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Supporting Information

# Multidimensional Correlations in Asymmetric Catalysis through Parameterization of Uncatalyzed Transition States

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**General Considerations:**

The experimental data and characterizations for all the compounds presented in the paper have been previously reported.[1] Geometry optimizations and frequency calculations were carried out using Gaussian 09 software, Revision D.01.14.[2] Vibrational frequencies and intensities were calculated at the M06-2X/def2TZVP level of theory, since such functional/basis-set combination was reported to provide a good accuracy for the calculation of organic molecules' properties in quantitative fashion.[3] π-interaction energies and distances were calculated using the B97D/def2TZVP level of theory.[4] Wheeler recently reported this functional to be an optimal compromise between accuracy and computational cost for the description of noncovalent interactions in sandwich complexes when coupled with a triple zeta basis set.[4a] Sterimol values were calculated for the M06/2X optimized geometries using Molecular Modeling Pro®. Multidimensional regression analyses were performed using Matlab®.

**IR, NBO, Sterimol and Geometrical Parameters**

Sterimol parameters **L**, **B1** and **B5,** respectively, represent the length, minimum and maximum widths of the considered substituent and they were computed using Molecular Modeling Pro®. Vibrational frequencies (**ν**) and intensities (***i***) were calculated from M06-2X/def2TZVP geometries. Parameters relative to chiral phosphoric acids in the enantiodivergent fluorination of allylic alcohols were calculated from the simplified model depicted in **Figure S1**. The BINOL scaffold is represented by a styrene moiety where the dihedral angle **β** is fixed at 60° in compliance with the structure of BINOL based phosphoric acids. This model allows the inclusion of the phosphate group, from which electronic parameters can be calculated, such as the symmetric and asymmetric stretching of the O=P-O$^-$ coordinating group. Geometrical properties such as the torsional angle **α** (**Figure S1**) were measured from the M06-2X optimized structures using GausView 5.0.
The parameters collected for the catalysts are depicted in **Figure S1**.

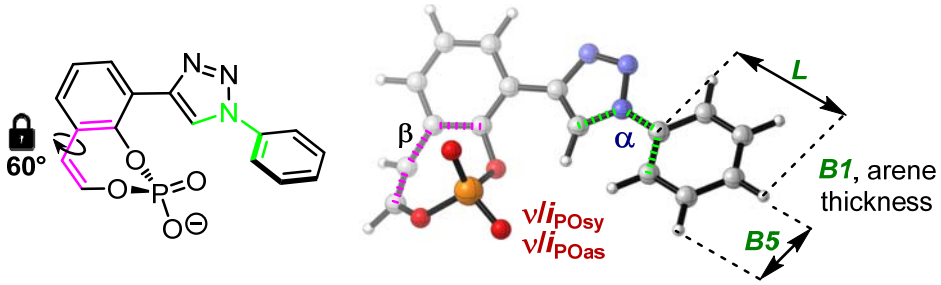



**Figure S1. Parameters collected for the catalysts 1a-1m.**

As catalysts **1k-1m** present an adamantly substituent instead of an aryl group, the angle **α** for these catalysts does not exist. Hence, we reasoned that **α** may describe the presence of sterics in an orthogonal position relative to the triazole ring. Thus, for modeling purposes, **sen(α)** has been used instead of **α** in order to evaluate the presence of sterics out of the triazol ring (Figure S2). Since the adamantly group presents an almost "spherical" symmetry, it always presents maximum sterics in orthogonal position with respect to the triazole. Hence, the value **sen(α)**=1 has been assigned to catalysts **1k-1m**.

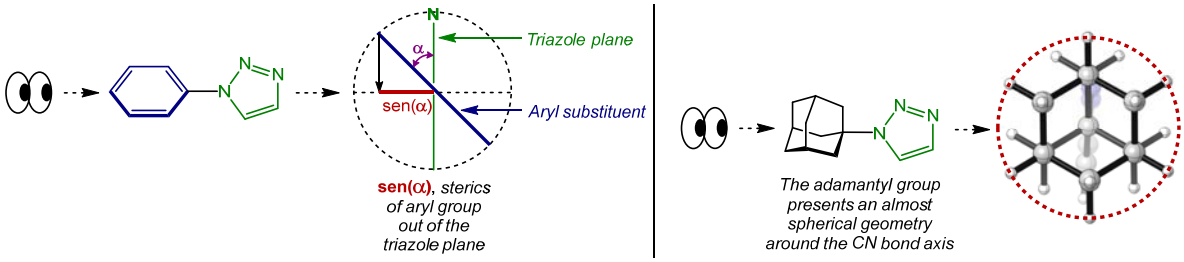



**Figure S2. Use of sen(α) as a parameter for sterics orthogonal to the triazole ring**

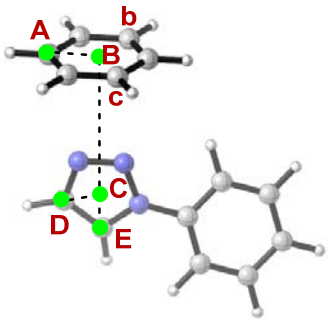
All the parameters measured are reported in the parameters tables (see below).

## Computed Interaction Energies and Distances

Interaction energies (***E***) and distances (***D***) were computed at the B97D/def2TZVP level of theory according with a previously reported procedure using the following geometrical requirements:

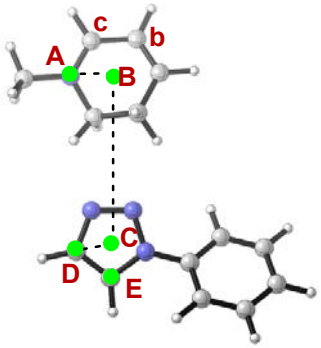
Geometrical requirements for the interaction with **PhH** (***E***/$\boldsymbol{D}_{\mathbf{PhH}}$):

- Probe: benzene **PhH**
- **ECB** = 180°
- The plane **Abc** is perpendicular to axis **BC**
- The dihedral angle **ABCD** = 0°




Geometrical requirements for the interaction with **ImC** (***E***/$\boldsymbol{D}_{\mathbf{ImC}}$):

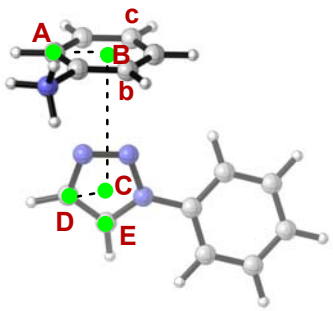
- Probe: Iminium **ImC**
- **ECB** = 180°
- **ABC** = 90°
- The plane **Bbc** and the axis **BC** are parallel
- The dihedral angle **ABCD** = 0°




Geometrical requirements for the interaction with **AnC** (***E***/$\boldsymbol{D}_{\mathbf{AnC}}$):

- Probe: anilinium **AnC**
- **ECB** = 180°

- The plane **Abc** is perpendicular to axis **BC**
- The dihedral angle **ABCD** = 0°




The interaction energies and distances calculated according with these structures are reported in the parameters tables (see below).

**Parametrization of uncatalyzed TSs and Electron Density Maps**

TSs of the uncatalyzed reactions **TS-A**, **TS-B**, and for substrates **2a-2k** were optimized at the M06-2X/def2TZVP level of theory. IR frequencies (**ν**) and intensities (***i***), NBO charges, and conformational energies ($E_{AB}$) were computed at the same level. The geometries of the computed structures are reported below (see Computed Geometries).

**TS-A** and **TS-B** differ in the tautomeric form in which the amide group acts as a nucleophile. In **TS-A** the amide is in iminolic form and presents a free OH group available for coordination. In **TS-B** the amide reacts in its most stable tautomeric form, yet shows distortion of the functional group out of planarity (Figure S3A). Thus, **TS-A** is favored by 5.9 kcal/mol, which suggests that intermediate **3** likely reacts in its iminol form.

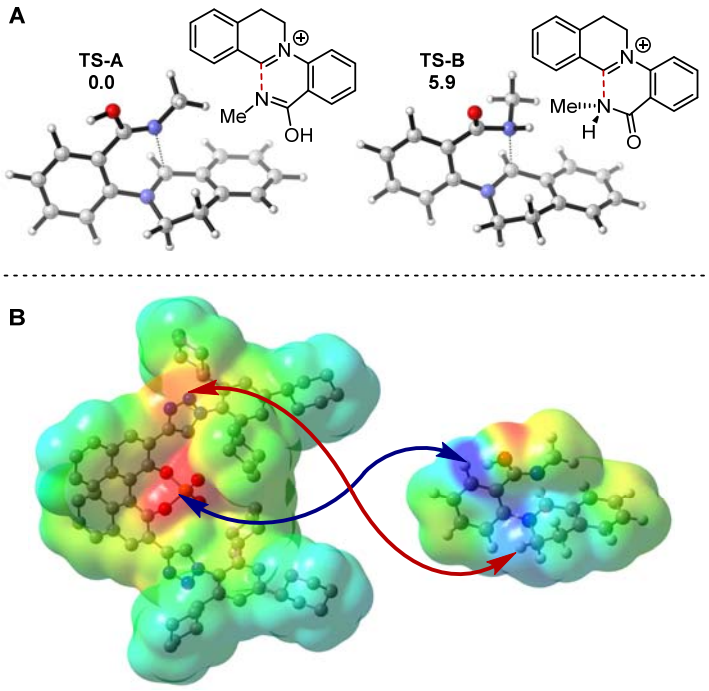



Figure S3. A) TS-A and TS-B. B) Electron density maps for **TS-A** (right) and catalyst **1b** (left).

Evaluation of the electron density map for **TS-A** highlighted the presence of two electron poor regions: the iminol OH group and the alkyl portion next to the iminium group. The same analysis for catalyst **1b** (geometry optimized at the M06-2X/6-31G level of theory) showed the presence of two electron rich regions: the phosphate group and the triazole ring. According with the model in Figure 2C, the electron poor regions in **TS-A** and the electron rich regions in **1b** match to give optimal molecular recognition. The distance between the two electron rich regions in the catalyst and the two electron poor regions in **TS-A** are similar, thus supporting the coordination mode

hypothesized.

The uncatalyzed TSs for substrates **2a-2k** presented two or four conformers depending on the substitution pattern of the benzyl substituent. Specifically, TSs for **2a-2d**, **2h** present only two conformers (A or B). Conformers A present the benzyl group folded towards the tetrahydroisoquinoline structure, while conformers B place the benzyl moiety in a free region of space. Their corresponding energies are $\mathbf{E_A}$ and $\mathbf{E_B}$ (Figure S4A).

**2e-2g**, **2i-2k** present 4 conformers (A1, A2, B1 and B2). A1 and A2 both have the benzyl group folded, and they differ from the rotation of the $H_2C$-Ar bond (Figure S4B). The rotation of the same bond also differentiate B1 and B2, in which the benzyl group is in a free region of space (Figure S4B). The energies of A1 and A2 (i.e. $\mathbf{E_{A1}}$ and $\mathbf{E_{A2}}$) were averaged according with the Boltzmann distribution in order to obtain the average energy of the "main conformers" A $\mathbf{E_A}$ (Figure S4B). The same procedure was followed to calculate $\mathbf{E_B}$ from $\mathbf{E_{B1}}$ and $\mathbf{E_{B2}}$. The conformation parameters $\mathbf{E_{AB}}$ were calculated as $\mathbf{E_{AB}}=\mathbf{E_B}-\mathbf{E_A}$. The relative energy values for the computed uncatalyzed TSs are reported in Table S1 in kcal/mol.

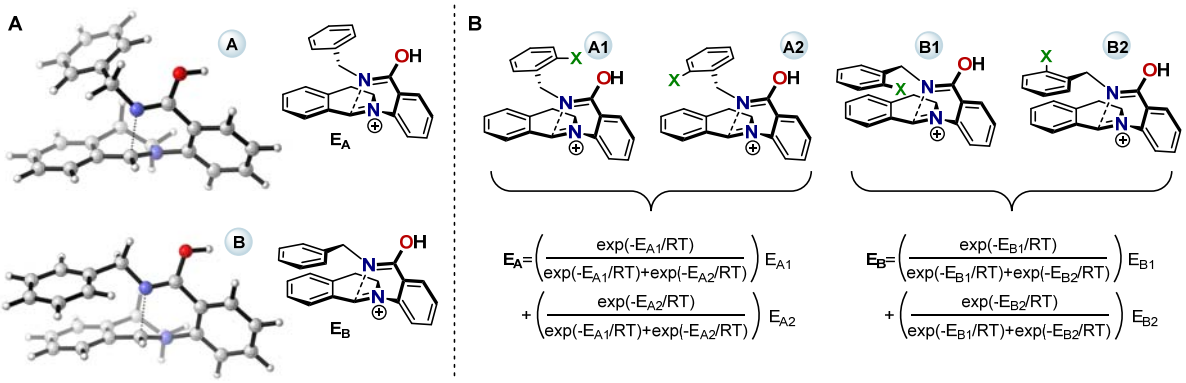



Figure S4. A) Conformers A and B. B) Conformers A1, A2, B1 and B2 and calculation of $\mathbf{E_A}$ and $\mathbf{E_B}$ for substrates **2e-2g**, **2i-2k**.

| Substrate | $E_{A1}$ | $E_{A2}$ | $E_{B1}$ | $E_{B2}$ | $E_A$ | $E_B$ | $E_{AB}$ |
|---|---|---|---|---|---|---|---|
| **1a** | | | | | 0.00 | 1.48 | 1.48 |
| **1b** | | | | | 0.00 | 1.53 | 1.53 |
| **1c** | | | | | 0.00 | 1.69 | 1.69 |
| **1d** | | | | | 0.00 | 1.29 | 1.29 |
| **1e** | 0.00 | 2.40 | 0.87 | 2.16 | 0.04 | 1.00 | 0.96 |
| **1f** | 0.00 | 0.29 | 1.11 | 1.42 | 0.11 | 1.22 | 1.11 |
| **1g** | 0.00 | 0.08 | 1.06 | 0.41 | 0.04 | 0.57 | 0.54 |
| **1h** | | | | | 0.00 | -0.64 | -0.64 |
| **1i** | 0.00 | -0.19 | 0.90 | 0.26 | -0.11 | 0.42 | 0.53 |
| **1j** | 0.00 | 0.05 | 1.09 | 0.46 | 0.02 | 0.63 | 0.60 |
| **1k** | 0.00 | 0.15 | 1.13 | 0.40 | 0.06 | 0.56 | 0.50 |

Table S1

Other parameters computed for the uncatalyzed TSs were acquired from the most stable conformer. They are listed in the parameters tables and summarized in Figure S5.

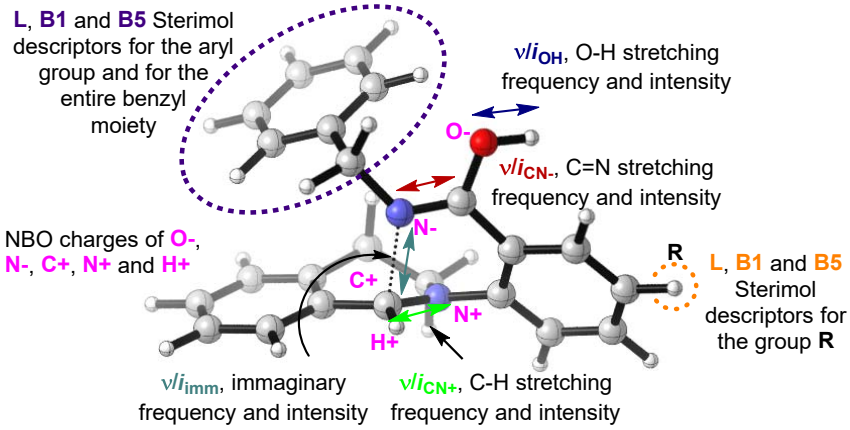



Figure S5

## Parameters Tables

| | | | | | Catalyst | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | cat | sub | ee (%) | ΔΔG‡ (kcal/mol) | $D_{AnC}$ | $E_{AnC}$ | $D_{PhH}$ | $E_{PhH}$ | $D_{ImC}$ | $E_{ImC}$ | sen(α) | L | B1 | B5 | $\nu_{POsy}$ | $i_{POsy}$ | $\nu_{POas}$ | $i_{POas}$ |
| *Training set* | 1h | 2a | 53 | 0.70 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1i | 2a | 74 | 1.13 | 4.277 | -9.876 | 4.706 | -0.449 | 5.420 | -13.521 | 0.810 | 7.026 | 1.770 | 3.847 | 1156.50 | 169.23 | 1388.50 | 268.96 |
| | 1e | 2a | 59 | 0.79 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1f | 2a | 63 | 0.88 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1a | 2a | 85 | 1.47 | 4.208 | -11.948 | 4.619 | -1.333 | 5.380 | -15.506 | 0.824 | 8.020 | 2.924 | 5.792 | 1155.68 | 207.91 | 1371.11 | 107.68 |
| | 1c | 2a | 80 | 1.28 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1j | 2b | 46 | 0.59 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1g | 2b | 46 | 0.58 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1e | 2b | 54 | 0.71 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1d | 2b | 80 | 1.30 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1c | 2b | 66 | 0.93 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1b | 2b | 49 | 0.63 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1j | 2d | 39 | 0.48 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1h | 2d | 48 | 0.62 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1e | 2d | 64 | 0.89 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1d | 2d | 84 | 1.45 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1b | 2d | 78 | 1.22 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1k | 2c | 78 | 1.22 | 4.204 | -13.373 | 4.839 | -0.279 | 5.366 | -17.487 | 1.000 | 6.338 | 3.318 | 3.707 | 1154.50 | 182.59 | 1378.32 | 264.87 |
| | 1h | 2c | 67 | 0.96 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1g | 2c | 38 | 0.47 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1f | 2c | 78 | 1.22 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1d | 2c | 84 | 1.45 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1b | 2c | 78 | 1.22 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1j | 2e | 52 | 0.67 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1h | 2e | 56 | 0.75 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1g | 2e | 33 | 0.40 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1f | 2e | 67 | 0.96 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1a | 2e | 93 | 1.96 | 4.208 | -11.948 | 4.619 | -1.333 | 5.380 | -15.506 | 0.824 | 8.020 | 2.924 | 5.792 | 1155.68 | 207.91 | 1371.11 | 107.68 |
| | 1c | 2e | 92 | 1.88 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1b | 2e | 91 | 1.81 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1j | 2f | 57 | 0.77 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1h | 2f | 62 | 0.85 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1e | 2f | 54 | 0.72 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1f | 2f | 63 | 0.88 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1a | 2f | 95 | 2.17 | 4.208 | -11.948 | 4.619 | -1.333 | 5.380 | -15.506 | 0.824 | 8.020 | 2.924 | 5.792 | 1155.68 | 207.91 | 1371.11 | 107.68 |
| | 1c | 2f | 94 | 2.01 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1j | 2g | 7 | 0.08 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1i | 2g | 60 | 0.82 | 4.277 | -9.876 | 4.706 | -0.449 | 5.420 | -13.521 | 0.810 | 7.026 | 1.770 | 3.847 | 1156.50 | 169.23 | 1388.50 | 268.96 |
| | 1e | 2g | 23 | 0.28 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1d | 2g | 70 | 1.03 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1a | 2g | 88 | 1.60 | 4.208 | -11.948 | 4.619 | -1.333 | 5.380 | -15.506 | 0.824 | 8.020 | 2.924 | 5.792 | 1155.68 | 207.91 | 1371.11 | 107.68 |
| | 1c | 2g | 83 | 1.41 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1b | 2g | 83 | 1.39 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1j | 2h | -54 | -0.71 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1h | 2h | -28 | -0.33 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1g | 2h | -33 | -0.41 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1i | 2h | 60 | 0.81 | 4.277 | -9.876 | 4.706 | -0.449 | 5.420 | -13.521 | 0.810 | 7.026 | 1.770 | 3.847 | 1156.50 | 169.23 | 1388.50 | 268.96 |
| | 1e | 2h | 39 | 0.49 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1f | 2h | 53 | 0.70 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1d | 2h | 71 | 1.05 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1b | 2h | 61 | 0.83 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1h | 2j | 34 | 0.42 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1g | 2j | 47 | 0.60 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1e | 2j | 74 | 1.11 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1d | 2j | 83 | 1.39 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1a | 2j | 91 | 1.78 | 4.208 | -11.948 | 4.619 | -1.333 | 5.380 | -15.506 | 0.824 | 8.020 | 2.924 | 5.792 | 1155.68 | 207.91 | 1371.11 | 107.68 |
| | 1c | 2j | 91 | 1.81 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1j | 2i | 11 | 0.13 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1g | 2i | 29 | 0.35 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1e | 2i | 32 | 0.39 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1d | 2i | 71 | 1.04 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1a | 2i | 93 | 1.96 | 4.208 | -11.948 | 4.619 | -1.333 | 5.380 | -15.506 | 0.824 | 8.020 | 2.924 | 5.792 | 1155.68 | 207.91 | 1371.11 | 107.68 |
| | 1b | 2i | 89 | 1.66 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1j | 2k | 0 | 0.00 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1h | 2k | 6 | 0.07 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1i | 2k | 55 | 0.73 | 4.277 | -9.876 | 4.706 | -0.449 | 5.420 | -13.521 | 0.810 | 7.026 | 1.770 | 3.847 | 1156.50 | 169.23 | 1388.50 | 268.96 |
| | 1e | 2k | 45 | 0.57 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1f | 2k | 68 | 0.97 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1a | 2k | 92 | 1.84 | 4.208 | -11.948 | 4.619 | -1.333 | 5.380 | -15.506 | 0.824 | 8.020 | 2.924 | 5.792 | 1155.68 | 207.91 | 1371.11 | 107.68 |
| | 1c | 2k | 89 | 1.66 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |

| | | | | | Substrate Benzyl | | | Substrate Aryl | | | Substrate group R | | | NBO charges | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | cat | sub | ee (%) | ΔΔG‡ (kcal/mol) | L | B1 | B5 | L | B1 | B5 | L | B1 | B5 | N+ | C+ | H+ | N- | O- |
| *Training set* | 1h | 2a | 53 | 0.70 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1i | 2a | 74 | 1.13 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1e | 2a | 59 | 0.79 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1f | 2a | 63 | 0.88 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1a | 2a | 85 | 1.47 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1c | 2a | 80 | 1.28 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1j | 2b | 46 | 0.59 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1g | 2b | 46 | 0.58 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1e | 2b | 54 | 0.71 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1d | 2b | 80 | 1.30 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1c | 2b | 66 | 0.93 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1b | 2b | 49 | 0.63 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1j | 2d | 39 | 0.48 | 4.979 | 1.701 | 7.697 | 7.805 | 1.770 | 3.149 | 2.081 | 1.000 | 1.000 | -0.361 | 0.321 | 0.237 | -0.436 | -0.661 |
| | 1h | 2d | 48 | 0.62 | 4.979 | 1.701 | 7.697 | 7.805 | 1.770 | 3.149 | 2.081 | 1.000 | 1.000 | -0.361 | 0.321 | 0.237 | -0.436 | -0.661 |
| | 1e | 2d | 64 | 0.89 | 4.979 | 1.701 | 7.697 | 7.805 | 1.770 | 3.149 | 2.081 | 1.000 | 1.000 | -0.361 | 0.321 | 0.237 | -0.436 | -0.661 |
| | 1d | 2d | 84 | 1.45 | 4.979 | 1.701 | 7.697 | 7.805 | 1.770 | 3.149 | 2.081 | 1.000 | 1.000 | -0.361 | 0.321 | 0.237 | -0.436 | -0.661 |
| | 1b | 2d | 78 | 1.22 | 4.979 | 1.701 | 7.697 | 7.805 | 1.770 | 3.149 | 2.081 | 1.000 | 1.000 | -0.361 | 0.321 | 0.237 | -0.436 | -0.661 |
| | 1k | 2c | 78 | 1.22 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1h | 2c | 67 | 0.96 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1g | 2c | 38 | 0.47 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1f | 2c | 78 | 1.22 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1d | 2c | 84 | 1.45 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1b | 2c | 78 | 1.22 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1j | 2e | 52 | 0.67 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1h | 2e | 56 | 0.75 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1g | 2e | 33 | 0.40 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1f | 2e | 67 | 0.96 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1a | 2e | 93 | 1.96 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1c | 2e | 92 | 1.88 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1b | 2e | 91 | 1.81 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1j | 2f | 57 | 0.77 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1h | 2f | 62 | 0.85 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1e | 2f | 54 | 0.72 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1f | 2f | 63 | 0.88 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1a | 2f | 95 | 2.17 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1c | 2f | 94 | 2.01 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1j | 2g | 7 | 0.08 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1i | 2g | 60 | 0.82 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1e | 2g | 23 | 0.28 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1d | 2g | 70 | 1.03 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1a | 2g | 88 | 1.60 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1c | 2g | 83 | 1.41 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1b | 2g | 83 | 1.39 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1j | 2h | -54 | -0.71 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1h | 2h | -28 | -0.33 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1g | 2h | -33 | -0.41 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1i | 2h | 60 | 0.81 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1e | 2h | 39 | 0.49 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1f | 2h | 53 | 0.70 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1d | 2h | 71 | 1.05 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1b | 2h | 61 | 0.83 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1h | 2j | 34 | 0.42 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1g | 2j | 47 | 0.60 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1e | 2j | 74 | 1.11 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1d | 2j | 83 | 1.39 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1a | 2j | 91 | 1.78 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1c | 2j | 91 | 1.81 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1j | 2i | 11 | 0.13 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1g | 2i | 29 | 0.35 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1e | 2i | 32 | 0.39 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1d | 2i | 71 | 1.04 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1a | 2i | 93 | 1.96 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1b | 2i | 89 | 1.66 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1j | 2k | 0 | 0.00 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |
| | 1h | 2k | 6 | 0.07 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |
| | 1i | 2k | 55 | 0.73 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |
| | 1e | 2k | 45 | 0.57 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |
| | 1f | 2k | 68 | 0.97 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |
| | 1a | 2k | 92 | 1.84 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |
| | 1c | 2k | 89 | 1.66 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |

| | cat | sub | ee (%) | $\Delta\Delta G^{\ddagger}$ (kcal/mol) | $E_{AB}$ | $\nu_{imm}$ | $i_{imm}$ | $\nu_{CN+}$ | $i_{CN+}$ | $\nu_{CN-}$ | $i_{CN-}$ | $\nu_{OH}$ | $i_{OH}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *Training set* | 1h | 2a | 53 | 0.70 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | 1i | 2a | 74 | 1.13 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | 1e | 2a | 59 | 0.79 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | 1f | 2a | 63 | 0.88 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | 1a | 2a | 85 | 1.47 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | 1c | 2a | 80 | 1.28 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | 1j | 2b | 46 | 0.59 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | 1g | 2b | 46 | 0.58 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | 1e | 2b | 54 | 0.71 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | 1d | 2b | 80 | 1.30 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | 1c | 2b | 66 | 0.93 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | 1b | 2b | 49 | 0.63 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | 1j | 2d | 39 | 0.48 | 1.287 | 143.47 | 59.35 | 1611.32 | 199.10 | 1767.11 | 424.58 | 3848.12 | 131.62 |
| | 1h | 2d | 48 | 0.62 | 1.287 | 143.47 | 59.35 | 1611.32 | 199.10 | 1767.11 | 424.58 | 3848.12 | 131.62 |
| | 1e | 2d | 64 | 0.89 | 1.287 | 143.47 | 59.35 | 1611.32 | 199.10 | 1767.11 | 424.58 | 3848.12 | 131.62 |
| | 1d | 2d | 84 | 1.45 | 1.287 | 143.47 | 59.35 | 1611.32 | 199.10 | 1767.11 | 424.58 | 3848.12 | 131.62 |
| | 1b | 2d | 78 | 1.22 | 1.287 | 143.47 | 59.35 | 1611.32 | 199.10 | 1767.11 | 424.58 | 3848.12 | 131.62 |
| | 1k | 2c | 78 | 1.22 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | 1h | 2c | 67 | 0.96 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | 1g | 2c | 38 | 0.47 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | 1f | 2c | 78 | 1.22 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | 1d | 2c | 84 | 1.45 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | 1b | 2c | 78 | 1.22 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | 1j | 2e | 52 | 0.67 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | 1h | 2e | 56 | 0.75 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | 1g | 2e | 33 | 0.40 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | 1f | 2e | 67 | 0.96 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | 1a | 2e | 93 | 1.96 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | 1c | 2e | 92 | 1.88 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | 1b | 2e | 91 | 1.81 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | 1j | 2f | 57 | 0.77 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | 1h | 2f | 62 | 0.85 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | 1e | 2f | 54 | 0.72 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | 1f | 2f | 63 | 0.88 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | 1a | 2f | 95 | 2.17 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | 1c | 2f | 94 | 2.01 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | 1j | 2g | 7 | 0.08 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | 1i | 2g | 60 | 0.82 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | 1e | 2g | 23 | 0.28 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | 1d | 2g | 70 | 1.03 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | 1a | 2g | 88 | 1.60 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | 1c | 2g | 83 | 1.41 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | 1b | 2g | 83 | 1.39 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | 1j | 2h | -54 | -0.71 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | 1h | 2h | -28 | -0.33 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | 1g | 2h | -33 | -0.41 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | 1i | 2h | 60 | 0.81 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | 1e | 2h | 39 | 0.49 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | 1f | 2h | 53 | 0.70 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | 1d | 2h | 71 | 1.05 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | 1b | 2h | 61 | 0.83 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | 1h | 2j | 34 | 0.42 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | 1g | 2j | 47 | 0.60 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | 1e | 2j | 74 | 1.11 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | 1d | 2j | 83 | 1.39 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | 1a | 2j | 91 | 1.78 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | 1c | 2j | 91 | 1.81 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | 1j | 2i | 11 | 0.13 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | 1g | 2i | 29 | 0.35 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | 1e | 2i | 32 | 0.39 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | 1d | 2i | 71 | 1.04 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | 1a | 2i | 93 | 1.96 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | 1b | 2i | 89 | 1.66 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | 1j | 2k | 0 | 0.00 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |
| | 1h | 2k | 6 | 0.07 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |
| | 1i | 2k | 55 | 0.73 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |
| | 1e | 2k | 45 | 0.57 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |
| | 1f | 2k | 68 | 0.97 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |
| | 1a | 2k | 92 | 1.84 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |
| | 1c | 2k | 89 | 1.66 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |

| | | | | | Catalyst | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | cat | sub | ee (%) | ΔΔG‡ (kcal/mol) | $D_{AnC}$ | $E_{AnC}$ | $D_{PhH}$ | $E_{PhH}$ | $D_{ImC}$ | $E_{ImC}$ | sen(α) | L | B1 | B5 | $\nu_{POsy}$ | $i_{POsy}$ | $\nu_{POas}$ | $i_{POas}$ |
| *Validation set* | 1j | 2a | 49 | 0.63 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1g | 2a | 48 | 0.61 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1d | 2a | 78 | 1.22 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1b | 2a | 77 | 1.19 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1h | 2b | 52 | 0.68 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1i | 2b | 66 | 0.93 | 4.277 | -9.876 | 4.706 | -0.449 | 5.420 | -13.521 | 0.810 | 7.026 | 1.770 | 3.847 | 1156.50 | 169.23 | 1388.50 | 268.96 |
| | 1f | 2b | 59 | 0.79 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1a | 2b | 75 | 1.15 | 4.208 | -11.948 | 4.619 | -1.333 | 5.380 | -15.506 | 0.824 | 8.020 | 2.924 | 5.792 | 1155.68 | 207.91 | 1371.11 | 107.68 |
| | 1g | 2d | 38 | 0.47 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1f | 2d | 78 | 1.22 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1c | 2d | 76 | 1.17 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1j | 2c | 49 | 0.63 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1e | 2c | 64 | 0.89 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1c | 2c | 76 | 1.17 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1i | 2e | 33 | 0.40 | 4.277 | -9.876 | 4.706 | -0.449 | 5.420 | -13.521 | 0.810 | 7.026 | 1.770 | 3.847 | 1156.50 | 169.23 | 1388.50 | 268.96 |
| | 1e | 2e | 54 | 0.71 | 4.245 | -12.474 | 4.737 | -0.302 | 5.391 | -16.298 | 0.809 | 6.310 | 1.770 | 3.835 | 1156.60 | 172.29 | 1389.85 | 271.24 |
| | 1d | 2e | 84 | 1.43 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1g | 2f | 32 | 0.39 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1d | 2f | 89 | 1.66 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1b | 2f | 93 | 1.96 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1h | 2g | 21 | 0.25 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1g | 2g | 10 | 0.12 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1f | 2g | 50 | 0.64 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1c | 2h | 58 | 0.78 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1j | 2j | 26 | 0.31 | 4.254 | -11.566 | 4.742 | -0.321 | 5.396 | -15.193 | 0.232 | 6.301 | 1.774 | 3.155 | 1155.04 | 175.96 | 1382.97 | 269.78 |
| | 1f | 2j | 81 | 1.32 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1b | 2j | 90 | 1.71 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |
| | 1h | 2i | 16 | 0.19 | 4.235 | -12.566 | 4.720 | -0.257 | 5.380 | -16.186 | 0.268 | 8.563 | 1.896 | 3.163 | 1155.59 | 172.19 | 1383.69 | 271.15 |
| | 1f | 2i | 65 | 0.91 | 4.193 | -14.711 | 4.766 | -0.091 | 5.357 | -19.294 | 0.746 | 6.287 | 1.965 | 5.526 | 1152.72 | 219.97 | 1368.79 | 226.28 |
| | 1c | 2i | 87 | 1.55 | 4.204 | -13.800 | 4.204 | -0.361 | 5.361 | -17.370 | 0.893 | 8.585 | 3.262 | 5.797 | 1152.34 | 205.71 | 1370.88 | 224.31 |
| | 1g | 2k | 31 | 0.38 | 4.285 | -6.075 | 4.740 | -0.510 | 5.416 | -12.105 | 0.080 | 8.661 | 2.095 | 3.155 | 1155.38 | 173.44 | 1381.11 | 262.64 |
| | 1d | 2k | 71 | 1.04 | 4.206 | -12.676 | 4.722 | -0.333 | 5.377 | -16.851 | 0.787 | 7.307 | 2.087 | 4.553 | 1154.60 | 196.62 | 1376.58 | 246.98 |
| | 1b | 2k | 86 | 1.51 | 4.169 | -14.404 | 4.646 | -0.907 | 5.357 | -18.087 | 0.914 | 10.661 | 3.334 | 7.648 | 1152.48 | 199.03 | 1375.76 | 121.38 |

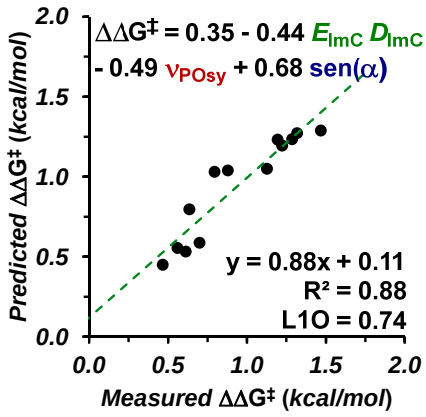
| | | | | | Substrate Benzyl | | | Substrate Aryl | | | Substrate group R | | | NBO charges | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | cat | sub | ee (%) | ΔΔG‡ (kcal/mol) | L | B1 | B5 | L | B1 | B5 | L | B1 | B5 | N+ | C+ | H+ | N- | O- |
| *Validation set* | 1j | 2a | 49 | 0.63 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1g | 2a | 48 | 0.61 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1d | 2a | 78 | 1.22 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1b | 2a | 77 | 1.19 | 4.370 | 1.705 | 6.107 | 6.382 | 1.770 | 3.171 | 2.081 | 1.000 | 1.000 | -0.353 | 0.327 | 0.239 | -0.445 | -0.664 |
| | 1h | 2b | 52 | 0.68 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1i | 2b | 66 | 0.93 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1f | 2b | 59 | 0.79 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1a | 2b | 75 | 1.15 | 4.804 | 1.715 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.356 | 0.326 | 0.238 | -0.439 | -0.663 |
| | 1g | 2d | 38 | 0.47 | 4.979 | 1.701 | 7.697 | 7.805 | 1.770 | 3.149 | 2.081 | 1.000 | 1.000 | -0.361 | 0.321 | 0.237 | -0.436 | -0.661 |
| | 1f | 2d | 78 | 1.22 | 4.979 | 1.701 | 7.697 | 7.805 | 1.770 | 3.149 | 2.081 | 1.000 | 1.000 | -0.361 | 0.321 | 0.237 | -0.436 | -0.661 |
| | 1c | 2d | 76 | 1.17 | 4.979 | 1.701 | 7.697 | 7.805 | 1.770 | 3.149 | 2.081 | 1.000 | 1.000 | -0.361 | 0.321 | 0.237 | -0.436 | -0.661 |
| | 1j | 2c | 49 | 0.63 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1e | 2c | 64 | 0.89 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1c | 2c | 76 | 1.17 | 4.980 | 1.705 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.355 | 0.325 | 0.238 | -0.436 | -0.664 |
| | 1i | 2e | 33 | 0.40 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1e | 2e | 54 | 0.71 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1d | 2e | 84 | 1.43 | 4.772 | 1.703 | 5.957 | 6.392 | 1.770 | 4.791 | 2.081 | 1.000 | 1.000 | -0.360 | 0.327 | 0.235 | -0.448 | -0.658 |
| | 1g | 2f | 32 | 0.39 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1d | 2f | 89 | 1.66 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1b | 2f | 93 | 1.96 | 4.804 | 1.712 | 5.949 | 6.378 | 1.863 | 4.514 | 2.081 | 1.000 | 1.000 | -0.359 | 0.329 | 0.236 | -0.447 | -0.664 |
| | 1h | 2g | 21 | 0.25 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1g | 2g | 10 | 0.12 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1f | 2g | 50 | 0.64 | 4.980 | 1.708 | 5.878 | 6.368 | 1.770 | 5.502 | 2.081 | 1.000 | 1.000 | -0.357 | 0.329 | 0.238 | -0.446 | -0.657 |
| | 1c | 2h | 58 | 0.78 | 5.062 | 1.714 | 5.901 | 6.344 | 1.860 | 5.501 | 2.081 | 1.000 | 1.000 | -0.365 | 0.324 | 0.238 | -0.424 | -0.655 |
| | 1j | 2j | 26 | 0.31 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1f | 2j | 81 | 1.32 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1b | 2j | 90 | 1.71 | 4.957 | 1.710 | 5.888 | 6.370 | 1.770 | 5.503 | 4.324 | 2.082 | 3.344 | -0.356 | 0.327 | 0.237 | -0.445 | -0.657 |
| | 1h | 2i | 16 | 0.19 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1f | 2i | 65 | 0.91 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1c | 2i | 87 | 1.55 | 5.888 | 1.700 | 6.107 | 6.381 | 1.819 | 5.505 | 3.800 | 1.920 | 1.920 | -0.352 | 0.329 | 0.239 | -0.438 | -0.665 |
| | 1g | 2k | 31 | 0.38 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |
| | 1d | 2k | 71 | 1.04 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |
| | 1b | 2k | 86 | 1.51 | 4.981 | 1.707 | 5.886 | 6.369 | 1.770 | 5.503 | 6.350 | 1.773 | 3.143 | -0.355 | 0.327 | 0.238 | -0.447 | -0.658 |

| | cat | sub | ee (%) | $\Delta\Delta G^{\ddagger}$ (kcal/mol) | $E_{AB}$ | $\nu_{imm}$ | $i_{imm}$ | $\nu_{CN+}$ | $i_{CN+}$ | $\nu_{CN-}$ | $i_{CN-}$ | $\nu_{OH}$ | $i_{OH}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *Validation set* | **1j** | **2a** | 49 | 0.63 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | **1g** | **2a** | 48 | 0.61 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | **1d** | **2a** | 78 | 1.22 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | **1b** | **2a** | 77 | 1.19 | 1.481 | 133.75 | 53.41 | 1623.65 | 201.32 | 1769.25 | 374.14 | 3852.18 | 120.67 |
| | **1h** | **2b** | 52 | 0.68 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | **1i** | **2b** | 66 | 0.93 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | **1f** | **2b** | 59 | 0.79 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | **1a** | **2b** | 75 | 1.15 | 1.527 | 146.88 | 61.05 | 1615.96 | 212.19 | 1774.81 | 368.94 | 3851.42 | 122.67 |
| | **1g** | **2d** | 38 | 0.47 | 1.287 | 143.47 | 59.35 | 1611.32 | 199.10 | 1767.11 | 424.58 | 3848.12 | 131.62 |
| | **1f** | **2d** | 78 | 1.22 | 1.287 | 143.47 | 59.35 | 1611.32 | 199.10 | 1767.11 | 424.58 | 3848.12 | 131.62 |
| | **1c** | **2d** | 76 | 1.17 | 1.287 | 143.47 | 59.35 | 1611.32 | 199.10 | 1767.11 | 424.58 | 3848.12 | 131.62 |
| | **1j** | **2c** | 49 | 0.63 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | **1e** | **2c** | 64 | 0.89 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | **1c** | **2c** | 76 | 1.17 | 1.694 | 138.46 | 58.78 | 1618.79 | 203.80 | 1771.48 | 359.30 | 3853.63 | 119.01 |
| | **1i** | **2e** | 33 | 0.40 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | **1e** | **2e** | 54 | 0.71 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | **1d** | **2e** | 84 | 1.43 | 0.959 | 129.94 | 61.51 | 1613.21 | 199.61 | 1756.18 | 395.19 | 3845.38 | 117.41 |
| | **1g** | **2f** | 32 | 0.39 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | **1d** | **2f** | 89 | 1.66 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | **1b** | **2f** | 93 | 1.96 | 1.114 | 134.82 | 62.62 | 1609.50 | 237.55 | 1764.99 | 370.43 | 3854.61 | 121.93 |
| | **1h** | **2g** | 21 | 0.25 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | **1g** | **2g** | 10 | 0.12 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | **1f** | **2g** | 50 | 0.64 | 0.536 | 125.73 | 61.56 | 1619.38 | 224.73 | 1771.87 | 376.58 | 3858.78 | 110.73 |
| | **1c** | **2h** | 58 | 0.78 | -0.636 | 135.71 | 82.86 | 1607.47 | 233.48 | 1758.26 | 420.05 | 3857.57 | 128.42 |
| | **1j** | **2j** | 26 | 0.31 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | **1f** | **2j** | 81 | 1.32 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | **1b** | **2j** | 90 | 1.71 | 0.533 | 125.68 | 60.63 | 1618.87 | 208.76 | 1768.99 | 409.98 | 3858.22 | 111.69 |
| | **1h** | **2i** | 16 | 0.19 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | **1f** | **2i** | 65 | 0.91 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | **1c** | **2i** | 87 | 1.55 | 0.499 | 135.00 | 52.38 | 1620.17 | 162.96 | 1770.25 | 355.50 | 3851.85 | 122.53 |
| | **1g** | **2k** | 31 | 0.38 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |
| | **1d** | **2k** | 71 | 1.04 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |
| | **1b** | **2k** | 86 | 1.51 | 0.602 | 136.19 | 55.96 | 1613.02 | 228.76 | 1765.88 | 424.93 | 3860.12 | 118.14 |

**Multivariate Correlation Analyses**

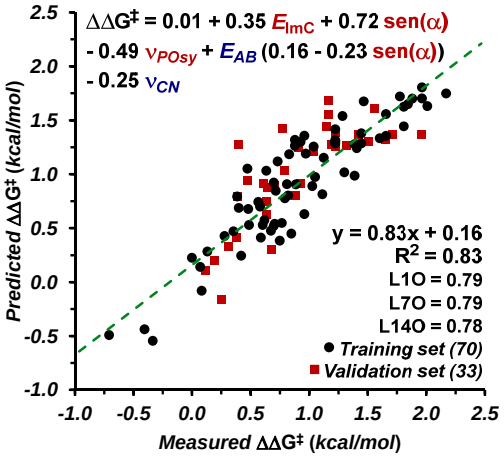
**Measured ΔΔG‡** values were calculated using the formula $\Delta\Delta G^{\ddagger} = -RT\ln(er)$ where R is the gas constant, T is temperature, and er is the enantiomeric ratio. The parameter sets and the **Measured ΔΔG‡** values were normalized by subtracting the mean and dividing by the standard deviation of each parameter set. Multiple linear regression models were developed using the functions LinearModel.stepwise and LinearModel.fit implemented in MATLAB® R2014a software in order to obtain the **predicted ΔΔG‡**. A good linear correlation ($R^2$ close to 1.0 and intercept close to 0.0) between the **Predicted ΔΔG‡** and the **Measured ΔΔG‡** indicates that the obtained model adequately approximates the system under study. Leave-K-Out cross validations (LKO) were also generated using MATLAB and are always reported below the $R^2$ value in the plots.

Model for substrate **2a** and catalysts **1a-1m** (Figure 2C):




| Measured ΔΔG‡ | Predicted ΔΔG‡ | L1O |
|---|---|---|
| 0.559 | 0.554 | 0.488 |
| 0.467 | 0.449 | -0.065 |
| 1.318 | 1.272 | 1.155 |
| 0.635 | 0.795 | 0.797 |
| 0.699 | 0.587 | 0.496 |
| 1.126 | 1.049 | 0.949 |
| 0.612 | 0.532 | 0.430 |
| 0.7934 | 1.0301 | 0.9757 |
| 0.878 | 1.0393 | 0.9671 |
| 1.2229 | 1.1937 | 1.0892 |
| 1.4665 | 1.2876 | 1.1405 |
| 1.2847 | 1.2338 | 1.122 |
| 1.1938 | 1.2319 | 1.1351 |

Model for substrates **2a-2k** and catalysts **1a-1k** (Figure 4C):



| | cat | sub | Measured ΔΔG | Predicted ΔΔG |
|---|---|---|---|---|
| Training set | 1h | 2a | 0.70 | 0.52 |
| | 1i | 2a | 1.13 | 1.15 |
| | 1e | 2a | 0.79 | 0.78 |
| | 1f | 2a | 0.88 | 1.27 |
| | 1a | 2a | 1.47 | 1.68 |
| | 1c | 2a | 1.28 | 1.54 |
| | 1j | 2b | 0.59 | 0.41 |
| | 1g | 2b | 0.58 | 0.70 |
| | 1e | 2b | 0.71 | 0.54 |
| | 1d | 2b | 1.30 | 1.02 |
| | 1c | 2b | 0.93 | 1.30 |
| | 1b | 2b | 0.63 | 1.03 |
| | 1j | 2d | 0.48 | 0.68 |
| | 1h | 2d | 0.62 | 0.57 |
| | 1e | 2d | 0.89 | 0.91 |
| | 1d | 2d | 1.45 | 1.38 |
| | 1b | 2d | 1.22 | 1.42 |
| | 1k | 2c | 1.22 | 1.32 |
| | 1h | 2c | 0.96 | 0.63 |
| | 1g | 2c | 0.47 | 1.05 |
| | 1f | 2c | 1.22 | 1.30 |
| | 1d | 2c | 1.45 | 1.29 |
| | 1b | 2c | 1.22 | 1.28 |
| | 1j | 2e | 0.67 | 0.48 |
| | 1h | 2e | 0.75 | 0.39 |
| | 1g | 2e | 0.40 | 0.69 |
| | 1f | 2e | 0.96 | 1.36 |
| | 1a | 2e | 1.96 | 1.81 |
| | 1c | 2e | 1.88 | 1.70 |
| | 1b | 2e | 1.81 | 1.44 |
| | 1j | 2f | 0.77 | 0.55 |
| | 1h | 2f | 0.85 | 0.45 |
| | 1e | 2f | 0.72 | 0.85 |
| | 1f | 2f | 0.88 | 1.32 |

| | cat | sub | Measured ΔΔG | Predicted ΔΔG |
|---|---|---|---|---|
| Training set | 1a | 2f | 2.17 | 1.75 |
| | 1c | 2f | 2.01 | 1.63 |
| | 1j | 2g | 0.08 | -0.08 |
| | 1i | 2g | 0.82 | 0.80 |
| | 1e | 2g | 0.28 | 0.43 |
| | 1d | 2g | 1.03 | 0.89 |
| | 1a | 2g | 1.60 | 1.34 |
| | 1c | 2g | 1.41 | 1.24 |
| | 1b | 2g | 1.39 | 0.99 |
| | 1j | 2h | -0.71 | -0.49 |
| | 1h | 2h | -0.33 | -0.54 |
| | 1g | 2h | -0.41 | -0.44 |
| | 1i | 2h | 0.81 | 0.91 |
| | 1e | 2h | 0.49 | 0.53 |
| | 1f | 2h | 0.70 | 0.92 |
| | 1d | 2h | 1.05 | 0.97 |
| | 1b | 2h | 0.83 | 1.18 |
| | 1h | 2j | 0.42 | 0.25 |
| | 1g | 2j | 0.60 | 0.53 |
| | 1e | 2j | 1.11 | 0.81 |
| | 1d | 2j | 1.39 | 1.28 |
| | 1a | 2j | 1.78 | 1.72 |
| | 1c | 2j | 1.81 | 1.63 |
| | 1j | 2i | 0.13 | 0.28 |
| | 1g | 2i | 0.35 | 0.47 |
| | 1e | 2i | 0.39 | 0.80 |
| | 1d | 2i | 1.04 | 1.26 |
| | 1a | 2i | 1.96 | 1.70 |
| | 1b | 2i | 1.66 | 1.36 |
| | 1j | 2k | 0.00 | 0.23 |
| | 1h | 2k | 0.07 | 0.14 |
| | 1i | 2k | 0.73 | 1.12 |
| | 1e | 2k | 0.57 | 0.74 |
| | 1f | 2k | 0.97 | 1.19 |
| | 1a | 2k | 1.84 | 1.65 |

| | cat | sub | Measured ΔΔG | Predicted ΔΔG |
|---|---|---|---|---|
| Validation set | 1c | 2k | 1.66 | 1.56 |
| | 1j | 2a | 0.63 | 0.63 |
| | 1g | 2a | 0.61 | 0.91 |
| | 1d | 2a | 1.22 | 1.25 |
| | 1b | 2a | 1.19 | 1.27 |
| | 1h | 2b | 0.68 | 0.30 |
| | 1i | 2b | 0.93 | 0.92 |
| | 1f | 2b | 0.79 | 1.03 |
| | 1a | 2b | 1.15 | 1.44 |
| | 1g | 2d | 0.47 | 0.94 |
| | 1f | 2d | 1.22 | 1.38 |
| | 1c | 2d | 1.17 | 1.68 |
| | 1j | 2c | 0.63 | 0.74 |
| | 1e | 2c | 0.89 | 0.80 |
| | 1c | 2c | 1.17 | 1.55 |
| | 1i | 2e | 0.40 | 1.28 |
| | 1e | 2e | 0.71 | 0.90 |
| | 1d | 2e | 1.43 | 1.37 |
| | 1g | 2f | 0.39 | 0.79 |
| | 1d | 2f | 1.66 | 1.32 |
| | 1b | 2f | 1.96 | 1.37 |
| | 1h | 2g | 0.25 | -0.19 |
| | 1g | 2g | 0.12 | 0.08 |
| | 1f | 2g | 0.64 | 0.87 |
| | 1c | 2h | 0.78 | 1.43 |
| | 1j | 2j | 0.31 | 0.28 |
| | 1f | 2j | 1.32 | 1.26 |
| | 1b | 2j | 1.71 | 1.38 |
| | 1h | 2i | 0.19 | 0.16 |
| | 1f | 2i | 0.91 | 1.24 |
| | 1c | 2i | 1.55 | 1.62 |
| | 1g | 2k | 0.38 | 0.43 |
| | 1d | 2k | 1.04 | 1.21 |
| | 1b | 2k | 1.51 | 1.30 |

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## Computed Geometries

*Catalyst 1b:*

| | x | y | z |
|---|---|---|---|
| C | 0.111024 | 7.592038 | 2.49615 |
| C | -0.12426 | 6.596592 | 1.577038 |
| C | 0.793196 | 5.520645 | 1.410166 |
| C | 1.947307 | 5.478807 | 2.248528 |
| C | 2.167201 | 6.52912 | 3.182855 |
| C | 1.275539 | 7.566905 | 3.303715 |
| H | -0.60471 | 8.398252 | 2.611728 |
| H | -1.02443 | 6.615756 | 0.974753 |
| C | 0.579579 | 4.463009 | 0.4655 |
| C | 2.839351 | 4.382215 | 2.15917 |
| H | 3.053912 | 6.483101 | 3.807464 |
| H | 1.449699 | 8.358937 | 4.023425 |
| C | 2.602467 | 3.334727 | 1.296934 |
| C | 1.453167 | 3.391438 | 0.457609 |
| H | 3.713277 | 4.344745 | 2.800228 |
| C | -0.57958 | 4.463019 | -0.46536 |
| C | -0.79319 | 5.520692 | -1.40998 |
| C | -1.45314 | 3.39142 | -0.45754 |
| C | 0.124227 | 6.596681 | -1.57677 |
| C | -1.94727 | 5.478855 | -2.24839 |
| C | -2.60238 | 3.334698 | -1.29695 |
| C | -0.11106 | 7.592166 | -2.49584 |
| H | 1.024378 | 6.615851 | -0.97446 |
| C | -2.16717 | 6.529208 | -3.18267 |
| C | -2.83926 | 4.382217 | -2.15914 |
| C | -1.27555 | 7.567035 | -3.30345 |
| H | 0.604644 | 8.398412 | -2.61135 |
| H | -3.05386 | 6.483185 | -3.80732 |
| H | -3.71315 | 4.344731 | -2.80026 |
| H | -1.44971 | 8.359099 | -4.02312 |
| O | 1.231897 | 2.333799 | -0.41296 |
| O | -1.23192 | 2.33377 | 0.413016 |
| P | 0.000032 | 1.134214 | 0.000136 |
| O | -0.39592 | 0.383439 | -1.33799 |
| O | 0.396051 | 0.383712 | 1.338395 |
| C | 3.505544 | 2.189779 | 1.261019 |
| C | 3.547639 | 1.076525 | 0.440339 |
| N | 4.591636 | 0.337414 | 0.899001 |
| H | 2.948048 | 0.784602 | -0.40111 |
| C | -3.50539 | 2.189687 | -1.26119 |
| C | -3.54763 | 1.076481 | -0.44045 |
| N | -4.59149 | 0.337299 | -0.89932 |
| H | -2.94823 | 0.784615 | 0.401154 |
| C | 5.063367 | -0.92555 | 0.423716 |
| C | 6.322836 | -0.97886 | -0.18896 |
| C | 4.249141 | -2.06336 | 0.590426 |
| C | 6.782035 | -2.22707 | -0.62457 |
| C | 4.748289 | -3.27917 | 0.117135 |
| C | 6.009656 | -3.3793 | -0.48355 |
| H | 7.760288 | -2.30357 | -1.08961 |
| H | 4.139509 | -4.17035 | 0.220562 |
| C | -5.06335 | -0.92559 | -0.42397 |

| | | | |
|---|---|---|---|
| C | -4.24917 | -2.06346 | -0.59042 |
| C | -6.3229 | -0.97875 | 0.188553 |
| C | -4.74847 | -3.2792 | -0.11706 |
| C | -6.78224 | -2.22688 | 0.624248 |
| C | -6.00992 | -3.37918 | 0.483439 |
| H | -4.13971 | -4.17041 | -0.22026 |
| H | -7.76055 | -2.30326 | 1.08919 |
| N | 5.198294 | 0.965313 | 1.966556 |
| N | 4.538987 | 2.080125 | 2.173048 |
| N | -4.53861 | 2.079937 | -2.17345 |
| N | -5.19791 | 0.965098 | -1.96705 |
| C | -6.5286 | -4.71743 | 0.970435 |
| C | -6.70116 | -5.72401 | -0.18622 |
| C | -5.63098 | -5.32403 | 2.068506 |
| H | -7.52323 | -4.5503 | 1.413167 |
| C | -7.2586 | -7.06364 | 0.314002 |
| H | -5.72336 | -5.88981 | -0.66006 |
| H | -7.3557 | -5.29182 | -0.95154 |
| C | -6.18745 | -6.66401 | 2.569053 |
| H | -4.62266 | -5.47799 | 1.659472 |
| H | -5.53183 | -4.61118 | 2.894651 |
| C | -6.36498 | -7.65755 | 1.411888 |
| H | -7.35684 | -7.7672 | -0.52049 |
| H | -8.26834 | -6.90496 | 0.719435 |
| H | -5.5254 | -7.08423 | 3.33442 |
| H | -7.16249 | -6.49307 | 3.047832 |
| H | -6.78563 | -8.60052 | 1.779663 |
| H | -5.37923 | -7.89021 | 0.984838 |
| C | 6.528188 | -4.71764 | -0.97044 |
| C | 6.700815 | -5.72409 | 0.186326 |
| C | 5.630411 | -5.32432 | -2.06833 |
| H | 7.522785 | -4.55063 | -1.4133 |
| C | 7.258123 | -7.06382 | -0.3138 |
| H | 5.723062 | -5.88978 | 0.660297 |
| H | 7.355473 | -5.29184 | 0.951504 |
| C | 6.18677 | -6.66439 | -2.56879 |
| H | 4.622129 | -5.4782 | -1.65917 |
| H | 5.531193 | -4.61157 | -2.89455 |
| C | 6.364357 | -7.6578 | -1.41152 |
| H | 7.356406 | -7.76728 | 0.520762 |
| H | 8.267831 | -6.90525 | -0.71935 |
| H | 5.524612 | -7.08467 | -3.33404 |
| H | 7.161765 | -6.49355 | -3.04768 |
| H | 6.784924 | -8.60083 | -1.77923 |
| H | 5.378638 | -7.89036 | -0.98435 |
| C | -7.17543 | 0.264968 | 0.3473 |
| C | -8.23609 | 0.357232 | -0.7713 |
| C | -7.85001 | 0.37255 | 1.727847 |
| H | -6.52243 | 1.141553 | 0.239961 |
| C | -9.03636 | 1.661041 | -0.65786 |
| H | -8.91279 | -0.50701 | -0.68681 |
| H | -7.733 | 0.297473 | -1.74087 |
| C | -8.63245 | 1.688789 | 1.842004 |
| H | -8.54799 | -0.46456 | 1.869304 |
| H | -7.09412 | 0.299659 | 2.518111 |
| C | -9.68289 | 1.803213 | 0.727651 |
| H | -9.80181 | 1.70379 | -1.44126 |

| | | | |
|---|---|---|---|
| H | -8.35503 | 2.505661 | -0.83151 |
| H | -9.11046 | 1.76059 | 2.825825 |
| H | -7.93077 | 2.530873 | 1.76443 |
| H | -10.2156 | 2.758168 | 0.804754 |
| H | -10.4303 | 1.006989 | 0.858521 |
| C | -2.90878 | -1.96658 | -1.30075 |
| C | -1.98562 | -3.17302 | -1.06679 |
| C | -3.10618 | -1.75752 | -2.82194 |
| H | -2.36074 | -1.08689 | -0.93674 |
| C | -0.6248 | -2.93892 | -1.73872 |
| H | -2.44208 | -4.07943 | -1.49503 |
| H | -1.85646 | -3.34511 | 0.009044 |
| C | -1.75235 | -1.53352 | -3.51077 |
| H | -3.60427 | -2.65049 | -3.2318 |
| H | -3.76954 | -0.90488 | -3.00324 |
| C | -0.79538 | -2.70496 | -3.24707 |
| H | 0.031354 | -3.79927 | -1.55474 |
| H | -0.15421 | -2.05092 | -1.29625 |
| H | -1.90156 | -1.39812 | -4.58888 |
| H | -1.30422 | -0.61608 | -3.10957 |
| H | 0.178835 | -2.50493 | -3.70725 |
| H | -1.19463 | -3.61958 | -3.71376 |
| C | 2.908899 | -1.96631 | 1.301013 |
| C | 1.98566 | -3.17277 | 1.067535 |
| C | 3.106637 | -1.75689 | 2.822115 |
| H | 2.360786 | -1.08669 | 0.936916 |
| C | 0.624984 | -2.93843 | 1.739673 |
| H | 2.442172 | -4.0791 | 1.495898 |
| H | 1.856271 | -3.34512 | -0.00823 |
| C | 1.752967 | -1.53265 | 3.511163 |
| H | 3.604769 | -2.64979 | 3.232078 |
| H | 3.770082 | -0.90424 | 3.003076 |
| C | 0.795871 | -2.7041 | 3.247934 |
| H | -0.03127 | -3.79879 | 1.556048 |
| H | 0.154354 | -2.05051 | 1.297083 |
| H | 1.902402 | -1.39702 | 4.589213 |
| H | 1.3048 | -0.61529 | 3.109851 |
| H | -0.17824 | -2.50387 | 3.708246 |
| H | 1.195148 | -3.61862 | 3.714784 |
| C | 7.175472 | 0.264764 | -0.34788 |
| C | 8.236263 | 0.356965 | 0.770592 |
| C | 7.849881 | 0.372222 | -1.72851 |
| H | 6.522564 | 1.141417 | -0.2405 |
| C | 9.036646 | 1.660691 | 0.657007 |
| H | 8.912875 | -0.50734 | 0.686068 |
| H | 7.733276 | 0.297294 | 1.740216 |
| C | 8.632454 | 1.688371 | -1.84281 |
| H | 8.54774 | -0.46497 | -1.87004 |
| H | 7.093874 | 0.299401 | -2.51867 |
| C | 9.683031 | 1.802737 | -0.72858 |
| H | 9.802186 | 1.703402 | 1.440316 |
| H | 8.355412 | 2.505382 | 0.830697 |
| H | 9.110362 | 1.760076 | -2.82669 |
| H | 7.930875 | 2.530534 | -1.7652 |
| H | 10.21587 | 2.757636 | -0.80578 |
| H | 10.43036 | 1.006436 | -0.8595 |

*Uncatalyzed TS for substrate 2a, conformer A:*

| | x | y | z |
|---|---|---|---|
| C | 2.978937 | -2.57173 | -1.59718 |
| C | 1.635682 | -2.2476 | -1.65943 |
| C | 1.000918 | -1.7322 | -0.52935 |
| C | 1.702791 | -1.5136 | 0.66032 |
| C | 3.043855 | -1.85284 | 0.712382 |
| C | 3.6747 | -2.3819 | -0.40741 |
| H | -0.96153 | -1.59503 | -1.48634 |
| H | 3.481721 | -2.97894 | -2.46353 |
| H | 1.073128 | -2.39957 | -2.57321 |
| C | -0.40806 | -1.40958 | -0.57698 |
| C | 0.976219 | -0.83439 | 1.785361 |
| H | 3.602468 | -1.69084 | 1.62602 |
| H | 4.723122 | -2.64639 | -0.35426 |
| C | -0.47088 | -1.29382 | 1.854914 |
| H | 1.45981 | -1.03326 | 2.741225 |
| H | -1.05505 | -0.66039 | 2.518916 |
| N | -1.10595 | -1.23767 | 0.519536 |
| H | 1.019347 | 0.24862 | 1.615401 |
| H | -0.53546 | -2.32507 | 2.211307 |
| C | -2.46136 | -0.81869 | 0.39017 |
| C | -3.45687 | -1.4978 | 1.074928 |
| C | -2.75813 | 0.291854 | -0.41131 |
| C | -4.77863 | -1.1106 | 0.930128 |
| H | -3.19185 | -2.34058 | 1.700707 |
| C | -4.09932 | 0.65036 | -0.55564 |
| C | -5.10096 | -0.04751 | 0.097621 |
| H | -5.55772 | -1.64933 | 1.452287 |
| H | -4.37382 | 1.469017 | -1.21053 |
| H | -6.13404 | 0.240139 | -0.04176 |
| C | -1.68871 | 1.140552 | -1.01082 |
| O | -1.97924 | 2.444669 | -1.17737 |
| N | -0.55568 | 0.678848 | -1.33378 |
| C | 0.526995 | 1.546452 | -1.79131 |
| H | 0.131454 | 2.455351 | -2.24775 |
| H | 1.086327 | 0.994702 | -2.5472 |
| H | -2.80488 | 2.683921 | -0.74149 |
| C | 1.434813 | 1.882513 | -0.63046 |
| C | 1.00176 | 2.769101 | 0.355483 |
| C | 2.688631 | 1.298195 | -0.51163 |
| C | 1.80499 | 3.05343 | 1.44838 |
| H | 0.03517 | 3.248255 | 0.253517 |
| C | 3.497307 | 1.58396 | 0.582602 |
| H | 3.035247 | 0.607645 | -1.27374 |
| C | 3.055972 | 2.456306 | 1.566087 |
| H | 1.463864 | 3.750567 | 2.20273 |
| H | 4.475936 | 1.127271 | 0.661455 |
| H | 3.688282 | 2.68559 | 2.413882 |

*Uncatalyzed TS for substrate 2a, conformer B:*

| | X | Y | Z |
|---|---|---|---|
| C | -3.14557 | 1.660203 | -1.10697 |
| C | -1.92595 | 1.056772 | -1.35224 |
| C | -0.84828 | 1.327999 | -0.51225 |
| C | -0.97578 | 2.194769 | 0.578394 |
| C | -2.20676 | 2.7789 | 0.822588 |
| C | -3.28256 | 2.513648 | -0.01892 |
| H | 0.530981 | -0.03692 | -1.53087 |
| H | -3.98999 | 1.455235 | -1.75036 |
| H | -1.80972 | 0.365316 | -2.17752 |
| C | 0.434317 | 0.693817 | -0.73959 |
| C | 0.242403 | 2.42078 | 1.433269 |
| H | -2.32749 | 3.452291 | 1.662187 |
| H | -4.23854 | 2.982329 | 0.176837 |
| C | 1.490155 | 2.45114 | 0.564573 |
| H | 0.163919 | 3.359028 | 1.981685 |
| H | 2.396392 | 2.460877 | 1.165995 |
| N | 1.543263 | 1.250346 | -0.29811 |
| H | 0.329949 | 1.617104 | 2.172359 |
| H | 1.487867 | 3.333299 | -0.07973 |
| C | 2.753409 | 0.51007 | -0.42404 |
| C | 3.874542 | 1.10115 | -0.98338 |
| C | 2.7888 | -0.80712 | 0.049917 |
| C | 5.039814 | 0.365315 | -1.12442 |
| H | 3.82018 | 2.127259 | -1.32462 |
| C | 3.967999 | -1.53394 | -0.11563 |
| C | 5.08005 | -0.9585 | -0.70701 |
| H | 5.911113 | 0.819796 | -1.5763 |
| H | 4.013388 | -2.5727 | 0.190596 |
| H | 5.979659 | -1.54327 | -0.84238 |
| C | 1.63927 | -1.39414 | 0.791677 |
| O | 1.921552 | -2.30532 | 1.735456 |
| N | 0.442044 | -1.04465 | 0.566382 |
| C | -0.66705 | -1.56344 | 1.35908 |
| H | -0.4114 | -2.54161 | 1.773802 |
| H | -0.82853 | -0.88712 | 2.203885 |
| H | 2.869068 | -2.36553 | 1.903319 |
| C | -1.92532 | -1.6522 | 0.53371 |
| C | -1.89918 | -2.26783 | -0.71434 |
| C | -3.12322 | -1.13849 | 1.011998 |
| C | -3.05378 | -2.36006 | -1.47683 |
| H | -0.96875 | -2.68071 | -1.08924 |
| C | -4.2831 | -1.23687 | 0.254209 |
| H | -3.15231 | -0.654 | 1.981574 |
| C | -4.24987 | -1.84257 | -0.99299 |
| H | -3.02521 | -2.84654 | -2.44349 |
| H | -5.21247 | -0.83654 | 0.638867 |
| H | -5.15378 | -1.92137 | -1.58292 |

*Uncatalyzed TS for substrate 2b, conformer A:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.28798 | 3.220938 | -1.47341 |
| C | -0.99498 | 2.729787 | -1.50135 |
| C | -0.52015 | 1.984848 | -0.42232 |
| C | -1.33513 | 1.705774 | 0.679563 |
| C | -2.62266 | 2.212872 | 0.699974 |
| C | -3.09343 | 2.967555 | -0.36765 |
| H | 1.482026 | 1.721781 | -1.26465 |
| H | -2.66627 | 3.80626 | -2.30016 |
| H | -0.34758 | 2.927702 | -2.34769 |
| C | 0.839194 | 1.486731 | -0.42847 |
| C | -0.78759 | 0.793122 | 1.73776 |
| H | -3.26675 | 2.004866 | 1.545644 |
| H | -4.1016 | 3.360736 | -0.33894 |
| C | 0.69174 | 1.055981 | 1.966281 |
| H | -1.3206 | 0.920509 | 2.679531 |
| H | 1.144104 | 0.273609 | 2.572032 |
| N | 1.424232 | 1.09862 | 0.680947 |
| H | -0.9421 | -0.24218 | 1.409377 |
| H | 0.842764 | 2.015271 | 2.467742 |
| C | 2.726705 | 0.529598 | 0.582157 |
| C | 3.746185 | 0.991504 | 1.399395 |
| C | 2.944355 | -0.50774 | -0.33314 |
| C | 5.018972 | 0.457828 | 1.279188 |
| H | 3.542184 | 1.781657 | 2.110891 |
| C | 4.238725 | -1.01688 | -0.44853 |
| C | 5.268927 | -0.53346 | 0.339831 |
| H | 5.818703 | 0.828666 | 1.905842 |
| H | 4.455959 | -1.78038 | -1.18653 |
| H | 6.267257 | -0.93193 | 0.221584 |
| C | 1.827514 | -1.12642 | -1.10119 |
| O | 1.961241 | -2.42835 | -1.41598 |
| N | 0.793743 | -0.47815 | -1.43673 |
| C | -0.33462 | -1.12805 | -2.10086 |
| H | -0.00791 | -2.02492 | -2.62961 |
| H | -0.72676 | -0.42106 | -2.83247 |
| H | 2.713333 | -2.82717 | -0.96393 |
| C | -1.40773 | -1.45825 | -1.09159 |
| C | -1.22763 | -2.50041 | -0.18096 |
| C | -2.57581 | -0.71427 | -1.02864 |
| C | -2.19188 | -2.77486 | 0.77309 |
| H | -0.3285 | -3.10432 | -0.23017 |
| C | -3.5427 | -0.99401 | -0.07031 |
| H | -2.73197 | 0.10149 | -1.72711 |
| C | -3.36816 | -2.0244 | 0.846106 |
| H | -2.04129 | -3.59176 | 1.469429 |
| H | -4.44968 | -0.40095 | -0.04004 |
| C | -4.422 | -2.35524 | 1.864647 |
| H | -3.97956 | -2.53882 | 2.844195 |
| H | -5.1499 | -1.55101 | 1.959463 |
| H | -4.96093 | -3.25988 | 1.576399 |

*Uncatalyzed TS for substrate 2b, conformer B:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.83025 | 1.961744 | -0.92002 |
| C | -1.69916 | 1.223231 | -1.21789 |
| C | -0.52587 | 1.451946 | -0.50278 |
| C | -0.47097 | 2.408065 | 0.518291 |
| C | -1.61587 | 3.124449 | 0.820216 |
| C | -2.78617 | 2.903417 | 0.100781 |
| H | 0.617627 | -0.14538 | -1.47964 |
| H | -3.74719 | 1.792624 | -1.46764 |
| H | -1.72602 | 0.461294 | -1.98731 |
| C | 0.666151 | 0.67412 | -0.77546 |
| C | 0.838714 | 2.581123 | 1.238857 |
| H | -1.59542 | 3.865858 | 1.609603 |
| H | -3.67297 | 3.475682 | 0.341279 |
| C | 1.989482 | 2.425585 | 0.257946 |
| H | 0.897003 | 3.561534 | 1.710717 |
| H | 2.951554 | 2.408461 | 0.764897 |
| N | 1.857582 | 1.152046 | -0.48526 |
| H | 0.928359 | 1.830159 | 2.031277 |
| H | 1.989458 | 3.243115 | -0.46678 |
| C | 2.979065 | 0.276679 | -0.59497 |
| C | 4.095005 | 0.665065 | -1.31782 |
| C | 2.940186 | -0.95316 | 0.072448 |
| C | 5.178026 | -0.19355 | -1.42322 |
| H | 4.100826 | 1.63049 | -1.80806 |
| C | 4.035537 | -1.80658 | -0.05761 |
| C | 5.140542 | -1.43615 | -0.80604 |
| H | 6.044014 | 0.101624 | -2.00019 |
| H | 4.017031 | -2.78813 | 0.401685 |
| H | 5.972506 | -2.11941 | -0.9079 |
| C | 1.799664 | -1.32636 | 0.953497 |
| O | 2.066827 | -2.12568 | 1.998393 |
| N | 0.624225 | -0.9085 | 0.737637 |
| C | -0.48565 | -1.23841 | 1.623289 |
| H | -0.27776 | -2.16599 | 2.162411 |
| H | -0.57701 | -0.44416 | 2.370603 |
| H | 3.015099 | -2.24808 | 2.122291 |
| C | -1.77054 | -1.34938 | 0.843114 |
| C | -1.81056 | -2.07542 | -0.34452 |
| C | -2.9312 | -0.73623 | 1.289047 |
| C | -2.98532 | -2.17338 | -1.071 |
| H | -0.91312 | -2.56837 | -0.70303 |
| C | -4.10986 | -0.84226 | 0.561655 |
| H | -2.91764 | -0.15905 | 2.206863 |
| C | -4.15714 | -1.55697 | -0.62988 |
| H | -3.00071 | -2.74545 | -1.99182 |
| H | -5.00709 | -0.35498 | 0.925198 |
| C | -5.43456 | -1.69382 | -1.40993 |
| H | -5.26317 | -1.55261 | -2.4775 |
| H | -5.85902 | -2.69098 | -1.27773 |
| H | -6.17911 | -0.97027 | -1.08096 |

*Uncatalyzed TS for substrate 2c, conformer A:*

| | X | Y | Z |
|---|---|---|---|
| C | -1.53934 | 3.83993 | -1.11615 |
| C | -0.32635 | 3.176375 | -1.15509 |
| C | -0.03867 | 2.215321 | -0.18633 |
| C | -0.96282 | 1.892049 | 0.811914 |
| C | -2.16805 | 2.572012 | 0.847029 |
| C | -2.45108 | 3.540874 | -0.10854 |
| H | 1.967388 | 1.802628 | -0.95452 |
| H | -1.77291 | 4.592469 | -1.85671 |
| H | 0.40306 | 3.40154 | -1.92439 |
| C | 1.237468 | 1.533508 | -0.20428 |
| C | -0.62324 | 0.755999 | 1.733005 |
| H | -2.89668 | 2.333044 | 1.612081 |
| H | -3.39637 | 4.067079 | -0.0697 |
| C | 0.857956 | 0.759955 | 2.07548 |
| H | -1.2029 | 0.811057 | 2.654039 |
| H | 1.152723 | -0.166 | 2.564806 |
| N | 1.680855 | 0.895109 | 0.853353 |
| H | -0.89111 | -0.1822 | 1.230757 |
| H | 1.102156 | 1.595807 | 2.735905 |
| C | 2.901829 | 0.172786 | 0.728908 |
| C | 3.905341 | 0.352446 | 1.66792 |
| C | 3.055721 | -0.72377 | -0.33613 |
| C | 5.10559 | -0.32482 | 1.530078 |
| H | 3.748039 | 1.039803 | 2.489397 |
| C | 4.28022 | -1.38151 | -0.46306 |
| C | 5.299452 | -1.17736 | 0.451903 |
| H | 5.894724 | -0.17275 | 2.25386 |
| H | 4.456703 | -2.03968 | -1.30593 |
| H | 6.24611 | -1.68392 | 0.322833 |
| C | 1.929761 | -1.05014 | -1.25665 |
| O | 1.918916 | -2.29189 | -1.77806 |
| N | 1.014711 | -0.2205 | -1.53079 |
| C | -0.14178 | -0.59432 | -2.34448 |
| H | 0.105057 | -1.429 | -3.00223 |
| H | -0.39022 | 0.268748 | -2.96293 |
| H | 2.577154 | -2.85716 | -1.35838 |
| C | -1.31358 | -0.9333 | -1.45581 |
| C | -1.35311 | -2.13721 | -0.76236 |
| C | -2.36679 | -0.03838 | -1.28789 |
| C | -2.4035 | -2.44732 | 0.091891 |
| H | -0.55516 | -2.85834 | -0.89845 |
| C | -3.42018 | -0.32857 | -0.44254 |
| H | -2.35902 | 0.906672 | -1.82155 |
| C | -3.4469 | -1.53594 | 0.256315 |
| H | -2.40905 | -3.39757 | 0.605587 |
| H | -4.24398 | 0.361144 | -0.31294 |
| O | -4.51346 | -1.73553 | 1.056095 |
| C | -4.62443 | -2.97672 | 1.725401 |
| H | -3.79634 | -3.12343 | 2.423658 |
| H | -5.55938 | -2.93988 | 2.276517 |
| H | -4.65382 | -3.8044 | 1.012737 |

*Uncatalyzed TS for substrate 2c, conformer B:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.53356 | 2.057096 | -0.90867 |
| C | -1.44629 | 1.24512 | -1.17673 |
| C | -0.2517 | 1.452835 | -0.49128 |
| C | -0.13143 | 2.464351 | 0.467431 |
| C | -1.23298 | 3.256878 | 0.740757 |
| C | -2.42497 | 3.05405 | 0.053417 |
| H | 0.808884 | -0.21602 | -1.4392 |
| H | -3.46874 | 1.902019 | -1.42947 |
| H | -1.52387 | 0.442557 | -1.89983 |
| C | 0.902916 | 0.613151 | -0.75115 |
| C | 1.200747 | 2.619723 | 1.149259 |
| H | -1.16 | 4.043481 | 1.481754 |
| H | -3.27825 | 3.683367 | 0.27156 |
| C | 2.319397 | 2.373681 | 0.149743 |
| H | 1.307424 | 3.618262 | 1.571885 |
| H | 3.291739 | 2.340431 | 0.63636 |
| N | 2.119911 | 1.07481 | -0.53088 |
| H | 1.282816 | 1.904723 | 1.974911 |
| H | 2.334326 | 3.158618 | -0.61024 |
| C | 3.211229 | 0.170147 | -0.66281 |
| C | 4.322162 | 0.520366 | -1.41357 |
| C | 3.15133 | -1.0551 | 0.010584 |
| C | 5.373425 | -0.37312 | -1.54166 |
| H | 4.34808 | 1.483604 | -1.90736 |
| C | 4.21398 | -1.94571 | -0.14392 |
| C | 5.310662 | -1.61379 | -0.92117 |
| H | 6.234863 | -0.10679 | -2.13911 |
| H | 4.175395 | -2.9247 | 0.319735 |
| H | 6.116849 | -2.32413 | -1.04246 |
| C | 2.032696 | -1.37282 | 0.937523 |
| O | 2.308057 | -2.17325 | 1.978438 |
| N | 0.865599 | -0.90407 | 0.776555 |
| C | -0.19761 | -1.18824 | 1.738802 |
| H | -0.01957 | -2.15932 | 2.206863 |
| H | -0.15115 | -0.43818 | 2.534059 |
| H | 3.253833 | -2.34154 | 2.060207 |
| C | -1.55151 | -1.15298 | 1.082501 |
| C | -1.80701 | -1.9092 | -0.05187 |
| C | -2.57931 | -0.37355 | 1.606342 |
| C | -3.04963 | -1.88578 | -0.67369 |
| H | -1.02407 | -2.5356 | -0.46646 |
| C | -3.82314 | -0.34389 | 1.008819 |
| H | -2.40242 | 0.222934 | 2.494512 |
| C | -4.06576 | -1.09319 | -0.14288 |
| H | -3.21715 | -2.49036 | -1.55345 |
| H | -4.62726 | 0.259211 | 1.409583 |
| O | -5.30236 | -0.98266 | -0.67209 |
| C | -5.62096 | -1.77775 | -1.79693 |
| H | -6.659 | -1.56377 | -2.03393 |
| H | -4.99242 | -1.51941 | -2.65339 |
| H | -5.51058 | -2.84096 | -1.57023 |

*Uncatalyzed TS for substrate 2d, conformer A:*

| | X | Y | Z |
|---|---|---|---|
| C | 1.363319 | 3.820263 | 1.186362 |
| C | 0.149212 | 3.156626 | 1.190681 |
| C | -0.11491 | 2.20147 | 0.209599 |
| C | 0.832771 | 1.887623 | -0.7692 |
| C | 2.039111 | 2.567394 | -0.77066 |
| C | 2.299796 | 3.528699 | 0.199625 |
| H | -2.14914 | 1.808796 | 0.909353 |
| H | 1.577277 | 4.56908 | 1.936612 |
| H | -0.59946 | 3.379465 | 1.942165 |
| C | -1.3926 | 1.517688 | 0.194003 |
| C | 0.514489 | 0.762207 | -1.71191 |
| H | 2.785141 | 2.337828 | -1.52227 |
| H | 3.245014 | 4.056265 | 0.186248 |
| C | -0.95821 | 0.76919 | -2.08825 |
| H | 1.116232 | 0.825639 | -2.61813 |
| H | -1.23906 | -0.14933 | -2.59926 |
| N | -1.80753 | 0.884777 | -0.88244 |
| H | 0.766362 | -0.18359 | -1.21616 |
| H | -1.18692 | 1.614776 | -2.7415 |
| C | -3.02739 | 0.159317 | -0.79075 |
| C | -3.9959 | 0.3086 | -1.7711 |
| C | -3.21755 | -0.71513 | 0.287656 |
| C | -5.19637 | -0.37332 | -1.66138 |
| H | -3.81267 | 0.976618 | -2.60311 |
| C | -4.44263 | -1.37698 | 0.386249 |
| C | -5.4275 | -1.20068 | -0.57062 |
| H | -5.95897 | -0.24321 | -2.41727 |
| H | -4.65043 | -2.01423 | 1.238128 |
| H | -6.37613 | -1.70882 | -0.46466 |
| C | -2.12299 | -1.01823 | 1.250497 |
| O | -2.13011 | -2.23627 | 1.816647 |
| N | -1.20727 | -0.18466 | 1.522318 |
| C | -0.08706 | -0.52693 | 2.394299 |
| H | -0.3523 | -1.34492 | 3.065908 |
| H | 0.137559 | 0.355378 | 2.994133 |
| H | -2.79213 | -2.81177 | 1.416014 |
| C | 1.11711 | -0.89049 | 1.556932 |
| C | 1.149992 | -2.107 | 0.873994 |
| C | 2.17621 | -0.002 | 1.425177 |
| C | 2.212063 | -2.42113 | 0.044093 |
| H | 0.339036 | -2.81407 | 0.999446 |
| C | 3.24659 | -0.29761 | 0.593788 |
| H | 2.159109 | 0.942267 | 1.957841 |
| C | 3.235251 | -1.49698 | -0.09006 |
| H | 2.262548 | -3.35703 | -0.49371 |
| H | 4.073866 | 0.385667 | 0.466112 |
| N | 4.350987 | -1.79997 | -1.01188 |
| O | 5.176916 | -0.93417 | -1.18146 |
| O | 4.351307 | -2.88475 | -1.54095 |

*Uncatalyzed TS for substrate 2d, conformer B:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.34878 | 2.067246 | -0.92299 |
| C | -1.26105 | 1.256427 | -1.19572 |
| C | -0.07484 | 1.443033 | -0.48989 |
| C | 0.039951 | 2.437314 | 0.487287 |
| C | -1.06327 | 3.226281 | 0.767159 |
| C | -2.24935 | 3.0405 | 0.064657 |
| H | 0.993739 | -0.2146 | -1.4513 |
| H | -3.27534 | 1.93748 | -1.46632 |
| H | -1.32903 | 0.479738 | -1.94788 |
| C | 1.083442 | 0.602941 | -0.74814 |
| C | 1.373907 | 2.589452 | 1.167824 |
| H | -0.99425 | 4.000606 | 1.521418 |
| H | -3.10279 | 3.668974 | 0.284662 |
| C | 2.488989 | 2.371146 | 0.156365 |
| H | 1.474334 | 3.581135 | 1.607724 |
| H | 3.465345 | 2.34523 | 0.63535 |
| N | 2.300386 | 1.077642 | -0.53811 |
| H | 1.468468 | 1.861109 | 1.980602 |
| H | 2.486604 | 3.166159 | -0.59283 |
| C | 3.390864 | 0.173176 | -0.66702 |
| C | 4.511164 | 0.522733 | -1.40393 |
| C | 3.319591 | -1.05838 | -0.005 |
| C | 5.556612 | -0.37776 | -1.53066 |
| H | 4.548456 | 1.489732 | -1.88954 |
| C | 4.376717 | -1.9563 | -0.15704 |
| C | 5.480906 | -1.62472 | -0.92306 |
| H | 6.42466 | -0.11231 | -2.11894 |
| H | 4.327521 | -2.9389 | 0.298279 |
| H | 6.283082 | -2.33925 | -1.04595 |
| C | 2.200978 | -1.3621 | 0.922995 |
| O | 2.464185 | -2.15624 | 1.96751 |
| N | 1.039475 | -0.87191 | 0.76552 |
| C | -0.01202 | -1.09048 | 1.752837 |
| H | 0.165061 | -2.02387 | 2.292587 |
| H | 0.029543 | -0.27968 | 2.486125 |
| H | 3.406707 | -2.34576 | 2.046514 |
| C | -1.36918 | -1.11549 | 1.099587 |
| C | -1.58714 | -1.9112 | -0.0229 |
| C | -2.40845 | -0.35009 | 1.612426 |
| C | -2.82224 | -1.92494 | -0.64703 |
| H | -0.7825 | -2.52283 | -0.41405 |
| C | -3.65154 | -0.34911 | 0.999376 |
| H | -2.24514 | 0.264531 | 2.48957 |
| C | -3.82779 | -1.1286 | -0.12687 |
| H | -3.01956 | -2.5319 | -1.51933 |
| H | -4.47072 | 0.251573 | 1.368123 |
| N | -5.13319 | -1.09248 | -0.81887 |
| O | -5.9491 | -0.29727 | -0.41593 |
| O | -5.28832 | -1.84856 | -1.74737 |

*Uncatalyzed TS for substrate 2e, conformer A1:*

| | X | Y | Z |
|---|---|---|---|
| C | 2.870713 | 3.024487 | 1.221866 |
| C | 1.541364 | 2.679265 | 1.388331 |
| C | 0.852067 | 2.075745 | 0.338834 |
| C | 1.481708 | 1.797693 | -0.8799 |
| C | 2.814304 | 2.139524 | -1.02894 |
| C | 3.500869 | 2.753347 | 0.013122 |
| H | -1.04353 | 1.981977 | 1.423545 |
| H | 3.4127 | 3.50748 | 2.023477 |
| H | 1.030693 | 2.882616 | 2.322471 |
| C | -0.54431 | 1.729652 | 0.498773 |
| C | 0.678716 | 1.116976 | -1.95302 |
| H | 3.320505 | 1.930429 | -1.9633 |
| H | 4.540002 | 3.025426 | -0.12195 |
| C | -0.77161 | 1.567162 | -1.92287 |
| H | 1.095672 | 1.326492 | -2.9379 |
| H | -1.39262 | 0.923458 | -2.54219 |
| N | -1.30983 | 1.510931 | -0.54775 |
| H | 0.72488 | 0.0354 | -1.80358 |
| H | -0.86831 | 2.596309 | -2.27825 |
| C | -2.65073 | 1.105145 | -0.31419 |
| C | -3.68273 | 1.700535 | -1.02295 |
| C | -2.90335 | 0.099493 | 0.628576 |
| C | -4.9944 | 1.341716 | -0.76176 |
| H | -3.45497 | 2.460306 | -1.7598 |
| C | -4.23624 | -0.2239 | 0.892697 |
| C | -5.27207 | 0.394323 | 0.21402 |
| H | -5.79996 | 1.818553 | -1.30369 |
| H | -4.47463 | -0.94923 | 1.661102 |
| H | -6.29617 | 0.135627 | 0.445926 |
| C | -1.81187 | -0.69238 | 1.264541 |
| O | -2.14455 | -1.91044 | 1.716271 |
| N | -0.62406 | -0.26135 | 1.383349 |
| C | 0.432582 | -1.11267 | 1.922824 |
| H | 0.066101 | -2.12765 | 2.084352 |
| H | 0.727556 | -0.70313 | 2.890407 |
| H | -2.95413 | -2.23484 | 1.30532 |
| C | 1.641139 | -1.13988 | 1.019905 |
| C | 1.637273 | -1.78308 | -0.21476 |
| C | 2.833674 | -0.54888 | 1.431034 |
| C | 2.766076 | -1.83507 | -1.01889 |
| C | 3.974039 | -0.59551 | 0.645906 |
| H | 2.864734 | -0.05419 | 2.394506 |
| C | 3.939201 | -1.23743 | -0.58319 |
| H | 2.727352 | -2.35279 | -1.96772 |
| H | 4.888413 | -0.13437 | 0.995511 |
| Br | 0.062154 | -2.63949 | -0.85501 |
| H | 4.825485 | -1.28688 | -1.20215 |

*Uncatalyzed TS for substrate 2e, conformer A2:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.27305 | 3.052737 | -1.08237 |
| C | -1.02876 | 2.499788 | -1.32534 |
| C | -0.34812 | 1.860315 | -0.29015 |
| C | -0.911 | 1.746448 | 0.986555 |
| C | -2.16566 | 2.285433 | 1.209615 |
| C | -2.83626 | 2.942202 | 0.182867 |
| H | 1.447643 | 1.498841 | -1.47781 |
| H | -2.80519 | 3.563726 | -1.87282 |
| H | -0.57317 | 2.576828 | -2.30556 |
| C | 0.997938 | 1.371223 | -0.503 |
| C | -0.11114 | 1.027823 | 2.036477 |
| H | -2.61856 | 2.204657 | 2.190263 |
| H | -3.81162 | 3.371547 | 0.373077 |
| C | 1.366116 | 1.370277 | 1.908442 |
| H | -0.45089 | 1.298023 | 3.035826 |
| H | 1.976898 | 0.716594 | 2.52804 |
| N | 1.823219 | 1.210472 | 0.511153 |
| H | -0.25414 | -0.05174 | 1.922141 |
| H | 1.550907 | 2.405502 | 2.206636 |
| C | 3.120138 | 0.707681 | 0.221543 |
| C | 4.238822 | 1.319229 | 0.766182 |
| C | 3.242866 | -0.40464 | -0.62194 |
| C | 5.503135 | 0.866228 | 0.428243 |
| H | 4.113346 | 2.164182 | 1.431261 |
| C | 4.528041 | -0.82714 | -0.96692 |
| C | 5.647914 | -0.19249 | -0.45881 |
| H | 6.3763 | 1.354477 | 0.839481 |
| H | 4.662481 | -1.64268 | -1.66806 |
| H | 6.633713 | -0.52481 | -0.75357 |
| C | 2.054524 | -1.20043 | -1.03717 |
| O | 2.257359 | -2.50809 | -1.27551 |
| N | 0.8938 | -0.69936 | -1.12972 |
| C | -0.28138 | -1.52858 | -1.38487 |
| H | 0.002175 | -2.47283 | -1.85259 |
| H | -0.92187 | -0.98212 | -2.07239 |
| H | 3.140815 | -2.78671 | -1.0086 |
| C | -1.00225 | -1.79251 | -0.08073 |
| C | -0.34213 | -2.52015 | 0.912358 |
| C | -2.28396 | -1.33202 | 0.204326 |
| C | -0.91818 | -2.75395 | 2.148831 |
| C | -2.87097 | -1.54634 | 1.447014 |
| C | -2.18444 | -2.2512 | 2.421189 |
| H | -0.38717 | -3.32975 | 2.895025 |
| H | -3.86806 | -1.17289 | 1.636506 |
| H | -2.64792 | -2.42282 | 3.383787 |
| H | 0.6432 | -2.91617 | 0.695144 |
| Br | -3.31829 | -0.41613 | -1.09503 |

*Uncatalyzed TS for substrate 2e, conformer B1:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.7974 | 2.078646 | -1.39431 |
| C | -1.63951 | 1.323458 | -1.45 |
| C | -0.55471 | 1.676834 | -0.6521 |
| C | -0.6134 | 2.779766 | 0.205358 |
| C | -1.78255 | 3.518972 | 0.262105 |
| C | -2.86593 | 3.170337 | -0.53707 |
| H | 0.71994 | 0.031391 | -1.34073 |
| H | -3.64554 | 1.817026 | -2.0119 |
| H | -1.57201 | 0.461029 | -2.10291 |
| C | 0.676103 | 0.906097 | -0.70395 |
| C | 0.611564 | 3.0871 | 1.022216 |
| H | -1.84612 | 4.377269 | 0.919638 |
| H | -3.77197 | 3.761065 | -0.49368 |
| C | 1.858049 | 2.843976 | 0.186897 |
| H | 0.602015 | 4.121086 | 1.365261 |
| H | 2.762039 | 2.916298 | 0.78801 |
| N | 1.823801 | 1.487178 | -0.40006 |
| H | 0.634984 | 2.44601 | 1.909839 |
| H | 1.921289 | 3.569454 | -0.6277 |
| C | 2.989645 | 0.675691 | -0.37757 |
| C | 4.148666 | 1.096045 | -1.00967 |
| C | 2.942645 | -0.5368 | 0.317579 |
| C | 5.26888 | 0.280928 | -0.9992 |
| H | 4.158948 | 2.048642 | -1.5241 |
| C | 4.074899 | -1.35279 | 0.295723 |
| C | 5.224614 | -0.95273 | -0.36315 |
| H | 6.170331 | 0.600012 | -1.50479 |
| H | 4.056658 | -2.32796 | 0.768032 |
| H | 6.087558 | -1.60404 | -0.38064 |
| C | 1.756899 | -0.91704 | 1.129266 |
| O | 1.96223 | -1.73886 | 2.167337 |
| N | 0.583506 | -0.50001 | 0.879929 |
| C | -0.52081 | -0.93567 | 1.734592 |
| H | -0.355 | -1.97629 | 2.025253 |
| H | -0.51334 | -0.34105 | 2.651454 |
| H | 2.901057 | -1.8652 | 2.346343 |
| C | -1.86417 | -0.81083 | 1.068525 |
| C | -2.21782 | -1.56953 | -0.04497 |
| C | -2.83001 | 0.036502 | 1.603457 |
| C | -3.48478 | -1.50327 | -0.60216 |
| C | -4.10233 | 0.118218 | 1.05908 |
| C | -4.43133 | -0.65773 | -0.04179 |
| H | -3.7295 | -2.11662 | -1.45867 |
| H | -4.83597 | 0.780689 | 1.498916 |
| H | -5.42521 | -0.6126 | -0.46749 |
| Br | -0.95357 | -2.73873 | -0.85096 |
| H | -2.57747 | 0.633105 | 2.472426 |

*Uncatalyzed TS for substrate 2e, conformer B2:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.2996 | 1.970657 | -1.96962 |
| C | -1.08586 | 1.308798 | -1.98691 |
| C | -0.26097 | 1.363592 | -0.86543 |
| C | -0.64015 | 2.071536 | 0.277328 |
| C | -1.86381 | 2.71924 | 0.287252 |
| C | -2.68622 | 2.670305 | -0.83146 |
| H | 1.369776 | 0.254933 | -1.80597 |
| H | -2.94607 | 1.939884 | -2.83601 |
| H | -0.77375 | 0.752749 | -2.86261 |
| C | 1.053519 | 0.735176 | -0.88925 |
| C | 0.321286 | 2.081875 | 1.431676 |
| H | -2.17415 | 3.268363 | 1.167539 |
| H | -3.63649 | 3.188533 | -0.81734 |
| C | 1.738451 | 2.253002 | 0.909302 |
| H | 0.089944 | 2.888787 | 2.125969 |
| H | 2.473205 | 2.121456 | 1.701187 |
| N | 2.023263 | 1.244252 | -0.13294 |
| H | 0.239542 | 1.138742 | 1.982611 |
| H | 1.868294 | 3.246396 | 0.473018 |
| C | 3.282638 | 0.602553 | -0.17362 |
| C | 4.455107 | 1.33981 | -0.25068 |
| C | 3.315265 | -0.79422 | -0.10595 |
| C | 5.671898 | 0.683619 | -0.3207 |
| H | 4.404182 | 2.420746 | -0.27826 |
| C | 4.551377 | -1.43759 | -0.19857 |
| C | 5.718941 | -0.706 | -0.31781 |
| H | 6.586574 | 1.25613 | -0.39707 |
| H | 4.606243 | -2.52014 | -0.20792 |
| H | 6.667725 | -1.21723 | -0.40545 |
| C | 2.082888 | -1.56016 | 0.197577 |
| O | 2.226181 | -2.71655 | 0.854638 |
| N | 0.912106 | -1.15602 | -0.10354 |
| C | -0.23466 | -1.95913 | 0.339708 |
| H | -0.00312 | -3.01286 | 0.170294 |
| H | -0.35851 | -1.82907 | 1.415137 |
| H | 3.131075 | -2.8429 | 1.163589 |
| C | -1.49826 | -1.61808 | -0.40071 |
| C | -1.61317 | -2.00644 | -1.73445 |
| C | -2.58646 | -0.97429 | 0.180756 |
| C | -2.76366 | -1.76357 | -2.46513 |
| C | -3.75003 | -0.72839 | -0.53516 |
| C | -3.83736 | -1.1251 | -1.85958 |
| H | -2.83078 | -2.08843 | -3.49496 |
| H | -4.58194 | -0.23527 | -0.05119 |
| H | -4.7496 | -0.94169 | -2.41204 |
| H | -0.78007 | -2.52531 | -2.19655 |
| Br | -2.55389 | -0.42606 | 2.00208 |

*Uncatalyzed TS for substrate 2f, conformer A1:*

| | X | Y | Z |
|---|---|---|---|
| C | 2.883081 | -2.38845 | -1.67552 |
| C | 1.55017 | -2.02755 | -1.76386 |
| C | 0.861993 | -1.66081 | -0.60892 |
| C | 1.496553 | -1.63473 | 0.638118 |
| C | 2.830501 | -1.99244 | 0.710799 |
| C | 3.515727 | -2.37059 | -0.4384 |
| H | -1.03537 | -1.32873 | -1.64438 |
| H | 3.42743 | -2.68538 | -2.56151 |
| H | 1.036872 | -2.03478 | -2.71838 |
| C | -0.5345 | -1.29464 | -0.6871 |
| C | 0.697575 | -1.17776 | 1.826064 |
| H | 3.341062 | -1.97416 | 1.66562 |
| H | 4.557903 | -2.65497 | -0.36712 |
| C | -0.7473 | -1.63064 | 1.715411 |
| H | 1.122857 | -1.56514 | 2.751534 |
| H | -1.37326 | -1.14103 | 2.458643 |
| N | -1.29696 | -1.29721 | 0.383712 |
| H | 0.743414 | -0.08625 | 1.877598 |
| H | -0.82768 | -2.71241 | 1.850201 |
| C | -2.63636 | -0.83797 | 0.251483 |
| C | -3.67141 | -1.58406 | 0.793195 |
| C | -2.8831 | 0.37009 | -0.41506 |
| C | -4.98147 | -1.1652 | 0.632616 |
| H | -3.44568 | -2.50262 | 1.319847 |
| C | -4.21416 | 0.756507 | -0.58517 |
| C | -5.25333 | -0.00371 | -0.07695 |
| H | -5.78922 | -1.75573 | 1.043414 |
| H | -4.45235 | 1.648949 | -1.15128 |
| H | -6.27566 | 0.311667 | -0.23431 |
| C | -1.7845 | 1.278688 | -0.85672 |
| O | -2.09873 | 2.580889 | -0.97605 |
| N | -0.61312 | 0.866515 | -1.10712 |
| C | 0.467591 | 1.775727 | -1.48116 |
| H | 0.108963 | 2.805275 | -1.53252 |
| H | 0.793168 | 1.487953 | -2.48226 |
| H | -2.92916 | 2.788529 | -0.53304 |
| C | 1.639953 | 1.665131 | -0.53382 |
| C | 1.542809 | 2.118867 | 0.788065 |
| C | 2.844736 | 1.14789 | -0.99783 |
| C | 2.663463 | 2.023037 | 1.60896 |
| C | 3.95475 | 1.065779 | -0.1716 |
| H | 2.915755 | 0.813572 | -2.02642 |
| C | 3.861521 | 1.501634 | 1.140787 |
| H | 2.599569 | 2.38423 | 2.628876 |
| H | 4.886651 | 0.669459 | -0.55395 |
| C | 0.268703 | 2.708727 | 1.330305 |
| H | -0.16976 | 3.427256 | 0.636303 |
| H | -0.48824 | 1.938063 | 1.513032 |
| H | 0.452947 | 3.217703 | 2.27473 |
| H | 4.722224 | 1.455061 | 1.795365 |

*Uncatalyzed TS for substrate 2f, conformer A2:*

| | X | Y | Z |
|---|---|---|---|
| C | 2.77016 | -2.94513 | -1.33771 |
| C | 1.461704 | -2.51392 | -1.46465 |
| C | 0.863808 | -1.81794 | -0.41366 |
| C | 1.563828 | -1.53694 | 0.764413 |
| C | 2.880791 | -1.9531 | 0.867355 |
| C | 3.475041 | -2.65773 | -0.17374 |
| H | -1.07327 | -1.64018 | -1.41203 |
| H | 3.242828 | -3.49694 | -2.13849 |
| H | 0.896326 | -2.72456 | -2.3648 |
| C | -0.5258 | -1.42073 | -0.50613 |
| C | 0.843587 | -0.77434 | 1.839494 |
| H | 3.442452 | -1.73595 | 1.767664 |
| H | 4.500223 | -2.9908 | -0.07427 |
| C | -0.61439 | -1.2037 | 1.918499 |
| H | 1.313064 | -0.93462 | 2.809565 |
| H | -1.18995 | -0.52453 | 2.544264 |
| N | -1.2365 | -1.20138 | 0.576363 |
| H | 0.906279 | 0.295692 | 1.618642 |
| H | -0.70232 | -2.21346 | 2.327377 |
| C | -2.58373 | -0.7817 | 0.399975 |
| C | -3.59773 | -1.40019 | 1.11455 |
| C | -2.85791 | 0.255665 | -0.50108 |
| C | -4.91457 | -1.03068 | 0.897938 |
| H | -3.35128 | -2.18609 | 1.817228 |
| C | -4.19503 | 0.593615 | -0.7186 |
| C | -5.21437 | -0.04883 | -0.03701 |
| H | -5.70811 | -1.52494 | 1.441953 |
| H | -4.45119 | 1.349321 | -1.45219 |
| H | -6.24366 | 0.217889 | -0.23431 |
| C | -1.76796 | 1.071371 | -1.10882 |
| O | -2.07113 | 2.34928 | -1.40342 |
| N | -0.60132 | 0.619281 | -1.30864 |
| C | 0.495991 | 1.493792 | -1.72428 |
| H | 0.1113 | 2.381247 | -2.22972 |
| H | 1.100958 | 0.934633 | -2.4348 |
| H | -2.92191 | 2.607599 | -1.03137 |
| C | 1.313518 | 1.889934 | -0.50931 |
| C | 0.698988 | 2.661497 | 0.476099 |
| C | 2.64128 | 1.484093 | -0.34421 |
| C | 1.368221 | 3.010679 | 1.63785 |
| C | 3.297905 | 1.832744 | 0.836449 |
| C | 2.675027 | 2.580474 | 1.823273 |
| H | 0.878906 | 3.618593 | 2.38734 |
| H | 4.325817 | 1.518246 | 0.973759 |
| H | 3.214177 | 2.84229 | 2.72434 |
| H | -0.31849 | 3.001352 | 0.321389 |
| C | 3.378176 | 0.706204 | -1.40019 |
| H | 4.378386 | 0.449114 | -1.05615 |
| H | 2.863292 | -0.2215 | -1.65219 |
| H | 3.480779 | 1.287195 | -2.31903 |

*Uncatalyzed TS for substrate 2f, conformer B1:*

| | X | Y | Z |
|---|---|---|---|
| C | -3.02093 | 1.72063 | -1.2913 |
| C | -1.80653 | 1.074328 | -1.43164 |
| C | -0.76921 | 1.369337 | -0.55071 |
| C | -0.93435 | 2.299651 | 0.479727 |
| C | -2.15874 | 2.930508 | 0.61741 |
| C | -3.19284 | 2.644178 | -0.26712 |
| H | 0.65488 | 0.001999 | -1.4938 |
| H | -3.83401 | 1.499288 | -1.96863 |
| H | -1.66019 | 0.34088 | -2.21545 |
| C | 0.520192 | 0.720831 | -0.69682 |
| C | 0.241351 | 2.54579 | 1.385622 |
| H | -2.30555 | 3.656587 | 1.407417 |
| H | -4.14402 | 3.148656 | -0.15536 |
| C | 1.527548 | 2.541634 | 0.574912 |
| H | 0.143018 | 3.500547 | 1.901062 |
| H | 2.404956 | 2.566978 | 1.217652 |
| N | 1.611903 | 1.312671 | -0.24239 |
| H | 0.290118 | 1.762688 | 2.149896 |
| H | 1.559874 | 3.403077 | -0.09648 |
| C | 2.835852 | 0.601847 | -0.34603 |
| C | 3.972415 | 1.228529 | -0.8327 |
| C | 2.86981 | -0.73345 | 0.072528 |
| C | 5.149423 | 0.510223 | -0.96022 |
| H | 3.921468 | 2.268283 | -1.13036 |
| C | 4.061061 | -1.44393 | -0.08393 |
| C | 5.187791 | -0.83255 | -0.60554 |
| H | 6.033156 | 0.992675 | -1.35548 |
| H | 4.106647 | -2.49533 | 0.17543 |
| H | 6.097909 | -1.40222 | -0.73406 |
| C | 1.70952 | -1.34981 | 0.768682 |
| O | 1.976716 | -2.31609 | 1.659554 |
| N | 0.509241 | -0.98533 | 0.569895 |
| C | -0.57297 | -1.58433 | 1.35629 |
| H | -0.32935 | -2.62985 | 1.562131 |
| H | -0.61414 | -1.0754 | 2.323254 |
| H | 2.921671 | -2.38882 | 1.836816 |
| C | -1.91092 | -1.48661 | 0.673167 |
| C | -2.14308 | -2.142 | -0.54282 |
| C | -2.93776 | -0.77581 | 1.282523 |
| C | -3.40938 | -2.05562 | -1.11303 |
| C | -4.19758 | -0.70424 | 0.706712 |
| H | -2.75194 | -0.28087 | 2.229314 |
| C | -4.43254 | -1.34682 | -0.49842 |
| H | -3.6013 | -2.57012 | -2.04739 |
| H | -4.98938 | -0.15573 | 1.200165 |
| H | -5.41287 | -1.30802 | -0.9558 |
| C | -1.06031 | -2.93044 | -1.22884 |
| H | -0.31392 | -2.27432 | -1.68515 |
| H | -0.5279 | -3.57869 | -0.52961 |
| H | -1.47788 | -3.55621 | -2.01533 |

*Uncatalyzed TS for substrate 2f, conformer B2:*

| | X | Y | Z |
|---|---|---|---|
| C | -3.00346 | 1.788991 | -1.13534 |
| C | -1.80933 | 1.13547 | -1.3832 |
| C | -0.68306 | 1.457176 | -0.62696 |
| C | -0.74436 | 2.412046 | 0.397943 |
| C | -1.94672 | 3.051 | 0.640244 |
| C | -3.06699 | 2.743503 | -0.12797 |
| H | 0.603589 | -0.05765 | -1.55186 |
| H | -3.88293 | 1.544995 | -1.71492 |
| H | -1.75065 | 0.363096 | -2.14137 |
| C | 0.564928 | 0.763365 | -0.8498 |
| C | 0.499295 | 2.646791 | 1.212167 |
| H | -2.01622 | 3.791328 | 1.427759 |
| H | -4.00131 | 3.253888 | 0.068395 |
| C | 1.735015 | 2.520628 | 0.338417 |
| H | 0.483047 | 3.634192 | 1.672773 |
| H | 2.647174 | 2.522728 | 0.930159 |
| N | 1.701552 | 1.249312 | -0.42016 |
| H | 0.546387 | 1.90967 | 2.021505 |
| H | 1.784165 | 3.339361 | -0.38347 |
| C | 2.868501 | 0.42201 | -0.46043 |
| C | 4.007056 | 0.881641 | -1.1007 |
| C | 2.852411 | -0.81582 | 0.195857 |
| C | 5.146157 | 0.091914 | -1.13293 |
| H | 3.989476 | 1.850852 | -1.58332 |
| C | 4.00685 | -1.59638 | 0.140678 |
| C | 5.13982 | -1.15341 | -0.52235 |
| H | 6.031221 | 0.444444 | -1.64503 |
| H | 4.015045 | -2.58143 | 0.592355 |
| H | 6.01788 | -1.78348 | -0.56285 |
| C | 1.667285 | -1.29521 | 0.964623 |
| O | 1.89876 | -2.10057 | 2.016891 |
| N | 0.495311 | -0.9695 | 0.629143 |
| C | -0.69094 | -1.4002 | 1.349094 |
| H | -0.49238 | -2.29358 | 1.948058 |
| H | -0.96103 | -0.60109 | 2.043883 |
| H | 2.835905 | -2.14136 | 2.238637 |
| C | -1.81811 | -1.64421 | 0.369569 |
| C | -1.5392 | -2.30194 | -0.82443 |
| C | -3.12071 | -1.2147 | 0.638063 |
| C | -2.5309 | -2.52872 | -1.76689 |
| C | -4.10828 | -1.4518 | -0.31577 |
| C | -3.82367 | -2.0946 | -1.51122 |
| H | -2.29918 | -3.04905 | -2.687 |
| H | -5.12078 | -1.12199 | -0.11412 |
| H | -4.61076 | -2.26759 | -2.23362 |
| C | -3.46589 | -0.48442 | 1.907904 |
| H | -4.53439 | -0.28289 | 1.955823 |
| H | -3.1944 | -1.05946 | 2.794942 |
| H | -2.94416 | 0.475651 | 1.962488 |
| H | -0.52809 | -2.64359 | -1.01658 |

*Uncatalyzed TS for substrate 2g, conformer A1:*

| | X | Y | Z |
|---|---|---|---|
| C | 2.7836 | -2.82458 | -1.24505 |
| C | 1.450088 | -2.49746 | -1.41769 |
| C | 0.749618 | -1.90448 | -0.37046 |
| C | 1.373119 | -1.61301 | 0.849765 |
| C | 2.709744 | -1.93051 | 1.002579 |
| C | 3.406693 | -2.5381 | -0.03691 |
| H | -1.12599 | -1.71507 | -1.48805 |
| H | 3.335825 | -3.29945 | -2.04446 |
| H | 0.946631 | -2.70538 | -2.35457 |
| C | -0.64089 | -1.54522 | -0.53756 |
| C | 0.550825 | -0.93847 | 1.91281 |
| H | 3.213938 | -1.70292 | 1.933482 |
| H | 4.451133 | -2.78822 | 0.099294 |
| C | -0.87875 | -1.44741 | 1.878081 |
| H | 0.976157 | -1.1116 | 2.900997 |
| H | -1.52724 | -0.85812 | 2.52231 |
| N | -1.41618 | -1.35254 | 0.503866 |
| H | 0.550935 | 0.140668 | 1.732932 |
| H | -0.93075 | -2.49374 | 2.189229 |
| C | -2.73277 | -0.858 | 0.281487 |
| C | -3.81235 | -1.49101 | 0.876877 |
| C | -2.90466 | 0.276694 | -0.52011 |
| C | -5.09692 | -1.03016 | 0.640617 |
| H | -3.63978 | -2.35516 | 1.506196 |
| C | -4.21058 | 0.707602 | -0.76085 |
| C | -5.29587 | 0.05915 | -0.19589 |
| H | -5.94086 | -1.53233 | 1.09386 |
| H | -4.39051 | 1.542778 | -1.42695 |
| H | -6.29794 | 0.404985 | -0.40987 |
| C | -1.75497 | 1.061342 | -1.06063 |
| O | -1.99144 | 2.358671 | -1.31689 |
| N | -0.62453 | 0.541113 | -1.29423 |
| C | 0.482471 | 1.338449 | -1.81828 |
| H | 0.17279 | 2.374097 | -1.96518 |
| H | 0.745824 | 0.9197 | -2.79132 |
| H | -2.79233 | 2.664694 | -0.87772 |
| C | 1.699257 | 1.295147 | -0.92989 |
| C | 1.664223 | 1.91712 | 0.324312 |
| C | 2.887246 | 0.724445 | -1.35651 |
| C | 2.799238 | 1.955188 | 1.125089 |
| C | 4.032664 | 0.766899 | -0.57044 |
| H | 2.921988 | 0.255626 | -2.33323 |
| C | 3.981241 | 1.380629 | 0.667747 |
| H | 2.782622 | 2.443413 | 2.088892 |
| H | 4.954627 | 0.329274 | -0.92907 |
| O | 0.465303 | 2.453115 | 0.682792 |
| C | 0.427507 | 3.268476 | 1.839162 |
| H | -0.57903 | 3.674163 | 1.893965 |
| H | 0.633948 | 2.687449 | 2.74231 |
| H | 1.147342 | 4.086026 | 1.76333 |
| H | 4.866051 | 1.428369 | 1.289398 |

*Uncatalyzed TS for substrate 2g, conformer A2:*

| | X | Y | Z |
|---|---|---|---|
| C | 2.625343 | -2.83144 | -1.28922 |
| C | 1.324198 | -2.39405 | -1.45491 |
| C | 0.655929 | -1.80582 | -0.38215 |
| C | 1.287181 | -1.61593 | 0.852419 |
| C | 2.59315 | -2.04865 | 1.001688 |
| C | 3.250421 | -2.66404 | -0.05888 |
| H | -1.22177 | -1.55912 | -1.47302 |
| H | 3.148974 | -3.30734 | -2.10696 |
| H | 0.816245 | -2.52034 | -2.40359 |
| C | -0.7269 | -1.41299 | -0.52374 |
| C | 0.517071 | -0.90549 | 1.928952 |
| H | 3.097818 | -1.91372 | 1.950682 |
| H | 4.264898 | -3.01778 | 0.077121 |
| C | -0.95074 | -1.30371 | 1.897216 |
| H | 0.92392 | -1.13319 | 2.913832 |
| H | -1.5511 | -0.64633 | 2.522534 |
| N | -1.49181 | -1.22024 | 0.522387 |
| H | 0.616248 | 0.175114 | 1.776398 |
| H | -1.08324 | -2.33148 | 2.244885 |
| C | -2.82376 | -0.76586 | 0.297085 |
| C | -3.88342 | -1.42409 | 0.901324 |
| C | -3.03479 | 0.346582 | -0.5283 |
| C | -5.1822 | -1.01416 | 0.649519 |
| H | -3.68506 | -2.26917 | 1.548443 |
| C | -4.3535 | 0.72679 | -0.78233 |
| C | -5.41721 | 0.049544 | -0.21086 |
| H | -6.00977 | -1.53661 | 1.110013 |
| H | -4.55847 | 1.546198 | -1.46139 |
| H | -6.43041 | 0.353421 | -0.43585 |
| C | -1.90581 | 1.179388 | -1.03473 |
| O | -2.16752 | 2.488421 | -1.22376 |
| N | -0.75424 | 0.704908 | -1.25403 |
| C | 0.375935 | 1.565135 | -1.59784 |
| H | 0.033083 | 2.500505 | -2.04283 |
| H | 0.98578 | 1.033122 | -2.32401 |
| H | -3.01972 | 2.737237 | -0.8489 |
| C | 1.184974 | 1.847936 | -0.35178 |
| C | 0.641655 | 2.624116 | 0.664525 |
| C | 2.476008 | 1.331802 | -0.18989 |
| C | 1.339604 | 2.880845 | 1.835534 |
| C | 3.184502 | 1.585712 | 0.983286 |
| C | 2.612539 | 2.352459 | 1.989142 |
| H | 0.903857 | 3.498272 | 2.608935 |
| H | 4.183692 | 1.195917 | 1.114581 |
| H | 3.177503 | 2.548566 | 2.891202 |
| H | -0.34671 | 3.045951 | 0.521934 |
| O | 2.969693 | 0.587551 | -1.21046 |
| C | 4.361589 | 0.332714 | -1.23275 |
| H | 4.662973 | -0.31242 | -0.40477 |
| H | 4.560196 | -0.17561 | -2.1726 |
| H | 4.925431 | 1.267534 | -1.19135 |

*Uncatalyzed TS for substrate 2g, conformer B1:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.9046 | 1.831615 | -1.35559 |
| C | -1.72053 | 1.125241 | -1.4611 |
| C | -0.644 | 1.469108 | -0.64732 |
| C | -0.74085 | 2.509749 | 0.281657 |
| C | -1.93542 | 3.200901 | 0.386852 |
| C | -3.00794 | 2.864799 | -0.43175 |
| H | 0.682126 | -0.0905 | -1.42874 |
| H | -3.74779 | 1.574504 | -1.98153 |
| H | -1.62558 | 0.307314 | -2.16507 |
| C | 0.609495 | 0.747089 | -0.74812 |
| C | 0.469329 | 2.796639 | 1.127102 |
| H | -2.03007 | 4.008991 | 1.101635 |
| H | -3.93598 | 3.415535 | -0.34698 |
| C | 1.729709 | 2.642727 | 0.291951 |
| H | 0.428333 | 3.804642 | 1.538394 |
| H | 2.625396 | 2.696628 | 0.907047 |
| N | 1.736895 | 1.328005 | -0.38596 |
| H | 0.502109 | 2.097715 | 1.969915 |
| H | 1.782921 | 3.421924 | -0.47238 |
| C | 2.926012 | 0.547553 | -0.40473 |
| C | 4.07345 | 1.039155 | -1.00633 |
| C | 2.913869 | -0.70224 | 0.221829 |
| C | 5.220318 | 0.262155 | -1.03284 |
| H | 4.054563 | 2.019434 | -1.46574 |
| C | 4.073525 | -1.47679 | 0.164137 |
| C | 5.21322 | -1.00432 | -0.46391 |
| H | 6.113795 | 0.638417 | -1.51246 |
| H | 4.084373 | -2.47462 | 0.586739 |
| H | 6.097921 | -1.62469 | -0.50751 |
| C | 1.737001 | -1.16885 | 1.003419 |
| O | 1.976718 | -2.01952 | 2.014733 |
| N | 0.55051 | -0.79714 | 0.756962 |
| C | -0.53878 | -1.30069 | 1.596179 |
| H | -0.35508 | -2.35642 | 1.809476 |
| H | -0.51873 | -0.76977 | 2.551855 |
| H | 2.918875 | -2.09474 | 2.203517 |
| C | -1.89046 | -1.14406 | 0.960664 |
| C | -2.19858 | -1.8707 | -0.19756 |
| C | -2.87045 | -0.35215 | 1.533886 |
| C | -3.47287 | -1.8081 | -0.74726 |
| C | -4.14788 | -0.27751 | 0.98974 |
| C | -4.44197 | -1.0118 | -0.14466 |
| H | -3.72606 | -2.37853 | -1.62917 |
| H | -4.90418 | 0.338096 | 1.457294 |
| H | -5.43561 | -0.97657 | -0.57271 |
| H | -2.63416 | 0.204476 | 2.433872 |
| O | -1.1808 | -2.60763 | -0.71543 |
| C | -1.47659 | -3.47673 | -1.79307 |
| H | -1.78406 | -2.91587 | -2.67949 |
| H | -0.55946 | -4.01769 | -2.00827 |
| H | -2.26285 | -4.18395 | -1.5202 |

*Uncatalyzed TS for substrate 2g, conformer B2:*

| | X | Y | Z |
|---|---|---|---|
| C | -2.69817 | 1.605434 | -1.89608 |
| C | -1.46199 | 0.985145 | -1.89547 |
| C | -0.59178 | 1.188633 | -0.82717 |
| C | -0.95414 | 1.994614 | 0.256011 |
| C | -2.19207 | 2.614006 | 0.241225 |
| C | -3.05634 | 2.422666 | -0.83081 |
| H | 1.057859 | 0.099778 | -1.75328 |
| H | -3.38117 | 1.45364 | -2.72034 |
| H | -1.16649 | 0.347582 | -2.72005 |
| C | 0.749768 | 0.624652 | -0.85931 |
| C | 0.036174 | 2.134374 | 1.376365 |
| H | -2.47897 | 3.260572 | 1.06198 |
| H | -4.01885 | 2.918338 | -0.83541 |
| C | 1.436011 | 2.289001 | 0.807423 |
| H | -0.19826 | 2.996199 | 2.000562 |
| H | 2.19001 | 2.228774 | 1.590048 |
| N | 1.716483 | 1.211243 | -0.16254 |
| H | -0.00841 | 1.238043 | 2.00348 |
| H | 1.540055 | 3.249161 | 0.295441 |
| C | 3.009005 | 0.638197 | -0.22582 |
| C | 4.130427 | 1.438109 | -0.38706 |
| C | 3.12532 | -0.74912 | -0.09772 |
| C | 5.381475 | 0.852427 | -0.48061 |
| H | 4.013701 | 2.511862 | -0.46093 |
| C | 4.393724 | -1.32091 | -0.2198 |
| C | 5.510719 | -0.52972 | -0.41976 |
| H | 6.255518 | 1.473792 | -0.62279 |
| H | 4.515042 | -2.39744 | -0.18963 |
| H | 6.483441 | -0.98969 | -0.52709 |
| C | 1.953852 | -1.58444 | 0.267713 |
| O | 2.201222 | -2.73427 | 0.909743 |
| N | 0.748382 | -1.26532 | 0.013375 |
| C | -0.30657 | -2.19205 | 0.455374 |
| H | -0.06111 | -3.18366 | 0.069252 |
| H | -0.28022 | -2.25313 | 1.544911 |
| H | 3.117326 | -2.78914 | 1.205611 |
| C | -1.67959 | -1.80957 | -0.01296 |
| C | -2.19785 | -2.32527 | -1.19061 |
| C | -2.48445 | -0.97481 | 0.771653 |
| C | -3.49183 | -2.02957 | -1.60101 |
| C | -3.78772 | -0.69107 | 0.383004 |
| C | -4.28232 | -1.22033 | -0.8033 |
| H | -3.88359 | -2.44854 | -2.51773 |
| H | -4.42203 | -0.06153 | 0.990447 |
| H | -5.30035 | -0.9965 | -1.09553 |
| O | -1.90791 | -0.4838 | 1.90171 |
| C | -2.73819 | 0.195946 | 2.823271 |
| H | -2.11456 | 0.43149 | 3.681928 |
| H | -3.131 | 1.119894 | 2.391198 |
| H | -3.56921 | -0.43753 | 3.14107 |
| H | -1.58013 | -2.98687 | -1.78795 |

*Uncatalyzed TS for substrate 2h, conformer A:*

| | X | Y | Z |
|---|---|---|---|
| C | 2.858944 | -3.0868 | -0.92167 |
| C | 1.54144 | -2.73527 | -1.14643 |
| C | 0.836605 | -2.04898 | -0.15787 |
| C | 1.444542 | -1.67945 | 1.046292 |
| C | 2.769719 | -2.02112 | 1.251197 |
| C | 3.46468 | -2.73246 | 0.278981 |
| H | -1.02898 | -1.99875 | -1.29205 |
| H | 3.413056 | -3.63473 | -1.67138 |
| H | 1.04861 | -2.99899 | -2.07453 |
| C | -0.5575 | -1.73937 | -0.35498 |
| C | 0.628462 | -0.8823 | 2.023423 |
| H | 3.260051 | -1.74083 | 2.175369 |
| H | 4.494865 | -3.01289 | 0.461145 |
| C | -0.82256 | -1.34057 | 2.024468 |
| H | 1.029205 | -0.97641 | 3.032332 |
| H | -1.45757 | -0.63702 | 2.558899 |
| N | -1.3452 | -1.44641 | 0.645123 |
| H | 0.688057 | 0.175605 | 1.745543 |
| H | -0.92041 | -2.32298 | 2.493861 |
| C | -2.70345 | -1.12458 | 0.353386 |
| C | -3.70888 | -1.74915 | 1.07445 |
| C | -2.99609 | -0.20305 | -0.66253 |
| C | -5.0361 | -1.51034 | 0.758508 |
| H | -3.44583 | -2.44137 | 1.86429 |
| C | -4.3417 | -0.00638 | -0.97986 |
| C | -5.35057 | -0.65551 | -0.28776 |
| H | -5.82006 | -2.00958 | 1.311649 |
| H | -4.60937 | 0.645715 | -1.802 |
| H | -6.3829 | -0.49097 | -0.5649 |
| C | -1.94935 | 0.646704 | -1.31154 |
| O | -2.38274 | 1.796705 | -1.86134 |
| N | -0.7286 | 0.31839 | -1.34344 |
| C | 0.305091 | 1.258828 | -1.77072 |
| H | -0.13386 | 2.166447 | -2.18443 |
| H | 0.910141 | 0.771253 | -2.53182 |
| H | -3.22083 | 2.077345 | -1.47878 |
| C | 1.173871 | 1.605723 | -0.58734 |
| C | 0.680134 | 2.464176 | 0.401689 |
| C | 2.472886 | 1.11262 | -0.45451 |
| C | 1.45641 | 2.826756 | 1.498569 |
| C | 3.262939 | 1.467911 | 0.639963 |
| C | 2.743103 | 2.318158 | 1.60026 |
| H | 1.080677 | 3.497963 | 2.255673 |
| H | 4.27118 | 1.09527 | 0.740091 |
| O | -0.59043 | 2.897328 | 0.210605 |
| C | -1.08718 | 3.902559 | 1.073412 |
| H | -2.06908 | 4.171093 | 0.692605 |
| H | -1.18294 | 3.533425 | 2.09749 |
| H | -0.442 | 4.783176 | 1.062035 |
| O | 2.902861 | 0.278458 | -1.43243 |
| C | 4.296426 | 0.059142 | -1.55283 |
| H | 4.68804 | -0.49958 | -0.70076 |
| H | 4.431645 | -0.52828 | -2.45734 |
| H | 4.829524 | 1.00799 | -1.64515 |
| H | 3.3567 | 2.599888 | 2.446153 |

*Uncatalyzed TS for substrate 2h, conformer B:*

| | X | Y | Z |
|---|---|---|---|
| C | 2.508849 | -1.43055 | -2.14734 |
| C | 1.309191 | -0.75961 | -2.00193 |
| C | 0.368441 | -1.22857 | -1.08739 |
| C | 0.625332 | -2.34912 | -0.29239 |
| C | 1.829225 | -3.01417 | -0.44911 |
| C | 2.761532 | -2.55823 | -1.37479 |
| H | -1.13264 | 0.271735 | -1.61265 |
| H | 3.247818 | -1.07589 | -2.85243 |
| H | 1.093499 | 0.124548 | -2.59032 |
| C | -0.92217 | -0.57842 | -0.97903 |
| C | -0.42796 | -2.73875 | 0.705983 |
| H | 2.039848 | -3.89516 | 0.145302 |
| H | 3.698426 | -3.08781 | -1.49267 |
| C | -1.81077 | -2.58115 | 0.093831 |
| H | -0.29667 | -3.76904 | 1.035542 |
| H | -2.59168 | -2.69273 | 0.843249 |
| N | -1.96045 | -1.23843 | -0.50613 |
| H | -0.3338 | -2.08991 | 1.583672 |
| H | -1.97207 | -3.32458 | -0.69082 |
| C | -3.19156 | -0.53739 | -0.38871 |
| C | -4.36409 | -1.09923 | -0.8692 |
| C | -3.18859 | 0.715256 | 0.232898 |
| C | -5.54999 | -0.38861 | -0.78232 |
| H | -4.33615 | -2.07945 | -1.32813 |
| C | -4.39083 | 1.422176 | 0.289517 |
| C | -5.55827 | 0.881651 | -0.2216 |
| H | -6.46368 | -0.81743 | -1.17124 |
| H | -4.4156 | 2.421093 | 0.7088 |
| H | -6.47611 | 1.452118 | -0.18265 |
| C | -1.97149 | 1.249199 | 0.901775 |
| O | -2.16571 | 2.086347 | 1.934805 |
| N | -0.79077 | 0.947166 | 0.551942 |
| C | 0.323505 | 1.508946 | 1.324373 |
| H | 0.185963 | 2.589734 | 1.384601 |
| H | 0.278525 | 1.110538 | 2.339007 |
| H | -3.08674 | 2.095759 | 2.219094 |
| C | 1.664926 | 1.217454 | 0.723241 |
| C | 2.179722 | 2.046279 | -0.27554 |
| C | 2.448893 | 0.163312 | 1.191613 |
| C | 3.470622 | 1.860578 | -0.7655 |
| C | 3.746411 | -0.02815 | 0.72258 |
| C | 4.238991 | 0.831186 | -0.24567 |
| H | 3.882649 | 2.509408 | -1.52313 |
| H | 4.365194 | -0.82947 | 1.096833 |
| H | 5.248226 | 0.691205 | -0.61122 |
| O | 1.339004 | 3.01438 | -0.71646 |
| C | 1.843827 | 3.960896 | -1.64026 |
| H | 2.120802 | 3.481001 | -2.58225 |
| H | 1.040697 | 4.670411 | -1.81731 |
| H | 2.710014 | 4.484062 | -1.22966 |
| O | 1.858291 | -0.64203 | 2.114559 |
| C | 2.662235 | -1.61137 | 2.758401 |
| H | 2.024718 | -2.09487 | 3.494294 |
| H | 3.028946 | -2.35475 | 2.045917 |
| H | 3.509678 | -1.14305 | 3.263543 |

*Uncatalyzed TS for substrate 2k, conformer A1:*

| | X | Y | Z |
|---|---|---|---|
| C | 4.360578 | -2.46974 | -1.54807 |
| C | 2.99369 | -2.26768 | -1.62956 |
| C | 2.298766 | -1.82678 | -0.50656 |
| C | 2.958764 | -1.5635 | 0.700357 |
| C | 4.326736 | -1.75486 | 0.763016 |
| C | 5.019922 | -2.21158 | -0.35301 |
| H | 0.35092 | -1.76239 | -1.51046 |
| H | 4.911147 | -2.82457 | -2.40862 |
| H | 2.461295 | -2.45782 | -2.55411 |
| C | 0.870763 | -1.60388 | -0.57659 |
| C | 2.135777 | -1.05847 | 1.853253 |
| H | 4.856875 | -1.54763 | 1.684238 |
| H | 6.089588 | -2.36507 | -0.28807 |
| C | 0.764784 | -1.70939 | 1.847401 |
| H | 2.631649 | -1.2604 | 2.802307 |
| H | 0.097951 | -1.24439 | 2.569826 |
| N | 0.141921 | -1.56631 | 0.514736 |
| H | 2.017557 | 0.025262 | 1.7609 |
| H | 0.837208 | -2.77631 | 2.073344 |
| C | -1.2262 | -1.19343 | 0.400522 |
| C | -2.20425 | -1.95599 | 1.019014 |
| C | -1.56263 | -0.03875 | -0.31502 |
| C | -3.5362 | -1.60858 | 0.891982 |
| H | -1.91728 | -2.83849 | 1.577192 |
| C | -2.9144 | 0.275934 | -0.44512 |
| C | -3.91598 | -0.49577 | 0.138793 |
| H | -4.29621 | -2.23068 | 1.346512 |
| H | -3.21353 | 1.140674 | -1.026 |
| C | -0.53207 | 0.89455 | -0.85973 |
| O | -0.90956 | 2.174558 | -1.0105 |
| N | 0.630422 | 0.512047 | -1.18655 |
| C | 1.618501 | 1.455465 | -1.70548 |
| H | 1.196172 | 2.459649 | -1.7623 |
| H | 1.868299 | 1.13315 | -2.71785 |
| H | -1.71755 | 2.363283 | -0.52071 |
| C | 2.881457 | 1.481531 | -0.8836 |
| C | 2.852482 | 2.000109 | 0.416994 |
| C | 4.096888 | 1.077753 | -1.41146 |
| C | 4.019964 | 2.098931 | 1.16379 |
| C | 5.273341 | 1.181476 | -0.67858 |
| H | 4.125281 | 0.691986 | -2.42403 |
| C | 5.227762 | 1.690566 | 0.606288 |
| H | 4.006132 | 2.506727 | 2.164298 |
| H | 6.213872 | 0.871137 | -1.11358 |
| O | 1.626445 | 2.376108 | 0.873416 |
| C | 1.564494 | 3.073272 | 2.102754 |
| H | 0.525299 | 3.360921 | 2.237954 |
| H | 1.875912 | 2.437212 | 2.936165 |
| H | 2.189734 | 3.96819 | 2.078121 |
| H | 6.135969 | 1.784367 | 1.187628 |
| C | -5.3412 | -0.14031 | -0.03349 |

| | | | |
|---|---|---|---|
| C | -5.81196 | 0.328055 | -1.26002 |
| C | -6.23393 | -0.26771 | 1.030235 |
| C | -7.14779 | 0.661271 | -1.41894 |
| H | -5.13728 | 0.400589 | -2.10469 |
| C | -7.56813 | 0.071575 | 0.871575 |
| H | -5.87828 | -0.6076 | 1.995368 |
| C | -8.02799 | 0.535707 | -0.35325 |
| H | -7.50407 | 1.011587 | -2.37863 |
| H | -8.24948 | -0.02094 | 1.706937 |
| H | -9.07042 | 0.797305 | -0.47732 |

*Uncatalyzed TS for substrate 2k, conformer A2:*

| | X | Y | Z |
|---|---|---|---|
| C | 4.179794 | -2.54647 | -1.58212 |
| C | 2.838861 | -2.21398 | -1.6474 |
| C | 2.188247 | -1.75794 | -0.50216 |
| C | 2.873362 | -1.59629 | 0.706704 |
| C | 4.217596 | -1.92235 | 0.755966 |
| C | 4.860141 | -2.40715 | -0.37824 |
| H | 0.232022 | -1.6134 | -1.46847 |
| H | 4.6925 | -2.91832 | -2.45861 |
| H | 2.288219 | -2.32073 | -2.57449 |
| C | 0.769555 | -1.48088 | -0.5406 |
| C | 2.111442 | -1.03144 | 1.871639 |
| H | 4.76383 | -1.80744 | 1.684378 |
| H | 5.907046 | -2.67877 | -0.32197 |
| C | 0.684342 | -1.5574 | 1.890299 |
| H | 2.59565 | -1.28607 | 2.813936 |
| H | 0.069383 | -1.00034 | 2.59395 |
| N | 0.055959 | -1.42845 | 0.557475 |
| H | 2.106431 | 0.061357 | 1.791249 |
| H | 0.662497 | -2.61423 | 2.168364 |
| C | -1.31849 | -1.07486 | 0.442024 |
| C | -2.28481 | -1.84342 | 1.071635 |
| C | -1.67652 | 0.059174 | -0.2979 |
| C | -3.6225 | -1.52475 | 0.930186 |
| H | -1.98515 | -2.70964 | 1.648156 |
| C | -3.03292 | 0.345936 | -0.43989 |
| C | -4.02182 | -0.43567 | 0.152332 |
| H | -4.37218 | -2.15295 | 1.393353 |
| H | -3.34393 | 1.198237 | -1.03372 |
| C | -0.65446 | 1.01778 | -0.80884 |
| O | -1.03305 | 2.308707 | -0.89211 |
| N | 0.518319 | 0.661241 | -1.1222 |
| C | 1.550683 | 1.637556 | -1.46413 |
| H | 1.104729 | 2.563211 | -1.83136 |
| H | 2.162798 | 1.20643 | -2.25258 |
| H | -1.88287 | 2.456511 | -0.46156 |
| C | 2.401784 | 1.918817 | -0.24602 |
| C | 1.852644 | 2.580694 | 0.845227 |
| C | 3.741377 | 1.516493 | -0.18596 |
| C | 2.592491 | 2.831063 | 1.991747 |

| | | | |
|---|---|---|---|
| C | 4.492281 | 1.765329 | 0.961633 |
| C | 3.914041 | 2.414835 | 2.043862 |
| H | 2.148465 | 3.357389 | 2.825521 |
| H | 5.528107 | 1.462307 | 1.014936 |
| H | 4.511242 | 2.608995 | 2.925386 |
| H | 0.824044 | 2.91692 | 0.782493 |
| O | 4.238472 | 0.88257 | -1.27699 |
| C | 5.641916 | 0.737227 | -1.37846 |
| H | 6.028598 | 0.063749 | -0.61059 |
| H | 5.830173 | 0.306688 | -2.3585 |
| H | 6.138161 | 1.707287 | -1.29904 |
| C | -5.45313 | -0.11375 | -0.03365 |
| C | -5.92559 | 0.327725 | -1.2694 |
| C | -6.34997 | -0.24635 | 1.026026 |
| C | -7.26734 | 0.629417 | -1.44142 |
| H | -5.24703 | 0.403856 | -2.11063 |
| C | -7.69022 | 0.061192 | 0.854077 |
| H | -5.99385 | -0.56497 | 1.99815 |
| C | -8.15178 | 0.498539 | -0.3799 |
| H | -7.6245 | 0.959566 | -2.40786 |
| H | -8.37498 | -0.03515 | 1.686181 |
| H | -9.19886 | 0.73525 | -0.51441 |

*Uncatalyzed TS for substrate 2k, conformer B1:*

| | X | Y | Z |
|---|---|---|---|
| C | 4.58835 | -1.11769 | -1.50574 |
| C | 3.260899 | -0.73112 | -1.53308 |
| C | 2.343686 | -1.37455 | -0.70641 |
| C | 2.741031 | -2.39893 | 0.157935 |
| C | 4.075092 | -2.76749 | 0.186281 |
| C | 4.99056 | -2.13204 | -0.645 |
| H | 0.633606 | -0.16395 | -1.35032 |
| H | 5.310068 | -0.62516 | -2.14253 |
| H | 2.931579 | 0.068388 | -2.18578 |
| C | 0.945575 | -0.98842 | -0.72377 |
| C | 1.680868 | -3.02557 | 1.021576 |
| H | 4.401941 | -3.55882 | 0.849575 |
| H | 6.030172 | -2.43286 | -0.62074 |
| C | 0.386473 | -3.15394 | 0.235147 |
| H | 1.992699 | -4.00973 | 1.369485 |
| H | -0.43909 | -3.46667 | 0.870632 |
| N | 0.017811 | -1.85091 | -0.35895 |
| H | 1.510191 | -2.40205 | 1.905819 |
| H | 0.499552 | -3.87976 | -0.5737 |
| C | -1.32619 | -1.39276 | -0.29147 |
| C | -2.3502 | -2.12663 | -0.86832 |
| C | -1.59723 | -0.20306 | 0.390694 |
| C | -3.64878 | -1.654 | -0.81879 |
| H | -2.11937 | -3.05193 | -1.38117 |
| C | -2.91034 | 0.262296 | 0.410487 |
| C | -3.94837 | -0.43914 | -0.19772 |
| H | -4.43843 | -2.21151 | -1.30563 |

| | | | |
|---|---|---|---|
| H | -3.14728 | 1.19993 | 0.9007 |
| C | -0.54041 | 0.504375 | 1.164409 |
| O | -0.94122 | 1.220537 | 2.227361 |
| N | 0.690224 | 0.446974 | 0.865296 |
| C | 1.663056 | 1.159537 | 1.694689 |
| H | 1.225683 | 2.108121 | 2.015002 |
| H | 1.854929 | 0.570896 | 2.596052 |
| H | -1.86719 | 1.054872 | 2.438704 |
| C | 2.958079 | 1.418371 | 0.978749 |
| C | 2.973473 | 2.270654 | -0.13379 |
| C | 4.154414 | 0.889487 | 1.431634 |
| C | 4.172338 | 2.58587 | -0.76114 |
| C | 5.360412 | 1.197199 | 0.811821 |
| C | 5.361641 | 2.047287 | -0.27897 |
| H | 4.195282 | 3.253549 | -1.61017 |
| H | 6.286756 | 0.784319 | 1.187686 |
| H | 6.292809 | 2.3073 | -0.76577 |
| H | 4.144987 | 0.2379 | 2.298234 |
| O | 1.761377 | 2.741224 | -0.52922 |
| C | 1.734859 | 3.722762 | -1.54827 |
| H | 2.110637 | 3.321612 | -2.49302 |
| H | 0.69396 | 4.010657 | -1.66655 |
| H | 2.32537 | 4.596711 | -1.26505 |
| C | -5.32928 | 0.090433 | -0.18351 |
| C | -6.41373 | -0.76801 | -0.00646 |
| C | -5.56625 | 1.454704 | -0.3492 |
| C | -7.70723 | -0.27085 | 0.008548 |
| H | -6.24388 | -1.82657 | 0.148593 |
| C | -6.8607 | 1.949772 | -0.33992 |
| H | -4.73631 | 2.129793 | -0.52087 |
| C | -7.93372 | 1.088324 | -0.15926 |
| H | -8.53955 | -0.94585 | 0.157641 |
| H | -7.03271 | 3.008405 | -0.48283 |
| H | -8.94418 | 1.474708 | -0.1505 |

*Uncatalyzed TS for substrate 2k, conformer B2:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.22313 | 1.023225 | -2.1537 |
| C | -2.91032 | 0.607563 | -2.02164 |
| C | -2.14437 | 1.07479 | -0.95687 |
| C | -2.68645 | 1.942949 | -0.00471 |
| C | -3.99999 | 2.356039 | -0.15077 |
| C | -4.76165 | 1.900978 | -1.22095 |
| H | -0.29665 | 0.168542 | -1.68262 |
| H | -4.82495 | 0.666691 | -2.97818 |
| H | -2.47577 | -0.07605 | -2.74131 |
| C | -0.73354 | 0.726821 | -0.86597 |
| C | -1.79777 | 2.373262 | 1.127131 |
| H | -4.42714 | 3.048983 | 0.564525 |
| H | -5.78483 | 2.237617 | -1.32908 |
| C | -0.40089 | 2.661485 | 0.605609 |
| H | -2.1915 | 3.26355 | 1.616814 |

| | | | |
|---|---|---|---|
| H | 0.303427 | 2.810555 | 1.421777 |
| N | 0.091272 | 1.528721 | -0.20246 |
| H | -1.75341 | 1.568574 | 1.867759 |
| H | -0.40135 | 3.556432 | -0.022 |
| C | 1.455566 | 1.16204 | -0.14878 |
| C | 2.456183 | 2.105424 | -0.33114 |
| C | 1.778674 | -0.17212 | 0.115216 |
| C | 3.781682 | 1.715103 | -0.31249 |
| H | 2.190267 | 3.137866 | -0.51962 |
| C | 3.122004 | -0.54577 | 0.106379 |
| C | 4.13842 | 0.377508 | -0.11877 |
| H | 4.555243 | 2.449987 | -0.49415 |
| H | 3.402362 | -1.58053 | 0.269405 |
| C | 0.731884 | -1.14272 | 0.52342 |
| O | 1.119416 | -2.17428 | 1.285529 |
| N | -0.49589 | -1.04038 | 0.201478 |
| C | -1.41554 | -2.07387 | 0.704723 |
| H | -1.01359 | -3.04672 | 0.413569 |
| H | -1.4149 | -2.0363 | 1.795669 |
| H | 2.021198 | -2.05901 | 1.607379 |
| C | -2.81508 | -1.94474 | 0.180158 |
| C | -3.22977 | -2.66502 | -0.92858 |
| C | -3.74553 | -1.14296 | 0.851852 |
| C | -4.54227 | -2.6026 | -1.38069 |
| C | -5.06468 | -1.08677 | 0.420913 |
| C | -5.45358 | -1.81801 | -0.69575 |
| H | -4.85095 | -3.18034 | -2.24114 |
| H | -5.79162 | -0.48025 | 0.941589 |
| H | -6.48463 | -1.77259 | -1.02246 |
| O | -3.26697 | -0.45312 | 1.922091 |
| C | -4.19932 | 0.216079 | 2.748499 |
| H | -3.63178 | 0.624853 | 3.580943 |
| H | -4.69372 | 1.028093 | 2.208741 |
| H | -4.95184 | -0.47753 | 3.129947 |
| H | -2.51386 | -3.30308 | -1.43478 |
| C | 5.554339 | -0.04825 | -0.14693 |
| C | 5.917312 | -1.25875 | -0.73662 |
| C | 6.546374 | 0.754724 | 0.414842 |
| C | 7.244218 | -1.6578 | -0.76381 |
| H | 5.162919 | -1.87749 | -1.20791 |
| C | 7.872319 | 0.352306 | 0.391142 |
| H | 6.27748 | 1.68578 | 0.89887 |
| C | 8.2242 | -0.85388 | -0.19873 |
| H | 7.514775 | -2.59302 | -1.23587 |
| H | 8.631598 | 0.979455 | 0.839335 |
| H | 9.260093 | -1.16564 | -0.21922 |

*Uncatalyzed TS for substrate 2j, conformer A1:*

| | X | Y | Z |
|---|---|---|---|
| C | 3.626706 | -2.82141 | -1.1765 |
| C | 2.285232 | -2.51992 | -1.33707 |
| C | 1.593697 | -1.90012 | -0.29982 |
| C | 2.233223 | -1.55705 | 0.897816 |
| C | 3.576944 | -1.85043 | 1.038892 |
| C | 4.265768 | -2.48441 | 0.009848 |
| H | -0.31121 | -1.80268 | -1.38045 |
| H | 4.172119 | -3.31613 | -1.96852 |
| H | 1.768568 | -2.76915 | -2.2565 |
| C | 0.190484 | -1.57823 | -0.45006 |
| C | 1.417683 | -0.86256 | 1.953294 |
| H | 4.092412 | -1.58563 | 1.953648 |
| H | 5.315664 | -2.71556 | 0.137151 |
| C | -0.00024 | -1.40464 | 1.966518 |
| H | 1.866644 | -0.99192 | 2.937755 |
| H | -0.64952 | -0.80603 | 2.601308 |
| N | -0.56798 | -1.37558 | 0.602363 |
| H | 1.389456 | 0.209371 | 1.736333 |
| H | -0.02108 | -2.43879 | 2.319308 |
| C | -1.90147 | -0.92489 | 0.391204 |
| C | -2.95643 | -1.55599 | 1.033413 |
| C | -2.12539 | 0.169889 | -0.44697 |
| C | -4.25273 | -1.13298 | 0.808796 |
| H | -2.75374 | -2.3906 | 1.693172 |
| C | -3.44871 | 0.558432 | -0.67134 |
| C | -4.52323 | -0.0797 | -0.0662 |
| H | -5.06853 | -1.6429 | 1.305984 |
| H | -3.66106 | 1.361756 | -1.36878 |
| C | -1.00968 | 0.962157 | -1.04276 |
| O | -1.28561 | 2.241456 | -1.34514 |
| N | 0.132213 | 0.465374 | -1.27706 |
| C | 1.20361 | 1.272957 | -1.8576 |
| H | 0.861741 | 2.2941 | -2.03138 |
| H | 1.452141 | 0.827826 | -2.82285 |
| H | -2.09561 | 2.535222 | -0.91428 |
| C | 2.444351 | 1.291598 | -1.00245 |
| C | 2.428317 | 1.955047 | 0.230818 |
| C | 3.632554 | 0.730187 | -1.44045 |
| C | 3.581781 | 2.040214 | 1.000931 |
| C | 4.795174 | 0.817034 | -0.68419 |
| H | 3.652292 | 0.232581 | -2.4031 |
| C | 4.762398 | 1.47058 | 0.534139 |
| H | 3.579908 | 2.559975 | 1.94819 |
| H | 5.715883 | 0.383368 | -1.05066 |
| O | 1.228808 | 2.480888 | 0.601529 |
| C | 1.202544 | 3.326718 | 1.735753 |
| H | 0.19127 | 3.718793 | 1.800794 |
| H | 1.436684 | 2.773155 | 2.649349 |
| H | 1.908146 | 4.152449 | 1.623318 |
| H | 5.66075 | 1.553445 | 1.132273 |
| C | -5.94526 | 0.345203 | -0.35161 |

| | | | |
|---|---|---|---|
| H | -5.89942 | 1.196442 | -1.0358 |
| C | -6.72198 | -0.77864 | -1.04105 |
| H | -6.81645 | -1.64531 | -0.38366 |
| H | -7.72764 | -0.44121 | -1.29214 |
| H | -6.22846 | -1.10011 | -1.95855 |
| C | -6.65524 | 0.796951 | 0.925877 |
| H | -6.1173 | 1.607157 | 1.418975 |
| H | -7.661 | 1.146002 | 0.691672 |
| H | -6.74855 | -0.02894 | 1.633663 |

*Uncatalyzed TS for substrate 2j, conformer A2:*

| | X | Y | Z |
|---|---|---|---|
| C | 3.47074 | -2.84907 | -1.19526 |
| C | 2.158714 | -2.44266 | -1.35554 |
| C | 1.498998 | -1.81917 | -0.29781 |
| C | 2.149126 | -1.56287 | 0.914435 |
| C | 3.465537 | -1.96492 | 1.058151 |
| C | 4.114832 | -2.61632 | 0.014277 |
| H | -0.40659 | -1.66184 | -1.35907 |
| H | 3.988396 | -3.35109 | -2.00114 |
| H | 1.635882 | -2.62049 | -2.28772 |
| C | 0.104389 | -1.46122 | -0.42847 |
| C | 1.384776 | -0.82039 | 1.973118 |
| H | 3.984799 | -1.77757 | 1.990209 |
| H | 5.138023 | -2.94546 | 0.146849 |
| C | -0.07418 | -1.25055 | 1.989061 |
| H | 1.816706 | -0.99214 | 2.958616 |
| H | -0.67669 | -0.5779 | 2.595817 |
| N | -0.64387 | -1.24139 | 0.623936 |
| H | 1.455987 | 0.25338 | 1.767618 |
| H | -0.1773 | -2.26352 | 2.386522 |
| C | -1.98727 | -0.81843 | 0.407135 |
| C | -3.02819 | -1.46081 | 1.061436 |
| C | -2.23854 | 0.25193 | -0.45663 |
| C | -4.33398 | -1.07552 | 0.824354 |
| H | -2.80787 | -2.2755 | 1.739939 |
| C | -3.57023 | 0.603224 | -0.69071 |
| C | -4.62964 | -0.04906 | -0.07449 |
| H | -5.13807 | -1.59434 | 1.33137 |
| H | -3.79926 | 1.390399 | -1.40192 |
| C | -1.13622 | 1.07953 | -1.02565 |
| O | -1.42405 | 2.374484 | -1.26667 |
| N | 0.019765 | 0.61608 | -1.24859 |
| C | 1.12673 | 1.478891 | -1.65577 |
| H | 0.757501 | 2.384632 | -2.13941 |
| H | 1.731934 | 0.922246 | -2.36724 |
| H | -2.27848 | 2.619225 | -0.8941 |
| C | 1.956139 | 1.837864 | -0.44307 |
| C | 1.419377 | 2.651436 | 0.547186 |
| C | 3.260608 | 1.355316 | -0.28588 |
| C | 2.136906 | 2.976163 | 1.689361 |
| C | 3.988551 | 1.677315 | 0.858499 |

| | | | |
|---|---|---|---|
| C | 3.422706 | 2.479376 | 1.839862 |
| H | 1.705724 | 3.621778 | 2.442035 |
| H | 4.997417 | 1.312371 | 0.986165 |
| H | 4.002653 | 2.727829 | 2.719228 |
| H | 0.420139 | 3.047417 | 0.406683 |
| O | 3.748479 | 0.573918 | -1.28118 |
| C | 5.143478 | 0.339752 | -1.31691 |
| H | 5.468597 | -0.26408 | -0.46707 |
| H | 5.334654 | -0.20612 | -2.23706 |
| H | 5.693267 | 1.28382 | -1.32601 |
| C | -6.06125 | 0.335754 | -0.3684 |
| H | -6.03512 | 1.16805 | -1.07654 |
| C | -6.77752 | 0.808469 | 0.898092 |
| H | -6.25462 | 1.641951 | 1.367955 |
| H | -7.79028 | 1.131279 | 0.656572 |
| H | -6.85365 | 0.000382 | 1.628243 |
| C | -6.81527 | -0.8235 | -1.02319 |
| H | -6.31684 | -1.1615 | -1.93202 |
| H | -6.89134 | -1.6722 | -0.34058 |
| H | -7.82806 | -0.51426 | -1.28177 |

*Uncatalyzed TS for substrate 2j, conformer B1:*

| | X | Y | Z |
|---|---|---|---|
| C | -3.85424 | 1.39281 | -1.54458 |
| C | -2.57496 | 0.86828 | -1.54389 |
| C | -1.60949 | 1.419271 | -0.70553 |
| C | -1.91056 | 2.489024 | 0.142223 |
| C | -3.1979 | 2.998172 | 0.141106 |
| C | -4.16117 | 2.453904 | -0.70114 |
| H | -0.02626 | 0.037173 | -1.32477 |
| H | -4.6126 | 0.972469 | -2.19041 |
| H | -2.31994 | 0.031335 | -2.18279 |
| C | -0.2605 | 0.88664 | -0.69766 |
| C | -0.80662 | 3.006011 | 1.023685 |
| H | -3.4505 | 3.827538 | 0.790204 |
| H | -5.16312 | 2.863502 | -0.69869 |
| C | 0.51231 | 2.983305 | 0.268534 |
| H | -1.01552 | 4.02296 | 1.35437 |
| H | 1.352107 | 3.204982 | 0.923626 |
| N | 0.747341 | 1.646142 | -0.31582 |
| H | -0.72802 | 2.379177 | 1.918405 |
| H | 0.501068 | 3.714289 | -0.54381 |
| C | 2.034085 | 1.046958 | -0.23797 |
| C | 3.136698 | 1.672238 | -0.80072 |
| C | 2.169454 | -0.17008 | 0.431803 |
| C | 4.374879 | 1.060741 | -0.74686 |
| H | 3.011597 | 2.627483 | -1.29541 |
| C | 3.428363 | -0.77477 | 0.451519 |
| C | 4.538071 | -0.18699 | -0.14041 |
| H | 5.225594 | 1.551388 | -1.20323 |
| H | 3.550807 | -1.75111 | 0.909481 |
| C | 1.03522 | -0.77025 | 1.185463 |

| | | | |
|---|---|---|---|
| O | 1.347983 | -1.53978 | 2.241072 |
| N | -0.18019 | -0.5743 | 0.881756 |
| C | -1.22994 | -1.1814 | 1.701849 |
| H | -0.90721 | -2.18089 | 2.002693 |
| H | -1.34644 | -0.59105 | 2.614802 |
| H | 2.285634 | -1.47942 | 2.456344 |
| C | -2.54951 | -1.27164 | 0.989112 |
| C | -2.67371 | -2.10217 | -0.13274 |
| C | -3.67052 | -0.60632 | 1.454899 |
| C | -3.90519 | -2.26221 | -0.7559 |
| C | -4.90757 | -0.75555 | 0.837252 |
| C | -5.01742 | -1.58792 | -0.26156 |
| H | -4.01404 | -2.91365 | -1.6109 |
| H | -5.77443 | -0.23551 | 1.221612 |
| H | -5.97596 | -1.72682 | -0.74504 |
| H | -3.5788 | 0.028021 | 2.329664 |
| O | -1.52905 | -2.70865 | -0.54313 |
| C | -1.62451 | -3.66857 | -1.57845 |
| H | -1.9534 | -3.2088 | -2.51419 |
| H | -0.6265 | -4.07762 | -1.70767 |
| H | -2.31469 | -4.47026 | -1.30649 |
| C | 5.882321 | -0.87732 | -0.13485 |
| H | 5.756881 | -1.82781 | 0.390445 |
| C | 6.348545 | -1.18162 | -1.56017 |
| H | 6.525937 | -0.2598 | -2.11775 |
| H | 7.284742 | -1.73955 | -1.53738 |
| H | 5.610495 | -1.77135 | -2.10445 |
| C | 6.925947 | -0.05007 | 0.617648 |
| H | 6.610104 | 0.158947 | 1.640136 |
| H | 7.873954 | -0.58693 | 0.654269 |
| H | 7.104398 | 0.902937 | 0.115847 |

*Uncatalyzed TS for substrate 2j, conformer B2:*

| | X | Y | Z |
|---|---|---|---|
| C | -3.53339 | 1.363781 | -2.05449 |
| C | -2.25641 | 0.840572 | -1.96123 |
| C | -1.45872 | 1.164243 | -0.86682 |
| C | -1.93292 | 1.993507 | 0.152894 |
| C | -3.21083 | 2.516734 | 0.045183 |
| C | -4.00349 | 2.205194 | -1.05398 |
| H | 0.308825 | 0.174663 | -1.67418 |
| H | -4.15977 | 1.118291 | -2.9009 |
| H | -1.87335 | 0.182075 | -2.7316 |
| C | -0.08181 | 0.69534 | -0.81045 |
| C | -1.0137 | 2.260986 | 1.311079 |
| H | -3.58613 | 3.181951 | 0.81376 |
| H | -4.99805 | 2.625836 | -1.13106 |
| C | 0.40574 | 2.468603 | 0.811263 |
| H | -1.33079 | 3.140854 | 1.870461 |
| H | 1.114307 | 2.493741 | 1.637157 |
| N | 0.804706 | 1.365844 | -0.08407 |
| H | -1.0393 | 1.400721 | 1.986965 |

| | | | |
|---|---|---|---|
| H | 0.484624 | 3.407274 | 0.256407 |
| C | 2.133377 | 0.879918 | -0.0686 |
| C | 3.213759 | 1.744062 | -0.18257 |
| C | 2.338049 | -0.49238 | 0.081253 |
| C | 4.498628 | 1.236375 | -0.20778 |
| H | 3.039011 | 2.808748 | -0.27315 |
| C | 3.646946 | -0.97982 | 0.026656 |
| C | 4.737941 | -0.13824 | -0.12991 |
| H | 5.332008 | 1.919971 | -0.31376 |
| H | 3.829847 | -2.04857 | 0.071247 |
| C | 1.21137 | -1.40302 | 0.403557 |
| O | 1.508942 | -2.52867 | 1.067293 |
| N | -0.00231 | -1.1711 | 0.096099 |
| C | -1.00465 | -2.16919 | 0.505095 |
| H | -0.68701 | -3.13744 | 0.112437 |
| H | -0.99458 | -2.24318 | 1.594236 |
| H | 2.414527 | -2.51486 | 1.398269 |
| C | -2.39249 | -1.87277 | 0.019138 |
| C | -2.88534 | -2.45537 | -1.13766 |
| C | -3.23846 | -1.05244 | 0.775125 |
| C | -4.19355 | -2.24028 | -1.55404 |
| C | -4.55276 | -0.8432 | 0.378074 |
| C | -5.02186 | -1.44028 | -0.78631 |
| H | -4.56495 | -2.7113 | -2.45377 |
| H | -5.21499 | -0.22089 | 0.962687 |
| H | -6.04918 | -1.27612 | -1.08551 |
| O | -2.68604 | -0.49977 | 1.888836 |
| C | -3.54499 | 0.178811 | 2.78425 |
| H | -2.93651 | 0.458018 | 3.640751 |
| H | -3.96392 | 1.077244 | 2.322708 |
| H | -4.35789 | -0.47144 | 3.114895 |
| H | -2.23649 | -3.10597 | -1.71365 |
| C | 6.141713 | -0.68953 | -0.22554 |
| H | 6.07322 | -1.77364 | -0.10168 |
| C | 7.035316 | -0.1385 | 0.886623 |
| H | 6.615817 | -0.3369 | 1.873323 |
| H | 8.022651 | -0.59759 | 0.834359 |
| H | 7.168008 | 0.940303 | 0.783984 |
| C | 6.743439 | -0.40547 | -1.60369 |
| H | 6.118177 | -0.80603 | -2.40204 |
| H | 6.853611 | 0.668898 | -1.76509 |
| H | 7.732764 | -0.85631 | -1.68322 |

*Uncatalyzed TS for substrate 2i, conformer A1:*

| | X | Y | Z |
|---|---|---|---|
| C | 3.932843 | -2.65273 | -1.38956 |
| C | 2.576714 | -2.39789 | -1.49502 |
| C | 1.891955 | -1.87333 | -0.40194 |
| C | 2.551935 | -1.57875 | 0.798004 |
| C | 3.909421 | -1.82633 | 0.88481 |
| C | 4.591859 | -2.36504 | -0.201 |
| H | -0.04159 | -1.78622 | -1.42734 |
| H | 4.474693 | -3.07348 | -2.22555 |
| H | 2.044142 | -2.61052 | -2.41459 |
| C | 0.476714 | -1.59394 | -0.49872 |
| C | 1.743529 | -0.97558 | 1.913415 |
| H | 4.440694 | -1.59746 | 1.800181 |
| H | 5.653286 | -2.56072 | -0.11702 |
| C | 0.342557 | -1.55974 | 1.929157 |
| H | 2.220815 | -1.14961 | 2.877399 |
| H | -0.3064 | -1.01811 | 2.613782 |
| N | -0.26034 | -1.46853 | 0.582178 |
| H | 1.679054 | 0.106314 | 1.762514 |
| H | 0.360009 | -2.61286 | 2.220548 |
| C | -1.61124 | -1.05383 | 0.428811 |
| C | -2.6248 | -1.75532 | 1.063181 |
| C | -1.89276 | 0.07688 | -0.3464 |
| C | -3.94489 | -1.37711 | 0.89545 |
| H | -2.37722 | -2.61472 | 1.673564 |
| C | -3.22912 | 0.433641 | -0.52652 |
| C | -4.24085 | -0.29294 | 0.080077 |
| H | -4.74046 | -1.92969 | 1.375658 |
| H | -3.49765 | 1.262397 | -1.16934 |
| C | -0.81944 | 0.938929 | -0.92676 |
| O | -1.14385 | 2.221296 | -1.15508 |
| N | 0.32779 | 0.488709 | -1.2166 |
| C | 1.362057 | 1.356134 | -1.77837 |
| H | 0.984596 | 2.37265 | -1.8963 |
| H | 1.603596 | 0.964007 | -2.76791 |
| H | -1.938 | 2.480303 | -0.67463 |
| C | 2.618388 | 1.373897 | -0.94626 |
| C | 2.602131 | 1.96659 | 0.322269 |
| C | 3.818999 | 0.888978 | -1.43921 |
| C | 3.767465 | 2.057759 | 1.073427 |
| C | 4.993551 | 0.985103 | -0.70264 |
| H | 3.837441 | 0.442907 | -2.42708 |
| C | 4.960485 | 1.567714 | 0.551116 |
| H | 3.76455 | 2.522477 | 2.048913 |
| H | 5.923342 | 0.612171 | -1.11076 |
| O | 1.390443 | 2.420361 | 0.745594 |
| C | 1.355913 | 3.20779 | 1.921536 |
| H | 0.333006 | 3.559853 | 2.023423 |
| H | 1.626551 | 2.61855 | 2.802016 |
| H | 2.029405 | 4.063224 | 1.838476 |
| H | 5.86787 | 1.656441 | 1.134536 |
| Br | -6.03392 | 0.191781 | -0.21362 |

*Uncatalyzed TS for substrate 2i, conformer A2:*

| | X | Y | Z |
|---|---|---|---|
| C | 3.763237 | -2.69589 | -1.42612 |
| C | 2.438313 | -2.31236 | -1.5237 |
| C | 1.793076 | -1.78262 | -0.4071 |
| C | 2.469194 | -1.59728 | 0.803826 |
| C | 3.797893 | -1.97584 | 0.885058 |
| C | 4.433614 | -2.53362 | -0.21938 |
| H | -0.1442 | -1.6178 | -1.40325 |
| H | 4.270482 | -3.12597 | -2.27878 |
| H | 1.894716 | -2.43673 | -2.45274 |
| C | 0.387756 | -1.45584 | -0.47674 |
| C | 1.71852 | -0.95115 | 1.933337 |
| H | 4.337513 | -1.84415 | 1.81504 |
| H | 5.46742 | -2.84558 | -0.13688 |
| C | 0.26951 | -1.41355 | 1.956266 |
| H | 2.179848 | -1.1861 | 2.892087 |
| H | -0.32928 | -0.79703 | 2.6234 |
| N | -0.3362 | -1.32339 | 0.609276 |
| H | 1.763003 | 0.136323 | 1.807674 |
| H | 0.198242 | -2.45381 | 2.284389 |
| C | -1.69611 | -0.93476 | 0.456183 |
| C | -2.69319 | -1.64943 | 1.10215 |
| C | -2.00715 | 0.174389 | -0.34089 |
| C | -4.02197 | -1.3097 | 0.922177 |
| H | -2.42689 | -2.49057 | 1.7296 |
| C | -3.35157 | 0.49288 | -0.53123 |
| C | -4.34548 | -0.25131 | 0.083191 |
| H | -4.80411 | -1.87377 | 1.41092 |
| H | -3.63786 | 1.307072 | -1.1857 |
| C | -0.94807 | 1.073455 | -0.88654 |
| O | -1.28233 | 2.369164 | -1.0424 |
| N | 0.213205 | 0.658608 | -1.16554 |
| C | 1.287443 | 1.573994 | -1.54476 |
| H | 0.882723 | 2.49922 | -1.95759 |
| H | 1.885419 | 1.080604 | -2.30716 |
| H | -2.12403 | 2.576351 | -0.62083 |
| C | 2.139861 | 1.873535 | -0.33189 |
| C | 1.608238 | 2.604097 | 0.723532 |
| C | 3.461572 | 1.421381 | -0.2419 |
| C | 2.348492 | 2.876626 | 1.864607 |
| C | 4.212328 | 1.69089 | 0.901258 |
| C | 3.652107 | 2.411047 | 1.947397 |
| H | 1.92029 | 3.458242 | 2.669384 |
| H | 5.23464 | 1.349594 | 0.978005 |
| H | 4.249826 | 2.621165 | 2.824889 |
| H | 0.594615 | 2.978275 | 0.635661 |
| O | 3.941642 | 0.722363 | -1.29987 |
| C | 5.340439 | 0.526073 | -1.38724 |
| H | 5.701478 | -0.12811 | -0.59067 |
| H | 5.518365 | 0.050826 | -2.34832 |
| H | 5.867918 | 1.481767 | -1.34384 |
| Br | -6.15034 | 0.172891 | -0.22807 |

*Uncatalyzed TS for substrate 2i, conformer B1:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.18477 | 1.31133 | -1.48688 |
| C | -2.88401 | 0.843041 | -1.50811 |
| C | -1.93583 | 1.418423 | -0.66605 |
| C | -2.27545 | 2.456164 | 0.20695 |
| C | -3.58383 | 2.907601 | 0.228246 |
| C | -4.53002 | 2.339424 | -0.61778 |
| H | -0.29946 | 0.123878 | -1.33124 |
| H | -4.9299 | 0.872593 | -2.13594 |
| H | -2.59893 | 0.032627 | -2.168 |
| C | -0.5642 | 0.949446 | -0.68444 |
| C | -1.18498 | 3.006799 | 1.084802 |
| H | -3.86633 | 3.711518 | 0.896674 |
| H | -5.54864 | 2.705027 | -0.59859 |
| C | 0.119441 | 3.067718 | 0.306713 |
| H | -1.43851 | 4.00385 | 1.443246 |
| H | 0.958529 | 3.322091 | 0.950768 |
| N | 0.412026 | 1.753373 | -0.30507 |
| H | -1.05831 | 2.363629 | 1.962256 |
| H | 0.053991 | 3.810263 | -0.49228 |
| C | 1.726632 | 1.219653 | -0.25627 |
| C | 2.784283 | 1.90719 | -0.83078 |
| C | 1.933197 | 0.001398 | 0.398041 |
| C | 4.057215 | 1.366065 | -0.80959 |
| H | 2.603959 | 2.859391 | -1.31366 |
| C | 3.215845 | -0.54546 | 0.395656 |
| C | 4.262361 | 0.128446 | -0.21228 |
| H | 4.883484 | 1.888806 | -1.27103 |
| H | 3.407252 | -1.51468 | 0.839565 |
| C | 0.840155 | -0.66626 | 1.158805 |
| O | 1.201924 | -1.43671 | 2.196445 |
| N | -0.38492 | -0.52518 | 0.867206 |
| C | -1.39966 | -1.20036 | 1.678954 |
| H | -1.01996 | -2.1825 | 1.970119 |
| H | -1.55106 | -0.626 | 2.596914 |
| H | 2.133189 | -1.32752 | 2.420196 |
| C | -2.70964 | -1.35635 | 0.960636 |
| C | -2.78199 | -2.1766 | -0.1733 |
| C | -3.86758 | -0.76064 | 1.430361 |
| C | -4.00017 | -2.39614 | -0.80473 |
| C | -5.09149 | -0.97047 | 0.805033 |
| C | -5.1501 | -1.79158 | -0.30636 |
| H | -4.06818 | -3.03972 | -1.66988 |
| H | -5.98784 | -0.50595 | 1.192781 |
| H | -6.09735 | -1.97623 | -0.79666 |
| H | -3.81485 | -0.13343 | 2.313417 |
| O | -1.60316 | -2.71172 | -0.58631 |
| C | -1.64158 | -3.66983 | -1.62798 |
| H | -1.99409 | -3.22395 | -2.56161 |
| H | -0.62158 | -4.02056 | -1.75699 |
| H | -2.2854 | -4.51074 | -1.36152 |
| Br | 5.978205 | -0.63933 | -0.2275 |

*Uncatalyzed TS for substrate 2i, conformer B2:*

| | X | Y | Z |
|---|---|---|---|
| C | -3.8463 | 1.277372 | -2.05942 |
| C | -2.55241 | 0.799245 | -1.95898 |
| C | -1.76869 | 1.159486 | -0.8653 |
| C | -2.27469 | 1.979838 | 0.147054 |
| C | -3.56933 | 2.457559 | 0.031877 |
| C | -4.34765 | 2.110385 | -1.06705 |
| H | 0.03673 | 0.246262 | -1.67394 |
| H | -4.46117 | 1.004961 | -2.90599 |
| H | -2.14475 | 0.149071 | -2.7238 |
| C | -0.37557 | 0.746 | -0.80789 |
| C | -1.37003 | 2.292696 | 1.305068 |
| H | -3.96924 | 3.11629 | 0.793545 |
| H | -5.35525 | 2.497303 | -1.15025 |
| C | 0.041814 | 2.547255 | 0.80741 |
| H | -1.72107 | 3.166712 | 1.853141 |
| H | 0.746642 | 2.605406 | 1.634886 |
| N | 0.482715 | 1.450659 | -0.07687 |
| H | -1.36608 | 1.439969 | 1.990386 |
| H | 0.088275 | 3.482436 | 0.2431 |
| C | 1.830031 | 1.028801 | -0.06649 |
| C | 2.864388 | 1.948087 | -0.1721 |
| C | 2.100971 | -0.33611 | 0.071124 |
| C | 4.177214 | 1.515305 | -0.20211 |
| H | 2.638433 | 3.003592 | -0.25328 |
| C | 3.427594 | -0.76453 | 0.012304 |
| C | 4.452323 | 0.154355 | -0.13281 |
| H | 4.985533 | 2.226448 | -0.30083 |
| H | 3.675597 | -1.81807 | 0.049182 |
| C | 1.019223 | -1.30454 | 0.388144 |
| O | 1.370593 | -2.42373 | 1.034587 |
| N | -0.20368 | -1.12194 | 0.087696 |
| C | -1.16132 | -2.16739 | 0.48699 |
| H | -0.80719 | -3.1149 | 0.075563 |
| H | -1.13723 | -2.2579 | 1.574703 |
| H | 2.269742 | -2.37553 | 1.379784 |
| C | -2.56369 | -1.91775 | 0.017916 |
| C | -3.05278 | -2.51768 | -1.13145 |
| C | -3.42491 | -1.12341 | 0.784393 |
| C | -4.37241 | -2.34339 | -1.53073 |
| C | -4.74921 | -0.95297 | 0.403306 |
| C | -5.2144 | -1.56655 | -0.75423 |
| H | -4.74102 | -2.82788 | -2.42439 |
| H | -5.4223 | -0.34904 | 0.994795 |
| H | -6.24975 | -1.43396 | -1.04101 |
| O | -2.8743 | -0.5548 | 1.891068 |
| C | -3.74086 | 0.101988 | 2.795882 |
| H | -3.13117 | 0.394632 | 3.647045 |
| H | -4.18537 | 0.990529 | 2.33882 |
| H | -4.53439 | -0.56796 | 3.133815 |
| H | -2.39227 | -3.14961 | -1.71486 |
| Br | 6.230795 | -0.44703 | -0.22911 |

*Molecular model for Catalyst 1a:*

| | X | Y | Z |
|---|---|---|---|
| C | -5.8417 | 1.313071 | 0.34773 |
| C | -5.09507 | 0.356438 | -0.33591 |
| C | -3.70108 | 0.622523 | -0.44237 |
| C | -3.0667 | 1.684117 | 0.177275 |
| C | -3.86527 | 2.605084 | 0.860461 |
| C | -5.23345 | 2.416825 | 0.941414 |
| H | -6.91657 | 1.188119 | 0.421072 |
| H | -3.38531 | 3.438632 | 1.35619 |
| H | -5.83981 | 3.13325 | 1.481313 |
| C | -5.76395 | -0.68096 | -1.10365 |
| H | -6.75644 | -0.40008 | -1.44432 |
| C | -5.54629 | -2.01657 | -1.1267 |
| H | -6.25546 | -2.71088 | -1.56065 |
| O | -3.00676 | -0.36935 | -1.08639 |
| O | -4.38454 | -2.59757 | -0.78163 |
| P | -2.92799 | -1.87484 | -0.3742 |
| O | -2.91838 | -1.68328 | 1.087167 |
| O | -1.8849 | -2.5907 | -1.12493 |
| C | -0.6783 | 0.900183 | -0.35414 |
| H | -0.7668 | 0.096521 | -1.06179 |
| C | -1.60661 | 1.730461 | 0.229594 |
| N | -0.93243 | 2.580372 | 1.057134 |
| N | 0.324457 | 2.304719 | 1.03221 |
| N | 0.497892 | 1.279371 | 0.179961 |
| C | 1.761742 | 0.626365 | 0.078223 |
| C | 1.858118 | -0.71942 | 0.479456 |
| C | 2.851041 | 1.358526 | -0.39264 |
| C | 3.114663 | -1.31131 | 0.407506 |
| C | 4.094611 | 0.731864 | -0.43061 |
| C | 4.205793 | -0.58237 | -0.03184 |
| H | 3.244227 | -2.34345 | 0.695975 |
| H | 4.967449 | 1.26617 | -0.77932 |
| C | 2.726727 | 2.797957 | -0.85157 |
| C | 3.415381 | 3.032056 | -2.19667 |
| C | 3.275239 | 3.747488 | 0.215352 |
| H | 1.666674 | 3.016955 | -0.97834 |
| H | 3.064362 | 2.325857 | -2.95007 |
| H | 3.203833 | 4.043527 | -2.54782 |
| H | 4.499816 | 2.933682 | -2.11702 |
| H | 2.734624 | 3.619737 | 1.152192 |
| H | 4.336032 | 3.549822 | 0.390698 |
| H | 3.171095 | 4.784427 | -0.11056 |
| C | 0.656999 | -1.50112 | 0.988668 |
| C | 0.156721 | -0.95776 | 2.332107 |
| C | 0.892818 | -3.00275 | 1.09203 |
| H | -0.15272 | -1.39706 | 0.267856 |
| H | -0.04843 | 0.111872 | 2.303194 |
| H | -0.77639 | -1.46278 | 2.582858 |
| H | 0.900771 | -1.14135 | 3.112664 |
| H | 1.246553 | -3.42177 | 0.148783 |
| H | 1.604624 | -3.25145 | 1.884868 |

| | | | |
|---|---|---|---|
| H | -0.06202 | -3.47519 | 1.32204 |
| Br | 5.91138 | -1.42601 | -0.11137 |

*Molecular model for Catalyst 1b:*

| | X | Y | Z |
|---|---|---|---|
| C | 6.425761 | 1.251622 | -0.71739 |
| C | 5.708866 | 0.578741 | 0.268637 |
| C | 4.29559 | 0.741002 | 0.227881 |
| C | 3.628096 | 1.429394 | -0.76809 |
| C | 4.399638 | 2.078449 | -1.73673 |
| C | 5.778781 | 1.982792 | -1.71074 |
| H | 7.508943 | 1.19957 | -0.70734 |
| H | 3.891573 | 2.622394 | -2.52195 |
| H | 6.363259 | 2.481383 | -2.47391 |
| C | 6.407655 | 0.007465 | 1.408091 |
| H | 7.360699 | 0.484458 | 1.618103 |
| C | 6.285891 | -1.21644 | 1.972901 |
| H | 7.021461 | -1.60331 | 2.667857 |
| O | 3.629507 | 0.013653 | 1.181187 |
| O | 5.187962 | -1.98683 | 1.894006 |
| P | 3.75106 | -1.64692 | 1.103603 |
| O | 3.928505 | -2.01586 | -0.31222 |
| O | 2.67924 | -2.1497 | 1.976476 |
| C | 1.246988 | 0.693854 | -0.10166 |
| H | 1.337037 | 0.036274 | 0.74642 |
| C | 2.168259 | 1.393936 | -0.84998 |
| N | 1.485965 | 2.050824 | -1.83037 |
| N | 0.227419 | 1.791832 | -1.73228 |
| N | 0.064804 | 0.967482 | -0.68873 |
| C | -1.23211 | 0.499508 | -0.32066 |
| C | -2.16483 | 1.432624 | 0.150703 |
| C | -1.52675 | -0.85904 | -0.43901 |
| C | -3.432 | 0.967759 | 0.469134 |
| C | -2.8112 | -1.27024 | -0.07939 |
| C | -3.77671 | -0.37692 | 0.358067 |
| H | -4.17974 | 1.668238 | 0.82654 |
| H | -3.04479 | -2.32427 | -0.14878 |
| C | -0.51875 | -1.88296 | -0.91143 |
| C | -0.07201 | -2.79396 | 0.243651 |
| C | -1.04815 | -2.72476 | -2.08126 |
| H | 0.372573 | -1.36621 | -1.2754 |
| C | 0.962341 | -3.81135 | -0.22559 |
| H | -0.95613 | -3.30929 | 0.641863 |
| H | 0.359892 | -2.20449 | 1.055409 |
| C | 0.006491 | -3.72563 | -2.54826 |
| H | -1.94127 | -3.27609 | -1.7662 |
| H | -1.35035 | -2.06784 | -2.90124 |
| C | 0.442949 | -4.63454 | -1.40095 |
| H | 1.244192 | -4.45107 | 0.612232 |
| H | 1.873852 | -3.27937 | -0.51479 |
| H | -0.38223 | -4.31406 | -3.3839 |
| H | 0.879764 | -3.17846 | -2.91774 |

| | | | |
|---|---|---|---|
| H | 1.212769 | -5.32924 | -1.74527 |
| H | -0.41494 | -5.24051 | -1.08174 |
| C | -1.82078 | 2.897779 | 0.292579 |
| C | -2.38887 | 3.712434 | -0.87798 |
| C | -2.27402 | 3.50148 | 1.626531 |
| H | -0.73278 | 2.997755 | 0.253362 |
| C | -1.97669 | 5.177837 | -0.77665 |
| H | -3.48288 | 3.630785 | -0.86313 |
| H | -2.03667 | 3.279179 | -1.81499 |
| C | -1.84036 | 4.962018 | 1.729997 |
| H | -3.3649 | 3.453271 | 1.708046 |
| H | -1.86527 | 2.917225 | 2.454124 |
| C | -2.38766 | 5.78275 | 0.564011 |
| H | -2.4119 | 5.748645 | -1.60042 |
| H | -0.88887 | 5.242642 | -0.88628 |
| H | -2.17112 | 5.385538 | 2.681396 |
| H | -0.7465 | 5.01177 | 1.722942 |
| H | -2.04564 | 6.818043 | 0.635841 |
| H | -3.48199 | 5.804365 | 0.626934 |
| C | -5.19654 | -0.79164 | 0.678274 |
| C | -6.13975 | -0.40936 | -0.47298 |
| C | -5.37024 | -2.27207 | 1.015637 |
| H | -5.51124 | -0.21538 | 1.55825 |
| C | -7.59403 | -0.73443 | -0.14168 |
| H | -5.82943 | -0.96077 | -1.36791 |
| H | -6.02587 | 0.652099 | -0.70404 |
| C | -6.8208 | -2.58848 | 1.373242 |
| H | -5.08833 | -2.87653 | 0.147219 |
| H | -4.69832 | -2.55227 | 1.830071 |
| C | -7.76147 | -2.20474 | 0.233101 |
| H | -8.23849 | -0.47989 | -0.98627 |
| H | -7.91524 | -0.11246 | 0.701488 |
| H | -6.92638 | -3.64918 | 1.611305 |
| H | -7.10087 | -2.03197 | 2.274573 |
| H | -8.79863 | -2.41325 | 0.506099 |
| H | -7.53178 | -2.82437 | -0.64082 |

*Molecular model for Catalyst 1c:*

| | X | Y | Z |
|---|---|---|---|
| C | -5.59324 | 1.239452 | 0.653225 |
| C | -4.88462 | 0.370582 | -0.1732 |
| C | -3.49603 | 0.646569 | -0.31804 |
| C | -2.82665 | 1.622904 | 0.396998 |
| C | -3.58788 | 2.459988 | 1.218365 |
| C | -4.95198 | 2.266821 | 1.340983 |
| H | -6.66382 | 1.104717 | 0.763471 |
| H | -3.07932 | 3.230483 | 1.782574 |
| H | -5.52848 | 2.91616 | 1.988129 |
| C | -5.598 | -0.56861 | -1.02293 |
| H | -6.60367 | -0.24865 | -1.28067 |
| C | -5.39052 | -1.8923 | -1.21415 |
| H | -6.12527 | -2.53008 | -1.69087 |

| | | | |
|---|---|---|---|
| O | -2.83925 | -0.25451 | -1.11593 |
| O | -4.21852 | -2.50946 | -0.99473 |
| P | -2.72942 | -1.83756 | -0.60805 |
| O | -2.61605 | -1.82792 | 0.861546 |
| O | -1.75655 | -2.45654 | -1.52076 |
| C | -0.44556 | 0.813963 | -0.15863 |
| H | -0.53207 | -0.05843 | -0.78399 |
| C | -1.36517 | 1.678473 | 0.392544 |
| N | -0.67527 | 2.595666 | 1.128542 |
| N | 0.586067 | 2.33598 | 1.076061 |
| N | 0.741896 | 1.255166 | 0.298869 |
| C | 2.015142 | 0.632526 | 0.137504 |
| C | 3.007771 | 1.298014 | -0.58431 |
| C | 2.218617 | -0.62691 | 0.713057 |
| C | 4.241878 | 0.668817 | -0.71443 |
| C | 3.466468 | -1.21365 | 0.532932 |
| C | 4.486813 | -0.58442 | -0.16897 |
| H | 5.035215 | 1.163254 | -1.26404 |
| H | 3.639805 | -2.19483 | 0.962076 |
| C | 1.156354 | -1.35896 | 1.5115 |
| C | 0.712648 | -2.63795 | 0.797962 |
| C | 1.651641 | -1.6637 | 2.927138 |
| H | 0.27601 | -0.72432 | 1.608169 |
| H | 1.544523 | -3.34522 | 0.725243 |
| H | 0.32908 | -2.43918 | -0.20387 |
| H | 2.500108 | -2.3521 | 2.911975 |
| H | 1.959633 | -0.75392 | 3.445351 |
| C | 2.770538 | 2.668219 | -1.18601 |
| C | 3.342717 | 3.754337 | -0.27103 |
| C | 3.340231 | 2.795868 | -2.59861 |
| H | 1.692103 | 2.821626 | -1.24837 |
| H | 4.422165 | 3.621262 | -0.1585 |
| H | 2.877779 | 3.706747 | 0.713087 |
| H | 4.432004 | 2.786521 | -2.59412 |
| H | 2.994997 | 1.985522 | -3.24175 |
| C | 5.83636 | -1.25029 | -0.33468 |
| C | 6.52562 | -1.44959 | 1.016339 |
| C | 5.717728 | -2.57907 | -1.08221 |
| H | 6.457589 | -0.57935 | -0.93536 |
| H | 5.937758 | -2.11567 | 1.651337 |
| H | 6.63813 | -0.50079 | 1.542333 |
| H | 5.113974 | -3.289 | -0.51362 |
| H | 5.242024 | -2.44181 | -2.05369 |
| H | 3.162647 | 4.744155 | -0.6963 |
| H | 3.02431 | 3.743272 | -3.03883 |
| H | 7.51442 | -1.89427 | 0.884647 |
| H | 6.7034 | -3.02364 | -1.23602 |
| H | 0.849848 | -2.1336 | 3.498479 |
| H | -0.10472 | -3.10233 | 1.350365 |

*Molecular model for Catalyst 1d:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.66582 | 1.532855 | 0.23457 |
| C | -3.98461 | 0.435248 | -0.28605 |
| C | -2.57985 | 0.601037 | -0.44256 |
| C | -1.8759 | 1.705946 | -0.00084 |
| C | -2.61152 | 2.772963 | 0.522541 |
| C | -3.98713 | 2.681338 | 0.636862 |
| H | -5.74501 | 1.485119 | 0.332587 |
| H | -2.07797 | 3.647045 | 0.872268 |
| H | -4.54422 | 3.510942 | 1.054363 |
| C | -4.72271 | -0.66731 | -0.87985 |
| H | -5.7083 | -0.38679 | -1.24054 |
| C | -4.58037 | -2.00096 | -0.6985 |
| H | -5.33971 | -2.70607 | -1.01548 |
| O | -1.94967 | -0.52512 | -0.90786 |
| O | -3.44613 | -2.60051 | -0.29923 |
| P | -1.97823 | -1.87682 | 0.069317 |
| O | -2.0485 | -1.42079 | 1.466922 |
| O | -0.93618 | -2.75906 | -0.48051 |
| C | 0.45515 | 0.664454 | -0.29558 |
| H | 0.314405 | -0.31135 | -0.72508 |
| C | -0.41429 | 1.678487 | 0.033754 |
| N | 0.324102 | 2.693265 | 0.569315 |
| N | 1.567609 | 2.358404 | 0.597607 |
| N | 1.665362 | 1.125741 | 0.076229 |
| C | 2.903085 | 0.422526 | 0.040416 |
| C | 2.980651 | -0.83622 | 0.643805 |
| C | 3.991378 | 1.008375 | -0.60917 |
| C | 4.20447 | -1.49756 | 0.580729 |
| C | 5.189574 | 0.306789 | -0.63249 |
| C | 5.314768 | -0.94555 | -0.04239 |
| H | 4.28514 | -2.47666 | 1.040878 |
| H | 6.042632 | 0.746548 | -1.13872 |
| C | 3.87731 | 2.346098 | -1.2852 |
| H | 2.948616 | 2.418795 | -1.85276 |
| H | 3.859451 | 3.154091 | -0.55391 |
| H | 4.717583 | 2.496743 | -1.96231 |
| C | 1.812091 | -1.48009 | 1.338946 |
| H | 1.196539 | -0.75226 | 1.867689 |
| H | 1.14654 | -1.99809 | 0.640128 |
| H | 2.173123 | -2.21598 | 2.056523 |
| C | 6.631037 | -1.67421 | -0.05668 |
| H | 7.227999 | -1.41277 | 0.820567 |
| H | 6.482689 | -2.754 | -0.04527 |
| H | 7.214229 | -1.41634 | -0.94121 |

*Molecular model for Catalyst 1e:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.22642 | 1.856389 | 0.234127 |
| C | -3.66426 | 0.691832 | -0.28283 |
| C | -2.24237 | 0.664139 | -0.33574 |
| C | -1.4332 | 1.67974 | 0.138783 |
| C | -2.05395 | 2.824214 | 0.648591 |
| C | -3.43311 | 2.900069 | 0.706673 |
| H | -5.30658 | 1.949536 | 0.262107 |
| H | -1.43317 | 3.629887 | 1.017431 |
| H | -3.90351 | 3.785083 | 1.116479 |
| C | -4.50174 | -0.25747 | -0.99729 |
| H | -5.40573 | 0.184893 | -1.40578 |
| C | -4.56855 | -1.6049 | -0.88895 |
| H | -5.39727 | -2.16826 | -1.30161 |
| O | -1.72934 | -0.52232 | -0.78577 |
| O | -3.56984 | -2.38885 | -0.45891 |
| P | -2.06662 | -1.8982 | 0.109309 |
| O | -2.25052 | -1.47837 | 1.507117 |
| O | -1.11024 | -2.90198 | -0.37468 |
| C | 0.798506 | 0.411521 | -0.03206 |
| H | 0.564432 | -0.62205 | -0.22599 |
| C | 0.021469 | 1.530064 | 0.141299 |
| N | 0.859707 | 2.586435 | 0.373578 |
| N | 2.079953 | 2.195584 | 0.347376 |
| N | 2.066075 | 0.870846 | 0.100419 |
| C | 3.265504 | 0.142908 | 0.023889 |
| C | 3.476395 | -0.98077 | 0.815942 |
| C | 4.287336 | 0.510189 | -0.84447 |
| C | 4.643266 | -1.71722 | 0.752834 |
| C | 5.47309 | -0.19391 | -0.92059 |
| C | 5.642209 | -1.31215 | -0.11822 |
| H | 4.746041 | -2.58568 | 1.387352 |
| H | 6.232057 | 0.136655 | -1.61516 |
| H | 6.562446 | -1.8774 | -0.1763 |
| F | 4.108432 | 1.560321 | -1.6404 |
| F | 2.522116 | -1.34536 | 1.662421 |

*Molecular model for Catalyst 1f:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.46565 | 1.931871 | 0.350681 |
| C | -3.88097 | 0.835163 | -0.27989 |
| C | -2.46327 | 0.874429 | -0.39789 |
| C | -1.66568 | 1.86657 | 0.146512 |
| C | -2.30976 | 2.936526 | 0.774606 |
| C | -3.68933 | 2.961063 | 0.877631 |
| H | -5.54628 | 1.979322 | 0.428842 |
| H | -1.70254 | 3.719088 | 1.21004 |
| H | -4.17275 | 3.791801 | 1.37657 |
| C | -4.71076 | -0.10586 | -1.01401 |
| H | -5.65056 | 0.31662 | -1.35765 |

| | | | |
|---|---|---|---|
| C | -4.70679 | -1.45918 | -0.99694 |
| H | -5.52299 | -2.03902 | -1.41107 |
| O | -1.93597 | -0.25023 | -0.98337 |
| O | -3.65305 | -2.21578 | -0.64995 |
| P | -2.11282 | -1.71358 | -0.21299 |
| O | -2.12719 | -1.47834 | 1.241731 |
| O | -1.17957 | -2.62423 | -0.89581 |
| C | 0.56152 | 0.678582 | -0.28071 |
| H | 0.335636 | -0.227 | -0.81259 |
| C | -0.21184 | 1.716696 | 0.169149 |
| N | 0.611478 | 2.580802 | 0.839324 |
| N | 1.813284 | 2.125963 | 0.842739 |
| N | 1.803095 | 0.967071 | 0.157946 |
| C | 2.893115 | 0.066236 | 0.143557 |
| C | 2.68116 | -1.22418 | 0.651905 |
| C | 4.123934 | 0.420559 | -0.40474 |
| C | 3.708808 | -2.16594 | 0.584568 |
| C | 5.158064 | -0.5145 | -0.43871 |
| C | 4.928979 | -1.79342 | 0.048838 |
| H | 3.549419 | -3.16727 | 0.95526 |
| H | 6.120484 | -0.2605 | -0.85551 |
| H | 5.729822 | -2.52097 | 0.005706 |
| O | 4.217311 | 1.673899 | -0.89996 |
| O | 1.478193 | -1.44895 | 1.182874 |
| C | 5.442165 | 2.067972 | -1.46451 |
| H | 5.305251 | 3.095069 | -1.79254 |
| H | 6.250111 | 2.026524 | -0.72835 |
| H | 5.705229 | 1.443017 | -2.32314 |
| C | 1.037149 | -2.78043 | 1.408502 |
| H | 1.099681 | -3.36015 | 0.486486 |
| H | 1.622904 | -3.24643 | 2.206596 |
| H | -0.00903 | -2.68711 | 1.690562 |

*Molecular model for Catalyst 1g:*

| | X | Y | Z |
|---|---|---|---|
| C | -5.70776 | 1.144607 | 0.242615 |
| C | -4.91205 | 0.090089 | -0.19895 |
| C | -3.54041 | 0.407804 | -0.40629 |
| C | -2.96896 | 1.628543 | -0.10127 |
| C | -3.81603 | 2.647923 | 0.343588 |
| C | -5.16568 | 2.399848 | 0.516628 |
| H | -6.77137 | 0.981006 | 0.37701 |
| H | -3.38988 | 3.613696 | 0.581105 |
| H | -5.81204 | 3.191882 | 0.873243 |
| C | -5.52445 | -1.13317 | -0.6905 |
| H | -6.54545 | -0.99903 | -1.03569 |
| C | -5.22039 | -2.42336 | -0.41717 |
| H | -5.89975 | -3.23174 | -0.65869 |
| O | -2.78485 | -0.67083 | -0.78032 |
| O | -4.01302 | -2.8633 | -0.02166 |
| P | -2.66635 | -1.92848 | 0.316203 |
| O | -2.849 | -1.36328 | 1.661924 |

| | | | |
|---|---|---|---|
| O | -1.49361 | -2.69417 | -0.13454 |
| C | -0.54331 | 0.822012 | -0.26383 |
| H | -0.59761 | -0.24389 | -0.39042 |
| C | -1.51641 | 1.782238 | -0.1543 |
| N | -0.8895 | 2.990551 | -0.00564 |
| N | 0.381845 | 2.825498 | -0.0166 |
| N | 0.619507 | 1.508543 | -0.17004 |
| C | 1.93147 | 1.001961 | -0.17883 |
| C | 2.140846 | -0.3768 | -0.19877 |
| C | 3.006222 | 1.888927 | -0.16279 |
| C | 3.435569 | -0.86406 | -0.19689 |
| H | 1.307623 | -1.0677 | -0.20613 |
| C | 4.296924 | 1.394192 | -0.14921 |
| H | 2.811016 | 2.950705 | -0.15785 |
| C | 4.504488 | 0.021407 | -0.16343 |
| H | 3.617317 | -1.93047 | -0.23029 |
| H | 5.147667 | 2.062719 | -0.14489 |
| S | 6.149081 | -0.60634 | -0.08138 |
| O | 6.193931 | -1.88345 | -0.74071 |
| O | 7.05844 | 0.440085 | -0.46863 |
| C | 6.387914 | -0.90041 | 1.652728 |
| H | 6.282063 | 0.04112 | 2.186199 |
| H | 5.655347 | -1.63045 | 1.988789 |
| H | 7.39895 | -1.29233 | 1.753992 |

*Molecular model for Catalyst 1h:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.78708 | 1.50175 | 0.077726 |
| C | -4.08728 | 0.359859 | -0.30516 |
| C | -2.67743 | 0.515306 | -0.42128 |
| C | -1.99441 | 1.673546 | -0.10025 |
| C | -2.74999 | 2.785925 | 0.282713 |
| C | -4.12658 | 2.692063 | 0.377522 |
| H | -5.86884 | 1.458654 | 0.142071 |
| H | -2.23291 | 3.702838 | 0.532951 |
| H | -4.70065 | 3.556248 | 0.68771 |
| C | -4.8037 | -0.78783 | -0.83673 |
| H | -5.77649 | -0.53882 | -1.25073 |
| C | -4.6698 | -2.10255 | -0.54458 |
| H | -5.4216 | -2.82757 | -0.83315 |
| O | -2.02505 | -0.64661 | -0.73799 |
| O | -3.55356 | -2.67662 | -0.06752 |
| P | -2.12762 | -1.90353 | 0.3598 |
| O | -2.33385 | -1.31684 | 1.692806 |
| O | -1.03566 | -2.81379 | -0.01661 |
| C | 0.353885 | 0.637798 | -0.17076 |
| H | 0.208898 | -0.41827 | -0.31102 |
| C | -0.53224 | 1.685793 | -0.0905 |
| N | 0.194556 | 2.828266 | 0.08027 |
| N | 1.449482 | 2.54265 | 0.110373 |
| N | 1.567133 | 1.215189 | -0.03776 |
| C | 2.834941 | 0.58669 | -0.02644 |

| | | | |
|---|---|---|---|
| C | 2.928303 | -0.79123 | 0.161982 |
| C | 3.981156 | 1.342622 | -0.20014 |
| C | 4.16811 | -1.39703 | 0.164317 |
| H | 2.03883 | -1.38983 | 0.313824 |
| C | 5.22986 | 0.732761 | -0.18687 |
| H | 3.890218 | 2.409788 | -0.34168 |
| C | 5.325958 | -0.64191 | -0.00803 |
| H | 4.259897 | -2.46504 | 0.30799 |
| H | 6.110509 | 1.343263 | -0.32301 |
| O | 6.500881 | -1.33243 | 0.014521 |
| C | 7.687019 | -0.59818 | -0.15409 |
| H | 8.501848 | -1.31643 | -0.10479 |
| H | 7.708475 | -0.09248 | -1.1242 |
| H | 7.811587 | 0.145819 | 0.638533 |

*Molecular model for Catalyst 1i:*

| | X | Y | Z |
|---|---|---|---|
| C | -5.05963 | 1.565083 | 0.35189 |
| C | -4.3948 | 0.507828 | -0.26419 |
| C | -2.97764 | 0.62424 | -0.32289 |
| C | -2.26414 | 1.661807 | 0.246326 |
| C | -2.98469 | 2.694631 | 0.853504 |
| C | -4.36463 | 2.635018 | 0.913123 |
| H | -6.14336 | 1.552236 | 0.390118 |
| H | -2.44057 | 3.518098 | 1.296655 |
| H | -4.9138 | 3.432466 | 1.397623 |
| C | -5.14325 | -0.45702 | -1.0528 |
| H | -6.0909 | -0.07373 | -1.41988 |
| C | -5.07711 | -1.80883 | -1.05646 |
| H | -5.85052 | -2.41614 | -1.51131 |
| O | -2.35796 | -0.46355 | -0.87507 |
| O | -3.99999 | -2.5228 | -0.69583 |
| P | -2.54953 | -1.93342 | -0.09195 |
| O | -2.75805 | -1.64275 | 1.334977 |
| O | -1.49733 | -2.79054 | -0.65348 |
| C | 0.060364 | 0.590865 | 0.014953 |
| H | -0.08865 | -0.44126 | -0.25764 |
| C | -0.80245 | 1.631346 | 0.254363 |
| N | -0.05129 | 2.730259 | 0.575087 |
| N | 1.195009 | 2.440203 | 0.543017 |
| N | 1.287081 | 1.137004 | 0.202095 |
| C | 2.540002 | 0.515395 | 0.103974 |
| C | 2.817807 | -0.63583 | 0.832857 |
| C | 3.533407 | 1.039181 | -0.71528 |
| C | 4.053963 | -1.25255 | 0.744759 |
| C | 4.776202 | 0.436402 | -0.7955 |
| C | 5.03473 | -0.71108 | -0.06703 |
| F | 3.303492 | 2.111371 | -1.45369 |
| F | 5.717974 | 0.943927 | -1.5831 |
| F | 6.224519 | -1.29201 | -0.14788 |
| F | 4.311743 | -2.34556 | 1.449619 |
| F | 1.905934 | -1.14933 | 1.635931 |

*Molecular model for Catalyst 1j:*

| | X | Y | Z |
|---|---|---|---|
| C | -3.97751 | 1.77878 | 0.110518 |
| C | -3.38594 | 0.580807 | -0.28326 |
| C | -1.96917 | 0.611961 | -0.41407 |
| C | -1.18292 | 1.703591 | -0.09661 |
| C | -1.83284 | 2.87747 | 0.296794 |
| C | -3.21122 | 2.905084 | 0.406325 |
| H | -5.05812 | 1.831654 | 0.185904 |
| H | -1.23425 | 3.744393 | 0.543465 |
| H | -3.7035 | 3.815521 | 0.724606 |
| C | -4.20686 | -0.49359 | -0.8169 |
| H | -5.15415 | -0.15301 | -1.22495 |
| C | -4.1959 | -1.81586 | -0.52836 |
| H | -5.01247 | -2.46815 | -0.81399 |
| O | -1.42667 | -0.60365 | -0.73791 |
| O | -3.13265 | -2.48995 | -0.06026 |
| P | -1.63886 | -1.85043 | 0.357084 |
| O | -1.78082 | -1.25077 | 1.692686 |
| O | -0.6373 | -2.8554 | -0.02963 |
| C | 1.061101 | 0.461752 | -0.18044 |
| H | 0.818585 | -0.57745 | -0.31032 |
| C | 0.274246 | 1.584602 | -0.10031 |
| N | 1.103448 | 2.659477 | 0.054686 |
| N | 2.32653 | 2.26387 | 0.073563 |
| N | 2.324167 | 0.928525 | -0.06468 |
| C | 3.529871 | 0.190096 | -0.05825 |
| C | 3.493185 | -1.19127 | 0.099347 |
| C | 4.741759 | 0.855504 | -0.20815 |
| C | 4.682504 | -1.90395 | 0.09573 |
| H | 2.55135 | -1.70801 | 0.232561 |
| C | 5.920752 | 0.128233 | -0.20048 |
| H | 4.739965 | 1.929218 | -0.32539 |
| C | 5.898799 | -1.25239 | -0.05234 |
| H | 4.650202 | -2.97872 | 0.217316 |
| H | 6.863833 | 0.647072 | -0.31636 |
| H | 6.822701 | -1.81587 | -0.05056 |

*Molecular model for Catalyst 1k:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.89215 | 1.646527 | 0.216942 |
| C | -4.25982 | 0.480878 | -0.20964 |
| C | -2.85605 | 0.583588 | -0.41988 |
| C | -2.11135 | 1.714755 | -0.13992 |
| C | -2.80089 | 2.853364 | 0.287375 |
| C | -4.17142 | 2.811558 | 0.470037 |
| H | -5.96839 | 1.641699 | 0.351795 |
| H | -2.23409 | 3.748847 | 0.506373 |
| H | -4.69204 | 3.696496 | 0.814911 |
| C | -5.0539 | -0.63467 | -0.69751 |
| H | -6.04045 | -0.3457 | -1.04818 |

| | | | |
|---|---|---|---|
| C | -4.95123 | -1.95573 | -0.4218 |
| H | -5.74643 | -2.65073 | -0.66537 |
| O | -2.26856 | -0.60244 | -0.77877 |
| O | -3.83008 | -2.57345 | -0.01627 |
| P | -2.34984 | -1.85916 | 0.317826 |
| O | -2.44162 | -1.27456 | 1.665267 |
| O | -1.32329 | -2.81336 | -0.12843 |
| C | 0.191589 | 0.583028 | -0.25637 |
| H | -0.00234 | -0.47198 | -0.32804 |
| C | -0.64966 | 1.673522 | -0.19962 |
| N | 1.371669 | 2.44171 | -0.0932 |
| N | 1.427103 | 1.11152 | -0.18564 |
| C | 2.71718 | 0.422775 | -0.10017 |
| C | 2.52503 | -1.07912 | -0.3308 |
| C | 3.310663 | 0.650525 | 1.297511 |
| C | 3.672443 | 0.988953 | -1.1582 |
| H | 1.83329 | -1.49085 | 0.408232 |
| H | 2.080048 | -1.24862 | -1.31515 |
| C | 3.882756 | -1.78437 | -0.22905 |
| H | 2.611162 | 0.263202 | 2.043366 |
| H | 3.415926 | 1.724875 | 1.46428 |
| C | 4.665528 | -0.05647 | 1.403325 |
| H | 3.233459 | 0.839784 | -2.14891 |
| H | 3.778105 | 2.064065 | -1.00109 |
| C | 5.027942 | 0.281765 | -1.05368 |
| H | 3.732852 | -2.85283 | -0.39706 |
| C | 4.474213 | -1.55849 | 1.166798 |
| C | 4.838538 | -1.22092 | -1.28622 |
| H | 5.081907 | 0.110871 | 2.399906 |
| C | 5.617415 | 0.510814 | 0.343494 |
| H | 5.704673 | 0.690556 | -1.80852 |
| H | 5.434068 | -2.07736 | 1.254524 |
| H | 3.804701 | -1.97448 | 1.924509 |
| H | 4.432881 | -1.39656 | -2.28692 |
| H | 5.804063 | -1.73367 | -1.22845 |
| H | 5.768852 | 1.580983 | 0.513056 |
| H | 6.594972 | 0.024294 | 0.420178 |
| N | 0.125187 | 2.786943 | -0.10272 |

*Molecular model for Catalyst 1l:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.93244 | 1.561974 | 0.26618 |
| C | -4.25977 | 0.428484 | -0.18649 |
| C | -2.86006 | 0.578658 | -0.39534 |
| C | -2.1461 | 1.728848 | -0.10021 |
| C | -2.8811 | 2.828743 | 0.355573 |
| C | -4.24943 | 2.742182 | 0.543606 |
| H | -6.00738 | 1.517524 | 0.40318 |
| H | -2.35727 | 3.742312 | 0.609618 |
| H | -4.79426 | 3.602475 | 0.912741 |
| C | -5.02002 | -0.69987 | -0.6982 |
| H | -6.0147 | -0.43345 | -1.0436 |

| | | | |
|---|---|---|---|
| C | -4.87667 | -2.0229 | -0.45161 |
| H | -5.65149 | -2.73527 | -0.71117 |
| O | -2.24105 | -0.58297 | -0.78104 |
| O | -3.74025 | -2.61526 | -0.05565 |
| P | -2.27948 | -1.86307 | 0.287188 |
| O | -2.3826 | -1.31021 | 1.647691 |
| O | -1.2297 | -2.78135 | -0.17837 |
| C | 0.187664 | 0.684225 | -0.154 |
| H | -0.00548 | -0.37215 | -0.09777 |
| C | -0.68449 | 1.757574 | -0.19669 |
| N | 1.450419 | 2.522607 | -0.26205 |
| N | 1.437876 | 1.183766 | -0.19189 |
| C | 2.700706 | 0.451976 | -0.09289 |
| C | 2.437876 | -1.05665 | -0.07056 |
| C | 3.416728 | 0.860995 | 1.202316 |
| C | 3.591274 | 0.796483 | -1.29435 |
| H | 1.796466 | -1.3164 | 0.775225 |
| H | 1.904946 | -1.35929 | -0.97576 |
| C | 3.771485 | -1.80487 | 0.03928 |
| H | 2.767393 | 0.627735 | 2.050903 |
| H | 3.573929 | 1.941723 | 1.18946 |
| C | 4.748062 | 0.112533 | 1.318178 |
| H | 3.067762 | 0.516317 | -2.21297 |
| H | 3.747993 | 1.87676 | -1.31735 |
| C | 4.924301 | 0.048635 | -1.18092 |
| H | 3.567174 | -2.87737 | 0.052976 |
| C | 4.483864 | -1.39703 | 1.333783 |
| C | 4.660486 | -1.46067 | -1.16044 |
| H | 5.250466 | 0.40984 | 2.242525 |
| C | 5.632437 | 0.46134 | 0.114916 |
| H | 5.552174 | 0.303041 | -2.03911 |
| H | 5.429121 | -1.94143 | 1.427582 |
| H | 3.865139 | -1.65974 | 2.196188 |
| H | 4.168812 | -1.76707 | -2.0883 |
| H | 5.607175 | -2.00676 | -1.0943 |
| H | 5.836445 | 1.53621 | 0.101803 |
| H | 6.594254 | -0.05545 | 0.195825 |
| C | 0.173997 | 2.874439 | -0.2656 |
| H | -0.08864 | 3.919582 | -0.3282 |

*Molecular model for Catalyst 1m:*

| | X | Y | Z |
|---|---|---|---|
| C | -4.94414 | 1.484372 | 0.117901 |
| C | -4.21599 | 0.358022 | -0.26175 |
| C | -2.81269 | 0.550669 | -0.39953 |
| C | -2.1541 | 1.733354 | -0.11055 |
| C | -2.9401 | 2.826286 | 0.266428 |
| C | -4.31245 | 2.695928 | 0.388774 |
| H | -6.0236 | 1.411201 | 0.197903 |
| H | -2.44289 | 3.761773 | 0.487674 |
| H | -4.90547 | 3.549617 | 0.694034 |
| C | -4.90896 | -0.8113 | -0.77701 |

| | | | |
|---|---|---|---|
| H | -5.89294 | -0.59158 | -1.18163 |
| C | -4.73542 | -2.12039 | -0.48043 |
| H | -5.47149 | -2.86689 | -0.75679 |
| O | -2.14009 | -0.60003 | -0.72522 |
| O | -3.59994 | -2.66238 | -0.0124 |
| P | -2.17477 | -1.8577 | 0.365623 |
| O | -2.34105 | -1.29229 | 1.714032 |
| O | -1.07988 | -2.74848 | -0.05247 |
| C | 0.203168 | 0.766116 | -0.18547 |
| H | 0.057685 | -0.29705 | -0.25291 |
| C | -0.69138 | 1.805146 | -0.13481 |
| N | 1.448717 | 1.327623 | -0.10456 |
| C | 2.684397 | 0.546571 | -0.06478 |
| C | 2.68026 | -0.34782 | 1.18624 |
| C | 3.907683 | 1.465817 | -0.01951 |
| C | 2.76804 | -0.34081 | -1.3175 |
| H | 2.604893 | 0.288077 | 2.073318 |
| H | 1.798099 | -0.99246 | 1.170107 |
| C | 3.958772 | -1.19012 | 1.227637 |
| H | 3.856947 | 2.103796 | 0.868108 |
| H | 3.910809 | 2.116516 | -0.89965 |
| C | 5.189053 | 0.623403 | 0.019545 |
| H | 1.890255 | -0.98905 | -1.36216 |
| H | 2.753239 | 0.298427 | -2.20534 |
| C | 4.045146 | -1.18507 | -1.27573 |
| H | 3.941876 | -1.82079 | 2.119345 |
| C | 5.179973 | -0.26515 | 1.268998 |
| C | 4.026005 | -2.07142 | -0.02495 |
| H | 6.05211 | 1.29376 | 0.050056 |
| C | 5.265026 | -0.25884 | -1.23166 |
| H | 4.087409 | -1.81185 | -2.16965 |
| H | 6.099798 | -0.85712 | 1.308719 |
| H | 5.150117 | 0.355529 | 2.169642 |
| H | 3.160285 | -2.7381 | -0.05484 |
| H | 4.925202 | -2.69516 | 0.003775 |
| H | 5.292306 | 0.366339 | -2.12945 |
| H | 6.186474 | -0.84916 | -1.2144 |
| N | -0.00755 | 2.995441 | -0.0281 |
| C | 1.259656 | 2.672557 | -0.01201 |
| H | 2.078155 | 3.369755 | 0.057615 |