108500 | -1.81376400 | 0.74497200  |
| C | -2.56864900 | -1.01214700 | -1.38513500 |
| C | -2.61571700 | -2.82452200 | 0.76858600  |
| H | -0.93329500 | -1.73664800 | 1.53496400  |
| C | -3.51939400 | -2.00694100 | -1.35525100 |
| H | -2.53587400 | -0.30857300 | -2.20954200 |
| C | -3.55147900 | -2.92379100 | -0.28054900 |
| H | -2.62407000 | -3.52972700 | 1.58954900  |
| H | -4.25141100 | -2.11491100 | -2.14765500 |
| O | -4.51314600 | -3.85817000 | -0.35174700 |
| C | -4.61803200 | -4.83958200 | 0.68792200  |
| H | -4.82337200 | -4.36712000 | 1.65354100  |
| H | -5.45616500 | -5.47514700 | 0.40560900  |
| H | -3.70590000 | -5.44057600 | 0.75315200  |

#### 5q-M1<sub>6-endo</sub>

|   |             |            |             |
|---|-------------|------------|-------------|
| C | 0.10480000  | 3.18826700 | 0.04233000  |
| C | 0.97234700  | 2.18667300 | -0.45105600 |
| C | 2.34030700  | 2.45671900 | -0.61430000 |
| C | 2.85285800  | 3.71180200 | -0.29677800 |
| C | 2.00109700  | 4.70710100 | 0.18355700  |
| C | 0.63975000  | 4.44284000 | 0.35136800  |
| C | -1.34988600 | 2.91842700 | 0.23621800  |
| C | -2.26164900 | 3.12105500 | -0.81391300 |
| C | -3.62219900 | 2.87836500 | -0.62627200 |
| C | -4.09022000 | 2.43196100 | 0.61240700  |
| C | -3.19383800 | 2.23598600 | 1.66542700  |
| C | -1.83276300 | 2.47869100 | 1.47999300  |
| H | 2.99209000  | 1.66732800 | -0.97372200 |
| H | 3.91236100  | 3.91026300 | -0.42315400 |
| H | 2.39302800  | 5.68893100 | 0.43085700  |
| H | -0.02069100 | 5.21770400 | 0.72823600  |
| H | -1.89768600 | 3.47355700 | -1.77447200 |
| H | -4.31749500 | 3.04347200 | -1.44392100 |
| H | -5.15003500 | 2.24558800 | 0.75809800  |
| H | -3.55439700 | 1.89765600 | 2.63218500  |
| H | -1.13515000 | 2.32810300 | 2.29842100  |
| C | 0.49239600  | 0.84419900 | -0.79975600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.64908000 | 0.25296500  | -0.66178800 |
| S | 2.68859100  | -2.09833600 | -0.47178100 |
| O | 3.16053400  | -3.42280600 | -0.91738700 |
| O | 2.65140200  | -1.05936600 | -1.54864200 |
| O | 1.49722900  | -2.09589000 | 0.40913400  |
| C | 4.04939600  | -1.47848900 | 0.63320300  |
| F | 5.22257200  | -1.45305900 | -0.01803900 |
| F | 4.18511800  | -2.26419900 | 1.71343200  |
| F | 3.78134300  | -0.22881000 | 1.05730700  |
| H | 1.24431400  | 0.14783900  | -1.24066800 |
| C | -1.70683700 | -0.59633900 | -0.51667300 |
| C | -1.72805100 | -1.50434000 | 0.59056500  |
| C | -2.77569000 | -0.64287700 | -1.47239700 |
| C | -2.74753800 | -2.41592500 | 0.73313600  |
| H | -0.89564800 | -1.48955700 | 1.28371900  |
| C | -3.79621100 | -1.54263500 | -1.32164300 |
| H | -2.76068100 | 0.04330200  | -2.31094600 |
| C | -3.79414400 | -2.44022800 | -0.22068800 |
| H | -2.73671700 | -3.11161700 | 1.56175200  |
| H | -4.61566100 | -1.60135700 | -2.02861800 |
| O | -4.82630000 | -3.27656700 | -0.17456400 |
| C | -4.92627700 | -4.24529800 | 0.88657500  |
| H | -4.99118500 | -3.74776300 | 1.85775400  |
| H | -5.84572000 | -4.79282300 | 0.68836700  |
| H | -4.07381800 | -4.92911400 | 0.86490100  |

#### 5q-TS2<sub>6-endo</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.74601200  | -0.08040100 | -0.00167400 |
| C | 3.33473200  | -0.43300200 | -1.31014100 |
| C | 4.18896300  | -0.18278800 | -2.39334500 |
| C | 5.42849400  | 0.42066200  | -2.19615400 |
| C | 5.83848700  | 0.76288200  | -0.90563200 |
| C | 5.00673700  | 0.50302700  | 0.18234000  |
| C | 2.85735600  | -0.37104000 | 1.13180800  |
| C | 1.46723800  | -0.10252600 | 1.00661700  |
| C | 0.59776200  | -0.38774200 | 2.09093800  |
| C | 1.08740500  | -0.96003800 | 3.24828900  |
| C | 2.46294000  | -1.24362100 | 3.35666600  |
| C | 3.33759200  | -0.95312500 | 2.31490700  |
| H | 3.87699700  | -0.46734700 | -3.39364300 |
| H | 6.07555200  | 0.61527100  | -3.04525700 |
| H | 6.80381100  | 1.23234600  | -0.74582200 |
| H | 5.31918600  | 0.78441700  | 1.18287600  |
| H | 1.11937800  | 0.63604900  | 0.28105100  |
| H | -0.45205600 | -0.13227600 | 1.99700200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.42391000  | -1.17795100 | 4.07863600  |
| H | 2.84611100  | -1.70143000 | 4.26365700  |
| H | 4.39189000  | -1.19259900 | 2.40624100  |
| C | 2.07348700  | -1.13715700 | -1.53952500 |
| C | 1.04540600  | -1.33889200 | -0.73892900 |
| S | -1.61751600 | 2.60585700  | -0.78806500 |
| O | -1.57738400 | 4.07162700  | -0.95849000 |
| O | -2.57542500 | 1.88306500  | -1.65944500 |
| O | -0.28810100 | 1.94902700  | -0.66715400 |
| C | -2.34027100 | 2.37958800  | 0.91223200  |
| F | -3.56471900 | 2.92167700  | 0.99710000  |
| F | -1.56429600 | 2.94408300  | 1.85177100  |
| F | -2.45403700 | 1.06417000  | 1.21309300  |
| H | 1.95972000  | -1.61768000 | -2.51413800 |
| C | -0.25893500 | -1.84645500 | -0.64082100 |
| C | -1.35245300 | -1.10290200 | -1.15461600 |
| C | -0.51123800 | -3.10119100 | -0.01562500 |
| C | -2.64156700 | -1.59737800 | -1.08164400 |
| H | -1.17931100 | -0.12696400 | -1.59063000 |
| C | -1.79049500 | -3.60050500 | 0.04573000  |
| H | 0.31730900  | -3.66627800 | 0.39764400  |
| C | -2.87104700 | -2.85220800 | -0.48442900 |
| H | -3.45287700 | -0.99813300 | -1.47333600 |
| H | -2.00306700 | -4.56293000 | 0.49761600  |
| O | -4.07647900 | -3.42510700 | -0.36284500 |
| C | -5.23528400 | -2.73675800 | -0.85768500 |
| H | -6.07628900 | -3.39575900 | -0.64740600 |
| H | -5.37345000 | -1.78331600 | -0.33974100 |
| H | -5.15790100 | -2.56797600 | -1.93576700 |

#### 5q-M2<sub>6-endo</sub>

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 3.83951200 | -0.28546500 | -0.00860600 |
| C | 3.35673500 | -1.38288000 | -0.77746400 |
| C | 4.22564300 | -2.04540200 | -1.67737000 |
| C | 5.53854600 | -1.64362400 | -1.82117900 |
| C | 6.02225500 | -0.56130100 | -1.06112500 |
| C | 5.19058200 | 0.10069700  | -0.17597100 |
| C | 2.92089900 | 0.38412600  | 0.90208600  |
| C | 1.57405700 | -0.08111200 | 1.02223300  |
| C | 0.68782800 | 0.61702400  | 1.88483900  |
| C | 1.10713300 | 1.71324500  | 2.62289600  |
| C | 2.43770200 | 2.15900100  | 2.51587300  |
| C | 3.31516300 | 1.50539100  | 1.67274500  |
| H | 3.83874800 | -2.88047400 | -2.25502500 |
| H | 6.19637800 | -2.15843500 | -2.51476400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 7.05473100  | -0.24295300 | -1.16875600 |
| H | 5.59615200  | 0.92822200  | 0.39442900  |
| H | -0.08647800 | 2.38205700  | 0.70480100  |
| H | -0.33443400 | 0.26830800  | 1.97552400  |
| H | 0.41196000  | 2.21989900  | 3.28596100  |
| H | 2.77345300  | 3.01601100  | 3.09095200  |
| H | 4.33085900  | 1.87552600  | 1.59889100  |
| C | 2.00262700  | -1.81852400 | -0.62018500 |
| C | 1.12688300  | -1.22445100 | 0.24656500  |
| S | -1.33937000 | 2.58727600  | -1.06062900 |
| O | -1.75193000 | 3.77666800  | -1.78419100 |
| O | -0.54786100 | 1.53177700  | -1.67791700 |
| O | -0.65518300 | 3.08542500  | 0.30811300  |
| C | -2.88773100 | 1.78704900  | -0.37861100 |
| F | -3.50953800 | 1.15562500  | -1.37169500 |
| F | -3.68561800 | 2.71909600  | 0.13360100  |
| F | -2.55489800 | 0.91146700  | 0.57124900  |
| H | 1.67324200  | -2.67480000 | -1.20237300 |
| C | -0.26230800 | -1.75468100 | 0.35757600  |
| C | -1.09168900 | -1.80851400 | -0.76929600 |
| C | -0.76954100 | -2.25969200 | 1.56999500  |
| C | -2.38395000 | -2.33572000 | -0.70579200 |
| H | -0.72995200 | -1.41002800 | -1.71177400 |
| C | -2.05034000 | -2.78991800 | 1.64889600  |
| H | -0.14482900 | -2.25072300 | 2.45840100  |
| C | -2.87007800 | -2.82973500 | 0.50998300  |
| H | -2.99540100 | -2.34901800 | -1.59983000 |
| H | -2.43623200 | -3.18680100 | 2.58229900  |
| O | -4.11273000 | -3.36264800 | 0.69122900  |
| C | -4.98688400 | -3.42821600 | -0.43111900 |
| H | -5.90961000 | -3.88086700 | -0.06688500 |
| H | -5.20567700 | -2.43015600 | -0.82915300 |
| H | -4.56912300 | -4.05143500 | -1.23068900 |