**Supporting Information**

# Systematic Functional Analysis of Active Site Residues in L-Threonine Dehydrogenase from *Thermoplasma Volcanium*

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**Figure S1.** SDS-PAGE gel of proteins purified through His-tag affinity chromatography. The wild type has a molecular weight of 35.9 kD. This gel indicates the presence and purity of reported proteins.

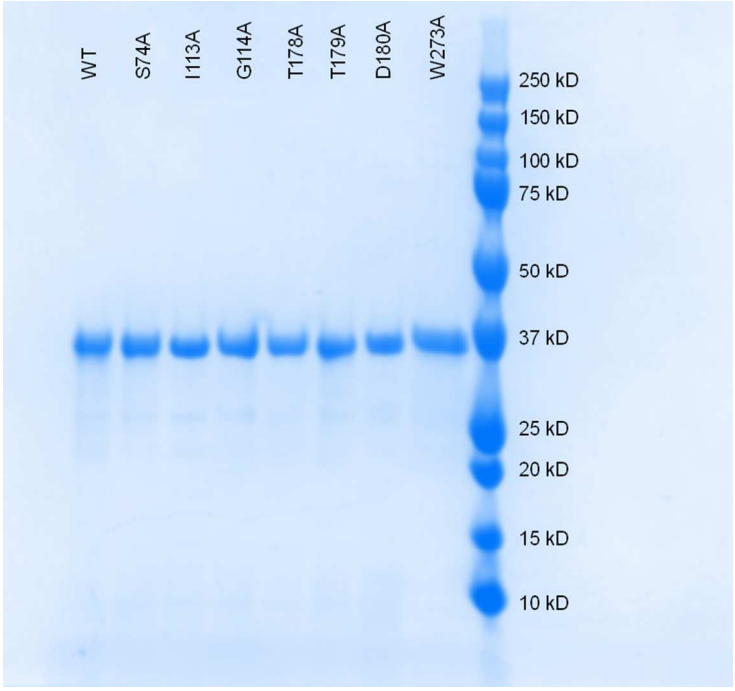
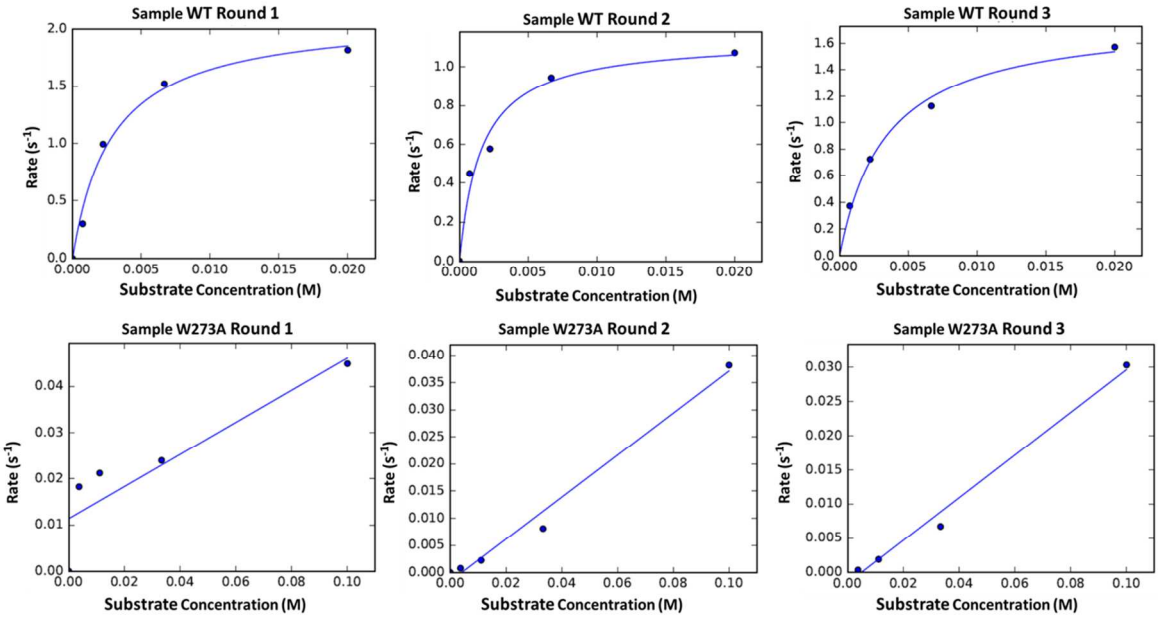
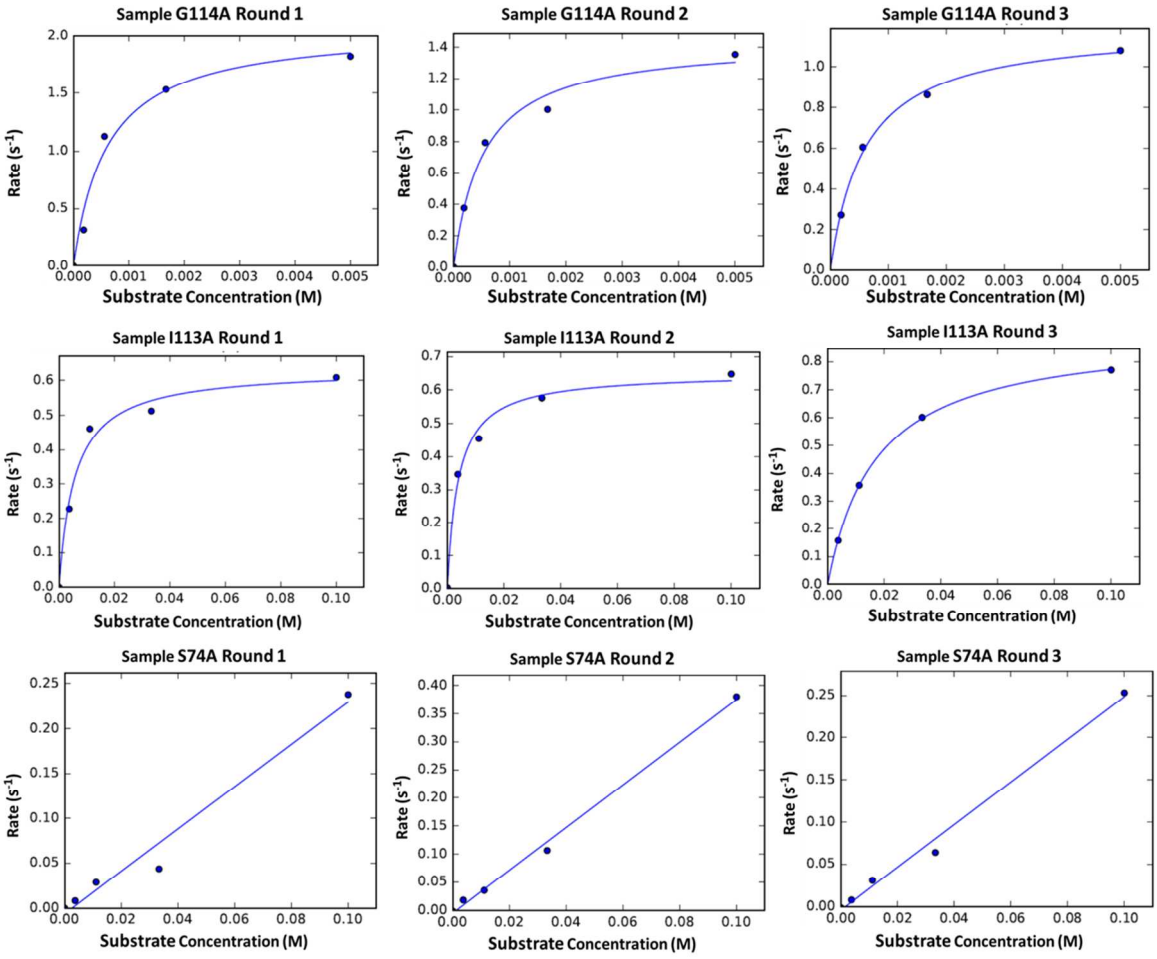


**Figure S2. Michaelis Menten and Linear Curve Fit On L-Threonine** The Michaelis Menten curves were fitted using a total of five points. WT and T179A data points were collected at L-threonine concentrations of 20 mM, 6.7 mM, 2.2 mM, 0.7 mM, and 0 mM. S74A, I113A, D180A, and W273A data points were collected at L-threonine concentrations of 100 mM, 33 mM, 11 mM, 3.7 mM, and 0 mM. G114A data points were collected at L-threonine concentrations of 5 mM, 1.7 mM, 0.6 mM, 0.2 mM, and 0 mM. T178A data points were collected at L-threonine concentrations of 40 mM, 13 mM, 4.4 mM, 1.8 mM, and 0 mM. In the case that the Michaelis Menten curve did not represent the data a linear fit was used and the slope was reported as the catalytic efficiency.




Sample G114A Round 1
Sample G114A Round 2
Sample G114A Round 3
Sample I113A Round 1
Sample I113A Round 2
Sample I113A Round 3
Sample S74A Round 1
Sample S74A Round 2
Sample S74A Round 3
Rate (s-1)
Substrate Concentration (M)

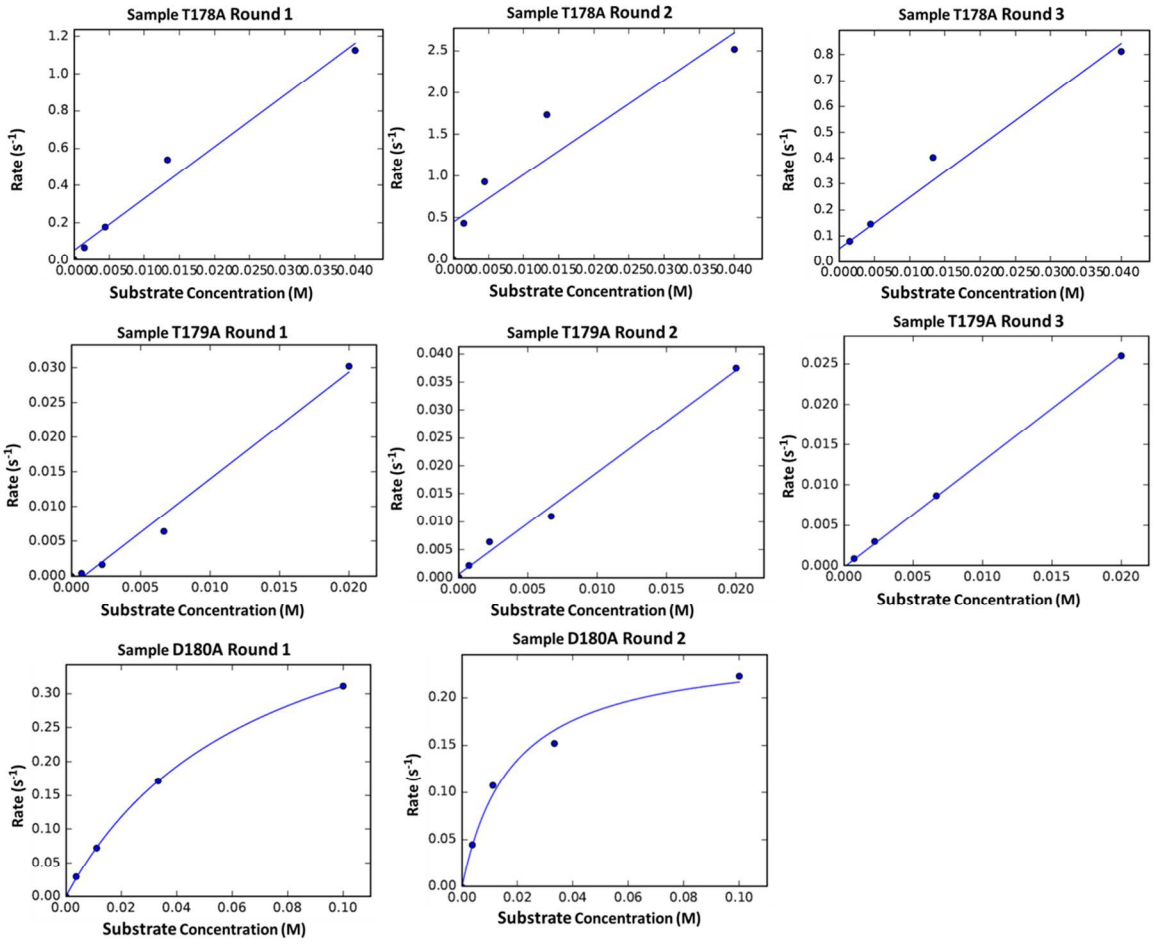

Sample T178A Round 1
Rate ($s^{-1}$)
Substrate Concentration (M)
Sample T178A Round 2
Rate ($s^{-1}$)
Substrate Concentration (M)
Sample T178A Round 3
Rate ($s^{-1}$)
Substrate Concentration (M)
Sample T179A Round 1
Rate ($s^{-1}$)
Substrate Concentration (M)
Sample T179A Round 2
Rate ($s^{-1}$)
Substrate Concentration (M)
Sample T179A Round 3
Rate ($s^{-1}$)
Substrate Concentration (M)
Sample D180A Round 1
Rate ($s^{-1}$)
Substrate Concentration (M)
Sample D180A Round 2
Rate ($s^{-1}$)
Substrate Concentration (M)

**Figure S3. Michaelis Menten and Linear Curve Fit On L-Serine.** The Michaelis Menten curves were fitted using a total of five points. WT and all mutants were tested at L-serine concentrations of 1 M, 0.25 M, 0.06 M, 0.02 M and 0 M. In the case that the Michaelis Menten curve did not represent the data a linear fit was used and the slope was reported as catalytic efficiency.

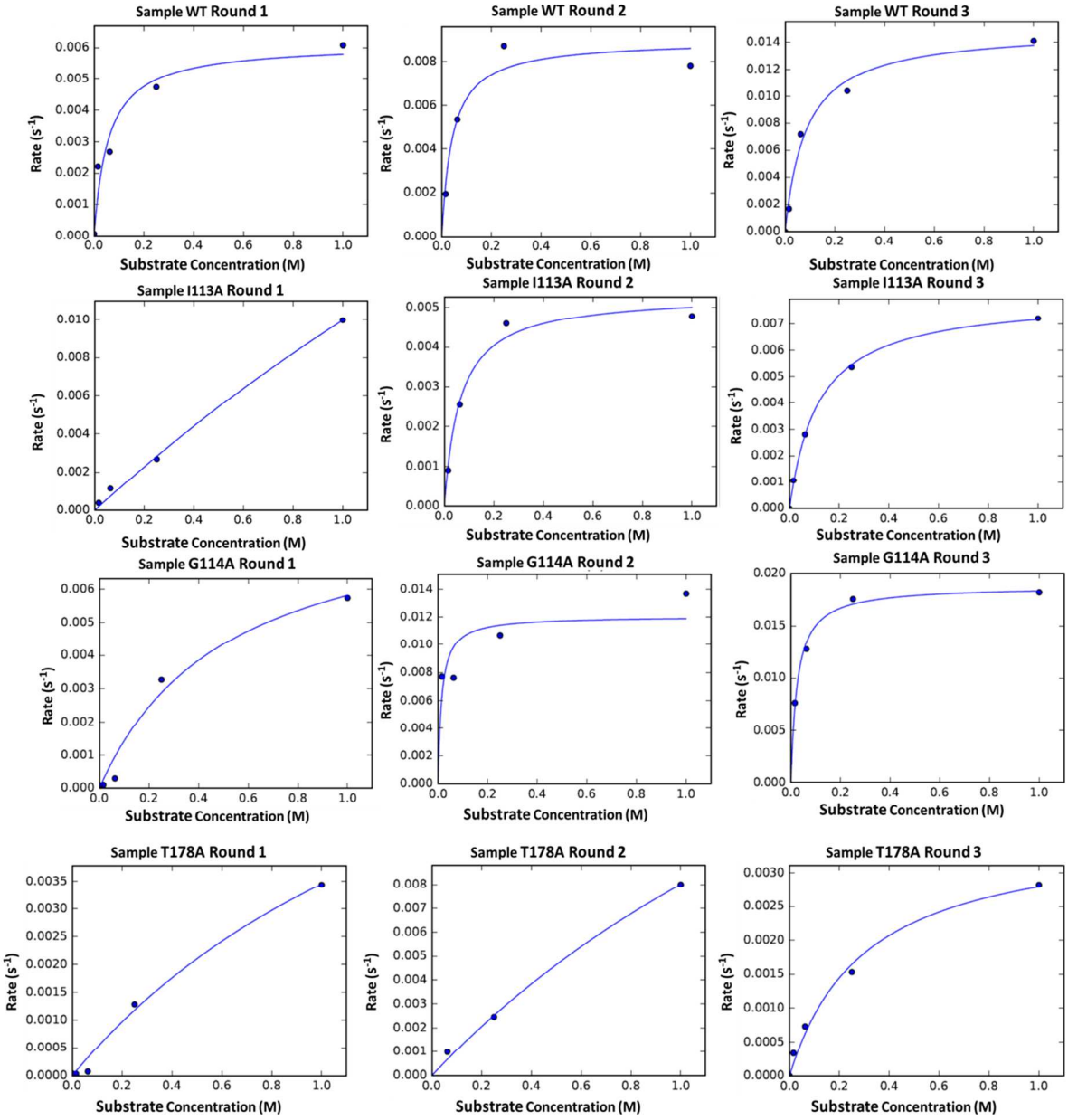


**Figure S4 Michaelis Menten and Linear Curve Fit On R-(-)-1-amino-2-propanol**

The Michaelis Menten curves were fitted using a total of five points. WT and all mutants were tested at R-(-)-1-amino-2-propanol concentrations of 1 M, 0.25 M, 0.06 M, 0.02 M and 0 M.

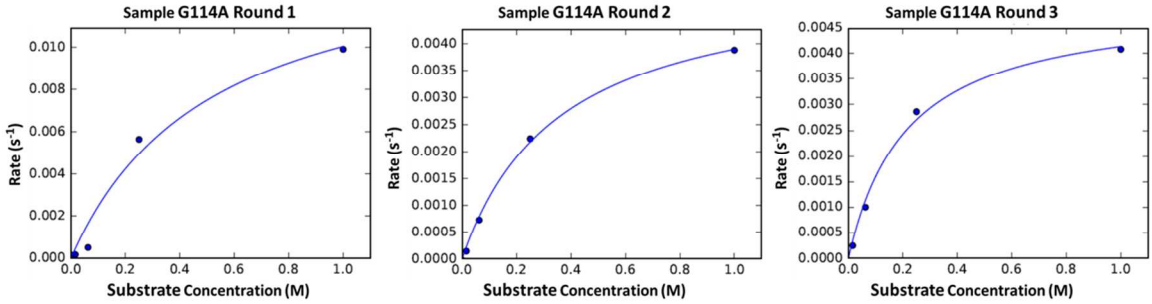


**Figure S5 Michaelis Menten and Linear Curve Fit On L-Threoninol.** The linear curves were fitted using a total of five points and the slope was reported. WT and all mutants were tested at L-threoninol concentrations of 1 M, 0.25 M, 0.06 M, 0.02 M and 0 M.

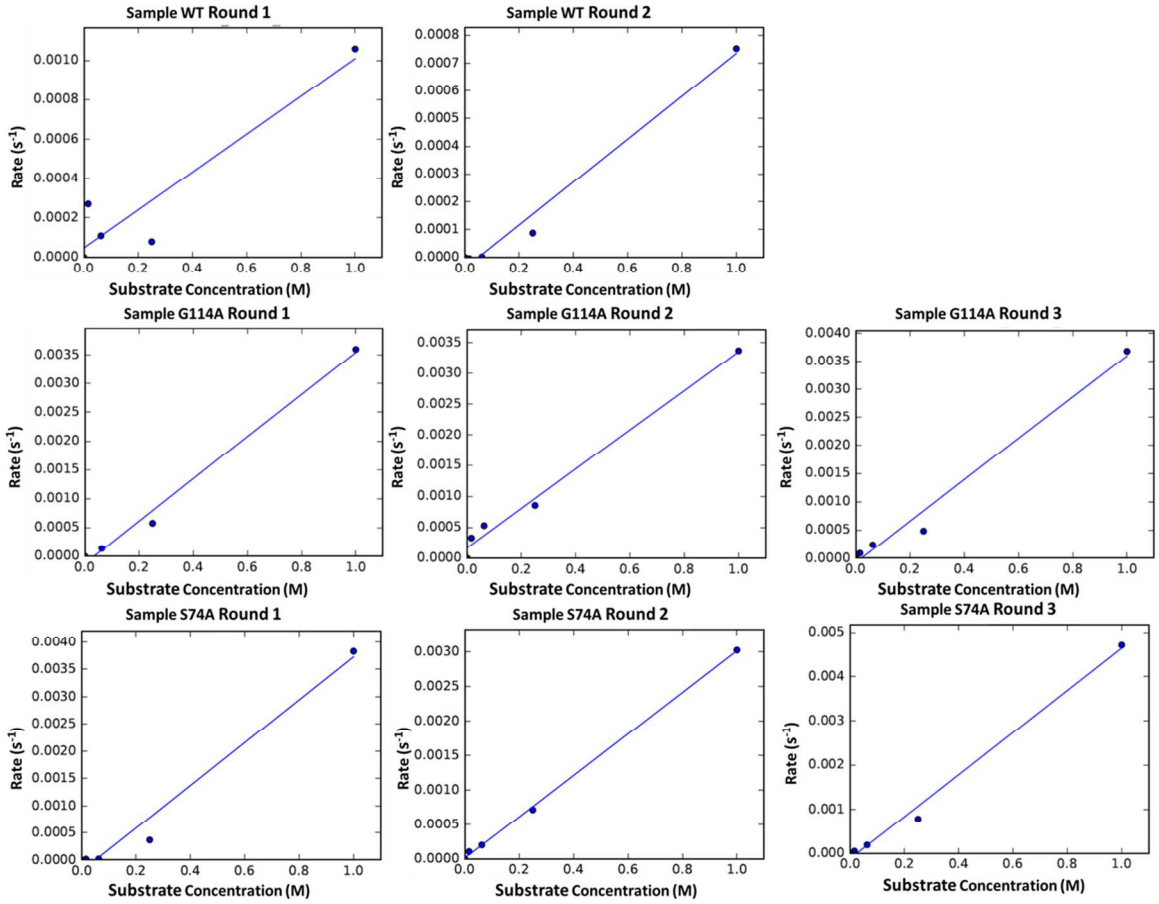


**Table S1 Amino acids profile of the seven mutated position in its protein family.** The amino acid conservation within the protein family was estimated for all mutated residues using the software Geneious. The presence of different residues at each position is reported as both an occurrence and a percentage.

| | S74 | | I113 | | G114 | | T178 | | T179 | | D180 | | W273 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Amino Acids | Number of Occurrences | Percent Presence | Number of Occurrences | Percent Presence | Number of Occurrences | Percent Presence | Number of Occurrences | Percent Presence | Number of Occurrences | Percent Presence | Number of Occurrences | Percent Presence | Number of Occurrences | Percent Presence |
| A | 0 | 0% | 2 | 3.20% | 23 | 36.50% | 4 | 6.90% | 3 | 5.20% | 2 | 3.30% | 0 | 0% |
| C | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% |
| D | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 53 | 88.30% | 0 | 0% |
| E | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% |
| F | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% |
| G | 0 | 0% | 0 | 0% | 0 | 60.30% | 0 | 0% | 1 | 1.70% | 0 | 0% | 0 | 0% |
| H | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 1 | 1.70% | 0 | 0% |
| I | 0 | 0% | 56 | 88.90% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 1 | 1.70% |
| K | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% |
| L | 0 | 0% | 1 | 1.60% | 0 | 0% | 1 | 1.70% | 0 | 0% | 0 | 0% | 2 | 3.40% |
| M | 1 | 1.60% | 1 | 1.60% | 0 | 0% | 1 | 1.70% | 0 | 0% | 0 | 0% | 0 | 0% |
| N | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 1 | 1.70% | 0 | 0% | 0 | 0% |
| P | 4 | 6.30% | 0 | 0% | 0 | 0% | 1 | 1.70% | 0 | 0% | 0 | 0% | 0 | 0% |
| Q | 0 | 0% | 2 | 3.20% | 0 | 0% | 0 | 0% | 0 | 0% | 4 | 6.70% | 1 | 1.70% |
| R | 1 | 1.60% | 0 | 0% | 0 | 0% | 2 | 3.40% | 1 | 1.70% | 0 | 0% | 1 | 1.70% |
| S | 57 | 89.10% | 0 | 0% | 0 | 3.20% | 3 | 5.25% | 9 | 15.50% | 0 | 0% | 0 | 0% |
| T | 1 | 1.60% | 0 | 0% | 0 | 0% | 45 | 77.60% | 43 | 74.10% | 0 | 0% | 0 | 0% |
| V | 0 | 0% | 1 | 1.60% | 0 | 0% | 1 | 1.70% | 0 | 0% | 0 | 0% | 0 | 0% |
| W | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 53 | 91.40% |
| Y | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% |
| U | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% |
| O | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% | 0 | 0% |

**Table S2 Kinetic characterization of tvTDH and mutants on L-threonine.** This table reports the $k_{cat}/K_M$ ($M^{-1}s^{-1}$), $k_{cat}$ ($s^{-1}$), and $K_M$ (M) values produced by the Michaelis Menten curves on L-Threonine. In the case of a straight linear fit the slope is reported as an estimate of $k_{cat}/K_M$ ($M^{-1}s^{-1}$).

| L-Threonine | | | |
|---|---|---|---|
| $k_{cat}/K_M$ ($M^{-1}s^{-1}$) | | | |
| WT | 6.6E+02 | ± | 9.4E+01 |
| I113A | 1.1E+02 | ± | 4.9E+01 |
| G114A | 2.7E+03 | ± | 5.7E+02 |
| T178A | 3.5E+01 | ± | 1.6E+01 |
| T179A | 1.6E+00 | ± | 2.1E-01 |
| D180A* | 1.1E+01 | ± | 3.6E+00 |
| W273A | 3.5E-01 | ± | 3.1E-02 |
| S74A | 2.9E+00 | ± | 6.4E-01 |
| $k_{cat}$ ($s^{-1}$) | | | |
| WT | 1.7E+00 | ± | 4.1E-01 |
| I113A | 7.3E-01 | ± | 1.2E-01 |
| G114A | 1.6E+00 | ± | 3.7E-01 |
| T178A | N.D. | ± | N.D. |
| T179A | N.D. | ± | N.D. |
| D180A* | 3.7E-01 | ± | 1.1E-01 |
| W273A | N.D. | ± | N.D. |
| S74A | N.D. | ± | N.D. |
| $K_M$ (M) | | | |
| WT | 2.6E-03 | ± | 7.6E-04 |
| I113A | 8.8E-03 | ± | 5.8E-03 |
| G114A | 5.7E-04 | ± | 3.6E-05 |
| T178A | N.D. | ± | N.D. |
| T179A | N.D. | ± | N.D. |
| D180A* | 4.3E-02 | ± | 2.5E-02 |
| W273A | N.D. | ± | N.D. |
| S74A | N.D. | ± | N.D. |

**Table S3 Kinetic characterization of tvTDH and mutants on L-serine.** This table reports the $k_{cat}/K_M$ ($M^{-1}s^{-1}$), $k_{cat}$ ($s^{-1}$), and $K_M$ (M) values produced by the Michaelis Menten curves on L-serine.

| L-Serine | | | |
|---|---|---|---|
| $k_{cat}/K_M$ ($M^{-1}s^{-1}$) | | | |
| WT | 1.7E-01 | ± | 4.4E-02 |
| I113A | 5.5E-02 | ± | 3.1E-02 |
| G114A | 5.4E-01 | ± | 3.7E-01 |
| T178A | 9.5E-03 | ± | 2.9E-03 |
| T179A | N.D. | ± | N.D. |
| D180A | N.D. | ± | N.D. |
| W273A | N.D. | ± | N.D. |
| S74A | N.D. | ± | N.D. |
| $k_{cat}$ ($s^{-1}$) | | | |
| WT | 1.0E-02 | ± | 3.7E-03 |
| I113A | 2.6E-02 | ± | 2.7E-02 |
| G114A | 1.3E-02 | ± | 4.2E-03 |
| T178A | 1.4E-02 | ± | 1.1E-02 |
| T179A | N.D. | ± | N.D. |
| D180A | N.D. | ± | N.D. |
| W273A | N.D. | ± | N.D. |
| S74A | N.D. | ± | N.D. |
| $K_M$ (M) | | | |
| WT | 6.1E-02 | ± | 1.8E-02 |
| I113A | 1.8E+00 | ± | 2.5E+00 |
| G114A | 1.8E-01 | ± | 2.3E-01 |
| T178A | 1.6E+00 | ± | 9.6E-01 |
| T179A | N.D. | ± | N.D. |
| D180A | N.D. | ± | N.D. |
| W273A | N.D. | ± | N.D. |
| S74A | N.D. | ± | N.D. |

**Table S4 Kinetic characterization of tvTDH and mutants on (R)-(-)-1-amino-2-propanol.** This table reports the $k_{cat}/K_M$ ($M^{-1}s^{-1}$), $k_{cat}$ ($s^{-1}$), and $K_M$ (M) values produced by the Michaelis Menten curves on R-(-)-1-amino-2-propanol.

| (R)-(-)-1-amino-2-propanol | | |
|---|---|---|
| $k_{cat}/K_M$ ($M^{-1}s^{-1}$) | | |
| WT | N.D. | ± N.D. |
| I113A | N.D. | ± N.D. |
| G114A | 2.3E-02 | ± 6.0E-03 |
| T178A | N.D. | ± N.D. |
| T179A | N.D. | ± N.D. |
| D180A | N.D. | ± N.D. |
| W273A | N.D. | ± N.D. |
| S74A | N.D. | ± N.D. |
| $k_{cat}$ ($s^{-1}$) | | |
| WT | N.D. | ± N.D. |
| I113A | N.D. | ± N.D. |
| G114A | 8.5E-03 | ± 4.7E-03 |
| T178A | N.D. | ± N.D. |
| T179A | N.D. | ± N.D. |
| D180A | N.D. | ± N.D. |
| W273A | N.D. | ± N.D. |
| S74A | N.D. | ± N.D. |
| $K_M$ (M) | | |
| WT | N.D. | ± N.D. |
| I113A | N.D. | ± N.D. |
| G114A | 3.6E-01 | ± 1.2E-01 |
| T178A | N.D. | ± N.D. |
| T179A | N.D. | ± N.D. |
| D180A | N.D. | ± N.D. |
| W273A | N.D. | ± N.D. |
| S74A | N.D. | ± N.D. |

**Table S5 Kinetic characterization of tvTDH and mutants on L-threoninol.** This table reports the slope of the linear fit as an estimate of $k_{cat}/K_M$ ($M^{-1}s^{-1}$) on L-threoninol.

| L-Threoninol $k_{cat}/K_M$ ($M^{-1}s^{-1}$) | | | |
|---|---|---|---|
| WT* | 8.7E-04 | ± | 9.4E-05 |
| I113A | N.D. | ± | N.D. |
| G114A | 3.5E-03 | ± | 2.3E-04 |
| T178A | N.D. | ± | N.D. |
| T179A | N.D. | ± | N.D. |
| D180A | N.D. | ± | N.D. |
| W273A | N.D. | ± | N.D. |
| S74A | 3.9E-03 | ± | 7.2E-04 |

| $k_{cat}$ ($s^{-1}$) | | | |
|---|---|---|---|
| WT | N.D. | ± | N.D. |
| I113A | N.D. | ± | N.D. |
| G114A | N.D. | ± | N.D. |
| T178A | N.D. | ± | N.D. |
| T179A | N.D. | ± | N.D |
| D180A | N.D. | ± | N.D. |
| W273A | N.D. | ± | N.D. |
| S74A | N.D. | ± | N.D. |

| $K_M$ (M) | | | |
|---|---|---|---|
| WT | N.D. | ± | N.D. |
| I113A | N.D. | ± | N.D. |
| G114A | N.D. | ± | N.D. |
| T178A | N.D. | ± | N.D. |
| T179A | N.D. | ± | N.D. |
| D180A | N.D. | ± | N.D. |
| W273A | N.D. | ± | N.D. |
| S74A | N.D. | ± | N.D. |

**Table S6 ΔΔG changes calculated with kinetic constants and Eyring's equation.** First order Arrhenius equations and constants were used to determine the change in free energy from wild type to the mutants. The ΔΔG changes were then calculated using Eyring's equation and reported in kcal.

| Mutant | ΔΔ G $k_{cat}$ of Threonine | ΔΔ G $K_M$ Threonine | ΔΔ G $k_{cat}$/ $K_M$ of Threonine |
|---|---|---|---|
| I113A | 4.97E-01 | 8.79E-03 | 1.05E+00 |
| G114A | 4.25E-02 | 5.73E-04 | -8.41E-01 |
| T178A | N.D. | N.D. | 1.75E+00 |
| T179A | N.D. | N.D. | 3.58E+00 |
| D180A | 9.06E-01 | 4.33E-02 | 2.45E+00 |
| W273 | N.D. | N.D. | 4.47E+00 |
| S74 | N.D. | N.D. | 3.22E+00 |

| Mutant | ΔΔ G $k_{cat}$ of Serine | ΔΔ G $K_M$ of Serine | ΔΔ G $k_{cat}$/ $K_M$ of Serine |
|---|---|---|---|
| I113A | -5.56E-01 | 2.02E+00 | 6.58E-01 |
| G114A | 6.53E-01 | -7.19E-01 | -6.99E-01 |
| T178A | -2.01E-01 | 1.92E+00 | 1.69E+00 |
| T179A | N.D. | N.D. | N. D. |
| D180A | N.D. | N.D. | N. D. |
| W273 | N.D. | N.D. | N. D. |
| S74 | N.D. | N.D. | N. D. |

**Table S7 Concentrations of purified proteins.** The protein concentrations are reported as an average of the biological triplicates after being measured with the spectrophotometer at an absorbance of 280 and converted to molar using the enzyme coefficient.

| | Protien Concentration in µM |
|---|---|
| WT | 68.0 |
| S74A | 59.2 |
| I113A | 55.2 |
| G114A | 61.7 |
| T178A | 56.2 |
| T179A | 38.8 |
| D180A | 32.3 |
| W273A | 42.5 |

**Document S1 Amino Acid Sequence of tvTDH.** Reported is the amino acid sequence of one subunit of the protein dimer tvTDH.

MILVTGSSGQIGTELVPYLAEKYGKKNVIASDIVQRDTGGIKFITLDVSNRDEIDRAVEKYSI
DAIFHLAGILSAKGEKDPALAYKVNMNGTYNILEAAKQHRVEKVVIPSTIGVFGPETPKNK
VPSITITRPRTMYGVTKIAAELLGQYYYEKFGLDVRSLRYPGIISYKAEPTAGTTDYAVEIFY
YAVKREKYKCYLAPNRALPMMYMPDALKALVDLYEADRDKLVLRNGYNVTAYTFTPSEL
YSKIKERIPEFEIEYKEDFRDKIAATWPESLDSSEASNEWGFSIEYDLDRTIDDMIDHISEKL
GIEGKHAL

**Document S2** First order Arrhenius equations and constants used to calculate changes in (A) $k_{cat}$, (B) $K_M$, and (C) $k_{cat}/K_M$. (D) Equation used to determine the change in free energy between WT and mutants.

**A.**

$$\Delta G = -RTln\left(\frac{kh}{k_B T}\right)$$

R = 8.314 J $mol^{-1}$ $K^{-1}$

T = 298 K

h = 6.626 x $10^{-34}$ J s

$k_B$ = 1.38 x 10-23 J $K^{-1}$

k = $k_{cat}$ ($s^{-1}$)

**B.**

$$\Delta G = -RTln(1/K_M)$$

R = 8.314 J $mol^{-1}$ $K^{-1}$

T = 298 K

**C.**

$$\Delta G = -RTln\left(\frac{khc^{\circ}}{k_B T}\right)$$

R = 8.314 J $mol^{-1}$ $K^{-1}$

T = 298 K

h = 6.626 x $10^{-34}$ J s

$k_B$ = 1.38 x 10-23 J $K^{-1}$

c° = 1 M

k = $k_{cat}/K_M$ ($M^{-1}s^{-1}$)

**D.**

$$\Delta\Delta G_{k_{cat}} = \Delta G_{Mutant\,k_{cat}} - \Delta G_{WT\,k_{cat}}$$

$$\Delta\Delta G_{K_M} = \Delta G_{Mutant\,K_M} - \Delta G_{WT\,K_M}$$

$$\Delta\Delta G_{k_{cat}/K_M} = \Delta G_{Mutant\,k_{cat}/K_M} - \Delta G_{WT\,k_{cat}/K_M}$$

**Document S3 Results of proton affinity calculations.**

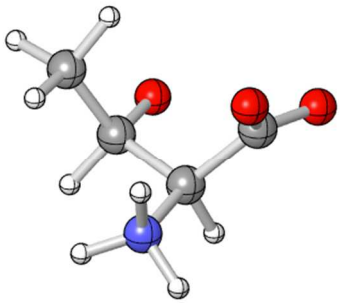
QM calculations were performed with Gaussian09.[1] Minima were located using B3LYP[2-6]/6-31+G(d,p) with the SMD continuum solvation[7] approach using water. All calculations were conducted without any protein present. Stationary points were confirmed as minima using harmonic vibrational analysis (no imaginary frequencies for minima). Structures used for calculations are provided in Supplemental Files, and computed structures and their resultant energies are reported below.

The energies reported in the main text (Relative Hydride Donation Propensities) were determined by first calculating the hydride donation propensity for each substrate (**1**), then comparing each substrates hydride donation propensity to that of the hydride donation propensity of the native substrate, threonine (**2**).

$$Hydride\ Donation\ Propensity\ \left(\frac{kcal}{mol}\right) = (Oxidized\ Substrate + NADH) - (Reduced\ Substrate + NAD)\ (\mathbf{1})$$

$$Relative\ Hydride\ Donation\ Propensity\ \left(\frac{kcal}{mol}\right) = Hydride\ Donation\ Propensity\ (substrate) - Hydride\ Donation\ Propensity\ (Threonine)\ \ (\mathbf{2})$$

**Deprotonated Threonine**



Charge = -1 Multiplicity = 1
mem = 800MB

Link 0: opt=modredundant freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 44 minutes 57.4 seconds.
File lengths (MBytes): RWF= 70 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 16:25:07 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000080 | 0.000450 | YES |
| RMS Force | 0.000017 | 0.000300 | YES |
| Maximum Displacement | 0.001736 | 0.001800 | YES |
| RMS Displacement | 0.000465 | 0.001200 | YES |

Predicted change in Energy=-7.663415D-08
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 13 minutes 44.9 seconds.
File lengths (MBytes): RWF= 94 Int= 0 D2E= 0 Chk= 7 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 16:38:53 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000080 | 0.000450 | YES |
| RMS Force | 0.000017 | 0.000300 | YES |
| Maximum Displacement | 0.002543 | 0.001800 | NO |
| RMS Displacement | 0.000730 | 0.001200 | YES |

Predicted change in Energy=-9.324847D-08

Values come from Link 1:
HF = -437.8549034 hartrees (-274758.330432534 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.128603 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =

-437.759941 hartrees (-274698.74057691 kcal/mol)

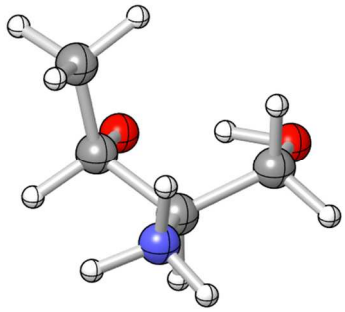
Comments:

*See deprot_threonine.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 7 | -0.348131 | 1.752005 | -0.681226 |
| 2 | 6 | -0.113080 | 0.262089 | -0.744234 |
| 3 | 6 | -1.217998 | -0.409083 | 0.094527 |
| 4 | 8 | -1.758267 | 0.294210 | 1.004873 |
| 5 | 6 | 1.352448 | -0.070376 | -0.268006 |
| 6 | 6 | 1.612204 | 0.422410 | 1.170682 |
| 7 | 8 | 1.625962 | -1.422162 | -0.415115 |
| 8 | 8 | -1.489447 | -1.613118 | -0.173717 |
| 9 | 1 | 1.982197 | 0.558324 | -0.938447 |
| 10 | 1 | 1.419141 | 1.494459 | 1.310683 |
| 11 | 1 | 1.001002 | -0.135502 | 1.889682 |
| 12 | 1 | 2.665539 | 0.245763 | 1.413473 |
| 13 | 1 | -0.205457 | -0.036455 | -1.788752 |
| 14 | 1 | -0.689985 | 1.978555 | 0.262114 |
| 15 | 1 | -1.068329 | 2.044995 | -1.347200 |
| 16 | 1 | 0.505386 | 2.284151 | -0.879121 |

**Deprotonated Threoninol**



Charge = 0 Multiplicity = 1
mem = 1600MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 44 minutes 3.7 seconds.
File lengths (MBytes): RWF= 68 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 22:00:01 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000032 | 0.000450 | YES |
| RMS Force | 0.000008 | 0.000300 | YES |
| Maximum Displacement | 0.001268 | 0.001800 | YES |
| RMS Displacement | 0.000286 | 0.001200 | YES |

Predicted change in Energy=-1.817658D-08
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 13 minutes 30.9 seconds.
File lengths (MBytes): RWF= 98 Int= 0 D2E= 0 Chk= 7 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 22:06:48 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000032 | 0.000450 | YES |
| RMS Force | 0.000008 | 0.000300 | YES |
| Maximum Displacement | 0.003485 | 0.001800 | NO |
| RMS Displacement | 0.000824 | 0.001200 | YES |

Predicted change in Energy=-5.231102D-08

Values come from Link 1:
HF = -364.269083 hartrees (-228582.49227333 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.160567 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-364.140537 hartrees (-228501.82837287 kcal/mol)

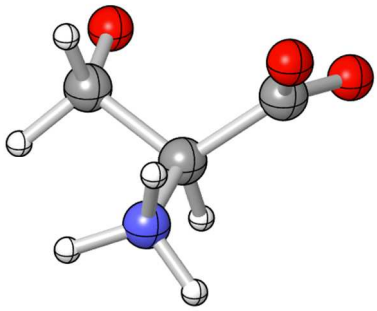
Comments:

*See deprot_threonol.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 7 | -1.533585 | -1.353100 | -0.218717 |
| 2 | 6 | -0.239274 | -0.621045 | -0.478163 |
| 3 | 6 | 0.825232 | -1.141725 | 0.496041 |
| 4 | 6 | -0.432337 | 0.922624 | -0.427885 |
| 5 | 6 | -1.028531 | 1.423960 | 0.898417 |
| 6 | 8 | 0.813651 | 1.516392 | -0.704568 |
| 7 | 1 | -1.170949 | 1.156732 | -1.221464 |
| 8 | 1 | -2.020828 | 1.002634 | 1.108251 |
| 9 | 1 | -0.368755 | 1.201003 | 1.744462 |
| 10 | 1 | -1.144378 | 2.511368 | 0.839533 |
| 11 | 1 | 0.045860 | -0.887551 | -1.498856 |
| 12 | 1 | -1.443383 | -2.351431 | -0.434596 |
| 13 | 1 | -2.288132 | -0.973203 | -0.799840 |
| 14 | 1 | 0.494054 | -0.978934 | 1.533121 |
| 15 | 1 | 0.964530 | -2.221299 | 0.358223 |
| 16 | 8 | 2.059767 | -0.473708 | 0.245692 |
| 17 | 1 | 1.755104 | 0.440207 | -0.118197 |
| 18 | 1 | -1.825912 | -1.272184 | 0.760927 |

**Deprotonated Serine**



Charge = -1 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 18 minutes 18.2 seconds.
File lengths (MBytes): RWF= 49 Int= 0 D2E= 0 Chk= 4 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 15:55:42 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000032 | 0.000450 | YES |
| RMS Force | 0.000007 | 0.000300 | YES |
| Maximum Displacement | 0.000471 | 0.001800 | YES |
| RMS Displacement | 0.000151 | 0.001200 | YES |

Predicted change in Energy=-6.891708D-09
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 7 minutes 31.6 seconds.
File lengths (MBytes): RWF= 62 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 16:03:15 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000032 | 0.000450 | YES |
| RMS Force | 0.000007 | 0.000300 | YES |
| Maximum Displacement | 0.000858 | 0.001800 | YES |
| RMS Displacement | 0.000227 | 0.001200 | YES |

Predicted change in Energy=-9.721896D-09
Optimization completed.
-- Stationary point found.

Values come from Link 1:
HF = -398.5355681 hartrees (-250085.054338431 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.100961 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-398.466547 hartrees (-250041.74290797 kcal/mol)

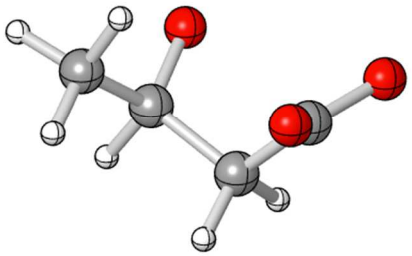
Comments:

*See deprot_serine.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 7 | -0.252833 | 1.851058 | -0.273834 |
| 2 | 6 | 0.191424 | 0.427872 | -0.491541 |
| 3 | 6 | -0.945804 | -0.495744 | -0.028449 |
| 4 | 8 | -1.656776 | -0.080618 | 0.938870 |
| 5 | 6 | 1.504821 | 0.201553 | 0.319391 |
| 6 | 8 | 2.036480 | -1.071400 | 0.175284 |
| 7 | 8 | -1.062942 | -1.606851 | -0.618150 |
| 8 | 1 | 2.196267 | 1.000480 | -0.029903 |
| 9 | 1 | 0.383298 | 0.302506 | -1.557865 |
| 10 | 1 | -0.742174 | 1.898188 | 0.629304 |
| 11 | 1 | -0.907851 | 2.157470 | -0.998597 |
| 12 | 1 | 1.261115 | 0.454508 | 1.374759 |
| 13 | 1 | 0.542439 | 2.498313 | -0.265308 |

**Deprotonated Hydroxybutyric acid**



Charge = -2 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 32 minutes 8.9 seconds.
File lengths (MBytes): RWF= 51 Int= 0 D2E= 0 Chk= 4 Scr= 1
Normal termination of Gaussian 09 at Mon Dec 5 14:04:09 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000039 | 0.000450 | YES |
| RMS Force | 0.000013 | 0.000300 | YES |
| Maximum Displacement | 0.001022 | 0.001800 | YES |
| RMS Displacement | 0.000406 | 0.001200 | YES |

Predicted change in Energy=-3.359417D-08
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 7 minutes 8.3 seconds.
File lengths (MBytes): RWF= 63 Int= 0 D2E= 0 Chk= 6 Scr= 1
Normal termination of Gaussian 09 at Mon Dec 5 14:11:18 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000039 | 0.000450 | YES |
| RMS Force | 0.000013 | 0.000300 | YES |
| Maximum Displacement | 0.001089 | 0.001800 | YES |
| RMS Displacement | 0.000333 | 0.001200 | YES |

Predicted change in Energy=-4.148163D-08
Optimization completed.
-- Stationary point found.

Values come from Link 1:
HF = -382.0208226 hartrees (-239721.886389726 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.097599 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-381.954921 hartrees (-239680.53247671 kcal/mol)

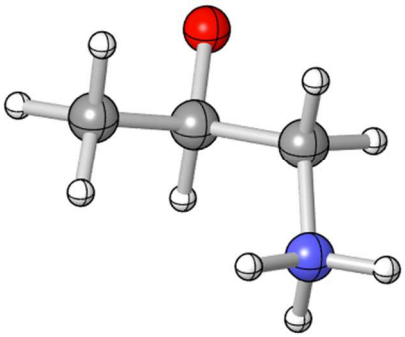
Comments:

*See deprot_hba.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.104430 | -0.137625 | 1.029096 |
| 2 | 6 | 1.278404 | 0.029706 | 0.067192 |
| 3 | 8 | 1.658690 | 1.213521 | -0.225453 |
| 4 | 6 | -1.304839 | -0.188246 | 0.339283 |
| 5 | 6 | -1.626436 | 1.136834 | -0.378170 |
| 6 | 8 | -1.464638 | -1.294554 | -0.506446 |
| 7 | 8 | 1.819063 | -1.021227 | -0.414673 |
| 8 | 1 | -2.007848 | -0.246251 | 1.200716 |
| 9 | 1 | -1.513553 | 2.006420 | 0.282859 |
| 10 | 1 | -0.972240 | 1.280668 | -1.246889 |
| 11 | 1 | -2.662126 | 1.117204 | -0.738372 |
| 12 | 1 | 0.229719 | -1.074688 | 1.582404 |
| 13 | 1 | 0.111763 | 0.690701 | 1.747450 |

**Deprotonated (R)-(-)-1-amino-2-propanol**



Charge = 0 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 6 minutes 2.5 seconds.
File lengths (MBytes): RWF= 48 Int= 0 D2E= 0 Chk= 4 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 14:50:58 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000018 | 0.000450 | YES |
| RMS Force | 0.000006 | 0.000300 | YES |
| Maximum Displacement | 0.000691 | 0.001800 | YES |
| RMS Displacement | 0.000189 | 0.001200 | YES |

Predicted change in Energy=-7.499463D-09
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 5 minutes 26.6 seconds.
File lengths (MBytes): RWF= 51 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 14:56:26 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000018 | 0.000450 | YES |
| RMS Force | 0.000006 | 0.000300 | YES |
| Maximum Displacement | 0.000651 | 0.001800 | YES |
| RMS Displacement | 0.000187 | 0.001200 | YES |

Predicted change in Energy=-9.444996D-09
Optimization completed.
-- Stationary point found.

Values come from Link 1:
HF = -249.7215181 hartrees (-156702.749822931 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.128137 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-249.622495 hartrees (-156640.61183745 kcal/mol)

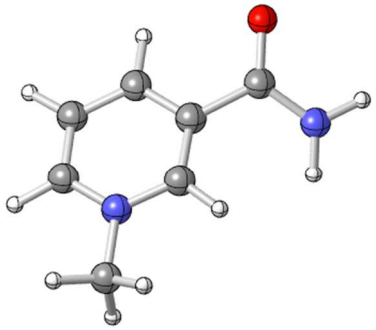
Comments:

*See deprot_ampropanol.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 7 | -1.926542 | 0.116038 | -0.126911 |
| 2 | 6 | -0.691853 | -0.620286 | 0.341331 |
| 3 | 6 | 0.605772 | -0.111235 | -0.317408 |
| 4 | 6 | 0.933477 | 1.325283 | 0.128795 |
| 5 | 8 | 1.636852 | -1.007530 | -0.015506 |
| 6 | 1 | 0.400797 | -0.075728 | -1.411588 |
| 7 | 1 | 0.143091 | 2.049151 | -0.114593 |
| 8 | 1 | 1.104081 | 1.353356 | 1.212659 |
| 9 | 1 | 1.848804 | 1.662389 | -0.369956 |
| 10 | 1 | -0.850949 | -1.668308 | 0.084309 |
| 11 | 1 | -2.773528 | -0.289439 | 0.282244 |
| 12 | 1 | -2.013237 | 0.063155 | -1.146629 |
| 13 | 1 | -0.655662 | -0.515752 | 1.428135 |
| 14 | 1 | -1.896794 | 1.106583 | 0.131534 |

**$NAD^+$ Analog**



Charge = 1 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 1 hours 32 minutes 11.4 seconds.
File lengths (MBytes): RWF= 78 Int= 0 D2E= 0 Chk= 7 Scr= 1
Normal termination of Gaussian 09 at Mon Dec 5 14:41:08 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000041 | 0.000450 | YES |
| RMS Force | 0.000006 | 0.000300 | YES |
| Maximum Displacement | 0.001156 | 0.001800 | YES |
| RMS Displacement | 0.000214 | 0.001200 | YES |

Predicted change in Energy=-8.682316D-09
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 1 hours 12 minutes 8.1 seconds.
File lengths (MBytes): RWF= 158 Int= 0 D2E= 0 Chk= 9 Scr= 1
Normal termination of Gaussian 09 at Mon Dec 5 15:53:18 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000042 | 0.000450 | YES |
| RMS Force | 0.000006 | 0.000300 | YES |
| Maximum Displacement | 0.001175 | 0.001800 | YES |
| RMS Displacement | 0.000291 | 0.001200 | YES |

Predicted change in Energy=-1.027654D-08
Optimization completed.
-- Stationary point found.

Values come from Link 1:
HF = -456.8034507 hartrees (-286648.733348757 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.157457 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-456.680295 hartrees (-286571.45191545 kcal/mol)

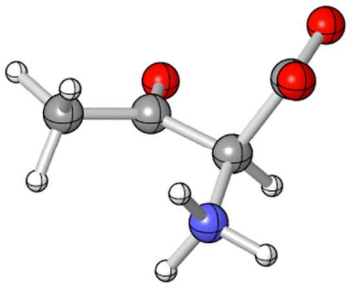
Comments:

*See NAD_analog.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.069430 | 0.872645 | 0.070991 |
| 2 | 6 | 1.111454 | 1.865225 | 0.181860 |
| 3 | 6 | -0.236904 | 1.519138 | 0.148119 |
| 4 | 6 | -0.602547 | 0.173267 | 0.021578 |
| 5 | 6 | 0.399218 | -0.783120 | -0.089005 |
| 6 | 7 | 1.702216 | -0.422762 | -0.068658 |
| 7 | 1 | -1.005168 | 2.280534 | 0.222186 |
| 8 | 1 | 3.133283 | 1.073969 | 0.084223 |
| 9 | 1 | 1.427870 | 2.895528 | 0.289167 |
| 10 | 1 | 0.204427 | -1.840473 | -0.219829 |
| 11 | 6 | 2.751756 | -1.467212 | -0.155673 |
| 12 | 1 | 3.610527 | -1.054371 | -0.682563 |
| 13 | 1 | 3.036498 | -1.764143 | 0.855223 |
| 14 | 1 | 2.354127 | -2.321241 | -0.700609 |
| 15 | 6 | -2.065164 | -0.181862 | -0.048714 |
| 16 | 8 | -2.876138 | 0.649870 | -0.493094 |
| 17 | 7 | -2.432560 | -1.399868 | 0.378571 |
| 18 | 1 | -1.791876 | -2.043347 | 0.823296 |
| 19 | 1 | -3.411628 | -1.655495 | 0.329334 |

**Threonone**



Charge = 0 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 43 minutes 20.4 seconds.
File lengths (MBytes): RWF= 69 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 16:23:39 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000009 | 0.000450 | YES |
| RMS Force | 0.000002 | 0.000300 | YES |
| Maximum Displacement | 0.000111 | 0.001800 | YES |
| RMS Displacement | 0.000030 | 0.001200 | YES |

Predicted change in Energy=-6.044474D-10
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 12 minutes 28.7 seconds.
File lengths (MBytes): RWF= 87 Int= 0 D2E= 0 Chk= 7 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 16:36:08 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000010 | 0.000450 | YES |
| RMS Force | 0.000002 | 0.000300 | YES |
| Maximum Displacement | 0.000243 | 0.001800 | YES |
| RMS Displacement | 0.000057 | 0.001200 | YES |

Predicted change in Energy=-7.727764D-10
Optimization completed.
-- Stationary point found.

Values come from Link 1:
HF = -437.134621 hartrees (-274306.34602371 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.118488 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-437.050451 hartrees (-274253.52850701 kcal/mol)

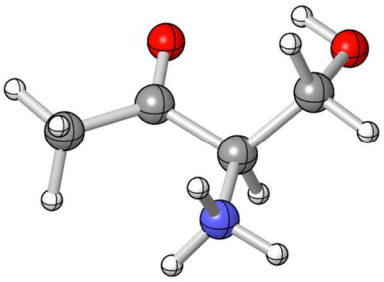
Comments:

*See threonone.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 7 | -0.111381 | 1.714647 | -0.641136 |
| 2 | 6 | -0.084419 | 0.217396 | -0.663572 |
| 3 | 6 | -1.331608 | -0.329439 | 0.122653 |
| 4 | 8 | -1.983692 | 0.523859 | 0.778778 |
| 5 | 6 | 1.207156 | -0.353201 | -0.079383 |
| 6 | 6 | 1.988528 | 0.462049 | 0.909295 |
| 7 | 8 | 1.541898 | -1.482186 | -0.420586 |
| 8 | 8 | -1.543523 | -1.560793 | 0.007250 |
| 9 | 1 | 2.458003 | 1.313744 | 0.400025 |
| 10 | 1 | 1.332294 | 0.869108 | 1.687567 |
| 11 | 1 | 2.767501 | -0.155108 | 1.358740 |
| 12 | 1 | -0.164105 | -0.096937 | -1.704508 |
| 13 | 1 | -0.203961 | 2.064891 | 0.318770 |
| 14 | 1 | -0.930661 | 2.050703 | -1.157720 |
| 15 | 1 | 0.725185 | 2.123194 | -1.072408 |

**Threonolone**



Charge = 1 Multiplicity = 1
mem = 1600MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 31 minutes 57.6 seconds.
File lengths (MBytes): RWF= 65 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 21:54:04 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000018 | 0.000450 | YES |
| RMS Force | 0.000004 | 0.000300 | YES |
| Maximum Displacement | 0.000773 | 0.001800 | YES |
| RMS Displacement | 0.000213 | 0.001200 | YES |

Predicted change in Energy=-5.673798D-09
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 12 minutes 21.3 seconds.
File lengths (MBytes): RWF= 90 Int= 0 D2E= 0 Chk= 7 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 22:00:16 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000018 | 0.000450 | YES |
| RMS Force | 0.000004 | 0.000300 | YES |
| Maximum Displacement | 0.000875 | 0.001800 | YES |
| RMS Displacement | 0.000255 | 0.001200 | YES |

Predicted change in Energy=-8.275428D-09
Optimization completed.
-- Stationary point found.

Values come from Link 1:
HF = -363.5382537 hartrees (-228123.889579287 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.150416 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-363.420320 hartrees (-228049.8850032 kcal/mol)

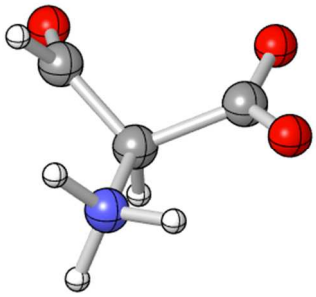
Comments:

*See threonolone.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 7 | 0.506488 | 1.862645 | -0.076479 |
| 2 | 6 | -0.143458 | 0.540142 | -0.366554 |
| 3 | 6 | -1.471474 | 0.449530 | 0.415987 |
| 4 | 6 | 0.781469 | -0.648569 | -0.076615 |
| 5 | 6 | 2.239534 | -0.437322 | 0.193565 |
| 6 | 8 | 0.268522 | -1.764503 | -0.091910 |
| 7 | 1 | 2.708141 | 0.103042 | -0.638393 |
| 8 | 1 | 2.376153 | 0.171740 | 1.095938 |
| 9 | 1 | 2.730214 | -1.401834 | 0.328557 |
| 10 | 1 | -0.358860 | 0.532068 | -1.439897 |
| 11 | 1 | -0.133943 | 2.629222 | -0.314470 |
| 12 | 1 | 1.361706 | 1.997035 | -0.627082 |
| 13 | 1 | -1.264922 | 0.296840 | 1.482865 |
| 14 | 1 | -2.015341 | 1.390213 | 0.295847 |
| 15 | 8 | -2.309200 | -0.576541 | -0.098168 |
| 16 | 1 | -1.811511 | -1.410376 | -0.042050 |
| 17 | 1 | 0.751947 | 1.959190 | 0.916361 |

**Seral**



Charge = 0 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 34 minutes 49.9 seconds.
File lengths (MBytes): RWF= 48 Int= 0 D2E= 0 Chk= 4 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 16:12:27 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000030 | 0.000450 | YES |
| RMS Force | 0.000010 | 0.000300 | YES |
| Maximum Displacement | 0.000342 | 0.001800 | YES |
| RMS Displacement | 0.000080 | 0.001200 | YES |

Predicted change in Energy=-1.262463D-08
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 6 minutes 12.0 seconds.
File lengths (MBytes): RWF= 55 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 16:18:40 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000030 | 0.000450 | YES |
| RMS Force | 0.000010 | 0.000300 | YES |
| Maximum Displacement | 0.000285 | 0.001800 | YES |
| RMS Displacement | 0.000084 | 0.001200 | YES |

Predicted change in Energy=-1.435879D-08
Optimization completed.
-- Stationary point found.

Values come from Link 1:
HF = -397.8045149 hartrees (-249626.311144899 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.089866 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-397.746797 hartrees (-249590.09258547 kcal/mol)

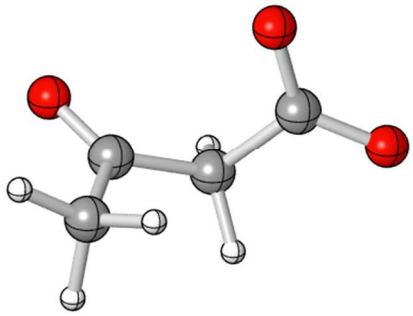
Comments:

*See seral.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 7 | 0.400083 | 1.804578 | 0.104075 |
| 2 | 6 | -0.179205 | 0.456669 | 0.393112 |
| 3 | 6 | 0.902661 | -0.638927 | 0.023318 |
| 4 | 8 | 2.024185 | -0.181768 | -0.320743 |
| 5 | 6 | -1.464993 | 0.233421 | -0.362881 |
| 6 | 8 | -2.322023 | -0.545866 | 0.015584 |
| 7 | 8 | 0.536479 | -1.828517 | 0.144404 |
| 8 | 1 | -0.363155 | 0.376987 | 1.466025 |
| 9 | 1 | 0.011033 | 2.231996 | -0.745089 |
| 10 | 1 | 1.412538 | 1.648844 | -0.056412 |
| 11 | 1 | -1.581632 | 0.794828 | -1.308581 |
| 12 | 1 | 0.260718 | 2.457533 | 0.880273 |

**Oxobutanoic acid**



Charge = -1 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 31 minutes 37.7 seconds.
File lengths (MBytes): RWF= 50 Int= 0 D2E= 0 Chk= 4 Scr= 1
Normal termination of Gaussian 09 at Mon Dec 5 14:04:03 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000012 | 0.000450 | YES |
| RMS Force | 0.000004 | 0.000300 | YES |
| Maximum Displacement | 0.000701 | 0.001800 | YES |
| RMS Displacement | 0.000260 | 0.001200 | YES |

Predicted change in Energy=-2.002621D-09
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 6 minutes 4.9 seconds.
File lengths (MBytes): RWF= 57 Int= 0 D2E= 0 Chk= 6 Scr= 1
Normal termination of Gaussian 09 at Mon Dec 5 14:10:08 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000012 | 0.000450 | YES |
| RMS Force | 0.000004 | 0.000300 | YES |
| Maximum Displacement | 0.000819 | 0.001800 | YES |
| RMS Displacement | 0.000276 | 0.001200 | YES |

Predicted change in Energy=-3.467508D-09
Optimization completed.
-- Stationary point found.

Values come from Link 1:
HF = -381.3158298 hartrees (-239279.496357798 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.086034 (Hartree/Particle)

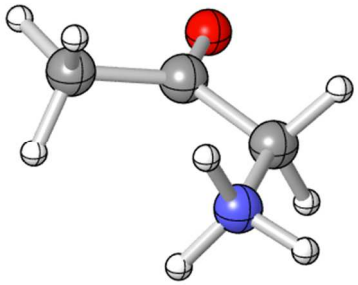
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-381.262672 hartrees (-239246.13930672 kcal/mol)

Comments:

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.126072 | 0.170525 | -0.903100 |
| 2 | 6 | -1.332332 | -0.066621 | 0.043637 |
| 3 | 8 | -2.393275 | 0.572854 | -0.219017 |
| 4 | 6 | 1.199336 | -0.052623 | -0.214667 |
| 5 | 6 | 1.745071 | 1.081185 | 0.609670 |
| 6 | 8 | 1.812659 | -1.116517 | -0.334583 |
| 7 | 8 | -1.187629 | -0.904938 | 0.982819 |
| 8 | 1 | 2.116194 | 1.855161 | -0.075191 |
| 9 | 1 | 0.955269 | 1.542263 | 1.211576 |
| 10 | 1 | 2.565158 | 0.745861 | 1.247386 |
| 11 | 1 | -0.223963 | -0.537563 | -1.733040 |
| 12 | 1 | -0.182726 | 1.188302 | -1.297734 |

**Aminopropanone**



Charge = 1 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 0 hours 7 minutes 12.6 seconds.
File lengths (MBytes): RWF= 46 Int= 0 D2E= 0 Chk= 4 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 14:52:22 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000022 | 0.000450 | YES |
| RMS Force | 0.000008 | 0.000300 | YES |
| Maximum Displacement | 0.001224 | 0.001800 | YES |
| RMS Displacement | 0.000383 | 0.001200 | YES |

Predicted change in Energy=-2.039165D-08
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 0 hours 4 minutes 41.5 seconds.
File lengths (MBytes): RWF= 47 Int= 0 D2E= 0 Chk= 5 Scr= 1
Normal termination of Gaussian 09 at Wed Dec 14 14:57:04 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000022 | 0.000450 | YES |
| RMS Force | 0.000008 | 0.000300 | YES |
| Maximum Displacement | 0.002350 | 0.001800 | NO |
| RMS Displacement | 0.000737 | 0.001200 | YES |

Predicted change in Energy=-4.089300D-08

Values come from Link 1:
HF = -248.9979952 hartrees (-156248.731967952 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.117018 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =

-248.910216 hartrees (-156193.64964216 kcal/mol)

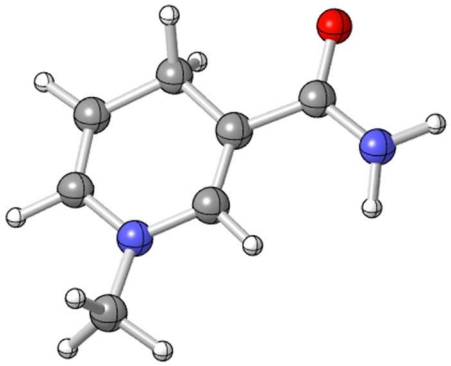
Comments:

*See ampropanone.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 7 | -1.836972 | 0.163712 | -0.027278 |
| 2 | 6 | -0.686232 | -0.789500 | 0.041778 |
| 3 | 6 | 0.691917 | -0.140265 | 0.000477 |
| 4 | 6 | 0.828947 | 1.351537 | 0.012753 |
| 5 | 8 | 1.654648 | -0.899693 | -0.028600 |
| 6 | 1 | 0.334423 | 1.784804 | -0.865689 |
| 7 | 1 | 0.337738 | 1.769239 | 0.900539 |
| 8 | 1 | 1.884378 | 1.626336 | 0.012097 |
| 9 | 1 | -0.777115 | -1.482504 | -0.796354 |
| 10 | 1 | -2.721726 | -0.352937 | 0.026711 |
| 11 | 1 | -1.840997 | 0.691516 | -0.907182 |
| 12 | 1 | -0.778199 | -1.352417 | 0.973133 |
| 13 | 1 | -1.824672 | 0.836887 | 0.746436 |

**NADH Analog**



Charge = 0 Multiplicity = 1
mem = 800MB

Link 0: opt freq rb3lyp/6-31+g(d,p) scrf=(smd,solvent=water)
Job cpu time: 0 days 2 hours 11 minutes 35.0 seconds.
File lengths (MBytes): RWF= 117 Int= 0 D2E= 0 Chk= 6 Scr= 1
Normal termination of Gaussian 09 at Mon Dec 5 15:20:42 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000015 | 0.000450 | YES |
| RMS Force | 0.000003 | 0.000300 | YES |
| Maximum Displacement | 0.000548 | 0.001800 | YES |
| RMS Displacement | 0.000121 | 0.001200 | YES |

Predicted change in Energy=-4.371668D-09
Optimization completed.
-- Stationary point found.

Link 1: N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31+G(d,p) Freq
Job cpu time: 0 days 1 hours 18 minutes 29.6 seconds.
File lengths (MBytes): RWF= 170 Int= 0 D2E= 0 Chk= 10 Scr= 1
Normal termination of Gaussian 09 at Mon Dec 5 16:39:13 2016.

| Item | Value | Threshold | Converged? |
|---|---|---|---|
| Maximum Force | 0.000015 | 0.000450 | YES |
| RMS Force | 0.000003 | 0.000300 | YES |
| Maximum Displacement | 0.005836 | 0.001800 | NO |
| RMS Displacement | 0.001176 | 0.001200 | YES |

Predicted change in Energy=-3.175607D-08

Values come from Link 1:
HF = -457.5344744 hartrees (-287107.458030744 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.165467 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and thermal Free Energies =
-457.405045 hartrees (-287026.23978795 kcal/mol)

Comments:

*See NADH_analog.mol2 file for easy access to the structure*

Coordinates (from last standard orientation):

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -2.098535 | 0.858590 | -0.058546 |
| 2 | 6 | -1.207062 | 1.859521 | -0.023588 |
| 3 | 6 | 0.286924 | 1.638003 | -0.022388 |
| 4 | 6 | 0.609523 | 0.149045 | -0.016615 |
| 5 | 6 | -0.382339 | -0.790668 | -0.034187 |
| 6 | 7 | -1.712889 | -0.493560 | -0.104825 |
| 7 | 1 | 0.742619 | 2.129655 | -0.896004 |
| 8 | 1 | -3.170010 | 1.025134 | -0.062912 |
| 9 | 1 | -1.576425 | 2.880380 | -0.001937 |
| 10 | 1 | -0.171714 | -1.853994 | 0.007591 |
| 11 | 6 | -2.721790 | -1.524695 | 0.138892 |
| 12 | 1 | -3.021472 | -1.549941 | 1.193620 |
| 13 | 1 | -3.604090 | -1.326497 | -0.474314 |
| 14 | 1 | -2.315616 | -2.498473 | -0.139183 |
| 15 | 6 | 2.024037 | -0.219862 | 0.019743 |
| 16 | 8 | 2.909833 | 0.668572 | 0.152464 |
| 17 | 7 | 2.405970 | -1.529221 | -0.060115 |
| 18 | 1 | 1.782436 | -2.244424 | -0.405297 |
| 19 | 1 | 3.397452 | -1.707342 | -0.152705 |
| 20 | 1 | 0.742049 | 2.136785 | 0.846161 |

## References:


1. Frisch, M.; Trucks, G.; Schlegel, H.; Scuseria, G.; Robb, M.; Cheeseman, J.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G., Gaussian 09, revision D. 01. Gaussian, Inc., Wallingford CT: 2009.
2. Becke, A. D., A new mixing of Hartree–Fock and local density‐functional theories. *The Journal of chemical physics* **1993,** *98* (2), 1372-1377.
3. Becke, A. D., Density‐functional thermochemistry. III. The role of exact exchange. *The Journal of chemical physics* **1993,** *98* (7), 5648-5652.
4. Tirado-Rives, J.; Jorgensen, W. L., Performance of B3LYP density functional methods for a large set of organic molecules. *Journal of Chemical Theory and Computation* **2008,** *4* (2), 297-306.
5. Stephens, P.; Devlin, F.; Chabalowski, C.; Frisch, M. J., Ab initio calculation of vibrational absorption and circular dichroism spectra using density functional force fields. *The Journal of Physical Chemistry* **1994,** *98* (45), 11623-11627.
6. Lee, C.; Yang, W.; Parr, R. G., Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Physical review B* **1988,** *37* (2), 785.
7. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *The Journal of Physical Chemistry B* **2009,** *113* (18), 6378-6396.